SMILES to Smell: Decoding Structure-Odor Relationship of Chemical Compounds using Deep Neural Network Approach

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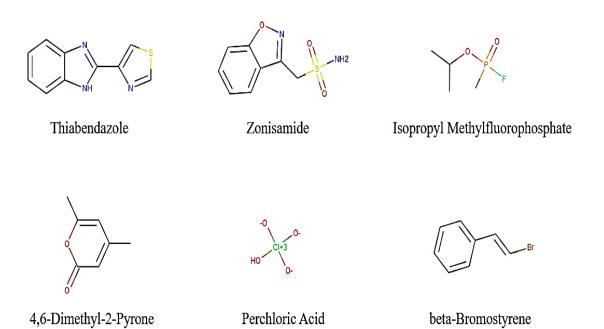


Figure S1: Example images of chemical structure generated by RDKit

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	1 : List of Chemical Compound				
	Common Name	IUPAC Name	SMILES	Smell Percepts	Source Database
1	2-Phenylpropyl butyrate	2-phenylpropyl butanoate	CCCC(=O)OCC(C)C1=CC=CC=	sweet fruity rummy apricot	OdorRactor ,TGSC
2	Formic acid	formic acid	C(=O)O	pungent acetic vinegar sharp fruity fermented penetrating	Sigma Aldrich, TGSC, Pubchem
3	cis-Aconitic acid	(Z)-prop-1-ene-1,2,3- tricarboxylic acid	C(C(=CC(=O)O)C(=O)O)C(=O)O	nutty musty vegetable dry toasted	OdorRactor ,TGSC
4	trans-Aconitic acid	(E)-prop-1-ene-1,2,3- tricarboxylic acid	C(C(=CC(=O)O)C(=O)O)C(=O)O	vegetable musty nutty caramel dry toasted	OdorRactor ,TGSC
5	Sodium mercaptopyruvate	sodium;2-oxo-3- sulfanylpropanoate	C(C(=O)C(=O)[O-])S.[Na+]	faint sulfurous cheese meaty	Sigma Aldrich, Flavorbase
6	3-Hydroxypyruvic acid	3-hydroxy-2-oxopropanoic acid	C(C(=O)C(=O)O)O	sour radish cabbage	OdorRactor ,TGSC
7	Dihydroxyacetone	1,3-dihydroxypropan-2-one	C(C(=O)CO)O	minty characteristic	OdorRactor ,TGSC, TGSC, PubChem
8	Citirc acid	2-hydroxypropane-1,2,3- tricarboxylic acid	C(C(=O)O)C(CC(=O)O)(C(=O)O) O	lemon	Sigma Aldrich
9	Cysteine	(2R)-2-amino-3- sulfanylpropanoic acid	C(C(C(=O)O)N)S	sulfurous	Sigma Aldrich, Flavorbase, TGSC
10	Tartaric acid	2,3-dihydroxybutanedioic acid	C(C(C(=O)O)O)(C(=O)O)O	mild caramel	Sigma Aldrich
11	Sorbitol	(2R ,3R ,4R ,5S)-hexane- 1,2,3,4,5,6-hexol	C(C(C(C(C(O)O)O)O)O)O	sweet caramel	Sigma Aldrich, TGSC
12	L-(+)-Arabinose	(2R, 3S, 4S)-2,3,4,5- tetrahydroxypentanal	C(C(C(C(C=O)O)O)O)O	woody	Sigma Aldrich
13	Ascorbic acid	(2R)-2-[(1S)-1,2- dihydroxyethyl]-3,4-dihydroxy-	C(C(C1C(=C(C(=O)O1)O)O)O)O	grassy mild	OdorRactor,
14	Ascorbic acid	2 <i>H</i> -furan-5-one (2 <i>R</i>)-2-[(1 <i>S</i>)-1,2- dihydroxyethyl]-3,4-dihydroxy- 2 <i>H</i> -furan-5-one	C(C(C1C(=C(C(=O)O1)O)O)O)O	green grassy mild	Sigma Aldrich
15	Mercaptoacetaldehyde	2-sulfanylacetaldehyde	C(C=O)S	cabbage	Flavornet, TGSC
16	Glutamine	(2S)-2,5-diamino-5-oxopentanoic acid	- (//-	milky custard cocoa oily	Sigma Aldrich, TGSC
17	Succinic acid	butanedioic acid	C(CC(=0)0)C(=0)0	acidic sour	Sigma Aldrich, Flavorbase
18	Glutamic acid	(2S)-2-aminopentanedioic acid	C(CC(=0)0)C(C(=0)0)N	bready yeasty	Sigma Aldrich, TGSC, OdoRactor
19	gamma-Aminobutyric acid	4-aminobutanoic acid	C(CC(=O)O)CN	savory meaty	OdorRactor ,TGSC
20	L-Ornithine hydrochloride	(2S)-2,5-diaminopentanoic acid;hydrochloride	C(CC(C(=O)O)N)CN.CI	green sweet cortex	Sigma Aldrich, TGSC
21	Arginine	(2S)-2-amino-5- (diaminomethylideneamino)pentan oic acid	C(CC(C(=O)O)N)CN=C(N)N	faint	Sigma Aldrich
22	Glutaraldehyde	pentanedial	C(CC=O)CC=O	medicinal pungent fruity sweet	Sigma Aldrich
23	Octanedinitrile	octanedinitrile	C(CCCC#N)CCC#N	sweet wax floral citrus mandarin fresh	OdorRactor ,TGSC
24	Sebacic acid	decanedioic acid	C(CCCCC(=O)O)CCCC(=O)O	characteristic	AOD, Pubchem
25	1,9-Nonanedithiol	nonane-1,9-dithiol	C(CCCS)CCCS	meaty sulfurous savory fatty lamb	Sigma Aldrich, TGSC, OdoRactor
26	1,8-Octanedithiol	octane-1,8-dithiol	C(CCCS)CCCS	meaty sulfurous mushroom earthy	Sigma Aldrich, TGSC, OdoRactor
27	1,6-Hexanedithiol	hexane-1,6-dithiol	C(CCCS)CCS	fatty meaty fungal sulfurous burnt	Sigma Aldrich, TGSC, OdoRactor
28	cadaverine	pentane-1,5-diamine	C(CCN)CCN	animal dead animal sperm characteristic urine	TGSC, PubChem
29	Putrescine	butane-1,4-diamine	C(CCN)CN	animal rotten fish strong piperidine rotten dead animal	TGSC
30	1,4-Butanedithiol	butane-1,4-dithiol	C(CCS)CS	meaty sulfurous	Sigma Aldrich, TGSC
31	beta-Alanine	3-aminopropanoic acid	C(CN)C(=0)O	fruity sweet	Sigma Aldrich
32	3-Mercaptopropionic acid	3-sulfanylpropanoic acid	C(CS)C(=0)O	sulfurous roasted strong acrid	TGSC, Pubchem
33	1,3-Propanedithiol	propane-1,3-dithiol	C(CS)CS	meaty sulfurous disagreeable	Sigma Aldrich, TGSC, OdoRactor, Pubchem
34	1,2-Ethanedithiol	ethane-1,2-dithiol	C(CS)S	sulfurous meaty onion garlic	OdorRactor ,Flavorbase, TGSC, Pubchem
35	Methanedithiol	methanedithiol	C(S)S	pungent	OdorRactor,
36	(+)-bicyclogermacrene	(1 <i>S</i> ,2 <i>Z</i> ,6 <i>Z</i> ,10 <i>R</i>)-3,7,11,11- tetramethylbicyclo[8.1	C/C/1=C/CC/C(=C\[C@H]2[C@H](C2(C)) C)CC1)/C	green woody weedy	TGSC
37	Isoeugenyl acetate	[2-methoxy-4-[(E)-prop-1-enyl]phenyl] acetate	C/C=C/C1=CC(=C(C=C1)OC(=O) C)OC	carnation spicy rose clove sweet floral balsamic powdery	Sigma Aldrich, AOD, TGSC
38	Rhodinyl phenylacetate	[(3S)-3,7-dimethyloct-7-enyl] 2-phenylacetate	C[C@@H](CCCC(=C)C)CCOC(= 0)CC1= CC=CC=C1	floral rose honey wax powdery geranium sweet green	OdorRactor ,TGSC
39	6-Methyl-3-nitro-2(5H)- pyridinone	(4R,5R)-2-hydroxy-3,4,5- trimethylcyclopent-2-en-	C[C@@H]1[C@H](C(=O)C(=C1 C)O)C	sweet milky dairy	TGSC
40	(2R)-4-Methoxy-2,5- dimethylfuran-3-one	(2R)-4-methoxy-2,5-dimethylfuran-3-one	C[C@@H]1C(=O)C(=C(O1)C)O C	burnt caramel	TGSC
41	N,N-Dimethyl menthyl succinamide	[(1R, 2S, 5R)-5-methyl-2-propan-2-ylcyclohexyl] 4-	C[C@@H]1CC[C@H]([C@@H](C1)OC(=O)CCC(=O)N(C)C)C(C)C	cooling minty	TGSC

42	(-)-Alloaromadendrene	(1aR ,4aS ,7R ,7aR ,7bS)-1,1,7-	C[C@@H]1CC[C@H]2[C@@H]	woody	OdorRactor,
		trimethyl-4-methyli	1[C@H] 3[C@H](C3(C)C)CCC2=C	•	,
43	Sclareolide	(3aR ,5aS ,9aS ,9bR)-3a ,6,6,9a -tetramethyl-1,4,5,	C[C@]12CCCC([C@@H]1CC[C @@]3([C@@H]2CC(=O)O3)C)(C)C	dry ambergis labdanum aromatic woody mossy cedar tobacco paper	OdorRactor ,TGSC
44	cis-2-Cyclopenten-1-one, 2- hydroxy-3,4,5- trimethyl	(4S ,5R)-2-hydroxy-3,4,5- trimethylcyclopent-2-en-		sweet maple caramel	TGSC
45	Trimethylamine oxide	N ,N -dimethylmethanamine oxide	C[N+](C)(C)[O-]	fishy	Sigma Aldrich, Pubchem
46	Betaine	2-(trimethylazaniumyl)acetate	C[N+](C)(C)CC(=O)[O-]	bland	OdorRactor,
47	Furtrethonium iodide	furan-2- ylmethyl(trimethyl)azanium;iodide	C[N+](C)(C)CC1=CC=CO1.[I-]	chicken	
48	Methylmethionine sulfonium chloride	[(3S)-3-amino-3-carboxypropyl]- dimethylsulfanium;chloride	C[S+](C)CCC(C(=O)O)N.[Cl-]	malty tomato potato sulfurous green	TGSC
49	Dehydrocostus lactone	(3aS ,6aR ,9aR ,9bS)-3,6,9- trimethylidene- 3a ,4,5,6a ,7,8,9a ,9b - octahydroazuleno[4,5-b]furan-2- one	C=C1CCC2C(C3C1CCC3=C)OC(=0)C2= C	nutty	TGSC
50	(2Z)-2,4-Pentadienal	(2Z)-penta-2,4-dienal	C=CC=CC=O	fruity	OdorRactor,
51	Acrolein	prop-2-enal	C=CC=O	almond cherry fruity sharp pungent acrid burnt sweet choking	OdorRactor ,TGSC
52	4-Vinylphenol	4-ethenylphenol	C=CC1=CC=C(C=C1)O	chemical phenolic medicinal sweet almond musty meaty	Flavornet, TGSC, OdoRactor
53	Styrene	styrene	C=CC1=CC=CC=C1	medicinal plastic balsamic gasoline sweet floral almond aromatic glue	Sigma Aldrich, Flavorbase, TGSC, Pubchem
54	2-Phenyl-4-pentenal	2-phenylpent-4-enal	C=CCC(C=O)C1=CC=CC=C1	fruity floral	OdorRactor ,TGSC
55	Magnolol	2-(2-hydroxy-5-prop-2- enylphenyl)-4-prop-2- enylphenol	C=CCC1=CC(=C(C=C1)O)C2=C(C=CC(= C2)CC=C)O	bitter	ADB, TGSC
56	4-Allylphenol	4-prop-2-enylphenol	C=CCC1=CC=C(C=C1)O	medicinal phenolic herbaceous	TGSC, OdoRactor
57	Allylbenzene	prop-2-enylbenzene	C=CCC1=CC=CC=C1	paint	
58	Safrole	5-prop-2-enyl-1,3-benzodioxole	C=CCC1=CC2=C(C=C1)OCO2	spice sweet warm woody floral sassafrass anisic	Flavornet, TGSC, Pubchem
59	1,6-Heptadien-3-one, 2- cyclohexyl-	2-cyclohexylhepta-1,6-dien-3-one	C=CCCC(=O)C(=C)C1CCCCC1	sweet green fruity pineapple tropical metallic weedy herbaceous galbanum orchid	OdorRactor ,TGSC
60	4-Pentenophenone	1-phenylpent-4-en-1-one	C=CCCC(=O)C1=CC=CC=C1	balsamic herbaceous lavender opoponax myrrh labdanum	OdorRactor ,TGSC
61	4-Penten-1-one, 1- spiro[4.5]dec-7-en-7-yl-	1-spiro[4.5]dec-8-en-9-ylpent-4- en-1-one	C=CCCC(=0)C1=CCCC2(C1)CC CC2	green galbanum fruity pineapple	TGSC
62	4-Pentenoic acid	pent-4-enoic acid	C=CCCC(=O)O	buttery cheese fruity dairy parmesan cheese caramel	Sigma Aldrich, TGSC, OdoRactor
63	4-Pentenal	pent-4-enal	C=CCCC=O	roasted	OdorRactor ,TGSC
64	9-Decen-5-olide	6-pent-4-enyloxan-2-one	C=CCCC1CCC(=0)01	sweet creamy nutty pleasant	TGSC, Flavorbase
65	9-Decenoic acid	dec-9-enoic acid	C=CCCCCCCC(=0)0	wax green fruity fatty soapy creamy cheese	Sigma Aldrich, TGSC, OdoRactor
66	(3E)-Trideca-3,12-dienenitrile	(3E)-trideca-3,12-dienenitrile	C=CCCCCCCCC=CCC#N	citrus sweet tangerine aldehydic fresh watery mandarin	OdorRactor ,TGSC
67	9-Decenal	dec-9-enal	C=CCCCCCCCC=0	aldehydic dewy rose wax floral fresh green citrus fatty	OdorRactor ,TGSC, Flavorbase
68 69	Undecylenic acid Allyl 10-undecenoate	undec-10-enoic acid prop-2-enyl undec-10-enoate	C=CCCCCCCCC(=0)O C=CCCCCCCCCC(=0)OCC=C	wax woody soapy sweet fruity pineapple wax	Sigma Aldrich OdorRactor ,TGSC, Pubchem
70	10-Undecenal	undec-10-enal	C=CCCCCCCCCC=O	fatty wax citrus rose sweet aldehydic mandarin soapy green floral marine orange	Sigma Aldrich, TGSC,OdoRactor
71	11-Dodecenoic acid	dodec-11-enoic acid	C=CCCCCCCCCC(=0)0	fatty citrus aldehydic	OdorRactor ,TGSC
72	10-Undecen-1-OL	undec-10-en-1-ol	C=CCCCCCCCCCC	floral clean fresh wax ozone citrus	OdorRactor ,TGSC TGSC
	Propanenitrile, 3-(10- undecenyloxy)- 9-Decen-1-OL	3-undec-10-enoxypropanenitrile dec-9-en-1-ol	C=CCCCCCCCCCCC#N	fruity pineapple	
74			C-CCCCCN-C-S	dewy rose wax aldehydic fresh clean floral	OdorRactor TGSC
75 76	5-Hexenyl isothiocyanate 5-Hexen-1-ol	6-isothiocyanatohex-1-ene hex-5-en-1-ol	C=CCCCCN=C=S C=CCCCCO	green pungent fatty wasabi	OdorRactor ,TGSC, Flavorbase Sigma Aldrich, OdoRactor
77	4-Pentenyl isothiocyanate	5-isothiocyanatopent-1-ene	C=CCCCCO C=CCCCN=C=S	green mustard horseradish green	Flavornet, Flavorbase, TGSC,
78	3-Butenyl isothiocyanate	4-isothiocyanatobut-1-ene	C=CCCN=C=S	pungent wasabi aromatic pungent green	OdoRactor OdorRactor ,Flavorbase
79	Allyl isothiocyanate	3-isothiocyanatoprop-1-ene	C=CCN=C=S	horseradish wasabi onion garlic sulfurous pungent	Sigma Aldrich, TGSC,
		, F . F	-	mustard penetrating sharp	Pubchem

80	Allyl alcohol	prop-2-en-1-ol	C=CCO	alliaceous pungent mustard	TGSC, OdoRactor, Pubchem
81	Allyl cinnamate	prop-2-enyl (E)-3-phenylprop-2-enoate	C=CCOC(=0)C=CC1=CC=CC=C	balsamic peach fruity apricot pineapple spicy cinnamyl plum weedy	Sigma Aldrich, TGSC, OdoRactor
82	Allyl benzoate	prop-2-enyl benzoate	C=CCOC(=0)C1=CC=CC=C1	sweet floral cherry berry fruity	OdorRactor ,TGSC
83	Allyl anthranilate	prop-2-enyl 2-aminobenzoate	C=CCOC(=O)C1=CC=CC=C1N	heliotrope green leafy floral grape	Sigma Aldrich, TGSC
84	Allyl salicylate	prop-2-enyl 2-hydroxybenzoate	C=CCOC(=0)C1=CC=CC=C10	fruity banana pineapple wintergreen	OdorRactor ,TGSC
85	Allyl 2-furoate	prop-2-enyl furan-2-carboxylate	C=CCOC(=O)C1=CC=CO1	caramel jammy fruity	Sigma Aldrich, TGSC, OdoRactor
86	Allyl phenylacetate	prop-2-enyl 2-phenylacetate	C=CCOC(=0)CC1=CC=CC=C1	honey sweet fruity rummy	Sigma Aldrich, AOD, TGSC, OdoRactor
87	Allyl cyclohexaneacetate	prop-2-enyl 2-cyclohexylacetate	C=CCOC(=0)CC1CCCCC1	sweet fruity pineapple green peach apricot ripe wax	·
88	Allyl cyclohexanepropionate	prop-2-enyl 3- cyclohexylpropanoate	C=CCOC(=0)CCC1CCCCC1	balsamic wax pineapple sweet tropical fruity candy apple green	Sigma Aldrich, TGSC, OdoRactor
89	Allyl cyclohexanebutyrate	prop-2-enyl 4-cyclohexylbutanoate	C=CCOC(=0)CCCC1CCCCC1	fatty fruity pineapple	OdorRactor ,TGSC
90	Allyl cyclohexanevalerate	prop-2-enyl 5- cyclohexylpentanoate	C=CCOC(=0)CCCCC1CCCCC1	fruity pineapple peach apricot apple	OdorRactor ,TGSC
91	Allyl cyclohexanehexanoate	prop-2-enyl 6- cyclohexylhexanoate	C=CCOC(=0)CCCCCC1CCCCC	fatty fruity	OdorRactor ,TGSC
92	Allyl phenoxyacetate	prop-2-enyl 2-phenoxyacetate	C=CCOC(=0)COC1=CC=CC=C1	honey pineapple sweet chamomile cocoa fruity fresh green camomile	Sigma Aldrich, Flavorbase, TGSC, OdoRactor
93	Acetic acid, (cyclohexyloxy)-, 2-propenyl ester	prop-2-enyl 2- cyclohexyloxyacetate	C=CCOC(=0)COC1CCCCC1	green herbaceous galbanum fruity pineapple leafy spicy woody	OdorRactor ,TGSC
94	Allyl formate	prop-2-enyl formate	C=CCOC=O	ethereal fruity	TGSC
95	4,7-Methano-1H-indene, 3a,4,5,6,7,7a- hexahydro-5-(2- propen-1-yloxy)-	9-prop-2- enoxytricyclo[5.2.1.02,6]dec-3- ene	C=CCOC1CC2CC1C3C2CC=C3	floral anisic fruity woody herbaceous	OdorRactor ,TGSC
96	Allyl phenethyl ether	2-prop-2-enoxyethylbenzene	C=CCOCCC1=CC=CC=C1	green fruity mushroom honey	TGSC
97	2-Allyloxyethanol	2-prop-2-enoxyethanol	C=CCOCCO	mushroom	TGSC
98	Allyl mercaptan	prop-2-ene-1-thiol	C=CCS	alliaceous sulfurous garlic onion roasted cooked onion grilled charred meaty	OdorRactor ,TGSC
99	S-Allyl-L-cysteine	(2R)-2-amino-3-prop-2- enylsulfanylpropanoic acid	C=CCSCC(C(=O)O)N	cooked roasted garlic allium	OdorRactor ,TGSC, Flavorbase
100	Diallyl sulfide	3-prop-2-enylsulfanylprop-1-ene	C=CCSCC=C	green horseradish sulfurous onion garlic metallic pungent	Sigma Aldrich, TGSC, Pubchem,OdoRactor
101	Allicin	3-prop-2-enylsulfinylsulfanylprop- 1-ene	C=CCSS(=O)CC=C	garlic	
102	Diallyl disulfide	3-(prop-2-enyldisulfanyl)prop-1- ene	C=CCSSCC=C	green sulfurous alliaceous onion garlic metallic	Sigma Aldrich, TGSC, OdoRactor, Pubchem
103	Diallyl trisulfide	3-(prop-2-enyltrisulfanyl)prop-1-ene		sulfurous alliaceous garlic green onion metallic	Sigma Aldrich, TGSC, OdoRactor
104	Diallyl tetrasulfide	3-(prop-2-enyltetrasulfanyl)prop-1-ene	-C=CCSSSSCC=C	garlic onion sulfurous	OdorRactor ,TGSC
105	Musk ketone	2.1.1IUPAC Name	C1=C(C(=C(C(=C1[N+](=O)[O-])C(C)(C)C)[N+](=O)[O-])C)C(=O)C	woody fatty soapy musk dry floral powdery sweet animal	Sigma Aldrich, TGSC, Pubchem
106	Tannic acid	[2,3-dihydroxy-5-[[(2R, 3R, 4S, 5R, 6S)-3,4,5,6- tetrakis[[3,4-dihydroxy-5-(3,4,5-trihydroxybenzoyl)oxybenzoyl]oxyloxan-2-yl]methoxycarbonyl]phenyl] 3,4,5-trihydroxybenzoate	C1=C(C=C(C(=C10)O)O)C(=O) OC2=CC(=CC(=C2O)O)C(=O)OCC3C(C(C (C(O3)O C(=O)C4=CC(=C(C(=C4)OC(=O) C5=CC(=C(C(=C5)O)O)O)O)O)OC(=O)C 6=CC(= C(C(=C6)OC(=O)C7=CC(=C(C(=C7)O)O) O)O)OC(=O)C8=CC(=C(C(=C S)OC(=O))C9=CC(=C(C(=C9)O)O)O)O)O OC(=O)C 1=CC(=C(C(=C1)OC(=O)C1=CC(=C(C(=C(C(=C))C)O)O)OC(=O)C1=CC(=C(C(=C(C(=C))C)O)O)OOO(=O)C(=O)C1=CC(=C(C(=C(=C(C(=C(=C(C(=C(=C(=C(=C(=C(medicinal woody faint	Sigma Aldrich, Flavorbase, Pubchem
107	Histidine	155.15 g/mol	C1=C(NC=N1)CC(C(=O)O)N	fishy	ADB
108	5-Hydroxymethylfurfural	5-(hydroxymethyl)furan-2- carbaldehyde	C1=C(OC(=C1)C=O)CO	buttery caramel musty cardboard fatty wax chamomile	Sigma Aldrich, TGSC, Pubchem, OdoRactor
109	3,4-dihydroxybenzoic acid	3,4-dihydroxybenzoic acid	C1=CC(=C(C=C1C(=O)O)O)O	mild phenolic balsamic	OdorRactor ,TGSC
110	3,4-Dihydroxybenzaldehyde	3,4-dihydroxybenzaldehyde	C1=CC(=C(C=C1C=O)O)O	medicinal bitter almond dry bitter	OdorRactor ,TGSC

111	2,4-Dihydroxybenzoic acid	2,4-dihydroxybenzoic acid	C1=CC(=C(C=C1O)O)C(=O)O	phenolic	Sigma Aldrich, TGSC ,
110	D 1	1	G1	h	Flavorbase
112	Resorcinol	benzene-1,3-diol	C1=CC(=CC(=C1)O)O	hawthorn nutty creamy phenolic musty vanilla characteristic	Sigma Aldrich, TGSC, Pubchem
113	4-Hydroxybenzoic acid	4-hydroxybenzoic acid	C1=CC(=CC=C1C(=O)O)O	phenolic nutty	SuperScent, TGSC
114	4-Hydroxycinnamic acid	(E)-3-(4-hydroxyphenyl)prop-2-enoic acid	C1=CC(=CC=C1C=CC(=O)O)O	balsamic	Flavornet, TGSC
115	4-Hydroxybenaldehyde	4-Hydroxybenaldehyde	C1=CC(=CC=C1C=O)O	sweet nutty almond balsamic woody vanilla brown honey	Sigma Aldrich, TGSC
				metallic	
116	Apigenin	5,7-dihydroxy-2-(4- hydroxyphenyl)chromen-4-one	C1=CC(=CC=C1C2=CC(=O)C3= C(C=C(C =C3O2)O)O)O	herbaceous camphoraceous balsamic woody	Sigma Aldrich, OdoRactor
117	[1,1'-Biphenyl]-4,4'- dicarboxylic acid	4-(4-carboxyphenyl)benzoic acid	C1=CC(=CC=C1C2=CC=C(C=C2)C(=O) O)C(=O)O	sandal wood woody	Sigma Aldrich,OdoRactor
118	Tyramine	4-(2-aminoethyl)phenol	C1=CC(=CC=C1CCN)O	phenolic meaty dirty cooked rubbery mild	Sigma Aldrich, TGSC
119	2-(4-Hydroxyphenyl)ethanol	4-(2-hydroxyethyl)phenol	C1=CC(=CC=C1CCO)O	sweet floral fruity	TGSC
120	1,4-Dichlorobenzene	1,4-dichlorobenzene	C1=CC(=CC=C1Cl)Cl	characteristic mothball aromatic	Pubchem
121	4-Hydroxybenzyl alcohol	4-(hydroxymethyl)phenol	C1=CC(=CC=C1CO)O	sweet fruity bitter almond coconut	Sigma Aldrich, TGSC
122	Coumalic acid	6-oxopyran-3-carboxylic acid	C1-CC(-0)CC-C1C(-0)O	bitter woody	OdorRactor,
123	Salicylic acid	2-hydroxybenzoic acid	C1=CC(=O)OC=C1C(=O)O C1=CC=C(C(=C1)C(=O)O)O	phenolic faint nutty	Sigma Aldrich, TGSC
123	Salicylaldehyde	2-hydroxybenzaldehyde	C1=CC=C(C(=C1)C(=0)0)0	pungent phenolic almond spicy	Sigma Aldrich, Flavorbase,
124	Buncymachyde	2 ilyaroxyoenzalaenyae	e1-ee-e(e(-e1)e-o)o	medicinal cinnamyl wintergreen cooling bitter irritating	TGSC, Pubchem
125	2-Bromophenol	2-bromophenol	C1=CC=C(C(=C1)O)Br	unpleasant medicinal	Pubchem
126	2-Chlorophenol	2-chlorophenol	C1=CC=C(C(=C1)O)C1	unpleasant penetrating	Pubchem
127	Benzonitrile	benzonitrile	C1=CC=C(C=C1)C#N	characteristic medicinal rancid almond	Flavornet, Pubchem
	2-Phenyl-3-(2-furyl)prop-2- enal	(E)-3-(furan-2-yl)-2-phenylprop- 2-enal	C1=CC=C(C=C1)C(=CC2=CC=C O2)C=O	warm spicy	OdorRactor ,TGSC
129	2,2-Dihydroxy-1-	2,2-dihydroxy-1-phenylethanone	C1=CC=C(C=C1)C(=O)C(O)O	vegetable green fatty nutty earthy	OdorRactor ,TGSC,
120	phenylethanone	1.1 1 1		powdery spicy	Flavorbase
130	Benzophenone	diphenylmethanone	C1=CC=C(C=C1)C(=O)C2=CC= CC=C2	apricot peach geranium sweet rose balsamic metallic powdery herbaceous	Sigma Aldrich, AOD, TGSC, Pubchem
131	2-Naphthyl phenyl ketone	naphthalen-2-yl(phenyl)methanone	C1=CC=C(C=C1)C(=O)C2=CC3= CC=CC =C3C=C2	naphthyl orange flower blossom floral	OdorRactor ,TGSC
132	2-Aminoacetophenone	2-amino-1-phenylethanone	C1=CC=C(C=C1)C(=O)CN	grape sweet	SuperScent, TGSC
133	2-Hydroxyacetophenone	2-hydroxy-1-phenylethanone	C1=CC=C(C=C1)C(=O)CO	phenolic sweet hawthorn tobacco honey herbaceous almond bitter cherry tropical melon	SuperScent, TGSC
134	2-(Benzoylamino)benzoic acid	2-benzamidobenzoic acid	C1=CC=C(C=C1)C(=O)NC2=CC =CC=C2 C(=O)O	fruity	OdorRactor,
135	Benzoic acid	benzoic acid	C1=CC=C(C=C1)C(=O)O	balsamic urine faint unpleasant	Sigma Aldrich, TGSC, Pubchem
136	Resorcinol dibenzoate	(3-benzoyloxyphenyl) benzoate	C1=CC=C(C=C1)C(=0)OC2=CC(=CC=C 2)OC(=0)C3=CC=CC=C3	pungent sweet creamy buttery fruity estery chemical pineapple apple banana ketonic	OdorRactor ,TGSC
137	Glyceryl tribenzoate	2,3-dibenzoyloxypropyl benzoate	C1=CC=C(C=C1)C(=O)OCC(CO C(=O)C2 =CC=CC=C2)OC(=O)C3=CC=CC =C3	plastic green balsamic herbaceous clean	OdorRactor ,TGSC
138	Benzoin	2-hydroxy-1,2-diphenylethanone	C1=CC=C(C=C1)C(C(=O)C2=CC =CC=C2)O	balsamic sweet vanilla woody medicinal camphoraceous	Sigma Aldrich, TGSC, Pubchem
139	Diphenylmethanol	diphenylmethanol		green weedy rose	TGSC
140	1-Phenyl-1,2-ethanediol	1-phenylethane-1,2-diol	C1=CC=C(C=C1)C(CO)O	sweet	Flavornet
141	Benzal glycerin	(Z)-4-phenylbut-3-ene-1,2,3-triol	C1=CC=C(C=C1)C=C(C(CO)O)O	fruity cherry bitter almond sweet musty bitter	OdorRactor ,TGSC
142	beta-Bromostyrene	[(E)-2-bromoethenyl]benzene	C1=CC=C(C=C1)C=CBr	green leafy hyacinth floral	OdorRactor ,TGSC, Pubchem
143	Cinnamonitrile	(E)-3-phenylprop-2-enenitrile	C1=CC=C(C=C1)C=CC#N	nitrile cinnamyl cassia cumin spicy	OdorRactor ,TGSC
144	Chalcone	(E)-1,3-diphenylprop-2-en-1-one	C1=CC=C(C=C1)C=CC(=0)C2=	floral balsamic herbaceous	TGSC
145	Cinnamic acid	(E)-3-phenylprop-2-enoic acid	CC=CC= C2 C1=CC=C(C=C1)C=CC(=O)O	cinnamyl honey floral spicy sweet	Sigma Aldrich, TGSC
146	Cinnamaldehyde	(E)-3-phenylprop-2-enal	C1=CC=C(C=C1)C=CC=O	balsamic storax cinnamyl clove spicy sweet paint	Sigma Aldrich, TGSC,
				candy warm aldehydic aromatic balsamic resinous honey powdery cassia pungent	Pubchem, OdoRactor

1.47	ois Cinnomoldobardo	(7) 2 phonylpro- 2 and	C1_CC_C(C_C1)C_CC_0	cniov oinnonvil	TCSC
147 148	cis-Cinnamaldehyde Cinnamyl alcohol	(Z)-3-phenylprop-2-enal (E)-3-phenylprop-2-en-1-ol	C1=CC=C(C=C1)C=CC=O C1=CC=C(C=C1)C=CCO	spicy cinnamyl balsamic hyacinth sweet oily spicy	TGSC Sigma Aldrich, TGSC,
	•		, , , , , , , , , , , , , , , , , , , ,	green powdery cinnamyl floral fermented	OdoRactor, Pubchem
149	Cinnamyl cinnamate	[(E)-3-phenylprop-2-enyl] (E)-3-phenylprop-2-enoate	C1=CC=C(C=C1)C=CCOC(=0)C =CC2=C C=CC=C2	almond balsamic berry carnation cinnamyl honey jasmine nutty rose sweet	Sigma Aldrich, TGSC, OdoRactor
1.50	25 : :12 : 12		at ag aya aya agaay aya	floral cassia spicy	o.t. D maga
150	2-Propenoic acid, 3-phenyl-, 3 phenyl-2- propenyl ester	phenylprop-2-enoate	C1=CC=C(C=C1)C=CCOC(=0)C =CC2=C C=CC=C2	sweet balsamic floral cinnamyl cassia spicy jasmine rose	OdorRactor ,TGSC
151	3-Phenylprop-2-en-1-yl benzoate	3-phenylprop-2-enyl benzoate	C1=CC=C(C=C1)C=CCOC(=0)C 2=CC=C C=C2	balsamic spicy buttery fruity	OdorRactor ,TGSC
152	Cinnamyl anthranilate	[(E)-3-phenylprop-2-enyl] 2-aminobenzoate	C1=CC=C(C=C1)C=CCOC(=0)C 2=CC=C C=C2N	balsamic fruity grape	OdorRactor ,TGSC, Pubchem
153	Cinnamyl formate	[(E)-3-phenylprop-2-enyl] formate	C1=CC=C(C=C1)C=CCOC=O	balsamic green floral herbaceous cinnamyl narcissus	Sigma Aldrich, TGSC, OdoRactor
154	Benzaldehyde	benzaldehyde	C1=CC=C(C=C1)C=O	almond cherry sweet burnt sugar bitter almond fruity sharp bitter powdery nutty maraschino aromatic spicy stinging powerful marzipan	Sigma Aldrich, Flavornet, AOD, TGSC, PubChem
155	Biphenyl	1,1'-biphenyl	C1=CC=C(C=C1)C2=CC=CC=C2	geranium green pungent rose metallic neroli bergamot cinnamyl	Sigma Aldrich, Flavorbase, TGSC, Pubchem
				pleasant buttery	1 os e, 1 usenem
156	Phenylacetate	2-phenylacetate	C1=CC=C(C=C1)CC(=O)[O-]	sweet	AOD
157	Phenylpyruvic acid	2-oxo-3-phenylpropanoic acid	C1=CC=C(C=C1)CC(=O)C(=O)O	sweet acidic honey almond weedy phenolic green	OdorRactor ,TGSC
158	1,3-Diphenylacetone	1,3-diphenylpropan-2-one	C1=CC=C(C=C1)CC(=0)CC2=C C=CC=C 2	plastic seedy fruity almond bitter almond cherry sweet powdery honey floral rose faint bitter	Sigma Aldrich, Flavorbase, TGSC
159	Phenylacetic acid	2-phenylacetic acid	C1=CC=C(C=C1)CC(=0)0	cheese chocolate green honey meaty musty herbaceous raspberry rose strawberry vanilla winey sweet honeysuckle sour wax civet floral tobacco animal powdery disagreeable	Sigma Aldrich, Flavorbase, TGSC, Pubchem
160	Cinnamyl phenylacetate	[(E)-3-phenylprop-2-enyl] 2-phenylacetate	C1=CC=C(C=C1)CC(=O)OCC=C C2=CC= CC=C2	floral chrysanthemum spicy tolu balsamic	OdorRactor ,TGSC
161	Benzyl phenylacetate	benzyl 2-phenylacetate	C1=CC=C(C=C1)CC(=0)OCC2= CC=CC= C2	honey floral sweet jasmine cocoa rose	Sigma Aldrich, TGSC, OdoRactor
162	DL-Phenylalanine	2-amino-3-phenylpropanoic acid	C1=CC=C(C=C1)CC(C(=O)O)N	cocoa chocolate sweet	Sigma Aldrich, Flavorbase
163	Phenylalanine	(2S)-2-amino-3-phenylpropanoic acid	C1=CC=C(C=C1)CC(C(=O)O)N	faint	Sigma Aldrich, Pubchem
164	1,2-Diphenylethanol		C1=CC=C(C=C1)CC(C2=CC=CC =C2)O	floral orris	TGSC
165	(2-Nitroethyl)benzene	2-nitroethylbenzene	C1=CC=C(C=C1)CC[N+](=O)[O-	floral spice	Flavornet
166	Phenylacetaldehyde	2-phenylacetaldehyde	C1=CC=C(C=C1)CC=O	apple apricot berry cherry chocolate grape grapefruit green honey hyacinth lemon melon orange vegetable peach peanut winey sweet hawthorn floral clover cocoa rose powdery fermented earthy	Sigma Aldrich, AOD, Flavorbase, TGSC
167	Diphenylmethane	benzylbenzene	C1=CC=C(C=C1)CC2=CC=CC= C2	sweet green plastic geranium wet orange herbaceous	OdorRactor ,TGSC, Pubchem
168	3-Phenylpropionic acid	3-Phenylpropionic acid	C1=CC=C(C=C1)CCC(=O)O	rose sweet balsamic musk cinnamyl fatty floral	Sigma Aldrich, TGSC
169	3-Phenylpropanal	3-phenylpropanal	C1=CC=C(C=C1)CCC=O	almond cherry chocolate cinnamyl clove green honey hyacinth meaty musty spicy peach plum strawberry sweet fresh cortex leafy foliage balsamic storax aldehydic floral melon	Sigma Aldrich, Flavorbase, TGSC, OdoRactor
170	2-(3-Phenylpropyl)Pyridine	2-(3-phenylpropyl)pyridine	C1=CC=C(C=C1)CCCC2=CC=C C=N2	fresh weedy cortex nasturtium bellpepper vegetable earthy pepper green metallic	Sigma Aldrich, TGSC, OdoRactor
171	5-Phenylpentan-1-ol	5-phenylpentan-1-ol	C1=CC=C(C=C1)CCCCCO	carnation medicinal floral rose lemon verbena	Sigma Aldrich, TGSC, OdoRactor
172	4-Phenyl-1-butanol	4-phenylbutan-1-ol	C1=CC=C(C=C1)CCCCO	floral rose	TGSC
173	3-Phenyl-1-propanol	3-phenylpropan-1-ol	C1=CC=C(C=C1)CCCO	balsamic hyacinth sweet cinnamyl anisic fruit spicy floral honey	Sigma Aldrich, TGSC, Pubchem, OdoRactor

174	Cinnamic acid, 3-	3-phenylpropyl (Z)-3-phenylprop-	C1=CC=C(C=C1)CCCOC(=O)C=	sweet balsamic spicy apricot rose	OdorRactor ,TGSC,
	phenylpropyl ester	2-enoate	CC2=CC =CC=C2	fruity	Flavorbase
175	3-Phenylpropyl phenylacetate	3-phenylpropyl 2-phenylacetate	2=CC=C C=C2	balsamic hyacinth rose green spicy floral	OdorRactor ,TGSC
176	3-Phenylpropyl formate	3-phenylpropyl formate	C1=CC=C(C=C1)CCCOC=O	sweet floral honey hyacinth cinnamyl	OdorRactor ,TGSC
177	Phenethylamine	2-phenylethanamine	C1=CC=C(C=C1)CCN	fishy ammonical	TGSC, Pubchem
178	Phenethyl isothiocyanate	2-isothiocyanatoethylbenzene	C1=CC=C(C=C1)CCN=C=S	green sulfurous horseradish gooseberry watercress	Sigma Aldrich, TGSC
179	2-Phenylethanol	2-phenylethanol	C1=CC=C(C=C1)CCO	honey rose spice lilac floral dried rose sweet fresh bready aromatic	Sigma Aldrich, Flavornet, Flavorbase, TGSC, Pubchem
180	2-Phenylethyl 3-phenylprop-2-enoate	2-phenylethyl 3-phenylprop-2- enoate	C2=CC= CC=C2	balsamic rose foliage spicy fruity sweet	OdorRactor ,Sigma Aldrich, TGSC
181	Phenethyl benzoate	2-phenylethyl benzoate	C1=CC=C(C=C1)CCOC(=0)C2= CC=CC= C2	honey balsamic floral rose	Flavornet, TGSC
182	Phenethyl anthranilate	2-phenylethyl 2-aminobenzoate	C1=CC=C(C=C1)CCOC(=0)C2= CC=CC= C2N	floral sweet rose grape orange orris honey	SuperScent, TGSC, Pubchem,OdoRactor
183	Phenethyl salicylate	2-phenylethyl 2-hydroxybenzoate	C1=CC=C(C=C1)CCOC(=0)C2= CC=CC= C2O	balsamic carnation hyacinth rose floral sweet spicy	Sigma Aldrich, Flavorbase, TGSC, OdoRactor
184	Phenethyl 2-furoate	2-phenylethyl furan-2-carboxylate	C1=CC=C(C=C1)CCOC(=0)C2= CC=CO2	honey rose musty mushroom	OdorRactor ,TGSC
185	Phenethyl phenylacetate	2-phenylethyl 2-phenylacetate	C1=CC=C(C=C1)CCOC(=0)CC2 =CC=CC =C2	apricot hyacinth rose sweet floral honey balsamic green powdery cinnamyl	Sigma Aldrich, TGSC
186	2-Phenylethyl 3- hydroxypropanoate	2-phenylethyl 3- hydroxypropanoate	C1=CC=C(C=C1)CCOC(=0)CCO	floral sweet rose	TGSC
187	2-Phenylethyl formate	2-phenylethyl formate	C1=CC=C(C=C1)CCOC=O	green herbaceous rose hyacinth watercress herbaceous floral	Sigma Aldrich, TGSC, Odoractor
188	(2- Phenylethoxy)acetaldehyde	2-(2-phenylethoxy)acetaldehyde	C1=CC=C(C=C1)CCOCC=O	hyacinth green rose	OdorRactor ,TGSC
189	2-Phenylethanethiol	2-phenylethanethiol	C1=CC=C(C=C1)CCS	camphoraceous rubbery sulfurous	Sigma Aldrich, TGSC
190	Benzyl isothiocyanate	isothiocyanatomethylbenzene	C1=CC=C(C=C1)CN=C=S	cabbage medicinal horseradish oily watercress dusty	Sigma Aldrich, TGSC
191	Benzyl alcohol	phenylmethanol	C1=CC=C(C=C1)CO	berry cherry grapefruit citrus walnut sweet rose floral phenolic balsamic chemical aromatic	Sigma Aldrich, TGSC, Pubchem
192	Cinnamein	benzyl (E)-3-phenylprop-2-enoate	C1=CC=C(C=C1)COC(=0)C=CC 2=CC=C C=C2	apricot cherry chocolate floral peach pineapple sweet balsamic fruity spicy powdery coumarinic	Sigma Aldrich, TGSC, Flavorbase
193	Benzyl benzoate	benzyl benzoate	C1=CC=C(C=C1)COC(=0)C2=C C=CC=C 2	almond cheese cherry floral pineapple strawberry sweet balsamic oily herbaceous fruity aromatic powdery pleasant	Sigma Aldrich, TGSC, Pubchem
194	Benzyl anthranilate	benzyl 2-aminobenzoate	C1=CC=C(C=C1)COC(=0)C2=C C=CC=C 2N	floral grapefruit lily muguet citrus	OdorRactor ,TGSC
195	Benzyl salicylate	benzyl 2-hydroxybenzoate	C1=CC=C(C=C1)COC(=0)C2=C C=CC=C 20	floral sweet balsamic herbaceous oily clean	Sigma Aldrich, TGSC, OdoRactor, Pubchem
196	Benzyl formate	benzyl formate	C1=CC=C(C=C1)COC=O	fruity spicy cranberry black tea chemical cherry almond apricot floral pineapple sweet	Sigma Aldrich, TGSC, OdoRactor
197	Dibenzyl ether	phenylmethoxymethylbenzene	C1=CC=C(C=C1)COCC2=CC=C C=C2	almond chocolate fruity spicy sweet earthy cherry mushroom rose plastic	Sigma Aldrich, TGSC, OdoRactor
198	Benzyl mercaptan	phenylmethanethiol	C1=CC=C(C=C1)CS	meaty sharp alliaceous onion sulfurous garlic horseradish minty coffee intense radish leek vegetable repulsive	Sigma Aldrich, Flavorbase, TGSC, Pubchem
199	Dibenzyl disulfide	(benzyldisulfanyl)methylbenzene	C=C2	green smoky earthy burnt caramel	Sigma Aldrich, TGSC,OdoRactor
200	Phenol	phenol	C1=CC=C(C=C1)O	antiseptic phenolic plastic rubbery medicinal aromatic acrid sweet tarry sickening	Sigma Aldrich, Flavorbase, TGSC, Pubchem
201	Phenyl salicylate	phenyl 2-hydroxybenzoate	C1=CC=C(C=C1)OC(=O)C2=CC =CC=C2 O	sweet fruity balsamic floral woody honey	Sigma Aldrich, Flavorbase, TGSC,OdoRactor
202	Diphenyl ether	phenoxybenzene	C1=CC=C(C=C1)OC2=CC=CC= C2	floral metallic geranium green leafy phenolic	Sigma Aldrich, Flavorbase, TGSC, Pubchem

203	Phenoxyacetic acid	2-phenoxyacetic acid	C1=CC=C(C=C1)OCC(=O)O	honey sour sweet	SuperScent, TGSC, Flavorbase, OdoRactor
204	Phenoxyacetaldehyde	2-phenoxyacetaldehyde	C1=CC=C(C=C1)OCC=O	green leafy hyacinth leathery fresh	
205	2-Phenoxyethanol	2-phenoxyethanol	C1=CC=C(C=C1)OCCO	ozone cortex floral nutty floral rose balsamic cinnamyl	SuperScent, TGSC, Pubchem,
206	Ethanol, 2-phenoxy-, formate	2-phenoxyethyl formate	C1=CC=C(C=C1)OCCOC=O	aromatic balsamic powdery cinnamyl sweet	OdorRactor ,TGSC
207	Benzenethiol	benzenethiol	C1=CC=C(C=C1)S	storax sulfurous meaty phenolic	Sigma Aldrich, TGSC,
20.				alliaceous rubbery garlic repulsive penetrating	OdoRactor, Pubchem
208	Diphenyl disulfide	(phenyldisulfanyl)benzene	C1=CC=C(C=C1)SSC2=CC=CC= C2	earthy sulfurous burnt	Sigma Aldrich, Flavorbase, TGSC,OdoRactor
209	2-Benzofurancarboxaldehyde	1-benzofuran-2-carbaldehyde	C1=CC=C2C(=C1)C=C(O2)C=O	nutty tonka bitter almond fruity bitter	OdorRactor ,TGSC
210	Coumarin	chromen-2-one	C1=CC=C2C(=C1)C=CC(=O)O2	spicy green sweet new mown hay tonka coumarinic hay pleasant vanilla	Sigma Aldrich, AOD, TGSC, Pubchem
211	Quinoline	quinoline	C1=CC=C2C(=C1)C=CC=N2	medicinal musty tobacco rubbery earthy leathery penetrating unpleasant	OdorRactor ,Sigma Aldrich, TGSC, Pubchem
212	Indole	1H -indole	C1=CC=C2C(=C1)C=CN2	buttery cheese chocolate fatty fishy grape green honey jasmine musty earthy vanilla winey mothball burnt animal floral naphthyl fecal pungent erogenic unpleasant sewage	Sigma Aldrich, Flavorbase, TGSC, Pubchem
213	Benzothiazole	1,3-benzothiazole	C1=CC=C2C(=C1)N=CS2	sulfurous gasoline rubbery vegetable cooked nutty coffee meaty brown unpleasant	Sigma Aldrich, TGSC, Pubchem
214	2-[(1h-Benzimidazol-2- ylmethyl)sulfanyl]-n- (naphthalen-2-yl)acetamide	2-(1 <i>H</i> -benzimidazol-2- ylmethylsulfanyl)- <i>N</i> - naphthalen- 2-ylacetamide	C1=CC=C2C=C(C=CC2=C1)NC(=O)CSC C3=NC4=CC=CC=C4N	alliaceous dairy sulfurous milky vegetable	OdorRactor ,TGSC
215	Naphthalen-2-yl 2- aminobenzoate	naphthalen-2-yl 2-aminobenzoate	C1=CC=C2C=C(C=CC2=C1)OC(=O)C3= CC=CC=C3N	floral neroli grape sweet candy fruity berry winey	OdorRactor ,TGSC
216	2-Naphthalenethiol	naphthalene-2-thiol	C1=CC=C2C=C(C=CC2=C1)S	sulfurous rubbery meaty roasted woody creamy oily brown brothy	Sigma Aldrich, TGSC
217	Naphthalene	naphthalene	C1=CC=C2C=CC=CC2=C1	mushroom tarry pungent dry resinous naphthyl aromatic mothball characteristic	Flavornet, TGSC
218	Isoquinoline	isoquinoline	C1=CC=C2C=NC=CC2=C1	sweet balsamic herbaceous anisic bitter almond penetrating unpleasant bitter	OdorRactor ,TGSC, Pubchem
219	Benzene	benzene	C1=CC=CC=C1	aromatic gasoline	AOD, ADB, TGSC, Pubchem
220	2-Pyridinemethanethiol	pyridin-2-ylmethanethiol	C1=CC=NC(=C1)CS	roasted roasted meat beefy sulfurous savory pork clean meaty	OdorRactor ,TGSC
221	Pyridine	pyridine	C1=CC=NC=C1	fishy sour putrid ammonical burnt sharp nauseating sickening	Sigma Aldrich, TGSC, Pubchem
222	5- (Pentafluorobenzoylamino)Fl uorescein	2,3,4,5,6-pentafluoro- <i>N</i> -(3,3',6'-trihydroxyspiro[3 <i>H</i> -2-benzofuran-1,9'-xanthene]-5- yl)benzamide	C1=CC2=C(C=C1NC(=O)C3=C(C(=C(C) C(=C3F)F)F)F)F)C(OC24C5=C(C=C (C=C5) O)OC6=C4C=CC(=C6)O)O	mentholic sweet fruity valerian root	OdorRactor ,TGSC
223	1-Furfurylpyrrole	1-(furan-2-ylmethyl)pyrrole	C1=CN(C=C1)CC2=CC=CO2	green vegetable earthy plastic wax fruity coffee cereal bready radish mushroom potato	Sigma Aldrich, OdoRactor
224	Pyrazineethanethiol	2-pyrazin-2-ylethanethiol	C1=CN=C(C=N1)CCS	cabbage green meaty sulfurous savory roasted burnt beefy chicken pork	Sigma Aldrich, TGSC, Flavorbase, OdoRactor
225	2-Mercaptomethylpyrazine	pyrazin-2-ylmethanethiol	C1=CN=C(C=N1)CS	roasted meat caramel roasted meaty	OdorRactor ,TGSC
226	Pyrazine	pyrazine	C1=CN=CC=N1	hazelnut pungent corn nutty sweet roasted roasted hazelnut roasted barley	Sigma Aldrich, TGSC,OdoRactor
227	Pyrrole-2-carboxaldehyde	1 <i>H</i> -pyrrole-2-carbaldehyde	C1=CNC(=C1)C=O	musty beefy coffee	OdorRactor ,TGSC
	2-Mercaptopyrimidine Pyrrole	1H-pyrimidine-2-thione 1H-pyrrole	C1=CNC(=S)N=C1 C1=CNC=C1	green onion nutty ethereal sweet warm	TGSC Sigma Aldrich, TGSC,
				chloroform nutty spicy woody green grassy	OdoRactor, Pubchem Sigma Aldrich, TGSC,
230	3-(2-Furyl)acrolein	(E)-3-(furan-2-yl)prop-2-enal	C1=COC(=C1)C=CC=O	fruity vanilla cinnamyl	OdoRactor, Pubchem
231	Furfural	furan-2-carbaldehyde	C1=COC(=C1)C=O	almond woody sweet bready bacon brown caramel phenolic	Sigma Aldrich, TGSC, Pubchem

232	2,4-Difurfurylfuran	2,4-bis(furan-2-ylmethyl)furan	C1=COC(=C1)CC2=CC(=CO2)C	floral fruity	OdorRactor ,TGSC
233	Furfuryl alcohol	furan-2-ylmethanol	C3=CC= CO3 C1=COC(=C1)CO	sulfurous estery brown burnt	TGSC, Pubchem
233	Turiuryi aconor	ruran-2-yimethanoi	e1-c0c(-c1)c0	coffee oily whiskey bready alcoholic chemical musty sweet caramel	Tose, rubenem
234	Furfuryl formate	furan-2-ylmethyl formate	C1=COC(=C1)COC=O	ethereal bready brown coffee	OdorRactor ,TGSC, Flavorbase
235	Difurfuryl ether	2-(furan-2-ylmethoxymethyl)furan	C1=COC(=C1)COCC2=CC=CO2	coffee nutty earthy	OdorRactor ,TGSC
236	Furfuryl mercaptan	furan-2-ylmethanethiol	C1=COC(=C1)CS	caramel chocolate coffee fishy meaty oily wax herbaceous smoky nutty sulfurous roasted coffee fatty burnt savory chicken cooked onion roasted	Sigma Aldrich, TGSC
237	2-Furanmethanethiol formate	S -(furan-2-ylmethyl) methanethioate	C1=COC(=C1)CSC=O	sulfurous butterscotch coffee horseradish ethereal spicy winey nutty	Sigma Aldrich, TGSC, OdoRactor
238	Difurfuryl sulfide	2-(furan-2- ylmethylsulfanylmethyl)furan	C1=COC(=C1)CSCC2=CC=CO2	cheese coffee green meaty nutty earthy sulfurous mushroom fungal roasted meat roasted cocoa	Sigma Aldrich, TGSC, OdoRactor
239	Difurfuryl disulfide	2-[(furan-2- ylmethyldisulfanyl)methyl]furan	C1=COC(=C1)CSSCC2=CC=CO 2	sulfurous onion coffee roasted chicken cabbage roasted meat roasted coffee potato meaty	Sigma Aldrich, Flavorbase, TGSC
240	Furan	furan	C1=COC=C1	ethereal strong	Pubchem
241	3-Furaldehyde	furan-3-carbaldehyde	C1=C0C=C1C=0	sulfurous	Sigma Aldrich
242	Thiophene-2-carbaldehyde 2-Thiophenemethanol	thiophene-2-carbaldehyde thiophen-2-ylmethanol	C1=CSC(=C1)C=O C1=CSC(=C1)CO	sulfurous savory coffee roasted coffee ethereal fermented burnt alliaceous roasted	Flavornet TGSC, Flavorbase
244	2-Thiophenemethanethiol	thiophen-2-ylmethanethiol	C1=CSC(=C1)CS	sulfurous coffee roasted coffee fishy roasted	Flavornet, TGSC, OdoRactor
245	Thiophene-2-thiol	thiophene-2-thiol	C1=CSC(=C1)S	caramel coffee burnt roasted coffee roasted	Sigma Aldrich, TGSC, Odoractor
246	2-Thienyl disulfide	2-(thiophen-2- yldisulfanyl)thiophene	C1=CSC(=C1)SSC2=CC=CS2	mushroom rubbery earthy	Sigma Aldrich, TGSC, OdoRactor
247	Thiophene	thiophene	C1=CSC=C1	garlic alliaceous sulfurous aromatic	Flavornet, TGSC, Pubchem, OdoRactor
248	3-Thiophenethiol	thiophene-3-thiol	C1=CSC=C1S	cooked meaty garlic	Flavornet, TGSC, OdoRactor
249	Thiazole	1,3-thiazole	C1=CSC=N1	nutty meaty pyridine fishy foul	Sigma Aldrich, TGSC,OdoRactor
250	Disodium 5'-inosinate	disodium;[(2R ,3S ,4R ,5R)-3,4-dihydroxy-5-(6- oxo-1H -purin-9-yl)oxolan-2-yl]methyl phosphate	C1=NC2=C(C(=O)N1)N=CN2C3 C(C(C(O 3)COP(=O)([O-])[O-])O)O.[Na+].[Na+]	salty meaty umami	Flavorbase
251	Cubenene	pentacyclo[4.2.0.02,5.03,8.04,7]o cta-1,3-diene	C12C3C4C1=C5C2C3=C45	spice fruit mango	Flavornet, TGSC
252	2,3-Dihydro-1,4-benzodioxin- 2-one		C1C(=0)OC2=CC=CC=C2O1	green coumarinic	TGSC
253	2-Benzyl-1,3-dioxan-5-ol	2-benzyl-1,3-dioxan-5-ol	C1C(COC(O1)CC2=CC=CC=C2) O	floral green honey dried rose tearose leafy powdery petitgrain lavender hyacinth rose	OdorRactor,
254	Styrene oxide	2-phenyloxirane	C1C(O1)C2=CC=CC=C2	faint sweet pleasant	Sigma Aldrich, Pubchem
255	Phenylacetaldehyde glyceryl acetal	(2-benzyl-1,3-dioxolan-4- yl)methanol	C1C(OC(O1)CC2=CC=CC=C2)C O	floral green honey dried rose tearose leafy powdery petitgrain lavender hyacinth rose	OdorRactor ,Sigma Aldrich, TGSC, Flavorbase
256	5,7-Dihydroxy-2-(4- hydroxyphenyl)chroman-4- one	5,7-dihydroxy-2-(4- hydroxyphenyl)-2,3- dihydrochromen-4-one	C1C(OC2=CC(=CC(=C2C1=O)O) O)C3=C C=C(C=C3)O	faint	Flavornet
257	1,3-Dihydroxyacetone dimer	2,5-bis(hydroxymethyl)-1,4- dioxane-2,5-diol	C1C(OCC(O1)(CO)O)(CO)O	cooling sweet mild fruity	OdorRactor ,TGSC, Flavorbase
258	1,4-Dithiane-2,5-diol	1,4-dithiane-2,5-diol	C1C(SCC(S1)O)O	meaty sulfurous eggy tomato toasted bready brothy grilled pungent	Sigma Aldrich,TGSC, Flavorbase, Pubchem, OdoRactor
259	2(5H)-Furanone	2H -furan-5-one	C1C=CC(=O)O1	buttery	OdorRactor ,TGSC
260	2H-Pyran Phthalide	2H -pyran 3H -2-benzofuran-1-one	C1C=CC=CO1 C1C2=CC=CC=C2C(=0)O1	smoky coconut coumarinic sweet tonka powdery phenolic lactonic	Sigma Aldrich, TGSC
262	1a,7b-Dihydro-1H- cyclopropa[c]chromen-2- one	1a ,7b -dihydro-1H - cyclopropa[c]chromen-2-one	C1C2C1C(=O)OC3=CC=CC=C23	sweet green spicy coumarinic nutty vanilla	OdorRactor ,TGSC
263	4,4a,5,9b- Tetrahydroindeno(1,2-d)-1,3- dioxin	4,4 <i>a</i> ,5,9 <i>b</i> -tetrahydroindeno[1,2-d][1,3]dioxine	C1C2COCOC2C3=CC=CC=C31	animal earthy jasmine fecal indole floral	OdorRactor ,TGSC, Flavorbase

264	2-Hydroxycyclopent-2-en-1-	2-hydroxycyclopent-2-en-1-one	C1CC(=O)C(=C1)O	maple caramel	TGSC
265	one L-Pyroglutamic acid	(2S)-5-oxopyrrolidine-2-	C1CC(=O)NC1C(=O)O	mild sweet ethereal	OdorRactor ,TGSC
266	gamma-Butyrolactone	carboxylic acid oxolan-2-one	C1CC(=O)OC1	caramel sweet oily fatty creamy	Sigma Aldrich, TGSC,
267	3,4-Dihydrocoumarin	3,4-dihydrochromen-2-one	C1CC(=O)OC2=CC=CC=C21	pleasant almond coconut creamy herbaceous tobacco sweet vanilla tonka coumarinic cinnamyl spicy herbaceous milky cocoa rose aromatic hay	Pubchem Sigma Aldrich, Flavorbase, TGSC, Pubchem
268	Dihydro-2(3H)-thiophenone	thiolan-2-one	C1CC(=O)SC1	burnt garlic	TGSC
269	2-(3- Phenylpropyl)tetrahydrofuran	2-(3-phenylpropyl)oxolane	C1CC(OC1)CCCC2=CC=CC=C2	sweet fruity green	OdorRactor,
270	Tetrahydrofurfuryl alcohol	oxolan-2-ylmethanol	C1CC(OC1)CO	vegetable cauliflower warm oily caramel	Sigma Aldrich, TGSC, Pubchem
271	Tetrahydrofurfuryl cinnamate	oxolan-2-ylmethyl (E)-3- phenylprop-2-enoate	C1CC(OC1)COC(=0)C=CC2=CC =CC=C2	balsamic sweet cortex	OdorRactor ,TGSC
272	(Tetrahydrofuryl)methyl phenylacetate	oxolan-2-ylmethyl 2-phenylacetate	C1CC(OC1)COC(=O)CC2=CC=C C=C2	,	OdorRactor ,TGSC
273 274	2-Cyclohexen-1-one 1-Pyrroline	cyclohex-2-en-1-one 3,4-dihydro-2 <i>H</i> -pyrrole	C1CC=CC(=0)C1 C1CC=NC1	pesticide roasted savory green ammonical shrimp seafood	Flavornet, TGSC OdorRactor ,TGSC
275	Indane	2,3-dihydro-1 <i>H</i> -indene	C1CC2=CC=CCC1	varnish	Subtractor, TODE
	1,2,3,4-Tetrahydroquinoline	1,2,3,4-tetrahydroquinoline	C1CC2=CC=CC=C2NC1	civet honey animal phenolic	Sigma Aldrich, TGSC, OdoRactor
277	Butanal, 4-(octahydro-4,7- methano-5H- inden-5- ylidene)-	(4E)-4-(8-tricyclo[5.2.1.02,6]decanylidene)b utanal	C1CC2C(C1)C3CC2CC3=CCCC =0	floral sweet muguet aldehydic wax	OdorRactor ,TGSC
278	Decahydrospiro[furan- 2(3H),5'- [4,7]methano[5h]indene]	spiro[oxolane-2,8'- tricyclo[5.2.1.02,6]decane]	C1CC2C(C1)C3CC2CC34CCCO4	fresh citrus grapefruit rhubarb vetiver floral gardenia	OdorRactor ,TGSC
279	4,7-Methano-1H-indene-5- acetaldehyde, octahydro-	2-(8- tricyclo[5.2.1.02,6]decanyl)acetal dehyde	C1CC2C(C1)C3CC2CC3CC=0	floral muguet lily	TGSC
280	Tricyclodecanedimethanol	[8-(hydroxymethyl)-3- tricyclo[5.2.1.02,6]decanyl]metha nol	C1CC2C3CC(C2C1CO)CC3CO	sweet amber musk floral sandal wood	OdorRactor ,TGSC
281	Octahydro-4,7-methano-1H-indenecarbaldehyde	tricyclo[5.2.1.02,6]decane-3- carbaldehyde	C1CC2CC1C3C2C(CC3)C=O	green melon aldehydic fresh	OdorRactor ,TGSC
282	2-Cyclohexylidene-2- phenylacetonitrile	2-cyclohexylidene-2- phenylacetonitrile	C1CCC(=C(C#N)C2=CC=CC=C2)CC1	floral geranium grapefruit peony fresh	OdorRactor ,TGSC
283	1,2-Cyclohexanedione	cyclohexane-1,2-dione	C1CCC(=0)C(=0)C1	sweet acorn nutty maple caramel brothy	OdorRactor ,TGSC
284	Cyclopentanone	cyclopentanone	C1CCC(=O)C1	minty peppermint ethereal	Sigma Aldrich, TGSC, OdoRactor, Pubchem
285	Cyclohexanone	cyclohexanone	C1CCC(=0)CC1	minty acetone pleasant	Sigma Aldrich, AOD, TGSC, OdoRactor, Pubchem
286	Caprolactam	azepan-2-one	C1CCC(=O)NCC1	faint unpleasant	Sigma Aldrich, TGSC, OdoRactor, Pubchem
287	2,5-Dicyclopentyl cyclopentanol	2,5-dicyclopentylcyclopentan-1-ol	C1CCC(C1)C2CCC(C2O)C3CCC C3	tropical fruity tropical fruit floral musk	TGSC
288	2-Cyclopentylcyclopentanone	2-cyclopentylcyclopentan-1-one	C1CCC(C1)C2CCCC2=O	fruity green minty aldehydic woody	TGSC
289	Cyclopentanethiol	cyclopentanethiol	CICCC(C1)S	green meaty sulfurous alliaceous onion garlic horseradish vegetable celery eggy	Flavornet, TGSC, OdoRactor
290	Cyclohexanecarboxylic acid	cyclohexanecarboxylic acid	C1CCC(CC1)C(=0)O	fruity acidic metallic cheese tropical fatty tropical fruit	OdorRactor ,SuperScent, Sigma Aldrich, TGSC
291	4-Cyclohexylcyclohexanone	4-cyclohexylcyclohexan-1-one	C1CCC(CC1)C2CCC(=0)CC2	floral orris woody cyclamen ozone fresh	OdorRactor ,TGSC
292	2-Cyclohexylcyclohexanone	2-cyclohexylcyclohexan-1-one	C1CCC(CC1)C2CCCCC2=O	sweet herbaceous cumin minty cyclamen woody orris ozone	OdorRactor ,TGSC
293	Cyclohexylacetic acid	2-cyclohexylacetic acid	C1CCC(CC1)CC(=0)O	acidic sharp acetic jasmine fatty cheese musty powdery honey caramel	Sigma Aldrich, TGSC, OdoRactor
294	(Cyclohexylmethyl)pyrazine	2-(cyclohexylmethyl)pyrazine	C1CCC(CC1)CC2=NC=CN=C2	green musty nutty earthy cocoa	OdorRactor ,TGSC, Flavorbase
295	3-Cyclohexylpropyl formate	3-cyclohexylpropyl formate	C1CCC(CC1)CCCOC=O	green metallic cinnamyl	TGSC
296	2-Cyclohexylethanol	2-cyclohexylethanol	C1CCC(CC1)CCO	floral wax cooling green peony lily dewy rose	SuperScent, TGSC
297	Cyclohexanol	cyclohexanol	C1CCC(CC1)O	camphoraceous mentholic phenolic	TGSC, Pubchem
298	Cyclohexyl cinnamate	cyclohexyl (E)-3-phenylprop-2-enoate	=CC=C2	fruity peach cherry bitter almond bitter	OdorRactor ,TGSC
299	Cyclohexyl benzoate	cyclohexyl benzoate	C1CCC(CC1)OC(=O)C2=CC=CC =C2	mild balsamic floral herbaceous	SuperScent, TGSC, OdoRactor

302 Cyclohe 303 Cyclohe 304 Benzen (cyclohe 305 Cyclohe 306 Dicyclo 307 Hexahy 308 5,6,7,8- Tetrahy 309 Octahyu 2-one 310 2-Naphi 311 Decahyu formate 312 8-Cyclo 313 Civeton 314 Isoambi 315 1-Oxasj 316 (7E)-Cy one 317 1,7-Dio one	exybenzoate nexyl phenylacetate nexyl formate nex, [2- hexyloxy)ethyl]- nexanethiol ohexyl disulfide ydrocoumarin 3- ydroquinoxaline ydro-2H-1-benzopyran- hthalenol, decahydro- ydro-2-naphthyl ite lohexadecenone nne brettolide spiro[4.7]dodecane	cyclohexyl 2-phenylacetate cyclohexyl formate 2-cyclohexyloxyethylbenzene cyclohexanethiol (cyclohexyldisulfanyl)cyclohexane 3,4,5,6,7,8-hexahydrochromen-2- one 5,6,7,8-tetrahydroquinoxaline 3,4,4a ,5,6,7,8,8a - octahydrochromen-2-one 1,2,3,4,4a ,5,6,7,8,8a - decahydronaphthalen-2-ol 1,2,3,4,4a ,5,6,7,8,8a - decahydronaphthalen-2-yl formate (8E)-cyclohexadec-8-en-1-one (9Z)-cycloheptadec-9-en-1-one	2 C1CCC(CC1)S C1CCC(CC1)SSC2CCCCC2 C1CCC2=C(C1)CCC(=0)O2 C1CCC2=NC=CN=C2C1 C1CCC2C(C1)CCC(=0)O2 C1CCC2C(CCC2C1)O C1CCC2CC(CCC2C1)O C1CCC2CC(CCCCCC(=0)CCC 1 C1CCCC=CCCCCCCC(=0)CCC	floral honey rose ethereal cooling sweet fruity banana cherry jammy floral hyacinth green metallic fruity raspberry balsamic sulfurous offensive disagreeable alliaceous onion eggy nutty coffee clam seafood coconut tonka coumarinic cheese musty nutty roasted beany cereal corn sweet herbaceous coumarinic tonka woody creamy lactonic coconut milky vanilla rose minty muguet clean floral	TGSC Sigma Aldrich, TGSC, OdoRactor OdorRactor ,TGSC Sigma Aldrich, TGSC,OdoRactor OdorRactor ,TGSC
302 Cyclohe 303 Cyclohe 304 Benzen (cyclohe 305 Cyclohe 306 Dicyclo 307 Hexahy 308 5,6,7,8- Tetrahy 309 Octahyu 2-one 310 2-Naphi 311 Decahyu formate 312 8-Cyclo 313 Civeton 314 Isoambi 315 1-Oxasj 316 (7E)-Cy one 317 1,7-Dio one	nexyl phenylacetate nexyl formate ne, [2- hexyloxy)ethyl]- nexanethiol ohexyl disulfide ydrocoumarin 3- ydroquinoxaline ydro-2H-1-benzopyran- hthalenol, decahydro- ydro-2-naphthyl ie lohexadecenone nne brettolide spiro[4.7]dodecane	cyclohexyl formate 2-cyclohexyloxyethylbenzene cyclohexanethiol (cyclohexyldisulfanyl)cyclohexane 3,4,5,6,7,8-hexahydrochromen-2- one 5,6,7,8-tetrahydroquinoxaline 3,4,4a ,5,6,7,8,8a - octahydrochromen-2-one 1,2,3,4,4a ,5,6,7,8,8a - decahydronaphthalen-2-ol 1,2,3,4,4a ,5,6,7,8,8a - decahydronaphthalen-2-yl formate (8E)-cyclohexadec-8-en-1-one (9Z)-cyclohexadec-9-en-1-one (10Z)-1-oxacycloheptadec-10-en-	C1CCC(CC1)OC(=0)CC2=CC=C C=C2 C1CCC(CC1)OCC=O C1CCC(CC1)OCC2=CC=CC=C 2 C1CCC(CC1)S C1CCC(CC1)SSC2CCCCC2 C1CCC2=C(C1)CCC(=0)O2 C1CCC2=NC=CN=C2C1 C1CCC2C(CC1)CCC(=0)O2 C1CCC2C(CCC2C1)O C1CCC2CC(CCC2C1)OC=O	ethereal cooling sweet fruity banana cherry jammy floral hyacinth green metallic fruity raspberry balsamic sulfurous offensive disagreeable alliaceous onion eggy nutty coffee clam seafood coconut tonka coumarinic cheese musty nutty roasted beany cereal corn sweet herbaceous coumarinic tonka woody creamy lactonic coconut milky vanilla rose minty muguet clean floral sandal wood woody oily floral dry musk laundered cloth dry balsamic	SuperScent, TGSC, OdoRactor OdorRactor ,TGSC TGSC, Pubchem OdorRactor ,TGSC TGSC Sigma Aldrich, TGSC, OdoRactor OdorRactor ,TGSC Sigma Aldrich, TGSC OdoRactor OdorRactor ,TGSC
303 Cyclohe 304 Benzen (cyclohe 305 Cyclohe 306 Dicyclo 307 Hexahy 308 5,6,7,8- Tetrahy 309 Octahyt 2-one 310 2-Napht 311 Decahyt formate 312 8-Cyclo 313 Civeton 314 Isoambt 315 1-Oxasp 316 (7E)-Cy one 317 1,7-Dio one	nexyl formate ne, [2- hexyloxy)ethyl]- nexanethiol ohexyl disulfide ydrocoumarin 3- ydroquinoxaline ydro-2H-1-benzopyran- hthalenol, decahydro- ydro-2-naphthyl ie lohexadecenone ne brettolide spiro[4.7]dodecane	cyclohexyl formate 2-cyclohexyloxyethylbenzene cyclohexanethiol (cyclohexyldisulfanyl)cyclohexane 3,4,5,6,7,8-hexahydrochromen-2- one 5,6,7,8-tetrahydroquinoxaline 3,4,4a ,5,6,7,8,8a - octahydrochromen-2-one 1,2,3,4,4a ,5,6,7,8,8a - decahydronaphthalen-2-ol 1,2,3,4,4a ,5,6,7,8,8a - decahydronaphthalen-2-yl formate (8E)-cyclohexadec-8-en-1-one (9Z)-cyclohexadec-9-en-1-one (10Z)-1-oxacycloheptadec-10-en-	C=C2 C1CCC(CC1)OC=O C1CCC(CC1)OCC2=CC=CC=C 2 C1CCC(CC1)S C1CCC(CC1)SSC2CCCCC2 C1CCC2=C(C1)CCC(=0)O2 C1CCC2=NC=CN=C2C1 C1CCC2C(C1)CCC(=0)O2 C1CCC2C(CCC2C1)O C1CCC2CC(CCC2C1)OC=O C1CCC2CC(CCCCCC(=0)CCC 1 C1CCCC=CCCCCCCCC(=0)CCC	ethereal cooling sweet fruity banana cherry jammy floral hyacinth green metallic fruity raspberry balsamic sulfurous offensive disagreeable alliaceous onion eggy nutty coffee clam seafood coconut tonka coumarinic cheese musty nutty roasted beany cereal corn sweet herbaceous coumarinic tonka woody creamy lactonic coconut milky vanilla rose minty muguet clean floral sandal wood woody oily floral dry musk laundered cloth dry balsamic	SuperScent, TGSC, OdoRactor OdorRactor, TGSC TGSC, Pubchem OdorRactor, TGSC TGSC Sigma Aldrich, TGSC, OdoRactor OdorRactor, TGSC Sigma Aldrich, TGSC OdoRactor OdorRactor, TGSC
304 Benzence (cyclohe) 305 Cyclohe 306 Dicyclo 307 Hexahy 308 5,6,7,8- Tetrahy 309 Octahyc 2-one 310 2-Naphi 311 Decahyc formate 312 8-Cyclo 313 Civeton 314 Isoambi 315 1-Oxasj 316 (7E)-Cy one 317 1,7-Dio one	ne, [2- hexyloxy)ethyl]- nexanethiol ohexyl disulfide ydrocoumarin 3- ydroquinoxaline ydro-2H-1-benzopyran- hthalenol, decahydro- ydro-2-naphthyl te lohexadecenone one brettolide spiro[4.7]dodecane	2-cyclohexyloxyethylbenzene cyclohexanethiol (cyclohexyldisulfanyl)cyclohexane 3,4,5,6,7,8-hexahydrochromen-2- one 5,6,7,8-tetrahydroquinoxaline 3,4,4a ,5,6,7,8,8a - octahydrochromen-2-one 1,2,3,4,4a ,5,6,7,8,8a - decahydronaphthalen-2-ol 1,2,3,4,4a ,5,6,7,8,8a - decahydronaphthalen-2-yl formate (8E)-cyclohexadec-8-en-1-one (9Z)-cycloheptadec-9-en-1-one (10Z)-1-oxacycloheptadec-10-en-	C1CCC(CC1)OCCC2=CC=CC=C 2 C1CCC(CC1)S C1CCC(CC1)SSC2CCCCC2 C1CCC2=C(C1)CCC(=0)O2 C1CCC2=NC=CN=C2C1 C1CCC2C(C1)CCC(=0)O2 C1CCC2C(CCC2C1)O C1CCC2CC(CCC2C1)O C1CCC2CC(CCCCCC1)OC=O C1CCCCCCCCCCCCCC(=0)CCC 1 C1CCCC=CCCCCCCCC(=0)CCC	banana cherry jammy floral hyacinth green metallic fruity raspberry balsamic sulfurous offensive disagreeable alliaceous onion eggy nutty coffee clam seafood coconut tonka coumarinic cheese musty nutty roasted beany cereal corn sweet herbaceous coumarinic tonka woody creamy lactonic coconut milky vanilla rose minty muguet clean floral sandal wood woody oily floral dry musk laundered cloth dry balsamic	OdoRactor OdorRactor ,TGSC TGSC, Pubchem OdorRactor ,TGSC TGSC Sigma Aldrich, TGSC, OdoRactor OdorRactor ,TGSC Sigma Aldrich, TGSC OdoRactor OdorRactor ,TGSC
(cyclohe 305 Cyclohe 306 Dicyclo 307 Hexahy 308 5,6,7,8- Tetrahy 309 Octahyo 2-one 310 2-Naphr 311 Decahyo formate 312 8-Cyclo 313 Civeton 314 Isoambr 315 1-Oxasp 316 (7E)-Cy one 317 1,7-Dio one	hexyloxy)ethyl]- nexanethiol ohexyl disulfide ydrocoumarin 3- ydroquinoxaline ydro-2H-1-benzopyran- hthalenol, decahydro- ydro-2-naphthyl ie lohexadecenone one brettolide spiro[4.7]dodecane	cyclohexanethiol (cyclohexyldisulfanyl)cyclohexane 3,4,5,6,7,8-hexahydrochromen-2- one 5,6,7,8-tetrahydroquinoxaline 3,4,4a ,5,6,7,8,8a - octahydrochromen-2-one 1,2,3,4,4a ,5,6,7,8,8a - decahydronaphthalen-2-ol 1,2,3,4,4a ,5,6,7,8,8a - decahydronaphthalen-2-yl formate (8E)-cyclohexadec-8-en-1-one (9Z)-cycloheptadec-9-en-1-one (10Z)-1-oxacycloheptadec-10-en-	2 C1CCC(CC1)S C1CCC(CC1)SSC2CCCCC2 C1CCC2=C(C1)CCC(=0)O2 C1CCC2=NC=CN=C2C1 C1CCC2C(C1)CCC(=0)O2 C1CCC2C(CCC2C1)O C1CCC2CC(CCC2C1)O C1CCC2CC(CCCCCC(=0)CCC 1 C1CCCC=CCCCCCCC(=0)CCC	fruity raspberry balsamic sulfurous offensive disagreeable alliaceous onion eggy nutty coffee clam seafood coconut tonka coumarinic cheese musty nutty roasted beany cereal corn sweet herbaceous coumarinic tonka woody creamy lactonic coconut milky vanilla rose minty muguet clean floral sandal wood woody oily floral dry musk laundered cloth dry balsamic	TGSC, Pubchem OdorRactor ,TGSC TGSC Sigma Aldrich, TGSC, OdoRactor OdorRactor ,TGSC Sigma Aldrich, TGSC OdorRactor ,TGSC OdorRactor ,TGSC
306 Dicyclo 307 Hexahy 308 5,6,7,8- Tetrahy 309 Octahyc 2-one 310 2-Naphi 311 Decahyc formate 312 8-Cyclo 313 Civeton 314 Isoambi 315 1-Oxasj 316 (7E)-Cy one 317 1,7-Dio one	ohexyl disulfide ydrocoumarin 3- ydroquinoxaline ydro-2H-1-benzopyran- hthalenol, decahydro- ydro-2-naphthyl ie lohexadecenone brettolide spiro[4.7]dodecane	(cyclohexyldisulfanyl)cyclohexane 3,4,5,6,7,8-hexahydrochromen-2- one 5,6,7,8-tetrahydroquinoxaline 3,4,4a ,5,6,7,8,8a - octahydrochromen-2-one 1,2,3,4,4a ,5,6,7,8,8a - decahydronaphthalen-2-ol 1,2,3,4,4a ,5,6,7,8,8a - decahydronaphthalen-2-yl formate (8E)-cyclohexadec-8-en-1-one (9Z)-cycloheptadec-9-en-1-one (10Z)-1-oxacycloheptadec-10-en-	C1CCC(CC1)SSC2CCCCC2 C1CCC2=C(C1)CCC(=0)O2 C1CCC2=NC=CN=C2C1 C1CCC2C(C1)CCC(=0)O2 C1CCC2CC(CCC2C1)O C1CCC2CC(CCC2C1)OC=O C1CCC2CC(CCCCCC(=0)CCC 1 C1CCCC=CCCCCCCC(=0)CCC	alliaceous onion eggy nutty coffee clam seafood coconut tonka coumarinic cheese musty nutty roasted beany cereal corn sweet herbaceous coumarinic tonka woody creamy lactonic coconut milky vanilla rose minty muguet clean floral sandal wood woody oily floral dry musk laundered cloth dry balsamic	OdorRactor ,TGSC TGSC Sigma Aldrich, TGSC, OdoRactor OdorRactor ,TGSC Sigma Aldrich, TGSC,OdoRactor OdorRactor ,TGSC
307 Hexahy 308 5,6,7,8 Tetrahy 309 Octahyo 2-one 310 2-Naphi 311 Decahyo formate 312 8-Cyclo 313 Civeton 314 Isoambi 315 1-Oxasj 316 (7E)-Cy one 317 1,7-Dio one	ydrocoumarin 3- ydroquinoxaline ydro-2H-1-benzopyran- hthalenol, decahydro- ydro-2-naphthyl te lohexadecenone one brettolide spiro[4.7]dodecane	3,4,5,6,7,8-hexahydrochromen-2- one 5,6,7,8-tetrahydroquinoxaline 3,4,4a ,5,6,7,8,8a - octahydrochromen-2-one 1,2,3,4,4a ,5,6,7,8,8a - decahydronaphthalen-2-ol 1,2,3,4,4a ,5,6,7,8,8a - decahydronaphthalen-2-yl formate (8E)-cyclohexadec-8-en-1-one (9Z)-cycloheptadec-9-en-1-one (10Z)-1-oxacycloheptadec-10-en-	C1CCC2=C(C1)CCC(=0)O2 C1CCC2=NC=CN=C2C1 C1CCC2C(C1)CCC(=0)O2 C1CCC2CC(CCC2C1)O C1CCC2CC(CCC2C1)OC=O C1CCCC=CCCCCCCC(=0)CCC 1 C1CCCC=CCCCCCCC(=0)CCC	clam seafood coconut tonka coumarinic cheese musty nutty roasted beany cereal corn sweet herbaceous coumarinic tonka woody creamy lactonic coconut milky vanilla rose minty muguet clean floral sandal wood woody oily floral dry musk laundered cloth dry balsamic	TGSC Sigma Aldrich, TGSC, OdoRactor OdorRactor ,TGSC Sigma Aldrich, TGSC,OdoRactor OdorRactor ,TGSC
308 5,6,7,8- Tetrahy 309 Octahyc 2-one 310 2-Naphi 311 Decahyc formate 312 8-Cyclo 313 Civeton 314 Isoambi 315 1-Oxasj 316 (7E)-Cy one 317 1,7-Dio one	3- ydroquinoxaline ydro-2H-1-benzopyran- hthalenol, decahydro- ydro-2-naphthyl te lohexadecenone one brettolide spiro[4.7]dodecane	one 5,6,7,8-tetrahydroquinoxaline 3,4,4a ,5,6,7,8,8a - octahydrochromen-2-one 1,2,3,4,4a ,5,6,7,8,8a - decahydronaphthalen-2-ol 1,2,3,4,4a ,5,6,7,8,8a - decahydronaphthalen-2-yl formate (8E)-cyclohexadec-8-en-1-one (9Z)-cycloheptadec-9-en-1-one (10Z)-1-oxacycloheptadec-10-en-	C1CCC2=NC=CN=C2C1 C1CCC2C(C1)CCC(=0)O2 C1CCC2CC(CCC2C1)O C1CCC2CC(CCC2C1)OC=O C1CCCC=CCCCCCCC(=0)CCC 1 C1CCCC=CCCCCCCC(=0)CCC	coconut tonka coumarinic cheese musty nutty roasted beany cereal corn sweet herbaceous coumarinic tonka woody creamy lactonic coconut milky vanilla rose minty muguet clean floral sandal wood woody oily floral dry musk laundered cloth dry balsamic	Sigma Aldrich, TGSC, OdoRactor OdorRactor ,TGSC Sigma Aldrich, TGSC,OdoRactor OdorRactor ,TGSC
Tetrahy 309 Octahyo 2-one	3- ydroquinoxaline ydro-2H-1-benzopyran- hthalenol, decahydro- ydro-2-naphthyl ie lohexadecenone brettolide spiro[4.7]dodecane	5,6,7,8-tetrahydroquinoxaline 3,4,4a ,5,6,7,8,8a - octahydrochromen-2-one 1,2,3,4,4a ,5,6,7,8,8a - decahydronaphthalen-2-ol 1,2,3,4,4a ,5,6,7,8,8a - decahydronaphthalen-2-yl formate (8E)-cyclohexadec-8-en-1-one (9Z)-cycloheptadec-9-en-1-one (10Z)-1-oxacycloheptadec-10-en-	C1CCC2C(C1)CCC(=0)02 C1CCC2CC(CCC2C1)0 C1CCC2CC(CCC2C1)0C=0 C1CCCC=CCCCCCCC(=0)CCC 1 C1CCCC=CCCCCCCC(=0)CCC	cereal corn sweet herbaceous coumarinic tonka woody creamy lactonic coconut milky vanilla rose minty muguet clean floral sandal wood woody oily floral dry musk laundered cloth dry balsamic	OdoRactor OdorRactor ,TGSC Sigma Aldrich, TGSC,OdoRactor OdorRactor ,TGSC
309 Octahyu 2-one 310 2-Naphi 311 Decahyu formate 312 8-Cyclo 313 Civeton 314 Isoambi 315 1-Oxasj 316 (7E)-Cy one 317 1,7-Dio one	hthalenol, decahydro- ydro-2H-1-benzopyran- hthalenol, decahydro- ydro-2-naphthyl ie lohexadecenone brettolide spiro[4.7]dodecane	1,2,3,4,4a ,5,6,7,8,8a - decahydronaphthalen-2-ol 1,2,3,4,4a ,5,6,7,8,8a - decahydronaphthalen-2-yl formate (8E)-cyclohexadec-8-en-1-one (9Z)-cycloheptadec-9-en-1-one (10Z)-1-oxacycloheptadec-10-en-	C1CCC2CC(CCC2C1)0 C1CCC2CC(CCC2C1)0C=0 C1CCCC=CCCCCCCC(=0)CCC 1 C1CCCC=CCCCCCCC(=0)CC	sweet herbaceous coumarinic tonka woody creamy lactonic coconut milky vanilla rose minty muguet clean floral sandal wood woody oily floral dry musk laundered cloth dry balsamic	OdorRactor ,TGSC Sigma Aldrich, TGSC,OdoRactor OdorRactor ,TGSC
310 2-Naphi 311 Decahy, formate 312 8-Cyclo 313 Civeton 314 Isoambi 315 1-Oxasj 316 (7E)-Cy one 317 1,7-Dio one	hthalenol, decahydro- ydro-2-naphthyl ie lohexadecenone ne brettolide spiro[4.7]dodecane	1,2,3,4,4a ,5,6,7,8,8a - decahydronaphthalen-2-ol 1,2,3,4,4a ,5,6,7,8,8a - decahydronaphthalen-2-yl formate (8E)-cyclohexadec-8-en-1-one (9Z)-cycloheptadec-9-en-1-one (10Z)-1-oxacycloheptadec-10-en-	C1CCC2CC(CCC2C1)OC=O C1CCCC=CCCCCCCC(=O)CCC 1 C1CCCC=CCCCCCCC(=O)CC	coconut milky vanilla rose minty muguet clean floral sandal wood woody oily floral dry musk laundered cloth dry balsamic	TGSC,OdoRactor OdorRactor ,TGSC
311 Decahy formate 312 8-Cyclo 313 Civeton 314 Isoambr 315 1-Oxasp 316 (7E)-Cyone 317 1,7-Dio one	ydro-2-naphthyl te lohexadecenone one brettolide spiro[4.7]dodecane	decahydronaphthalen-2-ol 1,2,3,4,4a ,5,6,7,8,8a - decahydronaphthalen-2-yl formate (8E)-cyclohexadec-8-en-1-one (9Z)-cycloheptadec-9-en-1-one (10Z)-1-oxacycloheptadec-10-en-	C1CCC2CC(CCC2C1)OC=O C1CCCC=CCCCCCCC(=O)CCC 1 C1CCCC=CCCCCCCC(=O)CC	sandal wood woody oily floral dry musk laundered cloth dry balsamic	TGSC,OdoRactor OdorRactor ,TGSC
312 8-Cyclo 313 Civeton 314 Isoambi 315 1-Oxasp 316 (7E)-Cy one 317 1,7-Dio one 317 1,7-Dio one	ydro-2-naphthyl de lohexadecenone one brettolide spiro[4.7]dodecane	1,2,3,4,4a ,5,6,7,8,8a - decahydronaphthalen-2-yl formate (8E)-cyclohexadec-8-en-1-one (9Z)-cycloheptadec-9-en-1-one (10Z)-1-oxacycloheptadec-10-en-	C1CCCC=CCCCCCCC(=0)CCC	musk laundered cloth dry balsamic	OdorRactor ,TGSC
312 8-Cyclo 313 Civeton 314 Isoambi 315 1-Oxasj 316 (7E)-Cy one 317 1,7-Dio one	one brettolide spiro[4.7]dodecane	(8E)-cyclohexadec-8-en-1-one (9Z)-cycloheptadec-9-en-1-one (10Z)-1-oxacycloheptadec-10-en-	1 C1CCCC=CCCCCCC(=O)CC	_	OdorRactor ,TGSC
313 Civeton 314 Isoambi 315 1-Oxası 316 (7E)-Cy one 317 1,7-Dio one	brettolide spiro[4.7]dodecane	(9Z)-cycloheptadec-9-en-1-one (10Z)-1-oxacycloheptadec-10-en-	1 C1CCCC=CCCCCCC(=O)CC	_	OdorRactor ,TGSC
314 Isoambi 315 1-Oxasj 316 (7E)-Cy one 317 1,7-Dio one	brettolide spiro[4.7]dodecane	(10Z)-1-oxacycloheptadec-10-en-	· ·		Î.
315 1-Oxası 316 (7E)-Cy one 317 1,7-Dio one	spiro[4.7]dodecane		C1	musk clean dry animal sweet	OdorRactor ,TGSC
316 (7E)-Cy one 317 1,7-Dio one	spiro[4.7]dodecane			musk sweet ambrette fruity wax fatty	OdorRactor ,TGSC
one 317 1,7-Dio one		1-oxaspiro[4.7]dodecane	C1CCCC2(CCC1)CCCO2	animal woody naphthyl saffron	OdorRactor ,TGSC
317 1,7-Dio one	Cyclohexadec-7-en-1-	(7E)-cyclohexadec-7-en-1-one	C1CCCCC(=0)CCCCCC=CCCC	cistus musk	TGSC
	oxacycloheptadecan-8-	1,7-dioxacycloheptadecan-8-one	C1CCCCC(=O)OCCCCCOCCCC	musk sweet oily amber animal	SuperScent, TGSC,
ļ ļ	cloheptadec-7-en-2-one	(7E)-1-oxacycloheptadec-7-en-2-	1 C1CCCCC=CCCCCC(=0)OCCC	incense fatty musty soapy sweet musk	OdoRactor OdorRactor,
319 (7E)-1-0	-Oxacycloheptadec-7-	one 1-oxacycloheptadec-7-en-2-one	C1 C1CCCCC=CCCCCC(=0)OCCC	amber fruity berry sweet soapy musk amber fruity	Sigma Aldrich, TGSC
en-2-on 320 Oxacyc		(12E)-1-oxacyclohexadec-12-en-	C1 C1CCCCC=CCCCOC(=0)CCCC	berry sweet musk wax dry laundered	TGSC, Pubchem
one, (12	12E)-	2-one	1	cloth metallic animal tropical	,
	ahydrocyclododeca[c]f	(4Z)-1,3,3a ,6,7,8,9,10,11,12,13,13a - dodecahydrocyclododeca[c]furan	C1CCCC2COCC2C=CCCC1	earthy animal natural musk	OdorRactor ,TGSC
322 Cyclope	pentadec-4-en-1-one	(4Z)-cyclopentadec-4-en-1-one	C1CCCCCC(=0)CCC=CCCCC1	musk animal natural	OdorRactor ,TGSC
323 5-Cyclo	lohexadecenone	(5Z)-cyclohexadec-5-en-1-one	C1CCCCC(=0)CCCC=CCCCC	dry powdery musk amber civet	OdorRactor ,TGSC
	•		C1CCCCC(=0)OCCC=CCCCC	musk	TGSC
	clohexadec-13-en-2-	2-one 1-oxacyclohexadec-13-en-2-one	C1CCCCC(=0)OCCC=CCCCC	musk	TGSC
		oxacyclohexadecane-2,13-dione	1 C1CCCCC(=O)OCCCC(=O)CC	musk	OdorRactor ,TGSC
dione 327 1,4-Dio	oxacyclohexadecane-		CC1 C1CCCCC(=0)OCCOC(=0)CC	sweet wax musk animal clean	OdorRactor ,TGSC
5,16-die	ione	dione 1,4-dioxacycloheptadecane-5,17-	CC1 C1CCCCC(=0)OCCOC(=0)CC	musty sweet powdery floral	Sigma Aldrich, Flavorbase,
5,17-die	ione	dione	CCC1	ambrette musk woody spicy vanilla fatty oily	TGSC
	-	cyclododecyl formate	C1CCCCC(CCCCC1)OC=O	sweet woody fresh laundered cloth clean	OdorRactor ,TGSC
	7,8,9,10,11,12,13-	4,5,6,7,8,9,10,11,12,13- decahydrocyclododeca[d][1,3]oxa zole	C1CCCCC2=C(CCCC1)N=CO2	green herbaceous terpenic earthy woody	TGSC
	ecahydrocyclododeca[c	1,3,3 <i>a</i> ,4,5,6,7,8,9,10,11,12,13,13 <i>a</i> - tetradecahydrocyclododeca[c]fura	C1CCCCC2COCC2CCCC1	warm woody amber old wood dry	OdorRactor ,TGSC
332 Cyclope	pentadecanone	cyclopentadecanone	C1CCCCCCC(=0)CCCCCC1	powdery musk animal natural	OdorRactor ,TGSC
333 Cyclohe	nexadecanone	cyclohexadecanone	C1CCCCCCC(=0)CCCCCCC1	greasy powdery musk animal	OdorRactor ,TGSC
334 Oxacyc	cloheptadecan-2-one	oxacycloheptadecan-2-one	C1CCCCCCC(=0)OCCCCCCC	musk sweet balsamic amber	OdorRactor ,TGSC
335 Cyclohe	neptadecanone	cycloheptadecanone	C1CCCCCCCC(=0)CCCCCCC	animal powdery musk	OdorRactor ,TGSC

336	Oxacyclohexadecan-2-one	oxacyclohexadecan-2-one	C1CCCCCCCCC(=0)CCCCCC1	musk animal powdery natural fruity berry tobacco coumarinic heliotrope licorice brown	Sigma Aldrich, TGSC, OdoRactor
337	Habanolide	(3E)-1-oxacyclohexadec-3-en-2-one	C1CCCCCCC(=0)C=CCCCCC	sweet musk wax	OdorRactor ,TGSC
338	1,6-Dioxacycloheptadecan-7-one	1,6-dioxacycloheptadecan-7-one	C1CCCCCCCCCCC(=0)CCCC	musk woody sweet fruity wax	OdorRactor ,TGSC
339	Ambrettolide	(8Z)-1-oxacycloheptadec-8-en-2- one	C1CCCCOC(=0)CCCCCC=CCC C1	sweet soapy musk amber fruity berry musty animal ambrette	SuperScent, TGSC, OdoRactor
340	1,8-Dioxacycloheptadecan-9- one	1,8-dioxacycloheptadecan-9-one	C1CCCCOCCCCCCC(=0)CCC	sweet musk oily fruity animal floral	OdorRactor ,TGSC
341	Piperine	(2E ,4E)-5-(1,3-benzodioxol-5-yl)-1-piperidin-1- ylpenta-2,4-dien-1-one	C1CCN(CC1)C(=0)C=CC=CC2= CC3=C(C=C2)OCO3	odorless	Sigma Aldrich, TGSC, Flavorbase, OdoRactor
342	Pyrrolidine	pyrrolidine	CICCNCI	fatty alkane ammonical animal eggy shellfish fishy seaweed unpleasant	Sigma Aldrich, TGSC, OdoRactor, Pubchem
343	Piperidine	piperidine	C1CCNCC1	fatty floral sweet animal ammonical fishy pepper	Sigma Aldrich, Flavorbase, TGSC,OdoRactor
344	Tetrahydrothiophene	thiolane	C1CCSC1	cabbage sulfurous stench	Flavornet, TGSC, Pubchem
345	1-(2-Chlorophenyl)piperazine hydrochloride	1-(2- chlorophenyl)piperazine;hydrochl oride	C1CN(CCN1)C2=CC=CC=C2Cl. C1	minty spearmint fruity	OdorRactor ,TGSC
346	Piperazine	piperazine	C1CNCCN1	ammonical	OdorRactor ,TGSC, Pubche
347	Cinnamaldehyde ethylene glycol acetal	2-[(E)-2-phenylethenyl]-1,3-dioxolane	C1COC(O1)C=CC2=CC=CC=C2	warm spicy cinnamyl allspice	OdorRactor ,TGSC
348	2-Benzyl-1,3-dioxolane	2-benzyl-1,3-dioxolane	C1COC(O1)CC2=CC=CC=C2	green wax sweet honey hyacinth	OdorRactor ,TGSC
349	Tetrahydrothiophen-3-one	thiolan-3-one	CICSCC1=0	buttery meaty sulfurous garlic green clam cooked vegetable alliaceous roasted cooked meat onion	Sigma Aldrich, Flavorbase, TGSC, OdoRactor
350	1,4-Dithiane	1,4-dithiane	C1CSCCS1	fishy sulfurous garlic onion pyridine seafood solvent fermented mushroom clam oyster turkey	Sigma Aldrich, Flavorbase, TGSC,OdoRactor
351	N-(2-Mercaptoethyl)-1,3- thiazolidine	2-(1,3-thiazolidin-3-yl)ethanethiol	C1CSCN1CCS	popcorn nutty	TGSC
352	1,3-Dithiolane	1,3-dithiolane	C1CSCS1	sulfurous sweet onion cooked onion	TGSC
353	1,3-Dithiane	1,3-dithiane	C1CSCSC1	alliaceous roasted	TGSC
354	Narciclasine	(2S ,3R ,4S ,4aR)-2,3,4,7- tetrahydroxy-3,4,4a ,5-tet	C1OC2=C(O1)C(=C3C(=C2)C4= CC(C(C(C4NC3=O)O)O)O)O	woody powdery musk fruity dry vetiver	OdorRactor ,TGSC
355	Piperonal	1,3-benzodioxole-5-carbaldehyde	C10C2=C(O1)C=C(C=C2)C=O	floral almond anisic balsamic berry cherry creamy herbaceous woody raspberry sweet vanilla violet winey heliotrope powdery coconut maraschino cinnamyl spicy	Sigma Aldrich, AOD, Flavorbase, TGSC, OdoRactor, Pubchem
356	Piperonyl alcohol	1,3-benzodioxol-5-ylmethanol	C1OC2=C(O1)C=C(C=C2)CO	powdery vanilla sweet	OdorRactor ,TGSC
357	Sesamol	1,3-benzodioxol-5-ol	C1OC2=C(O1)C=C(C=C2)O	phenolic spicy	Flavorbase
358	1,2,4-Trithiolane	1,2,4-trithiolane	C1SCSS1	sulfurous garlic roasted beef mushroom beefy roasted	Flavorbase
359 360	Lenthionine Benzyl 2,3-dimethylcrotonate	1,2,3,5,6-pentathiepane benzyl 2,3-dimethylbut-2-enoate	C1SSCSSS1 CC(=C(C)C(=O)OCC1=CC=CC= C1)C	mushroom herbaceous fruity spicy warm	TGSc OdorRactor ,TGSC
361	Methyl methacrylate	methyl 2-methylprop-2-enoate	CC(=C)C(=O)OC	fruity acrylic aromatic acrylate sulfurous sweet sharp unpleasant acrid plastic	Sigma Aldrich, TGSC, Pubchem
362	3-Isopropenylpentanedioic acid	3-prop-1-en-2-ylpentanedioic acid	CC(=C)C(CC(=O)O)CC(=O)O	savory cooked roasted	OdorRactor ,TGSC
363	2,6-Dimethylocta-1,5,7-trien-3-ol	2,6-dimethylocta-1,5,7-trien-3-ol	CC(=C)C(CC=C(C)C=C)O	camphoraceous lime	TGSC, OdoRactor
364	(E)-2,6-Dimethylocta-1,5,7-trien-3-ol	(5 <i>E</i>)-2,6-dimethylocta-1,5,7-trien-3-ol		camphoraceous lime terpenic	OdorRactor ,TGSC
365	3-Isopropenyl-6-oxoheptanoic acid	6-oxo-3-prop-1-en-2-ylheptanoic acid	CC(=C)C(CCC(=O)C)CC(=O)O	fatty floral	TGSC
366	Hotrienol	(5E)-3,7-dimethylocta-1,5,7-trien-3-ol	CC(=C)C=CCC(C)(C=C)O	hyacinth tropical sweet floral fennel ginger spicy moldy fungal	Flavornet, TGSC, Odoracto
367	Methacrolein	2-methylprop-2-enal	CC(=C)C=O	floral hyacinth green foliage high pungent	SuperScent, TGSC, Pubche

369	4-Acetyl-2-	1-(2-prop-1-en-2-ylpyridin-4-	CC(=C)C1=NC=CC(=C1)C(=O)C		TGSC
370	isopropenylpyridine Pyrazine, (1-methylethenyl)-	yl)ethanone 2-prop-1-en-2-ylpyrazine	CC(=C)C1=NC=CN=C1	roasted caramel chocolate nutty roasted	OdorRactor ,TGSC
				-	·
371	Elemol	2-[(1R ,3S ,4S)-4-ethenyl-4- methyl-3-prop-1-en-2- ylcyclohexyl]propan-2-ol	CC(=C)C1CC(CCC1(C)C=C)C(C) (C)O	green woody spicy rose sweet	Flavornet, TGSC
372	Carvone oxide	(1R, $4R$, $6R$)-1-methyl-4-prop-1-en-2-yl-7- oxabicyclo[4.1.0]heptan-2-one		minty spearmint	SuperScent, TGSC
373	Carvone-5,6-oxide, cis-(-)-	(1S, 4R, 6S)-1-methyl-4-prop-1- en-2-yl-7- oxabicyclo[4.1.0]heptan- 2-one	CC(=C)C1CC2C(O2)(C(=O)C1)C	sweet caraway minty spearmint spicy	OdorRactor ,TGSC
374	Menthadienyl acetate	(2-methylidene-5-prop-1-en-2- ylcyclohexyl) acetate	CC(=C)C1CCC(=C)C(C1)OC(=O)	minty spearmint fruity	OdorRactor ,TGSC
375	(-)-Perillaldehyde	(4S)-4-prop-1-en-2- ylcyclohexene-1-carbaldehyde	CC(=C)C1CCC(=CC1)C=O	cherry green oily fatty fresh grassy minty spicy herbaceous cumin dill	Sigma Aldrich, TGSC, Flavorbase, OdoRactor
376	Perillaldehyde	4-prop-1-en-2-ylcyclohexene-1- carbaldehyde	CC(=C)C1CCC(=CC1)C=0	spice green herbaceous grassy sweet minty cumin fresh cinnamyl pungent clove citrus orange lime fatty dill	Flavornet, Flavorbase, TGSC, OdoRactor
377	(-)-Perillyl alcohol	[(4S)-4-prop-1-en-2-ylcyclohexen- 1-yl]methanol	CC(=C)C1CCC(=CC1)CO	fatty green	Sigma Aldrich
378	Perillyl alcohol	(4-prop-1-en-2-ylcyclohexen-1- yl)methanol	CC(=C)C1CCC(=CC1)CO	green bois de rose lilac fatty sweet woody aromatic spicy cardamom cumin orange wax floral rose	TGSC,OdoRactor
379	Perillyl acetate	(4-prop-1-en-2-ylcyclohexen-1- yl)methyl acetate	CC(=C)C1CCC(=CC1)COC(=O)C	fruity woody raspberry berry	SuperScent, TGSC, OdoRactor
380	beta-Elemene		CC(=C)C1CCC(C(C1)C(=C)C)(C) C=C	herbaceous wax fresh	Flavornet, TGSC
381	1,2-Cyclohexanediol, 1-methyl-4-(1-methylethenyl)-	1-methyl-4-prop-1-en-2- ylcyclohexane-1,2-diol	CC(=C)C1CCC(C(C1)O)(C)O	minty	OdorRactor,
382	(1r,4r)-1-Methyl-4-(prop-1-en- 2- yl)cyclohex-2-en-1-ol	(1R,4R)-1-methyl-4-prop-1-en-2-ylcyclohex-2-en-1-ol	CC(=C)C1CCC(C=C1)(C)O	fresh minty	Flavornet, TGSC
383	P-Mentha-2,8-dien-1-ol	1-methyl-4-prop-1-en-2- ylcyclohex-2-en-1-ol	CC(=C)C1CCC(C=C1)(C)O	minty terpenic	OdorRactor ,TGSC
384			CC(=C)C1CCC(C1=C)(C)C(=O)C 2CCCC 2=O	woody cedar	TGSC
385	beta-Terpineol	1-methyl-4-prop-1-en-2- ylcyclohexan-1-ol	CC(=C)C1CCC(CC1)(C)O	musty woody earthy pungent	Flavornet, TGSC,OdoRactor
386	cis-1,2-Dihydroperillaldehyde	4-prop-1-en-2-ylcyclohexane-1- carbaldehyde	CC(=C)C1CCC(CC1)C=O	herbaceous fruity spicy	TGSC
387	Tetrahydro-5-isopropenyl-2- methyl-2- vinylfuran	2-ethenyl-2-methyl-5-prop-1-en-2-yloxolane	CC(=C)C1CCC(O1)(C)C=C	green minty spice herbaceous rosemary phenolic cooling spicy terpenic fresh dusty floral	OdorRactor ,TGSC, Flavorbase
388	(1R,4R,6S)-1-Methyl-4-(prop- 1-en-2-yl)-7- oxabicyclo[4.1.0]heptane	(1R,4R,6S)-1-methyl-4-prop-1- en-2-yl-7- oxabicyclo[4.1.0]heptane	CC(=C)C1CCC2(C(C1)O2)C	fresh citrus	Flavornet
389	Limonene-1,2-epoxide	(4R)-1-methyl-4-prop-1-en-2-yl-7-oxabicyclo[4.1.0]heptane	CC(=C)C1CCC2(C(C1)O2)C	fresh clean citrus minty spearmint herbaceous	SuperScent, TGSC
390	Limonene oxide	1-methyl-4-prop-1-en-2-yl-7-oxabicyclo[4.1.0]heptane	CC(=C)C1CCC2(C(C1)O2)C	fruit citrus minty spearmint herbaceous fresh clean	Flavornet, TGSC, OdoRactor, Pubchem
391	(+)-trans-Limonene oxide		CC(=C)C1CCC2(C(C1)O2)C	green	Flavornet
392	(+)-(E)-Limonene oxide	(1R, 4R)-1-methyl-4-prop-1-en-2-yl-7- oxabicyclo[4.1.0]heptane	CC(=C)C1CCC2(C(C1)O2)C	green	SuperScent, TGSC
393	beta-Selinene	(3R, 4aS, 8aR) -8a -methyl-5- methylidene-3-prop-1 en-2-yl- 1,2,3,4,4a,6,7,8- octahydronaphthalene	CC(=C)C1CCC2(CCCC(=C)C2C1)C	herbaceous	Flavornet
394	4-Penten-2-one, 4-methyl-	4-methylpent-4-en-2-one	CC(=C)CC(=0)C	pungent vegetable acrylate	TGSC
395	5-Methyl-5-hexen-2-one	5-methylhex-5-en-2-one	CC(=C)CCC(=O)C	green weedy foliage vegetable fatty	TGSC
396	alpha-Ocimene	(3E)-3,7-dimethylocta-1,3,7-triene	CC(=C)CCC=C(C)C=C	herbaceous fruity floral laundered cloth	Flavornet
397	3-Methyl-3-buten-1-OL	3-methylbut-3-en-1-ol	CC(=C)CCO	fruity sweet	Sigma Aldrich
398	3-Methyl-3-butenyl acetate	3-methylbut-3-enyl acetate	CC(=C)CCOC(=0)C	fruity	SuperScent, TGSC
399	Propanoic acid, 2,2-dimethyl-, 3-methyl-3- buten-1-yl ester	3-methylbut-3-enyl 2,2- dimethylpropanoate	CC(=C)CCOC(=O)C(C)(C)C	herbaceous fresh fruity floral chamomile rose	TGSC

400	Isopropenyl acetate	prop-1-en-2-yl acetate	CC(=C)OC(=O)C	fruity ethereal acetic sweet berry	Sigma Aldrich,
401	CID 53426765	prop-1-en-2-yl 4-oxopentanoate	CC(=C)OC(=O)CCC(=O)C	grape banana fruity green	TGSC,OdoRactor TGSC
402	gamma-Elemene	(1S,2S)-1-ethenyl-1-methyl-4- propan-2-ylidene-2- prop-1-en-2- ylcyclohexane	CC(=C1CCC(C(C1)C(=C)C)(C)C =C)C	green woody oily	Flavornet, TGSC
403	gamma-Terpineol	1-methyl-4-propan-2- ylidenecyclohexan-1-ol	CC(=C1CCC(CC1)(C)O)C	pine floral lilac terpenic	SuperScent, TGSC,OdoRactor
404	Piperitenone oxide	6-methyl-3-propan-2-ylidene-7- oxabicyclo[4.1.0]heptan-2-one	CC(=C1CCC2(C(C1=O)O2)C)C	herbaceous minty	OdorRactor ,TGSC
405	Selina-4(15),7(11)-diene	(4aS, 8aR) -8a -methyl-4- methylidene-6-propan-2- ylidene- 2,3,4a,5,7,8-hexahydro-1H - naphthalene	CC(=C1CCC2(CCCC(=C)C2C1)C)C	woody	Flavornet
406	(Z)-3-Methyl-5-phenylpent-2- enenitrile	(Z)-3-methyl-5-phenylpent-2- enenitrile	CC(=CC#N)CCC1=CC=CC=C1	citrus citral lemon	OdorRactor ,Pubchem
407	3-Methyl-5-phenylpent-2- enenitrile	(E)-3-methyl-5-phenylpent-2-enenitrile	CC(=CC#N)CCC1=CC=CC=C1	citrus citral lemon lemongrass fruity floral rose cinnamyl balsamic	OdorRactor ,TGSC
408	3,3,6-Trimethylhepta-1,5-dien- 4-one	3,3,6-trimethylhepta-1,5-dien-4- one	CC(=CC(=O)C(C)(C)C=C)C	green herbaceous minty berry herbaceous honey	Flavornet, TGSC, OdoRactor
409	Mesityl oxide	4-methylpent-3-en-2-one	CC(=CC(=0)C)C	musty mildew earthy chemical cardboard nutty chocolate woody vegetable vanilla sweet pungent acrylic acrylate spearmint unpleasant honey	Sigma Aldrich, TGSC, OdoRactor, Pubchem
410	3,3-Dimethylacrylic acid	3-methylbut-2-enoic acid	CC(=CC(=O)O)C	phenolic green dairy	SuperScent, TGSC,OdoRactor
411	2-Butenoic acid, 3-methyl-, 2-phenylethyl ester	2-phenylethyl 3-methylbut-2- enoate	CC(=CC(=O)OCCC1=CC=CC=C 1)C	sweet herbaceous winey	OdorRactor ,TGSC
412	3,3,6-Trimethylhepta-1,5-dien- 4-ol		CC(=CC(C(C)(C)C=C)O)C	herbaceous	Flavornet
413	Ipsdienol	(4S)-2-methyl-6-methylideneocta- 2,7-dien-4-ol		pine balsamic	OdorRactor ,TGSC
414	(5E)-3,5-Dimethylocta-1,5,7-trien-3-ol	(5 <i>E</i>)-3,5-dimethylocta-1,5,7-trien-3-ol	CC(=CC=C)CC(C)(C=C)O	sweet tropical floral fennel ginger spicy	OdorRactor,
	6-Methyl-3,5-heptadien-2-one	(3E)-6-methylhepta-3,5-dien-2-one	CC(=CC=CC(=O)C)C	cinnamyl spicy coconut woody sweet weedy green cooling herbaceous	SuperScent, TGSC, OdoRactor
416	3-Methyl-2-butenal	3-methylbut-2-enal	CC(=CC=O)C	cherry sweet fruity pungent nutty almond brown	Sigma Aldrich, TGSC, OdoRactor
417	(2E)-5-(2,2- Dimethylcyclopropyl)-3- methyl- pentenal	(E)-5-(2,2-dimethylcyclopropyl)-3-methylpent-2- enal	CC(=CC=0)CCC1CC1(C)C	citrus	TGSC
418	(Z)-p-Methoxy-alpha- methylcinnamaldehyde	(Z)-3-(4-methoxyphenyl)-2- methylprop-2-enal	CC(=CC1=CC=C(C=C1)OC)C=O	spicy cinnamyl floral	OdorRactor ,TGSC
419	3-Methyl-4-phenyl-3-buten-2- one	(E)-3-methyl-4-phenylbut-3-en-2- one	CC(=CC1=CC=CC=C1)C(=0)C	fruity berry camphoraceous sweet	OdorRactor ,TGSC, Flavorbase
420			CC(=CC1=CC=CC1)C=O	spicy cinnamyl cassia	TGSC
421	2-Methyl-3-phenyl-2- propenal	(Z)-2-methyl-3-phenylprop-2-enal	CC(=CC1=CC=CC1)C=O	spicy sweet cinnamyl cassia warm balsamic herbaceous	OdorRactor ,Sigma Aldrich, TGSC
422	2-Propen-1-ol, 2-methyl-3- phenyl-		CC(=CC1=CC=CC1)CO	balsamic sweet floral oriental storax	OdorRactor ,TGSC
423	2-Methyl-3(2-furyl)acrolein	(Z)-3-(furan-2-yl)-2-methylprop- 2-enal	CC(=CC1=CC=CO1)C=O	spicy cinnamyl woody herbaceous cassia medicinal	OdorRactor ,TGSC
424	6,6-Dimethoxy-2,5,5- trimethylhex-2-ene	6,6-dimethoxy-2,5,5-trimethylhex- 2-ene	CC(=CCC(C)(C)C(OC)OC)C	fresh citrus grapefruit soapy woody green violet fruity	OdorRactor ,TGSC
425	4-Hexen-1-ol, 5-methyl-2-(1-methylethenyl)-	5-methyl-2-prop-1-en-2-ylhex-4- en-1-ol	CC(=CCC(CO)C(=C)C)C	farnesol floral wax mimosa herbaceous	OdorRactor ,TGSC
426	(R)-Lavandulol	(2 <i>R</i>)-5-methyl-2-prop-1-en-2- ylhex-4-en-1-ol	CC(=CCC(CO)C(=C)C)C	herbaceous	Flavornet
427	(1E,6Z)-7,11-Dimethyl-3- methylidenedodeca-1,6,10- trien-1-ol	(1E,6Z)-7,11-dimethyl-3- methylidenedodeca-1,6,1	CC(=CCC/C(=C\CCC(=C)/C=C/O)/C)C	floral oily	Flavornet
428	(Z)-beta-Ocimene	(3Z)-3,7-dimethylocta-1,3,6- triene	CC(=CCC=C(C)C=C)C	citrus herbaceous floral warm herbaceous sweet	Flavornet, TGSC, OdoRactor
429	(E)-beta-Ocimene	(3E)-3,7-dimethylocta-1,3,6-triene	CC(=CCC=C(C)C=C)C	sweet herbaceous citrus floral tropical green terpenic woody vegetable	Sigma Aldrich, Flavornet, TGSC, OdoRactor
430	alpha-Sinensal	(2E,6E,9E)-2,6,10- trimethyldodeca-2,6,9,11- tetraenal	CC(=CCC=C(C)C=C)CCC=C(C) C=O	citrus orange mandarin	OdorRactor ,TGSC
431	3,6-Octadienal, 3,7-dimethyl-	(3E)-3,7-dimethylocta-3,6-dienal	CC(=CCC=C(C)CC=O)C	green	Flavornet
	1	(27) 27 1 1 1 2 2 5 1 1	CC(=CCC=C(C)CCO)C	rose	Flavornet
432	Isogeraniol	ol			
432	Isogeraniol trans-Isogeraniol			rose	Flavornet

435	2,2-Dimethyl-3-(3- methylpenta-2,4- dienyl)oxirane	2,2-dimethyl-3-(3-methylpenta-2,4-dienyl)oxirane	-CC(=CCC1C(O1)(C)C)C=C	sweet metallic herbaceous lavender pear fresh opoponax clary sage	OdorRactor ,TGSC
436	cis-Abienol	(1R ,2R ,4aS ,8aS)-2,5,5,8a -	CC(=CCC1C2(CCCC(C2CCC1(C	amber woody ambergis balsamic	TGSC
.50		tetramethyl-1-[(2Z)-3- methylpenta-2,4-dienyl]-3,4,4a ,6,7,8-hexahydro- 1H -naphthalen-2-ol)O)(C)C) C)C=C		
437	2-(3-Methyl-2- butenyl)cyclopentanone	2-(3-methylbut-2-enyl)cyclopentan 1-one	-CC(=CCC1CCCC1=0)C	floral jasmine	OdorRactor ,TGSC
438	Мугсепе	7-methyl-3-methylideneocta-1,6-diene	CC(=CCCC(=C)C=C)C	anisic grape green vegetable woody peach sweet vanilla winey balsamic musty spice plastic pepper terpenic herbaceous rose celery carrot pleasant	Sigma Aldrich, Flavornet, TGSC, Odoractor, Pubchem
439	(2Z,6E)-2,6-Dimethyl-10- methylidenedodeca-2,6,11- trienal	(2Z ,6E)-2,6-dimethyl-10- methylidenedodeca- 2,6,11-trienal	CC(=CCCC(=C)C=C)CCC=C(C) C=O	orange	Sigma Aldrich
440	beta-Sinensal	(2E,6E)-2,6-dimethyl-10-methylidenedodeca-2,6,11-trienal	CC(=CCCC(=C)C=C)CCC=C(C) C=O	sweet citrus orange fresh wax juicy	Flavornet, TGSC, Flavorbase
441	6-Octenal, 7-methyl-3- methylene-	7-methyl-3-methylideneoct-6-enal	CC(=CCCC(=C)CC=O)C	aldehydic juicy lemongrass floral lemon bois de rose rose	TGSC
442	(2Z)-3,7-Dimethylocta-2,6- dienenitrile	(2Z)-3,7-dimethylocta-2,6-dienenitrile	CC(=CCCC(=CC#N)C)C	citral lemon aldehydic metallic	OdorRactor,
443	3,7-Dimethylocta-2,6- dienenitrile	(2E)-3,7-dimethylocta-2,6-dienenitrile	CC(=CCCC(=CC#N)C)C	citrus lemon nitrile aldehydic metallic sharp	OdorRactor ,TGSC
444	4,8-Dimethyl-3,7-nonadien-2- one	(3E)-4,8-dimethylnona-3,7-dien- 2-one	CC(=CCCC(=CC(=O)C)C)C	floral fruity citrus fresh lemon rose grapefruit	OdorRactor ,TGSC, Flavorbase
445	Geranic acid	(2E)-3,7-dimethylocta-2,6-dienoic acid	CC(=CCCC(=CC(=O)O)C)C	dry weedy acidic moldy feet woody lemon rose winey green greasy sweet	Sigma Aldrich, TGSC, Olfactor
446	Methyl nerate	methyl (2Z)-3,7-dimethylocta-2,6-dienoate	CC(=CCCC(=CC(=O)OC)C)C	floral herbaceous citrus fruity green geranium	TGSC
447	Methyl geranate	methyl (2E)-3,7-dimethylocta-2,6-dienoate	CC(=CCCC(=CC(=O)OC)C)C	green fruit wax floral	Flavornet, TGSC, OdoRactor
448	trans-And cis-2,4,8-Trimethyl- 3,7-nona- dien-2-ol		CC(=CCCC(=CC(C)(C)O)C)C	earthy herbaceous pine melon	TGSC
449	Citral dimethyl acetal	(2 <i>E</i> _)-1,1-dimethoxy-3,7-dimethylocta-2,6-diene	CC(=CCCC(=CC(OC)OC)C)C	citrus green floral lemon lime natural aldehydic terpenic	Sigma Aldrich, TGSC
450	Lycopene	(6E ,8E ,10E ,12E ,14E ,16E ,18E ,20E ,22E ,24E , 26E)-2,6,10,14,19,23,27,31-octamethyldotriaconta-2,6,8,10,12,14,16,18,20,22,24,26, 30-tridecaene	CC(=CCCC(=CC=CC(=CC=CC(= CC=CC) =C(C)C=CC=C(C)C=CC=C(C)CC C=C(C) C)C)C)C)C	balsamic oriental	TGSC
451	Pseudoionone	(3E ,5E)-6,10-dimethylundeca- 3,5,9-trien-2-one		sweet wax citrus floral balsamic dry dusty powdery spicy berry orris fruity tea	OdorRactor ,TGSC, Flavorbase
452	Methyl 2-[(3,7-dimethyl-2,6-octadienylidene)amino]benzo ate	methyl 2-[[(2E)-3,7-dimethylocta- 2,6- dienylidene]amino]benzoate	CC(=CCCC(=CC=NC1=CC=CC= C1C(=O)OC)C)C	fresh sweet lemon orange flower fruity citrus	OdorRactor ,TGSC
453	Citral	(2E)-3,7-dimethylocta-2,6-dienal	CC(=CCCC(=CC=O)C)C	lemon minty sweet sharp citrus fresh juicy tart green	Sigma Aldrich, Flavornet, AOD, TGSC, Pubchem, OdoRactor
454	Neral	(2Z)-3,7-dimethylocta-2,6-dienal	CC(=CCCC(=CC=O)C)C	sweet citral lemon strong	Flavornet, TGSC, Pubchem, OdoRactor
455	1,3-Dioxolane, 2-(2,6-dimethyl-1,5-heptadienyl)-	2-[(1 <i>E</i>)-2,6-dimethylhepta-1,5-dienyl]-1,3- dioxolane	CC(=CCCC(=CC1OCCO1)C)C	citrus fresh clean floral lemon	OdorRactor ,TGSC
456	alpha-Farnesene	(3E,6E)-3,7,11-trimethyldodeca-1,3,6,10-tetraene	CC(=CCCC(=CCC=C(C)C=C)C) C	apple green lavender lie woody sweet fruity citrus herbaceous bergamot myrrh neroli vegetable floral juniperberry	Sigma Aldrich, Flavornet, TGSC, Flavorbase, OdoRactor
457	Apritone	2-[(2E)-3,7-dimethylocta-2,6-dienyl]cyclopentan-1-one	CC(=CCCC(=CCC1CCCC1=0)C) C	fruity fresh sweet apricot plum peach tropical warm ripe fleshy jammy davana floral	OdorRactor ,TGSC, Flavorbase
458	cis-beta-Farnesene	(6Z)-7,11-dimethyl-3- methylidenedodeca-1,6,10- triene	CC(=CCCC(=CCCC(=C)C=C)C)	citrus green	Flavornet, OdoRactor
459	cis-beta-Farnesene	(6Z)-7,11-dimethyl-3- methylidenedodeca-1,6,10- triene	CC(=CCCC(=CCCC(=C)C=C)C)	citrus green woody rose	OdorRactor ,TGSC
460	beta-Farnesene	(6E)-7,11-dimethyl-3-methylidenedodeca-1,6,10-triene	CC(=CCCC(=CCCC(=C)C=C)C)	herbaceous woody citrus sweet herbaceous green	Flavornet, TGSC, Flavorbase, OdoRactor
461	Farnesal	(2E,6E)-3,7,11-trimethyldodeca- 2,6,10-trienal	CC(=CCCC(=CCCC(=CC=O)C)C	floral minty	Sigma Aldrich, TGSC

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462	Geranylfarnesol	(2 <i>E</i> ,6 <i>E</i> ,10 <i>E</i> ,14 <i>E</i>)- 3,7,11,15,19-pentamethylicosa- 2,6,10,14,18-pentaen-1-ol	CC(=CCCC(=CCCC(=CCCC(=C CCC(=C CO)C)C)C)C)C	floral	OdorRactor ,TGSC
463	Farnesylacetone	(5 <i>E</i> ,9 <i>E</i>)-6,10,14- trimethylpentadeca-5,9,13-trien- 2-one	CC(=CCCC(=CCCC(=O) C)C)C)C	floral ethereal sweet creamy winey	Flavornet, Flavorbase
464	5,9,13-Pentadecatrien-2-one, 6,10,14- trimethyl-		CC(=CCCC(=CCCC(=CCCC(=O) C)C)C)C	fruity winey floral creamy	TGSC, OdoRactor
465	Geranyllinalool	(6E,10E)-3,7,11,15- tetramethylhexadeca- 1,6,10,14-tetraen-3-ol	CC(=CCCC(=CCCC(C)(C=C)0)C)C)C	floral rose mild balsamic	OdorRactor ,TGSC
466	Farnesol	(2E ,6E)-3,7,11-trimethyldodeca- 2,6,10-trien-1-ol	CC(=CCCC(=CCCC(=CCO)C)C)	anisic apricot balsamic clove grapefruit oily orange floral peach pear muguet sweet fresh linden flower angelica dry rose lily wax mild delicate citrus lime	Sigma Aldrich,Flavornet, TGSC, Flavorbase, OdoRactor, Pubchem
467	(2Z,6E)-Farnesol	(2Z ,6E)-3,7,11-trimethyldodeca- 2,6,10-trien-1-ol	CC(=CCCC(=CCC)C)C) C	rose	ADB
468	3,7,11-Trimethyldodeca- 2,6,10-trienyl acetate	3,7,11-trimethyldodeca-2,6,10- trienyl acetate	CC(=CCCC(=CCCC(=CCOC(=O)	green floral rose	OdorRactor ,TGSC
469	Farnesyl acetate	[(2E,6E)-3,7,11- trimethyldodeca-2,6,10-trienyl] acetate		oily wax faint green floral rose melon	Flavornet, TGSC, Flavorbase
470	Geranylacetone	(5E)-6,10-dimethylundeca-5,9-dien-2-one	CC(=CCCC(=CCCC(=O)C)C)C	apple green woody vegetable rose magnolia floral aldehydic fruity fresh leafy wax tropical pear guava	Sigma Aldrich, Flavornet, TGSC, OdoRactor
471	Nerylacetone	(5Z)-6,10-dimethylundeca-5,9-dien-2-one	CC(=CCCC(=CCCC(=O)C)C)C	fatty metallic	OdorRactor ,TGSC
472	Nerolidol	(6 <i>E</i>)-3,7,11-trimethyldodeca-1,6,10-trien-3-ol	CC(=CCCC(=CCCC(C)(C=C)O)C)C	apple green citrus woody rose wax floral	Sigma Aldrich, Flavornet, TGSC, OdoRactor
473	Peruviol	(3 <i>S</i> ,6 <i>Z</i>)-3,7,11-trimethyldodeca- 1,6,10-trien-3-ol	CC(=CCCC(=CCCC(C)(C=C)O)C)C	mild floral	OdorRactor,
474	cis-Nerolidol	(6Z)-3,7,11-trimethyldodeca- 1,6,10-trien-3-ol	CC(=CCCC(=CCCC(C)(C=C)O)C	wax rose floral	Flavornet, TGSC
475	Nerolidyl acetate	[(6E)-3,7,11-trimethyldodeca- 1,6,10-trien-3-yl] acetate	CC(=CCCC(=CCCC(C)(C=C)OC(=O)C)C) C	floral fresh citrus sweet wax freesia woody	OdorRactor ,TGSC
476	4,8-Decadienal, 5,9-dimethyl-	(4Z)-5,9-dimethyldeca-4,8-dienal	CC(=CCCC(=CCCC=O)C)C	citrus aldehydic marine floral ozone	OdorRactor ,TGSC
477	Pyridine, 4-(4,8-dimethyl-3,7-nonadienyl)-	4-[(3 <i>E</i>)-4,8-dimethylnona-3,7-dienyl]pyridine	CC(=CCCC(=CCCC1=CC=NC=C 1)C)C	fresh watery buttery clean wet costus metallic	OdorRactor ,TGSC
478		7 31 7		meaty cooked brown roasted	TGSC
479	Geraniol	(2E)-3,7-dimethylocta-2,6-dien-1- ol	-CC(=CCCC(=CCO)C)C	apple apricot berry rose sweet geranium floral fruity wax citrus citronella pleasant	Sigma Aldrich, AOD, TGSC, OdoRactor, Pubchem
480	Nerol	(2Z)-3,7-dimethylocta-2,6-dien-1- ol	CC(=CCCC(=CCO)C)C	citrus sweet natural neroli magnolia floral fresh green lemon lime wax spicy rose wet seashore	Sigma Aldrich, TGSC, Pubchem
481	3,7-Dimethyl-2,6-octadienyl 2,3- dimethylcrotonate	[(2E)-3,7-dimethylocta-2,6-dienyl] 2,3- dimethylbut-2-enoate	CC(=CCCC(=CCOC(=O)C(=C(C) C)C)C)C	sweet fruity tropical rose herbaceous rummy	OdorRactor ,TGSC
482	Neryl acetate	[(2Z)-3,7-dimethylocta-2,6-dienyl] acetate	CC(=CCCC(=CCOC(=O)C)C)C	apple apricot blossom chocolate grape green honey lemon lime oily orange wax peach pear raspberry rose sweet floral soapy citrus dewy grapefruit tropical fruity	Sigma Aldrich, TGSC, OdoRactor
483	Geranyl acetate	[(2E)-3,7-dimethylocta-2,6-dienyl] acetate	CC(=CCCC(=CCOC(=0)C)C)C	lavender fruity rose sweet floral green wax herbaceous cooling	Sigma Aldrich, TGSC, OdoRactor
484	(,6E)-3,7-Dimethyl-2,6- octadienyl cinnamate	[(2E)-3,7-dimethylocta-2,6-dienyl] (E)-3- phenylprop-2-enoate	CC(=CCCC(=CCOC(=O)C=CC1= CC=CC =C1)C)C	balsamic amber rose	TGSC
485	Geranyl benzoate	[(2E)-3,7-dimethylocta-2,6-dienyl] benzoate	CC(=CCCC(=CCOC(=O)C1=CC= CC=C1) C)C	balsamic ylang sweet amber rose	SuperScent, TGSC, OdoRactor
486	Geranyl anthranilate	[(2E)-3,7-dimethylocta-2,6-dienyl] 2- aminobenzoate		floral neroli rose geranium honeysuckle	OdorRactor ,TGSC
487	Geranyl acetoacetate	[(2E)-3,7-dimethylocta-2,6-	CC(=CCCC(=CCOC(=O)CC(=O) C)C)C	fruity sweet winey fermented apple	OdorRactor ,TGSC
		dienyl] 3- oxobutanoate	C/C/C	ирріс	<u> </u>

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489	Benzeneacetic acid, (2E)-3,7- dimethyl-2,6- octadien-1-yl ester	3,7-dimethylocta-2,6-dienyl 2- phenylacetate	CC(=CCCC(=CCOC(=O)CC1=C C=CC=C 1)C)C	floral tropical honey rose fruity sweet balsamic powdery dried fruit	OdorRactor ,TGSC
490	Geranyl phenylacetate	[(2E)-3,7-dimethylocta-2,6-dienyl] 2- phenylacetate	CC(=CCCC(=CCOC(=0)CC1=C C=CC=C 1)C)C	honey rose floral aromatic fruity geranium	Sigma Aldrich, TGSC, OdoRactor
491	(Z)-3,7-Dimethylocta-2,6- dienyl phenylacetate	[(2Z)-3,7-dimethylocta-2,6-dienyl] 2- phenylacetate	CC(=CCCC(=CCOC(=O)CC1=C C=CC=C 1)C)C	honey rose honeysuckle	TGSC
492	10-Undecenoic acid, 3,7- dimethyl-2,6- octadienyl ester	[(2E)-3,7-dimethylocta-2,6-dienyl] undec-10- enoate	CC(=CCCC(=CCOC(=O)CCCCC CCCC= C)C)C	wax floral leafy rose	TGSC
493	1,1-Digeranyloxy-2- phenylethane	2,2-bis[(2 <i>E</i>)-3,7-dimethylocta- 2,6- dienoxy]ethylbenzene	CC(=CCCC(=CCOC(CC1=CC=C C=C1)O CC=C(C)CCC=C(C)C)C)C	floral rose green powdery tropical	TGSC
494	2,6-Octadiene, 1-methoxy-3,7-dimethyl-	(2E)-1-methoxy-3,7-dimethylocta 2,6-diene		floral rose sweet	SuperScent, TGSC, OdoRactor
495	Geranyl formate	[(2E)-3,7-dimethylocta-2,6-dienyl] formate	CC(=CCCC(=CCOC=O)C)C	green fruity rose sweet fresh neroli tearose floral apple peach tropical	Sigma Aldrich, TGSC, OdoRactor
496	Neryl formate	[(2Z)-3,7-dimethylocta-2,6-dienyl] formate	CC(=CCCC(=CCOC=O)C)C	green rose geranium herbaceous fruity tea metallic sweet floral citrus tropical	OdorRactor ,TGSC
497	Digeranyl ether	(2E)-1-[(2E)-3,7-dimethylocta- 2,6-dienoxy]-3,7- dimethylocta- 2,6-diene	CC(=CCCC(=CCOCC=C(C)CCC =C(C)C) C)C	clean floral balsamic	TGSC
498	(E)-[(3,7-Dimethyl-2,6-octadienyl)oxy]acetaldehyde	2-[(2 <i>E</i>)-3,7-dimethylocta-2,6-dienoxy]acetaldehyde	CC(=CCCC(=CCOCC=O)C)C	wax clean aldehydic ozone rose sweet	OdorRactor ,TGSC
499	(Z)-3,7-Dimethylocta-2,6- diene-1-thiol	(2Z)-3,7-dimethylocta-2,6-diene- 1-thiol	CC(=CCCC(=CCS)C)C	green fruity berry minty sulfurous catty	OdorRactor ,TGSC
500	6-Methyl-5-hepten-2-one	6-methylhept-5-en-2-one	CC(=CCCC(=0)C)C	green oily pepper mushroom rubbery citrus musty lemongrass apple fruity ketonic creamy cheese banana nutty hazelnut filbert roasted coffee fatty powerful	Sigma Aldrich, TGSC,OdoRactor
501	3,7-Dimethyloct-6-en-1-yn-3- ol	3,7-dimethyloct-6-en-1-yn-3-ol	CC(=CCCC(C)(C#C)O)C	sweet musk wax woody ambrette dry	OdorRactor ,TGSC
502	2,6-Dimethyl-5,7-octadien-2-	(5E)-2,6-dimethylocta-5,7-dien-2-	CC(=CCCC(C)(C)O)C=C	citrus fresh lemon lime cologne sweet mace	SuperScent, TGSC, OdoRactor
503	1,1,5-Trimethylhepta-4,6- dienyl acetate	[(5E)-2,6-dimethylocta-5,7-dien-2-yl] acetate	CC(=CCCC(C)(C)OC(=O)C)C=C	fruity citrus lavender cologne bergamot floral	OdorRactor ,TGSC
504	(-)-Linalool	(3R)-3,7-dimethylocta-1,6-dien-3-	CC(=CCCC(C)(C=C)O)C	floral woody natural lavender fresh	Sigma Aldrich, TGSC, OdoRactor
505	Linalool	3,7-dimethylocta-1,6-dien-3-ol	CC(=CCCC(C)(C=C)O)C	lemon orange floral sweet lavender citrus bois de rose woody green blueberry terpenic wax rose fresh petitgrain spicy	Sigma Aldrich, TGSC, Pubchem
506	(+)-Linalool	(3S)-3,7-dimethylocta-1,6-dien-3-ol	CC(=CCCC(C)(C=C)O)C	sweet floral lavender petitgrain	OdorRactor ,TGSC
507	Linalyl acetate	3,7-dimethylocta-1,6-dien-3-yl acetate	CC(=CCCC(C)(C=C)OC(=O)C)C	fruity floral pear sweet green citrus spicy clean terpenic bergamot lavender woody	Sigma Aldrich, TGSC,OdoRactor
508	Linalyl cinnamate	3,7-dimethylocta-1,6-dien-3-yl (<i>E</i>)-3-phenylprop- 2-enoate	CC(=CCCC(C)(C=C)OC(=O)C=C C1=CC= CC=C1)C	balsamic sweet lily neroli labdanum amber	OdorRactor ,TGSC
509	Linalyl benzoate	3,7-dimethylocta-1,6-dien-3-yl benzoate	CC(=CCCC(C)(C=C)OC(=O)C1= CC=CC= C1)C	wax amber citrus musk fatty incense dry dairy creamy fishy fruity pear floral bergamot genet herbaceous tuberose tropical lily plum ylang grape	Sigma Aldrich, TGSC, OdoRactor
510	Linalyl anthranilate	3,7-dimethylocta-1,6-dien-3-yl 2- aminobenzoate	CC(=CCCC(C)(C=C)OC(=O)C1= CC=CC= C1N)C	linalool blossom herbaceous gardenia woody fresh bois de rose orange flower floral terpenic citrus petitgrain mandarin rose	OdorRactor ,TGSC
511	Linalyl phenylacetate	3,7-dimethylocta-1,6-dien-3-yl 2- phenylacetate	CC(=CCCC(C)(C=C)OC(=0)CC1 =CC=C C=C1)C	rose sweet honey neroli lily of the valley floral	OdorRactor ,TGSC
512	Linalyl formate	3,7-dimethylocta-1,6-dien-3-yl formate	CC(=CCCC(C)(C=C)OC=O)C	green citrus woody coriander herbaceous bergamot fruity rose	Sigma Aldrich, TGSC, OdoRactor
513	Linalool, oxide	6-methyl-2-(oxiran-2-yl)hept-5-en- 2-ol	CC(=CCCC(C)(C1CO1)O)C	woody floral herbaceous earthy green cooling terpenic	Flavornet, TGSC
514	alpha-Santalene	1,7-dimethyl-7-(4-methylpent-3-enyl)tricyclo[2.2.1.02,6]heptane	CC(=CCCC1(C2CC3C1(C3C2)C) C)C	sweet woody	Flavorbase
	<u> </u>				l

	i		İ	coffee meaty ammonical	İ
537	3-Methyl-2-butene-1-thiol	3-methylbut-2-ene-1-thiol	CC(=CCS)C	smoky sulfurous onion leek skunk	Flavornet, TGSC, Flavorbase
536	Prenyl formate	3-methylbut-2-enyl formate	CC(=CCOC=O)C	ethereal tomato fruity rummy	OdorRactor ,TGSC
535	Prenyl salicylate	3-methylbut-2-enyl 2- hydroxybenzoate	CC(=CCOC(=O)C1=CC=CC=C1 O)C	floral herbaceous green orchid woody metallic	OdorRactor ,TGSC
534	Prenyl benzoate	3-methylbut-2-enyl benzoate	CC(=CCOC(=O)C1=CC=CC=C1)	balsamic fruity chocolate tea ylang	SuperScent, TGSC, OdoRactor
533	2-Butenoic acid, 3-methyl-, 3-methyl-2- butenyl ester	3-methylbut-2-enyl 3-methylbut-2-enoate	CC(=CCOC(=O)C=C(C)C)C	heliotrope warm herbaceous green chervil	OdoRactor TGSC
532	Prenyl acetate	3-methylbut-2-enyl acetate	CC(=CCOC(=O)C)C	apple green lavender sweet banana fruity jasmine balsamic fresh ripe	Sigma Aldrich, AOD, Flavorbase, TGSC,
531	3-Methyl-2-buten-1-OL	3-methylbut-2-en-1-ol	CC(=CCO)C	green fruity herbaceous lavender sweet alcoholic yeasty	Sigma Aldrich, TGSC,OdoRactor
	dimethyl-6- methylidenecyclohexyl]-4- methylidenecyclohexyl]-4- methylhex-3- enyl]-2,5,5,8a- tetramethyl-3,4,4a,6,7,8- hexahydro-1H-naphthalen-2- ol	dimethyl-6- methylidenecyclohexyl]-4- methylidenecyclohexyl]-2,5,5,8 <i>a</i> -tetramethyl-3,4,4 <i>a</i> ,6,7,8-hexahydro-1 <i>H</i> - naphthalen-2-ol	C)O)(C) C)C)CCC3C(=C)CCCC3(C)C	and the second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second s	,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,
529 530	Perillene 2R,8As)-1-[(E)-6-[(1S)-2,2-	3-(4-methylpent-3-enyl)furan (2R ,8aS)-1-[(E)-6-[(1S)-2,2-	CC(=CCCC1=COC=C1)C CC(=CCCC1C2(CCCC(C2CCC1(woody amber ambergis labdanum woody	Flavornet OdorRactor ,TGSC
28	Myraldyl acetate	[(1S)-3-(4-methylpent-3-enyl)cyclohex-3-en-1-yl]methyl acetate	CC(=CCCC1=CCCC(C1)COC(=O)C)C	citrus freesia green	OdorRactor ,TGSC
527	3-Cyclohexene-1- carboxaldehyde, 3-(4- methyl- 3-pentenyl)-	3-(4-methylpent-3-enyl)cyclohex- 3-ene-1- carbaldehyde	CC(=CCCC1=CCCC(C1)C=O)C	aldehydic orange ozone fruity clean fresh	TGSC
526	3-(4-Methyl-3- pentenyl)cyclohex-3-ene-1- carbonitrile	,	CC(=CCCC1=CCCC(C1)C#N)C	ozone citrus linen laundered cloth marine	OdorRactor ,TGSC
:5	3-Cyclohexene-1- carboxaldehyde, 1-methyl- 3-(4-methyl-3-penten-1-yl)-	1-methyl-3-(4-methylpent-3- enyl)cyclohex-3-ene-1- carbaldehyde	CC(=CCCC1=CCCC(C1)(C)C=O)	citrus aldehydic grapefruit muguet ozone	OdorRactor ,TGSC
24	4-(4-Methyl-3- pentenyl)cyclohex-3-ene-1- carbaldehyde	4-(4-methylpent-3-enyl)cyclohex- 3-ene-1- carbaldehyde	CC(=CCCC1=CCC(CC1)C=O)C	citrus floral marine aldehydic greasy	OdorRactor ,TGSC
23	Methyl 2-(((4-(4-methyl-3-pentenyl)-3- cyclohexen-1-yl)methylene)amino)benzoate	methyl 2-[[4-(4-methylpent-3- enyl)cyclohex-3-en-1 yl]methylideneamino]benzoate	CC(=CCCC1=CCC(CC1)C=NC2= CC=CC =C2C(=0)OC)C	green fresh clean citrus fruity hyacinth	OdorRactor ,TGSC
22	1-Methyl-4-(4-methyl-3- pentenyl)cyclohex- 3-ene-1-carbaldehyde	1-methyl-4-(4-methylpent-3- enyl)cyclohex-3-ene-1- carbaldehyde	CC(=CCCC1=CCC(CC1)(C)C=O) C	aldehydic clean herbaceous ozone	TGSC
21	2-Methyl-2-(4-methylpent-3- enyl)cyclopropanecarbaldehy de	2-methyl-2-(4-methylpent-3- enyl)cyclopropane-1- carbaldehyde	CC(=CCCC1(CC1C=0)C)C	fruity citrus lemon	TGSC
		methylidene-2- bicyclo[2.2.1]heptanyl)pent-2- enyl] 2- phenylacetate)COC(= 0)CC3=CC=CC=C3	wood wood	
20	methyl-3- methylidene-2- bicyclo[2.2.1]heptanyl)pent- 2-enyl] acetate	3-methylidene-2- bicyclo[2.2.1]heptanyl)pent-2- enyl] acetate [(E)-2-methyl-5-(2-methyl-3-	CC(=CCCC1(C2CCC(C2)C1=C)C	wax woody honey floral sandal	TGSC, Flavorbase
19	5-(2,3-Dimethyl-3- tricyclo[2.2.1.02,6]heptanyl)- 2-methylpent- 2-enyl] acetate;[2-methyl-5-(2-	[5-(2,3-dimethyl-3- tricyclo[2.2.1.02,6]heptanyl)-2- methylpent-2-enyl] acetate;[2-	CC(=CCCC1(C2CCC(C2)C1=C)C)COC(= 0)C.CC(=CCCC1(C2CC3C1(C3C 2)C)C)C OC(=0)C	powdery orris violet acidic green	OdorRactor ,TGSC, Flavorbase
18	beta-SANTALOL	(Z)-2-methyl-5-[(1S,2R,4R)-2-methyl-3- methylidene-2-bicyclo[2.2.1]heptanyl]pent-2-en-1-ol	CC(=CCCC1(C2CCC(C2)C1=C)C)CO	woody sandal wood animal	Flavorbase
517	methyl-3-	the Jeannethyl-3-methylidene-2-bicyclo[2.2.1]heptanyl]pent-2-en-1-ol)CO	sweet sailual wood woody	Flavorbase
516	alpha-Santalyl acetate 2-Methyl-5-((1S,2S,4R)-2-	[(Z)-5-[(1S,3R,6R)-2,3-dimethyl-3-tricyclo[2.2.1.02,6]heptanyl]-2-methylpent-2-enyl] acetate (E)-2-methyl-5-[(1S,2S,4R)-2-	CC(=CCCC1(C2CC3C1(C3C2)C) C)COC(=0)C CC(=CCCC1(C2CCC(C2)C1=C)C		TGSC OdorRactor ,TGSC,
	ept-3-yl]-2- methyl-, (2Z)-	tricyclo[2.2.1.02,6]heptanyl)-2- methylpent-2-en-1-ol	C)CO		

538	(E)-2-Phenylpropenyl acetate		CC(=COC(=0)C)C1=CC=CC=C1	sweet honey neroli hyacinth floral	TGSC, OdoRactor
539	Acetone	acetate propan-2-one	CC(=O)C	apple ethereal pear solvent fruity	Flavornet, TGSC, PubChem
540	2,3-Butanedione	butane-2,3-dione	CC(=0)C(=0)C	characteristic buttery strong sweet creamy	Flavornet, TGSC, Pubchem
340	,	,	CC(-0)C(-0)C	pungent caramel fatty vanilla quinoline chlorine	
541	1-Phenyl-1,2-propanedione	1-phenylpropane-1,2-dione	CC(=0)C(=0)C1=CC=CC=C1	buttery green medicinal vegetable pepper pungent plastic honey	Sigma Aldrich, TGSC,OdoRactor
542	1-(2-Thienyl)propane-1,2- dione	1-thiophen-2-ylpropane-1,2-dione	CC(=O)C(=O)C1=CC=CS1	woody praline	TGSC
543	Pyruvic acid	2-oxopropanoic acid	CC(=O)C(=O)O	acidic sharp sour acetic caramel coffee creamy green meaty winey vinegar powerful	Sigma Aldrich, TGSC
544	3-Hydroxy-4-phenylbutan-2- one	3-hydroxy-4-phenylbutan-2-one	CC(=O)C(CC1=CC=CC=C1)O	creamy sweet fruity	OdorRactor ,TGSC
545	Dehydrozingerone	(E)-4-(4-hydroxy-3- methoxyphenyl)but-3-en-2- one	CC(=O)C=CC1=CC(=C(C=C1)O) OC	vanilla sweet powdery creamy balsamic	OdorRactor ,TGSC
546	Benzylideneacetone	(E)-4-phenylbut-3-en-2-one	CC(=O)C=CC1=CC=CC=C1	almond anisic balsamic buttery cherry cinnamyl spice creamy jammy herbaceous woody floral sweet vanilla rhubarb powdery phenolic fruity	Sigma Aldrich, TGSC, OdoRactor
547	Furfural acetone	(E)-4-(furan-2-yl)but-3-en-2-one	CC(=0)C=CC1=CC=CO1	sweet spicy warm balsamic cinnamyl vanilla nutty creamy coumarinic powdery anisic	OdorRactor ,TGSC
548	beta-Ionone epoxide	(E)-4-(2,2,6-trimethyl-7-oxabicyclo[4.1.0]heptan-1-yl)but-3-en-2-one	CC(=0)C=CC12C(CCCC1(O2)C) (C)C	fruit sweet woody berry violet orris powdery	Flavornet, TGSC, OdoRactor
549	3-Buten-2-one, 4-(2,2,6- trimethyl-7- oxabicyclo[4.1.0]hept-1-yl)-	4-(2,2,6-trimethyl-7- oxabicyclo[4.1.0]heptan-1- yl)but- 3-en-2-one	CC(=0)C=CC12C(CCCC1(O2)C) (C)C	fruity sweet berry woody orris violet powdery intense floral raspberry	OdorRactor ,TGSC, Flavorbase
550	gamma-Ionone	(E)-4-(2,2-dimethyl-6- methylidenecyclohexyl)but- 3-en-2-one	CC(=O)C=CC1C(=C)CCCC1(C)C	woody floral green fruity raspberry	TGSC, Flavorbase, ODoRactor
551	Methylglyoxal	2-oxopropanal	CC(=O)C=O	caramel sweet acidic ethereal brown rummy pungent	Sigma Aldrich, TGSC, Pubchem
552	3(2H)-Furanone, 5-acetyl-2- [(2- furanylmethyl)thio]dihydro- 2,5-dimethyl-	5-acetyl-2-(furan-2- ylmethylsulfanyl)-2,5- dimethyloxolan-3-one	CC(=0)C1(CC(=0)C(01)(C)SCC 2=CC=C 02)C	woody coffee	TGSC
553	Diacetyl trimer	1-(2-acetyl-6a -hydroxy-2,3a ,5- trimethyl-6H - furo[2,3- d][1,3]dioxol-5-yl)ethanone	CC(=O)C1(CC2(C(O1)(OC(O2)(C)C(=O)C)C)O)C	buttery roasted	OdorRactor ,TGSC
554	1-Acetylcyclohexyl acetate	(1-acetylcyclohexyl) acetate	CC(=O)C1(CCCCC1)OC(=O)C	honey floral fruity sweet rose nutty fig	ADB, TGSC, OdoRactor
555	Xanthoxylin	1-(2-hydroxy-4,6- dimethoxyphenyl)ethanone	CC(=0)C1=C(C=C(C=C10C)OC) O	·	TGSC
556	Isomaltol	1-(3-hydroxyfuran-2-yl)ethanone	CC(=0)C1=C(C=CO1)O	burnt caramel fruity	TGSC
557	Celestolide	1-(6- <i>tert</i> -butyl-1,1-dimethyl-2,3-dihydroinden-4- yl)ethanone	CC(=O)C1=C2CCC(C2=CC(=C1) C(C)(C) C)(C)C	animal musk cedar woody ambergis sweet	OdorRactor ,TGSC
557	Celestolide Acetovanillone			-	OdorRactor ,TGSC Sigma Aldrich, TGSC, Flavorbase
		dihydroinden-4- yl)ethanone 1-(4-hydroxy-3-	C(C)(C) C)(C)C	ambergis sweet almond hawthorn musty floral vanilla faint sweet powerful burnt coffee	Sigma Aldrich, TGSC,
558 559 560	Acetovanillone 3',4'-Dimethoxyacetophenone 4'-Chloroacetophenone	dihydroinden-4- yl)ethanone 1-(4-hydroxy-3- methoxyphenyl)ethanone 1-(3,4-dimethoxyphenyl)ethanone 1-(4-chlorophenyl)ethanone	C(C)(C) C)(C)C CC(=0)C1=CC(=C(C=C1)O)OC CC(=0)C1=CC(=C(C=C1)OC)OC CC(=0)C1=CC=C(C=C1)C1	ambergis sweet almond hawthorn musty floral vanilla faint sweet powerful burnt coffee woody sweet floral floral sweet hawthorn hay	Sigma Aldrich, TGSC, Flavorbase TGSC, OdoRactor
558 559 560 561	Acetovanillone 3',4'-Dimethoxyacetophenone 4'-Chloroacetophenone 4'-Hydroxyacetophenone	dihydroinden-4- yl)ethanone 1-(4-hydroxy-3- methoxyphenyl)ethanone 1-(3,4-dimethoxyphenyl)ethanone 1-(4-chlorophenyl)ethanone 1-(4-hydroxyphenyl)ethanone	C(C)(C) C)(C)C CC(=0)C1=CC(=C(C=C1)O)OC CC(=0)C1=CC(=C(C=C1)OC)OC CC(=0)C1=CC=C(C=C1)C1 CC(=0)C1=CC=C(C=C1)O	ambergis sweet almond hawthorn musty floral vanilla faint sweet powerful burnt coffee woody sweet floral floral sweet hawthorn hay mild sweet hawthorn balsamic mimosa floral	Sigma Aldrich, TGSC, Flavorbase TGSC, OdoRactor TGSC OdorRactor, TGSC
558 559 560	Acetovanillone 3',4'-Dimethoxyacetophenone 4'-Chloroacetophenone	dihydroinden-4- yl)ethanone 1-(4-hydroxy-3- methoxyphenyl)ethanone 1-(3,4-dimethoxyphenyl)ethanone 1-(4-chlorophenyl)ethanone	C(C)(C) C)(C)C CC(=0)C1=CC(=C(C=C1)O)OC CC(=0)C1=CC(=C(C=C1)OC)OC CC(=0)C1=CC=C(C=C1)C1	ambergis sweet almond hawthorn musty floral vanilla faint sweet powerful burnt coffee woody sweet floral floral sweet hawthorn hay mild sweet hawthorn balsamic	Sigma Aldrich, TGSC, Flavorbase TGSC, OdoRactor
558 559 560 561 562	Acetovanillone 3',4'-Dimethoxyacetophenone 4'-Chloroacetophenone 4'-Hydroxyacetophenone 4'-Methoxyacetophenone 5-Acetyl-2,3-dihydro-1H-	dihydroinden-4- yl)ethanone 1-(4-hydroxy-3- methoxyphenyl)ethanone 1-(3,4-dimethoxyphenyl)ethanone 1-(4-chlorophenyl)ethanone 1-(4-hydroxyphenyl)ethanone 1-(4-methoxyphenyl)ethanone	C(C)(C) C)(C)C CC(=0)C1=CC(=C(C=C1)O)OC CC(=0)C1=CC(=C(C=C1)OC)OC CC(=0)C1=CC=C(C=C1)C1 CC(=0)C1=CC=C(C=C1)O	ambergis sweet almond hawthorn musty floral vanilla faint sweet powerful burnt coffee woody sweet floral floral sweet hawthorn hay mild sweet hawthorn balsamic mimosa floral butter caramel fruity nutty sweet vanilla hawthorn anisic powdery balsamic acacia cherry maraschino pleasant heliotrope grassy hay smoky medicinal	Sigma Aldrich, TGSC, Flavorbase TGSC, OdoRactor TGSC OdorRactor,TGSC Sigma Aldrich, TGSC,
558 559 560 561 562	Acetovanillone 3',4'-Dimethoxyacetophenone 4'-Chloroacetophenone 4'-Hydroxyacetophenone 4'-Methoxyacetophenone	dihydroinden-4- yl)ethanone 1-(4-hydroxy-3- methoxyphenyl)ethanone 1-(3,4-dimethoxyphenyl)ethanone 1-(4-chlorophenyl)ethanone 1-(4-hydroxyphenyl)ethanone 1-(4-methoxyphenyl)ethanone	C(C)(C) C)(C)C CC(=0)C1=CC(=C(C=C1)O)OC CC(=0)C1=CC(=C(C=C1)OC)OC CC(=0)C1=CC=C(C=C1)C1 CC(=0)C1=CC=C(C=C1)OC CC(=0)C1=CC=C(C=C1)OC	ambergis sweet almond hawthorn musty floral vanilla faint sweet powerful burnt coffee woody sweet floral floral sweet hawthorn hay mild sweet hawthorn balsamic mimosa floral butter caramel fruity nutty sweet vanilla hawthorn anisic powdery balsamic acacia cherry maraschino pleasant heliotrope	Sigma Aldrich, TGSC, Flavorbase TGSC, OdoRactor TGSC OdorRactor ,TGSC Sigma Aldrich, TGSC, Pubchem

566	2'-Hydroxyacetophenone	1-(2-hydroxyphenyl)ethanone	CC(=O)C1=CC=CC=C1O	hawthorn herbaceous sweet phenolic tobacco honey herbaceous sharp bitter almond tropical melon bitter	Sigma Aldrich, TGSC,OdoRactor
567	2'-Methoxyacetophenone	1-(2-methoxyphenyl)ethanone	CC(=0)C1=CC=CC=C1OC	powdery anisic almond phenolic	OdorRactor ,TGSC
568	2-Acetylpyridine	1-pyridin-2-ylethanone	CC(=0)C1=CC=CC=N1	fatty oily tobacco popcorn corn musty nutty	Sigma Aldrich, Flavornet, TGSC, OdoRactor
569	1'-Acetonaphthone	1-naphthalen-1-ylethanone	CC(=O)C1=CC=CC2=CC=CC=C 21	sweet orange flower blossom powdery neroli floral	OdorRactor ,TGSC
570	2-Acetylpyrrole	1-(1H -pyrrol-2-yl)ethanone	CC(=O)C1=CC=CN1	walnut nutty bready musty nut cherry coumarinic licorice maraschino	TGSC, OdoRactor
571	2-Acetyl-1-methylpyrrole	1-(1-methylpyrrol-2-yl)ethanone	CC(=0)C1=CC=CN1C	earthy	Sigma Aldrich, TGSC, OdoRactor
572	2-Acetylfuran	1-(furan-2-yl)ethanone	CC(=0)C1=CC=C01	almond beefy caramel coffee musty potato tobacco balsamic sweet cocoa nutty brown toasted milky lactonic	Sigma Aldrich, OdoRactor
573	2-Acetylthiophene	1-thiophen-2-ylethanone	CC(=O)C1=CC=CS1	sulfurous nutty hazelnut walnut	Sigma Aldrich, TGSC
574	4-Acetylpyridine	1-pyridin-4-ylethanone	CC(=O)C1=CC=NC=C1	burnt coffee	SuperScent, TGSC, OdoRactor
575	1-(5,6,7,8- Tetrahydronaphthalen-2- yl)ethanone	1-(5,6,7,8-tetrahydronaphthalen-2-yl)ethanone	CC(=0)C1=CC2=C(CCCC2)C=C 1	floral musk grape orange flower	OdorRactor ,TGSC
576	2-Acetylnaphthalene	1-naphthalen-2-ylethanone	CC(=0)C1=CC2=CC=CC=C2C= C1	sweet neroli orange flower powdery honey floral	Sigma Aldrich, TGSC
577	2-Acetylbenzofuran	1-(1-benzofuran-2-yl)ethanone	CC(=0)C1=CC2=CC=CC=C201	sweet coumarinic floral orange flower honey tropical neroli lactonic honeysuckle	OdorRactor ,TGSC
578	1-[(3Ar,7aS)-3a,4,7,7a- tetrahydro-3H-inden 5-yl]ethanone	1-[(3aR,7aS)-3a,4,7,7a- tetrahydro-3H-inden-5- yl]ethanone	CC(=0)C1=CCC2C=CCC2C1	green fruity floral melon	TGSC
579	2-Acetyl-1,4,5,6- tetrahydropyridine	1-(1,2,3,4-tetrahydropyridin-6-yl)ethanone	CC(=O)C1=CCCCN1	caramel	Sigma Aldrich, TGSC
580	2-Acetyl-2-pyrroline	1-(2,3-dihydro-1 <i>H</i> -pyrrol-5-yl)ethanone	CC(=O)C1=CCCN1	popcorn toasted grain malty nutty ham roasted sweet	OdorRactor ,TGSC
581	3-Acetylpyridine	1-pyridin-3-ylethanone	CC(=O)C1=CN=CC=C1	nutty sweet hawthorn phenolic woody popcorn dry	Sigma Aldrich, TGSC,OdoRactor
582	5-Acetyl-2,3-dihydro-1,4-	1-(3,4-dihydro-2 <i>H</i> -1,4-thiazin-5-	CC(=O)C1=CSCCN1	nutty cooked roasted pocpcorn	OdorRactor ,TGSC
583	Acetylpyrazine	yl)ethanone 1-pyrazin-2-ylethanone	CC(=O)C1=NC=CN=C1	chocolate green nutty roasted hazelnut coffee popcorn corn bready musty potato	Sigma Aldrich, TGSC, Odoractor
584	1-(Oxazol-2-yl)ethanone	1-(1,3-oxazol-2-yl)ethanone	CC(=O)C1=NC=CO1	nutty popcorn	TGSC
585	2-Acetylthiazole	1-(1,3-thiazol-2-yl)ethanone	CC(=O)C1=NC=CS1	roasted chocolate hazelnut meaty fruity nutty sulfurous popcorn roasted peanut toasted corn raw bready	Sigma Aldrich, Flavornet, TGSC, OdoRactor
586	2-Acetyl-1-pyrroline	1-(3,4-dihydro-2 <i>H</i> -pyrrol-5-yl)ethanone	CC(=O)C1=NCCC1	nutty roasted malty grain popcorn toasted	Flavornet, TGSC, OdoRactor
587	1-(3,4,5,6-Tetrahydro-2- pyridinyl)ethanone	1-(2,3,4,5-tetrahydropyridin-6-yl)ethanone	CC(=0)C1=NCCCC1	roasted bready caramel	Flavornet, TGSC, OdoRactor
588	2-Acetyl-2-thiazoline	1-(4,5-dihydro-1,3-thiazol-2-yl)ethanone	CC(=O)C1=NCCS1	nutty roast popcorn potato chip bready corn taco toasted green onion chicken toasted grain roasted nut herbaceous grassy potato roasted	Sigma Aldrich, TGSC
589	1-(3,3- Dimethylbicyclo[2.2.1]hept-2- yl)ethan-1-one	1-(3,3-dimethyl-2-bicyclo[2.2.1]heptanyl)ethanone	CC(=0)C1C2CCC(C2)C1(C)C	camphoraceous herbaceous minty woody apple	OdorRactor ,TGSC
590	3,3-Dimethylcyclohexyl methyl ketone	1-(3,3- dimethylcyclohexyl)ethanone	CC(=O)C1CCCC(C1)(C)C	woody herbaceous minty cedar leafy thujonic	OdorRactor ,TGSC
591	Ethanone, 1-(3-cycloocten-1-yl)-	1-[(3Z)-cyclooct-3-en-1- yl]ethanone	CC(=O)C1CCCCC=CC1	aldehydic aromatic woody thujonic natural	TGSC
592	Benzoylacetone	1-phenylbutane-1,3-dione	CC(=O)CC(=O)C1=CC=CC=C1	balsamic woody dry vanilla hawthorn opoponax	OdorRactor ,TGSC
593	Acetoacetanilide	3-oxo-N -phenylbutanamide	CC(=O)CC(=O)NC1=CC=CC=C1	faint	Sigma Aldrich
594	Methyl acetoacetate	methyl 3-oxobutanoate	CC(=O)CC(=O)OC	fresh fruity citrus green agreeable	OdorRactor ,TGSC, Pubchem
595	Benzyl acetoacetate	benzyl 3-oxobutanoate	CC(=0)CC(=0)OCC1=CC=CC=C	floral sweet fruity banana	SuperScent, TGSC, OdoRactor
596	4-Methyl-4-phenylpentan-2-	4-methyl-4-phenylpentan-2-one	CC(=O)CC(C)(C)C1=CC=CC=C1	green sweet floral honey gardenia	OdorRactor ,TGSC
597	one 4-Cyclohexyl-4-methylpentan- 2-one	4-cyclohexyl-4-methylpentan-2- one	CC(=O)CC(C)(C)C1CCCCC1	floral woody wax vetiver	OdorRactor ,TGSC
598	4-Mercapto-4-methyl-2- pentanone	4-methyl-4-sulfanylpentan-2-one	CC(=O)CC(C)(C)S	sulfurous meaty green fruity catty black currant	SuperScent, TGSC, OdoRactor

599	4-Methyl-4-(methylthio)-2- pentanone	4-methyl-4-methylsulfanylpentan- 2-one	CC(=O)CC(C)(C)SC	fruity sulfurous green metallic musty rooty tropical black currant fermented	Sigma Aldrich, TGSC, Flavorbase
600	4,4-Dimethoxy-2-butanone	4,4-dimethoxybutan-2-one	CC(=O)CC(OC)OC	ethereal musty nutty alcoholic bitter	OdorRactor ,TGSC
601	4-Methoxyphenylacetone	1-(4-methoxyphenyl)propan-2-one	CC(=O)CC1=CC=C(C=C1)OC	caramel creamy vanilla sweet fruity spicy anisic balsamic licorice fennel green	Sigma Aldrich, TGSC
602	2-Furylacetone	1-(furan-2-yl)propan-2-one	CC(=O)CC1=CC=CO1	caramel fruity spicy radish herbaceous	OdorRactor ,TGSC
603	Levulinic acid	4-oxopentanoic acid	CC(=O)CCC(=O)O	winey sweet caramel acidic acetoin buttery guaiacol vanilla creamy weak	Sigma Aldrich, Flavorbase, TGSC,OdoRactor
604	Methyl levulinate	methyl 4-oxopentanoate	CC(=0)CCC(=0)OC	caramel	TGSC
605	5-Hexen-2-one Zingerone	hex-5-en-2-one 4-(4-hydroxy-3- methoxyphenyl)butan-2-one	CC(=0)CCC=C CC(=0)CCC1=CC(=C(C=C1)O)O C	ethereal floral clove creamy fatty spicy sweet phenolic ginger vanilla woody balsamic pungent characteristic	TGSC,OdoRactor Sigma Aldrich, Flavorbase, TGSC, Pubchem, OdoRactor
607	4-(4-Hydroxyphenyl)-2- butanone	4-(4-hydroxyphenyl)butan-2-one	CC(=0)CCC1=CC=C(C=C1)O	sweet berry jammy floral raspberry ripe woody seedy	Sigma Aldrich, Flavorbase, TGSC, Pubchem, OdoRactor
608	4-(4-Methoxyphenyl)-2- butanone	4-(4-methoxyphenyl)butan-2-one	CC(=0)CCC1=CC=C(C=C1)OC	cherry floral raspberry sweet rose fruity dry acacia woody powdery honey vanilla violet	Sigma Aldrich, TGSC, OdoRactor
609		[4-(3-oxobutyl)phenyl] acetate	=O)C	blueberry raspberry berry jammy	Sigma Aldrich, TGSC, OdoRactor
610	Benzylacetone	4-phenylbutan-2-one	CC(=0)CCC1=CC=CC=C1	floral balsamic	TGSC, OdoRactor
611	4-(2-Furyl)butan-2-one Piperonyl acetone	4-(furan-2-yl)butan-2-one 4-(1,3-benzodioxol-5-yl)butan-2- one	CC(=0)CCC1=CC=C01 CC(=0)CCC1=CC2=C(C=C1)OC O2	spicy caramel sweet floral raspberry cotton candy fruity jammy heliotrope powdery berry cassia mimosa	OdorRactor ,TGSC Sigma Aldrich, TGSC, Flavorbase, OdoRactor
613	4-(2,2-Dimethyl-6- methylenecyclohexyl)butan-2- one	4-(2,2-dimethyl-6- methylidenecyclohexyl)butan-2- one	CC(=0)CCC1C(=C)CCCC1(C)C	woody warm earthy ambergis tobacco amber violet	TGSC
614	5-Phenylpentan-2-one	5-phenylpentan-2-one	CC(=O)CCCC1=CC=CC=C1	floral sweetpea	OdorRactor ,TGSC
615	9-Decen-2-one	dec-9-en-2-one	CC(=0)CCCCCCC=C	fruity pineapple pear apple green fatty	TGSC, Flavorbase
616	4-Mercapto-2-butanone	4-sulfanylbutan-2-one	CC(=O)CCS	sulfurous onion	TGSC
617	4-(Methylthio)-2-butanone	4-methylsulfanylbutan-2-one	CC(=O)CCSC	sweet sulfurous vegetable potato earthy tomato metallic fatty cheese	Sigma Aldrich,TGSC, Flavorbase, OdoRactor
618	4,4'-Thiobis-2-butanone	4-(3-oxobutylsulfanyl)butan-2-one	CC(=O)CCSCCC(=O)C	spicy fresh green	OdorRactor ,TGSC
619	Hydroxyacetone	1-hydroxypropan-2-one	CC(=O)CO	pungent sweet caramel ethereal	OdorRactor ,TGSC
620	Acetoxyacetone	2-oxopropyl acetate	CC(=O)COC(=O)C	fruity buttery dairy nutty	OdorRactor ,TGSC
621	1-Methylthio-2-propanone	1-methylsulfanylpropan-2-one	CC(=O)CSC	melon	OdorRactor ,TGSC
	acetamide	acetamide	CC(=0)N	bland mousy	OdorRactor ,PubChem
623	N-Acetyl-2,3-dihydro-1H- pyrrole	1-(2,3-dihydropyrrol-1- yl)ethanone	CC(=O)N1CCC=C1	toasted	
624	Methyl N-acetylanthranilate	methyl 2-acetamidobenzoate	CC(=O)NC1=CC=CC=C1C(=O)O C		TGSC
625	Acetic acid	Acetic acid	CC(=O)O	sour pungent vinegar acidic sharp green herbaceous woody acetic	Sigma Aldrich, TGSC, PubChem
				8	1 doction
626	Acetic acid, sodium salt (2:1)	sodium;acetic acid;acetate	CC(=O)O.CC(=O)[O-].[Na+]	faint bland acetic	Sigma Aldrich, Pubchem
626	Acetic acid, sodium salt (2:1) Methyl acetate	sodium;acetic acid;acetate methyl acetate	CC(=O)O.CC(=O)[O-].[Na+] CC(=O)OC		
				faint bland acetic ethereal sweet fruity solvent estery	Sigma Aldrich, Pubchem Sigma Aldrich, TGSC,
627	Methyl acetate	methyl acetate	CC(=0)OC	faint bland acetic ethereal sweet fruity solvent estery winey cognac rummy pleasant	Sigma Aldrich, Pubchem Sigma Aldrich, TGSC, Pubchem
627	Methyl acetate 1-Phenylethenyl acetate	methyl acetate 1-phenylethenyl acetate	CC(=0)0C CC(=0)0C(=C)C1=CC=CC=C1	faint bland acetic ethereal sweet fruity solvent estery winey cognac rummy pleasant animal floral fecal phenolic acidic sharp vinegar acetic strong	Sigma Aldrich, Pubchem Sigma Aldrich, TGSC, Pubchem TGSC
627 628 629 630	Methyl acetate 1-Phenylethenyl acetate Acetic anhydride Tetrahydro-alpha,alpha,5-trimethyl-5- vinylfurfuryl	methyl acetate 1-phenylethenyl acetate acetyl acetate 2-(5-ethenyl-5-methyloxolan-2-	CC(=0)OC CC(=0)OC(=C)C1=CC=CC=C1 CC(=0)OC(=0)C CC(=0)OC(C)(C)C1CCC(01)(C)	faint bland acetic ethereal sweet fruity solvent estery winey cognac rummy pleasant animal floral fecal phenolic acidic sharp vinegar acetic strong pungent	Sigma Aldrich, Pubchem Sigma Aldrich, TGSC, Pubchem TGSC OdorRactor ,Pubchem
627 628 629 630	Methyl acetate 1-Phenylethenyl acetate Acetic anhydride Tetrahydro-alpha,alpha,5- trimethyl-5- vinylfurfuryl acetate Dimethylbenzylcarbinyl	methyl acetate 1-phenylethenyl acetate acetyl acetate 2-(5-ethenyl-5-methyloxolan-2-yl)propan-2-yl acetate (2-methyl-1-phenylpropan-2-yl)	CC(=0)OC(=C)C1=CC=CC=C1 CC(=0)OC(=O)C CC(=0)OC(C)(C)C1CCC(O1)(C) C=C CC(=0)OC(C)(C)C1=CC=CC=C1	faint bland acetic ethereal sweet fruity solvent estery winey cognac rummy pleasant animal floral fecal phenolic acidic sharp vinegar acetic strong pungent fruity woody sweet floral fruity pear rose green	Sigma Aldrich, Pubchem Sigma Aldrich, TGSC, Pubchem TGSC OdorRactor ,Pubchem OdorRactor,
627 628 629 630 631	Methyl acetate 1-Phenylethenyl acetate Acetic anhydride Tetrahydro-alpha,alpha,5- trimethyl-5- vinylfurfuryl acetate Dimethylbenzylcarbinyl acetate 1,1-Dimethyl-3-phenylpropyl	methyl acetate 1-phenylethenyl acetate acetyl acetate 2-(5-ethenyl-5-methyloxolan-2-yl)propan-2-yl acetate (2-methyl-1-phenylpropan-2-yl) acetate (2-methyl-4-phenylbutan-2-yl) acetate (2-methyl-6-methylideneoct-7-en-2-yl) acetate	CC(=0)OC(=C)C1=CC=CC=C1 CC(=0)OC(=O)C CC(=0)OC(C)(C)C1CCC(O1)(C) CC(=0)OC(C)(C)CC1=CC=CC=C1 CC(=0)OC(C)(C)CCC1=CC=CC=C1	faint bland acetic ethereal sweet fruity solvent estery winey cognac rummy pleasant animal floral fecal phenolic acidic sharp vinegar acetic strong pungent fruity woody sweet floral fruity pear rose green berry jasmine powdery rose green leafy sweet balsamic	Sigma Aldrich, Pubchem Sigma Aldrich, TGSC, Pubchem TGSC OdorRactor ,Pubchem OdorRactor, Sigma Aldrich, TGSC,OdoRactor
627 628 629 630 631	Methyl acetate 1-Phenylethenyl acetate Acetic anhydride Tetrahydro-alpha,alpha,5- trimethyl-5- vinylfurfuryl acetate Dimethylbenzylcarbinyl acetate 1,1-Dimethyl-3-phenylpropyl acetate	methyl acetate 1-phenylethenyl acetate acetyl acetate 2-(5-ethenyl-5-methyloxolan-2-yl)propan-2-yl acetate (2-methyl-1-phenylpropan-2-yl) acetate (2-methyl-4-phenylbutan-2-yl) acetate (2-methyl-6-methylideneoct-7-en-	CC(=0)OC CC(=0)OC(=C)C1=CC=CC=C1 CC(=0)OC(=0)C CC(=0)OC(C)(C)C1CCC(O1)(C) C=C CC(=0)OC(C)(C)CC1=CC=CC=C1 CC(=0)OC(C)(C)CCC1=CC=CC=C1	faint bland acetic ethereal sweet fruity solvent estery winey cognac rummy pleasant animal floral fecal phenolic acidic sharp vinegar acetic strong pungent fruity woody sweet floral fruity pear rose green berry jasmine powdery rose green leafy sweet balsamic narcissus floral citrus bergamot lavender floral woody nutmeg fresh herbaceous	Sigma Aldrich, Pubchem Sigma Aldrich, TGSC, Pubchem TGSC OdorRactor,Pubchem OdorRactor, Sigma Aldrich, TGSC,OdoRactor OdorRactor,TGSC

636 Styryl acetate	Sigma Aldrich, TGSC, OdoRactor Sigma Aldrich, AOD, Flavorbase, TGSC AOD, Flavorbase, TGSC, Pubchem, OdoRactor AOD Sigma Aldrich, TGSC, OdoRactor Cee OdorRactor ,TGSC SuperScent, TGSC
4-Formyl-2-methoxyphenyl acetate (2-methoxy-4-prop-2-enylphenyl) acetate (2-methoxy-4-prop-2-enylphenyl) acetate (2-methoxy-4-prop-2-enylphenyl) acetate (2-methoxy-4-prop-2-enylphenyl) acetate (2-methoxy-4-prop-2-enylphenyl) acetate (2-methoxy-4-prop-2-enylphenyl) acetate (2-methoxy-4-prop-2-enylphenyl) acetate (2-methoxy-4-prop-2-enylphenyl) acetate (2-methoxy-4-prop-2-enylphenyl) acetate (2-methoxy-4-prop-2-enylphenyl) acetate (2-methoxy-4-prop-2-enylphenyl) acetate (2-methoxy-4-prop-2-enylphenyl) acetate (2-methoxyphenyl) acetate (3-methoxyphenyl) acetate (4-4,8-trimethyl-1-tricyclol[6.3.1.02,5]dodecanyl) acetate (4-4,8-trimethyl-2-bicyclol[2.2.1]heptanyl] acetate (1,3,3-trimethyl-2-bicyclol[2.2.1]heptanyl) acetate (1,3,3-trimethyl-2-bicyclol[2.2.1]heptanyl) acetate (1,3,3-trimethyl-2-bicyclol[2.2.1]heptanyl) acetate (1,3,3-trimethyl-2-bicyclol[2.2.1]heptanyl) acetate (1,3,4-5,6,7,7a-hexahydro-acetate (1,3,4-5,6,7,7a-hexahydr	Sigma Aldrich, TGSC, OdoRactor Sigma Aldrich, AOD, Flavorbase, TGSC AOD, Flavorbase, TGSC, Pubchem, OdoRactor AOD ice Sigma Aldrich, TGSC, OdoRactor Ce OdorRactor ,TGSC SuperScent, TGSC
acetate Acetyleugenol Acetyleugenol C2-methoxy-4-prop-2-enylphenyl) acetate CC(=O)OC1=C(C=C(C=C)CC= fresh malty balsamic clove fru sweet spicy carnation woody f CC(=O)OC1=CC=CC=C1 phenolic lily jasmine metallic CC(=O)OC1=CC=CC=C1 phenolic lily jasmine metallic CC(=O)OC1=CC=CC=C1 phenolic lily jasmine metallic CC(=O)OC1=CC=CC=C1 musty woody walnut sweet spic ove powdery smoky dry phenolic guaiacol ham vanilla CC(=O)OC1=CC=CC=C1 musty woody walnut sweet spic ove powdery smoky dry phenolic guaiacol ham vanilla CC(=O)OC1=CC=CC=C1 musty woody walnut sweet spic ove powdery smoky dry phenolic guaiacol ham vanilla CC(=O)OC1=CC=CC=C1 musty woody walnut sweet spic ove powdery smoky dry phenolic guaiacol ham vanilla CC(=O)OC1=CCCCCIC3CCCCC green woody cedar pine licoric herbaceous acetate CC(=O)OC1=CCCCCIC3CCCCCC green woody cedar pine licoric herbaceous CC(=O)OC1CCCCC(C1)(CCC3C woody earthy amber fruity spic dry acetate CC(=O)OC1C(C2CCCI(C2)C)(C) balsamic fresh sweet pine herbaceous citrus fir CC(=O)OC1C(C2CCCI(C2)C)(C) bicyclo[2.2.1]heptanyl] acetate CC(=O)OC1C(C2CCCI(C2)C)(C) pine fir nreedle herbaceous citrus sweet balsamic fresh woody 648 4,7-Methano-1H-inden-5-ol, 3a,4,5,6,7,7a- hexahydro-, acetate 649 Octahydro-4,7-methano-1H- 8-tricyclo[5.2.1.02,6]dec-4-enyl acetate 649 Octahydro-4,7-methano-1H- 8-tricyclo[5.2.1.02,6]dec-4-enyl acetate 649 Octahydro-4,7-methano-1H- 8-tricyclo[5.2.1.02,6]dec-3-enyl acetate 649 Octahydro-4,7-methano-1H- 8-tricyclo[5.2.1.02,6]dec-4-enyl acetate 649 Octahydro-4,7-methano-1H- 8-tricyclo[5.2.1.02,6]dec-anyl acetate CC(=O)OC1CC2CC1C3C2CCC3 herbaceous green fruity basil	OdoRactor ity Sigma Aldrich, AOD, Flavorbase, TGSC AOD, Flavorbase, TGSC, Pubchem, OdoRactor AOD ice Sigma Aldrich, TGSC, OdoRactor Ce OdorRactor, TGSC SuperScent, TGSC Tus Sigma Aldrich, TGSC
acetate C)OC sweet spicy carnation woody f 640 Phenyl acetate phenyl acetate CC(=O)OC1=CC=CC=C1 phenolic lily jasmine metallic 641 Phenyl acetate phenyl acetate CC(=O)OC1=CC=CC=C1 sweet 642 2-Methoxyphenyl acetate (2-methoxyphenyl) acetate CC(=O)OC1=CC=CC=C1 cmusty woody walnut sweet spic clove powdery smoky dry phenolic guaiacol ham vanilla 643 4,7-Methano-1H-indenol, 3a,4,5,6,7,7a- hexahydro-, acetate 644 beta-Caryophyllene alcohol acetate clate 645 2-Norbornanol, 1,3,3- trimethyl-1- tricyclo[6.3.1.02,5]dodecanyl) acetate 646 Fenchyl acetate (1,3,3-trimethyl-2- bicyclo[2.2.1]heptanyl] acetate 647 Verdyl acetate (1,3,3-trimethyl-2- bicyclo[5.2.1.02,6]dec-3-enyl acetate S-tricyclo[5.2.1.02,6]dec-3-enyl acetate 648 4,7-Methano-1H-inden-5-ol, 3a,4,5,6,7,7a- hexahydro-, acetate 649 Octahydro-4,7-methano-1H- 8-tricyclo[5.2.1.02,6]dec-4-enyl acetate 649 Octahydro-4,7-methano-1H- 8-tricyclo[5.2.1.02,6]decanyl CC(=O)OC1CC2CC1C3C2CC3 herbaceous green fruity basil	AOD, Flavorbase, TGSC, Pubchem, OdoRactor AOD Sigma Aldrich, TGSC, OdoRactor CC OdorRactor ,TGSC SuperScent, TGSC Tus Sigma Aldrich, TGSC
641 Phenyl acetate phenyl acetate (2-methoxyphenyl) acetate (2-methoxyphenyl) acetate (2-methoxyphenyl) acetate (2-methoxyphenyl) acetate (2-methoxyphenyl) acetate (2-methoxyphenyl) acetate (2-methoxyphenyl) acetate (2-methoxyphenyl) acetate (2-methoxyphenyl) acetate (2-methoxyphenyl) acetate (2-methoxyphenyl) acetate (2-methoxyphenyl) acetate (2-methoxyphenyl) acetate (2-methoxyphenyl) acetate (2-methoxyphenyl) acetate (2-methoxyphenyl) acetate (2-methoxyphenyl) acetate (2-methoxyphenyl) acetate (2-methoxyphenyl) acetate (2-methoxyphenyl) acetate (2-methoxyphenyl) acetate (2-methoxyphenyl) acetate (2-methoxyphenyl) acetate (2-methoxyphenyl) acetate (2-methoxyphenyl) acetate (2-methoxyphenyl) acetate (2-methoxyphenyl) acetate (2-methoxyphenyl) acetate (2-methoxyphenyl) acetate (2-methoxyphenyl) acetate (2-methoxyphenyl) acetate (2-methoxyphenyl) acetate (2-methoxyphenyl) acetate (2-methoxyphenyl) acetate (2-methoxyphenyl) acetate (2-methoxyphenyl) acetate (2-methoxyphenyl) acetate (2-methoxyphenyl) acetate (2-methoxyphenyl) acetate (2-methoxyphenyl) acetate (2-methoxyphenyl) acetate (2-methoxyphenyl) acetate (2-methoxyphenyl) acetate (2-methoxyphenyl) acetate (2-methoxyphenyl) acetate (2-methoxyphenyl) acetate (2-methoxyphenyl) acetate (2-methoxyphenyl) acetate (2-methoxyphenyl) acetate (2-methoxyphenyl) acetate (2-methoxyphenyl) acetate (2-methoxyphenyl) acetate (2-methoxyphenyl) acetate (2-methoxyphenyl) acetate (2-methoxyphenyl) acetate (2-methoxyphenyl) acetate (2-methoxyphenyl) acetate (2-methoxyphenyl) acetate (2-methoxyphenyl) acetate (2-methoxyphenyl) acetate (2-methoxyphenyl) acetate (2-methoxyphenyl) acetate (2-methoxyphenyl) acetate (2-methoxyphenyl) acetate (2-methoxyphenyl) acetate (2-methoxyphenyl) acetate (2-methoxyphenyl) acetate (2-methoxyphenyl) acetate (2-methoxyphenyl) acetate (2-methoxyphenyl) acetate (2-methoxyphenyl) acetate (2-methoxyphenyl) acetate (2-methoxyphenyl) acetate (2-methoxyphenyl) acetate (2-methoxyphenyl) acetate (2-methoxyphenyl) acetate (2-methoxyphenyl) acetate (2-methoxy	Pubchem, OdoRactor AOD Sigma Aldrich, TGSC, OdoRactor Ce OdorRactor ,TGSC OdorRactor ,TGSC SuperScent, TGSC Tus Sigma Aldrich, TGSC
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clove powdery smoky dry phenolic guaiacol ham vanilla 4.7-Methano-1H-indenol, 3a,4.5,6,7,7a- hexahydro-, acetate 644 beta-Caryophyllene alcohol acetate 645 2-Norbornanol, 1,3,3- trimethyl-1- trimethyl-, acetate 646 Fenchyl acetate 647 Verdyl acetate 648 4,7-Methano-1H-inden-5-ol, 3a,4.5,6,7,7a- hexahydro-, acetate 649 Octahydro-4,7-methano-1H- 8-tricyclo[5.2.1.02,6]dec-a-enyl acetate 649 Octahydro-4,7-methano-1H- 8-tricyclo[5.2.1.02,6]dec-anyl acetate CC(=O)OC12CCCC(C1)(CCC3C woody earthy amber fruity spiral dry CC(=O)OC12CCCC(C1)(CCC3C woody earthy amber fruity spiral dry CC(=O)OC1C(C2CCC1(C2)C)(C) balsamic fresh sweet pine herbaceous citrus fir CC(=O)OC1C(C2CCC1(C2)C)(C) pine fi rneedle herbaceous citrus fir CC(=O)OC1C(C2CCC1(C2)C)(C) pine fi rneedle herbaceous citrus fir CC(=O)OC1C(C2CCC1(C2)C)(C) pine fi rneedle herbaceous citrus fir CC(=O)OC1CC2CC1C3C2C=C sweet balsamic fresh CC(=O)OC1CC2CC1C3C2C=C floral green soapy cedar pine woody CC(=O)OC1CC2CC1C3C2CC=C floral green herbaceous CC(=O)OC1CC2CC1C3C2CCC floral green herbaceous CC(=O)OC1CC2CC1C3C2CCC floral green herbaceous CC(=O)OC1CC2CC1C3C2CCC floral green herbaceous	OdoRactor Ce OdorRactor ,TGSC Cy OdorRactor ,TGSC SuperScent, TGSC Tus Sigma Aldrich, TGSC
3 herbaceous 644 beta-Caryophyllene alcohol acetate 645 2-Norbornanol, 1,3,3- trimethyl-1- bicyclo[2.2.1]heptanyl] acetate 646 Fenchyl acetate 647 Verdyl acetate 648 4,7-Methano-1H-inden-5-ol, 3a,4,5,6,7,7a- hexahydro-acetate 649 Octahydro-4,7-methano-1H- 8-tricyclo[5.2.1.02,6]dec-ay-update] 649 Octahydro-4,7-methano-1H- 640 beta-Caryophyllene alcohol (4,4,8-trimethyl-1- tricyclo[5.2.1.02,6]dec-ay-update) 642 CC(=O)OC1C(C2CCC1(C2)C)(C) balsamic fresh sweet pine herbaceous citrus fir 643 CC(=O)OC1C(C2CCC1(C2)C)(C) pine fi rneedle herbaceous citrus fir 644 CC(=O)OC1C(C2CCC1(C2)C)(C) pine fi rneedle herbaceous citrus fir 645 CC(=O)OC1C(C2CCC1(C2)C)(C) pine fi rneedle herbaceous citrus fir 646 CC(=O)OC1C(C2CCC1(C2)C)(C) pine fi rneedle herbaceous citrus fir 647 CC(=O)OC1C(C2CCC1(C2)C)(C) pine fi rneedle herbaceous citrus fir 648 CC(=O)OC1C(C2CCC1(C2)C)(C) pine fi rneedle herbaceous citrus fir 649 CC(=O)OC1CC2CC1C3C2CCCC displayed pine acetate 649 Octahydro-4,7-methano-1H- 8-tricyclo[5.2.1.02,6]dec-4-enyl acetate 649 Octahydro-4,7-methano-1H- 8-tricyclo[5.2.1.02,6]decanyl CC(=O)OC1CC2CC1C3C2CCC3 herbaceous green fruity basil	SuperScent, TGSC Sigma Aldrich, TGSC
acetate tricyclo[6.3.1.02,5]dodecanyl) acetate 645 2-Norbornanol, 1,3,3-	SuperScent, TGSC rus Sigma Aldrich, TGSC
trimethyl-, acetate bicyclo[2.2.1]heptanyl] acetate C herbaceous citrus fir 646 Fenchyl acetate (1,3,3-trimethyl-2-bicyclo[2.2.1]heptanyl) acetate CC(=O)OC1C(C2CCC1(C2)C)(C) pine fi rneedle herbaceous citrus fir 647 Verdyl acetate 8-tricyclo[5.2.1.02,6]dec-3-enyl acetate CC(=O)OC1CC2CC1C3C2C=CC floral green soapy cedar pine woody 648 4,7-Methano-1H-inden-5-ol, 3a,4,5,6,7,7a-hexahydro-, acetate CC(=O)OC1CC2CC1C3C2CC=C floral green herbaceous decate S-tricyclo[5.2.1.02,6]dec-4-enyl acetate CC(=O)OC1CC2CC1C3C2CC=C floral green herbaceous decate S-tricyclo[5.2.1.02,6]dec-4-enyl acetate CC(=O)OC1CC2CC1C3C2CCC floral green herbaceous decate S-tricyclo[5.2.1.02,6]decanyl CC(=O)OC1CC2CC1C3C2CCC herbaceous green fruity basil	rus Sigma Aldrich, TGSC
bicyclo[2.2.1]heptanyl) acetate 647 Verdyl acetate 8-tricyclo[5.2.1.02,6]dec-3-enyl acetate 4,7-Methano-1H-inden-5-ol, 3a,4,5,6,7,7a- hexahydro-, acetate 649 Octahydro-4,7-methano-1H- 8-tricyclo[5.2.1.02,6]dec-4-enyl acetate CC(=O)OC1CC2CC1C3C2C=CC floral green soapy cedar pine woody CC(=O)OC1CC2CC1C3C2CC=C floral green herbaceous CC(=O)OC1CC2CC1C3C2CC=C floral green herbaceous CC(=O)OC1CC2CC1C3C2CC=C floral green herbaceous CC(=O)OC1CC2CC1C3C2CC=C floral green fruity basil	
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3a,4,5,6,7,7a- hexahydro-, acetate 3 Octahydro-4,7-methano-1H- 8-tricyclo[5.2.1.02,6]decanyl CC(=O)OC1CC2CC1C3C2CCC3 herbaceous green fruity basil	
	OdorRactor ,TGSC, Pubchem
inden-5-yl acetate acetate	OdorRactor ,TGSC
Bornyl acetate (1,7,7-trimethyl-2-bicyclo[2,2,1]heptanyl) acetate (2,2,1]heptanyl) acetate (1,7,7-trimethyl-2-bicyclo[2,2,1]heptanyl) acetate (2,2,1]heptanyl) acetate (2,2,1]heptanyl) acetate (3,7,7-trimethyl-2-bicyclo[2,2,1]heptanyl) acetate (3,7,7-trimethyl-2-bicyclo[2,2,2]heptanyl) acetate (3,7,7-trimethyl-2-bicyclo[2,2,2]heptanyl) acetate (3,7,7-trimethyl-2-bicyclo[2,2,2]heptanyl) acetate (3,7,7-trimethyl-2	Sigma Aldrich, TGSC, Pubchem
651 Isobornyl acetate [(1S, 2S, 4R)-1,7,7-trimethyl-2-bicyclo[2.2.1]heptanyl] acetate [(1S, 2S, 4R)-1,7,7-trimethyl-2-bicyclo[2.2.1]heptanyl] acetate bicyclo[2.2.1]heptanyl] acetate bicyclo[OdorRactor ,TGSC, Pubchem
652 (1R,2S,4R)-1,7,7- Trimethylbicyclo[2,2.1]hepta n-2-yl acetate [(1R, 2S, 4R)-1,7,7-trimethyl-2-bicyclo[2,2.1]hepta n-2-yl acetate [(1R, 2S, 4R)-1,7,7-trimethyl-2-bicyclo[2,2.1]hepta n-2-yl acetate [(1R, 2S, 4R)-1,7,7-trimethyl-2-bicyclo[2,2.1]heptanyl] acetate [(1R, 2S, 4R)-1,7,7-trimethyl-2-bicyclo[2,2.1]heptanyl] acetate	TGSC
653 (-)-Bornyl acetate [(1S, 2R, 4S)-1,7,7-trimethyl-2-bicyclo[2.2.1]heptanyl] acetate capacitae (CC(=O)OC1CC2CCC1(C2(C)C)C pine woody sweet balsamic herbaceous fresh fi rneedle ceasibicy camphoraceous mentholic	Sigma Aldrich, TGSC, dar Flavorbase, OdoRactor
654 2-Oxabicyclo[2.2.2]octan-6- ol, 1,3,3- trimethyl-, acetate (1,3,3-trimethyl-2- oxabicyclo[2.2.2]octan-6-yl) acetate (1,3,3-trimethyl-2- oxabicyclo[2.2.2]octan-6-yl) CC(=O)OC1CC2CCC1(OC2(C)C) clean herbaceous fresh minty eucalyptus	OdorRactor ,TGSC
4-Tert-Butylcyclohexyl acetate (4-tert -butylcyclohexyl) acetate CC(=O)OC1CCC(CC1)C(C)(C)C creamy woody sweet cedar flo oily herbaceous balsamic green fruity fresh pine	
Decahydro-2-naphthyl acetate lacetate l	s OdorRactor ,TGSC
657 cis-3-Tert-Butylcyclohexyl [(1S, 3R)-3-tert - CC(=O)OC1CCC(C1)C(C)(C)C woody orris fresh floral camphoraceous	TGSC
658 Cyclohexyl acetate cyclohexyl acetate CC(=O)OC1CCCCC1 musty fruity fatty sweet ethere solvent banana apple	eal Sigma Aldrich, TGSC, OdoRactor, Pubchem
659 2-Tert-Butylcyclohexyl acetate CC(=O)OC1CCCCC1C(C)(C)C citrus fruity woody apple herbaceous powerful fresh	Sigma Aldrich, Flavorbase, TGSC, OdoRactor
660 cis-2-Tert-Butylcyclohexyl acetate [(1R, 2R)-2-tert - butylcyclohexyl] acetate CC(=O)OC1CCCCC1C(C)(C)C fruity bergamot lime woody camphoraceous spicy fi rneedl marjoram	OdorRactor ,TGSC
661 Cyclododecyl acetate cyclododecyl acetate CC(=O)OC1CCCCCCCC1 wax smoky metallic green	TGSC
662 1-Phenyl-1,2-ethanediol (2-acetyloxy-2-phenylethyl) CC(=O)OCC(C1=CC=CC=C1)OC gardenia muguet hyacinth diacetate (=O)C balsamic honey vetiver	OdorRactor ,TGSC
663 2-Hydroxypropane-1,3-diyl (3-acetyloxy-2-hydroxypropyl) CC(=O)OCC(COC(=O)C)O ethereal alcoholic diacetate	Sigma Aldrich
664 Triacetin 2,3-diacetyloxypropyl acetate CC(=O)OCC(COC(=O)C)OC(=O) mild fruity clean tropical crear acidic fatty	my Sigma Aldrich, TGSC, Pubchem
665 Allyl acetate prop-2-enyl acetate CC(=0)OCC=C fruity acrid	TGSC, Pubchem
666 (Z)-Cinnamyl acetate [(Z)-3-phenylprop-2-enyl] CC(=O)OCC=CC1=CC=CC1 floral spicy balsamic acetate	
$ \begin{array}{c cccc} 667 & Cinnamyl \ acetate & & & & & & & & & & & & & & & & & & &$	TGSC Sigma Aldrich, ADB, TGSC,

668	Veratryl acetate	(3,4-dimethoxyphenyl)methyl	CC(=O)OCC1=CC(=C(C=C1)OC)	sweet floral berry rose fresh	OdorRactor ,TGSC
669	4-Methoxybenzyl acetate	acetate (4-methoxyphenyl)methyl acetate	OC CC(=0)OCC1=CC=C(C=C1)OC	almond cherry coumarinic creamy	Sigma Aldrich, TGSC,
007	- Medionyoungs decide	(memonypheny)/memyr weemee		lilac plum sweet vanilla powdery balsamic fruity tonka spicy	OdoRactor
670	Benzyl acetate	benzyl acetate	CC(=0)OCC1=CC=CC=C1	apple apricot cherry jasmine plum sweet fresh boiled vegetable floral fruity pear boiled	Sigma Aldrich, AOD, TGSC OdoRactor, Pubchem
671	Furfuryl acetate	furan-2-ylmethyl acetate	CC(=0)OCC1=CC=CO1	banana sweet fruity horseradish pungent	Sigma Aldrich, TGSC, Odoractr, Pubchem
672	Piperonyl acetate	1,3-benzodioxol-5-ylmethyl acetate	CC(=O)OCC1=CC2=C(C=C1)OC O2	cherry strawberry sweet floral hawthorn metallic jammy jasmine aromatic powdery soapy	Sigma Aldrich, TGSC,OdoRactor
673	Myrtenyl acetate	(6,6-dimethyl-2-bicyclo[3.1.1]hept 2-enyl)methyl acetate	CC(=0)OCC1=CCC2CC1C2(C)C	herbaceous sweet fruity citrus fresh woody cedar floral green cooling	Sigma Aldrich, TGSC, OdoRactor
674	(5,5,11,11-Tetramethyl-2- tetracyclo[6.2.1.01,6.06,10]u ndecanyl)meth yl acetate	(5,5,11,11-tetramethyl-2-tetracyclo[6.2.1.01,6.06,10]undec anyl)methyl acetate	CC(=0)OCC1CCC(C23C14C2CC (C3)C4(C)C)(C)C	woody amber vetiver sandal wood clary sage	OdorRactor ,TGSC
675	Octahydro-4,7-methano-1H- indenemethyl acetate	3- tricyclo[5.2.1.02,6]decanylmethyl acetate	CC(=0)OCC1CCC2C1C3CCC2C 3	woody sandal wood fruity floral amber	TGSC
676	Tetrahydrofurfuryl acetate	oxolan-2-ylmethyl acetate	CC(=0)OCC1CCCO1	honey maple sweet fruity brown rummy ethereal caramel	Sigma Aldrich, TGSC,OdoRactor
677	3-Phenylbut-3-enyl acetate	3-phenylbut-3-enyl acetate	CC(=0)OCCC(=C)C1=CC=CC=C	sweet floral anisic acacia hawthorn	OdorRactor,
678	3-Mercapto-3-methyl-1-butyl acetate	(3-methyl-3-sulfanylbutyl) acetate	CC(=O)OCCC(C)(C)S	balsamic alcoholic fruity sulfurous sweet green tropical	TGSC, Flavorbase
679	Phenethyl acetate	2-phenylethyl acetate	CC(=0)OCCC1=CC=CC=C1	grape green honey melon citrus pineapple rose sweet winey tobacco floral fruity tropical yeasty cocoa balsamic	Sigma Aldrich, Flavorbase, TGSC, OdoRactor
680	Nopyl acetate	2-(6,6-dimethyl-2-bicyclo[3.1.1]hept-2-enyl)ethyl acetate	CC(=0)OCCC1=CCC2CC1C2(C) C	herbaceous linalyl woody pine lavender bergamot	OdorRactor ,TGSC
681	Nopyl acetate, (-)-	2-[(1R,5S)-6,6-dimethyl-2-bicyclo[3.1.1]hept-2-enyl]ethyl acetate	CC(=0)OCCC1=CCC2CC1C2(C) C	pine	Sigma Aldrich
682	2-Cyclohexylethyl acetate	2-cyclohexylethyl acetate	CC(=0)OCCC1CCCCC1	floral minty rose raspberry plastic green	SuperScent, TGSC, OdoRactor
683	4-Pentenyl acetate	pent-4-enyl acetate	CC(=0)OCCCC=C	green plastic weedy acrylate vegetable metallic cooked meaty sulfurous	OdorRactor ,TGSC
684	3-Phenylpropyl acetate	3-phenylpropyl acetate	CC(=0)OCCCC1=CC=CC=C1	spicy floral fruity sweet balsamic storax cinnamyl honey hay	Sigma Aldrich, TGSC, OdoRactor
	Cyclohexylpropyl acetate	3-cyclohexylpropyl acetate	CC(=0)OCCCC1CCCCC1	ethereal floral fruity	TGSC
686	9-Decenyl acetate	dec-9-enyl acetate	CC(=0)OCCCCCCCCCCCC	rose magnolia floral dewy petal peony ambrette	OdorRactor ,TGSC
687	10-Undecen-1-yl acetate	undec-10-enyl acetate	CC(=0)OCCCCCCCCCCCCCC	fresh clean laundered cloth rose fatty licorice fruity sharp wax meaty dairy cheese	OdorRactor ,TGSC
688	3-(Methylthio)propyl acetate	3-methylsulfanylpropyl acetate	CC(=0)OCCCSC	asparagus sulfurous herbaceous mushroom cabbage potato cheese herbaceous green sweet fruity	OdorRactor ,TGSC, Flavorbase
689	Ethylene glycol diacetate	2-acetyloxyethyl acetate	CC(=O)OCCOC(=O)C	green floral estery alcoholic acetic	TGSC, Pubchem
690	2-Phenoxyethyl acetate	2-phenoxyethyl acetate	CC(=O)OCCOC1=CC=CC=C1	sweet floral	TGSC
691	2-(Methylthio)ethyl acetate	2-methylsulfanylethyl acetate	CC(=0)OCCSC	tropical melon sweet rancid meaty	TGSC
692	Thioacetic acid	ethanethioic S-acid	CC(=O)S	alliaceous cooked roasted meaty burnt sulfurous savory herbaceous fruity fresh tropical fruit unpleasant	Sigma Aldrich, Flavorbase, TGSC,OdoRactor
693	S-Methyl thioacetate	S -methyl ethanethioate	CC(=O)SC	sulfurous eggy cheese dairy vegetable cabbage	OdorRactor ,TGSC
694	S-Furfuryl thioacetate	S -(furan-2-ylmethyl) ethanethioate	CC(=0)SCC1=CC=C01	sulfurous roasted nutty coffee burnt savory alliaceous vegetable garlic	Sigma Aldrich, Flavorbase, TGSC, OdoRactor
695	(Z)-3,4,5,6,6-Pentamethylhept- 3-en-2-one	(Z)-3,4,5,6,6-pentamethylhept-3-en-2-one	CC(C(=C(C)C(=O)C)C)C(C)(C)C	woody floral pine balsamic violet orris	OdorRactor ,TGSC
696	Sodium 2-(4- methoxyphenoxy)propanoate	sodium;2-(4- methoxyphenoxy)propanoate	CC(C(=O)[O-])OC1=CC=C(C=C1)OC.[Na+]	bland	OdorRactor,

697	Acetoin	3-hydroxybutan-2-one	CC(C(=0)C)O	buttery creamy sweet dairy milky fatty yogurt caramel green sour vanilla bland woody	Flavornet, TGSC, PubChem
698	Acetoin acetate	3-oxobutan-2-yl acetate	CC(C(=0)C)OC(=0)C	fruity pungent estery chemical pineapple apple banana ketonic fleshy grape rummy sweet creamy buttery	Sigma Aldrich, TGSC, Odoractor
699	Acetoin acetate	3-oxobutan-2-yl acetate	CC(C(=O)C)OC(=O)C	pungent sweet creamy buttery fruity estery chemical pineapple apple banana ketonic	OdorRactor ,TGSC
700	3-Mercapto-2-butanone	3-sulfanylbutan-2-one	CC(C(=O)C)S	chocolate coffee meaty sulfurous onion gassy roasted beefy fried	Sigma Aldrich, TGSC, OdoRactor
701	3-Mercapto-2-butanone	3-sulfanylbutan-2-one	CC(C(=O)C)S	sulfurous onion roasted meaty gassy beefy fried coffee chocolate	OdorRactor ,TGSC
702	3-(Methylthio)-2-butanone	3-methylsulfanylbutan-2-one	CC(C(=O)C)SC	sulfurous milky oily potato earthy fatty	OdorRactor ,TGSC
703	3-(Methylthio)-2-butanone	3-methylsulfanylbutan-2-one	CC(C(=O)C)SC	sulfurous milky oily potato earthy fatty	TGSC, OdoRactor
704	2-Hydroxy-N-(2- hydroxyethyl)propanamide	2-hydroxy-N -(2- hydroxyethyl)propanamide	CC(C(=O)NCCO)O	roasted cooked brown	OdorRactor ,Flavorbase
705	N-Lactoyl ethanolamine phosphate	2-(2- hydroxypropanoylamino)ethyl dihydrogen phosphate	CC(C(=O)NCCOP(=O)(O)O)O	roasted	OdorRactor,
706	Alanine	(2S)-2-aminopropanoic acid	CC(C(=O)O)N	sweet	Sigma Aldrich
707		2-hydroxypropanoic acid	CC(C(=0)0)0	sour weak unpleasant	Sigma Aldrich, Flavornet
708	2-Mercaptopropionic acid	2-sulfanylpropanoic acid	CC(C(=O)O)S	meaty sulfurous roasted savory brown unpleasant	Sigma Aldrich, TGSC, Pubchem, OdoRactor
709	Benzyl lactate	benzyl 2-hydroxypropanoate	CC(C(=0)OCC1=CC=CC=C1)O	floral fatty buttery fruity	OdorRactor ,TGSC
710	3,6-Dimethyl-3-vinylhept-5- en-2-ol	3-ethenyl-3,6-dimethylhept-5-en-2-ol	CC(C(C)(CC=C(C)C)C=C)O	herbaceous lavender	TGSC
711	3,4,5,6,6-Pentamethylheptan- 2-ol	3,4,5,6,6-pentamethylheptan-2-ol	CC(C(C)C(C)O)C(C)C(C)(C)C	woody amber fatty soapy raisin dry	OdorRactor ,TGSC
712	Kohinool	3,5,6,6-tetramethyl-4- methylideneheptan-2-ol	CC(C(C)O)C(=C)C(C)C(C)(C)C	woody clean dry amber vetiver	TGSC
713	2,3-Butanediol	butane-2,3-diol	CC(C(C)O)O	fruit onion creamy buttery	Flavornet, TGSC
714	3-Mercapto-2-butanol	3-sulfanylbutan-2-ol	CC(C(C)S)O	meaty sulfurous onion garlic	Sigma Aldrich, TGSC,
715	(R*,S*)-3-Mercaptobutan-2-	(2S ,3R)-3-sulfanylbutan-2-ol	CC(C(C)S)O	roasted alliaceous sulfurous roasted onion garlic	OdoRactor OdorRactor ,TGSC
716	ol 2,3-Butanedithiol	butane-2,3-dithiol	CC(C(C)S)S	meaty alliaceous roasted meat sulfurous meaty beefy alliaceous	Sigma Aldrich, TGSC
717	3-((2-Mercapto-1- methylpropyl)thio)-2- butanol	3-(3-sulfanylbutan-2- ylsulfanyl)butan-2-ol	CC(C(C)SC(C)C(C)S)O	coffee meaty fatty sulfurous roasted burnt brothy	OdorRactor ,TGSC
718	Pinacol	2,3-dimethylbutane-2,3-diol	CC(C)(C(C)(C)O)O	woody earthy warm bready patchouli	OdorRactor ,TGSC
719	Propanoic acid, 2,2-dimethyl-, 3a,4,5,6,7,7a hexahydro-4,7-methano-1H-inden-6-yl ester	8-tricyclo[5.2.1.02,6]dec-3-enyl 2,2- dimethylpropanoate	CC(C)(C)C(=0)OC1CC2CC1C3C 2C=CC3	fruity peach sweet powdery green floral	OdorRactor ,TGSC
720	Benzyl pivalate	benzyl 2,2-dimethylpropanoate	CC(C)(C)C(=0)OCC1=CC=CC= C1	floral herbaceous chamomile	TGSC
721	2-Phenylethyl pivalate	2-phenylethyl 2,2- dimethylpropanoate	CC(C)(C)C(=0)OCCC1=CC=CC =C1	rose spice geranium blueberry floral spicy	OdorRactor ,TGSC
722		2-tert -butyl-4-methoxyphenol	CC(C)(C)C1=C(C=CC(=C1)OC)O		Sigma Aldrich,OdoRactor
723	methoxyphenol 2-Tert-Butyl-1,4- dimethoxybenzene	2-tert -butyl-1,4- dimethoxybenzene	CC(C)(C)C1=C(C=CC(=C1)OC)O	woody vetiver forest	TGSC
724	Quinoline, (1,1-dimethylethyl)-	5-tert -butylquinoline	CC(C)(C)C1=C2C=CC=NC2=CC =C1	castoreum animal leathery earthy oakmoss vetiver	OdorRactor ,TGSC
725	2,4-Di-tert-butylphenol	2,4-di <i>tert</i> -butylphenol	CC(C)(C)C1=CC(=C(C=C1)O)C(C)(C)C	phenolic	TGSC
726	Methyl p-tert-	methyl 2-(4-tert -	CC(C)(C)C1=CC=C(C=C1)CC(=	creamy green hyacinth jasmine	Sigma Aldrich, TGSC, OdoRactor
727	butylphenylacetate 3-(4-Tert-	butylphenyl)acetate 3-(4- <i>tert</i> -butylphenyl)propanal	O)OC CC(C)(C)C1=CC=C(C=C1)CCC=	rose wax fruity honey leafy floral sweet watery fresh cyclamen	OdorRactor ,TGSC
728	butylphenyl)propanal 4-Tert-Butylphenol	4-tert -butylphenol	O CC(C)(C)C1=CC=C(C=C1)O	oakmoss leathery distinctive	Sigma Aldrich, TGSC,
729	Benzenepropanal, 3-(1,1-	3-(3-tert -butylphenyl)propanal	CC(C)(C)C1=CC=CC(=C1)CCC=	floral aldehydic rubbery	Pubchem TGSC
730	dimethylethyl)- 2-Tert-Butylpyrazine	2-tert -butylpyrazine	O CC(C)(C)C1=NC=CN=C1	minty green bellpepper nutty	TGSC
				roasted	
731	4-Tert-Butylcyclohexanone	4-tert -butylcyclohexan-1-one	CC(C)(C)C1CCC(=0)CC1	woody minty musk leathery patchouli	OdorRactor ,TGSC
732	4-Tert- Butylcyclohexanecarbaldehyd	4-tert -butylcyclohexane-1- carbaldehyde	CC(C)(C)C1CCC(CC1)C=O	floral woody	OdorRactor ,TGSC

733	4-Tert-Butylcyclohexanol	4-tert -butylcyclohexan-1-ol	CC(C)(C)C1CCC(CC1)O	woody musty camphoraceous	OdorRactor ,TGSC
				minty leathery patchouli	·
734	8-(1,1-Dimethylethyl)-1- oxaspiro(4.5)decan- 2-one	2-one	O2	urine woody lactonic	TGSC, OdoRactor
735	1,4-Dioxaspiro[4.5]decane, 8-(1,1- dimethylethyl)-	8-tert -butyl-1,4- dioxaspiro[4.5]decane	CC(C)(C)C1CCC2(CC1)OCCO2	mild woody balsamic patchouli	Flavorbase
736	2-Tert-Butylcyclohexanone	2-tert -butylcyclohexan-1-one	CC(C)(C)C1CCCCC1=O	woody camphoraceous orris minty	OdorRactor ,TGSC
737	2-Tert-Butylcyclohexanol	2-tert -butylcyclohexan-1-ol	CC(C)(C)C1CCCCC10	herbaceous pine camphoraceous minty phenolic patchouli earthy woody	OdorRactor ,TGSC
738	Tert-Butanol	2-methylpropan-2-ol	CC(C)(C)O	camphoraceous	OdorRactor ,Pubchem
739	Methyl tert-butyl ether	2-methoxy-2-methylpropane	CC(C)(C)OC	minty terpenic sweet solvent	TGSC, Pubchem
740	2-Methyl-2-propanethiol	2-methylpropane-2-thiol	CC(C)(C)S	sulfurous skunk offensive	TGSC, Pubchem
741	2-Methyl-3-buten-2-OL	2-methylbut-3-en-2-ol	CC(C)(C=C)O	oily herbaceous earthy	Sigma Aldrich, Flavornet, TGSC,OdoRactor
742	2- (Methyldithio)isobutyraldehy de	2-methyl-2- (methyldisulfanyl)propanal	CC(C)(C=O)SSC	smoky fatty aromatic cocoa dark chocolate chocolate tobacco	Flavornet, TGSC
743	2-Phenyl-2-propanol	2-phenylpropan-2-ol	CC(C)(C1=CC=CC=C1)O	green sweet earthy	SuperScent, TGSC
744	3-Mercapto-3-methylbutanal	3-methyl-3-sulfanylbutanal	CC(C)(CC=O)S	brothy cheese	TGSC
745	2,2-Dimethyl-3- phenylpropanal	2,2-dimethyl-3-phenylpropanal	CC(C)(CC1=CC=CC=C1)C=O	ocean fresh marine	TGSC
746	Dimethyl Phenylpropano		CC(C)(CC1=CC=CC=C1)CO	floral lily of the valley woody	OdorRactor ,TGSC
747	2-Methyl-1-phenylpropan-2- ol	2-methyl-1-phenylpropan-2-ol	CC(C)(CC1=CC=CC=C1)O	clean floral green rose oily rhubarb cortex	OdorRactor ,TGSC
748	alpha,alpha- Dimethylphenethyl formate	(2-methyl-1-phenylpropan-2-yl) formate		dry herbaceous green lily jasmine	OdorRactor ,TGSC
749	2-Methyl-4-phenyl-2-butanol	2-methyl-4-phenylbutan-2-ol	CC(C)(CCC1=CC=CC=C1)O	clean fresh green rose linalool lily violet floral bois de rose	OdorRactor ,TGSC
750	4-Cyclohexyl-2-methyl-2- butanol	4-cyclohexyl-2-methylbutan-2-ol	CC(C)(CCC1CCCC1)O	floral bois de rose coriander rose	TGSC
751	Myrcenol	2-methyl-6-methylideneoct-7-en-2- ol		fresh floral lavender citrus	OdorRactor ,TGSC
752	Myrcenyl methyl ether	7-methoxy-7-methyl-3- methylideneoct-1-ene	CC(C)(CCCC(=C)C=C)OC	pine resinous herbaceous	TGSC
753	Methyl 2-[[[4-(4-hydroxy-4-methylpentyl)-3-cyclohexenyl]methylene]amin o]benzoate	methyl 2-[[4-(4-hydroxy-4- methylpentyl)cyclohex- 3-en-1- yl]methylideneamino]benzoate	CC(C)(CCCC1=CCC(CC1)C=NC 2=CC=C C=C2C(=O)OC)O	fresh lily floral sweet orange flower	TGSC
754	Lyral	4-(4-hydroxy-4- methylpentyl)cyclohex-3-ene-1- carbaldehyde	CC(C)(CCCC1=CCC(CC1)C=O) O	floral muguet woody cyclamen rhubarb	AOD, TGSC, OdoRactor, Pubchem
755	3-Mercapto-3-methyl-1- butanol	3-methyl-3-sulfanylbutan-1-ol	CC(C)(CCO)S	sweet meaty roasted spicy vegetable	Sigma Aldrich, TGSC, Odoractor
756	4-Methoxy-2-methyl-2- butanethiol	4-methoxy-2-methylbutane-2-thiol	CC(C)(CCOC)S	catty black currant sulfurous minty tropical sweet skunk mango grapefruit	Flavornet, TGSC, OdoRactor
757	3-Mercapto-3-methylbutyl formate	(3-methyl-3-sulfanylbutyl) formate	CC(C)(CCOC=O)S	catty roasted sulfurous caramel onion roasted coffee roasted meat tropical coffee meaty	Flavornet, TGSC, OdoRactor
758	3-Benzyloxy-2,2- dimethylpropanal	2,2-dimethyl-3- phenylmethoxypropanal	CC(C)(COCC1=CC=CC=C1)C=O	aldehydic ozone floral green spicy coriander cardamom ginger	TGSC
759	2,5,6-Trimethylhept-4-enal	(E)-2,5,6-trimethylhept-4-enal	CC(C)C(=CCC(C)C=O)C	fresh green sweet ozone melon	OdorRactor ,TGSC
760	(NE)-N-[(6E)-2,4,4,7- tetramethylnona-6,8- dien-3- ylidene]hydroxylamine	(NE)-N -[(6E)-2,4,4,7- tetramethylnona-6,8-dien-3- ylidene]hydroxylamine		floral black currant green grapefruit herbaceous rose sage	OdorRactor ,TGSC
761	3-Methyl-2-butanone	3-methylbutan-2-one	CC(C)C(=O)C	camphoraceous acetone	Flavornet, OdoRactor, Pubchem
762	Acetyl isobutyryl	4-methylpentane-2,3-dione	CC(C)C(=O)C(=O)C	sweet fruity buttery creamy fatty brown	OdorRactor ,TGSC
763	3-methyl-2-oxobutanoic acid	2-oxobutanoic acid	CC(C)C(=O)C(=O)O	fruity	OdoRactor ,TGSC, Flavorbase
764	6-Octen-3-one, 2,4,4,7- tetramethyl-	2,4,4,7-tetramethyloct-6-en-3-one	CC(C)C(=O)C(C)(C)CC=C(C)C	sweet herbaceous tropical citrus clary sage bergamot petitgrain	OdorRactor ,TGSC
765	Methoxystyryl isopropyl ketone	(Z)-1-(4-methoxyphenyl)-4- methylpent-1-en-3-one	CC(C)C(=0)C=CC1=CC=C(C=C 1)OC	caramel fruity buttery	OdorRactor ,TGSC
766	Isobutyric acid	2-methylpropanoic acid	CC(C)C(=0)O	buttery acidic sour cheese dairy rancid strawberry pungent sharp stench	Sigma Aldrich, TGSC, Pubchem
767	Methyl isobutyrate	methyl 2-methylpropanoate	CC(C)C(=O)OC	floral fruity apple pineapple ethereal sweet tutti frutti	Sigma Aldrich, TGSC,OdoRactor
768	Cite	2-phenylpropan-2-yl 2- methylpropanoate	CC(C)C(=0)OC(C)(C)C1=CC=C C=C1	sweet fruity apricot peach plum green dry	OdorRactor ,TGSC
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769	Propanoic acid, 2-methyl-, 1,1-dimethyl-2- phenylethyl ester	(2-methyl-1-phenylpropan-2-yl) 2-methylpropanoate	CC(C)C(=0)OC(C)(C)CC1=CC= CC=C1	fruity jasmine jammy raisin black currant	OdorRactor ,TGSC
770	1,1-Dimethyl-3-phenylpropyl isobutyrate	(2-methyl-4-phenylbutan-2-yl) 2- methylpropanoate	CC(C)C(=0)OC(C)(C)CCC1=CC =CC=C1	floral green fruity papaya juicy sweet powdery honey	OdorRactor ,TGSC
771	Linalyl isobutyrate	3,7-dimethylocta-1,6-dien-3-yl 2- methylpropanoate		fruity lavender woody bergamot berry citrus juicy sweet fresh apple	OdorRactor ,TGSC
772	Nerolidyl isobutyrate	[(6E)-3,7,11-trimethyldodeca- 1,6,10-trien-3-yl] 2- methylpropanoate	CC(C)C(=0)OC(C)(CCC=C(C)C CC=C(C) C)C=C	fruity green oily bergamot pear woody	OdorRactor ,TGSC
773	Isopropyl isobutyrate	propan-2-yl 2-methylpropanoate	CC(C)C(=O)OC(C)C	pineapple sweet fruity citrus pear	OdorRactor ,TGSC
774	1-Phenylethyl isobutyrate	1-phenylethyl 2-methylpropanoate	CC(C)C(=O)OC(C)C1=CC=CC=C1	floral fruity tropical jasmine green mango	SuperScent, TGSC, OdoRactor
775	1-Phenylethyl isobutyrate	1-phenylethyl 2-methylpropanoate	CC(C)C(=O)OC(C)C1=CC=CC= C1	fruity tropical jasmine green mango floral woody	OdorRactor ,TGSC
776	4-Methylpent-4-en-2-yl 2- methylpropanoate	4-methylpent-4-en-2-yl 2- methylpropanoate	CC(C)C(=0)OC(C)CC(=C)C	herbaceous natural fruity floral chamomile	OdorRactor ,TGSC
777	Vanillin isobutyrate	(4-formyl-2-methoxyphenyl) 2-methylpropanoate	CC(C)C(=0)OC1=C(C=C(C=C1) C=0)OC	almond cherry chocolate creamy sweet vanilla fruity caramel cocoa	Sigma Aldrich, TGSC, Flavorbase
778	Guaiacol isobutyrate	(2-methoxyphenyl) 2- methylpropanoate	CC(C)C(=0)OC1=CC=CC=C1OC	fruity nutty	TGSC
779	3a,4,5,6,7,7a-Hexahydro-4,7- methano-1H- inden-6-yl isobutyrate	8-tricyclo[5.2.1.02,6]dec-3-enyl 2-methylpropanoate	CC(C)C(=0)OC1CC2CC1C3C2C =CC3	green weedy oily sweet woody floral gardenia jasmine tuberose	OdorRactor ,TGSC
780	3a,4,5,6,7,7a-Hexahydro-4,7- methano-1H- inden-5-yl isobutyrate	8-tricyclo[5.2.1.02,6]dec-4-enyl 2-methylpropanoate	CC(C)C(=0)OC1CC2CC1C3C2C C=C3	fruity amber chocolate anisic basil balsamic	OdorRactor ,TGSC
781	Isobornyl isobutyrate	[(1R ,2R ,4R)-1,7,7-trimethyl-2-bicyclo[2.2.1]heptanyl] 2-methylpropanoate	CC(C)C(=0)OC1CC2CCC1(C2(C)C)C	balsamic herbaceous spicy earthy woody fi rneedle nutty camphoraceous pine fruity	OdorRactor ,TGSC, Flavorbase
782	Bornyl isobutyrate	(1,7,7-trimethyl-2-bicyclo[2.2.1]heptanyl) 2-methylpropanoate	CC(C)C(=0)OC1CC2CCC1(C2(C)C)C	camphoraceous nutty pine fi rneedle	OdorRactor ,TGSC
783	Decahydro-2-naphthyl isobutyrate	1,2,3,4,4 <i>a</i> ,5,6,7,8,8 <i>a</i> - decahydronaphthalen-2-yl 2-methylpropanoate	CC(C)C(=0)OC1CCC2CCCCC2 C1	fruity apricot plum rose	OdorRactor ,TGSC
784	Propanoic acid, 2-methyl-, cyclohexyl ester	cyclohexyl 2-methylpropanoate	CC(C)C(=O)OC1CCCCC1	fruity	OdorRactor,
785	2-Phenylpropyl isobutyrate	2-phenylpropyl 2- methylpropanoate	CC(C)C(=O)OCC(C)C1=CC=CC =C1	fruity floral mango pineapple papaya mango tropical	OdorRactor ,TGSC
786	2-Phenylpropyl isobutyrate	2-phenylpropyl 2- methylpropanoate	CC(C)C(=0)OCC(C)C1=CC=CC =C1	fruity floral mango pineapple papaya tropical	Sigma Aldrich, TGSC, OdoRactor
787	Prenyl isobutyrate	3-methylbut-2-enyl 2- methylpropanoate	CC(C)C(=0)OCC=C(C)C	fruity blueberry raspberry pomegranate pineapple honey chrysanthemum dried fruit plum green wax	OdorRactor ,TGSC, Flavorbase
788	Geranyl isobutyrate	[(2E)-3,7-dimethylocta-2,6-dienyl] 2- methylpropanoate	CC(C)C(=O)OCC=C(C)CCC=C(C)C	floral sweet fruity green peach apricot rose citrus powdery	OdorRactor ,TGSC, Flavorbase
789	Neryl isobutyrate	[(2Z)-3,7-dimethylocta-2,6-dienyl] 2- methylpropanoate	CC(C)C(=0)OCC=C(C)CCC=C(C))C	fresh green fruity floral tutti frutti pear citrus melon berry lilac orange plum raspberry rose strawberry sweet	Sigma Aldrich, TGSC, OdoRactor
790	Cinnamyl isobutyrate	[(E)-3-phenylprop-2-enyl] 2-methylpropanoate	CC(C)C(=0)OCC=CC1=CC=CC=	balsamic fruity sweet almond spicy cinnamyl tropical pineapple floral	Sigma Aldrich, TGSC, OdoRactor
791	alpha-D-Glucopyranoside, beta-D- fructofuranosyl, diacetate hexakis(2- methylpropanoate)	[(2S ,3S ,4R ,5R)-5- (acetyloxymethyl)-2- [(2R ,3R ,4S ,5R ,6R)-6- (acetyloxymethyl)-3,4,5- tris(2- methylpropanoyloxy)oxan-2- yl]oxy-3,4- bis(2- methylpropanoyloxy)oxolan-2- yl]methyl 2- methylpropanoate	CC(C)C(=0)OCC1(C(C(C(O1)CO C(=0)C) OC(=0)C(C)C)OC(=0)C(C)C)OC 2C(C(C C(O2)COC(=0)C)OC(=0)C(C)C) OC(=0) C(C)C)OC(=0)C(C)C		Sigma Aldrich
792	Benzyl isobutyrate	benzyl 2-methylpropanoate	CC(C)C(=0)OCC1=CC=CC=C1	fruity herbaceous floral jasmine oily sweet rose tropical powdery woody juicy	Sigma Aldrich, Flavorbase, TGSC
793	Furfuryl isobutyrate	furan-2-ylmethyl 2- methylpropanoate	CC(C)C(=O)OCC1=CC=CO1	fruity coffee	TGSC
794	Piperonyl isobutyrate	1,3-benzodioxol-5-ylmethyl 2- methylpropanoate	CC(C)C(=O)OCC1=CC2=C(C=C 1)OCO2	fruity plum tropical powdery berry jammy heliotrope sweet	Sigma Aldrich, TGSC, Flavorbase, OdoRactor
795	2-Pinen-10-yl isobutyrate		CC(C)C(=0)OCC1=CCC2CC1C2 (C)C	fruity woody pine	OdorRactor,
796	Citronellyl isobutyrate	3,7-dimethyloct-6-enyl 2- methylpropanoate	CC(C)C(=O)OCCC(C)CCC=C(C)	fruity rose sweet floral geranium tropical citrus green	Sigma Aldrich, TGSC, OdoRactor

797	Rhodinyl isobutyrate	3,7-dimethyloct-7-enyl 2- methylpropanoate	CC(C)C(=O)OCCC(C)CCCC(=C)	sweet rose natural floral spicy fruity tropical geranium	OdorRactor ,TGSC
798	Phenethyl isobutyrate	V 1 1	CC(C)C(=0)OCCC1=CC=CC=C1	fruity tearose floral peach honey yeasty balsamic wax rose	Sigma Aldrich, TGSC, OdoRactor
799	3-Phenylpropyl isobutyrate	3-phenylpropyl 2- methylpropanoate	CC(C)C(=0)OCCCC1=CC=CC=	juicy honey tropical fermented sugar jammy osmanthus balsamic fruity sweet	Sigma Aldrich, TGSC, OdoRactor
800	3-Cyclohexylpropyl isobutyrate	3-cyclohexylpropyl 2- methylpropanoate	CC(C)C(=0)OCCCC1CCCCC1	green metallic fruity	TGSC
801	2-Phenoxyethyl isobutyrate	2-phenoxyethyl 2- methylpropanoate	CC(C)C(=0)OCCOC1=CC=CC=	honey rose sweet fruity green apple powdery tropical floral wax	Sigma Aldrich, Flavorbase, TGSC, OdoRactor
802	S-Prenyl thioisobutyrate	S -(3-methylbut-2-enyl) 2-methylpropanethioate	CC(C)C(=O)SCC=C(C)C	sulfurous fruity tropical durain passion fruit	TGSC
803	4-Methyl-3-sulfanylpentan-2- one	4-methyl-3-sulfanylpentan-2-one	CC(C)C(C(=O)C)S	black currant berry	Flavornet, TGSC
804	2-Isopropyl-N,2,3- trimethylbutanamide	N ,2,3-trimethyl-2-propan-2-ylbutanamide	CC(C)C(C)(C(C)C)C(=O)NC	mentholic minty cooling	OdorRactor ,TGSC
805	2,3,4-Trimethyl-3-pentanol	2,3,4-trimethylpentan-3-ol	CC(C)C(C)(C(C)C)O	fruity	OdorRactor,
806	2,5,6-Trimethyl-2-heptanol	2,5,6-trimethylheptan-2-ol	CC(C)C(C)CCC(C)(C)O	floral freesia fruity	TGSC
807	3-Methyl-2-butanol	3-methylbutan-2-ol	CC(C)C(C)O	fruity musty alcoholic fusel vegetable cider cocoa cheese	Sigma Aldrich, TGSC,OdoRactor
808	3-Methyl-2-butanethiol	3-methylbutane-2-thiol	CC(C)C(C)S	sulfurous beefy meaty repulsive savory burnt rubbery roasted chicken pork roasted coffee coffee cheese	Sigma Aldrich, TGSC, Odoractor
809	3-Methyl-2-phenylbutanal	3-methyl-2-phenylbutanal	CC(C)C(C=O)C1=CC=CC=C1	green fruity	OdorRactor,
810	(E)-5-Isopropyl-8-methylnona- 6,8-dien-2- one	(6E)-8-methyl-5-propan-2-ylnona-6,8-dien-2-one	CC(C)C(CCC(=0)C)C=CC(=C)C	fruity tobacco melon carrot hay tea	OdorRactor ,TGSC, Flavorbase
811	(2E)-2,4-Dimethylpent-2- enoic acid	(E)-2,4-dimethylpent-2-enoic acid	CC(C)C=C(C)C(=O)O	acidic fruity cheese honey tart sweaty floral animal	OdorRactor ,TGSC
812	2,4-Dimethyl-2-pentenoic acid	2,4-dimethylpent-2-enoic acid	CC(C)C=C(C)C(=O)O	sweet sour cheese creamy	ADB, TGSC
813	4-Methyl-2-phenylpent-2-enal	(E)-4-methyl-2-phenylpent-2-enal	CC(C)C=C(C=O)C1=CC=CC=C1	chocolate sweet cocoa nutty rose powdery floral honey	OdorRactor ,TGSC
814	Benzeneacetaldehyde, alpha- (2- methylpropylidene)-	4-methyl-2-phenylpent-2-enal	CC(C)C=C(C=0)C1=CC=CC=C1	chocolate sweet nutty rose powdery floral honey cocoa	Sigma Aldrich, TGSC
815	5-Methyl-3-hexen-2-one	(E)-5-methylhex-3-en-2-one	CC(C)C=CC(=O)C	fruity sweet berry cheese	OdorRactor ,TGSC
816	4-Methyl-2-pentenoic acid	(E)-4-methylpent-2-enoic acid	CC(C)C=CC(=O)O	fatty fruity black tea blackberry	OdorRactor ,TGSC
817	4-Methyl-2-pentenal	(E)-4-methylpent-2-enal	CC(C)C=CC=O	ethereal spicy green grassy aldehydic cooked apple cognac woody pungent fresh	OdorRactor ,TGSC
818	Capsaicin	(E)-N -[(4-hydroxy-3- methoxyphenyl)methyl]-8- methylnon-6-enamide	CC(C)C=CCCCCC(=0)NCC1=C C(=C(C=C1)O)OC	herbaceous burnt pungent	Flavorbase, Pubchem
819	Isobutyraldehyde	2-methylpropanal	CC(C)C=0	banana pungent malty green aldehydic fresh floral pleasant fruity cheese chocolate sharp	Sigma Aldrich, AOD, Flavorbase, TGSC, Pubchem
820	Propofol	2,6-di(propan-2-yl)phenol	CC(C)C1=C(C(=CC=C1)C(C)C)O	phenolic	TGSC
821	Isopropylphenylbutanal	3-(3-propan-2-ylphenyl)butanal	CC(C)C1=CC(=CC=C1)C(C)CC= 0	floral green flower lily muguet linden flower fresh	OdorRactor ,TGSC
822	2-Acetyl-4-isopropylpyridine	1-(4-propan-2-ylpyridin-2- yl)ethanone	CC(C)C1=CC(=NC=C1)C(=O)C	green grassy leafy herbaceous violet	TGSC, Flavorbase
823	Hinokitiol	2-hydroxy-6-propan-2- ylcyclohepta-2,4,6-trien-1- one	CC(C)C1=CC(=O)C(=CC=C1)O	phenolic woody mossy	OdorRactor ,TGSC
824	delta-Elemene	(3R,4R)-4-ethenyl-4-methyl-1- propan-2-yl-3-prop- 1-en-2-ylcyclohexene	CC(C)C1=CC(C(CC1)(C)C=C)C(=C)C	herbaceous sweet lavender woody	TGSC
825	(3S,4R)-4-Ethenyl-4-methyl-1- propan-2-yl- 3-prop-1-en-2-ylcyclohexene	(3S, 4R) -4-ethenyl-4-methyl-1- propan-2-yl-3-prop- 1-en-2-ylcyclohexene	CC(C)C1=CC(C(CC1)(C)C=C)C(=C)C	sweet lavender herbaceous woody	OdorRactor ,TGSC
826	4-Isopropylbenzonitrile	4-propan-2-ylbenzonitrile	CC(C)C1=CC=C(C=C1)C#N CC(C)C1=CC=C(C=C1)C(=O)C	spicy cumin green dry	OdorRactor ,TGSC
827 828	4-Isopropylacetophenone 2-(4- Isopropylphenyl)propionaldeh	1-(4-propan-2-ylphenyl)ethanone 2-(4-propan-2-ylphenyl)propanal	CC(C)C1=CC=C(C=C1)C(=O)C	spicy woody herbaceous orris green leafy aldehydic fresh	OdorRactor ,TGSC OdorRactor ,TGSC
829	yde 4-Isopropylcinnamaldehyde	(F)-3-(4-propan-2-ylphanyl)prop	CC(C)C1=CC=C(C=C1)C=CC=O	spicy amber	TGSC
	,	2-enal			
830	4-Isopropylbenzaldehyde	4-propan-2-ylbenzaldehyde	CC(C)C1=CC=C(C=C1)C=O	oily woody acidic sharp spicy cumin green herbaceous pungent herbaceous	Sigma Aldrich, Flavorbase, TGSC

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831	Benzoic acid, 2-[[2-methyl-3- [4-(1- methylethyl)phenyl]propylide ne]amino]-,	methyl 2-[[2-methyl-3-(4-propan- 2- ylphenyl)propylidene]amino]benz oate	CC(C)C1=CC=C(C=C1)CC(C)C= NC2=C C=CC=C2C(=0)OC	fresh lily of the valley neroli orange flower floral	TGSC
	methyl ester				
	3-(4-Isopropylphenyl)-2- methylpropanal	2-methyl-3-(4-propan-2- ylphenyl)propanal	О	floral vegetable rhubarb musty green cyclamen	Sigma Aldrich, TGSC, OdoRactor
833	4- Isopropylphenylacetaldehyde	2-(4-propan-2- ylphenyl)acetaldehyde	CC(C)C1=CC=C(C=C1)CC=O	earthy aldehydic cumin green cortex foliage	OdorRactor ,TGSC
834	Benzenepropanal, 4-(1-methylethyl)-	3-(4-propan-2-ylphenyl)propanal	CC(C)C1=CC=C(C=C1)CCC=O	floral fruity melon fresh muguet	OdorRactor ,TGSC
835	4-Isopropylbenzyl alcohol	(4-propan-2-ylphenyl)methanol	CC(C)C1=CC=C(C=C1)CO	floral strong cumin caraway spicy herbaceous leathery warm herbaceous sweet aromatic	Sigma Aldrich, TGSC
836	4-Isopropylbenzyl acetate	(4-propan-2-ylphenyl)methyl acetate	CC(C)C1=CC=C(C=C1)COC(=O)	fruity sweet herbaceous bergamot fresh	OdorRactor ,TGSC
837	4-Isopropylphenol	4-propan-2-ylphenol	CC(C)C1=CC=C(C=C1)O	woody warm spicy medicinal	TGSC
	1,3-p-Menthadien-7-al	4-propan-2-ylcyclohexa-1,3-diene- 1-carbaldehyde	CC(C)C1=CC=C(CC1)C=O	fatty spice cumin herbaceous	Flavornet, TGSC, Flavorbase, OdoRactor
839	Ar- Isopropylphenylacetaldehyde	2-(3-propan-2- ylphenyl)acetaldehyde	CC(C)C1=CC=CC(=C1)CC=O	green woody cortex foliage privet	OdorRactor ,TGSC
840	Cumene	cumene	CC(C)C1=CC=CC=C1	aromatic characteristic gasoline sharp penetrating	Pubchem
841	2-Isopropylphenol	2-propan-2-ylphenol	CC(C)C1=CC=CC=C10	medicinal phenolic solvent smoky toasted woody burnt rubbery	Sigma Aldrich, TGSC
842 843	2-Isopropylpyridine Quinoline, (1-methylethyl)-	2-propan-2-ylpyridine 4-propan-2-ylquinoline	CC(C)C1=CC=CC=N1 CC(C)C1=CC=NC2=CC=CC=C1	green vegetable cortex green metallic earthy leafy	OdorRactor ,TGSC OdorRactor ,TGSC
844	7-Isopropyl-1,1,4a-trimethyl-1,2,3,4,4a,9,10,10a-octahydrophenanthrene	1,1,4a -trimethyl-7-propan-2-yl- 2,3,4,9,10,10a - hexahydrophenanthrene	CC(C)C1=CC2=C(C=C1)C3(CCC C(C3CC 2)(C)C)C	woody spicy herbaceous	TGSC
845	6-Isopropylquinoline	6-propan-2-ylquinoline	CC(C)C1=CC2=C(C=C1)N=CC= C2	green weedy metallic earthy leafy phenolic nutty cortex	OdorRactor ,TGSC
846	Abietic acid	(1R, 4aR, 4bR, 10aR) -1,4a - dimethyl-7-propan-2- yl-2,3,4,4b,5,6,10,10a - octahydrophenanthrene-1-carboxylic acid		acetic	OdorRactor,
847	4-(Isopropyl)cyclohexadiene- 1-ethyl formate	2-(4-propan-2-ylcyclohexa-1,4-dien-1-yl)ethyl formate	CC(C)C1=CCC(=CC1)CCOC=O	sweet floral fruity herbaceous minty	OdorRactor ,TGSC
848	p-Menth-3-en-1-ol	1-methyl-4-propan-2-ylcyclohex-3- en-1-ol	CC(C)C1=CCC(CC1)(C)O	musty woody dry	Flavornet, TGSC,OdoRactor
849	1,2,5,6-Tetrahydrocuminic acid	4-propan-2-ylcyclohex-3-ene-1- carboxylic acid	CC(C)C1=CCC(CC1)C(=O)O	animal cumin sweaty spicy	OdorRactor ,TGSC
850	2-Isopropyl-6- methoxypyrazine	2-methoxy-6-propan-2-ylpyrazine	CC(C)C1=CN=CC(=N1)OC	green horseradish earthy peanut bellpepper raw raw potato galbanum green pea	Sigma Aldrich, TGSC
851	Isopropylpyrazine	2-propan-2-ylpyrazine	CC(C)C1=NC=CN=C1	minty green nutty honey	OdorRactor ,TGSC
852	2-Isopropyl-3- methoxypyrazine	2-methoxy-3-propan-2-ylpyrazine	CC(C)C1=NC=CN=C1OC	green pea chocolate beany green musty nutty earthy pepper	Sigma Aldrich, TGSC, OdoRactor
853	2-Isopropyl-3- methylthiopyrazine	2-methylsulfanyl-3-propan-2- ylpyrazine	CC(C)C1=NC=CN=C1SC	green vegetable roasted meat roasted	OdorRactor ,TGSC
854	Sabinene	4-methylidene-1-propan-2- ylbicyclo[3.1.0]hexane	CC(C)C12CCC(=C)C1C2	woody spicy pepper turpentine citrus terpenic pine green oily camphoraceous	Sigma Aldrich, Flavornet, TGSC, OdoRactor
855	cis-(+/-)-4-Thujanol	(1R ,2S ,5S)-2-methyl-5-propan- 2- ylbicyclo[3.1.0]hexan-2-ol	CC(C)C12CCC(C1C2)(C)O	balsamic	Flavornet, TGSC, OdoRactor
856	Sabinene hydrate	2-methyl-5-propan-2- ylbicyclo[3.1.0]hexan-2-ol	CC(C)C12CCC(C1C2)(C)O	minty eucalyptus green terpenic cooling spicy sweet camphoraceous	OdorRactor ,TGSC, Flavorbase
857	4-Thujanol	(1R, ,2R, ,5S)-2-methyl-5-propan- 2- ylbicyclo[3.1.0]hexan-2-ol	CC(C)C12CCC(C1C2)(C)O	woody balsamic	OdorRactor ,TGSC
858	1,4-Cineole	1-methyl-4-propan-2-yl-7- oxabicyclo[2.2.1]heptane	CC(C)C12CCC(O1)(CC2)C	spicy vanilla camphoraceous minty terpenic green cooling pine eucalyptus	Sigma Aldrich, AOD, TGSC, OdoRactor, Pubchem
859	4-Isopropyl-2,2,5,5- tetramethyl-1,3-dioxane	2,2,5,5-tetramethyl-4-propan-2-yl-1,3-dioxane	CC(C)C1C(COC(O1)(C)C)(C)C	woody old wood sawdust earthy fruity green herbaceous	OdorRactor ,TGSC
860	2,4-Diisopropyl-5,5-dimethyl- 1,3-dioxane	5,5-dimethyl-2,4-di(propan-2-yl)- 1,3-dioxane	CC(C)C1C(COC(O1)C(C)C)(C)C	spicy woody fruity	TGSC
861	4-Isopropyl-5,5-dimethyl-1,3-	5,5-dimethyl-4-propan-2-yl-1,3-dioxane	CC(C)C1C(COCO1)(C)C	green herbaceous camphoraceous woody	OdorRactor,

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862	beta-Phellandrene	3-methylidene-6-propan-2- ylcyclohexene	CC(C)C1CCC(=C)C=C1	minty terpenic pleasant	Flavornet, TGSC, Pubchem
863	4-Isopropyl-2-cyclohexenone	4-propan-2-ylcyclohex-2-en-1-one	CC(C)C1CCC(=0)C=C1	spicy cumin caraway woody herbaceous	SuperScent, TGSC, OdoRactor
864	2-Cyclohexen-1-ol, 1-methyl- 4-(1- methylethyl)-, trans-	(1R,4S)-1-methyl-4-propan-2-ylcyclohex-2-en-1- ol	CC(C)C1CCC(C=C1)(C)O	herbaceous	Flavornet
865	Cyclohexanemethanol, alpha- methyl-4-(1- methylethyl)-	1-(4-propan-2- ylcyclohexyl)ethanol	CC(C)C1CCC(CC1)C(C)O	floral muguet wax lily of the valley rose	OdorRactor ,TGSC
866	Cyclohexanemethanol, 4-(1-methylethyl)-, cis-	(4-propan-2- ylcyclohexyl)methanol	CC(C)C1CCC(CC1)CO	floral cumin grassy fresh clean magnolia muguet	OdorRactor ,TGSC
867	4-Isopropylcyclohexanol	4-propan-2-ylcyclohexan-1-ol	CC(C)C1CCC(CC1)O	leathery rose green dusty weedy metallic	OdorRactor ,TGSC
868	(-)-beta-Bourbonene	(15,2R,65,7R,85)-1-methyl-5-methylidene-8- propan-2-yltricyclo[5.3.0.02,6]decane	CC(C)C1CCC2(C1C3C2CCC3=C)C	buttery almond nutty caramel herbaceous woody floral balsamic	Flavornet, TGSC
869	1-Oxaspiro(4.5)decan-2-one, 8-(1- methylethyl)-, trans-	8-propan-2-yl-1- oxaspiro[4.5]decan-2-one	CC(C)C1CCC2(CC1)CCC(=O)O2	woody herbaceous celery lactonic	TGSC
870	Decatone	6-propan-2-yl-3,4,4 <i>a</i> ,5,6,7,8,8 <i>a</i> - octahydro-1 <i>H</i> - naphthalen-2-one	CC(C)C1CCC2CC(=0)CCC2C1	floral gardenia green grapefruit rhubarb vetiver woody	OdorRactor ,TGSC
871	3,5-Diisopropyl-1,2,4- trithiolane	3,5-di(propan-2-yl)-1,2,4- trithiolane	CC(C)C1SC(SS1)C(C)C	crispy bacon meaty smoky	OdorRactor ,TGSC
872	2,6-Decadienal, 3,7,9- trimethyl-	(2E ,6E)-3,7,9-trimethyldeca-2,6-dienal	CC(C)CC(=CCCC(=CC=O)C)C	fruity aldehydic wax floral	TGSC
873	Azanium;3-methylbutanoate	azanium;3-methylbutanoate	CC(C)CC(=O)[O-].[NH4+]	rancid fruity sharp cheese	TGSC
874	Methyl isobutyl ketone	4-methylpentan-2-one	CC(C)CC(=O)C	fruity ethereal spicy green sharp solvent herbaceous dairy sweet pleasant camphoraceous paint	Sigma Aldrich, Flavorbase, TGSC, Pubchem, OdoRactor
875	Sodium 4-methyl-2- oxovalerate	sodium;4-methyl-2-oxopentanoate	CC(C)CC(=O)C(=O)[O-].[Na+]	buttery fruity	Sigma Aldrich, TGSC
876	5-Methyl-2,3-hexanedione	5-methylhexane-2,3-dione	CC(C)CC(=O)C(=O)C	sweet fruity creamy buttery sharp brown	OdorRactor ,TGSC
877	4-methyl-2-oxopentanoic acid	4-methyl-2-oxopentanoic acid	CC(C)CC(=O)C(=O)O	fruity	OdoRactor ,TGSC
878	2-Hydroxy-5-methyl-3- hexanone	2-hydroxy-5-methylhexan-3-one	CC(C)CC(=O)C(C)O	sweet chocolate	OdorRactor ,TGSC
879	2,7-Dimethyloct-5-en-4-one	(E)-2,7-dimethyloct-5-en-4-one	CC(C)CC(=0)C=CC(C)C	chamomile animal fruity herbaceous tagette	OdorRactor ,TGSC
880	Diisobutyl ketone	2,6-dimethylheptan-4-one	CC(C)CC(=0)CC(C)C	ethereal fruity vanilla green metallic pineapple banana ketonic fermented sweet chemical peppermint mild	Sigma Aldrich, Flavorbase, TGSC, Pubchem, OdoRactor
881	4-Methyl-1-phenylpentan-2- one	4-methyl-1-phenylpentan-2-one	CC(C)CC(=O)CC1=CC=CC=C1	spicy woody sweet fruity burnt sugar burnt	Sigma Aldrich, TGSC, OdoRactor
882	Isovaleric acid	3-methylbutanoic acid	CC(C)CC(=0)0	cheese fatty sweet acidic rancid sour stinky sweaty tropical dairy pungent ripe fruity disagreeable	Sigma Aldrich, AOD, TGSC,OdoRactor
883	Methyl isovalerate	methyl 3-methylbutanoate	CC(C)CC(=O)OC	apple fruity pineapple sweet estery tutti frutti	Sigma Aldrich, TGSC, Pubchem, Odo Ractor
884	Linalyl isovalerate	3,7-dimethylocta-1,6-dien-3-yl 3-methylbutanoate	CC(C)CC(=0)OC(C)(CCC=C(C) C)C=C	apple sage sweet citrus bergamot lavender peach apricot herbaceous	Sigma Aldrich, TGSC, OdoRactor
885 886	Isopropyl isovalerate Eugenyl isovalerate	propan-2-yl 3-methylbutanoate (2-methoxy-4-prop-2-enylphenyl) 3- methylbutanoate)CC=C) OC	apple pineapple fruity winey fruity spicy clove	OdorRactor ,TGSC OdorRactor ,TGSC
887	1,3,3- Trimethylbicyclo[2.2.1]hept-2- yl 3- methylbutanoate	(1,3,3-trimethyl-2- bicyclo[2.2.1]heptanyl) 3- methylbutanoate	CC(C)CC(=0)OC1C(C2CCC1(C2)C)(C)C		TGSC
888	Isobornyl isovalerate	(1,7,7-trimethyl-2- bicyclo[2.2.1]heptanyl) 3- methylbutanoate	C)C)C	camphoraceous herbaceous earthy green tropical woody valerian root root apple pine cooling oily	Sigma Aldrich, OdoRactor
889	Bornyl isovalerate	[(1S, 2R, 4S)-1,7,7-trimethyl-2-bicyclo[2.2.1]heptanyl] 3-methylbutanoate	C)C)C	camphoraceous tropical valerian root	SuperScent, TGSC
890	Isovaleric acid, 2-bornyl ester	[(1S, 2R, 4R)-1,7,7-trimethyl-2-bicyclo[2.2.1]heptanyl] 3-methylbutanoate	C)C)C	camphoraceous tropical valerian root herbaceous root	OdorRactor ,TGSC
891	Cyclohexyl isovalerate	cyclohexyl 3-methylbutanoate	CC(C)CC(=0)OC1CCCCC1	fruity apple banana berry	SuperScent, TGSC, OdoRactor
892	Isobutyl isovalerate	2-methylpropyl 3-methylbutanoate	CC(C)CC(=O)OCC(C)C	apple ethereal raspberry winey sweet fruity green banana	Sigma Aldrich, TGSC,OdoRactor
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893	[(3E)-3,7-Dimethylocta-3,6-dienyl] 3- methylbutanoate	[(3E)-3,7-dimethylocta-3,6-dienyl] 3-methylbutano	CC(C)CC(=O)OCC/C(=C/CC=C(C)C)/C	fruity green apple blueberry pineapple sweet herbaceous melon	OdorRactor ,TGSC
894	Allyl isovalerate	prop-2-enyl 3-methylbutanoate	CC(C)CC(=0)OCC=C	apple cherry winey sweet fruity banana pineapple pungent	Sigma Aldrich, TGSC, OdoRactor, Pubchem
895	Geranyl isovalerate	[(2E)-3,7-dimethylocta-2,6-dienyl] 3- methylbutanoate	CC(C)CC(=0)OCC=C(C)CCC=C(C)C	apple berry green melon herbaceous rose fruity blueberry pineapple oily herbaceous	Sigma Aldrich, TGSC, Flavorbase, OdoRactor
896	Neryl isovalerate	[(2Z)-3,7-dimethylocta-2,6-dienyl] 3- methylbutanoate	CC(C)CC(=0)OCC=C(C)CCC=C(C)C	sweaty floral rose bergamot citrus fruity sour blueberry cranberry grape apple	SuperScent, TGSC, OdoRactor
897	Cinnamyl isovalerate	[(E)-3-phenylprop-2-enyl] 3-methylbutanoate	CC(C)CC(=0)OCC=CC1=CC=C C=C1	sweet spicy melon cherry apple blueberry sour fermented winey yeasty woody fruity	Sigma Aldrich, TGSC, OdoRactor
898	Benzyl isovalerate	benzyl 3-methylbutanoate	CC(C)CC(=0)OCC1=CC=CC=C1	fruity powdery musty apple herbaceous pineapple sweet herbaceous	Sigma Aldrich, TGSC, OdoRactor
899	Furfuryl isovalerate	furan-2-ylmethyl 3- methylbutanoate	CC(C)CC(=O)OCC1=CC=CO1	fruity grape plum berry ripe	Sigma Aldrich, TGSC, OdoRactor
900	3-Mercapto-3-methylbutyl isovalerate	(3-methyl-3-sulfanylbutyl) 3- methylbutanoate	CC(C)CC(=O)OCCC(C)(C)S	sulfurous tropical fruit grape	Flavorbase
901	Citronellyl isovalerate	3,7-dimethyloct-6-enyl 3- methylbutanoate	CC(C)CC(=O)OCCC(C)CCC=C(C)C	floral black currant honey rose herbaceous chamomile apple	OdorRactor ,TGSC
902	Rhodinyl isovalerate	3,7-dimethyloct-7-enyl 3- methylbutanoate	CC(C)CC(=O)OCCC(C)CCCC(= C)C	rose floral fruity	OdorRactor ,TGSC, Flavorbase
903	Phenethyl isovalerate	2-phenylethyl 3-methylbutanoate	CC(C)CC(=0)OCCC1=CC=CC=	fruity rose floral peach apricot sweet ripe pineapple tutti frutti apple blueberry balsamic	Sigma Aldrich, Flavorbase, TGSC,OdoRactor
904	3-Phenylpropyl isovalerate	3-phenylpropyl 3-methylbutanoate	CC(C)CC(=O)OCCCC1=CC=CC =C1	fruity strawberry raspberry plum	SuperScent, TGSC, Flavorbase
905	S-Methyl 3- methylbutanethioate	S -methyl 3-methylbutanethioate	CC(C)CC(=O)SC	sharp ripe cheese sulfurous acrid fermented tomato mushroom potato acidic vegetable dairy	OdorRactor ,TGSC
906	Butanethioic acid, 3-methyl-, S-(1- methylethyl) ester	S -propan-2-yl 3- methylbutanethioate	CC(C)CC(=0)SC(C)C	green galbanum sulfurous	TGSC
907	S-Prenyl thioisopentanoate	S -(3-methylbut-2-enyl) 3-methylbutanethioate	CC(C)CC(=O)SCC=C(C)C	sulfurous fruity tropical durain passion fruit dried fruit	TGSC
908	3-Hydroxy-5-methyl-2- hexanone	3-hydroxy-5-methylhexan-2-one	CC(C)CC(C(=O)C)O	sweet chocolate	TGSC
909	Methyl 2-hydroxy-4- methylpentanoate	methyl 2-hydroxy-4- methylpentanoate	CC(C)CC(C(=O)OC)O	sweet fruity musty	OdorRactor ,TGSC
910	6,8-Dimethylnonan-2-ol	6,8-dimethylnonan-2-ol	CC(C)CC(C)CCCC(C)O	chicken floral green fruity mushroom	OdorRactor ,TGSC
911	4-Methyl-2-pentanol	4-methylpentan-2-ol	CC(C)CC(C)O	pungent high alcoholic	SuperScent, TGSC
	1,3-Dimethylbutyl acetate 2,6-Dimethylheptan-4-ol	4-methylpentan-2-yl acetate 2,6-dimethylheptan-4-ol	CC(C)CC(C)OC(=0)C CC(C)CC(CC(C)C)O	sweet fruity banana pleasant ethereal fresh fermented yeasty	TGSC SuperScent, TGSC,OdoRactor
914	2,6-Dimethylheptan-4-yl acetate	2,6-dimethylheptan-4-yl acetate	CC(C)CC(CC(C)C)OC(=O)C	herbaceous floral lilac banana rhubarb	OdorRactor ,TGSC
915	4-Methyl-1-phenyl-2-pentanol	4-methyl-1-phenylpentan-2-ol	CC(C)CC(CC1=CC=CC=C1)O	green musty herbaceous floral creamy celery herbaceous	Sigma Aldrich, TGSC, Odoractor
916	2-Isopropyl-5-methyl-2- hexenal	(E)-5-methyl-2-propan-2-ylhex-2-enal	CC(C)CC=C(C=0)C(C)C	berry herbaceous lavender woody green blueberry tomato cocoa earthy	Sigma Aldrich, TGSC, Flavorbase
917	5-Methyl-2-phenyl-2-hexenal	(E)-5-methyl-2-phenylhex-2-enal	CC(C)CC=C(C=O)C1=CC=CC=C	•	Sigma Aldrich, OdoRactor
918	5-Methyl-2-phenylhex-2-enal	5-methyl-2-phenylhex-2-enal	CC(C)CC=C(C=O)C1=CC=CC=C	chocolate aldehydic bitter cocoa nutty green sweet fruity buttery rancid brown	AOD, TGSC, Flavorbase, OdoRactor
919	2-Isopropyl-5-methylhex-2-en- 1-ol	(E)-5-methyl-2-propan-2-ylhex-2-en-1-ol	CC(C)CC=C(CO)C(C)C	herbaceous fresh minty rosemary woody	OdorRactor ,TGSC
920	2-Isopropyl-5-methylhex-2- enyl acetate	[(Z)-5-methyl-2-propan-2-ylhex-2 enyl] acetate	CC(C)CC=C(COC(=O)C)C(C)C	herbaceous fresh minty woody	OdorRactor ,TGSC
921	5-Methyl-2- (methylthiomethyl)-2-hexenal	(E)-5-methyl-2- (methylsulfanylmethyl)hex-2-enal	CC(C)CC=C(CSC)C=O	onion meaty spicy herbaceous	Flavorbase
922	6-Methyl-3-hepten-2-one	(E)-6-methylhept-3-en-2-one	CC(C)CC=CC(=O)C	tropical oily green herbaceous fruity	TGSC
923	3-Methylbutanal	3-methylbutanal	CC(C)CC=O	fruity peach sour ethereal chocolate fatty aldehydic apple penetrating acrid buttery	Sigma Aldrich, TGSC, Pubchem,OdoRactor
924	2-Methyl-3-[4-(2- methylpropyl)phenyl]propana	2-methyl-3-[4-(2- methylpropyl)phenyl]propanal	CC(C)CC1=CC=C(C=C1)CC(C)C =O	floral muguet lily green tropical oily greasy marine balsamic	OdorRactor ,TGSC
925	2-Isobutylpyridine	2-(2-methylpropyl)pyridine	CC(C)CC1=CC=CC=N1	aromatic bellpepper	OdorRactor ,TGSC
926	4-Isobutylquinoline	4-(2-methylpropyl)quinoline	CC(C)CC1=CC=NC2=CC=CC=C 12	leathery animal herbaceous green	OdorRactor ,TGSC

927	6-Isobutylquinoline	6-(2-methylpropyl)quinoline	CC(C)CC1=CC2=C(C=C1)N=CC	earthy rooty nutty oakmoss vetiver	TGSC
721	o isocatyiqamomic	(2 metry propyr) quinomic	=C2	leathery green	Tobe
928	3-Isobutylpyridine	3-(2-methylpropyl)pyridine	CC(C)CC1=CN=CC=C1	aromatic	OdorRactor ,TGSC
929	2-Isobutylpyrazine	2-(2-methylpropyl)pyrazine	CC(C)CC1=NC=CN=C1	green vegetable fruity	TGSC
930	2-Isobutyl-3-methoxypyrazine	2-methoxy-3-(2- methylpropyl)pyrazine	CC(C)CC1=NC=CN=C1OC	green vegetable bellpepper earthy spice green pea galbanum	Sigma Aldrich, Flavorbase, TGSC, OdoRactor
931	2-Isobutylthiazole	2-(2-methylpropyl)-1,3-thiazole	CC(C)CC1=NC=CS1	green herbaceous tomato earthy vegetable metallic musty wax wasabi privet	Sigma Aldrich, Flavorbase, TGSC, OdoRactor
932	2-Isobutylquinoline	2-(2-methylpropyl)quinoline	CC(C)CC1=NC2=CC=CC=C2C= C1	animal leathery woody rooty tobacco oakmoss	OdorRactor ,TGSC
933	2H-Pyran-4-ol, tetrahydro-4-methyl-2-(2- methylpropyl)-	4-methyl-2-(2-methylpropyl)oxan- 4-ol	CC(C)CC1CC(CCO1)(C)O	fresh clean soft natural floral muguet linalool	OdorRactor ,TGSC, Pubchem
934	Cyclohexanol, 1-methyl-3-(2-methylpropyl)-	1-methyl-3-(2- methylpropyl)cyclohexan-1-ol	CC(C)CC1CCCC(C1)(C)O	floral muguet citrus	TGSC
935	Dihydro-2,4,6-tris(2- methylpropyl)-4h- 1,3,5-dithiazine	2,4,6-tris(2-methylpropyl)-1,3,5-dithiazinane	CC(C)CC1NC(SC(S1)CC(C)C)C C(C)C	meaty smoky bacon roasted savory fried	OdorRactor ,TGSC, Flavorbase
936	2,4,6-Triisobutyl-1,3,5- trioxane	2,4,6-tris(2-methylpropyl)-1,3,5-trioxane	CC(C)CC1OC(OC(O1)CC(C)C)C C(C)C	sweet dairy creamy vanilla berry milky chocolate cocoa	TGSC, OdoRactor
937	5-Hydroxy-2-(2- methylpropyl)-1,3-dioxane	2-(2-methylpropyl)-1,3-dioxan-5- ol	CC(C)CC1OCC(CO1)O	fruity fatty	TGSC
938	3,5-Diisobutyl-1,2,4- trithiolane	3,5-bis(2-methylpropyl)-1,2,4- trithiolane	CC(C)CC1SC(SS1)CC(C)C	roasted nutty bacon	OdorRactor ,TGSC
939	4-Methylpentanoic acid	4-methylpentanoic acid	CC(C)CCC(=O)O	pungent unpleasant sour	Sigma Aldrich, Flavorbase, TGSC,OdoRactor
940	Methyl 4-methylvalerate	methyl 4-methylpentanoate	CC(C)CCC(=0)OC	pineapple sweet fruity banana cheese	Sigma Aldrich, TGSC, OdoRactor
941	S-Methyl 4- methylpentanethioate	S -methyl 4-methylpentanethioate	CC(C)CCC(=0)SC	fermented tropical dairy creamy cheese vegetable	TGSC
942	7-Methyl-3-octen-2-one	(E)-7-methyloct-3-en-2-one	CC(C)CCC=CC(=0)C	creamy green earthy fruity fatty oily lactonic nutty meaty	OdorRactor ,TGSC, Flavorbase
943	1,3-Dioxepin, 4,7-dihydro-2-methyl-2-(3- methylbutyl)-	2-methyl-2-(3-methylbutyl)-4,7-dihydro-1,3- dioxepine	CC(C)CCC1(OCC=CCO1)C	lavender sweet herbaceous amber fresh	OdorRactor ,TGSC
944	2H-1,5-Benzodioxepin-3(4H)-one, 7-(3- methylbutyl)-	7-(3-methylbutyl)-1,5- benzodioxepin-3-one	CC(C)CCC1=CC2=C(C=C1)OCC (=O)CO 2	marine	TGSC
945	6-Methylheptan-2-one	6-methylheptan-2-one	CC(C)CCCC(=0)C	camphoraceous	OdorRactor,
946	5-Methylhexanoic acid	5-methylhexanoic acid	CC(C)CCCC(=0)0	fatty cheese oily fruity	OdorRactor ,TGSC
947	2,6-Dimethyl-2-heptanol	2,6-dimethylheptan-2-ol	CC(C)CCCC(C)(C)O	fresh floral woody citrus herbaceous bois de rose rose	OdorRactor ,TGSC
948	3,7-Dimethyl-1-octen-3-ol	3,7-dimethyloct-1-en-3-ol	CC(C)CCCC(C)(C=C)O	woody citrus camphoraceous	Flavornet, TGSC, OdoRactor
949	3,7-Dimethylocten-2-ol	3,7-dimethyloct-1-en-2-ol	CC(C)CCCC(C)C(=C)O	woody herbaceous pine	TGSC
950	3,7-Dimethyl-1-octene	3,7-dimethyloct-1-ene	CC(C)CCC(C)C=C	woody pine herbaceous	TGSC
951	3,7-Dimethyloctanenitrile	3,7-dimethyloctanenitrile	CC(C)CCC(C)CC#N	citrus aldehydic lemon fatty metallic	OdorRactor ,TGSC
952	1,1-Dimethoxy-3,7- dimethyloctane	1,1-dimethoxy-3,7-dimethyloctane	CC(C)CCCC(C)CC(OC)OC	ethereal rose	TGSC
953	3,7-Dimethyloctanal	3,7-dimethyloctanal	CC(C)CCCC(C)CC=O	citrus lemon green aldehydic	OdorRactor ,TGSC
954	6,10-Dimethylundecan-2-one	6,10-dimethylundecan-2-one	CC(C)CCCC(C)CCCC(=O)C	musty dry	OdorRactor ,TGSC
955	Phytol	(E ,7R ,11R)-3,7,11,15- tetramethylhexadec-2-en-1- ol	CC(C)CCCC(C)CCCC(C)CCCC(=CCO)C	floral balsamic powdery wax	Flavornet, TGSC, OdoRactor
956	3,7,11,15-Tetramethyl-2- hexadecen-1-OL	(E)-3,7,11,15-tetramethylhexadec- 2-en-1-ol	CC(C)CCCC(C)CCCC(C)CCCC(=CCO)C	green jasmine balsamic floral	Sigma Aldrich, TGSC
957	2-Hexadecen-1-ol, 3,7,11,15- tetramethyl-, acetate, (2E,7R,11R)-	[(E,7R,11R)-3,7,11,15- tetramethylhexadec-2-enyl] acetate	CC(C)CCCC(C)CCCC(C)CCCC(=CCOC(=O)C)C	mild wax fruity balsamic	OdorRactor ,TGSC
958	6,10,14-Trimethylpentadecan- 2-one	6,10,14-trimethylpentadecan-2- one	CC(C)CCCC(C)CCCC(C)CCCC(=O)C	fatty oily herbaceous jasmine celery woody fresh floral	Flavornet, Flavorbase, TGSC,OdoRactor
959	Isophytol	3,7,11,15-tetramethylhexadec-1-en-3-ol	CC(C)CCCC(C)CCCC(C)CCCC(C)(C=C)	chocolate herbaceous floral green	Sigma Aldrich, TGSC,OdoRactor
960	3,7-Dimethyloctan-1-o	3,7-dimethyloctan-1-ol	CC(C)CCCC(C)CCO	rose sweet wax soapy leathery musty citrus green aldehydic fresh fatty lemon lime orange woody floral plastic	Sigma Aldrich, TGSC, OdoRactor
961	3,7-Dimethyloctyl acetate	3,7-dimethyloctyl acetate	CC(C)CCCC(C)CCOC(=0)C	wax rose sweet fruity honey fresh clean	OdorRactor ,TGSC
962	3,7-Dimethyloctyl phenylacetate	3,7-dimethyloctyl 2-phenylacetate	CC(C)CCCC(C)CCOC(=0)CC1= CC=CC= C1	floral rose	TGSC
963	Vernaldehyde	1-methyl-4-(4- methylpentyl)cyclohex-3-ene-1- carbaldehyde	CC(C)CCCC1=CCC(CC1)(C)C= O	fresh wax green aldehydic metallic citrus	OdorRactor ,TGSC, Pubchem
064	6 Mathylhontonal	•	CC(C)CCCC-0	frach graan jujay awast areas	TCSC
964	6-Methylheptanal	6-methylheptanal	CC(C)CCCCC=O	fresh green juicy sweet orange	TGSC

965	Isodecanal	8-methylnonanal	CC(C)CCCCCCC=O	sweet floral rose lemon citrus green wax milky peely strong fruity	OdorRactor ,Flavorbase, Pubchem
966	12-Methyltridecanal	12-methyltridecanal	CC(C)CCCCCCCCCC=0	cooked fatty brothy tallow metallic sweaty meaty fruity wax citrus beefy	Flavornet, TGSC, Flavorbase, OdoRactor
967	Isotridecane, 1,1'-[(3,7-dimethyl-6-octenylidene)bis(oxy)]bis-	1-[3,7-dimethyl-1-(11-methyldodecoxy)oct-6-enoxy]-11-methyldodecane	CC(C)CCCCCCCCCCC(C)C CCC=C(C)C)OCCCCCCCCCCC(C)C	floral fresh rose fruity minty	TGSC
968	2-Octanol, 8,8- bis(isotridecyloxy)-2,6- dimethyl-	2,6-dimethyl-8,8-bis(11- methyldodecoxy)octan-2- ol	CC(C)CCCCCCCCCC(C)C	woody fresh sweet lily muguet milky	TGSC
969	Acetic acid, isodecyl ester	8-methylnonyl acetate	CC(C)CCCCCCCC(=0)C	fresh clean citrus green herbaceous cumin powdery	OdorRactor ,TGSC
970	Isononyl acetate	7-methyloctyl acetate	CC(C)CCCCCCC(=0)C	floral fruity violet sweet herbaceous cumin woody	OdorRactor ,TGSC
971	6-Methyl-1-heptanol	6-methylheptan-1-ol	CC(C)CCCCCO	fatty orange rose mild characteristic pleasant	TGSC, Pubchem
972	Isooctyl acetate	6-methylheptyl acetate	CC(C)CCCCCC(=0)C	sweet estery fruity	OdorRactor ,TGSC
973	5-Methylhexyl acetate	5-methylhexyl acetate	CC(C)CCCCOC(=0)C	sweet minty	TGSC, Pubchem
974	4-Methyl-1-pentanol	4-methylpentan-1-ol	CC(C)CCCO	nutty	TGSC
975	4-Methylpentyl 4-	4-methylpentyl 4-	CC(C)CCCOC(=0)CCC(C)C	fruity wax soapy herbaceous	TGSC
	methylpentanoate	methylpentanoate			
976	Isoamylamine	3-methylbutan-1-amine	CC(C)CCN	vanilla ammonical	Sigma Aldrich, Flavorbase, TGSC,OdoRactor
977	1-Isothiocyanato-3- methylbutane	1-isothiocyanato-3-methylbutane	CC(C)CCN=C=S	pungent horseradish cabbage green	OdorRactor ,Flavorbase
978	methylbutylidene)-	3-methyl- N -(3-methylbutyl)butan-1-imine		citrus fatty	OdorRactor ,TGSC
979	1-Butanamine, 3-methyl-N-(3-methylbutylidene)-	3-methyl- <i>N</i> -(3-methylbutyl)butan- 1-imine	CC(C)CCN=CCC(C)C	fishy oily sweet shellfish burnt cocoa	OdorRactor ,TGSC, Flavorbase
980	Isoamyl alcohol	3-methylbutan-1-ol	CC(C)CCO	oily whiskey malty burnt fusel alcoholic fruity banana fermented pungent ethereal cognac molasses winey brandy	Sigma Aldrich, Flavornet, Flavorbase, TGSC, OdoRactor
981	Isoamyl acetate	3-methylbutyl acetate	CC(C)CCOC(=O)C	banana pear sweet fruity solvent ripe estery	OdoRactor, Sigma Aldrich, Flavorbase, TGSC
982	Isoamyl pyruvate	3-methylbutyl 2-oxopropanoate	CC(C)CCOC(=O)C(=O)C	caramel balsamic rummy fruity arrack sweet	SuperScent, TGSC, Flavorbase, Odoractor
983	Isopentyl isobutyrate	3-methylbutyl 2-methylpropanoate	CC(C)CCOC(=0)C(C)C	fruity wax pineapple banana green apricot honey sweet estery	Sigma Aldrich, TGSC, Odoractor
984	Isoamyl lactate	3-methylbutyl 2- hydroxypropanoate	CC(C)CCOC(=0)C(C)O	fruity creamy nutty	TGSC
985	Isoamyl geranate	3-methylbutyl (2E)-3,7- dimethylocta-2,6-dienoate	CC(C)CCOC(=0)C=C(C)CCC=C(C)C		OdorRactor ,TGSC
986	Isopentyl cinnamate	3-methylbutyl (E)-3-phenylprop-2-enoate	CC(C)CCOC(=0)C=CC1=CC=C C=C1	chocolate balsamic floral amber cocoa orchid musty sweet berry fruity powdery carnation	Sigma Aldrich, TGSC, OdoRactor
987	Isopentyl benzoate	3-methylbutyl benzoate	CC(C)CCOC(=0)C1=CC=CC=C1	sweet balsamic green wax fruity	Sigma Aldrich, Flavorbase, TGSC
988	Isoamyl salicylate	3-methylbutyl 2-hydroxybenzoate	CC(C)CCOC(=0)C1=CC=CC=C1 0	grape green floral soapy sweet winey wintergreen herbaceous woody orchid metallic	Sigma Aldrich, TGSC
989	Isoamyl acetoacetate	3-methylbutyl 3-oxobutanoate	CC(C)CCOC(=0)CC(=0)C	ethereal sweet winey green fermented ripe banana ripe	OdorRactor ,TGSC
990	Diisopentyl thiomalate	bis(3-methylbutyl) 2- sulfanylbutanedioate	CC(C)CCOC(=0)CC(C(=0)OCC C(C)C)S	fermented coffee yeasty rye bready	OdorRactor ,TGSC, Flavorbase
991	Isoamyl isovalerate	3-methylbutyl 3-methylbutanoate	CC(C)CCOC(=0)CC(C)C	apple apricot banana green mango sweet winey tropical estery jammy ripe fruity pineapple cognac	Sigma Aldrich, Flavorbase, TGSC,OdoRactor
992	Isoamyl phenylacetate	3-methylbutyl 2-phenylacetate	CC(C)CCOC(=0)CC1=CC=CC=	honey rose chocolate sweet cocoa balsamic castoreum animal floral	Sigma Aldrich, TGSC
993	Isoamyl levulinate	3-methylbutyl 4-oxopentanoate	CC(C)CCOC(=O)CCC(=O)C	ethereal caramel	TGSC
993	Isoamyl 3-(2-	3-methylbutyl 3-(furan-2-	CC(C)CCOC(=0)CCC1=CC=CO	green sweet floral fruity apple rose	SuperScent, TGSC
995	furan)propionate Isoamyl 4-(2-furan)butyrate	yl)propanoate 3-methylbutyl 4-(furan-2- yl)butanoate	CC(C)CCOC(=O)CCCC1=CC=C	raisin caramel sour sweet buttery fruity caramel	TGSC
996	Acetaldehyde diisoamyl acetal	3-methyl-1-[1-(3- methylbutoxy)ethoxy]butane	CC(C)CCOC(C)OCCC(C)C	alcoholic fruity ethereal green fermented	OdorRactor ,TGSC
997		2,2-bis(3-	CC(C)CCOC(CC1=CC=CC=C1)O		TGSC
	acetal	methylbutoxy)ethylbenzene	CCC(C) C		

998	Isopentyl formate	3-methylbutyl formate	CC(C)CCOC=O	plum black currant ethereal vinous earthy fruity green cortex dry sharp estery apple wax sweet winey	Sigma Aldrich, Flavorbase, TGSC,OdoRactor
999	Allyl (3-methylbutoxy)acetate	prop-2-enyl 2-(3- methylbutoxy)acetate	CC(C)CCOCC(=0)OCC=C	fruity green pineapple galbanum fusel estery wax fatty	SuperScent, TGSC, PW
1000	Benzyl isoamyl ether	3-methylbutoxymethylbenzene	CC(C)CCOCC1=CC=CC=C1	green bean gardenia jasmine fruity weedy green pea floral	OdorRactor ,TGSC
1001	Isopentyl phenethyl ether	2-(3-methylbutoxy)ethylbenzene	CC(C)CCOCCC1=CC=CC=C1	green metallic hyacinth cooling leafy strong sweet watery tropical	OdorRactor ,Flavorbase
1002	3-Methylbutane-1-thiol	3-methylbutane-1-thiol	CC(C)CCS	sulfurous onion green onion garlic	Sigma Aldrich, TGSC,OdoRactor
1003	Methyl isopentyl disulfide	3-methyl-1- (methyldisulfanyl)butane	CC(C)CCSSC	sulfurous roasted	OdorRactor,
1004	Diisoamyl disulfide	3-methyl-1-(3- methylbutyldisulfanyl)butane	CC(C)CCSSCCC(C)C	sweet onion	TGSC
1005	Isobutylamine	2-methylpropan-1-amine	CC(C)CN	cheese fishy ammonical shellfish malty ripe	Sigma Aldrich, TGSC, Pubchem,OdorRactor ,Flavorbase
1006	Isobutyl isothiocyanate	1-isothiocyanato-2-methylpropane	CC(C)CN=C=S	green sweet chemical mild pungent wasabi horseradish	OdorRactor ,Flavorbase
1007	Isobutanol	2-methylpropan-1-ol	CC(C)CO	fruity whiskey winey bitter ethereal sweet musty penetrating disagreeable suffocating fusel	Sigma Aldrich, TGSC, Pubchem
1008	Isobutyl acetate	2-methylpropyl acetate	CC(C)COC(=O)C	apple banana ethereal pear pineapple sweet tropical fruity floral nail-polish	Sigma Aldrich, TGSC,OdoRactor
1009	Isobutyl isobutyrate	2-methylpropyl 2- methylpropanoate	CC(C)COC(=O)C(C)C	grape ethereal fruity tropical fruit pineapple banana ripe	Sigma Aldrich, TGSC, Pubchem
1010	Isobutyl lactate	2-methylpropyl 2- hydroxypropanoate	CC(C)COC(=O)C(C)O	buttery fruity caramel	TGSC
1011	Isobutyl cinnamate		CC(C)COC(=0)C=CC1=CC=CC=	peach sweet balsamic fruity labdanum spicy	Sigma Aldrich, TGSC
1012	Isobutyl benzoate	2-methylpropyl benzoate	CC(C)COC(=0)C1=CC=CC=C1	chocolate rose sweet fruity musty powdery balsamic chemical cherry	Sigma Aldrich, TGSC, OdoRactor
1013	Isobutyl anthranilate	2-methylpropyl 2-aminobenzoate	CC(C)COC(=0)C1=CC=CC=C1N	grape sweet fruity floral berry	OdorRactor ,TGSC
1014	Isobutyl 2- (methylamino)benzoate	2-methylpropyl 2- (methylamino)benzoate	CC(C)COC(=0)C1=CC=CC=C1N	fruity grapefruit grape sweet floral citrus	OdorRactor ,TGSC, Flavorbase
1015	Isobutyl salicylate	2-methylpropyl 2- hydroxybenzoate	CC(C)COC(=0)C1=CC=CC=C10	orchid floral clover herbaceous sweet spicy cooling wintergreen herbaceous	Sigma Aldrich, Flavorbase, TGSC, Pubchem
1016	Isobutyl acetoacetate	2-methylpropyl 3-oxobutanoate	CC(C)COC(=O)CC(=O)C	sweet winey brandy fruity	OdorRactor ,TGSC
1017	(+/-)-Isobutyl 3- methylthiobutyrate	2-methylpropyl 3- methylsulfanylbutanoate	CC(C)COC(=O)CC(C)SC	pungent dry strawberry sweet fruity sulfurous tropical ripe creamy cheese	OdorRactor ,TGSC, Flavorbase
1018	Isobutyl phenylacetate	2-methylpropyl 2-phenylacetate	CC(C)COC(=0)CC1=CC=CC=C1	chocolate honey musty spicy woody wax sweet floral amber fruity cocoa rose	Sigma Aldrich, Flavorbase, TGSC, OdoRactor
1019	Isobutyl 2-furanpropionate	2-methylpropyl 3-(furan-2- yl)propanoate	CC(C)COC(=0)CCC1=CC=CO1	fruity floral winey woody pineapple	OdorRactor ,TGSC
1020	Isobutyl 10-undecenoate	2-methylpropyl undec-10-enoate	CC(C)COC(=0)CCCCCCCCC=C	fatty fruity wax	OdorRactor ,TGSC
1021	[2,2-Bis(2-methylpropoxy)ethyl]benzen	2,2-bis(2- methylpropoxy)ethylbenzene	CC(C)COC(CC1=CC=CC=C1)OC C(C)C	sweet floral green almond rose cortex honey brown cocoa dried fruit powdery hyacinth	ADB, TGSC, Flavorbase, OdoRactor
1022	Isobutyl formate	2-methylpropyl formate	CC(C)COC=O	fruity ethereal sweet chemical	Sigma Aldrich, TGSC,OdoRactor
1023	2-Isobutoxynaphthalene	2-(2-methylpropoxy)naphthalene	CC(C)COC1=CC2=CC=CC=C2C =C1	sweet naphthyl strawberry fruity orange flower blossom musty floral	OdorRactor ,TGSC
l	l .	2-methylpropane-1-thiol	CC(C)CS	mustard cooked vegetable sulfurous rotten	Flavornet, Flavorbase, TGSC,OdoRactor
1024	2-Methyl-1-propanethiol	,		I DOMEST OUD I OUDII	- 000,0001001001
1024	2-Methyl-1-propanethiol Isopropylamine	propan-2-amine	CC(C)N	fishy ammonical	OdorRactor ,TGSC, Pubchem
	, , ,	,, ,	CC(C)N CC(C)N=C=S	fishy ammonical pungent mustard alliaceous	OdorRactor ,TGSC,
1025	Isopropylamine	propan-2-amine		fishy ammonical pungent mustard alliaceous chemical horseradish wasabi buttery alcoholic musty woody	
1025	Isopropylamine Isopropyl isothiocyanate	propan-2-amine 2-isothiocyanatopropane	CC(C)N=C=S	fishy ammonical pungent mustard alliaceous chemical horseradish wasabi	OdorRactor ,TGSC, Flavorbase

1030	Cinnamic Acid Isopropyl Ester	propan-2-yl 3-phenylprop-2- enoate	CC(C)OC(=0)C=CC1=CC=CC=C 1	balsamic fruity tropical cinnamyl berry strawberry peach amber	OdorRactor ,TGSC
1031	Isopropyl cinnamate	propan-2-yl (E)-3-phenylprop-2-enoate	CC(C)OC(=0)C=CC1=CC=CC=C	balsamic fruity tropical cinnamyl berry strawberry peach amber	Sigma Aldrich, TGSC
1032	Isopropyl benzoate	propan-2-yl benzoate	CC(C)OC(=0)C1=CC=CC=C1	sweet fruit floral balsamic	Flavornet, TGSC, OdoRactor
1033	Isopropyl anthranilate	propan-2-yl 2-aminobenzoate	CC(C)OC(=O)C1=CC=CC=C1N	hawthorn honey floral neroli	OdorRactor ,TGSC
1034	Isopropyl salicylate	propan-2-yl 2-hydroxybenzoate	CC(C)OC(=O)C1=CC=CC=C1O	vine clover orchid cortex green	OdorRactor ,TGSC
1035	Isopropyl phenylacetate	propan-2-yl 2-phenylacetate	CC(C)OC(=0)CC1=CC=CC=C1	honey ethereal rose winey sweet honeysuckle powdery cortex floral	Sigma Aldrich, TGSC, OdoRactor
1036	Isopropyl 1-cyclohexene-1-acetate	propan-2-yl 2-(cyclohexen-1-yl)acetate	CC(C)OC(=O)CC1=CCCCC1	sweet wax rose honey licorice	OdorRactor ,TGSC
1037	Isopropyl formate	propan-2-yl formate	CC(C)OC=O	ethereal cocoa tropical solvent sweet fruity pleasant	OdorRactor ,TGSC, Pubchem
1038	4-Hydroxy-3- isopropoxybenzaldehyde	4-hydroxy-3-propan-2- yloxybenzaldehyde	CC(C)OC1=C(C=CC(=C1)C=O)O		TGSC
1039	(2-Isopropoxyethyl)benzene	2-propan-2-yloxyethylbenzene	CC(C)OCCC1=CC=CC=C1	green rose plastic metallic spicy watercress foliage	OdorRactor ,TGSC
1040	2-Isopropoxyethyl salicylate	2-propan-2-yloxyethyl 2-	CC(C)OCCOC(=0)C1=CC=CC=	sweet floral balsamic herbaceous	OdorRactor ,TGSC
1041	2-Propanethiol	hydroxybenzoate propane-2-thiol	C10 CC(C)S	cherry meaty sulfurous alliaceous ripe onion gassy sharp pungent brothy chicken unpleasant skunk	Sigma Aldrich, TGSC, Pubchem
1042	S-Isopropyl 3-methylbut-2- enethioate	S -propan-2-yl 3-methylbut-2- enethioate	CC(C)SC(=O)C=C(C)C	sulfurous onion eggy meaty tropical galbanum alliaceous green earthy	OdorRactor ,TGSC, Flavorbase
1043 1044	Diisopropyl sulfide Furfuryl isopropyl sulfide	2-propan-2-ylsulfanylpropane 2-(propan-2- ylsulfanylmethyl)furan	CC(C)SC(C)C CC(C)SCC1=CC=CO1	sulfurous vegetable garlic coffee savory meaty floral	OdorRactor ,TGSC OdorRactor ,TGSC
1045	Diisopropyl disulfide	2-(propan-2-yldisulfanyl)propane	CC(C)SSC(C)C	meaty sulfurous onion alliaceous cabbage garlic burnt	Sigma Aldrich, TGSC, Flavorbase
1046	Diisopropyl trisulfide	2-(propan-2-yltrisulfanyl)propane	CC(C)SSSC(C)C	sulfurous garlic green leek onion	OdorRactor ,TGSC, Flavorbase
1047	4,8-Dimethyl-3,7-nonadien-2-	(3E)-4,8-dimethylnona-3,7-dien-2-ol	CC(C=C(C)CCC=C(C)C)O	woody pine lemon lime rose	OdorRactor ,TGSC, Flavorbase
1048	4,8-Dimethyl-3,7-nonadien-2-yl acetate, (3E)-	[(3E)-4,8-dimethylnona-3,7-dien-2-yl] acetate	CC(C=C(C)CCC=C(C)C)OC(=O)	citrus lemon earthy woody	OdorRactor ,TGSC
1049	3-Buten-2-OL	but-3-en-2-ol	CC(C=C)O	gassy green fermented	Flavorbase
1050	3-Buten-2-ol, 4-phenyl-	4-phenylbut-3-en-2-ol	CC(C=CC1=CC=CC=C1)O	floral sweet fruity balsamic	TGSC, OdoRactor
1051	(s)-2-Phenylpropanal	(2S)-2-phenylpropanal	CC(C=0)C1=CC=CC=C1	floral green hyacinth	TGSC
1052	2-Phenylpropanal	2-phenylpropanal	CC(C=O)C1=CC=CC=C1	fresh sharp green hyacinth leafy	Sigma Aldrich, TGSC
1053	Lilac aldehyde	2-(5-ethenyl-5-methyloxolan-2-	CC(C=0)C1CCC(O1)(C)C=C	lilac floral floral lilac	OdorRactor ,TGSC
1054	2-Cyclohexylpropanal	yl)propanal 2-cyclohexylpropanal	CC(C=0)C1CCCCC1	natural green fresh dusty fruity	OdorRactor ,TGSC
1055			CC(C1=CC=CC=C1)C(OC)OC	pollen floral leafy hyacinth green	Sigma Aldrich, TGSC,
1033	2-Phenylpropionaldehyde dimethyl acetal	1,1-dimenioxypropan-2-yroenzene	cc(c1-cc-cc-c1)c(0c)0c	mushroom earthy spicy walnut sweet citrus honey	OdoRactor
1056	(R)-(+)-N,N-Dimethyl-1- phenylethylamine	(1R)-N ,N -dimethyl-1- phenylethanamine	CC(C1=CC=CC=C1)N(C)C	fishy sweet ammonical	OdorRactor ,TGSC
1057	(R)-1-Phenylethanol	(1R)-1-phenylethanol	CC(C1=CC=CC=C1)O	floral earthy green honeysuckle	TGSC
1058	(S)-1-Phenylethanol	(1S)-1-phenylethanol	CC(C1=CC=CC=C1)O	floral hyacinth gardenia strawberry	TGSC
1059	1-Phenylethanol	1-phenylethanol	CC(C1=CC=CC=C1)O	hyacinth chemical fresh sweet almond gardenia naphthyl medicinal camphoraceous mild floral weak bitter	Sigma Aldrich, TGSC, Pubchem
1060	1-Phenylethyl acetate	0	CC(C1=CC=CC=C1)OC(=O)C	apple apricot gardenia green pineapple plum musty leafy rhubarb seedy berry sweet floral fruity herbaceous	Sigma Aldrich, TGSC, OdoRactor
1061	(R)-1-Phenylethyl acetate	[(1R)-1-phenylethyl] acetate	CC(C1=CC=CC=C1)OC(=O)C	fruity floral jasmine mimosa gardenia apricot apple	TGSC
1062	1-Phenylethyl formate	1-phenylethyl formate	CC(C1=CC=CC=C1)OC=O	green floral woody mimosa gardenia	OdorRactor ,TGSC
1063	1-Phenylethanethiol	1-phenylethanethiol	CC(C1=CC=CC=C1)S	sulfurous floral tropical meaty	OdorRactor ,TGSC
1064	1-(2-Thienyl)ethanethiol	1-thiophen-2-ylethanethiol	CC(C1=CC=CS1)S	strong mercaptan	OdorRactor,
1065	2-Norbornanemethanol, alpha,3,3-trimethyl-	1-(3,3-dimethyl-2-bicyclo[2.2.1]heptanyl)ethanol	CC(C1C2CCC(C2)C1(C)C)O	sweet fresh patchouli woody earthy vetiver herbaceous	OdorRactor ,TGSC
1066	alpha,3,3- Trimethylcyclohexanemethan ol		CC(C1CCCC(C1)(C)C)O	camphoraceous minty	OdorRactor ,TGSC

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1067	1-(3,3- Dimethylcyclohexyl)ethyl acetate	1-(3,3-dimethylcyclohexyl)ethyl acetate	CC(C1CCCC(C1)(C)C)OC(=O)C	floral rose musk fruity geranium	OdorRactor ,TGSC
1068	Cyclopropanecarboxylic acid, 2-[1-(3,3- dimethylcyclohexyl)ethoxy]-2- methylpropyl	[2-[1-(3,3- dimethylcyclohexyl)ethoxy]-2- methylpropyl] cyclopropanecarboxylate	CC(C1CCCC(C1)(C)C)OC(C)(C) COC(=0)C2CC2	musk	TGSC
1069	ester Cyclohexanemethanol, alpha,3,3-trimethyl-, formate	1-(3,3-dimethylcyclohexyl)ethyl formate	CC(C1CCCC(C1)(C)C)OC=O	woody herbaceous fruity apple fresh seashore	OdorRactor ,TGSC, Pubchem
1070	2-(1-Phenylethyl)-1,3- dioxolane	2-(1-phenylethyl)-1,3-dioxolane	CC(C1OCCO1)C2=CC=CC=C2	floral green mushroom earthy gardenia reseda rhubarb fungal	OdorRactor ,TGSC, Flavorbase
1071	4-Mercapto-2-pentanone	4-sulfanylpentan-2-one	CC(CC(=O)C)S	meaty pungent	TGSC
1072	4-Furfurylthio-2-pentanone	4-(furan-2- ylmethylsulfanyl)pentan-2-one	CC(CC(=0)C)SCC1=CC=CO1	meaty	OdorRactor ,Pubchem
1073	Methyl 3-hydroxybutyrate	methyl 3-hydroxybutanoate	CC(CC(=0)OC)O	apple fruity green winey	SuperScent, TGSC
1074	Methyl 3- (methylthio)butanoate	methyl 3-methylsulfanylbutanoate	CC(CC(=O)OC)SC	sweet cooked	OdorRactor ,TGSC
1075	Allyl 3,5,5- trimethylhexanoate	prop-2-enyl 3,5,5- trimethylhexanoate	CC(CC(=0)OCC=C)CC(C)(C)C	fruity pineapple spicy	OdorRactor ,TGSC
1076	2,2-Dimethyl-4- phenylpentanenitrile	2,2-dimethyl-4- phenylpentanenitrile	CC(CC(C)(C)C#N)C1=CC=CC=C	citrus gardenia grapefruit burnt leafy vetiver autumn	OdorRactor ,TGSC
1077	2-Methylene-3,5,5- trimethylhexanal	3,5,5-trimethyl-2- methylidenehexanal	CC(CC(C)(C)C)C(=C)C=O	minty camphoraceous	TGSC
1078	2,3,5,5-Tetramethylhexanal	2,3,5,5-tetramethylhexanal	CC(CC(C)(C)C)C(C)C=O	aldehydic floral citrus	OdorRactor ,TGSC
1079		4-methyl-4-phenylpentan-2-ol	CC(CC(C)(C)C1=CC=CC=C1)O	floral green hyacinth lilac muguet	TGSC
1080	1,3-Dimethyl-3-phenylbutyl acetate	(4-methyl-4-phenylpentan-2-yl) acetate	CC(CC(C)(C)C1=CC=CC=C1)OC (=0)C	green oily gardenia grapefruit woody balsamic fresh	OdorRactor ,TGSC
1081	4-Mercapto-4-methyl-2- pentanol	4-methyl-4-sulfanylpentan-2-ol	CC(CC(C)(C)S)O	floral grapefruit lemon	Flavornet, TGSC, Odorc
1082	2-Methyl-4-phenylpentanol	2-methyl-4-phenylpentan-1-ol	CC(CC(C)C1=CC=CC=C1)CO	citrus vetiver green grapefruit rhubarb floral	OdorRactor ,TGSC
1083	4,9-Decadienal, 2,5,9- trimethyl-	(4E)-2,5,9-trimethyldeca-4,9-dienal	CC(CC=C(C)CCCC(=C)C)C=O	floral aldehydic powdery citrus fruity animal wax sweet	OdorRactor ,TGSC
1084	2-Methyl-4-pentenoic acid	2-methylpent-4-enoic acid	CC(CC=C)C(=0)O	cheese fruity	Sigma Aldrich, TGSC
1085	4-Penten-2-OL	pent-4-en-2-ol	CC(CC=C)O	fruity	SuperScent, TGSC
1086		1	CC(CC=0)C1=CC(=CC=C1)C(= C)C	fresh ozone cortex green floral melon	TGSC
1087	3-Phenylbutanal	3-phenylbutanal	CC(CC=O)C1=CC=CC=C1	green herbaceous hyacinth foliage	OdorRactor ,TGSC
1088	3,5,5-Trimethylhexanal	3,5,5-trimethylhexanal	CC(CC=0)CC(C)(C)C	grassy weedy green citrus fatty natural earthy aldehydic dry powerful pungent fresh clean	Sigma Aldrich, Flavorbase, TGSC, OdoRactor
1089	3-(Methylthio)butanal	3-methylsulfanylbutanal	CC(CC=O)SC	green musk potato buchu potato chip sulfurous vegetable cabbage fishy potato chip	Sigma Aldrich, TGSC
1090	Benzoic acid, 2-((3-(4-(1,1-dimethylethyl)phenyl)-2-methylpropylidene)amino)-,	methyl 2-[[3-(4-tert -butylphenyl)-2- methylpropylidene]amino]benzoat	C=NC2	green orange flower lily floral citrus fresh muguet	OdorRactor ,TGSC
1091	methyl ester Butylphenyl methylpropional,	(2S)-3-(4-tert -butylphenyl)-2-	CC(CC1=CC=C(C=C1)C(C)(C)C)	floral lily	TGSC
1092	(+)- Butylphenyl methylpropional,	methylpropanal (2R)-3-(4-tert -butylphenyl)-2-	C=0 CC(CC1=CC=C(C=C1)C(C)(C)C)	floral lily of the valley	TGSC
1093	(-)- Lilial	methylpropanal 3-(4-tert -butylphenyl)-2- methylpropanal	C=O CC(CC1=CC=C(C=C1)C(C)(C)C) C=O	floral muguet watery green powdery cumin fresh light lily of the valley	AOD, TGSC, Flavorbase, Pubchem, OdoRactor
1094	Benzoic acid, 2-[[3-(4-methoxyphenyl)-2-methylpropylidene]amino]-, methyl ester	methyl 2-[[3-(4-methoxyphenyl)-2-methylpropylidene]amino]benzoat e		floral sweet anisic hawthorn green cortex mimosa spicy powdery	OdorRactor ,TGSC
1095	3-(4-Methoxyphenyl)-2- methylpropanal	3-(4-methoxyphenyl)-2- methylpropanal	CC(CC1=CC=C(C=C1)OC)C=O	sweet anisic basil fennel raspberry green	OdorRactor,
1096	2-Benzyl-2-methyl-3- butenitrile	2-benzyl-2-methylbut-3-enenitrile	CC(CC1=CC=CC=C1)(C=C)C#N	aldehydic spicy herbaceous green pepper sweet	OdorRactor ,TGSC
1097		3-methyl-4-phenylbutan-2-ol	CC(CC1=CC=CC=C1)C(C)O	floral muguet green rose mentholic	OdorRactor ,TGSC, Pubchem
1098	(3-Methoxy-2- methylpropyl)benzene	(3-methoxy-2- methylpropyl)benzene	CC(CC1=CC=CC=C1)COC	floral green rose petal fruity	TGSC
1099	1-Phenyl-2-propanol	1-phenylpropan-2-ol	CC(CC1=CC=CC=C1)O	floral rose	TGSC
1100	2-((3-(1,3-Benzodioxol-5-yl)- 2- methylpropylidene)amino)ben zoic acid	methyl 2-[[3-(1,3-benzodioxol-5-yl)-2-methylpropylidene]amino]benzoat e	CC(CC1=CC2=C(C=C1)OCO2)C =NC3=C C=CC=C3C(=O)OC	fresh green floral orange flower ozone leafy cortex	TGSC
	methyl ester		<u> </u>	<u> </u>	1

1101	Helional	3-(1,3-benzodioxol-5-yl)-2- methylpropanal	CC(CC1=CC2=C(C=C1)OCO2)C =O	herbaceous floral green watery fresh ozone cyclamen hay marine fruity cumin	Sigma Aldrich, TGSC, Pubchem
1102	3,7-Dimethyloct-7-ene-1,6-diol	3,7-dimethyloct-7-ene-1,6-diol	CC(CCC(C(=C)C)O)CCO	floral rose	TGSC
1103	3,7-Dimethyl-2- methyleneocta-6-enal	3,7-dimethyl-2-methylideneoct-6-enal	CC(CCC=C(C)C)C(=C)C=O	bergamot citrus fresh green woody petitgrain	OdorRactor ,TGSC, Pubchem
1104	Dihydromyrcene	3,7-dimethylocta-1,6-diene	CC(CCC=C(C)C)C=C	floral rose herbaceous citrus terpenic	TGSC
1105	Lemongrass oil	1,2-dimethoxy-4-prop-2- enylbenzene;(2Z)-3,7- dimethylocta-2,6-dienal;3,7- dimethylocta-1,6- diene;(2Z)-3,7- dimethylocta-2,6-dien-1- ol;(1S,4S)-1,7,7- trimethylbicyclo[2.2.1]heptan-2- ol	CC(CCC=C(C)C)C=C.CC(=CCC C(=CCO) C)C.CC(=CCCC(=CCC=O)C)C.CC I(C2CC C1(C(C2)O)C)C.COC1=C(C=C(C =C1)CC =C)OC	lemon	Sigma Aldrich
1106	2,6-Dimethyl-5-heptenal	2,6-dimethylhept-5-enal	CC(CCC=C(C)C)C=O	cantaloupe fruit green melon fresh ozone watermelon sweet clean oily floral strong watery characteristic	Sigma Aldrich, Flavorbase, TGSC
1107	3-(1,5-Dimethyl-4-hexenyl)-6- methylene-1- cyclohexene	3-(6-methylhept-5-en-2-yl)-6- methylidenecyclohexene	CC(CCC=C(C)C)C1CCC(=C)C= C1	sweet fruit herbaceous woody	Flavornet
1108	beta-Sesquiphellandrene	(3R)-3-[(2S)-6-methylhept-5-en-2-yl]-6- methylidenecyclohexene	CC(CCC=C(C)C)C1CCC(=C)C= C1	woody herbaceous fruity	Flavornet
1109	Zingiberenol	1-methyl-4-(6-methylhept-5-en-2-yl)cyclohex-2-en- 1-ol	CC(CCC=C(C)C)C1CCC(C=C1)(C)O	ginger metallic	Flavornet
1110	Citronellyl nitrile	3,7-dimethyloct-6-enenitrile	CC(CCC=C(C)C)CC#N	citrus fresh lemon metallic wax floral	OdorRactor ,TGSC
1111	(3R)-3,7-Dimethyloct-6- enenitrile	(3R)-3,7-dimethyloct-6-enenitrile	CC(CCC=C(C)C)CC#N	citrus green fruity floral	TGSC
1112	Citronellic acid	3,7-dimethyloct-6-enoic acid	CC(CCC=C(C)C)CC(=0)O	fatty cheese smoky grassy floral green citronella vegetable tobacco wax	Flavornet, TGSC,OdoRactor
1113	Methyl citronellate	methyl 3,7-dimethyloct-6-enoate	CC(CCC=C(C)C)CC(=O)OC	floral dry sweet weedy dusty wax geranium fatty fruity winey	OdorRactor ,TGSC
1114	2,4,8-Trimethyl-7-nonen-2- OL	2,4,8-trimethylnon-7-en-2-ol	CC(CCC=C(C)C)CC(C)(C)O	grapefruit citrus floral citronella	OdorRactor ,TGSC
1115	4,8-Dimethylnon-7-en-2-ol	4,8-dimethylnon-7-en-2-ol	CC(CCC=C(C)C)CC(C)O	citronella lemon grapefruit floral citrus	TGSC
1116	Citronellal methylanthranilate	methyl 2-(3,7-dimethyloct-6- enylideneamino)benzoate	CC(CCC=C(C)C)CC=NC1=CC=C C=C1C(=0)OC	fresh sharp citrus weedy grassy woody	OdorRactor ,TGSC
1117	3,7-Dimethyloct-6-enal oxime	N -(3,7-dimethyloct-6- enylidene)hydroxylamine	CC(CCC=C(C)C)CC=NO	citrus bergamot lime	TGSC
1118	Citronellal	3,7-dimethyloct-6-enal	CC(CCC=C(C)C)CC=O	cherry green lemon rose sweet fatty dry floral herbaceous wax aldehydic citrus	Sigma Aldrich, TGSC, Pubchem, OdoRactor
1119 1120	(S)-(-)-Citronellal (R)-(+)-Citronellal	(3S)-3,7-dimethyloct-6-enal (3R)-3,7-dimethyloct-6-enal	CC(CCC=C(C)C)CC=O CC(CCC=C(C)C)CC=O	herbaceous citrus citrus herbaceous fresh citrus	AOD, OdoRactor TGSC
1120	(3R)-3,7-Dimethyloct-6-en-1-	(3R)-3,7-dimethyloct-6-en-1-ol	CC(CCC=C(C)C)CCO	citronella petal rose leafy oily	AOD, TGSC, OdoRactor
1122	ol (-)-Citronellol	(3S)-3,7-dimethyloct-6-en-1-ol	CC(CCC=C(C)C)CCO	floral rose wax geranium oily	AOD, Sigma Aldrich, TGSC,
1123	Citronellol	3,7-dimethyloct-6-en-1-ol	CC(CCC=C(C)C)CCO	powdery geranium rose citrus floral wax leathery sweet green fatty terpenic	OdoRactor Sigma Aldrich, AOD, TGSC,OdoRactor
1124	(R)-3,7-Dimethyloct-6-enyl acetate	[(3R)-3,7-dimethyloct-6-enyl] acetate	CC(CCC=C(C)C)CCOC(=O)C	citrus lime dirty aldehydic	TGSC
1125	6-Octen-1-ol, 3,7-dimethyl-, acetate, (3S)-	[(3S)-3,7-dimethyloct-6-enyl] acetate	CC(CCC=C(C)C)CCOC(=0)C	floral fresh fruity bergamot rose sweet	OdorRactor ,TGSC
1126	Citronellyl acetate	3,7-dimethyloct-6-enyl acetate	CC(CCC=C(C)C)CCOC(=0)C	lemon rose dusty floral green fruity citrus woody tropical fruit fatty bois de rose wax pear apple	Sigma Aldrich, TGSC,OdoRactor
1127	3,7-Dimethyloct-6-en-1-yl (2R)-2- hydroxypropanoate	3,7-dimethyloct-6-enyl (2 <i>R</i>)-2- hydroxypropanoate	CC(CCC=C(C)C)CCOC(=0)C(C) O	floral lily of the valley warm natural	TGSC
1128	2-Butenoic acid, 3-methyl-, 3,7-dimethyl-6- octenyl ester	3,7-dimethyloct-6-enyl 3- methylbut-2-enoate	CC(CCC=C(C)C)CCOC(=0)C=C(C)C	floral rose geranium	TGSC
1129	Citronellyl cinnamate	3,7-dimethyloct-6-enyl (E)-3-phenylprop-2-enoate	CC(CCC=C(C)C)CCOC(=O)C=C C1=CC= CC=C1	palmarosa sweet cinnamyl rose floral	OdorRactor ,TGSC
1130	Citronellyl benzoate	3,7-dimethyloct-6-enyl benzoate	CC(CCC=C(C)C)CCOC(=0)C1= CC=CC= C1	verbena dried rose floral rose	OdorRactor ,TGSC
1131	Citronellyl anthranilate	3,7-dimethyloct-6-enyl 2- aminobenzoate	CC(CCC=C(C)C)CCOC(=0)C1= CC=CC= C1N	sweet rose fruity neroli floral petitgrain	OdorRactor ,TGSC

1132	Citronellyl phenylacetate	3,7-dimethyloct-6-enyl 2- phenylacetate	CC(CCC=C(C)C)CCOC(=0)CC1 =CC=CC =C1	sweet honey rose wax floral fresh herbaceous	OdorRactor ,TGSC
1133	8-(1-Methoxyethoxy)-2,6- dimethyloct-2-ene	8-(1-methoxyethoxy)-2,6- dimethyloct-2-ene	CC(CCC=C(C)C)CCOC(C)OC	citrus natural lemon	OdorRactor ,TGSC
1134	Citronellyl formate	3,7-dimethyloct-6-enyl formate	CC(CCC=C(C)C)CCOC=O	apricot honey peach plum rose floral bergamot cucumber sweet green wax citrus fruity mandarin	Sigma Aldrich, TGSC, OdoRactor
1135	Citronelloxyacetaldehyde	2-(3,7-dimethyloct-6- enoxy)acetaldehyde	CC(CCC=C(C)C)CCOCC=O	sweet wax floral aldehydic muguet fresh honeysuckle citrus melon green	OdorRactor ,TGSC
1136	6-Methylhept-5-en-2-ol	6-methylhept-5-en-2-ol	CC(CCC=C(C)C)O	sweet oily green coriander	Sigma Aldrich, TGSC, OdoRactor
1137	2,6,10-Trimethylundeca-5,9-dienal	2,6,10-trimethylundeca-5,9-dienal	CC(CCC=C(C)CCC=C(C)C)C=O	muguet wax watery hyacinth floral green aldehydic	OdorRactor ,TGSC
1138	3S,7,11-Trimethyl-6E,10- dodecadienal	(3S, 6E)-3,7,11-trimethyldodeca-6,10-dienal	CC(CCC=C(C)CCC=C(C)C)CC= O	floral green muguet creamy	TGSC
1139	Dihydrofarnesol	(6E)-3,7,11-trimethyldodeca-6,10-dien-1-ol	CC(CCC=C(C)CCC=C(C)C)CCO	floral green fruity	SuperScent, TGSC,
1140	6,10-Dodecadien-1-ol, 3,7,11-trimethyl-	3,7,11-trimethyldodeca-6,10-dien- 1-ol	CC(CCC=C(C)CCC=C(C)C)CCO	floral metallic cyclamen	TGSC, OdoRactor
1141	5,9-Undecadien-1-ol, 2,6,10-trimethyl-	2,6,10-trimethylundeca-5,9-dien-1-ol	CC(CCC=C(C)CCC=C(C)C)CO	wax aldehydic	OdorRactor ,TGSC
1142	(E)-6,10-Dimethylundeca-5,9-dien-2-yl acetate	[(5E)-6,10-dimethylundeca-5,9-dien-2-yl] acetate	CC(CCC=C(C)CCC=C(C)C)OC(= O)C	seaweed wax fresh bitter	OdorRactor ,TGSC
1143	4,8-Dimethyl-4,9-decadienal	(4E)-4,8-dimethyldeca-4,9-dienal	CC(CCC=C(C)CCC=O)C=C	floral aldehydic magnolia lily muguet	OdorRactor ,TGSC
1144	2-Methyl-4- phenylbutyraldehyde	2-methyl-4-phenylbutanal	CC(CCC1=CC=CC=C1)C=O	sweet floral earthy musty	OdorRactor ,TGSC
1145	3-Methyl-5- phenylpentanenitrile	3-methyl-5-phenylpentanenitrile	CC(CCC1=CC=CC=C1)CC#N	citrus floral muguet lily sweet metallic	OdorRactor ,TGSC
1146	3-Methyl-5-phenylpentanal	3-methyl-5-phenylpentanal	CC(CCC1=CC=CC1)CC=O	lily green wax woody aldehydic fresh	OdorRactor ,TGSC
1147	3-Methyl-5-phenylpentan-1-ol	3-methyl-5-phenylpentan-1-ol	CC(CCC1=CC=CC=C1)CCO	fresh floral rose geranium green muguet lily honey tropical	OdorRactor ,TGSC
1148	(R)-4-Phenyl-2-butanol	(2R)-4-phenylbutan-2-ol	CC(CCC1=CC=CC=C1)O	floral peony foliage sweet mimosa heliotrope	OdorRactor ,TGSC
1149	4-Phenyl-2-butyl acetate	4-phenylbutan-2-yl acetate	CC(CCC1=CC=CC=C1)OC(=O)C	-	OdorRactor ,TGSC
1150	3,7-Dimethyloct-7-en-1-ol	3,7-dimethyloct-7-en-1-ol	CC(CCCC(=C)C)CCO	floral rose spicy wax powdery geranium	OdorRactor,
1151	Rhodinol	(3S)-3,7-dimethyloct-7-en-1-ol	CC(CCCC(=C)C)CCO	floral spicy geranium lemon musty oily wax fruity rose sweet winey powdery fatty citronella fresh citrus mandarin lime metallic	Sigma Aldrich, TGSC, Flavorbase
1152	Rhodinyl acetate	3,7-dimethyloct-7-enyl acetate	CC(CCCC(=C)C)CCOC(=0)C	rose spicy geranium citrus leafy powdery floral fresh fruity	SuperScent, TGSC, Flavorbase,OdoRactor
1153	(-)-3,7-Dimethyloct-7-enyl benzoate	3,7-dimethyloct-7-enyl benzoate	CC(CCCC(=C)C)CCOC(=O)C1= CC=CC= C1	sweet floral rose ylang	TGSC
1154	Rhodinyl formate	3,7-dimethyloct-7-enyl formate	CC(CCCC(=C)C)CCOC=O	rose leafy green floral geranium dry	OdorRactor ,TGSC
1155	2,6-Dimethyl-6-hepten-1-ol	2,6-dimethylhept-6-en-1-ol	CC(CCCC(=C)C)CO	melon	OdorRactor ,TGSC
1156	6,10-Dimethylundec-9-en-2- one	6,10-dimethylundec-9-en-2-one	CC(CCCC(=0)C)CCC=C(C)C	sweet dry floral balsamic rose woody	OdorRactor ,TGSC
1157	Methyl 5-acetoxyhexanoate	methyl 5-acetyloxyhexanoate	CC(CCCC(=O)OC)OC(=O)C	fruity	OdorRactor,
1158	Dihydromyrcenol	2,6-dimethyloct-7-en-2-ol	CC(CCCC(C)(C)O)C=C	lime citrus cologne floral weedy fresh clean herbaceous watery marine	Sigma Aldrich, Flavorbase, TGSC
1159	7-Hydroxy-3,7- dimethyloctanenitrile	7-hydroxy-3,7- dimethyloctanenitrile	CC(CCCC(C)(C)O)CC#N	lily muguet woody fresh floral	TGSC
1160	Hydroxycitronellal dimethyl acetal	8,8-dimethoxy-2,6-dimethyloctan- 2-ol	CC(CCCC(C)(C)O)CC(OC)OC	floral lily rose muguet wax green tropical soapy	SuperScent, TGSC,OdoRactor
1161	Aurantiol	methyl 2-[(7-hydroxy-3,7-dimethyloctylidene)amino]benzoat e	CC(CCCC(C)(C)O)CC=NC1=CC =CC=C1 C(=O)OC	floral lily orange flower blossom sweet	OdorRactor ,TGSC
1162	(3R)-7-Hydroxy-3,7- dimethyloctanal	(3R)-7-hydroxy-3,7- dimethyloctanal	CC(CCCC(C)(C)O)CC=O	floral	TGSC
1163	(3S)-7-Hydroxy-3,7- dimethyloctanal	(3S)-7-hydroxy-3,7- dimethyloctanal	CC(CCCC(C)(C)O)CC=O	floral	TGSC
1164	Hydroxycitronellal	7-hydroxy-3,7-dimethyloctanal	CC(CCCC(C)(C)O)CC=O	lily sweet floral green wax tropical melon citrus	Sigma Aldrich, Flavorbase, TGSC,OdoRactor
1165	Octanal, 7-hydroxy-3,7- dimethyl-, reaction products with 1H-indole	7-hydroxy-3,7- dimethyloctanal;1 <i>H</i> -indole	CC(CCCC(C)(C)O)CC=O.C1=CC =C2C(= C1)C=CN2	animal fecal jasmine	TGSC

1166	3,7-Dimethyloctane-1,7-diol	3,7-dimethyloctane-1,7-diol	CC(CCCC(C)(C)O)CCO	floral lily green peony clean rose	OdorRactor ,TGSC,
1167	2,6-Dimethyloct-7-en-2-yl	2,6-dimethyloct-7-en-2-yl acetate	CC(CCCC(C)(C)OC(=O)C)C=C	weak sweet citrus bergamot lime lavender	Flavorbase OdorRactor ,TGSC
1168	acetate 7-Methoxy-3,7-dimethyloctan-	7-methoxy-3,7-dimethyloctan-2-ol	CC(CCCC(C)(C)OC)C(C)O	sweet sandal wood soapy floral	OdorRactor ,TGSC
1169	2-ol 6-Methoxy-2,6-	6-methoxy-2,6-dimethylheptanal	CC(CCCC(C)(C)OC)C=O	woody floral fruity watery citrus melon	OdorRactor ,TGSC,
1170	dimethylheptan-1-al 7-Methoxy-3,7-	7-methoxy-3,7-dimethyloctanal	CC(CCCC(C)(C)OC)CC=O	green melon floral lily sweet fresh	Flavorbase OdorRactor ,TGSC
1170	dimethyloctanal	, ·		meion norai my sweet iresn	Odorkactor, rosc
1171	2,6,10-Trimethylundec-9-enal	2,6,10-trimethylundec-9-enal	CC(CCCC(C)C=0)CCC=C(C)C	fresh marine rose lily of the valley incense floral aldehydic wax watery	OdorRactor ,TGSC
1172	3,5,5-Trimethyl-1-hexanol	3,5,5-trimethylhexan-1-ol	CC(CCO)CC(C)(C)C	oily herbaceous grassy green weedy floral earthy aldehydic leafy hay herbaceous cooling camphoraceous melon woody berry	Sigma Aldrich, TGSC, OdoRactor
1173	3,5,5-Trimethylhexyl acetate	3,5,5-trimethylhexyl acetate	CC(CCOC(=O)C)CC(C)(C)C	sweet orris cumin woody fruity spicy	OdorRactor ,TGSC
1174	3-Sulfanylbutyl acetate	3-sulfanylbutyl acetate	CC(CCOC(=O)C)S	pungent alliaceous hazelnut fruity cheese	OdorRactor ,Flavorbase
1175	3,5,5-Trimethylhexyl formate	3,5,5-trimethylhexyl formate	CC(CCOC=O)CC(C)(C)C	woody green herbaceous	OdorRactor,
1176	1,3-Butanedithiol	butane-1,3-dithiol	CC(CCS)S	alliaceous garlic meaty sulfurous onion spicy roasted nutty	AOD, TGSC, Flavorbase, OdoRactor
1177	1-Aminopropan-2-ol	1-aminopropan-2-ol	CC(CN)O	fishy ammonical	Sigma Aldrich, TGSC, PDB, OdoRactor
1178	(S)-(-)-2-Phenyl-1-propanol	(2S)-2-phenylpropan-1-ol	CC(CO)C1=CC=CC=C1	floral	TGSC
1179	(R)-2-Phenyl-1-propanol	(2R)-2-phenylpropan-1-ol	CC(CO)C1=CC=CC=C1	floral hyacinth hawthorn foliage fruity peony	SuperScent, TGSC, OdoRactor
1180	2-Phenylpropan-1-ol	2-phenylpropan-1-ol	CC(CO)C1=CC=CC=C1	hyacinth green spicy balsamic lilac honeysuckle sweet floral	Sigma Aldrich, Flavorbase, TGSC, OdoRactor
1181	2-Cyclohexylpropan-1-ol	2-cyclohexylpropan-1-ol	CC(CO)C1CCCCC1	floral minty green geranium balsamic muguet	OdorRactor ,TGSC
1182	2-Cyclododecylpropan-1-ol	2-cyclododecylpropan-1-ol	CC(CO)C1CCCCCCCCCC1	woody amber musk	OdorRactor ,TGSC
1183	1-Propanol, 2-methyl-3- [(1,7,7- trimethylbicyclo[2.2.1]hept-2- yl)oxy]-	2-methyl-3-[(1,7,7-trimethyl-2-bicyclo[2.2.1]heptanyl)oxy]propa n-1-ol	CC(CO)COC1CC2CCC1(C2(C)C) C	woody amber powdery warm dry	OdorRactor ,TGSC
	Propylene glycol	propane-1,2-diol	CC(CO)O	alcoholic	OdorRactor,
1185	2-Phenylpropyl acetate	2-phenylpropyl acetate	CC(COC(=0)C)C1=CC=CC=C1	sweet hyacinth lilac green earthy floral	OdorRactor ,TGSC
1186 1187	Propylene glycol diacetate Propylene glycol dibenzoate	2-acetyloxypropyl acetate 2-benzoyloxypropyl benzoate	CC(COC(=0)C)OC(=0)C CC(COC(=0)C1=CC=CC=C1)OC (=0)C2 =CC=CC=C2	fruity acetic salmon algae metallic shellfish ethereal	OdorRactor ,TGSC
1188	1,1'-Oxydi-2-propanol	1-(2-hydroxypropoxy)propan-2-ol	CC(COCC(C)O)O	alcoholic	OdorRactor ,TGSC
1189	4-Mercapto-3-methyl-2- butanol	3-methyl-4-sulfanylbutan-2-ol	CC(CS)C(C)O	sulfurous onion savory meaty fruity	TGSC, Flavorbase
1190	1,1-Dimethoxyethane	1,1-dimethoxyethane	CC(OC)OC	ethereal sharp sweet green new mown hay alcoholic aromatic strong vegetable	Sigma Aldrich, Flavorbase, TGSC,OdoRactor
1191	1-Benzyloxy-1-(2- methoxyethoxy)ethane	1-(2- methoxyethoxy)ethoxymethylbenz ene	CC(OCCOC)OCC1=CC=CC=C1	sweet green fruity bitter almond bitter	OdorRactor ,TGSC
1192	Ethanedithiol	ethane-1,1-dithiol	CC(S)S	sulfurous cheese onion savory meaty roasted	OdorRactor ,TGSC, Flavorbase
1193	1-(Methylthio)ethanethiol	1-methylsulfanylethanethiol	CC(S)SC	thiamine	Flavornet
1194	(Z)-3-Hexenyl cinnamate	[(E)-hex-3-enyl] (E)-3- phenylprop-2-enoate	=CC=C1	fresh balsamic green	OdorRactor ,TGSC
1195	(E)-3-Hydroxypent-3-en-2- one	(E)-3-hydroxypent-3-en-2-one	CC=C(C(=0)C)O	buttery caramel	TGSC
1196	3-Penten-2-one, 3-methyl-	(E)-3-methylpent-3-en-2-one	CC=C(C)C(=O)C	melon wax fresh green tropical mushroom	Sigma Aldrich, TGSC, OdoRactor
1197	3-Penten-2-one, 3-methyl-	(E)-3-methylpent-3-en-2-one	CC=C(C)C(=O)C	sweaty	TGSC
1198	Tiglic acid	(E)-2-methylbut-2-enoic acid	CC=C(C)C(=O)O	balsamic spicy sweet woody caramel dry pungent acidic brown ripe fruity	Sigma Aldrich, TGSC, Pubchem, OdoRactor
1199	Angelic acid	(Z)-2-methylbut-2-enoic acid	CC=C(C)C(=0)0	spicy sour	TGSC, Pubchem
1200	Methyl tiglate	methyl (E)-2-methylbut-2-enoate	CC=C(C)C(=O)OC	ethereal rummy	SuperScent, TGSC, OdoRactor
1201	Isopropyl tiglate	propan-2-yl (E)-2-methylbut-2-enoate	CC=C(C)C(=O)OC(C)C	sweet minty green vegetable spice cooling	SuperScent, TGSC, OdoRactor
1202	Isobutyl angelate	2-methylpropyl (Z)-2-methylbut-2-enoate	CC=C(C)C(=O)OCC(C)C	herbaceous green spicy woody caraway celery sweet cooling weedy	SuperScent, TGSC, OdoRactor

1203	Isobutyl tiglate	2-methylpropyl (E)-2-methylbut-2-enoate	CC=C(C)C(=O)OCC(C)C	herbaceous pungent chamomile	OdorRactor ,Sigma Aldrich, TGSC, Flavorbase
1204	Allyl tiglate	prop-2-enyl (E)-2-methylbut-2-enoate	CC=C(C)C(=O)OCC=C	green fruity berry	SuperScent, TGSC, OdoRactor
1205	3-Methyl-2-butenyl 2- methylcrotonate	3-methylbut-2-enyl (E)-2-methylbut-2-enoate	CC=C(C)C(=O)OCC=C(C)C	fruity jasmine ylang	TGSC
1206	Geranyl tiglate	[(2E)-3,7-dimethylocta-2,6-dienyl] (E)-2- methylbut-2-enoate	CC=C(C)C(=O)OCC=C(C)CCC= C(C)C	floral geranium fruity sweet herbaceous	Sigma Aldrich
1207	[(E)-3-Phenylprop-2-enyl] (Z)- 2-methylbut- 2-enoate	[(E)-3-phenylprop-2-enyl] (Z)-2-methylbut-2- enoate	CC=C(C)C(=0)OCC=CC1=CC=C C=C1	woody cinnamyl green herbaceous	OdorRactor ,TGSC
1208	Benzyl tiglate	benzyl (E)-2-methylbut-2-enoate	CC=C(C)C(=O)OCC1=CC=CC=C	balsamic earthy mushroom rose sweet cherry almond	SuperScent, TGSC
1209	Benzyl 2-methylbut-2-enoate	benzyl 2-methylbut-2-enoate	CC=C(C)C(=O)OCC1=CC=CC=C	earthy mushroom green	TGSC, OdoRactor
1210	Isoamyl angelate	3-methylbutyl (Z)-2-methylbut-2-enoate	CC=C(C)C(=O)OCCC(C)C	floral fruity chamomile	SuperScent, TGSC, OdoRactor
1211	Isoamyl tiglate	3-methylbutyl (E)-2-methylbut-2-enoate	CC=C(C)C(=O)OCCC(C)C	fruity winey herbaceous fresh angelica	Sigma Aldrich, TGSC
1212	3-Methyl-4-pentenyl 2- methylisocrotonate	3-methylpent-4-enyl (Z)-2- methylbut-2-enoate	CC=C(C)C(=O)OCCC(C)C=C	fruity green anisic	TGSC
1213	2-Butenoic acid, 2-methyl-, 3,7-dimethyl-6- octenyl ester, (2E)-	3,7-dimethyloct-6-enyl 2- methylbut-2-enoate	CC=C(C)C(=O)OCCC(C)CCC=C(C)C	fruity rose	Sigma Aldrich
1214	Citronellyl tiglate	3,7-dimethyloct-6-enyl (E)-2- methylbut-2-enoate	CC=C(C)C(=O)OCCC(C)CCC=C(C)C	rose fruity floral geranium leafy tea	SuperScent, TGSC, OdorRactor
1215	Phenethyl 2- methylisocrotonate		CC=C(C)C(=O)OCCC1=CC=CC=	floral rose woody orris	TGSC
1216	Phenethyl tiglate	2-phenylethyl (E)-2-methylbut-2-enoate	CC=C(C)C(=O)OCCC1=CC=CC= C1	green raspberry rose strawberry sweet natural oily leafy herbaceous dry	Sigma Aldrich, TGSC, Flavorbase, OdoRactor
1217	2,6-Dimethyl-2,4,6-octatriene	(4 <i>E</i> ,6 <i>E</i>)-2,6-dimethylocta-2,4,6-triene	CC=C(C)C=CC=C(C)C	terpenic sweet fresh floral grassy nutty pepper herbaceous tropical	ADB, TGSC, OdoRactor
	2-Methyl-2-butenal	2-methylbut-2-enal	CC=C(C)C=O	green fruity	Sigma Aldrich,OdoRactor
1219	Tiglic aldehyde	(E)-2-methylbut-2-enal	CC=C(C)C=O	pungent ethereal nutty anisic fruity green fruit	Flavornet, TGSC, OdoRactor
1220	(E)-Tetrahydro-2,2-dimethyl-5-(1-methyl-1- propenyl)furan	5-[(E)-but-2-en-2-yl]-2,2- dimethyloxolane	CC=C(C)C1CCC(O1)(C)C	citrus sweet herbaceous green celery spicy minty woody cooling camphoraceous fresh	Sigma Aldrich, TGSC, OdoRactor
1221	2-Buten-1-ol, 2-methyl-	2-methylbut-2-en-1-ol	CC=C(C)CO	green oily	TGSC
1222	Tiglyl tiglate	methylbut-2- enoate	CC=C(C)COC(=0)C(=CC)C	green forest humus fungal mushroom anisic floral leafy	TGSC
1223	2-ene	2-methyl-1-methylsulfanylbut-2- ene	CC=C(C)CSC	cooked roasted meaty	TGSC
1224	2-Phenyl-2-butenal	(E)-2-phenylbut-2-enal	CC=C(C=0)C1=CC=CC=C1	chocolate earthy floral musty sweet narcissus cortex beany honey cocoa nutty radish powdery	Sigma Aldrich, TGSC, Flavorbase, Odoractor
1225	2-((Methylthio)methyl)-2- butenal	(Z)-2-(methylsulfanylmethyl)but- 2-enal	CC=C(CSC)C=O	sulfurous burnt cooked cooked onion cabbage	OdorRactor ,TGSC
1226	9-Ethylidene-3- oxatricyclo(6.2.1.02,7)undeca ne-4-one	(9E)-9-ethylidene-3- oxatricyclo[6.2.1.02,7]undecan- 4-one	CC=C1CC2CC1C3C2OC(=0)CC 3	tonka sweet spicy balsamic woody tobacco green	OdorRactor ,TGSC
1227	Einecs 300-376-9	(9Z)-9-ethylidene-3- oxatricyclo[6.2.1.02,7]undecane	CC=C1CC2CC1C3C2OCCC3	fruity floral rhubarb costus woody rooty herbaceous berry	OdorRactor ,TGSC
1228	3-Penten-2-one	(E)-pent-3-en-2-one	CC=CC(=0)C	fruity phenolic fishy acetone chemical	Sigma Aldrich, TGSC, OdoRactor
1229	Pomarose	(2 <i>E</i> ,5 <i>Z</i>)-5,6,7-trimethylocta-2,5-dien-4-one	CC=CC(=O)C(=C(C)C(C)C)C	floral fruity rose apple plum raisin dried fruit	TGSC
1230	beta-Damascenone		CC=CC(=0)C1=C(C=CCC1(C)C) C	apple smoky nutty citrus woody herbaceous rose winey honey natural sweet fruity plum grape raspberry sugar earthy green floral tobacco tea	Sigma Aldrich, Flavornet, TGSC, Flavorbase
1231	beta-Damascone	(E)-1-(2,6,6-trimethylcyclohexen-1-yl)but-2-en-1- one	CC=CC(=0)C1=C(CCCC1(C)C)C	apple tea fruity floral berry plum black currant honey rose tobacco	Flavornet, ADB, TGSC
1232	(Z)-1-(2,6,6-Trimethyl-1-cyclohexen-1-yl)-2 buten-1-one	(Z)-1-(2,6,6-trimethylcyclohexen-1-yl)but-2-en-1- one	CC=CC(=0)C1=C(CCCC1(C)C)C	fruity floral black currant tobacco plum rose honey	TGSC, Flavorbase
1233	2-Buten-1-one, 1-(2,6,6-	1-(2,6,6-trimethylcyclohexen-1-yl)but-2-en-1-one	CC=CC(=O)C1=C(CCCC1(C)C)C	fruity floral plum rose honey tobacco black currant	OdorRactor ,TGSC
	, (2L)-				

1235	(Z)-1-(2,6,6-Trimethyl-2-cyclohexen-1-yl)-2 buten-1-	(Z)-1-(2,6,6-trimethylcyclohex-2-en-1-yl)but-2-en-	CC=CC(=O)C1C(=CCCC1(C)C)C	floral rose apple fruity	OdorRactor ,TGSC
	one	1-one			
1236	alpha-Damascone	(E)-1-(2,6,6-trimethylcyclohex-2-en-1-yl)but-2-en-1-one	CC=CC(=0)C1C(=CCCC1(C)C)C	fruity floral rose apple black currant	OdorRactor ,TGSC
1237	2-Buten-1-one, 1-(2,6,6- trimethyl-2- cyclohexen-1-yl)- , (2E)-		CC=CC(=0)C1C(=CCCC1(C)C)C	sweet floral metallic fruity apple spicy plum minty woody green berry rose black currant	OdorRactor ,TGSC, Flavorbase
1238	delta-Damascone	(E)-1-(2,6,6-trimethylcyclohex-3- en-1-yl)but-2-en- 1-one	CC=CC(=0)C1C(C=CCC1(C)C)C	floral sweet rose natural petal black currant tobacco woody minty fruity brown herbaceous	OdorRactor ,TGSC
1239	(2E)-1-[(1R,2S)-2,6,6- Trimethylcyclohex-3- en-1- yl]but-2-en-1-one	(E)-1-[(1R, 2S)-2,6,6- trimethylcyclohex-3-en-1-yl]but-2- en-1-one	CC=CC(=0)C1C(C=CCC1(C)C)C	fruity sweet rose natural petal black currant floral	TGSC
1240	2-Buten-1-one, 1-(2,2,6- trimethylcyclohexyl)-	1-(2,2,6-trimethylcyclohexyl)but-2-en-1-one	CC=CC(=0)C1C(CCCC1(C)C)C	fruity floral	TGSC
1241	2-Buten-1-one, 1-(2,4,4- trimethyl-2- cyclohexen-1-yl)-	1-(2,4,4-trimethylcyclohex-2-en-1-yl)but-2-en-1- one	CC=CC(=0)C1CCC(C=C1C)(C)C	floral plum rose	TGSC, OdoRactor
1242	(E)-1-(2,4,4-Trimethyl-2-cyclohexen-1-yl)-2-buten-1-one	(E)-1-(2,4,4-trimethylcyclohex-2-en-1-yl)but-2-en-1-one	CC=CC(=0)C1CCC(C=C1C)(C)C	fruity floral plum rose tobacco	OdorRactor ,TGSC
	Crotonic acid	(E)-but-2-enoic acid	CC=CC(=0)0	roasted milky burnt	OdorRactor ,TGSC
1244	Dimethylbenzyl carbinyl crotonate	(2-methyl-1-phenylpropan-2-yl) (E)-but-2-enoate	CC=CC(=O)OC(C)(C)CC1=CC= CC=C1	herbaceous fruity spicy warm	TGSC, Flavorbase
1245	1-Cyclohexylethyl 2-	1-cyclohexylethyl (E)-but-2-enoate	CC=CC(=0)OC(C)C1CCCCC1	fruity wax green date fig prune	OdorRactor ,TGSC
1246	butenoate 1,3-Dimethylbutyl 2-	4-methylpentan-2-yl (E)-but-2-	CC=CC(=O)OC(C)CC(C)C	grape brandy fruity juicy apple pear plum grape	OdorRactor ,TGSC
1247	butenoate 2-Cyclopentylcyclopentyl	enoate (2-cyclopentylcyclopentyl) (E)-	CC=CC(=0)OC1CCCC1C2CCC	fresh fruity plum peach tropical	OdorRactor ,TGSC
1240	crotonate	but-2-enoate	2	floral rose violet	Oder Design TCCC
1248 1249	Cyclohexyl crotonate Isobutyl crotonate	cyclohexyl (E)-but-2-enoate 2-methylpropyl (Z)-but-2-enoate	CC=CC(=0)OC1CCCCC1 CC=CC(=0)OCC(C)C	fruity sweet floral green woody fruity dry tropical rummy ripe	OdorRactor ,TGSC OdorRactor ,TGSC
1249	1sobuty1 crotonate	2-memypropyr (2)-out-2-enoate	cc=cc(=0)0cc(c)c	green pear caramel	Odorkacioi ,105C
1250	Isobutyl 2-butenoate	2-methylpropyl (E)-but-2-enoate	CC=CC(=O)OCC(C)C	fruity sweet pineapple apple banana	Sigma Aldrich, TGSC
1251	Geranyl crotonate	[(2E)-3,7-dimethylocta-2,6-dienyl] (E)-but-2-enoate)C	caramel sweet maple fruity almond acorn nutty	OdorRactor ,TGSC
1252	Benzyl crotonate	benzyl (E)-but-2-enoate	CC=CC(=O)OCC1=CC=CC=C1	warm herbaceous spicy balsamic	SuperScent, TGSC
1253	2-Methyl-3-pentenoic acid	(E)-2-methylpent-3-enoic acid	CC=CC(C)C(=O)O	nutty cranberry hazelnut	OdorRactor ,TGSC
1254	3-Penten-2-OL	(E)-pent-3-en-2-ol	CC=CC(C)O	green vinyl	Flavornet
	3-[(Hexa-1,4-dien-3- yl)disulfanyl]hexa-1,4- diene	3-(hexa-1,4-dien-3- yldisulfanyl)hexa-1,4-diene	CC=CC(C=C)SSC(C=C)C=CC	sulfurous alliaceous	TGSC
	1,3-Pentadiene Megastigmatrienone A	(3E)-penta-1,3-diene (4Z)-4-[(E)-but-2-enylidene]- 3,5,5- trimethylcyclohex-2-en-1- one	CC=CC=C CC=CC=C1C(=CC(=O)CC1(C)C) C	acrid petroleum tobacco sweet acorn nutty spicy fruity hay woody	Pubchem OdorRactor ,TGSC, Flavorbase
1258	Methyl sorbate	methyl (2E,4E)-hexa-2,4-dienoate	CC=CC=CC(=O)OC	fruity pungent licorice sweet brown spicy green anisic	OdorRactor ,TGSC
1259	Allyl sorbate	prop-2-enyl (2E,4E)-hexa-2,4-	CC=CC=CC(=O)OCC=C	fruity pineapple	OdorRactor ,TGSC
1260		dienoate			
	2,4-Hexadienal	(2E ,4E)-hexa-2,4-dienal	CC=CC=CC=O	green citrus floral sweet spicy aldehydic fruity wax fatty	Sigma Aldrich, Flavornet, TGSC, Pubchem, OdoRactor
1261	2,4-Hexadienal Sorbic alcohol	(2E ,4E)-hexa-2,4-dienal (2E ,4E)-hexa-2,4-dien-1-ol	CC=CC=CCO		
1261		(2E ,4E)-hexa-2,4-dien-1-ol [(2E ,4E)-hexa-2,4-dienyl]		aldehydic fruity wax fatty fresh almond apple green herbaceous winey musty sweet herbaceous nutty marzipan raw vegetable whiskey fresh green oily herbaceous	TGSC, Pubchem, OdoRactor Sigma Aldrich, TGSC, OdoRactor SuperScent, TGSC,
1262	Sorbic alcohol	(2E ,4E)-hexa-2,4-dien-1-ol	CC=CC=CCO	aldehydic fruity wax fatty fresh almond apple green herbaceous winey musty sweet herbaceous nutty marzipan raw vegetable whiskey	TGSC, Pubchem, OdoRactor Sigma Aldrich, TGSC, OdoRactor
1262	Sorbic alcohol Sorbyl acetate	(2E ,4E)-hexa-2,4-dien-1-ol [(2E ,4E)-hexa-2,4-dienyl] acetate hexa-2,4-dienyl 2- methylpropanoate [(2E ,4E)-hexa-2,4-dienyl] 2-	CC=CC=CCOC(=0)C	aldehydic fruity wax fatty fresh almond apple green herbaceous winey musty sweet herbaceous nutty marzipan raw vegetable whiskey fresh green oily herbaceous pumpkin parsley green fruity apple pear pineapple galbanum sweet tropical green fruity galbanum apple pear	TGSC, Pubchem, OdoRactor Sigma Aldrich, TGSC, OdoRactor SuperScent, TGSC, OdoRactor OdorRactor, TGSC,
1262	Sorbic alcohol Sorbyl acetate 2,4-Hexadienyl isobutyrate	(2E ,4E)-hexa-2,4-dien-1-ol [(2E ,4E)-hexa-2,4-dienyl] acetate hexa-2,4-dienyl 2- methylpropanoate	CC=CC=CCO CC=CC=CCOC(=0)C CC=CC=CCOC(=0)C(C)C	aldehydic fruity wax fatty fresh almond apple green herbaceous winey musty sweet herbaceous nutty marzipan raw vegetable whiskey fresh green oily herbaceous pumpkin parsley green fruity apple pear pineapple galbanum sweet tropical	TGSC, Pubchem, OdoRactor Sigma Aldrich, TGSC, OdoRactor SuperScent, TGSC, OdoRactor OdorRactor, TGSC, Flavorbase
1262 1263 1264 1265	Sorbic alcohol Sorbyl acetate 2,4-Hexadienyl isobutyrate Sorbyl isobutyrate	[(2E ,4E)-hexa-2,4-dien-1-ol [(2E ,4E)-hexa-2,4-dienyl] acetate hexa-2,4-dienyl 2- methylpropanoate [(2E ,4E)-hexa-2,4-dienyl] 2- methylpropanoate (E)-but-2-enal 1-methyl-4-propan-2-yl-2-prop-1-	CC=CC=CCO CC=CC=CCOC(=0)C CC=CC=CCOC(=0)C(C)C CC=CC=CCOC(=0)C(C)C	aldehydic fruity wax fatty fresh almond apple green herbaceous winey musty sweet herbaceous nutty marzipan raw vegetable whiskey fresh green oily herbaceous pumpkin parsley green fruity apple pear pineapple galbanum sweet tropical green fruity galbanum apple pear pineapple	TGSC, Pubchem, OdoRactor Sigma Aldrich, TGSC, OdoRactor SuperScent, TGSC, OdoRactor OdorRactor, TGSC, Flavorbase TGSC
1262 1263 1264 1265 1266	Sorbic alcohol Sorbyl acetate 2,4-Hexadienyl isobutyrate Sorbyl isobutyrate Crotonaldehyde	[(2E ,4E)-hexa-2,4-dien-1-ol [(2E ,4E)-hexa-2,4-dienyl] acetate hexa-2,4-dienyl 2- methylpropanoate [(2E ,4E)-hexa-2,4-dienyl] 2- methylpropanoate (E)-but-2-enal	CC=CC=CCO CC=CC=CCOC(=0)C CC=CC=CCOC(=0)C(C)C CC=CC=CCOC(=0)C(C)C	aldehydic fruity wax fatty fresh almond apple green herbaceous winey musty sweet herbaceous nutty marzipan raw vegetable whiskey fresh green oily herbaceous pumpkin parsley green fruity apple pear pineapple galbanum sweet tropical green fruity galbanum apple pear pineapple floral suffocating pungent green sweet carrot earthy dry	TGSC, Pubchem, OdoRactor Sigma Aldrich, TGSC, OdoRactor SuperScent, TGSC, OdoRactor OdorRactor, TGSC, Flavorbase TGSC Flavornet, Pubchem

1269	Isoeugenol	2-methoxy-4-[(E) -prop-1-enyl]phenol	CC=CC1=CC(=C(C=C1)O)OC	floral clove spicy woody sweet carnation phenolic eugenol	Sigma Aldrich, Flavornet, AOD, TGSC, Flavorbase, Pubchem, OdoRactor
1270	cis-Isoeugenol	2-methoxy-4-[(Z)-prop-1- enyl]phenol	CC=CC1=CC(=C(C=C1)O)OC	spicy clove	OdorRactor ,TGSC
1271	Isoeugenyl acetate	[2-methoxy-4-[(E)-prop-1-enyl]phenyl] acetate	CC=CC1=CC(=C(C=C1)OC(=O) C)OC	sweet spicy floral carnation balsamic powdery clove fruity	SuperScent, TGSC, Flavorbase, Odoractor
1272	Isoeugenyl phenylacetate	[2-methoxy-4-[(E)-prop-1-enyl]phenyl] 2- phenylacetate	CC=CC1=CC(=C(C=C1)OC(=O) CC2=CC =CC=C2)OC	apple cinnamyl honey spicy sweet clove floral	OdorRactor ,Sigma Aldrich, TGSC
1273	Isoeugenyl methyl ether	1,2-dimethoxy-4-[(Z)-prop-1-enyl]benzene	CC=CC1=CC(=C(C=C1)OC)OC	clove spicy blossom carnation woody	AOD, ADB
1274	Methyl isoeugenol	1,2-dimethoxy-4-prop-1- enylbenzene	CC=CC1=CC(=C(C=C1)OC)OC	spicy clove blossom carnation woody	AOD
1275	Methylisoeugenol	1,2-dimethoxy-4-[(E)-prop-1-enyl]benzene	CC=CC1=CC(=C(C=C1)OC)OC	spicy clove blossom carnation woody floral	Sigma Aldrich, TGSC, OdoRactor
1276	(E)-Isoeugenyl formate	[2-methoxy-4-[(E)-prop-1-enyl]phenyl] formate	CC=CC1=CC(=C(C=C1)OC=O)O C	orris green sweet woody clove	OdorRactor ,TGSC
1277	Benzyl isoeugenol	2-methoxy-1-phenylmethoxy-4- [(E)-prop-1-enyl]benzene	CC=CC1=CC(=C(C=C1)OCC2=C C=CC= C2)OC	spicy balsamic carnation magnolia powdery	OdorRactor ,TGSC
1278	trans-Anol	4-[(E)-prop-1-enyl]phenol	CC=CC1=CC=C(C=C1)O	warm spicy phenolic tea	Flavorbase
1279	cis-Anethole	1-methoxy-4-[(Z)-prop-1-enyl]benzene	CC=CC1=CC=C(C=C1)OC	anisic	OdorRactor ,TGSC
1280	Anethole	1-methoxy-4-[(E)-prop-1-enyl]benzene	CC=CC1=CC=C(C=C1)OC	anisic sweet spicy licorice mimosa medicinal	Sigma Aldrich, Flavornet, TGSC, Pubchem, OdoRactor
1281	Cassia oil	2-methoxy-4-prop-2- enylphenol;[(E)-prop-1- enyl]benzene	CC=CC1=CC=CC=C1.COC1=C(C=CC(= C1)CC=C)O	woody spicy sweet	Sigma Aldrich
1282	Isosafrole	5-[(E)-prop-1-enyl]-1,3- benzodioxole	CC=CC1=CC2=C(C=C1)OCO2	fragrant anisic sweet spicy sassafrass	AOD, TGSC, Pubchem, OdoRactor
1283	(3E,5E)-Octadien-2-one	(3E ,6E)-octa-3,6-dien-2-one	CC=CCC=CC(=O)C	fruity green grassy	OdorRactor ,TGSC
1284	Jasmine oil	1-[(Z)-but-2-enyl]-2- methylcyclopentene	CC=CCC1=C(CCC1)C	jasmine floral sweet indole wax oily jammy green tropical	Sigma Aldrich
1285	(2E,6E)-2,6-Octadienal	(2E ,6E)-octa-2,6-dienal	CC=CCCC=CC=O	green	OdorRactor,
1286	4-Hexenal	(E)-hex-4-enal	CC=CCCC=O	green vegetable	TGSC
1287	Tetrahydro-6-(3-pentenyl)-2H- pyran-2-one	6-[(E)-pent-3-enyl]oxan-2-one	CC=CCCC1CCCC(=0)O1	oily fruity coconut floral petal jasmine tuberose peach apricot	OdorRactor ,TGSC
1288	Hept-5-enoic acid	hept-5-enoic acid	CC=CCCCC(=O)O	rancid	ADB
1289	6-Octenal, (6Z)-	(Z)-oct-6-enal	CC=CCCCCC=O	fruity fresh green melon cucumber	TGSC
1290	Oct-6-enal	oct-6-enal	CC=CCCCCC=O	green melon	TGSC, Flavorbase, Odoractor
1291	Methyl 9-undecenoate	methyl (E)-undec-9-enoate	CC=CCCCCCCC(=0)OC	earthy fungal rose fatty floral wax	OdorRactor ,TGSC
1292	9-Undecenal	(E)-undec-9-enal	CC=CCCCCCCC=O	aldehydic mandarin citrus wax floral green	OdorRactor ,TGSC
1293	cis-4-Hexen-1-ol	(Z)-hex-4-en-1-ol	CC=CCCCO	green vegetable tomato turnip brothy gassy herbaceous musty metallic	OdorRactor ,TGSC
1294	4-Hexen-1-OL	(E)-hex-4-en-1-ol	CC=CCCCO	tomato green herbaceous musty metallic pungent vegetable oily	Sigma Aldrich, TGSC, OdoRactor
1295	(4Z)-4-Hexenyl acetate	[(Z)-hex-4-enyl] acetate	CC=CCCCOC(=O)C	green fruity banana	Flavorbase
1296	1-Propene, 1-(methylthio)-	1-methylsulfanylprop-1-ene	CC=CSC	acidic garlic	TGSC
1297	Di-1-propenyl sulfide	(E)-1-[(E)-prop-1-	CC=CSC=CC	savory brown	TGSC
		enyl]sulfanylprop-1-ene			
1298	Acetaldehyde	acetaldehyde	CC=0	coffee ethereal winey pungent aldehydic fruity fresh musty lifitng penetrating suffocating	
1299	Cyclopropanemethanol, 1-methyl-2-((1,2,2-trimethylbicyclo(3.1.0)hex-3-yl)methyl)-	[1-methyl-2-[(1,2,2-trimethyl-3-bicyclo[3.1.0]hexanyl)methyl]cycl opropyl]methano	CC1(C(CC2C1(C2)C)CC3CC3(C) CO)C	tropical woody fatty sandal wood herbaceous cologne floral creamy rose	OdorRactor ,TGSC, Flavorbase
1300	(3R,6R)-6-Ethenyl-2,2,6- trimethyloxan-3-ol	(3R, 6R)-6-ethenyl-2,2,6- trimethyloxan-3-ol	CC1(C(CCC(O1)(C)C=C)O)C	earthy	TGSC
1301	2H-Pyran-3-ol, 6- ethenyltetrahydro-2,2,6- trimethyl-	6-ethenyl-2,2,6-trimethyloxan-3-ol	CC1(C(CCC(O1)(C)C=C)O)C	honey floral	Flavornet, TGSC, OdoRactor
1302	Methyl 3-bicyclo(2.2.1)hept-5 en-2-yl-3- methyloxirane-2- carboxylate	methyl 3-(2-bicyclo[2.2.1]hept-5- enyl)-3- methyloxirane-2- carboxylate	CC1(C(O1)C(=O)OC)C2CC3CC2 C=C3	fruity floral sugar jasmine magnolia rose clover melon	TGSC
1303	Spathulenol	(1aR, 4aR, 7S, 7aR, 7bR)-1,1,7- trimethyl-4- methylidene-1a, 2,3,4a, 5,6,7a,7b - octahydrocyclopropa[h]azulen-7- ol	CC1(C2C1C3C(CCC3(C)O)C(=C) CC2)C	earthy herbaceous fruity	OdorRactor ,Flavornet
1304	beta-Carene	7,7-dimethyl-3- methylidenebicyclo[4.1.0]heptane	CC1(C2C1CC(=C)CC2)C	orange	Flavornet

1207	() Manufact 1	(1D 5C) (C	001/0200 0/01020 010	h	0: A11:1 FCCC
1305	(-)-Myrtenal	(1 <i>R</i> ,5 <i>S</i>)-6,6-dimethylbicyclo[3.1.1]hept-2-ene-2- carbaldehyde	CC1(C2CC=C(C1C2)C=0)C	berry honey lime minty woody pepper vanilla sweet cinnamyl tonka spicy terpenic camphoraceous jammy	Sigma Aldrich, TGSC
1306	Bicyclo(3.1.1)hept-2-ene-2- carboxaldehyde, 6,6-dimethyl-, (1S)-	(1 <i>S</i> ,5 <i>R</i>)-6,6-dimethylbicyclo[3.1.1]hept-2-ene-2-carbaldehyde	CC1(C2CC=C(C1C2)C=O)C	spicy	Flavornet
1307	Myrtenal	6,6-dimethylbicyclo[3.1.1]hept-2- ene-2- carbaldehyde	CC1(C2CC=C(C1C2)C=O)C	spicy cinnamyl terpenic camphoraceous jammy sweet tonka cooling green minty woody	SuperScent, TGSC, OdoRactor
1308	Bicyclo[3.1.1]hept-2-ene-2- acetaldehyde, 6,6-dimethyl-	2-(6,6-dimethyl-2- bicyclo[3.1.1]hept-2- enyl)acetaldehyde	CC1(C2CC=C(C1C2)CC=0)C	woody pine linseed oily fatty	OdorRactor ,TGSC
1309	Bicyclo(3.1.1)hept-2-ene-2- propanal, 6,6- dimethyl-	3-(6,6-dimethyl-2- bicyclo[3.1.1]hept-2- enyl)propanal	CC1(C2CC=C(C1C2)CCC=O)C	fresh clean watery balsamic pine nutty natural aldehydic	OdorRactor ,TGSC
1310	Nopol	2-(6,6-dimethyl-2-bicyclo[3.1.1]hept-2-enyl)ethanol	CC1(C2CC=C(C1C2)CCO)C	sweet balsamic citrus pine herbaceous	OdorRactor ,TGSC
1311	(-)-Myrtenol	[(1R,5S)-6,6-dimethyl-2-bicyclo[3.1.1]hept-2-enyl]methanol	CC1(C2CC=C(C1C2)CO)C	berry medicinal minty woody vanilla balsamic pine sweet	Sigma Aldrich, TGSC
1312	Myrtenol	(6,6-dimethyl-2-bicyclo[3.1.1]hept 2- enyl)methanol	CC1(C2CC=C(C1C2)CO)C	herbaceous woody pine balsamic sweet minty cooling medicinal camphoraceous	SuperScent, TGSC,OdoRactor,
1313	Myrtenyl formate	(6,6-dimethyl-2-bicyclo[3.1.1]hept 2-enyl)methyl formate	CC1(C2CC=C(C1C2)COC=O)C	woody pine oily	OdorRactor ,TGSC
1314	Pinocarvone	6,6-dimethyl-2- methylidenebicyclo[3.1.1]heptan- 3- one	CC1(C2CC1C(=C)C(=O)C2)C	minty	TGSC
1315	Pinocarveol	6,6-dimethyl-2- methylidenebicyclo[3.1.1]heptan- 3- ol	CC1(C2CC1C(=C)C(C2)O)C	floral herbaceous camphoraceous woody pine balsamic fresh cooling minty	Flavornet, TGSC, OdoRactor
1316	(-)-trans-Pinocarveol	(1 <i>S</i> ,3 <i>R</i> ,5 <i>S</i>)-6,6-dimethyl-2-methylidenebicyclo[3.1.1]heptan-3-ol	CC1(C2CC1C(=C)C(C2)O)C	warm woody balsamic fennel	TGSC
1317	alpha-Pinene oxide	2,7,7-trimethyl-3- oxatricyclo[4.1.1.02,4]octane	CC1(C2CC1C3(C(C2)O3)C)C	green	SuperScent, TGSC
1318	beta-Pinene	6,6-dimethyl-2- methylidenebicyclo[3.1.1]heptane	CC1(C2CCC(=C)C1C2)C	pine turpentine dry woody green herbaceous resinous hay cooling terpenic fresh minty eucalyptus camphoraceous spicy pepper nutmeg	Flavornet, OdoRactor, Pubchem
1319	(+)-beta-Pinene	(1R,5R)-6,6-dimethyl-2-methylidenebicyclo[3.1.1]heptane	CC1(C2CCC(=C)C1C2)C	sweet fresh pine woody hay green	TGSC
1320	(-)-beta-Pinene	(1 <i>S</i> ,5 <i>S</i>)-6,6-dimethyl-2-methylidenebicyclo[3.1.1]heptane	CC1(C2CCC(=C)C1C2)C	woody pine green resinous dry fresh hay	Sigma Aldrich, TGSC, Pubchem, OdoRactor
1321	Bornylcyclohexanol	4-(1,6,6-trimethyl-2-bicyclo[3.1.1]heptanyl)cyclohexan-1-ol	CC1(C2CCC(C1(C2)C)C3CCC(C C3)O)C	woody clean sandal wood balsamic	OdorRactor ,TGSC
1322	Bicyclo(3.1.1)heptan-2-ol, 2,6,6-trimethyl-, (1R,2S,5S)- rel-	(1R, 2S, 5S)-2,6,6- trimethylbicyclo[3.1.1]heptan-2- ol	CC1(C2CCC(C1C2)(C)O)C	pine woody fi rneedle camphoraceous incense	OdorRactor ,TGSC
1323	2-Mercaptopinane	2,6,6- trimethylbicyclo[3.1.1]heptane-2- thiol	CC1(C2CCC(C1C2)(C)S)C	grapefruit citrus sulfurous green tropical terpenic woody berry seedy buchu cooling	Sigma Aldrich, TGSC, OdoRactor
1324	(1r,2r,4r)-1,2,3,3- Tetramethylbicyclo[2.2.1]hep tan-2-ol	(1R, 2R, 4R)-1,2,3,3- tetramethylbicyclo[2.2.1]heptan-2- ol	CC1(C2CCC(C2)(C1(C)O)C)C	vegetable green mossy	TGSC
1325	(+)-Fenchone	(15,4R)-1,3,3- trimethylbicyclo[2.2.1]heptan-2- one	CC1(C2CCC(C2)(C1=O)C)C	balsamic camphoraceous thujonic cedar herbaceous earthy woody cooling mentholic pine terpenic fresh	AOD, TGSC, OdoRactor
1326	Fenchone	1,3,3- trimethylbicyclo[2.2.1]heptan-2- one	CC1(C2CCC(C2)(C1=O)C)C	camphoraceous herbaceous earthy	AOD
1327	(-)-Fenchone	(1R, 4S)-1,3,3- trimethylbicyclo[2.2.1]heptan-2- one	CC1(C2CCC(C2)(C1=O)C)C	sweet vanilla camphoraceous herbaceous earthy woody	Sigma Aldrich, AOD, TGSC, OdoRactor
1328	(1R)-Endo-(+)-Fenchyl alcohol	(1R, 2R, 4S)-1,3,3- trimethylbicyclo[2.2.1]heptan-2- ol	CC1(C2CCC(C2)(C10)C)C	camphoraceous	Flavornet
1329	alpha-Fenchol	(15 ,2S ,4R)-1,3,3- trimethylbicyclo[2.2.1]heptan-2- ol	CC1(C2CCC(C2)(C10)C)C	clean cooling camphoraceous pine eucalyptus green herbaceous minty earthy woody	OdorRactor ,TGSC

1330	Fenchol	1,3,3- trimethylbicyclo[2.2.1]heptan-2-ol	CC1(C2CCC(C2)(C10)C)C	earthy camphoraceous pine woody dry sweet lemon rooty	Sigma Aldrich, TGSC, OdoRactor
1331	Camphene hydrate	2,3,3- trimethylbicyclo[2.2.1]heptan-2-ol	CC1(C2CCC(C2)C1(C)O)C	camphoraceous mentholic musty minty	Flavornet
1332	Camphene	2,2-dimethyl-3- methylidenebicyclo[2.2.1]heptane	CC1(C2CCC(C2)C1=C)C	camphoraceous woody herbaceous fi meedle cooling pine terpenic citrus green minty spicy insipid	Flavornet, TGSC, Pubchem
1333	(+)-Camphene	(1R, 4S)-2,2-dimethyl-3-methylidenebicyclo[2.2.1]heptane	CC1(C2CCC(C2)C1=C)C	fresh fi rneedle minty cooling woody pine resinous medicinal citrus lime eucalyptus vanilla herbaceous camphoraceous	Sigma Aldrich, TGSC, OdoRactor
1334	(-)-Camphene	(1S ,4R)-2,2-dimethyl-3- methylidenebicyclo[2.2.1]heptane	CC1(C2CCC(C2)C1=C)C	woody fresh fi rneedle terpenic	TGSC, OdoRactor
1335	2,2-Dimethyl-1- norbornylideneethanol	(2Z)-2-(3,3-dimethyl-2-bicyclo[2.2.1]heptanylidene)ethan ol	CC1(C2CCC(C2)C1=CCO)C	woody dry sawdust patchouli camphoraceous minty	OdorRactor ,TGSC
1336	3,3- Dimethylbicyclo[2.2.1]heptan- 2-one	3,3-dimethylbicyclo[2.2.1]heptan- 2-one	CC1(C2CCC(C2)C1=0)C	camphoraceous	OdorRactor,
1337	1,3,3-Trimethyl-2- oxabicyclo[2.2.2]oct-5- ene	1,3,3-trimethyl-2- oxabicyclo[2.2.2]oct-5-ene	CC1(C2CCC(O1)(C=C2)C)C	minty lemon	Flavornet, TGSC
1338	Eucalyptol	1,3,3-trimethyl-2- oxabicyclo[2.2.2]octane	CC1(C2CCC(O1)(CC2)C)C	eucalyptus herbaceous camphoraceous medicinal minty fresh cooling fruity herbaceous woody citrus pepper sweet vanilla strong	OdorRactor ,TGSC, Pubchem,Sigma Aldrich, TGSC, Flavorbase
1339	Camphore	(1R,4S)-1,7,7- trimethylbicyclo[2.2.1]heptan-2- one	CC1(C2CCC1(C(=0)C2)C)C	camphoraceous minty phenolic herbaceous woody penetrating aromatic	AOD, Pubchem, OdoRactor
1340	D-Camphor	(1R,4R)-1,7,7- trimethylbicyclo[2.2.1]heptan-2- one	CC1(C2CCC1(C(=0)C2)C)C	ethereal minty warm fragrant penetrating camphoraceous phenolic herbaceous woody medicinal mentholic cooling green fresh	Sigma Aldrich, AOD, TGSC, Flavorbase, OdoRactor
1341	(-)-Camphor	(1S,4S)-1,7,7- trimethylbicyclo[2.2.1]heptan-2- one	CC1(C2CCC1(C(=0)C2)C)C	fragrant penetrating camphoraceous	AOD, Pubchem
1342	Camphor	1,7,7- trimethylbicyclo[2.2.1]heptan-2- one	CC1(C2CCC1(C(=0)C2)C)C	minty camphoraceous medicinal penetrating aromatic	Sigma Aldrich, TGSC, Pubchem
1343	1,7,7- Trimethylspiro[bicyclo[2.2.1] heptane- 3,1'-cyclopentane]-2-one	1,7,7- trimethylspiro[bicyclo[2.2.1]hepta ne-3,1'- cyclopentane]-2-one	CC1(C2CCC1(C(=0)C23CCCC3) C)C	herbaceous clary sage woody vetiver	TGSC
1344	Bicyclo[2.2.1]heptan-2-ol, 1,2,7,7- tetramethyl-, (1R,2R,4R)-rel-	(1R, 2R, 4R)-1,2,7,7- tetramethylbicyclo[2.2.1]heptan-2- ol	CC1(C2CCC1(C(C2)(C)O)C)C	earthy musty	Flavornet, TGSC
1345	2-Methylisoborneol	1,2,7,7- tetramethylbicyclo[2.2.1]heptan-2- ol	CC1(C2CCC1(C(C2)(C)O)C)C	earthy musty	SuperScent, TGSC, OdoRactor
1346	4-((1R,2R,4R)-Born-2- yl)cyclohexanol	4-(1,7,7-trimethyl-2-bicyclo[2.2.1]heptanyl)cyclohexan-1-ol	CC1(C2CCC1(C(C2)C3CCC(CC3)O)C)C	sandal wood sweet woody balsamic clean	OdorRactor ,TGSC
1347	(+)-Borneol	(1R ,2S ,4R)-1,7,7- trimethylbicyclo[2.2.1]heptan-2- ol	CC1(C2CCC1(C(C2)O)C)C	pine camphoraceous earthy balsamic	TGSC, Pubchem
1348	L-Borneol	(2R)-1,7,7- trimethylbicyclo[2.2.1]heptan-2-ol	CC1(C2CCC1(C(C2)O)C)C	pine woody camphoraceous earthy herbaceous musty minty pepper balsamic	OdorRactor ,TGSC, Pubchem
1349	Borneol	1,7,7- trimethylbicyclo[2.2.1]heptan-2-ol	CC1(C2CCC1(C(C2)O)C)C	sharp coniferous pepper camphoraceous woody balsamic pine	Flavornet, Flavorbase, TGSC, Pubchem
1350	Isoborneol	(1R,2R,4R)-1,7,7- trimethylbicyclo[2.2.1]heptan- 2-ol	CC1(C2CCC1(C(C2)O)C)C	woody vanilla musty camphoraceous balsamic herbaceous pine	Sigma Aldrich, TGSC, OdoRactor, Pubchem
1351	Isobornyl benzoate	(1,7,7-trimethyl-2-bicyclo[2.2.1]heptanyl) benzoate	CC1(C2CCC1(C(C2)OC(=O)C3= CC=CC= C3)C)C	pine balsamic herbaceous	Flavornet, TGSC
1352	(1s,2r,4r)-1,7,7- Trimethylbicyclo[2.2.1]hept-2- yl 2- hydroxybenzoate	[(1S, 2R, 4R)-1,7,7-trimethyl-2-	CC1(C2CCC1(C(C2)OC(=0)C3= CC=CC= C3O)C)C	green woody fresh orchid fi rneedle balsamic	OdorRactor ,TGSC
1353	Isobornyl phenylacetate	(1,7,7-trimethyl-2-bicyclo[2.2.1]heptanyl) 2-phenylacetate	CC1(C2CCC1(C(C2)OC(=0)CC3 =CC=CC =C3)C)C	balsamic cypress	OdorRactor ,TGSC

1354	Isobornyl methyl ether	2-methoxy-1,7,7-	CC1(C2CCC1(C(C2)OC)C)C	earthy musty pine woody	Flavornet, OdoRactor, TGSC
		trimethylbicyclo[2.2.1]heptane (1S, 2S, 4R)-2-methoxy-1,7,7-		camphoraceous borneol pine woody camphoraceous	, , ,
1355	(1S,2S,4R)-2-Methoxy-1,7,7-trimethylbicyclo[2.2.1]heptan e	(13,25,4 <i>K</i>)-2-methoxy-1,7,7-trimethylbicyclo[2.2.1]heptane	CC1(C2CCC1(C(C2)OC)C)C	borneol balsamic	OdorRactor ,TGSC
1356	Isobornyl formate	[(2S)-1,7,7-trimethyl-2-bicyclo[2.2.1]heptanyl] formate	CC1(C2CCC1(C(C2)OC=O)C)C	camphoraceous musty medicinal woody	OdorRactor,
1357	Bicyclo[2.2.1]heptan-2-ol, 1,7,7-trimethyl-, formate, (1R,2R,4R)-rel-	[(1R ,2R ,4R)-1,7,7-trimethyl-2-bicyclo[2.2.1]heptanyl] formate	CC1(C2CCC1(C(C2)OC=O)C)C	green earthy camphoraceous musty medicinal woody balsamic cooling minty pine	Flavornet, TGSC, Flavorbase
1358	Bornyl formate	(1,7,7-trimethyl-2-bicyclo[2.2.1]heptanyl) formate	CC1(C2CCC1(C(C2)OC=O)C)C	green earthy herbaceous balsamic pine	Flavornet, TGSC
	yl)oxy)-, rel-	2- bicyclo[2.2.1]heptanyl]oxy]ethano l		woody cedar balsamic pine	OdorRactor ,TGSC
1360	Cyclohexanol, 2(3 or 4)-(7,7-dimethylbicyclo(2.2.1)hept-2-yl)-	2-(7,7-dimethyl-2-bicyclo[2.2.1]heptanyl)cyclohexan-1-ol	CC1(C2CCC1C(C2)C3CCCCC3O)C	woody sweet oily sandal wood creamy	TGSC
1361	(1alpha,2alpha,5alpha)-6,6- Dimethylspiro(bicyclo(3.1.1) heptane-2,2'- oxirane)	(1R, 2R, 5S)-6,6-dimethylspiro[bicyclo[3.1.1]hepta ne-2,2'-oxirane]	CC1(C2CCC3(C1C2)CO3)C	rosemary sage herbaceous camphoraceous	OdorRactor ,TGSC
1362	(1R,5R,8R)-7,7-Dimethyl-6-methylidenetricyclo[6.2.1.01, 5]undecan-2-one	(1 <i>R</i> ,5 <i>R</i> ,8 <i>R</i>)-7,7-dimethyl-6-methylidenetricyclo[6.2.1.01,5]un decan-2-one		woody vetiver	TGSC
1363	Epoxyoxophorone	1,3,3-trimethyl-7- oxabicyclo[4.1.0]heptane-2,5- dione	CC1(CC(=O)C2C(C1=O)(O2)C)C	minty tobacco tea camphoraceous sweet	OdorRactor ,TGSC, Flavorbase
1364	3a,4,5,6-Tetrahydro-1,3,3- trimethylindancarbaldehyde	1,3,3-trimethyl-3 <i>a</i> ,4,5,6-tetrahydro-2 <i>H</i> -indene-1-carbaldehyde	CC1(CC(C2=CCCC21)(C)C=O) C	herbaceous black currant thujonic juniperberry	OdorRactor ,TGSC
1365	13-Oxabicyclo(10.1.0)trideca- 4,8-diene, trimethyl-	(4Z ,8Z)-1,2,2-trimethyl-13-oxabicyclo[10.1.0]trideca-4,8-diene	CC1(CC=CCCC=CCC2C1(O2) C)C	woody sweet dry powdery amber cedar patchouli sandal wood	OdorRactor ,TGSC
1366	4,8-Methanoazulen-9-ol, decahydro-2,2,4,8- tetramethyl-, stereoisomer	1,4,4,7- tetramethyltricyclo[5.3.1.02,6]und ecan-11- ol		earthy woody spice dusty balsamic	Flavornet, TGSC, Flavorbase, OdoRactor
1367	Caryophyllene oxide	(1R, 4R, 6R, 10S)-4,12,12- trimethyl-9-methylidene- 5-oxatricyclo[8.2.0.04,6]dodecane	CC1(CC2C1CCC3(C(O3)CCC2= C)C)C	sweet fresh dry woody spicy herbaceous spice	OdorRactor ,Flavornet, Pubchem
1368	Tricyclo(6.3.1.02,5)dodecan- 1-ol, 4,4,8- trimethyl-, (1R,2S,5R,8S)-	(1R, 2S, 5R, 8S)-4,4,8- trimethyltricyclo[6.3.1.02,5]dodec an-1-ol	CC1(CC2C1CCC3(CCCC2(C3)O) C)C	mossy earthy spice resinous	Flavornet, TGSC, Odoractor
1369	beta-Caryophyllene alcohol	4,4,8- trimethyltricyclo[6.3.1.02,5]dodec an-1-ol	CC1(CC2C1CCC3(CCCC2(C3)O) C)C	woody spicy earthy warm mossy	OdorRactor ,TGSC
1370	Caryophyllene formate	(4,4,8-trimethyl-1- tricyclo[6.3.1.02,5]dodecanyl) formate	CC1(CC2C1CCC3(CCCC2(C3)O C=O)C) C	woody spicy pepper camphoraceous	TGSC
1371	1,4,4- Trimethyltricyclo[5.3.1.02,6] undecan- 11-ol	1,4,4- trimethyltricyclo[5.3.1.02,6]undec an-11-ol	CC1(CC2C3CCCC(C2C1)(C3O)C)C	spicy mossy earthy resinous	OdorRactor ,TGSC
1372	Methylcamphenoate	methyl 6,6- dimethylbicyclo[2.2.1]heptane-2- carboxylate	CC1(CC2CC(C1C2)C(=0)OC)C	natural pine green fruity woody fi rneedle balsamic	OdorRactor ,TGSC
1373	2H-2,4a-Methanonaphthalen- 8(5H)-one, 1,3,4,6,7,8a-hexahydro- 1,1,5,5-tetramethyl-	2,2,8,8-tetramethyl-octahydro-1 <i>H</i> 2,4 <i>a</i> - methanonapthalen-10-one	CC1(CCC(=0)C2C13CCC(C3)C2 (C)C)C	woody cedar earthy tobacco incense dry patchouli	OdorRactor ,TGSC
1374	2(3H)-Furanone, 5- ethenyldihydro-5-methyl-	5-ethenyl-5-methyloxolan-2-one	CC1(CCC(=0)O1)C=C	fruity minty	OdorRactor ,TGSC
1375	Linalool oxide, pyrane, (Z)-	(2 <i>S</i> ,3 <i>S</i>)-2-ethenyl-2,6,6- trimethyloxan-3-ol	CC1(CCC(C(O1)(C)C=C)O)C	sweet floral creamy citrus green	Flavornet, TGSC, OdoRactor
1376	2,3b-Methano-3bH- cyclopenta[1,3]cyclopropa[1, 2]benzene-4- methanol, octahydro-7,7,8,8-tetramethyl-	(5,5,11,11-tetramethyl-2-tetracyclo[6,2.1.01,6.06,10]undec anyl)methanol	CC1(CCC(C23C14C2CC(C4)C3(C)C)CO) C	woody amber animal warm sage clary dry	OdorRactor ,TGSC

1377	(5,5,11,11-Tetramethyl-2- tetracyclo[6.2.1.01,6.06,10]u ndecanyl)meth yl formate	(5,5,11,11-tetramethyl-2- tetracyclo[6.2.1.01,6.06,10]undec anyl)methyl formate		woody amber cedar vetiver clary sage dry	OdorRactor ,TGSC
1378	1-Methoxy-4-(1-methoxy-1- methylethyl)-1- methylcyclohexane	1-methoxy-4-(2-methoxypropan-2-yl)-1- methylcyclohexane	CC1(CCC(CC1)C(C)(C)OC)OC	fruity minty green musty	TGSC
1379	2-[(2R,5S)-5-Ethenyl-5- methyloxolan-2- yl]propan-2- ol	2-[(2R ,5S)-5-ethenyl-5- methyloxolan-2-yl]propan- 2-ol	CC1(CCC(O1)C(C)(C)O)C=C	earthy floral sweet woody	OdorRactor ,TGSC
1380	Linalyl oxide	2-(5-ethenyl-5-methyloxolan-2-yl)propan-2-ol	CC1(CCC(O1)C(C)(C)O)C=C	earthy floral sweet woody lemon musty camphoraceous heral balsamic pine	Flavornet, TGSC, OdoRactor
1381	trans-Linalool oxide	2-[(2S,5S)-5-ethenyl-5- methyloxolan-2-yl]propan- 2-ol	CC1(CCC(O1)C(C)(C)O)C=C	floral citrus	Flavornet, SuperScent, TGSC
1382	1-(5,5-Dimethyl-1-cyclohexen-1-yl)-4- penten-1-one	1-(5,5-dimethylcyclohexen-1-yl)pent-4-en-1-one	CC1(CCC=C(C1)C(=0)CCC=C)C	green galbanum earthy weedy pineapple fresh narcissus hyacinth fruity	OdorRactor ,TGSC, Pubchem
1383	Isolongifolene	(1 <i>R</i> ,8 <i>S</i>)-2,2,7,7- tetramethyltricyclo[6.2.1.01,6]und ec-5-ene	CC1(CCC=C2C13CCC(C3)C2(C) C)C	woody dusty amber incense	TGSC
1384	1,2,3,4,4a,5,6,7-Octahydro- 2,5,5-trimethyl- 2-naphthol	2,5,5-trimethyl-1,3,4,4 <i>a</i> ,6,7-hexahydronaphthalen- 2-ol	CC1(CCC=C2C1CCC(C2)(C)O)C	amber musk animal old wood earthy natural ambergis seaweed	OdorRactor ,TGSC
1385	3-Cyclohexene-1-carboxylic acid, 1-methyl- , methyl ester	methyl 1-methylcyclohex-3-ene-1- carboxylate	CC1(CCC=CC1)C(=0)OC	tagette chrysanthemum natural thujonic herbaceous sweet	OdorRactor ,TGSC
1386	Amber spirolene	(3'S ,6'S ,9'S)-2',2',8',8'- tetramethylspiro[1,3-dioxol	CC1(CCC2([C@@H]3[C@@]14 CC[C@ @H](C4)C3(C)C)OCCO2)C	woody powdery musk fruity dry vetiver	OdorRactor ,TGSC
1387	4a,7-Methano-4aH- naphth[1,8a-b]oxirene, octahydro-4,4,8,8-tetramethyl-	2,2,8,8-tetramethyl-6- oxatetracyclo[7.2.1.01,7.05,7]dod ecane		rooty musty camphoraceous berry lime earthy vanilla humus patchouli	Sigma Aldrich, TGSC
1388	4a,7-Methano-4aH- naphth[1,8a-b]oxirene, octahydro-4,4,8,8-tetramethyl-	2,2,8,8-tetramethyl-6- oxatetracyclo[7.2.1.01,7.05,7]dod ecane		woody citrus linalyl dry herbaceous	OdorRactor ,TGSC
1389	Cyclohexanecarboxylic acid, 2,2-dimethyl-6- methylene-, methyl ester	methyl 2,2-dimethyl-6- methylidenecyclohexane-1- carboxylate	CC1(CCCC(=C)C1C(=O)OC)C	aromatic damascone rosemary fruity rose thujonic	OdorRactor ,TGSC
1390	1-(3,3- Dimethylcyclohexyl)pent-4- en-1-one	1-(3,3-dimethylcyclohexyl)pent-4- en-1-one	CC1(CCCC(C1)C(=0)CCC=C)C	green galbanum fruity pineapple herbaceous balsamic fi rneedle	TGSC
1391	2,6,6-Trimethyl-2- hydroxycyclohexanone	2-hydroxy-2,6,6- trimethylcyclohexan-1-one	CC1(CCCC(C1=O)(C)O)C	sweet tobacco herbaceous	TGSC
1392	2,6,6-Trimethyl-2- vinyltetrahydropyran	2-ethenyl-2,6,6-trimethyloxane	CC1(CCCC(O1)(C)C=C)C	camphoraceous herbaceous rosemary fresh sweet floral citrus woody cooling minty	OdorRactor ,TGSC
1393	Dihydroactinidiolide	4,4,7 <i>a</i> -trimethyl-6,7-dihydro-5 <i>H</i> -1-benzofuran-2- one	CC1(CCCC2(C1=CC(=O)O2)C)C	musk coumarinic ripe apricot fruity berry woody	SuperScent, TGSC, OdoRactor
1394	8Ah-2,4a-methanonaphthalen- 8a-ol, octahydro-1,1,5,5- tetramethyl-	2,2,8,8-tetramethyl-octahydro-1 <i>H</i> 2,4 <i>a</i> - methanonapthalen-9-ol	CC1(CCCC2(C13CCC(C3)C2(C) C)O)C	woody green mossy fi rneedle balsamic patchouli	TGSC
1395	Sclarene	(4aS ,8S ,8aS)-4,4,8a -trimethyl-7-methylidene-8- (3-methylidenepent-4-enyl)-2,3,4a ,5,6,8-hexahydro-1H -naphthalene	CC1(CCCC2(C1CCC(=C)C2CCC (=C)C= C)C)C	green terpenic woody amber sage clary	OdorRactor ,TGSC
1396	Labd-14-ene-8,13-diol, (13R)-	(1 <i>R</i> ,2 <i>R</i> ,8 <i>aS</i>)-1-[(3 <i>R</i>)-3- hydroxy-3-methylpent-4- enyl]- 2,5,5,8 <i>a</i> -tetramethyl-3,4,4 <i>a</i> ,6,7,8- hexahydro-1 <i>H</i> -naphthalen-2-ol	CC1(CCCC2(C1CCC(C2CCC(C)(C=C)O)(C)O)C)C	sweet balsamic amber woody weedy sage clary	OdorRactor ,TGSC, Flavorbase
1397	Sclareolide	(3aR ,5aS ,9aS ,9bR)-3a ,6,6,9a -tetramethyl- 1,4,5,5a ,7,8,9,9b - octahydrobenzo[e][1]benzofuran- 2-one	CC1(CCCC2(C1CCC3(C2CC(=O) O3)C)C)C	paper woody ambergis labdanum dry aromatic mossy cedar tobacco	Sigma Aldrich, TGSC, Flavorbase, OdoRactor
1398	Ambroxan	(3aR ,5aS ,9aS ,9bR)-3a ,6,6,9a -tetramethyl- 2,4,5,5a ,7,8,9,9b -octahydro-1H - benzo[e][1]benzofuran	CC1(CCCC2(C1CCC3(C2CCO3) C)C)C	floral sweet ambergis labdanum dry woody pine cedar green seedy tea paper	Sigma Aldrich, TGSC,Pubchem
1399	Ambrox	3a ,6,6,9a -tetramethyl-2,4,5,5a ,7,8,9,9b - octahydro-1 <i>H</i> - benzo[e][1]benzofuran	CC1(CCCC2(C1CCC3(C2CCO3) C)C)C	woody amber musk sweet dry ambergis	OdorRactor ,TGSC

1400		T	1		,
	5H-3,5a-Epoxynaphth[2,1-c]oxepin, dodecahydro-3,8,8,11a-tetramethyl-	5,5,9,13-tetramethyl-14,16-dioxatetracyclo[11.2.1.01,10.04,9]hexadecane	CC1(CCC2(C1CCC34C2CCC(O 3)(OC4) C)C)C	dry amber powdery woody musk	OdorRactor ,TGSC
1401	6,6,9a-Trimethyl- 1,2,3a,4,5,5a,7,8,9,9b- decahydrobenzo[e][1]benzof uran	6,6,9 <i>a</i> -trimethyl-1,2,3 <i>a</i> ,4,5,5 <i>a</i> ,7,8,9,9 <i>b</i> -decahydrobenzo[e][1]benzofuran	CC1(CCCC2(C1CCC3C2CCO3)C)C	amber ambergis musk woody cedar pine green seedy dry paper	OdorRactor ,TGSC
1402	Juniperol	(8S)-2,6,6,9- tetramethyltricyclo[5.4.0.02,9]und ecan 8-ol	CC1(CCCC2(C3C1C(C2(CC3)C) O)C)C	mossy woody	OdorRactor,
1403	Longifolene	3,3,7-trimethyl-8- methylidenetricyclo[5.4.0.02,9]un decane	CC1(CCCC2(C3C1C(C2=C)CC3) C)C	sweet woody rose medicinal fi rneedle	SuperScent, TGSC, OdoRactor
1404	Octahydro-8,8- dimethylnaphthalene-2- carbaldehyde	8,8-dimethyl-6,7-dihydro-5 <i>H</i> - naphthalene-2- carbaldehyde	CC1(CCCC2=C1C=C(C=C2)C=O)C	fresh dry muguet lily sweet melon floral green	OdorRactor ,TGSC
1405	2-Naphthalenecarbonitrile, 1,2,3,4,5,6,7,8- octahydro-8,8- dimethyl-	8,8-dimethyl-2,3,4,5,6,7- hexahydro-1 <i>H</i> - naphthalene-2- carbonitrile	CC1(CCCC2=C1CC(CC2)C#N)C	citrus marine earthy orris	OdorRactor ,TGSC
1406	1,2,3,4,5,6,7,8-Octahydro-8,8-dimethyl-2- naphthaldehyde	8,8-dimethyl-2,3,4,5,6,7- hexahydro-1 <i>H</i> - naphthalene-2- carbaldehyde	CC1(CCCC2=C1CC(CC2)C=0)C	floral clean muguet ozone marine sandy balsamic	OdorRactor ,TGSC
1407	3,8a-Ethano-8aH-1- benzopyran-2(3H)-one, hexahydro-3,5,5-trimethyl-	5,5,8-trimethyl-10- oxatricyclo[6.2.2.01,6]dodecan- 9-one	CC1(CCCC23C1CC(CC2)(C(=O) O3)C)C	animal musk ambergis dry amber civet	OdorRactor ,TGSC
1408	2H-2,4a-Methanonaphthalen- 1(5H)-one, hexahydro-5,5- dimethyl-	2,2-dimethyl-octahydro-1 <i>H</i> -2,4 <i>a</i> methanonapthalen-8-one	CC1(CCCC2C13CCC(C3)C2=0) C	tropical autumn fresh ozone orris woody earthy	TGSC
1409	Cycloheptanol, 2,2,7,7- tetramethyl-1-(2- propenyl)-	2,2,7,7-tetramethyl-1-prop-2- enylcycloheptan-1-ol	CC1(CCCCC(C1(CC=C)O)(C)C) C	woody camphoraceous patchouli earthy rooty	OdorRactor ,TGSC
1410	1-Methoxy-1- methylcyclododecane	1-methoxy-1- methylcyclododecane	CC1(CCCCCCCCCC1)OC	woody celery musk ambergis old wood	OdorRactor ,TGSC
1411	1-Oxaspiro[5.5]undecan-4-ol, 4-methyl-	4-methyl-1-oxaspiro[5.5]undecan- 4-ol	CC1(CCOC2(C1)CCCCC2)O	herbaceous rosemary minty camphoraceous tropical thujonic	OdorRactor ,TGSC
1412	Pantolactone	(3R)-3-hydroxy-4,4- dimethyloxolan-2-one	CC1(COC(=O)C1O)C	cotton candy	Flavornet
1413	2,5,5-Trimethyl-2-phenyl-1,3-dioxane	2,5,5-trimethyl-2-phenyl-1,3-dioxane	CC1(COC(OC1)(C)C2=CC=CC=C2)C	woody sandal wood camphoraceous sweet hawthorn	OdorRactor ,TGSC
1414	1,5-Dioxaspiro[5.5]undecane, 3,3-dimethyl-	3,3-dimethyl-1,5- dioxaspiro[5.5]undecane	CC1(COC2(CCCCC2)OC1)C	thyme herbaceous leathery tobacco animal sweet fresh	OdorRactor ,TGSC
			CC1/CCC/CC1)/C)O)O	meaty sulfurous herbaceous onion	Sigma Aldrich, ADB, TGSC,
1415	2,5-Dimethyl-1,4-dithiane-2,5-diol	2,5-dimethyl-1,4-dithiane-2,5-diol	cci(csc(csi)(c)0)0	chicken savory pork lamb bouillon	
			CC1(SC(SC(S1)(C)C)(C)C)C	1	OdoRactor Sigma Aldrich,
1416	diol 2,2,4,4,6,6-Hexamethyl-1,3,5-	2,2,4,4,6,6-hexamethyl-1,3,5-	CC1(SC(SC(S1)(C)C)(C)C)C	chicken savory pork lamb bouillon berry minty earthy citrus sulfurous blackberry green fruity burnt black currant cooling catty tropical grapefruit	OdoRactor Sigma Aldrich,
1416	diol 2,2,4,4,6,6-Hexamethyl-1,3,5- trithiane	2,2,4,4,6,6-hexamethyl-1,3,5-trithiane 1-tert -butyl-3,5-dimethyl-2,4,6-	CC1(SC(SC(S1)(C)C)(C)C)C CC1=C(C(=C(C(=C1[N+](=O)[O-])C)(C)(C)C)[N+](=O)[O-])C)[N+](=O)[O-] CC1=C(C(=C(C(=C1C)[N+](=O)[O-])C)[O-]	chicken savory pork lamb bouillon berry minty earthy citrus sulfurous blackberry green fruity burnt black currant cooling catty tropical grapefruit meaty	OdoRactor Sigma Aldrich, TGSC,OdoRactor
1416	diol 2,2,4,4,6,6-Hexamethyl-1,3,5- trithiane Musk xylene	2,2,4,4,6,6-hexamethyl-1,3,5-trithiane 1-tert -butyl-3,5-dimethyl-2,4,6-trinitrobenzene 1-tert -butyl-3,4,5-trimethyl-2,6-	CC1(SC(SC(S1)(C)C)(C)C)C CC1=C(C(=C(C(=C1[N+](=0)[0-])C(C)(C)C)[N+](=0)[0-])C)[N+](=0)[0-] CC1=C(C(=C(C(=C1C)[N+](=0)[0-])C(C)(C)C)[N+](=0)[0-])C	chicken savory pork lamb bouillon berry minty earthy citrus sulfurous blackberry green fruity burnt black currant cooling catty tropical grapefruit meaty fatty sweet soapy musk dry	OdoRactor Sigma Aldrich, TGSC,OdoRactor OdorRactor ,TGSC, Pubchem
1416	diol 2,2,4,4,6,6-Hexamethyl-1,3,5- trithiane Musk xylene Musk tibetene	2,2,4,4,6,6-hexamethyl-1,3,5-trithiane 1-tert -butyl-3,5-dimethyl-2,4,6-trinitrobenzene 1-tert -butyl-3,4,5-trimethyl-2,6-dinitrobenzene	CC1(SC(SC(S1)(C)C)(C)C)C CC1=C(C(=C(C(=C1[N+](=0)[0-])C(C)(C)C)[N+](=0)[0-]) CC1=C(C(=C(C(=C1C)[N+](=0)[0-])C(C)(C)C)[N+](=0)[0-])C	chicken savory pork lamb bouillon berry minty earthy citrus sulfurous blackberry green fruity burnt black currant cooling catty tropical grapefruit meaty fatty sweet soapy musk dry musk sweet powdery fatty	OdoRactor Sigma Aldrich, TGSC,OdoRactor OdorRactor ,TGSC, Pubchem OdorRactor ,TGSC
1416 1417 1418 1419 1420 1421	diol 2,2,4,4,6,6-Hexamethyl-1,3,5- trithiane Musk xylene Musk tibetene 2-Tert-Butyl-6-methylphenol 2,6-Dimethylbenzenethiolate 2,6-Dimethylstyrene	2,2,4,4,6,6-hexamethyl-1,3,5-trithiane 1-tert -butyl-3,5-dimethyl-2,4,6-trinitrobenzene 1-tert -butyl-3,4,5-trimethyl-2,6-dinitrobenzene 2-tert -butyl-6-methylphenol 2,6-dimethylbenzenethiolate 2-ethenyl-1,3-dimethylbenzene	CC1=C(C(=C(C(=C1[N+](=O)[O-])C(C)(C)C)[N+](=O)[O-])C(C)(C)C)[N+](=O)[O-])C(C)(C)(C)C)[N+](=O)[O-])C(C)(C)(C)C)[N+](=O)[O-])C(C1=C(C(=CC-C1)C(C)(C)C)O(C1=C(C(=CC-C1)C)[S-])C(C1=C(C(=CC-C1)C)C=C(C)C)C=C(C(=CC-C1)C)C=C(C(=CC-C1)C)C=C(C(=CC-C1)C)C=C(C(=CC-C1)C)C=C(C(=CC-C1)C)C=C(C(=CC-C1)C)C=C(C(=CC-C1)C)C=C(C(=CC-C1)C)C=C(C(=CC-C1)C)C=C(C(=CC-C1)C)C=C(C(=CC-C1)C)C=C(C(=CC-C1)C)C=C(C(=CC-C1)C)C=C(C(=CC-C1)C)C=C(C(=CC-C1)C)C=C(C(=CC-C1)C)C=C(C(=CC-C1)C)C=C(C(=CC-C1)C)C=C(C(=CC-C1)C)C=C(C(=CC-C1)C)C=C(C(=CC-C1)C)C=C(C(=CC-C1)C)C=C(C(=CC-C1)C)C=C(C(=CC-C1)C)C=C(C(=CC-C1)C)C=C(C(=CC-C1)C)C=C(C(=CC-C1)C)C=C(C(=CC-C1)C)C=C(C(=CC-C1)C)C=C(C(=CC-C1)C)C=C(C(=CC-C1)C)C=C(C(=CC-C1)C)C=C(C(=CC-C1)C)C=C(C(=CC-C1)C)C=C(C(=CC-C1)C)C=C(C(=CC-C1)C)C=C(C(=CC-C1)C)C=C(C(=CC-C1)C)C=C(C(=CC-C1)C)C=C(C(=CC-C1)C)C=C(C(=CC-C1)C)C=C(C(=CC-C1)C)C=C(C(=CC-C1)C)C=C(C(=CC-C1)C)C=C(C(=CC-C1)C)C=C(C(=CC-C1)C)C=C(C(=CC-C1)C)C=C(C(=CC-C1)C)C=C(C(=CC-C1)C)C=C(C(=CC-C1)C)C=C(C(=CC-C1)C)C=C(C(=CC-C1)C)C=C(C(=CC-C1)C)C=C(C(=CC-C1)C)C=C(C(=CC-C1)C)C=C(C(=CC-C1)C)C=C(C(=CC-C1)C)C=C(C(=CC-C1)C)C=C(C(=CC-C1)C)C=C(C(=CC-C1)C)C=C(C(=CC-C1)C)C=C(C(=CC-C1)C)C=C(C(=CC-C1)C)C=C((=CC-C1)C)C=C((=CC-C1)C)C=C((=CC-C1)C)C=C((=CC-C1)C)C=C((=CC-C1)C)C=C((=CC-C1)C)C=C((=CC-C1)C)C=C((=CC-C1)C)C=C((=CC-C1)C)C=C((=CC-C1)C)C=C((=CC-C1)C)C=C((=CC-C1)C)C=C((=CC-C1)C)C=C((=CC-C1)C)C=C((=CC-C1)C)C=C((=CC-C1)C)C=C((=CC-C1)C)C=C((=CC-C1)C)C=C((=CC-C1)C)C=C((=CC-C1)C)C=C((=CC-C1)C)C=C((=CC-C1)C)C=C((=CC-C1)C)C=C((=CC-C1)C)C=C((=CC-C1)C)C=C((=CC-C1)C)C=C((=CC-C1)C)C=C((=CC-C1)C)C=C((=CC-C1)C)C=C((=CC-C1)C)C=C((=CC-C1)C)C=C((=CC-C1)C)C=C((=CC-C1)C)C=C((=CC-C1)C)C=C((=CC-C1)C)C=C((=CC-C1)C)C=C((=CC-C1)C)C=C((=CC-C1)C)C=C((=CC-C1)C)C=C((=CC-C1)C)C=C((=CC-C1)C)C=C((=CC-C1)C)C=C((=CC-C1)C)C=C((=CC-C1)C)C=C((=CC-C1)C)C=C((=CC-C1)C)C=C((=CC-C1)C)C=C((=CC-C1)C)C=C((=CC-C1)C)C=C((=CC-C1)C)C=C((=CC-C1)C)C=C((=CC-C1)C)C=C((=CC-C1)C)C=C((=CC-C1)C)C=C((=CC-C1)C)C=C((=CC-C1)C)C=C((=CC-C1)C)C=C((=CC-C1)C)C=C((=CC-C1)C)C=C((=CC-C1)C)C=C((=CC-C1)C)C=C((=CC-C1)C)C=C((=CC-C1)C)C=C((=CC-C1)C)C=C((=CC	chicken savory pork lamb bouillon berry minty earthy citrus sulfurous blackberry green fruity burnt black currant cooling catty tropical grapefruit meaty fatty sweet soapy musk dry musk sweet powdery fatty leathery medicinal phenolic sulfurous meaty roasted phenolic metallic smoky gasoline	OdoRactor Sigma Aldrich, TGSC,OdoRactor OdorRactor ,TGSC, Pubchem OdorRactor ,TGSC TGSC OdorRactor ,TGSC
1416 1417 1418 1419 1420 1421 1422	diol 2,2,4,4,6,6-Hexamethyl-1,3,5- trithiane Musk xylene Musk tibetene 2-Tert-Butyl-6-methylphenol 2,6-Dimethylbenzenethiolate 2,6-Dimethylstyrene 2,6-Dimethylphenol	2,2,4,4,6,6-hexamethyl-1,3,5-trithiane 1-tert -butyl-3,5-dimethyl-2,4,6-trinitrobenzene 1-tert -butyl-3,4,5-trimethyl-2,6-dinitrobenzene 2-tert -butyl-6-methylphenol 2,6-dimethylbenzenethiolate 2-ethenyl-1,3-dimethylbenzene 2,6-dimethylphenol	CC1=C(C(=C(C(=C1[N+](=O)[O-])C(C)(C)C)[N+](=O)[O-])C(C)(C)C)[N+](=O)[O-])C(C)(C)C)[N+](=O)[O-])C(C)(C)C)[N+](=O)[O-])C(C)(C)C)[N+](=O)[O-])C(C)(C)C)C(C)C(C)C)O(CC1=C(C(=CC=C1)C)(C)(C)C)O(CC1=C(C(=CC=C1)C)C)C(C)C)C(C)C(C)C(C)C(C)C(C)C(C)C(C	chicken savory pork lamb bouillon berry minty earthy citrus sulfurous blackberry green fruity burnt black currant cooling catty tropical grapefruit meaty fatty sweet soapy musk dry musk sweet powdery fatty leathery medicinal phenolic sulfurous meaty roasted phenolic metallic smoky gasoline sweet phenolic rooty coffee medicinal tarry	OdoRactor Sigma Aldrich, TGSC,OdoRactor OdorRactor ,TGSC, Pubchem OdorRactor ,TGSC TGSC OdorRactor ,TGSC Flavornet Sigma Aldrich, TGSC, OdoRactor , Pubchem
1416 1417 1418 1419 1420 1421	diol 2,2,4,4,6,6-Hexamethyl-1,3,5- trithiane Musk xylene Musk tibetene 2-Tert-Butyl-6-methylphenol 2,6-Dimethylbenzenethiolate 2,6-Dimethylstyrene	2,2,4,4,6,6-hexamethyl-1,3,5-trithiane 1-tert -butyl-3,5-dimethyl-2,4,6-trinitrobenzene 1-tert -butyl-3,4,5-trimethyl-2,6-dinitrobenzene 2-tert -butyl-6-methylphenol 2,6-dimethylbenzenethiolate 2-ethenyl-1,3-dimethylbenzene	CC1=C(C(=C(C(=C1[N+](=O)[O-])C(C)(C)C)[N+](=O)[O-])C(C)(C)C)[N+](=O)[O-])C(C)(C)(C)C)[N+](=O)[O-])C(C)(C)(C)C)[N+](=O)[O-])C(C1=C(C(=CC-C1)C(C)(C)C)O(C1=C(C(=CC-C1)C)[S-])C(C1=C(C(=CC-C1)C)C=C(C)C)C=C(C(=CC-C1)C)C=C(C(=CC-C1)C)C=C(C(=CC-C1)C)C=C(C(=CC-C1)C)C=C(C(=CC-C1)C)C=C(C(=CC-C1)C)C=C(C(=CC-C1)C)C=C(C(=CC-C1)C)C=C(C(=CC-C1)C)C=C(C(=CC-C1)C)C=C(C(=CC-C1)C)C=C(C(=CC-C1)C)C=C(C(=CC-C1)C)C=C(C(=CC-C1)C)C=C(C(=CC-C1)C)C=C(C(=CC-C1)C)C=C(C(=CC-C1)C)C=C(C(=CC-C1)C)C=C(C(=CC-C1)C)C=C(C(=CC-C1)C)C=C(C(=CC-C1)C)C=C(C(=CC-C1)C)C=C(C(=CC-C1)C)C=C(C(=CC-C1)C)C=C(C(=CC-C1)C)C=C(C(=CC-C1)C)C=C(C(=CC-C1)C)C=C(C(=CC-C1)C)C=C(C(=CC-C1)C)C=C(C(=CC-C1)C)C=C(C(=CC-C1)C)C=C(C(=CC-C1)C)C=C(C(=CC-C1)C)C=C(C(=CC-C1)C)C=C(C(=CC-C1)C)C=C(C(=CC-C1)C)C=C(C(=CC-C1)C)C=C(C(=CC-C1)C)C=C(C(=CC-C1)C)C=C(C(=CC-C1)C)C=C(C(=CC-C1)C)C=C(C(=CC-C1)C)C=C(C(=CC-C1)C)C=C(C(=CC-C1)C)C=C(C(=CC-C1)C)C=C(C(=CC-C1)C)C=C(C(=CC-C1)C)C=C(C(=CC-C1)C)C=C(C(=CC-C1)C)C=C(C(=CC-C1)C)C=C(C(=CC-C1)C)C=C(C(=CC-C1)C)C=C(C(=CC-C1)C)C=C(C(=CC-C1)C)C=C(C(=CC-C1)C)C=C(C(=CC-C1)C)C=C(C(=CC-C1)C)C=C(C(=CC-C1)C)C=C(C(=CC-C1)C)C=C(C(=CC-C1)C)C=C(C(=CC-C1)C)C=C(C(=CC-C1)C)C=C(C(=CC-C1)C)C=C((=CC-C1)C)C=C((=CC-C1)C)C=C((=CC-C1)C)C=C((=CC-C1)C)C=C((=CC-C1)C)C=C((=CC-C1)C)C=C((=CC-C1)C)C=C((=CC-C1)C)C=C((=CC-C1)C)C=C((=CC-C1)C)C=C((=CC-C1)C)C=C((=CC-C1)C)C=C((=CC-C1)C)C=C((=CC-C1)C)C=C((=CC-C1)C)C=C((=CC-C1)C)C=C((=CC-C1)C)C=C((=CC-C1)C)C=C((=CC-C1)C)C=C((=CC-C1)C)C=C((=CC-C1)C)C=C((=CC-C1)C)C=C((=CC-C1)C)C=C((=CC-C1)C)C=C((=CC-C1)C)C=C((=CC-C1)C)C=C((=CC-C1)C)C=C((=CC-C1)C)C=C((=CC-C1)C)C=C((=CC-C1)C)C=C((=CC-C1)C)C=C((=CC-C1)C)C=C((=CC-C1)C)C=C((=CC-C1)C)C=C((=CC-C1)C)C=C((=CC-C1)C)C=C((=CC-C1)C)C=C((=CC-C1)C)C=C((=CC-C1)C)C=C((=CC-C1)C)C=C((=CC-C1)C)C=C((=CC-C1)C)C=C((=CC-C1)C)C=C((=CC-C1)C)C=C((=CC-C1)C)C=C((=CC-C1)C)C=C((=CC-C1)C)C=C((=CC-C1)C)C=C((=CC-C1)C)C=C((=CC-C1)C)C=C((=CC-C1)C)C=C((=CC-C1)C)C=C((=CC-C1)C)C=C((=CC-C1)C)C=C((=CC-C1)C)C=C((=CC-C1)C)C=C((=CC-C1)C)C=C((=CC-C1)C)C=C((=CC-C1)C)C=C((=CC-C1)C)C=C((=CC-C1)C)C=C((=CC-C1)C)C=C((=CC-C1)C)C=C((=CC-C1)C)C=C((=CC	chicken savory pork lamb bouillon berry minty earthy citrus sulfurous blackberry green fruity burnt black currant cooling catty tropical grapefruit meaty fatty sweet soapy musk dry musk sweet powdery fatty leathery medicinal phenolic sulfurous meaty roasted phenolic metallic smoky gasoline sweet phenolic rooty coffee	OdoRactor Sigma Aldrich, TGSC,OdoRactor OdorRactor ,TGSC, Pubchem OdorRactor ,TGSC TGSC OdorRactor ,TGSC Flavornet Sigma Aldrich, TGSC,
1416 1417 1418 1419 1420 1421 1422	diol 2,2,4,4,6,6-Hexamethyl-1,3,5- trithiane Musk xylene Musk tibetene 2-Tert-Butyl-6-methylphenol 2,6-Dimethylbenzenethiolate 2,6-Dimethylstyrene 2,6-Dimethylphenol	2,2,4,4,6,6-hexamethyl-1,3,5-trithiane 1-tert -butyl-3,5-dimethyl-2,4,6-trinitrobenzene 1-tert -butyl-3,4,5-trimethyl-2,6-dinitrobenzene 2-tert -butyl-6-methylphenol 2,6-dimethylbenzenethiolate 2-ethenyl-1,3-dimethylbenzene 2,6-dimethylphenol	CC1=C(C(=C(C(=C1[N+](=O)[O-])C(C)(C)C)[N+](=O)[O-])C(C)(C)C)[N+](=O)[O-])C(C)(C)C)[N+](=O)[O-])C(C)(C)C)[N+](=O)[O-])C(C)(C)C)[N+](=O)[O-])C(C)(C)C)C(C)C(C)C)O(CC1=C(C(=CC=C1)C)(C)(C)C)O(CC1=C(C(=CC=C1)C)C)C(C)C)C(C)C(C)C(C)C(C)C(C)C(C)C(C	chicken savory pork lamb bouillon berry minty earthy citrus sulfurous blackberry green fruity burnt black currant cooling catty tropical grapefruit meaty fatty sweet soapy musk dry musk sweet powdery fatty leathery medicinal phenolic sulfurous meaty roasted phenolic metallic smoky gasoline sweet phenolic rooty coffee medicinal tarry sulfurous herbaceous meaty roasted smoky phenolic metallic rosemary	OdoRactor Sigma Aldrich, TGSC,OdoRactor OdorRactor,TGSC, Pubchem OdorRactor,TGSC TGSC OdorRactor,TGSC Flavornet Sigma Aldrich, TGSC, OdoRactor, Pubchem Sigma Aldrich, TGSC,
1416 1417 1418 1419 1420 1421 1423	diol 2,2,4,4,6,6-Hexamethyl-1,3,5- trithiane Musk xylene Musk tibetene 2-Tert-Butyl-6-methylphenol 2,6-Dimethylbenzenethiolate 2,6-Dimethylphenol 2,6-Dimethylphenol 2,6-Dimethylphenol	2,2,4,4,6,6-hexamethyl-1,3,5-trithiane 1-tert -butyl-3,5-dimethyl-2,4,6-trinitrobenzene 1-tert -butyl-3,4,5-trimethyl-2,6-dinitrobenzene 2-tert -butyl-6-methylphenol 2,6-dimethylbenzenethiolate 2-ethenyl-1,3-dimethylbenzene 2,6-dimethylphenol 2,6-dimethylphenol	CC1=C(C(=C(C(=C1[N+](=O)[O-])C(C)(C)C)C)C CC1=C(C(=C(C(=C1[N+](=O)[O-])C(C)(C)C)[N+](=O)[O-])C(C)(C)(C)C)[N+](=O)[O-])C CC1=C(C(=C(C(=C1C)[N+](=O)[O-])C CC1=C(C(=CC=C1)C(C)(C)C)C CC1=C(C(=CC=C1)C)[S-] CC1=C(C(=CC=C1)C)C=C CC1=C(C(=CC=C1)C)C=C CC1=C(C(=CC=C1)C)S CC1=C(C(=CC=C1)C)S	chicken savory pork lamb bouillon berry minty earthy citrus sulfurous blackberry green fruity burnt black currant cooling catty tropical grapefruit meaty fatty sweet soapy musk dry musk sweet powdery fatty leathery medicinal phenolic sulfurous meaty roasted phenolic metallic smoky gasoline sweet phenolic rooty coffee medicinal tarry sulfurous herbaceous meaty roasted smoky phenolic metallic rosemary tobacco spicy phenolic chemical musty	OdoRactor Sigma Aldrich, TGSC,OdoRactor OdorRactor ,TGSC, Pubchem OdorRactor ,TGSC TGSC OdorRactor ,TGSC Flavornet Sigma Aldrich, TGSC, OdoRactor, Pubchem Sigma Aldrich, TGSC, OdoRactor OdoRactor OdorRactor ,TGSC

1428	Maltol	3-hydroxy-2-methylpyran-4-one	CC1=C(C(=O)C=CO1)O	caramel jammy sweet cotton candy fruity burnt bready burnt sugar	Sigma Aldrich, Flavorbase, TGSC,OdoRactor
1429	2-Methyl-4-oxo-4H-pyran-3-yl acetate	(2-methyl-4-oxopyran-3-yl) acetate	CC1=C(C(=0)C=CO1)OC(=0)C	fruity jammy berry tropical	OdorRactor ,TGSC
1430	Maltyl isobutyrate	(2-methyl-4-oxopyran-3-yl) 2- methylpropanoate	CC1=C(C(=O)C=CO1)OC(=O)C(C)C	caramel jammy sweet strawberry fruity tropical berry cotton candy dried fruit burnt sugar	Sigma Aldrich, TGSC, Flavorbase, OdoRactor
1431	2-Hydroxy-3,5,5-trimethyl-2-cyclohexen-1- one	2-hydroxy-3,5,5- trimethylcyclohex-2-en-1-one	CC1=C(C(=O)CC(C1)(C)C)O	phenolic woody dry clean nutty tobacco spicy powdery	OdorRactor ,TGSC
1432	2-Allyl-3-methylcyclopent-2- en-1-one	3-methyl-2-prop-2-enylcyclopent- 2-en-1-one	CC1=C(C(=O)CC1)CC=C	fenugreek lovage	TGSC
1433	Cyclotene	2-hydroxy-3-methylcyclopent-2-en- 1-one	CC1=C(C(=O)CC1)O	caramel seedy maple sugar coffee woody	SuperScent, TGSC
1434	4-Hydroxy-5-methylfuran- 3(2H)-one	4-hydroxy-5-methylfuran-3-one	CC1=C(C(=0)CO1)O	bready caramel sweet cotton candy burnt sugar sugar bready	OdorRactor ,Sigma Aldrich
1435	Safranal	2,6,6-trimethylcyclohexa-1,3- diene-1-carbaldehyde	CC1=C(C(CC=C1)(C)C)C=0	herbaceous herbaceous fresh camphoraceous powdery sweet phenolic metallic woody medicinal rosemary tobacco spicy	Sigma Aldrich, Flavorbase, TGSC, OdoRactor
1436	4-(2,6,6-Trimethyl-1,3- cyclohexadien-1-yl)- 2-butanone	4-(2,6,6-trimethylcyclohexa-1,3-dien-1-yl)butan-2- one	CC1=C(C(CC=C1)(C)C)CCC(=O) C	floral	OdorRactor,
1437	1-(3-(Methylthio)-butyryl)- 2,6,6- trimethylcyclohexene	3-methylsulfanyl-1-(2,6,6- trimethylcyclohexen-1- yl)butan-1- one		fruity sweet tobacco	TGSC
1438	delta-Iraldeine	(E)-3-methyl-4-(2,6,6-trimethylcyclohexen-1-yl)but-3-en-2-one		floral woody ambergis wax orris	OdorRactor ,TGSC
1439	3-Buten-2-ol, 3-methyl-4- (2,6,6-trimethyl-1- cyclohexen-1-yl)-	3-methyl-4-(2,6,6- trimethylcyclohexen-1-yl)but-3- en- 2-ol	CC1=C(C(CCC1)(C)C)C=C(C)C(C)O	woody vetiver acetic	OdorRactor ,TGSC
1440	beta-Ionone	(E)-4-(2,6,6-trimethylcyclohexen-1-yl)but-3-en-2- one	CC1=C(C(CCC1)(C)C)C=CC(=0) C	almond balsamic berry grape green jammy orange woody minty peach raspberry rose sweet violet winey seaweed floral orris dry seedy fruity powdery tropical beewax cedar	TGSC, Pubchem, OdoRactor
1441	4-(2,6,6-Trimethyl-cyclohex- 1-enyl)-but-3- en-2-one	4-(2,6,6-trimethylcyclohexen-1-yl)but-3-en-2-one	CC1=C(C(CCC1)(C)C)C=CC(=O) C	violet sweet floral woody	TGSC
1442	beta-Ionol	(E)-4-(2,6,6-trimethylcyclohexen-1-yl)but-3-en-2- ol	CC1=C(C(CCC1)(C)C)C=CC(C) 0	floral sweet herbaceous violet tropical balsamic woody berry powdery fruity	SuperScent, TGSC, Flavorbase, OdoRactor
1443	3-Buten-2-ol, 4-(2,6,6- trimethyl-1- cyclohexen-1-yl)- , 2-acetate	4-(2,6,6-trimethylcyclohexen-1-yl)but-3-en-2-yl acetate	CC1=C(C(CCC1)(C)C)C=CC(C) OC(=0)C		OdorRactor ,TGSC
1444	beta-Cyclocitral	2,6,6-trimethylcyclohexene-1- carbaldehyde	CC1=C(C(CCC1)(C)C)C=O	green fruity minty tropical herbaceous rose sweet tobacco damascone saffron clean hay sweet tobacco	Sigma Aldrich, Flavorbase, TGSC,OdoRactor
1445	(2S)-4-(2,6,6- Trimethylcyclohexen-1- yl)butan-2-ol	(2S)-4-(2,6,6- trimethylcyclohexen-1-yl)butan-2- ol	CC1=C(C(CCC1)(C)C)CC[C@H] (C)O	floral amber	TGSC
1446	Boronal	(E)-2-methyl-4-(2,6,6- trimethylcyclohexen-1- yl)but-2- enal	CC1=C(C(CCC1)(C)C)CC=C(C)C =O	floral dry sweet tobacco nutty violet boronia leafy hay woody	OdorRactor ,TGSC
1447	2,6,6-Trimethyl-1- cyclohexene-1- acetaldehyde	2-(2,6,6-trimethylcyclohexen-1-yl)acetaldehyde	CC1=C(C(CCC1)(C)C)CC=O	beefy camphoraceous cooling oily woody weedy fruity	Sigma Aldrich, TGSC
1448	Dihydro-beta-ionone	4-(2,6,6-trimethylcyclohexen-1-yl)butan-2-one	CC1=C(C(CCC1)(C)C)CCC(=0) C	woody earthy orris amber mahogany dry cedar berry seedy oily raspberry floral tea leafy	Sigma Aldrich, TGSC, OdoRactor
1449	Dihydro-beta-ionol	4-(2,6,6-trimethylcyclohexen-1-yl)butan-2-ol	CC1=C(C(CCC1)(C)C)CCC(C)O	woody floral amber sweet weak	OdorRactor ,TGSC, Flavorbase
1450	2,4,4-Trimethyl-3-(3-oxo-1-butenyl)cyclohex-2-en-1-one	5 7	CC1=C(C(CCC1=O)(C)C)C=CC(=O)C	woody	Flavornet
1451	3-(3-Butenyl)-2,4,4- trimethylcyclohex-2-en- 1-one	3-but-3-enyl-2,4,4- trimethylcyclohex-2-en-1-one	CC1=C(C(CCC1=O)(C)C)CCC=C	floral fruity woody tobacco	Flavorbase
1452	Musk ambrette	1- <i>tert</i> -butyl-2-methoxy-4-methyl-3,5- dinitrobenzene	CC1=C(C=C(C(=C1[N+](=O)[O-])OC)C(C)(C)C)[N+](=O)[O-]	musty sweet ambrette seedy musk floral	SuperScent, TGSC, Pubchem

1453	Carvacrol	2-methyl-5-propan-2-ylphenol	CC1=C(C=C(C=C1)C(C)C)O	woody spicy camphoraceous cooling thyme herbaceous smoky	Sigma Aldrich, Flavorbase, TGSC, OdoRactor, Pubchem
				medicinal phenolic origanum herbaceous	
1454	Carvacrol methyl ether	2-methoxy-1-methyl-4-propan-2-ylbenzene	CC1=C(C=C(C=C1)C(C)C)OC	herbaceous spicy leafy citrus	SuperScent, TGSC
1455	3,4-Dimethylphenol	3,4-dimethylphenol	CC1=C(C=C(C=C1)O)C	burnt dry	Sigma Aldrich
1456	Moskene	1,1,3,3,5-pentamethyl-4,6-dinitro- 2 <i>H</i> -indene	CC1=C(C=C2C(=C1[N+](=O)[O-])C(CC2(C)C)(C)C)[N+](=O)[O-]	sweet musk powdery ambrette dry	OdorRactor ,TGSC
1457	Methyl 2,4-dihydroxy-3- methylbenzoate	methyl 2,4-dihydroxy-3- methylbenzoate	CC1=C(C=CC(=C1O)C(=O)OC)O	oakmoss sweet seashore mossy phenolic	OdorRactor ,TGSC
1458	2-Methyl-3-furanthiol	2-methylfuran-3-thiol	CC1=C(C=CO1)S	buttery coconut coffee meaty	Sigma Aldrich, TGSC,
	,			sulfurous fishy metallic roasted chicken roasted chicken beefy	OdoRactor
1459	2-Methyl-3-(methylthio)furan	2-methyl-3-methylsulfanylfuran	CC1=C(C=CO1)SC	beefy minty spicy cheese coffee meaty nutty sulfurous pungent alliaceous dry brothy mustard	Sigma Aldrich, TGSC, Odoractor
1460	3-(Acetylthio)-2-methylfuran	S -(2-methylfuran-3-yl) ethanethioate	CC1=C(C=CO1)SC(=O)C	meaty sulfurous eggy burnt cooked roasted meat fried roasted	Sigma Aldrich, Flavornet, TGSC, OdoRactor
1461	2,6-Dimethyl-3-((2-methyl-3-furyl)thio)-4- heptanone	2,6-dimethyl-3-(2-methylfuran-3- yl)sulfanylheptan- 4-one	CC1=C(C=CO1)SC(C(C)C)C(=O) CC(C)C	sweet onion meaty roasted meat roasted	ADB, Flavorbase, TGSC, OdoRactor
1462	3-((2-Methyl-3-furyl)thio)-2-butanone	3-(2-methylfuran-3- yl)sulfanylbutan-2-one	CC1=C(C=CO1)SC(C)C(=O)C	spicy floral	OdorRactor ,TGSC
1463	3-((2-Methyl-3- furyl)thio)butanal	3-(2-methylfuran-3- yl)sulfanylbutanal	CC1=C(C=CO1)SC(C)CC=O	meaty roasted	TGSC
1464	Methyl 2-methyl-3-furyl disulfide	2-methyl-3- (methyldisulfanyl)furan	CC1=C(C=CO1)SSC	chocolate coffee fatty meaty peanut thiamine pepper sulfurous onion roasted beef vegetable chemical roasted beefy	Sigma Aldrich, TGSC, OdoRactor
1465	Bis(2-methyl-3-furyl)disulfide	2-methyl-3-[(2-methylfuran-3- yl)disulfanyl]furan	CC1=C(C=CO1)SSC2=C(OC=C2)C	sulfurous roasted meat onion meaty scallion savory chicken roasted	Sigma Aldrich, TGSC, OdoRactor
1466	Furfuryl 2-methyl-3-furyl disulfide	3-(furan-2-ylmethyldisulfanyl)-2- methylfuran	CC1=C(C=CO1)SSCC2=CC=CO 2	sulfurous meaty	OdorRactor ,TGSC
1467	Bis(2-methyl-3-furyl) tetrasulfide	2-methyl-3-[(2-methylfuran-3- yl)tetrasulfanyl]furan	CC1=C(C=CO1)SSSSC2=C(OC=C2)C	sulfurous meaty	TGSC
1468	2-Methylthiophene-3-thiol	2-methylthiophene-3-thiol	CC1=C(C=CS1)S	medicinal	Flavornet, TGSC
1469	Bicyclo[2.2.1]hept-5-ene-2-methanol, 5,6-dimethyl-1-(1-methylethenyl)-	(5,6-dimethyl-1-prop-1-en-2-yl-2-bicyclo[2,2.1]hept-5-enyl)methanol	CC1=C(C2(CC1CC2CO)C(=C)C) C	fresh ozone clean fresh woody	OdorRactor ,TGSC
1470	1,2,3,3,4,5,6- Heptamethylbicyclo(2.2.2)oct- 5-en-2-ol	1,2,3,3,4,5,6- heptamethylbicyclo[2.2.2]oct-5-en- 2- ol	CC1=C(C2(CCC1(C(C2(C)O)(C) C)C)C)C	woody camphoraceous patchouli	TGSC
1471	Bicyclo[2.2.1]hept-5-ene-2- carboxylic acid, 1,6-dimethyl-5-(1- methylethenyl)-, methyl ester	methyl 1,6-dimethyl-5-prop-1-en-2 ylbicyclo[2.2.1]hept-5-ene-2- carboxylate	CC1=C(C2CC(C1(C2)C)C(=0)O C)C(=C) C	woody pepper citrus dry	OdorRactor ,TGSC
1472	2-Methyl-5-(prop-1-en-2- yl)cyclohex-1-ene- 1-peroxol	2-hydroperoxy-1-methyl-4-prop-1- en-2- ylcyclohexene	CC1=C(CC(CC1)C(=C)C)OO	turpentine	Flavornet
1473	2-Methyl-4,5-dihydrofuran-3-thiol	5-methyl-2,3-dihydrofuran-4-thiol	CC1=C(CCO1)S	meaty roasted sulfurous savory	Flavornet, TGSC, Flavorbase
1474	Tetramethylpyrazine	2,3,5,6-tetramethylpyrazine	CC1=C(N=C(C(=N1)C)C)C	chocolate coffee fatty musty nutty burnt cocoa brown lard vanilla dry	Sigma Aldrich, TGSC
1475	6,7-Dihydro-2,3-dimethyl-5H-cyclopentapyrazine	2,3-dimethyl-6,7-dihydro-5 <i>H</i> - cyclopenta[b]pyrazine	CC1=C(N=C2CCCC2=N1)C	brown earthy burnt nutty roasted	OdorRactor ,TGSC, Flavorbase
	2-(5-Methyl-4-thiazolyl)ethyl isobutyrate	2-(5-methyl-1,3-thiazol-4-yl)ethyl 2- methylpropanoate	CC1=C(N=CS1)CCOC(=O)C(C)C		OdorRactor ,TGSC
1477	2,4,5-Trimethyloxazole	2,4,5-trimethyl-1,3-oxazole	CC1=C(OC(=N1)C)C	beefy chocolate nutty mustard vegetable roasted wasabi shellfish	Sigma Aldrich, TGSC, OdoRactor
1478	2-Isobutyl-4,5- dimethyloxazole	4,5-dimethyl-2-(2-methylpropyl)- 1,3-oxazole	CC1=C(OC(=N1)CC(C)C)C	burnt roasted	OdorRactor ,TGSC
	Furan, 3-methyl-2-(3-methyl-2-butenyl)-	3-methyl-2-(3-methylbut-2- enyl)furan	CC1=C(OC=C1)CC=C(C)C	minty caramel green	Flavornet, TGSC
	2-((3,3-Dimethyloxiran-2-yl)methyl)-3- methylfuran	2-[(3,3-dimethyloxiran-2- yl)methyl]-3-methylfuran	CC1=C(OC=C1)CC2C(O2)(C)C	green earthy citrus	Flavornet, TGSC, OdoRactor
1481	2,3-Dimethylbenzofuran	2,3-dimethyl-1-benzofuran	CC1=C(OC2=CC=CC=C12)C	chemical phenolic smoky tobacco resinous pungent licorice leathery bacon meaty	OdorRactor ,TGSC

1482	Ethanone, 1-(3-methyl-2-benzofuranyl)-	1-(3-methyl-1-benzofuran-2-yl)ethanone	CC1=C(OC2=CC=CC=C12)C(=O	floral orange flower	TGSC
	2,4,5-Trimethylthiazole	2,4,5-trimethyl-1,3-thiazole	CC1=C(SC(=N1)C)C	chocolate coffee hazelnut earthy musty nutty vegetable cocoa toasted brown herbaceous	Sigma Aldrich, Flavornet, Flavorbase, TGSC, OdoRactor
1484	5-Acetyl-2,4-dimethylthiazole	1-(2,4-dimethyl-1,3-thiazol-5-yl)ethanone	CC1=C(SC(=N1)C)C(=O)C	meaty nutty sulfurous boiled meaty musty earthy coffee boiled	Sigma Aldrich, TGSC, Odoractor
1485	2,4-Dimethyl-5-vinylthiazole	5-ethenyl-2,4-dimethyl-1,3- thiazole	CC1=C(SC(=N1)C)C=C	meaty nutty cocoa	OdorRactor ,TGSC, Flavorbase
1486	2-Isobutyl-4,5- dimethylthiazole	4,5-dimethyl-2-(2-methylpropyl)- 1,3-thiazole	CC1=C(SC(=N1)CC(C)C)C	geranium green rose nutty vegetable earthy beany tomato savory	OdorRactor ,TGSC, Flavorbase
1487	Thiamine hydrochloride	2-[3-[(4-amino-2-methylpyrimidin- 5-yl)methyl]-4- methyl-1,3-thiazol- 3-ium-5- yl]ethanol;chloride;hydrochloride		sour mild bitter characteristic	Sigma Aldrich, Pubchem
1488	2-Acetyl-3-methylthiophene	1-(3-methylthiophen-2- yl)ethanone	CC1=C(SC=C1)C(=O)C	phenolic wintergreen almond floral cananga	OdorRactor ,TGSC
1489	4,5-Dimethylthiazole	4,5-dimethyl-1,3-thiazole	CC1=C(SC=N1)C	meaty nutty smoky roasted fishy green shellfish ammonical seafood savory poultry	Sigma Aldrich, TGSC, Flavorbase, OdoRactor
1490	1-(4-Methylthiazol-5- yl)ethanone	1-(4-methyl-1,3-thiazol-5- yl)ethanone	CC1=C(SC=N1)C(=O)C	nutty roasted sulfurous	TGSC
1491	4-Methyl-5-vinylthiazole	5-ethenyl-4-methyl-1,3-thiazole	CC1=C(SC=N1)C=C	chocolate nutty musty vegetable cocoa rooty beer	Sigma Aldrich, TGSC, OdoRactor
1492	4-Methyl-5-thiazoleethanol	2-(4-methyl-1,3-thiazol-5- yl)ethanol	CC1=C(SC=N1)CCO	meaty fatty nutty sulfurous cooked beefy brothy yeasty bready oily sweet buttery cheese	Sigma Aldrich, Flavorbase, TGSC
1493	2-(4-Methylthiazol-5-yl)ethyl acetate	2-(4-methyl-1,3-thiazol-5-yl)ethyl acetate	CC1=C(SC=N1)CCOC(=O)C	meaty beefy brown brothy bready nutty chicken ham	Sigma Aldrich, Flavorbase, TGSC, OdoRactor
1494	2-(4-Methylthiazol-5-yl)ethyl formate	2-(4-methyl-1,3-thiazol-5-yl)ethyl formate	CC1=C(SC=N1)CCOC=O	nutty brown	OdorRactor ,TGSC
1495	(1R,4Ar,8aS)-1-Isopropyl-7- methyl-4- methylene- 1,2,3,4,4a,5,6,8a- octahydronaphthalene	(1R, 4aR, 8aS)-7-methyl-4- methylidene-1-propan-2	CC1=C[C@H]2[C@@H](CC1)C(=C)CC[C@@H]2C(C)C	herbaceous woody spicy	TGSC
1496	2-Acetyl-3,(5 or 6)- dimethylpyrazine	1-(3,5-dimethylpyrazin-1-ium-1-yl)ethanone	CC1=C[N+](=CC(=N1)C)C(=O)C	nutty roasted hazelnut roasted peanut popcorn corn toasted grain peanut butter peanut hazelnut roasted	OdorRactor ,TGSC
1497	5-Methylquinoxaline	5-methylquinoxaline	CC1=C2C(=CC=C1)N=CC=N2	coffee nutty toasted roasted corn burnt musty hazelnut potato	Sigma Aldrich, TGSC, OdoRactor
1498	Kahweofuran	6-methyl-2,3-dihydrothieno[2,3-c]furan	CC1=C2C(=CO1)CCS2	sulfurous roasted smoky	TGSC
1499	Ethanone, 1-(5(or 6)-methyl-7(or 8)-(1-methylethyl)bicyclo(2.2.2)oct-5-en-2-yl)-	1-(5-methyl-7-propan-2-yl-2-bicyclo[2.2.2]oct-4- enyl)ethanone		woody clean spicy balsamic	OdorRactor ,TGSC
1500	5(Or 6)-Methyl-7(or 8)-(1-methylethyl)bicyclo[2.2.2]oct-5-ene-2-carbaldehyde	5-methyl-7-propan-2- ylbicyclo[2.2.2]oct-4-ene-2- carbaldehyde	CC1=C2CC(C(C1)C(C2)C(C)C)C =0	aldehydic fatty green metallic	TGSC
1501	10-Epi-gamma-Eudesmol	2-[(2R,4aS)-4a,8-dimethyl- 2,3,4,5,6,7-hexahydro- 1H -naphthalen-2-yl]propan-2-ol	CC1=C2CC(CCC2(CCC1)C)C(C) (C)O	sweet woody floral	Flavornet, TGSC
1502	gamma-Eudesmol	2-[(2R,4aR)-4a,8-dimethyl- 2,3,4,5,6,7- hexahydro-1H - naphthalen-2-yl]propan-2-ol	CC1=C2CC(CCC2(CCC1)C)C(C) (C)O	wax sweet	Flavornet
1503	Butylated hydroxytoluene	2,6-di <i>tert</i> -butyl-4-methylphenol	CC1=CC(=C(C(=C1)C(C)(C)C)O) C(C)(C) C	camphoraceous phenolic	Sigma Aldrich, TGSC, Pubchem, OdoRactor
1504	2,4,6-Trimethylphenol	2,4,6-trimethylphenol	CC1=CC(=C(C(=C1)C)O)C	coffee phenolic	Flavornet, TGSC,OdoRactor
1505	2,6-Dimethoxy-4- methylphenol	2,6-dimethoxy-4-methylphenol	CC1=CC(=C(C(=C1)OC)O)OC	phenolic smoky medicinal woody spice eugenol root caramel clove rooty	Sigma Aldrich, TGSC, OdoRactor
1506	Methyl 2,4-dihydroxy-3,6-dimethylbenzoate	methyl 2,4-dihydroxy-3,6- dimethylbenzoate	CC1=CC(=C(C(=C1C(=O)OC)O) C)O	mossy woody phenolic earthy oakmoss	Sigma Aldrich, TGSC
1507	2',4'-Dimethylacetophenone	1-(2,4-dimethylphenyl)ethanone	CC1=CC(=C(C=C1)C(=O)C)C	woody floral sweet minty mimosa	Sigma Aldrich, TGSC
1508	6-Tert-Butyl-m-cresol	2-tert -butyl-5-methylphenol	CC1=CC(=C(C=C1)C(C)(C)C)O	animal leathery	TGSC

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1512 2.4.5 friendsylphenol 2.4.4 methylbenoxidehyde 2.4.4 methylbenoxidehydehydehydehydehydehydehydehydehydehy	1510	Thymol methyl ether		CC1=CC(=C(C=C1)C(C)C)OC	chocolate coffee green musty earthy vegetable nutty spicy woody smoky burnt	
	1511	1,2,4-Trimethylbenzene		CC1=CC(=C(C=C1)C)C	plastic aromatic distinctive	Flavornet, Pubchem
Al-Dimentylbeanzidelopies	1512	2,5-Dimethylphenol	2,5-dimethylphenol	CC1=CC(=C(C=C1)C)O	1 1 2	Flavornet, TGSC
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methylberoxilabylysis	1513	2,4-Dimethylbenzaldehyde	2,4-dimethylbenzaldehyde	CC1=CC(=C(C=C1)C=O)C		
1515 2.4-Pimerhylpha 1516 2.4-Jenneshylpha 1517 2.4-Jenneshylpha 1518 2.4-Jenneshylpha 1518 2.4-Jenneshylpha 1518 2.4-Jenneshylpha 2.4-Jenn	1514		2-hydroxy-4-methylbenzaldehyde	CC1=CC(=C(C=C1)C=O)O		
1516 1517 2-14-1518 1524 1525 1525 1525 1525 1525 1525 1525 1525 1525 1525 1525 1525 1525 1525 1525 1525 1525 1525 1525 1525 1525 1525 1525 1525 1525 1525 1525 1525 1525 1525 1525 1525 1525 1525 1525 1525 1525 1525 1525 1525 1525 1525 1525 1525 1525 1525 1525 1525 1525 1525 1525 1525 1525 1525 1525 1525 1525 1525 1525 1525 1525 1525 1525 1525 1525 1525 1525 1525 1525 1525 1525 1525 1525 1525 1525 1525 1525 1525 1525 1525 1525 1525 1525 1525 1525 1525 1525 1525 1525 1525 1525 1525 1525 1525 1525 1525 1525 1525 1525 1525 1525 1525 1525 1525 1525 1525 1525 1525 1525 1525 1525 1525 1525 1525 1525 1525 1525 1525 1525 1525 1525 1525 1525 1525 1525 1525 1525 1525 1525 1525 1525 1525 1525 1525 1525 1525 1525 1525 1525 1525 1525 1525 1525 1525 1525 1525 1525 1525 1525 1525 1525 1525 1525 1525 1525 1525 1525 1525 1525 1525 1525 1525 1525 1525 1525 1525 1525 1525 1525 1525 1525 1525 1525 1525 1525 1525 1525 1525 1525 1525 1525 1525 1525 1525 1525 1525 1525 1525 1525 1525 1525 1525 1525 1525 1525 1525 1525 1525 1525 1525 1525 1525 1525 1525 1525 1525 1525 1525 1525 1525 1525 1525 1525 1525 1525 1525 1525 1525 1525 1525 1525 1525 1525 1525 1525 1525 1525 1525 1525 1525 1525 1525 1525 1525 1525 1525 1525 1525 1525 1525 1525 1525 1525 1525 1525 1525 1525 1525 1525 1525 1525 1525 1525 1525 1525 1525 1525 1525 1525 1525 1525 1525 1525 1525 1525 1525 1525 1525 1525 1525 1525 1525 1525 1525 1525 1525 1525 1525 1525 1525 1525 1525 1525 1525 1525 1525 1525 15	1515		2.4-dimethylphenol	CC1-CC(-C(C-C1)O)C	·	
Methyl 3-methylaluseta		2'-Hydroxy-5'-	1-(2-hydroxy-5-			
	1517		methyl 2-hydroxy-5-	CC1=CC(=C(C=C1)O)C(=O)OC	minty fruity cherry leathery	TGSC
1520 2.4-Dimethylanisole 1-methoxy-2.4-dimethylbenzene CC1-CC4-CC1C/CCC spicy herbaceous Sigma Aldrich, TGSC	1518	2-Tert-Butyl-4-methylphenol	•	CC1=CC(=C(C=C1)O)C(C)(C)C	leathery medicinal	TGSC
1520 2.4-Dimethylanisole 1-methoxy-2.4-dimethylbenzene CC1-CC4-CC1C/CCC spicy herbaceous Sigma Aldrich, TGSC					-	
1521 1.2,4.5-trramethylbenzene 1.2,4.5-trramethylbenzene 1.2,4.5-trramethylbenzene 1.2.5-trrimethylphenol 2.4.5-trrimethylphenol 2.4.5-trrimethylphenol 1.6.5-trrimethylphenol 1.6	1519	2-Methoxy-4-methylphenol	2-methoxy-4-methylphenol	CC1=CC(=C(C=C1)O)OC	coffee green jasmine meaty woody smoky sweet vanilla winey coaltar medicinal spicy phenolic leathery	Sigma Aldrich, AOD, TGSC
1522 2.4.5-Trimethylphenol 2.4.5-trimethylphenol 1.7.5-dimethylfuran 1.7.5-dim	1520	2,4-Dimethylanisole	1-methoxy-2,4-dimethylbenzene	CC1=CC(=C(C=C1)OC)C	spicy herbaceous	Sigma Aldrich, TGSC
1523 2-Acetyl-3,5-dimethylfuran 1-3,5-dimethylfuran-2-ylethanone 1524 3-Acetyl-2,5-dimethylfuran 1-2,5-dimethylfuran-3-tylethanone 1525 2,5-Dimethylfuran-3-tylethanone 1526 2,5-dimethylfuran-3-tylethanone 1526 2,5-dimethylfuran-3-tylethanone 1526 2,5-dimethylfuran-3-tylethanone 1526 2,5-dimethylfuran-3-tylethanone 1527 3-(2,5-dimethylfuran-3-tylethanone) 1528 3-(2,5-dimethylfuran-3-tylethanone) 1528 3-(2,5-dimethylfuran-3-tylethanone) 1528 3-(2,5-dimethylfuran-3-tylethanone) 1529 2,5-dimethylfuran-3-tylethanone 1529 2,5-dimethylfuran-3-tylethanone 1529 2,5-dimethylfuran-3-ylethanone 1520 2,5-dimethylfuran-3-ylethan	1521	1,2,4,5-Tetramethylbenzene	1,2,4,5-tetramethylbenzene	CC1=CC(=C(C=C1C)C)C	rancid sweet camphoraceous	Flavornet, TGSC, Pubchem
1524 3-Acetyl-2,5-dimethylfuran 1-(2,5-dimethylfuran-3-ybehanone 1-(2,5-dimethylfuran-3-ybehanone 1-(2,5-dimethylfuran-3-ybehanone 1-(2,5-dimethylfuran-3-thiol 2,5-dimethylfuran-3-thiol 2,5-dimethylfuran-3-thiol 2,5-dimethylfuran-3-ybehanone 1-(2,5-dimethylfuran-3-ybehanone 1-(3,5-dimethylfuran-3-ybehanone	1522	2,4,5-Trimethylphenol		CC1=CC(=C(C=C1C)O)C	phenolic chemical	TGSC
1524 3-Acetyl-2.5-dimethylfuran 1-2.5-dimethylfuran-3-thiol 2.5-dimethylfuran-3-thiol 2.5-dimethylfuran-3-thiol 2.5-dimethylfuran-3-thiol 2.5-dimethylfuran-3-thiol 2.5-dimethylfuran-3-thiol 2.5-dimethylfuran-3-thiol CCI=CC(=C(0))C)SC(=O)C fruity floral tropical OdorRactor, TGSC	1523	2-Acetyl-3,5-dimethylfuran		CC1=CC(=C(O1)C(=O)C)C	sweet balsamic	OdorRactor ,TGSC
1525 2,5-Dimethylfuran-3-thiol 2,5-dimethylfuran-3-thiol 2,5-dimethylfuran-3-thiol CC1=CC(=C(O1)C)S meaty sulfurous lamb Flavornet, TGSC, OdoRacto CC1=CC(=C(O1)C)SC(=O)C fruity floral tropical OdorRactor, TGSC dimethyl-3-furanyl) ester dimethyl-3-furanyl) ester CC1=CC(=C(O1)C)SC(=O)C=C ceco CC2 ceco CC3 ceco CC4 ceco CC4 ceco c	1524	3-Acetyl-2,5-dimethylfuran	1-(2,5-dimethylfuran-3-	CC1=CC(=C(O1)C)C(=O)C	cocoa leathery corn powdery	
dimethyl-3-furanyl) ester	1525	2,5-Dimethylfuran-3-thiol	2,5-dimethylfuran-3-thiol	CC1=CC(=C(O1)C)S		Flavornet, TGSC, OdoRactor
1527 S-(2,5-Dimethyl-3-furanyl) 2 carbothioate 2-carbothioate 3-carbothioate 3-	1526			CC1=CC(=C(O1)C)SC(=O)C	fruity floral tropical	OdorRactor ,TGSC
1528 S-(2,5-Dimethylfuran-3-yl) S -(2,5-dimethylfuran-3-yl) furan-3-carbothioate Occ2 Coffee roasted meat meaty OdorRactor ,TGSC	1527	S-(2,5-Dimethyl-3-furanyl) 2-	S -(2,5-dimethylfuran-3-yl) furan-		vegetable	TGSC
1529 2,5-Dimethyl-3-	1528	S-(2,5-Dimethylfuran-3-yl)	S -(2,5-dimethylfuran-3-yl) furan-	CC1=CC(=C(O1)C)SC(=O)C2=C	coffee roasted meat meaty	OdorRactor ,TGSC
1530 2,5-Dimethyl-3- (methylditho)furan (methylditho)furan (methylditho)furan (methylditho)furan (methylditho)furan (methylditho)furan (methylditho)furan (methylditho)furan (methylditho)furan (methylditho)furan (methylditho)furan (methylditho)furan (methylditho)furan (methylditho)furan (methylditho)furan (methylditho)furan (methylditho)furan (methylditho)furan (methylditho)furan (methylditho)furan (methylditho)furan (methylditho)furan (methylditho)furan (methylditho)furan (methylditho)furan (methylditho)furan (methylditho)furan (methylditho)furan (methylditho)furan (methylditho)furan (methylditho)furan (methylditho)furan (methylditho)furan (methylditho)furan (methylditho)furan (methylditho)furan (methylditho)furan (methylditho)furan (methylditho)furan (methylditho)furan (methylditho)furan (methylditho)furan (methylditho)furan (methylditho)furan (methylditho)furan (methylditho)furan (methylditho)furan (methylditho)furan (methylditho)furan (methylditho)furan (methylditho)furan (methylditho)furan (methylditho)furan (methylditho)furan (methylditho)furan (methylditho)furan (methylditho)furan (methylditho)furan (methylditho)furan (methylditho)furan (methylditho)furan (methylditho)furan (methylditho)furan (methylditho)furan (methylditho)furan (methylditho)furan (methylditho)furan (methylditho)furan (methylditho)furan (methylditho)furan (methylditho)furan (methylditho)furan (methylditho)furan (methylditho)furan (methylditho)furan (methylditho)furan (methylditho)furan (methylditho)furan (methylditho)furan (methylditho)furan (methylditho)furan (methylditho)furan (methylditho)furan (methylditho)furan (methylditho)furan (methylditho)furan (methylditho)furan (methylditho)furan (methylditho)furan (methylditho)furan (methylditho)furan (methylditho)furan (methylditho)furan (methylditho)furan (methylditho)furan (methylditho)furan (methylditho)furan (methylditho)furan (methylditho)furan (methylditho)furan (methylditho)furan (methylditho)furan (methylditho)furan (methylditho)furan (methylditho)furan (methylditho)furan (methyl	1529	2,5-Dimethyl-3-	S -(2,5-dimethylfuran-3-yl) 3-	CC1=CC(=C(O1)C)SC(=O)CC(C)	roasted creamy cocoa	OdorRactor ,TGSC
1531 3,3'-Dithiobis(2,5-dimethylfuran) 3-4(2,5-dimethylfuran) 2-2 3-4(2,5-dimethylfuran) 3-4 3-4 3-4 3-4 3-4 3-4 3-4 3-4 3-4 3-4 3-4 3-4 3-4 3-4 3-4 3-4 3-4 3-4 3-4 3-4 3-4 3-4 3-4 3-4 3-4 3-4 3-4 3-4 3-4 3-4 3-4 3-4 3-4 3-4 3-4 3-4 3-4 3-4 3-4 3-4 3-4 3-4 3-4 3-4 3-4 3-4 3-4 3-4 3-4 3-4 3-4 3-4 3-4 3-4 3-4 3-4 3-4 3-4 3-4 3-4 3-4 3-4 3-4 3-4 3-4 3-4 3-4 3-4 3-4 3-4 3-4 3-4 3-4 3-4 3-4 3-4 3-4 3-4 3-4 3-4 3-4 3-4 3-4 3-4 3-4 3-4 3-4 3-4 3-4 3-4 3-4 3-4 3-4 3-4 3-4 3-4 3-4 3-4 3-4 3-4 3-4 3-4 3-4 3-4 3-4 3-4 3-4 3-4 3-4 3-4 3-4 3-4 3-4 3-4 3-4 3-4 3-4 3-4 3-4 3-4 3-4 3-4 3-4 3-4 3-4 3-4 3-4 3-4 3-4 3-4 3-4 3-4 3-4 3-4 3-4 3-4 3-4 3-4 3-4 3-4 3-4 3-4 3-4 3-4 3-4 3-4 3-4 3-4 3-4 3-4 3-4 3-4 3-4 3-4 3-4 3-4 3-4 3-4 3-4 3-4 3-4 3-4 3-4 3-4 3-4 3-4 3-4 3-4 3-4 3-4 3-4 3-4 3-4 3-4 3-4 3-4 3-4 3-4 3-4 3-4 3-4 3-4 3-4 3-4 3-4 3-4 3-4 3-4 3-4 3-4 3-4 3-4 3-4 3-4 3-4 3-4 3-4 3-4 3-4 3-4 3-4 3-4 3-4 3-4 3-4 3-4 3-4 3-4 3-4 3-4 3-4 3-4 3-4 3-4 3-4 3-4 3-4 3-4 3-4 3-4 3-4 3-4 3-4 3-4 3-4 3-4 3-4 3-4 3-4 3-4 3-4 3-4 3-4 3-4 3-4 3-4 3-4 3-4 3-4 3-4 3-4 3-4 3-4 3-4 3-4 3-4 3-4 3-4 3-4 3-4 3-4 3-4 3-4 3-4 3-4 3-4 3-4 3-4 3-4 3-4 3-4 3-4 3-4 3-4 3-4 3-4 3-4 3-4 3-4 3-4 3-4 3-4 3-4 3-4 3-4 3-4 3-4 3-4 3-4 3-4 3-4 3-4 3-4 3-4 3-4 3-4 3-4 3-4 3-4 3-4 3-4 3-4 3-4 3-4 3-4 3-4 3-4 3-4 3-4 3-4 3-4 3-4 3-4 3-4 3-4 3-4 3-4 3-4 3-4 3-4 3-4 3-4 3-4 3-4 3-4 3-4 3-4 3-4 3-4 3-4 3-4 3-4 3-4 3-4 3	1530	2,5-Dimethyl-3-	2,5-dimethyl-3-		roasted meat meaty	Flavorbase
dimethylfuran) yl)disulfanyl]-2,5- dimethylfuran 1-(3-Hydroxy-5-methyl-2-thienyl)ethanone	1531			CC1=CC(=C(O1)C)SSC2=C(OC(meaty	OdorRactor .TGSC
thienyl)ethanone yl)ethanone CCl=CC(=C(S1)C)C(=O)C nutty meaty roasted burnt ADB, TGSC, OdoRactor						
3-Acetyl-2,5-dimethylthiophene 1-(2,5-dimethylthiophen-3-ylbethanone 1-(2,5-dimethylthiophene	1532			CC1=CC(=C(S1)C(=O)C)O	meaty brown roasted cooked	OdorRactor ,TGSC
3-methoxy-5-methylphenol 3-methoxy-5-methylphenol 3-methoxy-5-methylphenol CC1=CC(=CC(=C1)OC)O fruity woody hay oakmoss marine mossy OdorRactor ,TGSC	1533	3-Acetyl-2,5-	1-(2,5-dimethylthiophen-3-	CC1=CC(=C(S1)C)C(=O)C	nutty meaty roasted burnt	ADB, TGSC, OdoRactor
1-(4-tert -butyl-2,6-dimethylacetophenone 1-(4-tert -butyl-2,6-dimethylacetophenone 1-(3-xylene 1,3-xylene 1,3-xylene 1,3-xylene CC1=CC(=CC1)C CC1=CC(=CC1)C Sweet aromatic solvent sweet organic chemical Flavornet, Pubchem Flavornet, Pubchem 1537 3-Methylbenzaldehyde 3-methylbenzaldehyde CC1=CC(=CC=C1)C=O fruity sweet cherry bitter almond phenolic bitter TGSC,OdoRactor TGSC T	1534			CC1=CC(=CC(=C1)OC)O		OdorRactor ,TGSC
1536 M-Xylene 1,3-xylene CC1=CC(=CC=C1)C plastic sweet aromatic solvent sweet organic chemical fruity sweet cherry bitter almond phenolic bitter divided phenolic bitter almond phenolic bitter almond phenolic bitter almond phenolic bitter almond phenolic bitter divided phenolic bitter almond phenol	1535	• '			woody rose musk orange flower	OdorRactor ,TGSC
3-Methylbenzaldehyde 3-methylbenzaldehyde CC1=CC(=CC=C1)C=O fruity sweet cherry bitter almond phenolic bitter TGSC,OdoRactor TGSC	1536	, i			plastic sweet aromatic solvent	Flavornet, Pubchem
Majantol 2,2-dimethyl-3-(3-methylphenyl)propan-1-ol pol polymethylphenyl)propan-1-ol pol polymethylphenyl)pentan-1-ol pol polymethylphenyl)pentan-1-ol pol polymethylphenyl)pentan-1-ol pol polymethylphenyl)pentan-1-ol pol polymethylphenyl)pentan-1-ol pol polymethylphenyl)pentan-1-ol polymethylphenyl polymethylphenyl)pentan-1-ol polymethylphenyl henylphenylphenylphenylphenylphenylphenylphenylphenylphenylphenylphenylphenylphenylphenylphenylphenylphenylphenylphenylphenylphenylphenylphenylphenylphenylphenylphenylphenylphenylphenylphenylphenylphenylphenylphenylphenylphenylphenylphenylphenylphenylphenylphenylphenylphenylphenylphenylphenylphenylphenylphenylphenylphenylphenylphenylphenylphenylphenylphenylphenylphenylphenylphenylphenylphenylphenylphenylphenylphenylphenylphenylphenylphenylphenylphenylphenylphenylphenylphenylphenylphenylphenylphenylphenylphenylphenylphenylphenylphenylphenylphenylphenylphenylphenylphenylphenylphenylphenylphenylphenylphenylphenylphenylphenylphenylphenylphenylphenylphenylphenylphe	1537	3-Methylbenzaldehyde	3-methylbenzaldehyde	CC1=CC(=CC=C1)C=O	fruity sweet cherry bitter almond	-
1539 5-(3-Methylphenyl)pentan-1- ol OdorRactor ,TGSC ol Picture ol Picture ol Picture ol Picture ol Picture ol Picture ol Picture ol Picture ol Picture ol Picture ol Picture ol Picture ol Picture ol Picture ol Picture ol Picture ol Picture ol Picture ol Picture ol Picture ol Picture ol Picture ol Picture ol Picture ol Picture ol Picture ol Picture ol Picture ol Picture ol Picture ol Picture ol Picture ol Picture ol Picture ol Picture ol Picture ol Picture ol Picture ol Picture ol Picture ol Picture ol Picture ol Picture ol Picture ol Picture ol Picture ol Picture ol Picture ol Picture ol Picture ol Picture ol Picture ol Picture ol Picture ol Picture ol Picture ol Picture ol Picture ol Picture ol Picture ol Picture ol Picture ol Picture ol Picture ol Picture ol Picture ol Picture ol Picture ol Picture ol Picture ol Picture ol Picture ol Picture ol Picture ol Picture ol Picture ol Picture ol Picture ol Picture ol Picture ol Picture ol Picture ol Picture ol Picture ol Picture ol Picture ol Picture ol Picture ol Picture ol Picture ol Picture ol Picture ol Picture ol Picture ol Picture ol Picture ol Picture ol Picture ol Picture ol Picture ol Picture ol Picture ol Picture ol Picture ol Picture ol Picture ol Picture ol Picture ol Picture ol Picture ol Picture ol Picture ol Picture ol Picture ol Picture ol Picture ol Picture ol Picture ol Picture ol Picture ol Picture ol Picture ol Picture ol Picture ol Picture ol Picture ol Picture ol Picture ol Picture ol Picture ol Picture ol Picture ol Picture ol Picture ol Picture ol Picture ol Picture ol Picture ol Picture ol Picture ol Picture ol Picture ol Picture ol Picture ol Picture ol Picture ol Picture ol Picture ol Picture ol Picture ol Picture ol Picture ol Picture ol Picture ol Picture ol Picture ol Picture ol Picture ol Picture ol Picture ol Picture ol Picture ol Picture ol Picture ol Picture ol Picture ol Picture ol Picture ol Picture ol Picture ol Picture ol Picture ol Picture ol Picture ol Picture ol Picture ol Picture ol Picture ol Picture ol Picture ol Picture ol	1538	Majantol		CC1=CC(=CC=C1)CC(C)(C)CO	*	
muguet 1541 m-Cresol 3-methylphenol CC1=CC(=CC=C1)O medicinal woody ethereal fecal plastic leathery phenolic dry tarry coaltar sweet 1542 3-Methylanisole 1-methoxy-3-methylbenzene CC1=CC(=CC=C1)OC floral narcissus TGSC 1543 M-Tolyl acetate (3-methylphenyl) acetate CC1=CC(=CC=C1)OC(=O)C pungent floral phenolic narcissus OdorRactor ,TGSC 1544 m-Cresyl phenylacetate (3-methylphenyl) 2-phenylacetate CC1=CC(=CC=C1)OC(=O)CC2= floral ylang OdorRactor ,TGSC 1545 m-Cresyl phenylacetate (3-methylphenyl) 2-phenylacetate CC1=CC(=CC=C1)OC(=O)CC2= floral ylang OdorRactor ,TGSC 1546 m-Cresyl phenylacetate (3-methylphenyl) 2-phenylacetate CC1=CC(=CC=C1)OC(=O)CC2= floral ylang OdorRactor ,TGSC 1547 m-Cresyl phenylacetate (3-methylphenyl) 2-phenylacetate CC1=CC(=CC=C1)OC(=O)CC2= floral ylang OdorRactor ,TGSC 1548 m-Cresyl phenylacetate (3-methylphenyl) 2-phenylacetate CC1=CC(=CC=C1)OC(=O)CC2= floral ylang OdorRactor ,TGSC 1549 m-Cresyl phenylacetate (3-methylphenyl) 2-phenylacetate CC1=CC(=CC=C1)OC(=O)CC2= floral ylang OdorRactor ,TGSC 1540 m-Cresyl phenylacetate (3-methylphenyl) 2-phenylacetate CC1=CC(=CC=C1)OC(=O)CC2= floral ylang OdorRactor ,TGSC 1541 m-Cresyl phenylacetate (3-methylphenyl) 2-phenylacetate CC1=CC(=CC=C1)OC(=O)CC2= floral ylang OdorRactor ,TGSC floral ylang 1539	5-(3-Methylphenyl)pentan-1-		CC1=CC(=CC=C1)CCCCCO	rose floral blossom wax geranium	OdorRactor ,TGSC	
1541 m-Cresol 3-methylphenol CC1=CC(=CC=C1)O medicinal woody ethereal fecal plastic leathery phenolic dry tarry coaltar sweet 1542 3-Methylanisole 1-methoxy-3-methylbenzene CC1=CC(=CC=C1)OC floral narcissus TGSC, Pubchem Coaltar sweet 1543 M-Tolyl acetate (3-methylphenyl) acetate CC1=CC(=CC=C1)OC(=O)C pungent floral phenolic narcissus OdorRactor ,TGSC 1544 m-Cresyl phenylacetate (3-methylphenyl) 2-phenylacetate CC1=CC(=CC=C1)OC(=O)CC2= floral ylang OdorRactor ,TGSC	1540	01 2-(3-Methylphenyl)ethanol	2-(3-methylphenyl)ethanol	CC1=CC(=CC=C1)CCO	floral rose jasmine lilac woody	OdorRactor ,TGSC
1542 3-Methylanisole 1-methoxy-3-methylbenzene CC1=CC(=CC=C1)OC floral narcissus TGSC 1543 M-Tolyl acetate (3-methylphenyl) acetate CC1=CC(=CC=C1)OC(=O)C pungent floral phenolic narcissus OdorRactor ,TGSC 1544 m-Cresyl phenylacetate (3-methylphenyl) 2-phenylacetate CC1=CC(=CC=C1)OC(=O)CC2= floral ylang OdorRactor ,TGSC CC=CC=CC C2	1541	m-Cresol	3-methylphenol	CC1=CC(=CC=C1)O	medicinal woody ethereal fecal plastic leathery phenolic dry tarry	Sigma Aldrich, Flavornet, Flavorbase, TGSC, Pubchem
1543 M-Tolyl acetate (3-methylphenyl) acetate CC1=CC(=CC=C1)OC(=O)C pungent floral phenolic narcissus OdorRactor ,TGSC 1544 m-Cresyl phenylacetate (3-methylphenyl) 2-phenylacetate CC1=CC(=CC=C1)OC(=O)CC2= floral ylang OdorRactor ,TGSC CC=CC=C2	1542	3-Methylanisole	1-methoxy-3-methylbenzene	CC1=CC(=CC=C1)OC		TGSC
CC=CC= C2			·			
	1544	m-Cresyl phenylacetate	(3-methylphenyl) 2-phenylacetate		floral ylang	OdorRactor ,TGSC
=C2	1545	3-Phenoxytoluene	1-methyl-3-phenoxybenzene	CC1=CC(=CC=C1)OC2=CC=CC	floral fruity rose geranium	TGSC

1546	2,4,6-Trimethylpyridine	2,4,6-trimethylpyridine	CC1=CC(=NC(=C1)C)C	fishy animal leathery tobacco	Flavorbase,OdoRactor
10.0				musty aromatic	·
1547	2,4-Dimethylpyridine	2,4-dimethylpyridine	CC1=CC(=NC=C1)C	smoky phenolic	OdorRactor ,TGSC
1548	Piperitenone	3-methyl-6-propan-2- ylidenecyclohex-2-en-1-one	CC1=CC(=0)C(=C(C)C)CC1	minty phenolic	OdorRactor ,TGSC
1549	d-Piperitone	(6S)-3-methyl-6-propan-2- ylcyclohex-2-en-1-one	CC1=CC(=O)C(CC1)C(C)C	herbaceous minty mentholic peppermint strong fresh	OdoRactor ,TGSC, Flavorbase
1550	(R)-6-(Isopropyl)-3- methylcyclohex-2-en-1- one	(6R)-3-methyl-6-propan-2-ylcyclohex-2-en-1-one	CC1=CC(=O)C(CC1)C(C)C	pungent minty peppermint harsh herbaceous	OdorRactor ,TGSC, Flavorbase
1551	Piperitone	3-methyl-6-propan-2-ylcyclohex-2- en-1-one	CC1=CC(=O)C(CC1)C(C)C	sweet fruit minty fresh herbaceous camphoraceous medicinal	TGSC, Flavornet
1552	Umbellulon	4-methyl-1-propan-2- ylbicyclo[3.1.0]hex-3-en-2- one	CC1=CC(=O)C2(C1C2)C(C)C	minty pungent	SuperScent, TGSC
1553	(+)-Verbenone	(1 <i>R</i> ,5 <i>R</i>)-4,6,6- trimethylbicyclo[3.1.1]hept-3-en-2- one	CC1=CC(=O)C2CC1C2(C)C	camphoraceous mentholic celery	OdorRactor ,TGSC
1554	Verbenone	4,6,6-trimethylbicyclo[3.1.1]hept- 3-en-2-one	CC1=CC(=O)C2CC1C2(C)C	spicy minty camphoraceous	OdorRactor ,TGSC
1555	(-)-Verbenone	(1 <i>S</i> ,5 <i>S</i>)-4,6,6- trimethylbicyclo[3.1.1]hept-3-en-2- one	CC1=CC(=0)C2CC1C2(C)C	spicy minty vanilla camphoraceous	Sigma Aldrich, TGSC
1556	2-Cyclohexen-1-one, 4- hydroxy-4-(3- hydroxy-1- butenyl)-3,5,5-trimethyl-	4-hydroxy-4-(3-hydroxybut-1-enyl)-3,5,5- trimethylcyclohex-2-en-1-one	CC1=CC(=0)CC(C1(C=CC(C)0) 0)(C)C	fruity floral woody	Flavorbase
1557	Isophorone	3,5,5-trimethylcyclohex-2-en-1- one	CC1=CC(=0)CC(C1)(C)C	berry green woody vegetable citrus nutty camphoraceous wax herbaceous sweet tobacco winey cooling fruity musty cedar leathery sharp peppermint	Sigma Aldrich, Flavorbase, TGSC, Pubchem
1558	2,6,6-Trimethylcyclohex-2- ene-1,4-dione	2,6,6-trimethylcyclohex-2-ene-1,4-dione	CC1=CC(=O)CC(C1=O)(C)C	musty woody sweet tea tobacco leafy citrus lemon brown	Sigma Aldrich, TGSC, Odoractor
1559	3-Oxo-alpha-ionol	4-[(E)-3-hydroxybut-1-enyl]-3,5,5- trimethylcyclohex-2-en-1-one	CC1=CC(=O)CC(C1C=CC(C)O)(C)C	spice	Flavornet, TGSC
1560	3-Methyl-2-cyclopenten-1- one	3-methylcyclopent-2-en-1-one	CC1=CC(=O)CC1	sweet fruity fatty	Sigma Aldrich, TGSC, OdoRactor
1561	3-Methyl-2-cyclohexen-1-one	3-methylcyclohex-2-en-1-one	CC1=CC(=O)CCC1	sweet walnut almond benzoin caramel cherry medicinal nutty phenolic fruity	Sigma Aldrich, OdoRactor
1562	4,6-Dimethyl-2H-pyran-2-one	4,6-dimethylpyran-2-one	CC1=CC(=O)OC(=C1)C	sweet caramel sugar green licorice balsamic gourmand	OdorRactor ,TGSC
1563	p-Menth-1-en-3-ol	3-methyl-6-propan-2-ylcyclohex-2- en-1-ol	CC1=CC(C(CC1)C(C)C)O	herbaceous	Flavornet,OdoRactor
1564	2,4,4,6-Tetramethylcyclohexa- 2,5-dien-1- one	2,4,4,6-tetramethylcyclohexa-2,5-dien-1-one	CC1=CC(C=C(C1=O)C)(C)C	warm sweet minty woody natural green hay	TGSC
1565	(S)-cis-Verbenol	(1 <i>S</i> ,2 <i>S</i> ,5 <i>S</i>)-4,6,6- trimethylbicyclo[3.1.1]hept-3- en- 2-ol	CC1=CC(C2CC1C2(C)C)O	balsamic	TGSC
1566	Verbenol	4,6,6-trimethylbicyclo[3.1.1]hept-3-en-2-ol	CC1=CC(C2CC1C2(C)C)O	pine herbaceous fresh ozone	OdorRactor ,TGSC
1567	4,6,6- Trimethylbicyclo[3.1.1]hept-3- en-2-yl acetate	(4,6,6-trimethyl-2-bicyclo[3.1.1]hept-3-enyl) acetate	CC1=CC(C2CC1C2(C)C)OC(=O) C	spicy	OdorRactor ,TGSC
1568	2,3-Dihydro-5-methyl-3- thiophenethiol	5-methyl-2,3-dihydrothiophene-3-thiol	CC1=CC(CS1)S	rubbery meaty	TGSC
1569	1-Methyl-4-(prop-1-en-2- yl)benzene	1-methyl-4-prop-1-en-2-ylbenzene	CC1=CC=C(C=C1)C(=C)C	clove citrus pine phenolic spicy styrene musty coffee nutty guaiacol lemon	Sigma Aldrich, Flavorbase, TGSC, OdoRactor
1570	4'-Methylacetophenone	1-(4-methylphenyl)ethanone	CC1=CC=C(C=C1)C(=O)C	hawthorn fruity bitter almond floral sweet mimosa coumarinic cherry acacia powdery naphthyl vanilla bitter	Sigma Aldrich, TGSC,OdoRactor
1571	Methyl 4-methylbenzoate	methyl 4-methylbenzoate	CC1=CC=C(C=C1)C(=O)OC	sweet anisic floral ylang unpleasant	TGSC, Pubchem
1572	2-(4-Methylphenyl)propan-2- ol	2-(4-methylphenyl)propan-2-ol	CC1=CC=C(C=C1)C(C)(C)O	walnut citrus musty sweet fruity cherry coumarinic cooling floral camphoraceous celery herbaceous	Sigma Aldrich, OdoRactor, Pubchem
1573	P-Cymene	1-methyl-4-propan-2-ylbenzene	CC1=CC=C(C=C1)C(C)C	citrus gasoline solvent terpenic fresh woody spicy chemical lemon cumin origanum cilantro strong sweet aromatic pleasant	Sigma Aldrich, Flavorbase, TGSC, Pubchem

1574	Cumin oil	(1R, 5S)-6,6-dimethyl-2-methylidenebicyclo[3,1,1]heptane; 1-methyl-4-propan-2-ylbenzene;4-	CC1=CC=C(C=C1)C(C)C.CC(C) C1=CCC (=CC1)C=O.CC(C)C1=CC=C(C=	sweet cumin fatty sweaty pepper green vegetable	Sigma Aldrich, TGSC
		propan-2-ylbenzaldehyde;4- propan-2-ylcyclohexa-1,4-diene-1- carbaldehyde	C1)C=O.		
1575	2-(4-Methylphenyl)propanal	2-(4-methylphenyl)propanal	CC1=CC=C(C=C1)C(C)C=O	floral green sweet woody herbaceous powdery	OdorRactor ,TGSC
1576	alpha-Curcumene	1-methyl-4-(6-methylhept-5-en-2-yl)benzene	CC1=CC=C(C=C1)C(C)CCC=C(C)C	herbaceous	Flavornet
1577	1-(4-Methylphenyl)ethanol	1-(4-methylphenyl)ethanol	CC1=CC=C(C=C1)C(C)O	sweet hawthorn floral nutty powdery	OdorRactor ,TGSC
1578	p-Methylcinnamaldehyde	(E)-3-(4-methylphenyl)prop-2-enal	CC1=CC=C(C=C1)C=CC=O	spicy cinnamyl	OdorRactor ,TGSC
1579 1580	4-Methylbenzaldehyde 4-Methylbiphenyl	4-methylbenzaldehyde 1-methyl-4-phenylbenzene	CCI=CC=C(C=C1)C=O CCI=CC=C(C=C1)C2=CC=CC= C2	fruity phenolic cherry floral chocolate fennel spicy minty herbaceous floral wintergreen anisic wax tarragon cooling	Sigma Aldrich, TGSC Sigma Aldrich, TGSC,OdoRactor
1581	Benzeneethanol, alpha,alpha,4-trimethyl-	2-methyl-1-(4- methylphenyl)propan-2-ol	CC1=CC=C(C=C1)CC(C)(C)O	floral green cumin muguet	OdorRactor ,TGSC
1582	2-Methyl-3-(p- tolyl)propionaldehyde	2-methyl-3-(4- methylphenyl)propanal	CC1=CC=C(C=C1)CC(C)C=0	orange sweet amber woody aldehydic fresh cyclamen dry costus floral fruity citrus green powdery melon velvet muguet	OdorRactor ,TGSC, Flavorbase
1583	(4- Methylphenyl)acetaldehyde	2-(4-methylphenyl)acetaldehyde	CC1=CC=C(C=C1)CC=O	sweet green lilac fresh cortex narcissus nutty phenolic fruity	OdorRactor ,TGSC
1584	4-(4-Methylphenyl)-2- butanone	4-(4-methylphenyl)butan-2-one	CC1=CC=C(C=C1)CCC(=O)C	sweet fruity floral raspberry plum gardenia	OdorRactor ,TGSC
	Benzenepropanal, 4-methyl- 2-(4-Methylphenyl)ethanol	3-(4-methylphenyl)propanal 2-(4-methylphenyl)ethanol	CC1=CC=C(C=C1)CCC=O CC1=CC=C(C=C1)CCO	lily lilac floral heliotrope floral balsamic rose green	OdorRactor, TGSC
1586 1587	4-Methylbenzyl alcohol	(4-methylphenyl)methanol	CC1=CC=C(C=C1)CC0	floral pleasant green rose leafy	TGSC, Flavorbase
1588	4-Methylbenzyl acetate	(4-methylphenyl)methyl acetate	CC1=CC=C(C=C1)COC(=O)C	sweet balsamic sweet floral fruity green hyacinth hawthorn cilantro herbaceous privet	OdorRactor ,TGSC
1589	P-Cresol	4-methylphenol	CC1=CC=C(C=C1)O	medicinal phenolic smoky animal mimosa narcissus sweet tarry	Sigma Aldrich, TGSC, Pubchem
1590	1-Methoxy-4-methylbenzene	1-methoxy-4-methylbenzene	CC1=CC=C(C=C1)OC	cedar camphoraceous sweet vanilla naphthyl narcissus ylang powdery nutty minty strong floral pungent sharp fruity	Sigma Aldrich, TGSC, OdoRactor, Pubchem
1591	p-Tolyl acetate	(4-methylphenyl) acetate	CC1=CC=C(C=C1)OC(=O)C	anisic phenolic animal narcissus floral	Sigma Aldrich, TGSC,OdoRactor
1592	p-Tolyl isobutyrate	(4-methylphenyl) 2- methylpropanoate	CC1=CC=C(C=C1)OC(=O)C(C)C	animal floral lily narcissus green fruity	OdorRactor ,TGSC
1593	p-Cresyl isovalerate	(4-methylphenyl) 3- methylbutanoate	CC1=CC=C(C=C1)OC(=O)CC(C) C	tobacco animal sweet herbaceous	OdorRactor ,TGSC
1594	p-Tolyl phenylacetate	(4-methylphenyl) 2-phenylacetate	CC1=CC=C(C=C1)OC(=O)CC2= CC=CC= C2	hyacinth animal rose honey lily narcissus	Sigma Aldrich, TGSC, OdoRactor
1595	1-Methyl-4-phenoxybenzene	1-methyl-4-phenoxybenzene	CC1=CC=C(C=C1)OC2=CC=CC =C2	rose floral narcissus	OdorRactor ,TGSC
1596	Methyl (p-tolyloxy)acetate	methyl 2-(4- methylphenoxy)acetate	CC1=CC=C(C=C1)OCC(=O)OC	wild fruity fatty	SuperScent, TGSC, OdoRactor
1597	(4- Methylphenoxy)acetaldehyde	2-(4-methylphenoxy)acetaldehyde	CC1=CC=C(C=C1)OCC=O	hay melon ozone floral seaweed marine	OdorRactor ,TGSC
1598	2-(4-Methylphenoxy)ethanol	2-(4-methylphenoxy)ethanol	CC1=CC=C(C=C1)OCCO	floral jasmine animal	TGSC
1599	Benzene, 1-(2- methoxyethoxy)-4-methyl-	1-(2-methoxyethoxy)-4- methylbenzene	CC1=CC=C(C=C1)OCCOC	fresh green privet cortex earthy nasturtium phenolic melon animal	TGSC
1600	2-(p-Tolyloxy)ethyl acetate	2-(4-methylphenoxy)ethyl acetate	CC1=CC=C(C=C1)OCCOC(=O)C	floral jasmine gardenia fruity balsamic	TGSC
1601	p-Mentha-1,3,8-triene	1-methyl-4-prop-1-en-2- ylcyclohexa-1,3-diene	CC1=CC=C(CC1)C(=C)C	turpentine camphoraceous herbaceous woody oily chemical cooling pine thyme tropical terpenic	OdorRactor ,TGSC
1602	alpha-Terpinene	1-methyl-4-propan-2-ylcyclohexa- 1,3-diene	CCI=CC=C(CCI)C(C)C	berry green lemon medicinal woody pepper sweet terpenic citrus camphoraceous thyme spicy juicy	Sigma Aldrich, Flavornet, TGSC
1603	2-Methyl-5-prop-1-en-2- ylcyclohexa-2,4- dien-1-ol	2-methyl-5-prop-1-en-2- ylcyclohexa-2,4-dien-1-ol	CC1=CC=C(CC1O)C(=C)C	oily herbaceous	Flavornet
1604	1-(5-Methyl-1h-pyrrol-2-yl)ethanone	1-(5-methyl-1 <i>H</i> -pyrrol-2-yl)ethanone	CC1=CC=C(N1)C(=O)C	earthy roasted	OdorRactor ,TGSC

1605	2,5-Dimethylfuran	2,5-dimethylfuran	CC1=CC=C(O1)C	chemical ethereal meaty roasted beefy bacon gravy juicy	OdorRactor ,TGSC
1606	2-Acetyl-5-methylfuran	1-(5-methylfuran-2-yl)ethanone	CC1=CC=C(O1)C(=O)C	musty hay coconut coumarinic sweet caramel milky nutty	Sigma Aldrich, OdoRactor
1607	3-(5-Methyl-2-furyl)butanal	3-(5-methylfuran-2-yl)butanal	CC1=CC=C(O1)C(C)CC=O	green vegetable fruity fatty watermelon cucumber cyclamen floral	OdorRactor ,TGSC, Sigma Aldrich
1608	3-(5-Methyl-2-furyl)prop-2-enal	(E)-3-(5-methylfuran-2-yl)prop-2-enal	CC1=CC=C(O1)C=CC=O	sweet spicy	OdorRactor,
1609	5-Methylfurfural	5-methylfuran-2-carbaldehyde	CC1=CC=C(O1)C=O	almond caramel spicy sweet burnt sugar maple bready brown coffee	Sigma Aldrich, TGSC,OdoRactor
1610	5-Methyl-2-furanmethanethiol	(5-methylfuran-2-yl)methanethiol	CC1=CC=C(O1)CS	sulfurous roasted coffee coffee roasted	Flavornet, TGSC
1611	2-Methyl-5-(methylthio)furan	2-methyl-5-methylsulfanylfuran	CC1=CC=C(O1)SC	sulfurous onion garlic coffee mustard horseradish pungent	OdorRactor ,TGSC
1612	2,5-Dimethylthiophene	2,5-dimethylthiophene	CC1=CC=C(S1)C	pepper nutty sulfurous	Sigma Aldrich, TGSC,OdoRactor
1613	2-Acetyl-5-methylthiophene	1-(5-methylthiophen-2- yl)ethanone	CC1=CC=C(S1)C(=O)C	spicy sweet honey hawthorn almond acacia hyacinth caramel	TGSC,OdoRactor
1614	5-Methyl-2- thiophenecarboxaldehyde	5-methylthiophene-2-carbaldehyde	CC1=CC=C(S1)C=O	graham cracker sweet bitter almond furfural woody cherry sulfurous bready bitter	Sigma Aldrich, TGSC, OdoRactor
1615	Cycloionone	2,5,5,8 <i>a</i> -tetramethyl-7,8-dihydro-6 <i>H</i> -chromene	CC1=CC=C2C(CCCC2(O1)C)(C)	woody cedar raspberry orris root	OdorRactor ,TGSC
1616	Eucarvone	2,6,6-trimethylcyclohepta-2,4-dien- 1-one	CC1=CC=CC(CC1=O)(C)C	minty	SuperScent, TGSC
1617	Toluene	toluene	CC1=CC=CC=C1	paint sweet pungent benzene solvent	Flavornet
1618	O-Xylene	1,2-xylene	CC1=CC=CC=C1C	geranium sweet aromatic	Flavornet, Pubchem
1619	2'-Methylacetophenone	1-(2-methylphenyl)ethanone	CC1=CC=C1C(=0)C	sweet hawthorn powdery anisic coumarinic phenolic burnt nutty honey almond cherry floral	Sigma Aldrich, TGSC,OdoRactor
1620	1,4-Bis(2- methylbenzoyl)piperazine	[4-(2-methylbenzoyl)piperazin-1-yl]-(2-methylphen	CC1=CC=CC=C1C(=O)N2CCN(CC2)C(= O)C3=CC=CC=C3C	citrus metallic green aldehydic	OdorRactor,
1621	Methyl o-toluate	methyl 2-methylbenzoate	CC1=CC=CC=C1C(=O)OC	floral ylang orange flower grape	TGSC
1622	1,2,3-Propanetriol, cyclic ether with (2- methylphenyl)methanediol	(2- methylphenyl)methanediol;propan e-1,2,3-triol	CC1=CC=CC=C1C(O)O.C(C(CO) O)O	fruity bitter almond bitter	TGSC
1623	2-Methylbenzaldehyde	2-methylbenzaldehyde	CC1=CC=CC=C1C=O	fruity sweet cherry chemical coumarinic powdery	Sigma Aldrich, TGSC
1624	2-Methylphenethyl alcohol	2-(2-methylphenyl)ethanol	CC1=CC=CC=C1CCO	natural floral rose wax mimosa peony green earthy cyclamen	OdorRactor ,TGSC
1625	o-Cresol	2-methylphenol	CC1=CC=CC=C10	medicinal musty phenolic plastic herbaceous leathery sweet tarry	Sigma Aldrich, TGSC, PubChem
1626	2-Methylanisole	1-methoxy-2-methylbenzene	CC1=CC=CC=C10C	floral earthy walnut warm sweet nutty naphthyl camphoraceous phenolic woody orchid	Sigma Aldrich, TGSC, OdoRactor
1627	o-Tolyl acetate	(2-methylphenyl) acetate	CC1=CC=CC=C1OC(=O)C	fruit medicinal sweet floral dried fruit	OdorRactor ,TGSC
1628	o-Tolyl isobutyrate	(2-methylphenyl) 2- methylpropanoate	CC1=CC=CC=C1OC(=O)C(C)C	phenolic berry medicinal	OdorRactor ,TGSC
1629	o-Tolyl salicylate	(2-methylphenyl) 2- hydroxybenzoate	CC1=CC=CC=C1OC(=O)C2=CC =CC=C2 O	herbaceous eucalyptus	OdorRactor ,TGSC
1630	2-Methylbenzenethiol	2-methylbenzenethiol	CC1=CC=CC=C1S	meaty sulfurous onion garlic eggy rubbery chemical naphthyl musty	Sigma Aldrich, TGSC,OdoRactor
1631	2-Methylpyridine	2-methylpyridine	CC1=CC=CC=N1	sweaty strong unpleasant	Flavornet, TGSC, Pubchem
1632	1-Methylnaphthalene	1-methylnaphthalene	CC1=CC=CC2=CC=CC12	earthy naphthyl chemical medicinal camphoraceous	Sigma Aldrich, Pubchem
1633	1-Methyl-1,3-cyclohexadiene	1-methylcyclohexa-1,3-diene	CC1=CC=CCC1	fruity lemon lime truffle citrus	ADB, TGSC, OdoRactor
1634	2-Methylfuran	2-methylfuran	CC1=CC=CO1	ethereal acetone chocolate	Sigma Aldrich, TGSC, Pubchem,OdoRactor
1635	2-Methylthiophene	2-methylthiophene	CC1=CC=CS1	sulfurous alliaceous onion roasted	Flavornet, TGSC,OdoRactor
1636	4-Methylquinoline	4-methylquinoline	CC1=CC=NC2=CC=CC=C12	faint oily herbaceous floral sweet	Flavornet, TGSC, Pubchem, OdoRactor
1637	tau-Muurolol	(1 <i>S</i> ,4 <i>S</i>)-1,6-dimethyl-4-propan- 2-yl-3,4,4 <i>a</i> ,7,8,8 <i>a</i>	CC1=CC2[C@@H](CC[C@](C2 CC1)(C) O)C(C)C	burnt quinoline herbaceous	Flavornet
				i.	1

1638	2- Naphthalenecarboxaldehyde, 5,6,7,8- tetrahydro-1-methoxy- 3,5,5,8,8-pentamethyl	6,7- dihydronaphthalene-2-	CC1=CC2=C(C(=C1C=O)OC)C(CCC2(C) C)(C)C	sweet musk powdery woody	OdorRactor ,TGSC
1639	1,1,6-Trimethyl-1,2- dihydronaphthalene	1,1,6-trimethyl-2 <i>H</i> -naphthalene	CC1=CC2=C(C=C1)C(CC=C2)(C)C	anisic licorice	Flavornet, TGSC
1640	2,6-Dimethylnaphthalene	2,6-dimethylnaphthalene	CC1=CC2=C(C=C1)C=C(C=C2) C	grassy	Flavornet
1641	7-Methylcoumarin	7-methylchromen-2-one	CC1=CC2=C(C=C1)C=CC(=O)O	sweet coumarinic tonka coconut powdery	OdorRactor ,TGSC
1642	6-Methylquinoline	6-methylquinoline	CC1=CC2=C(C=C1)N=CC=C2	leathery animal tonka castoreum tobacco civet fecal	Sigma Aldrich, Flavorbase, TGSC
1643	6-Methyl-1,2,3,4-	6-methyl-1,2,3,4-	CC1=CC2=C(C=C1)NCCC2	animal leathery civet ambergis	OdorRactor ,TGSC
	tetrahydroquinoline	tetrahydroquinoline			
1644	6-Methylcoumarin	6-methylchromen-2-one	CC1=CC2=C(C=C1)OC(=O)C=C 2	anisic coconut creamy herbaceous vanilla sweet powdery floral	Sigma Aldrich, TGSC, Pubchem
1645	2H-1,5-Benzodioxepin-3(4H)-one, 7- methyl-	•	2	fresh watery clean melon green marine ozone phenolic	OdorRactor ,TGSC
1646	1H-Indene-2-methanol, 2,3-dihydro-2,5-dimethyl-	(2,5-dimethyl-1,3-dihydroinden-2-yl)methanol	CC1=CC2=C(CC(C2)(C)CO)C=C	floral lily muguet	TGSC
1647	7-Methyl-4,4a,5,6-tetrahydro- 2(3H)- naphthalenone	7-methyl-4,4 <i>a</i> ,5,6-tetrahydro-3 <i>H</i> -naphthalen-2- one	CC1=CC2=CC(=0)CCC2CC1	coconut tonka toasted coumarinic fruity	OdorRactor ,TGSC, Flavorbase
1648	2-Methylnaphthalene	2-methylnaphthalene	CC1=CC2=CC=CC=C2C=C1	sweet floral woody	TGSC
	2-Methylindole	2-methyl-1 <i>H</i> -indole	CC1=CC2=CC=CC2N1	animal indole fresh naphthyl	OdorRactor ,TGSC
1650	2-Methylbenzofuran	2-methyl-1-benzofuran	CC1=CC2=CC=CC=C2O1	burnt phenolic	TGSC, Flavorbase
1651	Linden ether	3,6-dimethyl-2,4,5,7 <i>a</i> -tetrahydro-1-benzofuran	CC1=CC2C(=C(CO2)C)CC1	floral minty	Flavornet, TGSC
1652	Ethanone, 1-(4,7,7-trimethylbicyclo[4.1.0]hept-4-en-3-yl)-	1-(4,7,7-trimethyl-3-bicyclo[4.1.0]hept-4-enyl)ethanone	CC1=CC2C(C2(C)C)CC1C(=0)C	herbaceous woody thyme dry clary sage petitgrain lavender	OdorRactor ,TGSC
1653	gamma-Muurolene	(1S, 4aS, 8aR)-7-methyl-4- methylidene-1-propan- 2-yl-2,3,4a,5,6,8a -hexahydro- 1H -naphthalene	CC1=CC2C(CC1)C(=C)CCC2C(C)C	herbaceous woody spice	Flavornet
1654	(-)-gamma-Cadinene	(1R, 4aS, 8aS)-7-methyl-4- methylidene-1-propan- 2-yl-2,3,4a,5,6,8a-hexahydro- 1H-naphthalene	CC1=CC2C(CC1)C(=C)CCC2C(C)C	woody herbaceous	Flavornet
1655	alpha-Muurolene	(15,4aS,8aR)-4,7-dimethyl-1- propan-2-yl- 1,2,4a,5,6,8a - hexahydronaphthalene	CC1=CC2C(CC1)C(=CCC2C(C)C)C	woody	Flavornet
1656	(+)-alpha-Cadinene	(1 <i>S</i> ,4 <i>aR</i> ,8 <i>aR</i>)-4,7-dimethyl-1- propan-2-yl- 1,2,4 <i>a</i> ,5,6,8 <i>a</i> - hexahydronaphthalene	CC1=CC2C(CC1)C(=CCC2C(C)C)C	woody dry	TGSC
1657	Bicyclo[2.2.2]oct-5-ene-2- carbonitrile, 5- methyl-7-(1- methylethyl)-	5-methyl-7-propan-2- ylbicyclo[2.2.2]oct-5-ene-2- carbonitrile	CC1=CC2C(CC1CC2C(C)C)C#N	green woody ozone	TGSC
1658	7-Isopropyl-5- methylbicyclo[2.2.2]oct-5- ene-2-carbaldehyde	5-methyl-7-propan-2- ylbicyclo[2.2.2]oct-5-ene-2- carbaldehyde	CC1=CC2C(CC1CC2C(C)C)C=0	fatty green metallic aldehydic	OdorRactor ,TGSC
1659	Cadina-1(10),4-diene	4,7-dimethyl-1-propan-2-yl- 1,2,3,5,6,8 <i>a</i> - hexahydronaphthalene	CC1=CC2C(CCC(=C2CC1)C)C(C)C	thyme herbaceous woody dry	OdorRactor,
1660	(+)-delta-Cadinene	(15,8aR)-4,7-dimethyl-1-propan- 2-yl- 1,2,3,5,6,8a - hexahydronaphthalene	CC1=CC2C(CCC(=C2CC1)C)C(C)C	thyme medicinal woody	Flavornet, OdoRactor
1661	Cedrelanol	(15,4S,4aR,8aR)-1,6-dimethyl- 4-propan-2-yl- 3,4,4a,7,8,8a-hexahydro-2H- naphthalen-1-ol	CC1=CC2C(CCC(C2CC1)(C)O)C (C)C	balsamic earthy	OdorRactor ,TGSC
1662	delta-Cadinol	(1 <i>R</i> ,4 <i>S</i> ,4 <i>aR</i> ,8 <i>aS</i>)-1,6-dimethyl- 4-propan-2-yl- 3,4,4 <i>a</i> ,7,8,8 <i>a</i> -hexahydro-2 <i>H</i> - naphthalen-1-ol	CC1=CC2C(CCC(C2CC1)(C)O)C (C)C	herbaceous	SuperScent, TGSC
1663	T-Muurolol	-	CC1=CC2C(CCC(C2CC1)(C)O)C (C)C	herbaceous weak spice honey	Flavornet , TGSC
1664	alpha-Cadinol	-	CC1=CC2C(CCC(C2CC1)(C)O)C (C)C	herbaceous woody	Flavornet
1665	Bicyclo[2.2.2]oct-5-ene-2- carboxaldehyde, 6-methyl-8-(1-methylethyl)-	6-methyl-8-propan-2- ylbicyclo[2.2.2]oct-5-ene-2- carbaldehyde	CC1=CC2CC(C1CC2C(C)C)C=O	fresh grassy oily green spicy	OdorRactor ,TGSC

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1666	2-[8-Isopropyl-6- methylbicyclo[2.2.2]oct-5- en- 2-yl]-1,3-dioxolane	2-(6-methyl-8-propan-2-yl-2-bicyclo[2.2.2]oct-5- enyl)-1,3-dioxolane	CC1=CC2CC(C1CC2C(C)C)C3O CCO3	privet cortex floral rose green woody milky	OdorRactor ,TGSC
1667	Terpinolene	1-methyl-4-propan-2- ylidenecyclohexene	CC1=CCC(=C(C)C)CC1	plastic pine woody sweet citrus fresh herbaceous lemon	Sigma Aldrich, TGSC,OdoRactor
1668	(E)-gamma-Bisabolene	(4E)-1-methyl-4-(6-methylhept-5-en-2-ylidene)cyclohexene	CC1=CCC(=C(C)CCC=C(C)C)C C1	sweet	ADB
1669	(Z)-gamma-Bisabolene	(4Z)-1-methyl-4-(6-methylhept-5- en-2- ylidene)cyclohexene	CC1=CCC(=C(C)CCC=C(C)C)C C1	sweet fruity balsamic citrus myrrh opoponax spicy woody tropical terpenic green banana	OdorRactor ,TGSC, Flavorbase
1670	4-(4-Methyl-3-cyclohexen-1- ylidene)pentanal	(4E)-4-(4-methylcyclohex-3-en-1-vlidene)pentanal	CC1=CCC(=C(C)CCC=O)CC1	floral lily of the valley	TGSC
1671	gamma-Terpinene	1.4-diene	CC1=CCC(=CC1)C(C)C	citrus herbaceous gasoline turpentine terpenic oily woody lemon lime tropical herbaceous sweet	Sigma Aldrich, TGSC
1672	alpha-Angelica lactone	5-methyl-3 <i>H</i> -furan-2-one	CC1=CCC(=0)01	oily nutty sweet tonka coumarinic tobacco solvent coconut	Sigma Aldrich, TGSC,OdoRactor
1673	p-Mentha-1,5,8-triene	2-methyl-5-prop-1-en-2- ylcyclohexa-1,3-diene	CC1=CCC(C=C1)C(=C)C	roasted	SuperScent, TGSC
1674	(+)-alpha-Phellandrene	(5S)-2-methyl-5-propan-2- ylcyclohexa-1,3-diene	CC1=CCC(C=C1)C(C)C	chilli	Flavornet
1675	alpha-Phellandrene	2-methyl-5-propan-2-ylcyclohexa- 1,3-diene	CC1=CCC(C=C1)C(C)C	herbaceous minty spice turpentine citrus herbaceous terpenic green woody black pepper medicinal	Sigma Aldrich, TGSC
1676	Zingiberene	(5R)-2-methyl-5-[(2S)-6-methylhept-5-en-2-yl]cyclohexa-1,3-diene	CC1=CCC(C=C1)C(C)CCC=C(C) C	spice fresh sharp	Flavornet, TGSC
1677	Humulene		CC1=CCC(C=CCC(=CCC1)C)(C)	woody spice	Flavornet, TGSC, OdoRactor
1678	3-Cyclopentene-1-butanol, beta,2,2,3- tetramethyl-delta- methylene-	2-methyl-4-(2,2,3- trimethylcyclopent-3-en-1- yl)pent- 4-en-1-ol	CC1=CCC(C1(C)C)C(=C)CC(C)C	woody natural sandal wood	TGSC
1679	1-(2,2,3-Trimethylcyclopent- 3-en-1- yl)ethanone	1-(2,2,3-trimethylcyclopent-3-en-1-yl)ethanone	CC1=CCC(C1(C)C)C(=O)C	herbaceous green woody amber leafy fatty sweet pine camphoraceous	OdorRactor ,TGSC, Flavorbase
1680	4-Penten-2-ol, 3,3-dimethyl-5- (2,2,3- trimethyl-3- cyclopenten-1-yl)-	(E)-3,3-dimethyl-5-(2,2,3- trimethylcyclopent-3-en- 1-yl)pent-4-en-2-ol	CC1=CCC(C1(C)C)C=CC(C)(C)C (C)O	woody sandal wood herbaceous tropical	OdorRactor ,TGSC
1681	Ebanol	(Z)-3-methyl-5-(2,2,3- trimethylcyclopent-3-en-1- yl)pent- 4-en-2-ol	CC1=CCC(C1(C)C)C=CC(C)C(C)	woody sandal wood musk	OdorRactor ,TGSC, Flavorbase
1682	3-Cyclopentene-1-acetonitrile, 2,2,3- trimethyl-	2-(2,2,3-trimethylcyclopent-3-en-1-yl)acetonitrile	CC1=CCC(C1(C)C)CC#N	pine rosemary hay	OdorRactor ,TGSC
1683	3-Penten-2-one, 3-methyl-5- (2,2,3-trimethyl- 3-cyclopenten-1-yl)-	(E)-3-methyl-5-(2,2,3-trimethylcyclopent-3-en-1-yl)pent-3-en-2-one	CC1=CCC(C1(C)C)CC=C(C)C(= O)C	woody orris floral powdery sandal wood	OdorRactor ,TGSC
1684	3-Methyl-5-(2,2,3-trimethyl-3-cyclopenten- 1-yl)pent-3-en-2-ol	(E)-3-methyl-5-(2,2,3-trimethylcyclopent-3-en-1-yl)pent-3-en-2-ol	CC1=CCC(C1(C)C)CC=C(C)C(C) O	woody oily spicy powdery sandal wood	TGSC
1685	2-Methyl-4-(2,2,3-trimethyl-3-cyclopenten- 1-yl)-2-buten-1-ol	(E)-2-methyl-4-(2,2,3-trimethylcyclopent-3-en-1-yl)but-2-en-1-ol	CC1=CCC(C1(C)C)CC=C(C)CO	woody sandal wood creamy milky wax greasy musk	OdorRactor ,TGSC
1686	Sandalore	3-methyl-5-(2,2,3- trimethylcyclopent-3-en-1- yl)pentan-2-ol	CC1=CCC(C1(C)C)CCC(C)C(C) O	sweet sandal wood woody wax greasy creamy cedar	OdorRactor ,TGSC, Pubchem
1687	3-Cyclopentene-1-butanol, beta,2,2,3- tetramethyl-	2-methyl-4-(2,2,3- trimethylcyclopent-3-en-1- yl)butan-1-ol	CC1=CCC(C1(C)C)CCC(C)CO	herbaceous sandal wood wax nutty woody	OdorRactor ,TGSC
1688	alpha-Campholenol	2-(2,2,3-trimethylcyclopent-3-en-1-yl)ethanol	CC1=CCC(C1(C)C)CCO	sweet berry camphoraceous	OdorRactor ,TGSC
1689	Campholene acetate	2-[(1S)-2,2,3-trimethylcyclopent- 3-en-1-yl]ethyl acetate	CC1=CCC(C1(C)C)CCOC(=O)C	sweet lavender floral berry herbaceous	OdorRactor ,TGSC
1690	2,2,3-Trimethylcyclopent-3- ene-1-ethyl acetate	2-(2,2,3-trimethylcyclopent-3-en-1-yl)ethyl acetate	CC1=CCC(C1(C)C)CCOC(=O)C	sweet woody floral violet	TGSC
1691	alpha-Calacorene	(1 <i>S</i>)-4,7-dimethyl-1-propan-2-yl-1,2- dihydronaphthalene	CC1=CCC(C2=C1C=CC(=C2)C) C(C)C	woody	Flavornet, OdoRactor
1692	3,4-Dihydrocadalene	4,7-dimethyl-1-propan-2-yl-1,2-dihydronaphthalene	CC1=CCC(C2=C1C=CC(=C2)C) C(C)C	woody	OdorRactor,
1693	Terpinen-4-ol	4-methyl-1-propan-2-ylcyclohex-3- en-1-ol	CC1=CCC(CC1)(C(C)C)O	grapefruit lemon lime woody herbaceous pepper turpentine nutmeg musty spicy earthy sweet mentholic citrus terpenic fresh pine	Sigma Aldrich, Flavorbase, TGSC, OdoRactor, Pubchem

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1694	(+)-Terpinen-4-ol	(1S)-4-methyl-1-propan-2-ylcyclohex-3-en-1-ol	CC1=CCC(CC1)(C(C)C)O	musty dusty	TGSC
1695	3-Cyclohexen-1-ol, 1-(1,5-dimethyl-4-hexenyl)-4-methyl-	4-methyl-1-(6-methylhept-5-en-2-yl)cyclohex-3-en- 1-ol	CC1=CCC(CC1)(C(C)CCC=C(C) C)O	sweet herbaceous citrus floral lemon herbaceous tart fresh	Flavornet, TGSC, OdoRactor
1696	4-Acetyl-1,4-dimethyl-1- cyclohexene	1-(1,4-dimethylcyclohex-3-en-1-yl)ethanone	CC1=CCC(CC1)(C)C(=O)C	fruity	OdorRactor ,TGSC
1697	(-)-Limonene	(4S)-1-methyl-4-prop-1-en-2- ylcyclohexene	CC1=CCC(CC1)C(=C)C	camphoraceous herbaceous minty terpenic pine pepper	Sigma Aldrich, TGSC, OdoRactor
1698	Limonene	1-methyl-4-prop-1-en-2- ylcyclohexene	CC1=CCC(CC1)C(=C)C	citrus lemon orange penetrating herbaceous terpenic camphoraceous woody petroleum phenolic aromatic resinous paint	Sigma Aldrich, AOD, TGSC, OdoRactor, Pubchem
1699	D-Limonene	(4R)-1-methyl-4-prop-1-en-2-ylcyclohexene	CC1=CCC(CC1)C(=C)C	fresh peely lemon orange sweet citrus minty	Sigma Aldrich, AOD, TGSC, Pubchem, OdoRactor
1700	beta-Bisabolene	(4S)-1-methyl-4-(6-methylhepta- 1,5-dien-2- yl)cyclohexene	CC1=CCC(CC1)C(=C)CCC=C(C) C	balsamic woody	Flavornet, TGSC, Odoractor
1701	(R)-beta-Bisabolene	(4R)-1-methyl-4-(6-methylhepta- 1,5-dien-2-yl)cyclohexene	CC1=CCC(CC1)C(=C)CCC=C(C)	balsamic woody	OdorRactor,
1702	4-Methyl-beta- methylenecyclohex-3-ene-1- ethanol	2-(4-methylcyclohex-3-en-1-yl)prop-2-en-1-ol	CC1=CCC(CC1)C(=C)CO	clean citrus minty	TGSC
1703	p-Mentha-1,8(10)-dien-9-yl acetate	2-(4-methylcyclohex-3-en-1- yl)prop-2-enyl acetate	CC1=CCC(CC1)C(=C)COC(=O)C	sweet fruity minty	OdorRactor ,TGSC
1704	alpha-Bisabolene	1-methyl-4-(6-methylhepta-2,5-dien-2- yl)cyclohexene	CC1=CCC(CC1)C(=CCC=C(C)C)	balsamic spicy floral	OdorRactor ,TGSC
1705	(Z)-alpha-Bisabolene	1-methyl-4-[(2Z)-6-methylhepta- 2,5-dien-2-yl]cyclohexene		coconut	ADB
1706	4-Acetyl-1- methylcyclohexene	1-(4-methylcyclohex-3-en-1-yl)ethanone	CC1=CCC(CC1)C(=O)C	spice	Flavornet
1707	4-Methylcyclohex-3-ene-1- carboxylic acid	4-methylcyclohex-3-ene-1- carboxylic acid	CC1=CCC(CC1)C(=O)O	sweaty cumin castoreum cedar leathery	TGSC, Flavorbase
1708	(+)-alpha-Terpineol	2-[(1R)-4-methylcyclohex-3-en-1-	CC1=CCC(CC1)C(C)(C)O	lilac floral	OdorRactor ,TGSC
1709	(-)-alpha-Terpineol	yl]propan-2-ol 2-[(1S)-4-methylcyclohex-3-en-1-	CC1=CCC(CC1)C(C)(C)O	lilac floral terpenic	Sigma Aldrich, TGSC,
1710	alpha-TERPINEOL	yl]propan-2-ol 2-(4-methylcyclohex-3-en-1- yl)propan-2-ol	CC1=CCC(CC1)C(C)(C)O	lilac oily anisic minty pine terpenic resinous cooling lemon lime citrus woody floral	OdoRactor Sigma Aldrich, TGSC, OdoRactor
1711	Thyme oil	3,7-dimethylocta-1,6-dien-3-ol;2- (4- methylcyclohex-3-en-1- yl)propan-2-ol;1-methyl-4- propan- 2-ylbenzene;2-methyl-5-propan-2- ylbicyclo[3,1,0]hexan-2-ol;5- methyl-2-propan-2- ylphenol		green honey floral spicy citrus fruity minty woody	Sigma Aldrich
1712	Cyclohexene, 4-(1-methoxy-1-methylethyl)- 1-methyl-	4-(2-methoxypropan-2-yl)-1- methylcyclohexene	CC1=CCC(CC1)C(C)(C)OC	citrus grapefruit bergamot orange flower vegetable celery spicy earthy	SuperScent, TGSC
1713	alpha-Terpinyl acetate	2-(4-methylcyclohex-3-en-1- yl)propan-2-yl acetate	CC1=CCC(CC1)C(C)(C)OC(=O) C	citrus fruity pear apple spicy herbaceous bergamot lavender herbaceous lime woody floral wax clean sweet pine	Sigma Aldrich, TGSC
1714	Terpinyl isobutyrate	2-(4-methylcyclohex-3-en-1- yl)propan-2-yl 2- methylpropanoate	CC1=CCC(CC1)C(C)(C)OC(=O) C(C)C	green floral herbaceous spice fatty pepper bergamot fruity refreshing lavender	SuperScent, TGSC, Flavorbase, Odoractor
1715	Terpinyl cinnamate	2-(4-methylcyclohex-3-en-1-yl)propan-2-yl (E)-3-phenylprop-2-enoate	CC1=CCC(CC1)C(C)(C)OC(=0) C=CC2= CC=CC=C2	sweet balsamic winey nutmeg	OdorRactor ,TGSC
1716	p-Menth-1-en-8-yl benzoate	2-(4-methylcyclohex-3-en-1- yl)propan-2-yl benzoate	CC1=CCC(CC1)C(C)(C)OC(=O) C2=CC= CC=C2	fi rneedle balsamic ylang woody floral cypress	OdorRactor ,TGSC
1717	alpha-Terpinyl anthranilate	2-(4-methylcyclohex-3-en-1-yl)propan-2-yl 2- aminobenzoate	C2=CC=CC2 CC1=CCC(CC1)C(C)(C)OC(=0) C2=CC= CC=C2N	orange flower floral lily fruity neroli	OdorRactor ,TGSC
1718	alpha-Terpinyl isovalerate	2-(4-methylcyclohex-3-en-1-yl)propan-2-yl 3- methylbutanoate	CC1=CCC(CC1)C(C)(C)OC(=O) CC(C)C	sweet pine incense orange citrus balsamic frankincense	OdorRactor ,TGSC
1719	Terpinyl formate	2-(4-methylcyclohex-3-en-1- yl)propan-2-yl formate	CC1=CCC(CC1)C(C)(C)OC=O	citrus floral sweet lavender fruity herbaceous woody cypress	Flavornet, TGSC, OdoRactor
1720	(S)-alpha,alpha,4- Trimethylcyclohex-3-ene- 1-methanethiol	2-[(1S)-4-methylcyclohex-3-en-1-yl]propane-2- thiol	CC1=CCC(CC1)C(C)(C)S	grapefruit citrus	TGSC

1721	1-p-Menthene-8-thiol	2-(4-methylcyclohex-3-en-1-	CC1=CCC(CC1)C(C)(C)S	grapefruit citrus sulfurous	Flavornet, TGSC, OdoRactor
	-	yl)propane-2-thiol		aromatic naphthyl resinous woody alliaceous onion garlic tropical	
1722	(+)-Epi-alpha-bisabolol	(2S)-6-methyl-2-[(1R)-4-methylcyclohex-3-en-1-yl]hept-5-en-2-ol	CC1=CCC(CC1)C(C)(CCC=C(C) C)O	floral pepper balsamic clean	OdorRactor ,TGSC
1723	Levomenol	(2S)-6-methyl-2-[(1S)-4-methylcyclohex-3-en-1-yl]hept-5-en-2-ol	CC1=CCC(CC1)C(C)(CCC=C(C) C)O	herbaceous fruity nutty coconut floral	Flavornet, TGSC
1724	alpha-Bisabolol	6-methyl-2-(4-methylcyclohex-3- en-1-yl)hept-5-en- 2-ol	CC1=CCC(CC1)C(C)(CCC=C(C) C)O	spice pepper balsamic clean floral	Flavornet, TGSC,OdoRactor
1725	P-Menth-1-en-9-al	2-(4-methylcyclohex-3-en-1- yl)propanal	CC1=CCC(CC1)C(C)C=O	spicy herbaceous	OdorRactor ,TGSC
1726	3-(4-Methylcyclohex-3-en-1-yl)butanal	3-(4-methylcyclohex-3-en-1- yl)butanal	CC1=CCC(CC1)C(C)CC=O	citrus green aldehydic herbaceous	OdorRactor ,TGSC
1727	2-(2-(4-Methyl-3-cyclohexen- 1- yl)propyl)cyclopentanone	2-[2-(4-methylcyclohex-3-en-1-yl)propyl]cyclopentan-1-one	CC1=CCC(CC1)C(C)CC2CCCC2 =0	fruity tropical lactonic peach apricot oily wax custard coconut	OdorRactor ,TGSC
1728	3-(4-Methylcyclohex-3-en-1-yl)butan-1-ol	3-(4-methylcyclohex-3-en-1-yl)butan-1-ol	CC1=CCC(CC1)C(C)CCO	sweet citrus rose herbaceous fresh clean warm	OdorRactor ,TGSC
1729	p-Menth-1-en-9-ol	2-(4-methylcyclohex-3-en-1-yl)propan-1-ol	CC1=CCC(CC1)C(C)CO	fruity herbaceous	Flavornet, Flavorbase
1730	P-Menth-1-en-9-yl acetate	2-(4-methylcyclohex-3-en-1- yl)propyl acetate	CC1=CCC(CC1)C(C)COC(=0)C	fruit herbaceous spicy warm	Flavornet, TGSC, OdoRactor
1731	2-Methyl-2-(4-methyl-3- cyclohexen-1- yl)oxirane	2-methyl-2-(4-methylcyclohex-3- en-1-yl)oxirane	CC1=CCC(CC1)C2(CO2)C	fresh citrus	Flavornet
1732	Carvone	2-methyl-5-prop-1-en-2- ylcyclohex-2-en-1-one	CC1=CCC(CC1=O)C(=C)C	green minty camphoraceous basil fennel licorice	Sigma Aldrich, Flavornet, TGSC
1733	(-)-Carvone	(5R)-2-methyl-5-prop-1-en-2- ylcyclohex-2-en-1- one	CC1=CCC(CC1=0)C(=C)C	herbaceous spearmint minty sweet	Sigma Aldrich, AOD, Flavorbase, Pubchem, OdoRactor
1734	d-Carvone	(5S)-2-methyl-5-prop-1-en-2-ylcyclohex-2-en-1- one	CC1=CCC(CC1=0)C(=C)C	spice minty bready caraway	Sigma Aldrich, AOD, Flavorbase, TGSC, OdoRactor
1735	2-Cyclohexen-1-one, 2- methyl-5-(1- methylethyl)-, (S)-	(5S)-2-methyl-5-propan-2- ylcyclohex-2-en-1-one	CC1=CCC(CC1=0)C(C)C	minty	TGSC
1736	(-)-trans-Carveol	(1 <i>S</i> ,5 <i>R</i>)-2-methyl-5-prop-1-en-2-ylcyclohex-2-en-1-ol	CC1=CCC(CC10)C(=C)C	caraway solvent spearmint spicy	Flavornet, TGSC, OdoRactor, Pubchem
1737	Carveol	2-methyl-5-prop-1-en-2- ylcyclohex-2-en-1-ol	CC1=CCC(CC1O)C(=C)C	minty herbaceous fresh spearmint caraway	Sigma Aldrich, TGSC
1738	(-)-cis-Carveol	(1R,5R)-2-methyl-5-prop-1-en-2-ylcyclohex-2-en-	CC1=CCC(CC10)C(=C)C	minty spearmint	OdorRactor ,Flavornet, TGSC
1739	Carvyl acetate	(2-methyl-5-prop-1-en-2- ylcyclohex-2-en-1-yl) acetate	CC1=CCC(CC1OC(=O)C)C(=C)C	green minty sweet spearmint fruity herbaceous sour	Sigma Aldrich, Flavorbase, TGSC
1740	1-Methyl-1,4-cyclohexadiene	1-methylcyclohexa-1,4-diene	CC1=CCC=CC1	faint	Sigma Aldrich
1741	alpha-Thujene	2-methyl-5-propan-2- ylbicyclo[3.1.0]hex-2-ene	CC1=CCC2(C1C2)C(C)C	woody green herbaceous	Flavornet
1742	Carotol		CC1=CCC2(CCC(C2(CC1)O)C(C)C)C	pleasant mild	SuperScent, TGSC
1743	Naphthalene, 1,2,4a,5,8,8a- hexahydro-4,7- dimethyl-1-(1- methylethyl)-	4,7-dimethyl-1-propan-2-yl-1,2,4 <i>a</i> ,5,8,8 <i>a</i> - hexahydronaphthalene	CC1=CCC2C(C1)C(CC=C2C)C(C)C	fresh herbaceous vetiver woody longifolone	OdorRactor ,TGSC
1744	beta-Cadinene	(15,4aR,8aS)-4,7-dimethyl-1-propan-2-yl-1,2,4a,5,8,8a - hexahydronaphthalene	CC1=CCC2C(C1)C(CC=C2C)C(C)C	green woody pleasant	SuperScent, TGSC, Pubchem
1745	3-Carene	3,7,7-trimethylbicyclo[4.1.0]hept- 3-ene	CC1=CCC2C(C1)C2(C)C	lemon sweet citrus terpenic herbaceous pine solvent resinous phenolic cypress medicinal woody pungent	Sigma Aldrich, TGSC, Pubchem, OdoRactor
1746	4,11,11-Trimethyl-8- methylenebicyclo[7.2.0]undec 3-en-5-yl acetate	[(3Z)-4,11,11-trimethyl-8-methylidene-5-bicyclo[7.2.0]undec-3-enyl] acetate	CC1=CCC2C(CC2(C)C)C(=C)CC C1OC(= 0)C	woody fresh sharp cedar spicy	OdorRactor ,TGSC
1747	8-Isopropyl-1,3- dimethyltricyclo[4.4.0.02,7]d ec-3-ene	(2 <i>R</i> ,6 <i>R</i>)-1,3-dimethyl-8-propan-2- yltricyclo[4.4.0.02,7]dec-3-ene	CC1=CCC2C3C1C2(CCC3C(C)C)C	woody spice honey	Flavornet, TGSC
1748	(-)-alpha-Copaene	(1 <i>R</i>)-1,3-dimethyl-8-propan-2- yltricyclo[4.4.0.02,7]dec-3-ene	CC1=CCC2C3C1C2(CCC3C(C)C	woody spicy honey	OdorRactor,
1749	Pinenol	2,6,6-trimethylbicyclo[3.1.1]hept- 2-en-1-ol	CC1=CCC2CC1(C2(C)C)O	musty dusty	OdorRactor ,TGSC, Flavornet

1750	(+)-alpha-Pinene	(1R,5R)-2,6,6- trimethylbicyclo[3.1.1]hept-2-ene	CC1=CCC2CC1C2(C)C	pine terpenic aromatic minty herbaceous	Sigma Aldrich, TGSC
1751	alpha-Pinene	2,6,6-trimethylbicyclo[3.1.1]hept- 2-ene	CC1=CCC2CC1C2(C)C	pine turpentine fresh camphoraceous sweet earthy woody terpenic cooling herbaceous	Flavornet, TGSC, Pubchem
1752	alpha-Pinene	2,6,6-trimethylbicyclo[3.1.1]hept- 2-ene	CC1=CCC2CC1C2(C)C	turpentine characteristic pine	Pubchem
1753	(-)-alpha-Pinene	(1 <i>S</i> ,5 <i>S</i>)-2,6,6- trimethylbicyclo[3.1.1]hept-2-ene	CC1=CCC2CC1C2(C)C	woody pine resinous sharp warm fresh terpenic earthy	Sigma Aldrich, TGSC
1754	trans-alpha-Bergamotene	(1S,5S,6R)-2,6-dimethyl-6-(4-methylpent-3-enyl)bicyclo[3.1.1]hept-2-ene	CC1=CCC2CC1C2(C)CCC=C(C)	woody warm tea	Flavornet, OdoRactor
1755	(1S,5S)-2,6-Dimethyl-6-(4-methylpent-3-enyl)bicyclo[3.1.1]hept-2-ene	(1 <i>S</i> ,5 <i>S</i>)-2,6-dimethyl-6-(4-methylpent-3-	CC1=CCC2CC1C2(C)CCC=C(C)	woody warm tea	OdorRactor ,TGSC
1756	(-)-Germacrene D	(1E ,6E ,8S)-1-methyl-5- methylidene-8-propan-2- ylcyclodeca-1,6-diene	CC1=CCCC(=C)C=CC(CC1)C(C)	woody spice	Flavornet, TGSC
1757	(4Z)-4,11,11-Trimethyl-8- methylidenebicyclo[7.2.0]und ec-4-ene	(4Z)-4,11,11-trimethyl-8-	CC1=CCCC(=C)C2CC(C2CC1)(C)C	spicy sweet woody clove dry terpenic	OdorRactor ,TGSC
1758	beta-Caryophyllene	(1 <i>R</i> ,4 <i>E</i> ,9 <i>S</i>)-4,11,11-trimethyl-8-methylidenebicyclo[7.2.0]undec-4-ene	CC1=CCCC(=C)C2CC(C2CC1)(C)C	spicy woody sweet clove dry turpentine	Sigma Aldrich, TGSC, Pubchem, OdoRactor
1759	Isocaryophyllene	(1R,4Z,9S)-4,11,11-trimethyl-	CC1=CCCC(=C)C2CC(C2CC1)(C	woody spicy	Flavornet, TGSC, OdoRactor
1760	Germacrene B	(1E ,5E)-1,5-dimethyl-8-propan- 2- ylidenecyclodeca-1,5-diene	CC1=CCCC(=CCC(=C(C)C)CC1)	woody earthy spice	Flavornet, TGSC, OdoRactor
1761	Ethanone, 1-(2,6,10-trimethyl-2,5,9- cyclododecatrien-1-yl)-	1-[(2Z ,5Z ,9Z)-2,6,10- trimethylcyclododeca-2,5,9- trien- 1-yl]ethanone	CC1=CCCC(=CCC=C(C(CC1)C(=0)C)C) C	woody ambergis musk vetiver tobacco	OdorRactor ,TGSC
1762	1,5,5-Trimethylcyclohexene	1,5,5-trimethylcyclohexene	CC1=CCCC(C1)(C)C	lime citrus lemon herbaceous terpenic	OdorRactor ,TGSC
1763	Methyl 2,6,6- trimethylcyclohex-2-ene-1- carboxylate	methyl 2,6,6-trimethylcyclohex-2- ene-1- carboxylate	CC1=CCCC(C1C(=0)OC)(C)C	natural herbaceous floral fruity woody camphoraceous	OdorRactor ,TGSC
1764	Cyclohexenebutanal, alpha,2,2,6- tetramethyl-	4-(2,6,6-trimethylcyclohex-2-en-1-yl)pentanal	CC1=CCCC(C1C(C)CCC=O)(C)	orris woody leathery tobacco animal	OdorRactor ,TGSC
1765	3-Methyl-4-(2,6,6-trimethyl-2-cyclohexen-1-yl)-3-buten-2-one	* - *	CC1=CCCC(C1C=C(C)C(=0)C)(C)C	floral violet sweet orris powdery woody	OdorRactor ,TGSC, Pubchem
1766	3-Methyl-alpha-ionyl acetate	[(E)-3-methyl-4-(2,6,6-trimethylcyclohex-2-en-1-yl)but-3-en-2-yl] acetate	CC1=CCCC(C1C=C(C)C(C)OC(= O)C)(C) C	floral powdery violet woody vetiver fruity	OdorRactor ,TGSC
1767	1-Penten-3-one, 4-methyl-1- (2,6,6-trimethyl- 2-cyclohexen-1-yl)-	(E)-4-methyl-1-(2,6,6-trimethylcyclohex-2-en-1-yl)pent-1-en-3-one	CC1=CCCC(C1C=CC(=O)C(C)C) (C)C	sweet floral violet woody	TGSC
1768	alpha-Ionone	(E)-4-(2,6,6-trimethylcyclohex-2-en-1-yl)but-3-en-2-one	CC1=CCCC(C1C=CC(=0)C)(C)C	berry cherry woody raspberry violet sweet floral orris tropical fruity balsamic	Sigma Aldrich, TGSC, Flavorbase, Pubchem, OdoRactor
1769	4-(2,6,6-Trimethylcyclohex-2-en-1-yl)but-3- en-2-one	4-(2,6,6-trimethylcyclohex-2-en-1-yl)but-3-en-2- one	CC1=CCCC(C1C=CC(=O)C)(C)C	floral	OdorRactor ,TGSC, Pubchem
1770	(E)-5-Methyl-1-(2,6,6- trimethylcyclohex-2- en-1- yl)hex-1-en-3-one	(E)-5-methyl-1-(2,6,6-trimethylcyclohex-2-en-1-yl)hex-1-en-3-one	CC1=CCCC(C1C=CC(=O)CC(C) C)(C)C	woody vetiver earthy rooty	OdorRactor ,TGSC
1771	Allyl alpha-ionone	(1E)-1-(2,6,6-trimethylcyclohex- 2-en-1-yl)hepta- 1,6-dien-3-one	CC1=CCCC(C1C=CC(=0)CCC= C)(C)C	meaty woody spicy fruity floral green orris tropical weedy wax leathery vanilla	Sigma Aldrich, TGSC, OdoRactor
1772	alpha-Ionol	(E)-4-(2,6,6-trimethylcyclohex-2-en-1-yl)but-3-en- 2-ol	CC1=CCCC(C1C=CC(C)O)(C)C	floral tropical sweet violet woody berry powdery	OdorRactor ,TGSC
1773	3-Buten-2-ol, 4-(2,6,6- trimethyl-2- cyclohexen-1-yl)-, acetate	4-(2,6,6-trimethylcyclohex-2-en-1-	CC1=CCCC(C1C=CC(C)OC(=O) C)(C)C	sweet woody floral violet berry	OdorRactor ,TGSC
1774	Oxiranecarboxylic acid, 3- methyl-3-(2- (2,6,6-trimethyl- 2-cyclohexen-1-yl)ethenyl)- , methyl ester	methyl 3-methyl-3-[(E)-2-(2,6,6-trimethylcyclohex 2-en-1-yl)ethenyl]oxirane-2-carboxylate	CC1=CCCC(C1C=CC2(C(O2)C(= O)OC)C)(C)C	fruity raspberry prune	OdorRactor ,TGSC
1775	2-Methyl-4-(2,6,6-trimethyl-2- cyclohexen-1- yl)-2-butenal	(E)-2-methyl-4-(2,6,6- trimethylcyclohex-2-en-1- yl)but-2- enal	CC1=CCCC(C1CC=C(C)C=O)(C)	tobacco dry sweet nutty violet	OdorRactor ,TGSC

1776	Dihydro-alpha-ionone	4-(2,6,6-trimethylcyclohex-2-en-1-yl)butan-2-one	CC1=CCCC(C1CCC(=O)C)(C)C	woody earthy herbaceous orris raspberry floral warm violet berry fruity powdery	OdorRactor ,TGSC
1777	(4E,7E)-1,5,9,9-Tetramethyl- 12- oxabicyclo[9.1.0]dodeca- 4,7-diene	(4Z ,7Z)-1,5,9,9-tetramethyl-12-oxabicyclo[9.1.0]dodeca-4,7-diene	CC1=CCCC2(C(O2)CC(C=CC1)(C)C)C	herbaceous	Flavornet
1778	Humulene epoxide	(4E ,7E)-1,5,9,9-tetramethyl-12-oxabicyclo[9.1.0]dodeca-4,7-diene	CC1=CCCC2(C(O2)CC(C=CC1)(C)C)C	herbaceous	SuperScent, TGSC
1779	13-Oxabicyclo[10.1.0]trideca- 4,8-diene, 1,5,9-trimethyl-	1,5,9-trimethyl-13- oxabicyclo[10.1.0]trideca-4,8- diene	CC1=CCCC2(C(O2)CCC(=CCC1)C)C	woody amber	TGSC
1780	7-Epi-alpha-Selinene	5,8a -dimethyl-3-prop-1-en-2-yl-2,3,4,4a ,7,8- hexahydro-1H - naphthalene	CC1=CCCC2(C1CC(CC2)C(=C)C)C	amber	OdorRactor ,TGSC
1781	7-Epi-alpha-Eudesmol	2-[(2 <i>S</i> ,4 <i>aR</i> ,8 <i>aR</i>)-4 <i>a</i> ,8- dimethyl-2,3,4,5,6,8 <i>a</i> - hexahydro- 1 <i>H</i> -naphthalen-2-yl]propan-2-ol		sweet woody	Flavornet, Odoractor
1782	5,7-Diepi-alpha-eudesmol	2-[(2S ,4aR)-4a ,8-dimethyl- 2,3,4,5,6,8a - hexahydro-1H - naphthalen-2-yl]propan-2-ol	CC1=CCCC2(C1CC(CC2)C(C)(C)O)C	sweet woody	OdorRactor,
1783	1-Methylcyclohexene	1-methylcyclohexene	CC1=CCCCC1	lime citrus	OdorRactor ,TGSC
1784	Methylcyclopentadecenone	2-methylcyclopentadec-2-en-1-one		musk ketonic animal soapy	OdorRactor ,TGSC
1785	Nerol oxide	4-methyl-2-(2-methylprop-1-enyl)- 3,6-dihydro-2 <i>H</i> - pyran	CC1=CCOC(C1)C=C(C)C	oily green weedy herbaceous celery cortex narcissus vegetable floral minty	Flavornet, TGSC, OdoRactor
1786	3,6-Dihydro-4-methyl-2- phenyl-2H-pyran	4-methyl-2-phenyl-3,6-dihydro- 2 <i>H</i> -pyran	CC1=CCOC(C1)C2=CC=CC=C2	floral rose geranium metallic green	OdorRactor ,TGSC
1787	2-Acetyl-3,6-	1-(3,6-dimethylpyrazin-2-	CC1=CN=C(C(=N1)C(=O)C)C	popcorn roasted hazelnut caramel	OdorRactor ,TGSC
1788	dimethylpyrazine 2,3,5-Trimethylpyrazine	yl)ethanone 2,3,5-trimethylpyrazine	CC1=CN=C(C(=N1)C)C	roasted hazelnut chocolate hazelnut peanut potato roasted musty nutty earthy powdery cocoa baked potato roasted nut coffee baked	Sigma Aldrich, Flavorbase, TGSC, OdoRactor
1789	2-Acetyl-3,5- dimethylpyrazine	1-(3,5-dimethylpyrazin-2- yl)ethanone	CC1=CN=C(C(=N1)C)C(=O)C	caramel roasted hazelnut nutty roasted hazelnut	Sigma Aldrich, TGSC, OdoRactor
1790	2-Ethenyl-3,5- dimethylpyrazine	2-ethenyl-3,5-dimethylpyrazine	CC1=CN=C(C(=N1)C)C=C	earthy musty	Flavornet, TGSC, OdoRactor
1791	2-Methoxy-3,5- dimethylpyrazine	2-methoxy-3,5-dimethylpyrazine	CC1=CN=C(C(=N1)C)OC	earthy	TGSC
1792	Pyrazine, 2,5-dimethyl-3-(3-methylbutyl)-	2,5-dimethyl-3-(3- methylbutyl)pyrazine	CC1=CN=C(C(=N1)CCC(C)C)C	fruit	TGSC, Sigma Aldrich
1793	3-Methoxy-2,5- dimethylpyrazine	3-methoxy-2,5-dimethylpyrazine	CC1=CN=C(C(=N1)OC)C	earthy	Flavornet
1794	2,5-Dimethylpyrazine	2,5-dimethylpyrazine	CC1=CN=C(C=N1)C	meaty medicinal nutty woody cocoa roasted nut beefy grassy chocolate peanut musty earthy powdery baked potato roasted baked	Sigma Aldrich, TGSC, Odoractor
1795	2-Acetyl-5-methylpyrazine	1-(5-methylpyrazin-2-yl)ethanone	CC1=CN=C(C=N1)C(=O)C	nutty popcorn	TGSC, OdoRactor
1796	2-Isopropyl-5-methylpyrazine	2-methyl-5-propan-2-ylpyrazine	CC1=CN=C(C=N1)C(C)C	green coffee nutty earthy sweaty roasted	Flavornet, TGSC, OdoRactor
1797	2-Methyl-5- (methylthio)pyrazine	2-methyl-5- methylsulfanylpyrazine	CC1=CN=C(C=N1)SC	almond caramel coffee green musty nutty earthy peanut vegetable toasted popcorn roasted hazelnut cashewnut corn	Sigma Aldrich, TGSC, OdoRactor
1798	2,5-Dimethylthiazole	2,5-dimethyl-1,3-thiazole	CC1=CN=C(S1)C	nutty roasted roasted meat earthy	TGSC, Flavorbase, Odoractor
1799	2-Isobutyl-5-methylthiazole	5-methyl-2-(2-methylpropyl)-1,3-	CC1=CN=C(S1)CC(C)C	green pepper cabbage tropical fruit fruity green nutty	TGSC
1000	2 (Dimed: 1	thiazole	CCL CN CC/ NL)C	CC	O' A11' 1 E1 '
1800	2,6-Dimethylpyrazine	2,6-dimethylpyrazine	CC1=CN=CC(=N1)C	coffee roasted meat meaty nutty chocolate cocoa roasted fried potato roasted nut fried	Sigma Aldrich, Flavorbase, TGSC,OdoRactor
1801	1-(6-Methyl-2- pyrazinyl)ethanone	1-(6-methylpyrazin-2-yl)ethanone	CC1=CN=CC(=N1)C(=O)C	roasted roasted coffee cocoa popcorn coffee	TGSC
1802	2-Methoxy-6-methylpyrazine	2-methoxy-6-methylpyrazine	CC1=CN=CC(=N1)OC	roasted hazelnut roasted almond roasted peanut nutty roasted	TGSC
1803	3-Methylindole	3-methyl-1 <i>H</i> -indole	CC1=CNC2=CC=CC12	fatty fecal mothball jasmine animal civet naphthyl offensive strong manure	Sigma Aldrich, Flavorbase, TGSC, Pubchem

1804	Octanal, 7-hydroxy-3,7- dimethyl-, reaction products with 3-methyl-1H-indole	7-hydroxy-3,7-dimethyloctanal;3-methyl-1 H - indole	CC1=CNC2=CC=CC=C12.CC(C CCC(C)(C)O)CC=O	animal fecal	TGSC
1805	2,4-Dimethylthiazole	2,4-dimethyl-1,3-thiazole	CC1=CSC(=N1)C	coffee meaty rubbery moldy tea beefy roasted barley roasted barley	Sigma Aldrich, TGSC,OdoRactor
1806	2-Acetyl-4-methylthiazole	1-(4-methyl-1,3-thiazol-2-yl)ethanone	CC1=CSC(=N1)C(=O)C	cooked meaty	TGSC
1807	2-Isopropyl-4-methylthiazole	4-methyl-2-propan-2-yl-1,3- thiazole	CC1=CSC(=N1)C(C)C	musty alliaceous sulfurous coffee meaty green nutty earthy tropical fruit fruity vegetable rooty peach	Sigma Aldrich, Flavorbase, TGSC, OdoRactor
1808	4-Methylthiazole	4-methyl-1,3-thiazole	CC1=CSC=N1	green vegetable tomato nutty roasted meat alliaceous ripe tropical roasted meaty	Sigma Aldrich, TGSC, OdoRactor, Pubchem,OdoRactor
1809	2,6-Dimethylpyridine	2,6-dimethylpyridine	CC1=NC(=CC=C1)C	coffee green nutty baked potato ammonical woody bready cocoa oily fishy vegetable herbaceous pyridine musty baked	Sigma Aldrich, Flavorbase, TGSC,OdoRactor
1810	2,5-Dihydro-2-isopropyl-4-	4-methyl-2-propan-2-yl-2,5-	CC1=NC(SC1)C(C)C	toasted sulfurous sweet cocoa	TGSC, Flavorbase
1811	methylthiazole 1-(5,6-Dimethylpyrazin-2- yl)ethanone	dihydro-1,3-thiazole 1-(5,6-dimethylpyrazin-2- yl)ethanone	CC1=NC=C(N=C1C)C(=O)C	chocolate roasted aromatic green	TGSC
1812	5-Isobutyl-2,3-	2,3-dimethyl-5-(2-	CC1=NC=C(N=C1C)CC(C)C	green leafy nutty	Sigma Aldrich, TGSC
1813	dimethylpyrazine 1-(2-Methyloxazol-5-	methylpropyl)pyrazine 1-(2-methyl-1,3-oxazol-5-	CC1=NC=C(O1)C(=O)C	nutty	TGSC
1814	yl)ethanone 5-Methoxy-2-methylthiazole	yl)ethanone 5-methoxy-2-methyl-1,3-thiazole	CC1=NC=C(S1)OC	green cabbage vegetable sulfurous	OdorRactor ,TGSC
1815	2-Methyl-5,7-dihydrofuro[3,4-d]pyrimidine	2-methyl-5,7-dihydrofuro[3,4-d]pyrimidine	CC1=NC=C2COCC2=N1	sweet popcorn	TGSC
1816	2-Methyl-5,7- dihydrothieno[3,4- d]pyrimidine	2-methyl-5,7-dihydrothieno[3,4-d]pyrimidine	CC1=NC=C2CSCC2=N1	popcorn roasted corn taco toasted nutty	OdorRactor ,TGSC, Flavorbase
1817	4-Acetyl-2-methylpyrimidine	1-(2-methylpyrimidin-4- yl)ethanone	CC1=NC=CC(=N1)C(=O)C	burnt meaty roasted	OdorRactor ,TGSC
1818	2-Methylpyrazin	2-methylpyrazine	CC1=NC=CN=C1	chocolate green meaty nutty cocoa roasted peanut brown musty earthy	Sigma Aldrich, TGSC,OdoRactor
1819	2,3-Dimethylpyrazine	2,3-dimethylpyrazine	CC1=NC=CN=C1C	almond coffee green meaty nutty peanut buttery cocoa baked potato walnut caramel roasted potato musty baked	Sigma Aldrich, TGSC, OdoRactor
1820	2-Acetyl-3-methylpyrazine	1-(3-methylpyrazin-2-yl)ethanone	CC1=NC=CN=C1C(=O)C	roasted nutty roasted hazelnut vegetable caramel toasted grain corn hazelnut	Sigma Aldrich, TGSC, OdoRactor
1821	2-Isopropyl-3-methylpyrazine	2-methyl-3-propan-2-ylpyrazine	CC1=NC=CN=C1C(C)C	woody coffee	TGSC
1822	2-Isobutyl-3-methylpyrazine	2-methyl-3-(2- methylpropyl)pyrazine	CC1=NC=CN=C1CC(C)C	herbaceous sugar green caramel	Sigma Aldrich, TGSC, OdoRactor
1823	2-Methoxy-3-methylpyrazine	2-methoxy-3-methylpyrazine	CC1=NC=CN=C1OC	roasted almond hazelnut peanut chocolate nutty cocoa roasted almond roasted hazelnut roasted peanut	Sigma Aldrich, TGSC, OdoRactor
1824	2-Methyl-3- (methylthio)pyrazine	2-methyl-3- methylsulfanylpyrazine	CC1=NC=CN=C1SC	roasted roasted meat nutty almond vegetable	OdorRactor ,TGSC
1825	2-Furfurylthio-3- methylpyrazine	2-(furan-2-ylmethylsulfanyl)-3- methylpyrazine	CC1=NC=CN=C1SCC2=CC=CO	nutty roasted coffee sulfurous coffee cooked meaty roasted	Sigma Aldrich, TGSC, OdoRactor
1826 1827	2-Methylthiazole 2-Methylquinoxaline	2-methyl-1,3-thiazole 2-methylquinoxaline	CC1=NC=CS1 CC1=NC2=CC=CC=C2N=C1	green vegetable burnt roasted nutty fruit coffee	TGSC Sigma Aldrich, TGSC
1828	2,3-Dimethylquinoxaline	2,3-dimethylquinoxaline	CC1=NC2=CC=CC=C2N=C1C	toasted roasted coffee fatty earthy	OdorRactor ,TGSC
1829	2-Methylbenzoxazole	2-methyl-1,3-benzoxazole	CC1=NC2=CC=CC=C2O1	almond musty vanilla tobacco burnt phenolic meaty powdery	Sigma Aldrich, TGSC
1830	2-Methyl-2-thiazoline	2-methyl-4,5-dihydro-1,3-thiazole	CC1=NCCS1	capers sulfurous musty meaty nutty beefy	TGSC
1831	4-Methyl-3-thiazoline	4-methyl-2,5-dihydro-1,3-thiazole	CC1=NCSC1	vegetable garlic carbide	Flavornet, Flavorbase
1832	Limonene dioxide	1-methyl-4-(2-methyloxiran-2-yl)- 7- oxabicyclo[4.1.0]heptane	CC12CCC(CC102)C3(CO3)C	mentholic	TGSC, Pubchem, OdoRactor

1833	Androstenol	10,13-dimethyl- 2,3,4,5,6,7,8,9,11,12,14,15- dodecahydro-1 <i>H</i> -	CC12CCC3C(C1CC=C2)CCC4C3 (CCC(C 4)O)C	faint animal musk natural	Sigma Aldrich, TGSC, OdoRactor
1834	Zingiberol	cyclopenta[a]phenanthren-3-ol 2-[(2R, 4aR) -4a -methyl-8- methylidene- 1,2,3,4,5,6,7,8a - octahydronaphthalen-2-yl]propan- 2-ol	CC12CCCC(=C)C1CC(CC2)C(C) (C)O	ginger spicy	TGSC
1835	beta-Eudesmol	2-[(2R,4aR,8aS)-4a-methyl-8-methylidene- 1,2,3,4,5,6,7,8a-octahydronaphthalen-2-yl]propan- 2-ol	CC12CCCC(=C)C1CC(CC2)C(C) (C)O	woody green	Flavornet, OdoRactor, TGSC
1836	1,5- Dimethylbicyclo[3.2.1]octan- 8-one oxime	N -(1,5-dimethyl-8-bicyclo[3.2.1]octanylidene)hydrox ylamine	CC12CCCC(C1=NO)(CC2)C	fresh buchu fruity natural leafy oily clean herbaceous	OdorRactor ,TGSC
1837	2H-4,7a-Ethanonaphth[1,2-b]oxirene, octahydro-3a,4,7b-trimethyl-	2,7,8-trimethyl-3- oxatetracyclo[6.3.2.01,7.02,4]trid ecane		dry laundered cloth soft musk	OdorRactor ,TGSC
1838	3-Hydroxy-4,5-dimethylfuran- 2(5H)-one	4-hydroxy-2,3-dimethyl-2 <i>H</i> -furan- 5-one	CC1C(=C(C(=O)O1)O)C	caramel celery green maple meaty nutty earthy seedy tobacco winey spice sweet burnt sugar coffee brown sugar cotton candy chicken	Sigma Aldrich, Flavorbase, TGSC, OdoRactor
1839	2,4,5-Trimethyl-3-oxazoline	2,4,5-trimethyl-2,5-dihydro-1,3-oxazole	CC1C(=NC(O1)C)C	nutty musty green woody caramel vegetable cocoa brown bready	OdorRactor ,TGSC
1840	4,5-Dimethyl-2-isobutyl-3-thiazoline	4,5-dimethyl-2-(2-methylpropyl)- 2,5-dihydro-1,3- thiazole	CC1C(=NC(S1)CC(C)C)C	green nutty sulfurous burnt cocoa corn sweet roasted meaty chocolate vegetable	Sigma Aldrich, TGSC, Flavorbase, OdoRactor
1841	4-Acetyl-2,5-dimethylfuran- 3(2H)-one	4-acetyl-2,5-dimethylfuran-3-one	CC1C(=0)C(=C(O1)C)C(=O)C	caramel fruity	TGSC
1842	Furaneol	4-hydroxy-2,5-dimethylfuran-3-one	CC1C(=0)C(=C(O1)C)O	beefy buttery	
1843	Furaneol	4-hydroxy-2,5-dimethylfuran-3- one	CC1C(=0)C(=C(01)C)O	strawberry sweet caramel cotton candy brown sugar burnt brown savory fruity pineapple	Sigma Aldrich, TGSC, Flavorbase, OdoRactor
1844	2,5-Dimethyl-4-methoxy- 3(2H)-furanone	4-methoxy-2,5-dimethylfuran-3-one	CC1C(=O)C(=C(O1)C)OC	caramel coffee grape maple meaty mossy mushroom nutty potato sweet mildew vegetable fruity brandy moldy burnt sugar wasabi musty beany cocoa	Sigma Aldrich, Flavornet, TGSC, Odoractor
1845	2,5-Dimethyl-4-oxo-4,5-dihydrofuran-3-yl acetate	(2,5-dimethyl-4-oxofuran-3-yl) acetate	CC1C(=0)C(=C(O1)C)OC(=0)C	berry caramel sweet tropical fruity bready brown sugar toffee molasses fatty burnt sugar bready baked fatty	Sigma Aldrich, TGSC, OdoRactor,
1846	4-Hydroxy-2,5- dimethylthiophen-3(2H)-one	4-hydroxy-2,5-dimethylthiophen-3- one	CC1C(=0)C(=C(S1)C)O	meaty bready	OdorRactor ,TGSC
1847	2,5-Dimethyl-3(2H)-furanone	2,5-dimethylfuran-3-one	CC1C(=O)C=C(O1)C	fruity estery caramel	OdorRactor ,TGSC
1848	1H-Inden-1-one, 2,3-dihydro- 2,3,3- trimethyl-	2,3,3-trimethyl-2 <i>H</i> -inden-1-one	CC1C(=0)C2=CC=CC=C2C1(C) C	herbaceous leathery saffron marine tobacco woody phenolic	OdorRactor ,TGSC
1849	8,9-Dehydrotheaspirone	2,6,6,10-tetramethyl-1- oxaspiro[4.5]deca-7,9-dien-	CC1C(=0)CC2(O1)C(=CC=CC2(C)C)C	woody floral	OdorRactor ,TGSC
1850	2-Methyltetrahydrofuran-3- one	2-methyloxolan-3-one	CC1C(=0)CCO1	buttery sweet bready nutty solvent brown rummy roasted caramel	Flavornet, Flavorbase, TGSC, OdoRactor
1851	(2S)-2-Methyloxolan-3-one	(2S)-2-methyloxolan-3-one	CC1C(=0)CCO1	sweet buttery nutty solvent bready brown rummy	OdorRactor ,TGSC
1852	2-Methyltetrahydrothiophen-3- one	2-methylthiolan-3-one	CC1C(=O)CCS1	buttery balsamic cabbage onion musty fruity berry sulfurous	Sigma Aldrich, Flavornet, TGSC, Odoractor
1853	2-Hydroxy-3,4,5-trimethyl-2-cyclopenten-1- one	2-hydroxy-3,4,5- trimethylcyclopent-2-en-1-one	CC1C(C(=0)C(=C1C)O)C	sweet burnt spicy caramel maple coffee bready licorice	TGSC
1854	Galactoarabinan	4-[6-[(3,5-dihydroxy-4- methoxyoxan-2-yl)oxymethyl]- 3,5-dihydroxy-4-methoxyoxan-2- yl]oxy-2-(hydroxymethyl)-6- methyloxane-3,5-diol	CC1C(C(C(C(O1)CO)O)OC2C(C(C(C(O2) COC3C(C(C(CO3)O)OC)O)O)OC)O)O	balsamic resinous pine	TGSC

1855	Neohesperidin dihydrochalcone	1-[4-[(2 <i>S</i> ,3 <i>R</i> ,4 <i>S</i> ,5 <i>S</i> ,6 <i>R</i>)-4,5-dihydroxy-6- (hydroxymethyl)-3-	CC1C(C(C(C(O1)OC2C(C(C(OC 2OC3=C	orange sweet	Sigma Aldrich, TGSC
	чинучноснавсопе	dinydroxy-6- (hydroxymethyl)-3- [(2S ,3R ,4R ,5R ,6S)-3,4,5- trihydroxy-6-methyloxan-2-	20C3=C C(=C(C(=C3)O)C(=O)CCC4=CC(=C(C=C		
		yl]oxyoxan-2-yl]oxy-	4)OC)O)O)O)O)O)O)O		
		2,6-dihydroxyphenyl]-3-(3-hydroxy-4-			
		methoxyphenyl)propan-1-one			
1856	Cashmeran	1,1,2,3,3-pentamethyl-2,5,6,7- tetrahydroinden-4- one	CC1C(C2=C(C1(C)C)C(=O)CCC 2)(C)C	spicy musk woody clean	OdorRactor ,TGSC, Pubchem
1857	Traseolide	1-(1,1,2,6-tetramethyl-3-propan-2-yl-2,3- dihydroinden-5-	CC1C(C2=C(C1(C)C)C=C(C(=C2)C(=O)C	sweet amber musk herbaceous creamy dry	OdorRactor ,TGSC, Pubchem
1050	N P.I	yl)ethanone)C)C(C)C		O.L. B
1858	Phantolide	1-(1,1,2,3,3,6-hexamethyl-2 <i>H</i> - inden-5- yl)ethanone	CC1C(C2=C(C1(C)C)C=C(C(=C2)C)C(=0)C)(C)C	sweet musk amber powdery fruity	OdorRactor ,TGSC
1859	1-(2,3-Dihydro-1,1,2,3,3- pentamethyl-1H- inden-5- yl)ethan-1-one	1-(1,1,2,3,3-pentamethyl-2 <i>H</i> - inden-5-yl)ethanone	CC1C(C2=C(C1(C)C)C=C(C=C2) C(=O)C) (C)C	musk	TGSC
1860	Decahydro-2,2,6,6,7,8,8- heptamethyl-2H- indeno(4,5-	2,2,6,6,7,8,8-heptamethyl-3,3 <i>a</i> ,4,5,5 <i>a</i> ,7,8 <i>a</i> ,8 <i>b</i> -	CC1C(C2CCC3CC(OC3C2C1(C) C)(C)C)(C)C	animal musk woody spicy	TGSC
	b)furan	octahydrocyclopenta[g][1]benzofu ran			
1861	Cyclopentanol, 1,2-dimethyl-3-(1- methylethenyl)-	1,2-dimethyl-3-prop-1-en-2- ylcyclopentan-1-ol	CC1C(CCC1(C)O)C(=C)C	camphoraceous citrus spicy	TGSC
1862	1,2-Dimethyl-3-(1- methylethenyl)cyclopentyl	[(1S,2R,3R)-1,2-dimethyl-3-prop- 1-en-2- ylcyclopentyl] acetate	CC1C(CCC1(C)OC(=O)C)C(=C) C	warm herbaceous clary sage woody	OdorRactor ,TGSC
1863	acetate 2-Methyl-3-	O -(2-methyloxolan-3-yl)	CC1C(CCO1)OC(=S)C	sulfurous meaty roasted meat	TGSC, Flavorbase
1864	thioacetoxytetrahydrofuran (2S,3R)-2-	ethanethioate (2S, 3R)-2-methyloxolane-3-thiol	CC1C(CCO1)S	onion	Flavornet
	Methyltetrahydrofuran-3-thiol				
1865	2-Methyltetrahydrofuran-3- thiol	2-methyloxolane-3-thiol	CC1C(CCO1)S	roasted meaty caramel coffee sulfurous roasted beef chicken	Sigma Aldrich, TGSC, OdoRactor
				beefy roasted meat alliaceous	
1866	2,3,5,6-Tetramethyl-1,4- dioxane-2,5-diol	2,3,5,6-tetramethyl-1,4-dioxane- 2,5-diol	CC1C(OC(C(O1)(C)O)C)(C)O	buttery milky creamy dairy	TGSC
1867		4-(4,5-dimethyl-1,3-dioxolan-2-yl)- 2- methoxyphenol	CC1C(OC(O1)C2=CC(=C(C=C2) O)OC)C	vanilla creamy chocolate powdery caramel dairy custard gourmand	TGSC
	2-yı)-2- memoxypnenoi	2- methoxyphenol	Ojocje	balsamic malty	
1868	1,3-Dioxolane, 4,5-dimethyl- 2-phenyl-	4,5-dimethyl-2-phenyl-1,3-dioxolane	CC1C(OC(O1)C2=CC=CC=C2)C	weak animal	OdorRactor ,Flavorbase
1869	2-Benzyl-4,5-dimethyl-1,3-dioxolane	2-benzyl-4,5-dimethyl-1,3-dioxolane	CC1C(OC(O1)CC2=CC=CC=C2)	floral sweet earthy herbaceous	TGSC, Flavorbase, OdoRactor
1870	1-(3,5,6-Trimethyl-3- cyclohexen-1- yl)ethanone	1-(3,5,6-trimethylcyclohex-3-en-1-yl)ethanone	CC1C=C(CC(C1C)C(=O)C)C	green floral earthy woody dry	OdorRactor ,TGSC
1871	3,5,6-Trimethyl-3- cyclohexene-1-	3,5,6-trimethylcyclohex-3-ene-1-carbaldehyde	CC1C=C(CC(C1C)C=O)C	green leafy herbaceous fresh clean chrysanthemum	OdorRactor ,TGSC
1872	carboxaldehyde Methyl 2-(((2,4(or 3,5)-	methyl 2-[[(E)-(2,4-	CC1C=C(CCC1=CNC2=CC=CC=	fresh green sweet floral orange	OdorRactor ,TGSC
10/2	dimethyl-3- cyclohexen-1- yl)methylene)amino)benzoate	dimethylcyclohex-3-en-1- ylidene)methyl]amino]benzoate	C2C(=O)OC)C	flower leafy	Odorkacioi , rose
1873		1-(2,4-dimethylcyclohex-3-en-1-	CC1C=C(CCC1C(=O)C(C)(C)C)	herbaceous floral grapefruit	OdorRactor ,TGSC
	1-yl)-2,2- dimethyl-1- propanone	yl)-2,2- dimethylpropan-1-one	С	chrysanthemum	
1874	Benzoic acid, 2-(((2,4-dimethyl-3- cyclohexen-1-	methyl 2-[(2,4-dimethylcyclohex- 3-en-1-	CC1C=C(CCC1C=NC2=CC=CC=C2C(=O	aldehydic green natural leafy fresh cortex narcissus	OdorRactor ,TGSC
	yl)methylene)amino)-, methyl ester	yl)methylideneamino]benzoate)OC)C		
1875	2,4-Dimethylcyclohex-3-ene- 1-carbaldehyde	2,4-dimethylcyclohex-3-ene-1- carbaldehyde	CC1C=C(CCC1C=O)C	green leafy cortex tart floral peely aldehydic	SuperScent, TGSC, OdoRactor, Pubchem
1876	3-Cyclohexene-1-methanol, 2,4-dimethyl-	(2,4-dimethylcyclohex-3-en-1- yl)methanol	CC1C=C(CCC1CO)C	floral fresh herbaceous green petal gardenia minty	OdorRactor,
1877	5-Methyl-2(5H)-furanone	2-methyl-2 <i>H</i> -furan-5-one	CC1C=CC(=O)O1	sweet herbaceous tobacco nutty	Flavorbase
1878	1-Oxaspiro[4.5]deca-3,6-	2,9-dimethyl-6-propan-2-yl-1-	CC1C=CC2(O1)C=C(CCC2C(C)	tonka coumarinic fruity black currant tropical	TGSC
	diene, 2,7- dimethyl-10-(1- methylethyl)-	oxaspiro[4.5]deca- 3,9-diene	C)C		
1879	5-Methyl-5(H)- cyclopentapyrazine	5-methyl-5 <i>H</i> - cyclopenta[b]pyrazine	CC1C=CC2=NC=CN=C12	roasted	Flavornet, TGSC
1880	3-Cyclohexene-1-carboxylic acid, 2,6,6- trimethyl-, methyl	methyl 2,6,6-trimethylcyclohex-3- ene-1- carboxylate	CC1C=CCC(C1C(=0)OC)(C)C	floral rose fruity saffron	TGSC
1881	ester Trivertal	1,2-dimethylcyclohex-3-ene-1-	CC1C=CCCC1(C)C=O	ethereal green aldehydic weedy	Sigma Aldrich, TGSC,
		carbaldehyde		herbaceous soapy cortex	OdorRactor,

1882	Spiro(1,3-dithiolo(4,5-b)furan- 2,3'(2'H)- furan), hexahydro- 2',3a-dimethyl-	2',3a -dimethylspiro[6,6a - dihydro-5H - [1,3]dithiolo[4,5- b]furan-2,3'-oxolane]	CC1C2(CCO1)SC3CCOC3(S2)C	meaty ham	OdorRactor ,Flavorbase, TGSC
1883	Spiro(1,4-	3,4-dimethylspiro[oxirane-2,10'-tricyclo[6.2.1.02,7]undec-4-ene]	CC1C2(O1)CC3CC2C4C3CC=C(C4)C	fresh floral fruity rhubarb zesty woody spicy	OdorRactor ,TGSC
1884	https://pubchem.ncbi.nlm.nih. gov/compoun d/642887	(3S)-3,6-dimethyl-3H-1- benzofuran-2-one	CC1C2=C(C=C(C=C2)C)OC1=O	coconut	OdorRactor ,TGSC
1885	Georgywood	1-[(1 <i>R</i> ,2 <i>S</i>)-1,2,8,8-tetramethyl-1,3,4,5,6,7- hexahydronaphthalen-2-yl]ethanone	CC1C2=C(CCCC2(C)C)CCC1(C) C(=O)C	woody amber floral	TGSC, Flavorbase
1886	2,7-Dimethyl-5,7- dihydrofuro[3,4- d]pyrimidine	2,7-dimethyl-5,7-dihydrofuro[3,4-d]pyrimidine	CC1C2=NC(=NC=C2CO1)C	popcorn cereal	TGSC
1887	3a,4,5,6,7,7a- Hexahydromethoxydimethyl- 4,7-methano-1H-indene	3-methoxy-4,5- dimethyltricyclo[5.2.1.02,6]dec-3- ene	CC1C2C3CCC(C3)C2C(=C1C)O C	herbaceous woody rosemary juniper	TGSC
1888	Cyclohexanol, 4-(5,5,6-trimethylbicyclo(2.2.1)hept-2-yl)-	4-(5,5,6-trimethyl-2-bicyclo[2.2.1]heptanyl)cyclohexan-1-ol	CC1C2CC(C1(C)C)CC2C3CCC(CC3)O	sandal wood sweet woody balsamic clean	OdorRactor ,TGSC
1889	3-(5,5,6-	3-(5,5,6-trimethyl-2-bicyclo[2.2.1]heptanyl)cyclohexan-1-ol	CC1C2CC(C1(C)C)CC2C3CCCC (C3)O	sandal wood clean sweet woody ethereal	Sigma Aldrich, TGSC, Pubchem
1890	3,5,5- Trimethylbicyclo[2.2.1]hepta n-2-one	3,5,5- trimethylbicyclo[2.2.1]heptan-2- one	CC1C2CC(C1=O)CC2(C)C	camphoraceous cedar woody	OdorRactor ,TGSC
1891	(1S,7S)-5,9-	(1 <i>S</i> ,7 <i>S</i>)-5,9- dimethyltricyclo[5.2.1.02,6]dec-4- en-8	CC1C2CC(C10)C3C2CC=C3C	camphoraceous earthy patchouli woody herbaceous	TGSC
1892	(+)-Pinanone	(1R, 2R, 5S)-2,6,6- trimethylbicyclo[3.1.1]heptan-3- one	CC1C2CC(C2(C)C)CC1=O	camphoraceous fi rneedle spruce pine	TGSC
1893	Pinocamphone	(1S, 2R, 5R)-2,6,6- trimethylbicyclo[3.1.1]heptan-3- one	CC1C2CC(C2(C)C)CC1=O	spicy	TGSC
1894	Thujone	(1S, 4R, 5R)-4-methyl-1-propan- 2-ylbicyclo[3.1.0]hexan-3-one	CC1C2CC2(CC1=O)C(C)C	cedar thujonic	TGSC
1895	3-Thujanone	4-methyl-1-propan-2- ylbicyclo[3.1.0]hexan-3-one	CC1C2CC2(CC1=0)C(C)C	thujonic cedar spicy woody	TGSC
1896	Thujyl alcohol	4-methyl-1-propan-2- ylbicyclo[3.1.0]hexan-3-ol	CC1C2CC2(CC10)C(C)C	camphoraceous spicy minty	SuperScent, TGSC,OdoRactor
1897	Bicyclo(3.1.0)hexan-3-ol, 4-methyl-1-(1-methylethyl)-, (1S,3S,4R,5R)-	(1S, 3S, 4R, 5R)-4-methyl-1- propan-2- ylbicyclo[3.1.0]hexan-3- ol	CC1C2CC2(CC10)C(C)C	spicy minty camphoraceous	OdorRactor ,TGSC
1898	Indeno[1,2-d]-1,3-dioxin, 4,4a,5,9b- tetrahydro-2,4- dimethyl-	2,4-dimethyl-4,4 <i>a</i> ,5,9 <i>b</i> - tetrahydroindeno[1,2-d][1,3]dioxine	CC1C2CC3=CC=CC=C3C2OC(O 1)C	floral narcissus green grapefruit geranium mangnolia gardenia	OdorRactor ,TGSC
1899	Tricyclo[3.3.1.13,7]decan-2-ol, 4-methyl-8- methylene-	4-methyl-8-methylideneadamantan- 2-ol	CC1C2CC3CC1C(C(C2)C3=C)O	woody spicy ginger cardamom	TGSC
1900	4-Methyl-8- methyleneadamantan-2-yl acetate	(4-methyl-8-methylidene-2- adamantyl) acetate	CC1C2CC3CC1C(C(C2)C3=C)O C(=O)C	woody amber vetiver	TGSC
1901	(3R,3Ar,7aS)-3,6-dimethyl- 3a,4,5,7a- tetrahydro-3H-1- benzofuran-2-one	(3R, 3aR, 7aS)-3,6-dimethyl-3a,4,5,7a -tetrahydro-3H -1-benzofuran-2-one	CC1C2CCC(=CC2OC1=0)C	coconut dill spicy sweet	OdorRactor,
1902	Wine lactone	3,6-dimethyl-3 <i>a</i> ,4,5,7 <i>a</i> - tetrahydro-3 <i>H</i> -1- benzofuran-2- one	CC1C2CCC(=CC2OC1=0)C	coconut spice dill sweet woody	Flavornet, TGSC, Odoractor
1903	Indisan	1-(2,2,3-trimethyl-1- bicyclo[2.2.1]heptanyl)cyclohexan- 1-ol	CC1C2CCC(C2)(C1(C)C)C3(CC CCC3)O	woody sandal wood clean sweet	TGSC
1904	2-Methoxy-3,5- dimethylcyclopent-2-en-1- one	2-methoxy-3,5-dimethylcyclopent- 2-en-1-one	CC1CC(=C(C1=O)OC)C	caramel maple	TGSC
1905	2-Methyl-4-methylidene-6- phenyltetrahydro- 2H-pyran	2-methyl-4-methylidene-6- phenyloxane	CC1CC(=C)CC(O1)C2=CC=CC= C2	geranium floral green leafy herbaceous	OdorRactor ,TGSC
1906	4-(2,4,6-Trimethyl-3- cyclohexen-1-yl)-3- buten-2- one	(E)-4-(2,4,6-trimethylcyclohex-3-en-1-yl)but-3-en-2-one	CC1CC(=CC(C1C=CC(=0)C)C)C	floral orris violet woody	OdorRactor ,TGSC

1907	2,4,6-Trimethylcyclohex-3- ene-1- carbaldehyde;3,5,6-	2,4,6-trimethylcyclohex-3-ene-1-carbaldehyde;3,5,6-	CC1CC(=CC(C1C=O)C)C.CC1C =C(CC(C	green aldehydic earthy woody herbaceous leafy foliage wet	OdorRactor ,TGSC, Flavorbase
	trimethylcyclohex-3-ene- 1-carbaldehyde	trimethylcyclohex-3-ene-1- carbaldehyde	1C)C=O)C	grassy hay vegetable	
	Isocyclogeraniol	(2,4,6-trimethylcyclohex-3-en-1-yl)methanol	CC1CC(=CC(C1CO)C)C	spice floral carnation herbaceous green woody	OdorRactor ,TGSC
	2-Cyclopenten-1-one, 2-hydroxy-3,4- dimethyl-	2-hydroxy-3,4-dimethylcyclopent- 2-en-1-one	CC1CC(=0)C(=C1C)O	caramel	Flavornet, TGSC, OdoRactor
1910	3,4-Dimethyl-1,2- cyclopentanedione	3,4-dimethylcyclopentane-1,2-dione	CC1CC(=O)C(=O)C1C	sweet maple caramel fenugreek licorice anisic herbaceous sugar	Sigma Aldrich, TGSC, OdoRactor
1911	Dehydronootkatone	(4R,4aS,6S)-4,4a -dimethyl-6- prop-1-en-2-yl- 3,4,5,6-tetrahydronaphthalen-2- one	CC1CC(=O)C=C2C1(CC(C=C2)C (=C)C)C	citrus fruity grapefruit tropical juicy	TGSC, Flavorbase
1912	Nootkatone	(4R,4aS,6R)-4,4a -dimethyl-6-prop-1-en-2-yl-3,4,5,6,7,8-hexahydronaphthalen-2-one	CC1CC(=0)C=C2C1(CC(CC2)C(=C)C)C	grapefruit citrus gardenia woody orange sweet peely powerful	Flavornet, TGSC, Pubchem
1913	Nookatone	4,4 <i>a</i> -dimethyl-6-prop-1-en-2-yl-3,4,5,6,7,8- hexahydronaphthalen-2-one	CC1CC(=0)C=C2C1(CC(CC2)C(=C)C)C	grapefruit citrus woody gardenia orange sweet peely	OdorRactor ,TGSC, Pubchem
1914	(-)-Nootkatone	(4 <i>S</i> ,4 <i>aR</i> ,6 <i>S</i>)-4,4 <i>a</i> -dimethyl-6-prop-1-en-2-yl-3,4,5,6,7,8-hexahydronaphthalen-2-one	CC1CC(=0)C=C2C1(CC(CC2)C(=C)C)C	terpenic grapefruit citrus orange sweet woody powerful	Flavornet, Pubchem
1915	Dihydronootkatone	(4 <i>R</i> ,4 <i>aS</i> ,6 <i>R</i> ,8 <i>aS</i>)-4,4 <i>a</i> - dimethyl-6-prop-1-en-2- yl-1,3,4,5,6,7,8,8 <i>a</i> - octahydronaphthalen-2-one	CC1CC(=0)CC2C1(CC(CC2)C(= C)C)C	citrus fruit grapefruit strong	OdorRactor ,TGSC, Flavorbase
1916	4,4a-Dimethyl-6-propan-2-yl- 1,3,4,5,6,7,8,8a- octahydronaphthalen-2-one	4,4a -dimethyl-6-propan-2-yl- 1,3,4,5,6,7,8,8a - octahydronaphthalen-2-one	CC1CC(=O)CC2C1(CC(CC2)C(C)C)C	woody dusty fresh green sour spicy herbaceous fruity animal	
1917	5-Methyldihydro-3(2H)- furanone	5-methyloxolan-3-one	CC1CC(=O)CO1	hay sweet coumarinic	OdorRactor ,TGSC
1918	3,5-Dimethyl-1,2- cyclopentanedione	3,5-dimethylcyclopentane-1,2-dione	CC1CC(C(=O)C1=O)C	coffee sweet maple caramel brown sugar burnt sugar	Sigma Aldrich, TGSC, OdoRactor, Pubchem
1919	2,5-Dimethyltetrahydrofuran- 3-thiol	2,5-dimethyloxolane-3-thiol	CC1CC(C(O1)C)S	sulfurous roasted meaty onion	TGSC, Flavorbase
1920	6-Azulenol, 1,2,3,3a,4,5,6,8a- octahydro-4,8 dimethyl-2-(1- methylethylidene)-	4,8-dimethyl-2-propan-2-ylidene- 3,3a ,4,5,6,8a - hexahydro-1H - azulen-6-ol	CC1CC(C=C(C2C1CC(=C(C)C)C 2)C)O	sweet balsamic woody root sandal wood	OdorRactor ,TGSC
1921	Vetiveryl acetate	(4,8-dimethyl-2-propan-2-ylidene- 3,3a ,4,5,6,8a - hexahydro-1 <i>H</i> - azulen-6-yl) acetate	CC1CC(C=C(C2C1CC(=C(C)C)C 2)C)OC(=0)C	woody powdery rooty vetiver sweet dry sandal wood	Sigma Aldrich, TGSC
1922	1,2,3,3a,4,5,6,8a-Octahydro-2- isopropylidene-4,8- dimethylazulen-6-yl formate	(4,8-dimethyl-2-propan-2-ylidene-3,3a ,4,5,6,8a - hexahydro-1 <i>H</i> - azulen-6-yl) formate	CC1CC(C=C(C2C1CC(=C(C)C)C 2)C)OC =0	sandal wood fresh woody	TGSC
1923	Tonalid	1-(3,5,5,6,8,8-hexamethyl-6,7-dihydronaphthalen- 2-yl)ethanone	CC1CC(C2=C(C1(C)C)C=C(C(= C2)C(=O) C)C)(C)C	ethereal musk sweet amber fruity powdery	Sigma Aldrich, OdoRactor, Pubchem
1924	Ethanone, 1-(2,3,4,5,6,7-hexahydro-1,1,3-trimethyl-1H-inden-5-yl)-	1-[(3 <i>R</i> ,3 <i>aS</i> ,5 <i>R</i> ,7 <i>aR</i>)-1,1,3- trimethyl- 2,3,3 <i>a</i> ,4,5,6,7,7 <i>a</i> - octahydroinden-5-yl]propan-2- one	CC1CC(C2C1CC(CC2)CC(=0)C) (C)C	woody dry tobacco leafy thujonic	OdorRactor ,TGSC
1925	3-Cyclohexene-1-carbonitrile, 3,5-dimethyl-	3,5-dimethylcyclohex-3-ene-1-carbonitrile	CC1CC(CC(=C1)C)C#N	coumarinic tonka tobacco	OdorRactor ,TGSC
1926	3,5-Dimethylcyclohex-3-ene- 1-carbaldehyde	3,5-dimethylcyclohex-3-ene-1- carbaldehyde	CC1CC(CC(=C1)C)C=O	green aldehydic leafy	TGSC
1927	3-Cyclohexene-1-methanol, 3,5-dimethyl-	(3,5-dimethylcyclohex-3-en-1-yl)methanol	CC1CC(CC(=C1)C)CO	fresh petal floral herbaceous green gardenia minty	OdorRactor ,TGSC
1928	3,5-Dimethylcyclohex-3-ene- 1-methyl acetate	(3,5-dimethylcyclohex-3-en-1-yl)methyl acetate	CC1CC(CC(=C1)C)COC(=O)C	citrus floral green grapefruit gardenia petal	OdorRactor ,TGSC
1929	2H-Pyran-2-one, tetrahydro- 4,4,6(or 4,6,6)- trimethyl-	4,4,6-trimethyloxan-2-one	CC1CC(CC(=0)01)(C)C	walnut nutty saffron citrus herbaceous bitter acorn	OdorRactor ,TGSC
1930	2-[(3,3,5- Trimethylcyclohexyl)acetyl]c yclopentan-1- one	2-[2-(3,3,5- trimethylcyclohexyl)acetyl]cyclop entan- 1-one	CC1CC(CC(C1)(C)C)CC(=0)C2C CCC2= 0	woody animal aromatic	TGSC
1931	cis-3,3,5- Trimethylcyclohexanol	(1S,5S)-3,3,5- trimethylcyclohexan-1-ol	CC1CC(CC(C1)(C)C)O	minty	TGSC, Pubchem
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1933	3,3,5-Trimethylcyclohexyl acetate	(3,3,5-trimethylcyclohexyl) acetate	CC1CC(CC(C1)(C)C)OC(=O)C	mild fruity sweet minty spicy clove floral herbaceous green mentholic lavender	OdorRactor ,TGSC, Flavorbase
1934	4-[(3,3- Dimethylbicyclo[2.2.1]hept-2- yl)methyl]-2- methylcyclohexan-1-one	4-[(3,3-dimethyl-2-bicyclo[2.2.1]heptanyl)methyl]-2-methylcyclohexan-1-one	CC1CC(CCC1=0)CC2C3CCC(C3)C2(C) C		OdorRactor ,TGSC
1935	Rhubafuran	2,4-dimethyl-4-phenyloxolane	CC1CC(CO1)(C)C2=CC=CC=C2	green rhubarb grapefruit citrus herbaceous eucalyptus woody	OdorRactor ,TGSC
1936	2,4,6-Trimethyl-4-phenyl-1,3-dioxane	2,4,6-trimethyl-4-phenyl-1,3-dioxane	CC1CC(OC(O1)C)(C)C2=CC=CC =C2	floral fresh citrus gardenia green natural	OdorRactor ,TGSC
1937		2-methoxy-4-(4,4,6-trimethyl-1,3-dioxan-2- yl)phenol			OdorRactor ,TGSC
1938	4,4,6-Trimethyl-2-phenyl-1,3-dioxane	4,4,6-trimethyl-2-phenyl-1,3-dioxane	CC1CC(OC(O1)C2=CC=CC=C2)(C)C	herbaceous reseda green rose	TGSC
1939	2-Benzyl-4,4,6-trimethyl-1,3-dioxane	2-benzyl-4,4,6-trimethyl-1,3-dioxane	CC1CC(OC(O1)CC2=CC=CC=C2)(C)C	hyacinth sweetpea green bean balsamic narcissus reseda floral	OdorRactor ,TGSC
1940	(2S,4R)-4-Methyl-2-[(1E)-3-methylbuta-1,3 dienyl]oxolane	(2S,4R)-4-methyl-2-[(1E)-3-methylbuta-1,3-dienyl]oxolane	CC1CC(OC1)C=CC(=C)C	quince fruit	Flavorbase
	3,5-Dimethyl-1,2-dithiolane	3,5-dimethyldithiolane	CC1CC(SS1)C	sulfurous cooked onion	TGSC
1942	alpha-Irone	(E)-4-(2,5,6,6-tetramethylcyclohex-2-en-1-yl)but-3-en-2-one	CC1CC=C(C(C1(C)C)C=CC(=0) C)C	floral orris berry violet woody powdery raspberry sweet	OdorRactor ,TGSC, Flavorbase
1943	2,6,9,10-Tetramethyl-1- oxaspiro[4.5]deca- 3,6-diene	2,6,9,10-tetramethyl-1-oxaspiro[4.5]deca-3,6- diene	CC1CC=C(C2(C1C)C=CC(O2)C) C	fruity black currant berry	TGSC
1944	3,6-Dimethylcyclohex-3-ene- 1-carbaldehyde	3,6-dimethylcyclohex-3-ene-1- carbaldehyde	CC1CC=C(CC1C=O)C	green tart citrus herbaceous aldehydic cortex	OdorRactor ,TGSC
1945	3,6-Dimethyl-5,6,7,7a- tetrahydro-3H-1- benzofuran- 2-one	3,6-dimethyl-5,6,7,7 <i>a</i> -tetrahydro-3 <i>H</i> -1- benzofuran-2-one	CC1CC=C2C(C(=O)OC2C1)C	sweet creamy coumarinic coconut powdery tobacco spearmint tonka	SuperScent, TGSC
1946	CID 11855994	(5Z)-3-methylcyclotetradec-5-en- 1-one	CC1CC=CCCCCCCCC(=0)C1	musk	TGSC
1947	CID 66823518	(5E)-3-methylcyclotetradec-5-en-1-one	CC1CC=CCCCCCCCC(=0)C1	musk animal powdery fatty laundered cloth ambergis anisic	TGSC
1948	4-Methyl-1- oxaspiro(5.5)undecene	4-methyl-1-oxaspiro[5.5]undec-2- ene	CC1CC2(CCCCC2)OC=C1	herbaceous rosemary minty camphoraceous thujonic tropical	OdorRactor,
1949	1-(2,3,8,8-Tetramethyl- 1,2,3,4,5,6,7,8- octahydronaphthalen-2- yl)ethanone	1-(2,3,8,8-tetramethyl-1,3,4,5,6,7-hexahydronaphthalen-2-yl)ethanone	CC1CC2=C(CC1(C)C(=O)C)C(C CC2)(C) C	woody dry ambergis cedar old wood phenolic ketonic	OdorRactor ,TGSC
1950		(3Z)-3-(4,7,7-trimethyl-3-bicyclo[4.1.0]heptanylidene)propa nenitrile		rose geranium woody sandal wood	TGSC
1951	Octahydro-7-methyl-1,4- methanonaphthalen 6(2H)-one	5- methyltricyclo[6.2.1.02,7]undecan- 4-one	CC1CC2C3CCC(C3)C2CC1=0	natural herbaceous woody fruity pine cedar raspberry absinthe juniperberry	OdorRactor ,TGSC
1952	3,4,4a,5,8,8a(Or 3,4,4a,7,8,8a)-hexahydro- 3,3,6,7-tetramethyl-1H-2- benzopyran	(4aS ,6R ,7S ,8aR)-3,3,6,7- tetramethyl- 2,4,4a ,5,6,7,8,8a - octahydrochromene	CC1CC2CC(COC2CC1C)(C)C	floral petitgrain neroli grapefruit woody herbaceous cranberry	OdorRactor ,TGSC
1953	Pulegone	(5R)-5-methyl-2-propan-2- ylidenecyclohexan-1- one	CC1CCC(=C(C)C)C(=O)C1	cinnamyl lime minty fruity spicy herbaceous vanilla camphoraceous peppermint fresh buchu sulfurous metallic	Sigma Aldrich, TGSC, OdoRactor
1954	(-)-Pulegone	(5S)-5-methyl-2-propan-2- ylidenecyclohexan-1- one	CC1CCC(=C(C)C)C(=O)C1	minty pleasant camphoraceous	TGSC, Pubchem
1955	p-Menth-4(8)-en-3-one	5-methyl-2-propan-2- ylidenecyclohexan-1-one	CC1CCC(=C(C)C)C(=O)C1	peppermint camphoraceous herbaceous fresh buchu minty sulfurous sweet metallic pleasant	SuperScent, TGSC, Flavorbase, Pubchem
1956	Guaiene	1,4-dimethyl-7-propan-2-ylidene- 2,3,4,5,6,8- hexahydro-1 <i>H</i> - azulene	CC1CCC(=C(C)C)CC2=C1CCC2 C	woody spice sweet dry guaiacwood powdery balsamic	Flavornet, TGSC
1957	beta-Irone	(E)-4-(2,5,6,6-tetramethylcyclohexen-1-yl)but-3-en-2-one	CC1CCC(=C(C1(C)C)C=CC(=0) C)C	floral fresh sweet violet berry woody powdery	OdorRactor ,TGSC
1958	3-(Isopropyl)-6- methylcyclohex-2-en-1-one	6-methyl-3-propan-2-ylcyclohex-2- en-1-one	CC1CCC(=CC1=O)C(C)C	minty spearmint	TGSC
1959	3-Methylcyclopentane-1,2-dione	3-methylcyclopentane-1,2-dione	CC1CCC(=0)C1=0	caramel coffee maple nutty smoky sweet woody sugar burnt bready	Sigma Aldrich, TGSC, OdoRactor

1960	4-Methylcyclohexanone	4-methylcyclohexan-1-one	CC1CCC(=O)CC1	musty animal	Sigma Aldrich, TGSC,OdoRactor
1961	gamma-Valerolactone	5-methyloxolan-2-one	CC1CCC(=0)01	anisic herbaceous herbaceous sweet warm tobacco cocoa woody hay coumarinic coconut	Sigma Aldrich, Flavorbase, TGSC
1962	Tetrahydro-5,6-dimethyl-2H- pyran-2-one	5,6-dimethyloxan-2-one	CC1CCC(=0)OC1C	fruity minty	TGSC
1963	Isopulegone	5-methyl-2-prop-1-en-2- ylcyclohexan-1-one	CC1CCC(C(=O)C1)C(=C)C	peppermint herbaceous minty fresh	OdorRactor ,TGSC
1964	Menthone-8-thioacetate	O -[2-[(1S)-4-methyl-2- oxocyclohexyl]propan-2- yl] ethanethioate	CC1CCC(C(=O)C1)C(C)(C)OC(= S)C	black currant fruity herbaceous tropical catty	OdorRactor ,TGSC
1965	p-Mentha-8-thiol-3-one	5-methyl-2-(2-sulfanylpropan-2- yl)cyclohexan-1- one	CC1CCC(C(=O)C1)C(C)(C)S	berry grape sulfurous minty green fruity tropical peach buchu raspberry natural passion fruit	Sigma Aldrich, TGSC, OdoRactor
1966	cis-2-(1-Mercapto-1- methylethyl)-5- methylcyclohexan-1-one	(2R ,5S)-5-methyl-2-(2- sulfanylpropan-2- yl)cyclohexan-1- one	CC1CCC(C(=O)C1)C(C)(C)S	rubbery	TGSC
1967	p-Mentha-8-thiol-3-one	5-methyl-2-(2-sulfanylpropan-2-yl)cyclohexan-1-on	CC1CCC(C(=O)C1)C(C)(C)S	sulfurous minty green fruity berry buchu fruity tropical peach raspberry herbaceous	OdorRactor ,TGSC
1968	(+)-Menthone	(2R ,5S)-5-methyl-2-propan-2-ylcyclohexan-1-one	CC1CCC(C(=O)C1)C(C)C	mentholic minty peppermint	TGSC, Pubchem
1969	Menthone	(2S, 5R)-5-methyl-2-propan-2-ylcyclohexan-1-one	CC1CCC(C(=0)C1)C(C)C	mentholic peppermint cooling herbaceous anisic berry herbaceous camphoraceous woody minty peach raspberry sweet fresh green	Sigma Aldrich, Flavornet, TGSC, Odoractor, Pubchem
1970	(+)-Isomenthone	(2R ,5R)-5-methyl-2-propan-2-ylcyclohexan-1-one	CC1CCC(C(=O)C1)C(C)C	minty	TGSC
1971	Isomenthone	(2S,5S)-5-methyl-2-propan-2-ylcyclohexan-1-one	CC1CCC(C(=O)C1)C(C)C	minty	TGSC
1972	p-Menthan-3-one	5-methyl-2-propan-2-ylcyclohexan- 1-one	CC1CCC(C(=O)C1)C(C)C	minty mentholic cooling peppermint sweet camphoraceous ethereal	Flavornet, TGSC, Pubchem
1973	(1R,2S,5R)-5-Methyl-2- (propan-2-yl)-N-[2- (pyridin- 2- yl)ethyl]cyclohexanecarboxa mide	5-methyl-2-propan-2-yl- <i>N</i> -(2-pyridin-2- ylethyl)cyclohexane-1-carboxamide	CC1CCC(C(C1)C(=0)NCCC2=C C=CC=N 2)C(C)C	cooling	TGSC
1974	Cyclohexanol, 2-(1,1-dimethylethyl)-4- methyl-	2-tert -butyl-4-methylcyclohexan-1-ol	CC1CCC(C(C1)C(C)(C)C)O	minty earthy vetiver fresh marine patchouli	OdorRactor ,TGSC
1975	2-Tert-butyl-4- methylcyclohexyl acetate		CC1CCC(C(C1)C(C)(C)C)OC(=O)C	floral rose tropical fruity	TGSC
1976	(2,4- Dimethylcyclohexyl)methanol	(2,4-dimethylcyclohexyl)methanol	CC1CCC(C(C1)C)CO	floral minty earthy leathery	OdorRactor ,TGSC
1977	2,4- Dimethylcyclohexylmethyl acetate	(2,4-dimethylcyclohexyl)methyl acetate	CC1CCC(C(C1)C)COC(=O)C	floral woody carvone sweet grapefruit cortex	OdorRactor ,TGSC
1978	Cyclopropanecarboxylic acid (2-isopropyl-5- methyl-cyclohexyl)-amide, (1S,2S,5R)-	N -[(1S ,2S ,5R)-5-methyl-2- propan-2- ylcyclohexyl]cyclopropanecarboxa mide	(C)C	savory brothy umami	TGSC
1979	Isopulegol	5-methyl-2-prop-1-en-2- ylcyclohexan-1-ol	CC1CCC(C(C1)O)C(=C)C	minty medicinal woody cooling green grassy herbaceous	OdorRactor ,TGSC, Sigma Aldrich
1980	(-)-Isopulegol	(1R ,2S ,5R)-5-methyl-2-prop-1- en-2-ylcyclohexan- 1-ol	CC1CCC(C(C1)O)C(=C)C	minty medicinal woody cooling herbaceous	Sigma Aldrich, TGSC, Flavorbase, OdoRactor
1981	1-(2-Hydroxy-4- methylcyclohexyl)ethan-1- one	1-(2-hydroxy-4- methylcyclohexyl)ethanone	CC1CCC(C(C1)O)C(=O)C	floral hawthorn	TGSC
1982	p-Menthane-3,8-diol	2-(2-hydroxypropan-2-yl)-5- methylcyclohexan-1- ol	CC1CCC(C(C1)O)C(C)(C)O	geranium rose fruity herbaceous floral green lavender tea minty eucalyptus	OdorRactor ,TGSC
1983	Menthoglycol	(1R ,2R ,5R)-2-(2- hydroxypropan-2-yl)-5- methylcyclohexan-1-ol	CC1CCC(C(C1)O)C(C)(C)O	herbaceous minty eucalyptus	OdorRactor ,TGSC
1984	(+)-Isomenthol	(1S, 2R, 5R)-5-methyl-2-propan-2-ylcyclohexan-1- ol	CC1CCC(C(C1)O)C(C)C	herbaceous earthy camphoraceous hay musty sweet peppermint	TGSC, Pubchem
1985	Menthol	5-methyl-2-propan-2-ylcyclohexan- 1-ol	CC1CCC(C(C1)O)C(C)C	mentholic cooling minty peppermint	TGSC, Pubchem
1986	(+)-Neomenthol	(1S, 2S, 5R)-5-methyl-2-propan-2-ylcyclohexan-1- ol	CC1CCC(C(C1)O)C(C)C	mentholic minty sweet cooling	SuperScent, TGSC, Pubchem, OdoRactor
1987	Neoisomenthol	(1R, 2R, 5R)-5-methyl-2-propan- 2-ylcyclohexan-1- ol	CC1CCC(C(C1)O)C(C)C	mentholic musty woody camphoraceous	Flavornet, TGSC

1988	l-Menthol	(1R ,2S ,5R)-5-methyl-2-propan-2-ylcyclohexan-1- ol	CC1CCC(C(C1)O)C(C)C	woody minty camphoraceous cooling mentholic peppermint	Sigma Aldrich, TGSC, Pubchem, OdoRactor
1989	(-)-Menthyl isobutyrate	(5-methyl-2-propan-2- ylcyclohexyl) 2- methylpropanoate	CC1CCC(C(C1)OC(=O)C(C)C)C(C)C	sweet herbaceous clary sage rose	TGSC
1990	Menthyl lactate	[(1R, ,2S, ,5R)-5-methyl-2-propan- 2-ylcyclohexyl] 2- hydroxypropanoate	CC1CCC(C(C1)OC(=O)C(C)O)C(C)C	alcoholic minty cooling	Sigma Aldrich, TGSC
1991	Propanoic acid, 2-hydroxy-, 5-methyl-2-(1-methylethyl)cyclohexyl ester	(5-methyl-2-propan-2- ylcyclohexyl) 2-	CC1CCC(C(C1)OC(=O)C(C)O)C(C)C	minty mentholic	SuperScent, TGSC
1992	l-Menthyl lactate	[(1R, ,2S, ,5R)-5-methyl-2-propan- 2-ylcyclohexyl] (2R)-2- hydroxypropanoate	CC1CCC(C(C1)OC(=O)C(C)O)C(C)C	minty mentholic cooling	OdorRactor ,TGSC
1993	Isopulegol acetate	(5-methyl-2-prop-1-en-2- ylcyclohexyl) acetate	CC1CCC(C(C1)OC(=O)C)C(=C)	minty leafy	Flavornet, TGSC
1994	Isopulegyl acetate	[(1R ,2S ,5R)-5-methyl-2-prop-1-en-2- ylcyclohexyl] acetate	CC1CCC(C(C1)OC(=O)C)C(=C) C	woody sweet peppermint tropical mentholic camphoraceous cooling medicinal seedy berry	OdorRactor ,TGSC
1995	L-Menthyl acetate	[(1R ,2S ,5R)-5-methyl-2-propan- 2-ylcyclohexyl] acetate	CC1CCC(C(C1)OC(=0)C)C(C)C	berry mango melon oily orange woody minty camphoraceous herbaceous raspberry sweet tea fruity floral mentholic herbaceous	Sigma Aldrich, TGSC, OdoRactor
1996	Menthyl acetate	(5-methyl-2-propan-2- ylcyclohexyl) acetate	CC1CCC(C(C1)OC(=0)C)C(C)C	berry melon oily orange woody herbaceous spicy camphoraceous minty raspberry tea fruity mentholic cooling earthy weedy	Sigma Aldrich, TGSC, Pubchem, OdoRactor
1997	Menthyl acetate	(5-methyl-2-propan-2- ylcyclohexyl) acetate	CC1CCC(C(C1)OC(=O)C)C(C)C	mentholic tea minty fruity cooling	OdorRactor ,TGSC, Pubchem
1998	Menthyl anthranilate	(5-methyl-2-propan-2- ylcyclohexyl) 2- aminobenzoate	CC1CCC(C(C1)OC(=0)C2=CC= CC=C2N)C(C)C	fruity grape mentholic	TGSC
1999	(-)-Menthyl (-)-2-pyrrolidone- 5-carboxylate	(5-methyl-2-propan-2- ylcyclohexyl) 5- oxopyrrolidine-2- carboxylate	7 7 7	minty mentholic	OdorRactor,
2000	Menthyl isovalerate	(5-methyl-2-propan-2- ylcyclohexyl) 3- methylbutanoate	CC1CCC(C(C1)OC(=O)CC(C)C) C(C)C	woody fruity sweet cooling	Sigma Aldrich, TGSC, OdoRactor
2001	Butanoic acid, 3-hydroxy-, 5-methyl-2-(1-methylethyl)cyclohexyl ester	(5-methyl-2-propan-2- ylcyclohexyl) 3- hydroxybutanoate	CC1CCC(C(C1)OC(=O)CC(C)O) C(C)C	cooling minty	TGSC
2002	l-Monomenthyl glutarate	5-[(1R, 2S, 5R)-5-methyl-2-propan-2-ylcyclohexyl]oxy-5-oxopentanoic acid	CC1CCC(C(C1)OC(=0)CCCC(= 0)O)C(C) C	minty mentholic	TGSC
2003		2-hydroxypropyl (5-methyl-2- propan-2- ylcyclohexyl) carbonate	CC1CCC(C(C1)OC(=O)OCC(C)O)C(C)C	mentholic	TGSC
2004	1-Menthyl methyl ether	2-methoxy-4-methyl-1-propan-2- ylcyclohexane	CC1CCC(C(C1)OC)C(C)C	minty	OdorRactor ,TGSC
2005	Isopulegyl formate	(5-methyl-2-prop-1-en-2- ylcyclohexyl) formate	CC1CCC(C(C1)OC=O)C(=C)C	minty green leafy tuberose	OdorRactor ,TGSC
2006	1,2-Propanediol, 2-methyl-3- [[(1R,2S,5R)- 5-methyl-2-(1- methylethyl)cyclohexyl]oxy]-	2-methyl-3-[(1R, 2S, 5R)-5-methyl-2-propan-2-ylcyclohexyl]oxypropane-1,2-diol	CC1CCC(C(C1)OCC(C)(CO)O)C (C)C	minty cooling	OdorRactor ,TGSC
2007	3-[[5-Methyl-2-(1-methylethyl)cyclohexyl]oxy]p ropane-1,2-diol	3-(5-methyl-2-propan-2- ylcyclohexyl)oxypropane- 1,2-diol	CC1CCC(C(C1)OCC(CO)O)C(C) C	minty vanilla	OdorRactor ,TGSC
2008	(+)-gamma-Gurjunene	(1 <i>R</i> ,3 <i>aR</i> ,4 <i>R</i> ,7 <i>R</i>)-1,4-dimethyl-7-prop-1-en-2-yl-1,2,3,3 <i>a</i> ,4,5,6,7-octahydroazulene	CC1CCC(C=C2C1CCC2C)C(=C) C	musty	TGSC
2009	2-[(1R,4R,5S)-1,8- Dimethylspiro[4.5]dec-8- en- 4-yl]propan-2-ol	2-[(1R ,4R ,5S)-1,8- dimethylspiro[4.5]dec-8-en-4- yl]propan-2-ol	CC1CCC(C12CCC(=CC2)C)C(C) (C)O	fruity sweet powdery floral ripe	TGSC
2010	cis,cis-Photocitral A	(1R ,2R ,5S)-2-methyl-5-prop-1- en-2- ylcyclopentane-1- carbaldehyde	CC1CCC(C1C=0)C(=C)C	minty camphoraceous herbaceous	OdorRactor ,TGSC
2011	3,9-Dimethyl-6-(1- methylethyl)-1,4- dioxaspiro(4.5)decan-2-one	2,9-dimethyl-6-propan-2-yl-1,4-dioxaspiro[4.5]decan-3-one	CC1CCC(C2(C1)OC(C(=O)O2)C) C(C)C	minty	TGSC, Flavorbase

2012	1,6-Dimethyl-4-	1,6-dimethyl-4-propan-2-yl-	CC1CCC(C2=C1C=CC(=C2)C)C(herbaceous spice	Flavornet, TGSC
2013	isopropyltetralin 1-Naphthalenol, 5,6,7,8-	1,2,3,4- tetrahydronaphthalene 2,5-dimethyl-8-propan-2-yl-	C)C CC1CCC(C2=C1C=CC(=C2O)C)	herbaceous	Flavornet
	tetrahydro-2,5- dimethyl-8-(1-methylethyl)-	5,6,7,8-tetrahydronaph	C(C)C		
2014	Cubenol	4,7-dimethyl-1-propan-2-yl- 2,3,4,5,6,8a - hexahydro-1H - naphthalen-4a -ol	CC1CCC(C2C1(CCC(=C2)C)O)C (C)C	spice herbaceous green tea	Flavornet, TGSC, OdoRactor
2015	Cadina-1,4-diene-3-ol	3,8-dimethyl-5-propan-2-yl-2,4 <i>a</i> ,5,6,7,8-hexahydr	CC1CCC(C2C1=CC(C(=C2)C)O) C(C)C	woody spicy	OdorRactor ,TGSC
2016	beta-Cubebene	(1R ,5S ,6R ,7S ,10R)-10- methyl-4-methylidene-7- propan-2- yltricyclo[4.4.0.01,5]decane	CC1CCC(C2C13C2C(=C)CC3)C(citrus fruit radish	Flavornet, TGSC, OdoRactor
2017	Caswell No. 264AB	(1 <i>R</i> ,5 <i>S</i> ,6 <i>R</i> ,7 <i>S</i> ,10 <i>R</i>)-4,10- dimethyl-7-propan-2- yltricyclo[4.4.0.01,5]dec-3-ene	CC1CCC(C2C13C2C(=CC3)C)C(C)C	herbaceous wax herbaceous	Flavornet, TGSC, OdoRactor
2018	Cubebol		CC1CCC(C2C13C2C(CC3)(C)O) C(C)C	spicy minty cooling	TGSC, Flavorbase
2019	p-MENTHAN-8-OL	2-(4-methylcyclohexyl)propan-2- ol	CC1CCC(CC1)C(C)(C)O	sweet pine herbaceous terpenic lime woody citrus floral	OdorRactor ,TGSC
2020	p-Menthan-8-yl acetate	2-(4-methylcyclohexyl)propan-2- yl acetate	CC1CCC(CC1)C(C)(C)OC(=0)C	pine citrus woody lime cologne herbaceous fresh soapy coniferous floral fruity	Flavornet, Flavorbase, TGSC
2021	Dihydrocarvone	2-methyl-5-prop-1-en-2- ylcyclohexan-1-one	CC1CCC(CC1=0)C(=C)C	herbaceous minty warm herbaceous spearmint cooling woody terpenic rye bready hay camphoraceous	Sigma Aldrich, Flavorbase, TGSC, OdoRactor
2022	(+)-Isodihydrocarvone	(2S ,5R)-2-methyl-5-prop-1-en-2-ylcyclohexan-1- one	CC1CCC(CC1=0)C(=C)C	herbaceous warm	Flavornet
2023	(1S,4S)-Dihydrocarvone	(2S ,5S)-2-methyl-5-prop-1-en-2-ylcyclohexan-1- one	CC1CCC(CC1=0)C(=C)C	warm herbaceous	Flavornet, OdoRactor
2024	(+)-Dihydrocarvone	(2R,5R)-2-methyl-5-prop-1-en-2-ylcyclohexan-1- one	CC1CCC(CC1=0)C(=C)C	warm herbaceous minty spearmint mentholic	AOD
2025	Cyclohexanone, 2-methyl-5- (1-methylethyl)-	2-methyl-5-propan-2-ylcyclohexan- 1-one	CC1CCC(CC1=O)C(C)C	minty spearmint herbaceous woody cooling green	OdorRactor ,TGSC
2026	Dihydrocarveol	2-methyl-5-prop-1-en-2- ylcyclohexan-1-ol	CC1CCC(CC10)C(=C)C	mentholic spearmint herbaceous minty spice cooling sweet camphoraceous fresh terpenic	Flavornet, TGSC,OdoRactor
2027	(-)-Isodihydrocarveol	(1R, 2R, 5S)-2-methyl-5-prop-1-en-2-ylcyclohexan-1-ol	CC1CCC(CC1O)C(=C)C	woody spice	Flavornet, TGSC
2028	Dihydrocarvyl acetate	(2-methyl-5-prop-1-en-2- ylcyclohexyl) acetate	CC1CCC(CC10C(=0)C)C(=C)C	medicinal minty vanilla camphoraceous floral rose cumin sweet green fruity vegetable pine beany	Sigma Aldrich, TGSC, OdoRactor
2029	Rotundone	(3 <i>S</i> ,5 <i>R</i> ,8 <i>S</i>)-3,8-dimethyl-5-prop-1-en-2-yl- 3,4,5,6,7,8-hexahydro-2 <i>H</i> -azulen-1-one	(=C)C	woody pepper agarwood	TGSC
2030	Azulene, 1,2,3,4,5,6,7,8- octahydro-1,4- dimethyl-7-(1- methylethenyl)-, (1S,4S,7R)-	1,4-dimethyl-7-prop-1-en-2-yl- 1,2,3,4,5,6,7,8- octahydroazulene	CC1CCC(CC2=C1CCC2C)C(=C) C	sweet woody balsamic pepper	OdorRactor ,TGSC
2031	alpha-Guaiene	(15,4S,7R)-1,4-dimethyl-7-prop-1-en-2-yl-1,2,3,4,5,6,7,8-octahydroazulene	CC1CCC(CC2=C1CCC2C)C(=C) C	woody balsamic	Flavornet, OdoRactor
2032	Guaiol	2-[(3S,5R,8S)-3,8-dimethyl- 1,2,3,4,5,6,7,8- octahydroazulen-5- yl]propan-2-ol	CCICCC(CC2=C1CCC2C)C(C)(C)O	woody balsamic tearose guaiacwood rose floral pleasant	Sigma Aldrich, Flavornet, TGSC, Pubchem, OdoRactor
2033	Guaiol acetate	2-[(3 <i>S</i> ,5 <i>R</i> ,8 <i>S</i>)-3,8-dimethyl- 1,2,3,4,5,6,7,8- octahydroazulen-5- yl]propan-2-yl acetate	CC1CCC(CC2=C1CCC2C)C(C)(C)OC(=0)C	tearose woody spicy green fatty balsamic rose	OdorRactor ,TGSC
2034	7-Isopropyl-4-methyloxepan- 2-one	4-methyl-7-propan-2-yloxepan-2-one	CC1CCC(OC(=O)C1)C(C)C	caramel maple brown sugar molasses	OdorRactor ,TGSC, Pubchem
2035	2-[(3R,5S,6S)-6,10- Dimethylspiro[4.5]dec- 9-en-3-yl]propan-2-ol	2-[(3R ,5S ,6S)-6,10- dimethylspiro[4.5]dec-9-en-3- yl]propan-2-ol	CC1CCC=C(C12CCC(C2)C(C)(C)O)C	spicy pepper woody	OdorRactor ,TGSC
2036	Valencene	(3 <i>R</i> ,4 <i>aS</i> ,5 <i>R</i>)-4 <i>a</i> ,5-dimethyl-3- prop-1-en-2-yl- 2,3,4,5,6,7-hexahydro-1 <i>H</i> - naphthalene	CC1CCC=C2C1(CC(CC2)C(=C)C)C	grapefruit green oily sweet fresh citrus woody orange	Sigma Aldrich

2037	4a,5-Dimethyl-3-(prop-1-en-2-yl)- 1,2,3,4,4a,5,6,7- octahydronaphthalene	4a ,5-dimethyl-3-prop-1-en-2-yl- 2,3,4,5,6,7- hexahydro-1 <i>H</i> - naphthalene	CC1CCC=C2C1(CC(CC2)C(=C)C)C	sweet citrus grapefruit woody orange green oily fresh dry	OdorRactor ,TGSC
2038	4-Methylcyclohexene	4-methylcyclohexene	CC1CCC=CC1	citrus	OdorRactor, ,OdoRactor
2039	1-Naphthalenol, 1,2,3,4,4a,7,8,8a- octahydro- 2,4a,5,8a-tetramethyl-, 1- formate	(2,4a ,5,8a -tetramethyl- 1,2,3,4,7,8- hexahydronaphthalen- 1-yl) formate	CC1CCC2(C(=CCCC2(C1OC=O) C)C)C	woody amber dusty powdery dry	OdorRactor ,TGSC
2040	Patchouli alcohol	(1 <i>R</i> ,3 <i>R</i> ,6 <i>S</i> ,7 <i>S</i> ,8 <i>S</i>)-2,2,6,8- tetramethyltricyclo[5.3.1.03,8]und ecan-3-ol	CC1CCC2(C(C3CCC2(C1C3)C)(C)C)O	earthy camphoraceous powdery woody patchouli	OdorRactor ,TGSC
2041	8-Methyl-1- oxaspiro[4.5]decan-2-one	8-methyl-1-oxaspiro[4.5]decan-2-one	CC1CCC2(CC1)CCC(=0)O2	lactonic coconut tropical creamy coumarinic dairy plum	OdorRactor ,TGSC
2042	Vitispirane	2,6,6-trimethyl-10-methylidene-1- oxaspiro[4.5]dec 8-ene	CC1CCC2(O1)C(=C)C=CCC2(C) C	floral fruity earthy woody green chrysanthemum winey	OdorRactor ,TGSC, Flavorbase
2043	Theaspirane	2,6,6,10-tetramethyl-1- oxaspiro[4.5]dec-9-ene	CC1CCC2(O1)C(=CCCC2(C)C)C	berry green woody minty vanilla winey herbaceous tobacco leafy metallic spicy tea wet cooling camphoraceous fresh	Sigma Aldrich, TGSC, OdoRactor
2044	6-Hydroxydihydrotheaspirane	2,6,10,10-tetramethyl-1- oxaspiro[4.5]decan-6-ol	CC1CCC2(O1)C(CCCC2(C)O)(C) C	camphoraceous pine woody earthy green herbaceous cooling	OdorRactor ,TGSC, Pubchem
2045	6-Acetoxydihydrotheaspirane	(2,6,10,10-tetramethyl-1- oxaspiro[4.5]decan-6-yl) acetate	CC1CCC2(O1)C(CCCC2(C)OC(= O)C)(C) C	citrus herbaceous green tea tangerine grapefruit mango passion fruit	SuperScent, TGSC, OdoRactor
2046	Dehydromenthofurolactone	(6R)-3,6-dimethyl-5,6-dihydro- 4H-1-benzofuran- 2-one	CC1CCC2=C(C(=0)0C2=C1)C	lactonic coumarinic sweet coconut	OdorRactor ,TGSC
2047	5,6-Dihydro-3,6- dimethylbenzofuran-2(4h)- one	3,6-dimethyl-5,6-dihydro-4 <i>H</i> -1-benzofuran-2-one	CC1CCC2=C(C(=0)OC2=C1)C	tonka hay coumarinic coconut	OdorRactor ,TGSC
2048	Isomintlactone	3,6-dimethyl-5,6,7,7 <i>a</i> -tetrahydro-4 <i>H</i> -1- benzofuran-2-one	CC1CCC2=C(C(=0)0C2C1)C	sweet creamy coumarinic coconut powdery tobacco spearmint tonka	OdorRactor ,TGSC
2049	(-)-Menthofuran	(6S)-3,6-dimethyl-4,5,6,7- tetrahydro-1-benzofuran	CC1CCC2=C(C1)OC=C2C	herbaceous fatty thyme terpenic	TGSC
2050	(+)-Menthofuran	(6R)-3,6-dimethyl-4,5,6,7- tetrahydro-1- benzofuran	CC1CCC2=C(C1)OC=C2C	minty leafy herbaceous camphoraceous	TGSC
2051	Menthofuran	3,6-dimethyl-4,5,6,7-tetrahydro-1- benzofuran	CC1CCC2=C(C1)OC=C2C	musty minty nutty earthy coffee pungent	Sigma Aldrich, TGSC, OdoRactor
2052	Bulnesol		CC1CCC2=C(CCC(CC12)C(C)(C)O)C	spice	Flavornet, TGSC
2053	6,7-Dihydro-2,5-dimethyl-5H-cyclopentapyrazine	3,7-dimethyl-6,7-dihydro-5 <i>H</i> - cyclopenta[b]pyrazine	CC1CCC2=NC(=CN=C12)C	burnt earthy nutty roasted coffee coffee roasted	OdorRactor ,TGSC
2054	5-Methyl-6,7-dihydro-5H- cyclopenta[b]pyrazine	5-methyl-6,7-dihydro-5 <i>H</i> -cyclopenta[b]pyrazine	CC1CCC2=NC=CN=C12	earthy baked potato roasted peanut sweet nutty roasted toasted grain coffee corn savory meaty baked	OdorRactor ,TGSC
2055	5-Methyl-6,7-dihydro-5H- cyclopenta[b]pyrazine	5-methyl-6,7-dihydro-5 <i>H</i> - cyclopenta[b]pyrazine	CC1CCC2=NC=CN=C12	earthy peanut roast baked potato sweet nutty roasted toasted grain coffee corn savory meaty baked	Sigma Aldrich, TGSC, OdoRactor
2056	(1Z)-1-[(1S,5S,7R,8R)-6,6,8- Trimethyl-2- tricyclo[5.3.1.01,5]undecanyli dene]propan- 2-one	(1Z)-1-[(1S ,5S ,7R ,8R)-6,6,8-trimethyl-2-tricyclo[5.3.1.01,5]undecanyliden e]propan-2-one	CC1CCC23CC1C(C2CCC3=CC(=0)C)(C) C	woody warm amber musk	OdorRactor ,TGSC
2057	2(3H)-Benzofuranone, hexahydro-3,6- dimethyl-	3,6-dimethyl-3a ,4,5,6,7,7a - hexahydro-3H -1- benzofuran-2- one	CC1CCC2C(C(=0)0C2C1)C	tonka coumarinic lactonic phenolic tobacco gourmand sweet	TGSC, Flavorbase
2058	7-Methylhexahydro-2H- benzo[b][1,4]dioxepin-3(4H)- one	7-methyl-5 <i>a</i> ,6,7,8,9,9 <i>a</i> - hexahydrobenzo[b][1,4]dioxepin-3-one	CC1CCC2C(C1)OCC(=0)CO2	sweet strawberry fruity tropical berry cotton candy	OdorRactor,
2059	Spiro(bicyclo(4.1.0)heptane-2,5'- (1,3)dioxane), 2',2',3,7,7-pentamethyl-, (1R,3R,6S)-rel-	(1'R ,3'R ,6'S)-2,2,3',7',7'- pentamethylspiro[1,3- dioxane- 5,2'-bicyclo[4.1.0]heptane]	CC1CCC2C(C2(C)C)C13COC(O C3)(C)C	amber woody spicy aldehydic green seaweed	OdorRactor ,TGSC
2060	(1Ar,4R,7bS)-1,1,4,7- tetramethyl- 1a,2,3,4,4a,5,6,7b- octahydrocyclopropa[e]azule ne	(1aR ,4R ,7bS)-1,1,4,7- tetramethyl- 1a ,2,3,4,4a ,5,6,7b - octahydrocyclopropa[e]azulene	CC1CCC2C(C2(C)C)C3=C(CCC1 3)C	woody balsamic	Flavornet, TGSC
2061	1H-Cycloprop(e)azulene, 1a,2,3,4,4a,5,6,7b-octahydro- 1,1,4,7- tetramethyl-, (1aR,4R,4aR,7bS)-	(4R,4aR)-1,1,4,7-tetramethyl- 1a,2,3,4,4a,5,6,7b - octahydrocyclopropa[e]azulene	CC1CCC2C(C2(C)C)C3=C(CCC1 3)C	woody balsamic	OdorRactor,

2062	4,7-Dimethyl- 3,4,4a,5,6,7,8,8a- octahydroisochromen-1-one	4,7-dimethyl-3,4,4 <i>a</i> ,5,6,7,8,8 <i>a</i> - octahydroisochromen-1-one	CC1CCC2C(COC(=0)C2C1)C	cherry creamy minty sweet coumarinic coconut powdery tobacco spearmint	Sigma Aldrich, TGSC
2063	4,9,12,12-Tetramethyl-5-oxatricyclo[8.2.0.04,6]dodeca	4,9,12,12-tetramethyl-5- oxatricyclo[8.2.0.04,6]dodecane	CC1CCC2C(O2)(CCC3C1CC3(C) C)C	amber woody nutmeg tobacco dusty	OdorRactor ,TGSC
2064	(1S,2S,5S,8R)-2,6-Dimethyl- 9-propan-2- ylidene-11- oxatricyclo[6.2.1.01,5]undec- 6- en-8-ol	(15 ,2S ,5S ,8R)-2,6-dimethyl-9-propan-2-ylidene- 11-oxatricyclo[6.2.1.01,5]undec-6-en-8-ol	CC1CCC2C13CC(=C(C)C)C(O3)(C=C2C) O	fresh fatty	TGSC
2065	1-((3R,3Ar,7R,8aS)-3,6,8,8- Tetramethyl- 2,3,4,7,8,8a-hexahydro-1H- 3a,7- methanoazulen-5- yl)ethanone	1-[(1 <i>R</i> ,2 <i>R</i> ,5 <i>S</i> ,7 <i>R</i>)-2,6,6,8- tetramethyl-9- tricyclo[5.3.1.01,5]undec-8- enyl]ethanone	CC1CCC2C13CC(C2(C)C)C(=C(C3)C(=O)C)C	woody amber leathery musk cedar vetiver	OdorRactor ,TGSC
2066	Cedrenol	2,6,6-trimethyl-8- methylidenetricyclo[5.3.1.01,5]un decan-9-ol		fruit cedar woody sweet soft	TGSC
2067	1H-3a,7-Methanoazulen- 5(4H)-one, hexahydro-3,6,8,8- tetramethyl-	2,6,6,8- tetramethyltricyclo[5.3.1.01,5]und ecan-9- one	CC1CCC2C13CC(C2(C)C)C(C(= 0)C3)C	woody cedar	OdorRactor ,TGSC
2068	alpha-Cedrene epoxide	2,6,6,8-tetramethyl-9-oxatetracyclo[5.4.1.01,5.08,10]do decane	CC1CCC2C13CC(C2(C)C)C4(C(C3)O4)C	woody amber tobacco sandal wood linalyl patchouli fresh herbaceous	OdorRactor ,TGSC
2069	4H-4a,9-Methanoazuleno[5,6-d]-1,3- dioxole, octahydro-2,2,5,8,8,9a-hexamethyl-, (4aR,5R,7aS,9R)-	(1R ,8R ,10S ,13R)-5,5,7,9,9,13- hexamethyl-4,6- dioxatetracyclo[6.5.1.01,10.03,7]t etradecane	C3)OC(O	woody amber agarwood	TGSC
2070	(1S,2R,5S)-2,6,6,8- Tetramethyltricyclo[5.3.1.01, 5]undec-8-ene	(1 <i>S</i> ,2 <i>R</i> ,5 <i>S</i>)-2,6,6,8- tetramethyltricyclo[5.3.1.01,5]und ec-8-ene	CC1CCC2C13CC=C(C(C3)C2(C) C)C	woody cedar sweet fresh	OdorRactor ,TGSC
2071	Cedrenyl acetate	[(1S ,2R ,5S ,7R)-2,6,6- trimethyl-8- tricyclo[5.3.1.01,5]undec-8- enyl]methyl acetate	CC1CCC2C13CC=C(C(C3)C2(C) C)COC(=O)C	woody cedar peanut wax vetiver sharp dry	OdorRactor ,TGSC
2072	Ethanone, 1- ((3R,3aS,6S,7R,8aS)- octahydro-3,6,8,8-tetramethyl- 1H-3a,7- methanoazulen-6-yl)-	1-[(1 <i>S</i> ,2 <i>R</i> ,5 <i>S</i> ,7 <i>R</i> ,8 <i>S</i>)-2,6,6,8- tetramethyl-8- tricyclo[5.3.1.01,5]undecanyl]etha none	CC1CCC2C13CCC(C(C3)C2(C)C)(C)C(= O)C	woody vetiver	TGSC
2073	Cedrol	(1 <i>S</i> ,2 <i>R</i> ,5 <i>S</i> ,7 <i>R</i> ,8 <i>R</i>)-2,6,6,8- tetramethyltricyclo[5.3.1.01,5]und ecan-8-ol	CC1CCC2C13CCC(C(C3)C2(C)C)(C)O	woody sweet cedar dry earthy	Sigma Aldrich, TGSC, OdoRactor, Pubchem
2074	Methyl cedryl ether	(2R,5S,7R,8R)-8-methoxy- 2,6,6,8- tetramethyltricyclo[5.3.1.01,5]und ecane	CC1CCC2C13CCC(C(C3)C2(C)C)(C)OC	woody dusty dry ambergis	OdorRactor ,TGSC
2075	Cedryl methyl ether	(1 <i>S</i> ,2 <i>R</i> ,5 <i>S</i> ,7 <i>R</i> ,8 <i>S</i>)-8-methoxy-2,6,6,8- tetramethyltricyclo[5.3.1.01,5]und ecane	CC1CCC2C13CCC(C(C3)C2(C)C)(C)OC	woody earthy dry cedar ambergis vetiver	Sigma Aldrich, TGSC, OdoRactor
2076	Cedranyl acetate	(2,6,6,8-tetramethyl-8-tricyclo[5.3.1.01,5]undecanyl) acetate	CC1CCC2C13CCC(C(C3)C2(C)C)(C)OC(=0)C	dry woody cedar powdery	OdorRactor ,TGSC
2077	Cedrol formate	[(1S,2R,5S,7R,8R)-2,6,6,8- tetramethyl-8- tricyclo[5.3.1.01,5]undecanyl] formate	CC1CCC2C13CCC(C(C3)C2(C)C)(C)OC= O	amber woody vetiver cedar	OdorRactor ,TGSC
2078	Globulol	1,1,4,7-tetramethyl-2,3,4 <i>a</i> ,5,6,7,7 <i>a</i> ,7 <i>b</i> -octahydro-	CC1CCC2C1C3C(C3(C)C)CCC2(C)O	floral rose	OdorRactor ,TGSC
2079	Viridiflorol	(1aR, 4S, 4aS, 7R, 7aS, 7bS) - 1,1,4,7-tetramethyl-2,3,4a,5,6,7,7a,7b-octahydro-1aH - cyclopropa[e]azulen-4-ol	CC1CCC2C1C3C(C3(C)C)CCC2(C)O	green sweet herbaceous fruity tropical minty	Flavornet, TGSC
2080	(-)-Alloaromadendrene	(1aR, 4aS, 7R, 7aR, 7bS) -1,1,7-trimethyl-4- methylidene-2,3,4a,5,6,7,7a,7b-octahydro-1aH-cyclopropa[e]azulene	CC1CCC2C1C3C(C3(C)C)CCC2 =C	woody	Flavornet
2081	(+)-Aromadendrene	(1 <i>aR</i> ,4 <i>aR</i> ,7 <i>R</i> ,7 <i>aR</i> ,7 <i>bS</i>)-1,1,7- trimethyl-4- methylidene-2,3,4 <i>a</i> ,5,6,7,7 <i>a</i> ,7 <i>b</i> -octahydro-1 <i>aH</i> - cyclopropa[e]azulene	CC1CCC2C1C3C(C3(C)C)CCC2 =C	woody	Flavornet
2082	Calarene epoxide	6,7,9,9-tetramethyl-2- oxatetracyclo[5.5.0.01,3.08,10]do decane	CC1CCC2C3(C1(C4C(C4(C)C)C C3)C)O2	woody patchouli ambergis	TGSC

2083	cis-Pinane	(1S ,2R ,5S)-2,6,6-	CC1CCC2CC1C2(C)C	fresh pine balsamic herbaceous	OdorRactor ,TGSC
2083	CIS-F IIIalie	trimethylbicyclo[3.1.1]heptane	ccrcczccrcz(c)c	_	Odorkaciói , i osc
2084	4,7,7-Trimethyl-6- thiabicyclo[3.2.1]octane	4,7,7-trimethyl-6- thiabicyclo[3.2.1]octane	CC1CCC2CC1SC2(C)C	sulfurous minty fresh fi rneedle vegetable passion fruit papaya peach apricot grapefruit tropical seedy soupy	OdorRactor ,TGSC, Flavorbase
2085	3-Methylcyclohexanone	3-methylcyclohexan-1-one	CC1CCCC(=O)C1	medicinal minty camphoraceous	Sigma Aldrich, TGSC,OdoRactor
2086	3-Methylcyclohexane-1,2- dione	3-methylcyclohexane-1,2-dione	CC1CCCC(=O)C1=O	coffee caramel burnt sugar	Sigma Aldrich, TGSC, Odoractor,
2087	(R)-6-Methyltetrahydro-2H- pyran-2-one	(6R)-6-methyloxan-2-one	CC1CCCC(=0)01	creamy fruity coconut	OdorRactor ,TGSC
2088	delta-Hexalactone	6-methyloxan-2-one	CC1CCCC(=0)01	sweet creamy fruity coconut herbaceous	Sigma Aldrich, TGSC,OdoRactor
2089	3-Methylcyclohexanol	3-methylcyclohexan-1-ol	CC1CCCC(C1)O	solvent dry musty rummy fusel fruity	TGSC
2090	2,2,6- Trimethylcyclohexanone	2,2,6-trimethylcyclohexan-1-one	CC1CCCC(C1=O)(C)C	tobacco pungent honey citrus thujonic labdanum cistus	ADB, TGSC, OdoRactor
2091	Cyclohexanepropanol, alpha,beta,2,2,6- pentamethyl-	3-methyl-4-(2,2,6- trimethylcyclohexyl)butan-2-ol	CC1CCCC(C1CC(C)C(C)O)(C)C	woody violet cedar floral ambergis	OdorRactor ,TGSC
2092	Cyclohexanepropanol, alpha,beta,2,2,6- pentamethyl-, acetate	[3-methyl-4-(2,2,6- trimethylcyclohexyl)butan-2-yl] acetate	CC1CCCC(C1CC(C)C(C)OC(=0) C)(C)C	woody vetiver powdery	OdorRactor ,TGSC
2093	Cyclohexanepropanol, alpha,2,2,6- tetramethyl-	4-(2,2,6- trimethylcyclohexyl)butan-2-ol	CC1CCCC(C1CCC(C)O)(C)C	floral violet woody leathery	OdorRactor ,TGSC
2094	Tetrahydroionyl acetate	4-(2,2,6- trimethylcyclohexyl)butan-2-yl acetate	CC1CCCC(C1CCC(C)OC(=O)C)(C)C	fruity floral berry	OdorRactor ,TGSC
2095	3-Methylcyclohexene	3-methylcyclohexene	CC1CCCC=C1	citrus	TGSC
2096	Geosmin	(4 <i>S</i> ,4 <i>aS</i> ,8 <i>aR</i>)-4,8 <i>a</i> -dimethyl-1,2,3,4,5,6,7,8-octahydronaphthalen-4 <i>a</i> -ol	CC1CCCC2(C1(CCCC2)O)C	beefy earthy musty soil fresh humus plowed	Flavornet, TGSC, OdorRactor,
2097	Octahydro-4,8a-dimethyl- 4a(2H)-naphthol	4,8a -dimethyl-1,2,3,4,5,6,7,8- octahydronaphthalen-4a -ol	CC1CCCC2(C1(CCCC2)O)C	earthy humus dirty	TGSC
2098	(4s,4Ar,8ar)-4,8a- dimethyloctahydronaphthalen- 4a(2h)-ol	(4 <i>S</i> ,4 <i>aR</i> ,8 <i>aR</i>)-4,8 <i>a</i> -dimethyl-1,2,3,4,5,6,7,8-octahydronaphthalen-4 <i>a</i> -ol	CC1CCCC2(C1(CCCC2)O)C	earthy musty dirty humus	OdorRactor ,TGSC
2099	(+)-Geosmin	(4R, 4aR, 8aS)-4,8a -dimethyl- 1,2,3,4,5,6,7,8- octahydronaphthalen-4a -ol	CC1CCCC2(C1(CCCC2)O)C	earthy musty humus	TGSC
2100	Cycloeudesmol	2-[(1aR ,3aR ,7S ,7aR)-3a ,7-dimethyl-2,3,4,5,6,7-hexahydro-1H -cyclopropa[i]inden-1a -yl]propan-2-ol	CC1CCC2(C13CC3(CC2)C(C)(C)O)C	algae	TGSC
	2-Methylcyclohexanone	2-methylcyclohexan-1-one	CC1CCCCC1=0	peppermint minty cooling	Sigma Aldrich, TGSC,OdoRactor
2102	3-Methylcyclopentadecanone	3-methylcyclopentadecan-1-one	CC1CCCCCCCCCCC(=0)C1	fruity lactonic fatty	Flavorbase
2103	Cyclopentadecanone, 3- methyl-, (3R)-	(3R)-3-methylcyclopentadecan-1-one	CC1CCCCCCCCCCC(=0)C1	musk animal powdery	TGSC
2104	3-Methylcyclopentadecanone	3-methylcyclopentadecan-1-one	CC1CCCCCCCCCCC(=0)C1	sweet musk animal powdery floral soapy fatty natural	OdorRactor ,TGSC
2105	2-Methylpiperidine	2-methylpiperidine	CCICCCCNI	ammonical seafood taco corn fishy popcorn brown nutty shellfish roasted cheese	Sigma Aldrich, Flavorbase, TGSC,OdoRactor
2106	trans-Rose oxide	(2R ,4R)-4-methyl-2-(2-methylprop-1-enyl)oxane	CC1CCOC(C1)C=C(C)C	floral	Flavornet
2107	Rose oxide	4-methyl-2-(2-methylprop-1- enyl)oxane	CC1CCOC(C1)C=C(C)C	geranium green honey earthy raspberry rose spicy fresh vegetable floral camphoraceous	Sigma Aldrich, Flavorbase, TGSC, OdoRactor
2108	(2R-cis)-Tetrahydro-4-methyl- 2-(2-methyl-1 propenyl)-2H- pyran	(2R ,4S)-4-methyl-2-(2-methylprop-1-enyl)oxane	CC1CCOC(C1)C=C(C)C	green floral	Flavornet
2109	(2S,4R)-4-Methyl-2-(2- methylprop-1-en-1- yl)tetrahydro-2H-pyran	(2S ,4R)-4-methyl-2-(2-methylprop-1-enyl)oxane	CC1CCOC(C1)C=C(C)C	rose green floral geranium powdery metallic cortex strong	OdorRactor ,TGSC, Flavorbase
2110	Tetrahydro-4-methyl-2- phenyl-2H-pyran	4-methyl-2-phenyloxane	CC1CCOC(C1)C2=CC=CC=C2	floral rose fresh green herbaceous phenolic bitter parsley	OdorRactor ,TGSC
2111	2H-Pyran, tetrahydro-4- methyl-2-(2- methylpropyl)-	4-methyl-2-(2-methylpropyl)oxane	CC1CCOC(C1)CC(C)C	rose geranium green herbaceous metallic	OdorRactor ,TGSC
	m-Dioxane, 4-methyl-2-styryl-	4-methyl-2-[(E)-2-phenylethenyl]-1,3-dioxane	CC1CCOC(O1)C=CC2=CC=CC=	spicy sweet candy cinnamyl warm	TGSC
2113	2-Methyl-1,5- dioxaspiro[5.5]undecane	4-methyl-1,5- dioxaspiro[5.5]undecane	CC1CCOC2(O1)CCCCC2	herbaceous eucalyptus woody thujonic	OdorRactor ,TGSC

2114	2,2,4-Trimethyl-1,3-dioxolane	2,2,4-trimethyl-1,3-dioxolane	CC1COC(O1)(C)C	earthy ethereal green vegetable potato tomato asparagus musty raw raw potato	OdorRactor ,TGSC
2115	Acetoin propyleneglycol ketal	1-(2,4-dimethyl-1,3-dioxolan-2-yl)ethanol	CC1COC(O1)(C)C(C)O	fatty buttery mild fruity	TGSC, Flavorbase
2116	1,3-Dioxolane, 2,4-dimethyl- 2-(5,6,7,8- tetrahydro-5,5,8,8- tetramethyl-2- naphthalenyl)-	2,4-dimethyl-2-(5,5,8,8- tetramethyl-6,7- dihydronaphthalen-2-yl)-1,3- dioxolane	CC1COC(O1)(C)C2=CC3=C(C=C 2)C(CC C3(C)C)(C)C	woody dry amber powdery musk	OdorRactor ,TGSC
2117	2,4-Dimethyl-2-(4-methylpent- 3-enyl)-1,3- dioxolane	2,4-dimethyl-2-(4-methylpent-3-enyl)-1,3- dioxolane	CC1COC(O1)(C)CCC=C(C)C	fatty green citrus	OdorRactor ,TGSC
2118	2,4-Dimethyl-1,3-dioxolane	2,4-dimethyl-1,3-dioxolane	CC1COC(O1)C	fruity green grassy	ADB, TGSC
2119	2-Isopropyl-4-methyl-1,3-dioxolane	4-methyl-2-propan-2-yl-1,3- dioxolane	CC1COC(O1)C(C)C	winey	OdorRactor ,TGSC
2120	4-Methyl-2-(1-phenylethyl)- 1,3-dioxolane	4-methyl-2-(1-phenylethyl)-1,3-dioxolane	CC1COC(O1)C(C)C2=CC=CC=C 2	green mushroom chicken herbaceous earthy new mown hay	OdorRactor ,TGSC
2121	2,6-Dimethyl-5-heptenal propyleneglycol acetal	4-methyl-2-(6-methylhept-5-en-2-yl)-1,3- dioxolane	CC1COC(O1)C(C)CCC=C(C)C	green citrus	OdorRactor ,TGSC
2122	Citral propylene glycol acetal	2-[(1E)-2,6-dimethylhepta-1,5-dienyl]-4-methyl-1,3-dioxolane	CC1COC(O1)C=C(C)CCC=C(C) C	citrus sweet lemon orange	TGSC
2123	1,3-Dioxolane, 4-methyl-2- styryl-		CC1COC(O1)C=CC2=CC=CC=C	spicy cinnamyl	TGSC
2124	2-Methoxy-4-(4-methyl-1,3-dioxolan-2-yl)phenol	2-methoxy-4-(4-methyl-1,3-dioxolan-2-yl)phenol	CC1COC(O1)C2=CC(=C(C=C2) O)OC	sweet vanilla chocolate creamy dairy powdery cocoa	OdorRactor ,TGSC
2125	1,3-Dioxolane, 4-methyl-2-(4-methylphenyl)-	4-methyl-2-(4-methylphenyl)-1,3-dioxolane	CC1COC(O1)C2=CC=C(C=C2)C	floral bitter almond cherry fruity bitter	TGSC
2126	4-Methyl-2-phenyl-1,3- dioxolane	4-methyl-2-phenyl-1,3-dioxolane	CC1COC(O1)C2=CC=CC=C2	bitter sweet naphthyl woody narcissus fruity floral	Sigma Aldrich, TGSC, OdoRactor
2127	Perillaldehyde propyleneglycol acetal	4-methyl-2-(4-prop-1-en-2-ylcyclohexen-1-yl)-1,3- dioxolane	CC1COC(O1)C2=CCC(CC2)C(= C)C	fatty spicy herbaceous	TGSC
2128	2-Isobutyl-4-methyl-1,3- dioxolane	4-methyl-2-(2-methylpropyl)-1,3-dioxolane	CC1COC(O1)CC(C)C	apple creamy musty woody pineapple sweet ethereal tropical fruity sour dairy buttery rummy ripe	TGSC, OdoRactor
2129	Hydroxycitronellal propyleneglycol acetal	2,6-dimethyl-7-(4-methyl-1,3-dioxolan-2-yl)heptan 2-ol	CC1COC(O1)CC(C)CCCC(C)(C) O	green floral lily muguet	TGSC
2130	1,3-Dioxolane, 4-methyl-2-[2-(methylthio)ethyl]-	4-methyl-2-(2- methylsulfanylethyl)-1,3- dioxolane	CC1COC(O1)CCSC	meaty	TGSC
2131	Anethofuran	(3 <i>S</i> ,3 <i>aS</i> ,7 <i>aR</i>)-3,6-dimethyl- 2,3,3 <i>a</i> ,4,5,7 <i>a</i> - hexahydro-1- benzofuran	CC1COC2C1CCC(=C2)C	minty dill	Flavornet, TGSC, OdoRactor
2132	3,6-Dimethyl-2,3,3a,4,5,7a- hexahydro-1- benzofuran	3,6-dimethyl-2,3,3a ,4,5,7a - hexahydro-1- benzofuran	CC1COC2C1CCC(=C2)C	minty floral herbaceous dill	OdorRactor ,TGSC, Flavorbase
2133	Galaxolide	4,6,6,7,8,8-hexamethyl-1,3,4,7- tetrahydrocyclopenta[g]isochrome ne	CC1COCC2=CC3=C(C=C12)C(C (C3(C)C)C)(C)C	ethereal sweet floral musk	OdoRactor, Pubchem, Sigma Aldrich
2134	Galaxolide	4,6,6,7,8,8-hexamethyl-1,3,4,7-tetrahydrocyclopenta[g]isochrome ne	CC1COCC2=CC3=C(C=C12)C(C (C3(C)C)C)(C)C	floral musk sweet	OdorRactor ,Pubchem, TGSC
2135	3,4,6,7,8,9-Hexahydro- 4,6,6,9,9- pentamethyl-1H- naphtho[2,3-c]pyran	4,6,6,9,9-pentamethyl-3,4,7,8- tetrahydro-1 <i>H</i> - benzo[g]isochromene	CC1COCC2=CC3=C(C=C12)C(C CC3(C) C)(C)C	musk	TGSC
2136 2137	4-Methyl-1,3-dithiolane 2,4-Dimethyl-3-oxazoline	4-methyl-1,3-dithiolane 2,4-dimethyl-2,5-dihydro-1,3- oxazole	CC1CSCS1 CC1N=C(CO1)C	sulfurous alliaceous tomato boiled beefy	TGSC OdorRactor ,TGSC
2138	4H-1,3,5-Dithiazine, 2,4,6-trimethyl-	2,4,6-trimethyl-4 <i>H</i> -1,3,5-dithiazine	CC1N=C(SC(S1)C)C	meaty beefy	TGSC
2139	Pyrrolidino[1,2-e]-4H-1,3,5-dithiazine, 2,4- dimethyl	2,4-dimethyl-6,7,8,8 <i>a</i> -tetrahydro-4 <i>H</i> -pyrrolo[2,1-d	CC1N2CCCC2SC(S1)C	meaty cooked roasted	OdorRactor ,TGSC
2140	2-Isopropyl-4,6-dimethyl- 1,3,5-dithiazinane	4,6-dimethyl-2-propan-2-yl-1,3,5-dithiazinane	CC1NC(SC(S1)C(C)C)C	sulfurous groundnut cocoa roasted	Flavorbase
2141	Thialdine	2,4,6-trimethyl-1,3,5-dithiazinane	CC1NC(SC(S1)C)C	sulfurous nutty hazelnut corn meaty earthy clam	OdorRactor ,TGSC
2142	4-Isopropyl-2,6-dimethyl-1,3,5-dithiazinane	2,4-dimethyl-6-propan-2-yl-1,3,5-dithiazinane	CC1NC(SC(S1)C)C(C)C	leek nutty onion peanut meaty	OdorRactor ,TGSC
2143		4,6-dimethyl-2-(2-methylpropyl)- 1,3,5- dithiazinane	CC1NC(SC(S1)CC(C)C)C	nutty roasted cocoa peanut groundnut hazelnut meaty	TGSC, Flavorbase
2144	2-Methylthiazolidine	2-methyl-1,3-thiazolidine	CC1NCCS1	meaty cooked bouillon soupy brothy sweet fishy	OdorRactor ,TGSC, Flavorbase
2145	Paraldehyde	2,4,6-trimethyl-1,3,5-trioxane	CC1OC(OC(O1)C)C	sweet aromatic	OdorRactor ,TGSC, Pubchem

2146	2-Methyl-4-phenyl-1,3-	2-methyl-4-phenyl-1,3-dioxolane	CC1OCC(O1)C2=CC=CC=C2	floral jasmine hyacinth animal	OdorRactor ,TGSC
	dioxolane		` '		·
2147	2'- Methylspiro[bicyclo[2.2.1]he ptane-2,5'- [1,3]dioxane]	2-methylspiro[1,3-dioxane-5,2'-bicyclo[2.2.1]heptane]	CC10CC2(CC3CCC2C3)CO1	fruity green rhubarb celery galbanum	OdorRactor ,TGSC
2148	2,4,4-Trimethyl-1,3-oxathiane	2,4,4-trimethyl-1,3-oxathiane	CC1OCCC(S1)(C)C	green woody terpenic	TGSC
2149	2,4,6-Trimethyl-1,3,5- trithiane	2,4,6-trimethyl-1,3,5-trithiane	CC1SC(SC(S1)C)C	sulfurous green onion onion	TGSC
2150	3,5-Dimethyl-1,2,4-trithiolane	3,5-dimethyl-1,2,4-trithiolane	CC1SC(SS1)C	meaty beefy sulfurous cooked chicken onion	OdorRactor ,TGSC, Flavorbase
2151	2-Methyl-1,3-dithiolane	2-methyl-1,3-dithiolane	CC1SCCS1	sulfurous alliaceous smoky savory vegetable	Flavornet, TGSC, OdoRactor
2152	3-Methyl-1,2,4-trithiane	3-methyl-1,2,4-trithiane	CC1SCCSS1	meaty	OdorRactor,
2153	3-Methyl-1,2,4-trithiolane	3-methyl-1,2,4-trithiolane	CC1SCSS1	alliaceous roasted onion cooked seafood sulfurous	Flavorbase, TGSC
2154	2-Benzylidene-butyraldehyde	2-benzylidenebutanal	CCC(=CC1=CC=CC=C1)C=O	spicy	TGSC
2155	2-Furfurylidenebutyraldehyde	(2E)-2-(furan-2- ylmethylidene)butanal	CCC(=CC1=CC=CO1)C=O	spicy cinnamyl leathery	OdorRactor ,TGSC
2156	6-Ethyl-3-methyloct-5-en-1-ol	6-ethyl-3-methyloct-5-en-1-ol	CCC(=CCC(C)CCO)CC	floral aldehydic muguet lily of the valley	TGSC
2157	2-Ethyl-4-(2,2,3- trimethylcyclopent-3-en-1- yl)but-2-en-1-ol	(E)-2-ethyl-4-(2,2,3- trimethylcyclopent-3-en-1- yl)but- 2-en-1-ol	CCC(=CCC1CC=C(C1(C)C)C)C O	woody sandal wood greasy oily wax	OdorRactor ,TGSC, Flavorbase
2158	3,7-Dimethylnona-2,6- dienenitrile	3,7-dimethylnona-2,6-dienenitrile	CCC(=CCCC(=CC#N)C)C	lemon cologne metallic citrus	OdorRactor ,TGSC
2159	1,6-Nonadien-3-OL, 3,7-dimethyl-	(6E)-3,7-dimethylnona-1,6-dien-3-ol	CCC(=CCCC(C)(C=C)O)C	floral fresh bois de rose herbaceous wet green lavender bergamot rose	OdorRactor ,TGSC
2160	1,6-Nonadien-3-OL, 3,7-dimethyl-, acetate	[(6E)-3,7-dimethylnona-1,6-dien-3-yl] acetate	CCC(=CCCC(C)(C=C)OC(=O)C)	floral bergamot fruity tropical rose	OdorRactor ,TGSC
2161	Sodium propionate	sodium;propanoate	CCC(=O)[O-].[Na+]	bland faint acetic	Sigma Aldrich, TGSC, Flavorbase, Pubchem
2162	Methyl ethyl ketone	butan-2-one	CCC(=O)C	ethereal acetone fruity camphoraceous sweet solvent ketonic pleasant pungent minty	Sigma Aldrich, AOD, Flavorbase, TGSC, Pubchem
2163	Dimethylionone	(E)-2-methyl-1-(2,6,6-trimethylcyclohex-2-en-1-yl)pent-1-en-3-one	CCC(=0)C(=CC1C(=CCCC1(C)C)C)C	floral violet sweet powdery woody	OdorRactor ,TGSC
2164	1-Penten-3-one, 2-methyl-1- (2,2,6- trimethylcyclohexenyl)	(E)-2-methyl-1-(2,2,6-trimethylcyclohex-3-en-1-yl)pent-1-en-3-one	CCC(=0)C(=CC1C(CC=CC1(C)C)C)C	powdery woody orris violet berry	OdorRactor ,TGSC
2165	2,3-Pentanedione	pentane-2,3-dione	CCC(=0)C(=0)C	almond buttery caramel cheese chocolate coffee creamy fruity sweet pungent nutty toasted	Sigma Aldrich, TGSC, OdoRactor, Pubchem
2166	3,4-Hexanedione	hexane-3,4-dione	CCC(=0)C(=0)CC	buttery almond nutty caramel coffee creamy toasted	Sigma Aldrich, AOD, TGSC, OdoRactor
2167	2-Oxobutyric acid	2-Oxobutyric acid	CCC(=0)C(=0)0	caramel creamy sweet lactonic brown	Sigma Aldrich, TGSC, OdorRactor
2168	2-Methyl-3-pentanone	2-methylpentan-3-one	CCC(=O)C(C)C	minty	Flavornet
	4,7-Dimethyloct-6-en-3-one	4,7-dimethyloct-6-en-3-one	CCC(=0)C(C)CC=C(C)C	grapefruit fruity bitter fresh citrus	OdorRactor ,TGSC
2170	2-Hydroxy-3-pentanone	2-hydroxypentan-3-one	CCC(=O)C(C)O	truffle earthy nutty	Flavornet, TGSC
2171	2-Mercapto-3-pentanone	2-sulfanylpentan-3-one	CCC(=O)C(C)S	roasted meat meaty roasted	Flavornet, TGSC
2172	Ethyl vinyl ketone	pent-1-en-3-one	CCC(=0)C=C	green fishy pungent pepper mustard garlic onion spicy	Sigma Aldrich, TGSC, OdoRactor
2173	2-Hexen-4-one	(E)-hex-4-en-3-one	CCC(=0)C=CC	ethereal acidic pungent spicy green tropical metallic	Sigma Aldrich, TGSC, OdoRactor
2174	4,6,10-Dodecatrien-3-one,	(4E ,6E)-7,11-dimethyldodeca-	CCC(=0)C=CC=C(C)CCC=C(C)	sweet violet citronella	TGSC
2174	7,11-dimethyl-, reaction products with acetone, ionone	4,6,10-trien-3- one;propan-2-one;(<i>E</i>)-4-(2,6,6-	C.CC1=C CCC(C1C=CC(=O)C)(C)C.CC(=	sweet violet chronena	Tusc
	fraction	trimethylcyclohex- 2-en-1-yl)but-3-en-2-one	O)C		
2175	beta-Methylionone	(E)-1-(2,6,6-trimethylcyclohexen-1-yl)pent-1-en-3- one	CCC(=0)C=CC1=C(CCCC1(C)C)	orris woody powdery floral violet tropical tobacco creamy	OdorRactor ,TGSC
2176	1-Penten-3-one, 1-(4-methoxyphenyl)-, (1E)	1-(4-methoxyphenyl)pent-1-en-3- one	CCC(=0)C=CC1=CC=C(C=C1)O C	sweet powdery cherry fruity almond anisic vanilla dry heliotrope coumarinic	OdorRactor ,TGSC
2177	1-(2,6,6-Trimethyl-2- cyclohexen-1-yl)-1- penten-3- one	(E)-1-(2,6,6-trimethylcyclohex-2-en-1-yl)pent-1-en-3-one	CCC(=0)C=CC1C(=CCCC1(C)C)	sweet powdery fruity floral violet beewax orris woody powdery tea	OdorRactor ,TGSC
2178	Methyl-delta-ionone	(E)-1-(2,6,6-trimethylcyclohex-3-en-1-yl)pent-1-en-3-one	CCC(=O)C=CC1C(C=CCC1(C)C)	woody musk patchouli oakmoss	OdorRactor ,TGSC
2179	1-[4-(Morpholin-4- yl)phenyl]propan-1-one	1-(4-morpholin-4-ylphenyl)propan- 1-one	CCC(=O)C1=CC=C(C=C1)N2CC OCC2	spicy citrus woody resinous	TGSC, OdoRactor

2180	4'-Methoxypropiophenone	1-(4-methoxyphenyl)propan-1-one	CCC(=O)C1=CC=C(C=C1)OC	musty anisic	TGSC
2181	Propiophenone	1-phenylpropan-1-one	CCC(=0)C1=CC=CC=C1	cherry hawthorn lilac floral	Sigma Aldrich, TGSC,
	• •		, ,	aromatic herbaceous strong	Pubchem
2182	2-Propionylpyrrole	1-(1H -pyrrol-2-yl)propan-1-one	CCC(=0)C1=CC=CN1	roasted popcorn	Flavornet, TGSC, OdoRactor
2183	2-Propionylthiophene	1-thiophen-2-ylpropan-1-one	CCC(=0)C1=CC=CS1	creamy caramel	TGSC
2184	2-Propionylthiazole	1-(1,3-thiazol-2-yl)propan-1-one	CCC(=O)C1=NC=CS1	nutty popcorn bready cereal	OdorRactor ,TGSC
2185	2-Propionyl-1-pyrroline	1-(3,4-dihydro-2 <i>H</i> -pyrrol-5-yl)propan-1-one	CCC(=O)C1=NCCC1	roasted fishy	Flavornet, TGSC
2186	2-Propionyl-2-thiazoline	1-(4,5-dihydro-1,3-thiazol-2-yl)propan-1-one	CCC(=0)C1=NCCS1	meaty nutty cooked roasted	OdorRactor ,TGSC
2187	Nerone	1-(2-methyl-5-propan-2- ylcyclohex-2-en-1- yl)propan-1- one	CCC(=0)C1CC(CC=C1C)C(C)C	leafy green woody herbaceous phenolic floral cortex citrus	OdorRactor ,TGSC
2188	3-Pentanone	pentan-3-one	CCC(=0)CC	ethereal acetone	Sigma Aldrich, TGSC, Pubchem
2189	Ethyl 2,4-dioxohexanoate	ethyl 2,4-dioxohexanoate	CCC(=0)CC(=0)C(=0)OCC	burnt sugar caramel fruity floral	OdorRactor ,Flavorbase
2190	5-Methyl-5-phenylhexan-3- one	5-methyl-5-phenylhexan-3-one	CCC(=0)CC(C)(C)C1=CC=CC=C	spicy pepper woody rose floral	TGSC
2191	3-Hexanone, 5-mercapto-5-methyl-	5-methyl-5-sulfanylhexan-3-one	CCC(=0)CC(C)(C)S	citrus grape fruity watery tropical earthy dewy	Flavorbase, TGSC
2192	Yuzunone	(6Z ,8E)-undeca-6,8,10-trien-3- one	CCC(=0)CCC=CC=CC=C	peely balsamic floral	TGSC
2193	3-Pentanone, 1-(2,6,6- trimethyl-2- cyclohexen-1-yl)-, reaction products with 2- propyn-1-ol	prop-2-yn-1-ol;1-(2,6,6- trimethylcyclohex-2-en-1- yl)pentan-3-one	CCC(=0)CCC1C(=CCCC1(C)C) C.C#CC 0	amber ambergis animal dry fresh metallic	TGSC
2194	1-Hydroxybutan-2-one	1-hydroxybutan-2-one	CCC(=O)CO	sweet coffee musty grain malty butterscotch brown	OdorRactor ,TGSC
2195	1-(Methylthio)-2-butanone	1-methylsulfanylbutan-2-one	CCC(=O)CSC	mushroom garlic oily fishy fresh radish mustard horseradish wasabi alliaceous onion savory metallic vegetable	OdorRactor ,TGSC, Flavorbase
2196	Propionic acid	propanoic acid	CCC(=0)O	dairy acidic rancid sour soy vinegar cheese pungent disagreeable	Sigma Aldrich, TGSC, Pubchem
2197	Methyl propionate	methyl propanoate	CCC(=O)OC	apple banana strawberry fresh rummy fruity sweet	Sigma Aldrich, TGSC, OdoRactor, Pubchem
2198	Terpinyl propionate	2-(4-methylcyclohex-3-en-1- yl)propan-2-yl propanoate)C	herbaceous green old wood citrus geranium tropical sweet	SuperScent, TGSC, OdoRactor
2199	Benzylisopropyl propionate	(2-methyl-1-phenylpropan-2-yl) propanoate	CCC(=0)OC(C)(C)CC1=CC=CC =C1	sweet jasmine hairy tea natural floral	OdorRactor ,TGSC
2200	Linalyl propionate	3,7-dimethylocta-1,6-dien-3-yl propanoate		herbaceous pear sweet bergamot lily woody rose rummy floral fresh	Sigma Aldrich, TGSC
2201	Nerolidyl propionate	3,7,11-trimethyldodeca-1,6,10- trien-3-yl propanoate	CCC(=0)OC(C)(CCC=C(C)CCC= C(C)C) C=C	floral	TGSC
2202	Isopropyl propionate	propan-2-yl propanoate	CCC(=O)OC(C)C	fruity ethereal sweet pineapple banana	SuperScent, TGSC,OdoRactor
2203	1-Phenylethyl propionate	1-phenylethyl propanoate	CCC(=0)OC(C)C1=CC=CC=C1	gardenia green musty sweet floral rose weedy fresh fruity tropical citrus	Sigma Aldrich, TGSC,OdoRactor
2204	Cyclotene propionate	(2-methyl-5-oxocyclopenten-1-yl) propanoate	CCC(=0)OC1=C(CCC1=0)C	nutty creamy caramel buttery maple	TGSC, Flavorbase
2205	Maltol propionate	(2-methyl-4-oxopyran-3-yl) propanoate	CCC(=0)OC1=C(OC=CC1=0)C	fruity sweet caramel bready jammy strawberry berry baked cookie pineapple tropical	OdorRactor ,TGSC, Flavorbase
2206	Propanoic acid, 4- methylphenyl ester	(4-methylphenyl) propanoate	CCC(=0)OC1=CC=C(C=C1)C	animal	OdorRactor,
2207	Guaiacol propionate	(2-methoxyphenyl) propanoate	CCC(=0)OC1=CC=CC=C1OC	fruity nutty vanilla	TGSC
2208	3a,4,5,6,7,7a-Hexahydro-4,7- methano-1H- indenyl propionate	3-tricyclo[5.2.1.02,6]dec-4-enyl propanoate	CCC(=0)0C1C=CC2C1C3CCC2 C3	fruity herbaceous woody jasmine oily basil green	OdorRactor ,TGSC
2209		(4,8-dimethyl-2-propan-2-ylidene-3,3a ,4,5,6,8a - hexahydro-1 <i>H</i> - azulen-6-yl) propanoate	CCC(=0)0C1CC(C2CC(=C(C)C) CC2C(= C1)C)C	rooty woody cedar	TGSC
2210	Carvyl propionate	(2-methyl-5-prop-1-en-2- ylcyclohex-2-en-1-yl) propanoate	CCC(=0)OC1CC(CC=C1C)C(=C) C	minty sweet warm fruity	Sigma Aldrich, TGSC
2211	l-Menthyl propionate		CCC(=0)OC1CC(CCC1C(C)C)C	herbaceous sweet floral rose peony	TGSC
2212	Tricyclodecenyl propionate	8-tricyclo[5.2.1.02,6]dec-3-enyl propanoate	CCC(=O)OC1CC2CC1C3C2C=C C3	fruity herbaceous woody jasmine oily basil	OdorRactor ,TGSC

2213	Isobornyl propionate	(1,7,7-trimethyl-2-	CCC(=0)0C1CC2CCC1(C2(C)C)	pungent pine camphoraceous	OdorRactor ,TGSC,Sigma
		bicyclo[2.2.1]heptanyl) propanoate	c	woody lavender balsamic fruity herbaceous earthy herbaceous floral vanilla fruit	Aldrich
2214	Cyclobayyl propiorata	cyclohavyl proponosto	CCC(=0)OC1CCCCC1	turpentine	Sigma Aldrich, TGSC,
2214	Cyclohexyl propionate	cyclohexyl propanoate	CCC(=0)0CTCCCCCT	banana pineapple sweet fruity wax green	Sigma Aldrich, TGSC, OdoRactor
2215	Ethyl propionate	ethyl propanoate	CCC(=0)OCC	ethereal pineapple sweet winey fruity rummy juicy grape fermented eggy	Sigma Aldrich, TGSC, OdoRactor, Pubchem
2216	Acetic acid, 2-(1- oxopropoxy)-, 1-(3,3- dimethylcyclohexyl)ethyl ester	[2-[1-(3,3- dimethylcyclohexyl)ethoxy]-2- oxoethyl] propanoate	CCC(=0)OCC(=0)OC(C)C1CCC C(C1)(C) C	musk ambrette fruity berry	TGSC
2217	Cyclopentenyl propionate musk	[2,2-dimethyl-3-(2-methyl-5-prop- 1-en-2- ylcyclopenten-1-yl)propyl] propanoate			SuperScent, TGSC
2218	1-Propanol, 2-[1-(3,3-dimethylcyclohexyl)ethoxy]-2-methyl-, 1-propanoate	[2-[1-(3,3- dimethylcyclohexyl)ethoxy]-2- methylpropyl] propanoate	CCC(=0)OCC(C)(C)OC(C)C1CC CC(C1)(C)C	musk ambrette fruity pear	TGSC
2219	Isobutyl propionate	2-methylpropyl propanoate	CCC(=0)OCC(C)C	banana floral sweet fruity green ethereal tutti frutti rummy pungent bubblegum tropical estery	Sigma Aldrich, Flavorbase, TGSC,OdoRactor
2220	Propylene glycol dipropionate	2-propanoyloxypropyl propanoate	CCC(=O)OCC(C)OC(=O)CC	winey fruity	TGSC
2221	Tripropionin	2,3-di(propanoyloxy)propyl propanoate	CCC(=O)OCC(COC(=O)CC)OC(=O)CC	oily fatty fruity chemical	Sigma Aldrich, TGSC.OdoRactor
2222	Allyl propionate	prop-2-enyl propanoate	CCC(=0)OCC=C	apricot apple fruity tropical ripe ethereal sharp acrylate alliaceous	SuperScent, TGSC, OdoRactor
2223	Geranyl propionate	[(2E)-3,7-dimethylocta-2,6-dienyl] propanoate	CCC(=0)OCC=C(C)CCC=C(C)C	floral fresh wax tropical fruity rose sweet honey vegetable powdery	Sigma Aldrich, TGSC, OdoRactor
2224	Neryl propionate	[(2Z)-3,7-dimethylocta-2,6-dienyl] propanoate	CCC(=0)OCC=C(C)CCC=C(C)C	fruity floral green jammy berry sweet tutti frutti powdery	OdorRactor ,TGSC
2225	2,4-Hexadienol monopropionate	[(2Z,4E)-hexa-2,4-dienyl] propanoate	CCC(=0)OCC=CC=CC	fruity sweet tropical pineapple winey	OdorRactor ,TGSC
2226	Cinnamyl propionate	[(E)-3-phenylprop-2-enyl] propanoate	CCC(=0)OCC=CC1=CC=CC=C1	sweet spicy fruity balsamic grape floral green cherry bubblegum	Sigma Aldrich, TGSC, OdoRactor
2227	Anisyl propionate	(4-methoxyphenyl)methyl propanoate	CCC(=O)OCC1=CC=C(C=C1)OC	herbaceous anisic cherry floral fruity vanilla peach	Sigma Aldrich, TGSC, OdoRactor
2228	Benzyl propionate	benzyl propanoate	CCC(=0)OCC1=CC=CC=C1	berry jasmine sweet fruity floral banana balsamic apple jammy	Sigma Aldrich, TGSC, OdoRactor
2229	Furfuryl propionate	furan-2-ylmethyl propanoate	CCC(=O)OCC1=CC=CO1	floral spicy sweet fruity green banana oily coffee	Sigma Aldrich, TGSC, OdoRactor
2230	Tetrahydrofurfuryl propionate	oxolan-2-ylmethyl propanoate	CCC(=0)OCC1CCCO1	violet leaf oily paint fruity tropical musty nutty fermented fatty banana violet	
2231	Isoamyl propionate	3-methylbutyl propanoate	CCC(=0)OCCC(C)C	apple pear fruity sweet banana pineapple ripe tropical fruit estery green fresh apricot plum	Sigma Aldrich, Flavorbase, TGSC, OdoRactor
2232	Citronellyl propionate	3,7-dimethyloct-6-enyl propanoate	CCC(=O)OCCC(C)CCC=C(C)C	fruity rose wax floral green neroli citrus	Sigma Aldrich, TGSC,OdoRactor
2233	Rhodinyl propionate	3,7-dimethyloct-7-enyl propanoate	CCC(=0)OCCC(C)CCCC(=C)C	rose geranium verbena floral	OdorRactor ,TGSC
2234	2-(4-Methyl-5-thiazolyl)ethyl propionate	2-(4-methyl-1,3-thiazol-5-yl)ethyl propanoate	CCC(=0)OCCC1=C(N=CS1)C	roasted nutty	TGSC
2235	2-Phenylethyl propionate	2-phenylethyl propanoate	CCC(=0)OCCC1=CC=CC=C1	rose sweet floral fruity honey balsamic storax	Sigma Aldrich, TGSC, Pubchem, OdoRactor
2236	3-Phenylpropyl propionate	3-phenylpropyl propanoate	CCC(=0)OCCCC1=CC=CC=C1	floral balsamic hyacinth mimosa fruity	SuperScent, TGSC, OdoRactor
2237	Cyclohexylpropyl propionate	3-cyclohexylpropyl propanoate	CCC(=0)OCCCC1CCCCC1	green fruity fresh blueberry	TGSC
2238	Isononyl propionate	7-methyloctyl propanoate	CCC(=0)OCCCCCC(C)C	floral lavender herbaceous woody	OdorRactor ,TGSC
2239	9-Decenyl propionate	dec-9-enyl propanoate	CCC(=0)OCCCCCCCCCC	dewy wax rose amber fresh floral petal	OdorRactor ,TGSC
2240	2-Phenoxyethyl propionate	2-phenoxyethyl propanoate	CCC(=0)OCCOC1=CC=CC=C1	lavender fruity resinous myrrh opoponax hay	Sigma Aldrich, TGSC, OdoRactor
2241	Allyl thiopropionate	S-prop-2-enyl propanethioate	CCC(=0)SCC=C	fresh onion garlic green alliaceous gassy	OdorRactor ,TGSC
2242	Furfuryl thiopropionate	S -(furan-2-ylmethyl) propanethioate	CCC(=0)SCC1=CC=CO1	coffee sulfurous onion garlic savory alliaceous	Sigma Aldrich, TGSC, OdoRactor,
2243	1-Penten-3-ol, 2-methyl-1- (methylbicyclo(2.2.1)hept-5- en-2-yl)-	(E)-2-methyl-1-(2-methyl-2-	CCC(C(=CC1(CC2CC1C=C2)C)C)O	woody autumn sweet sandal wood sawdust	OdorRactor ,TGSC

2244	Ethyl 2-ethylacetoacetate	ethyl 2-ethyl-3-oxobutanoate	CCC(C(=O)C)C(=O)OCC	fruity winey green herbaceous	OdorRactor ,TGSC
2245	3-Hydroxy-2-pentanone	3-hydroxypentan-2-one	CCC(C(=O)C)O	earthy ethereal root beer herbaceous truffle	Sigma Aldrich, TGSC,
2246	3-Mercapto-2-pentanone	3-sulfanylpentan-2-one	CCC(C(=O)C)S	sulfurous onion meaty metallic roasted horseradish potato nutty roasted meat tropical fruit alliaceous catty savory hazelnut grapefruit	OdoRactor Flavornet, TGSC, OdoRactor
2247	Methyl 2- (methylthio)butyrate	methyl 2-methylsulfanylbutanoate	CCC(C(=O)OC)SC	sulfurous musty onion fruity tropical green	OdorRactor ,TGSC
2248	n-Ethyl-2,2- diisopropylbutanamide	<i>N</i> ,2-diethyl-3-methyl-2-propan-2-ylbutanamide	CCC(C(C)C)(C(C)C)C(=O)NCC	cooling minty	TGSC
2249	1 10	2-methyl-3-sulfanylpentanal	CCC(C(C)C=0)S	savory grilled roasted sulfurous onion tropical fruit dairy beefy cooked chicken alliaceous garlic	OdorRactor ,TGSC
2250	3-Mercapto-2-methylpentan-1- ol	2-methyl-3-sulfanylpentan-1-ol	CCC(C(C)CO)S	sulfurous onion	OdorRactor ,TGSC
2251	Ethyl 2-hydroxy-2- methylbutanoate	ethyl 2-hydroxy-2- methylbutanoate	CCC(C)(C(=O)OCC)O	caramel nutty	OdorRactor ,TGSC
2252	4-Tert-Pentylcyclohexanone	4-(2-methylbutan-2-yl)cyclohexan- 1-one	CCC(C)(C)C1CCC(=O)CC1	woody dry orris earthy camphoraceous	OdorRactor ,TGSC
2253	Cyclohexane, 1-(1,1-dimethylpropyl)-4- ethoxy-, cis-	1-ethoxy-4-(2-methylbutan-2- yl)cyclohexane	CCC(C)(C)C1CCC(CC1)OCC	fresh bellpepper ozone marine green	OdorRactor ,TGSC
2254	2-Tert-Pentylcyclohexyl acetate	[2-(2-methylbutan-2- yl)cyclohexyl] acetate	CCC(C)(C)C1CCCCC1OC(=O)C	balsamic woody sweet fi rneedle raspberry jammy	OdorRactor ,TGSC
2255		prop-2-enyl 5,5- dimethylheptanoate	CCC(C)(C)CCCC(=0)OCC=C	fruity rose sweet musk	OdorRactor ,TGSC
2256		3,7-dimethylocta-4,6-dien-3-ol	CCC(C)(C=CC=C(C)C)O	sweet floral lily citrus fresh	OdorRactor ,TGSC
2257	4-Mercapto-4-methyl-2- hexanone	4-methyl-4-sulfanylhexan-2-one	CCC(C)(CC(=O)C)S	catty floral fruity black currant sulfurous meaty	Flavorbase
2258	3-Methyl-3-pentanol	3-methylpentan-3-ol	CCC(C)(CC)O	leafy green fruity powerful	Sigma Aldrich, TGSC
		3,7-dimethyloct-6-en-3-ol	CCC(C)(CCC=C(C)C)O	bois de rose woody citrus blueberry weedy floral rose	OdorRactor ,TGSC
2260	6,10,14-Hexadecatrien-3-ol, 3,7,11,15- tetramethyl-	(6E,10E)-3,7,11,15- tetramethylhexadeca-6,10,14- trien-3-ol	CCC(C)(CCC=C(C)CCC=C(C)CC C=C(C) C)O		OdorRactor ,TGSC
2261	3-Methyl-1-phenyl-3-pentanol	3-methyl-1-phenylpentan-3-ol	CCC(C)(CCC1=CC=CC=C1)O	floral sweet lilac anisic earthy fresh narcissus peony rose fruity	Sigma Aldrich, TGSC, Flavorbase, OdoRactor
2262	1-Ethyl-1-methyl-3- phenylpropyl acetate	(3-methyl-1-phenylpentan-3-yl) acetate	CCC(C)(CCC1=CC=CC=C1)OC(=O)C	fresh narcissus floral hyacinth tea sweet fruity	OdorRactor ,TGSC
2263		3,7-dimethyloctan-3-ol	CCC(C)(CCCC(C)C)O	lilac floral lily bois de rose woody tea oily fatty citrus fresh sweet earthy rose	Sigma Aldrich, TGSC
2264	3,7-Dimethyloctan-3-yl acetate	3,7-dimethyloctan-3-yl acetate	CCC(C)(CCCC(C)C)OC(=O)C	herbaceous citrus weedy cologne woody fresh bergamot floral	OdorRactor ,TGSC
2265	6-Methoxy-2,6- dimethyloctanal	6-methoxy-2,6-dimethyloctanal	CCC(C)(CCCC(C)C=0)OC	marine seashore ozone green fruity citrus	TGSC
2266	5-Methylheptane-3,4-dione	5-methylheptane-3,4-dione	CCC(C)C(=O)C(=O)CC	fruity chemical	TGSC
	Pentanoic acid, 3-methyl-2- oxo-, ethyl ester	ethyl 3-methyl-2-oxopentanoate	CCC(C)C(=0)C(=0)OCC	nutty walnut woody herbaceous	TGSC
2268	5-Methyl-2-hepten-4-one	(E)-5-methylhept-2-en-4-one	CCC(C)C(=0)C=CC	buttery hazelnut raw pungent ketonic sweet filbert nutty roasted coffee	Sigma Aldrich, Flavornet, TGSC, OdoRactor
2269	(S)-5-Methyl-2-hepten-4-one	(E,5S)-5-methylhept-2-en-4-one	CCC(C)C(=0)C=CC	hazelnut metallic fatty nutty	TGSC
2270	5-Methylhept-2-en-4-one	5-methylhept-2-en-4-one	CCC(C)C(=0)C=CC	nutty hazelnut soft buttery chocolate metallic	TGSC
2271	N,2-Dimethyl-N- phenylbutanamide	N ,2-dimethyl-N - phenylbutanamide	CCC(C)C(=O)N(C)C1=CC=CC= C1	fresh floral woody citrus oily natural cedar grapefruit	OdorRactor ,TGSC
2272	2-Methylbutanoic acid	2-methylbutanoic acid	CCC(C)C(=0)O	apple apricot berry cheese chocolate creamy grape woody peach pineapple sour strawberry winey pungent acidic roquefort cheese fruity dirty fermented	Sigma Aldrich, TGSC,OdoRactor
2273	(R)-2-Methylbutanoic acid	(2R)-2-methylbutanoic acid	CCC(C)C(=0)0	cheese sweaty	SuperScent, TGSC
2274	Methyl 2-methylbutyrate	methyl 2-methylbutanoate	CCC(C)C(=O)OC	apple sweet ethereal estery fruity lily fatty tutti frutti powdery ripe	Sigma Aldrich, TGSC,OdoRactor
2275	Methyl (2S)-2- methylbutanoate	methyl (2S)-2-methylbutanoate	CCC(C)C(=0)OC	fruity apple	TGSC
2276	Methyl (R)-2- methylbutanoate	methyl (2R)-2-methylbutanoate	CCC(C)C(=O)OC	fruity dairy	TGSC
2277	•	propan-2-yl 2-methylbutanoate	CCC(C)C(=O)OC(C)C	green oily ethereal pineapple sweet fruity tropical	Sigma Aldrich, TGSC, Pubchem

2278	Ethyl 2-methylbutyrate	ethyl 2-methylbutanoate	CCC(C)C(=0)OCC	apple green plum sweet fruity sharp estery berry fresh tropical cognac phenolic strong	TGSC, Sigma Aldrich, Flavorbase, Pubchem, OdoRactor
2279	Ethyl (2R)-2-methylbutanoate	ethyl (2R)-2-methylbutanoate	CCC(C)C(=O)OCC	apple peach fruity fresh	Flavornet, TGSC
2280	Isobutyl 2-methylbutyrate	2-methylpropyl 2-methylbutanoate	CCC(C)C(=O)OCC(C)C	sweet fruity citrus	OdorRactor ,TGSC, Flavorbase
2281	Propylene glycol 1-(2- methylbutyrate)	2-hydroxypropyl 2- methylbutanoate	CCC(C)C(=O)OCC(C)O	fruity ethereal	TGSC
2282	Geranyl 2-methylbutyrate	[(2E)-3,7-dimethylocta-2,6-dienyl] 2- methylbutanoate	CCC(C)C(=0)OCC=C(C)CCC=C(C)C	fruity apple rose	OdorRactor ,TGSC
2283	3-Methylbutyl 2- methylbutanoate	3-methylbutyl 2-methylbutanoate	CCC(C)C(=0)OCCC(C)C	fruity sweet citrus cherry blueberry apple winey strong ripe banana tropical ripe	Sigma Aldrich, TGSC, Flavorbase, OdoRactor
2284	Phenethyl 2-methylbutyrate	2-phenylethyl 2-methylbutanoate	CCC(C)C(=0)OCCC1=CC=CC= C1	floral green sweet tropical wax rose fruity pear	OdorRactor ,TGSC, Flavorbase, Sigma Aldrich,
2285	S-Methyl 2- methylbutanethioate	S -methyl 2-methylbutanethioate	CCC(C)C(=O)SC	sulfurous sweet cabbage tropical fruity	OdorRactor ,TGSC
2286	D-Isoleucine methyl ester hydrochloride	methyl (2R, 3R)-2-amino-3- methylpentanoate;hydrochloride	CCC(C)C(C(=O)OC)N.Cl	onion sulfurous	Sigma Aldrich
2287	Methyl 2-hydroxy-3- methylpentanoate	methyl 2-hydroxy-3- methylpentanoate	CCC(C)C(C(=O)OC)O	fruity estery caramel	SuperScent, TGSC
2288	Ethyl 2-hydroxy-3- methylpentanoate	ethyl 2-hydroxy-3- methylpentanoate	CCC(C)C(C(=O)OCC)O	fruity berry	OdorRactor ,TGSC
2289	2,3-Dimethylpentanal	2,3-dimethylpentanal	CCC(C)C(C)C=O	green ethereal	TGSC
2290	4-Methyl-2- (methylthiomethyl)-2-hexenal	(E)-4-methyl-2- (methylsulfanylmethyl)hex-2-enal	CCC(C)C=C(CSC)C=O	onion meaty soupy	TGSC
2291	(R)-2-Methylbutyraldehyde	(2R)-2-methylbutanal	CCC(C)C=O	burnt cocoa coffee	TGSC
2292	2-Methylbutyraldehyde	2-methylbutanal	CCC(C)C=O	chocolate coffee almond cocoa musty nutty malty fermented	Sigma Aldrich, TGSC
2293	(S)-2-Methylbutanal	(2S)-2-methylbutanal	CCC(C)C=O	fruity fresh cocoa coffee	TGSC
2294	1,3-Dioxane, 2-(2,4-dimethyl- 3-cyclohexen- 1-yl)-5-methyl-5-(1- methylpropyl)-	5-butan-2-yl-2-(2,4- dimethylcyclohex-3-en-1-yl)-5- methyl-1,3-dioxane	CCC(C)C1(COC(OC1)C2CCC(= CC2C)C) C	dusty woody mahogany amber resinous earthy floral dry	OdorRactor ,TGSC
2295	6-Sec-Butylquinoline	6-butan-2-ylquinoline	CCC(C)C1=CC2=C(C=C1)N=CC =C2	castoreum animal leathery earthy oakmoss vetiver	OdorRactor ,TGSC
2296	5-(Sec-Butyl)-2,3- dimethylpyrazine	5-butan-2-yl-2,3-dimethylpyrazine	CCC(C)C1=CN=C(C(=N1)C)C	nutty marine burnt roasted	Sigma Aldrich, TGSC
2297	2-Sec-Butyl-3- methoxypyrazine	2-butan-2-yl-3-methoxypyrazine	CCC(C)C1=NC=CN=C1OC	green vegetable pepper carrot earthy musty green pea galbanum bellpepper potato nutty	Sigma Aldrich, TGSC, Odoractor
2298	2-(1-Methylpropyl)thiazole	2-butan-2-yl-1,3-thiazole	CCC(C)C1=NC=CS1	chocolate green musty nutty minty vegetable pepper sulfurous herbaceous green bean spicy tomato	Sigma Aldrich, TGSC, Odoractor
2299	1-Ethynyl-2-(1- methylpropyl)cyclohexyl acetate	(2-butan-2-yl-1- ethynylcyclohexyl) acetate	CCC(C)C1CCCCC1(C#C)OC(=O)C	woody amber guaiacwood dry	OdorRactor ,TGSC
2300	2-Sec-Butylcyclohexanone	2-butan-2-ylcyclohexan-1-one	CCC(C)C1CCCCC1=0	musty green spicy minty woody	Sigma Aldrich, TGSC,
				vanilla camphoraceous fresh peppermint cooling mentholic	Odoractor
	2-(2-Butyl)-4,5-dimethyl-3-thiazoline	2-butan-2-yl-4,5-dimethyl-2,5-dihydro-1,3- thiazole	CCC(C)C1N=C(C(S1)C)C	peppermint cooling mentholic meaty spicy vegetable	OdorRactor ,TGSC
	thiazoline 5-Methylheptan-3-one oxime	dihydro-1,3- thiazole N -(5-methylheptan-3- ylidene)hydroxylamine	CCC(C)CC(=NO)CC	peppermint cooling mentholic meaty spicy vegetable leafy fig green weedy cortex galbanum	OdorRactor ,TGSC OdorRactor ,TGSC
2302	thiazoline 5-Methylheptan-3-one oxime 5-Methylheptan-3-one	dihydro-1,3- thiazole N -(5-methylheptan-3- ylidene)hydroxylamine 5-methylheptan-3-one	CCC(C)CC(=NO)CC CCC(C)CC(=O)CC	peppermint cooling mentholic meaty spicy vegetable leafy fig green weedy cortex galbanum herbaceous sweet oily	OdorRactor ,TGSC OdorRactor ,TGSC TGSC,OdoRactor
2302 2303 2304	thiazoline 5-Methylheptan-3-one oxime 5-Methylheptan-3-one 3-Methylvaleric acid	dihydro-1,3- thiazole N -(5-methylheptan-3- ylidene)hydroxylamine 5-methylheptan-3-one 3-methylpentanoic acid	CCC(C)CC(=NO)CC CCC(C)CC(=O)CC CCC(C)CC(=O)O	peppermint cooling mentholic meaty spicy vegetable leafy fig green weedy cortex galbanum herbaceous sweet oily animal sharp acidic cheese green fruity sweaty berry creamy herbaceous	OdorRactor ,TGSC OdorRactor ,TGSC TGSC,OdoRactor Sigma Aldrich, TGSC, OdoRactor
2302 2303 2304 2305	thiazoline 5-Methylheptan-3-one oxime 5-Methylheptan-3-one 3-Methylvaleric acid Ethyl 3-methylpentanoate	dihydro-1,3- thiazole N -(5-methylheptan-3- ylidene)hydroxylamine 5-methylheptan-3-one 3-methylpentanoic acid ethyl 3-methylpentanoate	CCC(C)CC(=NO)CC CCC(C)CC(=O)CC CCC(C)CC(=O)O CCC(C)CC(=O)OCC	peppermint cooling mentholic meaty spicy vegetable leafy fig green weedy cortex galbanum herbaceous sweet oily animal sharp acidic cheese green fruity sweaty berry creamy	OdorRactor ,TGSC OdorRactor ,TGSC TGSC,OdoRactor Sigma Aldrich, TGSC, OdoRactor OdorRactor ,TGSC, Flavorbase
2302 2303 2304 2305 2306	thiazoline 5-Methylheptan-3-one oxime 5-Methylheptan-3-one 3-Methylvaleric acid Ethyl 3-methylpentanoate 2,3-Dimethyl-5-(2-methylbutyl)pyrazine	dihydro-1,3- thiazole N -(5-methylheptan-3- ylidene)hydroxylamine 5-methylheptan-3-one 3-methylpentanoic acid ethyl 3-methylpentanoate 2,3-dimethyl-5-(2- methylbutyl)pyrazine	CCC(C)CC(=NO)CC CCC(C)CC(=O)CC CCC(C)CC(=O)O CCC(C)CC(=O)OCC CCC(C)CC1=CN=C(C(=N1)C)C	peppermint cooling mentholic meaty spicy vegetable leafy fig green weedy cortex galbanum herbaceous sweet oily animal sharp acidic cheese green fruity sweaty berry creamy herbaceous pineapple fruity natural tropical nutty	OdorRactor ,TGSC OdorRactor ,TGSC TGSC,OdoRactor Sigma Aldrich, TGSC, OdoRactor OdorRactor ,TGSC, Flavorbase Sigma Aldrich
2302 2303 2304 2305 2306 2307	thiazoline 5-Methylheptan-3-one oxime 5-Methylheptan-3-one 3-Methylvaleric acid Ethyl 3-methylpentanoate 2,3-Dimethyl-5-(2-	dihydro-1,3- thiazole N -(5-methylheptan-3- ylidene)hydroxylamine 5-methylheptan-3-one 3-methylpentanoic acid ethyl 3-methylpentanoate 2,3-dimethyl-5-(2-	CCC(C)CC(=NO)CC CCC(C)CC(=O)CC CCC(C)CC(=O)O CCC(C)CC(=O)OCC	peppermint cooling mentholic meaty spicy vegetable leafy fig green weedy cortex galbanum herbaceous sweet oily animal sharp acidic cheese green fruity sweaty berry creamy herbaceous pineapple fruity natural tropical nutty sour cheese linalool woody blueberry sweet	OdorRactor ,TGSC OdorRactor ,TGSC TGSC,OdoRactor Sigma Aldrich, TGSC, OdoRactor OdorRactor ,TGSC, Flavorbase
2303 2304 2305 2306 2307 2308	thiazoline 5-Methylheptan-3-one oxime 5-Methylheptan-3-one 3-Methylvaleric acid Ethyl 3-methylpentanoate 2,3-Dimethyl-5-(2-methylbutyl)pyrazine 4-Methylhexanoic acid	dihydro-1,3- thiazole N -(5-methylheptan-3- ylidene)hydroxylamine 5-methylheptan-3-one 3-methylpentanoic acid ethyl 3-methylpentanoate 2,3-dimethyl-5-(2- methylbutyl)pyrazine 4-methylhexanoic acid	CCC(C)CC(=N0)CC CCC(C)CC(=0)CC CCC(C)CC(=0)O CCC(C)CC(=0)OCC CCC(C)CC1=CN=C(C(=N1)C)C CCC(C)CCC(=0)O	peppermint cooling mentholic meaty spicy vegetable leafy fig green weedy cortex galbanum herbaceous sweet oily animal sharp acidic cheese green fruity sweaty berry creamy herbaceous pineapple fruity natural tropical nutty sour cheese	OdorRactor ,TGSC OdorRactor ,TGSC TGSC,OdoRactor Sigma Aldrich, TGSC, OdoRactor OdorRactor ,TGSC, Flavorbase Sigma Aldrich TGSC
2302 2303 2304 2305 2306 2307	thiazoline 5-Methylheptan-3-one oxime 5-Methylheptan-3-one 3-Methylvaleric acid Ethyl 3-methylpentanoate 2,3-Dimethyl-5-(2-methylbutyl)pyrazine 4-Methylhexanoic acid 3,6-Dimethyl-3-octanol	dihydro-1,3- thiazole N -(5-methylheptan-3- ylidene)hydroxylamine 5-methylheptan-3-one 3-methylpentanoic acid ethyl 3-methylpentanoate 2,3-dimethyl-5-(2- methylbutyl)pyrazine 4-methylhexanoic acid 3,6-dimethyloctan-3-ol	CCC(C)CC(=NO)CC CCC(C)CC(=O)CC CCC(C)CC(=O)O CCC(C)CC(=O)OCC CCC(C)CC1=CN=C(C(=N1)C)C CCC(C)CCC(=O)O CCC(C)CCC(=O)O	peppermint cooling mentholic meaty spicy vegetable leafy fig green weedy cortex galbanum herbaceous sweet oily animal sharp acidic cheese green fruity sweaty berry creamy herbaceous pineapple fruity natural tropical nutty sour cheese linalool woody blueberry sweet bois de rose fresh floral rose	OdorRactor ,TGSC OdorRactor ,TGSC TGSC,OdoRactor Sigma Aldrich, TGSC, OdorRactor ,TGSC, Flavorbase Sigma Aldrich TGSC OdorRactor ,TGSC

Semethylocanal Semethylocanal CCC(C)CCCCO Survey and provential TGSC					T	T
Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Sect	2312	2,6-Dimethyloctanal	2,6-dimethyloctanal	CCC(C)CCCC(C)C=O	green dry grassy weedy wax rose	TGSC
CCCC/CCCC Cocco Cocco CCCC/CCCC Cocco Cocco CCCC/CCC Cocco CCCC Cocco	2313		-			TGSC
2317 3-Modyl-1-postupal 4-methylmean 1-el CCCC/CCCO concease favor wasny found concease favor formers ToSC Coloration ToSC C	2314	8-Methyldecanal	8-methyldecanal	CCC(C)CCCCCCC=0	C	Flavorbase
Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Section Sect	2315	(S)-(+)-4-Methyl-1-hexanol	(4S)-4-methylhexan-1-ol	CCC(C)CCCO	spicy nutty green sour	TGSC
2318	2316	4-Methyl-1-hexanol	,	CCC(C)CCCO	·	,
Patternois acid, 2-methyl, 3-methylpequyl (2 p-2-methylben) CCCC/CCCC_CCC_CCC_CCCC_CCCC_CCCC_CCCC	2317	3-Methyl-1-pentanol	3-methylpentan-1-ol	CCC(C)CCO	cognac cocoa fruity fermented	
2321 Andrey hypersystemics April Spetials 1-amine CCCCCCC April Spetials April	2318	(S)-(+)-3-Methyl-1-pentanol	(3S)-3-methylpentan-1-ol	CCC(C)CCO		OdorRactor ,TGSC
2222 62-4-0-3-4-1-1-1-1-1-1-1-1-1-1-1-1-1-1-1-1-1-1	2319			CCC(C)CCOC(=O)C(=CC)C	, , , ,	TGSC
methylhutylamine		, ,			- J	
2323 2.2 2.2 2.2 2.2 2.2 2.2 2.2 2.2 2.2 2.2 2.2 2.2 2.2 2.2 2.2 2.2 2.2 2.2 2.2 2.2 2.2 2.2 2.2 2.2 2.2 2.2 2.2 2.2 2.2 2.2 2.2 2.2 2.2 2.2 2.2 2.2 2.2 2.2 2.2 2.2 2.2 2.2 2.2 2.2 2.2 2.2 2.2 2.2 2.2 2.2 2.2 2.2 2.2 2.2 2.2 2.2 2.2 2.2 2.2 2.2 2.2 2.2 2.2 2.2 2.2 2.2 2.2 2.2 2.2 2.2 2.2 2.2 2.2 2.2 2.2 2.2 2.2 2.2 2.2 2.2 2.2 2.2 2.2 2.2 2.2 2.2 2.2 2.2 2.2 2.2 2.2 2.2 2.2 2.2 2.2 2.2 2.2 2.2 2.2 2.2 2.2 2.2 2.2 2.2 2.2 2.2 2.2 2.2 2.2 2.2 2.2 2.2 2.2 2.2 2.2 2.2 2.2 2.2 2.2 2.2 2.2 2.2 2.2 2.2 2.2 2.2 2.2 2.2 2.2 2.2 2.2 2.2 2.2 2.2 2.2 2.2 2.2 2.2 2.2 2.2 2.2 2.2 2.2 2.2 2.2 2.2 2.2 2.2 2.2 2.2 2.2 2.2 2.2 2.2 2.2 2.2 2.2 2.2 2.2 2.2 2.2 2.2 2.2 2.2 2.2 2.2 2.2 2.2 2.2 2.2 2.2 2.2 2.2 2.2 2.2 2.2 2.2 2.2 2.2 2.2 2.2 2.2 2.2 2.2 2.2 2.2 2.2 2.2 2.2 2.2 2.2 2.2 2.2 2.2 2.2 2.2 2.2 2.2 2.2 2.2 2.2 2.2 2.2 2.2 2.2 2.2 2.2 2.2 2.2 2.2 2.2 2.2 2.2 2.2 2.2 2.2 2.2 2.2 2.2 2.2 2.2 2.2 2.2 2.2 2.2 2.2 2.2 2.2 2.2 2.2 2.2 2.2 2.2 2.2 2.2 2.2 2.2 2.2 2.2 2.2 2.2 2.2 2.2 2.2 2.2 2.2 2.2 2.2 2.2 2.2 2.2 2.2 2.2 2.2 2.2	2321	• .		CCC(C)CNCN=O	green fruity floral anisic	Flavorbase
2323 2-3-2-4-4-4-4-4-4-4-4-4-4-4-4-4-4-4-4-4-	2322	(S)-(-)-2-Methyl-1-butanol	(2S)-2-methylbutan-1-ol	CCC(C)CO	ethereal fresh malty	Flavornet, TGSC
Activation CCCCCCC Contemporary CCCCCCCC Contemporary CCCCCCCCC Contemporary CCCCCCCCCCC Contemporary CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC	2323	(+)-2-Methyl-1-butanol	(2R)-2-methylbutan-1-ol	CCC(C)CO		
	2324	2-Methyl-1-butanol	2-methylbutan-1-ol	CCC(C)CO		TGSC,OdoRactor
contail	2325	2-Methylbutyl acetate	2-methylbutyl acetate	CCC(C)COC(=O)C		,
2.222 2.222 2.222 2.222 2.222 2.222 2.222 2.2222 2.2222 2.2222 2.2222 2.2222 2.2222 2.2222 2.22222 2.22222 2.22222 2.22222 2.22222 2.22222 2.22222 2.22222 2.22222 2.22222 2.22222 2.22222 2.22222 2.222222 2.222222 2.222222 2.222222 2.222222 2.222222 2.222222 2.222222 2.222222 2.222222 2.222222 2.222222 2.222222 2.222222 2.222222 2.222222 2.222222 2.22222 2.222222 2.222222 2.222222 2.222222 2.222222 2.222222 2.222222 2.222222 2.222222 2.222222 2.22222 2.222222 2.22222 2.22222 2.22222 2.22222 2.22222 2.22222 2.22222 2.22222 2.22222 2.22222 2.22222 2.22222 2.22222 2.22222 2.22222 2.22222 2.22222 2.22222 2.22222 2.22222 2.22222 2.22222 2.22222 2.22222 2.22222 2.22222 2.22222 2.22222 2.22222 2.22222 2.22222 2.22222 2.22222 2.22222 2.22222 2.22222 2.22222 2.22222 2.22222 2.22222 2.22222 2.22222 2.22222 2.22222 2.22222 2.22222 2.22222 2.22222 2.22222 2.22222 2.22222 2.22222 2.22222 2.22222 2.22222 2.22222 2.22222 2.22222 2.22222 2.22222 2.22222 2.22222 2.22222 2.22222 2.22222 2.22222 2.22222 2.22222 2.22222 2.22222 2.22222 2.22222 2.22222 2.22222 2.22222 2.22222 2.22222 2.22222 2.22222 2.22222 2.22222 2.22222 2.22222 2.22222 2.22222 2.22222 2.22222 2.22222 2.22222 2.22222 2.22222 2.22222 2.22222 2.22222 2.22222 2.22222 2.22222 2.22222 2.22222 2.22222 2.22222 2.22222 2.22222 2.22222 2.22222 2.22222 2.22222 2.22222 2.22222 2.22222 2.22222 2.22222 2.22222 2.22222 2.22222 2.22222 2.22222 2.22222 2.22222 2.22222 2.22222 2.22222 2.22222 2.22222 2.22222 2.22222 2.22222 2.22222 2.22222 2.22222 2.22222 2.22222 2.22222 2.22222 2.22222 2.22222 2.22222 2.22222 2.22222 2.22222 2.22222 2.22222 2.22222 2.22222 2.22222 2.22222 2.22222	2326	2-Methylbutyl angelate		CCC(C)COC(=O)C(=CC)C	floral fruity	SuperScent, TGSC
2322 2.Methylbutyl acceptable 2.	2327	2-Methylbutyl isobutyrate		CCC(C)COC(=O)C(C)C	fruity ethereal tropical banana	1
2323 2-Methylburyl 3-methylburyl 2-methylburyl 2-hydroxybenzoate onoate ono	2328		2-methylbutyl 2-methylbutanoate	CCC(C)COC(=O)C(C)CC	11	Sigma Aldrich, TGSC,
2331 2-Methylbutyl salicylate 2-methylbutyl 2-hydroxybenzoate OCCC(C)COC(-O)CC 3 sweet fruity effected mining green halsaming	2329	2-Methylbutyl 3-methyl-2-		CCC(C)COC(=O)C=C(C)C	blackberry peely tobacco metallic	
2.34 2.4methylbutyl propionate 2-methylbutyl propaneate 2.5methylbutyl 3-methylbutanoate 2.5methylbutanoate 2.5methylbutano	2330				herbaceous woody orchid floral	TGSC
2332 2-Methylbutyl isovalerate	2331	2-Methylbutyl propionate	2-methylbutyl propanoate	-	0	OdorRactor .TGSC
2.333 2.4Methyl-1-butanethiol 2-methylbutane-1-thiol CCC(C)CS meany bloody sulfurous OdorRactor (TGSC OdoRactor CCC(C)N fish y ammonical OdorRactor (TGSC OdoRactor TGSC Pubchem CCC(C)N fish y ammonical OdorRactor (TGSC TGSC CCC(C)O fish y winey TGSC CCC(C)O fish y fish y fish y fish y fish y fish y fish y fish y fish y fish y fish y fish y fish y fish y fish y fish y fish y fish y fish y fish y fish y fish y fish y fish y fish y fish y fish y fish y fish y fish y fish y fish y fish y fish y fish y fish y fish y fish y fish y fish y fish y fish y fish y fish y fish y fish y fish y fish y fish y fish y fish y fish y fish y fish y fish y fish y fish y fish y fish y fish y fish y fish y fish y fish y fish y fish y fish y fish y fish y fish y fish y fish y fish y fish y fish y fish y fish y fish y fish y fish y fish y fish y fish y fish y fish y fish y fish y fish y fish y fish y fish y fish y fish y fish y fish y fish y fish y fish y fish y fish y fish y fish y fish y fish y fish y fish y fish y fish y fish y fish y fish y fish y fish y fish y fish y fish y fish y fish y fish y fish y fish y fish y fish y fish y fish y fish y fish y fish y fish y fish y fish y fish y fish y fish y fish y fish y fish y fish y fish y fish y fish y fish y fish y fish y fish					herbaceous fruity earthy cheese apple green peppermint scotch spearmint cherry whiskey sweaty	Sigma Aldrich, TGSC,
2335 Sec-butylamine Sec-butylamine Sec-butylamine CCC(C)N Sec-butylamine Sec-butylamine CCC(C)N Sec-butylamine Sec-butylamine CCC(C)N Sec-butylamine Sec-butylamine Sec-butylamine CCC(C)N Sec-butylamine Se	2333	2-Methyl-1-butanethiol	2-methylbutane-1-thiol	CCC(C)CS		
2336 (2R)-2-Isothiocyanatobutane (2R) -2-isothiocyanatobutane (2R) -2-isothiocyanatobutane (2R) -2-isothiocyanatobutane (2R) -2-isothiocyanatobutane (2CC(C)N=C=S green OdorRactor ,Flavorbase (2338 (S)+(+)2-Butanol (2S) -butan-2-ol CCC(C)O oily winey TGSC	2334				sulfurous meaty bloody	
See-Butyl isothiocyanate	2335	Sec-butylamine	butan-2-amine	CCC(C)N	fishy ammonical	OdorRactor ,TGSC, Pubchem
Acceptable CCC Coccord CCC CCCCOCC CCCCOCCOCC CCCCOCCOCC CCCCOCCOCC CCCCCOCCC CCCCCCCC	2336	(2R)-2-Isothiocyanatobutane	(2R)-2-isothiocyanatobutane	CCC(C)N=C=S	chemical mild pungent horseradish	OdorRactor ,Flavorbase
2340 2-Butanol	2337	Sec-Butyl isothiocyanate	2-isothiocyanatobutane	CCC(C)N=C=S	green	OdorRactor ,Flavorbase
2-Butanol Dutan-2-ol CCC(C)O winey sweet apricot fruity pleasant Flavornet, TGSC, Pubchem strong Solvent fruity banana pleasant SuperScent, TGSC					oily winey	
2341 Sec-butyl acetate butan-2-yl acetate CCC(C)OC(=O)C solvent fruity banana pleasant SuperScent, TGSC 2342 2-Ethoxybutane CCC(C)OCC berry floral woody OdorRactor, TGSC 2343 2-Butanethiol butane-2-thiol CCC(C)S sulfurous beefy poultry leek onion obnoxious skunk 2344 S-Sec-Butyl 3-methylbut-2-enthioate S-butan-2-yl 3-methylbut-2-enthioate S-butan-2-yl 3-methylbut-2-enthioate S-butan-2-yl 3-methylbut-2-enthioate S-butan-2-yl 3-methylbut-2-enthioate S-butan-2-yl 3-methylbut-2-enthioate S-butan-2-yl 3-methylbutanethioate Sigma Aldrich, CCC(C=C)OC(C)OC(C)C Sulfurous TGSC Sigma Aldrich, CTGSC Sulfurous Supersonation Sigma Aldrich, CTGSC Sulfurous Sigma Aldrich, CTGSC Sigma Aldrich, CTGSC Sigma Aldrich, CTGSC Sigma Aldrich, CCC(C=CC=CC=CCCCCCCCCCCCC)C(C=CC=CC=CC=CC=CCCCCCCC					winey sweet apricot fruity pleasant	
2342 2-Ethoxybutane 2-ethoxybutane CCC(C)OCC berry floral woody OdorRactor ,TGSC 2343 2-Butanethiol butane-2-thiol CCC(C)S sulfurous beefy poultry leek onion obnoxious skunk 2344 S-Sec-Butyl 3-methylbut-2- enethioate CCC(C)SC(=O)C=C(C)C green grassy herbaceous spicy OdorRactor ,TGSC 2345 Butanethioic acid, 3-methyl-, S-butan-2-yl 3-methylbut-2- enethioate CCC(C)SC(=O)CC(C)C green grassy herbaceous spicy OdorRactor ,TGSC 2346 Di-sec-butyl disulfide 2-(butan-2-yldisulfanyl)butane CCC(C)SSC(C)CC sulfurous butter ethereal radish chrysanthemum green horseradish pungent vegetable tropical fruity berry OdorRactor ,TGSC 2348 1-(2.6.6-Trimethyl-1- cyclohexen-1-yl)pent-1-en-3-ol [(E-)-1-(2.6.6-trimethylcyclohexen-1-yl)pent-1-en-3-yl] acetate [4-(1-acetyloxypropyl)phenyl] acetate Di-sec-butyl double acetate [4-(1-acetyloxypropyl)phenyl] acetate [4-(1-acetyloxypropyl)phenyl] acetate [4-(1-acetyloxypropyl)phenyl] acetate [4-(1-acetyloxypropyl)propan-1-ol] CCC(C=CC=CC) balsamic floral sweet Sigma Aldrich, TGSC 2350 [R)-(+)-1-Phenyl-1-propanol] [IR)-1-phenylpropan-1-ol] CCC(C=CC=CC1)OC [floral] TGSC	2341	Sec-butyl acetate	butan-2-yl acetate	CCC(C)OC(=O)C	C	SuperScent, TGSC
2-Butanethiol butane-2-thiol CCC(C)S sulfurous beefy poultry leek onion obnoxious skunk S-Sec-Butyl 3-methylbut-2- enethioate enethioate 2-345 Sec-Butyl 3-methylbut-2- enethioate 2-346 Di-sec-butyl disulfide 2-(butan-2-yl 3-methylbutanethioate) 2-(butan-2-yl 3-methylbutanethioate) S-butan-2-yl 3-methylbut-2- enethioate 2-(butan-2-yl 3-methylbutanethioate) CCC(C)SC(=O)CC(C)C spicy galbanum green herbaceous OdorRactor ,TGSC 2-346 Di-sec-butyl disulfide 2-(butan-2-yldisulfanyl)butane 2-(b		•	•			1
enethioate enethioate enethioate Butanethioic acid, 3-methyl-, S-butan-2-yl 3-methylbutanethioate 2345 Butanethioic acid, 3-methyl-, S-(1-methylpropyl) ester Butanethioic acid, 3-methyl-, S-(1-methylpropyl) ester Butanethioic acid, 3-methyl-, S-(1-methylpropyl) ester Butanethioic acid, 3-methyl-, S-(1-methylpropyl) ester Butanethioic acid, 3-methyl-, S-(1-methylpropyl) ester Butanethioic acid, 3-methyl-, S-(1-methylpropyl) ester Butanethioate CCC(C)SC(C)CC Sulfurous TGSC CCC(C=C)O Butter ethereal radish chrysanthemum green horseradish pungent vegetable tropical fruity Butanethiological fruity CCC(C=CC1=C(CCCC1(C)C)C) Butter ethereal radish Chrysanthemum green horseradish pungent vegetable tropical fruity Butanethiological fruity CCC(C=CC1=C(CCCC1(C)C)C) Butter ethereal radish Chrysanthemum green horseradish pungent vegetable tropical fruity CCC(C=CC1=C(CCCC1(C)C)C) Butter ethereal radish Chrysanthemum green horseradish pungent vegetable tropical fruity CCC(C=CC1=C(CCCC1(C)C)C) Butter ethereal radish Chrysanthemum green horseradish pungent vegetable tropical fruity CCC(C=CC1=C(CCC1(C)C)C) Butter ethereal radish Chrysanthemum green horseradish pungent vegetable tropical fruity CCC(C=CC1=C(CCC1(C)C)C) Butter ethereal radish Chrysanthemum green horseradish pungent vegetable tropical fruity CCC(C=CC1=C(CCC1(C)C)C) Butter ethereal radish Chrysanthemum green horseradish pungent vegetable tropical fruity CCC(C=CC1=C(CCC1(C)C)C) Butter ethereal radish Chrysanthemum green horseradish pungent vegetable tropical fruity CCC(C=CC1=C(CCC1(C)C)C) Butter ethereal radish Chrysanthemum green horseradish pungent vegetable tropical fruity CCC(C=CC1=C(CCC1(C)C)C) Butter ethereal radish Chrysanthemum green horseradish pungent vegetable tropical fruity CCC(C=CC1=C(CCC1(C)C)C) Butter ethereal radish Chrysanthemum green horseradish pungent vegetable tropical fruity CCC(C=CC1=C(CCC1(C)C)C) Butter ethereal radish Crysanthemum green horseradish pungent vegetable TGSC CCC(C=CC1=CC1CCC1(C)C)C Butter e	2343	2-Butanethiol	butane-2-thiol	CCC(C)S		TGSC, Flavorbase, Pubchem
S-(1- methylpropyl) ester methylbutanethioate	2344			CCC(C)SC(=O)C=C(C)C	green grassy herbaceous spicy	OdorRactor ,TGSC
2347 1-Penten-3-OL pent-1-en-3-ol CCC(C=C)O butter ethereal radish chrysanthemum green horseradish pungent vegetable tropical fruity TGSC,OdoRactor pungent vegetable tropical fruity TGSC,OdoRactor pungent vegetable tropical fruity OdorRactor,TGSC cyclohexen-1-yl)pent-1-en-3-ol CCC(C=CC1=C(CCCC1(C)C)C) fruity berry OdorRactor,TGSC cyclohexen-1-yl)pent-1-en-3-ol CCC(C=CC1=C(CCCC1(C)C)C) Derry raspberry TGSC cyclohexen-1-yl)pent-1-en-3-yl] acetate CCC(C=CC1=C(C=C1)OC(=O)C) Derry raspberry TGSC cyclohexen-1-yl)pent-1-propanol 1-phenylpropan-1-ol CCC(C1=CC=CC1)OC(=O)C) Derry raspberry TGSC cyclohexen-1-yl)pent-1-en-3-yl] acetate CCC(C1=CC=CC1)OC(=O)C Derry raspberry TGSC cyclohexen-1-yl)pent-1-en-3-yl] acetate CCC(C1=CC=CC1)OC(=O)C Derry raspberry TGSC cyclohexen-1-yl)pent-1-en-3-yl] acetate CCC(C1=CC=CC=C1)OC(=O)C Derry raspberry TGSC cyclohexen-1-yl)pent-1-en-3-yl] acetate CCC(C1=CC=C1)OC(=O)C Derry raspberry TGSC Derry raspberry TGSC Derry raspberry TGSC Derry raspberry TGSC Derry raspberry Derry raspberry TGSC Derry raspberry Derr	2345			CCC(C)SC(=0)CC(C)C	spicy galbanum green herbaceous	OdorRactor ,TGSC
2347 1-Penten-3-OL pent-1-en-3-ol CCC(C=C)O butter ethereal radish chrysanthemum green horseradish pungent vegetable tropical fruity TGSC,OdoRactor pungent vegetable tropical fruity TGSC,OdoRactor pungent vegetable tropical fruity OdorRactor,TGSC cyclohexen-1-yl)pent-1-en-3-ol CCC(C=CC1=C(CCCC1(C)C)C) fruity berry OdorRactor,TGSC cyclohexen-1-yl)pent-1-en-3-ol CCC(C=CC1=C(CCCC1(C)C)C) Derry raspberry TGSC cyclohexen-1-yl)pent-1-en-3-yl] acetate CCC(C=CC1=C(CCCC1(C)C)C) Derry raspberry TGSC cyclohexen-1-yl)pent-1-en-3-yl] acetate CCC(C=CC1=C(CCCC1(C)C)C) Derry raspberry TGSC cyclohexen-1-yl)pent-1-en-3-yl] acetate CCC(C=CC1=C(C=CC1)OC(=O)C) Derry raspberry TGSC cyclohexen-1-yl)pent-1-en-3-yl] acetate CCC(C=CC1=C(C=C1)OC(=O)C) Derry raspberry TGSC cyclohexen-1-yl)pent-1-en-3-yl] acetate CCC(C=CC1=C(C=C1)OC(=O)C) Derry raspberry TGSC cyclohexen-1-yl)pent-1-en-3-yl] acetate CCC(C=CC=CC1)OC(=O)C Derry raspberry TGSC cyclohexen-1-yl)pent-1-en-3-yl] acetate CCC(C=CC=CC1)OC(=O)C Derry raspberry TGSC cyclohexen-1-yl)pent-1-en-3-yl] acetate CCC(C=CC=CC1)OC(=O)C Derry raspberry TGSC cyclohexen-1-yl)pent-1-en-3-yl] acetate CCC(C=CC=CC=C1)OC(=O)C Derry raspberry TGSC cyclohexen-1-yl)pent-1-en-3-yl] acetate CCC(C=C=CC=C1)OC(=O)C Derry raspberry TGSC cyclohexen-1-yl)pent-1-en-3-yl] acetate CCC(C=C=CC=C1)OC(=O)C Derry raspberry TGSC cyclohexen-1-yl)pent-1-en-3-yl] acetate CCC(C=C=CC=C1)OC(=O)C Derry raspberry TGSC cyclohexen-1-yl)pent-1-en-3-yl] acetate CCC(C=C=C=C1)OC(=O)C Derry raspberry TGSC Derry ras	2346	Di-sec-butyl disulfide	2-(butan-2-yldisulfanyl)butane	CCC(C)SSC(C)CC	sulfurous	TGSC
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$					chrysanthemum green horseradish pungent vegetable	Sigma Aldrich,
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$	2348	cyclohexen-1-yl)pent-				OdorRactor ,TGSC
2350 Dihydrogalangal acetate [4-(1-acetyloxypropyl)phenyl] acetate OC(C1=CC=C(C=C1)OC(=O)C) pungent spicy TGSC 2351 1-Phenyl-1-propanol 1-phenylpropan-1-ol CCC(C1=CC=CC=C1)O balsamic floral sweet Sigma Aldrich, TGSC 2352 (R)-(+)-1-Phenyl-1-propanol (1R)-1-phenylpropan-1-ol CCC(C1=CC=CC=C1)O floral TGSC	2349	[(E)-1-(2,6,6- Trimethylcyclohexen-1-	trimethylcyclohexen-1-yl)pent-1-en-		berry raspberry	TGSC
2351 1-Phenyl-1-propanol 1-phenylpropan-1-ol CCC(C1=CC=CC1)O balsamic floral sweet Sigma Aldrich, TGSC 2352 (R)-(+)-1-Phenyl-1-propanol (1R)-1-phenylpropan-1-ol CCC(C1=CC=CC1)O floral TGSC	2350	Dihydrogalangal acetate	[4-(1-acetyloxypropyl)phenyl]		pungent spicy	TGSC
2352 (R)-(+)-1-Phenyl-1-propanol (1R)-1-phenylpropan-1-ol CCC(C1=CC=CC1)O floral TGSC		,	acetate			
2353 (S)-(-)-1-Phenyl-1-propanol (1S)-1-phenylpropan-1-ol CCC(C1=CC=CC=C1)O floral TGSC	2351				balsamic floral sweet	Sigma Aldrich, TGSC
		1-Phenyl-1-propanol	1-phenylpropan-1-ol	CCC(C1=CC=CC=C1)O		

2555 All J. J. edge (husyane) 2 edge (husyane) 2 edge (husyane) 2 edge (husyane) 2 edge (husyane) 2 edge (husyane) 2 edge (husyane) 2 edge (husyane) 2 edge (husyane) 2 edge (husyane) 2 edge (husyane) 2 edge (husyane) 2 edge (husyane) 2 edge (husyane) 2 edge (husyane) 2 edge (husyane) 2 edge (husyane) 2 edge (husyane) 2 edge (husyane) 2 edge (husyane) 2 edge (husyane) 2 edge (husyane) 2 edge (husyane) 2 edge (husyane) 2 edge (husyane) 2 edge (husyane) 2 edge (husyane) 2 edge (husyane) 2 edge (husyane) 2 edge (husyane) 2 edge (husyane) 2 edge (husyane) 2 edge (husyane) 2 edge (husyane) 2 edge (husyane) 2 edge (husyane) 2 edge (husyane) 2 edge (husyane) 2 edge (husyane) 2 edge (husyane) 2 edge (husyane) 2 edge (husyane) 2 edge (husyane) 2 edge (husyane) 2 edge (husyane) 2 edge (husyane) 2 edge (husyane) 2 edge (husyane) 2 edge (husyane) 2 edge (husyane) 2 edge (husyane) 2 edge (husyane) 2 edge (husyane) 2 edge (husyane) 2 edge (husyane) 2 edge (husyane) 2 edge (husyane) 2 edge (husyane) 2 edge (husyane) 2 edge (husyane) 2 edge (husyane) 2 edge (husyane) 2 edge (husyane) 2 edge (husyane) 2 edge (husyane) 2 edge (husyane) 2 edge (husyane) 2 edge (husyane) 2 edge (husyane) 2 edge (husyane) 2 edge (husyane) 2 edge (husyane) 2 edge (husyane) 2 edge (husyane) 2 edge (husyane) 2 edge (husyane) 2 edge (husyane) 2 edge (husyane) 2 edge (husyane) 2 edge (husyane) 2 edge (husyane) 2 edge (husyane) 2 edge (husyane) 2 edge (husyane) 2 edge (husyane) 2 edge (husyane) 2 edge (husyane) 2 edge (husyane) 2 edge (husyane) 2 edge (husyane) 2 edge (husyane) 2 edge (husyane) 2 edge (husyane) 2 edge (husyane) 2 edge (husyane) 2 edge (husyane) 2 edge (husyane) 2 edge (husyane) 2 edge (husyane) 2 edge (husyane) 2 edge (husyane) 2 edge (husyane) 2 edge (husyane) 2 edge (husyane) 2 edge (husyane) 2 edge (husyane) 2 edge (husyane	2354	Butanamide, 2-ethyl-N-methyl-N-(3- methylphenyl)-	2-ethyl-N -methyl-N -(3-methylphenyl)butanamide	CCC(CC)C(=O)N(C)C1=CC=CC(=C1)C	bitter tropical grapefruit rhubarb guava	TGSC
2505 All-Designation	2355	2-Ethylbutyric acid	2-ethylbutanoic acid	CCC(CC)C(=O)O		Sigma Aldrich
2-255 2-24(b) 2-	2356	Allyl 2-ethylbutyrate	prop-2-enyl 2-ethylbutanoate	CCC(CC)C(=O)OCC=C		
2509 24-bity-blue) aceane 2-adipt-buyl aceane 2-adipt-buyl aceane 2-adipt-buyl-aceane 2-adipt-buyl	2357	2-Ethylbutanal	2-ethylbutanal	CCC(CC)C=O	green sweet ethereal cocoa fruity	SuperScent, TGSC
2509 24-bity-blue) aceane 2-adipt-buyl aceane 2-adipt-buyl aceane 2-adipt-buyl-aceane 2-adipt-buyl	2358	2-Ethyl-1-butanol	2-ethylbutan-1-ol	CCC(CC)CO	sweet musty alcoholic	OdorRactor ,TGSC
2560 3-Postanelud postano-3-tiled CCC/CCS fails sweet behaviours only antly Patronec, TGSC						
2561 3-Pontanechiol 2001 2-Earthylo-fo-pera-3-one 4-ehylly-fo-fo-n3-one CCCICCS fishly 2-Earthylo-fo-pera-3-one CCCICCS CCCICCS fishly 2-Earthylo-fo-pera-3-one CCCICCS CCCICCS fishly 2-Earthylo-fo-pera-3-one CCCICCS CCCICCS CCCICCS CCCICCS CCCICCS Cocide Cocide Cacide Cac		. , ,	,,			
1.502 3-bisyle-6-bergean-3-one 4-estylepe-6-en-3-one CCCCCC-CCC-CDCC Code	2360	3-Pentanol	pentan-3-ol	CCC(CC)O	fruit sweet herbaceous oily nutty	Flavornet, TGSC
1836 http://doi.org/10.10.10.10.10.10.10.10.10.10.10.10.10.1	2361	3-Pentanethiol	pentane-3-thiol	CCC(CC)S		TGSC, OdoRactor
Flavorskee Flavorskee Flavorskee Flavorskee Flavorskee Flavorskee Flavorskee Flavorskee Flavorskee Flavorskee Flavorskee Flavorskee Flavorskee Flavorskee Flavorskee Flavorskee Flavorskee Flavorskee Flavorskee Flavorskee Flavorskee Flavorskee Flavorskee Flavorskee Flavorskee Flavorskee Flavorskee Flavorskee Flavorskee Flavorskee Flavorskee Flavorskee Flavorskee Flavorskee Flavorskee Flavorskee Flavorskee Flavorskee Flavorskee Flavorskee Flavorskee Flavorskee Flavorskee Flavorskee Flavorskee Flavorskee Flavorskee Flavorskee Flavorskee Flavorskee Flavorskee Flavorskee Flavorskee Flavorskee Flavorskee Flavorskee Flavorskee Flavorskee Flavorskee Flavorskee Flavorskee Flavorskee Flavorskee Flavorskee Flavorskee Flavorskee Flavorskee Flavorskee Flavorskee Flavorskee Flavorskee Flavorskee Flavorskee Flavorskee Flavorskee Flavorskee Flavorskee Flavorskee Flavorskee Flavorskee Flavorskee Flavorskee Flavorskee Flavorskee Flavorskee Flavorskee Flavorskee Flavorskee Flavorskee Flavorskee Flavorskee Flavorskee Flavorskee Flavorskee Flavorskee Flavorskee Flavorskee Flavorskee Flavorskee Flavorskee Flavorskee Flavorskee Flavorskee Flavorskee Flavorskee Flavorskee Flavorskee Flavorskee Flavorskee Flavorskee Flavorskee Flavorskee Flavorskee Flavorskee Flavorskee Flavorskee Flavorskee Flavorskee Flavorskee Flavorskee Flavorskee Flavorskee Flavorskee Flavorskee Flavorskee Flavorskee Flavorskee Flavorskee Flavorskee Flavorskee Flavorskee Flavorskee Flavorskee Flavorskee Flavorskee Flavorskee Flavorskee Flavorskee Flavorskee Flavorskee Flavorskee Flavorskee Flavorskee Flavorskee Flavorskee Flavorskee Flavorskee Flavorskee Flavorskee Flavorskee Flavorskee Flavorskee Flavorskee Flavorskee Flavorskee Flavorskee Flavorskee Fla	2362	4-Ethyl-6-hepten-3-one	4-ethylhept-6-en-3-one	CCC(CC=C)C(=O)CC	fishy	Flavornet, TGSC
2366 DSST0s_CID_5186 1-(2-2ert - minds)sycholocytlops 200 1-2ert - minds)sycholocytlops 1-2ert - minds 1-2ert -	2363	Ethyl 2-benzylbutanoate	ethyl 2-benzylbutanoate		green floral fruity sweet	
cdp1-2_6_c timenthy -	2364	1-Phenyl-2-butanol	1-phenylbutan-2-ol	CCC(CC1=CC=CC=C1)O		TGSC
dimethylethylicyclohexylloxy buspleyclohexyloxybutan-2-ol	2365			CCC(CCC1C(CCCC1(C)C)C)O	, ,	TGSC
meat bunt roasted Flavorbase 2368 DSTSx, CID, 5186 1-(1-alydroxypropoxypropau-1-ol CCCQ)OC(CC)O alcoholic OdoRactor,	2366			CCC(COC1CCCCC1C(C)(C)C)O	woody amber ambrette	OdorRactor ,TGSC
2360 DSSTox_CID_5186	2367	1,2-Butanedithiol	butane-1,2-dithiol	CCC(CS)S		
Savoyy Suffanylpropyslatfanylpropassaffanylpropassaffanylpropassaffanylpropassaffanylpropassaffanylpropassaffanylpropassaffanylpropassaffanylpropassaffanylpropassaffanylpropassaffanylpropassaffanylpropassaffanylpropassaffanylpropassaffanylpropassaffanylpropassaffanylpropassaffanylpropassaffanylpropassaffanylpropassaffanylpropassaffanylpropassaffanylpropassaffanylpropassaffanylpropassaffanylpropassaffanylpropassaffanylpropassaffanylpropassaffanylpropassaffanylpropassaffanylpropassaffanylpropassaffanylpropassaffanylpropassaffanylpropassaffanylpropassaffanylpropassaffanylpropassaffanylpropassaffanylpropassaffanylpropassaffanylpropassaffanylpropassaffanylpropassaffanylpropassaffanylpropassaffanylpropassaffanylpropassaffanylpropassaffanylpropassaffanylpropassaffanylpropassaffanylpropassaffanylpropassaffanylpropassaffanylpropassaffanylpropassaffanylpropassaffanylpropassaffanylpropassaffanylpropassaffanylpropassaffanylpropassaffanylpropassaffanylpropassaffanylpropassaffanylpropassaffanylpropassaffanylpropassaffanylpropassaffanylpropassaffanylpropassaffanylpropassaffanylpropassaffanylpropassaffanylpropassaffanylpropassaffanylpropassaffanylpropassaffanylpropassaffanylpropassaffanylpropassaffanylpropassaffanylpropassaffanylpropassaffanylpropassaffanylpropassaffanylpropassaffanylpropassaffanylpropassaffanylpropassaffanylpropassaffanylpropassaffanylpropassaffanylpropassaffanylpropassaffanylpropassaffanylpropassaffanylpropassaffanylpropassaffanylpropassaffanylpropassaffanylpropassaffanylpropassaffanylpropassaffanylpropassaffanylpropassaffanylpropassaffanylpropassaffanylpropassaffanylpropassaffanylpropassaffanylpropassaffanylpropassaffanylpropassaffanylpropassaffanylpropassaffanylpropassaffanylpropassaffanylpropassaffanylpropassaffanylpropassaffanylpropassaffanylpropassaffanylpropassaffanylpropassaffanylpropassaffanylpropassaffanylpropassaffanylpropassaffanylpropassaffanylpropassaffanylpropassaffanylpropassaffanylpropassaffanylpropassaffanylpropassaffanylpropassaffanylpropassaffanylpropassaffanylpropassaffanylpropassaffanylp	2368	DSSTox_CID_5186	1-(1-hydroxypropoxy)propan-1-ol	CCC(O)OC(CC)O		
Suffanylpropylsalifanylpropylsalifanylpropylsalifanylpropylsalifanylpropylsalifanylpropylsalifanylpropylsalifanylpropylsalifanylpropylsalifanylpropylsalifanylpropylsalifanylpropylsalifanylpropane-1 fibiol fibiol fibiol fibiol fibiol fibiol fibiol fibiol fibiol fibiol fibiol fibiol fibiol fibiol fibiol fibiol fibiol fibiol fibiol fibiol fibiol fibiol fibiol fibiol fibiol fibiol fibiol fibiol fibiol fibiol fibiol fibiol fibiol fibiol fibiol fibiol fibiol fibiol fibiol fibiol fibiol fibiol fibiol fibiol fibiol fibiol fibiol fibiol fibiol fibiol fibiol fibiol fibiol fibiol fibiol fibiol fibiol fibiol fibiol fibiol fibiol fibiol fibiol fibiol fibiol fibiol fibiol fibiol fibiol fibiol fibiol fibiol fibiol fibiol fibiol fibiol fibiol fibiol fibiol fibiol fibiol fibiol fibiol fibiol fibiol fibiol fibiol fibiol fibiol fibiol fibiol fibiol fibiol fibiol fibiol fibiol fibiol fibiol fibiol fibiol fibiol fibiol fibiol fibiol fibiol fibiol fibiol fibiol fibiol fibiol fibiol fibiol fibiol fibiol fibiol fibiol fibiol fibiol fibiol fibiol fibiol fibiol fibiol fibiol fibiol fibiol fibiol fibiol fibiol fibiol fibiol fibiol fibiol fibiol fibiol fibiol fibiol fibiol fibiol fibiol fibiol fibiol fibiol fibiol fibiol fibiol fibiol fibiol fibiol fibiol fibiol fibiol fibiol fibiol fibiol fibiol fibiol fibiol fibiol fibiol fibiol fibiol fibiol fibiol fibiol fibiol fibiol fibiol fibiol fibiol fibiol fibiol fibiol fibiol fibiol fibiol fibiol fibiol fibiol fibiol fibiol fibiol fibiol fibiol fibiol fibiol fibiol fibiol fibiol fibiol fibiol fibiol fibiol fibiol fibiol fibiol fibiol fibiol fibiol fibiol fibiol fibiol fibiol fibiol fibiol fibiol fibiol fibiol fibiol fibiol fibiol fibiol fibiol fibiol fibiol fibiol fibiol fibiol fibiol fibiol fibiol fibiol fibiol fibiol fibiol fibiol fibiol fibiol fibiol fibiol fibiol fibiol fibiol fibiol fibiol fibiol fibiol fibiol fibiol fibiol fibiol fibiol fibiol fibiol fibiol fibiol fibiol fibiol fibiol fibiol fibiol fibiol fibiol fibiol fibiol fibiol fibiol fibiol fibiol fibiol fibiol fibiol fibiol fibiol	2369	1,1-Propanedithiol	propane-1,1-dithiol	CCC(S)S		TGSC
ceal 2-y-liprop-2-enal CCO CCC-C(C)C(C)O) acidic dry sweaty strawberry woody fruity jammy sour woody fruity jammy sour CCC-C(C)C(C)O)O acidic dry sweaty strawberry woody fruity jammy sour to Sigma Aldrich, Flavomet, ToSC. OdoRactor delty lesser commendation acid, 2-pentenoic acid, 2-pentenoic acid, 2-pentenoic acid, 2-pentenoic acid, 2-pentenoic acid, 2-pentenoic acid, 2-pentenoic acid, 2-pentenoic acid, 2-pentenoic acid, 2-pentenoic acid, 2-pentenoic acid, 2-pentenoic acid, 2-pentenoic acid, 2-pentenoic acid, 2-pentenoic acid, 2-pentenoic acid, 2-pentenoic acid, 2-pentenoic acid, 2-pentenoic acid, 2-pentenoic acid, 2-pentenoic acid, 2-pentenoic acid, 2-pentenoic acid, 2-pentenoic acid, 2-pentenoic acid, 2-pentenoic acid, 2-pentenoic acid, 2-pentenoic acid, 2-pentenoic acid, 2-pentenoic acid, 2-pentenoic acid, 2-pentenoic acid, 2-pentenoic acid, 2-pentenoic acid, 2-pentenoic acid, 2-pentenoic acid, 2-pentenoic acid, 2-pentenoic acid, 2-pentenoic acid, 2-pentenoic acid, 2-pentenoic acid, 2-pentenoic acid, 2-pentenoic acid, 2-pentenoic acid, 2-pentenoic acid, 2-pentenoic acid, 2-pentenoic acid, 2-pentenoic acid, 2-pentenoic acid, 2-pentenoic acid, 2-pentenoic acid, 2-pentenoic acid, 2-pentenoic acid, 2-pentenoic acid, 2-pentenoic acid, 2-pentenoic acid, 2-pentenoic acid, 2-pentenoic acid, 2-pentenoic acid, 2-pentenoic acid, 2-pentenoic acid, 2-pentenoic acid, 2-pentenoic acid, 2-pentenoic acid, 2-pentenoic acid, 2-pentenoic acid, 2-pentenoic acid, 2-pentenoic acid, 2-pentenoic acid, 2-pentenoic acid, 2-pentenoic acid, 2-pentenoic acid, 2-pentenoic acid, 2-pentenoic acid, 2-pentenoic acid, 2-pentenoic acid, 2-pentenoic acid, 2-pentenoic acid, 2-pentenoic acid, 2-pentenoic acid, 2-pentenoic acid, 2-pentenoic acid, 2-pentenoic acid, 2-pentenoic acid, 2-pentenoic acid, 2-pentenoic acid, 2-pentenoic acid, 2-pentenoic acid, 2-pentenoic acid, 2-pentenoic acid, 2-pentenoic acid, 2-pentenoic acid, 2-pentenoic acid, 2-pentenoic acid, 2-pentenoic acid, 2-pentenoic acid, 2-pentenoic acid, 2-pentenoic acid, 2-pentenoic acid,	2370	Sulfanylpropylsulfanyl)propa ne-1-thiol	sulfanylpropylsulfanyl)propane-1-	CCC(S)SC(CC)S	• 0	TGSC
woody fruity jammy sour acidic dry sweety strawberry Sigma Aldrich, Flavomet, TGSC 2379 2-Pentenoic acid, 2-methyl-, ethyl (E)-2-methylpent-2-enoate CCC=C(C)C(=O)OCC fruity berry runnny jammy sweet TGSC OdoRactor TGSC CdoRactor TGSC	2371				metallic	Flavornet, TGSC
Pentenoic acid, 2-methyl-, ethyl (E)-2-methylpent-2-enoate chyl ester CCC-C(C)C(C)-O)OCC fruity jammy sweet OdorRactor, TGSC CodoRactor CCC-C(C)C(C)-O)OCC fruity perny runmy jammy sweet OdorRactor, TGSC CodoRactor CCC-C(C)C(C)-O CodoRactor CCC-C(C)-O CodoRactor CCC-C(C)-C(C)-C(C)-C(C)-C(C)-C(C)-C(C)-				CCC=C(C)C(=0)O	woody fruity jammy sour	·
ethyl ester	2373	2-Methyl-2-pentenoic acid		CCC=C(C)C(=O)O		
cccccccccccccccccccccccccccccccccccc		ethyl ester				·
2-Penten-1-ol, 2-methyl- acetate CCC=C(C)COC(=O)C pear melon banana fruity TGSC				, ,	ripe aldehydic	OdoRactor
acetate acetate acetate acetate (E)-2-phenyl-pent-2-enal CCC=C(C=O)C1=CC=CCC=C1 floral hyacinth green narcissus foliage radish honey sweetpea (E)-2-phenyl-pent-2-enal CCC=C1C2=CC=CC=CC=CC=CO)O celery sweet lovage maple herbaceous floral sweet horage maple herbaceous floral sweet herbaceous floral sweet herbaceous floral sweet herbaceous floral sweet herbaceous floral sweet herbaceous floral sweet herbaceous clery maple fenugreek sweet lovage brown vegetable acidic cheese feta cheese buttery rancid sour fatty pungent (E)-pent-2-enoic acid (E)-pent-2-enoic acid (CC=CC=CC=CC=O)O acidic cheese feta cheese buttery rancid sour fatty pungent GAB (EE)-3,5-Octadien-2-one octa-3,5-dien-2-one CCC=CC=CC=O)C fatty fruity hay green herbaceous floral sweet herbaceous floral sweet herbaceous floral sweet herbaceous condition from the flavormet, TGSC flavormet, TGSC (SZ, 4Z)-bepta-2,4-dienal CCC=CC=CC=CC=O)C fruity fatty mushroom Flavormet, TGSC green cucumber melon aldehydic OdorRactor, TGSC 2385 Nona-2,4,6-trienal (2E, 4E)-hepta-2,4-dienal CCC=CC=CC=O fired pungent fruity spicy citrus greasy rancid rancid fish (E)-pent-2-enal (CC=CC=CC=O) fired flavormet, TGSC flavormet, TGSC pungent fruity spicy citrus greasy rancid rancid fish (E)-pent-2-dien-1-ol (CC=CC=CCO) green flavormet, TGSC flavormet, TGSC pungent fruity spicy citrus greasy rancid rancid fish flavormet, TGSC flavormet, TGSC flavormet, TGSC pungent fruity spicy citrus greasy rancid rancid fish flavormet, TGSC flavormet, TGSC flavormet, TGSC pungent fruity spicy citrus greasy rancid rancid fish flavormet, TGSC flavormet, TGSC flavormet, TGSC flavormet, TGSC flavormet, TGSC flavormet, TGSC flavormet, TGSC flavormet, TGSC flavormet, TGSC flavormet, TGSC flavormet, TGSC flavormet, TGSC flavormet, TGSC flavormet, TGSC flavormet, TGSC flavormet, TGSC flavormet, TGSC flavormet, TGSC flavormet, TGSC flavormet, TGSC flavormet, TGSC flavormet, TGSC flavormet, TGSC flavormet, TGSC flavormet, TGSC flavormet, TGSC flavormet, TGSC flavormet, TGSC flavormet, TGSC flavormet, TGSC fla		7.1		CCC=C(C)C=O		
Same Aldrich, TGSC	2377			CCC=C(C)COC(=0)C	pear melon banana fruity	TGSC
isobenzofuranone 1-one 1 herbaceous brown vegetable Sigma Aldrich, TGSC Sproyylidene-2-benzofuran-1-one 1 herbaceous brown vegetable Sproyylidene-2-benzofuran-1-one 1 Sproyylidene-2-benzofuran-1-one 1 Sproyylidene-2-benzofuran-1-one 1 Sproyylidene-2-benzofuran-1-one 1 Sproyylidene-2-benzofuran-1-one 1 Sproyylidene-2-benzofuran-1-one CCC=CCC=CC=CC=COO Sproyy woody herbaceous clery maple fenugreek sweet lovage brown vegetable Sigma Aldrich, TGSC Sproyylidene-2-one CCC=CCC=CC=COO Sproyylidene-2-one Sigma Aldrich, TGSC, OdoRactor CCC=CC=CC=COO Sproyylidene-2-one CCC=CC=CC=CC=COO Sproyylidene-2-one CCC=CC=CC=CC=CC=CC=CC=CC=CC=CC=CC=CC=CC	2378	2-Phenyl-2-pentenal		, ,		TGSC
propylidene- 2381 2-Pentenoic acid (E)-pent-2-enoic acid (CC=CC(=O)O acidic cheese feta cheese buttery rancid sour fatty pungent (DoRactor acidic cheese feta cheese buttery rancid sour fatty pungent (DoRactor acidic cheese feta cheese buttery rancid sour fatty pungent (DoRactor acidic cheese feta cheese buttery rancid sour fatty pungent (DoRactor acidic cheese feta cheese buttery rancid sour fatty pungent (DoRactor acidic cheese feta cheese buttery rancid sour fatty pungent (DoRactor acidic cheese feta cheese buttery rancid sour fatty pungent (DoRactor acidic cheese feta cheese buttery rancid sour fatty pungent (DoRactor acidic cheese feta cheese buttery rancid sour fatty pungent (DoRactor acidic cheese feta cheese buttery rancid sour fatty pungent (DoRactor acidic cheese feta cheese buttery rancid sour fatty pungent (DoRactor acidic fatty fruity hay green herbaceous (DoRactor acidic fatty fruity fatty mushroom plants) (DoRactor acidic fatty hazelnut nutty green plastic preen oily aldehydic vegetable pungent fruity spicy citrus greasy rancid rancid fish pungent fruity spicy citrus greasy rancid rancid fish (E.Z)-2.4-Heptadienal (DoRactor acidic fatty fatty hazelnut nutty preen oily aldehydic vegetable pungent fruity spicy citrus greasy rancid rancid fish pungent fruity spicy citrus greasy rancid rancid fish pungent fruity spicy citrus greasy rancid rancid fish pungent fruity acid pungent fruity acid pungent fruity acid pungent fruity acid pungent fruity acid pungent fruity acid pungent fruity cheese fruity pungent fruity orange tomato pungent fruity orange tomato pungent fruity orange tomato pungent fruity orange tomato pungent fruity orange tomato pungent fruity orange tomato pungent fruity orange tomato pungent fruity orange tomato pungent fruity orange tomato pungent fruity orange tomato pungent fruity orange tomato pungent fruity orange tomato pungent fruity orange tomat	2379		1-one	1	3 0 1	OdorRactor,
rancid sour fatty pungent OdoRactor 2382 3,5-Octadiene-2-one octa-3,5-dien-2-one CCC=CC=CC(=O)C fatty fruity hay green herbaceous TGSC 2383 (E,E)-3,5-Octadien-2-one (3E,5E)-octa-1,3,5-dien-2-one CCC=CC=CC(=O)C fruity fatty mushroom Flavornet, TGSC Flavornet, TGSC Green plastic Flavornet, TGSC CCC=CC=CC=CC green plastic Flavornet, TGSC OdorRactor, TGSC CCC=CC=CC=CC green cucumber melon aldehydic OdorRactor, TGSC CCC=CC=CC=O cinnamyl fatty hazelnut nutty green oily aldehydic vegetable pungent fruity spicy citrus greasy rancid rancid fish CCC=CC=CC=O fishy (2E,4E)-hepta-2,4-dienal CCC=CC=CC=O fried Sigma Aldrich, Flavornet, TGSC, Flavorbase, OdoRactor CCC=CC=CC=O firity fatty mushroom Flavornet, TGSC CCC=CC=CC=O fishy CCC=CC=CC=O fishy CCC=CC=CC=O fried Flavornet, TGSC CCC=CC=CC=O fried Flavornet, TGSC CCC=CC=CC=O fatty cheese nutty almond TGSC SuperScent, TGSC, Odoractor CCC=CC=CC=CC 2390 Hepta-2,4-dien-1-ol (E)-pent-2-enal CCC=CC=CC pungent fruity orange tomato apple green vegetable strawberry Sigma Aldrich, TGSC, OdoRactor CCC=CCC=CC OdoRactor CCC=CCC=CC CCC=CCC=CC CCC=CCC=CCC=C	2380	. ,	3-propylidene-2-benzofuran-1-one	CCC=C1C2=CC=C2C(=0)0 1	sweet herbaceous celery maple fenugreek sweet	Sigma Aldrich, TGSC
2383 (E,E)-3,5-Octadien-2-one (3E,5E)-octa-3,5-dien-2-one CCC=CC=CC green plastic Flavornet, TGSC 2384 1,3,5-Octatriene (3E,5E)-octa-1,3,5-triene CCC=CC=CC green plastic Flavornet, TGSC 2385 Nona-2,4,6-trienal (2Z,4Z,6Z)-nona-2,4,6-trienal CCC=CC=CC=O green cucumber melon aldehydic OdorRactor, TGSC 2386 2,4-Heptadienal (2E,4E)-hepta-2,4-dienal CCC=CC=CC=O cinnamyl fatty hazelnut nutty green oily aldehydic vegetable pungent fruity spicy citrus greasy rancid rancid fish 2387 2,4-Heptadienal (2E,4E)-hepta-2,4-dienal CCC=CC=CC=O fried Flavornet, TGSC 2389 2,4-Heptadienal (2E,4Z)-hepta-2,4-dienal CCC=CC=CC=O fried Flavornet, TGSC 2389 2,4-Heptadienal (2E,4Z)-hepta-2,4-dien-1-ol CCC=CC=CCO green fatty cheese nutty almond TGSC 2390 Hepta-2,4-dien-1-ol (2E,4E)-hepta-2,4-dien-1-ol CCC=CC=CCO green fatty nutty cheese fruity SuperScent, TGSC, Odoractor 2391 2-Pentenal (E)-pent-2-enal CCC=CC=O pungent fruity orange tomato apple green vegetable strawberry OdorRactor, TGSC, OdoRactor 2392 1,5-Octadien-3-one (5E)-octa-1,5-dien-3-one CCC=CCC(=O)C=C earthy musty	2381	2-Pentenoic acid	(E)-pent-2-enoic acid	CCC=CC(=O)O	-	
2384 1,3,5-Octatriene (3E,5E)-octa-1,3,5-triene CCC=CC=CC green plastic Flavornet, TGSC	2382	3,5-Octadiene-2-one	octa-3,5-dien-2-one	CCC=CC=CC(=O)C	fatty fruity hay green herbaceous	TGSC
2385 Nona-2,4,6-trienal (2Z ,4Z ,6Z)-nona-2,4,6-trienal CCC=CC=CC=O green cucumber melon aldehydic OdorRactor ,TGSC	2383	(E,E)-3,5-Octadien-2-one	(3E ,5E)-octa-3,5-dien-2-one	CCC=CC=CC(=O)C	fruity fatty mushroom	Flavornet, TGSC
2386 2,4-Heptadienal (2E ,4E)-hepta-2,4-dienal CCC=CC=CC=O cinnamyl fatty hazelnut nutty green oily aldehydic vegetable pungent fruity spicy citrus greasy rancid rancid fish 2387 2,4-Heptadienal (2E ,4E)-hepta-2,4-dienal CCC=CC=CC=O fishy 2388 (E,Z)-2,4-Heptadienal (2E ,4Z)-hepta-2,4-dienal CCC=CC=CC=O fried Flavornet, TGSC 2389 2,4-Heptadien-1-ol, (E,Z)- hepta-2,4-dien-1-ol CCC=CCCCO fatty cheese nutty almond TGSC 2390 Hepta-2,4-dien-1-ol (2E,4E)-hepta-2,4-dien-1-ol CCC=CCCCO green fatty nutty cheese fruity SuperScent, TGSC, Odoractor 2391 2-Pentenal (E)-pent-2-enal CCC=CC=O pungent fruity orange tomato apple green vegetable strawberry OdoRactor CCC=CCC=CCCO earthy musty OdorRactor, TGSC, Odoractor, TGSC, Odoractor CCC=CCC=CCO CCC=CCCO CCCC=CCCO CCCC=CCCO CCCC=CCCO CCCC=CCCO CCCC=CCCC=CCCO CCCC=CCCC=CCCC=CCCC=CCCC=CCCC=CCCC=CCCC=CCCC	2384	1,3,5-Octatriene		CCC=CC=CC=C	green plastic	Flavornet, TGSC
green oily aldehydic vegetable pungent fruity spicy citrus greasy rancid rancid fish 2387 2,4-Heptadienal (2E ,4E)-hepta-2,4-dienal CCC=CC=CC=O fishy 2388 (E,Z)-2,4-Heptadienal (2E ,4Z)-hepta-2,4-dienal CCC=CC=CC=O fried Flavornet, TGSC 2389 2,4-Heptadien-1-ol, (E,Z)- hepta-2,4-dien-1-ol CCC=CCCCO fatty cheese nutty almond TGSC 2390 Hepta-2,4-dien-1-ol (2E,4E)-hepta-2,4-dien-1-ol CCC=CCCO green fatty nutty cheese fruity SuperScent, TGSC, Odoractor 2391 2-Pentenal (E)-pent-2-enal CCC=CC=O pungent fruity orange tomato apple green vegetable strawberry OdoRactor 2392 1,5-Octadien-3-one (5E)-octa-1,5-dien-3-one CCC=CCC(=O)C=C earthy musty OdorRactor, TGSC,						·
2388 (E,Z)-2,4-Heptadienal (2E, 4Z)-hepta-2,4-dienal CCC=CC=CC fried Flavornet, TGSC 2389 2,4-Heptadien-1-ol, (E,Z)-hepta-2,4-dien-1-ol CCC=CCCC fatty cheese nutty almond TGSC 2390 Hepta-2,4-dien-1-ol (2E,4E)-hepta-2,4-dien-1-ol CCC=CCCO green fatty nutty cheese fruity SuperScent, TGSC, Odoractor 2391 2-Pentenal (E)-pent-2-enal CCC=CC=O pungent fruity orange tomato apple green vegetable strawberry OdoRactor 2392 1,5-Octadien-3-one (5E)-octa-1,5-dien-3-one CCC=CCC(=O)C=C earthy musty OdorRactor, TGSC,		_			green oily aldehydic vegetable pungent fruity spicy citrus greasy rancid rancid fish	TGSC, Flavorbase,
2389 2,4-Heptadien-1-ol, (E,Z)- hepta-2,4-dien-1-ol CCC=CCCO fatty cheese nutty almond TGSC 2390 Hepta-2,4-dien-1-ol (2E,4E)-hepta-2,4-dien-1-ol CCC=CCO green fatty nutty cheese fruity SuperScent, TGSC, Odoractor 2391 2-Pentenal (E)-pent-2-enal CCC=CCO pungent fruity orange tomato apple green vegetable strawberry OdorRactor 2392 1,5-Octadien-3-one (5E)-octa-1,5-dien-3-one CCC=CCC(=O)C=C earthy musty OdorRactor, TGSC,					-	
2390 Hepta-2,4-dien-1-ol (2E,4E)-hepta-2,4-dien-1-ol CCC=CCO green fatty nutty cheese fruity SuperScent, TGSC, Odoractor 2391 2-Pentenal (E)-pent-2-enal CCC=CCO pungent fruity orange tomato apple green vegetable strawberry Sigma Aldrich, TGSC, OdoRactor 2392 1,5-Octadien-3-one (5E)-octa-1,5-dien-3-one CCC=CCC(=O)C=C earthy musty OdorRactor, TGSC,			•			
2391 2-Pentenal (E)-pent-2-enal CCC=CC=O pungent fruity orange tomato apple green vegetable strawberry OdoRactor 2392 1,5-Octadien-3-one (5E)-octa-1,5-dien-3-one CCC=CCC(=O)C=C earthy musty OdorRactor, TGSC,		•	*			SuperScent, TGSC,
	2391	2-Pentenal	(E)-pent-2-enal	CCC=CC=O		Sigma Aldrich, TGSC,
ITIarra ··· · · ·	2392	1,5-Octadien-3-one	(5E)-octa-1,5-dien-3-one	CCC=CCC(=0)C=C	earthy musty	OdorRactor ,TGSC, Flavornet

2302	(7)-1 5-Octodian 3 and	(5Z)-octa-1,5-dien-3-one	CCC=CCC(=O)C=C	geranium metallic green	Flavornet, TGSC
2393 2394	(Z)-1,5-Octadien-3-one 3-Hexenoic acid	(5Z)-octa-1,5-dien-3-one (E)-hex-3-enoic acid	CCC=CCC(=0)C=C CCC=CCC(=0)0	cheese fruity honey acidic green	Sigma Aldrich, TGSC,
		,	` ′	dairy wax powerful	OdoRactor
2395	cis-3-Hexenoic acid	(Z)-hex-3-enoic acid	CCC=CCC(=0)0	fruity green grassy sweaty cheese acidic	ADB, TGSC, OdoRactor
2396	Methyl (Z)-3-hexenoate	methyl (Z)-hex-3-enoate	CCC=CCC(=0)OC	floral fruity	TGSC
2397		methyl (E)-hex-3-enoate	CCC=CCC(=0)OC	green honey fruity hyacinth cortex papaya guava pineapple tropical sharp sweet fresh apple pear floral earthy estery	Sigma Aldrich, TGSC, OdoRactor
2398	Ethyl 3-hexenoate	ethyl (E)-hex-3-enoate	CCC=CCC(=O)OCC	sweet metallic fresh fruity green passion fruit guava pineapple papaya weedy honey	Sigma Aldrich, TGSC, Flavorbase
2399	Ethyl (E)-3-hexenoate	ethyl (Z)-hex-3-enoate	CCC=CCC(=0)OCC	tropical green pear apple	OdorRactor ,TGSC
2400		[(Z)-hept-4-en-2-yl] 2- hydroxybenzoate	CCC=CCC(C)OC(=0)C1=CC=C C=C1O	floral green lily muguet	TGSC
2401	Octa-1,5-dien-3-ol	(5E)-octa-1,5-dien-3-ol	CCC=CCC(C=C)O	earthy	OdorRactor ,TGSC
2402	1,5-Octadien-3-ol, (E)-	octa-1,5-dien-3-ol	CCC=CCC(C=C)O	earthy herbaceous mushroom geranium leafy green marine	Flavornet, TGSC
2403	1,5Z-Octadien-3-ol	(5Z)-octa-1,5-dien-3-ol	CCC=CCC(C=C)O	green marine mushroom metallic	OdorRactor ,TGSC
2404	3-Hexene, 1,1-dimethoxy-, (3Z)-	(Z)-1,1-dimethoxyhex-3-ene	CCC=CCC(OC)OC	fruity apple	OdorRactor ,TGSC
2405	(Z)-1,1-Diethoxyhex-3-ene	(Z)-1,1-diethoxyhex-3-ene	CCC=CCC(OCC)OCC	green natural apple juicy	OdorRactor ,TGSC
	Ethyl 2,4,7-decatrienoate	ethyl (2E,4E,7E)-deca-2,4,7-trienoate	CCC=CCC=CC(=0)OCC	mild fatty pear green	OdorRactor ,TGSC, Flavorbase
2407	(2e,4e,7z)-2,4,7-Decatrienal	(2E ,4E ,7Z)-deca-2,4,7-trienal	CCC=CCC=CC=O	green citrus	OdorRactor ,TGSC, Flavorbase
2408	2,4,7-Decatrienal	(2E ,4E ,7E)-deca-2,4,7-trienal	CCC=CCC=CC=CC=O	green citrus oily fatty fishy	OdorRactor ,TGSC, Flavorbase
2409	8,11,14-Heptadecatrienal	heptadeca-8,11,14-trienal	CCC=CCC=CCC=CCCCCCC=	seaweed	TGSC
2410	9,12,15-Octadecatrienoic	methyl octadeca-9,12,15-trienoate	CCC=CCC=CCC=CCCCCCCC(oily fruity fatty	OdorRactor ,TGSC
2410	9,12,15-Octadecatrienoic acid, methyl ester, (9Z,12Z,15Z)-	memyi octadeca-9,12,15-trienoate	=0)0C	iony rrunty ranty	Ouorkactor, rGSC
2411	Ethyl linolenate	ethyl (9Z,12Z,15Z)-octadeca- 9,12,15-trienoate	CCC=CCC=CCC=CCCCCCCC(=0)OC	mild oily fatty	Flavorbase
2412	(3Z,6Z)-3,6-Nonadienal	(3Z ,6Z)-nona-3,6-dienal	CCC=CCC=CCC=O	fatty soapy cucumber	TGSC
2413	Tuberose lactone	5-[(2Z ,5Z)-octa-2,5- dienyl]oxolan-2-one	CCC=CCC=CCC1CCC(=0)01	spicy herbaceous	TGSC
2414	Deca-4,7-dienal	deca-4,7-dienal	CCC=CCC=CCCC=O	citrus aldehydic tangerine	TGSC
2415	(3E,6Z)-3,6-Nonadien-1-ol	(3E ,6Z)-nona-3,6-dien-1-ol	CCC=CCC=CCCO	fishy fatty raw green cucumber bellpepper fruity watermelon sweet wax fresh melon pear apple banana	Flavornet, TGSC, Flavorbase
2416	(3Z,6Z)-3,6-Nonadien-1-ol	(3Z ,6Z)-nona-3,6-dien-1-ol	CCC=CCC=CCCO	fresh watermelon green sweet cucumber melon honeydew wax oily vegetable	OdorRactor ,TGSC, Flavorbase
2417	trans,cis-3,6-Nonadien-1-ol	(3E,6E)-nona-3,6-dien-1-ol	CCC=CCC=CCCO	green fresh violet cucumber fatty oily mushroom fishy melon watermelon chicken	OdorRactor ,TGSC, Flavorbase
2418	Nona-3,6-dienyl acetate	[(3E,6E)-nona-3,6-dienyl] acetate	CCC=CCC=CCCOC(=O)C	sweet wax fresh green melon fruity pear cucumber	OdorRactor ,TGSC, Flavorbase
2419	3,6-Nonadien-1-ol, acetate, (3E,6Z)-	[(3E,6Z)-nona-3,6-dienyl] acetate	CCC=CCC=CCCOC(=O)C	sweet wax green melon fruity pear fresh	OdorRactor ,TGSC, Flavorbase
2420	cis-3-Hexenal	(Z)-hex-3-enal	CCC=CCC=0	apple grape green lilac orange vegetable pear pineapple strawberry fatty grassy weedy fruity strong green tomato pungent	Sigma Aldrich, TGSC, Flavorbase, Pubchem
2421	3-Hexenal	(E)-hex-3-enal	CCC=CCC=0	leafy green tomato melon apple sharp vegetable tropical natural fruity strong pungent	OdorRactor ,TGSC, Flavorbase
2422	Isojasmone	2-methyl-3-[(E)-pent-2-enyl]cyclopent-2-en-1-one	CCC=CCC1=C(C(=0)CC1)C	sweet herbaceous jasmine wax lactonic floral fruity creamy spicy	OdorRactor ,TGSC, Flavorbase
2423	Jasmone	3-methyl-2-[(Z)-pent-2-enyl]cyclopent-2-en-1-one	CCC=CCC1=C(CCC1=O)C	jasmine fruity woody herbaceous floral spicy celery citrus	Sigma Aldrich, TGSC, Flavorbase, Pubchem, OdoRactor
2424	(E)-Jasmone	3-methyl-2-[(E)-pent-2-enyl]cyclopent-2-en-1-one	CCC=CCC1=C(CCC1=O)C	mushroom fungal jasmine	TGSC, Pubchem
2425	Cyclopentaneacetic acid, 3- oxo-trans-2-(cis- 2-pentenyl), methyl ester	methyl 2-[(1R, 2R)-3-oxo-2-[(E	CCC=CCC1C(CCC1=O)CC(=O) OC	floral fresh oily wax fruity green sweet petal magnolia	TGSC
2426	Methyl jasmonate	methyl 2-[$(1R,2R)$ -3-oxo-2-[(Z) -pent-2- enyl]cyclopentyl]acetate	CCC=CCC1C(CCC1=0)CC(=0) OC	floral fresh petal magnolia oily wax sweet fruity green jasmine sharp	Flavornet, TGSC, Pubchem, OdoRactor

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2427	Cyclopentaneacetic acid, 3- oxo-2-(2- pentenyl)-, methyl ester	methyl 2-(3-oxo-2-pent-2- enylcyclopentyl)acetate	CCC=CCC1C(CCC1=O)CC(=O) OC	floral jasmine oily green greasy petal soft sharp penetrating	SuperScent, TGSC, Pubchem, OdoRactor
2428	Methyl {3-oxo-2-[(2Z)-pent-2-en-1-yl]cyclopentyl}acetate	methyl 2-[3-oxo-2-[(Z)-pent-2-enyl]cyclopentyl]acetate	CCC=CCC1C(CCC1=O)CC(=O) OC	floral jasmine sharp persistent	OdorRactor ,TGSC, Pubchem
2429	Methyl 2-(3-oxo-2-(pent-2-en- 1- yl)cyclopentyl)acetate	methyl 2-[3-oxo-2-[(E)-pent-2-enyl]cyclopentyl]acetate	CCC=CCC1C(CCC1=0)CC(=0) OC	jasmine melon herbaceous sweet floral lily oily green petal greasy soft	Sigma Aldrich, TGSC, OdoRactor
2430	Jasmine lactone	6-[(Z)-pent-2-enyl]oxan-2-one	CCC=CCC1CCCC(=0)01	creamy wax jasmine peach coconut lactonic fatty dairy tropical fruity	OdorRactor ,TGSC
2431	2H-Pyran-2-one, tetrahydro-6- (2-pentenyl)-	6-[(E)-pent-2-enyl]oxan-2-one	CCC=CCC1CCCC(=0)01	oily fruity petal floral jasmine tuberose peach apricot coconut	OdorRactor ,TGSC
2432	2-(trans-2- Pentenyl)cyclopentanone	2-[(E)-pent-2-enyl]cyclopentan-1- one	CCC=CCC1CCCC1=0	fruity floral balsamic dairy lactonic coconut creamy peach apricot coumarinic	OdorRactor ,TGSC, Flavorbase
2433	Ethyl cis-4-heptenoate	ethyl (Z)-hept-4-enoate	CCC=CCCC(=0)OCC	fruity green apple tropical grape papaya passion fruit pineapple	TGSC
2434	4-Heptenal diethyl acetal	(Z)-7,7-diethoxyhept-3-ene	CCC=CCCC(OCC)OCC	green oily cucumber seedy wax fatty creamy dry salty fishy fruity vegetable apple herbaceous	OdorRactor ,TGSC
2435	(2E,6Z)-Nona-2,6-dienenitrile	(2E ,6Z)-nona-2,6-dienenitrile	CCC=CCCC=CC#N	green violet leaf floral walnut	OdorRactor ,TGSC
2436	(2E,6Z)-N-Cyclopropylnona-	(2E ,6Z)-N -cyclopropylnona-2,6	CCC=CCCC=CC(=O)NC1CC1	leafy violet meaty herbaceous	TGSC
	2,6-dienamide	dienamide			
2437	(2E,6Z)-N-Ethylnona-2,6- dienamide	(2E ,6Z)-N -ethylnona-2,6- dienamide	CCC=CCCC=CC(=O)NCC	meaty spicy	TGSC, Flavorbase
2438	(2E,6E)-1,1-Diethoxynona- 2,6-diene	(2 <i>E</i> ,6 <i>E</i>)-1,1-diethoxynona-2,6-diene	CCC=CCCC=CC(OCC)OCC	green cucumber fresh oily paint	OdorRactor ,TGSC
2439	2,6-Nonadienal	nona-2,6-dienal	CCC=CCCC=CC=O	cucumber violet leaf green violet	OdorRactor ,TGSC, Sigma Aldrich
2440	2,6-Nonadienal, (E,E)-	(2E ,6E)-nona-2,6-dienal	CCC=CCCC=CC=O	green vegetable citrus cucumber melon fresh fatty violet leaf leafy violet	Sigma Aldrich, TGSC, Flavorbase, OdoRactor
2441	trans-2,cis-6-Nonadienal	(2E ,6Z)-nona-2,6-dienal	CCC=CCCC=CC=O	green wax vegetable violet cucumber fatty dry violet leaf melon	Sigma Aldrich, TGSC, Flavorbase, OdoRactor, Pubchem
2442	(2E,6Z)-Nona-2,6-dien-1-ol	(2E ,6Z)-nona-2,6-dien-1-ol	CCC=CCCC=CCO	green cucumber oily violet leaf leafy fatty nutty violet	OdorRactor ,TGSC
2443	(2E,6Z)-Nona-2,6-dien-1-ol	(2E ,6Z)-nona-2,6-dien-1-ol	CCC=CCCC=CCO	green melon vegetable violet leaf cucumber oily leafy fatty nutty violet flower violet	Sigma Aldrich, TGSC, Flavorbase,
2444	Nona-2,6-dien-1-ol	nona-2,6-dien-1-ol	CCC=CCCC=CCO	powerful melon cucumber green vegetable	Flavornet, Flavorbase, TGSC, OdoRactor
2445	(e,z)-2,6-Nonadienyl acetate	[(2E ,6Z)-nona-2,6-dienyl] acetate	CCC=CCCC=CCOC(=0)C	apple green oily leafy fatty nutty melon spicy cucumber violet	Sigma Aldrich, TGSC, Flavorbase, OdoRactor
2446	cis-4-Heptenal	(Z)-hept-4-enal	CCC=CCCC=O	buttery potato vegetable fishy green minty biscuit creamy oily dairy milky	Sigma Aldrich, TGSC, OdoRactor
2447	(Z)-5-Hex-3-enyldihydro-5- methylfuran- 2(3H)-one	5-[(E)-hex-3-enyl]-5- methyloxolan-2-one	CCC=CCCC1(CCC(=0)01)C	coconut creamy oily fruity rich wax green paint jasmine buttery cookie fatty milky nutty	OdorRactor ,Sigma Aldrich, TGSC
2448	gamma-Jasmolactone	5-[(Z)-hex-3-enyl]oxolan-2-one	CCC=CCCC1CCC(=0)01	creamy coconut buttery	OdorRactor ,TGSC
2449	7-Decen-4-olide	5-hex-3-enyloxolan-2-one	CCC=CCCC1CCC(=O)O1	fatty buttery oily nutty	TGSC
2450	Jasmolactone	6-[(E)-hex-3-enyl]oxan-2-one	CCC=CCCC1CCCC(=0)01	creamy fruity peach plum dairy coconut buttery sweet milky floral	OdorRactor ,TGSC, Flavorbase
2451	cis-5-Octenoic acid	(Z)-oct-5-enoic acid	CCC=CCCCC(=0)0	greasy fatty	ADB, TGSC, OdoRactor
2452	5-Octenoic acid, methyl ester, (5Z)-	methyl (Z)-oct-5-enoate	CCC=CCCCC(=O)OC	sweet fruity woody creamy	OdorRactor ,TGSC
2453	5-Octenal, (5Z)-	(Z)-oct-5-enal	CCC=CCCCC=O	fruity	OdorRactor,
2454	(Z)-9,9-Dimethoxynon-3-ene	(Z)-9,9-dimethoxynon-3-ene	CCC=CCCCCC(OC)OC	fruity green melon cucumber	OdorRactor ,TGSC
2455	cis-6-Nonenal	(Z)-non-6-enal	CCC=CCCCCC=0	melon citrus green cucumber cantaloupe wax woody orris	Sigma Aldrich, TGSC, OdoRactor
2456	cis-7-Decen-1-al	(Z)-dec-7-enal	CCC=CCCCCCC=O	citrus aldehydic cucumber	OdorRactor ,TGSC
2457	8-Undecenal, (8Z)-	(Z)-undec-8-enal	CCC=CCCCCCCC=0	aldehydic citrus wax floral clean	Sigma Aldrich, TGSC
2458	(Z)-Non-6-en-1-ol	(Z)-non-6-en-1-ol	CCC=CCCCCCO	green melon fresh wax honeydew cantaloupe cucumber clean vegetable juicy fatty	Sigma Aldrich, TGSC, OdoRactor

2459	cis-6-Nonenyl Acetate	[(Z)-non-6-enyl] acetate	CCC=CCCCCCC(=0)C	melon honeydew cantaloupe green tropical fruit pear kiwi metallic	OdorRactor ,TGSC
2460	cis-5-Octen-1-ol	(Z)-oct-5-en-1-ol	CCC=CCCCCO	fatty green melon watery watermelon earthy mushroom violet leafy fishy soapy	Sigma Aldrich, TGSC, OdoRactor
2461	5-Octen-1-ol, acetate, (Z)-	acetic acid;oct-5-en-1-ol	CCC=CCCCO.CC(=0)O	fruity banana melon green fleshy fermented estery juicy pineapple	TGSC, Flavorbase
2462	5-Octenyl propanoate	[(Z)-oct-5-enyl] propanoate	CCC=CCCCCCC(=O)CC	green leafy woody apple banana watermelon cucumber tropical	OdorRactor ,TGSC
2463	cis-4-Hepten-1-ol	(Z)-hept-4-en-1-ol	CCC=CCCCO	fresh oily fatty creamy vegetable dairy green grassy	OdorRactor ,TGSC
2464	cis-3-Hexen-1-ol	(Z)-hex-3-en-1-ol	CCC=CCCO	green grassy fresh foliage vegetable oily herbaceous melon pungent strong sharp	Sigma Aldrich, TGSC, Flavorbase, OdoRactor, Pubchem
2465	3-Hexen-1-ol	(E)-hex-3-en-1-ol	CCC=CCCO	green mossy fresh cortex privet leafy floral petal oily earthy	Sigma Aldrich, TGSC, OdoRactor
2466	(Z)-1-Methoxyhex-3-ene	(Z)-1-methoxyhex-3-ene	CCC=CCCOC	green fruity pear apple fig fresh	TGSC
2467	cis-3-Hexenyl acetate	[(Z)-hex-3-enyl] acetate	CCC=CCCOC(=0)C	banana green vegetable fresh sweet fruity apple grassy melon pear strong	Sigma Aldrich, Flavornet, TGSC, Flavorbase, OdoRactor
2468	trans-3-Hexenyl acetate	[(E)-hex-3-enyl] acetate	CCC=CCCOC(=O)C	fruity sharp green banana pear cortex hyacinth narcissus rummy apple	OdorRactor ,TGSC
2469	cis-3-Hexenyl tiglate	[(Z)-hex-3-enyl] (E)-2- methylbut-2-enoate	CCC=CCCOC(=0)C(=CC)C	banana fatty green vegetable earthy pepper herbaceous cortex mushroom radish	Sigma Aldrich, TGSC
2470	(Z)-3-Hexenyl Angelate	[(Z)-hex-3-enyl] (Z)-2- methylbut-2-enoate	CCC=CCCOC(=0)C(=CC)C	green floral herbaceous apple pear	TGSC
2471	2-Butenoic acid, 2-methyl-, (3Z)-3-hexenyl ester, (2E)-	[(E)-hex-3-enyl] (Z)-2- methylbut-2-enoate	CCC=CCCOC(=0)C(=CC)C	herbaceous vegetable fruity green vegetable banana earthy cortex mushroom radish	OdorRactor ,TGSC, Flavorbase
2472	cis-3-Hexen-1yl 2-methylpent- 2-en-1-oate	[(E)-hex-3-enyl] (Z)-2- methylpent-2-enoate	CCC=CCCOC(=O)C(=CCC)C	fruity fresh green natural metallic tropical wax	OdorRactor ,TGSC
2473	cis-3-Hexenyl pyruvate	[(Z)-hex-3-enyl] 2- oxopropanoate	CCC=CCCOC(=0)C(=0)C	green oily melon banana cucumber tea fatty vegetable fruity floral spicy caramel	OdorRactor ,TGSC, Flavorbase
2474	cis-3-Hexenyl isobutyrate	[(Z)-hex-3-enyl] 2- methylpropanoate	CCC=CCCOC(=0)C(C)C	apple orange minty ethereal nutty sweet winey fruity green pear tropical mango tomato violet leaf cut grass violet	Sigma Aldrich, TGSC, Flavorbase, OdoRactor
2475	cis-3-Hexenyl 2- methylbutanoate	[(Z)-hex-3-enyl] 2- methylbutanoate	CCC=CCCOC(=O)C(C)CC	vegetable juicy pineapple fresh apple sweet fruity pear acidic herbaceous minty wax pepper berry sweaty almond gardenia hyacinth chemical naphthyl medicinal camphoraceous herbaceous apple	Sigma Aldrich, TGSCGSC, Flavorbase, OdoRactor
2476	cis-3-Hexenyl lactate	[(Z)-hex-3-enyl] 2- hydroxypropanoate	CCC=CCCOC(=O)C(C)O	green fruity leafy sweet melon wax violet leaf tropical vegetable fresh	Sigma Aldrich, TGSC, Flavorbase, OdoRactor
2477	Hex-3-enyl 2-ethylbutanoate	hex-3-enyl 2-ethylbutanoate	CCC=CCCOC(=O)C(CC)CC	violet green fruity apple	Flavorbase
2478	(E)-3-Hexenyl crotonate	[(E)-hex-3-enyl] (E)-but-2-enoate	CCC=CCCOC(=0)C=CC	fruity apple tropical green vegetable fresh dirty chemical metallic	OdorRactor ,TGSC, Flavorbase
2479	cis-3-Hexenyl benzoate	[(Z)-hex-3-enyl] benzoate	CCC=CCCOC(=O)C1=CC=CC=C	fresh green leafy floral orchid balsamic fatty sweet spicy fruity mild herbaceous woody	OdorRactor ,TGSC, Flavorbase
2480	cis-3-Hexenyl anthranilate	[(Z)-hex-3-enyl] 2- aminobenzoate	CCC=CCCOC(=0)C1=CC=CC=C	fruity sweet green grape jasmine orange flower grape floral lilac naphthyl	OdorRactor ,TGSC
2481	3-Hexenyl salicylate	[(E)-hex-3-enyl] 2- hydroxybenzoate	CCC=CCCOC(=O)C1=CC=CC=C	balsamic green floral metallic herbaceous	OdorRactor,
2482	cis-3-Hexenyl salicylate	[(Z)-hex-3-enyl] 2- hydroxybenzoate	CCC=CCCOC(=0)C1=CC=CC=C	balsamic green floral metallic herbaceous sweet woody	Sigma Aldrich, TGSC, Flavorbase
2483	(3Z)-Hex-3-en-1-yl	[(Z)-hex-3-enyl]	CCC=CCCOC(=O)C1CC1	fresh floral green tropical fruit	OdorRactor ,TGSC
2484	cyclopropanecarboxylate cis-3-Hexenyl propionate	cyclopropanecarboxylate [(Z)-hex-3-enyl] propanoate	CCC=CCCOC(=O)CC	natural green fresh fruity apple pear vegetable melon banana peach wax leafy sweet citrus	Sigma Aldrich, TGSCGSC, Flavorbase, OdoRactor
				green earthy floral	ļ

2486	cis-3-Hexenyl isovalerate	[(Z)-hex-3-enyl] 3- methylbutanoate	CCC=CCCOC(=O)CC(C)C	apple green fresh fruity tropical pineapple floral dirty	Sigma Aldrich, TGSC
2487	cis-3-Hexenyl 3- methylbutanoate	hex-3-enyl 3-methylbutanoate	CCC=CCCOC(=O)CC(C)C	sweet apple fruity	TGSC, Flavorbase, Odoractor
2488	cis-3-Hexenyl cis-3-hexenoate	[(Z)-hex-3-enyl](Z)-hex-3-enoate	CCC=CCCOC(=0)CC=CCC	green tomato pear melon metallic fennel tropical fruity violet leaf apple leafy violet	Sigma Aldrich, TGSC, Flavorbase
2489	cis-3-Hexenyl phenylacetate		CCC=CCCOC(=0)CC1=CC=CC= C1	mossy herbaceous woody sweet green rose honey sweetpea tropical kiwi beany floral vegetable melon wax	
2490	(3Z)-Hex-3-en-1-yl methyl carbonate	[(Z)-hex-3-enyl] methyl carbonate	CCC=CCCOC(=0)OC	green natural floral violet leafy wax apple fruity pear	OdorRactor ,TGSC, Flavorbase
2491	Acetaldehyde ethyl cis-3- hexenyl acetal	(Z)-1-(1-ethoxyethoxy)hex-3-ene	CCC=CCCOC(C)OCC	green mushroom musty vegetable violet leafy natural earthy radish raw fruity	Sigma Aldrich, TGSC
2492	Acetaldehyde di-cis-3- hexenyl acetal	(Z)-1-[1-[(Z) -hex-3-enoxy]ethoxy]hex-3-ene	CCC=CCCOC(C)OCCC=CCC	green leafy herbaceous sweet vegetable	OdorRactor ,TGSC, Flavorbase
2493	(E)-1-(1- Methoxypropoxy)hex-3-ene	(E)-1-(1-methoxypropoxy)hex-3-ene	CCC=CCCOC(CC)OC	green fresh dusty weedy cortex green bean tomato	OdorRactor ,TGSC
2494	cis-3-Hexenyl formate	[(Z)-hex-3-enyl] formate	CCC=CCCOC=O	green vegetable fresh wax sweet grassy sharp fruity citrus melon strong apple	Sigma Aldrich, TGSC, Flavorbase, OdoRactor
	3-Hexen-1-ol, formate	[(E)-hex-3-enyl] formate	CCC=CCCOC=O	strong sharp green fruity apple	Flavorbase
2496	3-Hexene, 1-[(2-methyl-2-propenyl)oxy]-, (3Z)-	$(Z\)$ -1-(2-methylprop-2-enoxy)hex-3-ene		green fresh floral pear bellpepper tropical radish	TGSC
2497		2-[(Z)-hex-3-enoxy]acetaldehyde	CCC=CCCOCC=O	green fresh watery ozone wax citrus aldehydic	OdorRactor ,TGSC
2498		3-[(Z)-hex-3- enoxy]propanenitrile	CCC=CCCOCCC#N	green fruity tropical floral violet oily cucumber fatty	OdorRactor ,TGSC
2499	cis-2-Penten-1-ol	(Z)-pent-2-en-1-ol	CCC=CCO	ethereal green plastic rubbery phenolic nasturtium medicinal aldehydic cherry narcissus metallic fruity	TGSC, Flavorbase, ODoRactor
2500	2-Penten-1-OL	(E)-pent-2-en-1-ol	CCC=CCO	mushroom	Flavornet, TGSC, OdoRactor
2501	1-Butene, 1-(methylthio)-, (E)-	(E)-1-methylsulfanylbut-1-ene	CCC=CSC	alliaceous onion garlic savory	Flavorbase
2502	Propionaldehyde	propanal	CCC=0	almond apple banana cheese chocolate grape green meaty musty ethereal winey cocoa whiskey pungent choking earthy alcoholic nutty cognac brandy suffocating fruity unpleasant	Sigma Aldrich, TGSC, PubChem
2503	5-Ethyl-3,4,5,6-tetramethyl-2-cyclohexen-1- one	5-ethyl-3,4,5,6- tetramethylcyclohex-2-en-1-one	CCC1(C(C(=CC(=O)C1C)C)C)C	caramel fruity spicy warm	OdorRactor ,TGSC
2504	2-Ethyl-1,3,3-trimethyl-2- norbornanol	2-ethyl-1,3,3- trimethylbicyclo[2.2.1]heptan-2-ol	CCC1(C(C2CCC1(C2)C)(C)C)O	earthy humus	TGSC
2505	Ethyl alpha-ethyl-beta-methyl- beta- phenylglycidate	ethyl (2R, 3S)-2-ethyl-3-methyl-3- phenyloxirane-2- carboxylate	CCC1(C(O1)(C)C2=CC=CC=C2) C(=O)O CC	fruity berry jammy raspberry strawberry	TGSC
2506	8-Ethyl-1,5- dimethylbicyclo[3.2.1]octan- 8- ol	8-ethyl-1,5- dimethylbicyclo[3.2.1]octan-8-ol	CCC1(C2(CCCC1(CC2)C)C)O	earthy rooty humus dirty	OdorRactor ,TGSC
2507	5-Ethyl-2,3,4,5-tetramethyl-2-cyclohexenone	5-ethyl-2,3,4,5- tetramethylcyclohex-2-en-1-one	CCC1(CC(=0)C(=C(C1C)C)C)C	caramel fruity spicy	OdorRactor ,TGSC
2508	2-Ethyl-2,5,5-trimethyl-4- (propan-2-yl)-1,3- dioxane	2-ethyl-2,5,5-trimethyl-4-propan-2- yl-1,3-dioxane	CCC1(OCC(C(O1)C(C)C)(C)C)C	minty leathery	TGSC
2509	5-Ethyl-4-hydroxy-2- methylfuran-3(2H)- one	5-ethyl-4-hydroxy-2-methylfuran- 3-one	CCC1=C(C(=O)C(O1)C)O	caramel fruity cotton candy sweet bready maple brown sugar burnt	Sigma Aldrich, TGSC, Flavorbase
2510	Ethyl maltol	2-ethyl-3-hydroxypyran-4-one	CCC1=C(C(=O)C=CO1)O	caramel sweet jammy strawberry cotton candy berry sugar	Sigma Aldrich, TGSC, OdoRactor
2511	Ethyl maltol isobutyrate	(2-ethyl-4-oxopyran-3-yl) 2- methylpropanoate	CCC1=C(C(=0)C=CO1)OC(=0)C (C)C	sweet caramel strawberry tropical	Flavorbase
2512	3-Ethyl-2-hydroxy-2- cyclopenten-1-one	3-ethyl-2-hydroxycyclopent-2-en- 1-one	CCC1=C(C(=O)CC1)O	chocolate coffee maple smoky sweet caramel fenugreek brown brown sugar rummy whiskey	Sigma Aldrich, Flavorbase, TGSC, OdoRactor
2513	3-Ethyl-2-hydroxy-4- methylcyclopent-2-en- 1-one	3-ethyl-2-hydroxy-4- methylcyclopent-2-en-1-one	CCC1=C(C(=0)CC1C)O	sweet maple caramel	OdorRactor ,TGSC
2514	5-Ethyl-2,4-dimethylthiazole	5-ethyl-2,4-dimethyl-1,3-thiazole	CCC1=C(N=C(S1)C)C	nutty roasted meaty earthy	Flavornet, TGSC

	2 5 Diathrol 4 mathroldhianala	2.5 diathrol 4 mosthrol 1.2 thiomala	CCC1_C(N_C(C1)CC)C	and an acceptant	TCCC
2515	2,5-Diethyl-4-methylthiazole	2,5-diethyl-4-methyl-1,3-thiazole	CCC1=C(N=C(S1)CC)C	green nutty	TGSC
2516	5-Ethyl-4-methylthiazole	5-ethyl-4-methyl-1,3-thiazole	CCC1=C(N=CS1)C	nutty fleshy green earthy	TGSC, OdoRactor
2517	2,5-Dimethyl-4-ethyloxazole	4-ethyl-2,5-dimethyl-1,3-oxazole	CCC1=C(OC(=N1)C)C	burnt roasted	OdorRactor ,TGSC
2518	4-Ethyl-2-methoxyphenol	4-ethyl-2-methoxyphenol	CCC1=CC(=C(C=C1)O)OC	meaty smoky spice clove phenolic bacon medicinal woody sweet	Sigma Aldrich, AOD, TGSC, OdoRactor
2519	4-Ethyl-1,2- dimethoxybenzene	4-ethyl-1,2-dimethoxybenzene	CCC1=CC(=C(C=C1)OC)OC	musty earthy	TGSC
2520	3-Ethylphenol	3-ethylphenol	CCC1=CC(=CC=C1)O	musty	Flavornet, TGSC
2521	4'-Ethylacetophenone	1-(4-ethylphenyl)ethanone	CCC1=CC=C(C=C1)C(=O)C	floral hawthorn	SuperScent, TGSC, OdoRactor
2522	4-Ethylbenzaldehyde	4-ethylbenzaldehyde	CCC1=CC=C(C=C1)C=O	bitter almond sweet anisic fruity cherry bitter	Sigma Aldrich, TGSC, Odoractor
	3-(4-Ethylphenyl)-2,2- dimethylpropanenitrile	3-(4-ethylphenyl)-2,2- dimethylpropanenitrile	CCC1=CC=C(C=C1)CC(C)(C)C# N	ozone marine anisic herbaceous	OdorRactor ,TGSC
2524	3-(4-Ethylphenyl)-2,2- dimethylpropanal	3-(4-ethylphenyl)-2,2- dimethylpropanal	CCC1=CC=C(C=C1)CC(C)(C)C=	ozone fresh green marine clean	OdorRactor ,TGSC
	4-Ethylphenol	4-ethylphenol	CCC1=CC=C(C=C1)O	alcoholic medicinal phenolic spice smoky guaiacol castoreum savory powerful woody	Sigma Aldrich, TGSC, OdoRactor, Pubchem
2526	4-Ethylanisole	1-ethyl-4-methoxybenzene	CCC1=CC=C(C=C1)OC	anisic	OdorRactor ,TGSC
	2-Ethyl-5-methylfuran	2-ethyl-5-methylfuran	CCC1=CC=C(O1)C	fresh gassy burnt	TGSC
2528	2-Ethyl-5-methylthiophene	2-ethyl-5-methylthiophene	CCC1=CC=C(S1)C	sulfurous ethereal solvent fruity burnt	TGSC
2529	5-Ethylthiophene-2- carbaldehyde	5-ethylthiophene-2-carbaldehyde	CCC1=CC=C(S1)C=O	bitter almond cherry sweet fruity bitter	OdorRactor ,TGSC
2530	2-Ethylbenzenethiol	2-ethylbenzenethiol	CCC1=CC=CC=C1S	sulfurous roasted meaty smoky	Sigma Aldrich, TGSC,
				allium roasted meat	Flavorbase, OdoRactor,
	2-Ethylpyridine	2-ethylpyridine	CCC1=CC=CC=N1	green grassy	Flavornet, TGSC
2532	2-Ethylfuran	2-ethylfuran	CCC1=CC=CO1	chemical coffee ethereal sweet burnt earthy malty beany bready	Sigma Aldrich, TGSC, OdoRactor
2533	Versalide		CCC1=CC2=C(C=C1C(=0)C)C(C CC2(C) C)(C)C	musk sweet ambrette	SuperScent, TGSC
2534	2(3H)-Furanone, 5-ethyl-	5-ethyl-3H -furan-2-one	CCC1=CCC(=O)O1	spice	Flavornet, OdoRactor
2535	6-Ethyl-2,10,10-trimethyl-1-oxaspiro[4.5]deca-3,6-diene	10-ethyl-2,6,6-trimethyl-1- oxaspiro[4.5]deca-3,9- diene	CCC1=CCCC(C12C=CC(O2)C)(C)C	fruity black currant berry	TGSC
	Ethyl 2-ethyl-6,6- dimethylcyclohex-2-ene-1- carboxylate	ethyl 2-ethyl-6,6- dimethylcyclohex-2-ene-1- carboxylate	CCC1=CCCC(C1C(=0)OCC)(C) C	rose spicy fruity berry damascone floral warm woody	OdorRactor ,TGSC
2537	5-Ethyl-2,3-dimethylpyrazine	5-ethyl-2,3-dimethylpyrazine	CCC1=CN=C(C(=N1)C)C	burnt popcorn roasted cocoa	Flavornet, TGSC, Odoractor
2538	2,5-Diethyl-3-methylpyrazine	2,5-diethyl-3-methylpyrazine	CCC1=CN=C(C(=N1)C)CC	toasted roasted hazelnut meaty nutty hazelnut roasted	OdorRactor ,TGSC
2539	3,5-Diethyl-2-methylpyrazine	3,5-diethyl-2-methylpyrazine	CCC1=CN=C(C(=N1)CC)C	nutty meaty vegetable baked	Flavornet, TGSC, OdoRactor
2540	5-Ethyl-2-methylpyridine	5-ethyl-2-methylpyridine	CCC1=CN=C(C=C1)C	roasted nutty raw raw potato earthy sharp penetrating strong aromatic	Sigma Aldrich, TGSC, OdoRactor, Pubchem
2541	5-Ethyl-2-methylthiazole	5-ethyl-2-methyl-1,3-thiazole	CCC1=CN=C(S1)C	chocolate fishy pyrazine	OdorRactor,
2542	2,5-Diethylthiazole	2,5-diethyl-1,3-thiazole	CCC1=CN=C(S1)CC	meaty musty nutty	TGSC
	2-Ethyl-6-vinylpyrazine	2-ethenyl-6-ethylpyrazine	CCC1=CN=CC(=N1)C=C	buttery baked potato baked	TGSC
2544	3-Ethylpyridine	3-ethylpyridine	CCC1=CN=CC=C1	caramel coffee green meaty musty smoky peanut tobacco leathery oakmoss strong roasted nutty	Sigma Aldrich, Flavorbase, TGSC,OdoRactor
2545	2-Ethyl-4,5-dimethyloxazole	2-ethyl-4,5-dimethyl-1,3-oxazole	CCC1=NC(=C(O1)C)C	green creamy vegetable earthy	OdorRactor ,TGSC
2546	2-Ethyl-4,5-dimethylthiazole	2-ethyl-4,5-dimethyl-1,3-thiazole	CCC1=NC(=C(S1)C)C	hazelnut cocoa nutty burnt	OdorRactor ,TGSC
2547	2-Ethyl-6-methylpyrazine	2-ethyl-6-methylpyrazine	CCC1=NC(=CN=C1)C	roasted potato	OdorRactor ,TGSC
	2-Ethyl-5(6)-methylpyrazine		CCC1=NC(=CN=C1)C.CCC1=N C=C(N= C1)C	potato nutty roasted coffee hazelnut cocoa roasted barley	Sigma Aldrich, TGSC
2549	3-Ethyl-2,5-dimethylpyrazine	3-ethyl-2,5-dimethylpyrazine	CCC1=NC(=CN=C1C)C	potato roasted nutty cocoa	Flavornet, TGSC, Pubchem
	2-Ethenyl-3-ethyl-5- methylpyrazine	2-ethenyl-3-ethyl-5- methylpyrazine	CCC1=NC(=CN=C1C=C)C	earthy	Flavornet, TGSC
	2-Ethyl-4-methylthiazole	2-ethyl-4-methyl-1,3-thiazole	CCC1=NC(=CS1)C	green nutty pistachio brown savory coffee sulfurous meaty	Sigma Aldrich, TGSC, OdoRactor
2552	2-Ethyl-5-methylpyrazine	2-ethyl-5-methylpyrazine	CCC1=NC=C(N=C1)C	fruit sweet coffee beany nutty grassy roasted toffee cocoa green	Flavornet, Flavorbase, TGSC, OdoRactor

2553	2-Ethyl-3,5-dimethylpyrazine	2-ethyl-3,5-dimethylpyrazine	CCC1=NC=C(N=C1C)C	almond beefy caramel cheese coffee corn woody earthy tobacco potato nutty burnt roasted peanut musty cocoa hazelnut chocolate brown sweet roasted peanut burnt almond burnt hazelnut	Sigma Aldrich, Flavornet, Flavorbase, OdoRactor
2554	2,3-Diethyl-5-methylpyrazine	2,3-diethyl-5-methylpyrazine	CCC1=NC=C(N=C1CC)C	hazelnut meaty vegetable potato roasted musty roasted hazelnut nutty earthy toasted green	Sigma Aldrich, TGSC, OdoRactor
2555	Pyridine, 2-ethyl-4-(1- methylethenyl)	2-ethyl-4-prop-1-en-2-ylpyridine	CCC1=NC=CC(=C1)C(=C)C	nutty bitter herbaceous	TGSC
2556	2-Ethylpyrazine	2-ethylpyrazine	CCC1=NC=CN=C1	buttery musty nutty woody peanut roasted cocoa fermented coffee meaty	Sigma Aldrich, TGSC, Pubchem, OdoRactor
2557	2-Ethyl-3-methylpyrazine	2-ethyl-3-methylpyrazine	CCC1=NC=CN=C1C	hazelnut earthy potato roasted sweaty nutty peanut musty corn raw bready cereal green	Sigma Aldrich, Flavornet, Flavorbase, TGSC, OdoRactor
2558	2-Acetyl-3-ethylpyrazine	1-(3-ethylpyrazin-2-yl)ethanone	CCC1=NC=CN=C1C(=O)C	green meaty oily nutty earthy potato popcorn corn	Sigma Aldrich, TGSC, OdoRactor
2559	2,3-Diethylpyrazine	2,3-diethylpyrazine	CCC1=NC=CN=C1CC	hazelnut meaty earthy baked potato green nutty raw bellpepper baked	Sigma Aldrich, TGSC, OdoRactor
2560	2-Ethyl-3-methoxypyrazine	2-ethyl-3-methoxypyrazine	CCC1=NC=CN=C1OC	earthy bellpepper nutty raw raw potato green	Sigma Aldrich, TGSC, OdoRactor
2561	2-Ethoxy-3-ethylpyrazine	2-ethoxy-3-ethylpyrazine	CCC1=NC=CN=C1OCC	raw raw potato earthy nutty roasted weak woody	Sigma Aldrich, TGSC, Flavorbase
2562	2-Ethyl-3- (methylthio)pyrazine	2-ethyl-3-methylsulfanylpyrazine	CCC1=NC=CN=C1SC	roasted cooked meaty roasted meat	Sigma Aldrich, TGSC
2563	2-Ethylthiazole	2-ethyl-1,3-thiazole	CCC1=NC=CS1	green nutty	TGSC
2564	Magnol	1-(4-ethyl-2- bicyclo[2.2.1]heptanyl)cyclohexan- 1- ol	CCC12CCC(C1)C(C2)C3(CCCC C3)O	magnolia muguet floral lily	OdorRactor ,TGSC
2565	5-Ethyl-3-hydroxy-4- methylfuran-2(5H)- one	2-ethyl-4-hydroxy-3-methyl-2 <i>H</i> - furan-5-one	CCC1C(=C(C(=O)O1)O)C	caramel maple spice sweet fruity fenugreek nutty butterscotch brown sugar chicory praline powerful	Sigma Aldrich, Flavorbase, TGSC, OdoRactor
2566	5-Ethyl-2,5-dihydro-4-methyl- 2-(1- methylpropyl)-thiazole	2-butan-2-yl-5-ethyl-4-methyl-2,5-dihydro-1,3- thiazole	CCC1C(=NC(S1)C(C)CC)C	meaty nutty cooked roasted	TGSC
2567	Thiazole, 5-ethyl-2,5-dihydro-4-methyl-2-(2- methylpropyl)-	5-ethyl-4-methyl-2-(2- methylpropyl)-2,5-dihydro- 1,3-thiazole	CCC1C(=NC(S1)CC(C)C)C	meaty nutty cooked roasted chocolate vegetable	Flavorbase, TGSC
2568	2-Ethyl-4-hydroxy-5-methyl-3(2H)- furanone	2-ethyl-4-hydroxy-5-methylfuran- 3-one	CCC1C(=0)C(=C(01)C)O	caramel sweet candy butterscotch	Flavornet, TGSC, Odoractor
2569	2(Or 5)-Ethyl-4-hydroxy-5(or 2)-methyl- 3(2H)-furanone	2-ethyl-4-(hydroxymethyl)furan-3- one	CCC1C(=O)C(=CO1)CO	caramel	Flavornet, TGSC
2570	Diethyldimethylcyclohex-2-en- 1-one	3,4-diethyl-2,5-dimethylcyclohex- 2-en-1-one	CCC1C(CC(=O)C(=C1CC)C)C	dry chrysanthemum woody phenolic powdery orris	OdorRactor ,TGSC
2571	5-Ethyl-2(5H)-furanone	2-ethyl-2H -furan-5-one	CCC1C=CC(=0)O1	spice	Flavornet, TGSC
2572	5-Ethyl-2-hydroxy-3- methylcyclopent-2-en- 1-one	5-ethyl-2-hydroxy-3- methylcyclopent-2-en-1-one	CCC1CC(=C(C1=O)O)C	caramel malty	OdorRactor ,TGSC
2573	4-Ethyl-2-hydroxy-3- methylcyclopent-2-en- 1-one	4-ethyl-2-hydroxy-3- methylcyclopent-2-en-1-one	CCC1CC(=0)C(=C1C)O	sweet malty	TGSC, Pubchem
2574	Bicyclo[2.2.1]heptane, 2- ethyl-5-methoxy-	2-ethyl-5- methoxybicyclo[2.2.1]heptane	CCC1CC2CC1CC2OC	herbaceous green leafy citrus	OdorRactor ,TGSC
2575	1,2-Cyclopentanedione, 3- ethyl-	3-ethylcyclopentane-1,2-dione	CCC1CCC(=O)C1=O	sweet caramel maple	TGSC
2576	gamma-Caprolactone	5-ethyloxolan-2-one	CCC1CCC(=0)01	herbaceous sweet coumarinic coconut tobacco creamy lactonic green tonka hay herbaceous	Sigma Aldrich, TGSC,OdoRactor
2577	2(3H)-Furanone, 5- ethyldihydro-, (S)-	(5S)-5-ethyloxolan-2-one	CCC1CCC(=O)O1	sweet coconut creamy woody	TGSC
2578	2,5-Diethyltetrahydrofuran	2,5-diethyloxolane	CCC1CCC(O1)CC	caramel sweet herbaceous	ADB, TGSC
2579	1-Oxaspiro(4.5)decan-2-one, 8-ethyl-, cis-	8-ethyl-1-oxaspiro[4.5]decan-2-one	CCC1CCC2(CC1)CCC(=0)O2	spicy cinnamyl creamy lactonic aldehydic peach	OdorRactor ,TGSC
2580	6-Ethyltetrahydro-2H-pyran-2- one	6-ethyloxan-2-one	CCC1CCCC(=0)O1	coconut oily green earthy lactonic coumarinic	OdorRactor ,TGSC, Flavorbase
2581	4,5-Dimethyl-2-ethyl-3- thiazoline	2-ethyl-4,5-dimethyl-2,5-dihydro- 1,3-thiazole	CCC1N=C(C(S1)C)C	nutty meaty musty sulfurous coffee chocolate raw vegetable	OdorRactor ,TGSC
2582	3-Thiazoline, 2-ethyl-4- methyl-	2-ethyl-4-methyl-2,5-dihydro-1,3-thiazole	CCC1N=C(CS1)C	nutty roasted vegetable tropical peach creamy dairy tomato meaty	TGSC, Flavorbase

2583	2,4,6-Triethyl-1,3,5-dithiazinane	2,4,6-triethyl-1,3,5-dithiazinane	CCC1NC(SC(S1)CC)CC	sulfurous alliaceous roasted fried onion leek fatty scallion meaty savory seafood fried	TGSC, Flavorbase
2584	2-Ethyl-5,5-dimethyl-1,3-dioxane	2-ethyl-5,5-dimethyl-1,3-dioxane	CCC1OCC(CO1)(C)C	tutti frutti	
2585	2-Ethyl-4-methyl-1,3- dioxolane	2-ethyl-4-methyl-1,3-dioxolane	CCC1OCC(O1)C	medicinal sweet sweet medicinal	
2586	3-Ethyl-8,11(or 9,11)- dimethyl-2,4- dioxaspiro(5.5)undec-8-ene	3-ethyl-8,11-dimethyl-2,4-dioxaspiro[5.5]undec-8- ene	CCC10CC2(CC(=CCC2C)C)C01	aromatic herbaceous natural celery cumin forest humus	OdorRactor ,TGSC
2587	2,4-Dioxaspiro[5.5]undec-8-ene, 3-ethyl-	3-ethyl-2,4-dioxaspiro[5.5]undec- 9-ene	CCC1OCC2(CCC=CC2)CO1	rose cashewnut herbaceous sweet fruity floral	OdorRactor ,TGSC
2588	1,3-Oxathiane, 2-ethyl-4,4- dimethyl-	2-ethyl-4,4-dimethyl-1,3- oxathiane	CCC1OCCC(S1)(C)C	herbaceous sage tagette black currant minty sulfurous onion	TGSC
2589	3,5-Diethyl-1,2,4-trithiolane	3,5-diethyl-1,2,4-trithiolane	CCC1SC(SS1)CC	cooked roasted sulfurous garlic seafood	OdorRactor ,TGSC, Flavorbase
2590	2-Pentanone	pentan-2-one	CCCC(=0)C	alcoholic apple banana cheese chocolate fishy ethereal musty pineapple potato strawberry sweet winey fruity woody fermented acetone	Sigma Aldrich, AOD, TGSC,OdoRactor
2591	2,3-Hexanedione	hexane-2,3-dione	CCCC(=0)C(=0)C	sharp penetrating sweet aromatic caramel buttery oily fatty creamy phenolic fruity dry jammy dry	AOD, TGSC, OdoRactor,Sigma Aldrich,Pubchem
2592	4,5-Octanedione	octane-4,5-dione	CCCC(=0)C(=0)CCC	fatty buttery creamy	TGSC
2593 2594	3-Benzyl-4-heptanone	3-benzylheptan-4-one 3-sulfanylheptan-4-one	CCCC(=0)C(CC)CC1=CC=CC=C 1 CCCC(=0)C(CC)S	fruity berry woody herbaceous minty plum raisin buchu herbaceous grapefruit green	OdorRactor ,TGSC TGSC
	3-Mercaptoheptan-4-one	• •		black currant	
2595	3-(Methylsulfanyl)heptan-4- one	3-methylsulfanylheptan-4-one	CCCC(=O)C(CC)SC	green minty herbaceous vegetable basil	TGSC
2596	3-(2-Methyl-3-furylthio)-4- heptanone	3-(2-methylfuran-3- yl)sulfanylheptan-4-one	CCCC(=O)C(CC)SC1=C(OC=C1)	roasted meat roasted meaty	OdorRactor ,TGSC
2597	1-Hexen-3-one	hex-1-en-3-one	CCCC(=0)C=C	vegetable metal cooked metallic	Flavornet, TGSC
2598	2-Hepten-4-one	(E)-hept-2-en-4-one	CCCC(=O)C=CC	ethereal	OdorRactor ,TGSC
2599	Butyrophenone	1-phenylbutan-1-one	CCCC(=O)C1=CC=CC=C1	cherry vanilla camphoraceous walnut hazelnut	Sigma Aldrich, TGSC,OdoRactor
2600	2-Butyrylfuran	1-(furan-2-yl)butan-1-one	CCCC(=0)C1=CC=CO1	balsamic	OdorRactor ,TGSC
2601	1-(Thiophen-2-yl)butan-1-one	1-thiophen-2-ylbutan-1-one	CCCC(=O)C1=CC=CS1	roasted meaty grilled roasted beef beefy	OdorRactor ,TGSC
2602	3-Hexanone	hexan-3-one	CCCC(=O)CC	grape earthy ethereal winey sweet wax rummy fruity	Sigma Aldrich, TGSC,OdoRactor
2603	Glyceryl 3-oxohexanoate	3-oxohexanoic acid;propane-1,2,3-triol	CCCC(=0)CC(=0)O.C(C(C0)O) O	mild fatty	OdorRactor ,TGSC
2604	Ethyl 3-oxohexanoate	ethyl 3-oxohexanoate	CCCC(=0)CC(=0)OCC	berry green mossy sweet fruity sweaty	Sigma Aldrich, TGSC, OdoRactor
2605	4-Heptanone	heptan-4-one	CCCC(=0)CCC	apple banana cheese peanut pineapple strawberry fruity sweet cognac tutti frutti pleasant	Sigma Aldrich, TGSC, OdoRactor, Pubchem
2606	5-Oxooctanoic acid	5-oxooctanoic acid	CCCC(=O)CCCC(=O)O	fruity musk	Flavorbase, TGSC
2607	Butyramide	butanamide	CCCC(=O)N	nutty	OdorRactor ,TGSC
2608	Butyric acid	butanoic acid	CCCC(=O)O	sharp dairy cheese rancid sweaty acetic buttery fruit acidic caprylic penetrating obnoxious unpleasant	Sigma Aldrich, TGSC, Pubchem
2609	Methyl butyrate	methyl butanoate	CCCC(=0)OC	apple ethereal sweet fruit banana pineapple pungent fusel fermented creamy	Sigma Aldrich, TGSC, OdoRactor, Pubchem
2610	Butyric anhydride	butanoyl butanoate	CCCC(=O)OC(=O)CCC	buttery pungent	Sigma Aldrich, TGSC, OdoRactor, Pubchem
2611	Butanoic acid, 1-methyl-1-(4-methyl-3- cyclohexen-1-yl)ethyl ester	2-(4-methylcyclohex-3-en-1- yl)propan-2-yl butanoate	CCCC(=O)OC(C)(C)C1CCC(=CC 1)C	apple sour rosemary fruity balsamic floral	Flavornet, TGSC, OdoRactor
2612	Guaiyl butyrate	2-[(3 <i>S</i> ,5 <i>R</i> ,8 <i>S</i>)-3,8-dimethyl-1,2,3,4,5,6,7,8- octahydroazulen-5-yl]propan-2-yl butanoate		rose plum animal balsamic woody	OdorRactor ,TGSC
2613	Butanoic acid, 1,1-dimethyl-2- phenylethyl ester	butanoate	C=C1	herbaceous plum floral green herbaceous fruity prune spicy wax seedy berry	Sigma Aldrich, TGSC, OdoRactor
2614	Linalyl butyrate	3,7-dimethylocta-1,6-dien-3-yl butanoate	CCCC(=0)OC(C)(CCC=C(C)C)C =C	banana pear sweet fruity berry floral bergamot blueberry pineapple citrus spicy	Sigma Aldrich, TGSC, OdoRactor
2615	Isopropyl butyrate	propan-2-yl butanoate	CCCC(=O)OC(C)C	creamy green wax pineapple sweet fruity ethereal estery ripe	Sigma Aldrich, TGSC, OdoRactor

2616	1-Methyl-2-oxopropyl	3-oxobutan-2-yl butanoate	CCCC(=O)OC(C)C(=O)C	berry cheese sweet fruity creamy	Sigma Aldrich, TGSC
2617	butyrate Ethyl butyryl lactate	(1-ethoxy-1-oxopropan-2-yl)	CCCC(=0)OC(C)C(=0)OCC	buttery acetic musty fruity buttery creamy sweet sour	Flavorbase, TGSC
		butanoate		buttermilk	
2618	alpha-Methylbenzyl butyrate	1-phenylethyl butanoate	CCCC(=0)0C(C)C1=CC=CC=C1	fruity earthy sweet berry juicy floral jasmine bubblegum tropical pulpy fruit ripe tutti frutti	Sigma Aldrich, TGSC, OdoRactor
2619	Sec-Butyl butyrate	butan-2-yl butanoate	CCCC(=O)OC(C)CC	sweet fruity banana apple pear apricot pineapple rummy	Flavorbase
2620	1-Phenylpropyl butyrate	1-phenylpropyl butanoate	CCCC(=0)OC(CC)C1=CC=CC=	fruity floral jasmine apricot plum	SuperScent, TGSC, OdoRactor
2621	2-Methyl-5-oxo-1- cyclopenten-1-yl butyrate	(2-methyl-5-oxocyclopenten-1-yl) butanoate	CCCC(=0)OC1=C(CCC1=0)C	fruity nutty caramel maple	TGSC
2622	4-Butyroxy-2,5-dimethyl-3(2H)-furanone	(2,5-dimethyl-4-oxofuran-3-yl) butanoate	CCCC(=0)OC1=C(OC(C1=0)C) C	fruity sweet ethereal tropical green weedy earthy wasabi	TGSC
2623	Maltyl butyrate	(2-methyl-4-oxopyran-3-yl) butanoate	CCCC(=0)OC1=C(OC=CC1=0)C	sweet fruity strawberry berry	TGSC
2624	p-Tolyl butyrate	(4-methylphenyl) butanoate	CCCC(=O)OC1=CC=C(C=C1)C	narcissus phenolic animal	OdorRactor ,TGSC
2625	Phenyl butyrate	phenyl butanoate	CCCC(=0)OC1=CC=CC=C1	sweet floral	TGSC, Flavorbase
2626	Guaiacol butyrate	(2-methoxyphenyl) butanoate	CCCC(=0)OC1=CC=CC=C1OC	fruity nutty	TGSC
2627	3-Tricyclo[5.2.1.02,6]dec-4-enyl butanoate	3-tricyclo[5.2.1.02,6]dec-4-enyl butanoate	CCCC(=0)OC1C=CC2C1C3CCC 2C3	fruity green peach orchid balsamic woody	OdorRactor ,TGSC
2628	Bornyl butyrate	(1,7,7-trimethyl-2-bicyclo[2.2.1]heptanyl) butanoate	CCCC(=0)OC1CC2CCC1(C2(C) C)C	herbaceous woody fruity fir cone- like	Flavornet, Flavorbase, TGSC, OdoRactor,
2629	Cyclohexyl butyrate	cyclohexyl butanoate	CCCC(=0)OC1CCCCC1	fresh sweet apple pineapple fruity floral	Sigma Aldrich, Flavorbase, TGSC, OdoRactor
2630	Ethyl butyrate	ethyl butanoate	CCCC(=0)OCC	apple banana ethereal pineapple fruity juicy cognac sweet tutti frutti buttery	Sigma Aldrich, Flavorbase, TGSC, OdoRactor
2631	2-Methylallyl butyrate	2-methylprop-2-enyl butanoate	CCCC(=O)OCC(=C)C	fruity ethereal sweet pineapple apple plum	OdorRactor ,TGSC
2632	Butanoic acid, 5-(2,3-dimethyltricyclo(2.2.1.02,6)h ept-3-yl)-2- methyl-2-pentenyl ester	[(E)-5-(2,3-dimethyl-3-tricyclo[2.2.1.02,6]heptanyl)-2-methylpent-2-enyl] butanoate	CCCC(=0)OCC(=CCCC1(C2CC3 C1(C3C 2)C)C)C	woody balsamic fruity rose nutty	OdorRactor ,TGSC
2633	Isobutyl butyrate	2-methylpropyl butanoate	CCCC(=0)OCC(C)C	fruity ethereal pineapple sweet rummy cherry apple tutti frutti ripe bubblegum candy berry	Sigma Aldrich, TGSC,OdoRactor
2634	2-Methylbutyl butyrate	2-methylbutyl butanoate	CCCC(=0)OCC(C)CC	fruity pear apricot apple tropical gooseberry spicy rummy	TGSC
2635	Propylene glycol dibutyrate	2-butanoyloxypropyl butanoate	CCCC(=O)OCC(C)OC(=O)CCC	sweet fruity buttery	TGSC
	[(2S)-2-Hydroxy-2- phenylethyl] butanoate	[(2S)-2-hydroxy-2-phenylethyl] butanoate	CCCC(=O)OCC(C1=CC=CC=C1) O	fruity hyacinth	TGSC
2637	Tributyrin	2,3-di(butanoyloxy)propyl butanoate	CCCC(=0)OCC(COC(=0)CCC)O C(=0)C CC	caramel creamy fatty cheese wax acidic fruity buttery	Sigma Aldrich, TGSC, Pubchem
2638	Allyl butyrate	prop-2-enyl butanoate	CCCC(=0)OCC=C	apricot peach sweet pungent fruity green pineapple wax tropical	Sigma Aldrich, TGSC, OdoRactor
2639	Geranyl butyrate	[(2E)-3,7-dimethylocta-2,6-dienyl] butanoate	CCCC(=O)OCC=C(C)CCC=C(C)	apple apricot sweet fruit rose wax raspberry tropical fresh peach green	Sigma Aldrich, TGSC, OdoRactor
2640	Neryl butyrate	[(2Z)-3,7-dimethylocta-2,6-dienyl] butanoate	CCCC(=0)OCC=C(C)CCC=C(C)	green orange floral sweet wax oily fatty leafy	Sigma Aldrich, TGSC, OdoRactor
2641	2,4-Hexadienyl butyrate	[(2E,4E)-hexa-2,4-dienyl] butanoate	CCCC(=0)OCC=CC=CC	fruity green winey cheese dairy	TGSC
2642	Hexa-2,4-dienyl butyrate	hexa-2,4-dienyl butanoate	CCCC(=0)OCC=CC=CC	fruity winey green cheese dairy	OdorRactor ,TGSC
2643	Cinnamyl butyrate	[(E)-3-phenylprop-2-enyl] butanoate	CCCC(=0)OCC=CC1=CC=CC=C		OdorRactor ,Sigma Aldrich
	Butanoic acid, 3-phenyl-2- propenyl ester	3-phenylprop-2-enyl butanoate	1	balsamic winey fruity cognac cinnamyl	TGSC, OdoRactor
2645	Anisyl butyrate	(4-methoxyphenyl)methyl butanoate	CCCC(=0)OCC1=CC=C(C=C1)O C	plum sweet buttery anisic floral tropical fruity	Sigma Aldrich, TGSC, OdoRactor
2646	Benzyl butyrate	2-phenylethyl acetate	CCCC(=0)OCC1=CC=CC=C1	apricot berry plum buttery cheese jasmine peach pear fruity fresh loganberry sweet wax tropical pineapple apple	Sigma Aldrich, TGSC, OdoRac
2647	Furfuryl butyrate	furan-2-ylmethyl butanoate	CCCC(=0)OCC1=CC=CO1	grape fruity green	Sigma Aldrich, TGSC, OdoRactor
2648	Tetrahydrofurfuryl butyrate	oxolan-2-ylmethyl butanoate	CCCC(=0)OCC1CCC01	cheese pineapple fruity green sweet musty tropical apricot creamy	Sigma Aldrich, TGSC, Pubchem, OdoRactor

2649	Propyl butyrate	propyl butanoate	CCCC(=O)OCCC	apple creamy honey wax winey pineapple solvent fruity sweet apricot rancid sweaty bubblegum tutti frutti ethereal	Sigma Aldrich, TGSC, OdoRactor
2650	Isoamyl butyrate	3-methylbutyl butanoate	CCCC(=0)OCCC(C)C	apricot banana pineapple fruity pear sweet estery green tropical melon tutti frutti	Sigma Aldrich, TGSC, OdoRactor
2651	Citronellyl butyrate	3,7-dimethyloct-6-enyl butanoate	CCCC(=0)OCCC(C)CCC=C(C)C	honey fruity sweet rose floral tropical green geranium wax bois de rose citrus	Sigma Aldrich, TGSC,OdoRactor
2652	Rhodinyl butyrate	3,7-dimethyloct-7-enyl butanoate	CCCC(=0)OCCC(C)CCCC(=C)C	fruity rose tropical berry geranium floral	OdorRactor ,TGSC
2653	cis-3-Hexenyl butyrate	[(Z)-hex-3-enyl] butanoate	CCCC(=0)OCCC=CCC	winey green fresh apple fruity metallic buttery vegetable grape	Flavornet, TGSC, Flavorbase, OdoRactor
2654	2-(4-Methylthiazol-5-yl)ethyl butyrate	2-(4-methyl-1,3-thiazol-5-yl)ethyl butanoate	CCCC(=O)OCCC1=C(N=CS1)C	roasted nutty	OdorRactor ,TGSC
2655	Phenethyl butyrate	2-phenylethyl butanoate	CCCC(=0)OCCC1=CC=CC=C1	musty sweet yeasty grape floral strawberry rose fruity green	Sigma Aldrich, Flavorbase, TGSC, OdoRactor
2656	3-Cyclohexylpropyl butyrate	3-cyclohexylpropyl butanoate	CCCC(=0)OCCCC1CCCCC1	cooling green wax	TGSC
2657	Methionyl butyrate	3-methylsulfanylpropyl butanoate	CCCC(=0)OCCCSC	fruity pineapple mushroom cheese sulfurous savory tropical fruit	OdorRactor ,TGSC, Flavorbase
2658	2-Phenoxyethyl butyrate	2-phenoxyethyl butanoate	CCCC(=0)OCCOC1=CC=CC=C1	fruity floral honey wax apple chamomile	Flavorbase
2659	Methylthiomethyl butyrate	methylsulfanylmethyl butanoate	CCCC(=0)OCSC	sulfurous musty onion fruity tropical metallic vegetable	OdorRactor ,TGSC
2660	S-Methyl butanethioate	S -methyl butanethioate	CCCC(=O)SC	cheese fatty green musty sulfurous cabbage garlic eggy tomato tropical fruit	Sigma Aldrich, TGSC
2661	5-Hydroxy-4-octanone	5-hydroxyoctan-4-one	CCCC(C(=0)CCC)O	buttery sweet pungent nutty	SuperScent, TGSC, OdoRactor
2662	2-Methylpentan-2-ol	2-methylpentan-2-ol	CCCC(C)(C)O	pungent	Flavornet
2663	1-Hexanol, 3-mercapto-3-methyl- (3R)-	(3R)-3-methyl-3-sulfanylhexan-1-	CCCC(C)(CCO)S	grapefruit passion fruit black	TGSC
2664	methyl-, (3R)- 2-Methylpentanoic acid	2-methylpentanoic acid	CCCC(C)C(=O)O	currant onion cheese sour strong pungent	Sigma Aldrich, Flavorbase,
2665	M d 10 d 1	4.10 4.1	agagyayay oyog		TGSC
2665	Methyl 2-methylpentanoate	methyl 2-methylpentanoate	CCCC(C)C(=O)OC	fruity berry apple tropical pineapple banana melon grape sweet green	SuperScent, TGSC, OdoRactor,
2666	2-Pentyl 2-methylpentanoate	pentan-2-yl 2-methylpentanoate	CCCC(C)C(=0)OC(C)CCC	fruity pear	TGSC
2667	Valeric acid, 2-methyl-, ethyl ester, (+)-	ethyl (2S)-2-methylpentanoate	CCCC(C)C(=0)OCC	green fresh fruity green melon apple pineapple natural wax fatty pear	OdorRactor ,TGSC, Flavorbase
2668	Ethyl 2-methylpentanoate	ethyl 2-methylpentanoate	CCCC(C)C(=0)OCC	pineapple fruity green melon apple natural wax fresh fatty	
2669	Methyl 2-[(2- methylpentylidene)amino]ben zoate	methyl 2-(2- methylpentylideneamino)benzoate	CCCC(C)C=NC1=CC=CC=C1C(=O)OC	sweet fruity citrus green grape cumin	OdorRactor ,TGSC
2670	2-Methylpentanal	2-methylpentanal	CCCC(C)C=O	ethereal fruity earthy green vegetable cocoa cheese ham	Sigma Aldrich, Flavorbase, TGSC, OdoRactor, Pubchem
2671	5-Methyl-2-(1-methylbutyl)-5- propyl-1,3- dioxane	5-methyl-2-pentan-2-yl-5-propyl- 1,3-dioxane	CCCC(C)C1OCC(CO1)(C)CCC	oily green jasmine herbaceous spicy fresh blossom	OdorRactor ,TGSC
2672	3-Methylhexanal	3-methylhexanal	CCCC(C)CC=O	sweet green	OdorRactor,
2673	2-Methylpentyl 2- methylpentanoate	2-methylpentyl 2- methylpentanoate	CCCC(C)COC(=0)C(C)CCC	fruity clean sweet pear oily jasmine natural	OdorRactor ,TGSC
2674	2-Pentanol	pentan-2-ol	CCCC(C)O	fermented alcoholic fusel musty sweet winey ripe banana apple green oily disagreeable strong ripe	Sigma Aldrich, AOD, TGSC, OdoRactor
2675	1-Methylbutyl acetate	pentan-2-yl acetate	CCCC(C)OC(=O)C	herbaceous weedy musty green vegetable nutty beany ketonic juicy banana fruity orange animal	SuperScent, TGSC, Pubchem
2676	(2S)-Pentan-2-yl 3- methylbutanoate	[(2S)-pentan-2-yl] 3- methylbutanoate	CCCC(C)OC(=O)CC(C)C	fruity apple brandy cooling metallic	TGSC
2677	2-Pentyl butyrate	pentan-2-yl butanoate	CCCC(C)OC(=O)CCC	fruity sweet banana apricot herbaceous cashewnut	SuperScent, TGSC, OdoRactor
2678	2-Pentanethiol	pentane-2-thiol	CCCC(C)S	sulfurous gassy	OdorRactor ,TGSC
2679	1-Hexen-3-OL	hex-1-en-3-ol	CCCC(C=C)O	banana ethereal winey green metallic earthy rummy acidic meaty	Sigma Aldrich, TGSC, Flavorbase, OdoRactor
2680	1-Hexen-3-yl acetate	hex-1-en-3-yl acetate	CCCC(C=C)OC(=O)C	green fruity rummy	OdorRactor ,TGSC
2681	Methyl 3-hydroxyhexanoate	methyl 3-hydroxyhexanoate	CCCC(CC(=0)OC)O	sweet woody ripe fruity ripe	Sigma Aldrich, TGSC,
	. y y y	y : y ::-::y:::::	((-//	tropical pineapple juicy oily ethereal winey	Odoractor

2682	Methyl R-3-acetoxyhexanoate	methyl (3R)-3- acetyloxyhexanoate	CCCC(CC(=O)OC)OC(=O)C	fruity green lettuce	OdorRactor ,TGSC
2683	Ethyl (S)-3-hydroxyhexanoate	ethyl (3S)-3-hydroxyhexanoate	CCCC(CC(=0)OCC)O	fruity grape burnt wood spicy	OdorRactor ,TGSC
				pineapple cranberry woody hay dusty burnt	, , , , , , , , , , , , , , , , , , , ,
2684	Ethyl 3-hydroxyhexanoate	ethyl 3-hydroxyhexanoate	CCCC(CC(=O)OCC)O	grape citrus smoky fresh fruity	Sigma Aldrich, Flavorbase,
ļ				woody spicy pineapple cranberry dusty burnt wood hay green sweet	TGSC, OdoRactor
ļ				strong winey burnt	
2685	4-Ethylheptanoic acid	4-ethylheptanoic acid	CCCC(CC)CCC(=0)O	goaty	TGSC
2686	3-Hexanol	hexan-3-ol	CCCC(CC)O	fusel green alcoholic medicinal ethereal tropical fruit pineapple	Sigma Aldrich, TGSC,OdoRactor
				apple cider	1 GSC, OdoRacioi
				rummy solvent fruity	
2687	3-Mercaptohexanal	3-sulfanylhexanal	CCCC(CC=O)S	onion green citrus tropical fruit	TGSC, Flavorbase
2688	3-(Methylthio)hexanal	3-methylsulfanylhexanal	CCCC(CC=O)SC	sharp fruity buttery green grassy privet fatty	OdorRactor ,TGSC
2000	o (wearynano)nomanar	, ,	0000(00 0)50		Suomantoi ,1 GBC
2689	S-(1-Oxohexan-3-yl)	S -(1-oxohexan-3-yl) ethanethioate	CCCC(CC=O)SC(=O)C	grapefruit citrus sweet	Flavorbase
2690	ethanethioate 1-Phenyl-2-pentanol	1-phenylpentan-2-ol	CCCC(CC1=CC=CC=C1)O	green sweet earthy	OdorRactor ,TGSC
2691	Cyclohexanepropanol, 2,2,6-	1-(2,2,6-	CCCC(CCC1C(CCCC1(C)C)C)O	dry sawdust woody powdery	OdorRactor ,TGSC
	trimethyl-alpha propyl-	trimethylcyclohexyl)hexan-3-ol		amber sandal wood	
2602	Ethyl 5-hydroxyoctanoate	ethyl 5-hydroxyoctanoate	CCCC(CCCC(=0)OCC)O	sweet fatty pineapple fruity apple	TGSC, Flavorbase
2692	Emyr 5-nydroxyoctanoate	emyr 5-nyuroxyocianoate		sweet ratty pineappie fruity apple	1 OSC, Flavoroase
2693	Ethyl 5-acetoxyoctanoate	ethyl 5-acetyloxyoctanoate	CCCC(CCCC(=O)OCC)OC(=O)C	musk fruity	TGSC
2694	(s) 2 Marcontohavanal	(2C) 2 culfonulhavan 1 al	CCCC(CCO)s	iviou fruity tranical fruit granafruit	TGSC
2094	(s)-3-Mercaptohexanol	(3S)-3-sulfanylhexan-1-ol	CCCC(CCO)S	juicy fruity tropical fruit grapefruit black currant buchu mango guava	1030
2695	3-Mercapto-1-hexanol	3-sulfanylhexan-1-ol	CCCC(CCO)S	sulfurous fruity tropical fruit	Flavornet, TGSC, OdoRactor
ļ				savory chicken meaty roasted coffee coffee	
ļ				roasted	
2696	3-(Methylthio)-1-hexanol	3-methylsulfanylhexan-1-ol	CCCC(CCO)SC	green melon vegetable earthy	Sigma Aldrich, TGSC,
ļ				pepper sulfurous metallic leafy pungent spicy	OdoRactor,
				wasabi	
2697	3-Mercaptohexyl acetate	3-sulfanylhexyl acetate	CCCC(CCOC(=O)C)S	boxtree floral fruity pear tropical	Flavornet, TGSC, OdoRactor
				blackberry raspberry black currant bud	
2698	3-(Methylthio)hexyl acetate	3-methylsulfanylhexyl acetate	CCCC(CCOC(=O)C)SC	sulfurous green spicy vegetable	Sigma Aldrich, TGSC,
				tropical pungent	OdoRactor
2699	3-(Acetylmercapto)hexyl acetate	3-acetylsulfanylhexyl acetate	CCCC(CCOC(=O)C)SC(=O)C	sulfurous metallic buchu catty sweet fruity tropical apricot peach	TGSC
ļ	acetate			green	
ļ				vegetable onion garlic burnt	
2500	227	0 10 11 11	aggavage av evage a	rubbery	o.t. p maga
2700	3-Mercaptohexyl butyrate	3-sulfanylhexyl butanoate	CCCC(CCOC(=O)CCC)S	sulfurous fruity tropical passion fruit tropical fruit ripe	OdorRactor ,TGSC
2701	2-Hexenoic acid, 2-methyl-	(E)-2-methylhex-2-enoic acid	CCCC=C(C)C(=O)O	fruity cheese	OdorRactor ,TGSC
2702	Butylidenephthalide	(3Z)-3-butylidene-2-benzofuran-1	CCCC=C1C2=CC=CC=C2C(=O)	herbaceous celery lovage	Sigma Aldrich, TGSC
2703	3-Hepten-2-one	one (E)-hept-3-en-2-one	O1 CCCC=CC(=O)C	herbaceous green vegetable coconut creamy grassy green nutty	Sigma Aldrich, TGSC,
2703	5-Hepten-2-one	(E)-nept-3-en-2-one	CCCC=CC(=0)C	wax caraway sweet fruity ketonic	OdoRactor
ļ				cheese	
2704	4 Octon 2 one (E)	oct-4-en-3-one	CCCC=CC(=O)CC	woody	OdorRactor ,TGSC
2704 2705	4-Octen-3-one, (E)- 2-Hexenoic acid	oct-4-en-3-one (E)-hex-2-enoic acid	CCCC=CC(=0)CC CCCC=CC(=0)0	coconut fruity fatty fruity musty sweet warm	Sigma Aldrich, TGSC,
				herbaceous	OdoRactor
2706	Methyl 2-hexenoate	methyl (E)-hex-2-enoate	CCCC=CC(=O)OC	fatty green fruity pineapple earthy	OdorRactor ,TGSC
2707	Methyl 2-hexenoate	methyl (E)-hex-2-enoate	CCCC=CC(=0)OC	fruity fatty green banana honey	SuperScent, TGSC,
2,01					OdoRactor
2708	Ethyl hex-2-enoate	ethyl (E)-hex-2-enoate	CCCC=CC(=O)OCC	green sweet fruity vegetable	OdorRactor ,TGSC,
2709	cis-3-Hexenyl trans-2-	[(Z)-hex-3-enyl] (E)-hex-2-enoate	CCCC=CC(=0)OCCC=CCC	rummy juicy green grassy fruity tropical pear	Flavorbase OdorRactor ,TGSC,
2107	hexenoate	L(2)-nex-3-enyij (15)-nex-2-enoate		kiwi berry artichoke melon apple	Flavorbase
				pineapple	
2710	trans-2-Hexenal dimethyl acetal	(E)-1,1-dimethoxyhex-2-ene	CCCC=CC(OC)OC	fruity apple	OdorRactor ,TGSC
2711	2-Hexene, 1,1-diethoxy-, (2E)-	(E)-1,1-diethoxyhex-2-ene	CCCC=CC(OCC)OCC	fruity green pepper dry rooty fatty	OdorRactor ,TGSC
		•		spicy celery caraway	·
	1,1-Diethoxyhex-2-ene	1,1-diethoxyhex-2-ene	CCCC=CC(OCC)OCC	green fruity apple	OdorRactor ,TGSC
2713	1,3,5,7-Undecatetraene, (Z,Z,E)-	undeca-1,3,5,7-tetraene	CCCC=CC=CC=C	woody earthy leafy galbanum	TGSC
2714	2,4-Octadienal	(2E ,4E)-octa-2,4-dienal	CCCC=CC=CC=O	fatty green vegetable seaweed	Sigma Aldrich, Flavornet,
				cucumber oily citrus melon pear	TGSC, OdoRactor
2715	2.4 Octodien 1 ol. (2E.4E)	(2F AF) note 2 A diam 1 of	CCCC-CC-CCO	peely fatty chicken creamy wax	OdorPactor TCSC
2/13	2,4-Octadien-1-ol, (2E,4E)-	(2E ,4E)-octa-2,4-dien-1-ol	CCCC=CC=CCO	rany chicken creamy wax	OdorRactor ,TGSC

2716	2-Hexenal	(E)-hex-2-enal	CCCC=CC=O	almond apple green vegetable plum sweet leafy banana aldehydic fatty cheese sharp fresh clean spicy herbaceous	Sigma Aldrich, Flavornet, TGSC, OdoRactor, Pubchem
2717	Hexenal	hex-2-enal	CCCC=CC=O	fatty rancid sweet bitter almond fruity green leafy apple plum vegetable bitter	Flavornet, TGSC,OdoRactor
2718	(Z)-2-Hexenal	(Z)-hex-2-enal	CCCC=CC=O	green fresh strong grassy	SuperScent, TGSC, Flavorbase
2719	(E)-4-Methyl-2-(pent-1-enyl)- 1,3-dioxolane	4-methyl-2-[(E)-pent-1-enyl]-1,3-dioxolane	CCCC=CC1OCC(O1)C	green fruity apple	TGSC
2720	Hept-3-enoic acid	hept-3-enoic acid	CCCC=CCC(=O)O	rancid	ADB
2721	Cyclopentanone, 2-(2-	2-[(E)-hex-2-enyl]cyclopentan-1-	CCCC=CCC1CCCC1=O	floral oily jasmine coconut milky	OdorRactor ,TGSC
2722	hexenyl)- Cyclopentanol, 2-(2-hexenyl)-	one 2-[(E)-hex-2-enyl]cyclopentan-1-	CCCC=CCC1CCCC1O	dairy floral green fruity natural wax	OdorRactor ,TGSC
2723	5-Nonen-2-one	ol (E)-non-5-en-2-one	CCCC=CCCC(=O)C	jasmine tropical banana fruity berry cheese dairy	OdorRactor ,TGSC,
				herbaceous	Flavorbase
2724	(E)-4-Octenoic acid	(E)-oct-4-enoic acid	CCCC=CCCC(=O)O	greasy	OdorRactor ,TGSC
2725	Methyl (Z)-oct-4-enoate	methyl (Z)-oct-4-enoate	CCCC=CCCC(=O)OC	fresh pineapple fruity	SuperScent, TGSC, OdoRactor
2726	Ethyl cis-4-octenoate	ethyl (Z)-oct-4-enoate	CCCC=CCCC(=0)OCC	fresh pineapple juicy pear fruity fatty green	OdorRactor ,TGSC, Flavorbase
2727	Ethyl trans-4-octenoate	ethyl (E)-oct-4-enoate	CCCC=CCCC(=O)OCC	fruity pear citrus	SuperScent, TGSC, Flavorbase, OdoRactor
2728	6-Decenoic acid	(E)-dec-6-enoic acid	CCCC=CCCCCC(=0)0	milky buttery dairy	TGSC
2729	(E)-6-Decenal	(E)-dec-6-enal	CCCC=CCCCCC=O	cucumber green	OdorRactor ,TGSC
2730	(Z)-6-Decenal	(Z)-dec-6-enal	CCCC=CCCCCC=O	tallow green cucumber	OdorRactor ,Flavornet, TGSC
2731	(Z)-4-Octen-1-ol	(Z)-oct-4-en-1-ol	CCCC=CCCCO	earthy sweet herbaceous	OdorRactor ,TGSC
2732	4-Octen-1-ol, acetate, (Z)-	acetic acid;oct-4-en-1-ol	CCCC=CCCCO.CC(=O)O	estery fishy fruity pear	TGSC
2733	cis-3-Hepten-1-ol	(Z)-hept-3-en-1-ol	CCCC=CCCO	green dry earthy grassy oily fatty wax herbaceous	Sigma Aldrich, TGSC, OdoRactor
2734	3-Hepten-1-ol, (3Z)-	hept-3-en-1-ol	CCCC=CCCO	resinous	TGSC
2735	cis-3-Heptenyl acetate	[(Z)-hept-3-enyl] acetate	CCCC=CCCOC(=O)C	green tropical banana vegetable fatty passion fruit	TGSC
2736	cis-2-Hexen-1-ol	(Z)-hex-2-en-1-ol	CCCC=CCO	alcoholic almond apple green vegetable leafy pepper winey fruit cortex green bean nasturtium herbaceous soapy aldehydic narcissus phenolic fresh fatty fusel whiskey	Sigma Aldrich, TGSC
2737	2-Hexen-1-OL	(E)-hex-2-en-1-ol	CCCC=CCO	apple unripe banana fatty green orange walnut herbaceous minty vegetable raspberry strawberry winey fruity leafy fresh herbaceous unripe fruit	Sigma Aldrich, TGSC, OdoRactor
2738	Hex-2-enyl acetate	hex-2-enyl acetate	CCCC=CCOC(=0)C	apple banana grape green sweet privet fresh wax peach pear pineapple strawberry leafy fruity strong	Sigma Aldrich, Flavorbase, TGSC, OdoRactor
2739	trans-2-Hexenyl acetate	[(E)-hex-2-enyl] acetate	CCCC=CCOC(=0)C	green privet fresh apple banana wax sweet leafy fruity	SuperScent, TGSC, OdoRactor
2740	(Z)-Hex-2-enyl acetate	[(Z)-hex-2-enyl] acetate	CCCC=CCOC(=O)C	green sweet privet fresh apple banana wax leafy fruity	OdorRactor ,TGSC
2741	trans-2-Hexenyl 2- methylbutyrate	[(E)-hex-2-enyl] 2- methylbutanoate	CCCC=CCOC(=O)C(C)CC	fruity	OdorRactor ,TGSC
2742	trans-2-Hexenyl salicylate	[(E)-hex-2-enyl] 2- hydroxybenzoate	CCCC=CCOC(=O)C1=CC=CC=C	green woody floral orchid balsamic	OdorRactor ,TGSC
2743	trans-2-Hexenyl propionate	[(E)-hex-2-enyl] propanoate	CCCC=CCOC(=0)CC	green fruity apple pear pulpy fruit creamy powdery unripe banana tropical rhubarb ripe apple ripe	OdorRactor, ,TGSC, Flavorbase
2744	trans-2-Hexenyl isovalerate	[(E)-hex-2-enyl] 3-methylbutanoate	CCCC=CCOC(=0)CC(C)C	green wax apple pear banana grape fresh cortex fusel vegetable fruity buttery tropical	OdorRactor ,TGSC, Flavorbase
2745	2-Hexenyl phenylacetate	[(E)-hex-2-enyl] 2-phenylacetate	CCCC=CCOC(=O)CC1=CC=CC=	green mossy rummy honey	OdorRactor ,TGSC, Flavorbase
2746	2-Hexenyl	[(E)-hex-2-enyl] 2-	CCCC=CCOC(=O)CC1CCCC1	fruity jasmine pear lactonic	OdorRactor ,TGSC
2747	cyclopentanylacetate trans-2-Hexenyl butyrate	cyclopentylacetate [(E)-hex-2-enyl] butanoate	CCCC=CCOC(=O)CCC	green fruity apricot ripe banana cortex orchid fermented apple fatty fresh	OdorRactor ,TGSC, Flavorbase
2748	trans-2-Hexenyl formate	[(E)-hex-2-enyl] formate	CCCC=CCOC=O	green fruity rummy	OdorRactor ,TGSC, Flavorbase
2749	Butyraldehyde	butanal	CCCC=O	apple chocolate creamy green meaty ethereal pear pungent cocoa musty malty bready fruity characteristic garbage sweet garbage	Sigma Aldrich, TGSC, PubChem

2750	2-Tert-butyl-5-methyl-2- propyl-2,5- dihydrofuran	5-tert -butyl-2-methyl-5-propyl- 2H -furan	CCCC1(C=CC(O1)C)C(C)(C)C	fruity black currant natural eucalyptus anisic buchu leafy green	TGSC, Flavorbase
2751	2,6-Dimethoxy-4-	2,6-dimethoxy-4-propylphenol	CCCC1=CC(=C(C(=C1)OC)O)O	phenolic	TGSC
2752	propylphenol 2-Methoxy-4-propylphenol	2-methoxy-4-propylphenol	CCCC1=CC(=C(C=C1)O)OC	anisic apricot clove fishy meaty oily spicy floral woody pepper sharp sweet powdery allspice soapy winey phenolic balsamic	Sigma Aldrich, Flavorbase, TGSC, OdoRactor
2753	4-Propylphenol	4-propylphenol	CCCC1=CC=C(C=C1)O	medicinal phenolic	Sigma Aldrich, TGSC,OdoRactor
2754	1-Methoxy-4-propylbenzene	1-methoxy-4-propylbenzene	CCCC1=CC=C(C=C1)OC	anisic herbaceous sweet licorice sassafrass fennel herbaceous root beer	Sigma Aldrich, TGSC, OdoRactor
2755	2-Propylphenol	2-propylphenol	CCCC1=CC=CC=C1O	medicinal smoky phenolic	Flavornet, TGSC,OdoRactor
2756	2-Propylpyridine	2-propylpyridine	CCCC1=CC=CC=N1	green minty floral roasted tobacco nutty fatty	Sigma Aldrich, TGSC, OdoRactor
2757	Dihydrosafrole	5-propyl-1,3-benzodioxole	CCCC1=CC2=C(C=C1)OCO2	spicy sassafrass	TGSC, Pubchem
2758	3-Propylpyridine	3-propylpyridine	CCCC1=CN=CC=C1	sweet musty beany earthy woody green	OdorRactor ,TGSC
2759	4,5-Dimethyl-2- propyloxazole	4,5-dimethyl-2-propyl-1,3-oxazole	CCCC1=NC(=C(O1)C)C	roasted burnt	OdorRactor ,TGSC
2760	2,5-Dimethyl-3- propylpyrazine	2,5-dimethyl-3-propylpyrazine	CCCC1=NC(=CN=C1C)C	nutty hazelnut	TGSC
2761	3,5-Dimethyl-2- propylpyrazine	3,5-dimethyl-2-propylpyrazine	CCCC1=NC=C(N=C1C)C	nutty hazelnut burnt	TGSC
2762	2-Propylpyrazine	2-propylpyrazine	CCCC1=NC=CN=C1	green nutty vegetable hazelnut roasted barley corn roasted barley	Sigma Aldrich, TGSC, Flavorbase, Pubchem, OdoRactor
2763	2-Methyl-3-propylpyrazine	2-methyl-3-propylpyrazine	CCCC1=NC=CN=C1C	nutty	OdorRactor ,TGSC
2764	2-Methoxy-3-propylpyrazine	2-methoxy-3-propylpyrazine	CCCC1=NC=CN=C1OC	earthy bellpepper raw raw potato galbanum	OdorRactor ,TGSC
2765	2-Propylthiazole	2-propyl-1,3-thiazole	CCCC1=NC=CS1	green vegetable herbaceous nutty	Flavorbase, TGSC
2766	1-Phenyl-3-propyl-pyrazole	1-phenyl-3-propylpyrazole	CCCC1=NN(C=C1)C2=CC=CC= C2	roasted cooked	TGSC
2767	3-Propylbicyclo[2.2.1]hept-5- ene-2- carbaldehyde	3-propylbicyclo[2.2.1]hept-5-ene- 2-carbaldehyde	CCCC1C2CC(C1C=O)C=C2	green aldehydic sweaty chrysanthemum wet	OdorRactor ,TGSC
2768	3-Methyl-5-propyl-2- cyclohexen-1-one	3-methyl-5-propylcyclohex-2-en-1- one	CCCC1CC(=CC(=O)C1)C	herbaceous fresh celery green cumin	OdorRactor ,TGSC
2769	Clarycet	(4-methyl-2-propyloxan-4-yl) acetate	CCCC1CC(CCO1)(C)OC(=O)C	herbaceous clary sage saffron tea fruity floral	OdorRactor ,TGSC
2770	2,6-Dipropyl-5,6-dihydro-2H- thiopyran-3- carbaldehyde	2,6-dipropyl-3,6-dihydro-2 <i>H</i> - thiopyran-5- carbaldehyde	CCCC1CC=C(C(S1)CCC)C=O	green mango tropical	TGSC
2771	gamma-Heptalactone	5-propyloxolan-2-one	CCCC1CCC(=0)01	caramel coconut herbaceous sweet fatty nutty fruit tonka hay coumarinic lactonic creamy powdery	Sigma Aldrich, Flavorbase, TGSC, OdoRactor
2772	(5S)-5-Propyloxolan-2-one	(5S)-5-propyloxolan-2-one	CCCC1CCC(=0)O1	fatty coconut fruity sweet	TGSC
2773	(5R)-5-Propyloxolan-2-one	(5R)-5-propyloxolan-2-one	CCCC1CCC(=O)O1	sweet spicy herbaceous hay coumarinic	TGSC
2774	delta-Octalactone	6-propyloxan-2-one	CCCC1CCCC(=0)01	buttery coconut peach sweet fatty tonka tropical dairy creamy coumarinic green lactonic	Sigma Aldrich, TGSC,OdoRactor
2775	cis-2-Methyl-4-propyl-1,3- oxathiane	(2R,4S)-2-methyl-4-propyl-1,3-oxathiane	CCCC1CCOC(S1)C	green tropical galbanum pineapple	OdorRactor ,TGSC
2776	trans-2-Methyl-4-propyl-1,3- oxathiane	(2R, 4R)-2-methyl-4-propyl-1,3-oxathiane	CCCC1CCOC(S1)C	passion fruit tropical sulfurous green onion garlic	OdorRactor ,TGSC, Flavorbase
2777	2-Methyl-4-propyl-1,3- oxathiane	2-methyl-4-propyl-1,3-oxathiane	CCCC1CCOC(S1)C	strong green passion fruit black currant galbanum pineapple tropical sulfurous fruity onion	Sigma Aldrich, Flavorbase, TGSC, Pubchem
2778	4-Methyl-2-propyl-1,3- oxathiane	4-methyl-2-propyl-1,3-oxathiane	CCCC1OCCC(S1)C	onion garlic fruity sweet lychee pear	TGSC, Flavorbase
2779	2-Butyl-2-butenal	(2Z)-2-ethylidenehexanal	CCCCC(=CC)C=O	roasted cooked	OdorRactor ,TGSC
2780	alpha-Butylcinnamaldehyde	(2E)-2-benzylidenehexanal	CCCCC(=CC1=CC=CC=C1)C=O	floral green jasmine lily herbaceous	OdorRactor ,TGSC
2781	2-Hexanone	hexan-2-one	CCCCC(=O)C	pungent acetone characteristic fruity fungal meaty buttery	AOD, TGSC, Pubchem,OdoRactor
2782	2,3-Heptanedione	heptane-2,3-dione	CCCCC(=O)C(=O)C	apple berry buttery cheese oily pineapple yogurt	Sigma Aldrich, TGSC, OdoRactor
2783	2-Methyl-3-heptanone	2-methylheptan-3-one	CCCCC(=O)C(C)C	fruity green leafy	TGSC, OdoRactor
2784	4-Sulfanylnonan-5-one	4-sulfanylnonan-5-one	CCCCC(=0)C(CCC)S	green fruity grapefruit minty leafy	TGSC
2785	4-((2-Methyl-3-furyl)thio)-5- nonanone	4-(2-methylfuran-3- yl)sulfanylnonan-5-one	CCCCC(=O)C(CCC)SC1=C(OC=C1)C	roasted meat meaty	OdorRactor ,TGSC
2786	1-Hepten-3-one	hept-1-en-3-one	CCCCC(=0)C=C	metallic	Flavornet

2787	Propenyl butyl ketone	(E)-oct-2-en-4-one	CCCCC(=0)C=CC	yeasty jammy tropical fruity mushroom metallic bready pineapple horseradish earthy	OdorRactor ,TGSC
2788	Valerophenone	1-phenylpentan-1-one	CCCCC(=0)C1=CC=CC=C1	valerian root root balsamic	OdorRactor ,TGSC
2789	2-Pentanoylfuran	1-(furan-2-yl)pentan-1-one	CCCCC(=0)C1=CC=CO1	sweet caramel fruity	OdorRactor ,TGSC
2790	3-Heptanone	heptan-3-one	CCCC(=0)CC	fatty green ethereal fruity sweet	Sigma Aldrich, AOD,
	-	•	, ,	ketonic musty cheese	TGSC,OdoRactor
2791	Valeric acid	pentanoic acid	CCCCC(=O)O	cheese acidic rancid fatty earthy	Sigma Aldrich, AOD,
				sweaty sharp sour milky tobacco	Flavorbase, TGSC,
				fruity	OdoRactor, Pubchem
				unpleasant penetrating sewage	
2792	Endo-1,7,7-	[(2R)-1,7,7-trimethyl-2-	CCCCC(=O)O[C@@H]1CC2CC	woody sawdust berry seedy spice	OdorRactor ,TGSC
	trimethylbicyclo[2.2.1]hept-2-yl valerate	bicyclo[2.2.1]heptanyl] pen	C1(C2(C) C)C	camphoraceous	
2793	Methyl valerate	methyl pentanoate	CCCCC(=0)OC	fruity nutty sweet green apple	Sigma Aldrich,
				pineapple tutti frutti juicy bubblegum sweaty estery	TGSC,OdoRactor
2794	1-Methyl-1-(4-	2-(4-methylcyclohex-3-en-1-	CCCCC(=O)OC(C)(C)C1CCC(=C		OdorRactor ,TGSC
2194	methylcyclohex-3-enyl)ethyl valerate	yl)propan-2-yl pentanoate	C1)C	inuity norai	Odorkacioi ,103C
2705		2.7. finantialism 1.6 fina.2 at	GGGGG(, D)OG(G)(GGG, G(G)G)	siamo la conde Cosian e di ca	Flores A TOSC O La Posta
2795	Linalyl valerate	3,7-dimethylocta-1,6-dien-3-yl	CCCCC(=O)OC(C)(CCC=C(C)C)	citrus lavender fruity apricot	Flavornet, TGSC, OdoRactor
		pentanoate	C=C		
2796	Isopropyl valerate	propan-2-yl pentanoate	CCCCC(=0)OC(C)C	fruity pineapple	TGSC
2797	Bornyl valerate	(1,7,7-trimethyl-2-		woody sawdust berry seedy spice	SuperScent, TGSC,
		bicyclo[2.2.1]heptanyl) pentanoate)C)C	camphoraceous	OdoRactor
2798	Ethyl valerate	ethyl pentanoate	CCCCC(=O)OCC	apple yeasty sweet fruity pineapple	Sigma Aldrich, Flavorbase,
				green tropical acidic berry strong	TGSC,OdoRactor
2799	Isobutyl valerate	2-methylpropyl pentanoate	CCCCC(=0)OCC(C)C	ethereal fruity apple sweet	OdorRactor ,TGSC, Flavorbase
2800	Allyl valerate	prop-2-enyl pentanoate	CCCCC(=O)OCC=C	pineapple	TGSC
2801	Geranyl valerate	[(2E)-3,7-dimethylocta-2,6-		rose fruit pineapple floral apple	Flavornet, TGSC, Flavorbase,
2801	Geranyi valerate				OdoRactor
2002	0.77	dienyl] pentanoate)C	tobacco	
2802	trans-2-Hexenyl valerate	[(E)-hex-2-enyl] pentanoate	CCCCC(=0)OCC=CCCC	green fruity apple banana pineapple cognac estery unripe banana winey unripe fruit	OdorRactor ,TGSC, Flavorbase
2803	Benzyl valerate	benzyl pentanoate	CCCCC(=0)OCC1=CC=CC=C1	fruity floral apple strong faint musk tobacco	OdorRactor ,TGSC
2804	Furfuryl pentanoate	furan-2-ylmethyl pentanoate	CCCCC(=O)OCC1=CC=CO1	musty fruity sweet pineapple apple tropical cheese ripe caramel	Sigma Aldrich, TGSC, OdoRactor
2805	Propyl valerate	propyl pentanoate	CCCCC(=O)OCCC	ethereal fruity pineapple metallic animal	SuperScent, TGSC
2806	Isoamyl valerate	3-methylbutyl pentanoate	CCCCC(=0)OCCC(C)C	fruity apple green ripe	OdorRactor ,TGSC
2807	Citronellyl valerate	3,7-dimethyloct-6-enyl		warm honey herbaceous rose floral	
2007	Chronolly valerate	pentanoate	C	warm noney neroaceous rose moral	racyonaci, rese, eueriaeier
2808	cis-3-	hex-3-enyl pentanoate	CCCCC(=0)OCCC=CCC	apple green fruity pear kiwi unripe	ADR TGSC
2000	HEXENYLVALERATE	nex-5-enyi pentanoate	CCCCC(-0)0CCC-CCC	banana tropical estery fresh grape unripe fruit	ADB, TOSC
2809	(E)-Hex-3-enyl valerate	[(E)-hex-3-enyl] pentanoate	CCCCC(=0)OCCC=CCC	green fruity apple pear kiwi unripe banana tropical estery fresh grape buttery	OdorRactor ,TGSC, Flavorbase
				juicy unripe fruit	
2810	cis-3-Hexenyl valerate	[(Z)-hex-3-enyl] pentanoate	CCCCC(=0)OCCC=CCC	green fruity vegetable apple pear kiwi unripe banana tropical estery fresh grape banana unripe fruit	Sigma Aldrich, TGSC, OdoRactor
2811	Phenethyl valerate	2-phenylethyl pentanoate	CCCCC(=0)OCCC1=CC=CC=C1	floral fruity rose leafy	SuperScent, TGSC, OdoRactor
2812	Butyl valerate	butyl pentanoate	CCCCC(=0)OCCCC	apple ethereal raspberry sweet fruity pineapple green tropical tutti frutti	TGSC
				11111111	İ
2813	3-Phenylpropyl valerate	3-phenylpropyl pentanoate	CCCCC(=0)OCCCC1=CC=CC=	fruity strawberry floral	OdorRactor ,TGSC
2813 2814	3-Phenylpropyl valerate 2-Phenylhexanenitrile	3-phenylpropyl pentanoate 2-phenylhexanenitrile		fruity strawberry floral orchid clover balsamic narcissus	OdorRactor ,TGSC OdorRactor ,TGSC
2814	2-Phenylhexanenitrile	2-phenylhexanenitrile	C1 CCCCC(C#N)C1=CC=CC=C1	fruity strawberry floral orchid clover balsamic narcissus storax	OdorRactor ,TGSC
2814 2815	2-Phenylhexanenitrile Ethyl 2-acetylhexanoate	2-phenylhexanenitrile ethyl 2-acetylhexanoate	C1 CCCCC(C#N)C1=CC=CC=C1 CCCCC(C(=0)C)C(=0)OCC	fruity strawberry floral orchid clover balsamic narcissus storax fruity winey	OdorRactor ,TGSC TGCS
2814 2815 2816	2-Phenylhexanenitrile Ethyl 2-acetylhexanoate Ethyl 2-hydroxyhexanoate	2-phenylhexanenitrile ethyl 2-acetylhexanoate ethyl 2-hydroxyhexanoate	C1 CCCCC(C#N)C1=CC=CC=C1 CCCCC(C(=0)C)C(=0)OCC CCCCC(C(=0)OCC)O	fruity strawberry floral orchid clover balsamic narcissus storax fruity winey green fruity	OdorRactor ,TGSC TGCS Sigma Aldrich
2814 2815 2816 2817	2-Phenylhexanenitrile Ethyl 2-acetylhexanoate Ethyl 2-hydroxyhexanoate 4-Methyl-5-nonanol	2-phenylhexanenitrile ethyl 2-acetylhexanoate ethyl 2-hydroxyhexanoate 4-methylnonan-5-ol	C1 CCCCC(C#N)C1=CC=CC=C1 CCCCC(C(=0)C)C(=0)OCC CCCCC(C(=0)OCC)O CCCCC(C(C)CCC)O	fruity strawberry floral orchid clover balsamic narcissus storax fruity winey green fruity spicy herbaceous	OdorRactor ,TGSC TGCS Sigma Aldrich TGSC
2814 2815 2816 2817 2818	2-Phenylhexanenitrile Ethyl 2-acetylhexanoate Ethyl 2-hydroxyhexanoate 4-Methyl-5-nonanol 4-Sulfanylnonan-5-ol	2-phenylhexanenitrile ethyl 2-acetylhexanoate ethyl 2-hydroxyhexanoate 4-methylnonan-5-ol 4-sulfanylnonan-5-ol	C1 CCCCC(C#N)C1=CC=CC=C1 CCCCCC(C(=0)C)C(=0)OCC CCCCC(C(=0)OCC)O CCCCC(C(C)CCC)O CCCCC(C(C)CCC)O	fruity strawberry floral orchid clover balsamic narcissus storax fruity winey green fruity spicy herbaceous grapefruit bellpepper	OdorRactor ,TGSC TGCS Sigma Aldrich TGSC TGSC
2814 2815 2816 2817 2818 2819	2-Phenylhexanenitrile Ethyl 2-acetylhexanoate Ethyl 2-hydroxyhexanoate 4-Methyl-5-nonanol 4-Sulfanylnonan-5-ol 2,2-Dimethyl-1-hexanol	2-phenylhexanenitrile ethyl 2-acetylhexanoate ethyl 2-hydroxyhexanoate 4-methylnonan-5-ol 4-sulfanylnonan-5-ol 2,2-dimethylhexan-1-ol	C1 CCCCC(C#N)C1=CC=CC=C1 CCCCC(C(=0)C)C(=0)OCC CCCCC(C(=0)OCC)O CCCCC(C(C)CCC)O CCCCC(C(CCC)S)O CCCCC(C(CCC)SO	fruity strawberry floral orchid clover balsamic narcissus storax fruity winey green fruity spicy herbaceous grapefruit bellpepper herbaceous pungent	OdorRactor ,TGSC TGCS Sigma Aldrich TGSC TGSC TGSC
2814 2815 2816 2817 2818	2-Phenylhexanenitrile Ethyl 2-acetylhexanoate Ethyl 2-hydroxyhexanoate 4-Methyl-5-nonanol 4-Sulfanylnonan-5-ol 2.2-Dimethyl-1-hexanol 2-Methylhexanoic acid	2-phenylhexanenitrile ethyl 2-acetylhexanoate ethyl 2-hydroxyhexanoate 4-methylnonan-5-ol 4-sulfanylnonan-5-ol	C1 CCCCC(C#N)C1=CC=CC=C1 CCCCCC(C(=0)C)C(=0)OCC CCCCC(C(=0)OCC)O CCCCC(C(C)CCC)O CCCCC(C(C)CCC)O	fruity strawberry floral orchid clover balsamic narcissus storax fruity winey green fruity spicy herbaceous grapefruit bellpepper herbaceous pungent lard fruity cheese oily fatty acidic chicken roasted savory	OdorRactor ,TGSC TGCS Sigma Aldrich TGSC TGSC TGSC Sigma Aldrich, TGSC, OdoRactor,
2814 2815 2816 2817 2818 2819	2-Phenylhexanenitrile Ethyl 2-acetylhexanoate Ethyl 2-hydroxyhexanoate 4-Methyl-5-nonanol 4-Sulfanylnonan-5-ol 2,2-Dimethyl-1-hexanol	2-phenylhexanenitrile ethyl 2-acetylhexanoate ethyl 2-hydroxyhexanoate 4-methylnonan-5-ol 4-sulfanylnonan-5-ol 2,2-dimethylhexan-1-ol	C1 CCCCC(C#N)C1=CC=CC=C1 CCCCC(C(=0)C)C(=0)OCC CCCCC(C(=0)OCC)O CCCCC(C(C)CCC)O CCCCC(C(CCC)S)O CCCCC(C(CCC)SO	fruity strawberry floral orchid clover balsamic narcissus storax fruity winey green fruity spicy herbaceous grapefruit bellpepper herbaceous pungent lard fruity cheese oily fatty acidic	OdorRactor ,TGSC TGCS Sigma Aldrich TGSC TGSC TGSC Sigma Aldrich, TGSC,

2823	Octanoic acid, 4-methyl-, (4S)-	(4S)-4-methyloctanoic acid	CCCCC(C)CCC(=O)O	mutton goaty meaty	TGSC,
2824	(R)-(-)-2-Hexanol	(2R)-hexan-2-ol	CCCCC(C)O	earthy mushroom dusty oily	TGSC
	(S)-(+)-2-Hexanol	(2S)-hexan-2-ol	CCCCC(C)O	earthy mushroom green ripe berry astringent metallic	TGSC
2826	2-Hexanol	hexan-2-ol	CCCCC(C)O	winey grassy chemical fruity fatty	Sigma Aldrich, ADB,
2025	43444		agaggga og cola	terpenic cauliflower	TGSC,OdoRactor
	1-Methylpentyl acetate	hexan-2-yl acetate	CCCCC(C)OC(=0)C	fruity apple pear sour	TGSC TGSC
	2-Hexanol butanoate 1-Hepten-3-OL	hexan-2-yl butanoate hept-1-en-3-ol	CCCCC(C)OC(=0)CCC CCCCC(C=C)O	banana fruity fleshy ripe tomato buttery oily green metallic	Sigma Aldrich, TGSC,
2029	1-Hepten-5-OL	пере-1-еп-3-от	CCCC(C=C)0	spicy acrylate earthy fruity mushroom	OdoRactor
2830	Oct-2-en-4-ol	oct-2-en-4-ol	CCCCC(C=CC)O	fruity berry	OdorRactor,
	2-Octen-4-ol	(E)-oct-2-en-4-ol	CCCCC(C=CC)O	fruity berry	SuperScent, TGSC, OdoRactor
	Methyl 2-butyl-2- ethylhexanoate	methyl 2-butyl-2-ethylhexanoate	CCCCC(CC)(CCCC)C(=0)OC	fatty	TGSC
	2-Ethylhexanoic acid	2-ethylhexanoic acid	CCCCC(CC)C(=O)O	cucumber mild	Sigma Aldrich, Pubchem
	(R)-2-Ethylhexanoic acid	(2R)-2-ethylhexanoic acid	CCCC(CC)C(=0)O	herbaceous earthy	TGSC
	(S)-2-Ethylhexanoic acid	(2S)-2-ethylhexanoic acid	CCCC(CC)C(=O)O	sweet herbaceous musty	TGSC
	Ethyl 2-ethylhexanoate	ethyl 2-ethylhexanoate	CCCC(CC)C(=0)OCC	orris fruity herbaceous cumin fresh carrot	
2837	2-Octenoic acid, 4-ethyl-, (2Z)-	(Z)-4-ethyloct-2-enoic acid	CCCCC(CC)C=CC(=O)O	fatty	ADB
2838	1,3-Dioxolane, 2-(1-	2-heptan-3-yl-1,3-dioxolane	CCCCC(CC)C1OCCO1	green fruity radish gardenia	OdorRactor ,TGSC,
	ethylpentyl)-	Y J /-		metallic chrysanthemum	Flavorbase
				herbaceous vegetable	
				woody	
2839	4-Ethyloctanoic acid	4-ethyloctanoic acid	CCCCC(CC)CCC(=0)0	fatty goaty mutton	OdorRactor,
2840	4-Ethyloctanoic acid	4-ethyloctanoic acid	CCCC(CC)CCC(=O)O	meaty fatty goaty lamb mutton	Sigma Aldrich, TGSC
2841	4-Ethyloctanal	4-ethyloctanal	CCCCC(CC)CCC=O	floral wax fatty milky lactonic citrus fruity orange	TGSC, Flavorbase
2842	2-Ethylhexan-1-ol	2-ethylhexan-1-ol	CCCCC(CC)CO	oily rose sweet green citrus fresh floral mild	Sigma Aldrich, TGSC, OdoRactor, Pubchem
2843	2-Ethylhexyl acetate	2-ethylhexyl acetate	CCCCC(CC)COC(=0)C	earthy herbaceous humus dirty pleasant	Sigma Aldrich, TGSC, Pubchem
2844	2-Ethylhexyl benzoate	2-ethylhexyl benzoate	CCCCC(CC)COC(=0)C1=CC=C C=C1	ethereal	TGSC
2845	2-Ethylhexyl salicylate	2-ethylhexyl 2-hydroxybenzoate	CCCCC(CC)COC(=0)C1=CC=C C=C10	orchid sweet balsamic floral	Sigma Aldrich, TGSC, OdoRactor, Pubchem
2846	2-Ethylhexyl propionate	2-ethylhexyl propanoate	CCCCC(CC)COC(=0)CC	winey pear grape	TGSC
	2-Ethylhexyl 3- mercaptopropionate	2-ethylhexyl 3-sulfanylpropanoate	CCCCC(CC)COC(=O)CCS	sulfurous tropical fruit savory	Flavorbase
	2-Ethyl-1-hexanethiol	2-ethylhexane-1-thiol	CCCCC(CC)CS	sulfurous alliaceous roasted vegetable meaty tropical roasted	OdorRactor ,Flavorbase
2849	3-Heptanol	heptan-3-ol	CCCCC(CC)O	banana buttery coffee green meaty minty herbaceous herbaceous bitter pungent	Sigma Aldrich, TGSC,OdoRactor
2850	(3S)-Heptan-3-ol	(3S)-heptan-3-ol	CCCCC(CC)O	lavender medicinal	TGSC
		heptan-3-yl acetate	CCCCC(CC)OC(=O)C	sweet floral rose pear	OdorRactor ,TGSC
	3-(Methylthio)heptanal	3-methylsulfanylheptanal	CCCC(CC=O)SC	cooked roasted fatty green	OdorRactor ,TGSC
	3-Mercaptoheptyl acetate	3-sulfanylheptyl acetate	CCCC(CCOC(=O)C)S	fruit peach citrus tea	OdorRactor ,Flavorbase
	, , ,	(3S)-1-methoxyheptane-3-thiol	CCCCC(CCOC)S	sulfurous black currant green tropical fruit	Flavorbase, TGSC
2855	3-(Hydroxymethyl)heptan-2- one	3-(hydroxymethyl)heptan-2-one	CCCCC(CO)C(=O)C	fruity herbaceous spicy	OdorRactor ,TGSC
2856	Valeraldehyde dibutyl acetal	1,1-dibutoxypentane	CCCCC(OCCCC)OCCCC	sweet nutty	OdorRactor ,TGSC
2857	(2E,5Z)-2,5-Undecadien-1-ol	(2E ,5Z)-undeca-2,5-dien-1-ol	CCCCC/C=C\C/C=C/CO	fatty wax	TGSC
2858	cis-4-Decenal	(Z)-dec-4-enal	CCCCC/C=C\CCC=O	citrus aldehydic orange watery cardamom	OdorRactor,
2859	(2S)-2-Methylheptanoate	(2S)-2-methylheptanoate	CCCCC[C@H](C)C(=O)[O-]	wax green cheese sweaty buttermilk	OdorRactor ,TGSC
2960	2-Heptenal, 2-ethyl-	(E)-2-ethylhept-2-enal	CCCCC=C(CC)C=O	sharp green	OdorRactor ,TGSC
2860	Bovolide	(5E)-3,4-dimethyl-5- pentylidenefuran-2-one	CCCCC=C1C(=C(C(=O)O1)C)C	spicy herbaceous minty celery lovage dairy lactonic	TGSC
	Bovonde	pentyndeneruran-2-one		berry buttery green lemon spicy	Sigma Aldrich, Flavornet,
2861	3-Octen-2-one	(E)-oct-3-en-2-one	CCCCC=CC(=0)C	nutty herbaceous earthy sweet herbaceous mushroom hay blueberry oily ketonic	TGSC
2861 2862 2863	3-Octen-2-one (Z)-3-Octen-2-one	1 0	CCCCC=CC(=0)C	nutty herbaceous earthy sweet herbaceous mushroom hay	
2861 2862 2863	3-Octen-2-one	(E)-oct-3-en-2-one		nutty herbaceous earthy sweet herbaceous mushroom hay blueberry oily ketonic	TGSC

2866	trans,trans-2,4-Nonadienal	(2E ,4E)-nona-2,4-dienal	CCCCC=CC=CC=O	fishy fatty green meaty melon floral vegetable wax watermelon violet leaf cucumber tropical fruit chicken strong violet	Sigma Aldrich, Flavornet, AOD, TGSC, Flavorbase, OdoRactor
2867	(E,Z)-2,4-Nonadienal	(2E ,4Z)-nona-2,4-dienal	CCCCC=CC=CC=O	geranium pungent	Flavornet
2868	Nona-2,4-dien-1-ol	nona-2,4-dien-1-ol	CCCCC=CC=CCO	wax fatty green melon cucumber vegetable chicken aldehydic	OdorRactor ,TGSC, Flavorbase
2869	2-Heptenal	(E)-hept-2-enal	CCCCC=CC=O	apple fatty green lemon spicy soapy almond pungent vegetable fresh oily fruity	Sigma Aldrich, Flavornet, TGSC, OdoRactor
	5-(Hex-1-EN-1-YL)-4- methyloxolan-2-one	5-hex-1-enyl-4-methyloxolan-2- one	CCCCC=CC1C(CC(=0)01)C	green nutty milky lactonic	Flavorbase
	3-Octenoic acid	(E)-oct-3-enoic acid	CCCCC=CCC(=O)O	oily fatty	OdorRactor ,TGSC
2872	Ethyl oct-3-enoate	ethyl (E)-oct-3-enoate	CCCCC=CCC(=0)OCC	fruity fatty winey tropical pineapple passion fruit	OdorRactor ,TGSC, Flavorbase
2873	Ethyl 3-octenoate	ethyl oct-3-enoate	CCCCC=CCC(=O)OCC	fruity tropical winey fatty pineapple passion fruit	TGSC, Flavorbase
2874	trans-4-Nonenal	(E)-non-4-enal	CCCCC=CCCC=O	fruity	OdorRactor,
	5-Decenoic acid	(E)-dec-5-enoic acid	CCCCC=CCCCC(=0)0	buttery milky fatty	OdorRactor ,TGSC
	(Z)-5-Decenoic acid	(Z)-dec-5-enoic acid	CCCCC=CCCCC(=0)0	fatty green	TGSC
2877	1-Butyl-5-carboxypentyl 5- decenoate	6-[(E)-dec-5-enoyl]oxydecanoic acid	CCCCC=CCCCC(=0)OC(CCCC) CCCCC(=0)O	milky green fruity jasmine lactonic gardenia peach	TGSC
2878	9-Tetradecen-5-olide	6-non-4-enyloxan-2-one	CCCCC=CCCCC1CCCC(=0)01	fruit buttery dairy	Flavorbase
2879	Undecenoic acid, 3- methylbutyl ester	3-methylbutyl (E)-undec-6-enoate	CCCCC=CCCCCC(=0)OCCC(C)	floral rose wax	OdorRactor ,TGSC
2880	(Z)-11-Hexadecenal	(Z)-hexadec-11-enal	CCCCC=CCCCCCCCCCC=O	wax	TGSC
2881	(Z)-13-Octadecenal	(Z)-octadec-13-enal	CCCCC=CCCCCCCCCCCC=O	wax	TGSC
2882	Z-5-Decen-1-ol	(Z)-dec-5-en-1-ol	CCCCC=CCCCCO	wax fatty rose	OdorRactor ,TGSC
2883	(E)-5-Decen-1-ol	(E)-dec-5-en-1-ol	CCCCC=CCCCCO	wax floral rose	TGSC
2884	cis-3-Octen-1-ol	(Z)-oct-3-en-1-ol	CCCCC=CCCO	fatty fresh greasy melon green cortex herbaceous earthy fusel spicy	OdorRactor ,TGSC
2885	cis-3-Octenyl propionate	[(Z)-oct-3-enyl] propanoate	CCCCC=CCCOC(=0)CC	pear honeydew melon fruity green cortex cantaloupe artichoke	OdorRactor ,TGSC
2886	trans-2-Hepten-1-ol	(E)-hept-2-en-1-ol	CCCCC=CCO	pungent fatty plastic green	OdorRactor ,TGSC
2887	trans-2-Heptenyl acetate	[(E)-hept-2-enyl] acetate	CCCCC=CCOC(=O)C	fruity sweet wax tropical kiwi pineapple	OdorRactor ,TGSC
2888	Pentanal	pentanal	CCCCC=O	fruity woody nutty vanilla malty almond pungent acrid strong fermented bready berry powerful	Sigma Aldrich, AOD, TGSC, OdoRactor, Pubchem
2889	2(3H)-Furanone, 5,5- dibutyldihydro-	5,5-dibutyloxolan-2-one	CCCCC1(CCC(=0)01)CCCC	oily coconut buttery	OdorRactor ,TGSC
2890	2H-Pyran-2-one, 5-butyl-5- ethyltetrahydro-	5-butyl-5-ethyloxan-2-one	CCCCC1(CCC(=0)OC1)CC	warm costus fatty animal root coconut	OdorRactor ,TGSC
2891	4-Butyl-5-methylthiazole	4-butyl-5-methyl-1,3-thiazole	CCCCC1=C(SC=N1)C	green bellpepper	TGSC, Pubchem
2892	2-Butyl-5-ethylthiophene	2-butyl-5-ethylthiophene	CCCCC1=CC=C(S1)CC	fruity berry earthy	OdorRactor ,TGSC
2893	2-Butylfuran	2-butylfuran	CCCCC1=CC=CO1	spicy fruity winey sweet	SuperScent, TGSC, OdoRactor
2894	2-Butylthiophene	2-butylthiophene	CCCCC1=CC=CS1	fruity floral milky fried chicken	TGSC
2895 2896	5-Butyloxazole 4-Butylthiazole	5-butyl-1,3-oxazole 4-butyl-1,3-thiazole	CCCCC1=CN=CO1 CCCCC1=CSC=N1	bacon fatty animal meaty green herbaceous minty vegetable	TGSC TGSC
2897	2-Butyl-3,5-dimethylpyrazine	2-butyl-3,5-dimethylpyrazine	CCCCC1=NC=C(N=C1C)C	sweet earthy	TGSC
2898	2-Butyl-3-methylpyrazine	2-butyl-3-methylpyrazine	CCCCC1=NC=CN=C1C	anisic licorice	OdorRactor ,TGSC
2899	5-Butyl-4-methyldihydro- 2(3H)-furanone, cis-(-)-	(4S,5S)-5-butyl-4-methyloxolan- 2-one	CCCCC1C(CC(=0)01)C	coconut	Flavornet
2900	Whiskey lactone	5-butyl-4-methyloxolan-2-one	CCCCC1C(CC(=0)01)C	coconut green tonka coumarinic toasted nutty celery burnt lactonic woody maple lovage	Sigma Aldrich, Flavorbase, TGSC, OdoRactor
2901	trans-3-Methyl-4-octanolide	(4S, 5R)-5-butyl-4-methyloxolan-2-one	CCCCC1C(CC(=O)O1)C	floral lactonic coconut	Flavornet
2902	cis-3-Methyl-4-octanolide	(4R,5R)-5-butyl-4-methyloxolan-2-one	, , , ,	spice sweet coconut vanilla	Flavornet, TGSC, OdoRactor
	2,3-Epoxyheptanal	3-butyloxirane-2-carbaldehyde	CCCCC1C(O1)C=O	citrus fatty green	OdorRactor ,TGSC
2904	6-Butyl-3,6-dihydro-2,4- dimethyl-2H-pyran	6-butyl-2,4-dimethyl-3,6-dihydro- 2 <i>H</i> -pyran	CCCCC1C=C(CC(O1)C)C	floral green earthy spicy geranium vegetable	OdorRactor ,TGSC
	3-N-Butyl-4,5- dihydrophthalide	3-butyl-4,5-dihydro-3 <i>H</i> -2- benzofuran-1-one	1	herbaceous celery	TGSC
2906	Butylphthalide	3-butyl-3 <i>H</i> -2-benzofuran-1-one	CCCCC1C2=CC=CCC(=O)O	herbaceous phenolic celery	OdorRactor ,TGSC

2907	Sedanolide	3-butyl-3a ,4,5,6-tetrahydro-3H -	CCCCC1C2CCCC=C2C(=O)O1	herbaceous celery	TGSC
2908	3-Acetyl-5-butyldihydro-	2-benzofuran-1- one (3R, 5S)-3-acetyl-5-butyloxolan-	CCCC1CC(C(=0)O1)C(=0)C	floral jasmine gardenia tuberose	OdorRactor ,TGSC
	2(3H)-furanone	2-one			
2909	gamma-Octalactone	5-butyloxolan-2-one	CCCCC1CCC(=0)01	caramel fruity almond coconut creamy herbaceous peach sweet wax tonka dairy fatty milky soapy coumarinic apricot spicy green	Sigma Aldrich, TGSC
2910	delta-Nonalactone	6-butyloxan-2-one	CCCCCICCCC(=0)01	apricot buttery meaty nutty sweet winey coconut creamy milky coumarinic fatty oily	Sigma Aldrich, Flavorbase, TGSC, OdoRactor
2911	7-Butyloxepan-2-one	7-butyloxepan-2-one	CCCCC1CCCCC(=0)01	buttery sweet tonka creamy coconut milky celery fatty dry lactonic cheese coumarinic	Sigma Aldrich, TGSC, OdoRactor
	2-Butyl-1,4- dioxaspiro[4.4]nonane	3-butyl-1,4-dioxaspiro[4.4]nonane	CCCCC1COC2(O1)CCCC2	jasmine green fungal	OdorRactor ,TGSC
2913	5-Methyl-3- butyltetrahydropyran-4-yl acetate	(3-butyl-5-methyloxan-4-yl) acetate	CCCCC1COCC(C1OC(=O)C)C	floral jasmine jasmone parsley spicy	OdorRactor ,TGSC
2914	2-Butyl-4,4,6-trimethyl-1,3-dioxane	2-butyl-4,4,6-trimethyl-1,3-dioxane	CCCCC1OC(CC(O1)(C)C)C	herbaceous spice chamomile green basil	OdorRactor ,TGSC
2915	2-Butyl-4-methyl-1,3- dioxolane	2-butyl-4-methyl-1,3-dioxolane	CCCCC1OCC(O1)C	nutty fatty	OdorRactor ,TGSC
2916	Hexane	hexane	CCCCCC	alkane gasoline	Flavornet, Pubchem
2917	Methyl 2-octynoate	methyl oct-2-ynoate	CCCCCC#CC(=O)OC	green vegetable leafy wax violet cucumber fruity fatty melon violet leaf floral	Sigma Aldrich, TGSC,OdoRactor
2918 2919	Ethyl 2-octynoate Isoamyl 2-octynoate	ethyl oct-2-ynoate 3-methylbutyl oct-2-ynoate	CCCCC#CC(=0)OCC CCCCC#CC(=0)OCCC(C)C	violet violet leaf oily wax leafy green sweet leafy violet	TGSC TGSC
2920	cis-3-Hexenyl 2-octynoate	[(Z)-hex-3-enyl] oct-2-ynoate	CCCCCC#CC(=0)OCCC=CCC	green violet	TGSC, OdoRactor
2921	1,3-Undecadien-5-yne	(3E)-undeca-1,3-dien-5-yne	CCCCCC#CC=CC=C	green violet leaf floral violet greasy tropical fruity chicken	OdorRactor ,TGSC
2922	3-Nonyne	non-3-yne	CCCCC#CCC	cucumber marine	TGSC
2923	2-Pentyl-1-buten-3-one	3-methylideneoctan-2-one	CCCCCC(=C)C(=O)C	musty mushroom fungal	OdorRactor ,TGSC
2924	2-((4- Methylphenyl)methylene)hept an-1-al	al	CCCCCC(=CC1=CC=C(C=C1)C) C=O	floral heliotrope tropical mimosa berry green	OdorRactor ,TGSC
2925	(2-(Dimethoxymethyl)-1- heptenyl)benzene	enyl]benzene	OC)OC	floral jasmine lily green lemon	OdorRactor ,TGSC
2926	1,1-Diethoxy-2-amyl-3-	2-(diethoxymethyl)hept-1-		ethereal jasmine floral aldehydic	OdorRactor ,TGSC
2927	phenyl-2-propene Amylcinnamaldehyde	enylbenzene (2E)-2-benzylideneheptanal	OCC)OC C CCCCCC(=CC1=CC=CC=C1)C=	green fruity floral jasmine	OdorRactor ,TGSC, Pubchem
2928	alpha-Amylcinnamaldehyde		O		
		2-benzylideneheptanal	CCCCCC(=CC1=CC=CC1)C= O	jasmine lily sweet floral oily fruity herbaceous tropical green powdery	Sigma Aldrich, TGSC, Pubchem, OdoRactor
2929	2-Benzylideneheptanal	2-benzylideneheptanal (2Z)-2-benzylideneheptanal	0	herbaceous tropical green powdery sweet floral oily fruity herbaceous jasmine	
2929 2930	2-Benzylideneheptanal 1-Heptanol, 2- (phenylmethylene)-	(2Z)-2-benzylideneheptanal (2E)-2-benzylideneheptan-1-ol	O CCCCCC(=CC1=CC=CC1)C= O CCCCCC(=CC1=CC=CC=C1)CO	herbaceous tropical green powdery sweet floral oily fruity herbaceous jasmine spicy floral jasmine wax fruity cinnamyl alcoholic	Pubchem, OdoRactor OdorRactor, SuperScent, TGSC, Sigma Aldrich
	2-Benzylideneheptanal 1-Heptanol, 2- (phenylmethylene)- alpha-Amylcinnamyl isovalerate	(2Z)-2-benzylideneheptanal (2E)-2-benzylideneheptan-1-ol [(2Z)-2-benzylideneheptyl] 3-methylbutanoate	O CCCCCC(=CC1=CC=CC=C1)C=O CCCCCC(=CC1=CC=CC=C1)CO CCCCCC(=CC1=CC=CC=C1)CO C(=O)C C(C)C	herbaceous tropical green powdery sweet floral oily fruity herbaceous jasmine spicy floral jasmine wax fruity cinnamyl alcoholic fruity tobacco oily hay	Pubchem, OdoRactor OdorRactor, SuperScent, TGSC, Sigma Aldrich OdorRactor ,TGSC
2930	2-Benzylideneheptanal 1-Heptanol, 2- (phenylmethylene)- alpha-Amylcinnamyl	(2Z)-2-benzylideneheptanal (2E)-2-benzylideneheptan-1-ol [(2Z)-2-benzylideneheptyl] 3-methylbutanoate	0 CCCCCC(=CC1=CC=CC=C1)C= 0 CCCCCC(=CC1=CC=CC=C1)C0 CCCCCC(=CC1=CC=CC=C1)C0	herbaceous tropical green powdery sweet floral oily fruity herbaceous jasmine spicy floral jasmine wax fruity cinnamyl alcoholic fruity tobacco oily hay	Pubchem, OdoRactor OdorRactor, SuperScent, TGSC, Sigma Aldrich
2930 2931	2-Benzylideneheptanal 1-Heptanol, 2- (phenylmethylene)- alpha-Amylcinnamyl isovalerate	(2Z)-2-benzylideneheptanal (2E)-2-benzylideneheptan-1-ol [(2Z)-2-benzylideneheptyl] 3-methylbutanoate [(2Z)-2-benzylideneheptyl]	O CCCCCC(=CC1=CC=CC=C1)C= O CCCCCC(=CC1=CC=CC=C1)CO CCCCC(=CC1=CC=CC=C1)CO C(=O)C C(C)C CCCCC(=CC1=CC=CC=C1)CO CCCCCC(=CC1=CC=CC=C1)CO	herbaceous tropical green powdery sweet floral oily fruity herbaceous jasmine spicy floral jasmine wax fruity cinnamyl alcoholic fruity tobacco oily hay	Pubchem, OdoRactor OdorRactor, SuperScent, TGSC, Sigma Aldrich OdorRactor ,TGSC
2930 2931 2932	2-Benzylideneheptanal 1-Heptanol, 2- (phenylmethylene)- alpha-Amylcinnamyl isovalerate alpha-Amylcinnamyl formate	(2Z)-2-benzylideneheptanal (2E)-2-benzylideneheptan-1-ol [(2Z)-2-benzylideneheptyl] 3-methylbutanoate [(2Z)-2-benzylideneheptyl] formate	O CCCCCC(=CC1=CC=CC=C1)C= O CCCCCC(=CC1=CC=CC=C1)CO CCCCCC(=CC1=CC=CC=C1)CO C(=0)C C(C)C CCCCC(=CC1=CC=CC=C1)CO C=O	herbaceous tropical green powdery sweet floral oily fruity herbaceous jasmine spicy floral jasmine wax fruity cinnamyl alcoholic fruity tobacco oily hay herbaceous sweet oily green banana cinnamyl spicy soapy fruity sweet herbaceous coconut woody cheese ketonic green	Pubchem, OdoRactor OdorRactor, SuperScent, TGSC, Sigma Aldrich OdorRactor, TGSC OdorRactor, TGSC Sigma Aldrich, AOD,
2930 2931 2932 2933	2-Benzylideneheptanal 1-Heptanol, 2- (phenylmethylene)- alpha-Amylcinnamyl isovalerate alpha-Amylcinnamyl formate 2-Heptanone 2,3-Octanedione 3-Hydroxy-3-methyl-2,4- nonanedione	(2Z)-2-benzylideneheptanal (2E)-2-benzylideneheptan-1-ol [(2Z)-2-benzylideneheptyl] 3- methylbutanoate [(2Z)-2-benzylideneheptyl] formate heptan-2-one octane-2,3-dione 3-hydroxy-3-methylnonane-2,4-dione	0 CCCCCC(=CC1=CC=CC=C1)C= 0 CCCCCC(=CC1=CC=CC=C1)C0 CCCCCC(=CC1=CC=CC=C1)C0 C(=0)C C(C)C CCCCCC(=CC1=CC=CC=C1)C0 CCCCCC(=CC1=CC=CC=C1)C0 CCCCCC(=CC1=CC=CC=C1)C0 CCCCCC(=O)C	herbaceous tropical green powdery sweet floral oily fruity herbaceous jasmine spicy floral jasmine wax fruity cinnamyl alcoholic fruity tobacco oily hay herbaceous sweet oily green banana cinnamyl spicy soapy fruity sweet herbaceous coconut woody cheese ketonic green creamy penetrating dill asparagus cilantro herbaceous	Pubchem, OdoRactor OdorRactor, SuperScent, TGSC, Sigma Aldrich OdorRactor ,TGSC OdorRactor ,TGSC Sigma Aldrich, AOD, TGSC,OdoRactor
2930 2931 2932 2933 2934	2-Benzylideneheptanal 1-Heptanol, 2- (phenylmethylene)- alpha-Amylcinnamyl isovalerate alpha-Amylcinnamyl formate 2-Heptanone 2,3-Octanedione 3-Hydroxy-3-methyl-2,4-	(2Z)-2-benzylideneheptanal (2E)-2-benzylideneheptan-1-ol [(2Z)-2-benzylideneheptyl] 3- methylbutanoate [(2Z)-2-benzylideneheptyl] formate heptan-2-one octane-2,3-dione 3-hydroxy-3-methylnonane-2,4-	O CCCCCC(=CC1=CC=CC=C1)C= O CCCCCC(=CC1=CC=CC=C1)CO CCCCCC(=CC1=CC=CC=C1)CO C(=O)C C(C)C CCCCCC(=CC1=CC=CC=C1)CO C=O CCCCCC(=CC1=CC=CC=C1)CO CCCCCC(=O)C CCCCCC(=O)C	herbaceous tropical green powdery sweet floral oily fruity herbaceous jasmine spicy floral jasmine wax fruity cinnamyl alcoholic fruity tobacco oily hay herbaceous sweet oily green banana cinnamyl spicy soapy fruity sweet herbaceous coconut woody cheese ketonic green creamy penetrating dill asparagus cilantro herbaceous earthy fatty cortex aldehydic rubbery earthy plastic strawberry fruity caramel burnt hay	Pubchem, OdoRactor OdorRactor, SuperScent, TGSC, Sigma Aldrich OdorRactor, TGSC OdorRactor, TGSC Sigma Aldrich, AOD, TGSC, OdoRactor OdorRactor, TGSC
2930 2931 2932 2933 2934	2-Benzylideneheptanal 1-Heptanol, 2- (phenylmethylene)- alpha-Amylcinnamyl isovalerate alpha-Amylcinnamyl formate 2-Heptanone 2,3-Octanedione 3-Hydroxy-3-methyl-2,4- nonanedione	(2Z)-2-benzylideneheptanal (2E)-2-benzylideneheptan-1-ol [(2Z)-2-benzylideneheptyl] 3- methylbutanoate [(2Z)-2-benzylideneheptyl] formate heptan-2-one octane-2,3-dione 3-hydroxy-3-methylnonane-2,4-dione	O CCCCCC(=CC1=CC=CC=C1)C= O CCCCCC(=CC1=CC=CC=C1)CO CCCCCC(=CC1=CC=CC=C1)CO C(=O)C C(C)C CCCCCC(=CC1=CC=CC=C1)CO C=O CCCCCC(=O)C CCCCCC(=O)C CCCCCC(=O)C(C)(C(=O)C)O	herbaceous tropical green powdery sweet floral oily fruity herbaceous jasmine spicy floral jasmine wax fruity cinnamyl alcoholic fruity tobacco oily hay herbaceous sweet oily green banana cinnamyl spicy soapy fruity sweet herbaceous coconut woody cheese ketonic green creamy penetrating dill asparagus cilantro herbaceous earthy fatty cortex aldehydic rubbery earthy plastic strawberry fruity caramel burnt	Pubchem, OdoRactor OdorRactor, SuperScent, TGSC, Sigma Aldrich OdorRactor, TGSC OdorRactor, TGSC Sigma Aldrich, AOD, TGSC, OdoRactor TGSC Flavornet, TGSC, OdoRactor TGSC
2930 2931 2932 2933 2934 2935 2936	2-Benzylideneheptanal 1-Heptanol, 2- (phenylmethylene)- alpha-Amylcinnamyl isovalerate alpha-Amylcinnamyl formate 2-Heptanone 2,3-Octanedione 3-Hydroxy-3-methyl-2,4- nonanedione 3-Methyl-2,4-nonanedione	(2Z)-2-benzylideneheptanal (2E)-2-benzylideneheptan-1-ol [(2Z)-2-benzylideneheptyl] 3- methylbutanoate [(2Z)-2-benzylideneheptyl] formate heptan-2-one octane-2,3-dione 3-hydroxy-3-methylnonane-2,4- dione 3-methylnonane-2,4-dione	O CCCCCC(=CC1=CC=CC=C1)C= O CCCCCC(=CC1=CC=CC=C1)CO CCCCCC(=CC1=CC=CC=C1)CO C(=O)C C(C)C CCCCCC(=CC1=CC=CC=C1)CO CCCCCC(=O)C CCCCCC(=O)C CCCCCC(=O)C(C)(C(=O)C) CCCCCC(=O)C(C)(C(=O)C)	herbaceous tropical green powdery sweet floral oily fruity herbaceous jasmine spicy floral jasmine wax fruity cinnamyl alcoholic fruity tobacco oily hay herbaceous sweet oily green banana cinnamyl spicy soapy fruity sweet herbaceous coconut woody cheese ketonic green creamy penetrating dill asparagus cilantro herbaceous earthy fatty cortex aldehydic rubbery earthy plastic strawberry fruity caramel burnt hay	Pubchem, OdoRactor OdorRactor, SuperScent, TGSC, Sigma Aldrich OdorRactor, TGSC OdorRactor, TGSC Sigma Aldrich, AOD, TGSC, OdoRactor OdorRactor, TGSC TGSC TGSC Flavornet, TGSC, OdoRactor
2930 2931 2932 2933 2934 2935 2936 2937	2-Benzylideneheptanal 1-Heptanol, 2- (phenylmethylene)- alpha-Amylcinnamyl isovalerate alpha-Amylcinnamyl formate 2-Heptanone 2,3-Octanedione 3-Hydroxy-3-methyl-2,4- nonanedione 3-Methyl-2,4-nonanedione 5-Sulfanylundecan-6-one	(2Z)-2-benzylideneheptanal (2E)-2-benzylideneheptan-1-ol [(2Z)-2-benzylideneheptyl] 3- methylbutanoate [(2Z)-2-benzylideneheptyl] formate heptan-2-one octane-2,3-dione 3-hydroxy-3-methylnonane-2,4-dione 3-methylnonane-2,4-dione 5-sulfanylundecan-6-one	O CCCCCC(=CC1=CC=CC=C1)C= O CCCCCC(=CC1=CC=CC=C1)CO CCCCCC(=CC1=CC=CC=C1)CO CCCCCC(=CC1=CC=CC=C1)CO CCCCCC(=CC1=CC=CC=C1)CO CCCCCC(=O)C CCCCCC(=O)C CCCCCC(=O)C CCCCCC(=O)C(C)(C(=O)C) CCCCCC(=O)C(C)C(=O)C CCCCCC(=O)C(C)C(=O)C	herbaceous tropical green powdery sweet floral oily fruity herbaceous jasmine spicy floral jasmine wax fruity cinnamyl alcoholic fruity tobacco oily hay herbaceous sweet oily green banana cinnamyl spicy soapy fruity sweet herbaceous coconut woody cheese ketonic green creamy penetrating dill asparagus cilantro herbaceous earthy fatty cortex aldehydic rubbery earthy plastic strawberry fruity caramel burnt hay herbaceous grapefruit vetiver cucumber green mushroom metallic herbaceous earthy musty dirty vegetable cabbage brocolli	Pubchem, OdoRactor OdorRactor, SuperScent, TGSC, Sigma Aldrich OdorRactor, TGSC OdorRactor, TGSC Sigma Aldrich, AOD, TGSC, OdoRactor TGSC Flavornet, TGSC, OdoRactor TGSC Sigma Aldrich, TGSC,

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2941	3-Octanone	octan-3-one	CCCCCC(=0)CC	banana berry buttery cheese green musty earthy vegetable spicy herbaceous butter resinous lavender sweet mushroom fresh herbaceous ketonic moldy	Sigma Aldrich, AOD, TGSC, OdoRactor
				fermented	
2942	3-Oxooctanoic acid glyceride	3-oxooctanoic acid;propane-1,2,3-triol	CCCCCC(=0)CC(=0)O.C(C(CO) O)O	fatty	TGSC
2943	5-Oxodecanoic acid	5-oxodecanoic acid	CCCCCC(=0)CCCC(=0)O	creamy peach	TGSC, Flavorbase
2944	1-(Methylthio)-3-octanone	1-methylsulfanyloctan-3-one	CCCCC(=0)CCSC	citrus tomato vegetable cheese blue cheese meaty dairy sulfurous	Flavorbase
2945	Hexanoic acid	hexanoic acid	CCCCCC(=O)O	cheese fatty sour sweaty	Sigma Aldrich, AOD, TGSC,OdoRactor
2946	ethyl hexanoate	methyl hexanoate	CCCCC(=0)OC	ethereal pineapple fruit fresh sweet	Sigma Aldrich, TGSC,OdoRactor
2947	Linalyl hexanoate	3,7-dimethylocta-1,6-dien-3-yl hexanoate	CCCCCC(=O)OC(C)(CCC=C(C) C)C=C	green fruity animal pear pineapple warm	OdorRactor ,TGSC
2948	Isopropyl hexanoate	propan-2-yl hexanoate	CCCCCC(=O)OC(C)C	fresh fruity pineapple loganberry berry	Flavornet, TGSC, OdoRactor
2949	Cyclohexyl hexanoate	cyclohexyl hexanoate	CCCCC(=0)OC1CCCCC1	fruity pineapple	TGSC
2950	Ethyl hexanoate	ethyl hexanoate	CCCCCC(=O)OCC	apple banana pineapple winey fruit sweet wax green fatty estery strong strawberry pear	Sigma Aldrich, Flavorbase, TGSC, Pubchem, OdoRactor
2951	Isobutyl hexanoate	2-methylpropyl hexanoate	CCCCCC(=0)OCC(C)C	fruity peach tropical estery apple apple chocolate green pineapple sweet	Sigma Aldrich, TGSC, OdoRactor
2952	2-Methylbutyl hexanoate	2-methylbutyl hexanoate	CCCCCC(=0)OCC(C)CC	ethereal	OdorRactor ,TGSC
2953	2-Hydroxypropyl hexanoate	2-hydroxypropyl hexanoate	CCCCCC(=0)OCC(C)O	fruity green ethereal	TGSC
2954	Allyl hexanoate	prop-2-enyl hexanoate	CCCCCC(=0)OCC=C	pineapple sweet fruity tropical ethereal rummy fatty cognac arrack juicy estery	Sigma Aldrich, TGSC, OdoRactor
2955	Prenyl caproate	3-methylbut-2-enyl hexanoate	CCCCCC(=0)OCC=C(C)C	fruity green cheese	SuperScent, TGSC, OdoRactor
2956	Geranyl hexanoate	[(2E)-3,7-dimethylocta-2,6-	CCCCCC(=0)OCC=C(C)CCC=C(Sigma Aldrich, TGSC,
2957	Hexanoic acid, 3-phenyl-2-	dienyl] hexanoate [(E)-3-phenylprop-2-enyl]	C)C CCCCC(=0)OCC=CC1=CC=C	geranium wax fruity green spicy	OdoRactor TGSC
	propenyl ester	hexanoate	C=C1		
2958 2959	Pent-2-enyl hexanoate (E)-2-Hexenyl hexanoate	[(Z)-pent-2-enyl] hexanoate [(E)-hex-2-enyl] hexanoate	CCCCC(=0)OCC=CCC CCCCC(=0)OCC=CCCC	banana bergamot green natural cognac herbaceous	OdorRactor ,TGSC OdorRactor ,TGSC,
2939	(E)-2-Hexenyl nexanoate	[(E)-iicx-2-effyi] fickanoate		wax clean fruity pear berry tea apple	Flavorbase
2960	Benzyl hexanoate	benzyl hexanoate	CCCCCC(=0)OCC1=CC=CC=C1	green apricot fruity gardenia jasmine	OdorRactor ,TGSC
2961	Furfuryl hexanoate	furan-2-ylmethyl hexanoate	CCCCCC(=0)OCC1=CC=CO1	green fatty musty wax	OdorRactor ,TGSC
2962	Propyl hexanoate	propyl hexanoate	CCCCCC(=0)OCCC	cheese winey fruit sweet pineapple green tropical juicy	Sigma Aldrich, TGSC,OdoRactor
2963	Isopentyl hexanoate	3-methylbutyl hexanoate	CCCCCC(=0)OCCC(C)C	fruity banana apple pineapple green pungent sour cheese sweet	SuperScent, TGSC, OdoRactor
2964	Citronellyl hexanoate	3,7-dimethyloct-6-enyl hexanoate	CCCCCC(=O)OCCC(C)CCC=C(C)C	floral rose fruity	SuperScent, TGSC, OdoRactor
2965	3-Mercaptohexyl hexanoate	3-sulfanylhexyl hexanoate	CCCCCC(=0)OCCC(CCC)S	fruity sulfurous tropical passion fruit	OdorRactor ,TGSC
2966	(Z)-3-Hexenyl hexanoate	[(Z)-hex-3-enyl] hexanoate	CCCCCC(=0)0CCC=CCC	apple green vegetable fruit prune wax pear winey tropical grassy pineapple balsamic pulpy fruit fatty	Sigma Aldrich, TGSC, Flavorbase, OdoRactor
2967	Hex-3-enyl hexanoate	[(E)-hex-3-enyl] hexanoate	CCCCCC(=0)OCCC=CCC	fruity green fatty apple pear	Flavorbase
2968	2-(4-Methyl-5-thiazolyl)ethyl Hexanoate	2-(4-methyl-1,3-thiazol-5-yl)ethyl hexanoate	CCCCCC(=O)OCCC1=C(N=CS1)	roasted nutty	OdorRactor ,TGSC
2969	2-Phenylethyl hexanoate	2-phenylethyl hexanoate	CCCCCC(=0)OCCC1=CC=CC=	banana green rose sweet honey floral wax woody sweaty pineapple fruity	Sigma Aldrich, Flavorbase, TGSC, OdoRactor
2970	Butyl hexanoate	butyl hexanoate	CCCCCC(=O)OCCCC	fruity winey berry pineapple wax green juicy apple	Sigma Aldrich, TGSC,OdoRactor
2971	3-Phenylpropyl hexanoate	3-phenylpropyl hexanoate	CCCCCC(=O)OCCCC1=CC=CC =C1	sweet fruity green	OdorRactor ,TGSC
2972	Pentyl hexanoate	pentyl hexanoate	CCCCCC(=0)OCCCCC	pineapple fruity green sweet pear fatty estery apple wax cognac	Sigma Aldrich, AOD, TGSC,OdoRactor
2973	Methylthiomethyl hexanoate	methylsulfanylmethyl hexanoate	CCCCC(=O)OCSC	pineapple fruity	OdorRactor ,TGSC
2974	S-Methyl hexanethioate	S -methyl hexanethioate	CCCCC(=O)SC	fruity ethereal green tropical cabbage cheese rancid floral	OdorRactor ,TGSC
2975	O-Ethyl hexanethioate	O -ethyl hexanethioate	CCCCCC(=S)OCC	fruity green sulfurous	Flavorbase
2976	S-Prop-2-en-1-yl	O -prop-2-enyl hexanethioate	CCCCCC(=S)OCC=C	sulfurous fruity tropical	TGSC
	butanethioate				

2977	4-Methyl-3-decen-5-ol	(E)-4-methyldec-3-en-5-ol	CCCCCC(C(=CCC)C)O	green oily violet lily seedy fruity kiwi	OdorRactor ,TGSC
2978	3-Hydroxy-2-octanone	3-hydroxyoctan-2-one	CCCCC(C(=O)C)O	nutty brown	OdorRactor ,TGSC
2979	5-Sulfanylundecan-6-ol	5-sulfanylundecan-6-ol	CCCCC(C(CCCC)S)O	herbaceous grapefruit buchu oily	TGSC
				minty	
2980	2,4-Dimethyl-4-nonanol	2,4-dimethylnonan-4-ol	CCCCC(C)(CC(C)C)O	fruity	OdorRactor,
2981	2-Methylheptanoic acid	2-methylheptanoic acid	CCCCCC(C)C(=O)O	buttery cheese creamy wax sweaty	Sigma Aldrich, TGSC,
2002	43641 1 11	4 4 1	adagaayayaaay oyo	buttermilk green	OdoRactor
2982	4-Methylnonanoic acid	4-methylnonanoic acid	CCCCC(C)CCC(=0)0	chicken meaty pork lamb	Sigma Aldrich, TGSC, OdoRactor
2983	4-Methylnonanoic acid	4-methylnonanoic acid	CCCCCC(C)CCC(=0)0	meaty pork lamb chicken	OdorRactor ,TGSC
2984	(R)-(-)-2-Heptanol	(2R)-heptan-2-ol	CCCCC(C)O	fruity sweet oily fatty	TGSC
2985	(S)-(+)-2-Heptanol	(2S)-heptan-2-ol	CCCCC(C)O	mushroom oily fatty cheese blue cheese moldy	OdorRactor ,TGSC
2986	2-Heptanol	heptan-2-ol	CCCCCC(C)O	oily earthy mushroom fresh lemongrass herbaceous sweet floral fruity green alcoholic	Sigma Aldrich, Flavornet, TGSC,OdoRactor
2987	1-Methylhexyl acetate	heptan-2-yl acetate	CCCCC(C)OC(=O)C	fenugreek fruity brown	SuperScent, TGSC, OdoRactor
2988	2-Heptyl butyrate	heptan-2-yl butanoate	CCCCC(C)OC(=0)CCC	fruity green vegetable cheese walnut	OdorRactor ,TGSC
2989	2-Heptanethiol	heptane-2-thiol	CCCCC(C)S	pungent sulfurous sweaty skunk onion vegetable	OdorRactor ,TGSC
2990	1-Octen-3-OL	oct-1-en-3-ol	CCCCCC(C=C)O	cheese creamy fishy green meaty mushroom herbaceous earthy oily fungal raw chicken raw	Sigma Aldrich, TGSC, OdoRactor
2991	(S)-1-Octen-3-ol	(3S)-oct-1-en-3-ol	CCCCC(C=C)O	earthy moldy grassy herbaceous	TGSC, OdoRactor
2992	(3R)-Oct-1-en-3-ol	(3R)-oct-1-en-3-ol	CCCCCC(C=C)O	mushroom fungal fruity earthy	OdorRactor ,TGSC
2993	1-Octen-3-yl acetate	oct-1-en-3-yl acetate	CCCCCC(C=C)OC(=O)C	violet melon humus herbaceous green fruity oily	Sigma Aldrich, TGSC,
				lavender fresh	OdoRactor
2994 2995	1-Octen-3-yL propionate 1-Octen-3-yl butyrate	oct-1-en-3-yl propanoate oct-1-en-3-yl butanoate	CCCCCC(C=C)OC(=0)CCC	mushroom fungal buttery fatty fishy green musty wax strawberry mushroom fruity floral orchid privet watery metallic	TGSC Sigma Aldrich, TGSC, OdoRactor
2996	Amyl cinnamyl acetate	[(E)-1-phenyloct-1-en-3-yl]	CCCCCC(C=CC1=CC=CC=C1)O	floral jasmine chocolate leathery	OdorRactor ,TGSC
2990	Annyi chinamyi acetate	acetate	C(=0)C	fruity balsamic spicy cinnamyl sweet tropical	odorkaciór, rose
2997	Methyl 3-acetoxyoctanoate	methyl 3-acetyloxyoctanoate	CCCCCC(CC(=O)OC)OC(=O)C	winey fruity green	TGSC
2998	Ethyl 3-hydroxyoctanoate	ethyl 3-hydroxyoctanoate	CCCCC(CC(=0)OCC)O	winey fruity floral	TGSC
2999	3-Octanol	octan-3-ol	ccccc(cc)o	melon musty oily herbaceous spicy woody wax nutty minty mossy mushroom earthy herbaceous citrus dairy creamy fermented	Sigma Aldrich, AOD, Flavornet, TGSC,OdoRactor
3000	3-Octyl acetate	octan-3-yl acetate	CCCCC(CC)OC(=0)C	bergamot woody green grapefruit rose apple herbaceous fresh wax aldehydic fatty citrus minty anisic herbaceous fruity floral warm	OdorRactor ,TGSC, Sigma Aldrich
3001	1-Ethylhexyl tiglate	octan-3-yl (E)-2-methylbut-2-enoate	CCCCCC(CC)OC(=O)C(=CC)C	spicy dried fruit pepper	Sigma Aldrich, TGSC
3002	3-Octyl butyrate	octan-3-yl butanoate	CCCCCC(CC)OC(=O)CCC	fruity green herbaceous citrus musty	OdorRactor ,TGSC
3003	Octan-3-yl formate	octan-3-yl formate	CCCCC(CC)OC=O	fruity green vegetable green juicy apple pear wax tropical citrus	OdorRactor ,TGSC
3004	3-Mercaptooctanal	3-sulfanyloctanal	CCCCC(CC=O)S	citrus fruity grapefruit green peely	OdorRactor ,TGSC
3005	Glyceryl 5-hydroxydecanoate	2,3-dihydroxypropyl 5- hydroxydecanoate	O	buttery tropical fresh peach coconut oily	OdorRactor ,TGSC, Flavorbase
3006	Ethyl 5-hydroxydecanoate	ethyl 5-hydroxydecanoate	CCCCC(CCCC(=0)OCC)O	sweet fatty peach	TGSC
3007	(2,2-Dimethyl-1,3-dioxolan-4-yl)methyl 5-	(2,2-dimethyl-1,3-dioxolan-4-yl)methyl 5- hydroxydecanoate	CCCCCC(CCCC(=O)OCC1COC(O1)(C)C	sweet fatty peach	TGSC, Flavorbase
3008	hydroxydecanoate 3-(Hydroxymethyl)octan-2-	3-(hydroxymethyl)octan-2-one)O CCCCCC(CO)C(=O)C	musty herbaceous sweet earthy	OdorRactor ,TGSC
3009	one 1,1-Dimethoxyhexane	1,1-dimethoxyhexane	CCCCCC(OC)OC	fungal green sweet musty dry cooked	OdorRactor ,TGSC,
3010	1,1-Diethoxyhexane	1,1-diethoxyhexane	CCCCCC(OCC)OCC	apple leafy mild cognac pear floral hyacinth apple	Flavorbase OdorRactor ,TGSC
3011	(6S)-6-Hexyloxan-2-one	(6S)-6-hexyloxan-2-one	CCCCCC[C@H]1CCCC(=0)01	fruity fermented fruity sweet milky	TGSC
3012	2-Methyl-2-octenal	(E)-2-methyloct-2-enal	CCCCCC=C(C)C=O	fruity green	OdorRactor,
3012	(E)-2-Butyl-2-octenal	(E)-2-methyloct-2-enal	CCCCC=C(CCCC)C=0	grassy	ADB
2013	(L)-2-Duty1-2-Octolial	(12) 2-out yiott-2-tilai		Brussy	יעעיי

3014	2-Hexylidene cyclopentanone	2-hexylidenecyclopentan-1-one	CCCCCC=C1CCCC1=O	strong green herbaceous warm jasmine spicy fruity floral	OdorRactor ,TGSC, Flavorbase
3015	3-Nonen-2-one	(E)-non-3-en-2-one	CCCCCC=CC(=O)C	berry mushroom spicy fruity fatty oily ketonic weedy licorice	Sigma Aldrich, TGSC, OdoRactor
3016	2-Octenoic acid	(E)-oct-2-enoic acid	CCCCCC=CC(=O)O	butterscotch acidic musty sour fatty wax dirty vegetable cheese aldehydic	ADB, TGSC, OdoRactor
3017	Methyl oct-2-enoate	methyl (E)-oct-2-enoate	CCCCCC=CC(=0)OC	green fruity animal hairy costus sweet pear oily wax violet fresh melon violet leaf cooked leafy	Sigma Aldrich, TGSC, OdoRactor
3018	2-Octenoic acid, ethyl ester	ethyl (E)-oct-2-enoate	CCCCCC=CC(=0)OCC	fatty green fruity musty oily fruit pungent wax tropical plum pineapple juicy hairy pear	TGSC, Flavorbase, ODoRactor
3019	Ethyl (2Z)-oct-2-enoate	ethyl (Z)-oct-2-enoate	CCCCCC=CC(=0)OCC	fruity pear green wax tropical plum fatty	SuperScent, TGSC
3020	1,5-Undecadien-4-ol	undeca-1,5-dien-4-ol	CCCCC=CC(CC=C)O	green earthy mushroom	TGSC
3021	1,5-Undecadien-4-ol, 4-	undeca-1,5-dien-4-yl acetate	CCCCCC=CC(CC=C)OC(=O)C	green fatty galbanum	TGSC
3022	acetate 3,5-Undecadien-2-one	(3E ,5E)-undeca-3,5-dien-2-one	CCCCCC=CC=CC(=0)C	cucumber green tallow fatty fruity	TGSC
				fried	
3023	Pellitorine	(2E ,4E)-N -(2- methylpropyl)deca-2,4-dienamide	CCCCCC=CC=CC(=O)NCC(C)C	spicy herbaceous	OdorRactor ,TGSC, Flavorbase
3024	Methyl (2E,4Z)-2,4- decadienoate	methyl (2 E ,4 Z)-deca-2,4-dienoate	CCCCCC=CC=CC(=O)OC	fruity wax pear lemon	OdorRactor ,TGSC
3025	Ethyl (2E,4Z)-deca-2,4-dienoate	ethyl (2 E ,4 Z)-deca-2,4-dienoate	CCCCCC=CC=CC(=0)OCC	apple fatty green winey wax pear sweet fruity tropical vegetable	Sigma Aldrich, TGSC, Flavorbase, OdoRactor
3026	Propyl 2,4-decadienoate	propyl (2E,4E)-deca-2,4-dienoate	CCCCCC=CC=CC(=0)OCCC	fruity fatty melon green pear fresh vegetable	OdorRactor ,TGSC
3027	Propyl (2E,4Z)-2,4- decadienoate	propyl (2E ,4Z)-deca-2,4- dienoate	CCCCCC=CC=CC(=0)OCCC	pear wax tropical	Flavorbase
3028	1,3,5-Undecatriene	(3E,5E)-undeca-1,3,5-triene	CCCCCC=CC=CC=C	green pineapple fresh greasy resinous galbanum bellpepper cucumber wax melon vegetable citrus powerful diffusive	Sigma Aldrich, TGSCGSC, Flavorbase, OdoRactor
3029	2,4-Decadienal	(2E ,4E)-deca-2,4-dienal	CCCCCC=CC=CC=O	fatty meaty citrus fried wax oily cucumber melon pumpkin nutty chicken coriander brothy orange sweet fresh green strong	Sigma Aldrich,Flavornet, Flavorbase, TGSC, OdoRactor
3030	2,4-Decadienal	(2E ,4E)-deca-2,4-dienal	CCCCCC=CC=CC=O	fatty oily cucumber melon citrus pumpkin nutty fried chicken coriander brothy	ADB, OdoRactor
	2,4-Decadienal (E,Z)-2,4-Decadienal	(2E ,4E)-deca-2,4-dienal (2E ,4Z)-deca-2,4-dienal	CCCCCC=CC=CC=O	fishy fried fatty geranium green wax	Flavornet, TGSC,
3033	Deca-2,4-dienal	deca-2,4-dienal	CCCCCC=CC=CC=O	orange sweet fresh citrus fatty green oily chicken roasty	OdorRactor
3034	Deca-2,4-dienal	deca-2,4-dienal	CCCCCC=CC=CC=O	seaweed	Flavornet
3035	(2E,4E)-2,4-Decadien-1-ol	(2E,4E)-deca-2,4-dien-1-ol	CCCCCC=CC=CCO	fatty wax citrus melon fruity dairy	OdorRactor ,TGSC
3036	Deca-2,4-dien-1-ol	deca-2,4-dien-1-ol	CCCCC=CC=CCO	fatty wax citrus melon meaty chicken turkey dairy fruity	ADB, TGSC
3037	2-Octenal, (2Z)-	(Z)-oct-2-enal	CCCCC=CC=O	green leafy walnut fatty fruity	Flavornet, TGSC, OdoRactor
3038	2-Octenal	(E)-oct-2-enal	CCCCCC=CC=O	green spicy nutty fatty fresh cucumber herbaceous banana wax leafy	Sigma Aldrich, Flavornet, TGSC, OdoRactor
3039	3-Nonenoic acid, methyl ester	methyl (E)-non-3-enoate	CCCCCC=CCC(=O)OC	melon fruity green watermelon pear honeydew juicy fatty dry	Sigma Aldrich, TGSC, OdoRactor
3040	(E,Z,Z)-Trideca-2,4,7-trienal	(2E ,4Z ,7Z)-trideca-2,4,7-trienal	CCCCCC=CCC=CC=CC=O	fatty citrus wax oily fruity	OdorRactor ,TGSC
3041	Linoleic acid	acid	CCCCCC=CCC=CCCCCCCC(= 0)O	, ,	Sigma Aldrich, Flavorbase, OdoRactor
3042	Methyl linoleate	methyl (9 Z ,12 Z)-octadeca-9,12-dienoate	CCCCCC=CCC=CCCCCCCC(= 0)OC		SuperScent, TGSC, OdoRactor
	Ethyl linoleate	ethyl (9Z ,12Z)-octadeca-9,12- dienoate	CCCCCC=CCC=CCCCCCCC(= 0)OCC		TGSC
3044	(Z)-3-Nonenal	(Z)-non-3-enal	CCCCCC=CCC=O	cucumber green	Flavornet, TGSC
3045	3-Nonenal, (3E)-	non-3-enal	CCCCC=CCC=O	fatty	Flavornet, TGSC, OdoRactor
3046	3-Nonenal	(E)-non-3-enal	CCCCC=CCC=O	fatty	OdorRactor,
3047	(5R)-5-[(Z)-Oct-2- enyl]oxolan-2-one	(5R)-5-[(Z)-oct-2-enyl]oxolan-2-one		soapy	Flavornet
3048	(Z)-4-Hydroxy-6-dodecenoic acid lactone	5-[(Z)-oct-2-enyl]oxolan-2-one	CCCCCC=CCC1CCC(=0)O1	sweet fatty wax dairy creamy fruity lactonic buttery peach	OdorRactor ,TGSC, Flavorbase

3049	(E)-2-(2- Octenyl)cyclopentanone	2-[(E)-oct-2-enyl] cyclopentan-1-one	CCCCCC=CCC1CCCC1=0	fruity green fatty peach jasmine melon sweet apple apricot lactonic	OdorRactor ,TGSC
3050	(Z)-4-Decenoic acid	(Z)-dec-4-enoic acid	CCCCC=CCCC(=0)0	fatty green	SuperScent, TGSC
3051	Obtusilic acid	(E)-dec-4-enoic acid	CCCCC=CCC(=0)0	oily fatty meaty savory	OdorRactor ,Flavorbase
3052	Methyl (Z)-4-decenoate	methyl (Z)-dec-4-enoate	CCCCCC=CCCC(=0)OC	fruity pear mango fishy peach green	SuperScent, TGSC, OdoRactor
3053	Ethyl trans-4-decenoate	ethyl (E)-dec-4-enoate	CCCCCC=CCCC(=0)OCC	fatty pear green fruity wax cognac	OdorRactor, ,TGSC, Flavorbase
3054	(Z)-1,1-Diethoxy-4-decene	(Z)-1,1-diethoxydec-4-ene	CCCCCC=CCCC(OCC)OCC	oily pineapple apple citrus bitter orange orange bitter	OdorRactor ,TGSC
3055	2,6-Dodecadienal, (2E,6Z)-	dodeca-2,6-dienal	CCCCCC=CCCC=CC=O	citrus mandarin orange melon fatty green aldehydic spicy wax	OdorRactor ,TGSC, Flavorbase
3056	4-Decenal	dec-4-enal	CCCCC=CCCC=O	aldehydic fatty citrus orange	TGSC, OdoRactor
3057	4-Decenal	(E)-dec-4-enal	CCCCC=CCCC=O	citrus fresh aldehydic orange	OdorRactor ,TGSC,
3058	cis-4-Decenal	(Z)-dec-4-enal	CCCCCC=CCCC=O	mandarin tangerine green fatty orange green musty aldehydic citrus watery cardamom rancid	Flavorbase Flavornet, TGSC, Flavorbase
3059	(Z)-8-Tetradecenal	(Z)-tetradec-8-enal	CCCCC=CCCCCCCC=O	wax floral fruity citrus	OdorRactor ,TGSC
3060	cis-4-Decen-1-ol	(Z)-tetradec-8-enai (Z)-dec-4-en-1-ol	CCCCC=CCCCO	fruity	Sigma Aldrich, OdoRactor
3061	Dec-4-en-1-ol	(E)-dec-4-en-1-ol	CCCCC=CCCO	wax fatty fruity	OdorRactor ,TGSC
			CCCCC=CCCCC(=0)C	wax fatty herbaceous citrus floral	OdorRactor ,TGSC,
3062	cis-4-Decenyl acetate	[(Z)-dec-4-enyl] acetate	ccccc=ccccoc(=o)c	oily estery fruity juicy orange rose spicy	Flavorbase
3063	(E)-3-Nonen-1-ol	(E)-non-3-en-1-ol	CCCCC=CCCO	green wax melon cucumber	TGSC
3064	(Z)-3-Nonenyl acetate	[(Z)-non-3-enyl] acetate	CCCCCC=CCCOC(=0)C	fruity fleshy pear green tropical herbaceous	TGSC
3065	trans-2-Octen-1-Ol	(E)-oct-2-en-1-ol	CCCCC=CCO	green meaty fruity vegetable citrus earthy soapy plastic fatty	Sigma Aldrich, TGSC, OdoRactor
3066	trans-2-Octen-1-yl acetate	[(E)-oct-2-enyl] acetate	CCCCCC=CCOC(=0)C	green aldehydic melon pear tropical earthy fatty oily wax	OdorRactor ,TGSC
3067	(E)-Oct-2-enyl butyrate	[(E)-oct-2-enyl] butanoate	CCCCCC=CCOC(=0)CCC	wax fruity berry buttery	OdorRactor ,TGSC
3068	Hexanal	hexanal	CCCCC=0	fatty green tallow strong	Sigma Aldrich, AOD, TGSC,
3008	Hexanai	пехана	cccc-o	penetrating grassy leafy sweaty vegetable clean woody unripe fruit fresh aldehydic fruity sharp	Pubchem
3069	2,2,5-Trimethyl-5- pentylcyclopentan-1-one	2,2,5-trimethyl-5- pentylcyclopentan-1-one	CCCCCC1(CCC(C1=0)(C)C)C	fruity peach apricot jasmine herbaceous lavender lactonic	OdorRactor ,TGSC
3070	Dihydrojasmone	3-methyl-2-pentylcyclopent-2-en-1- one	CCCCCC1=C(CCC1=0)C	green floral fruity jasmine woody spice herbaceous fresh myrrh powdery sweet	Sigma Aldrich, ADB, TGSC, OdoRactor
3071	6-Pentyl-2H-pyran-2-one	6-pentylpyran-2-one	CCCCCC1=CC=CC(=0)O1	almond coconut mushroom sweet tonka lactonic creamy fatty wax brown	Sigma Aldrich, TGSC, OdoRactor
3072	2-Pentylpyridine	2-pentylpyridine	CCCCCC1=CC=CC=N1	green melon vegetable fat tallow bellpepper mushroom herbaceous fatty meaty	Sigma Aldrich, Flavorbase, TGSC, OdoRactor
3073	2-Pentylfuran	2-pentylfuran	CCCCCC1=CC=CO1	green vegetable buttery beany fruity earthy metallic	Sigma Aldrich, Flavornet, TGSC
3074	2-Pentylthiophene	2-pentylthiophene	CCCCCC1=CC=CS1	sweet fruit fatty roasted hazelnut fermented meaty bloody chicken cranberry corn roasted barley barley	Flavornet, Odoractor
2075	5 D + 1 2H 6 2	5 . 1211 6 . 2	gaagaa gaay oyot	hazelnut roasted	O.I. D
3075	5-Pentyl-3H-furan-2-one	5-pentyl-3 <i>H</i> -furan-2-one	CCCCCC1=CCC(=0)01	fruity milky dairy tropical coconut coumarinic tobacco	OdorRactor ,TGSC, Flavorbase
3076	2-Pentyl-2-cyclopenten-1-one	2-pentylcyclopent-2-en-1-one	CCCCCC1=CCCC1=O	woody floral jasmine tuberose isojasmone	OdorRactor ,TGSC
3077	2-Pentylcyclohex-2-en-1-one	2-pentylcyclohex-2-en-1-one	CCCCCC1=CCCCC1=O	muguet orange coconut lactonic jasmine floral	OdorRactor ,TGSC
3078	3,4-Dimethyl-5-pentylfuran- 2(5H)-one	3,4-dimethyl-2-pentyl-2 <i>H</i> -furan-5-one	CCCCCC1C(=C(C(=O)O1)C)C	celery green tea	Flavorbase
3079	2(3H)-Furanone, dihydro-4- methyl-5-pentyl-	4-methyl-5-pentyloxolan-2-one	CCCCCC1C(CC(=O)O1)C	wax lactonic metallic plum tuberose	OdorRactor ,TGSC
3080	Cyclopentanone, 3-methyl-2- pentyl-	3-methyl-2-pentylcyclopentan-1- one	CCCCCC1C(CCC1=0)C	coconut sweet jasmine spicy fruity	OdorRactor ,TGSC
3081	Methyl trans-3-oxo-2- pentylcyclopentanecarboxylat	methyl (1R, ,2S)-3-oxo-2- pentylcyclopentane-1- carboxylate	CCCCCC1C(CCC1=0)C(=0)OC	floral jasmine rose green muguet	TGSC
3082	Cyclopentanone, 3-(2-	3-(2-oxopropyl)-2-	CCCCCC1C(CCC1=0)CC(=0)C	floral magnolia jasmine	OdorRactor ,TGSC
3083	oxopropyl)-2-pentyl- Methyl dihydrojasmonate, (+-	pentylcyclopentan-1-one methyl 2-[(1R,2S)-3-oxo-2-	CCCCCC1C(CCC1=O)CC(=O)O	floral jasmine	Flavornet, TGSC
3084)-cis- Methyl dihydrojasmonate	pentylcyclopentyl]acetate methyl 2-(3-oxo-2- pentylcyclopentyl)acetate	CCCCCC1C(CCC1=0)CC(=0)O	jasmine sweet floral oily green lactonic tropical natural powerful	Sigma Aldrich, TGSC, Flavorbase, Pubchem
3085	trans-4,5-Epoxy-2(E)-	3-(3-pentyloxiran-2-yl)prop-2-enal	CCCCCC1C(O1)C=CC=O	fruity citrus metallic green aldehydic	OdorRactor,
	Decenal Decenal	. I J Joygraf - Cim	(- /- /- /-		,

3086	4,5-Epoxy-(E)-dec-2-enal	(E)-3-[(2S,3R)-3-pentyloxiran-2-yl]prop-2-enal	CCCCCC1C(O1)C=CC=O	strong green bean citrus metallic green aldehydic	OdorRactor ,TGSC, Flavorbase
3087	2,3-Epoxyoctanal	3-pentyloxirane-2-carbaldehyde	CCCCCC1C(O1)C=O	citrus fatty fruity soapy	TGSC
3088	2-Nonenoic acid gamma- lactone	2-pentyl-2 <i>H</i> -furan-5-one	CCCCCC1C=CC(=O)O1	minty fruity coconut fatty coumarinic hay deep fried	OdorRactor ,TGSC, Flavorbase
3089	2-Cyclohexene-1-carboxylic acid, 2-methyl- 4-oxo-6-pentyl-, ethyl ester	ethyl 2-methyl-4-oxo-6- pentylcyclohex-2-ene-1- carboxylate	CCCCCC1CC(=O)C=C(C1C(=O) OCC)C	sweet anisic floral jasmine clean autumn	OdorRactor ,TGSC
3090	Massoia lactone	2-pentyl-2,3-dihydropyran-6-one	CCCCCC1CC=CC(=O)O1	peach sweet creamy coconut herbaceous lactonic fruity powerful buttery	Flavornet, Flavorbase, TGSC, OdoRactor
3091	2H-Pyran-2-one, 5,6-dihydro-6-pentyl-, (R)-	(2R)-2-pentyl-2,3-dihydropyran-6	-CCCCCC1CC=CC(=0)O1	sweet coconut meaty lactonic creamy milky wax	OdorRactor ,TGSC
3092	(S)-4-Nonanolide	(5S)-5-pentyloxolan-2-one	CCCCCC1CCC(=0)O1	coconut fatty moldy	TGSC
3093	gamma-Nonalactone	5-pentyloxolan-2-one	CCCCCCICCC(=0)01	strong anisic coconut fatty herbaceous peach tropical creamy wax sweet buttery oily	Sigma Aldrich, Flavorbase, TGSC, OdoRactor, Pubchem
3094 3095	(5R)-5-Pentyloxolan-2-one 5-Pentyltetrahydrofuran-2-ol	(5R)-5-pentyloxolan-2-one 5-pentyloxolan-2-ol	CCCCCCICCC(=0)01 CCCCCCICCC(01)0	sweet coconut soft fatty milky fruity green melon	TGSC TGSC
3096	delta-Decalactone	6-pentyloxan-2-one	CCCCC1CCCC(=0)01	apricot buttery coconut creamy fatty peach plum sweet winey dairy oily fresh fruity lactonic milky nutty	Sigma Aldrich, Flavorbase, TGSC,OdoRactor
3097	(S)-delta-Decanolide	(6S)-6-pentyloxan-2-one	CCCCC1CCCC(=0)O1	fruity sweet peach fatty buttery	TGSC
3098	delta-Decalactone, (+)-	(6R)-6-pentyloxan-2-one	CCCCC1CCCC(=0)01	peach sweet fruity milky	Flavornet, TGSC
3099	2-Pentylcyclopentanone	2-pentylcyclopentan-1-one	CCCCC1CCCC1=0	coconut jasmine oily foliage rose fern green herbaceous floral	OdorRactor ,TGSC
3100	2-Pentylcyclopentan-1-ol	2-pentylcyclopentan-1-ol	CCCCC1CCCC10	floral jasmine magnolia tea fruity	TGSC
3101	Acetaldehyde 1,3-octanediol acetal	2-methyl-4-pentyl-1,3-dioxane	CCCCC1CCOC(01)C	green ethereal musty	OdorRactor ,TGSC
3102	Hexanal octane-1,3-diol acetal	2,4-dipentyl-1,3-dioxane	CCCCCC1CCOC(01)CCCCC	fatty green	TGSC
3103	5-Pentyl-1,4-dioxan-2-one	5-pentyl-1,4-dioxan-2-one	CCCCC1COC(=0)CO1	fruity winey ethereal	TGSC
3104	Tetrahydro-3-pentyl-2H- pyran-4-yl acetate	(3-pentyloxan-4-yl) acetate	CCCCC1COCCC1OC(=0)C	floral herbaceous oily green jasmine mushroom lactonic tea	OdorRactor ,TGSC
3105	Hexanal butane-2,3-diol acetal	4,5-dimethyl-2-pentyl-1,3-dioxolane	CCCCCC1OC(C(O1)C)C	sweet fatty green	OdorRactor ,TGSC
3106	4-Methyl-2-pentyl-1,3- dioxolane	4-methyl-2-pentyl-1,3-dioxolane	CCCCCC1OCC(O1)C	green wax vegetable licorice fruity rue clean petroleum sweet pineapple	OdorRactor ,TGSC
3107	trans-4-Methyl-2-pentyl-1,3- dioxolane	(2S ,4S)-4-methyl-2-pentyl-1,3-dioxolane	CCCCCC1OCC(O1)C	wax green fruity vegetable	TGSC
3108	Octane	heptane	CCCCCCC	alkane gasoline	Flavornet, TGSC, pUBCHEM
3109	Heptane	heptane	CCCCCCC	sweet ethereal gasoline	Flavornet, TGSC, Pubchem
3110	Methyl 2-nonynoate	methyl non-2-ynoate	CCCCCC#CC(=0)OC	peach violet leaf floral green melon cucumber violet	Sigma Aldrich, TGSC,OdoRactor
3111	Ethyl 2-nonynoate	ethyl non-2-ynoate	CCCCCC#CC(=0)OCC	leafy floral violet leaf green cucumber violet	SuperScent, TGSC, Flavorbase, OdoRactor
3112	2-Nonynoic Acid cis-3-Hexen- 1-yl Ester	[(Z)-hex-3-enyl] non-2-ynoate	CCCCCC#CC(=0)OCCC=CCC	green	TGSC
3113	1,1-Dimethoxynon-2-yne	1,1-dimethoxynon-2-yne	CCCCCC#CC(OC)OC	fresh green violet foliage sweet	OdorRactor ,TGSC
3114	Benzoic acid, 2-((2- (phenylmethylene)octylidene) amino)-, methyl ester	methyl 2-[[(2E)-2-benzylideneoctylidene]amino]benz oate		floral fresh fatty wax	OdorRactor ,TGSC
3115	alpha-Hexylcinnamaldehyde	(2E)-2-benzylideneoctanal	CCCCCCC(=CC1=CC=CC=C1)C =O	jasmine lily sweet floral green herbaceous wax fresh citrus powdery fruity tropical spicy	Sigma Aldrich, TGSC, Pubchem, OdoRactor
3116	2-Octanone, oxime	(NE)-N -octan-2- ylidenehydroxylamine	CCCCCC(=NO)C	clean earthy floral fresh green	TGSC
3117	2-Octanone	octan-2-one	CCCCCCC(=0)C	green earthy fruity floral herbaceous soapy gasoline weedy natural woody herbaceous musty ketonic cheese blue cheese parmesan cheese dairy fatty bitter pleasant	Sigma Aldrich, AOD, TGSC, OdoRactor, Pubchem
3118	1-Nonen-3-one	non-1-en-3-one	CCCCCC(=0)C=C	pungent mushroom	Flavornet, TGSC
3119	3-Nonanone	nonan-3-one	CCCCCCC(=0)CC	cheese green fruity sweet jasmine spicy leafy herbaceous fresh floral	Sigma Aldrich, TGSC, OdoRactor
3120	4-Oxodecanal	4-oxodecanal	CCCCCC(=0)CCC=0	fatty	Flavornet, OdoRactor
3121	7-Tridecanone	tridecan-7-one	CCCCCC(=0)CCCCCC	floral	TGSC
3122	3-Nonanon-1-yl acetate	3-oxononyl acetate	CCCCCC(=0)CCOC(=0)C	floral fruity wax reseda	TGSC

3124 Mo 3125 Etl	fethyl heptanoate	heptanoic acid methyl heptanoate	CCCCCCC(=0)0C	cheese sour rancid pungent sweaty wax fermented pineapple fruity disagreeable berry green fruity sweet orris wax	Sigma Aldrich, AOD, TGSC, OdoRactor, Pubchem Sigma Aldrich,
3125 Etl		methyl heptanoate	CCCCCC(=0)OC	berry green fruity sweet orris wax	Sigma Aldrich
3126 Iso	thyl heptanoate			floral apple	TGSC,OdoRactor
		ethyl heptanoate	CCCCCCC(=O)OCC	berry melon peach pineapple plum fruity cognac rummy winey sweet estery green seedy strong	Sigma Aldrich, Flavorbase, TGSC, OdoRactor
3127 Al	sobutyl heptanoate	2-methylpropyl heptanoate	CCCCCC(=0)OCC(C)C	green herbaceous fruity	OdorRactor,
	llyl heptanoate	prop-2-enyl heptanoate	CCCCCCC(=0)OCC=C	apricot banana berry pineapple sweet wax fruity fusel cognac ripe fermented	Sigma Aldrich, TGSC,OdoRactor
3128 Ge	eranyl heptanoate	[(2E)-3,7-dimethylocta-2,6-dienyl] heptanoate	C(C)C	floral cognac fusel winey	OdorRactor ,TGSC
3129 Be	enzyl heptanoate	benzyl heptanoate	CCCCCCC(=0)OCC1=CC=CC=	fruity apricot herbaceous sage	OdorRactor ,TGSC
3130 Fu	urfuryl heptanoate	furan-2-ylmethyl heptanoate	CCCCCCC(=0)OCC1=CC=C01	green	SuperScent, TGSC, OdoRactor
3131 Pro	ropyl heptanoate	propyl heptanoate	CCCCCCC(=O)OCCC	sweet fruity apple pear pineapple grape strawberry winey green ripe fermented cognac juicy tutti frutti	SuperScent, TGSC, OdoRactor
3132 3-1	-Methylbutyl heptanoate	3-methylbutyl heptanoate	CCCCCC(=0)OCCC(C)C	fruity herbaceous grassy unripe banana unripe fruit	OdorRactor ,TGSC
3133 cis	is-3-Hexenyl heptanoate	[(Z)-hex-3-enyl] heptanoate	CCCCCC(=0)OCCC=CCC	green fruity wax tropical	Flavorbase
	-Phenylethyl heptanoate	2-phenylethyl heptanoate		floral rose apricot	OdorRactor ,TGSC
3135 Bu	utyl heptanoate	butyl heptanoate	CCCCCC(=0)OCCCC	green fruity licorice grassy oily winey pear tropical starfruit	SuperScent, TGSC, OdoRactor
3136 Pe	entyl heptanoate	pentyl heptanoate	CCCCCC(=0)OCCCCC	ethereal fruity unripe banana coconut lemon unripe fruit	OdorRactor ,TGSC
3137 He	lexyl heptanoate	hexyl heptanoate	CCCCCC(=0)OCCCCCC	green foliage leafy cognac	TGSC, OdoRactor
	thyl 2-acetyloctanoate	ethyl 2-acetyloctanoate	CCCCCC(C(=0)C)C(=0)OCC	dihydrojasmone fruity jasmine wax herbaceous celery floral strong winey	OdorRactor ,TGSC, Flavorbase
3139 2-1	-Methyloctanal	2-methyloctanal	CCCCCC(C)C=0	floral rose lily muguet	OdorRactor ,TGSC, Flavorbase
3140 (R	R)-(-)-2-Octanol	(2R)-octan-2-ol	CCCCCC(C)O	creamy cucumber fatty sour	TGSC
	-Octanol	octan-2-ol	CCCCCC(C)O	green oily woody spicy earthy herbaceous mushroom fatty fresh	Sigma Aldrich, AOD, TGSC, OdoRactor
3142 (S)	S)-(+)-2-Octanol	(2S)-octan-2-ol	CCCCCC(C)O	mushroom oily fatty creamy grape	OdorRactor ,TGSC
3143 1-1	-Methylheptyl acetate	octan-2-yl acetate	CCCCCC(C)OC(=0)C	fruit	Flavornet, TGSC
3144 1-1	-Nonen-3-ol	non-1-en-3-ol	CCCCCC(C=C)O	oily creamy green earthy mushroom	OdorRactor ,TGSC
3145 3-1	-Nonanol	nonan-3-ol	CCCCCC(CC)O	spice herbaceous oily	OdorRactor ,TGSC
3146 No	Ionan-3-yl acetate	nonan-3-yl acetate	CCCCCC(CC)OC(=0)C	herbaceous fruity ethereal floral	OdorRactor ,TGSC
	-Acetyloxynonyl cetate;nonane-1,3-diol	3-acetyloxynonyl acetate;nonane- 1,3-diol	CCCCCC(CCO)O.CCCCCCC(C COC(= O)C)OC(=O)C	floral fresh sweet oily jasmine watery	OdorRactor ,TGSC
3148 3-1	-Hydroxynonyl acetate	3-hydroxynonyl acetate	CCCCCC(CCOC(=0)C)O	floral fresh sweet oily jasmine watery	SuperScent, TGSC, OdoRactor
	-Nonanone, 3- nydroxymethyl)-	3-(hydroxymethyl)nonan-2-one	CCCCCC(CO)C(=O)C	fresh sweet green weedy earthy herbaceous	OdorRactor ,TGSC
3150 2-1	-Hydroperoxy-1-oct-1-en-3- loxyperoxyoctane	2-hydroperoxy-1-oct-1-en-3- yloxyperoxyoctane	CCCCCC(COOOC(CCCCC)C= C)OO	metallic mushroom	Flavornet
	astor oil	2,3-bis[[(Z)-12-hydroxyoctadec- 9- enoyl]oxy]propyl (Z)-12- hydroxyoctadec-9-enoate		faint mild	Sigma Aldrich, Pubchem
3152 1,1	,1-Dimethoxyheptane	1,1-dimethoxyheptane	CCCCCC(OC)OC	green fruity tropical orange privet oily fatty wax vegetable coconut	OdorRactor ,TGSC, Flavorbase
3153 1,1	,1-Diethoxyheptane	1,1-diethoxyheptane	CCCCCC(OCC)OCC	creamy buttery fresh herbaceous winey green leafy wax citrus	OdorRactor,
3154 1-0	-Octene	oct-1-ene	CCCCCCC=C	camphoraceous gasoline	Flavornet,OdoRactor
	rans-2-Nonen-1-ol	(E)-non-2-en-1-ol	CCCCCC=CC	fatty green melon wax sweet violet oily tallow	Sigma Aldrich, TGSC, OdoRactor
3156 2-1	-Nonenenitrile	(E)-non-2-enenitrile	CCCCCC=CC#N	green fatty orris	TGSC
3130 2-	-Decen-2-one	(E)-dec-3-en-2-one	CCCCCCC=CC(=O)C	fatty green jasmine meaty citrus earthy vegetable wax pear fruity	Sigma Aldrich, TGSC, OdoRactor
				apple fresh	Odokaciói
3157 3-1	E)-Non-2-enoic acid	(E)-non-2-enoic acid	CCCCCCC=CC(=0)O		ADB, TGSC, OdoRactor

3159	Methyl 2-nonenoate	methyl (E)-non-2-enoate	CCCCCC=CC(=O)OC	green violet sweet wax pear fruity melon vegetable	Sigma Aldrich, TGSC, OdoRactor
3160	2,4-Undecadienal	(2E ,4E)-undeca-2,4-dienal	CCCCCCC=CC=CC=O	green oily caramel spicy citrus buttery baked fatty wax chicken sweet fruity	Sigma Aldrich, TGSC, OdoRactor
				aldehydic	
3161	(2Z,4Z)-Undeca-2,4-dien-1-ol	(2Z ,4Z)-undeca-2,4-dien-1-ol	CCCCCC=CC=CCO	fatty	OdorRactor ,TGSC
3162	2-Nonenal	(E)-non-2-enal	cccccc=cc=o	fatty wax cucumber green paper aldehydic citrus melon vegetable cereal chicken	Sigma Aldrich, Flavornet, TGSC, OdoRactor
3163	Non-2-enal	(Z)-non-2-enal	CCCCCC=CC=O	orris fatty cucumber wax	Flavornet, TGSC, OdoRactor
3164	3-Decenoic acid	(E)-dec-3-enoic acid	CCCCCCC=CCC(=0)0	fatty	TGSC
3165	(E)-4-Undecenal	(E)-undec-4-enal	CCCCCCC=CCCC=O	fatty aldehydic floral herbaceous citrus	TGSC
3166	7-Tetradecen-2-one, (7E)-	tetradec-7-en-2-one	CCCCCC=CCCCC(=0)C	fruity jasmine orris	TGSC
3167	cis-2-Nonen-1-ol	(Z)-non-2-en-1-ol	CCCCCCC=CCO	melon wax sweet green cucumber tallow	Sigma Aldrich, TGSC, OdoRactor
3168	2-Nonen-1-ol	non-2-en-1-ol	CCCCCC=CCO	sweet fatty melon cucumber vegetable	TGSC
3169	trans-2-Nonenyl acetate	[(E)-non-2-enyl] acetate	CCCCCC=CCOC(=O)C	fruity wax citrus rue carrot oily earthy fatty	OdorRactor ,TGSC
3170	Heptanal	heptanal	CCCCCCC=0	fatty oily nutty woody fruity citrus rancid green herbaceous winey ozone aldehydic fresh cognac pungent penetrating	Flavornet, AOD, TGSC, OdoRactor, Pubchem
3171	Dihydrojasmone lactone	5-hexyl-5-methyloxolan-2-one	CCCCCC1(CCC(=O)O1)C	coconut creamy jasmine oily cheese peach wax spicy natural fresh sweet lactonic fatty powdery coumarinic fruity floral buttery	Sigma Aldrich, TGSC, Flavorbase, OdoRactor
3172	Hexyl-1,1-dimethoxy-3- phenylprop-2-ene	1-[(E)-3,3-dimethoxyprop-1-enyl]-4-hexylbenzene	CCCCCCC1=CC=C(C=C1)C=CC (OC)OC	fresh green fatty foliage woody	OdorRactor ,TGSC
3173	2-Hexylpyridine	2-hexylpyridine	CCCCCC1=CC=CC=N1	green fatty mutton vegetable nutty	OdorRactor ,TGSC, Flavorbase
3174	2-Hexylthiophene	2-hexylthiophene	CCCCCCC1=CC=CS1	floral fruity gassy green meaty sulfurous	OdorRactor ,TGSC
3175	2-Hexyl-2-cyclopenten-1-one	2-hexylcyclopent-2-en-1-one	CCCCCC1=CCCC1=O	sweet floral herbaceous woody jasmine celery wax fresh dry	OdorRactor ,TGSC
3176	5-Hexyl-4- methyldihydrofuran-2(3H)- one	5-hexyl-4-methyloxolan-2-one	CCCCCCC1C(CC(=0)01)C	fruity floral lactonic green peach wax oily tropical buttery	OdorRactor ,TGSC
3177	Methyl 2-hexyl-3- oxocyclopentanecarboxylate	methyl 2-hexyl-3-oxocyclopentane- 1-carboxylate	CCCCCCC1C(CCC1=O)C(=O)O C	green fresh jasmine floral oily herbaceous	OdorRactor ,TGSC
3178	(E)-4,5-Epoxy-2-undecenal	(E)-3-(3-hexyloxiran-2-yl)prop-2-	CCCCCC1C(O1)C=CC=O	metallic	Flavornet, TGSC
3179	2-Hexyl-4- acetoxytetrahydrofuran	(5-hexyloxolan-3-yl) acetate	CCCCCC1CC(CO1)OC(=O)C	sweet floral fruity	OdorRactor ,TGSC
3180	gamma-Decalactone	5-hexyloxolan-2-one	CCCCCC1CCC(=O)O1	peach fat sweet oily wax coconut buttery fresh fruity creamy fatty	Sigma Aldrich, Flavorbase, TGSC,OdoRactor
3181	(5S)-5-Hexyloxolan-2-one	(5S)-5-hexyloxolan-2-one	CCCCCC1CCC(=0)01	soft sweet coconut fruity fatty	TGSC
3182	delta-Undecalactone	6-hexyloxan-2-one	CCCCCCICCC(=0)01	buttery coconut wax peach creamy fatty fruity milky lactonic green sweet	Sigma Aldrich, TGSC, OdoRactor
3183	2-Hexylcyclopentanone	2-hexylcyclopentan-1-one	CCCCCC1CCCC1=0	jasmine fruity floral	OdorRactor ,TGSC
3184	7-Hexyloxepan-2-one	7-hexyloxepan-2-one	CCCCCC1CCCCC(=0)01	sweet peach fruity celery milky fatty apricot	OdorRactor ,TGSC, Flavorbase
3185	alpha-Hexyl-gamma- butyrolactone	3-hexyloxolan-2-one	CCCCCC1CCOC1=0	floral sweet grassy fruity green coconut	OdorRactor ,TGSC
3186	2-Hexyl-5-keto-1,4-dioxane	5-hexyl-1,4-dioxan-2-one	CCCCCC1COC(=0)CO1	fatty creamy buttery sweet nutty	OdorRactor ,TGSC, Flavorbase
3187	2-Hexyl-4,5-dimethyl-1,3-dioxolane	2-hexyl-4,5-dimethyl-1,3-dioxolane	CCCCCC1OC(C(O1)C)C	creamy dairy fruity green	OdorRactor ,TGSC
3188	2-Hexyl-4-methyl-1,3- dioxolane	2-hexyl-4-methyl-1,3-dioxolane	CCCCCC1OCC(O1)C	green fatty	OdorRactor ,TGSC
3189	2-Hexyl-1,3-dioxolane-4-	(2-hexyl-1,3-dioxolan-4-	CCCCCC10CC(01)C0	earthy fungal mossy green sweet	OdorRactor ,TGSC
3190	methanol 2-Hexyl-4-methyl-1,3-	yl)methanol 2-hexyl-4-methyl-1,3-dioxane	CCCCCC10CCC(01)C	floral geranium rose	TGSC
3191	dioxane 2-Hexyl-1,3-dioxolane	2-hexyl-1,3-dioxolane	CCCCCC1OCCO1	green oily plastic fatty fruity fresh cortex wet narcissus herbaceous woody basil	OdorRactor ,TGSC, Flavorbase
3192	Octanenitrile	octanenitrile	CCCCCCC#N	fatty aldehydic green	OdorRactor ,TGSC
3193	(phenylmethylene)-	2-benzylidenenonanal	C=0	fruity green leafy	TGSC
3194	N-Nonan-2-	N -nonan-2-ylidenehydroxylamine	CCCCCCC(=NO)C	cucumber floral fresh green	TGSC

3195	2-Nonanone	nonan-2-one	CCCCCCC(=O)C	fatty green melon cucumber weedy earthy herbaceous fruity fresh	Sigma Aldrich, AOD, TGSC,OdoRactor
				sweet wax soapy	
3196	3-Decanone	decan-3-one	CCCCCCC(=O)CC	cheese coconut wax fruity citrus fatty green orange floral	Sigma Aldrich, Flavorbase, TGSC, OdoRactor
3197	1-Hydroxypropan-2-olate;3- oxodecanoic acid	1-hydroxypropan-2-olate;3- oxodecanoic acid	CCCCCCC(=0)CC(=0)0.CC(C 0)[0-]	weak oily	Flavorbase
3198	Paradol	1-(4-hydroxy-3- methoxyphenyl)decan-3-one	CCCCCCC(=0)CCC1=CC(=C(C=C1)O) OC	spicy pungent pepper	TGSC, Flavorbase
3199	5-Oxododecanoic Acid	5-oxododecanoic acid	CCCCCCC(=0)CCCC(=0)O	creamy peach	Flavorbase
3200	N,N-Diethyloctanamide	N ,N -diethyloctanamide	CCCCCCC(=0)N(CC)CC	spice sweet mint tobacco woody fruity fresh	OdorRactor ,TGSC
3201	Octanoic acid	octanoic acid	CCCCCCC(=0)0	cheese oily sweaty fatty wax rancid vegetable acidic fruity soapy sour unpleasant faint irritating	Sigma Aldrich, AOD, TGSC, Pubchem
3202	Methyl octanoate	methyl octanoate	CCCCCCC(=0)OC	green citrus fruity orange wax sweet aldehydic vegetable herbaceous powerful winey	Sigma Aldrich, TGSC, OdoRactor, Pubchem
3203	Linalyl octanoate	3,7-dimethylocta-1,6-dien-3-yl octanoate	CCCCCCC(=0)OC(C)(CCC=C(C)C)C= C	fruity herbaceous sweet green natural dry	OdorRactor ,TGSC
3204	Isopropyl octanoate	propan-2-yl octanoate	CCCCCCC(=0)OC(C)C	banana coconut cognac fruity	OdorRactor ,TGSC
3205	p-Tolyl octanoate	(4-methylphenyl) octanoate	CCCCCCC(=O)OC1=CC=C(C=C1)C	animal fecal ylang jasmine indole green naphthyl hay	OdorRactor ,TGSC
3206	Ethyl octanoate	ethyl octanoate	CCCCCCC(=0)OCC	apricot banana floral pear pineapple winey fruit fatty wax sweet brandy musty creamy dairy fermented	Sigma Aldrich, Flavorbase, TGSC, OdoRactor
3207	Isobutyl octanoate	2-methylpropyl octanoate	CCCCCCC(=O)OCC(C)C	fruity green oily floral weak fatty winey	TGSC, Flavorbase
3208	Propylene glycol dicaprylate	2-octanoyloxypropyl octanoate	CCCCCCC(=O)OCC(C)OC(=O)	fatty fruity	TGSC
3209	Allyl octanoate	prop-2-enyl octanoate	CCCCCCC(=O)OCC=C	banana buttery fatty pineapple wax sweet fruity green tropical	Sigma Aldrich, TGSC, OdoRactor
3210	Geranyl octanoate	[(2E)-3,7-dimethylocta-2,6-dienyl] octanoate	CCCCCCC(=O)OCC=C(C)CCC =C(C)C	herbaceous rose fruity cognac	OdorRactor ,TGSC
3211	(E)-2-Hexenyl octanoate	[(E)-hex-2-enyl] octanoate	CCCCCCC(=0)OCC=CCCC	pear green fruity oily winey earthy	OdorRactor ,TGSC, Flavorbase
3212	Benzyl octanoate	benzyl octanoate	CCCCCCC(=O)OCC1=CC=CC =C1	herbaceous fatty fruity peach pineapple	SuperScent, TGSC
3213	Furfuryl octanoate	furan-2-ylmethyl octanoate	CCCCCCC(=O)OCC1=CC=CO	wax sweet metallic fruity peach caramel bready	SuperScent, TGSC, OdoRactor
3214	Propyl octanoate	propyl octanoate	CCCCCCC(=O)OCCC	coconut cocoa cognac winey fatty	OdorRactor ,TGSC
3215	Isopentyl octanoate	3-methylbutyl octanoate	CCCCCCCC(=0)OCCC(C)C	apple coconut green wax pineapple sweet oily soapy fruity	Sigma Aldrich, TGSC, OdoRactor
3216	(Z)-3-Hexenyl octanoate	[(Z)-hex-3-enyl] octanoate	CCCCCCC(=0)OCCC=CCC	green leafy orchid kiwi metallic fruity asparagus lettuce winey wax fatty tropical	OdorRactor ,TGSC, Flavorbase
3217	Phenethyl octanoate	2-phenylethyl octanoate	CCCCCCC(=O)OCCC1=CC=C C=C1	green floral fruity sweet wax cocoa caramel winey cognac	Sigma Aldrich, TGSC, OdoRactor
3218	Butyl octanoate	butyl octanoate	CCCCCCC(=0)OCCCC	fruit buttery ethereal herbaceous dank	Flavornet, TGSC,OdoRactor
3219	Pentyl octanoate	pentyl octanoate	CCCCCCC(=0)OCCCCC	sweet winey orris cognac fatty elderflower	Sigma Aldrich, TGSC, OdoRactor
3220	Hexyl octanoate	hexyl octanoate	CCCCCCC(=0)OCCCCCC	green vegetable oily herbaceous fruity wax berry apple estery	Sigma Aldrich, TGSC, OdoRactor
3221	Heptyl octanoate	heptyl octanoate	CCCCCCC(=0)OCCCCCCC	wax oily green tropical fresh fatty fruity musty	OdorRactor ,TGSC
3222	2-Nonanol	nonan-2-ol	CCCCCCC(C)O	fatty green melon cucumber wax creamy citrus orange cheese fruity	Sigma Aldrich, TGSC,OdoRactor
3223	1-Decen-3-ol	dec-1-en-3-ol	CCCCCCCC(C=C)O	cheese green fruity earthy wax fungal mushroom ketonic vegetable	Sigma Aldrich, TGSC, OdoRactor
3224	3-Decanol	decan-3-ol	CCCCCCC(CC)O	floral fatty orange musty mushroom	OdorRactor ,TGSC
3225	2,3-Dihydroxypropyl 5- hydroxydodecanoate	2,3-dihydroxypropyl 5- hydroxydodecanoate	CCCCCCC(CCCC(=0)OCC(CO	peach fruity coconut oily fresh tropical	OdorRactor ,TGSC
3226	Octanol, acetate, mono((acetyloxy)methyl) deriv.	2-acetyloxynonyl acetate		watery floral muguet fresh	OdorRactor ,TGSC
3227	1,1-Dimethoxyoctane	1,1-dimethoxyoctane	CCCCCCC(OC)OC	citrus floral green leafy rose violet ozone clean fresh	OdorRactor ,TGSC
		1,1-diethoxyoctane	CCCCCCC(OCC)OCC	green citrus oily fatty woody spicy	OdorRactor ,TGSC

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3229	Decenoic acid 2-Decenoic acid	dec-2-enoic acid	CCCCCCCC=CC(=0)0 CCCCCCCC=CC(=0)0	fatty wax buttery oily creamy dairy	OdorRactor ,TGSC
3230	2-Decenoic acid	(E)-dec-2-enoic acid	CCCCCC=CC(=0)0	green lactonic plum fatty milky fruity sweet fresh	OdorRactor ,TGSC, Flavorbase
3231	Methyl 2-decenoate	methyl (E)-dec-2-enoate	CCCCCCCC=CC(=O)OC	fresh green soapy fatty earthy	TGSC
3232	Ethyl trans-2-decenoate	ethyl (E)-dec-2-enoate	CCCCCCCC=CC(=0)OCC	fatty wax fruity green apple pear violet melon soapy citrus	Sigma Aldrich, TGSC, GSC, Flavorbase, OdoRactor
3233	Butyl 2-decenoate	butyl (E)-dec-2-enoate	CCCCCCC=CC(=0)OCCCC	fruity fatty oily green dairy nasturtium clean citrus peach apricot	OdorRactor ,TGSC, Pubchem
3234	(2E,4E)-2,4-Dodecadienal	(2E ,4E)-dodeca-2,4-dienal	CCCCCCCC=CC=CC=O	spice fatty grapefruit orange citrus strong fried meat fried	ADB, TGSCGSC, Flavorbase, OdoRactor
3235	2,4-Dodecadien-1-ol	(2E ,4E)-dodeca-2,4-dien-1-ol	CCCCCCC=CC=CCO	wax fruity green	OdorRactor ,TGSC
3236	2-Decenal	(E)-dec-2-enal	CCCCCCCC=CC=O	fatty green meaty oily orange citrus wax floral earthy coriander mushroom aldehydic chicken pork rose strong	Sigma Aldrich, TGSC, Flavorbase, OdoRactor
3237	(Z)-2-Decenal	(Z)-dec-2-enal	CCCCCCCC=CC=O	tallow fatty	Flavornet, TGSC, OdoRactor
3238 3239	(Z)-4-Dodecenal 2-Decen-1-ol	(Z)-dodec-4-enal (E)-dec-2-en-1-ol	CCCCCCC=CCC=O	aldehydic citrus fruity fatty wax ozone citrus rose rue	OdorRactor ,TGSC OdorRactor ,TGSC
3240	2-Decenol	dec-2-en-1-ol	CCCCCCC=CCO	wax citrus rose fresh ozone rue fatty	OdorRactor ,TGSC
3241	2-Decenyl acetate	dec-2-enyl acetate	CCCCCCCC=CCOC(=O)C	wax fatty	OdorRactor ,TGSC
3242	Methyl 2- (octylideneamino)benzoate	methyl 2- (octylideneamino)benzoate		floral grape oily fatty fresh	OdorRactor ,TGSC
3243	Octanal	octanal	CCCCCCCC=0	fatty honey citrus fruity soapy green lemon aldehydic wax orange peely orange strong pungent	Sigma Aldrich, AOD, TGSC, Pubchem
3244	2-Heptyl-2,4-dimethyl-1,3-dioxolane	2-heptyl-2,4-dimethyl-1,3-dioxolane	CCCCCCC1(OCC(O1)C)C	fruity floral fatty herbaceous	TGSC
3245	(E)-3-[(2R,3S)-3- Pentyloxiran-2-yl]prop-2- enal	3-heptyloxirene-2-carbaldehyde	CCCCCCC1=C(O1)C=O	metallic green	Flavornet
3246	2-Heptylpyridine	2-heptylpyridine	CCCCCCC1=CC=CC=N1	green floral geranium earthy	TGSC
3247	2-Heptylfuran	2-heptylfuran	CCCCCCC1=CC=CO1	green fatty lactonic oily nutty	OdorRactor ,TGSC
3248	trans-2,3-Epoxydecanal	(2S, 3R)-3-heptyloxirane-2-	CCCCCCC1C(O1)C=O	roasted meaty dairy beefy	,
		carbaldehyde 3-heptyloxirane-2-carbaldehyde		,	OdorRactor ,TGSC,
	2,3-Epoxydecanal		CCCCCCC1C(O1)C=O	citrus fatty soapy	Flavorbase
3250	3-Heptyldihydro-5-methyl- 2(3H)-furanone	3-heptyl-5-methyloxolan-2-one	CCCCCCC1CC(OC1=O)C	creamy green wax lactonic citrus fruity	OdorRactor ,TGSC
3251	6-Heptyl-5,6-dihydro-2H- pyran-2-one	2-heptyl-2,3-dihydropyran-6-one	CCCCCCC1CC=CC(=0)O1	coconut creamy fatty lactonic wax buttery dairy	OdorRactor ,TGSC, Flavorbase
3252	(s)-gamma-Undecalactone	(5S)-5-heptyloxolan-2-one	CCCCCCC1CCC(=0)01	fatty sweet aldehydic	TGSC
3253	(5R)-5-Heptyloxolan-2-one	(5R)-5-heptyloxolan-2-one	CCCCCCC1CCC(=0)01	fatty sweet peach	TGSC
3254	gamma-Undecalactone	5-heptyloxolan-2-one	CCCCCCC1CCC(=0)01	musty earthy peach sweet apricot fruity creamy fatty lactonic ketonic coconut	Sigma Aldrich, TGSC, OdoRactor
3255	delta-Dodecalactone	6-heptyloxan-2-one	CCCCCCC1CCCC(=0)01	buttery cheese coconut creamy oily peach winey fruit sweet tropical fresh metallic fatty dairy milky powerful	Sigma Aldrich, Flavorbase, TGSC, OdoRactor, Pubchem
3256	2H-Pyran-2-one, 6- heptyltetrahydro-, (6R)-	(6R)-6-heptyloxan-2-one	CCCCCCCICCCC(=0)01	fruity apricot lactonic	TGSC
3257	2-Heptylcyclopentanone	2-heptylcyclopentan-1-one	CCCCCCCICCCC1=0	fruity peach oily tropical fresh jasmine	OdorRactor ,TGSC
3258	2-Heptyltetrahydrofuran	2-heptyloxolane	CCCCCCC1CCCO1	natural green pea wax rose floral	OdorRactor ,TGSC
3259	2-Heptyl-4-methyl-1,3- dioxolane	2-heptyl-4-methyl-1,3-dioxolane	CCCCCCC1OCC(O1)C	green woody	OdorRactor,
3260	2-Heptyl-1,3-dioxolane	2-heptyl-1,3-dioxolane	CCCCCCC1OCCO1	citrus orange fatty fresh aldehydic	OdorRactor ,TGSC
3261	Nonane	nonane	CCCCCCCC	gasoline	Flavornet, TGSC
	Methyl 2-undecynoate	methyl undec-2-ynoate	CCCCCCCC#CC(=0)OC	wax fruity green floral violet meaty fatty milky	OdorRactor ,TGSC
3263	Ethyl undec-2-ynoate	ethyl undec-2-ynoate	CCCCCCCC#CC(=O)OCC	green reseda wax	TGSC
3264	2-Decanone	decan-2-one	CCCCCCCC(=0)C	floral fatty peach orange	Sigma Aldrich, AOD, Flavorbase, TGSC,OdoRactor
3265	Undecane-2,3-dione	undecane-2,3-dione	CCCCCCCC(=O)C(=O)C	wax creamy fatty dairy aldehydic rancid vegetable	OdorRactor ,TGSC
3266	Nonivamide	N -[(4-hydroxy-3- methoxyphenyl)methyl]nonanamid e		bland	OdorRactor,

3267	Nonanoic acid	nonanoic acid	CCCCCCCC(=0)O	cheese wax tallow green fatty	Sigma Aldrich, AOD,
3268	Methyl nonanoate	methyl nonanoate	CCCCCCCC(=0)OC	dairy dirty sweet fruity pear wax tropical	TGSC,OdoRactor Sigma Aldrich, TGSC,
3206	Methyl nonanoate	metnyi nonanoate	CCCCCCC(=0)0C	coconut nutty winey	OdoRactor, Pubchem
3269	Ethyl nonanoate	ethyl nonanoate	CCCCCCCC(=0)OCC	oily fruity nutty rose wax rummy winey tropical natural cognac estery apple banana fatty grape	Sigma Aldrich, Flavorbase, TGSC, OdoRactor
3270	Isobutyl nonanoate	2-methylpropyl nonanoate	CCCCCCCC(=0)OCC(C)C	oily rose fruity winey	Flavorbase
3271	Allyl nonanoate	prop-2-enyl nonanoate	CCCCCCCC(=0)OCC=C	sweet wax fruity winey creamy cortex pineapple	SuperScent, TGSC, Pubchem, OdoRactor
3272	Geranyl nonanoate	[(2E)-3,7-dimethylocta-2,6-dienyl] nonanoate	CCCCCCCC(=0)OCC=C(C)CC C=C(C)	floral geranium green rose	OdorRactor ,TGSC
3273	Benzyl nonanoate	benzyl nonanoate	CCCCCCCC(=0)OCC1=CC=C C=C1	floral sweet elemi winey	TGSC
3274 3275	Propyl nonanoate 3-Methylbutyl nonanoate	propyl nonanoate 3-methylbutyl nonanoate	CCCCCCCC(=0)OCCC CCCCCCCC(=0)OCCC(C)C	yeasty melon fermented fruity oily apricot floral	OdorRactor ,TGSC SuperScent, TGSC, OdoRactor
3276	Butyl nonanoate	butyl nonanoate	CCCCCCCC(=0)OCCCC	orange apricot rose	OdorRactor ,TGSC
3277	Amyl nonanoate	pentyl nonanoate	CCCCCCCC(=0)OCCCCC	apricot floral cognac	OdorRactor ,TGSC
3278	Hexyl nonanoate	hexyl nonanoate	CCCCCCCC(=0)OCCCCCC	brandy green vegetable fruity floral	OdorRactor ,TGSC
3279	Heptyl nonan-1-oate	heptyl nonanoate	CCCCCCCC(=0)OCCCCCCC	winey sweet oily floral orange flower rose	TGSC
3280	2-Methyldecanenitrile	2-methyldecanenitrile	CCCCCCCC(C)C#N	peach fruity floral jasmine lactonic	·
3281	2-Methyldecanal	2-methyldecanal	CCCCCCCC(C)C=0	citrus wax watery fresh dry	OdorRactor ,TGSC
	2-Ethyldecanoic acid	2-ethyldecanoic acid	CCCCCCCC(CC)C(=0)0	soapy wax citrus woody	TGSC
3283	1,1-Dimethoxynonane	1,1-dimethoxynonane	CCCCCCCC(OC)OC	floral plastic citrus green fresh	OdorRactor ,TGSC
3284	1,1-Diethoxynonane	1,1-diethoxynonane	CCCCCCCC(OCC)OCC	aldehydic floral rose	OdorRactor ,TGSC
3285	2-Undecenal	(E)-undec-2-enal	cccccccc=cc=0	orange herbaceous fruity green soapy sweet fresh citrus aldehydic wax fatty rose clean	Sigma Aldrich, Flavornet, TGSC, OdoRactor
3286	3-Dodecenal	(E)-dodec-3-enal	CCCCCCCC=CCC=O	citrus orange bitter mandarin coriander	TGSC
3287	Oleic acid	(Z)-octadec-9-enoic acid	CCCCCCCC=CCCCCCCC(= O)O	fatty wax lard fried oily tallow savory	Sigma Aldrich, TGSC. Pubchem, OdoRactor
3288	Methyl oleate	methyl (Z)-octadec-9-enoate	CCCCCCCC=CCCCCCCC(= O)OC	mild fatty	OdorRactor ,TGSC, Pubchem
3289	Ethyl octadec-9-enoate	ethyl octadec-9-enoate	CCCCCCCC=CCCCCCCC(= 0)OCC	fatty oily dairy milky wax tallow	OdorRactor ,TGSC
3290	Ethyl oleate	ethyl (Z)-octadec-9-enoate	CCCCCCCC=CCCCCCCC(= 0)OCC	wax fatty oily dairy milky tallow	Sigma Aldrich, TGSC, OdoRactor
3291	Sorbitan monooleate	[(2R)-2-[(2R,3R,4S)-3,4-dihydroxyoxolan-2-yl]-2-hydroxyethyl] (Z)-octadec-9-enoate	CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC	fatty oily wax	TGSC
3292	9-Octadecenoic acid (9Z)-, 2,3- bis(acetyloxy)propyl ester	2,3-diacetyloxypropyl octadec-9- enoate	CCCCCCCCC=CCCCCCCC(= O)OCC(C OC(=O)C)OC(=O)C	bland	TGSC
3293	Butyl oleate	butyl (Z)-octadec-9-enoate	CCCCCCCCC=CCCCCCCC(= 0)OCCC	fatty	OdorRactor ,TGSC, Pubchem
3294	Polyoxyethylene sorbitan	2-[2-[3,4-bis(2-	CCCCCCCCC=CCCCCCCCC(=	alcoholic characteristic	Sigma Aldrich, Pubchem
	monooleate	hydroxyethoxy)oxolan-2-yl]-2-(2- hydroxyethoxy)ethoxy]ethyl (E)- octadec-9-enoate	0)0CC0 CC(C1C(C(C01)0CC0)0CC0)0 CC0		
3295	9-Octadecenal	(E)-octadec-9-enal	CCCCCCCC=CCCCCCCC=O	fatty	OdorRactor ,TGSC
3296	Oleyl alcohol	(Z)-octadec-9-en-1-ol	CCCCCCCC=CCCCCCCCO	fatty animal	OdorRactor ,TGSC
3297	Oleyl acetate	[(Z)-octadec-9-enyl] acetate	CCCCCCCC=CCCCCCCCCCCCCCCCCCCCCCCCCCCCC	fatty	OdorRactor ,TGSC
3298	trans-2-Undecen-1-ol	(E)-undec-2-en-1-ol	CCCCCCCC=CCO	floral rose wax fresh fruity	OdorRactor ,TGSC
3299	2-Undecenyl acetate	[(E)-undec-2-enyl] acetate	CCCCCCCCC=CCOC(=O)C	fresh wax rose	OdorRactor ,TGSC
3300	1-Decene, 1-methoxy-, (1E)-	170.29 g/mol	CCCCCCCCC=COC	fruity floral citrus fatty	TGSC
3301	Methyl 2- (nonylideneamino)benzoate	methyl 2- (nonylideneamino)benzoate	CCCCCCCC=NC1=CC=CC=C1 C(=0)0 C	sweet floral orange flower rose aldehydic	OdorRactor ,TGSC
3302	Nonanal	nonanal	CCCCCCCC=0	apple coconut fatty fishy grape grapefruit green lemon lime meaty melon oily orange wax nutty peach rose floral citrus aldehydic fresh orris peely cucumber	Sigma Aldrich, AOD, TGSC, OdoRactor
3303	2-Octylthiophene	2-octylthiophene	CCCCCCCC1=CC=CS1	green grassy musty	TGSC
3304	(s)-gamma-Dodecalactone	(5S)-5-octyloxolan-2-one	CCCCCCCC1CCC(=0)01	fatty fruity milky	TGSC
3305	gamma-Dodecalactone	5-octyloxolan-2-one	CCCCCCCC1CCC(=0)01	fatty fruity peach pear sweet floral	Sigma Aldrich, TGSC,
				metallic milky	OdoRactor

3306	R-(+)-gamma-Dodecalactone	(5R)-5-octyloxolan-2-one	CCCCCCCC1CCC(=0)O1	fruity floral sweet aldehydic	TGSC
3307	6-Octyltetrahydro-2H-pyran-2-	6-octyloxan-2-one	CCCCCCCC1CCCC(=0)O1	woody creamy milky oily dairy buttery	OdorRactor ,TGSC
3308	one 4-Methyl-2-octyl-1,3-	4-methyl-2-octyl-1,3-dioxolane	CCCCCCCC1OCC(O1)C	musty fruity	OdorRactor ,TGSC
3309	dioxolane Decanenitrile	decanenitrile		,	·
			CCCCCCCCC#N	fresh musty fatty wax oily cognac	OdorRactor ,TGSC
3310	2-Undecanone	undecan-2-one	CCCCCCCCC(=0)C	orris citrus orange fresh green wax fruity creamy fatty floral ketonic pineapple rose rue	Sigma Aldrich, Flavorbase, TGSC, Pubchem,OdoRactor
3311	Glycerides, palm-oil mono- and di-, hydrogenated, 3- oxododecanoates	1-hydroxypropan-2-olate;3- oxododecanoic acid	CCCCCCCCC(=0)CC(=0)O.C C(CO)[O-]	mild fatty	TGSC
3312	Decanoic acid	decanoic acid	CCCCCCCC(=0)0	fatty citrus rancid sour unpleasant wax cheese soapy	Sigma Aldrich, AOD, Flavorbase
3313	Methyl decanoate	methyl decanoate	CCCCCCCCC(=0)OC	oily fruity winey floral fermented	Sigma Aldrich, TGSC,OdoRactor
3314	Isopropyl decanoate	propan-2-yl decanoate	CCCCCCCCC(=0)OC(C)C	green vegetable woody oily fruity	TGSC
3315	Ethyl decanoate	ethyl decanoate	CCCCCCCCC(=0)OCC	grape oily pear winey sweet wax fruity apple brandy fatty nutty cognac	Sigma Aldrich, Flavorbase, TGSC,OdoRactor
3316	Isobutyl decanoate	2-methylpropyl decanoate	CCCCCCCCC(=0)OCC(C)C	oily sweet brandy apricot fermented cognac	OdorRactor ,TGSC
3317	Allyl decanoate Furfuryl decanoate	prop-2-enyl decanoate furan-2-ylmethyl decanoate	CCCCCCCCC(=0)OCC=C CCCCCCCCC(=0)OCC1=CC=	fatty sweet fruity pineapple fatty caramel	TGSC TGSC
3318			CO1	,	
3319	Propyl decanoate	propyl decanoate	CCCCCCCCC(=0)OCCC	wax fruity fatty green vegetable woody oily fruit	OdorRactor ,TGSC
3320	Isoamyl decanoate	3-methylbutyl decanoate	CCCCCCCCC(=0)OCCC(C)C	wax banana fruity sweet cognac green dirty	OdorRactor ,TGSC
3321	(Z)-3-Hexenyl decanoate	[(Z)-hex-3-enyl] decanoate	CCCCCCCCC(=0)OCCC=CCC	gree fruity fatty wax	Flavorbase
3322	2-(4-Methyl-5-thiazolyl)ethyl decanoate	2-(4-methyl-1,3-thiazol-5-yl)ethyl decanoate	CCCCCCCCC(=0)OCCC1=C(N =CS1)C	roasted nutty	TGSC
3323	Butyl decanoate	butyl decanoate	CCCCCCCCC(=0)OCCCC	whiskey	Flavornet, TGSC
3324	Pentyl decanoate	pentyl decanoate	CCCCCCCC(=0)OCCCCC	fruity cognac winey	TSGC
3325	Heptyl decanoate	heptyl decanoate	CCCCCCCCC(=0)OCCCCCCC	winey brandy cognac	TGSC
3326	Octyl decanoate	octyl decanoate	CCCCCCCCC(=0)OCCCCCCC	fatty wax	TGSC
3327	1,1-Dimethoxy-2-	1,1-dimethoxy-2-methylundecane	C CCCCCCCCC(C)C(OC)OC	aldehydic amber lemon green wax	OdorRactor ,TGSC
3328	methylundecane 2-Methylundecanal	2-methylundecanal	CCCCCCCCC(C)C=O	fresh amber mossy citrus metallic	SuperScent, TGSC,
3320	2 Methyrandectana	2 menyanacenna		wax coumarinic aldehydic tuberose gassy	OdoRactor
3329	3-Methyldodecanonitrile	3-methyldodecanenitrile	CCCCCCCC(C)CC#N	orange green algae watery oily marine laundered cloth citrus	OdorRactor ,TGSC
3330	2-Undecanol	undecan-2-ol	CCCCCCCCC(C)O	wax fruity fresh laundered cloth sarsaparilla	Sigma Aldrich, TGSC, OdoRactor
3331	(10)-Gingerol	(5S)-5-hydroxy-1-(4-hydroxy-3-methoxyphenyl)tetradecan-3-one	CCCCCCCCC(CC(=0)CCC1=C C(=C(C =C1)0)OC)O	musk woody	TGSC
3332	1,1-Dimethoxydecane	1,1-dimethoxydecane	CCCCCCCC(OC)OC	wax herbaceous citrus green neroli	OdorRactor ,TGSC
3333	1,1-Diethoxydecane	1,1-diethoxydecane	CCCCCCCC(OCC)OCC	mossy aldehydic wax green orange	OdorRactor ,TGSC
3334	Dodecenal	dodec-2-enal	CCCCCCCCC=CC=O	fresh cognac coconut citrus herbaceous mandarin orange wax bitter fatty cilantro green fruity strong tallow tangerine	SuperScent, TGSC, Flavorbase, OdoRactor
3335	2-Dodecenal	(E)-dodec-2-enal	CCCCCCCCC=CC=0	fatty orange herbaceous green sweet herbaceous citrus metallic mandarin wax aldehydic coriander	Sigma Aldrich, TGSC, Flavorbase, OdoRactor
3336	(Z)-2-Dodecenal	(Z)-dodec-2-enal	CCCCCCCCC=CC=O	herbaceous green citrus fruity mandarin orange	OdorRactor,
3337	Heptadec-7-ene	heptadec-7-ene	CCCCCCCCC=CCCCCCC	alkane	Flavornet
3338	2-Dodecen-1-ol	dodec-2-en-1-ol	CCCCCCCCC=CCO	fatty	OdorRactor ,TGSC
3339	trans-2-Dodecen-1-ol	(E)-dodec-2-en-1-ol	CCCCCCCCCC=CCO	oil fatty	Flavornet, TGSC, OdoRactor
3340	Dodec-2-enyl acetate	[(E)-dodec-2-enyl] acetate	CCCCCCCCCC=CCOC(=0)C	fresh fatty	OdorRactor ,TGSC
3341	Methyl 2- (decylideneamino)benzoate	methyl 2- (decylideneamino)benzoate	CCCCCCCCCC=NC1=CC=CC=C 1C(=0) OC	fatty wax sweet orange blossom fresh dry orange flower	OdorRactor ,TGSC
3342	Decanal	decanal	CCCCCCCCC=O	floral citrus sweet soapy orange tallow strong penetrating wax aldehydic fatty	Sigma Aldrich, AOD, Flavorbase, TGSC,OdoRactor

3343	4-Nonylphenol	4-nonylphenol	CCCCCCCCC1=CC=C(C=C1)O	phenolic	Pubchem
3344	delta-Tetradecalactone	6-nonyloxan-2-one	CCCCCCCCC1CCCC(=0)01	creamy wax buttery oily fatty	Sigma Aldrich, TGSC
		•	, ,	cheese milky dairy	
3345	4-Methyl-2-nonyl-1,3- dioxolane	4-methyl-2-nonyl-1,3-dioxolane	CCCCCCCCC1OCC(01)C	green floral herbaceous	TGSC
3346	Undecane	undecane	CCCCCCCCC	faint alkane	Sigma Aldrich
3347	2-Dodecanone	dodecan-2-one	CCCCCCCCC(=0)C	fruity citrus floral orange	TGSC, ODoRactor
3348	Undecanoic acid	undecanoic acid	CCCCCCCCCC(=0)0	oily wax creamy cheese fatty coconut	Sigma Aldrich, AOD, TGSC,OdoRactor
3349	Methyl undecanoate	methyl undecanoate	CCCCCCCCC(=0)OC	fatty wax fruity rose	SuperScent, TGSC, OdoRactor
3350	Ethyl undecanoate	ethyl undecanoate	CCCCCCCCCC(=0)OCC	coconut cognac soapy wax fatty buttery	Sigma Aldrich, TGSC.OdoRactor
3351	Undecane, 1,1-dimethoxy-	1,1-dimethoxyundecane	CCCCCCCCCC(OC)OC	floral citrus fresh	OdorRactor ,TGSC
3352	2-Tridecenenitrile	tridec-2-enenitrile	CCCCCCCCCCC+CC#N	citrus wax mandarin fresh aldehydic seashore	OdorRactor ,TGSC
3353	2-Tridecenal	(E)-tridec-2-enal	CCCCCCCCCCC=CC=O	citrus tangerine powdery soapy creamy wax aldehydic fatty watery cilantro	Sigma Aldrich, TGSC, OdoRactor
3354	trans-2-Tridecen-1-ol	(E)-tridec-2-en-1-ol	CCCCCCCCCCC	wax clean watery cilantro rue	OdorRactor ,TGSC, Flavorbase
3355	2-Tridecenyl acetate	[(E)-tridec-2-enyl] acetate	CCCCCCCCCCC=CCOC(=O)C	citrus laundered cloth fatty wax fruity pear apple	OdorRactor ,TGSC
2255			0000000000		g:
3356	Undecanal	undecanal	ccccccccc=0	fatty orange wax rose oily pungent sweet floral citrus soapy aldehydic green laundered cloth watermelon pineapple cilantro	Sigma Aldrich, AOD, TGSC,OdoRactor
3357	2-Decylfuran	2-decylfuran	CCCCCCCCCC1=CC=CO1	spicy aldehydic fatty	OdorRactor ,TGSC
3358	2-Decyl-4-methyl-1,3- dioxolane	2-decyl-4-methyl-1,3-dioxolane	CCCCCCCCCC1OCC(O1)C	sweet fatty floral	OdorRactor ,TGSC
3359	Dodecane	dodecane	CCCCCCCCCC	alkane	Flavornet
3360	Dodecanenitrile	dodecanenitrile	CCCCCCCCCC#N	citrus orange metallic spicy dry	OdorRactor ,TGSC
3361	2-Tridecanone	tridecan-2-one	CCCCCCCCCC(=0)C	spicy herbaceous fatty wax dairy	Sigma Aldrich,
				milky coconut nutty herbaceous earthy mushroom chicken fat	TGSC,OdoRactor
3362	Lauric acid	dodecanoic acid	CCCCCCCCCCC(=0)0	fatty metallic coconut bay weak wax	Sigma Aldrich, AOD, Flavorbase, Pubchem
3363	Methyl dodecanoate	methyl dodecanoate	CCCCCCCCCCC(=0)OC	coconut creamy fatty soapy wax mushroom floral winey oily	Sigma Aldrich, TGSC, OdoRactor, Pubchem
3364	p-Tolyl laurate	(4-methylphenyl) dodecanoate	CCCCCCCCCCC(=0)OC1=CC =C(C=C 1)C	floral sweet nutty vanilla balsamic oily floral	OdorRactor ,TGSC, Pubchem
3365	Ethyl laurate	ethyl dodecanoate	CCCCCCCCCC(=0)OCC	green floral fruity leafy sweet wax soapy clean rummy creamy mild fatty oily	Sigma Aldrich, Flavorbase, TGSC, OdoRactor
3366	(2R)-2-[(2R,3R,4S)-3,4-Bis(2-hydroxyethoxy)oxolan-2-yl]- 2-hydroxyethyl dodecanoate	[(2R)-2-[(2R ,3R ,4S)-3,4-bis(2-hydroxyethoxy)oxolan-2-yl]-2-hydroxyethyl] dodecanoate	CCCCCCCCCCC(=0)OCC(C1 C(C(C01)OCCO)OCCO)O	alcoholic characteristic	Sigma Aldrich, PubChem, TGSC
3367	Benzyl laurate	benzyl dodecanoate	CCCCCCCCCCC(=0)OCC1=C C=CC=C	fatty wax soapy	OdorRactor ,TGSC
3368	Isoamyl laurate	3-methylbutyl dodecanoate	CCCCCCCCCCC(=0)OCCC(C)	beer brandy creamy grape wax plum rummy winey oily fatty peach alcoholic yeasty fusel	Sigma Aldrich, TGSC, OdoRactor
3369	Butyl laurate	butyl dodecanoate	CCCCCCCCCC(=0)OCCCC	fermented dairy oily wax soapy fruity peanut	Sigma Aldrich, TGSC
3370	Amyl laurate	pentyl dodecanoate	CCCCCCCCCC(=0)OCCCCC	V 1	TGSC
3371	Polysorbate 20	2-[2-[3,4-bis(2-	CCCCCCCCCCC(=0)OCCOCC	alcoholic characteristic	Sigma Aldrich, Pubchem
22		hydroxyethoxy)oxolan-2-yl]-2-(2-	(C1C(C(C01)OCCO)OCCO)OCCO		
3372	Dodecanal dimethyl acetal	1,1-dimethoxydodecane	CCCCCCCCCC(OC)OC		OdorRactor,
3373	2-Tetradecenal	(E)-tetradec-2-enal	CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC	citrus wax green pepper soapy fatty cilantro chicken cucumber herbaceous lemon floral	OdorRactor ,TGSC
3374	Dodecanal	dodecanal	CCCCCCCCCCC=0	floral wax herbaceous sweet lily fatty citrus soapy aldehydic green orange clean woody fruity	Sigma Aldrich, AOD, Flavorbase, TGSC,OdoRactor
3375	Tetrahydro-6-undecyl-2H- pyran-2-one	6-undecyloxan-2-one	CCCCCCCCCCCCC(=0)O	fatty wax dairy buttery	TGSC
3376	Tridecane	tridecane	cccccccccc	wax hydrocarbon	Flavornet, Pubchem

3377	Tridecanoic acid	tridecanoic acid	CCCCCCCCCCC(=0)0	woody wax	Sigma Aldrich,
			` ′	•	TGSC,OdoRactor
3378	Tridecanal	tridecanal	CCCCCCCCCCCCC=0	grapefruit floral sweet musty soapy citrus wax fresh clean aldehydic petal	Sigma Aldrich, TGSC, OdoRactor
3379	Tetradecane	tetradecane	CCCCCCCCCCCC	wax	Flavornet, TGSC,OdoRactor
3380	Tetradecanenitrile	tetradecanenitrile	CCCCCCCCCCC#N	clean fresh wet orange flower green floral	OdorRactor ,TGSC
3381	2-Pentadecanone	pentadecan-2-one	CCCCCCCCCCCC(=0)C	celery jasmine fatty spicy fresh oily wax burnt floral	Sigma Aldrich, TGSC, OdoRactor
3382	Myristic acid	tetradecanoic acid	CCCCCCCCCCCC(=0)0	oily wax soapy fatty coconut pineapple citrus	Sigma Aldrich, TGSC,OdoRactor
3383	Methyl tetradecanoate	methyl tetradecanoate	CCCCCCCCCCCC(=0)OC	fatty honey wax petal orris coconut cognac	Sigma Aldrich, TGSC, OdoRactor, Pubchem
3384	Isopropyl myristate	propan-2-yl tetradecanoate	CCCCCCCCCCCC(=0)OC(C)	cheese cherry cinnamyl wax winey oily fatty	Sigma Aldrich, TGSC,OdoRactor
3385	Ethyl tetradecanoate	ethyl tetradecanoate	CCCCCCCCCCCC(=0)OCC	coconut soapy ethereal wax sweet orris violet fatty	Sigma Aldrich, Flavorbase, TGSC, OdoRactor
3386	Isobutyl myristate	2-methylpropyl tetradecanoate	CCCCCCCCCCCC(=O)OCC(C)C	mild fatty wax	Flavorbase
3387	Butyl myristate	butyl tetradecanoate	CCCCCCCCCCCC(=O)OCCC	oily fatty	TGSC
3388	(Z)-9-Tricosene	(Z)-tricos-9-ene	cccccccccccccccccccccccccccccccccccccc	fatty wax	TGSC
3389	Tetradecanal	tetradecanal	CCCCCCCCCCCCC=0	floral wax amber citrus musk fatty incense dry dairy creamy fishy fruity pear	Flavornet, TGSC, OdoRactor
3390	2H-Pyran-2-one, tetrahydro-6- tridecyl-	6-tridecyloxan-2-one	CCCCCCCCCCCCCCCC(=O	fatty wax savory mild creamy dairy	TGSC, Flavorbase
3391	Pentadecane	pentadecane	ccccccccccc	wax	Flavornet, TGSC,OdoRactor
3392	Hexadecan-2-one	hexadecan-2-one	CCCCCCCCCCCC(=0)C	fruit	Flavornet, TGSC
3393	Pentadecanoic acid	pentadecanoic acid	CCCCCCCCCCCCC(=0)0	wax	Sigma Aldrich, TGSC, OdoRactor
3394	Ethyl pentadecanoate	ethyl pentadecanoate	CCCCCCCCCCCC(=0)OCC	sweet honey	TGSC
3395	Pentadecanal	pentadecanal	CCCCCCCCCCCCCCC	fresh wax	Flavornet, TGSC
3396	gamma-Stearolactone	5-tetradecyloxolan-2-one	CCCCCCCCCCCCCC1CCC(=O)O1	wax fatty	TGSC
3397 3398	Hexadecane Palmitic acid	hexadecane hexadecanoic acid	CCCCCCCCCCCCCCC(=0)0	alkane faint fatty wax creamy	Flavornet Sigma Aldrich, TGSC,
3398	Paimiuc acid	nexadecanoic acid	CCCCCCCCCCC(=0)0	ramit ratty wax creamy	Pubchem
3399	Methyl palmitate	methyl hexadecanoate	CCCCCCCCCCCCCC(=0)OC	,	Sigma Aldrich, TGSC,OdoRactor
3400	Isopropyl palmitate	propan-2-yl hexadecanoate	CCCCCCCCCCCCCC(=0)OC (C)C		Sigma Aldrich,OdoRactor
3401	Ethyl palmitate	ethyl hexadecanoate	CCCCCCCCCCCCC(=0)OC	wax fruity creamy milky balsamic	Sigma Aldrich, TGSC,OdoRactor
3402	Hex-3-enyl hexadecanoate	hex-3-enyl hexadecanoate	CCCCCCCCCCCCCC(=0)OC CC=CC	mild fatty wax	Flavorbase
3403	Hexadecanal	hexadecanal	CCCCCCCCCCCCCCC	cardboard	Flavornet
3404	Octadecane	octadecane	CCCCCCCCCCCCCCCC	alkane fuel	Flavornet, Pubchem
3405	Stearic acid	octadecanoic acid	CCCCCCCCCCCCCCC(=0)	fatty wax lard fried oily savory tallow	SuperScent, TGSC, Pubchem
3406	Butyl stearate	octadecanoic acid	CCCCCCCCCCCCCCC(=0) 0.CCCC CCCCCCCCCCCCC(=0)0	fatty oily fruity	OdorRactor ,Pubchem, TGSC
3407	Methyl stearate	methyl octadecanoate	CCCCCCCCCCCCCC(=0)	wax oily fatty	Sigma Aldrich, TGSC
3408	Ethyl stearate	ethyl octadecanoate	OC CCCCCCCCCCCCCCCC(=O) OCC	wax	Sigma Aldrich, TGSC
3409	Isobutyl stearate	2-methylpropyl octadecanoate	CCCCCCCCCCCCCCC(=0) OCC(C) C	mild fatty	OdorRactor ,TGSC
3410	Propylene glycol monostearate	2-hydroxypropyl octadecanoate	OCC(C) C OCC(C) C OCC(C) O	fatty	OdorRactor ,TGSC
3411	Glyceryl monostearate	2,3-dihydroxypropyl octadecanoate	CCCCCCCCCCCCCCC(=0)	fatty wax	TGSC
3412	Octadecanal	octadecanal	CCCCCCCCCCCCCCCCC	oily	Flavornet
3413	Eicosane	icosane	ccccccccccccccc	wax	Flavornet
3414	Heneicosane	henicosane	ccccccccccccccc	wax	Flavornet, TGSC
3415	2-Methyldocosane	2-methyldocosane	CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC	wax	TGSC
3416	Docosane	docosane	cccccccccccccccc	wax	Flavornet, TGSC
3410	Bocosume				

3417	Tricosane	tricosane	cccccccccccccccc	wax	Flavornet, TGSC
	Stearyl alcohol	ootodooon 1 ol	CC		Flavornet, Pubchm.
3418	1-Hexadecanol	octadecan-1-ol hexadecan-1-ol	cccccccccccccc	oily bland wax clean floral fruity greasy oily	OdoRactor Sigma Aldrich, Flavornet,
3420	Cetyl lactate	hexadecyl 2-hydroxypropanoate		fatty buttery	TGSC, Pubchem TGSC, OdoRactor
3421	1-Tetradecanol	tetradecan-1-ol	C(C)O CCCCCCCCCCCCCO	fruity wax orris coconut	Flavornet, TGSC
3422	Tetradecyl acetate	tetradecyl acetate	CCCCCCCCCCCCCCC(=0)C	wax fatty	SuperScent,
3423	1-Tridecanol	tridecan-1-ol	CCCCCCCCCCCC	musty pleasant	TGSC,OdoRactor Flavornet, Pubchem
	1-Dodecanol	dodecan-1-ol	cccccccccc	coconut fatty honey earthy soapy	Sigma Aldrich, Flavorbase,
				wax oily floral citrus sweet repulsive	TGSC,OdoRactor
3425	Dodecyl acetate	dodecyl acetate	CCCCCCCCCCCCCC(=0)C	citrus rose wax sweet fresh laundered cloth clean fruity	Sigma Aldrich, Flavorbase, TGSC,OdoRactor
3426	Dodecyl isobutyrate	dodecyl 2-methylpropanoate	CCCCCCCCCCCCCC(=0)C(C)C	oily fatty fruity wax milky buttery	OdorRactor ,TGSC, Flavorbase
3427	Propanoic acid, 2-hydroxy-, dodecyl ester	dodecyl 2-hydroxypropanoate	CCCCCCCCCCCCC(=0)C(C)O	fatty buttery	TGSC
3428	Dodecyl propionate	dodecyl propanoate	CCCCCCCCCCCC(=0)CC	fruity winey ambrette	OdorRactor ,TGSC
3429	Dodecyl butyrate	dodecyl butanoate	CCCCCCCCCCCC(=0)CCC	fatty fruity rancid	OdorRactor ,TGSC
3430	1-Dodecanethiol	dodecane-1-thiol	cccccccccs	sulfurous skunk cooked meaty fatty	TGSC, Flavorbase, Pubchem
3431	1-Undecanol	undecan-1-ol	ccccccccco	grape green lemon lime sweet wax rose soapy floral citrus fresh laundered cloth	Sigma Aldrich, TGSC, Pubchem,OdoRactor
3432	Undecyl acetate	undecyl acetate	CCCCCCCCCCCC(=0)C	oily wax clean	SuperScent, TGSC, OdoRactor
3433	Undecyl butyrate	undecyl butanoate	CCCCCCCCCCCC(=0)CCC	fruity wax	TGSC
3434	1-Decanol	decan-1-ol	cccccccco	orange fatty wax sweet fruity rose clean watery floral oily	AOD, Sigma Aldrich, Flavorbase, TGSC,OdoRactor
3435	1-Methoxydecane	1-methoxydecane	CCCCCCCCCC	sweet clean fresh marine laundered cloth	OdorRactor ,TGSC
3436	Decyl acetate	decyl acetate	CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC	pineapple rose orange oily wax sweet creamy citrus soapy clean fresh laundered cloth	Sigma Aldrich, TGSC,OdoRactor
3437	Decyl anthranilate	decyl 2-aminobenzoate	CCCCCCCCCCC(=0)C1=CC= CC=C1N	floral grape neroli	OdorRactor ,TGSC
3438	Decyl propionate	decyl propanoate	CCCCCCCCCCC(=0)CC	fruity ethereal winey fatty cognac rummy	Sigma Aldrich, TGSC, OdoRactor
3439	Decyl butyrate	decyl butanoate	CCCCCCCCCCC(=0)CCC	sweet fruity rose fatty wax citrus	Sigma Aldrich, TGSC
3440	Decane, 1-(ethenyloxy)-	1-ethenoxydecane	CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC	wax rose laundered cloth powdery clean fresh	OdorRactor ,TGSC
3441	Decyl formate	decyl formate	CCCCCCCCCCCOC=O	honeysuckle floral orange blossom	OdorRactor ,TGSC
3442	(Decyloxy)acetaldehyde	2-decoxyacetaldehyde	CCCCCCCCCCCCC	fatty rose wax	TGSC
3443	1-Nonanol	nonan-1-ol	ccccccco	fresh clean floral dusty wet citrus rose fatty green orange oily fruity citronella	Sigma Aldrich, AOD, TGSC, OdoRactor, Pubchem
3444	Nonyl acetate	nonyl acetate	CCCCCCCCCC(=O)C	gardenia fruity soapy sweet wax green tropical fruit clean	Sigma Aldrich, TGSC,OdoRactor
3445	Nonyl benzoate	nonyl benzoate	CCCCCCCCCC(=O)C1=CC=C C=C1	myrrh sweet orange wintergreen minty balsamic	OdorRactor ,TGSC
3446	Nonyl anthranilate	nonyl 2-aminobenzoate	CCCCCCCCCC(=O)C1=CC=C C=C1N	citrus sweet orange mandarin	TGSC
3447	Nonyl isovalerate	nonyl 3-methylbutanoate	CCCCCCCCCC(=O)CC(C)C	fruity apple hazelnut citrus	OdorRactor ,TGSC
3448	Nonyl heptanoate	nonyl heptanoate	CCCCCCCCCC(=O)CCCCCC	floral orange herbaceous cognac	TGSC
3449	Nonyl octanoate	nonyl octanoate	CCCCCCCCCC(=0)CCCCCCC	sweet rose mushroom floral cognac	OdorRactor ,TGSC
3450	Nonyl nonan-1-oate	nonyl nonanoate	CCCCCCCCCC(=0)CCCCCCC C	floral orange rose fruity oily aldehydic	TGSC
3451	1-Nonanethiol	nonane-1-thiol	CCCCCCCCS	bad characteristic	AOD, OdoRactor, Pubchem
3452	1-Octanol	octan-1-ol	ccccccco	fatty woody citrus wax chemical metallic burnt mossy nutty mushroom green orange aldehydic rose floral sweet coconut penetrating aromatic	Sigma Aldrich, AOD, TGSC, Pubchem
3453	Octyl acetate	octyl acetate	CCCCCCCCC(=0)C	jasmine melon fruity herbaceous green earthy mushroom wax floral apple	Sigma Aldrich, TGSC,OdoRactor

3454	Octyl isobutyrate	octyl 2-methylpropanoate	CCCCCCCCC(=0)C(C)C	creamy green woody earthy oily wax soapy fruity clean aldehydic	Sigma Aldrich, TGSC, OdoRactor
	Octyl 2-methylbutyrate 2-Butenoic acid, octyl ester	octyl 2-methylbutanoate octyl but-2-enoate	CCCCCCCCCC(=0)C(C)CC	wax fruity green musty lactonic fruity hay winey mushroom chemical	OdorRactor ,TGSC TGSC
3457	Octyl cinnamate	octyl (E)-3-phenylprop-2-enoate	CCCCCCCCC(=0)C=CC1=CC =CC=C1	balsamic cinnamyl opoponax	OdorRactor ,TGSC
3458	Octyl benzoate	octyl benzoate		fruity balsamic	OdorRactor ,TGSC
3459	Octyl 2-furoate	octyl furan-2-carboxylate	CCCCCCCCC(=0)C1=CC=C0	oily wax earthy mushroom creamy tallow	OdorRactor ,TGSC
3460	Octyl propionate	octyl propanoate	CCCCCCCCCC(=0)CC	sweet fruity mushroom floral raspberry green jammy wax woody	Sigma Aldrich, TGSC, OdoRactor
3461	Dioctyl malonate	dioctyl propanedioate	CCCCCCCCC(=0)CC(=0)OCC		OdorRactor,
3462	Octyl isovalerate	octyl 3-methylbutanoate	CCCCCCCCC(=0)CC(C)C	honey rose warm floral apple pineapple	Sigma Aldrich, TGSC
3463	Octyl phenylacetate	octyl 2-phenylacetate	CCCCCCCCC(=0)CC1=CC=C C=C1	orange basil bois de rose earthy honey rooty rose	OdorRactor ,TGSC
3464	Octyl butyrate	octyl butanoate	CCCCCCCCCC(=0)CCC	green musty orange citrus fruity wax oily earthy creamy jasmine fresh natural sweet	Sigma Aldrich, TGSC, OdoRactor
3465	Octyl heptanoate	octyl heptanoate	CCCCCCCCC(=0)CCCCCC	honey fruity fatty	OdorRactor ,TGSC
3466	Octyl octanoate	octyl octanoate	CCCCCCCCC(=0)CCCCCCC	coconut oily fruity sweet	Sigma Aldrich, TGSC, OdoRactor
3467	Octyl formate	octyl formate	CCCCCCCCCC=O	orange fruity rose wax cucumber	Sigma Aldrich, TGSC,OdoRactor
3468	Acetaldehyde, (octyloxy)-	2-octoxyacetaldehyde	CCCCCCCCCCC=O	green floral sweet	OdorRactor ,TGSC
	1-Octanethiol	octane-1-thiol	CCCCCCCS	characteristic mild sulfurous	AOD, OdoRactor, Pubchem
3470	Methyl octyl sulfide	1-methylsulfanyloctane	CCCCCCCSC	earthy baked potato roasted peanut roasted baked	TGSC
3471	1-Heptanol	heptan-1-ol	CCCCCCCO	apple apricot coconut green chemical meaty musty oily nutty citrus woody strawberry vanilla winey leafy violet herbaceous sweet peony pungent vegetable fruity banana aromatic fatty violet leaf	Flavornet, AOD, TGSC, OdoRactor, Pubchem
3472	Heptyl acetate	heptyl acetate	CCCCCCCCC(=O)C	apricot oily citrus woody pear fresh green rummy fruity ripe wax fatty aldehydic winey	Sigma Aldrich, TGSC,OdoRactor
3473	Heptyl isobutyrate	heptyl 2-methylpropanoate	CCCCCCCCC(=0)C(C)C	sweet green fruity floral apple cherry apricot warm estery pineapple peach tropical herbaceous	SuperScent, TGSC, Flavorbase, OdoRactor
3474	Heptyl 2-methylbutyrate	heptyl 2-methylbutanoate	CCCCCCCC(=O)C(C)CC	fruity apple	OdorRactor,
3475	Heptyl cinnamate	heptyl (E)-3-phenylprop-2-enoate	CCCCCCCCC(=0)C=CC1=CC= CC=C1	green leafy hyacinth	OdorRactor ,TGSC
3476	Heptyl benzoate	heptyl benzoate	CCCCCCCCC(=0)C1=CC=CC= C1	green leafy metallic herbaceous sage balsamic	OdorRactor ,TGSC
	Heptyl propionate	heptyl propanoate	CCCCCCCC(=0)CC	floral rose apricot	OdorRactor ,TGSC
	Heptyl isovalerate	heptyl 3-methylbutanoate	CCCCCCCCC(=0)CC(C)C	fruity woody animal	TGSC
	Heptyl phenylacetate	heptyl 2-phenylacetate	CCCCCCCOC(=0)CC1=CC=CC =C1	lemongrass honey citrus sweet verbena foliage	OdorRactor ,TGSC
3480	Heptyl butyrate	heptyl butanoate	CCCCCCCC(=0)CCC	green sweet fruity tropical chamomile green tea floral clean hay	Sigma Aldrich, TGSC, Odoractor
	Heptyl valerate	heptyl pentanoate	CCCCCCCC(=0)CCCC	fruity apple	OdorRactor ,TGSC
	Heptyl hexanoate	heptyl hexanoate	CCCCCCCCC(=0)CCCCC	green leafy sappy	OdorRactor,
	Heptyl heptanoate	heptyl heptanoate	CCCCCCCCC(=0)CCCCCC	grassy green fruity	Sigma Aldrich, TGSC, OdoRactor
3484	Heptyl formate	heptyl formate	CCCCCCCCCC	apple fatty plum green wax floral herbaceous cucumber vegetable fruity	Sigma Aldrich, TGSC,OdoRactor
3485	Heptanal, cyclic acetal with 1,2,3- propanetriol	1-heptoxy-3-hydroxypropan-2-one	CCCCCCCCC(=0)CO	earthy fungal green oily sweet	OdorRactor ,TGSC
3486	Tea tree oil	zinc;diheptoxy-sulfanylidene- sulfido-λ5-phosphane	CCCCCCCOP(=S)(OCCCCCC)[S-].CCCCCCCOP(=S)(OCCCCCCC)[S-].[Zn+2]	spicy warm citrus terpenic nutmeg pine earthy	Sigma Aldrich, TGSC, Pubchem
3487	1-Heptanethiol	heptane-1-thiol	CCCCCCS	sulfurous onion unpleasant	Sigma Aldrich, TGSC, OdoRactor
3488	Hexylamine	hexan-1-amine	CCCCCCN	ammonical musty fishy	TGSC, Pubchem, OdoRactor, ADB

3490 I-Hex 3491 I-Met 3492 Hexyl 3493 Hexyl 3494 Hexyl 3495 Hexyl 3496 Hexyl 3497 Hexyl 3498 Hexyl 3499 Hexyl 3500 Hexyl 3501 Dihex 3502 Hexyl 3504 Hexyl 3504 Hexyl 3505 Hexyl 3506 Hexyl 3507 Hexyl 3508 Hexyl 3508 Hexyl 3510 Hexyl 3511 Hexyl 3511 Hexyl 3512 Hexyl	cyl angelate cyl pivalate cyl isobutyrate cyl 2-methyl-3-pentenoate cyl 2-methylbutanoate cyl lactate cyl crotonate cyl cinnamate cyl cinnamate cyl cinnamate cyl cinnamate cyl cyl alicylate cyl salicylate cyl 2-furoate cyl propionate	1-isothiocyanatohexane hexan-1-ol 1-methoxyhexane hexyl acetate hexyl (E)-2-methylbut-2-enoate hexyl (Z)-2-methylbut-2-enoate hexyl 2,2-dimethylpropanoate hexyl 2-methylpropanoate hexyl 2-methylpropanoate hexyl 2-methylput-3-enoate hexyl 2-methylbutanoate hexyl 2-hydroxypropanoate hexyl (E)-but-2-enoate dihexyl (E)-but-2-enoate hexyl (E)-a-phenylprop-2-enoate hexyl (E)-hex-2-enoate hexyl benzoate hexyl 2-hydroxybenzoate hexyl y-hydroxybenzoate hexyl furan-2-carboxylate hexyl propanoate	CCCCCCOCCOC CCCCCCCCCCCCCCCCCCCCCCCCC	green pungent horseradish watercress green herbaceous woody sweet resinous floral ethereal fusel oily fruity alcoholic musty pungent pleasant sweet paint herbaceous lavender fruity apple banana cherry floral pear sweet herbaceous fruity green fatty fresh estery fresh green oily herbaceous fruity natural green floral gardenia jasmine sweet floral fatty musty green fruity woody grape winey sweet green apple pear berry fruity ripe berry peach ripe fruity tropical sweet wax spicy guaiacwood green cantaloupe rindy green fruity strawberry wax apple spicy tropical banana woody sweet floral green fruity pineapple fruity sweet caramel green walnut oily radish apple pear vegetable celery tropical herbaceous fresh floral green magnolia plastic cortex cypress cumin fruity balsamic fruity green fatty balsamic green woody fresh sappy clean green orchid herbaceous fresh floral wax green sweet pear apple apple apricot cheese creamy fatty green melon musty oily floral wax	SuperScent, TGSC, OdoRactor TGSC OdorRactor, TGSC, OdoRactor Sigma Aldrich, TGSC, OdoRactor OdorRactor, TGSC Sigma Aldrich, TGSC, OdoRactor OdorRactor, TGSC OdoRactor OdorRactor, TGSC Sigma Aldrich, TGSC,
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3500 Hexyl 3501 Dihex 3502 Hexyl 3503 Hexyl 3504 Hexyl 3505 Hexyl 3506 Hexyl 3507 Hexyl 3508 Hexyl 3509 Hexyl 3510 Hexyl 3511 Hexyl 3511 Hexyl	exyl fumarate exyl fumarate exyl cinnamate exyl (E)-2-hexenoate exyl benzoate exyl salicylate exyl 2-furoate exyl 2-furoate	hexyl (E) -but-2-enoate dihexyl (E) -but-2-enedioate hexyl (E) -3-phenylprop-2-enoate hexyl (E) -hex-2-enoate hexyl benzoate hexyl 2-hydroxybenzoate hexyl furan-2-carboxylate	CCCCCCOC(=0)C=CC CCCCCCCOC(=0)C=CC(=0)OCC CCCCCCCCC(=0)C=CC1=CC=C CCCCCCCCC(=0)C1=CC=CC=C1 CCCCCCCCC(=0)C1=CC=CC=C1 CCCCCCCCC(=0)C1=CC=CC=C1 CCCCCCCCC(=0)C1=CC=CC=C1	pineapple fruity sweet caramel green walnut oily radish apple pear vegetable celery tropical herbaceous fresh floral green magnolia plastic cortex cypress cumin fruity balsamic fruity green fatty balsamic green woody fresh sappy clean green orchid herbaceous fresh floral wax green sweet pear apple apple apricot cheese creamy fatty	Sigma Aldrich, TGSC, OdoRactor OdorRactor ,TGSC OdorRactor ,TGSC OdorRactor ,TGSC Sigma Aldrich, TGSC, OdoRactor Sigma Aldrich, TGSC, OdoRactor SuperScent, TGSC, OdoRactor Sigma Aldrich, TGSC,
3501 Dihex 3502 Hexyl 3503 Hexyl 3504 Hexyl 3505 Hexyl 3506 Hexyl 3507 Hexyl 3508 Hexyl 3509 Hexyl 3510 Hexyl 3511 Hexyl 3512 Hexyl	exyl fumarate kyl cinnamate kyl (E)-2-hexenoate kyl benzoate kyl salicylate kyl 2-furoate kyl propionate	dihexyl (E)-but-2-enedioate hexyl (E)-3-phenylprop-2-enoate hexyl (E)-hex-2-enoate hexyl benzoate hexyl 2-hydroxybenzoate hexyl furan-2-carboxylate	CCCCCCOC(=0)C=CC(=0)OCC CCCC CCCCC CCCCCCCC(=0)C=CC1=CC=C CCCCCCCC(=0)C1=CC=CC=C1 CCCCCCCCC(=0)C1=CC=CC=C1 CCCCCCCCC(=0)C1=CC=CC=C1 CCCCCCCC(=0)C1=CC=CC=C1	green walnut oily radish apple pear vegetable celery tropical herbaceous fresh floral green magnolia plastic cortex cypress cumin fruity balsamic fruity green fatty balsamic green woody fresh sappy clean green orchid herbaceous fresh floral wax green sweet pear apple apple apricot cheese creamy fatty	OdorRactor ,TGSC OdorRactor ,TGSC OdorRactor ,TGSC Sigma Aldrich, TGSC, OdoRactor Sigma Aldrich, TGSC, OdoRactor SuperScent, TGSC, OdoRactor Sigma Aldrich, TGSC,
3502 Hexyl 3503 Hexyl 3504 Hexyl 3505 Hexyl 3506 Hexyl 3507 Hexyl 3508 Hexyl 3509 Hexyl 3510 Hexyl 3511 Hexyl 3512 Hexyl	cyl cinnamate cyl (E)-2-hexenoate cyl benzoate cyl salicylate cyl 2-furoate cyl propionate	hexyl (E)-3-phenylprop-2-enoate hexyl (E)-hex-2-enoate hexyl benzoate hexyl 2-hydroxybenzoate hexyl furan-2-carboxylate	CCCC CCCCCCCC(=0)C=CC1=CC=C C=C1 CCCCCCCC(=0)C=CCCC CCCCCCC(=0)C1=CC=CC=C1 CCCCCCCC(=0)C1=CC=CC=C1 0 CCCCCCCC(=0)C1=CC=CO1	magnolia plastic cortex cypress cumin fruity balsamic fruity green fatty balsamic green woody fresh sappy clean green orchid herbaceous fresh floral wax green sweet pear apple apple apricot cheese creamy fatty	OdorRactor ,TGSC OdorRactor ,TGSC Sigma Aldrich, TGSC, OdoRactor Sigma Aldrich, TGSC, OdoRactor SuperScent, TGSC, OdoRactor Sigma Aldrich, TGSC,
3503 Hexyl 3504 Hexyl 3505 Hexyl 3506 Hexyl 3507 Hexyl 3508 Hexyl 3509 Hexyl 3510 Hexyl 3511 Hexyl	cyl (E)-2-hexenoate cyl benzoate cyl salicylate cyl 2-furoate cyl propionate	hexyl (E)-hex-2-enoate hexyl benzoate hexyl 2-hydroxybenzoate hexyl furan-2-carboxylate	C=C1 CCCCCCCC(=0)C=CCCC CCCCCCCC(=0)C1=CC=CC=C1 CCCCCCCCC(=0)C1=CC=CC=C1 CCCCCCCCC(=0)C1=CC=CO1	cypress cumin fruity balsamic fruity green fatty balsamic green woody fresh sappy clean green orchid herbaceous fresh floral wax green sweet pear apple apple apricot cheese creamy fatty	OdorRactor ,TGSC Sigma Aldrich, TGSC, OdoRactor Sigma Aldrich, TGSC, OdoRactor SuperScent, TGSC, OdoRactor Sigma Aldrich, TGSC,
3504 Hexyl 3505 Hexyl 3506 Hexyl 3507 Hexyl 3508 Hexyl 3509 Hexyl 3510 Hexyl 3511 Hexyl 3512 Hexyl	cyl benzoate cyl salicylate cyl 2-furoate cyl propionate	hexyl benzoate hexyl 2-hydroxybenzoate hexyl furan-2-carboxylate	CCCCCCOC(=0)C1=CC=CC=C1 CCCCCCCC(=0)C1=CC=CC=C1 CCCCCCCCC(=0)C1=CC=C01	balsamic green woody fresh sappy clean green orchid herbaceous fresh floral wax green sweet pear apple apple apricot cheese creamy fatty	Sigma Aldrich, TGSC, OdoRactor Sigma Aldrich, TGSC, OdoRactor SuperScent, TGSC, OdoRactor Sigma Aldrich, TGSC,
3505 Hexyl 3506 Hexyl 3507 Hexyl 3508 Hexyl 3509 Hexyl 3510 Hexyl 3511 Hexyl	cyl salicylate cyl 2-furoate cyl propionate	hexyl 2-hydroxybenzoate hexyl furan-2-carboxylate	CCCCCCOC(=O)C1=CC=CC=C1 O CCCCCCOC(=O)C1=CC=CO1	clean green orchid herbaceous fresh floral wax green sweet pear apple apple apricot cheese creamy fatty	OdoRactor Sigma Aldrich, TGSC, OdoRactor SuperScent, TGSC, OdoRactor Sigma Aldrich, TGSC,
3506 Hexyl 3507 Hexyl 3508 Hexyl 3509 Hexyl 3510 Hexyl 3511 Hexyl 3512 Hexyl	xyl 2-furoate xyl propionate	hexyl furan-2-carboxylate	O CCCCCCCC(=O)C1=CC=CO1	floral wax green sweet pear apple apple apricot cheese creamy fatty	OdoRactor SuperScent, TGSC, OdoRactor Sigma Aldrich, TGSC,
3507 Hexyl 3508 Hexyl 3509 Hexyl 3510 Hexyl 3511 Hexyl 3512 Hexyl	xyl propionate			apple apricot cheese creamy fatty	OdoRactor Sigma Aldrich, TGSC,
3508 Hexyl 3509 Hexyl 3510 Hexyl 3511 Hexyl 3512 Hexyl		hexyl propanoate	CCCCCCOC(=0)CC		
3510 Hexyl 3511 Hexyl 3512 Hexyl	and managing of the			pear fruity rotting fruit rotten	OdoKacioi
3510 Hexyl 3511 Hexyl 3512 Hexyl	xyl propionate	hexyl propanoate	CCCCCCOC(=O)CC	pear green fruity musty rotting fruit ripe rotten	OdorRactor ,TGSC
3511 Hexyl 3512 Hexyl	xyl isovalerate	hexyl 3-methylbutanoate	CCCCCCOC(=0)CC(C)C	sweet green fruity strawberry apple juicy fresh unripe fruit	Sigma Aldrich, TGSC, OdoRactor, Pubchem
3512 Hexyl	xyl 3-mercaptobutanoate	hexyl 3-sulfanylbutanoate	CCCCCCOC(=O)CC(C)S	fruity spicy herbaceous	TGSC
	xyl phenylacetate	hexyl 2-phenylacetate	CCCCCCCC(=0)CC1=CC=CC=	green sweet wax fruity rose winey foliage honey floral powdery	SuperScent, TGSC, OdoRactor
2512 77 1	xyl butyrate	hexyl butanoate	CCCCCCOC(=0)CCC	apricot pineapple sweet fruity apple wax soapy green estery vegetable strong	Sigma Aldrich, Flavorbase, TGSC, OdoRactor
3513 Hexyl	xyl valerate	hexyl pentanoate	CCCCCCOC(=0)CCCC	oily fruity green brandy	SuperScent, TGSC
3514 Hexyl	xyl hexanoate	hexyl hexanoate	CCCCCCOC(=0)CCCCC	green vegetable fruity herbaceous grassy fresh sweet wax tropical berry	Sigma Aldrich, TGSC, OdoRactor
3515 1-(1-N	-Methoxyethoxy)hexane	1-(1-methoxyethoxy)hexane	CCCCCCC(C)OC	green cortex herbaceous nasturtium	OdorRactor ,TGSC
3516 1-(1-H	-Ethoxyethoxy)hexane	1-(1-ethoxyethoxy)hexane	CCCCCCC(C)OCC	natural green floral earthy fungal	OdorRactor ,TGSC
acetal		1-[1-(3- methylbutoxy)ethoxy]hexane	CCCCCCOC(C)OCCC(C)C	fruity sweet apple	TGSC
	vane, 1,1'-	1-(1-hexoxyethoxy)hexane	CCCCCCOC(C)OCCCCCC	sweet green ethereal wax herbaceous	OdorRactor ,TGSC
	ylidenebis(oxy)]bis- canal dihexyl acetal	1,1-dihexoxyhexane	CCCCCCOC(CCCCC)OCCCCCC		OdorRactor ,TGSC
3520 Hexyl	xyl formate	hexyl formate	CCCCCCOC=O	plum green ethereal fruity apple banana sweet	Sigma Aldrich, TGSC, Odoractor
		2-hexoxyacetonitrile	CCCCCCCC#N	floral herbaceous fatty violet	TGSC
3522 1-(2,2 Dimet	2,2- nethoxyethoxy)hexane	1-(2,2-dimethoxyethoxy)hexane	CCCCCCOCC(OC)OC	green leafy sweet floral fruity fresh	OdorRactor ,TGSC
		hexane-1-thiol	CCCCCCS	sulfurous burnt fat meaty fatty garlic roasted alliaceous nutty	Flavornet, TGSC, OdoRactor, Pubchem
3524 Thioc	exanethiol			unpleasant	1

3525	Amylamine	pentan-1-amine	CCCCCN	fishy ammonical	Sigma Aldrich, TGSC, Pubchem,OdoRactor
3526	Pentyl isothiocyanate	1-isothiocyanatopentane	CCCCCN=C=S	green pungent vegetable radish	OdorRactor ,Flavorbase
3527		4-methyl-3-pentyl-1,3-oxazolidin-	CCCCCN1C(COC1=0)C	horseradish herbaceous celery jasmine	TGSC
3528	2-one 1-Pentanol	2-one pentan-1-ol	cccco	sweet vanilla balsamic fermented fusel oily pungent bready yeasty winey solvent alcoholic ethereal chemical	Sigma Aldrich, AOD, Flavorbase, TGSC, Pubchem
3529	Pentyl acetate	pentyl acetate	CCCCCOC(=0)C	banana earthy ethereal fruity pear apple	Sigma Aldrich, AOD, TGSC, OdoRactor, Pubchem
3530	Pentyl 2-methylisocrotonate	pentyl (Z)-2-methylbut-2-enoate	CCCCCOC(=O)C(=CC)C	floral fruity	OdorRactor ,TGSC
3531	Pentyl isobutyrate	pentyl 2-methylpropanoate	CCCCCOC(=0)C(C)C	fruity apple banana apricot buttery	OdorRactor ,TGSC
	Pentyl 2-methylbutyrate	pentyl 2-methylbutanoate	CCCCCOC(=0)C(C)CC	apple fruity tropical	TGSC, OdoRactor
	Amyl lactate	pentyl 2-hydroxypropanoate	CCCCCOC(=0)C(C)O CCCCCOC(=0)C=CC1=CC=CC=	fruity cognac brandy balsamic amber cocoa orchid	TGSC OdorRactor ,TGSC
	cis-Amyl cinnamate	pentyl (Z)-3-phenylprop-2-enoate	C1	labdanum	·
3535	Pentyl benzoate	pentyl benzoate	CCCCCOC(=0)C1=CC=CC=C1	floral green musty amber balsamic	SuperScent, TGSC, OdoRactor
3536	Pentyl anthranilate	pentyl 2-aminobenzoate	CCCCCOC(=0)C1=CC=CC=C1N	floral orchid grape	OdorRactor ,TGSC
3537	Pentyl salicylate	pentyl 2-hydroxybenzoate	CCCCCOC(=0)C1=CC=CC=C10	herbaceous floral clover green sweet chocolate	SuperScent, TGSC, OdoRactor
3538	Amyl 2-furoate	pentyl furan-2-carboxylate	CCCCCOC(=O)C1=CC=CO1	anisic fennel oily caramel winey fruity herbaceous sweet	SuperScent, TGSC, OdoRactor
3539	Pentyl propionate	pentyl propanoate	CCCCCOC(=O)CC	herbaceous fermented sweet fruity apricot pineapple apple	OdorRactor ,TGSC
	Pentyl 3-methylbutanoate Pentyl phenylacetate	pentyl 3-methylbutanoate pentyl 2-phenylacetate	CCCCCOC(=0)CC(C)C CCCCCOC(=0)CC1=CC=CC=C1	apple fruity fresh balsamic chocolate animal tobacco	OdorRactor ,TGSC OdorRactor ,TGSC
3542	Pentyl butyrate	pentyl butanoate	CCCCCOC(=O)CCC	banana cherry pineapple tropical sweet fruity	Sigma Aldrich, Flavornet, TGSC,OdoRactor
3543	Pentyl valerate	pentyl pentanoate	CCCCCOC(=0)CCCC	fruity apple pear sweet pineapple green peach pungent ripe	SuperScent, TGSC, OdoRactor
3544	Pentyl 3- (methylthio)propionate	pentyl 3-methylsulfanylpropanoate	CCCCCOC(=O)CCSC	pineapple tropical fruit sulfurous fruity	OdorRactor ,TGSC
3545	Pentyl formate	pentyl formate	CCCCCOC=O	earthy ethereal fruity powerful green unripe banana plum ripe	Sigma Aldrich, TGSC. Pubchem,OdoRactor
3546	Amyl isoeugenol	2-methoxy-1-pentoxy-4-[(E)-	CCCCCOC1=C(C=C(C=C1)C=C	tea clove sweet balsamic floral	OdorRactor ,TGSC,
3547	1-Pentanethiol	prop-1-enyl]benzene pentane-1-thiol	COCCCCS	spicy carnation alliaceous sulfurous fatty roasted meat vegetable green cabbage brocolli tropical penetrating unpleasant meaty strong offensive garlic roasted	Flavorbase Sigma Aldrich, Flavorbase, TGSC,OdoRactor
	Methyl pentyl disulfide	1-(methyldisulfanyl)pentane	CCCCCSSC	sulfurous onion	OdorRactor ,TGSC
3549	Butylamine	butan-1-amine	CCCCN	fishy meaty ammonical	Sigma Aldrich, ADB, TGSC, OdoRactor, Pubchem
3550	Butyl isothiocyanate	1-isothiocyanatobutane	CCCCN=C=S	sulfurous pungent green	Flavornet, TGSC,OdoRactor
3551	1-Butanol	butan-1-ol	cccco	banana vanilla medicinal fusel oily sweet balsamic whiskey fermented winey alcoholic	Sigma Aldrich, Flavorbase, TGSC
3552	Butyl acetate	butyl acetate	CCCCOC(=0)C	solvent sharp banana green sweet pear ethereal fruity strong pineapple	Sigma Aldrich, Flavorbase, TGSC, OdoRactor, Pubchem
3553	Butyl tiglate	butyl (E)-2-methylbut-2-enoate	CCCCOC(=0)C(=CC)C	floral herbaceous fruity warm	SuperScent, TGSC, Flavorbase, OdoRactor
3554	Butyl angelate	butyl (Z)-2-methylbut-2-enoate	CCCCOC(=0)C(=CC)C	winey fruity spicy rose sweet herbaceous chamomile caramel	TGSC, Flavorbase
3555	Butyl isobutyrate	butyl 2-methylpropanoate	CCCCOC(=0)C(C)C	apple banana fruity sweet green tropical fruit tutti frutti melon citrus cheese	Sigma Aldrich, TGSC
3556	Butyl 2-methylbutyrate	butyl 2-methylbutanoate	CCCCOC(=O)C(C)CC	apple chocolate pineapple sweet fruit cocoa green	Sigma Aldrich, TGSC, OdoRactor
3557	Butyl 2-methylvalerate	butyl 2-methylpentanoate	CCCCOC(=0)C(C)CCC	aromatic floral fruity chamomile rose herbaceous	OdorRactor ,TGSC
3558	Butyl lactate	butyl 2-hydroxypropanoate	CCCCOC(=O)C(C)O	creamy fruity fermented mushroom wax milky dairy earthy ketonic lactonic vanilla cheese	OdorRactor ,TGSC, Pubchem
				CHCCSC	

3560	Butanoic acid, 2-butoxy-1- methyl-2- oxoethyl ester	(1-butoxy-1-oxopropan-2-yl) butanoate	CCCCOC(=O)C(C)OC(=O)CCC	buttery cheese creamy buttermilk dairy fatty wax sweaty green sweet sour fruity	Sigma Aldrich, Flavorbase, TGSC, OdoRactor
3561	Butyl cinnamate	butyl (E)-3-phenylprop-2-enoate	CCCCOC(=0)C=CC1=CC=CC=C	milky balsamic sweet cocoa spicy fruity	OdorRactor ,TGSC, Flavorbase
3562	Butylparaben	butyl 4-hydroxybenzoate	CCCCOC(=0)C1=CC=C(C=C1)O	camphoraceous phenolic	Sigma Aldrich, TGSC
3563	Butyl benzoate	butyl benzoate	CCCCOC(=0)C1=CC=CC=C1	fruity balsamic amber woody spicy	Sigma Aldrich, Flavorbase, TGSC, OdoRactor, Pubchem
3564	Butyl anthranilate	butyl 2-aminobenzoate	CCCCOC(=0)C1=CC=CC=C1N	plum sweet grape fruity winey floral berry powdery petitgrain	Sigma Aldrich, Flavorbase, TGSC, OdoRactor
3565	Butyl salicylate	butyl 2-hydroxybenzoate	CCCCOC(=0)C1=CC=CC=C10	floral orchid herbaceous medicinal clover	Sigma Aldrich, TGSC, OdoRactor
3566	Butyl 2-furoate	butyl furan-2-carboxylate	CCCCOC(=0)C1=CC=CO1	floral orchid	TGSC
3567	Butyl propionate	butyl propanoate	CCCCOC(=0)CC	estery banana ripe tutti frutti cherry rummy earthy sweet rose fruity apple	SuperScent, TGSC,OdoRactor
3568	Butyl acetoacetate	butyl 3-oxobutanoate	CCCCOC(=0)CC(=0)C	sweet fruity brandy fermented winey	OdorRactor ,Flavorbase, TGSC
3569	Butyl isovalerate	butyl 3-methylbutanoate	CCCCOC(=0)CC(C)C	fruity apple pear sweet pineapple green peach pungent ethereal	Sigma Aldrich, SuperScent, TGSC,OdoRactor
3570	Acetyl tributyl citrate	tributyl 2-acetyloxypropane-1,2,3- tricarboxylate	CCCCOC(=0)CC(CC(=0)OCCC C)(C(=0) OCCCC)OC(=0)C	herbaceous sweet winey herbaceous	Sigma Aldrich, TGSC, Pubchem
3571	Butyl (E)-pent-3-enoate	butyl pent-3-enoate	CCCCOC(=O)CC=CC	herbaceous chamomile	TGSC
3572	Butyl phenylacetate	butyl 2-phenylacetate		honey rose chocolate floral cocoa	Sigma Aldrich, TGSC, OdoRactor
3573	Butyl butyrate	butyl butanoate	CCCCOC(=0)CCC	strong sweet apple banana peach pear fruity green cherry tropical fruit ripe juicy pineapple	Sigma Aldrich, Flavorbase, TGSC,OdoRactor
3574	Butyl levulinate	butyl 4-oxopentanoate	CCCCOC(=O)CCC(=O)C	fruity herbaceous wax caramel savory	Sigma Aldrich, TGSC, OdoRactor
3575	Dibutyl sebacate	dibutyl decanedioate	CCCCOC(=0)CCCCCCCC(=0) OCCCC	fruity oily	TGSC
3576	Butyl undec-10-enoate	butyl undec-10-enoate	CCCCOC(=0)CCCCCCCCCCC	buttery winey floral fruity fatty fusel soapy wax	Sigma Aldrich, TGSC, OdoRactor
3577	1-Butoxy-1-ethoxyethane	1-(1-ethoxyethoxy)butane	CCCCOC(C)OCC	winey brandy rummy	TGSC
3578	(2-(1- Butoxyethoxy)ethyl)benzene	2-(1-butoxyethoxy)ethylbenzene	CCCCOC(C)OCCC1=CC=CC=C1		OdorRactor ,TGSC, Flavorbase
3579	1,1-Dibutoxyethane	1-(1-butoxyethoxy)butane	CCCCOC(C)OCCCC	floral rose green seaweed algae	TGSC
3580	Butyl formate	butyl formate	CCCCOC=O	fruity rummy brandy plum winey	Sigma Aldrich, TGSC, Pubchem,OdoRactor
	p-Butoxytoluene	1-butoxy-4-methylbenzene	CCCCOC1=CC=C(C=C1)C	ylang floral	TGSC
	Butyl phenyl ether	butoxybenzene		licorice anisic	TGSC
3583	2-Butoxynaphthalene	2-butoxynaphthalene	C1	sweet fruity floral berry strawberry raspberry	
3584	Vanillyl butyl ether	4-(butoxymethyl)-2- methoxyphenol	CCCCOCC1=CC(=C(C=C1)O)O	creamy vanilla fruity	Sigma Aldrich, TGSC, OdoRactor
3585 3586	Benzyl butyl ether Benzene, (2-butoxyethyl)-	butoxymethylbenzene 2-butoxyethylbenzene	CCCCOCC1=CC=CC=C1 CCCCOCCC1=CC=CC=C1	floral rose mushroom gardenia green metallic	OdorRactor ,TGSC OdorRactor ,TGSC
2507	0.D		gggggggggg, ovg	watercress floral	TORG
3587 3588	2-Butoxyethyl acetate 1-Butanethiol	2-butoxyethyl acetate butane-1-thiol	CCCCOCCOC(=0)C CCCCS	pleasant sweet fruity sulfurous garlic onion eggy coffee fatty roasted beef cooked onion savory cheese strong obnoxious skunk cabbage roasted	TGSC Sigma Aldrich, Flavorbase, TGSC, OdoRactor, Pubchem
3589	Butyl methyl sulfide	1-methylsulfanylbutane	CCCCSC	sulfurous garlic onion vegetable	TGSC
3590	Dibutyl sulfide	1-butylsulfanylbutane	ccccsccc	green sulfurous grassy violet leaf herbaceous rose geranium alliaceous onion garlic horseradish rubbery savory vegetable violet	Sigma Aldrich, TGSC,OdoRactor
3591	Butyl ethyl disulfide	1-(ethyldisulfanyl)butane	CCCCSSCC	sulfurous onion garlic cooked onion	OdorRactor ,TGSC
3592	Butyl propyl disulfide	1-(propyldisulfanyl)butane	CCCCSSCCC	sulfurous	TGSC
3593 3594	Dibutyl disulfide Propylamine	1-(butyldisulfanyl)butane propan-1-amine	CCCCSSCCCC CCCN	sulfurous ammonical strong	OdorRactor ,TGSC OdorRactor ,TGSC, Pubchem
3595	Tripropylamine	N ,N -dipropylpropan-1-amine	CCCN(CCC)CCC	fishy ammonical	OdorRactor ,TGSC, Pubchem
3596	Propanol	propan-1-ol	CCCO	alcoholic apple musty earthy	Sigma Aldrich, TGSC,
23,0	· · · · · ·	ı r		peanut pear sweet weak fusel fermented tequila yeasty fruity	Pubchem

3597	Propyl acetate	propyl acetate	CCCOC(=O)C	celery pear fruity solvent fusel raspberry pungent sweet pleasant	Sigma Aldrich, TGSC, Pubchem, OdoRactor
3598	Propyl 2-methylisocrotonate	propyl (Z)-2-methylbut-2-enoate	CCCOC(=O)C(=CC)C	fruity winey rose	TGSC
3599	Propyl tiglate	propyl (E)-2-methylbut-2-enoate	CCCOC(=0)C(=CC)C	green seedy apple fruity	SuperScent, TGSC,OdoRactor
3600	Propyl pyruvate	propyl 2-oxopropanoate	CCCOC(=O)C(=O)C	sweet caramel floral	TGSC
3601	Propyl isobutyrate	propyl 2-methylpropanoate	CCCOC(=0)C(C)C	sweet ripe fruity tropical melon berry pineapple estery juicy tutti frutti	Sigma Aldrich, TGSC,OdoRactor
3602	Propyl 2-methylbutyrate	propyl 2-methylbutanoate	CCCOC(=O)C(C)CC	fruity winey apple pineapple	TGSC
3603	Propyl lactate	propyl 2-hydroxypropanoate	CCCOC(=O)C(C)O	winey yogurt milky	TGSC
3604	Propanoic acid, 2-(1,1-dimethylpropoxy)-, propyl ester, (2S)-	propyl (2S)-2-(2-methylbutan-2-yloxy)propanoate	CCCOC(=0)C(C)OC(C)(C)CC	floral clary sage bois de rose bergamot natural rose	TGSC
3605	Propyl 2-mercaptopropionate	propyl 2-sulfanylpropanoate	CCCOC(=O)C(C)S	cooked roasted meat baked potato fruity tropical ripe strawberry meaty baked	OdorRactor ,TGSC, Flavorbase
3606	Propyl cinnamate		CCCOC(=0)C=CC1=CC=CC=C1	balsamic musty cortex amber	OdorRactor ,TGSC
3607	Propyl 2-furanacrylate	propyl (Z)-3-(furan-2-yl)prop-2-enoate	CCCOC(=0)C=CC1=CC=CO1	sweet spicy fruity caramel strawberry apple pear honey tropical	OdorRactor ,TGSC, Flavorbase
3608	Propylparaben	propyl 4-hydroxybenzoate	CCCOC(=0)C1=CC=C(C=C1)O	burnt smoky sweet woody hawthorn	Sigma Aldrich, TGSC
3609 3610	Propyl benzoate Propyl anthranilate	propyl benzoate propyl 2-aminobenzoate	CCCOC(=0)C1=CC=CC=C1 CCCOC(=0)C1=CC=CC=C1N	balsamic nutty floral orange flower cortex	SuperScent, TGSC TGSC
3611	Propyl salicylate	propyl 2-hydroxybenzoate	CCCOC(=0)C1=CC=CC=C10	herbaceous clover fruity plum floral foliage	OdorRactor ,TGSC
3612	Propyl 2-furoate	propyl furan-2-carboxylate	CCCOC(=0)C1=CC=CO1	sweet herbaceous earthy chocolate mushroom	,
3613	Propyl propionate	propyl propanoate	CCCOC(=0)CC	oily fruity winey pineapple sharp chemical pungent sweet	Sigma Aldrich, TGSC,OdoRactor
3614	Propyl isovalerate	propyl 3-methylbutanoate	CCCOC(=O)CC(C)C	fruity bitter apple blueberry ethereal pear sweet strong	Sigma Aldrich, Flavorbase, TGSC,OdoRactor
3615	Propyl phenylacetate	propyl 2-phenylacetate	CCCOC(=0)CC1=CC=CC=C1	sweet honey floral apricot rose	SuperScent, TGSC, OdoRactor
3616	Propyl levulinate	propyl 4-oxopentanoate	CCCOC(=0)CCC(=0)C	sweet caramel	TGSC
3617	1,1-Dipropoxyethane	1-(1-propoxyethoxy)propane	CCCOC(C)OCCC	green leafy herbaceous fresh	OdorRactor ,TGSC
3618	(2-(1- Propoxyethoxy)ethyl)benzene	2-(1-propoxyethoxy)ethylbenzene	CCCOC(C)OCCC1=CC=CC=C1	chrysanthemum green leafy ethereal hyacinth herbaceous reseda floral lilac	Sigma Aldrich, TGSC, Flavorbase, OdoRactor
3619	Propyl formate	propyl formate	CCCOC=O	sweetpea berry green ethereal sweet fruity rummy	Sigma Aldrich, TGSC,OdoRactor
3620	2-Methyl-6-propoxypyrazine	2-methyl-6-propoxypyrazine	CCCOC1=NC(=CN=C1)C	green vegetable	TGSC
3621	1-Propanethiol	propane-1-thiol	CCCS	vegetable sulfurous cabbage gassy sweet onion alliaceous offensive	Sigma Aldrich, TGSC,OdoRactor
3622	Methyl propanesulfinate	methyl propane-1-sulfinate	CCCS(=O)OC	cooked onion fruity sweet	TGSC
	Methyl propyl sulfide	1-methylsulfanylpropane	CCCSC	alliaceous creamy green leek	OdorRactor ,TGSC
3624	S-Propyl thioacetate	S -propyl ethanethioate	CCCSC(=O)C	sulfurous green onion green garlic fresh vegetable scallion fresh vegetable	OdorRactor ,TGSC
3625	Allyl propyl sulfide	1-prop-2-enylsulfanylpropane	CCCSCC=C	alliaceous green onion garlic	OdorRactor ,TGSC
3626	Dipropyl sulfide	1-propylsulfanylpropane	CCCSCCC	garlic onion alliaceous	OdorRactor ,TGSC
	1-Propanesulfonothioic acid, S-propyl ester	1-propylsulfonylsulfanylpropane	CCCSS(=0)(=0)CCC	roasted alliaceous onion leek	OdorRactor ,TGSC, Flavorbase, Pubchem
3628	trans-Propenyl propyl disulfide	1-[[(E)-prop-1-enyl]disulfanyl]propane	CCCSS/C=C/C	sulfurous cooked onion	OdorRactor ,TGSC
3629	Methyl propyl disulfide	1-(methyldisulfanyl)propane	CCCSSC	alliaceous sulfurous onion radish mustard tomato potato garlic	Sigma Aldrich, TGSC, OdoRactor
	Propyl 2-methyl-3-furyl disulfide	2-methyl-3- (propyldisulfanyl)furan	CCCSSC1=C(OC=C1)C	meaty	OdorRactor ,TGSC
3631	Ethyl propyl disulfide	1-(ethyldisulfanyl)propane	CCCSSCC	alliaceous garlic green onion onion sulfurous roasted savory gamey fatty green vegetable	OdorRactor ,TGSC, Flavorbase
3632	Allyl propyl disulfide	1-(prop-2-enyldisulfanyl)propane	CCCSSCC=C	alliaceous garlic green onion sulfurous pungent	OdorRactor ,TGSC, Pubchem
3633	Furfuryl propyl disulfide	2-[(propyldisulfanyl)methyl]furan	CCCSSCC1=CC=CO1	sulfurous alliaceous garlic	OdorRactor ,TGSC
3634	Dipropyl disulfide	1-(propyldisulfanyl)propane	CCCSSCCC	alliaceous green onion earthy sulfurous burnt scallion metallic tropical fresh	Sigma Aldrich, TGSC,OdoRactor
	Methyl propyl trisulfide	1-(methyltrisulfanyl)propane	CCCSSSC	sulfurous onion garlic green	Sigma Aldrich, TGSC,

3636	Ethyl propyl trisulfide	1_(ethyltriculfonyl)propone	CCCSSSCC	alliaceous sulfurous garlic onion	TGSC
3636	Euryi propyi trisuinde	1-(ethyltrisulfanyl)propane		green	TUSC
3637	Allyl propyl trisulfide	1-(prop-2-enyltrisulfanyl)propane	CCCSSSCC=C	sulfurous alliaceous garlic onion	OdorRactor ,TGSC
3638	Dipropyl trisulfide	1-(propyltrisulfanyl)propane	CCCSSSCCC	alliaceous sulfurous green onion garlic tropical pungent green vegetable strong durain	OdorRactor ,TGSC, Flavorbase
3639	Ethylamine	ethanamine	CCN	ripe cheese ammonical fishy	SuperScent, TGSC, Flavorbase, Pubchem
3640	Triethylamine	N ,N -diethylethanamine	CCN(CC)CC	fishy ammonical strong	Sigma Aldrich, TGSC, OdoRactor, Pubchem
3641	Ethyl isothiocyanate	isothiocyanatoethane	CCN=C=S	garlic mustard pungent	Sigma Aldrich, TGSC,OdoRactor
3642	2-Acetyl-1-ethylpyrrole	1-(1-ethylpyrrol-2-yl)ethanone	CCN1C=CC=C1C(=O)C	nutty roasted	OdorRactor ,TGSC
3643	1-Ethyl-1H-pyrrole-2- carbaldehyde	1-ethylpyrrole-2-carbaldehyde	CCN1C=CC=C1C=O	burnt roasted smoky	OdorRactor ,TGSC
3644	N-Ethyl-p-menthane-3- carboxamide	N -ethyl-5-methyl-2-propan-2- ylcyclohexane-1- carboxamide	CCNC(=0)C1CC(CCC1C(C)C)C	mentholic minty alcoholic cooling	Sigma Aldrich, TGSC, OdoRactor
3645	Ethyl 2-(ethylamino)benzoate	ethyl 2-(ethylamino)benzoate	CCNC1=CC=CC=C1C(=O)OCC	fruity neroli tangerine petitgrain floral	OdorRactor ,TGSC
3646	Diethylamine	N -ethylethanamine	CCNCC	ammonical fishy	SuperScent, TGSC, Pubchem
3647	Ethanol	ethanol	CCO	sweet strong alcoholic ethereal medicinal pleasant fragrant weak vinous	Flavornet, Flavorbase, TGSC, Pubchem
3648	4-(1-Ethoxyvinyl)-3,3,5,5- tetramethylcyclohexanone	4-(1-ethoxyethenyl)-3,3,5,5- tetramethylcyclohexan- 1-one	CCOC(=C)C1C(CC(=O)CC1(C)C)(C)C	woody old wood amber tobacco herbaceous	OdorRactor ,TGSC
3649	Ethyl acetate	ethyl acetate	CCOC(=O)C	anisic ethereal pineapple fruity sweet weedy green grape rummy sharp winey brandy	Sigma Aldrich, Flavorbase, TGSC, OdoRactor, Pubchem
3650	Ethyl methacrylate	ethyl 2-methylprop-2-enoate	CCOC(=O)C(=C)C	acrylate pungent apple chamomile acrid	OdorRactor ,Flavorbase, Pubchem
3651	Ethyl tiglate	ethyl (E)-2-methylbut-2-enoate	CCOC(=O)C(=CC)C	caramel fruity raspberry sweet tutti frutti tropical berry floral	Sigma Aldrich, TGSC, OdoRactor
3652	Ethyl 2-	ethyl (2E)-2-benzylidene-3-		balsamic tropical fruity tropical	TGSC
3653	benzylideneacetoacetate Ethyl pyruvate	oxobutanoate ethyl 2-oxopropanoate	C(=0)C CCOC(=0)C(=0)C	fruit green balsamic vegetable ethereal fruity sweet rummy caramel sharp	Sigma Aldrich, TGSC,OdoRactor
3654	Citronellyl ethyl oxalate	2-O -(3,7-dimethyloct-6-enyl) 1-O -ethyl oxalate	CCOC(=0)C(=0)OCCC(C)CCC= C(C)C	sweet lily muguet rose aldehydic lychee wax floral	OdorRactor ,TGSC
3655	Diethyl tartrate	diethyl 2,3-dihydroxybutanedioate	CCOC(=O)C(C(C(=O)OCC)O)O	fruity winey caramel	OdorRactor ,TGSC
3656	Diethyl L-tartrate	diethyl (2R, 3R)-2,3- dihydroxybutanedioate	CCOC(=O)C(C(C(=O)OCC)O)O	fruity winey earthy musty	Sigma Aldrich
3657	Ethyl 2-hydroxy-3- methylbutanoate	ethyl 2-hydroxy-3- methylbutanoate	CCOC(=0)C(C(C)C)O	fruity pineapple strawberry tea honey	TGSC
3658	Ethyl 2-mercapto-2- methylpropionate	ethyl 2-methyl-2- sulfanylpropanoate	CCOC(=O)C(C)(C)S	sulfurous tropical fruity meaty	Flavorbase, TGSC
3659	Ethyl 2-methyl-2-	ethyl 2-methyl-2-	CCOC(=O)C(C)(C)SC	green minty sulfurous fruity ethereal	TGSC, OdoRactor
3660	(methylthio)propionate Ethyl isobutyrate	methylsulfanylpropanoate ethyl 2-methylpropanoate	CCOC(=O)C(C)C	citrus strawberry sweet rubbery fruity ethereal alcoholic fusel rummy pungent	Sigma Aldrich, AOD, Flavorbase, TGSC
3661	Ethyl 3-hydroxy-2- methylbutyrate	ethyl 3-hydroxy-2- methylbutanoate	CCOC(=0)C(C)C(C)O	fruity	Flavorbase
3662	Ethyl 2-methyl-3,4- pentadienoate	InChI=1S/C8H12O2/c1-4-6- 7(3)8(9)10-5-2/h6- 7H,1,5H2,2-3H3	CCOC(=0)C(C)C=C=C	green sweet tutti frutti fruity tropical rummy strawberry	OdorRactor ,TGSC
3663	Ethyl (E)-2-methylpent-3- enoate	ethyl (E)-2-methylpent-3-enoate	CCOC(=0)C(C)C=CC	fruity green pineapple cherry cooling pungent sweet strawberry melon	OdorRactor ,TGSC, Flavorbase
3664	Ethyl 2-cyclohexylpropionate	ethyl 2-cyclohexylpropanoate	CCOC(=0)C(C)C1CCCCC1	fruity green pear	OdorRactor ,TGSC
3665	Ethyl 2-methyl-4-pentenoate	ethyl 2-methylpent-4-enoate	CCOC(=O)C(C)CC=C	fruity green cooling sweet pungent pineapple banana estery tropical spicy cooling	OdorRactor ,TGSC
3666	Ethyl 2-methyl-4-pentenoate	ethyl 2-methylpent-4-enoate	CCOC(=0)C(C)CC=C	pineapple fruity green pungent banana cooling sweet estery tropical spicy tiglate	Sigma Aldrich, Flavorbase, OdoRactor
I			CCOC(=O)C(C)O	buttery fruity sharp tart	Sigma Aldrich, Flavornet,
3667	Ethyl lactate	ethyl 2-hydroxypropanoate		butterscotch sweet acidic ethereal brown rummy milky	Flavorbase, TGSC, Pubchem
	Ethyl lactate Ethyl 2-mercaptopropionate	ethyl 2-hydroxypropanoate ethyl 2-sulfanylpropanoate	CCOC(=0)C(C)S		Flavorbase, TGSC, Pubchem Sigma Aldrich, TGSC, Flavorbase, OdoRactor

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3670	Ethyl 2-hydroxy-4- methylvalerate	ethyl 2-hydroxy-4- methylpentanoate	CCOC(=O)C(CC(C)C)O	fresh blackberry	TGSC, OdoRactor
3671	(S)-(-)-Ethyl Leucate	ethyl (2S)-2-hydroxy-4- methylpentanoate	CCOC(=O)C(CC(C)C)O	fruity blackberry fresh	TGSC
3672	Ethyl 2-hydroxy-4- methylvalerate, (2R)-	ethyl (2R)-2-hydroxy-4- methylpentanoate	CCOC(=O)C(CC(C)C)O	fruity fresh blackberry	TGSC
3673	Ethyl 2-benzylacetoacetate	ethyl 2-benzyl-3-oxobutanoate	CCOC(=O)C(CC1=CC=CC=C1)C (=O)C	balsamic jasmine fruity sweet floral spicy tropical berry davana tropical fruit musty vanilla	Sigma Aldrich,TGSC, Flavorbase, OdoRactor
3674	Ethyl 2-hydroxy-3- phenylpropanoate	ethyl 2-hydroxy-3- phenylpropanoate	CCOC(=0)C(CC1=CC=CC=C1)O	spicy pepper bellpepper	TGSC
3675	Ethyl acrylate	ethyl prop-2-enoate	CCOC(=O)C=C	harsh plastic acrylate fruity sharp irritating acrid penetrating sour pungent	Sigma Aldrich, Flavorbase, TGSC,OdoRactor
3676	Ethyl geranate	ethyl (2E)-3,7-dimethylocta-2,6-dienoate	CCOC(=O)C=C(C)CCC=C(C)C	woody rose green fruity mild	OdorRactor ,TGSC, Flavorbase
3677	Ethyl aconitate	(2E)-2-(2-ethoxy-2- oxoethylidene)butanedioic acid	CCOC(=O)C=C(CC(=O)O)C(=O) O	sweet fruity winey caramel rummy	OdorRactor ,TGSC, Flavorbase
3678	Ethyl crotonate	ethyl (\overline{E})-but-2-enoate	CCOC(=O)C=CC	pungent fruity acrid estery acidic sharp rummy cognac pineapple meaty caramel ethereal sweet winey alliaceous chemical fermented	SuperScent, TGSC, Sigma Aldrich, Flavorbase, Pubchem, OdoRactor
3679	Diethyl maleate	diethyl (Z)-but-2-enedioate	CCOC(=O)C=CC(=O)OCC	banana citrus fruity	Sigma Aldrich, TGSC, OdoRactor
3680	2-Butenedioic acid (2E)-, 1,4-diethyl ester	diethyl but-2-enedioate	CCOC(=0)C=CC(=0)OCC	fruity banana citrus	OdorRactor ,TGSC
3681	Ethyl sorbate	ethyl (2E,4E)-hexa-2,4-dienoate	CCOC(=0)C=CC=CC	ethereal fruity anisic licorice warm green tropical sweet pineapple	Sigma Aldrich, TGSC, OdoRactor
3682	Ethyl cinnamate	ethyl (E)-3-phenylprop-2-enoate	CCOC(=0)C=CC1=CC=CC=C1	cinnamyl spicy plum sweet honey floral balsamic fruity powdery berry	Sigma Aldrich, Flavornet, TGSC, Flavorbase, OdoRactor
3683	Ethyl 3-(2-furyl)acrylate	ethyl (E)-3-(furan-2-yl)prop-2-enoate	CCOC(=0)C=CC1=CC=CO1	balsamic floral fruity berry apple	Flavorbase
3684	2-Propenoic acid, 3- (methylthio)-, ethyl ester, (E)-	ethyl 3-methylsulfanylprop-2- enoate	CCOC(=O)C=CSC	sweet onion sulfurous fruity plum grape rotten sour	TGSC, Flavorbase
3685	Ethyl 2-hydroxy-4- methylbenzoate	ethyl 2-hydroxy-4-methylbenzoate	CCOC(=0)C1=C(C=C(C=C1)C)O	animal floral ylang licorice	TGSC, Flavorbase
3686	1,3-Cyclohexadiene-1- carboxylic acid, 2,6,6-trimethyl-, ethyl ester	ethyl 2,6,6-trimethylcyclohexa-1,3- diene-1- carboxylate	CCOC(=0)C1=C(C=CCC1(C)C)C	natural herbaceous rose apple woody floral fresh	OdorRactor ,TGSC
3687	2-Phenyl-3-carbethoxyfuran	ethyl 2-phenylfuran-3-carboxylate	CCOC(=O)C1=C(OC=C1)C2=CC =CC=C2	cherry fruity	OdorRactor ,TGSC
3688	Ethyl vanillate	ethyl 4-hydroxy-3- methoxybenzoate	CCOC(=0)C1=CC(=C(C=C1)O)O C	floral fruit sweet vanilla phenolic burnt smoky powdery metallic guaiacol	Flavornet, TGSC,OdoRactor
3689	Ethyl 4-methoxybenzoate	ethyl 4-methoxybenzoate	CCOC(=0)C1=CC=C(C=C1)OC	anisic fruity tarragon sweet licorice spicy cherry floral powdery fennel	Sigma Aldrich, Flavorbase, TGSC, OdoRactor
3690	Ethyl benzoate	ethyl benzoate	CCOC(=0)C1=CC=CC=C1	anisic banana berry cherry grape floral camomile minty plum vanilla celery fruity dry musty wintergreen sweet medicinal ylang	Sigma Aldrich, Flavorbase, TGSC
3691	Diethyl phthalate	diethyl benzene-1,2-dicarboxylate	CCOC(=0)C1=CC=CC=C1C(=0)	faint aromatic faint	Sigma Aldrich, Pubchem
3692	Ethyl anthranilate	ethyl 2-aminobenzoate	CCOC(=0)C1=CC=CC=C1N	blossom grape sweet orange flower wintergreen fruity green floral	Sigma Aldrich, Flavorbase, TGSC, Pubchem
3693	Ethyl 2- (methylamino)benzoate	ethyl 2-(methylamino)benzoate	CCOC(=0)C1=CC=CC=C1NC	grape petitgrain sweet mandarin fruity	OdorRactor ,TGSC, Flavorbase
3694	Ethyl 2-[(2-chloro-4- nitrobenzoyl)amino]benzoate	ethyl 2-[(2-chloro-4- nitrobenzoyl)amino]benzoate	CCOC(=0)C1=CC=CC=C1NC(= 0)C2=C(C=C(C=C2)[N+](=0)[O-])C1	woody cedar raspberry orris root	OdorRactor ,TGSC
3695	Ethyl 2-[[[2,4(or3,5)-dimethyl-3-cyclohexen 1-yl]methyl]amino]benzoate	ethyl 2-[(2,4-dimethylcyclohex-3- en-1- yl)methylamino]benzoate		fresh green herbaceous leafy cortex natural	OdorRactor ,TGSC
3696	Ethyl salicylate	ethyl 2-hydroxybenzoate	CCOC(=O)C1=CC=CC=C1O	minty fruity floral sweet wintergreen spicy balsamic tutti frutti cooling	Sigma Aldrich, TGSC,OdoRactor
3697	Ethyl 2-methoxybenzoate	ethyl 2-methoxybenzoate	CCOC(=0)C1=CC=CC=C1OC	floral ylang tuberose fruity raspberry sweet grape	OdorRactor ,TGSC, Flavorbase
3698	Ethyl 2-furoate	ethyl furan-2-carboxylate	CCOC(=O)C1=CC=CO1	floral plum fruity balsamic orchid burnt	Sigma Aldrich, Flavorbase, TGSC,OdoRactor

3699	Ethyl nicotinate	ethyl pyridine-3-carboxylate	CCOC(=O)C1=CN=CC=C1	floral fruity tobacco herbaceous	Flavorbase
	Ethyl (1R,2R,6R,7S)-	ethyl (1R,2R,6R,7S)-	, ,	sweet fruity rummy candy floral	OdorRactor ,TGSC
	tricyclo[5.2.1.02,6]decane-2-carboxylate	tricyclo[5.2.1.02,6]decane-2- carboxylate	3	ripe	,
3701	Ethyl 2,3,6,6- tetramethylcyclohex-2-ene-1- carboxylate	ethyl 2,3,6,6-tetramethylcyclohex- 2-ene-1- carboxylate	CCOC(=0)C1C(=C(CCC1(C)C)C)C	rose warm spicy fruity berry woody floral	OdorRactor ,TGSC
3702	Ethyl chrysanthemate	ethyl 2,2-dimethyl-3-(2- methylprop-1- enyl)cyclopropane-	CCOC(=O)C1C(C1(C)C)C=C(C)	herbaceous ethereal sweet winey herbaceous fruity immortelle floral	Sigma Aldrich, TGSC
		1-carboxylate		chrysanthemum	
3703	Cyclohexanecarboxylic acid, 2,2,6-trimethyl-, ethyl ester, (1R,6S)-rel-	ethyl (1 <i>R</i> ,6 <i>S</i>)-2,2,6- trimethylcyclohexane-1- carboxylate	CCOC(=0)C1C(CCCC1(C)C)C	fruity floral rose amber	TGSC
3704	Ethyl methyl-p-tolylglycidate	ethyl 3-methyl-3-(4- methylphenyl)oxirane-2- carboxylate	CCOC(=0)C1C(O1)(C)C2=CC=C (C=C2) C	almond vanilla fruity floral green sweet berry cherry powdery	OdorRactor ,TGSC, Flavorbase
3705	Ethyl methylphenylglycidate	ethyl 3-methyl-3-phenyloxirane-2- carboxylate	CCOC(=0)C1C(O1)(C)C2=CC=C C=C2	strawberry sweet fruity floral honey fatty candy strong berry	Sigma Aldrich, Flavorbase, TGSC, Pubchem
3706	Ethyl 3-p-tolyloxirane-2- carboxylate	ethyl 3-(4-methylphenyl)oxirane-2- carboxylate	CCOC(=0)C1C(O1)C2=CC=C(C =C2)C	fruity sweet raspberry floral rose	TGSC
3707	Ethyl 3-phenylglycidate	ethyl 3-phenyloxirane-2- carboxylate	CCOC(=0)C1C(O1)C2=CC=CC= C2	caramel strawberry floral tropical sweet fruity berry honey rose strong	Sigma Aldrich, TGSC, OdoRactor, Pubchem
3708	Bicyclo[2.2.1]hept-5-ene-2- carboxylic acid, ethyl ester	ethyl bicyclo[2.2.1]hept-5-ene-2- carboxylate	CCOC(=O)C1CC2CC1C=C2	fruity green watery honeydew	TGSC, Flavorbase
	Ethyl 5-oxooxolane-2- carboxylate	ethyl 5-oxooxolane-2-carboxylate	CCOC(=0)C1CCC(=0)O1	roasted smoky	Flavornet
3710	Diethyl 1,4- cyclohexanedicarboxylate	diethyl cyclohexane-1,4- dicarboxylate	CCOC(=0)C1CCC(CC1)C(=0)O	fruity raspberry apple ethereal	TGSC
3711	3-Cyclohexene-1-carboxylic acid, ethyl ester	ethyl cyclohex-3-ene-1- carboxylate	CCOC(=0)C1CCC=CC1	sweet fruity floral ylang	TGSC
3712	Ethyl cyclohexanecarboxylate	ethyl cyclohexanecarboxylate	CCOC(=0)C1CCCCC1	fruity cheese winey fermented apple brandy berry	Flavornet, Flavorbase, TGSC, OdoRactor
3713	Ethyl acetoacetate	ethyl 3-oxobutanoate	CCOC(=O)CC(=O)C	fruity ethereal green apple fatty fresh estery tutti frutti berry rummy pleasant	Sigma Aldrich, Flavorbase, TGSC, OdoRactor, Pubchem
3714	Ethyl benzoylacetate	ethyl 3-oxo-3-phenylpropanoate	CCOC(=0)CC(=0)C1=CC=CC=C 1	sweet fruity cherry naphthyl hawthorn phenolic brandy berry woody jammy	SuperScent, TGSC, Flavorbase
3715	Diethyl malonate	diethyl propanedioate	CCOC(=O)CC(=O)OCC	fruity sweet green apple	Sigma Aldrich, TGSC, OdoRactor
3716	Benzyl ethyl malonate	3-O -benzyl 1-O -ethyl propanedioate	CCOC(=0)CC(=0)OCC1=CC=C C=C1	fruity winey apple	TGSC
3717	Diethyl malate	diethyl 2-hydroxybutanedioate	CCOC(=O)CC(C(=O)OCC)O	fruity sweet brown sugar winey herbaceous caramel	Sigma Aldrich, OdoRactor
3718	Ethyl isovalerate	ethyl 3-methylbutanoate	CCOC(=O)CC(C)C	apple fruity sweet pineapple tutti frutti estery sharp orange green strong banana blueberry	Sigma Aldrich, Flavorbase, TGSC,OdoRactor
3719	Ethyl 3,5,5- trimethylhexanoate	ethyl 3,5,5-trimethylhexanoate	CCOC(=0)CC(C)CC(C)(C)C	fruity apple winey yeasty floral	OdorRactor ,TGSC
3720	Ethyl 3,7-dimethyloct-6-enoate	ethyl 3,7-dimethyloct-6-enoate	CCOC(=0)CC(C)CCC=C(C)C	fruity citrus sweet licorice rose spicy fennel dry dusty	OdorRactor ,TGSC
3721	Ethyl 3-hydroxybutyrate	ethyl 3-hydroxybutanoate	CCOC(=0)CC(C)O	grape sweet marshmallow fruity green tropical apple wax	Sigma Aldrich, Flavornet, TGSC, Odoractor
	Ethyl 3-mercaptobutyrate Ethyl 3-(methylthio)butyrate	ethyl 3-sulfanylbutanoate ethyl 3-methylsulfanylbutanoate	CCOC(=O)CC(C)S CCOC(=O)CC(C)SC	sulfurous roasted sweet sour tropical fruity pineapple sulfurous earthy fatty wax ripe vegetable cheese	TGSC OdorRactor, ,TGSC, Flavorbase
	Ethyl 3-(ethylthio)butyrate	ethyl 3-ethylsulfanylbutanoate	CCOC(=O)CC(C)SCC	metallic fruity	TGSC, OdoRactor
3725	Ethyl 3-hydroxy-3- phenylpropanoate	ethyl 3-hydroxy-3- phenylpropanoate		fruity leathery strawberry animal dry hay	OdorRactor ,TGSC
	Triethyl citrate	triethyl 2-hydroxypropane-1,2,3- tricarboxylate	O)OCC) O	fruity winey	Sigma Aldrich, Pubchem
	Ethyl 2,4-dimethyl-1,3-dioxolane-2-acetate	ethyl 2-(2,4-dimethyl-1,3-dioxolan- 2-yl)acetate	CCOC(=0)CC1(OCC(01)C)C	fruity strawberry licorice apple fresh plum	Sigma Aldrich, TGSC, Flavorbase, OdoRactor
	1,3-Dioxolane-2-acetic acid, 2-methyl-, ethyl ester	ethyl 2-(2-methyl-1,3-dioxolan-2- yl)acetate	CCOC(=0)CC1(OCCO1)C	sweet fruity apple green tropical plum woody pear berry	OdorRactor ,TGSC, Flavorbase
3729	Ethyl phenylacetate	ethyl 2-phenylacetate	CCOC(=0)CC1=CC=CC=C1	anisic apple apricot cherry chocolate grapefruit honey melon wax pineapple raspberry rose sweet winey floral balsamic cocoa dark chocolate licorice pleasant	Sigma Aldrich, TGSC, Pubchem
	2-Cyclopentene-1-acetic acid, ethyl ester	ethyl 2-cyclopent-2-en-1-ylacetate	CCOC(=O)CC1CCC=C1	fruity pineapple pear plum jackfruit	TGSC

3731	Ethyl levulinate	ethyl 4-oxopentanoate	CCOC(=O)CCC(=O)C	apple green ethereal pineapple sweet fruity floral berry rhubarb mild caramel tropical	Flavornet, Flavorbase, TGSC,OdoRactor
3732	Diethyl succinate	diethyl butanedioate	CCOC(=0)CCC(=0)OCC	cooked apple apricot chocolate cranberry grape winey fruit musty wax floral peach pear ylang	Sigma Aldrich, TGSC, Odoractor
3733	Diethyl 2- hydroxypentanedioate	diethyl 2-hydroxypentanedioate	CCOC(=0)CCC(C(=0)OCC)O	cotton candy caramel	TGSC
3734	Ethyl 4-methylpentanoate	ethyl 4-methylpentanoate	CCOC(=O)CCC(C)C	fruit	Flavornet, OdoRactor
3735	Ethyl 4-pentenoate	ethyl pent-4-enoate	CCOC(=0)CCC=C	green herbaceous fruity caramel	OdorRactor ,TGSC,
2726	Ed. 147 - 1	4 1/45) + 47 5	ggogy ovaga agg g	warm ethereal fruity sweet ethereal juicy	Flavorbase TGSC
3736	Ethyl 4,7-octadienoate	ethyl (4E)-octa-4,7-dienoate	CCOC(=0)CCC=CCC=C	pineapple pear mango passion fruit	TOSC
3737	Ethyl (Z)-4,7-octadienoate	ethyl (4Z)-octa-4,7-dienoate	CCOC(=0)CCC=CCC=C	pineapple fruity pear	OdorRactor ,TGSC, Flavorbase
3738	1,3-Dioxolane-2-propanoic acid, 2,4- dimethyl-, ethyl ester	ethyl 3-(2,4-dimethyl-1,3-dioxolan- 2- yl)propanoate	CCOC(=0)CCC1(OCC(O1)C)C	oily caramel	TGSC
3739	Ethyl 3-phenylpropionate	ethyl 3-phenylpropanoate	CCOC(=0)CCC1=CC=CC=C1	ethereal fruity winey hyacinth rose honey rummy floral	Sigma Aldrich, TGSC, OdoRactor
3740	Ethyl 3-(2-	ethyl 3-(2-	CCOC(=0)CCC1=CC=CC=C10	spicy	TGSC
3741	hydroxyphenyl)propanoate Ethyl 2-furanpropionate	hydroxyphenyl)propanoate ethyl 3-(furan-2-yl)propanoate	CCOC(=0)CCC1=CC=CO1	sweet fruity balsamic green	Sigma Aldrich, Flavorbase,
3741	Emyi z-imanpropionate	emyi 5-(iman-2-yi)piopanoate	ccoc(-0)ccc1-cc-co1	pineapple ripe acrylate rummy horseradish cooked jammy woody chamomile	TGSC, OdoRactor
3742	Ethyl 3-cyclohexylpropanoate	ethyl 3-cyclohexylpropanoate	CCOC(=0)CCC1CCCCC1	fruity sweet pineapple peach pear	SuperScent, TGSC,
27.12	T. 151		2224 0,222	strong	Flavorbase, OdoRactor
3743 3744	Ethyl 5-hexenoate Ethyl 4-phenylbutanoate	ethyl hex-5-enoate ethyl 4-phenylbutanoate	CCOC(=0)CCCC=C CCOC(=0)CCCC1=CC=CC=C1	fruity pineapple sweet fruity plum	TGSC OdorRactor ,TGSC
			` '		·
3745	Ethyl 9-decenoate	ethyl dec-9-enoate	CCOC(=0)CCCCCCCC=C	fruity fatty oily elderberry woody quince	TGSC, Flavorbase
3746	Diethyl sebacate	diethyl decanedioate	С	melon quince winey fruity	Sigma Aldrich, TGSC,OdoRactor
3747	Ethyl 10-undecenoate	ethyl undec-10-enoate	CCOC(=0)CCCCCCCCCCC	cognac soapy fatty musty fruity wax clean creamy sweet	Sigma Aldrich, TGSC,OdoRactor
3748	Hexanoic acid, 6-(acetyloxy)-, ethyl ester	ethyl 6-acetyloxyhexanoate	CCOC(=0)CCCCCOC(=0)C	fruity floral anisic fresh raspberry jasmine balsamic	OdorRactor ,TGSC
3749	Ethyl 4-hydroxybutanoate	ethyl 4-hydroxybutanoate	CCOC(=0)CCCO	caramel	Flavornet, TGSC
3750	Ethyl 4-(methylthio)butyrate	ethyl 4-methylsulfanylbutanoate	CCOC(=0)CCCSC	sulfurous pineapple	OdorRactor ,TGSC, Flavorbase
3751	Ethyl 4-(acetylthio)butyrate	ethyl 4-acetylsulfanylbutanoate	CCOC(=O)CCCSC(=O)C	sulfurous meaty	TGSC
3752	Ethyl 3-mercaptopropionate	ethyl 3-sulfanylpropanoate	CCOC(=O)CCS	sulfurous animal fruity grape skunk meaty fresh foxy durain	TGSC, Flavorbase
3753	Ethyl 3- (methylthio)propionate	ethyl 3-methylsulfanylpropanoate	CCOC(=O)CCSC	sulfurous metallic pineapple fruity tomato ripe pulpy fruit caramel	Sigma Aldrich, TGSC, Flavorbase, OdoRactor
	, , ,1 1			milky cheese	ŕ
3754	Ethyl 3- (furfurylthio)propionate	ethyl 3-(furan-2- ylmethylsulfanyl)propanoate	CCOC(=0)CCSCC1=CC=CO1	coffee fatty meaty onion garlic sulfurous vegetable animal alliaceous roasted nutty	Sigma Aldrich, TGSC, Flavorbase
3755	N-((Ethoxycarbonyl)methyl)- P-menthane-3- carboxamide	ethyl 2-[[(1R, ,2S, ,5R))-5-methyl- 2-propan-2- ylcyclohexanecarbonyl]amino]acet ate	CCOC(=0)CNC(=0)C1CC(CCC1 C(C)C)C	cooling mentholic	TGSC
3756	Ethyl (4- methylphenoxy)acetate	ethyl 2-(4-methylphenoxy)acetate	CCOC(=O)COC1=CC=C(C=C1)C	fruity cherry hay powdery brown	OdorRactor ,TGSC
3757	Ethyl phenoxyacetate	ethyl 2-phenoxyacetate	CCOC(=O)COC1=CC=CC=C1	green floral rose	TGSC
3758	Ethyl thioglycolate	ethyl 2-sulfanylacetate	CCOC(=O)CS	sulfurous alliaceous green fruity	Flavorbase
3759	Ethyl (methylthio)acetate	ethyl 2-methylsulfanylacetate	CCOC(=O)CSC	apricot coffee green ethereal sulfurous sweet winey tropical fruity onion radish	Sigma Aldrich, Flavorbase, TGSC
3760	Ethyl 2,5-Dimethyl-3-oxo- 4(2H)-furyl carbonate	(2,5-dimethyl-4-oxofuran-3-yl) ethyl carbonate	CCOC(=O)OC1=C(OC(C1=O)C)	caramel cotton candy brown sugar burnt sugar	TGSC, Flavorbase
3761	Carbonic acid, ethyl 2,3,6-	ethyl (2,3,6-trimethylcyclohexyl)	CCOC(=0)OC1C(CCC(C1C)C)C	warm floral rose leathery metallic	OdorRactor ,TGSC
3762	trimethylcyclohexyl ester 2-Tert-Butylcyclohexyl ethyl	carbonate (2-tert -butylcyclohexyl) ethyl	CCOC(=0)OC1CCCCC1C(C)(C)	fruity spice woody floral green	OdorRactor ,TGSC
3763	Carbonate O-Ethyl S-(2-	ethyl furan-2-	CCOC(=O)SCC1=CC=CO1	herbaceous spicy floral	TGSC
3703		ylmethylsulfanylformate		C-1	TORG
	furylmethyl)thiocarbonate 2-(3-Ethoxybuten-1-yl)-1,3,3- trimethylcyclohexene	2-[(E)-3-ethoxybut-1-enyl]-1,3,3-trimethylcyclohexene	CCOC(C)C=CC1=C(CCCC1(C)C)C	fruity apricot raspberry woody cedar floral	TGSC

	1-Ethoxyethyl acetate	1-ethoxyethyl acetate	CCOC(C)OC(=O)C	fresh fruity blueberry acetic estery	OdorRactor ,TGSC
27.67	1.60 + 11 2.41	2 (1 .4) 2.7	adodkayodkaykada akayaya	.6.16.1	O.I. P
3767	1,6-Octadiene, 3-(1- ethoxyethoxy)-3,7- dimethyl-	3-(1-ethoxyethoxy)-3,7- dimethylocta-1,6-diene	CCOC(C)OC(C)(CCC=C(C)C)C= C	sweet fresh floral tropical herbaceous muguet natural	OdorRactor ,TGSC
	3-(1-Ethoxyethoxy)-3,7- dimethyloct-1-ene	3-(1-ethoxyethoxy)-3,7- dimethyloct-1-ene	CCOC(C)OC(C)(CCCC(C)C)C=C	sweet cardamom floral fruity tropical fresh	OdorRactor ,TGSC
3769	2-(1-Ethoxyethoxy)-5-(1- propenyl)anisole	1-(1-ethoxyethoxy)-2-methoxy-4- [(E)-prop-1-enyl]benzene	CCOC(C)OC1=C(C=C(C=C1)C= CC)OC	sweet carnation floral spicy tropical	OdorRactor ,TGSC
3770	Benzene, (1-ethoxyethoxy)-	1-ethoxyethoxybenzene	CCOC(C)OC1=CC=CC=C1	green leafy rose cortex fresh	OdorRactor ,TGSC
	Acetal	1,1-diethoxyethane	ccoc(c)occ	ethereal green nutty earthy sweet vegetable honey floral tart fruit creamy fruity choking alcoholic nut whiskey pungent woody	Sigma Aldrich, TGSC, OdoRactor, Pubchem
3772	4,6,9-Trimethyl-3,5,8,10- tetraoxadodecane	1,2-bis(1-ethoxyethoxy)propane	CCOC(C)OCC(C)OC(C)OCC	fruity	OdorRactor ,TGSC
3773	1,2,3-Tris((1- ethoxy)ethoxy)propane	1,2,3-tris(1-ethoxyethoxy)propane	CCOC(C)OCC(COC(C)OCC)OC(C)OCC	fruity	TGSC
3774	(E)-1-(1-Ethoxyethoxy)-3,7-dimethylocta- 2,6-diene	(2E)-1-(1-ethoxyethoxy)-3,7-dimethylocta-2,6-diene	CCOC(C)OCC=C(C)CCC=C(C)C	sweet creamy vanilla caramel	TGSC
3775	(2-(1- Ethoxyethoxy)ethyl)benzene	2-(1-ethoxyethoxy)ethylbenzene	CCOC(C)OCCC1=CC=CC=C1	green leafy nasturtium fresh floral hyacinth lilac	TGSC, Flavorbase
3776	Citral diethyl acetal	(2E)-1,1-diethoxy-3,7- dimethylocta-2,6-diene	CCOC(C=C(C)CCC=C(C)C)OCC	green oily citrus fresh lemon wax sweet floral	Sigma Aldrich, TGSC, OdoRactor
3777	Cinnamaldehyde diethyl acetal	[(E)-3,3-diethoxyprop-1-enyl]benzene	CCOC(C=CC1=CC=CC1)OCC	spicy cinnamyl	OdorRactor ,TGSC
3778	(Diethoxymethyl)benzene	diethoxymethylbenzene	CCOC(C1=CC=CC=C1)OCC	green bitter almond bitter	OdorRactor ,TGSC
	2-(Diethoxymethyl)furan	2-(diethoxymethyl)furan	CCOC(C1=CC=CO1)OCC	fruity earthy mushroom	OdorRactor ,TGSC
	1,3-Benzodioxole, 5- (diethoxymethyl)-	5-(diethoxymethyl)-1,3- benzodioxole	CCOC(C1=CC2=C(C=C1)OCO2) OCC	floral sweet spicy heliotrope	OdorRactor ,TGSC
3781	4,7-Methano-1H-indene, 5- (diethoxymethyl)- 3a,4,5,6,7,7a-hexahydro-	6]dec-3-ene	CCOC(C1CC2CC1C3C2CC=C3) OCC	herbaceous fruity anisic basil fennel hyacinth	OdorRactor ,TGSC
3782	1,1-Diethoxy-3-methylbutane	1,1-diethoxy-3-methylbutane	CCOC(CC(C)C)OCC	fruity fatty	TGSC
3783	Hydroxycitronellal diethyl acetal	8,8-diethoxy-2,6-dimethyloctan-2-ol	CCOC(CC(C)CCCC(C)(C)O)OCC	green lily muguet floral	ADB, TGSC
3784	(2,2-Diethoxyethyl)benzene	2,2-diethoxyethylbenzene	CCOC(CC1=CC=CC=C1)OCC	fresh green almond sweet hyacinth linden flower floral	OdorRactor ,TGSC
3785	Methional diethyl acetal	1,1-diethoxy-3-	CCOC(CCSC)OCC	cabbage pungent	TGSC
·		methylsulfanylpropane			
3786	Ethyl formate	methylsulfanylpropane ethyl formate	CCOC=O	fruity ethereal sweet winey pungent alcoholic rose cognac fermented rummy	Sigma Aldrich, Flavorbase, TGSC, Pubchem,OdoRactor
	Ethyl formate 2-Ethoxy-2,6,6-trimethyl-9- methylenebicyclo[3.3.1]nona ne		CCOC=0 CCOC1(CCC2C(=C)C1CCC2(C) C)C	pungent alcoholic rose cognac	
	2-Ethoxy-2,6,6-trimethyl-9-methylenebicyclo[3.3.1]nona	ethyl formate 2-ethoxy-2,6,6-trimethyl-9-	CCOC1(CCC2C(=C)C1CCC2(C)	pungent alcoholic rose cognac fermented rummy	TGSC, Pubchem,OdoRactor
3787 3788 3789	2-Ethoxy-2,6,6-trimethyl-9-methylenebicyclo[3.3.1]nona ne 1,1-Diethoxycyclohexane 4-(Diethoxymethyl)-1-ethoxy-2-methoxybenzene	ethyl formate 2-ethoxy-2,6,6-trimethyl-9- methylidenebicyclo[3.3.1]nonane 1,1-diethoxycyclohexane 4-(diethoxymethyl)-1-ethoxy-2- methoxybenzene	CCOC1(CCC2C(=C)C1CCC2(C) C)C CCOC1(CCCCC1)OCC CCOC1=C(C=C(C=C1)C(OCC)O CC)OC	pungent alcoholic rose cognac fermented rummy woody amber orris tobacco fruity rummy tobacco woody vanilla milky creamy caramel powdery	TGSC, Pubchem, OdoRactor OdorRactor , TGSC OdorRactor , TGSC TGSC
3787	2-Ethoxy-2,6,6-trimethyl-9-methylenebicyclo[3.3.1]nona ne 1,1-Diethoxycyclohexane 4-(Diethoxymethyl)-1-ethoxy-	ethyl formate 2-ethoxy-2,6,6-trimethyl-9- methylidenebicyclo[3.3.1]nonane 1,1-diethoxycyclohexane 4-(diethoxymethyl)-1-ethoxy-2-	CCOC1(CCC2C(=C)C1CCC2(C) C)C CCOC1(CCCCC1)OCC CCOC1=C(C=C(C=C1)C(OCC)O	pungent alcoholic rose cognac fermented rummy woody amber orris tobacco fruity rummy tobacco woody vanilla milky creamy caramel	TGSC, Pubchem, OdoRactor OdorRactor , TGSC OdorRactor , TGSC TGSC Sigma Aldrich, TGSC,
3787 3788 3789 3790	2-Ethoxy-2,6,6-trimethyl-9-methylenebicyclo[3.3.1]nona ne 1,1-Diethoxycyclohexane 4-(Diethoxymethyl)-1-ethoxy-2-methoxybenzene	ethyl formate 2-ethoxy-2,6,6-trimethyl-9- methylidenebicyclo[3.3.1]nonane 1,1-diethoxycyclohexane 4-(diethoxymethyl)-1-ethoxy-2- methoxybenzene 2-ethoxy-5-[(E)-prop-1- enyl]phenol 1-ethoxy-2-methoxy-4-[(E)-prop-	CCOC1(CCC2C(=C)C1CCC2(C) C)C CCOC1(CCCCC1)OCC CCOC1=C(C=C(C=C1)C(OCC)O CC)OC	pungent alcoholic rose cognac fermented rummy woody amber orris tobacco fruity rummy tobacco woody vanilla milky creamy caramel powdery caramel creamy medicinal nutty spicy sweet vanilla woody tobacco phenolic	TGSC, Pubchem, OdoRactor OdorRactor , TGSC OdorRactor , TGSC TGSC Sigma Aldrich, TGSC,
3787 3788 3789 3790	2-Ethoxy-2,6,6-trimethyl-9-methylenebicyclo[3,3,1]nona ne 1,1-Diethoxycyclohexane 4-(Diethoxymethyl)-1-ethoxy-2-methoxybenzene Vanitrope Ethyl isoeugenol 4-Ethoxy-3-	ethyl formate 2-ethoxy-2,6,6-trimethyl-9- methylidenebicyclo[3.3.1]nonane 1,1-diethoxycyclohexane 4-(diethoxymethyl)-1-ethoxy-2- methoxybenzene 2-ethoxy-5-[(E)-prop-1- enyl]phenol	CCOC1(CCC2C(=C)C1CCC2(C) C)C CCOC1(CCCCC1)OCC CCOC1=C(C=C(C=C1)C(OCC)O CC)OC CCOC1=C(C=C(C=C1)C=CC)O CCOC1=C(C=C(C=C1)C=CC)O	pungent alcoholic rose cognac fermented rummy woody amber orris tobacco fruity rummy tobacco woody vanilla milky creamy caramel powdery caramel creamy medicinal nutty spicy sweet vanilla woody tobacco phenolic powdery anisic floral	TGSC, Pubchem,OdoRactor OdorRactor ,TGSC OdorRactor ,TGSC TGSC Sigma Aldrich, TGSC, OdoRactor
3787 3788 3789 3790	2-Ethoxy-2,6,6-trimethyl-9-methylenebicyclo[3.3.1]nona ne 1,1-Diethoxycyclohexane 4-(Diethoxymethyl)-1-ethoxy-2-methoxybenzene Vanitrope Ethyl isoeugenol	ethyl formate 2-ethoxy-2,6,6-trimethyl-9- methylidenebicyclo[3.3.1]nonane 1,1-diethoxycyclohexane 4-(diethoxymethyl)-1-ethoxy-2- methoxybenzene 2-ethoxy-5-[(E)-prop-1- enyl]phenol 1-ethoxy-2-methoxy-4-[(E)-prop-1- enyl]benzene 4-ethoxy-3-methoxybenzaldehyde 2-ethoxy-1-methyl-4-propan-2-	CCOC1(CCC2C(=C)C1CCC2(C) C)C CCOC1(CCCCC1)OCC CCOC1=C(C=C(C=C1)C(OCC)O CC)OC CCOC1=C(C=C(C=C1)C=CC)O CCOC1=C(C=C(C=C1)C=CC)O	pungent alcoholic rose cognac fermented rummy woody amber orris tobacco fruity rummy tobacco woody vanilla milky creamy caramel powdery caramel creamy medicinal nutty spicy sweet vanilla woody tobacco phenolic powdery anisic floral spicy carnation clove sweet floral vanilla powdery spicy herbaceous carrot earthy	TGSC, Pubchem,OdoRactor OdorRactor ,TGSC OdorRactor ,TGSC TGSC Sigma Aldrich, TGSC, OdoRactor OdorRactor ,TGSC TGSC SuperScent, TGSC,
3787 3788 3789 3790 3791 3792 3793	2-Ethoxy-2,6,6-trimethyl-9-methylenebicyclo[3.3.1]nona ne 1,1-Diethoxycyclohexane 4-(Diethoxymethyl)-1-ethoxy-2-methoxybenzene Vanitrope Ethyl isoeugenol 4-Ethoxy-3-methoxybenzaldehyde Carvacryl ethyl ether	ethyl formate 2-ethoxy-2,6,6-trimethyl-9- methylidenebicyclo[3.3.1]nonane 1,1-diethoxycyclohexane 4-(diethoxymethyl)-1-ethoxy-2- methoxybenzene 2-ethoxy-5-[(E)-prop-1- enyl]phenol 1-ethoxy-2-methoxy-4-[(E)-prop-1- enyl]benzene 4-ethoxy-3-methoxybenzaldehyde 2-ethoxy-1-methyl-4-propan-2- ylbenzene	CCOC1(CCC2C(=C)C1CCC2(C) C)C CCOC1(CCCCC1)OCC CCOC1=C(C=C(C=C1)C(OCC)O CCOC1=C(C=C(C=C1)C=CC)O CCOC1=C(C=C(C=C1)C=CC)OC CCOC1=C(C=C(C=C1)C=C)OC CCOC1=C(C=C(C=C1)C=O)OC	pungent alcoholic rose cognac fermented rummy woody amber orris tobacco fruity rummy tobacco woody vanilla milky creamy caramel powdery caramel creamy medicinal nutty spicy sweet vanilla woody tobacco phenolic powdery anisic floral spicy carnation clove sweet floral vanilla powdery spicy herbaceous carrot earthy carrot	TGSC, Pubchem,OdoRactor OdorRactor ,TGSC OdorRactor ,TGSC TGSC Sigma Aldrich, TGSC, OdoRactor OdorRactor ,TGSC TGSC SuperScent, TGSC, Flavorbase, Odoractor
3787 3788 3789 3790 3791 3792 3793 3794	2-Ethoxy-2,6,6-trimethyl-9-methylenebicyclo[3.3.1]nona ne 1,1-Diethoxycyclohexane 4-(Diethoxymethyl)-1-ethoxy-2-methoxybenzene Vanitrope Ethyl isoeugenol 4-Ethoxy-3-methoxybenzaldehyde	ethyl formate 2-ethoxy-2,6,6-trimethyl-9- methylidenebicyclo[3.3.1]nonane 1,1-diethoxycyclohexane 4-(diethoxymethyl)-1-ethoxy-2- methoxybenzene 2-ethoxy-5-[(E)-prop-1- enyl]phenol 1-ethoxy-2-methoxy-4-[(E)-prop-1- enyl]benzene 4-ethoxy-3-methoxybenzaldehyde 2-ethoxy-1-methyl-4-propan-2-	CCOC1(CCC2C(=C)C1CCC2(C) C)C CCOC1(CCCCC1)OCC CCOC1=C(C=C(C=C1)C(OCC)O CC)OC CCOC1=C(C=C(C=C1)C=CC)O CCOC1=C(C=C(C=C1)C=C)OC CCOC1=C(C=C(C=C1)C=C)OC	pungent alcoholic rose cognac fermented rummy woody amber orris tobacco fruity rummy tobacco woody vanilla milky creamy caramel powdery caramel creamy medicinal nutty spicy sweet vanilla woody tobacco phenolic powdery anisic floral spicy carnation clove sweet floral vanilla powdery spicy herbaceous carrot earthy	TGSC, Pubchem,OdoRactor OdorRactor ,TGSC OdorRactor ,TGSC TGSC Sigma Aldrich, TGSC, OdoRactor OdorRactor ,TGSC TGSC SuperScent, TGSC, Flavorbase, Odoractor TGSC Sigma Aldrich, AOD,
3787 3788 3789 3790 3791 3792 3793 3794	2-Ethoxy-2,6,6-trimethyl-9-methylenebicyclo[3.3.1]nona ne 1,1-Diethoxycyclohexane 4-(Diethoxymethyl)-1-ethoxy-2-methoxybenzene Vanitrope Ethyl isoeugenol 4-Ethoxy-3-methoxybenzaldehyde Carvacryl ethyl ether 2-Ethoxy-4-methylphenol	ethyl formate 2-ethoxy-2,6,6-trimethyl-9- methylidenebicyclo[3,3,1]nonane 1,1-diethoxycyclohexane 4-(diethoxymethyl)-1-ethoxy-2- methoxybenzene 2-ethoxy-5-[(E)-prop-1- enyl]phenol 1-ethoxy-2-methoxy-4-[(E)-prop-1- enyl]benzene 4-ethoxy-3-methoxybenzaldehyde 2-ethoxy-1-methyl-4-propan-2- ylbenzene 2-ethoxy-4-methylphenol	CCOC1(CCC2C(=C)C1CCC2(C) C)C CCOC1(CCCCC1)OCC CCOC1=C(C=C(C=C1)C(OCC)O CCOC1=C(C=C(C=C1)C=CC)O CCOC1=C(C=C(C=C1)C=CC)OC CCOC1=C(C=C(C=C1)C=O)OC CCOC1=C(C=C(C=C1)C=O)OC CCOC1=C(C=C(C=C1)C(C)C)C CCOC1=C(C=CC(C=C1)C(C)C)C	pungent alcoholic rose cognac fermented rummy woody amber orris tobacco fruity rummy tobacco woody vanilla milky creamy caramel powdery caramel creamy medicinal nutty spicy sweet vanilla woody tobacco phenolic powdery anisic floral spicy carnation clove sweet floral vanilla powdery spicy herbaceous carrot earthy carrot vanilla woody spicy guaiacol	TGSC, Pubchem,OdoRactor OdorRactor ,TGSC OdorRactor ,TGSC TGSC Sigma Aldrich, TGSC, OdoRactor OdorRactor ,TGSC TGSC SuperScent, TGSC, Flavorbase, Odoractor TGSC
3787 3788 3789 3790 3791 3792 3793 3794 3795	2-Ethoxy-2,6,6-trimethyl-9-methylenebicyclo[3.3.1]nona ne 1,1-Diethoxycyclohexane 4-(Diethoxymethyl)-1-ethoxy-2-methoxybenzene Vanitrope Ethyl isoeugenol 4-Ethoxy-3-methoxybenzaldehyde Carvacryl ethyl ether 2-Ethoxy-4-methylphenol	ethyl formate 2-ethoxy-2,6,6-trimethyl-9- methylidenebicyclo[3.3.1]nonane 1,1-diethoxycyclohexane 4-(diethoxymethyl)-1-ethoxy-2- methoxybenzene 2-ethoxy-5-[(E)-prop-1- enyl]phenol 1-ethoxy-2-methoxy-4-[(E)-prop-1- enyl]benzene 4-ethoxy-3-methoxybenzaldehyde 2-ethoxy-1-methyl-4-propan-2- ylbenzene 2-ethoxy-4-methylphenol 3-ethoxy-4-hydroxybenzaldehyde	CCOC1(CCC2C(=C)C1CCC2(C) C)C CCOC1(CCCCC1)OCC CCOC1=C(C=C(C=C1)C(OCC)O CCOC1=C(C=C(C=C1)C=CC)O CCOC1=C(C=C(C=C1)C=CC)OC CCOC1=C(C=C(C=C1)C=O)OC CCOC1=C(C=C(C=C1)C=O)OC CCOC1=C(C=C(C=C1)C(C)C)C CCOC1=C(C=CC(C=C1)C(C)C)C	pungent alcoholic rose cognac fermented rummy woody amber orris tobacco fruity rummy tobacco woody vanilla milky creamy caramel powdery caramel creamy medicinal nutty spicy sweet vanilla woody tobacco phenolic powdery anisic floral spicy carnation clove sweet floral vanilla powdery spicy herbaceous carrot earthy carrot vanilla woody spicy guaiacol sweet vanilla creamy caramel root	TGSC, Pubchem,OdoRactor OdorRactor ,TGSC OdorRactor ,TGSC TGSC Sigma Aldrich, TGSC, OdoRactor OdorRactor ,TGSC TGSC SuperScent, TGSC, Flavorbase, Odoractor TGSC Sigma Aldrich, AOD, Flavorbase, TGSC,
3787 3788 3789 3790 3791 3792 3793 3794 3795	2-Ethoxy-2,6,6-trimethyl-9-methylenebicyclo[3,3,1]nona ne 1,1-Diethoxycyclohexane 4-(Diethoxymethyl)-1-ethoxy-2-methoxybenzene Vanitrope Ethyl isoeugenol 4-Ethoxy-3-methoxybenzaldehyde Carvacryl ethyl ether 2-Ethoxy-4-methylphenol Ethyl vanillin	ethyl formate 2-ethoxy-2,6,6-trimethyl-9- methylidenebicyclo[3.3.1]nonane 1,1-diethoxycyclohexane 4-(diethoxymethyl)-1-ethoxy-2- methoxybenzene 2-ethoxy-5-[(E)-prop-1- enyl]phenol 1-ethoxy-2-methoxy-4-[(E)-prop-1- enyl]benzene 4-ethoxy-3-methoxybenzaldehyde 2-ethoxy-1-methyl-4-propan-2- ylbenzene 2-ethoxy-4-methylphenol 3-ethoxy-4-hydroxybenzaldehyde (2-ethoxy-4-formylphenyl) acetate	CCOC1(CCC2C(=C)C1CCC2(C) C)C CCOC1(CCCCC1)OCC CCOC1=C(C=C(C=C1)C(OCC)O CCOC1=C(C=C(C=C1)C=CC)O CCOC1=C(C=C(C=C1)C=C)OC CCOC1=C(C=C(C=C1)C=O)OC CCOC1=C(C=C(C=C1)C=O)OC CCOC1=C(C=CC(C=C1)C(C)C)C CCOC1=C(C=CC(C=C1)C(C)C)C CCOC1=C(C=CC(C=C1)CO)O CCOC1=C(C=CC(C=C1)C=O)OC	pungent alcoholic rose cognac fermented rummy woody amber orris tobacco fruity rummy tobacco woody vanilla milky creamy caramel powdery caramel creamy medicinal nutty spicy sweet vanilla woody tobacco phenolic powdery anisic floral spicy carnation clove sweet floral vanilla powdery spicy herbaceous carrot earthy carrot vanilla woody spicy guaiacol sweet vanilla creamy caramel root beer powerful vanilla milky creamy caramel	TGSC, Pubchem,OdoRactor OdorRactor ,TGSC OdorRactor ,TGSC TGSC Sigma Aldrich, TGSC, OdoRactor OdorRactor ,TGSC TGSC SuperScent, TGSC, Flavorbase, Odoractor TGSC Sigma Aldrich, AOD, Flavorbase, TGSC, OdoRactor, Pubchem
3787 3788 3789 3790 3791 3792 3793 3794 3795 3796 3797 3798	2-Ethoxy-2,6,6-trimethyl-9-methylenebicyclo[3,3,1]nona ne 1,1-Diethoxycyclohexane 4-(Diethoxymethyl)-1-ethoxy-2-methoxybenzene Vanitrope Ethyl isoeugenol 4-Ethoxy-3-methoxybenzaldehyde Carvacryl ethyl ether 2-Ethoxy-4-methylphenol Ethyl vanillin 2-Ethoxy-4-formylphenyl acetate Ethyl vanillin isobutyrate Ethyl vanillin beta-D-glucopyranoside	ethyl formate 2-ethoxy-2,6,6-trimethyl-9- methylidenebicyclo[3.3.1]nonane 1,1-diethoxycyclohexane 4-(diethoxymethyl)-1-ethoxy-2- methoxybenzene 2-ethoxy-5-[(E)-prop-1- enyl]phenol 1-ethoxy-2-methoxy-4-[(E)-prop-1- enyl]benzene 4-ethoxy-3-methoxybenzaldehyde 2-ethoxy-1-methyl-4-propan-2- ylbenzene 2-ethoxy-4-methylphenol 3-ethoxy-4-hydroxybenzaldehyde (2-ethoxy-4-formylphenyl) acetate (2-ethoxy-4-formylphenyl) 2- methylpropanoate 3-ethoxy-4-[(2S, 3R, 4S, 5S, 6R))-3,4,5-trihydroxy- 6-(hydroxymethyl)oxan-2- yl]oxybenzaldehyde	CCOC1(CCC2C(=C)C1CCC2(C) C)C CCOC1(CCCCC1)OCC CCOC1=C(C=C(C=C1)C(OCC)O CCOC1=C(C=C(C=C1)C=CC)O CCOC1=C(C=C(C=C1)C=C)OC CCOC1=C(C=C(C=C1)C=O)OC CCOC1=C(C=CC(C=C1)C=O)OC CCCCC1=C(C=CC(C=C1)C=O)OC2 CC(C(C(C(CC)CO)OO)OO)	pungent alcoholic rose cognac fermented rummy woody amber orris tobacco fruity rummy tobacco woody vanilla milky creamy caramel powdery caramel creamy medicinal nutty spicy sweet vanilla woody tobacco phenolic powdery anisic floral spicy carnation clove sweet floral vanilla powdery spicy herbaceous carrot earthy carrot vanilla woody spicy guaiacol sweet vanilla creamy caramel root beer powerful vanilla milky creamy caramel powdery sweet creamy vanilla chocolate milky caramel rummy vanilla	TGSC, Pubchem,OdoRactor OdorRactor ,TGSC OdorRactor ,TGSC TGSC Sigma Aldrich, TGSC, OdoRactor OdorRactor ,TGSC TGSC SuperScent, TGSC, Flavorbase, Odoractor TGSC Sigma Aldrich, AOD, Flavorbase, TGSC, OdoRactor, Pubchem TGSC TGSC TGSC
3787 3788 3789 3790 3791 3792 3793 3794 3795 3796 3797 3798	2-Ethoxy-2,6,6-trimethyl-9-methylenebicyclo[3.3.1]nona ne 1,1-Diethoxycyclohexane 4-(Diethoxymethyl)-1-ethoxy-2-methoxybenzene Vanitrope Ethyl isoeugenol 4-Ethoxy-3-methoxybenzaldehyde Carvacryl ethyl ether 2-Ethoxy-4-methylphenol Ethyl vanillin 2-Ethoxy-4-formylphenyl acetate Ethyl vanillin isobutyrate Ethyl vanillin beta-D-	ethyl formate 2-ethoxy-2,6,6-trimethyl-9- methylidenebicyclo[3.3.1]nonane 1,1-diethoxycyclohexane 4-(diethoxymethyl)-1-ethoxy-2- methoxybenzene 2-ethoxy-5-[(E)-prop-1- enyl]phenol 1-ethoxy-2-methoxy-4-[(E)-prop-1- enyl]benzene 4-ethoxy-3-methoxybenzaldehyde 2-ethoxy-1-methyl-4-propan-2- ylbenzene 2-ethoxy-4-methylphenol 3-ethoxy-4-hydroxybenzaldehyde (2-ethoxy-4-formylphenyl) acetate (2-ethoxy-4-formylphenyl) 2- methylpropanoate 3-ethoxy-4-[(2S, 3R, 4S, 5S, 6R))-3,4,5-trihydroxy- 6-(hydroxymethyl)oxan-2-	CCOC1(CCC2C(=C)C1CCC2(C) C)C CCOC1(CCCCC1)OCC CCOC1=C(C=C(C=C1)C(OCC)O CCOC1=C(C=C(C=C1)C=CC)O CCOC1=C(C=C(C=C1)C=C)OC CCOC1=C(C=C(C=C1)C=O)OC CCOC1=C(C=CC(C=C1)C=O)OC CCCCC1=C(C=CC(C=C1)C=O)OC2 CC(C(C(C(CC)CO)OO)OO)	pungent alcoholic rose cognac fermented rummy woody amber orris tobacco fruity rummy tobacco woody vanilla milky creamy caramel powdery caramel creamy medicinal nutty spicy sweet vanilla woody tobacco phenolic powdery anisic floral spicy carnation clove sweet floral vanilla powdery spicy herbaceous carrot earthy carrot vanilla woody spicy guaiacol sweet vanilla creamy caramel root beer powerful vanilla milky creamy caramel powdery sweet creamy vanilla chocolate milky caramel rummy vanilla sweet creamy vanilla phenolic	TGSC, Pubchem,OdoRactor OdorRactor ,TGSC OdorRactor ,TGSC TGSC Sigma Aldrich, TGSC, OdoRactor OdorRactor ,TGSC TGSC SuperScent, TGSC, Flavorbase, Odoractor TGSC Sigma Aldrich, AOD, Flavorbase, TGSC, OdoRactor, Pubchem TGSC TGSC

3801	2-Ethoxy-4-	2-ethoxy-4-	CCOC1=C(C=CC(=C1)COC)O	sweet floral spicy carnation clove	OdorRactor ,TGSC, Pubchem
	(methoxymethyl)phenol	(methoxymethyl)phenol		powdery vanilla custard woody burnt	
				wood balsamic burnt	
3802	2,5-Dimethyl-4-ethoxy-3(2H)-furanone	4-ethoxy-2,5-dimethylfuran-3-one	CCOC1=C(OC(C1=O)C)C	caramel fruity brandy strawberry	у
3803	4-Methylphenetole	1-ethoxy-4-methylbenzene	CCOC1=CC=C(C=C1)C	ylang floral cananga	OdorRactor ,TGSC
3804	4-Ethoxybenzaldehyde	4-ethoxybenzaldehyde	CCOC1=CC=C(C=C1)C=O	spicy sweet floral anisic cherry almond	OdoRactor, Sigma Aldrich, TGSC, Flavorbase
3805	4-Ethoxyphenol	4-ethoxyphenol	CCOC1=CC=C(C=C1)O	mild hawthorn phenolic plastic nutty animal	OdorRactor ,TGSC
3806	7-Ethoxy-4-methylcoumarin		O)O2)C	nutty walnut	TGSC
3807	2-Ethoxynaphthalene	2-ethoxynaphthalene	CCOC1=CC2=CC=CC=C1	grape naphthyl floral orange flower powdery citrus	Sigma Aldrich, TGSC
3808	2-Ethoxy-6-methylpyrazine	2-ethoxy-6-methylpyrazine	CCOC1=NC(=CN=C1)C	nutty roasted pineapple	OdorRactor ,TGSC, Pubchem
3809	2-Ethoxy-5-methylpyrazine	2-ethoxy-5-methylpyrazine	CCOC1=NC=C(N=C1)C	nutty roasted chocolate	OdorRactor ,TGSC, Pubchem
3810	2-Ethoxy-3-methylpyrazine	2-ethoxy-3-methylpyrazine	CCOC1=NC=CN=C1C	almond earthy pineapple nutty hazelnut roasted almond peanut cocoa roasted	Sigma Aldrich, TGSC, Flavorbase, OdoRactor
3811	2-Ethoxy-3-isopropylpyrazine	2-ethoxy-3-propan-2-ylpyrazine	CCOC1=NC=CN=C1C(C)C	roasted nutty earthy green vegetable	TGSC, Flavorbase
3812	2-Ethoxythiazole	2-ethoxy-1,3-thiazole	CCOC1=NC=CS1	meaty nutty musty vegetable phenolic roasted burnt green coffee brothy sweet roasted onion	Sigma Aldrich, Flavorbase, TGSC, OdoRactor
3813	cis-3-Ethoxy-1,1,5- trimethylcyclohexane	(3R, 5R)-3-ethoxy-1,1,5- trimethylcyclohexane	CCOC1CC(CC(C1)(C)C)C	fresh green herbaceous natural citrus woody	OdorRactor ,TGSC
3814	Ethoxybornane	2-ethoxy-1,7,7- trimethylbicyclo[2.2.1]heptane	CCOC1CC2CCC1(C2(C)C)C	camphoraceous woody cedar eucalyptus blueberry	TGSC
	Ether	ethoxyethane	CCOCC	ethereal sweet pungent	AOD, Pubhcem
3816	Acetic acid, ethoxy-, (1R,2S,5R)-5-methyl- 2-(1-methylethyl)cyclohexyl ester, rel-	5-methyl-2-propan-2- ylcyclohexyl) 2-ethoxyacetate	CCOCC(=0)0C1CC(CCC1C(C)C)C	moldy	TGSC
3817	1-Ethoxy-3-methyl-2-butene	1-ethoxy-3-methylbut-2-ene	CCOCC=C(C)C	fruity green grassy	OdorRactor ,TGSC
3818	Ethyl geranyl ether	(2E)-1-ethoxy-3,7-dimethylocta- 2,6-diene	CCOCC=C(C)CCC=C(C)C	ethereal fruity green light spicy natural floral rose	TGSC, Flavorbase
3819	3,7-Dimethyl-1-ethoxy-2,6-octadiene	(2Z)-1-ethoxy-3,7-dimethylocta- 2,6-diene	CCOCC=C(C)CCC=C(C)C	floral clean rose cologne	OdorRactor ,TGSC
3820	4-(Ethoxymethyl)-2- methoxyphenol	4-(ethoxymethyl)-2- methoxyphenol	CCOCC1=CC(=C(C=C1)O)OC	alcoholic rummy sweet chocolate creamy vanilla spicy nutmeg smoky	OdorRactor, ,TGSC
	Benzyl ethyl ether	ethoxymethylbenzene	CCOCC1=CC=CC=C1	fruity pineapple tropical	OdorRactor ,TGSC
		2-(ethoxymethyl)phenol	CCOCC1=CC=CC=C1O	phenolic animal smoky sweet vanilla castoreum	OdorRactor ,TGSC, Flavorbase
3823	o-(Ethoxymethyl)anisole	1-(ethoxymethyl)-2- methoxybenzene	CCOCC1=CC=CC=C1OC	green spicy floral fruity tearose rose	OdorRactor ,TGSC
3824	2-(Ethoxymethyl)furan	2-(ethoxymethyl)furan	CCOCC1=CC=CO1	sweet spicy nutty coffee ethereal fermented buttery	OdorRactor ,TGSC, Flavorbase
3825	Pyrazine, 2-ethoxymethyl-	2-(ethoxymethyl)pyrazine	CCOCC1=NC=CN=C1	nutty hazelnut almond earthy pineapple	OdorRactor ,TGSC
3826	8-Ethoxy-2,6-dimethyloct-2-ene	8-ethoxy-2,6-dimethyloct-2-ene	CCOCCC(C)CCC=C(C)C	rose citrus cologne floral fresh clean	OdorRactor ,TGSC
	Octane, 1-ethoxy-3,7- dimethyl-	1-ethoxy-3,7-dimethyloctane	CCOCCC(C)CCCC(C)C	rose citrus green floral fresh clean herbaceous	OdorRactor ,TGSC
3828 3829	3-Ethoxy-1-propanol 2-Ethoxyethyl acetate	3-ethoxypropan-1-ol 2-ethoxyethyl acetate	CCOCCCO CCOCCOC(=0)C	fruit mild weak sweet estery fruity	Flavornet Flavorbase, Pubchem
3830	Diethylene glycol monoethyl	2-(2-ethoxyethoxy)ethanol	CCOCCOCCO	pleasant faint ethereal mild pleasant	Sigma Aldrich, OdoRactor,
3830	ether (Ethoxymethoxy)cyclododeca	ethoxymethoxycyclododecane	CCOCOCICCCCCCCCCC	woody cedar dusty amber	Pubchem OdorRactor, TGSC, Pubchem
3831	ne	ethyl nitrite	CCON=0	ambergis dry ethereal sweet rummy fruit	OdorRactor , Flavorbase,
3034	Ethyl nitrite	curyi mune	CCON=0	fermented	TGSC, Pubchem
3833	Ethanethiol	ethanethiol	CCS	sulfurous alliaceous fruity rubbery vegetable onion garlic meaty coffee	Sigma Aldrich, Flavorbase, TGSC, Pubchem
3834	Ethyl methyl sulfide	methylsulfanylethane	CCSC	tropical skunk leek penetrating sulfurous garlic tomato coffee cabbage vegetable meaty metallic bloody alliaceous corn calm savory	Flavornet, Flavorbase, TGSC,OdoRactor
3835	S-Ethyl thioacetate	S -ethyl ethanethioate	CCSC(=O)C	coffee sulfurous fruity onion garlic meaty	Sigma Aldrich, TGSC, OdoRactor
3836	N-Acetylthioglycine S-ethyl	S -ethyl 2-acetamidoethanethioate	CCSC(=O)CNC(=O)C	pungent meaty	TGSC
0000	ester	5 Striyi 2-acetamidoethanetinoate	CCSC(=O)CNC(=O)C	pungent meaty	1000

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3837	3-(Ethylthio)-1-butanol	3-ethylsulfanylbutan-1-ol	CCSC(C)CCO	cooked roasted nutty	OdorRactor ,TGSC
3838	Ethane, 1,1-bis(ethylthio)-	1,1-bis(ethylsulfanyl)ethane	CCSC(C)SCC	burnt rubbery alliaceous	TGSC
3839	Diethyl sulfide	ethylsulfanylethane	CCSCC	sulfurous ethereal garlic	Sigma Aldrich, TGSC, OdoRactor, Pubchem
3840	3-(Ethylthio)propanoic acid	3-ethylsulfanylpropanoic acid	CCSCCC(=O)O	savory dairy	TGSC
3841	3-(Ethylthio)propanol	3-ethylsulfanylpropan-1-ol	CCSCCCO	sulfurous vegetable potato	TGSC
3842	Ethyl methyl disulfide	(methyldisulfanyl)ethane	CCSSC	sulfurous truffle alliaceous green vegetable	OdorRactor ,TGSC
3843	Diethyl disulfide	(ethyldisulfanyl)ethane	CCSSCC	sulfurous onion greasy garlic gassy ripe alliaceous	Sigma Aldrich, TGSC,OdoRactor
3844	Methyl ethyl trisulfide	(methyltrisulfanyl)ethane	CCSSSC	alliaceous garlic green onion onion sulfurous	OdorRactor ,TGSC, Flavorbase
3845	Diethyl trisulfide	(ethyltrisulfanyl)ethane	CCSSSCC	sulfurous garlic onion	OdorRactor ,TGSC
3846	Iodomethane	iodomethane	CI	ethereal pungent medicinal	Pubchem
3847	Hydrochloric acid	chlorane	Cl	faint pungent irritating	Sigma Aldrich, Pubchem
3848	Chlorine	molecular chlorine	CICI	irritating strong suffocating pungent	Pubchem
3849	Methylamine	methanamine	CN	pungent fishy ammonical	Pubchem
3850	Trimethylamine	N ,N -dimethylmethanamine	CN(C)C	fishy meaty oily rancid sweaty	Sigma Aldrich, TGSC,
3630	Trincuryamine	iv ,iv -unitettiyinettiananine		fruity pungent ammonical rotten rotten fish	Pubchem
3851	Methyl 2- (dimethylamino)benzoate	methyl 2- (dimethylamino)benzoate	CN(C)C1=CC=CC=C1C(=O)OC	fruity orange leafy petitgrain	OdorRactor ,TGSC
3852	Methyl isothiocyanate	methylimino(sulfanylidene)methan e	CN=C=S	pungent mustard horseradish	Sigma Aldrich, Flavorbase, OdoRactor, Pubchem
3853	1-Methylpyrrole	1-methylpyrrole	CN1C=CC=C1	herbaceous woody smoky	Sigma Aldrich, TGSC
3854	1-Methylpyrrole-2- carboxaldehyde	1-methylpyrrole-2-carbaldehyde	CN1C=CC=C1C=O	roasted nutty burnt	OdorRactor ,Flavorbase, TGSC
3855	1-Methylpyrrolidine	1-methylpyrrolidine	CN1CCCC1	ammonical	OdorRactor ,TGSC
3856	N-Methylpiperidine	1-methylpiperidine	CN1CCCC1	faint pepper	Sigma Aldrich, Pubchem,OdoRactor
3857	[4-(4-Methylpiperazin-1-yl)phenyl]methanol	[4-(4-methylpiperazin-1-yl)phenyl]methanol	CN1CCN(CC1)C2=CC=C(C=C2)	almond nutty	OdorRactor,
3858	Dimethylamine	N -methylmethanamine	CNC	pungent ammonical fishy	
3859	Methyl 2-	methyl 2-(methylamino)benzoate	CNC1=CC=CC=C1C(=0)OC	fruity musty sweet neroli powdery	Sigma Aldrich, TGSC,
5057	(methylamino)benzoate	memyr 2 (memyrammo)semzsare		phenolic winey clean fresh floral blossom	Pubchem
				grape orange mandarin	
3860	Methyl cyclopentylideneacetate	methyl 2-cyclopentylideneacetate	COC(=0)C=C1CCCC1	tuberose ylang sweet dry floral fruity weedy	OdorRactor ,TGSC
3861	Methyl cinnamate	methyl (E)-3-phenylprop-2-enoate	COC(=0)C=CC1=CC=CC=C1	balsamic fruity strawberry honey sweet cherry cinnamyl	Sigma Aldrich, TGSC, Flavorbase, OdoRactor
3862	Methyl furfuracrylate	methyl (E)-3-(furan-2-yl)prop-2-enoate	COC(=O)C=CC1=CC=CO1	fruity cherry clove cinnamyl	OdorRactor ,TGSC
3863	Methyl benzoate	methyl benzoate	COC(=O)C1=CC=CC=C1	fruity sweet herbaceous cherry lettuce prune phenolic wintergreen	Sigma Aldrich, TGSC, Pubchem
				almond floral cananga chemical medicinal	Tubenem
3864	Dimethyl phthalate	dimethyl benzene-1,2- dicarboxylate	COC(=0)C1=CC=CC=C1C(=0)O C	aromatic ethereal	Sigma Aldrich, Pubchem,OdoRactor
3865	Methyl anthranilate	methyl 2-aminobenzoate	COC(=0)C1=CC=CC=C1N	chocolate coffee grape grapefruit jasmine lemon lime medicinal musty floral herbaceous strawberry sweet orange flower neroli fruity powdery	Sigma Aldrich, Flavorbase, TGSC, OdoRactor, Pubchem
3866	Methyl 2- [cinnamylideneamino]benzoat	methyl 2-[[(E)-3-phenylprop-2-enylidene]amino]benzoate	COC(=0)C1=CC=CC=C1N=CC= CC2=CC =CC=C2	sweet cinnamyl cypress spicy	OdorRactor ,TGSC
3867	Methyl 2- [(phenylmethylene)amino]ben zoate	methyl 2- (benzylideneamino)benzoate		bitter almond sweet benzaldehyde cherry fruity floral bitter	OdorRactor ,TGSC
3868	Benzoic acid, 2-[(2- phenylethylidene)amino]-, methyl ester	methyl 2-(2- phenylethylideneamino)benzoate		hyacinth green floral foliage mandarin sweetpea	OdorRactor ,TGSC
3869	Methyl N-formylanthranilate	methyl 2-formamidobenzoate	COC(=O)C1=CC=CC=C1NC=O	fruity grape	OdorRactor ,TGSC
3870	Methyl salicylate	methyl 2-hydroxybenzoate	COC(=O)C1=CC=CC=C1O	beer minty spicy sweet peppermint vanilla wintergreen root beer aromatic phenolic camphoraceous	Sigma Aldrich, TGSC, Pubchem
3871	Methyl 2-furoate	methyl furan-2-carboxylate	COC(=0)C1=CC=CO1	berry mushroom fruity sweet tobacco fungal winey	Sigma Aldrich, TGSC,OdoRactor
3872	Methyl nicotinate	methyl pyridine-3-carboxylate	COC(=0)C1=CN=CC=C1	herbaceous tobacco warm herbaceous	Sigma Aldrich, TGSC
3873	Methyl cyclohexanecarboxylate	methyl cyclohexanecarboxylate	COC(=0)C1CCCCC1	fruity estery pineapple cooling minty milky berry creamy	Sigma Aldrich, TGSC, OdoRactor
3874	Trimethyl citrate	trimethyl 2-hydroxypropane-1,2,3-		ethereal fruity	TGSC
		tricarboxylate	OC)O		

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3875	Methyl phenylacetate	methyl 2-phenylacetate	COC(=O)CC1=CC=CC=C1	honey jasmine sweet floral spicy wax almond fruity	Sigma Aldrich, TGSC, Pubchem
3876	Methyl cyclohexylacetate	methyl 2-cyclohexylacetate	COC(=0)CC1CCCCC1	fruity tropical banana mango pineapple honey	TGSC
3877	Dimethyl succinate	dimethyl butanedioate	COC(=0)CCC(=0)OC	fruity winey green sweet floral pleasant ethereal	Sigma Aldrich, TGSC, Pubchem, OdoRactor
3878	Methyl (4E)-octa-4,7- dienoate	methyl (4E)-octa-4,7-dienoate	COC(=0)CCC=CCC=C	fruity green pear	TGSC
3879	Methyl 3-phenylpropionate	methyl 3-phenylpropanoate	COC(=O)CCC1=CC=CC=C1	honey fruity winey balsamic floral	SuperScent, TGSC
3880	Dimethyl glutarate	dimethyl pentanedioate	COC(=O)CCCC(=O)OC	floral estery faint agreeable	OdorRactor ,SuperScent, TGSC, Pubchem
3881	Methyl 4-phenylbutyrate	methyl 4-phenylbutanoate	COC(=0)CCCC1=CC=CC=C1	sweet fruity honey floral dried fruit	OdorRactor ,TGSC
3882	Dimethyl adipate	dimethyl hexanedioate	COC(=0)CCCCC(=0)OC	nutty	SuperScent, TGSC
	Methyl 10-undecenoate	methyl undec-10-enoate	COC(=0)CCCCCCCCCCC	banana honey oily citrus earthy	Sigma Aldrich,
3003	Mediyi 10-dildecelloate	inchiyi undec-10-enoate	coc(-o)ccccccc-c	rose soapy winey fatty wax fungal floral	TGSC,OdoRactor
3884	Methyl 4- (methylthio)butyrate	methyl 4-methylsulfanylbutanoate	COC(=0)CCCSC	sulfurous cabbage fruity pineapple cheese	OdorRactor ,TGSC
3885	Methyl 3-	methyl 3-	COC(=O)CCSC	vegetable onion sweet garlic	Sigma Aldrich, TGSC,
	(methylthio)propionate	methylsulfanylpropanoate	. ,	tomato fruity sulfurous pungent rooty horseradish	OdoRactor
3886	Methyl 3- (furfurylthio)propionate	methyl 3-(furan-2- ylmethylsulfanyl)propanoate	COC(=0)CCSCC1=CC=CO1	earthy fruity sweet	TGSC
3887	Methyl (methylthio)acetate	methyl 2-methylsulfanylacetate	COC(=0)CSC	potato sulfurous nutty fruity tropical baked potato cooked roasted baked	Sigma Aldrich, TGSC, OdoRactor
3888	Methyl indole-1-carboxylate	methyl indole-1-carboxylate	COC(=O)N1C=CC2=CC=CC=C2	citrus orange grape orange flower lily	TGSC
3889	Cyclooctyl methyl carbonate	cyclooctyl methyl carbonate	COC(=0)OC1CCCCCC1	fresh herbaceous natural oily jasmine wax	OdorRactor ,TGSC
3890	Cinnamaldehyde dimethyl acetal	[(E)-3,3-dimethoxyprop-1-enyl]benzene	COC(C=CC1=CC=CC=C1)OC	fresh green spicy cinnamyl herbaceous	TGSC
3891		dimethoxymethylbenzene	COC(C1=CC=CC=C1)OC	nutty floral bitter almond fruity winey green sharp bitter	Sigma Aldrich, TGSC, OdoRactor
3892	(2,2-Dimethoxyethyl)benzene	2,2-dimethoxyethylbenzene	COC(CC1=CC=CC=C1)OC	green hyacinth spicy floral rose earthy mushroom foliage strong	Sigma Aldrich, Flavorbase, TGSC, OdoRactor
3893	Methyl formate	methyl formate	COC=O	fruity estery plum agreeable pleasant	Sigma Aldrich, TGSC, Pubchem
3894	1,1-Dimethoxycyclododecane	1,1-dimethoxycyclododecane	COC1(CCCCCCCCCC1)OC	woody cedar patchouli ambergis	OdorRactor ,TGSC
3895	2,6-Dimethoxyphenol	2,6-dimethoxyphenol	COC1=C(C(=CC=C1)OC)O	meaty smoky phenolic balsamic bacon powdery woody sweet medicinal	Sigma Aldrich, TGSC
3896	3,4-Dimethoxystyrene	4-ethenyl-1,2-dimethoxybenzene	COC1=C(C=C(C=C1)C=C)OC	green floral weedy fruity cortex	OdorRactor ,TGSC
3897	Veratraldehyde	3,4-dimethoxybenzaldehyde	COC1=C(C=C(C=C1)C=O)OC	caramel cherry creamy woody citrus minty sweet vanilla powdery herbaceous phenolic	Sigma Aldrich, TGSC, OdoRactor, Pubchem
3898	Chavibetol	2-methoxy-5-prop-2-enylphenol	COC1=C(C=C(C=C1)CC=C)O	spicy carnation	TGSC
3899	Methyleugenol	1,2-dimethoxy-4-prop-2- enylbenzene	COC1=C(C=C(C=C1)CC=C)OC	anisic apricot banana chocolate cinnamyl clove coconut creamy green musty oily spicy fruity earthy woody peach plum raspberry sweet vanilla fresh warm carnation vegetable wax pepper phenolic herbaceous	Sigma Aldrich, AOD, TGSC, Pubchem
3900	N-(2-(3,4- Dimethoxyphenyl)ethyl)-3,4- dimethoxycinnamic acid amide	3-(3,4-dimethoxyphenyl)- <i>N</i> -[2-(3,4-dimethoxyphenyl)ethyl]prop-2-enamide	COC1=C(C=C(C=C1)CCNC(=O) C=CC2= CC(=C(C=C2)OC)OC)OC	savory meaty	TGSC
3901	2,4,6-Trichloroanisole	1,3,5-trichloro-2-methoxybenzene	COC1=C(C=C(C=C1Cl)Cl)Cl	moldy	
3902	Vanillic acid	4-hydroxy-3-methoxybenzoic acid	COC1=C(C=CC(=C1)C(=O)O)O	chocolate creamy grape nutty winey pleasant vanilla dairy milky sweet powdery beany phenolic brown	Sigma Aldrich, AOD, TGSC, OdoRactor, Pubchem
3903	Methyl vanillate	methyl 4-hydroxy-3- methoxybenzoate	COC1=C(C=CC(=C1)C(=O)OC)O	spicy phenolic carnation vanilla butterscotch caramel warm guaiacol	Sigma Aldrich, TGSC, Odoractor
3904	Vanillylmandelic acid	2-hydroxy-2-(4-hydroxy-3- methoxyphenyl)acetic acid	COC1=C(C=CC(=C1)C(C(=O)O) O)O	sweet vanilla	TGSC, Flavorbase
3905	2-Methoxy-4-vinylphenol	4-ethenyl-2-methoxyphenol	COC1=C(C=CC(=C1)C=C)O	apple spicy roasted peanut winey clove curry woody amber dry fresh cedar smoky sweet warm phenolic roasted	Sigma Aldrich, TGSC

3906	Sodium ferulate	sodium;(E)-3-(4-hydroxy-3-methoxyphenyl)prop-2 enoate	COC1=C(C=CC(=C1)C=CC(=O)[O-])O.[Na+]	sweet spicy clove phenolic	TGSC
3907	Ferulic acid	(E)-3-(4-hydroxy-3- methoxyphenyl)prop-2-enoic acid	COC1=C(C=CC(=C1)C=CC(=O) O)O	faint	Sigma Aldrich
3908	4-Hydroxy-3- methoxycinnamaldehyde	(E)-3-(4-hydroxy-3- methoxyphenyl)prop-2-enal	COC1=C(C=CC(=C1)C=CC=O)O	cookie toasted grain roasted barley vanilla custard dairy roasted barley	TGSC
3909	Vanillin	4-hydroxy-3- methoxybenzaldehyde	COC1=C(C=CC(=C1)C=O)O	caramel chocolate sweet vanilla creamy phenolic dry eugenol strong	Sigma Aldrich, AOD, TGSC, Pubchem
3910	Glucovanillin	3-methoxy-4-[(2S ,3R ,4S ,5S ,6R)-3,4,5-trihydroxy 6-(hydroxymethyl)oxan-2-yl]oxybenzaldehyde	COC1=C(C=CC(=C1)C=O)OC2C (C(C(C(O2)CO)O)O)O	vanilla	Flavorbase, TGSC
3911	Eugenol	2-methoxy-4-prop-2-enylphenol	COC1=C(C=CC(=C1)CC=C)O		Sigma Aldrich, AOD, Flavorbase, TGSC, Pubchem
3912	Eugenyl benzoate	(2-methoxy-4-prop-2-enylphenyl) benzoate	COC1=C(C=CC(=C1)CC=C)OC(=O)C2= CC=CC=C2	balsamic clove spicy	OdorRactor ,TGSC
3913	Eugenyl phenylacetate	(2-methoxy-4-prop-2-enylphenyl) 2-phenylacetate	COC1=C(C=CC(=C1)CC=C)OC(=0)CC2 =CC=CC=C2	spicy honey sweet carnation	OdorRactor ,TGSC
3914	Eugenyl formate	(2-methoxy-4-prop-2-enylphenyl) formate	COC1=C(C=CC(=C1)CC=C)OC= O	woody orris warm dry	OdorRactor ,TGSC
3915	Eugenyl glucoside	(2R, 3S, 4S, 5R, 6S)-2- (hydroxymethyl)-6-(2- methoxy-4- prop-2-enylphenoxy)oxane-3,4,5- triol	COC1=C(C=CC(=C1)CC=C)OC2 C(C(C(C (O2)CO)O)O)O	eugenol	Flavorbase
3916	Benzyl eugenol	2-methoxy-1-phenylmethoxy-4- prop-2- enylbenzene	COC1=C(C=CC(=C1)CC=C)OCC 2=CC=C C=C2	warm spicy hay balsamic floral	TGSC
3917	Homovanillin	2-(4-hydroxy-3- methoxyphenyl)acetaldehyde	COC1=C(C=CC(=C1)CC=O)O	floral vanilla	TGSC
3918	Vanillyl alcohol	4-(hydroxymethyl)-2- methoxyphenol	COC1=C(C=CC(=C1)CO)O	anisic sweet creamy vanilla caramel coconut tonka milky powdery graham cracker phenolic	Sigma Aldrich, TGSC, OdoRactor
3919	Dillapiol	4,5-dimethoxy-6-prop-2-enyl-1,3-benzodioxole	COC1=C(C2=C(C=C1CC=C)OC O2)OC	woody spice	Flavornet, TGSC
3920	Apiole	4,7-dimethoxy-5-prop-2-enyl-1,3- benzodioxole	COC1=C2C(=C(C(=C1)CC=C)O C)OCO2	herbaceous parsley	TGSC
3921	2-Hydroxy-4- methoxybenzaldehyde	2-hydroxy-4- methoxybenzaldehyde	COC1=CC(=C(C=C1)C=O)O	vanilla	TGSC
3922	Dehydrodivanillin	3-(5-formyl-2-hydroxy-3- methoxyphenyl)-4- hydroxy-5- methoxybenzaldehyde	COC1=CC(=CC(=C1O)C2=C(C(= CC(=C2)C=O)OC)O)C=O	fruity vanilla creamy	TGSC, Flavorbase
3923	2,6-Dimethoxy-4-vinylphenol	4-ethenyl-2,6-dimethoxyphenol	COC1=CC(=CC(=C1O)OC)C=C	phenolic animal leathery	OdorRactor ,TGSC
3924	Syringaldehyde	4-hydroxy-3,5- dimethoxybenzaldehyde	COC1=CC(=CC(=C1O)OC)C=O	chocolate grape woody smoky winey plastic tonka sweet	Sigma Aldrich, TGSC,OdoRactor
3925	4-Allyl-2,6-dimethoxyphenol	2,6-dimethoxy-4-prop-2- enylphenol	COC1=CC(=CC(=C10)OC)CC=C	7.1	Sigma Aldrich, TGSC, OdoRactor
3926	Elemicin	1,2,3-trimethoxy-5-prop-2- enylbenzene	COC1=CC(=CC(=C1OC)OC)CC=	spice floral	Flavornet, TGSC
3927	1,3-Dimethoxybenzene	1,3-dimethoxybenzene	COC1=CC(=CC=C1)OC	acidic medicinal fruity nutmeg neroli cooling sweet root beer coconut hazelnut earthy nutty	Sigma Aldrich, Flavorbase, TGSC,OdoRactor
3928	Myristicin	4-methoxy-6-prop-2-enyl-1,3- benzodioxole	COC1=CC(=CC2=C1OCO2)CC=	spice warm balsamic woody	Flavornet, TGSC
3929	4-Methoxybenzonitrile	4-methoxybenzonitrile	COC1=CC=C(C=C1)C#N	sweet floral hawthorn coumarinic hay	OdorRactor ,TGSC
3930	4-Methoxybenzoic acid	4-methoxybenzoic acid	COC1=CC=C(C=C1)C(=O)O	fecal phenolic animal medicinal fatty	Sigma Aldrich, TGSC
3931	Methyl 4-methoxybenzoate	methyl 4-methoxybenzoate	COC1=CC=C(C=C1)C(=0)OC	anisic chocolate creamy melon woody spicy sweet vanilla herbaceous	Sigma Aldrich, TGSC,OdoRactor
3932	Sodium (4- methoxybenzoyloxy)acetate	sodium;2-(4- methoxybenzoyl)oxyacetate	COC1=CC=C(C=C1)C(=O)OCC(=O)[O-].[Na+]	brown cooked roasted	TGSC
3933	((4- Methoxybenzoyl)oxy)acetic acid	2-(4-methoxybenzoyl)oxyacetic acid	COC1=CC=C(C=C1)C(=0)OCC(=0)O	cooked roasted brown	OdorRactor ,TGSC
3934	1-(Dimethoxymethyl)-4- methoxybenzene	1-(dimethoxymethyl)-4- methoxybenzene	COC1=CC=C(C=C1)C(OC)OC	floral hawthorn jasmine lilac elderflower	OdorRactor ,TGSC
3935	4-Methoxycinnamaldehyde	(E)-3-(4-methoxyphenyl)prop-2-enal	COC1=CC=C(C=C1)C=CC=O	cinnamyl creamy herbaceous spicy floral fruity sweet cherry vanilla smoky	Sigma Aldrich, TGSC, OdoRactor

3936	Methyl 2-[[(4- methoxyphenyl)methylene]am ino]benzoate	methyl 2-[(4- methoxyphenyl)methylideneamino benzoate	` ,	floral sweet hawthorn mimosa powdery	OdorRactor ,TGSC
3937	4-Methoxybenzaldehyde	4-methoxybenzaldehyde	COC1=CC=C(C=C1)C=O	anisic sweet floral hawthorn balsamic vanilla woody coumarinic creamy spicy powdery mimosa fruity hay almond	SuperScent, TGSC, OdoRacor, Pubchem
3938	Estragole	1-methoxy-4-prop-2-enylbenzene	COC1=CC=C(C=C1)CC=C	alcoholic green minty sweet vanilla licorice herbaceous fennel anisic spice sassafrass phenolic harsh herbaceous ammonical	Sigma Aldrich, Flavorbase, TGSC, OdoRactor, Pubchem
3939	4- Methoxyphenylacetaldehyde	2-(4-methoxyphenyl)acetaldehyde	COC1=CC=C(C=C1)CC=O	floral hawthorn anisic powdery	TGSC
3940	1-(Cyclopropylmethyl)-4- methoxybenzene	1-(cyclopropylmethyl)-4- methoxybenzene	COC1=CC=C(C=C1)CC2CC2	anisic sweet root beer licorice herbaceous tarragon sassafrass	TGSC
3941	4-Methoxybenzyl alcohol	(4-methoxyphenyl)methanol	COC1=CC=C(C=C1)CO	caramel chocolate hyacinth fruit sweet vanilla powdery hawthorn lilac rose creamy balsamic coumarinic lactonic cherry licorice	Sigma Aldrich, TGSC, OdoRactor
3942	4-Methoxybenzyl	(4-methoxyphenyl)methyl 2-	COC1=CC=C(C=C1)COC(=O)CC	anisic honey balsamic woody	Sigma Aldrich, TGSC
3943	phenylacetate 4-Methoxybenzyl formate	phenylacetate (4-methoxyphenyl)methyl formate	2=CC= CC=C2 COC1=CC=C(C=C1)COC=O	floral sweet fruity anisic vanilla	Sigma Aldrich, TGSC,
3944	4-Methoxy-alpha-toluenethiol	(4-methoxyphenyl)methanethiol	COC1=CC=C(C=C1)CS	seaweed spicy powdery sulfurous burnt floral balsamic	OdoRactor TGSC
		, J1 J ,	` '	anisic	
3945	1,4-Dimethoxybenzene	1,4-dimethoxybenzene	COC1=CC=C(C=C1)OC	fatty fennel sweet green new mown hay nutty tobacco phenolic earthy clover	Sigma Aldrich, Flavorbase, TGSC,OdoRactor
	3-Methoxybenzaldehyde	3-methoxybenzaldehyde	COC1=CC=CC(=C1)C=O	anisic	Sigma Aldrich, TGSC
	3-Methoxyphenol 2-Allyl-6-methoxyphenol	3-methoxyphenol 2-methoxy-6-prop-2-enylphenol	COC1=CC=CC(=C1)O COC1=CC=CC(=C1O)CC=C	phenolic spicy sweet smoky phenolic	TGSC TGSC, Flavorbase
			0001 00 00 01		o: All'i mono
3949	Anisole	anisole	COC1=CC=CC=C1	alcoholic buttery cheese ethereal phenolic gasoline anisic musty moldy nail-polish	Sigma Aldrich, TGSC
3950	Methyl 2-methoxybenzoate	methyl 2-methoxybenzoate	COC1=CC=CC=C1C(=O)OC	hyacinth herbaceous herbaceous floral fruity black currant cananga	Sigma Aldrich, TGSC, OdoRactor
3951	1-Methoxy-2-vinylbenzene	1-ethenyl-2-methoxybenzene	COC1=CC=CCCCCC	green herbaceous nutty ethereal	OdorRactor ,TGSC
3952	2-Methoxycinnamaldehyde	(E)-3-(2-methoxyphenyl)prop-2-enal	COC1=CC=CC=C1C=CC=O	floral spicy sweet cinnamyl oily woody paper cassia resinous	Sigma Aldrich, TGSC, OdoRactor
3953	2-Methoxybenzaldehyde	2-methoxybenzaldehyde	COC1=CC=CC=C1C=O	almond balsamic hawthorn spicy sweet vanilla anisic powdery guaiacol	Sigma Aldrich, TGSC,OdoRactor
3954	2-Methoxybiphenyl	1-methoxy-2-phenylbenzene	COC1=CC=CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC	floral rose fruity	TGSC
3955	Guaiacol	2-methoxyphenol	COC1=CC=CC=C10	medicinal smoky woody sweet phenolic spice vanilla savory meaty bacon aromatic	Sigma Aldrich, TGSC, Pubchem
3956	1,2-Dimethoxybenzene	1,2-dimethoxybenzene	COC1=CC=CC=C1OC	vanilla sweet creamy phenolic musty earthy nutty	Sigma Aldrich, Flavorbase, TGSC
3957	Guaiacyl phenylacetate	(2-methoxyphenyl) 2- phenylacetate	COC1=CC=CC=C1OC(=O)CC2= CC=CC= C2	meaty smoky balsamic phenolic spice floral woody powdery honey smoky sausage chemical	Sigma Aldrich, TGSC, OdoRactor
3958	2-Methoxybenzenethiol	2-methoxybenzenethiol	COC1=CC=CC=C1S	caramel coffee smoky meaty powdery sweet spicy phenolic sulfurous sausage	Sigma Aldrich, TGSC
	2-Methoxypyridine	2-methoxypyridine	COC1=CC=CC=N1	green fermented tea	TGSC
3960	7-Methoxycoumarin	7-methoxychromen-2-one	COC1=CC2=C(C=C1)C=CC(=O) O2	balsamic sweet tonka	Sigma Aldrich, TGSC,OdoRactor
3961	Sarisan	5-methoxy-6-prop-2-enyl-1,3-	COC1=CC2=C(C=C1CC=C)OCO	spice pepper	Flavornet, TGSC
3962	2-Methoxynaphthalene	benzodioxole 2-methoxynaphthalene	2 COC1=CC2=CC=CC=C2C=C1	floral strawberry sweet naphthyl orange flower acacia neroli	Sigma Aldrich, TGSC
3963 3964	1-Methoxycyclohexene 2-Methoxypyrazine	1-methoxycyclohexene 2-methoxypyrazine	COC1=CCCCC1 COC1=NC=CN=C1	herbaceous spicy chocolate nutty sweet cocoa	Flavornet, TGSC Sigma Aldrich, TGSC, OdoRactor
3965	2-Methoxythiazole	2-methoxy-1,3-thiazole	COC1=NC=CS1	cereal bready caramel	TGSC
3966	Scentenal	8- methoxytricyclo[5.2.1.02,6]decan e-4- carbaldehyde	COC1CC2CC1C3C2CC(C3)C=O	watery floral ozone fresh marine seashore aldehydic woody mossy magnolia	OdorRactor ,TGSC

4,7-Methano-1H-indene, 3a,4,5,6,7,7a- hexahydro-5- methoxy-	9-methoxytricyclo[5.2.1.02,6]dec- 3-ene	COC1CC2CC1C3C2CC=C3	fruity sweet green herbaceous melon	OdorRactor ,TGSC
1-Methoxyindan	1-methoxy-2,3-dihydro-1 <i>H</i> - indene	COC1CCC2=CC=CC2	floral minty earthy hawthorn animal anisic	OdorRactor ,TGSC
Cyclododecane, methoxy-	methoxycyclododecane	COC1CCCCCCCCCC1	woody musk tobacco cedar dry amber patchouli	OdorRactor ,TGSC
1,6-Octadiene, 8-methoxy-	8-methoxyocta-1,6-diene	COCC=CCCCC=C	green fatty violet fruity	TGSC
Benzyl methyl ether	methoxymethylbenzene	COCC1=CC=CC=C1	metallic fruity ethereal ylang green	Flavornet, TGSC,OdoRactor
			floral hyacinth	
				OdorRactor ,TGSC
Pyrazine, methoxymethyl-	2-(methoxymethyl)pyrazine	COCC1=NC=CN=C1		TGSC
(2-Methoxyethyl)benzene	2-methoxyethylbenzene	COCCC1=CC=CC=C1	green floral jasmine metallic rose	OdorRactor ,TGSC
2-(2-Methoxyethoxy)ethanol	2-(2-methoxyethoxy)ethanol	COCCOCCO	mild musty pleasant ethereal	SuperScent, TGSC, Pubchem
	methoxymethoxycyclododecane	COCOC1CCCCCCCCCC1	woody cedar amber ambergis dry	OdorRactor ,TGSC
Methanethiol	methanethiol	CS	sulfurous gasoline garlic decomposing cabbage vegetable oily alliaceous eggy creamy savory alcoholic powerful unpleasant disagreeable pungent decayed solvent	Flavornet, AOD, TGSC, Pubchem
Dimethyl sulfone	methylsulfonylmethane	CS(=O)(=O)C	sulfurous burnt	Flavornet
Dimethyl sulfoxide	methylsulfinylmethane	CS(=0)C	buttery sulfurous garlic fatty oily	Sigma Aldrich, TGSC,
			cheese mushroom salty oyster	PubChem
Dimethyl sulfide	methylsulfanylmethane	CSC	green sulfurous onion sweet corn vegetable cabbage tomato radish creamy fishy seafood berry fruity potato unpleasant rotten vegetables rotten	Sigma Aldrich, TGSC, Pubchem
Methyl thiocyanate	methyl thiocyanate	CSC#N	sulfurous onion	Flavornet, TGSC, Pubchem
S-Methyl thiobenzoat	S -methyl benzenecarbothioate	CSC(=0)C1=CC=CC=C1	sulfurous cabbage garlic potato vegetable fermented cheese milky	OdorRactor ,TGSC, Flavorbase
Methyl 2-thiofuroate	S -methyl furan-2-carbothioate	CSC(=O)C1=CC=CO1	creamy sulfurous milky cooked onion fried alliaceous	Sigma Aldrich, TGSC, Pubchem, OdoRactor
Tris(methylthio)methane	tris(methylsulfanyl)methane	CSC(SC)SC	sulfurous earthy mushroom musty truffle	Sigma Aldrich, TGSC, OdoRactor
Thioanisole	methylsulfanylbenzene	CSC1=CC=CC=C1	sulfurous solvent spicy woody sawdust pungent	Sigma Aldrich, TGSC
2-(Methylthio)phenol	2-methylsulfanylphenol	CSC1=CC=CC=C10	meaty onion garlic sulfurous eggy	OdorRactor ,TGSC
	2-methylsulfanylpyrazine 2-methylsulfanyl-1,3- benzothiazole	CSC1=NC=CN=C1 CSC1=NC2=CC=CC=C2S1	corn nutty sulfurous ethereal fatty woody smoky	OdorRactor ,TGSC TGSC
2-(Methylthiomethyl)-3- phenylpropenal	(E)-2-(methylsulfanylmethyl)-3- phenylprop-2-enal	CSCC(=CC1=CC=CC=C1)C=0	green weedy brocolli green bean vegetable sauerkraut kimchi cabbage green onion	OdorRactor ,TGSC
Allyl methyl sulfide	3-methylsulfanylprop-1-ene	CSCC=C	alliaceous garlic onion sulfurous	OdorRactor ,TGSC
(Methylthio)acetaldehyde	2-methylsulfanylacetaldehyde	CSCC=O	sulfurous vegetable onion garlic mustard nutty potato	OdorRactor ,TGSC
Benzyl methyl sulfide	methylsulfanylmethylbenzene	CSCC1=CC=CC=C1	roasted burnt beefy pork lamb chicken	OdorRactor ,TGSC
Furfuryl methyl sulfide	2-(methylsulfanylmethyl)furan	CSCC1=CC=CO1	coffee onion garlic sulfurous pungent vegetable horseradish alliaceous radish mustard	Sigma Aldrich, TGSC, Flavorbase, OdoRactor
3- (Methylthio)methylthiophene	3- (methylsulfanylmethyl)thiophene	CSCC1=CSC=C1	cooked roasted dairy sulfurous allium watercress truffle mushroom onion savory	OdorRactor ,TGSC, Flavorbase
L-Methionylglycine	tic acid		savory meaty cheese	TGSC
DL-Methionine	2-amino-4-methylsulfanylbutanoic acid	CSCCC(C(=O)O)N	sulfurous acidic	Sigma Aldrich
5-(Methylthio)-2- [(methylthio)methyl]-2- pentenal	$(E\)$ -5-methylsulfanyl-2- (methylsulfanylmethyl)pent-2-enal	CSCCC=C(CSC)C=O	meaty potato cabbage vegetable sweet	Flavorbase
	3a,4,5,6,7,7a- hexahydro-5-methoxy- 1-Methoxyindan Cyclododecane, methoxy- 1,6-Octadiene, 8-methoxy- Benzyl methyl ether 2-(Methoxymethyl)furan Pyrazine, methoxymethyl- (2-Methoxyethyl)benzene 2-(2-Methoxyethoxy)ethanol (Methoxymethoxy)cyclodode cane Methanethiol Dimethyl sulfone Dimethyl sulfone Dimethyl sulfore Dimethyl sulfore Tris(methylthio)methane Thioanisole 2-(Methylthio)phenol 2-(Methylthio)benzothiazole 2-(Methylthio)benzothiazole 2-(Methylthio)benzothiazole 2-(Methylthio)benzothiazole 3-(Methylthio)acetaldehyde Benzyl methyl sulfide Furfuryl methyl sulfide Furfuryl methyl sulfide Furfuryl methyl sulfide 5-(Methylthio)penol L-Methionipelyl-2- [(methylthio)-2-	3a-4s,5,6,7,7a- hexahydro-5- methoxy- 1-Methoxyindan	3a.4.5.6.7.a hexalydro-5- methoxy- 1-Methoxyindan 1-methoxy-2.3-dillydro-1H -	3-a/se 3-a/se 3-a/se 3-a/se 3-a/se 3-a/se 3-a/se 3-a/se 3-a/se 3-a/se 3-a/se 3-a/se 3-a/se 3-a/se 3-a/se 3-a/se 3-a/se 3-a/se 3-a/se 3-a/se 3-a/se 3-a/se 3-a/se 3-a/se 3-a/se 3-a/se 3-a/se 3-a/se 3-a/se 3-a/se 3-a/se 3-a/se 3-a/se 3-a/se 3-a/se 3-a/se 3-a/se 3-a/se 3-a/se 3-a/se 3-a/se 3-a/se 3-a/se 3-a/se 3-a/se 3-a/se 3-a/se 3-a/se 3-a/se 3-a/se 3-a/se 3-a/se 3-a/se 3-a/se 3-a/se 3-a/se 3-a/se 3-a/se 3-a/se 3-a/se 3-a/se 3-a/se 3-a/se 3-a/se 3-a/se 3-a/se 3-a/se 3-a/se 3-a/se 3-a/se 3-a/se 3-a/se 3-a/se 3-a/se 3-a/se 3-a/se 3-a/se 3-a/se 3-a/se 3-a/se 3-a/se 3-a/se 3-a/se 3-a/se 3-a/se 3-a/se 3-a/se 3-a/se 3-a/se 3-a/se 3-a/se 3-a/se 3-a/se 3-a/se 3-a/se 3-a/se 3-a/se 3-a/se 3-a/se 3-a/se 3-a/se 3-a/se 3-a/se 3-a/se 3-a/se 3-a/se 3-a/se 3-a/se 3-a/se 3-a/se 3-a/se 3-a/se 3-a/se 3-a/se 3-a/se 3-a/se 3-a/se 3-a/se 3-a/se 3-a/se 3-a/se 3-a/se 3-a/se 3-a/se 3-a/se 3-a/se 3-a/se 3-a/se 3-a/se 3-a/se 3-a/se 3-a/se 3-a/se 3-a/se 3-a/se 3-a/se 3-a/se 3-a/se 3-a/se 3-a/se 3-a/se 3-a/se 3-a/se 3-a/se 3-a/se 3-a/se 3-a/se 3-a/se 3-a/se 3-a/se 3-a/se 3-a/se 3-a/se 3-a/se 3-a/se 3-a/se 3-a/se 3-a/se 3-a/se 3-a/se 3-a/se 3-a/se 3-a/se 3-a/se 3-a/se 3-a/se 3-a/se 3-a/se 3-a/se 3-a/se 3-a/se 3-a/se 3-a/se 3-a/se 3-a/se 3-a/se 3-a/se 3-a/se 3-a/se 3-a/se 3-a/se 3-a/se 3-a/se 3-a/se 3-a/se 3-a/se 3-a/se 3-a/se 3-a/se 3-a/se 3-a/se 3-a/se 3-a/se 3-a/se 3-a/se 3-a/se 3-a/se 3-a/se 3-a/se 3-a/se 3-a/se 3-a/se 3-a/se 3-a/se 3-a/se 3-a/se 3-a/se 3-a/se 3-a/se 3-a/se 3-a/se 3-a/se 3-a/se 3-a/se 3-a/se 3-a/se 3-a/se 3-a/se 3-a/se 3-a/se 3-a/se 3-a/se 3-a/se 3-a/se 3-a/se 3-a/se 3-a/se 3

3998	3- (Methylthio)propionaldehyde	3-methylsulfanylpropanal	CSCCC=O	cooked potato pungent beefy cheese creamy fishy green meaty oily fruity nutty peanut sulfurous tomato potato musty earthy vegetable yeasty bready limburger savory brothy onion malty	Sigma Aldrich, Flavorbase, TGSC, OdoRactor
3999	4 (Mothylthio)hutanal	4 mothylaulfanylhutanal	CSCCCC-O	cabbage garlic sulfurous	OdorRactor ,TGSC
4000	4-(Methylthio)butanal 5-	4-methylsulfanylbutanal 5-methylsulfanylpentanenitrile	CSCCCC=O CSCCCCC#N	brocolli cabbage	Flavornet, TGSC
4000	(Methylsulfanyl)pentanenitril	3-methylsunanylpentanemtrie	CSCCCC#IN	brocom cabbage	Flavoriet, 105C
4001	1-Isothiocyanato-6- (methylthio)hexane	1-isothiocyanato-6- methylsulfanylhexane	CSCCCCCN=C=S	radish sweet fatty mild pungent horseradish	OdorRactor ,TGSC
4002	Berteroin	1-isothiocyanato-5- methylsulfanylpentane	CSCCCCN=C=S	cabbage radish	Flavornet, TGSC, OdoRactor
4003	Erucin	1-isothiocyanato-4- methylsulfanylbutane	CSCCCCN=C=S	cabbage radish pungent	Flavornet, Flavorbase, TGSC
4004	4-(Methylthio)buta	4-methylsulfanylbutan-1-ol	CSCCCCO	cabbage sulfurous garlic potato green alliaceous vegetable	Sigma Aldrich, TGSC, Odoractor
4005	3-Methylthiopropylamine	3-methylsulfanylpropan-1-amine	CSCCCN	sulfurous vegetable ripe cheese	OdorRactor ,TGSC
4006	3-(Methylthio)propyl isothiocyanate	1-isothiocyanato-3- methylsulfanylpropane	CSCCCN=C=S	green sulfurous earthy vegetable horseradish rooty metallic pungent radish	Sigma Aldrich, TGSC, OdoRactor
4007	Methionol	3-methylsulfanylpropan-1-ol	CSCCCO	green meaty earthy sulfurous sweet potato onion vegetable soupy savory cooked	Sigma Aldrich, TGSC,OdoRactor
4008	3-(Methylthio)propyl mercaptoacetate	3-methylsulfanylpropyl 2- sulfanylacetate	CSCCCOC(=0)CS	radish nutty meaty fatty lettuce creamy brothy savory alliaceous onion	TGSC, Flavorbase
4009	2-(Methylthio)ethanol	2-methylsulfanylethanol	CSCCO	meaty sulfurous	Sigma Aldrich, TGSC, OdoRactor
4010	1,2-Bis(methylthio)ethane	1,2-bis(methylsulfanyl)ethane	CSCCSC	sulfurous dairy	OdorRactor ,TGSC
4011	Methylthiomethylmercaptan	methylsulfanylmethanethiol	CSCS	pungent sulfurous	AOD
4012	Bis(methylthio)methane	bis(methylsulfanyl)methane	CSCSC	cheese horseradish spicy earthy sulfurous garlic mushroom green pungent metallic alliaceous mustard	Sigma Aldrich, TGSC, OdoRactor
4013	2,4,6-Trithiaheptane	methylsulfanyl(methylsulfanylmet hylsulfanyl)meth ane	CSCSCSC	sulfurous cooked roasted onion leek cress radish horseradish	OdorRactor ,TGSC, Flavorbase
4014	2,3,5-Trithiahexane	(methyldisulfanyl)- methylsulfanylmethane	CSCSSC	sulfurous onion cabbage burnt rubber garlic burnt	SuperScent, TGSC, Flavorbase, Odoractor
4015	S-Methyl methanethiosulfonate	methylsulfonylsulfanylmethane	CSS(=O)(=O)C	sulfurous pungent roasted	TGSC
4016	Dimethyl disulfide	(methyldisulfanyl)methane	CSSC	green putrid cabbage onion sulfurous vegetable garlic corn rotten cabbage	Sigma Aldrich, TGSC, OdoRactor, Pubchem,OdoRactor
4017	Methyl phenyl disulfide	(methyldisulfanyl)benzene	CSSC1=CC=CC=C1	pungent radish turnip	OdorRactor ,TGSC
4018	Allyl methyl disulfide	3-(methyldisulfanyl)prop-1-ene	CSSCC=C	alliaceous garlic onion green sulfurous	OdorRactor ,TGSC
4019	Benzyl methyl disulfide	(methyldisulfanyl)methylbenzene	CSSCC1=CC=CC=C1	sulfurous cabbage vegetable green metallic	OdorRactor ,TGSC
4020	Methyl furfuryl disulfide	2-[(methyldisulfanyl)methyl]furan	CSSCC1=CC=CO1	caramel coffee fishy meaty vegetable fruity nutty sulfurous smoky alliaceous roasted roasted coffee roasted meat eggy onion garlic	Sigma Aldrich, TGSC, OdoRactor
4021	Dimethyl trisulfide	(methyltrisulfanyl)methane	CSSSC	alliaceous meaty savory cooked onion sulfurous fishy cabbage eggy vegetable fresh green onion marshy swampy	Sigma Aldrich, TGSC, OdoRactor
4022	Allyl methyl trisulfide	3-(methyltrisulfanyl)prop-1-ene	CSSSCC=C	sulfurous alliaceous creamy garlic onion	SuperScent, TGSC, OdoRactor
4023	Dimethyl tetrasulfide	(methyltetrasulfanyl)methane	CSSSSC	cabbage sulfurous garlic meaty	Flavornet
4024	1,1,6-Trimethyltetralin	4,4,7-trimethyl-2,3-dihydro-1 <i>H</i> - naphthalene	LTMQZVLXCLQPCT- UHFFFAOYSA-N	woody camphoraceous naphthyl fruity	OdorRactor ,Flavorbase
4025	Ammonia	azane	N	ammonical pungent suffocating sharp cloying repellent irritating	SuperScent, TGSC, Pubchem
4026	Chlorimide	???????	N(Cl)Cl	swimming pool chlorinous	
4027	Chloramine	??????	NCI	strong pungent	Pubchem
4028	Magnesium phosphate hydrate	trimagnesium;diphosphate;hydrate]P(=O)([O-])[O-	faint	Sigma Aldrich
	in article].[Mg+2].[Mg+2].[Mg+2]		
4029	2-(4-Methyl-5-thiazolyl)ethyl octanoate	2-(4-methyl-1,3-thiazol-5-yl)ethyl octanoate].[Mg+2].[Mg+2] OGJATLSJIMPQBD- UHFFFAOYSA-N	roasted nutty	TGSC

4031	Sodium 3-methyl-2- oxobutanoate	sodium;3-methyl-2-oxobutanoate	vCC(C)C(=O)C(=O)[O-].[Na+]	fruity	Sigma Aldrich
4032	2-(1-Methylpropyl)-1- vinylcyclohexyl acetate		vCCC(C)C1CCCCC1(C=C)OC(= O)C	woody amber dry ambrette	OdorRactor ,TGSC
4033	Diisopropyl adipate	dipropan-2-yl hexanedioate	ZDQWESQEGGJUCH- UHFFFAOYSA-N	estery fatty sour	OdorRactor ,TGSC
4034	Diammonium sulfide	diazanium;sulfide	[NH4+].[NH4+].[S-2]	sulfurous eggy ammonical	Sigma Aldrich, TGSC, Pubchem
4035	Ammonium hydroxide	azanium;hydroxide	[NH4+].[OH-]	ammonical pungent suffocating	TGSC, Pubchem
4036	Ozone	ozone	[O-][O+]=O	characteristic pungent	Pubchem
4037	Ferrous sulfate	iron(2+);sulfate	[O-]S(=O)(=O)[O-].[Fe+2]	metallic	
4038	Propargyl alcohol	prop-2-yn-1-ol	C#CCO	floral geranium	TGSC,Pubchem, OdoRactor
4039	DL-Xylose	(2R, 3S, 4R)-2,3,4,5- tetrahydroxypentanal	C([C@H]([C@@H]([C@H](C=O)O)O)O) O	smoky woody sweet caramel	OdorRactor ,Flavorbase, TGSC
4040	Glucuronolactone	(2R)-2-[(2S ,3R ,4S)-3,4- dihydroxy-5-oxooxolan- 2-yl]-2-hydroxyacetaldehyde	C(=O)C(C1C(C(C(=O)O1)O)O)O	mentholic	TGSC

Table S2: Features used for the development of prediction models

Descriptor	Count
1D and 2 D Properties	1444

Fingerprint	Count	Fingerprii
MACCS fingerprint	166	Substructu
		fingerprint

Count 307

Sr. No		
1	Descriptor	Description Number of acidic groups. The list of acidic groups is defined by
1	nAcid	Number of acidic groups. The list of acidic groups is defined by these SMARTS "\$([O;H1]-[C,S,P]=O)", "\$([*;-;!\$(*~[*;+])])",
		" $\{(NH)(S(=O)=O)C(F)(F)F\}$ ", and " $\{(n1nnnc1)\}$ " originally
		presented in JOELib
	ALogP	Ghose-Crippen LogKow
-	ALogP2	Square of ALogP
	AMR apol	Molar refractivity Sum of the atomic polarizabilities (including implicit hydrogens)
	фог	Sum of the atomic polarizationaes (merating implicit hydrogens)
	naAromAtom	Number of aromatic atoms
	nAromBond	Number of aromatic bonds
	nAtom nHeavyAtom	Number of atoms Number of heavy atoms (i.e. not hydrogen)
	nH	Number of hydrogen atoms
	nB	Number of boron atoms
12	nC	Number of carbon atoms
12	NT	No. 1 and 6 miles and 6 miles and 6 miles and 6 miles and 6 miles and 6 miles and 6 miles and 6 miles and 6 miles and 6 miles and 6 miles and 6 miles and 6 miles and 6 miles and 6 miles and 6 miles and 6 miles and 6 miles and 6 miles and 6 miles and 6 miles and 6 miles and 6 miles and 6 miles and 6 miles and 6 miles and 6 miles and 6 miles and 6 miles and 6 miles and 6 miles and 6 miles and 6 miles and 6 miles and 6 miles and 6 miles and 6 miles and 6 miles and 6 miles and 6 miles and 6 miles and 6 miles and 6 miles and 6 miles and 6 miles and 6 miles and 6 miles and 6 miles and 6 miles and 6 miles and 6 miles and 6 miles and 6 miles and 6 miles and 6 miles and 6 miles and 6 miles and 6 miles and 6 miles and 6 miles and 6 miles and 6 miles and 6 miles and 6 miles and 6 miles and 6 miles and 6 miles and 6 miles and 6 miles and 6 miles and 6 miles and 6 miles and 6 miles and 6 miles and 6 miles and 6 miles and 6 miles and 6 miles and 6 miles and 6 miles and 6 miles and 6 miles and 6 miles and 6 miles and 6 miles and 6 miles and 6 miles and 6 miles and 6 miles and 6 miles and 6 miles and 6 miles and 6 miles and 6 miles and 6 miles and 6 miles and 6 miles and 6 miles and 6 miles and 6 miles and 6 miles and 6 miles and 6 miles and 6 miles and 6 miles and 6 miles and 6 miles and 6 miles and 6 miles and 6 miles and 6 miles and 6 miles and 6 miles and 6 miles and 6 miles and 6 miles and 6 miles and 6 miles and 6 miles and 6 miles and 6 miles and 6 miles and 6 miles and 6 miles and 6 miles and 6 miles and 6 miles and 6 miles and 6 miles and 6 miles and 6 miles and 6 miles and 6 miles and 6 miles and 6 miles and 6 miles and 6 miles and 6 miles and 6 miles and 6 miles and 6 miles and 6 miles and 6 miles and 6 miles and 6 miles and 6 miles and 6 miles and 6 miles and 6 miles and 6 miles and 6 miles and 6 miles and 6 miles and 6 miles and 6 miles and 6 miles and 6 miles and 6 miles and 6 miles and 6 miles and 6 miles and 6 miles and 6 miles and 6 miles and 6 miles and 6 miles and 6 miles and 6 miles and 6 miles and 6 miles
13	nN	Number of nitrogen atoms
14	nO	Number of oxygen atoms
15	nS	Number of sulphur atoms
16	nP	Number of phosphorus etems
10	III P	Number of phosphorus atoms
17	nF	Number of fluorine atoms
10	n C1	Number of chloring stoms
18	nCl	Number of chlorine atoms
19	nBr	Number of bromine atoms
	nI	Number of iodine atoms
	V	N 1 61 1 7 7 7 7 7 7 7 7 7 7 7 7 7 7 7 7
	nX ATS0m	Number of halogen atoms (F, Cl, Br, I, At, Uus)
	TY ISOIII	Broto-Moreau autocorrelation - lag 0 / weighted by mass
23	ATS1m	Broto-Moreau autocorrelation - lag 1 / weighted by mass
24	ATS2m	Broto-Moreau autocorrelation - lag 2 / weighted by mass
25	ATS3m	Proto Morony autocorrelation, log 2 / weighted by mass
23	A185III	Broto-Moreau autocorrelation - lag 3 / weighted by mass
26	ATS4m	Broto-Moreau autocorrelation - lag 4 / weighted by mass
27	ATS5m	Broto-Moreau autocorrelation - lag 5 / weighted by mass
28	ATS6m	Broto-Moreau autocorrelation - lag 6 / weighted by mass
	ATS7m	Broto-Moreau autocorrelation - lag 7 / weighted by mass
		The state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the s
30	ATS8m	Broto-Moreau autocorrelation - lag 8 / weighted by mass
21	A TEGO	
31	ATS0v	Broto-Moreau autocorrelation - lag 0 / weighted by van der Waals volumes
32	ATS1v	Broto-Moreau autocorrelation - lag 1 / weighted by van der
		Waals volumes
33	ATS2v	Broto-Moreau autocorrelation - lag 2 / weighted by van der
		Waals volumes
34	ATS3v	Broto-Moreau autocorrelation - lag 3 / weighted by van der
	,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,	Waals volumes
35	ATS4v	Broto-Moreau autocorrelation - lag 4 / weighted by van der
2.5	A FDG F	Waals volumes
36	ATS5v	Broto-Moreau autocorrelation - lag 5 / weighted by van der Waals volumes
37	ATS6v	Broto-Moreau autocorrelation - lag 6 / weighted by van der
		Waals volumes
38	ATS7v	Broto-Moreau autocorrelation - lag 7 / weighted by van der Waals volumes
30	ATS8v	Broto-Moreau autocorrelation - lag 8 / weighted by van der
	,	Waals volumes
40	ATS0e	Broto-Moreau autocorrelation - lag 0 / weighted by Sanderson
		electronegativities
41	ATS1e	Broto-Moreau autocorrelation - lag 1 / weighted by Sanderson
		electronegativities
	AFFCC	
42	ATS2e	Broto-Moreau autocorrelation - lag 2 / weighted by Sanderson
13	ATS3e	electronegativities Broto-Moreau autocorrelation - lag 3 / weighted by Sanderson
		electronegativities
44	ATS4e	Broto-Moreau autocorrelation - lag 4 / weighted by Sanderson
	A TEG 5	electronegativities
45	ATS5e	Broto-Moreau autocorrelation - lag 5 / weighted by Sanderson electronegativities
46	ATS6e	Broto-Moreau autocorrelation - lag 6 / weighted by Sanderson
		electronegativities
47	ATS7e	Broto-Moreau autocorrelation - lag 7 / weighted by Sanderson
		electronegativities
10	ATS8e	Broto-Moreau autocorrelation - lag 8 / weighted by Sanderson
48	AISOC	electronegativities
49	ATS0p	Broto-Moreau autocorrelation - lag 0 / weighted by
	·	polarizabilities
50	ATS1p	Broto-Moreau autocorrelation - lag 1 / weighted by
- 51	ATC2~	Proto Morony autocorrelation log 2 / weighted by
	ATS2p	Broto-Moreau autocorrelation - lag 2 / weighted by polarizabilities
51		IDOIAITZAUIILIES
	ATS3p	Broto-Moreau autocorrelation - lag 3 / weighted by
	ATS3p	X

Bit	
MACCSFP1	
MACCSFP2	
MACCSFP3	
MACCSFP4 MACCSFP5	
MACCSFP6	
MACCSFP7 MACCSFP8	
MACCSFP9	
MACCSFP10 MACCSFP11	
MACCSFP12	
MACCSFP13	
MACCSFP14	
MACCSFP15	
MACCSFP16	
MACCSFF10	
MACCSFP17	
MACCSFP18	
MACCSFP19	
MACCSFP20	
MACCSFP21	
MACCSFP22	
MACCSFP23	
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MACCSFP40	
MACCSFP41	
WACCSI I 41	
MACCSFP42	
MACCSFP43	
MACCSFP44	
MACCSFP45	
MACCSFP46	
MACCSFP47	
MACCSFP48	
MACCSFP49	
MACCSFP50	
MACCSFP51	
MACCSFP52	
WACCSIT 32	

		I
Bit SubFP1	Description Primary carbon	SMARTS [CX4H3][#6]
Suorti	i iiiiai y carbon	[CA4113][#0]
SubFP2	Canadam, ankan	(CV 41131/(1461)/(461
SubFP3	Secondary carbon Tertiary carbon	[CX4H2]([#6])[#6] [CX4H1]([#6])([#6])[#6]
SubFP4	Quaternary carbon	[CX4]([#6])([#6])([#6])[#6]
SubFP5	Alkene	[CX3;\$([H2]),\$([H1][#6]),\$(C([#6
])[#6])]=[CX3;\$([H2]),\$([H1][#6]) ,\$(C([#6])[#6])]
SubFP6	Alkyne	[CX2]#[CX2]
SubFP7 SubFP8	Allene Alkylchloride	[CX3]=[CX2]=[CX3] [CIX1][CX4]
SubFP9	Alkylfluoride	[FX1][CX4]
SubFP10	Alkylbromide	[BrX1][CX4]
SubFP11 SubFP12	Alkyliodide Alcohol	[IX1][CX4] [OX2H][CX4;!\$(C([OX2H])[O,S,
Subit 12	Alcohol	#7,#15])]
SubFP13	Primary alcohol	[OX2H][CX4H2;!\$(C([OX2H])[O,
SubFP14	Secondary alcohol	S,#7,#15])] [OX2H][CX4H;!\$(C([OX2H])[O,S
	seesman areanar	[,#7,#15])]
SubFP15	Tertiary alcohol	[OX2H][CX4D4;!\$(C([OX2H])[O,
SubFP16	Dialkylether	S,#7,#15])] [OX2]([CX4;!\$(C([OX2])[O,S,#7,
		#15,F,Cl,Br,I])])[CX4;!\$(C([OX2]
SubFP17	Dialkylthioether)[O,S,#7,#15])] [SX2]([CX4;!\$(C([OX2])[O,S,#7,
SUUTETI	Diarkylinoether	#15,F,Cl,Br,I])])[CX4;!\$(C([OX2])
)[O,S,#7,#15])]
SubFP18	Alkylarylether	[OX2](c)[CX4;!\$(C([OX2])[O,S,# 7,#15,F,Cl,Br,I])]
SubFP19	Diarylether	[c][OX2][c]
SubFP20	Alkylarylthioether	[SX2](c)[CX4;!\$(C([OX2])[O,S,#
SubFP21	Diarylthioether	7,#15,F,Cl,Br,I])] [c][SX2][c]
SubFP22	Oxonium	[O+;!\$([O]~[!#6]);!\$([S]*~[#7,#8,
		#15,#16])]
SubFP23	Amine	[NX3+0,NX4+;!\$([N]~[!#6]);!\$([N]*~[#7,#8,#15,#16])]
SubFP24	Primary aliph amine	[NX3H2+0,NX4H3+;!\$([N][!C]);!
G 1 FD25	G 1 1:1 :	\$([N]*~[#7,#8,#15,#16])]
SubFP25	Secondary aliph amine	[NX3H1+0,NX4H2+;!\$([N][!C]);! \$([N]*~[#7,#8,#15,#16])]
SubFP26	Tertiary aliph amine	[NX3H0+0,NX4H1+;!\$([N][!C]);!
SubFP27	Quaternary aliph ammonium	\$([N]*~[#7,#8,#15,#16])] [NX4H0+;!\$([N][!C]);!\$([N]*~[#7
SUUFF27	Quaternary ampir animomum	[NA4H0+,:\$([N][:C]),:\$([N] ~[#/],#8,#15,#16])]
SubFP28	Primary arom amine	[NX3H2+0,NX4H3+]c
SubFP29	Secondary arom amine	[NX3H1+0,NX4H2+;!\$([N][!c]);!\$ ([N]*~[#7,#8,#15,#16])]
SubFP30	Tertiary arom amine	[NX3H0+0,NX4H1+;!\$([N][!c]);!\$
G 1 FD21		([N]*~[#7,#8,#15,#16])]
SubFP31	Quaternary arom ammonium	[NX4H0+;!\$([N][!c]);!\$([N]*~[#7, #8,#15,#16])]
SubFP32	Secondary mixed amine	[NX3H1+0,NX4H2+;\$([N]([c])[C]
SubFP33	Tertiary mixed amine);!\$([N]*~[#7,#8,#15,#16])] [NX3H0+0,NX4H1+;\$([N]([c])([C
])[#6]);!\$([N]*~[#7,#8,#15,#16])]
SubFP34	Quaternary mixed ammonium	 [NX4H0+;\$([N]([c])([C])[#6][#6])
	Quaternary manea animientani	;!\$([N]*~[#7,#8,#15,#16])]
SubFP35	Ammonium	[N+;!\$([N]~[!#6]);!\$(N=*);!\$([N]*
SubFP36	Alkylthiol	~[#7,#8,#15,#16])] [SX2H][CX4;!\$(C([SX2H])~[O,S,
		#7,#15])]
SubFP37	Dialkylthioether	[SX2]([CX4;!\$(C([SX2])[O,S,#7,# 15,F,Cl,Br,I])])[CX4;!\$(C([SX2])[
		O,S,#7,#15])]
SubFP38	Alkylarylthioether	[SX2](c)[CX4;!\$(C([SX2])[O,S,#7
SubFP39	Disulfide	,#15])] [SX2D2][SX2D2]
SubFP40	1,2-Aminoalcohol	[OX2H][CX4;!\$(C([OX2H])[O,S, #7,#15,F,Cl,Br,I])][CX4;!\$(C([N])
		[O,S,#7,#15])][NX3;!\$(NC=[O,S,
C-1-FD41	1.2 D'-1	N])]
SubFP41	1,2-Diol	[OX2H][CX4;!\$(C([OX2H])[O,S, #7,#15])][CX4;!\$(C([OX2H])[O,S
		,#7,#15])][OX2H]
SubFP42	1,1-Diol	[OX2H][CX4;!\$(C([OX2H])([OX 2H])[O,S,#7,#15])][OX2H]
SubFP43	Hydroperoxide	[OX2H][OX2]
C 1 ED44	D	LONADALIONADAL
SubFP44	Peroxo	[OX2D2][OX2D2]
SubFP45	Organolithium compounds	[LiX1][#6,#14]
SubFP46	Organomagnesium	[MgX2][#6,#14]
54011 10	compounds	[[11g112][[10],[11]]
SubFP47	Organometallic compounds	[!#1;!#5;!#6;!#7;!#8;!#9;!#14;!#15; !#16;!#17;!#33;!#34;!#35;!#52;!#5
		3;!#85]~[#6;!-]
SubFP48	Aldehyde	[\$([CX3H][#6]),\$([CX3H2])]=[O
SubFP49	Ketone	X1] [#6][CX3](=[OX1])[#6]
SubFP50	Thioaldehyde	[\$([CX3H][#6]),\$([CX3H2])]=[SX 1]
SubFP51	Thioketone	[#6][CX3](=[SX1])[#6]
SubFP52	Imine	[NX2;\$([N][#6]),\$([NH]);!\$([N][C
		X3]=[#7,#8,#15,#16])]=[CX3;\$([
		CH2]),\$([CH][#6]),\$([C]([#6])[#6])]
L		l ₁₁

53	ATS4p	Broto-Moreau autocorrelation - lag 4 / weighted by polarizabilities	MACCSFP53
54	ATS5p	Broto-Moreau autocorrelation - lag 5 / weighted by	MACCSFP54
		polarizabilities	
55	ATS6p	Broto-Moreau autocorrelation - lag 6 / weighted by polarizabilities	MACCSFP55
56	ATS7p	Broto-Moreau autocorrelation - lag 7 / weighted by polarizabilities	MACCSFP56
57	ATS8p	Broto-Moreau autocorrelation - lag 8 / weighted by	MACCSFP57
37	Атзор	polarizabilities	WACCSFF3/
58	ATS0i	Broto-Moreau autocorrelation - lag 0 / weighted by first ionization potential	MACCSFP58
59	ATS1i	Broto-Moreau autocorrelation - lag 1 / weighted by first ionization potential	MACCSFP59
60	ATS2i	Broto-Moreau autocorrelation - lag 2 / weighted by first ionization potential	MACCSFP60
61	ATS3i	Broto-Moreau autocorrelation - lag 3 / weighted by first	MACCSFP61
62	ATS4i	ionization potential Broto-Moreau autocorrelation - lag 4 / weighted by first ionization potential	MACCSFP62
63	ATS5i	Broto-Moreau autocorrelation - lag 5 / weighted by first ionization potential	MACCSFP63
64	ATS6i	Broto-Moreau autocorrelation - lag 6 / weighted by first	MACCSFP64
		ionization potential	
65	ATS7i	Broto-Moreau autocorrelation - lag 7 / weighted by first ionization potential	MACCSFP65
	A maga:		14.665-14
66	ATS8i	Broto-Moreau autocorrelation - lag 8 / weighted by first ionization potential	MACCSFP66
67	ATS0s	Broto-Moreau autocorrelation - lag 0 / weighted by I-state	MACCSFP67
68	ATS1s	Broto-Moreau autocorrelation - lag 1 / weighted by I-state	MACCSFP68
69	ATS2s	Broto-Moreau autocorrelation - lag 2 / weighted by I-state	MACCSFP69
	ATS3s ATS4s	Broto-Moreau autocorrelation - lag 3 / weighted by I-state Broto-Moreau autocorrelation - lag 4 / weighted by I-state	MACCSFP70 MACCSFP71
	ATS5s	Broto-Moreau autocorrelation - lag 5 / weighted by I-state	MACCSFP72
73	ATS6s	Broto-Moreau autocorrelation - lag 6 / weighted by I-state	MACCSFP73
74	ATS7s	Broto-Moreau autocorrelation - lag 7 / weighted by I-state	MACCSFP74
75	ATS8s	Broto-Moreau autocorrelation - lag 8 / weighted by I-state	MACCSFP75
76	AATS0m	Average Broto-Moreau autocorrelation - lag 0 / weighted by mass	MACCSFP76
77	AATS1m	Average Broto-Moreau autocorrelation - lag 1 / weighted by	MACCSFP77
70	A A TS2	mass	MACCCED70
/8	AATS2m	Average Broto-Moreau autocorrelation - lag 2 / weighted by mass	MACCSFP78
79	AATS3m	Average Broto-Moreau autocorrelation - lag 3 / weighted by mass	MACCSFP79
80	AATS4m	Average Broto-Moreau autocorrelation - lag 4 / weighted by	MACCSFP80
91	AATS5m	mass Average Broto-Moreau autocorrelation - lag 5 / weighted by	MACCSFP81
		mass	
82	AATS6m	Average Broto-Moreau autocorrelation - lag 6 / weighted by mass	MACCSFP82
83	AATS7m	Average Broto-Moreau autocorrelation - lag 7 / weighted by	MACCSFP83
84	AATS8m	mass Average Broto-Moreau autocorrelation - lag 8 / weighted by mass	MACCSFP84
85	AATS0v	Average Broto-Moreau autocorrelation - lag 0 / weighted by van der Waals volumes	MACCSFP85
86	AATS1v	Average Broto-Moreau autocorrelation - lag 1 / weighted by van	MACCSFP86
87	AATS2v	der Waals volumes Average Broto-Moreau autocorrelation - lag 2 / weighted by van der Waals volumes	MACCSFP87
88	AATS3v	Average Broto-Moreau autocorrelation - lag 3 / weighted by van	MACCSFP88
	AATS4v	der Waals volumes Average Broto-Moreau autocorrelation - lag 4 / weighted by van der Waals volumes	MACCSFP89
90	AATS5v	Average Broto-Moreau autocorrelation - lag 5 / weighted by van der Waals volumes	MACCSFP90
01	AATS6v	Average Broto-Moreau autocorrelation - lag 6 / weighted by van	MACCSFP91
	AATS7v	der Waals volumes Average Broto-Moreau autocorrelation - lag 7 / weighted by van der Waals volumes	MACCSFP92
93	AATS8v	Average Broto-Moreau autocorrelation - lag 8 / weighted by van	MACCSFP93
04	AATS0e	der Waals volumes Average Broto-Moreau autocorrelation - lag 0 / weighted by	MACCSFP94
74		Sanderson electronegativities	1711 ICCOI I /T

SubFP53	Immonium	[NX3+;!\$([N][!#6]);!\$([N][CX3]=
SubFP54	Oxime	[#7,#8,#15,#16])] [NX2](=[CX3;\$([CH2]),\$([CH][#
		6]),\$([C]([#6])[#6])])[OX2H]
SubFP55	Oximether	[NX2](=[CX3;\$([CH2]),\$([CH][# 6]),\$([C]([#6])[#6])])[OX2][#6;!\$(C=[#7,#8])]
SubFP56	Acetal	[OX2]([#6;!\$(C=[O,S,N])])[CX4;! \$(C(O)(O)[!#6])][OX2][#6;!\$(C=[O,S,N])]
SubFP57	Hemiacetal	[OX2H][CX4;!\$(C(O)(O)[!#6])][O X2][#6;!\$(C=[O,S,N])]
SubFP58	Aminal	[NX3v3;!\$(NC=[#7,#8,#15,#16])]([#6])[CX4;!\$(C(N)(N)[!#6])][NX3 v3;!\$(NC=[#7,#8,#15,#16])][#6]
SubFP59	Hemiaminal	[NX3v3;!\$(NC=[#7,#8,#15,#16])](
SubFP60	Thioacetal	[#6])[CX4;!\$(C(N)(N)[!#6])][OX2 H] [SX2]([#6;!\$(C=[O,S,N])])[CX4;!
5401100	Timodectui	\$(C(S)(S)[!#6])][SX2][#6;!\$(C=[O ,S,N])]
SubFP61	Thiohemiacetal	[SX2]([#6;!\$(C=[O,S,N])])[CX4;! \$(C(S)(S)[!#6])][OX2H]
SubFP62	Halogen acetal like	[NX3v3,SX2,OX2;!\$(*C=[#7,#8,# 15,#16])][CX4;!\$(C([N,S,O])([N,S ,O])[!#6])][FX1,ClX1,BrX1,IX1]
SubFP63	Acetal like	[NX3v3,SX2,OX2;!\$(*C=[#7,#8,#
		15,#16])][CX4;!\$(C([N,S,O])([N,S,O])[!#6])][FX1,CIX1,BrX1,IX1,N X3v3,SX2,OX2;!\$(*C=[#7,#8,#15
SubFP64	Halogenmethylen ester and	,#16])] [NX3v3,SX2,OX2;\$(**=[#7,#8,#1
	similar	5,#16])][CX4;!\$(C([N,S,O])([N,S,O])([N,S,O])[!#6])][FX1,ClX1,BrX1,IX1]
SubFP65	NOS methylen ester and	[NX3v3,SX2,OX2;\$(**=[#7,#8,#1
G LEDGG	similar	5,#16])][CX4;!\$(C([N,S,O])([N,S,O])([N,S,O])[!#6])][NX3v3,SX2,OX2;!\$(*C=[#7,#8,#15,#16])]
SubFP66	Hetero methylen ester and similar	[NX3v3,SX2,OX2;\$(**=[#7,#8,#1 5,#16])][CX4;!\$(C([N,S,O])([N,S,O])[!#6])][FX1,ClX1,BrX1,IX1,N
		X3v3,SX2,OX2;!\$(*C=[#7,#8,#15,#16])]
SubFP67	Cyanhydrine	[NX1]#[CX2][CX4;\$([CH2]),\$([C H]([CX2])[#6]),\$(C([CX2])([#6])[
SubFP68	Chloroalkene	#6])][OX2H] [CIX1][CX3]=[CX3]
SubFP69 SubFP70	Fluoroalkene Bromoalkene	[FX1][CX3]=[CX3] [BrX1][CX3]=[CX3]
SubFP71	Iodoalkene	[IX1][CX3]=[CX3]
SubFP72	Enol	[OX2H][CX3;\$([H1]),\$(C[#6])]=[CX3]
SubFP73	Endiol	[OX2H][CX3;\$([H1]),\$(C[#6])]=[CX3;\$([H1]),\$(C[#6])][OX2H]
SubFP74	Enolether	[OX2]([#6;!\$(C=[N,O,S])])[CX3;\$ ([H0][#6]),\$([H1])]=[CX3]
SubFP75	Enolester	[OX2]([CX3]=[OX1])[#6X3;\$([#6][#6]),\$([H1])]=[#6X3;!\$(C[OX2H])]
SubFP76	Enamine	[NX3;\$([NH2][CX3]),\$([NH1]([C X3])[#6]),\$([N]([CX3])([#6])[#6]) ;!\$([N]*=[#7,#8,#15,#16])][CX3;\$ ([CH]),\$([C][#6])]=[CX3]
SubFP77	Thioenol	[SX2H][CX3;\$([H1]),\$(C[#6])]=[
SubFP78	Thioenolether	CX3]
		[SX2]([#6;!\$(C=[N,O,S])])[CX3;\$ (C[#6]),\$([CH])]=[CX3]
SubFP79	Acylchloride	[CX3;\$([R0][#6]),\$([H1R0])](=[O X1])[ClX1]
SubFP80	Acylfluoride	[CX3;\$([R0][#6]),\$([H1R0])](=[O X1])[FX1]
SubFP81	Acylbromide	[CX3;\$([R0][#6]),\$([H1R0])](=[O X1])[BrX1]
SubFP82	Acyliodide	[CX3;\$([R0][#6]),\$([H1R0])](=[O X1])[IX1]
SubFP83	Acylhalide	[CX3;\$([R0][#6]),\$([H1R0])](=[O X1])[FX1,CIX1,BrX1,IX1]
SubFP84	Carboxylic acid	[CX3;\$([R0][#6]),\$([H1R0])](=[O X1])[\$([OX2H]),\$([OX1-])]
SubFP85	Carboxylic ester	[CX3;\$([R0][#6]),\$([H1R0])](=[O X1])[OX2][#6;!\$(C=[O,N,S])]
SubFP86	Lactone	[#6][#6X3R](=[OX1])[#8X2][#6;! \$(C=[O,N,S])]
SubFP87	Carboxylic anhydride	[CX3;\$([H0][#6]),\$([H1])](=[OX1])[#8X2][CX3;\$([H0][#6]),\$([H1])](=[OX1])
SubFP88	Carboxylic acid derivative	[\$([#6X3H0][#6]),\$([#6X3H])](=[!#6])[!#6]
SubFP89	Carbothioic acid	[CX3;!R;\$([C][#6]),\$([CH]);\$([C] (=[OX1])[\$([SX2H]),\$([SX1-])]),\$([C](=[SX1])[\$([OX2H]),\$([OX1-])])]
SubFP90	Carbothioic S ester	[CX3;\$([R0][#6]),\$([H1R0])](=[O X1])[SX2][#6;!\$(C=[O,N,S])]
SubFP91	Carbothioic S lactone	[#6][#6X3R](=[OX1])[#16X2][#6
SubFP92	Carbothioic O ester	;!\$(C=[O,N,S])] [CX3;\$([H0][#6]),\$([H1])](=[SX1
SubFP93	Carbothioic O lactone])[OX2][#6;!\$(C=[O,N,S])] [#6][#6X3R](=[SX1])[#8X2][#6;!
SubFP94	Carbothioic halide	\$(C=[O,N,S])] [CX3;\$([H0][#6]),\$([H1])](=[SX1
5uUIT 74	Caroonnoic nande])[FX1,ClX1,BrX1,IX1]

Societies declares particular	95	AATS1e	Average Broto-Moreau autocorrelation - lag 1 / weighted by	MACCSFP95
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Solution of communications Solution So				
Solution of communications Solution So	99	AATS5e	Average Broto-Moreau autocorrelation - lag 5 / weighted by	MACCSFP99
Sancheros of corromogrativities Average Brook Marrana autocorrelation - lag 7 / weighted by Average Brook Marrana autocorrelation - lag 8 / weighted by MACCSFP102 ANTS09 Average Brook Marrana autocorrelation - lag 1 / weighted by MACCSFP103 ANTS09 Average Brook Marrana autocorrelation - lag 1 / weighted by Podurabelities ANTS09 Average Brook Marrana autocorrelation - lag 2 / weighted by Podurabelities ANTS09 Average Brook Marrana autocorrelation - lag 1 / weighted by Podurabelities ANTS09 Average Brook Marrana autocorrelation - lag 6 / weighted by Podurabelities ANTS09 Average Brook Marrana autocorrelation - lag 6 / weighted by Podurabelities ANTS09 Average Brook Marrana autocorrelation - lag 6 / weighted by Podurabelities ANTS09 Average Brook Marrana autocorrelation - lag 6 / weighted by Podurabelities ANTS09 Average Brook Marrana autocorrelation - lag 6 / weighted by Podurabelities ANTS09 Average Brook Marrana autocorrelation - lag 7 / weighted by Podurabelities AVERAGE Prook Marrana autocorrelation - lag 8 / weighted by Podurabelities AVERAGE Prook Marrana autocorrelation - lag 8 / weighted by Podurabelities AVERAGE Prook Marrana autocorrelation - lag 8 / weighted by Podurabelities AVERAGE Prook Marrana autocorrelation - lag 9 / weighted by first Podurabelities AVERAGE Prook Marrana autocorrelation - lag 9 / weighted by first Prook ANTS01 Average Brook Marrana autocorrelation - lag 9 / weighted by first Prook ANTS01 Average Brook Marrana autocorrelation - lag 9 / weighted by first Prook ANTS01 Average Brook Marrana autocorrelation - lag 9 / weighted by first Prook ANTS01 Average Brook Marrana autocorrelation - lag 9 / weighted by first Prook ANTS01 Average Brook Marrana autocorrelation - lag 9 / weighted by first Prook ANTS01 Average Brook Marrana autocorrelation - lag 1 / weighted by first Prook ANTS01 Average Brook Marrana autocorrelation - lag 1 / weighted by first Prook ANTS01 Average Brook Marrana autocorrelation - lag 1 / weighted by first Proo			Sanderson electronegativities	
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Dolar Act S2p	103	AATSOP		WACCSTF 103
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Doc AATS0 Average Broot-Morean autocorrelation lag 3 / weighted by polarizabilities		•	polarizabilities	
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ionization potential 121 AATS0s Average Broto-Moreau autocorrelation - lag 0 / weighted by I-state 122 AATS1s Average Broto-Moreau autocorrelation - lag 1 / weighted by I-state 123 AATS2s Average Broto-Moreau autocorrelation - lag 2 / weighted by I-state 124 AATS3s Average Broto-Moreau autocorrelation - lag 3 / weighted by I-state 125 AATS4s Average Broto-Moreau autocorrelation - lag 4 / weighted by I-state 126 AATS5s Average Broto-Moreau autocorrelation - lag 4 / weighted by I-state MACCSFP125 MACCSFP125 MACCSFP125				
121 AATS0s Average Broto-Moreau autocorrelation - lag 0 / weighted by I-state 122 AATS1s Average Broto-Moreau autocorrelation - lag 1 / weighted by I-state 123 AATS2s Average Broto-Moreau autocorrelation - lag 2 / weighted by I-state 124 AATS3s Average Broto-Moreau autocorrelation - lag 3 / weighted by I-state 125 AATS4s Average Broto-Moreau autocorrelation - lag 4 / weighted by I-state 126 AATS5s Average Broto-Moreau autocorrelation - lag 5 / weighted by I-state MACCSFP125 MACCSFP125 MACCSFP125 MACCSFP126	120	AATS8i	• • • • • • • • • • • • • • • • • • • •	MACCSFP120
state 122 AATS1s Average Broto-Moreau autocorrelation - lag 1 / weighted by I-state 123 AATS2s Average Broto-Moreau autocorrelation - lag 2 / weighted by I-state 124 AATS3s Average Broto-Moreau autocorrelation - lag 3 / weighted by I-state 125 AATS4s Average Broto-Moreau autocorrelation - lag 4 / weighted by I-state 126 AATS5s Average Broto-Moreau autocorrelation - lag 5 / weighted by I-state MACCSFP125 MACCSFP125 MACCSFP125 MACCSFP126				
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state 123 AATS2s				
state 123 AATS2s				
state 123 AATS2s	122	AATS1s	Average Broto-Moreau autocorrelation - lag 1 / weighted by I-	MACCSFP122
state 124 AATS3s Average Broto-Moreau autocorrelation - lag 3 / weighted by I- state 125 AATS4s Average Broto-Moreau autocorrelation - lag 4 / weighted by I- state MACCSFP124 MACCSFP125 MACCSFP125 MACCSFP126				
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state 125 AATS4s Average Broto-Moreau autocorrelation - lag 4 / weighted by I- state MACCSFP125 MACCSFP126	123	IAA182s		MACCSFP123
state 125 AATS4s Average Broto-Moreau autocorrelation - lag 4 / weighted by I- state MACCSFP125 MACCSFP126	124	AATS3s	Average Broto-Moreau autocorrelation - lag 3 / weighted by I-	MACCSFP124
state 126 AATS5s Average Broto-Moreau autocorrelation - lag 5 / weighted by I- MACCSFP126	124			
state 126 AATS5s Average Broto-Moreau autocorrelation - lag 5 / weighted by I- MACCSFP126				
state 126 AATS5s Average Broto-Moreau autocorrelation - lag 5 / weighted by I- MACCSFP126	125	AATS4s	Average Broto-Moreau autocorrelation - lag 4 / weighted by L	MACCSFP125
	123			
state	126	AATS5s	Average Broto-Moreau autocorrelation - lag 5 / weighted by I-	MACCSFP126
			state	

SubFP95	Carbodithioic acid	[CX3;!R;\$([C][#6]),\$([CH]);\$([C]
SubFP96	Carbodithioic ester	(=[SX1])[SX2H])] [CX3;!R;\$([C][#6]),\$([CH]);\$([C] (=[SX1])[SX2][#6;!\$(C=[O,N,S])]
SubFP97	Carbodithiolactone)] [#6][#6X3R](=[SX1])[#16X2][#6;
SubFP98	Amide	!\$(C=[O,N,S])] [CX3;\$([R0][#6]),\$([H1R0])](=[O
		X1])[#7X3;\$([H2]),\$([H1][#6;!\$(C=[O,N,S])]),\$([#7]([#6;!\$(C=[O,
		N,S])])[#6;!\$(C=[O,N,S])])]
SubFP99	Primary amide	[CX3;\$([R0][#6]),\$([H1R0])](=[O X1])[NX3H2]
SubFP100	Secondary amide	[CX3;\$([R0][#6]),\$([H1R0])](=[O X1])[#7X3H1][#6;!\$(C=[O,N,S])]
SubFP101	Tertiary amide	[CX3;\$([R0][#6]),\$([H1R0])](=[O X1])[#7X3H0]([#6;!\$(C=[O,N,S])
SubFP102	Lactam])[#6;!\$(C=[O,N,S])] [#6R][#6X3R](=[OX1])[#7X3;\$([
		H1][#6;!\$(C=[O,N,S])]),\$([H0]([# 6;!\$(C=[O,N,S])])[#6;!\$(C=[O,N,S])])]
SubFP103	Alkyl imide	[#6X3;\$([H0][#6]),\$([H1])](=[OX 1])[#7X3H0]([#6])[#6X3;\$([H0][#
SubFP104	N hetero imide	6]),\$([H1])](=[OX1]) [#6X3;\$([H0][#6]),\$([H1])](=[OX
		1])[#7X3H0]([!#6])[#6X3;\$([H0][#6]),\$([H1])](=[OX1])
SubFP105	Imide acidic	[#6X3;\$([H0][#6]),\$([H1])](=[OX 1])[#7X3H1][#6X3;\$([H0][#6]),\$(
SubFP106	Thioamide	[H1])](=[OX1]) [\$([CX3;!R][#6]),\$([CX3H;!R])](=
		[SX1])[#7X3;\$([H2]),\$([H1][#6;!\$ (C=[O,N,S])]),\$([#7]([#6;!\$(C=[O, N,S])])[#6;!\$(C=[O,N,S])])]
SubFP107	Thiolactam	[#6R][#6X3R](=[SX1])[#7X3;\$([H1][#6;!\$(C=[O,N,S])]),\$([H0]([#
		6;!\$(C=[O,N,S])])[#6;!\$(C=[O,N,S])])]
SubFP108	Oximester	[#6X3;\$([H0][#6]),\$([H1])](=[OX 1])[#8X2][#7X2]=,:[#6X3;\$([H0](
		[#6])[#6]),\$([H1][#6]),\$([H2])]
SubFP109	Amidine	[NX3;!\$(NC=[O,S])][CX3;\$([CH]),\$([C][#6])]=[NX2;!\$(NC=[O,S])]
SubFP110	Hydroxamic acid	[CX3;\$([H0][#6]),\$([H1])](=[OX1])[#7X3;\$([H1]),\$([H0][#6;!\$(C=[O,N,S])])][\$([OX2H]),\$([OX1-])]
SubFP111	Hydroxamic acid ester	[CX3;\$([H0][#6]),\$([H1])](=[OX1
])[#7X3;\$([H1]),\$([H0][#6;!\$(C=[O,N,S])])][OX2][#6;!\$(C=[O,N,S]
SubFP112	Imidoacid)] [CX3R0;\$([H0][#6]),\$([H1])](=[N X2;\$([H1]),\$([H0][#6;!\$(C=[O,N,
		S])])]\$([OX2H]),\$([OX1-])]
SubFP113	Imidoacid cyclic	[#6R][#6X3R](=,:[#7X2;\$([H1]),\$ ([H0][#6;!\$(C=[O,N,S])])])[\$([OX
SubFP114	Imidoester	2H]),\$([OX1-])] [CX3R0;\$([H0][#6]),\$([H1])](=[N
		X2;\$([H1]),\$([H0][#6;!\$(C=[O,N, S])])])[OX2][#6;!\$(C=[O,N,S])]
SubFP115	Imidolactone	[#6R][#6X3R](=,:[#7X2;\$([H1]),\$ ([H0][#6;!\$(C=[O,N,S])])]OX2][
SubFP116	Imidothioacid	#6;!\$(C=[O,N,S])] [CX3R0;\$([H0][#6]),\$([H1])](=[N
Subitito	midounoacid	X2;\$([H1]),\$([H0][#6;!\$(C=[O,N, S])])]\$([SX2H]),\$([SX1-])]
SubFP117	Imidothioacid cyclic	[#6R][#6X3R](=,:[#7X2;\$([H1]),\$
		([H0][#6;!\$(C=[O,N,S])])])[\$([SX 2H]),\$([SX1-])]
SubFP118	Imidothioester	[CX3R0;\$([H0][#6]),\$([H1])](=[N X2;\$([H1]),\$([H0][#6;!\$(C=[O,N,
		S])])])[SX2][#6;!\$(C=[O,N,S])]
SubFP119	Imidothiolactone	[#6R][#6X3R](=,:[#7X2;\$([H1]),\$ ([H0][#6;!\$(C=[O,N,S])])])[SX2][#6;!\$(C=[O,N,S])]
SubFP120	Amidine	[#7X3v3;!\$(N([#6X3]=[#7X2])C= [O,S])][CX3R0;\$([H1]),\$([H0][#6
])]=[NX2v3;!\$(N(=[#6X3][#7X3]) C=[O,S])]
SubFP121	Imidolactam	[#6][#6X3R;\$([H0](=[NX2;!\$(N(= [#6X3][#7X3])C=[O,S]))]#7X3;!
		\$(N([#6X3]=[#7X2])C=[O,S])]),\$([H0](-
		[NX3;!\$(N([#6X3]=[#7X2])C=[O, S])])=,:[#7X2;!\$(N(=[#6X3][#7X3
SubFP122	Imidoylhalide])C=[O,S])]) [CX3R0;\$([H0][#6]),\$([H1])](=[N
		X2;\$([H1]),\$([H0][#6;!\$(C=[O,N, S])])])[FX1,ClX1,BrX1,IX1]
SubFP123	Imidoylhalide cyclic	[#6R][#6X3R](=,:[#7X2;\$([H1]),\$ ([H0][#6;!\$(C=[O,N,S])])]FX1,C
SubFP124	Amidrazone	[HU][#6;:\$(C=[U,N,S])])][FX1,C [X1,BrX1,IX1] [\$([\$([#6X3][#6]),\$([#6X3H])](=[
20011127	2 Mindrazone	#7X2v3])[#7X3v3][#7X3v3]),\$([\$ ([#6X3][#6]),\$([#6X3H])]([#7X3v
		3])=[#7X2v3][#7X3v3])]
SubFP125	Alpha aminoacid	[NX3,NX4+;!\$([N]~[!#6]);!\$([N]* ~[#7,#8,#15,#16])][C][CX3](=[O
SubFP126	Alpha hydroxyacid	[OX2H][C][CX3](=[OX1])[OX2H
		,OX1-]

127	AATS6s	Average Ducto Mousey entercompletion, leg 6 / weighted by I
127	AA130s	Average Broto-Moreau autocorrelation - lag 6 / weighted by I-state
128	AATS7s	Average Broto-Moreau autocorrelation - lag 7 / weighted by I-state
129	AATS8s	Average Broto-Moreau autocorrelation - lag 8 / weighted by I-state
130	ATSC0c	Centered Broto-Moreau autocorrelation - lag 0 / weighted by
131	ATSC1c	charges Centered Broto-Moreau autocorrelation - lag 1 / weighted by
	ATSC2c	charges Centered Broto-Moreau autocorrelation - lag 2 / weighted by charges
133	ATSC3c	Centered Broto-Moreau autocorrelation - lag 3 / weighted by
	ATSC4c	charges Centered Broto-Moreau autocorrelation - lag 4 / weighted by
	ATSC5c	charges Centered Broto-Moreau autocorrelation - lag 5 / weighted by
	ATSC6c	charges Centered Broto-Moreau autocorrelation - lag 6 / weighted by
		charges
	ATSC7c	Centered Broto-Moreau autocorrelation - lag 7 / weighted by charges
138	ATSC8c	Centered Broto-Moreau autocorrelation - lag 8 / weighted by charges
139	ATSC0m	Centered Broto-Moreau autocorrelation - lag 0 / weighted by
140	ATSC1m	mass Centered Broto-Moreau autocorrelation - lag 1 / weighted by mass
141	ATSC2m	Centered Broto-Moreau autocorrelation - lag 2 / weighted by
142	ATSC3m	mass Centered Broto-Moreau autocorrelation - lag 3 / weighted by
		mass
	ATSC4m	Centered Broto-Moreau autocorrelation - lag 4 / weighted by mass
144	ATSC5m	Centered Broto-Moreau autocorrelation - lag 5 / weighted by mass
145	ATSC6m	Centered Broto-Moreau autocorrelation - lag 6 / weighted by mass
146	ATSC7m	Centered Broto-Moreau autocorrelation - lag 7 / weighted by mass
147	ATSC8m	Centered Broto-Moreau autocorrelation - lag 8 / weighted by
148	ATSC0v	Centered Broto-Moreau autocorrelation - lag 0 / weighted by van
149	ATSC1v	der Waals volumes Centered Broto-Moreau autocorrelation - lag 1 / weighted by van der Waals volumes
150	ATSC2v	Centered Broto-Moreau autocorrelation - lag 2 / weighted by van der Waals volumes
151	ATSC3v	Centered Broto-Moreau autocorrelation - lag 3 / weighted by van der Waals volumes
152	ATSC4v	Centered Broto-Moreau autocorrelation - lag 4 / weighted by van
153	ATSC5v	der Waals volumes Centered Broto-Moreau autocorrelation - lag 5 / weighted by van
154	ATSC6v	der Waals volumes Centered Broto-Moreau autocorrelation - lag 6 / weighted by van
155	ATSC7v	der Waals volumes Centered Broto-Moreau autocorrelation - lag 7 / weighted by van der Waals volumes
156	ATSC8v	Centered Broto-Moreau autocorrelation - lag 8 / weighted by van der Waals volumes
157	ATSC0e	Centered Broto-Moreau autocorrelation - lag 0 / weighted by Sanderson electronegativities
158	ATSC1e	Centered Broto-Moreau autocorrelation - lag 1 / weighted by Sanderson electronegativities
159	ATSC2e	Centered Broto-Moreau autocorrelation - lag 2 / weighted by Sanderson electronegativities
160	ATSC3e	Centered Broto-Moreau autocorrelation - lag 3 / weighted by Sanderson electronegativities
161	ATSC4e	Centered Broto-Moreau autocorrelation - lag 4 / weighted by Sanderson electronegativities
162	ATSC5e	Centered Broto-Moreau autocorrelation - lag 5 / weighted by
163	ATSC6e	Sanderson electronegativities Centered Broto-Moreau autocorrelation - lag 6 / weighted by Sanderson electronegativities
164	ATSC7e	Sanderson electronegativities Centered Broto-Moreau autocorrelation - lag 7 / weighted by
165	ATSC8e	Sanderson electronegativities Centered Broto-Moreau autocorrelation - lag 8 / weighted by Sanderson electronegativities
166	ATSC0p	Sanderson electronegativities Centered Broto-Moreau autocorrelation - lag 0 / weighted by
167	ATSC1p	polarizabilities Centered Broto-Moreau autocorrelation - lag 1 / weighted by polarizabilities
168	ATSC2p	Centered Broto-Moreau autocorrelation - lag 2 / weighted by polarizabilities
169	ATSC3p	Centered Broto-Moreau autocorrelation - lag 3 / weighted by polarizabilities
170	ATSC4p	Centered Broto-Moreau autocorrelation - lag 4 / weighted by polarizabilities
171	ATSC5p	Centered Broto-Moreau autocorrelation - lag 5 / weighted by polarizabilities
172	ATSC6p	Centered Broto-Moreau autocorrelation - lag 6 / weighted by polarizabilities
173	ATSC7p	Centered Broto-Moreau autocorrelation - lag 7 / weighted by polarizabilities
	ATSC8p	Centered Broto-Moreau autocorrelation - lag 8 / weighted by

M	ACCSFP1	127
M	ACCSFP1	128
M	ACCSFP1	129
M	ACCSFP1	130
M	ACCSFP1	131
M	ACCSFP1	132
M	ACCSFP1	133
M	ACCSFP1	134
M	ACCSFP1	135
M	ACCSFP1	136
M	ACCSFP1	137
M	ACCSFP1	138
M	ACCSFP1	139
M	ACCSFP1	140
M	ACCSFP1	141
M	ACCSFP1	142
M	ACCSFP1	143
M	ACCSFP1	144
M	ACCSFP1	145
M	ACCSFP1	146
M	ACCSFP1	147
M	ACCSFP1	148
M	ACCSFP1	149
M	ACCSFP1	150
M	ACCSFP1	151
M	ACCSFP1	152
M	ACCSFP1	153
M	ACCSFP1	154
M	ACCSFP1	155
M	ACCSFP1	156
M	ACCSFP1	157
M	ACCSFP1	158
M	ACCSFP1	159
M	ACCSFP1	160
M	ACCSFP1	161
M	ACCSFP1	162
M	ACCSFP1	163
M	ACCSFP1	164
l	ACCSFP1	165
M	ACCSITI	

SubFP127	Peptide middle	[NX3;\$([N][CX3](=[OX1])[C][N X3,NX4+])][C][CX3](=[OX1])[N X3;\$([N][C][CX3](=[OX1])[NX3, OX2,OX1-])]
SubFP128	Peptide C term	[NX3;\$([N][CX3](=[OX1])[C][N X3,NX4+])][C][CX3](=[OX1])[O
SubFP129	Peptide N term	X2H,OX1-] [NX3,NX4+;!\$([N]~[!#6]);!\$([N]* ~[#7,#8,#15,#16])][C][CX3](=[O X1])[NX3;\$([N][C][CX3](=[OX1])[NX3,OX2,OX1-])]
SubFP130	Carboxylic orthoester	[#6][OX2][CX4;\$(C[#6]),\$([CH]) ([OX2][#6])[OX2][#6]
SubFP131	Ketene	[CX3]=[CX2]=[OX1]
SubFP132	Ketenacetal	[#7X2,#8X3,#16X2;\$(*[#6,#14])] [#6X3]([#7X2,#8X3,#16X2;\$(*[#6,#14])])=[#6X3]
SubFP133	Nitrile	[NX1]#[CX2]
SubFP134	Isonitrile	[CX1-]#[NX2+]
SubFP135	Vinylogous carbonyl or carboxyl derivative	[#6X3](=[OX1])[#6X3]=,:[#6X3] #7,#8,#16,F,Cl,Br,I]
SubFP136	Vinylogous acid	[#6X3](=[OX1])[#6X3]=,:[#6X3] \$([OX2H]),\$([OX1-])]
SubFP137	Vinylogous ester	[#6X3](=[OX1])[#6X3]=,:[#6X3]
SubFP138	Vinylogous amide	#6;!\$(C=[O,N,S])] [#6X3](=[OX1])[#6X3]=,:[#6X3] #7X3;\$([H2]),\$([H1][#6;!\$(C=[O, N,S])]),\$([#7]([#6;!\$(C=[O,N,S])]
SubFP139	Vinylogous halide	[#6;!\$(C=[O,N,S])])] [#6X3](=[OX1])[#6X3]=,:[#6X3]
SubFP140	Carbonic acid dieester	FX1,ClX1,BrX1,IX1] [#6;!\$(C=[O,N,S])][#8X2][#6X3](=[OX1])[#8X2][#6;!\$(C=[O,N,S])
SubFP141	Carbonic acid esterhalide	[#6;!\$(C=[O,N,S])][OX2;!R][CX3](=[OX1])[OX2][FX1,CIX1,BrX1
SubFP142	Carbonic acid monoester	[#6;!\$(C=[O,N,S])][OX2;!R][CX3](=[OX1])[\$([OX2H]),\$([OX1-])]
SubFP143	Carbonic acid derivatives	[!#6][#6X3](=[!#6])[!#6]
SubFP144	Thiocarbonic acid dieester	[#6;!\$(C=[O,N,S])][#8X2][#6X3](=[SX1])[#8X2][#6;!\$(C=[O,N,S])
SubFP145	Thiocarbonic acid esterhalide	[#6;!\$(C=[O,N,S])][OX2;!R][CX3](=[SX1])[OX2][FX1,ClX1,BrX1, IX1]
SubFP146	Thiocarbonic acid monoester	-
SubFP147	Urea	[#7X3;!\$([#7][!#6])][#6X3](=[OX 1])[#7X3;!\$([#7][!#6])]
SubFP148	Thiourea	[#7X3;!\$([#7][!#6])][#6X3](=[SX
SubFP149	Isourea	1])[#7X3;!\$([#7][!#6])] [#7X2;!\$([#7][!#6])]=,:[#6X3]([#8 X2&!\$([#8][!#6]),OX1-])[#7X3;!\$([#7][!#6])]
SubFP150	Isothiourea	[#7X2;!\$([#7][!#6])]=,:[#6X3]([#1 6X2&!\$([#16][!#6]),SX1-])[#7X3;!\$([#7][!#6])]
SubFP151	Guanidine	[N;v3X3,v4X4+][CX3](=[N;v3X2 v4X3+])[N;v3X3,v4X4+]
SubFP152	Carbaminic acid	[NX3]C(=[OX1])[O;X2H,X1-]
SubFP153	Urethan	[#7X3][#6](=[OX1])[#8X2][#6]
SubFP154	Biuret	[#7X3][#6](=[OX1])[#7X3][#6](= [OX1])[#7X3]
SubFP155	Semicarbazide	[#7X3][#7X3][#6X3]([#7X3;!\$([#7][#7]])=[OX1]
SubFP156	Carbazide	[#7X3][#7X3][#6X3]([#7X3][#7X
SubFP157	Semicarbazone	3])=[OX1] #7X2](=[#6])[#7X3][#6X3]([#7X
SubFP158	Carbazone	3;!\$([#7][#7])]=[OX1] [#7X2](=[#6])[#7X3][#6X3]([#7X
SubFP159	Thiosemicarbazide	3][#7X3])=[OX1] [#7X3][#7X3][#6X3]([#7X3;!\$([#
SubFP160	Thiocarbazide	7][#7])])=[SX1] [#7X3][#7X3][#6X3]([#7X3][#7X
SubFP161	Thiosemicarbazone	3])=[SX1] [#7X2](=[#6])[#7X3][#6X3]([#7X
SubFP162	Thiocarbazone	3;!\$([#7][#7])])=[SX1] [#7X2](=[#6])[#7X3][#6X3]([#7X
SubFP162	Isocyanate	
SubFP163 SubFP164	·	[NX2]=[CX2]=[OX1] [OX2][CX2]#[NX1]
SubFP164 SubFP165	Cyanate Isothiocyanate	[NX2]=[CX2]=[SX1]
SubFP166	Thiocyanate	[SX2][CX2]#[NX1]
SubFP167	Carbodiimide	[NX2]=[CX2]=[NX2]
SubFP168	Orthocarbonic derivatives	[CX4H0]([O,S,#7])([O,S,#7])([O,
		S,#7])[O,S,#7,F,Cl,Br,I]
SubFP169 SubFP170	Phenol 1,2-Diphenol	[OX2H][c] [OX2H][c][c][OX2H]
SubFP171	Arylchloride	[CI][c]
SubFP172	Arylfluoride	[F][c]
SubFP173	Arylbromide	[Br][c]
SubFP174	Aryliodide	[I][c]

175	ATSC0i	Centered Broto-Moreau autocorrelation - lag 0 / weighted by first ionization potential
176	ATSC1i	Centered Broto-Moreau autocorrelation - lag 1 / weighted by first ionization potential
177	ATSC2i	Centered Broto-Moreau autocorrelation - lag 2 / weighted by
178	ATSC3i	first ionization potential Centered Broto-Moreau autocorrelation - lag 3 / weighted by
179	ATSC4i	first ionization potential Centered Broto-Moreau autocorrelation - lag 4 / weighted by
180	ATSC5i	first ionization potential Centered Broto-Moreau autocorrelation - lag 5 / weighted by
181	ATSC6i	first ionization potential Centered Broto-Moreau autocorrelation - lag 6 / weighted by
182	ATSC7i	first ionization potential Centered Broto-Moreau autocorrelation - lag 7 / weighted by
	ATSC8i	first ionization potential Centered Broto-Moreau autocorrelation - lag 8 / weighted by
	ATSC0s	first ionization potential
		Centered Broto-Moreau autocorrelation - lag 0 / weighted by I-state
	ATSC1s	Centered Broto-Moreau autocorrelation - lag 1 / weighted by I-state
	ATSC2s	Centered Broto-Moreau autocorrelation - lag 2 / weighted by I-state
187	ATSC3s	Centered Broto-Moreau autocorrelation - lag 3 / weighted by I-state
188	ATSC4s	Centered Broto-Moreau autocorrelation - lag 4 / weighted by I-
	ATSC5s	state Centered Broto-Moreau autocorrelation - lag 5 / weighted by I-
		state
	ATSC6s	Centered Broto-Moreau autocorrelation - lag 6 / weighted by I-state
	ATSC7s	Centered Broto-Moreau autocorrelation - lag 7 / weighted by I-state
	ATSC8s	Centered Broto-Moreau autocorrelation - lag 8 / weighted by I-state
193	AATSC0c	Average centered Broto-Moreau autocorrelation - lag 0 / weighted by charges
194	AATSC1c	Average centered Broto-Moreau autocorrelation - lag 1 / weighted by charges
195	AATSC2c	Average centered Broto-Moreau autocorrelation - lag 2 / weighted by charges
196	AATSC3c	Average centered Broto-Moreau autocorrelation - lag 3 / weighted by charges
197	AATSC4c	Average centered Broto-Moreau autocorrelation - lag 4 /
		weighted by charges
108	AATSC5c	Average centered Broto-Moreau autocorrelation - lag 5 /
196	AAISCSC	weighted by charges
199	AATSC6c	Average centered Broto-Moreau autocorrelation - lag 6 /
		weighted by charges
200	AATSC7c	Average centered Broto-Moreau autocorrelation - lag 7 /
		weighted by charges
	AATSC8c	Average centered Broto-Moreau autocorrelation - lag 8 / weighted by charges
	AATSC0m	Average centered Broto-Moreau autocorrelation - lag 0 / weighted by mass
203	AATSC1m	Average centered Broto-Moreau autocorrelation - lag 1 / weighted by mass
204	AATSC2m	Average centered Broto-Moreau autocorrelation - lag 2 /
		weighted by mass
205	AATSC3m	Average centered Broto-Moreau autocorrelation - lag 3 / weighted by mass
206	AATSC4m	Average centered Broto-Moreau autocorrelation - lag 4 /
		weighted by mass
207	AATSC5m	Average centered Broto-Moreau autocorrelation - lag 5 / weighted by mass
200	A ATRICIC	Aviana an anti-mad Director Man
208	AATSC6m	Average centered Broto-Moreau autocorrelation - lag 6 / weighted by mass
209	AATSC7m	Average centered Broto-Moreau autocorrelation - lag 7 /
210	AATSC8m	weighted by mass Average centered Broto-Moreau autocorrelation - lag 8 /
_	A A TOTAL CO.	weighted by mass
211	AATSC0v	Average centered Broto-Moreau autocorrelation - lag 0 / weighted by van der Waals volumes
212	AATSC1v	Average centered Broto-Moreau autocorrelation - lag 1 /
		weighted by van der Waals volumes
213	AATSC2v	Average centered Broto-Moreau autocorrelation - lag 2 / weighted by van der Waals volumes
214	AATSC3v	Average centered Broto-Moreau autocorrelation - lag 3 /
215	AATSC4v	weighted by van der Waals volumes Average centered Broto-Moreau autocorrelation - lag 4 /
		weighted by van der Waals volumes

SubFP175	Arylthiol	[SX2H][c]
SubFP176	Iminoarene	[c]=[NX2;\$([H1]),\$([H0][#6;!\$([C
SubFP177	Oxoarene	[c]=[N,S,O])])] [c]=[OX1]
SubFP178	Thioarene	
		[c]=[SX1]
SubFP179	Hetero N basic H	[nX3H1+0]
SubFP180	Hetero N basic no H	[nX3H0+0]
SubFP181	Hetero N nonbasic	[nX2,nX3+]
SubFP182	Hetero O	[o]
SubFP183	Hetero S	[sX2]
SubFP184	Heteroaromatic	[a;!c]
SubFP185	Nitrite	[NX2](=[OX1])[O;\$([X2]),\$([X1-])]
SubFP186	Thionitrite	[SX2][NX2]=[OX1]
SubFP187	Nitrate	[\$([NX3](=[OX1])(=[OX1])[O;\$([X2]),\$([X1-])]),\$([NX3+]([OX1-])(=[OX1])[O;\$([X2]),\$([X1-])])]
SubFP188	Nitro	[\$([NX3](=O)=O),\$([NX3+](=O)[
SubFP189	Nitroso	O-])][!#8] [NX2](=[OX1])[!#7;!#8]
SubFP190	Azide	[NX1]~[NX2]~[NX2,NX1]
SubFP191	Acylazide	[CX3](=[OX1])[NX2]~[NX2]~[N
SubFP192	Diazo	X1] [\$([#6]=[NX2+]=[NX1-]),\$([#6-]-
SubFP193	Diazonium	[NX2+]#[NX1])] [#6][NX2+]#[NX1]
SubFP194	Nitrosamine	[#7;!\$(N*=O)][NX2]=[OX1]
SubFP195	Nitrosamide	[NX2](=[OX1])N-*=O
SubFP196	N-Oxide	[\$([#7+][OX1-
]),\$([#7v5]=[OX1]);!\$([#7](~[O])~ [O]);!\$([#7]=[#7])]
SubFP197	Hydrazine	[NX3;\$([H2]),\$([H1][#6]),\$([H0]([#6])[#6]);!\$(NC=[O,N,S])][NX3; \$([H2]),\$([H1][#6]),\$([H0]([#6])[
SubFP198	Hydrazone	#6]);!\$(NC=[O,N,S])] [NX3;\$([H2]),\$([H1][#6]),\$([H0]([#6])[#6]);!\$(NC=[O,N,S])][NX2]
SubFP199	Hydroxylamine	=[#6] [NX3;\$([H2]),\$([H1][#6]),\$([H0]([#6])[#6]);!\$(NC=[O,N,S])][OX2;
		\$([H1]),\$(O[#6;!\$(C=[N,O,S])])]
SubFP200	Sulfon	\$([H1]),\$(O[#6;!\$(C=[N,O,S])])] [\$([SX4](=[OX1])(=[OX1])([#6])[#6]),\$([SX4+2]([OX1-])([OX1-
	Sulfon Sulfoxide	[\$([SX4](=[OX1])(=[OX1])([#6])[#6]),\$([SX4+2]([OX1-])([OX1-])([#6])[#6])] [\$([SX3](=[OX1])([#6])[#6]),\$([S
SubFP201		[\$([SX4](=[OX1])(=[OX1])([#6])[#6]),\$([SX4+2]([OX1-])([OX1-])([#6])[#6])]
SubFP200 SubFP201 SubFP202 SubFP203	Sulfoxide	[\$([SX4](=[OX1])(=[OX1])([#6])[#6]),\$([SX4+2]([OX1-])([OX1-])([#6])[#6])] [\$([SX3](=[OX1])([#6])[#6]),\$([S X3+]([OX1-])([#6])[#6])]
SubFP201 SubFP202	Sulfoxide Sulfonium	[\$([SX4](=[OX1])(=[OX1])([#6])[#6]),\$([SX4+2]([OX1-])([OX1-])([#6])[#6])] [\$([SX3](=[OX1])([#6])[#6]),\$([S X3+]([OX1-])([#6])[#6])] [S+;!\$([S]~[!#6]);!\$([S]*~[#7,#8,# 15,#16])]
SubFP201 SubFP202 SubFP203	Sulfoxide Sulfonium	[\$([SX4](=[OX1])(=[OX1])([#6])[#6]),\$([SX4+2]([OX1-])([OX1-])([#6])[#6])] [\$([SX3](=[OX1])([#6])[#6]),\$([S X3+]([OX1-])([#6])[#6])] [S+;!\$([S]~[!#6]);!\$([S]*~[#7,#8,# 15,#16])] [SX4](=[OX1])(=[OX1])([\$([OX2 H]),\$([OX1-
SubFP201 SubFP202 SubFP203 SubFP204	Sulfoxide Sulfonium Sulfuric acid	[\$([SX4](=[OX1])(=[OX1])([#6])[#6]),\$([SX4+2]([OX1-])([OX1-])([#6])[#6])] [\$([SX3](=[OX1])([#6])[#6]),\$([S X3+]([OX1-])([#6])[#6])] [S+;!\$([S]~[!#6]);!\$([S]*~[#7,#8,# 15,#16])] [SX4](=[OX1])(=[OX1])([\$([OX2 H]),\$([OX1-])])[\$([OX2H]),\$([OX1-])] [SX4](=[OX1])(=[OX1])([\$([OX2 H]),\$([OX1-])])[\$([OX2- H]),\$([OX1-])])[OX2][#6;!\$(C=[O,N,S])]
SubFP201 SubFP202 SubFP203 SubFP204	Sulfoxide Sulfonium Sulfuric acid Sulfuric monoester	[\$([SX4](=[OX1])(=[OX1])([#6])[#6]),\$([SX4+2]([OX1-])([OX1-])([#6])[#6])] [\$([SX3](=[OX1])([#6])[#6]),\$([S X3+]([OX1-])([#6])[#6])] [S+;!\$([S]~[!#6]);!\$([S]*~[#7,#8,# 15,#16])] [SX4](=[OX1])(=[OX1])([\$([OX2 H]),\$([OX1-])])[\$([OX2H]),\$([OX1-])] [SX4](=[OX1])(=[OX1])([\$([OX2 H]),\$([OX1-
SubFP201 SubFP202 SubFP203 SubFP204 SubFP205	Sulfoxide Sulfonium Sulfuric acid Sulfuric monoester	[\$([SX4](=[OX1])(=[OX1])([#6])[#6]),\$([SX4+2]([OX1-])([OX1-])([#6])[#6])] [\$([SX3](=[OX1])([#6])[#6]),\$([SX3+]([OX1-])([#6])[#6])] [S+;!\$([S]~[!#6]);!\$([S]*~[#7,#8,#15,#16])] [SX4](=[OX1])(=[OX1])([\$([OX2H]),\$([OX1-])])[\$([OX2H]),\$([OX1-])] [SX4](=[OX1])(=[OX1])([\$([OX2H]),\$([OX1-])] [SX4](=[OX1])(=[OX1])([\$([OX2H]),\$([OX1-])] [SX4](=[OX1])(=[OX1])([\$([OX2H]),\$([OX1-])]] [SX4](=[OX1])(=[OX1])([OX2][#6;!\$(C=[O,N,S])]
SubFP201 SubFP202 SubFP203 SubFP204 SubFP205	Sulfoxide Sulfonium Sulfuric acid Sulfuric monoester Sulfuric diester	[\$([SX4](=[OX1])(=[OX1])([#6])[#6]),\$([SX4+2]([OX1-])([OX1-])([#6])[#6])] [\$([SX3](=[OX1])([#6])[#6]),\$([S X3+]([OX1-])([#6])[#6])] [S+;!\$([S]~[!#6]);!\$([S]*~[#7,#8,# 15,#16])] [SX4](=[OX1])(=[OX1])([\$([OX2 H]),\$([OX1-])])[\$([OX2H]),\$([OX1-])] [SX4](=[OX1])(=[OX1])([\$([OX2 H]),\$([OX1-])])[OX2][#6;!\$(C=[O,N,S])] [SX4](=[OX1])(=[OX1])([OX2][# 6;!\$(C=[O,N,S])])[OX2][#6;!\$(C= [O,N,S])] [SX4](=[OX1])(=[OX1])([#7X3;\$
SubFP201 SubFP202 SubFP203 SubFP204 SubFP205 SubFP206	Sulfonium Sulfuric acid Sulfuric monoester Sulfuric diester Sulfuric monoamide	[\$([SX4](=[OX1])(=[OX1])([#6])[#6]),\$([SX4+2]([OX1-])([OX1-])([#6])[#6])] [\$([SX3](=[OX1])([#6])[#6]),\$([SX3+]([OX1-])([#6])[#6])] [\$+;!\$([S]~[!#6]);!\$([S]*~[#7,#8,#15,#16])] [\$X4](=[OX1])(=[OX1])([\$([OX2H]),\$([OX1-])] [\$X4](=[OX1])(=[OX1])([\$([OX2H]),\$([OX1-])] [\$X4](=[OX1])(=[OX1])([\$([OX2H]),\$([OX1-])] [\$X4](=[OX1])(=[OX1])([\$([OX2H]),\$([OX1-])]] [\$X4](=[OX1])(=[OX1])([OX2][#6;!\$(C=[O,N,S])] [\$X4](=[OX1])(=[OX1])([OX2][#6;!\$(C=[O,N,S])]) [\$X4](=[OX1])(=[OX1])([#7X3;\$([H2]),\$([H1][#6;!\$(C=[O,N,S])]),\$([#7]([#6;!\$(C=[O,N,S])])[#6;!\$(C=[O,N,S])])][#6;!\$(C=[O,N,S])])][\$([OX2H]),\$([OX1-])]
SubFP201 SubFP202 SubFP203 SubFP204 SubFP205 SubFP206	Sulfoxide Sulfonium Sulfuric acid Sulfuric monoester Sulfuric diester	[\$([SX4](=[OX1])(=[OX1])([#6])[#6]),\$([SX4+2]([OX1-])([OX1-])([#6])[#6])] [\$([SX3](=[OX1])([#6])[#6]),\$([SX3+]([OX1-])([#6])[#6])] [\$x3+]([OX1-])([#6])[#6])] [\$x4](=[OX1])(=[OX1])([\$([OX2H]),\$([OX1-])] [\$x4](=[OX1])(=[OX1])([\$([OX2H]),\$([OX1-])] [\$x4](=[OX1])(=[OX1])([\$([OX2H]),\$([OX1-])] [\$x4](=[OX1])(=[OX1])([\$([OX2H]),\$([OX1-])] [\$x4](=[OX1])(=[OX1])([OX2][#6;!\$(C=[O,N,S])] [\$x4](=[OX1])(=[OX1])([OX2][#6;!\$(C=[O,N,S])],\$([H2]),\$([H1][#6;!\$(C=[O,N,S])]),\$([#7]([#6;!\$(C=[O,N,S])])[#6;!\$(C=[O,N,S])])] [\$x4](=[OX1])(=[OX1])([#7X3;\$([H2]),\$([H1][#6;!\$(C=[O,N,S])]),\$([#7]([#6;!\$(C=[O,N,S])])[#6;!\$(C=[O,N,S])])] [\$x4](=[OX1])(=[OX1])([#7X3;\$([H2]),\$([OX1-])]]
SubFP201 SubFP202 SubFP203 SubFP204 SubFP205	Sulfonium Sulfuric acid Sulfuric monoester Sulfuric diester Sulfuric monoamide	[\$([SX4](=[OX1])(=[OX1])([#6])[#6]),\$([SX4+2]([OX1-])([OX1-])([#6])[#6])] [\$([SX3](=[OX1])([#6])[#6]),\$([SX3+]([OX1-])([#6])[#6])] [\$x3+]([OX1-])([#6])[#6])] [\$x4](=[OX1])(=[OX1])([\$([OX2H]),\$([OX1-])] [\$x4](=[OX1])(=[OX1])([\$([OX2H]),\$([OX1-])] [\$x4](=[OX1])(=[OX1])([\$([OX2H]),\$([OX1-])] [\$x4](=[OX1])(=[OX1])([\$([OX2H]),\$([OX1-])] [\$x4](=[OX1])(=[OX1])([OX2][#6;!\$(C=[O,N,S])] [\$x4](=[OX1])(=[OX1])([OX2][#6;!\$(C=[O,N,S])]) [\$x4](=[OX1])(=[OX1])([#7X3;\$([H2]),\$([H1][#6;!\$(C=[O,N,S])]),\$([#7]([#6;!\$(C=[O,N,S])])[#6;!\$(C=[O,N,S])])] [\$x4](=[OX1])(=[OX1])([#7X3;\$([H2]),\$([OX1-])] [\$x4](=[OX1])(=[OX1])([#7X3;\$([H2]),\$([OX1-])]] [\$x4](=[OX1])(=[OX1])([#7X3;\$([H2]),\$([H1][#6;!\$(C=[O,N,S])]),\$([#7]([#6;!\$(C=[O,N,S])]),\$([#7]([#6;!\$(C=[O,N,S])])]#6;!\$(C=[O,N,S])])]#6;!\$(C=[O,N,S])])]#6;!\$(C=[O,N,S])])]#6;!\$(C=[O,N,S])]]]#6;!\$(C=[O,N,S])]]]#6;!\$(C=[O,N,S])]]]#6;!\$(C=[O,N,S])]]]#6;!\$(C=[O,N,S])]]]#6;!\$(C=[O,N,S])]]]#6;!\$(C=[O,N,S])]]]#6;!\$(C=[O,N,S])]]]#7X3;\$([H2]),\$([H1][#6;!\$(C=[O,N,S])]]]#6;!\$(C=[O,N,S])]]]#6;!\$(C=[O,N,S])]]]#7X3;\$([H2]),\$([H1][#6;!\$(C=[O,N,S])]]]#7X3;\$([H2]),\$([H1][#6;!\$(C=[O,N,S])]]]#6;!\$(C=[O,N,S])]]]#7X3;\$([H2]),\$([H1][#6;!\$(C=[O,N,S])]]]#7X3;\$([H2]),\$([H1][#6;!\$(C=[O,N,S])]]]#6;!\$(C=[O,N,S])]]]#7X3;\$([H2]),\$([H1][#6;!\$(C=[O,N,S])]]]#7X3;\$([H2]),\$([H1][#6;!\$(C=[O,N,S])]]]#7X3;\$([H2]),\$([H1][#6;!\$(C=[O,N,S])]]]#7X3;\$([H2]),\$([H1][#6;!\$(C=[O,N,S])]]]#7X3;\$([H2]),\$([H1][#6;!\$(C=[O,N,S])]]]#1]#1X3;\$([H2]),\$([H1][#6;!\$(C=[O,N,S])]]]#1X1]#1X1]#1X1]#1X1]#1X1]#1X1]#1X1]
SubFP201 SubFP202 SubFP203 SubFP204 SubFP205 SubFP206	Sulfonium Sulfuric acid Sulfuric monoester Sulfuric diester Sulfuric monoamide	[\$([SX4](=[OX1])(=[OX1])([#6])[#6]),\$([SX4+2]([OX1-])([OX1-])([#6])[#6])] [\$([SX3](=[OX1])([#6])[#6]),\$([SX3+]([OX1-])([#6])[#6])] [\$x3+]([OX1-])([#6])[#6])] [\$x4](=[OX1])(=[OX1])([\$([OX2H]),\$([OX1-])] [\$x4](=[OX1])(=[OX1])([\$([OX2H]),\$([OX1-])] [\$x4](=[OX1])(=[OX1])([\$([OX2H]),\$([OX1-])] [\$x4](=[OX1])(=[OX1])([OX2][#6;!\$(C=[O,N,S])] [\$x4](=[OX1])(=[OX1])([OX2][#6;!\$(C=[O,N,S])] [\$x4](=[OX1])(=[OX1])([#7X3;\$([H2]),\$([H1][#6;!\$(C=[O,N,S])]),\$([#7]([#6;!\$(C=[O,N,S])]),\$([#7]([#6;!\$(C=[O,N,S])]),\$([#7]([#6;!\$(C=[O,N,S])]),\$([H2]),\$([H1][#6;!\$(C=[O,N,S])]),\$([H2]),\$([H1][#6;!\$(C=[O,N,S])]),\$([#7]([#6;!\$(C=[O,N,S])]),\$([#7]([#6;!\$(C=[O,N,S])]),\$([#7]([#6;!\$(C=[O,N,S])]),\$([#7]([#6;!\$(C=[O,N,S])]),\$([#7]([#6;!\$(C=[O,N,S])]),\$([#7]([#6;!\$(C=[O,N,S])]),\$([#7]([#6;!\$(C=[O,N,S])]),\$([#7]([#6;!\$(C=[O,N,S])]),\$([#7]([#6;!\$(C=[O,N,S])]),\$([#7]([#6;!\$(C=[O,N,S])]),\$([#7]([#6;!\$(C=[O,N,S])]),\$([#7]([#6;!\$(C=[O,N,S])]),\$([#7]([#6;!\$(C=[O,N,S])]),\$([#7]([#6;!\$(C=[O,N,S])]),\$([#7]([#6;!\$(C=[O,N,S])]),\$([#7]([#6;!\$(C=[O,N,S])]),\$([#7]([#6;!\$(C=[O,N,S])]),\$([#7]([#6;!\$(C=[O,N,S])]),\$([#7]([#6;!\$(C=[O,N,S])]),\$([#7]([#6;!\$(C=[O,N,S])]),\$([#7]([#6;!\$(C=[O,N,S])]),\$([#7]([#6;!\$(C=[O,N,S])]),\$([#7]([#6;!\$(C=[O,N,S])]),\$([#7]([#6;!\$(C=[O,N,S])]),\$([#7]([#6;!\$(C=[O,N,S])]),\$([#7]([#6;!\$(C=[O,N,S])]),\$([#7]([#6;!\$(C=[O,N,S])]),\$([#7]([#6;!\$(C=[O,N,S])]),\$([#7]([#6;!\$(C=[O,N,S])]),\$([#7]([#6;!\$(C=[O,N,S])]),\$([#7]([#6;!\$(C=[O,N,S])]),\$([#7]([#6;!\$(C=[O,N,S])]),\$([#7]([#6;!\$(C=[O,N,S])]),\$([#7]([#6;!\$(C=[O,N,S])]),\$([#7]([#6;!\$(C=[O,N,S])]),\$([#7]([#6;!\$(C=[O,N,S])]),\$([#7]([#6;!\$(C=[O,N,S])]),\$([#7]([#6;!\$(C=[O,N,S])]),\$([#7]([#6;!\$(C=[O,N,S])]),\$([#7]([#6;!\$(C=[O,N,S])]),\$([#7]([#6;!\$(C=[O,N,S])]),\$([#7]([#6;!\$(C=[O,N,S])]),\$([#7]([#6;!\$(C=[O,N,S])]),\$([#7]([#6;!\$(C=[O,N,S])]),\$([#7]([#6;!\$(C=[O,N,S])]),\$([#7]([#6;!\$(C=[O,N,S])]),\$([#7]([#6;!\$(C=[O,N,S])]),\$([#7]([#6;!\$(C=[O,N,S])]),\$([#7]([#6;!\$(C=[O,N,S])]),\$([#7]([#6;!\$(C=[O,N,S])]),\$([#7]([#6;!\$(C=[O,N,S])]),\$([#7]([#6;!\$(C=[O,N,S])]),\$([#7]([#6;!\$(C=[O,N,S])]),\$([#7]([#6;!\$(
SubFP201 SubFP203 SubFP204 SubFP205 SubFP206 SubFP207	Sulfonium Sulfuric acid Sulfuric monoester Sulfuric diester Sulfuric monoamide	[\$([SX4](=[OX1])(=[OX1])([#6])[#6]),\$([SX4+2]([OX1-])([OX1-])([#6])[#6])] [\$([SX3](=[OX1])([#6])[#6])] [\$([SX3](=[OX1])([#6])[#6])] [\$X3+]([OX1-])([#6])[#6])] [\$X4](=[OX1])(=[OX1])([\$([OX2H]),\$([OX1-])]] [\$X4](=[OX1])(=[OX1])([\$([OX2H]),\$([OX1-])]] [\$X4](=[OX1])(=[OX1])([\$([OX2H]),\$([OX1-])]] [\$X4](=[OX1])(=[OX1])([OX2][#6;!\$(C=[O,N,S])]] [\$X4](=[OX1])(=[OX1])([OX2][#6;!\$(C=[O,N,S])]],\$([H1][#6;!\$(C=[O,N,S])]),\$([#7]([#6;!\$(C=[O,N,S])]),\$([#7]([#6;!\$(C=[O,N,S])]),\$([#7]([#6;!\$(C=[O,N,S])]),\$([#7]([#6;!\$(C=[O,N,S])]),\$([#7]([#6;!\$(C=[O,N,S])]),\$([#7]([#6;!\$(C=[O,N,S])]),\$([#7]([#6;!\$(C=[O,N,S])]),\$([#7]([#6;!\$(C=[O,N,S])]),\$([#7]([#6;!\$(C=[O,N,S])]),\$([#7]([#6;!\$(C=[O,N,S])]),\$([#7]([#6;!\$(C=[O,N,S])]),\$([#7]([#6;!\$(C=[O,N,S])]),\$([#7]([#6;!\$(C=[O,N,S])]),\$([#7]([#6;!\$(C=[O,N,S])]),\$([#7]([#6;!\$(C=[O,N,S])]),\$([#7]([#6;!\$(C=[O,N,S])]),\$([#7]([#6;!\$(C=[O,N,S])]),\$([#7]([#6;!\$(C=[O,N,S])]),\$([#7]([#6;!\$(C=[O,N,S])]),\$([#7]([#6;!\$(C=[O,N,S])]),\$([#7]([#6;!\$(C=[O,N,S])]),\$([#7]([#6;!\$(C=[O,N,S])])]][[SX4](=[OX1])(=[OX1])([#7X3][
SubFP201 SubFP203 SubFP204 SubFP205 SubFP206 SubFP207	Sulfonium Sulfuric acid Sulfuric monoester Sulfuric diester Sulfuric monoamide Sulfuric diamide Sulfuric diamide	[\$([SX4](=[OX1])(=[OX1])([#6])[#6]),\$([SX4+2]([OX1-])([OX1-])([#6])[#6])] [\$([SX3](=[OX1])([#6])[#6]),\$([SX3+]([OX1-])([#6])[#6])] [\$x3+]([OX1-])([#6])[#6])] [\$x4](=[OX1])(=[OX1])([\$([OX2H]),\$([OX2H]),\$([OX1-])] [\$x4](=[OX1])(=[OX1])([\$([OX2H]),\$([OX2H]),\$([OX1-])] [\$x4](=[OX1])(=[OX1])([\$([OX2H]),\$([OX2H]),\$([OX1-])] [\$x4](=[OX1])(=[OX1])([OX2][#6;!\$(C=[O,N,S])] [\$x4](=[OX1])(=[OX1])([#7X3;\$([H2]),\$([H1][#6;!\$(C=[O,N,S])]),\$([#7]([#6;!\$(C=[O,N,S])]),\$([#7]([#6;!\$(C=[O,N,S])]),\$([#7]([#6;!\$(C=[O,N,S])]),\$([#7]([#6;!\$(C=[O,N,S])]),\$([#7]([#6;!\$(C=[O,N,S])]),\$([#7]([#6;!\$(C=[O,N,S])]),\$([#7]([#6;!\$(C=[O,N,S])]),\$([#7]([#6;!\$(C=[O,N,S])]),\$([#7]([#6;!\$(C=[O,N,S])]),\$([#7]([#6;!\$(C=[O,N,S])]),\$([#7]([#6;!\$(C=[O,N,S])]),\$([#7]([#6;!\$(C=[O,N,S])]),\$([#7]([#6;!\$(C=[O,N,S])]),\$([#7]([#6;!\$(C=[O,N,S])]),\$([#7]([#6;!\$(C=[O,N,S])]),\$([#7]([#6;!\$(C=[O,N,S])]),\$([#7]([#6;!\$(C=[O,N,S])])]] [\$x4](=[OX1])(=[OX1])([#7X3][#6;!\$(C=[O,N,S])]),\$([#7]([#6;!\$(C=[O,N,S])])]] [\$x4](=[OX1])(=[OX1])([#7X3][#6;!\$(C=[O,N,S])])]] [\$x4](=[OX1])(=[OX1])([#7X3][#6;!\$(C=[O,N,S])])]
SubFP201 SubFP202 SubFP203 SubFP204 SubFP205 SubFP206 SubFP207 SubFP207	Sulfonium Sulfuric acid Sulfuric monoester Sulfuric diester Sulfuric monoamide Sulfuric diamide Sulfuric diamide Sulfuric derivative	[\$([SX4](=[OX1])(=[OX1])([#6])[#6]),\$([SX4+2]([OX1-])([OX1-])([#6]),\$([S X3+]([OX1-])([#6])[#6])] [\$([SX3](=[OX1])([#6])[#6])] [\$x+;!\$([S]~[!#6]);!\$([S]*~[#7,#8,# 15,#16])] [\$X4](=[OX1])(=[OX1])([\$([OX2 H]),\$([OX1-])] [\$X4](=[OX1])(=[OX1])([\$([OX2 H]),\$([OX1-])] [\$X4](=[OX1])(=[OX1])([\$([OX2 H]),\$([OX1-])] [\$X4](=[OX1])(=[OX1])([OX2][#6;!\$(C=[O,N,S])] [\$X4](=[OX1])(=[OX1])([OX2][#6;!\$(C=[O,N,S])]) [\$X4](=[OX1])(=[OX1])([#7X3;\$([H2]),\$([H1][#6;!\$(C=[O,N,S])]),\$([#7]([#6;!\$(C=[O,N,S])])[#6;!\$(C=[O,N,S])])] [\$X4](=[OX1])(=[OX1])([#7X3;\$([H2]),\$([H1][#6;!\$(C=[O,N,S])]),\$([#7]([#6;!\$(C=[O,N,S])]),\$([#7]([#6;!\$(C=[O,N,S])]),\$([#7]([#6;!\$(C=[O,N,S])]),\$([#7]([#6;!\$(C=[O,N,S])])] [\$X4](=[OX1])(=[OX1])([#7X3;\$([H2]),\$([H1][#6;!\$(C=[O,N,S])]),\$([#7]([#6;!\$(C=[O,N,S])])] [\$X4](=[OX1])(=[OX1])([#7X3][#6;!\$(C=[O,N,S])])] [\$X4](=[OX1])(=[OX1])([#7X3][#6;!\$(C=[O,N,S])]] [\$X4](=[OX1])(=[OX1])([#7X3][#6;!\$(C=[O,N,S])]] [\$X4](=[OX1])(=[OX1])([#7X3][#6;!\$(C=[O,N,S])]] [\$X4](=[OX1])(=[OX1])([#7X3][#6;!\$(C=[O,N,S])]] [\$X4](=[OX1])(=[OX1])([#7X3][#6;!\$(C=[O,N,S])]] [\$X4](=[OX1])(=[OX1])([#7X3][#6;!\$(C=[O,N,S])]] [\$X4](=[OX1])(=[OX1])([#7X3][#6;!\$(C=[O,N,S])]] [\$X4](=[OX1])(=[OX1])([#7X3][#6;!\$(C=[O,N,S])]]
SubFP201 SubFP202 SubFP203 SubFP204 SubFP205 SubFP206 SubFP207 SubFP207	Sulfonium Sulfuric acid Sulfuric monoester Sulfuric diester Sulfuric monoamide Sulfuric diamide Sulfuric diamide	[\$([SX4](=[OX1])(=[OX1])([#6])[#6]),\$([SX4+2]([OX1-])([OX1-])([#6])[#6])] [\$([SX3](=[OX1])([#6])[#6]),\$([SX3+]([OX1-])([#6])[#6])] [\$+;\\$([S]~[\fieb]);\\$([S]*~[\fi-7,\fieb])] [\$X4](=[OX1])(=[OX1])([\fi([OX2H]),\\$([OX1-])] [\$X4](=[OX1])(=[OX1])([\fi([OX2H]),\\$([OX1-])] [\$X4](=[OX1])(=[OX1])([\fi([OX2H]),\\$([OX1-])] [\$X4](=[OX1])(=[OX1])([\fi([OX2H]),\\$([OX1-])] [\$X4](=[OX1])(=[OX1])([\fi-7])([\fi-7])[\fi-7]) [\$X4](=[OX1])(=[OX1])([\fi-7])([\fi-7])([\fi-7])([\fi-7])([\fi-7])([\fi-7])([\fi-7])([\fi-7])([\fi-7])([\fi-7])([\fi-7])([\fi-7])([\fi-7])([\fi-7])([\fi-7])([\fi-7])([\fi-7])([\fi-7])([\fi-7])([\fi-7])([\fi-7])([\fi-7])([\fi-7])([\fi-7])([\fi-7])([\fi-7])([\fi-7])([\fi-7])([\fi-7])([\fi-7])([\fi-7])([\fi-7])([\fi-7])([\fi-7])([\fi-7])([\fi-7])([\fi-7])([\fi-7])([\fi-7])([\fi-7])([\fi-7])([\fi-7])([\fi-7])([\fi-7])([\fi-7])([\fi-7])([\fi-7])([\fi-7])([\fi-7])([\fi-7])([\fi-7])([\fi-7])([\fi-7])([\fi-7])([\fi-7])([\fi-7])([\fi-7])([\fi-7])([\fi-7])([\fi-7])([\fi-7])([\fi-7])([\fi-7])([\fi-7])([\fi-7])([\fi-7])([\fi-7])([\fi-7])([\fi-7])([\fi-7])([\fi-7])([\fi-7])([\fi-7])([\fi-7])([\fi-7])([\fi-7])([\fi-7])([\fi-7])([\fi-7])([\fi-7])([\fi-7])([\fi-7])([\fi-7])([\fi-7])([\fi-7])([\fi-7])([\fi-7])([\fi-7])([\fi-7])([\fi-7])([\fi-7])([\fi-7])([\fi-7])([\fi-7])([\fi-7])([\fi-7])([\fi-7])([\fi-7])([\fi-7])([\fi-7])([\fi-7])([\fi-7])([\fi-7])([\fi-7])([\fi-7])([\fi-7])([\fi-7])([\fi-7])([\fi-7])([\fi-7])([\fi-7])([\fi-7])([\fi-7])([\fi-7])([\fi-7])([\fi-7])([\fi-7])([\fi-7])([\fi-7])([\fi-7])([\fi-7])([\fi-7])([\fi-7])([\fi-7])([\fi-7])([\fi-7])([\fi-7])([\fi-7])([\fi-7])([\fi-7])([\fi-7])([\fi-7])([\fi-7])([\fi-7])([\fi-7])([\fi-7])([\fi-7])([\fi-7])([\fi-7])([\fi-7])([\fi-7])([\fi-7])([\fi-7])([\fi-7])([\fi-7])([\fi-7])([\fi-7])([\fi-7])([\fi-7])([\fi-7])([\fi-7])([\fi-7])([\fi-7])([\fi-7])([\fi-7])([\fi-7])([\fi-7])([\fi-7])([\fi-7])([\fi-7])([\fi-7])([\fi-7])([\fi-7])([\fi-7])([\fi-7])([\fi-7])([\fi-7])([\fi-7])([\fi-7])([\fi-7])([\fi-7])([\fi-7])([\fi-7])([\fi-7])([\fi-7])([\fi-7])([\fi-7])([\fi-7])([\f
SubFP202 SubFP203 SubFP204 SubFP205 SubFP206 SubFP207 SubFP207 SubFP208 SubFP209 SubFP210	Sulfonium Sulfuric acid Sulfuric monoester Sulfuric diester Sulfuric monoamide Sulfuric diamide Sulfuric diamide Sulfuric derivative	[\$([SX4](=[OX1])(=[OX1])([#6])[#6]),\$([SX4+2]([OX1-])([OX1-])([#6])[#6])] [\$([SX3](=[OX1])([#6])[#6]),\$([SX3+]([OX1-])([#6])[#6])] [\$x3+]([OX1-])([#6])[#6])] [\$x4](=[OX1])(=[OX1])([\$([OX2H]),\$([OX1-])]] [\$x4](=[OX1])(=[OX1])([\$([OX2H]),\$([OX1-])]] [\$x4](=[OX1])(=[OX1])([\$([OX2H]),\$([OX1-])]] [\$x4](=[OX1])(=[OX1])([OX2][#6;!\$(C=[O,N,S])]] [\$x4](=[OX1])(=[OX1])([OX2][#6;!\$(C=[O,N,S])]] [\$x4](=[OX1])(=[OX1])([#7X3;\$([H2]),\$([H1][#6;!\$(C=[O,N,S])]),\$([#7]([#6;!\$(C=[O,N,S])])[#6;!\$(C=[O,N,S])])] [\$x4](=[OX1])(=[OX1])([#7X3;\$([H2]),\$([H1][#6;!\$(C=[O,N,S])]),\$([#7]([#6;!\$(C=[O,N,S])]),\$([#7]([#6;!\$(C=[O,N,S])]),\$([#7]([#6;!\$(C=[O,N,S])]),\$([#7]([#6;!\$(C=[O,N,S])])] [\$x4](=[OX1])(=[OX1])([#7X3;\$([H2]),\$([H1][#6;!\$(C=[O,N,S])])] [\$x4](=[OX1])(=[OX1])([#7X3][#6;!\$(C=[O,N,S])])] [\$x4](=[OX1])(=[OX1])([#7X3][#6;!\$(C=[O,N,S])])] [\$x4](=[OX1])(=[OX1])([#7X3][#6;!\$(C=[O,N,S])])] [\$x4](=[OX1])(=[OX1])([#7X3][#6;!\$(C=[O,N,S])])[SX4](=[OX1])(=[OX1])([#7X3][#6;!\$(C=[O,N,S])])[OX2][#6;!\$(C=[O,N,S])]] [\$x4](=[OX1])(=[OX1])([#7X3][#6;!\$(C=[O,N,S])])[SX4](=[!#6])([!#6])([!#6])[!#6]][[SX4;\$([H1]),\$([H0][#6])](=[OX1])[[SX4;\$([H1]),\$([H0][#6])](=[OX1])[[SX4;\$([H1]),\$([H0][#6])](=[OX1])[[SX4;\$([H1]),\$([H0][#6])](=[OX1])[[SX4;\$([H1]),\$([H0][#6])](=[OX1])[[SX4;\$([H1]),\$([H0][#6])](=[OX1])[[SX4;\$([H1]),\$([H0][#6])](=[OX1])[[SX4;\$([H1]),\$([H0][#6])](=[OX1])[[SX4;\$([H1]),\$([H0][#6])](=[OX1])[[SX4;\$([H1]),\$([H0][#6])](=[OX1])[[SX4;\$([H1]),\$([H0][#6])](=[OX1])[[SX4;\$([H1]),\$([H0][#6])](=[OX1])[[SX4;\$([H1]),\$([H0][#6])](=[OX1])[[SX4;\$([H1]),\$([H0][#6])](=[OX1])[[SX4;\$([H1]),\$([H0][#6])](=[OX1])[[SX4;\$([H1]),\$([H0][#6])](=[OX1])[[SX4;\$([H1]),\$([H0][#6])](=[OX1])[[SX4;\$([H1]),\$([H0][#6])](=[OX1])[[SX4;\$([H1]),\$([H0][#6])](=[OX1])[[SX4;\$([H1]),\$([H0][#6])](=[OX1])[[SX4;\$([H1]),\$([H0][#6])](=[OX1])[[SX4;\$([H1]),\$([H0][#6])](=[OX1])[[SX4;\$([H1]),\$([H0][#6])](=[OX1])[[SX4;\$([H1]),\$([H0][#6])](=[OX1])[[SX4;\$([H1]),\$([H0][#6])](=[OX1])[[SX4;\$([H1]),\$([H0][#6])](=[OX1])[[SX4;\$([H1]),\$([H0][#6])](=[OX1])[[SX4;\$([H1]),\$([H0][#6])](=[OX1])[[SX4;\$([H1]),\$([H
SubFP201 SubFP202 SubFP203 SubFP204 SubFP205 SubFP206	Sulfonium Sulfuric acid Sulfuric monoester Sulfuric diester Sulfuric monoamide Sulfuric diamide Sulfuric diamide Sulfuric esteramide Sulfuric derivative Sulfonic acid	[\$([SX4](=[OX1])(=[OX1])([#6])[#6]),\$([SX4+2]([OX1-])([OX1-])([#6])[#6])] [\$([SX3](=[OX1])([#6])[#6]),\$([SX3+]([OX1-])([#6])[#6])] [\$x;!\$([S]~[!#6]);!\$([S]*~[#7,#8,#15,#16])] [\$X4](=[OX1])(=[OX1])([\$([OX2H]),\$([OX1-])] [\$X4](=[OX1])(=[OX1])([\$([OX2H]),\$([OX1-])] [\$X4](=[OX1])(=[OX1])([OX2][#6;!\$(C=[O,N,S])] [\$X4](=[OX1])(=[OX1])([OX2][#6;!\$(C=[O,N,S])]) [\$X4](=[OX1])(=[OX1])([#7X3;\$([H2]),\$([H1][#6;!\$(C=[O,N,S])]),\$([#7]([#6;!\$(C=[O,N,S])]),\$([#7]([#6;!\$(C=[O,N,S])]),\$([#7]([#6;!\$(C=[O,N,S])]),\$([#7]([#6;!\$(C=[O,N,S])]),\$([#7]([#6;!\$(C=[O,N,S])]),\$([#7]([#6;!\$(C=[O,N,S])]),\$([#7]([#6;!\$(C=[O,N,S])]),\$([#7]([#6;!\$(C=[O,N,S])]),\$([#7]([#6;!\$(C=[O,N,S])]),\$([#7]([#6;!\$(C=[O,N,S])]),\$([#7]([#6;!\$(C=[O,N,S])]),\$([#7]([#6;!\$(C=[O,N,S])]),\$([#7]([#6;!\$(C=[O,N,S])]),\$([#7]([#6;!\$(C=[O,N,S])]),\$([#7]([#6;!\$(C=[O,N,S])]),\$([#7]([#6;!\$(C=[O,N,S])]),\$([#7]([#6;!\$(C=[O,N,S])]),\$([#7]([#6;!\$(C=[O,N,S])]),\$([#7]([#6;!\$(C=[O,N,S])]),\$([#7]([#6;!\$(C=[O,N,S])]),\$([#7]([#6;!\$(C=[O,N,S])]),\$([#7]([#6;!\$(C=[O,N,S])]),\$([#7]([#6;!\$(C=[O,N,S])]),\$([#7]([#6;!\$(C=[O,N,S])]),\$([#7]([#6;!\$(C=[O,N,S])]),\$([#7]([#6;!\$(C=[O,N,S])]),\$([#7]([#6;!\$(C=[O,N,S])]),\$([#7]([#6;!\$(C=[O,N,S])]),\$([#7]([#6;!\$(C=[O,N,S])]),\$([#7]([#6;!\$(C=[O,N,S])]),\$([#7]([#6]),[[#6]),[[#6]),[[#6]),[[#6]),[[#6]],[[#6]],[[[OX1]],[[OX1]],[[OX1]],[[[OX1]],[[[OX1]],[[[OX1]],[[[OX1]],[[[OX1]],[[[OX1]],[[[OX1]],[[[OX1]],[[[OX1]],[[[OX1]]],[[[OX1]],[[[OX1]],[[[OX1]]],[[[OX1]],[[[OX1]],[[[OX1]]],[[[OX1]],[[[OX1]]],[[[OX1]],[[[OX1]],[[[OX1]],[[[OX1]],[[[OX1]],[[[OX1]]],[[[OX1]],[[[OX1]],[[[OX1]],[[[OX1]],[[[OX1]],[[[OX1]]],[[[OX1]],[[[OX1]]],[[[OX1]],[[[OX1]]],[[[OX1]],[[[OX1]]],[[[OX1]],[[[OX1]],[[[OX1]],[[[OX1]],[[[OX1]],[[[OX1]]],[[[OX1]],[[[OX1]],[[[OX1]],[[[OX1]]],[[[OX1]],[[[OX1]]],[[[OX1]],[[[OX1]]],[[[OX1]]],[[[OX1]],[[[OX1]]],[[[OX1]],[[[OX1]]],[[[OX1]],[[[OX1]]],[[[OX1]]],[[[OX1]]],[[[OX1]],[[[OX1]]],[[[OX1]]],[[[OX1]],[[[OX1]]],[[[OX1]]],[[[OX1]]],[[[OX1]]],[[[OX1]]],[[[OX1]]],[[[OX1]]],[[[OX1]]],[[[OX1]]],[[[OX1]]],[[[OX1]]],[[[OX1]]],[[[OX1]]],[[[OX1]]],[[[
SubFP202 SubFP203 SubFP204 SubFP205 SubFP206 SubFP207 SubFP207 SubFP208 SubFP209 SubFP210	Sulfonium Sulfuric acid Sulfuric monoester Sulfuric diester Sulfuric monoamide Sulfuric diamide Sulfuric diamide Sulfuric esteramide Sulfuric derivative Sulfonic acid	[\$([SX4](=[OX1])(=[OX1])([#6])[#6]),\$([SX4+2]([OX1-])([OX1-])([#6])[#6])] [\$([SX3](=[OX1])([#6])[#6]),\$([SX3+]([OX1-])([#6])[#6])] [\$([SX3](=[OX1])([#6])[#6])] [\$([SX3](=[OX1])([#6])[#6])] [\$([SX3-](=[OX1])([S)[]*~[#7,#8,#15,#16])] [\$([OX1-])([OX1])([S)([OX2-H]),\$([OX1-])] [\$([OX2H]),\$([OX1-])] [\$([OX2H]),\$([OX1])([\$([OX2-H]),\$([OX1-])]] [\$([OX1-])([OX1])([OX1])([OX2][#6;!\$(C=[O,N,S])]) [\$([OX1-])([OX1])([OX1])([OX2][#6;!\$(C=[O,N,S])]),\$([#7]([#6;!\$(C=[O,N,S])])[#6;!\$(C=[O,N,S])]),\$([#7]([#6;!\$(C=[O,N,S])]),\$([#7]([#6;!\$(C=[O,N,S])]),\$([#7]([#6;!\$(C=[O,N,S])]),\$([#7]([#6;!\$(C=[O,N,S])]),\$([#7]([#6;!\$(C=[O,N,S])]),\$([#7]([#6;!\$(C=[O,N,S])])] [\$([A1])([A1])([A1])([A1])([A1])([A1])([A1])([A1])([A1])([A1])([A1])([A1])([A1])([A1])([A1])([A1])([A1])([A1])([A1])([A1])([A1])([A1])([A1])([A1])([A1])([A1])([A1])([A1])([A1])([A1])([A1])([A1])([A1])([A1])([A1])([A1])([A1])([A1])([A1])([A1])([A1])([A1])([A1])([A1])([A1])([A1])([A1])([A1])([A1])([A1])([A1])([A1])([A1])([A1])([A1])([A1])([A1])([A1])([A1])([A1])([A1])([A1])([A1])([A1])([A1])([A1])([A1])([A1])([A1])([A1])([A1])([A1])([A1])([A1])([A1])([A1])([A1])([A1])([A1])([A1])([A1])([A1])([A1])([A1])([A1])([A1])([A1])([A1])([A1])([A1])([A1])([A1])([A1])([A1])([A1])([A1])([A1])([A1])([A1])([A1])([A1])([A1])([A1])([A1])([A1])([A1])([A1])([A1])([A1])([A1])([A1])([A1])([A1])([A1])([A1])([A1])([A1])([A1])([A1])([A1])([A1])([A1])([A1])([A1])([A1])([A1])([A1])([A1])([A1])([A1])([A1])([A1])([A1])([A1])([A1])([A1])([A1])([A1])([A1])([A1])([A1])([A1])([A1])([A1])([A1])([A1])([A1])([A1])([A1])([A1])([A1])([A1])([A1])([A1])([A1])([A1])([A1])([A1])([A1])([A1])([A1])([A1])([A1])([A1])([A1])([A1])([A1])([A1])([A1])([A1])([A1])([A1])([A1])([A1])([A1])([A1])([A1])([A1])([A1])([A1])([A1])([A1])([A1])([A1])([A1])([A1])([A1])([A1])([A1])([A1])([A1])([A1])([A1])([A1])([A1])([A1])([A1])([A1])([A1])([A1])([A1])([A1])([A1])([A1])([A1])([A1])([A1])([A1])([A1])([A1])([A1])([A1])([A1])([A1])([A1])([A1])([A1])([A1])([A1])([A1])([A1])([A1])([A1])([A1])([A1])([A1])([A1])([A1])([A1])([A1])([A1]
SubFP202 SubFP203 SubFP204 SubFP205 SubFP206 SubFP207 SubFP207 SubFP208 SubFP210 SubFP211	Sulfonium Sulfuric acid Sulfuric monoester Sulfuric diester Sulfuric monoamide Sulfuric diamide Sulfuric diamide Sulfuric esteramide Sulfuric derivative Sulfonic acid Sulfonamide	[\$([SX4](=[OX1])(=[OX1])([#6])[#6]),\$([SX4+2]([OX1-])([OX1-])([#6])[#6])] [\$([SX3](=[OX1])([#6])[#6]),\$([SX3+]([OX1-])([#6])[#6])] [\$([SX3](=[OX1])([#6])[#6])] [\$([SX3](=[OX1])([#6])[#6])] [\$([OX1-])([#6])[*]([OX1])([\$([OX2H]),\$([OX1-])] [\$([OX2H]),\$([OX1-])] [\$([OX2H]),\$([OX1-])] [\$([OX2H]),\$([OX1-])] [\$([OX2H]),\$([OX1-])] [\$([OX2H]),\$([OX1-])] [\$([OX1-]))]([OX2][#6;!\$(C=[O,N,S])] [\$([OX1-]))]([OX2][#6;!\$(C=[O,N,S])] [\$([A1]),\$([A1])([A1])([A1])([A1])([A1]),\$([OX1-])] [\$([A1]),\$([A1])([A1])([A1])([A1]),\$([OX1-])] [\$([A1]),\$([A1])([A1])([A1])([A1]),\$([A1]),\$([A1]),\$([A1]),\$([A1]),\$([A1]),\$([A1]),\$([A1]),\$([A1]),\$([A1]),\$([A1]),\$([A1]),\$([A1]),\$([A1]),\$([A1]),\$([A1]),\$([A1]),\$([A1]),\$([A1]),\$([A1]),\$([A1]),\$([A1]),\$([A1]),\$([A1]),\$([A1]),\$([A1]),\$([A1]),\$([A1]),\$([A1]),\$([A1]),\$([A1]),\$([A1]),\$([A1]),\$([A1]),\$([A1]),\$([A1]),\$([A1]),\$([A1]),\$([A1]),\$([A1]),\$([A1]),\$([A1]),\$([A1]),\$([A1]),\$([A1]),\$([A1]),\$([A1]),\$([A1]),\$([A1]),\$([A1]),\$([A1]),\$([A1]),\$([A1]),\$([A1]),\$([A1]),\$([A1]),\$([A1]),\$([A1]),\$([A1]),\$([A1]),\$([A1]),\$([A1]),\$([A1]),\$([A1]),\$([A1]),\$([A1]),\$([A1]),\$([A1]),\$([A1]),\$([A1]),\$([A1]),\$([A1]),\$([A1]),\$([A1]),\$([A1]),\$([A1]),\$([A1]),\$([A1]),\$([A1]),\$([A1]),\$([A1]),\$([A1]),\$([A1]),\$([A1]),\$([A1]),\$([A1]),\$([A1]),\$([A1]),\$([A1]),\$([A1]),\$([A1]),\$([A1]),\$([A1]),\$([A1]),\$([A1]),\$([A1]),\$([A1]),\$([A1]),\$([A1]),\$([A1]),\$([A1]),\$([A1]),\$([A1]),\$([A1]),\$([A1]),\$([A1]),\$([A1]),\$([A1]),\$([A1]),\$([A1]),\$([A1]),\$([A1]),\$([A1]),\$([A1]),\$([A1]),\$([A1]),\$([A1]),\$([A1]),\$([A1]),\$([A1]),\$([A1]),\$([A1]),\$([A1]),\$([A1]),\$([A1]),\$([A1]),\$([A1]),\$([A1]),\$([A1]),\$([A1]),\$([A1]),\$([A1]),\$([A1]),\$([A1]),\$([A1]),\$([A1]),\$([A1]),\$([A1]),\$([A1]),\$([A1]),\$([A1]),\$([A1]),\$([A1]),\$([A1]),\$([A1]),\$([A1]),\$([A1]),\$([A1]),\$([A1]),\$([A1]),\$([A1]),\$([A1]),\$([A1]),\$([A1]),\$([A1]),\$([A1]),\$([A1]),\$([A1]),\$([A1]),\$([A1]),\$([A1]),\$([A1]),\$([A1]),\$([A1]),\$([A1]),\$([A1]),\$([A1]),\$([A1]),\$([A1]),\$([A1]),\$([A1]),\$([A1]),\$([A1]),\$([A1]),\$([A1]),\$([A1]),\$([A1]),\$([A1]),\$([A1]),\$([A1]),\$([A1]),\$([A1]),\$([A1]),\$([A1]),\$([A1]),\$([A1
SubFP202 SubFP203 SubFP204 SubFP205 SubFP206 SubFP207 SubFP207 SubFP208 SubFP210 SubFP211	Sulfonium Sulfuric acid Sulfuric monoester Sulfuric diester Sulfuric monoamide Sulfuric diamide Sulfuric diamide Sulfuric esteramide Sulfuric derivative Sulfonic acid Sulfonamide	[\$([SX4](=[OX1])(=[OX1])([#6])[#6]),\$([SX4+2]([OX1-])([OX1-])([#6])[#6])] [\$([SX3](=[OX1])([#6])[#6]),\$([SX3+]([OX1-])([#6])[#6])] [\$x+;!\$([S]~[!#6]);!\$([S]*~[#7,#8,#15,#16])] [\$X4](=[OX1])(=[OX1])([\$([OX2H]),\$([OX1-])]] [\$X4](=[OX1])(=[OX1])([\$([OX2H]),\$([OX1-])]] [\$X4](=[OX1])(=[OX1])([OX2][#6;!\$(C=[O,N,S])]] [\$X4](=[OX1])(=[OX1])([OX2][#6;!\$(C=[O,N,S])]] [\$X4](=[OX1])(=[OX1])([#7X3;\$([H2]),\$([H1][#6;!\$(C=[O,N,S])]),\$([#7]([#6;!\$(C=[O,N,S])]),\$([#7]([#6;!\$(C=[O,N,S])]),\$([#7]([#6;!\$(C=[O,N,S])]),\$([#7]([#6;!\$(C=[O,N,S])]),\$([#7]([#6;!\$(C=[O,N,S])]),\$([#7]([#6;!\$(C=[O,N,S])]),\$([#7]([#6;!\$(C=[O,N,S])]),\$([#7]([#6;!\$(C=[O,N,S])]),\$([#7]([#6;!\$(C=[O,N,S])]),\$([#7]([#6;!\$(C=[O,N,S])]),\$([#7]([#6;!\$(C=[O,N,S])]),\$([#7]([#6;!\$(C=[O,N,S])]),\$([#7]([#6;!\$(C=[O,N,S])]),\$([#7]([#6;!\$(C=[O,N,S])]),\$([#7]([#6;!\$(C=[O,N,S])]),\$([#7]([#6;!\$(C=[O,N,S])]),\$([#7]([#6;!\$(C=[O,N,S])]),\$([#7]([#6;!\$(C=[O,N,S])]),\$([#7]([#6;!\$(C=[O,N,S])]),\$([#7]([#6;!\$(C=[O,N,S])]),\$([#7]([#6;!\$(C=[O,N,S])]),\$([#7]([#6;!\$(C=[O,N,S])]),\$([#7]([#6;!\$(C=[O,N,S])]),\$([#7]([#6;!\$(C=[O,N,S])]),\$([#7]([#6;!\$(C=[O,N,S])]),\$([#7]([#6;!\$(C=[O,N,S])]),\$([#7]([#6;!\$(C=[O,N,S])]),\$([#7]([#6;!\$(C=[O,N,S])]),\$([#7]([#6;!\$(C=[O,N,S])]),\$([#7]([#6;!\$(C=[O,N,S])]),\$([#7]([#6;!\$(C=[O,N,S])]),\$([#7]([#6;!\$(C=[O,N,S])]),\$([#7]([#6;!\$(C=[O,N,S])]),\$([#7]([#6;!\$(C=[O,N,S])]),\$([#7]([#6;!\$(C=[O,N,S])]),\$([#7]([#6;!\$(C=[O,N,S])]),\$([#7]([#6;!\$(C=[O,N,S])]),\$([#7]([#6;!\$(C=[O,N,S])]),\$([#7]([#6;!\$(C=[O,N,S])]),\$([#7]([#6;!\$(C=[O,N,S])])],\$([#7]([#6;!\$(C=[O,N,S])]),\$([#7]([#6;!\$(C=[O,N,S])]),\$([#7]([#6;!\$(C=[O,N,S])])],\$([#7]([#6;!\$(C=[O,N,S])])]]
SubFP202 SubFP203 SubFP204 SubFP205 SubFP206 SubFP207 SubFP208 SubFP210 SubFP211	Sulfonium Sulfuric acid Sulfuric monoester Sulfuric diester Sulfuric monoamide Sulfuric diamide Sulfuric derivative Sulfuric derivative Sulfonic acid Sulfonic acid Sulfonic ester	[\$([SX4](=[OX1])(=[OX1])([#6])[#6]),\$([SX4+2]([OX1-])([OX1-])([#6])]#6]),\$([SX3](=[OX1])([#6])[#6]),\$([SX3+]([OX1-])([#6])[#6])] [\$([SX3](=[OX1])([#6])[#6]),\$([SX3+]([OX1-])([#6])[#6])] [\$([SX3](=[OX1])([#6])[#6])] [\$([SX3](=[OX1])(=[OX1])([\$([OX2+1]),\$([OX1-1])]] [\$([OX1-1])([OX1])([S([OX2+1]),\$([OX1-1])]] [\$([OX1-1])([OX1])([OX1])([OX2+1]),\$([OX1-1])] [\$([OX1-1])([OX1])([OX1])([OX2][#6;\$(C=[O,N,S])]),\$([H1][#6;!\$(C=[O,N,S])]),\$([H7]([#6;!\$(C=[O,N,S])]),\$([H7]([#6;!\$(C=[O,N,S])]),\$([H7]([#6;!\$(C=[O,N,S])]),\$([H7]([#6;!\$(C=[O,N,S])]),\$([H7]([#6;!\$(C=[O,N,S])]),\$([H7]([#6;!\$(C=[O,N,S])]),\$([H7]([#6;!\$(C=[O,N,S])]),\$([H7]([#6;!\$(C=[O,N,S])]),\$([H7]([#6;!\$(C=[O,N,S])]),\$([H7]([#6;!\$(C=[O,N,S])]),\$([H7]([#6;!\$(C=[O,N,S])]),\$([H7]([#6;!\$(C=[O,N,S])]),\$([H7]([#6;!\$(C=[O,N,S])]),\$([H7]([#6;!\$(C=[O,N,S])]),\$([H7]([#6;!\$(C=[O,N,S])]),\$([H7]([H0][#6])([=[OX1]([OX1-])]] [\$X4](=[OX1])([OX2H]),\$([OX1-])] [\$X4;\$([H1]),\$([H0][#6])([=[OX1]([H0][#6]),\$([OX1-])] [\$X4;\$([H1]),\$([H0][#6]),\$([OX1-])] [\$X4;\$([H1]),\$([H0][#6]),\$([OX1-])] [\$X4;\$([H1]),\$([H0][#6]),\$([OX1-])] [\$X4;\$([H1]),\$([H0][#6]),\$([OX1-])] [\$X4;\$([H1]),\$([H0][#6]),\$([OX1-])] [\$X4;\$([H1]),\$([H0][#6]),\$([OX1-])] [\$X4;\$([H1]),\$([H0][#6]),\$([H0][#6]),\$([OX1-])] [\$X4;\$([H1]),\$([H0][#6]),\$([OX1-])] [\$X4;\$([H1]),\$([H0][#6]),\$([OX1-])] [\$X4;\$([H1]),\$([H0][#6]),\$([OX1-])] [\$X4;\$([H1]),\$([H0][#6]),\$([OX1-])] [\$X4;\$([H1]),\$([H0][#6]),\$([OX1-])]
SubFP202 SubFP203 SubFP204 SubFP205 SubFP206 SubFP207 SubFP208 SubFP210 SubFP211 SubFP212	Sulfonium Sulfuric acid Sulfuric monoester Sulfuric diester Sulfuric monoamide Sulfuric diamide Sulfuric derivative Sulfonic acid Sulfonic acid Sulfonic acid	[\$([SX4](=[OX1])(=[OX1])([#6])[#6]),\$([SX4+2]([OX1-])([OX1-])([#6])[#6]),\$([SX3](=[OX1])([#6])[#6]),\$([SX3+]([OX1-])([#6])[#6])] [\$([SX3](=[OX1])([#6])[#6]),\$([SX3+]([OX1-])([#6])[#6])] [\$([SX3](=[OX1])([#6])[#6])] [\$([SX3](=[OX1])(=[OX1])([\$([OX2+1]),\$([OX1-1])]] [\$([OX1-1])([OX1])([S([OX2+1]),\$([OX1-1])]] [\$([OX2+1]),\$([OX1-1])[] [\$([OX1-1])([OX1])([OX1])([OX2][#6;1\$(C=[O,N,S])]] [\$([OX1-1])([OX1])([OX1])([OX2][#6;1\$(C=[O,N,S])]),\$([H1][#6;1\$(C=[O,N,S])]),\$([H7]([#6;1\$(C=[O,N,S])]),\$([H7]([#6;1\$(C=[O,N,S])]),\$([H7]([#6;1\$(C=[O,N,S])]),\$([H7]([#6;1\$(C=[O,N,S])]),\$([H7]([#6;1\$(C=[O,N,S])]),\$([H7]([#6;1\$(C=[O,N,S])]),\$([H7]([#6;1\$(C=[O,N,S])]),\$([H7]([#6;1\$(C=[O,N,S])]),\$([H7]([#6;1\$(C=[O,N,S])]),\$([H7]([#6;1\$(C=[O,N,S])]),\$([H7]([#6;1\$(C=[O,N,S])]),\$([H7]([H6],1\$(C=[O,N,S])]),\$([H7]([H6],1\$(C=[O,N,S])]),\$([H7]([H6],1\$([OX1])([H7X3][[H6;1\$(C=[O,N,S])]),\$([H7]([H6],1\$([IH0][H6])](=[OX1])([IH0][H6]),\$([OX1-])] [\$X4]([H1]),\$([H0][H6]),\$([OX1-])] [\$X4;\$([H1]),\$([H0][H6]),\$([OX1-])] [\$X4;\$([H1]),\$([H0][H6]),\$([OX1-])] [\$X4;\$([H1]),\$([H0][H6]),\$([OX1-])] [\$X4;\$([H1]),\$([H0][H6]),\$([OX1-])] [\$X4;\$([H1]),\$([H0][H6]),\$([OX1-])] [\$X4;\$([H1]),\$([H0][H6]),\$([OX1-])] [\$X4;\$([H1]),\$([H0][H6]),\$([OX1-])] [\$X4;\$([H1]),\$([H0][H6]),\$([OX1-])] [\$X4;\$([H1]),\$([H0][H6]),\$([OX1-])]

216	AATSC5v	Average centered Broto-Moreau autocorrelation - lag 5 / weighted by van der Waals volumes
217	AATSC6v	Average centered Broto-Moreau autocorrelation - lag 6 / weighted by van der Waals volumes
218	AATSC7v	Average centered Broto-Moreau autocorrelation - lag 7 / weighted by van der Waals volumes
219	AATSC8v	Average centered Broto-Moreau autocorrelation - lag 8 / weighted by van der Waals volumes
220	AATSC0e	Average centered Broto-Moreau autocorrelation - lag 0 / weighted by Sanderson electronegativities
221	AATSC1e	Average centered Broto-Moreau autocorrelation - lag 1 / weighted by Sanderson electronegativities
222	AATSC2e	Average centered Broto-Moreau autocorrelation - lag 2 /
223	AATSC3e	weighted by Sanderson electronegativities Average centered Broto-Moreau autocorrelation - lag 3 /
224	AATSC4e	weighted by Sanderson electronegativities Average centered Broto-Moreau autocorrelation - lag 4 /
225	AATSC5e	weighted by Sanderson electronegativities Average centered Broto-Moreau autocorrelation - lag 5 / weighted by Sanderson electronegativities
226	AATSC6e	Average centered Broto-Moreau autocorrelation - lag 6 / weighted by Sanderson electronegativities
227	AATSC7e	Average centered Broto-Moreau autocorrelation - lag 7 /
228	AATSC8e	weighted by Sanderson electronegativities Average centered Broto-Moreau autocorrelation - lag 8 / weighted by Sanderson electronegativities
229	AATSC0p	Average centered Broto-Moreau autocorrelation - lag 0 / weighted by polarizabilities
230	AATSC1p	Average centered Broto-Moreau autocorrelation - lag 1 / weighted by polarizabilities
231	AATSC2p	Average centered Broto-Moreau autocorrelation - lag 2 / weighted by polarizabilities
232	AATSC3p	Average centered Broto-Moreau autocorrelation - lag 3 / weighted by polarizabilities
233	AATSC4p	Average centered Broto-Moreau autocorrelation - lag 4 / weighted by polarizabilities
234	AATSC5p	Average centered Broto-Moreau autocorrelation - lag 5 / weighted by polarizabilities
235	AATSC6p	Average centered Broto-Moreau autocorrelation - lag 6 /
236	AATSC7p	weighted by polarizabilities Average centered Broto-Moreau autocorrelation - lag 7 / weighted by polarizabilities
237	AATSC8p	Average centered Broto-Moreau autocorrelation - lag 8 / weighted by polarizabilities
238	AATSC0i	Average centered Broto-Moreau autocorrelation - lag 0 / weighted by first ionization potential
239	AATSC1i	Average centered Broto-Moreau autocorrelation - lag 1 / weighted by first ionization potential
240	AATSC2i	Average centered Broto-Moreau autocorrelation - lag 2 / weighted by first ionization potential
241	AATSC3i	Average centered Broto-Moreau autocorrelation - lag 3 / weighted by first ionization potential
242	AATSC4i	Average centered Broto-Moreau autocorrelation - lag 4 / weighted by first ionization potential
243	AATSC5i	Average centered Broto-Moreau autocorrelation - lag 5 / weighted by first ionization potential

SubFP216	Sulfinic amide	[SX3;\$([H1]),\$([H0][#6])](=[OX1])[#7X3;\$([H2]),\$([H1][#6;!\$(C=[O,N,S])]),\$([#7]([#6;!\$(C=[O,N,S])])[#6;!\$(C=[O,N,S])])
SubFP217	Sulfinic ester	[SX3;\$([H1]),\$([H0][#6])](=[OX1
SubFP218	Sulfinic halide])[OX2][#6;!\$(C=[O,N,S])] [SX3;\$([H1]),\$([H0][#6])](=[OX1])[FX1,CIX1,BrX1,IX1]
SubFP219	Sulfinic derivative	[SX3;\$([H1]),\$([H0][#6])](=[!#6])
SubFP220	Sulfenic acid	[!#6] [SX2;\$([H1]),\$([H0][#6])][\$([OX
SubFP221	Sulfenic amide	2H]),\$([OX1-])] [SX2;\$([H1]),\$([H0][#6])][#7X3;\$ ([H2]),\$([H1][#6;!\$(C=[O,N,S])]), \$([#7]([#6;!\$(C=[O,N,S])])[#6;!\$(
SubFP222	Sulfenic ester	C=[O,N,S])]) [SX2;\$([H1]),\$([H0][#6])][OX2][
SubFP223	Sulfenic halide	#6;!\$(C=[O,N,S])] [SX2;\$([H1]),\$([H0][#6])][FX1,Cl
SubFP224	Sulfenic derivative	X1,BrX1,IX1] [SX2;\$([H1]),\$([H0][#6])][!#6]
SubFP225	Phosphine	[PX3;\$([H3]),\$([H2][#6]),\$([H1]([
		#6])[#6]),\$([H0]([#6])([#6])[#6])]
SubFP226	Phosphine oxide	[PX4;\$([H3]=[OX1]),\$([H2](=[O X1])[#6]),\$([H1](=[OX1])([#6])[# 6]),\$([H0](=[OX1])([#6])([#6])[#6])]
SubFP227	Phosphonium	[P+;!\$([P]~[!#6]);!\$([P]*~[#7,#8,# 15,#16])]
SubFP228	Phosphorylen	[PX4;\$([H3]=[CX3]),\$([H2](=[CX 3])[#6]),\$([H1](=[CX3])([#6])[#6]),\$([H0](=[CX3])([#6])([#6])[#6])]
SubFP229	Phosphonic acid	[PX4;\$([H1]),\$([H0][#6])](=[OX1])([\$([OX2H]),\$([OX1-])])[\$([OX2H]),\$([OX1-])]
SubFP230	Phosphonic monoester	[PX4;\$([H1]),\$([H0][#6])](=[OX1])([\$([OX2H]),\$([OX1-])])[OX2][#6;!\$(C=[O,N,S])]
SubFP231	Phosphonic diester	[PX4;\$([H1]),\$([H0][#6])](=[OX1])([OX2][#6;!\$(C=[O,N,S])])[OX2]
SubFP232	Phosphonic monoamide][#6;!\$(C=[O,N,S])] [PX4;\$([H1]),\$([H0][#6])](=[OX1
])([\$([OX2H]),\$([OX1-])])[#7X3;\$([H2]),\$([H1][#6;!\$(C =[O,N,S])]),\$([#7]([#6;!\$(C=[O,N, S])])[#6;!\$(C=[O,N,S])])]
SubFP233	Phosphonic diamide	[PX4;\$([H1]),\$([H0][#6])](=[OX1])([#7X3;\$([H2]),\$([H1][#6;!\$(C=[O,N,S])]),\$([#7]([#6;!\$(C=[O,N,S])])][#7X3;\$([H2]),\$([H1][#6;!\$(C=[O,N,S])]),\$([#7]([#6;!\$(C=[O,N,S])])[#6;!\$(C=[O,N,S])])]
SubFP234	Phosphonic esteramide	[PX4;\$([H1]),\$([H0][#6])](=[OX1])([OX2][#6;!\$(C=[O,N,S])])[#7X]3;\$([H2]),\$([H1][#6;!\$(C=[O,N,S])]),\$([#7]([#6;!\$(C=[O,N,S])])[#6;
SubFP235	Phosphonic acid derivative	!\$(C=[O,N,S])]) [PX4;\$([H1]),\$([H0][#6])](=[!#6])
SubFP236	Phosphoric acid	([!#6])[!#6] [PX4D4](=[OX1])([\$([OX2H]),\$([OX1-])])([\$([OX2H]),\$([OX1-])])[\$([OX2H]),\$([OX1-])]
SubFP237	Phosphoric monoester	[PX4D4](=[OX1])([\$([OX2H]),\$([OX1-])])([\$([OX2H]),\$([OX1-])])[OX2][#6;!\$(C=[O,N,S])]
SubFP238	Phosphoric diester	[PX4D4](=[OX1])([\$([OX2H]),\$([
		OX1-])])([OX2][#6;!\$(C=[O,N,S])])[O
SubFP239	Phosphoric triester	X2][#6;!\$(C=[O,N,S])] [PX4D4](=[OX1])([OX2][#6;!\$(C =[O,N,S])])([OX2][#6;!\$(C=[O,N,
		S])])[OX2][#6;!\$(C=[O,N,S])]
SubFP240	Phosphoric monoamide	[PX4D4](=[OX1])([\$([OX2H]),\$([OX1-])])([\$([OX2H]),\$([OX1-])])[#7X3;\$([H2]),\$([H1][#6;!\$(C=[O,N,S])]),\$([#7]([#6;!\$(C=[O,N,S])])[#6;!\$(C=[O,N,S])])]
SubFP241	Phosphoric diamide	[PX4D4](=[OX1])([\$([OX2H]),\$([OX1-])])([#7X3;\$([H2]),\$([H1][#6;!\$(C=[O,N,S])]),\$([#7]([#6;!\$(C=[O,N,S])])[#7X3;\$([H2]),\$([H1][#6;!\$(C=[O,N,S])]),\$([#7]([#6;!\$(C=[O,N,S])]),\$([#7]([#6;!\$(C=[O,N,S])])[#6;!\$(
SubFP242	Phosphoric triamide	C=[O,N,S])])] [PX4D4](=[OX1])([#7X3;\$([H2]), \$([H1][#6;!\$(C=[O,N,S])]),\$([#7]([#6;!\$(C=[O,N,S])])[#6;!\$(C=[O, N,S])])])([#7X3;\$([H2]),\$([H1][#6 ;!\$(C=[O,N,S])]),\$([#7]([#6;!\$(C= [O,N,S])])[#6;!\$(C=[O,N,S])])][# 7X3;\$([H2]),\$([H1][#6;!\$(C=[O,N,S])])[#7X3;\$([H2]),\$([H1][#6;!\$(C=[O,N,S])])[#6;!\$(C=[O,N,S])])[
SubFP243	Phosphoric monoestermonoamide	[PX4D4](=[OX1])([\$([OX2H]),\$([OX1-])])([OX2][#6;!\$(C=[O,N,S])])[#7 X3;\$([H2]),\$([H1][#6;!\$(C=[O,N,S])])[# S])]),\$([#7]([#6;!\$(C=[O,N,S])])[# 6;!\$(C=[O,N,S])])

244	AATSC6i	Average centered Broto-Moreau autocorrelation - lag 6 /
244	AATSCOI	weighted by first ionization potential
245	AATSC7i	Average centered Broto-Moreau autocorrelation - lag 7 /
		weighted by first ionization potential
246	AATSC8i	Average centered Broto-Moreau autocorrelation - lag 8 / weighted by first ionization potential
247	AATSC0s	Average centered Broto-Moreau autocorrelation - lag 0 /
		weighted by I-state
248	AATSC1s	Average centered Broto-Moreau autocorrelation - lag 1 / weighted by I-state
249	AATSC2s	Average centered Broto-Moreau autocorrelation - lag 2 / weighted by I-state
250	AATSC3s	Average centered Broto-Moreau autocorrelation - lag 3 / weighted by I-state
251	AATSC4s	Average centered Broto-Moreau autocorrelation - lag 4 / weighted by I-state
252	AATSC5s	Average centered Broto-Moreau autocorrelation - lag 5 / weighted by I-state
252	AATSC6s	
253	JAA I DC08	Average centered Broto-Moreau autocorrelation - lag 6 / weighted by I-state
254	AATSC7s	Average centered Broto-Moreau autocorrelation - lag 7 /
		weighted by I-state
255	AATSC8s	Average centered Broto-Moreau autocorrelation - lag 8 /
		weighted by I-state
256	MATS1c	Moran autocorrelation - lag 1 / weighted by charges
257	MATS2c	Moran autocorrelation - lag 2 / weighted by charges
258	MATS3c	Moran autocorrelation - lag 3 / weighted by charges
230	William	iviorali autocorrelation - lag 57 weighted by charges
259	MATS4c	Moran autocorrelation - lag 4 / weighted by charges
260	MATS5c	Moran autocorrelation - lag 5 / weighted by charges
261	MATS6c	Moran autocorrelation - lag 6 / weighted by charges
262	MATS7c	Moran autocorrelation - lag 7 / weighted by charges
263	MATS8c	Moran autocorrelation - lag 8 / weighted by charges
264	MATS1m	Moran autocorrelation - lag 1 / weighted by mass
	MATS2m	Moran autocorrelation - lag 2 / weighted by mass
267	MATS4m MATS4m	Moran autocorrelation - lag 3 / weighted by mass Moran autocorrelation - lag 4 / weighted by mass
268	MATS5m	Moran autocorrelation - lag 5 / weighted by mass
	MATS6m	Moran autocorrelation - lag 6 / weighted by mass
271	MATS7m MATS8m	Moran autocorrelation - lag 7 / weighted by mass Moran autocorrelation - lag 8 / weighted by mass
272	MATS1v	Moran autocorrelation - lag 1 / weighted by van der Waals volumes
273	MATS2v	Moran autocorrelation - lag 2 / weighted by van der Waals
274	MATS3v	wolumes Moran autocorrelation - lag 3 / weighted by van der Waals
275	MATS4v	volumes Moran autocorrelation - lag 4 / weighted by van der Waals
		volumes
	MATS5v	Moran autocorrelation - lag 5 / weighted by van der Waals volumes
277	MATS6v	Moran autocorrelation - lag 6 / weighted by van der Waals volumes
278	MATS7v	Moran autocorrelation - lag 7 / weighted by van der Waals
279	MATS8v	wolumes Moran autocorrelation - lag 8 / weighted by van der Waals
		volumes
280	MATS1e	Moran autocorrelation - lag 1 / weighted by Sanderson electronegativities
281	MATS2e	Moran autocorrelation - lag 2 / weighted by Sanderson
	-	electronegativities
1		

SubFP244		
	Phosphoric diestermonoamide	[PX4D4](=[OX1])([OX2][#6;!\$(C =[O,N,S])])([OX2][#6;!\$(C=[O,N,
	diestermonoamide	S])])[#7X3;\$([H2]),\$([H1][#6;!\$(
		C=[O,N,S])]),\$([#7]([#6;!\$(C=[O, N,S])])[#6;!\$(C=[O,N,S])])]
		11,3]/]/[#0,:\$(C=[O,11,3]/]/]
SubFP245	Phosphoric	[PX4D4](=[OX1])([OX2][#6;!\$(C
	monoesterdiamide	=[O,N,S])])([#7X3;\$([H2]),\$([H1] [#6;!\$(C=[O,N,S])]),\$([#7]([#6;!\$(
		C=[O,N,S])])[#6;!\$(C=[O,N,S])])]
)[#7X3;\$([H2]),\$([H1][#6;!\$(C=[O,N,S])]),\$([#7]([#6;!\$(C=[O,N,S]
)])[#6;!\$(C=[O,N,S])])]
SubFP246	Phosphoric acid derivative	[PX4D4](=[!#6])([!#6])([!#6])[!#6]
SubFP247		
SubFP247	Phosphinic acid	[PX4;\$([H2]),\$([H1][#6]),\$([H0]([#6])[#6])](=[OX1])[\$([OX2H]),\$([
G 1 FD2 10	Di Li i	OX1-])]
SubFP248	Phosphinic ester	[PX4;\$([H2]),\$([H1][#6]),\$([H0]([#6])[#6])](=[OX1])[OX2][#6;!\$(C
SubFP249	Phosphinic amide	=[O,N,S])] [PX4;\$([H2]),\$([H1][#6]),\$([H0]([
	F	#6])[#6])](=[OX1])[#7X3;\$([H2]),
		\$([H1][#6;!\$(C=[O,N,S])]),\$([#7]([#6;!\$(C=[O,N,S])])[#6;!\$(C=[O,
		N,S])])]
SubFP250	Phosphinic acid derivative	[PX4;\$([H2]),\$([H1][#6]),\$([H0]([#6])[#6])](=[!#6])[!#6]
SubFP251	Phosphonous acid	[PX3;\$([H1]),\$([H0][#6])]([\$([OX
		2H]),\$([OX1-])])[\$([OX2H]),\$([OX1-])]
SubFP252	Phosphonous monoester	[PX3;\$([H1]),\$([H0][#6])]([\$([OX
		2H]),\$([OX1-
SubFP253	Phosphonous diester])])[OX2][#6;!\$(C=[O,N,S])] [PX3;\$([H1]),\$([H0][#6])]([OX2][
		#6;!\$(C=[O,N,S])])[OX2][#6;!\$(C
SubFP254	Phosphonous monoamide	=[O,N,S])] [PX3;\$([H1]),\$([H0][#6])]([\$([OX
2011201	I nospiionous monoumus	2H]),\$([OX1-
])])[#7X3;\$([H2]),\$([H1][#6;!\$(C =[O,N,S])]),\$([#7]([#6;!\$(C=[O,N,
		S])])[#6;!\$(C=[O,N,S])])]
SubFP255	Phosphonous diamide	[PX3;\$([H1]),\$([H0][#6])]([#7X3;
Suoff 233	r nosphonous diamide	\$([H2]),\$([H1][#6;!\$(C=[O,N,S])]
),\$([#7]([#6;!\$(C=[O,N,S])])[#6;!\$
		(C=[O,N,S])])]#7X3;\$([H2]),\$([H1][#6;!\$(C=[O,N,S])]),\$([#7]([#
		6;!\$(C=[O,N,S])])[#6;!\$(C=[O,N,S
SubFP256	Phosphonous esteramide])])] [PX3;\$([H1]),\$([H0][#6])]([OX2][
54011250	Thosphonous esteramae	#6;!\$(C=[O,N,S])])[#7X3;\$([H2]),
		\$([H1][#6;!\$(C=[O,N,S])]),\$([#7]([#6;!\$(C=[O,N,S])])[#6;!\$(C=[O,
		[n, 0, 0, 0, 0, 0]
SubFP257	Phosphonous derivatives	[PX3;\$([D2]),\$([D3][#6])]([!#6])[!
SubFP258	Phosphinous acid	#6] [PX3;\$([H2]),\$([H1][#6]),\$([H0]([
		#6])[#6])][\$([OX2H]),\$([OX1-])]
SubFP259	Phosphinous ester	[PX3;\$([H2]),\$([H1][#6]),\$([H0]([
		#6])[#6])][OX2][#6;!\$(C=[O,N,S])
SubFP260	Phosphinous amide	[PX3;\$([H2]),\$([H1][#6]),\$([H0]([
		#6])[#6])][#7X3;\$([H2]),\$([H1][# 6;!\$(C=[O,N,S])]),\$([#7]([#6;!\$(C
		= [O,N,S])])[#6;!\$(C=[O,N,S])])
SubFP261	Phosphinous derivatives	[PX3;\$([H2]),\$([H1][#6]),\$([H0]([
	r nospinnous derivatives	#6])[#6])][!#6]
SubFP262 SubFP263		
3u011 203	Quart silane	[SiX4]([#6])([#6])[#6]
	Quart silane Non-quart silane	
SubED264	Non-quart silane	[SiX4]([#6])([#6])([#6])[#6] [SiX4;\$([H1]([#6])([#6]),\$([H2]([#6])[#6]),\$([H3][#6]),\$([H4])]
SubFP264		[SiX4]([#6])([#6])([#6])[#6] [SiX4;\$([H1]([#6])([#6])[#6]),\$([H2]([#6])[#6]),\$([H3][#6]),\$([H4]
SubFP265	Non-quart silane Silylmonohalide Het trialkylsilane	[SiX4]([#6])([#6])([#6])[#6] [SiX4;\$([H1]([#6])([#6]),\$([H2]([#6])[#6]),\$([H3][#6]),\$([H4])] [SiX4]([FX1,CIX1,BrX1,IX1])([# 6])([#6])[#6] [SiX4]([!#6])([#6])([#6])[#6]
	Non-quart silane Silylmonohalide	[SiX4]([#6])([#6])([#6])[#6] [SiX4;\$([H1]([#6])([#6]),\$([H2]([#6])[#6]),\$([H3][#6]),\$([H4])] [SiX4]([FX1,ClX1,BrX1,IX1])([# 6])([#6])[#6]
SubFP265 SubFP266	Non-quart silane Silylmonohalide Het trialkylsilane Dihet dialkylsilane	[SiX4]([#6])([#6])([#6])[#6] [SiX4;\$([H1]([#6])([#6]),\$([H2]([#6])[#6]),\$([H3][#6]),\$([H4])] [SiX4]([FX1,ClX1,BrX1,IX1])([# 6])([#6])[#6] [SiX4]([!#6])([#6])([#6])[#6] [SiX4]([!#6])([#6])([#6])[#6]
SubFP265 SubFP266 SubFP267	Non-quart silane Silylmonohalide Het trialkylsilane Dihet dialkylsilane Trihet alkylsilane Silicic acid derivative	[SiX4]([#6])([#6])([#6])[#6] [SiX4;\$([H1]([#6])([#6]),\$([H4]),\$([H4])] [H2]([#6])[#6]),\$([H3][#6]),\$([H4])] [SiX4]([FX1,ClX1,BrX1,IX1])([#6])([#6])[#6] [SiX4]([!#6])([#6])([#6])[#6] [SiX4]([!#6])([!#6])([#6])[#6] [SiX4]([!#6])([!#6])([!#6])[#6] [SiX4]([!#6])([!#6])([!#6])[#6]
SubFP265 SubFP266 SubFP267 SubFP268 SubFP269 SubFP270	Non-quart silane Silylmonohalide Het trialkylsilane Dihet dialkylsilane Trihet alkylsilane Silicic acid derivative Trialkylborane Boric acid derivatives	[SiX4]([#6])([#6])([#6])[#6] [SiX4;\$([H1]([#6])([#6]),\$([H4]),\$([H4])] [H2]([#6])[#6]),\$([H3][#6]),\$([H4])] [SiX4]([FX1,ClX1,BrX1,IX1])([#6])([#6])[#6] [SiX4]([!#6])([#6])([#6])[#6] [SiX4]([!#6])([!#6])([#6])[#6] [SiX4]([!#6])([!#6])([!#6])[#6] [SiX4]([!#6])([!#6])([!#6])[!#6] [SiX4]([!#6])([!#6])([!#6])[!#6] [BX3]([#6])([#6])[#6]
SubFP265 SubFP266 SubFP267 SubFP268 SubFP269	Non-quart silane Silylmonohalide Het trialkylsilane Dihet dialkylsilane Trihet alkylsilane Silicic acid derivative Trialkylborane Boric acid derivatives Boronic acid derivative	[SiX4]([#6])([#6])([#6])[#6] [SiX4;\$([H1]([#6])([#6]),\$([H4]),\$([H4])] [H2]([#6])[#6]),\$([H3][#6]),\$([H4])] [SiX4]([FX1,ClX1,BrX1,IX1])([#6])([#6])[#6] [SiX4]([!#6])([#6])([#6])[#6] [SiX4]([!#6])([!#6])([#6])[#6] [SiX4]([!#6])([!#6])([!#6])[#6] [SiX4]([!#6])([!#6])([!#6])[!#6] [BX3]([#6])([#6])[#6] [BX3]([!#6])([!#6])[!#6]
SubFP265 SubFP266 SubFP267 SubFP268 SubFP269 SubFP270 SubFP271 SubFP272	Non-quart silane Silylmonohalide Het trialkylsilane Dihet dialkylsilane Trihet alkylsilane Silicic acid derivative Trialkylborane Boric acid derivatives Boronic acid derivative Borohydride	[SiX4]([#6])([#6])([#6])[#6] [SiX4;\$([H1]([#6])([#6]),\$([H4]),\$([H4])] [H2]([#6])[#6]),\$([H3][#6]),\$([H4])] [SiX4]([FX1,ClX1,BrX1,IX1])([#6])([#6])[#6] [SiX4]([!#6])([#6])([#6])[#6] [SiX4]([!#6])([!#6])([#6])[#6] [SiX4]([!#6])([!#6])([!#6])[#6] [SiX4]([!#6])([!#6])([!#6])[#6] [SiX4]([!#6])([!#6])([!#6])[!#6] [BX3]([#6])([#6])[#6] [BX3]([!#6])([!#6])[!#6] [BX3]([!#6])([!#6])[!#6]
SubFP265 SubFP266 SubFP267 SubFP268 SubFP269 SubFP270 SubFP271	Non-quart silane Silylmonohalide Het trialkylsilane Dihet dialkylsilane Trihet alkylsilane Silicic acid derivative Trialkylborane Boric acid derivatives Boronic acid derivative	[SiX4]([#6])([#6])([#6])[#6] [SiX4;\$([H1]([#6])([#6]),\$([H4]),\$([H4])] [H2]([#6])[#6]),\$([H3][#6]),\$([H4])] [SiX4]([FX1,ClX1,BrX1,IX1])([#6])([#6])[#6] [SiX4]([!#6])([#6])([#6])[#6] [SiX4]([!#6])([!#6])([#6])[#6] [SiX4]([!#6])([!#6])([!#6])[#6] [SiX4]([!#6])([!#6])([!#6])[!#6] [BX3]([#6])([#6])[#6] [BX3]([!#6])([!#6])[!#6]
SubFP265 SubFP266 SubFP267 SubFP268 SubFP269 SubFP270 SubFP271 SubFP272	Non-quart silane Silylmonohalide Het trialkylsilane Dihet dialkylsilane Trihet alkylsilane Silicic acid derivative Trialkylborane Boric acid derivatives Boronic acid derivative Borohydride	[SiX4]([#6])([#6])([#6])[#6] [SiX4;\$([H1]([#6])([#6]),\$([H4]),\$([H4])] [H2]([#6])[#6]),\$([H3][#6]),\$([H4])] [SiX4]([FX1,CIX1,BrX1,IX1])([#6])([#6])[#6] [SiX4]([!#6])([#6])([#6])[#6] [SiX4]([!#6])([!#6])([#6])[#6] [SiX4]([!#6])([!#6])([!#6])[#6] [SiX4]([!#6])([!#6])([!#6])[!#6] [SiX4]([!#6])([!#6])([!#6])[!#6] [BX3]([#6])([#6])[#6] [BX3]([!#6])([!#6])[!#6] [BX3]([!#6])([!#6])[!#6]
SubFP265 SubFP266 SubFP267 SubFP268 SubFP269 SubFP270 SubFP271 SubFP272 SubFP273	Non-quart silane Silylmonohalide Het trialkylsilane Dihet dialkylsilane Trihet alkylsilane Silicic acid derivative Trialkylborane Boric acid derivatives Boronic acid derivative Borohydride Quaternary boron	[SiX4]([#6])([#6])([#6])[#6] [SiX4;\$([H1]([#6])([#6]),\$([H4]),\$([H4])] [H2]([#6])[#6]),\$([H3][#6]),\$([H4])] [SiX4]([FX1,ClX1,BrX1,IX1])([#6])([#6])[#6] [SiX4]([!#6])([#6])([#6])[#6] [SiX4]([!#6])([!#6])([#6])[#6] [SiX4]([!#6])([!#6])([!#6])[#6] [SiX4]([!#6])([!#6])([!#6])[!#6] [BX3]([#6])([#6])[#6] [BX3]([!#6])([!#6])[!#6] [BX3]([!#6])([!#6])[!#6] [BX3]([!#6])([!#6])[!#6] [BX3]([!#6])([!#6])[!#6]
SubFP265 SubFP266 SubFP267 SubFP268 SubFP269 SubFP270 SubFP271 SubFP272 SubFP273	Non-quart silane Silylmonohalide Het trialkylsilane Dihet dialkylsilane Trihet alkylsilane Silicic acid derivative Trialkylborane Boric acid derivatives Boronic acid derivative Borohydride Quaternary boron Aromatic	[SiX4]([#6])([#6])([#6])[#6] [SiX4;\$([H1]([#6])([#6]),\$([H4]),\$([H4])] [SiX4]([#6]),\$([H3][#6]),\$([H4])] [SiX4]([FX1,CIX1,BrX1,IX1])([#6])([#6])[#6] [SiX4]([!#6])([#6])([#6])[#6] [SiX4]([!#6])([!#6])([#6])[#6] [SiX4]([!#6])([!#6])([!#6])[#6] [SiX4]([!#6])([!#6])([!#6])[!#6] [BX3]([#6])([#6])[#6] [BX3]([#6])([!#6])[!#6] [BX3]([!#6])([!#6])[!#6] [BX3]([!#6])([!#6])[!#6] [BX3]([!#6])([!#6])[!#6]
SubFP265 SubFP266 SubFP267 SubFP268 SubFP269 SubFP270 SubFP271 SubFP272 SubFP273 SubFP274 SubFP275 SubFP276	Non-quart silane Silylmonohalide Het trialkylsilane Dihet dialkylsilane Trihet alkylsilane Silicic acid derivative Trialkylborane Boric acid derivatives Boronic acid derivative Borohydride Quaternary boron Aromatic Heterocyclic Epoxide	[SiX4]([#6])([#6])([#6])[#6] [SiX4;\$([H1]([#6])([#6]),\$([H4]),\$([H4])] [SiX4]([#6]),\$([H3][#6]),\$([H4])] [SiX4]([FX1,ClX1,BrX1,IX1])([#6])([#6])[#6] [SiX4]([!#6])([#6])([#6])[#6] [SiX4]([!#6])([!#6])([#6])[#6] [SiX4]([!#6])([!#6])([!#6])[!#6] [SiX4]([!#6])([!#6])([!#6])[!#6] [BX3]([#6])([#6])[#6] [BX3]([!#6])([!#6])[!#6] [BX3]([!#6])([!#6])[!#6] [BX4] [BX4] [BX4] [BX4]
SubFP265 SubFP266 SubFP267 SubFP268 SubFP269 SubFP270 SubFP271 SubFP272 SubFP273 SubFP274 SubFP275 SubFP276 SubFP277	Non-quart silane Silylmonohalide Het trialkylsilane Dihet dialkylsilane Trihet alkylsilane Silicic acid derivative Trialkylborane Boric acid derivatives Boronic acid derivative Borohydride Quaternary boron Aromatic Heterocyclic Epoxide NH aziridine	[SiX4]([#6])([#6])([#6])[#6] [SiX4;\$([H1]([#6])([#6]),\$([H4]),\$([H4])] [SiX4]([#6]),\$([H3][#6]),\$([H4])] [SiX4]([FX1,C1X1,BrX1,IX1])([#6])([#6])[#6] [SiX4]([!#6])([#6])([#6])[#6] [SiX4]([!#6])([!#6])([#6])[#6] [SiX4]([!#6])([!#6])([!#6])[#6] [SiX4]([!#6])([!#6])([!#6])[!#6] [BX3]([#6])([#6])[#6] [BX3]([!#6])([!#6])[!#6] [BX3]([!#6])([!#6])[!#6] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4]
SubFP265 SubFP266 SubFP267 SubFP268 SubFP269 SubFP270 SubFP271 SubFP272 SubFP273 SubFP274 SubFP275 SubFP276	Non-quart silane Silylmonohalide Het trialkylsilane Dihet dialkylsilane Trihet alkylsilane Silicic acid derivative Trialkylborane Boric acid derivatives Boronic acid derivative Borohydride Quaternary boron Aromatic Heterocyclic Epoxide	[SiX4]([#6])([#6])([#6])[#6] [SiX4;\$([H1]([#6])([#6]),\$([H4]),\$([H4])] [SiX4]([#6]),\$([H3][#6]),\$([H4])] [SiX4]([FX1,ClX1,BrX1,IX1])([#6])([#6])[#6] [SiX4]([!#6])([#6])([#6])[#6] [SiX4]([!#6])([!#6])([#6])[#6] [SiX4]([!#6])([!#6])([!#6])[!#6] [SiX4]([!#6])([!#6])([!#6])[!#6] [BX3]([#6])([#6])[#6] [BX3]([!#6])([!#6])[!#6] [BX3]([!#6])([!#6])[!#6] [BX4] [BX4] [BX4] [BX4]
SubFP265 SubFP266 SubFP267 SubFP268 SubFP269 SubFP270 SubFP271 SubFP272 SubFP273 SubFP274 SubFP275 SubFP276 SubFP277	Non-quart silane Silylmonohalide Het trialkylsilane Dihet dialkylsilane Trihet alkylsilane Silicic acid derivative Trialkylborane Boric acid derivatives Boronic acid derivative Borohydride Quaternary boron Aromatic Heterocyclic Epoxide NH aziridine	[SiX4]([#6])([#6])([#6])[#6] [SiX4;\$([H1]([#6])([#6]),\$([H4]),\$([H4])] [SiX4]([FX1,C1X1,BrX1,IX1])([#6])([#6])[#6] [SiX4]([!#6])([#6])([#6])[#6] [SiX4]([!#6])([!#6])([#6])[#6] [SiX4]([!#6])([!#6])([!#6])[#6] [SiX4]([!#6])([!#6])([!#6])[!#6] [BX3]([#6])([#6])[#6] [BX3]([#6])([#6])[!#6] [BX3]([!#6])([!#6])[!#6] [BX3]([!#6])([!#6])[!#6] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4]
SubFP265 SubFP266 SubFP267 SubFP268 SubFP269 SubFP270 SubFP271 SubFP272 SubFP273 SubFP274 SubFP275 SubFP276 SubFP277	Non-quart silane Silylmonohalide Het trialkylsilane Dihet dialkylsilane Trihet alkylsilane Silicic acid derivative Trialkylborane Boric acid derivatives Boronic acid derivative Borohydride Quaternary boron Aromatic Heterocyclic Epoxide NH aziridine Spiro	[SiX4]([#6])([#6])([#6])[#6] [SiX4;\$([H1]([#6])([#6]),\$([H4]),\$([H4])] [SiX4]([#6]),\$([H3][#6]),\$([H4])] [SiX4]([FX1,CIX1,BrX1,IX1])([#6])([#6])[#6] [SiX4]([!#6])([#6])([#6])[#6] [SiX4]([!#6])([!#6])([#6])[#6] [SiX4]([!#6])([!#6])([!#6])[!#6] [SiX4]([!#6])([!#6])([!#6])[!#6] [BX3]([#6])([#6])[#6] [BX3]([!#6])([!#6])[!#6] [BX3]([!#6])([!#6])[!#6] [BX3]([!#6])([!#6])[!#6] [BX4] a [!#6;!R0] [OX2r3]1[#6r3][#6r3]1 [NX3H1r3]1[#6r3][#6r3]1
SubFP265 SubFP266 SubFP267 SubFP268 SubFP269 SubFP270 SubFP271 SubFP272 SubFP273 SubFP274 SubFP275 SubFP276 SubFP276 SubFP277 SubFP278	Non-quart silane Silylmonohalide Het trialkylsilane Dihet dialkylsilane Trihet alkylsilane Silicic acid derivative Trialkylborane Boric acid derivatives Boronic acid derivative Borohydride Quaternary boron Aromatic Heterocyclic Epoxide NH aziridine Spiro Annelated rings	[SiX4]([#6])([#6])([#6])[#6] [SiX4;\$([H1]([#6])([#6])[#6]),\$([H4])] [SiX4;\$([H1]([#6]),\$([H3][#6]),\$([H4])] [SiX4]([FX1,CIX1,BrX1,IX1])([#6])([#6])[#6] [SiX4]([!#6])([#6])([#6])[#6] [SiX4]([!#6])([!#6])([#6])[#6] [SiX4]([!#6])([!#6])([!#6])[!#6] [SiX4]([!#6])([!#6])([!#6])[!#6] [BX3]([#6])([#6])[!#6] [BX3]([!#6])([!#6])[!#6] [BX3]([!#6])([!#6])[!#6] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [B
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SubFP265 SubFP266 SubFP267 SubFP268 SubFP269 SubFP270 SubFP271 SubFP272 SubFP273 SubFP274 SubFP275 SubFP276 SubFP276 SubFP277 SubFP278	Non-quart silane Silylmonohalide Het trialkylsilane Dihet dialkylsilane Trihet alkylsilane Silicic acid derivative Trialkylborane Boric acid derivatives Boronic acid derivative Borohydride Quaternary boron Aromatic Heterocyclic Epoxide NH aziridine Spiro Annelated rings	[SiX4]([#6])([#6])([#6])[#6] [SiX4;\$([H1]([#6])([#6])[#6]),\$([H4])] [SiX4;\$([H1]([#6]),\$([H3][#6]),\$([H4])] [SiX4]([FX1,CIX1,BrX1,IX1])([#6])([#6])[#6] [SiX4]([!#6])([#6])([#6])[#6] [SiX4]([!#6])([!#6])([#6])[#6] [SiX4]([!#6])([!#6])([!#6])[!#6] [SiX4]([!#6])([!#6])([!#6])[!#6] [BX3]([#6])([#6])[!#6] [BX3]([!#6])([!#6])[!#6] [BX3]([!#6])([!#6])[!#6] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [B
SubFP265 SubFP266 SubFP267 SubFP268 SubFP269 SubFP270 SubFP271 SubFP272 SubFP273 SubFP274 SubFP275 SubFP276 SubFP276 SubFP277 SubFP278	Non-quart silane Silylmonohalide Het trialkylsilane Dihet dialkylsilane Trihet alkylsilane Silicic acid derivative Trialkylborane Boric acid derivatives Boronic acid derivative Borohydride Quaternary boron Aromatic Heterocyclic Epoxide NH aziridine Spiro Annelated rings	[SiX4]([#6])([#6])([#6])[#6] [SiX4;\$([H1]([#6])([#6])[#6]),\$([H4])] [SiX4]([#6]),\$([H3][#6]),\$([H4])] [SiX4]([FX1,CIX1,BrX1,IX1])([#6])([#6])[#6] [SiX4]([!#6])([#6])([#6])[#6] [SiX4]([!#6])([!#6])([#6])[#6] [SiX4]([!#6])([!#6])([!#6])[#6] [SiX4]([!#6])([!#6])([!#6])[#6] [BX3]([#6])([!#6])[!#6] [BX3]([!#6])([!#6])[!#6] [BX3]([!#6])([!#6])[!#6] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX
SubFP265 SubFP266 SubFP267 SubFP268 SubFP269 SubFP270 SubFP271 SubFP272 SubFP273 SubFP274 SubFP275 SubFP276 SubFP276 SubFP277 SubFP278	Non-quart silane Silylmonohalide Het trialkylsilane Dihet dialkylsilane Trihet alkylsilane Silicic acid derivative Trialkylborane Boric acid derivatives Boronic acid derivative Borohydride Quaternary boron Aromatic Heterocyclic Epoxide NH aziridine Spiro Annelated rings	[SiX4]([#6])([#6])([#6])[#6] [SiX4;\$([H1]([#6])([#6])[#6]),\$([H4])] [SiX4]([FX1,CIX1,BrX1,IX1])([#6])([#6])[#6] [SiX4]([!#6])([#6])([#6])[#6] [SiX4]([!#6])([!#6])([#6])[#6] [SiX4]([!#6])([!#6])([#6])[#6] [SiX4]([!#6])([!#6])([!#6])[#6] [SiX4]([!#6])([!#6])([!#6])[!#6] [BX3]([#6])([!#6])[!#6] [BX3]([!#6])([!#6])[!#6] [BX3]([!#6])([!#6])[!#6] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4] [BX4]
SubFP265 SubFP266 SubFP267 SubFP268 SubFP269 SubFP270 SubFP271 SubFP272 SubFP273 SubFP274 SubFP275 SubFP276 SubFP276 SubFP277 SubFP278	Non-quart silane Silylmonohalide Het trialkylsilane Dihet dialkylsilane Trihet alkylsilane Silicic acid derivative Trialkylborane Boric acid derivatives Boronic acid derivative Borohydride Quaternary boron Aromatic Heterocyclic Epoxide NH aziridine Spiro Annelated rings	[SiX4]([#6])([#6])([#6])[#6] [SiX4;\$([H1]([#6])([#6]),\$([H4]),\$([H4])] [SiX4]([#6]),\$([H3][#6]),\$([H4])] [SiX4]([FX1,CIX1,BrX1,IX1])([#6])([#6])[#6] [SiX4]([!#6])([#6])([#6])([#6])[#6] [SiX4]([!#6])([!#6])([!#6])[#6] [SiX4]([!#6])([!#6])([!#6])[#6] [BX3]([#6])([#6])[#6] [BX3]([!#6])([!#6])[!#6] [BX3]([!#6])([!#6])[!#6] [BX4] [

282	MATS3e	Moran autocorrelation - lag 3 / weighted by Sanderson electronegativities
		electionegui vides
283	MATS4e	Moran autocorrelation - lag 4 / weighted by Sanderson
		electronegativities
294	MATS5e	Moran autocorrelation - lag 5 / weighted by Sanderson
204	WATSSE	electronegativities
295	MATS6e	Managed and the Company of the Company of the Company of the Company of the Company of the Company of the Company of the Company of the Company of the Company of the Company of the Company of the Company of the Company of the Company of the Company of the Company of the Company of the Company of the Company of the Company of the Company of the Company of the Company of the Company of the Company of the Company of the Company of the Company of the Company of the Company of the Company of the Company of the Company of the Company of the Company of the Company of the Company of the Company of the Company of the Company of the Company of the Company of the Company of the Company of the Company of the Company of the Company of the Company of the Company of the Company of the Company of the Company of the Company of the Company of the Company of the Company of the Company of the Company of the Company of the Company of the Company of the Company of the Company of the Company of the Company of the Company of the Company of the Company of the Company of the Company of the Company of the Company of the Company of the Company of the Company of the Company of the Company of the Company of the Company of the Company of the Company of the Company of the Company of the Company of the Company of the Company of the Company of the Company of the Company of the Company of the Company of the Company of the Company of the Company of the Company of the Company of the Company of the Company of the Company of the Company of the Company of the Company of the Company of the Company of the Company of the Company of the Company of the Company of the Company of the Company of the Company of the Company of the Company of the Company of the Company of the Company of the Company of the Company of the Company of the Company of the Company of the Company of the Company of the Company of the Company of the Company of the Company of the Company of the Company of the Company of the Company of the Company of the Company of the Company of the Compa
283	MAISOE	Moran autocorrelation - lag 6 / weighted by Sanderson electronegativities
286	MATS7e	Moran autocorrelation - lag 7 / weighted by Sanderson electronegativities
287	MATS8e	Moran autocorrelation - lag 8 / weighted by Sanderson
288	MATS1p	electronegativities Moran autocorrelation - lag 1 / weighted by polarizabilities
	MATS2p	Moran autocorrelation - lag 2 / weighted by polarizabilities
	MATS3p MATS4p	Moran autocorrelation - lag 3 / weighted by polarizabilities Moran autocorrelation - lag 4 / weighted by polarizabilities
291	MA134p	ivioran autocorrelation - rag 4 / weighted by polarizabilities
292	MATS5p	Moran autocorrelation - lag 5 / weighted by polarizabilities
293	MATS6p	Moran autocorrelation - lag 6 / weighted by polarizabilities
294	MATS7p	Moran autocorrelation - lag 7 / weighted by polarizabilities
	MATS8p MATS1i	Moran autocorrelation - lag 8 / weighted by polarizabilities Moran autocorrelation - lag 1 / weighted by first ionization
		potential
297	MATS2i	Moran autocorrelation - lag 2 / weighted by first ionization potential
298	MATS3i	Moran autocorrelation - lag 3 / weighted by first ionization
200	MATS4i	potential Moran autocorrelation - lag 4 / weighted by first ionization
		potential
300	MATS5i	Moran autocorrelation - lag 5 / weighted by first ionization potential
301	MATS6i	Moran autocorrelation - lag 6 / weighted by first ionization
301	141711501	potential
302	MATS7i	Moran autocorrelation - lag 7 / weighted by first ionization
202	MATS8i	potential
303	WA1561	Moran autocorrelation - lag 8 / weighted by first ionization potential
304	MATS1s	Moran autocorrelation - lag 1 / weighted by I-state
305	MATS2s	Moran autocorrelation - lag 2 / weighted by I-state
306	MATS3s	Moran autocorrelation - lag 3 / weighted by I-state
307	MATS4s	Moran autocorrelation - lag 4 / weighted by I-state
308	MATS5s	Moran autocorrelation - lag 5 / weighted by I-state
	MATS6s	Moran autocorrelation - lag 6 / weighted by I-state
	MATS7s MATS8s	Moran autocorrelation - lag 7 / weighted by I-state Moran autocorrelation - lag 8 / weighted by I-state
312	GATS1c	Geary autocorrelation - lag 1 / weighted by charges
	GATS2c GATS3c	Geary autocorrelation - lag 2 / weighted by charges Geary autocorrelation - lag 3 / weighted by charges
315	GATS4c	Geary autocorrelation - lag 4 / weighted by charges
	GATS5c GATS6c	Geary autocorrelation - lag 5 / weighted by charges Geary autocorrelation - lag 6 / weighted by charges
318	GATS7c	Geary autocorrelation - lag 7 / weighted by charges
	GATS8c GATS1m	Geary autocorrelation - lag 8 / weighted by charges Geary autocorrelation - lag 1 / weighted by mass
321	GATS2m	Geary autocorrelation - lag 2 / weighted by mass
	GATS3m GATS4m	Geary autocorrelation - lag 3 / weighted by mass Geary autocorrelation - lag 4 / weighted by mass
324	GATS5m	Geary autocorrelation - lag 5 / weighted by mass
	GATS6m GATS7m	Geary autocorrelation - lag 6 / weighted by mass
	GATS/m GATS8m	Geary autocorrelation - lag 7 / weighted by mass Geary autocorrelation - lag 8 / weighted by mass
328	GATS1v	Geary autocorrelation - lag 1 / weighted by van der Waals volumes
329	GATS2v	Geary autocorrelation - lag 2 / weighted by van der Waals
330	GATS3v	volumes Geary autocorrelation - lag 3 / weighted by van der Waals
330		volumes

SubFP282	Sugar pattern 2	[OX2;\$([r5]1@C(!@[OX2,NX3,S X2,FX1,ClX1,BrX1,IX1])@C@C @C1),\$([r6]1@C(!@[OX2,NX3,S X2,FX1,ClX1,BrX1,IX1])@C@C @C@C1)]
SubFP283	Sugar pattern combi	[OX2;\$([r5]1@C(!@[OX2,NX3,S X2,FX1,ClX1,BrX1,IX1])@C@C(O)@C1),\$([r6]1@C(!@[OX2,NX 3,SX2,FX1,ClX1,BrX1,IX1])@C @C(O)@C(O)@C1)]
SubFP284	Sugar pattern 2 reducing	[OX2;\$([r5]1@C(!@[OX2H1])@ C@C@C1),\$([r6]1@C(!@[OX2H 1])@C@C@C@CC1)]
SubFP285	Sugar pattern 2 alpha	[OX2;\$([r5]1@[C@@](!@[OX2, NX3,SX2,FX1,ClX1,BrX1,IX1]) @C@C@C1),\$([r6]1@[C@@](! @[OX2,NX3,SX2,FX1,ClX1,BrX 1,IX1])@C@C@C@C1)]
SubFP286	Sugar pattern 2 beta	[OX2;\$([r5]1@[C@](!@[OX2,NX 3,SX2,FX1,ClX1,BrX1,IX1])@C @C@C1),\$([r6]1@[C@](!@[OX2,NX3,SX2,FX1,ClX1,BrX1,IX1]) @C@C@C@C@C1)]
SubFP287	Conjugated double bond	*=*[*]=,#,:[*]
SubFP288	Conjugated tripple bond	*#*[*]=,#,:[*]
SubFP289	Cis double bond	*/[D2]=[D2]/*
SubFP290 SubFP291	Trans double bond Mixed anhydrides	*/[D2]=[D2]/* [\$(*=O),\$([#16,#14,#5]),\$([#7]([#6]=[OX1]))][#8X2][\$(*=O),\$([#16,#14,#5]),\$([#7]([#6]=[OX1]))]
SubFP292	Halogen on hetero	[FX1,ClX1,BrX1,IX1][!#6]
SubFP293	Halogen multi subst	[F,Cl,Br,I;!\$([X1]);!\$([X0-])]
SubFP294	Trifluoromethyl	[FX1][CX4;!\$([H0][Cl,Br,I]);!\$([F][C]([F])([F])]([FX1])([FX1])
SubFP295 SubFP296	C ONS bond Charged	[#6]~[#7,#8,#16] [!+0]
SubFP297	Anion	[-1,-2,-3,-4,-5,-6,-7]
SubFP298	Kation	[+1,+2,+3,+4,+5,+6,+7]
SubFP299	Salt	([-1,-2,-3,-4,-5,-6,-
SubFP300	1,3-Tautomerizable	7]).([+1,+2,+3,+4,+5,+6,+7]) [\$([#7X2,OX1,SX1]=*[!H0;!\$([a;!n])]),\$([#7X3,OX2,SX2;!H0]*=*),\$([#7X3,OX2,SX2;!H0]*:n)]
SubFP301	1,5-Tautomerizable	[\$([#7X2,OX1,SX1]=,:**=,:*[!H0 !\$([a;!n])]),\$([#7X3,OX2,SX2;!H0]]*=**=*),\$([#7X3,OX2,SX2;!H0] *=,:**:n)]
SubFP302	Rotatable bond	[!\$(*#*)&!D1]-!@[!\$(*#*)&!D1]
SubFP303	Michael acceptor	[CX3]=[CX3][\$([CX3]=[O,N,S]), \$(C#[N]),\$([S,P]=[OX1]),\$([NX3] =O),\$([NX3+](=O)[O-])]
SubFP304	Dicarbodiazene	[CX3](=[OX1])[NX2]=[NX2][CX 3](=[OX1])
SubFP305	CH-acidic	[\$([CX4;!\$([H0]);!\$(C[!#6;!\$([P,S]=O);!\$(N(~O)~O)])][\$([CX3]=[O,N,S]),\$(C#[N]),\$([S,P]=[OX1]),\$([NX3]=O),\$([NX3+](=O)[O-]);!\$(*[S,O,N;H1,H2]);!\$([*+0][S,O;X1-])]),\$([CX4;!\$([H0])]1[CX3]=[CX3][CX3]=[CX3]1)]
SubFP306	CH-acidic strong	[CX4;!\$([H0]);!\$(C[!#6;!\$([P,S]=O);!\$(N(~O)~O)])]([\$([CX3]=[O, N,S]),\$(C#[N]),\$([S,P]=[OX1]),\$([NX3]=O),\$([NX3+](=O)[O-]);!\$(*[S,O,N;H1,H2]);!\$([*+0][S,O;X1-])])[\$([CX3]=[O,N,S]),\$(C#[N]),\$([S,P]=[OX1]),\$([NX3]=O),\$([NX3+](=O)[O-]);!\$(*[S,O,N;H1,H2]);!\$([*+0][S,O;X1-])]
SubFP307	Chiral center specified	[\$([*@](~*)(~*)(*)*),\$([*@H](*)(*)*),\$([*@](~*)(*)*),\$([*@H](~*) ~*)]

221	GATS4v	Geary autocorrelation - lag 4 / weighted by van der Waals
		volumes
332	GATS5v	Geary autocorrelation - lag 5 / weighted by van der Waals volumes
333	GATS6v	Geary autocorrelation - lag 6 / weighted by van der Waals volumes
334	GATS7v	Geary autocorrelation - lag 7 / weighted by van der Waals
335	GATS8v	Volumes Geary autocorrelation - lag 8 / weighted by van der Waals
336	GATS1e	volumes Geary autocorrelation - lag 1 / weighted by Sanderson
	GATS2e	electronegativities Geary autocorrelation - lag 2 / weighted by Sanderson
		electronegativities
338	GATS3e	Geary autocorrelation - lag 3 / weighted by Sanderson electronegativities
339	GATS4e	Geary autocorrelation - lag 4 / weighted by Sanderson electronegativities
340	GATS5e	Geary autocorrelation - lag 5 / weighted by Sanderson
341	GATS6e	Geary autocorrelation - lag 6 / weighted by Sanderson
342	GATS7e	electronegativities Geary autocorrelation - lag 7 / weighted by Sanderson
3/13	GATS8e	electronegativities Geary autocorrelation - lag 8 / weighted by Sanderson
		electronegativities
	GATS1p GATS2p	Geary autocorrelation - lag 1 / weighted by polarizabilities Geary autocorrelation - lag 2 / weighted by polarizabilities
	GATS4n	Geary autocorrelation - lag 3 / weighted by polarizabilities
	GATS4p GATS5p	Geary autocorrelation - lag 4 / weighted by polarizabilities Geary autocorrelation - lag 5 / weighted by polarizabilities
	GATS6p	Geary autocorrelation - lag 6 / weighted by polarizabilities
	GATS7p	Geary autocorrelation - lag 7 / weighted by polarizabilities
	GATS1:	Geary autocorrelation - lag 8 / weighted by polarizabilities
	GATS1i	Geary autocorrelation - lag 1 / weighted by first ionization potential
353	GATS2i	Geary autocorrelation - lag 2 / weighted by first ionization potential
354	GATS3i	Geary autocorrelation - lag 3 / weighted by first ionization potential
355	GATS4i	Geary autocorrelation - lag 4 / weighted by first ionization potential
356	GATS5i	Geary autocorrelation - lag 5 / weighted by first ionization
357	GATS6i	potential Geary autocorrelation - lag 6 / weighted by first ionization
358	GATS7i	potential Geary autocorrelation - lag 7 / weighted by first ionization
	GATS8i	potential Geary autocorrelation - lag 8 / weighted by first ionization
		potential
	GATS1s	Geary autocorrelation - lag 1 / weighted by I-state
	GATS2s	Geary autocorrelation - lag 2 / weighted by I-state
	GATS3s GATS4s	Geary autocorrelation - lag 3 / weighted by I-state Geary autocorrelation - lag 4 / weighted by I-state
		Geary autocorrelation - lag 47 weighted by 1-state
104	(†ATS5s	Geary autocorrelation - lag 5 / weighted by I-state
	GATS5s GATS6s	Geary autocorrelation - lag 5 / weighted by I-state Geary autocorrelation - lag 6 / weighted by I-state
365	GATS5s GATS6s GATS7s	Geary autocorrelation - lag 6 / weighted by I-state
365 366	GATS6s	Geary autocorrelation - lag 6 / weighted by I-state Geary autocorrelation - lag 7 / weighted by I-state Geary autocorrelation - lag 8 / weighted by I-state
365 366 367	GATS6s GATS7s	Geary autocorrelation - lag 6 / weighted by I-state Geary autocorrelation - lag 7 / weighted by I-state
365 366 367 368	GATS6s GATS7s GATS8s	Geary autocorrelation - lag 6 / weighted by I-state Geary autocorrelation - lag 7 / weighted by I-state Geary autocorrelation - lag 8 / weighted by I-state Graph energy from Barysz matrix / weighted by atomic number Leading eigenvalue from Barysz matrix / weighted by atomic
365 366 367 368 369	GATS6s GATS7s GATS8s SpAbs_DzZ	Geary autocorrelation - lag 6 / weighted by I-state Geary autocorrelation - lag 7 / weighted by I-state Geary autocorrelation - lag 8 / weighted by I-state Graph energy from Barysz matrix / weighted by atomic number Leading eigenvalue from Barysz matrix / weighted by atomic number Spectral diameter from Barysz matrix / weighted by atomic
365 366 367 368 369	GATS6s GATS7s GATS8s SpAbs_DzZ SpMax_DzZ	Geary autocorrelation - lag 6 / weighted by I-state Geary autocorrelation - lag 7 / weighted by I-state Geary autocorrelation - lag 8 / weighted by I-state Graph energy from Barysz matrix / weighted by atomic number Leading eigenvalue from Barysz matrix / weighted by atomic number Spectral diameter from Barysz matrix / weighted by atomic number Spectral absolute deviation from Barysz matrix / weighted by
365 366 367 368 369 370	GATS6s GATS7s GATS8s SpAbs_DzZ SpMax_DzZ SpDiam_DzZ	Geary autocorrelation - lag 6 / weighted by I-state Geary autocorrelation - lag 7 / weighted by I-state Geary autocorrelation - lag 8 / weighted by I-state Graph energy from Barysz matrix / weighted by atomic number Leading eigenvalue from Barysz matrix / weighted by atomic number Spectral diameter from Barysz matrix / weighted by atomic number
365 366 367 368 369 370 371	GATS6s GATS7s GATS8s SpAbs_DzZ SpMax_DzZ SpDiam_DzZ SpAD_DzZ SpMAD_DzZ	Geary autocorrelation - lag 6 / weighted by I-state Geary autocorrelation - lag 7 / weighted by I-state Geary autocorrelation - lag 8 / weighted by I-state Graph energy from Barysz matrix / weighted by atomic number Leading eigenvalue from Barysz matrix / weighted by atomic number Spectral diameter from Barysz matrix / weighted by atomic number Spectral absolute deviation from Barysz matrix / weighted by atomic number Spectral mean absolute deviation from Barysz matrix / weighted by atomic number
365 366 367 368 369 370 371 372	GATS6s GATS7s GATS8s SpAbs_DzZ SpMax_DzZ SpDiam_DzZ SpAD_DzZ SpMAD_DzZ EE_DzZ	Geary autocorrelation - lag 6 / weighted by I-state Geary autocorrelation - lag 7 / weighted by I-state Geary autocorrelation - lag 8 / weighted by I-state Graph energy from Barysz matrix / weighted by atomic number Leading eigenvalue from Barysz matrix / weighted by atomic number Spectral diameter from Barysz matrix / weighted by atomic number Spectral absolute deviation from Barysz matrix / weighted by atomic number Spectral mean absolute deviation from Barysz matrix / weighted by atomic number Spectral mean absolute deviation from Barysz matrix / weighted by atomic number Estrada-like index from Barysz matrix / weighted by atomic number (ln(1+x))
365 366 367 368 369 370 371 372 373	GATS6s GATS7s GATS8s SpAbs_DzZ SpMax_DzZ SpDiam_DzZ SpAD_DzZ SpMAD_DzZ EE_DzZ SM1_DzZ	Geary autocorrelation - lag 6 / weighted by I-state Geary autocorrelation - lag 7 / weighted by I-state Geary autocorrelation - lag 8 / weighted by I-state Graph energy from Barysz matrix / weighted by atomic number Leading eigenvalue from Barysz matrix / weighted by atomic number Spectral diameter from Barysz matrix / weighted by atomic number Spectral absolute deviation from Barysz matrix / weighted by atomic number Spectral mean absolute deviation from Barysz matrix / weighted by atomic number Spectral mean absolute deviation from Barysz matrix / weighted by atomic number Estrada-like index from Barysz matrix / weighted by atomic number (ln(1+x)) Spectral moment of order 1 from Barysz matrix / weighted by atomic number
365 366 367 368 369 370 371 372 373 374	GATS6s GATS7s GATS8s SpAbs_DzZ SpMax_DzZ SpDiam_DzZ SpAD_DzZ SpMAD_DzZ EE_DzZ SM1_DzZ VE1_DzZ	Geary autocorrelation - lag 6 / weighted by I-state Geary autocorrelation - lag 7 / weighted by I-state Geary autocorrelation - lag 8 / weighted by I-state Graph energy from Barysz matrix / weighted by atomic number Leading eigenvalue from Barysz matrix / weighted by atomic number Spectral diameter from Barysz matrix / weighted by atomic number Spectral absolute deviation from Barysz matrix / weighted by atomic number Spectral mean absolute deviation from Barysz matrix / weighted by atomic number Estrada-like index from Barysz matrix / weighted by atomic number (ln(1+x)) Spectral moment of order 1 from Barysz matrix / weighted by atomic number Coefficient sum of the last eigenvector from Barysz matrix / weighted by atomic number
365 366 367 368 369 370 371 372 373 374	GATS6s GATS7s GATS8s SpAbs_DzZ SpMax_DzZ SpDiam_DzZ SpAD_DzZ SpMAD_DzZ EE_DzZ SM1_DzZ	Geary autocorrelation - lag 6 / weighted by I-state Geary autocorrelation - lag 7 / weighted by I-state Geary autocorrelation - lag 8 / weighted by I-state Graph energy from Barysz matrix / weighted by atomic number Leading eigenvalue from Barysz matrix / weighted by atomic number Spectral diameter from Barysz matrix / weighted by atomic number Spectral absolute deviation from Barysz matrix / weighted by atomic number Spectral mean absolute deviation from Barysz matrix / weighted by atomic number Estrada-like index from Barysz matrix / weighted by atomic number (ln(1+x)) Spectral moment of order 1 from Barysz matrix / weighted by atomic number Coefficient sum of the last eigenvector from Barysz matrix / weighted by atomic number Average coefficient sum of the last eigenvector from Barysz matrix / weighted by atomic number
365 366 367 368 369 370 371 372 373 374 375	GATS6s GATS7s GATS8s SpAbs_DzZ SpMax_DzZ SpDiam_DzZ SpAD_DzZ SpMAD_DzZ EE_DzZ SM1_DzZ VE1_DzZ	Geary autocorrelation - lag 6 / weighted by I-state Geary autocorrelation - lag 7 / weighted by I-state Geary autocorrelation - lag 8 / weighted by I-state Graph energy from Barysz matrix / weighted by atomic number Leading eigenvalue from Barysz matrix / weighted by atomic number Spectral diameter from Barysz matrix / weighted by atomic number Spectral absolute deviation from Barysz matrix / weighted by atomic number Spectral mean absolute deviation from Barysz matrix / weighted by atomic number Estrada-like index from Barysz matrix / weighted by atomic number (ln(1+x)) Spectral moment of order 1 from Barysz matrix / weighted by atomic number Coefficient sum of the last eigenvector from Barysz matrix / weighted by atomic number Average coefficient sum of the last eigenvector from Barysz matrix / weighted by atomic number Logarithmic coefficient sum of the last eigenvector from Barysz
365 366 367 368 369 370 371 372 373 374 375 376	GATS6s GATS7s GATS8s SpAbs_DzZ SpMax_DzZ SpDiam_DzZ SpAD_DzZ SpMAD_DzZ EE_DzZ SM1_DzZ VE1_DzZ VE2_DzZ	Geary autocorrelation - lag 6 / weighted by I-state Geary autocorrelation - lag 7 / weighted by I-state Geary autocorrelation - lag 8 / weighted by I-state Graph energy from Barysz matrix / weighted by atomic number Leading eigenvalue from Barysz matrix / weighted by atomic number Spectral diameter from Barysz matrix / weighted by atomic number Spectral absolute deviation from Barysz matrix / weighted by atomic number Spectral mean absolute deviation from Barysz matrix / weighted by atomic number Spectral mean absolute deviation from Barysz matrix / weighted by atomic number Estrada-like index from Barysz matrix / weighted by atomic number (ln(1+x)) Spectral moment of order 1 from Barysz matrix / weighted by atomic number Coefficient sum of the last eigenvector from Barysz matrix / weighted by atomic number Average coefficient sum of the last eigenvector from Barysz matrix / weighted by atomic number Logarithmic coefficient sum of the last eigenvector from Barysz matrix / weighted by atomic number Randic-like eigenvector-based index from Barysz matrix /
365 366 367 368 369 370 371 372 373 374 375 376 377	GATS6s GATS7s GATS8s SpAbs_DzZ SpMax_DzZ SpDiam_DzZ SpAD_DzZ SpMAD_DzZ EE_DzZ SM1_DzZ VE1_DzZ VE2_DzZ VE3_DzZ	Geary autocorrelation - lag 6 / weighted by I-state Geary autocorrelation - lag 7 / weighted by I-state Geary autocorrelation - lag 8 / weighted by I-state Graph energy from Barysz matrix / weighted by atomic number Leading eigenvalue from Barysz matrix / weighted by atomic number Spectral diameter from Barysz matrix / weighted by atomic number Spectral absolute deviation from Barysz matrix / weighted by atomic number Spectral mean absolute deviation from Barysz matrix / weighted by atomic number Spectral mean absolute deviation from Barysz matrix / weighted by atomic number Estrada-like index from Barysz matrix / weighted by atomic number (ln(1+x)) Spectral moment of order 1 from Barysz matrix / weighted by atomic number Coefficient sum of the last eigenvector from Barysz matrix / weighted by atomic number Average coefficient sum of the last eigenvector from Barysz matrix / weighted by atomic number Logarithmic coefficient sum of the last eigenvector from Barysz matrix / weighted by atomic number Randic-like eigenvector-based index from Barysz matrix / weighted by atomic number Normalized Randic-like eigenvector-based index from Barysz
365 366 367 368 369 370 371 372 373 374 375 376 377 378	GATS6s GATS7s GATS8s SpAbs_DzZ SpMax_DzZ SpDiam_DzZ SpAD_DzZ SpMAD_DzZ EE_DzZ SM1_DzZ VE1_DzZ VE2_DzZ VE3_DzZ VR1_DzZ	Geary autocorrelation - lag 6 / weighted by I-state Geary autocorrelation - lag 7 / weighted by I-state Geary autocorrelation - lag 8 / weighted by I-state Graph energy from Barysz matrix / weighted by atomic number Leading eigenvalue from Barysz matrix / weighted by atomic number Spectral diameter from Barysz matrix / weighted by atomic number Spectral absolute deviation from Barysz matrix / weighted by atomic number Spectral mean absolute deviation from Barysz matrix / weighted by atomic number Estrada-like index from Barysz matrix / weighted by atomic number (ln(1+x)) Spectral moment of order 1 from Barysz matrix / weighted by atomic number Coefficient sum of the last eigenvector from Barysz matrix / weighted by atomic number Logarithmic coefficient sum of the last eigenvector from Barysz matrix / weighted by atomic number Logarithmic coefficient sum of the last eigenvector from Barysz matrix / weighted by atomic number Randic-like eigenvector-based index from Barysz matrix / weighted by atomic number Normalized Randic-like eigenvector-based index from Barysz matrix / weighted by atomic number Logarithmic Randic-like eigenvector-based index from Barysz matrix / weighted by atomic number
365 366 367 368 369 370 371 372 373 374 375 376 377 378 379 380	GATS6s GATS7s GATS8s SpAbs_DzZ SpMax_DzZ SpMam_DzZ SpAD_DzZ SpMAD_DzZ EE_DzZ SM1_DzZ VE1_DzZ VE2_DzZ VR3_DzZ VR3_DzZ VR3_DzZ	Geary autocorrelation - lag 6 / weighted by I-state Geary autocorrelation - lag 7 / weighted by I-state Geary autocorrelation - lag 8 / weighted by I-state Graph energy from Barysz matrix / weighted by atomic number Leading eigenvalue from Barysz matrix / weighted by atomic number Spectral diameter from Barysz matrix / weighted by atomic number Spectral absolute deviation from Barysz matrix / weighted by atomic number Spectral mean absolute deviation from Barysz matrix / weighted by atomic number Estrada-like index from Barysz matrix / weighted by atomic number (ln(1+x)) Spectral moment of order 1 from Barysz matrix / weighted by atomic number Coefficient sum of the last eigenvector from Barysz matrix / weighted by atomic number Average coefficient sum of the last eigenvector from Barysz matrix / weighted by atomic number Logarithmic coefficient sum of the last eigenvector from Barysz matrix / weighted by atomic number Randic-like eigenvector-based index from Barysz matrix / weighted by atomic number Normalized Randic-like eigenvector-based index from Barysz matrix / weighted by atomic number Logarithmic Randic-like eigenvector-based index from Barysz matrix / weighted by atomic number
365 366 367 368 369 370 371 372 373 374 375 376 377 378 379 380 381	GATS6s GATS7s GATS8s SpAbs_DzZ SpMax_DzZ SpMam_DzZ SpAD_DzZ SpMAD_DzZ SpMAD_DzZ EE_DzZ SM1_DzZ VE1_DzZ VE2_DzZ VE3_DzZ VR1_DzZ VR2_DzZ VR2_DzZ	Geary autocorrelation - lag 6 / weighted by I-state Geary autocorrelation - lag 7 / weighted by I-state Geary autocorrelation - lag 8 / weighted by I-state Graph energy from Barysz matrix / weighted by atomic number Leading eigenvalue from Barysz matrix / weighted by atomic number Spectral diameter from Barysz matrix / weighted by atomic number Spectral absolute deviation from Barysz matrix / weighted by atomic number Spectral mean absolute deviation from Barysz matrix / weighted by atomic number Estrada-like index from Barysz matrix / weighted by atomic number (ln(1+x)) Spectral moment of order 1 from Barysz matrix / weighted by atomic number Coefficient sum of the last eigenvector from Barysz matrix / weighted by atomic number Logarithmic coefficient sum of the last eigenvector from Barysz matrix / weighted by atomic number Logarithmic coefficient sum of the last eigenvector from Barysz matrix / weighted by atomic number Randic-like eigenvector-based index from Barysz matrix / weighted by atomic number Normalized Randic-like eigenvector-based index from Barysz matrix / weighted by atomic number Logarithmic Randic-like eigenvector-based index from Barysz matrix / weighted by atomic number
365 366 367 368 369 370 371 372 373 374 375 376 377 378 379 380 381 382	GATS6s GATS7s GATS8s SpAbs_DzZ SpAbs_DzZ SpMax_DzZ SpAD_DzZ SpAD_DzZ SpMAD_DzZ EE_DzZ SM1_DzZ VE1_DzZ VE2_DzZ VE3_DzZ VR1_DzZ VR2_DzZ VR3_DzZ VR3_DzZ SpAbs_Dzm	Geary autocorrelation - lag 6 / weighted by I-state Geary autocorrelation - lag 7 / weighted by I-state Geary autocorrelation - lag 8 / weighted by I-state Graph energy from Barysz matrix / weighted by atomic number Leading eigenvalue from Barysz matrix / weighted by atomic number Spectral diameter from Barysz matrix / weighted by atomic number Spectral absolute deviation from Barysz matrix / weighted by atomic number Spectral mean absolute deviation from Barysz matrix / weighted by atomic number Estrada-like index from Barysz matrix / weighted by atomic number (ln(1+x)) Spectral moment of order 1 from Barysz matrix / weighted by atomic number Coefficient sum of the last eigenvector from Barysz matrix / weighted by atomic number Average coefficient sum of the last eigenvector from Barysz matrix / weighted by atomic number Logarithmic coefficient sum of the last eigenvector from Barysz matrix / weighted by atomic number Randic-like eigenvector-based index from Barysz matrix / weighted by atomic number Normalized Randic-like eigenvector-based index from Barysz matrix / weighted by atomic number Logarithmic Randic-like eigenvector-based index from Barysz matrix / weighted by atomic number Logarithmic Randic-like eigenvector-based index from Barysz matrix / weighted by atomic number
365 366 367 368 369 370 371 372 373 374 375 376 377 378 379 380 381 382 383	GATS6s GATS7s GATS8s SpAbs_DzZ SpMax_DzZ SpMam_DzZ SpAD_DzZ SpMAD_DzZ EE_DzZ SM1_DzZ VE1_DzZ VE2_DzZ VE3_DzZ VR1_DzZ VR2_DzZ VR3_DzZ VR3_DzZ SpAbs_Dzm SpMax_Dzm	Geary autocorrelation - lag 6 / weighted by I-state Geary autocorrelation - lag 7 / weighted by I-state Geary autocorrelation - lag 8 / weighted by I-state Graph energy from Barysz matrix / weighted by atomic number Leading eigenvalue from Barysz matrix / weighted by atomic number Spectral diameter from Barysz matrix / weighted by atomic number Spectral absolute deviation from Barysz matrix / weighted by atomic number Spectral mean absolute deviation from Barysz matrix / weighted by atomic number Estrada-like index from Barysz matrix / weighted by atomic number (ln(1+x)) Spectral moment of order 1 from Barysz matrix / weighted by atomic number Coefficient sum of the last eigenvector from Barysz matrix / weighted by atomic number Average coefficient sum of the last eigenvector from Barysz matrix / weighted by atomic number Logarithmic coefficient sum of the last eigenvector from Barysz matrix / weighted by atomic number Randic-like eigenvector-based index from Barysz matrix / weighted by atomic number Normalized Randic-like eigenvector-based index from Barysz matrix / weighted by atomic number Logarithmic Randic-like eigenvector-based index from Barysz matrix / weighted by atomic number Logarithmic Randic-like eigenvector-based index from Barysz matrix / weighted by atomic number Logarithmic Randic-like eigenvector-based index from Barysz matrix / weighted by atomic number
365 366 367 368 370 371 372 373 374 375 376 377 378 379 380 381 382 383 384	GATS6s GATS7s GATS8s SpAbs_DzZ SpAbs_DzZ SpMax_DzZ SpAD_DzZ SpAD_DzZ SpMAD_DzZ EE_DzZ SM1_DzZ VE1_DzZ VE2_DzZ VE3_DzZ VR1_DzZ VR2_DzZ VR3_DzZ SpAbs_Dzm SpMax_Dzm SpDiam_Dzm	Geary autocorrelation - lag 6 / weighted by I-state Geary autocorrelation - lag 7 / weighted by I-state Geary autocorrelation - lag 8 / weighted by I-state Graph energy from Barysz matrix / weighted by atomic number Leading eigenvalue from Barysz matrix / weighted by atomic number Spectral diameter from Barysz matrix / weighted by atomic number Spectral absolute deviation from Barysz matrix / weighted by atomic number Spectral mean absolute deviation from Barysz matrix / weighted by atomic number Estrada-like index from Barysz matrix / weighted by atomic number Estrada-like index from Barysz matrix / weighted by atomic number (ln(1+x)) Spectral moment of order 1 from Barysz matrix / weighted by atomic number Coefficient sum of the last eigenvector from Barysz matrix / weighted by atomic number Average coefficient sum of the last eigenvector from Barysz matrix / weighted by atomic number Logarithmic coefficient sum of the last eigenvector from Barysz matrix / weighted by atomic number Randic-like eigenvector-based index from Barysz matrix / weighted by atomic number Romalized Randic-like eigenvector-based index from Barysz matrix / weighted by atomic number Logarithmic Randic-like eigenvector-based index from Barysz matrix / weighted by atomic number Logarithmic Randic-like eigenvector-based index from Barysz matrix / weighted by atomic number Spectral diameter from Barysz matrix / weighted by mass Leading eigenvalue from Barysz matrix / weighted by mass Spectral absolute deviation from Barysz matrix / weighted by mass Spectral absolute deviation from Barysz matrix / weighted by mass
365 366 367 368 369 370 371 372 373 374 375 376 377 378 379 380 381 382 383 384	GATS6s GATS7s GATS8s SpAbs_DzZ SpMax_DzZ SpMax_DzZ SpAD_DzZ SpAD_DzZ SpMAD_DzZ EE_DzZ SM1_DzZ VE1_DzZ VE2_DzZ VE3_DzZ VR3_DzZ VR3_DzZ VR3_DzZ SpAbs_Dzm SpMax_Dzm SpAD_Dzm SpAD_Dzm	Geary autocorrelation - lag 6 / weighted by I-state Geary autocorrelation - lag 7 / weighted by I-state Geary autocorrelation - lag 8 / weighted by I-state Graph energy from Barysz matrix / weighted by atomic number Leading eigenvalue from Barysz matrix / weighted by atomic number Spectral diameter from Barysz matrix / weighted by atomic number Spectral absolute deviation from Barysz matrix / weighted by atomic number Spectral mean absolute deviation from Barysz matrix / weighted by atomic number Spectral mean absolute deviation from Barysz matrix / weighted by atomic number Estrada-like index from Barysz matrix / weighted by atomic number (In(1+x)) Spectral moment of order 1 from Barysz matrix / weighted by atomic number Coefficient sum of the last eigenvector from Barysz matrix / weighted by atomic number Average coefficient sum of the last eigenvector from Barysz matrix / weighted by atomic number Logarithmic coefficient sum of the last eigenvector from Barysz matrix / weighted by atomic number Randic-like eigenvector-based index from Barysz matrix / weighted by atomic number Normalized Randic-like eigenvector-based index from Barysz matrix / weighted by atomic number Logarithmic Randic-like eigenvector-based index from Barysz matrix / weighted by atomic number Cograph energy from Barysz matrix / weighted by mass Leading eigenvalue from Barysz matrix / weighted by mass Spectral diameter from Barysz matrix / weighted by mass Spectral absolute deviation from Barysz matrix / weighted by mass Spectral mean absolute deviation from Barysz matrix / weighted by mass Spectral mean absolute deviation from Barysz matrix / weighted by mass
365 366 367 368 369 370 371 372 373 374 375 376 377 378 379 380 381 382 383 384 385	GATS6s GATS7s GATS8s SpAbs_DzZ SpMax_DzZ SpMax_DzZ SpAD_DzZ SpAD_DzZ SpMAD_DzZ EE_DzZ SM1_DzZ VE1_DzZ VE2_DzZ VE3_DzZ VR1_DzZ VR2_DzZ VR3_DzZ SpAbs_Dzm SpMax_Dzm SpDiam_Dzm SpMAD_Dzm	Geary autocorrelation - lag 6 / weighted by I-state Geary autocorrelation - lag 7 / weighted by I-state Geary autocorrelation - lag 8 / weighted by I-state Graph energy from Barysz matrix / weighted by atomic number Leading eigenvalue from Barysz matrix / weighted by atomic number Spectral diameter from Barysz matrix / weighted by atomic number Spectral absolute deviation from Barysz matrix / weighted by atomic number Spectral mean absolute deviation from Barysz matrix / weighted by atomic number Spectral mean absolute deviation from Barysz matrix / weighted by atomic number Estrada-like index from Barysz matrix / weighted by atomic number (ln(1+x)) Spectral moment of order 1 from Barysz matrix / weighted by atomic number Coefficient sum of the last eigenvector from Barysz matrix / weighted by atomic number Average coefficient sum of the last eigenvector from Barysz matrix / weighted by atomic number Logarithmic coefficient sum of the last eigenvector from Barysz matrix / weighted by atomic number Randic-like eigenvector-based index from Barysz matrix / weighted by atomic number Normalized Randic-like eigenvector-based index from Barysz matrix / weighted by atomic number Logarithmic Randic-like eigenvector-based index from Barysz matrix / weighted by atomic number Graph energy from Barysz matrix / weighted by mass Leading eigenvalue from Barysz matrix / weighted by mass Spectral diameter from Barysz matrix / weighted by mass Spectral diameter from Barysz matrix / weighted by mass Spectral mean absolute deviation from Barysz matrix / weighted by mass Estrada-like index from Barysz matrix / weighted by mass Estrada-like index from Barysz matrix / weighted by mass
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365 366 367 368 369 370 371 372 373 374 375 376 377 378 379 380 381 382 383 384 385 386 387 388	GATS6s GATS7s GATS8s SpAbs_DzZ SpAbs_DzZ SpMax_DzZ SpDiam_DzZ SpAD_DzZ SpMAD_DzZ EE_DzZ SM1_DzZ VE1_DzZ VE2_DzZ VE3_DzZ VR3_DzZ VR3_DzZ VR3_DzZ SpAbs_Dzm SpMax_Dzm SpAD_Dzm SpMAD_Dzm EE_Dzm SM1_Dzm VE1_Dzm VE2_Dzm	Geary autocorrelation - lag 6 / weighted by I-state Geary autocorrelation - lag 7 / weighted by I-state Geary autocorrelation - lag 8 / weighted by I-state Graph energy from Barysz matrix / weighted by atomic number Leading eigenvalue from Barysz matrix / weighted by atomic number Spectral diameter from Barysz matrix / weighted by atomic number Spectral absolute deviation from Barysz matrix / weighted by atomic number Spectral mean absolute deviation from Barysz matrix / weighted by atomic number Spectral mean absolute deviation from Barysz matrix / weighted by atomic number Estrada-like index from Barysz matrix / weighted by atomic number (ln(1+x)) Spectral moment of order 1 from Barysz matrix / weighted by atomic number Coefficient sum of the last eigenvector from Barysz matrix / weighted by atomic number Average coefficient sum of the last eigenvector from Barysz matrix / weighted by atomic number Logarithmic coefficient sum of the last eigenvector from Barysz matrix / weighted by atomic number Randic-like eigenvector-based index from Barysz matrix / weighted by atomic number Normalized Randic-like eigenvector-based index from Barysz matrix / weighted by atomic number Logarithmic Randic-like eigenvector-based index from Barysz matrix / weighted by atomic number Graph energy from Barysz matrix / weighted by mass Leading eigenvalue from Barysz matrix / weighted by mass Spectral diameter from Barysz matrix / weighted by mass Spectral mean absolute deviation from Barysz matrix / weighted by mass Spectral mean absolute deviation from Barysz matrix / weighted by mass Coefficient sum of the last eigenvector from Barysz matrix / weighted by mass Coefficient sum of the last eigenvector from Barysz matrix / weighted by mass Logarithmic coefficient sum of the last eigenvector from Barysz matrix / weighted by mass Logarithmic coefficient sum of the last eigenvector from Barysz matrix / weighted by mass
365 366 367 368 369 370 371 372 373 374 375 376 377 378 379 380 381 382 383 384 385 386 387 388	GATS6s GATS7s GATS8s SpAbs_DzZ SpMax_DzZ SpMax_DzZ SpAD_DzZ SpAD_DzZ SpMAD_DzZ EE_DzZ SM1_DzZ VE1_DzZ VE2_DzZ VE3_DzZ VR1_DzZ VR2_DzZ VR3_DzZ VR3_DzZ SpAbs_Dzm SpMax_Dzm SpMaD_Dzm SpMAD_Dzm SpMAD_Dzm SpMAD_Dzm SpMAD_Dzm SpM1_Dzm SpM1_Dzm VE1_Dzm VE2_Dzm	Geary autocorrelation - lag 6 / weighted by I-state Geary autocorrelation - lag 7 / weighted by I-state Geary autocorrelation - lag 8 / weighted by I-state Graph energy from Barysz matrix / weighted by atomic number Leading eigenvalue from Barysz matrix / weighted by atomic number Spectral diameter from Barysz matrix / weighted by atomic number Spectral absolute deviation from Barysz matrix / weighted by atomic number Spectral mean absolute deviation from Barysz matrix / weighted by atomic number Spectral mean absolute deviation from Barysz matrix / weighted by atomic number Estrada-like index from Barysz matrix / weighted by atomic number (ln(1+x)) Spectral moment of order 1 from Barysz matrix / weighted by atomic number Coefficient sum of the last eigenvector from Barysz matrix / weighted by atomic number Average coefficient sum of the last eigenvector from Barysz matrix / weighted by atomic number Logarithmic coefficient sum of the last eigenvector from Barysz matrix / weighted by atomic number Logarithmic coefficient sum of the last eigenvector from Barysz matrix / weighted by atomic number Normalized Randic-like eigenvector-based index from Barysz matrix / weighted by atomic number Logarithmic Randic-like eigenvector-based index from Barysz matrix / weighted by atomic number Cogarithmic Randic-like eigenvector-based index from Barysz matrix / weighted by mass Leading eigenvalue from Barysz matrix / weighted by mass Spectral diameter from Barysz matrix / weighted by mass Spectral mean absolute deviation from Barysz matrix / weighted by mass Spectral mean absolute deviation from Barysz matrix / weighted by mass Estrada-like index from Barysz matrix / weighted by mass Estrada-like index from Barysz matrix / weighted by mass Coefficient sum of the last eigenvector from Barysz matrix / weighted by mass Logarithmic coefficient sum of the last eigenvector from Barysz matrix / weighted by mass Logarithmic coefficient sum of the last eigenvector from Barysz
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365 366 367 368 370 371 372 373 374 375 376 377 378 379 380 381 382 383 384 385 386 387 388 389 390 391	GATS6s GATS7s GATS8s SpAbs_DzZ SpMax_DzZ SpMax_DzZ SpAD_DzZ SpMAD_DzZ SpMAD_DzZ EE_DzZ SM1_DzZ VE1_DzZ VE2_DzZ VE3_DzZ VR1_DzZ VR2_DzZ VR3_DzZ VR3_DzZ SpMax_Dzm SpMax_Dzm SpAD_Dzm SpAD_Dzm SpMAD_Dzm SpMAD_Dzm VE1_Dzm VE2_Dzm VE3_Dzm VE1_Dzm VE1_Dzm	Geary autocorrelation - lag 6 / weighted by I-state Geary autocorrelation - lag 8 / weighted by I-state Geary autocorrelation - lag 8 / weighted by I-state Graph energy from Barysz matrix / weighted by atomic number Leading eigenvalue from Barysz matrix / weighted by atomic number Spectral diameter from Barysz matrix / weighted by atomic number Spectral absolute deviation from Barysz matrix / weighted by atomic number Spectral mean absolute deviation from Barysz matrix / weighted by atomic number Spectral mean absolute deviation from Barysz matrix / weighted by atomic number Estrada-like index from Barysz matrix / weighted by atomic number (ln(1+x)) Spectral moment of order 1 from Barysz matrix / weighted by atomic number Coefficient sum of the last eigenvector from Barysz matrix / weighted by atomic number Average coefficient sum of the last eigenvector from Barysz matrix / weighted by atomic number Logarithmic coefficient sum of the last eigenvector from Barysz matrix / weighted by atomic number Randic-like eigenvector-based index from Barysz matrix / weighted by atomic number Normalized Randic-like eigenvector-based index from Barysz matrix / weighted by atomic number Logarithmic Randic-like eigenvector-based index from Barysz matrix / weighted by atomic number Graph energy from Barysz matrix / weighted by mass Leading eigenvalue from Barysz matrix / weighted by mass Spectral diameter from Barysz matrix / weighted by mass Spectral mean absolute deviation from Barysz matrix / weighted by mass Estrada-like index from Barysz matrix / weighted by mass Coefficient sum of the last eigenvector from Barysz matrix / weighted by mass Logarithmic coefficient sum of the last eigenvector from Barysz matrix / weighted by mass Coefficient sum of the last eigenvector from Barysz matrix / weighted by mass Logarithmic coefficient sum of the last eigenvector from Barysz matrix / weighted by mass Logarithmic coefficient sum of the last eigenvector from Barysz matrix / weighted by mass Logarithmic Randic-like eigenvector-
365 366 367 368 369 370 371 372 373 374 375 376 377 378 379 380 381 382 383 384 385 386 387 388 389 390 391 392 393	GATS6s GATS7s GATS8s SpAbs_DzZ SpMax_DzZ SpMax_DzZ SpAD_DzZ SpAD_DzZ SpMAD_DzZ EE_DzZ SM1_DzZ VE1_DzZ VE2_DzZ VE3_DzZ VR3_DzZ VR3_DzZ VR3_DzZ SpMax_Dzm SpMax_Dzm SpMax_Dzm SpMaD_Dzm SpMaD_Dzm SpMaD_Dzm SpMaD_Dzm VE1_Dzm VE2_Dzm VE3_Dzm VE3_Dzm	Geary autocorrelation - lag 6 / weighted by I-state Geary autocorrelation - lag 7 / weighted by I-state Gery autocorrelation - lag 8 / weighted by I-state Graph energy from Barysz matrix / weighted by atomic number Leading eigenvalue from Barysz matrix / weighted by atomic number Spectral diameter from Barysz matrix / weighted by atomic number Spectral absolute deviation from Barysz matrix / weighted by atomic number Spectral mean absolute deviation from Barysz matrix / weighted by atomic number Spectral mean absolute deviation from Barysz matrix / weighted by atomic number Estrada-like index from Barysz matrix / weighted by atomic number Coefficient sum of order 1 from Barysz matrix / weighted by atomic number Coefficient sum of the last eigenvector from Barysz matrix / weighted by atomic number Average coefficient sum of the last eigenvector from Barysz matrix / weighted by atomic number Logarithmic coefficient sum of the last eigenvector from Barysz matrix / weighted by atomic number Logarithmic coefficient sum of the last eigenvector from Barysz matrix / weighted by atomic number Randic-like eigenvector-based index from Barysz matrix / weighted by atomic number Logarithmic Randic-like eigenvector-based index from Barysz matrix / weighted by atomic number Cogarithmic Randic-like eigenvector-based index from Barysz matrix / weighted by atomic number Cogarithmic Randic-like eigenvector-based index from Barysz matrix / weighted by atomic number Cogarithmic Randic-like eigenvector-based by mass Spectral diameter from Barysz matrix / weighted by mass Spectral diameter from Barysz matrix / weighted by mass Spectral mean absolute deviation from Barysz matrix / weighted by mass Coefficient sum of the last eigenvector from Barysz matrix / weighted by mass Logarithmic Randic-like eigenvector-based index from Barysz matrix / weighted by mass Logarithmic coefficient sum of the last eigenvector from Barysz matrix / weighted by mass Normalized Randic-like eigenvector-based index from Barysz matrix / weighted by mass G
365 366 367 368 369 370 371 372 373 374 375 376 377 378 379 380 381 382 383 384 385 386 387 388 389 390 391 392	GATS6s GATS7s GATS8s SpAbs_DzZ SpAbs_DzZ SpMax_DzZ SpAD_DzZ SpAD_DzZ SpMAD_DzZ EE_DzZ SM1_DzZ VE1_DzZ VE2_DzZ VE3_DzZ VR3_DzZ VR3_DzZ VR3_DzZ SpAbs_Dzm SpAb_Dzm SpAD_Dzm SpMAD_Dzm EE_Dzm SM1_Dzm VE1_Dzm VE2_Dzm VR3_Dzm VR3_Dzm	Geary autocorrelation - lag 6 / weighted by I-state Geary autocorrelation - lag 8 / weighted by I-state Geary autocorrelation - lag 8 / weighted by I-state Graph energy from Barysz matrix / weighted by atomic number Leading eigenvalue from Barysz matrix / weighted by atomic number Spectral diameter from Barysz matrix / weighted by atomic number Spectral absolute deviation from Barysz matrix / weighted by atomic number Spectral mean absolute deviation from Barysz matrix / weighted by atomic number Spectral mean absolute deviation from Barysz matrix / weighted by atomic number Estrada-like index from Barysz matrix / weighted by atomic number (ln(1+x)) Spectral moment of order 1 from Barysz matrix / weighted by atomic number Coefficient sum of the last eigenvector from Barysz matrix / weighted by atomic number Average coefficient sum of the last eigenvector from Barysz matrix / weighted by atomic number Logarithmic coefficient sum of the last eigenvector from Barysz matrix / weighted by atomic number Randic-like eigenvector-based index from Barysz matrix / weighted by atomic number Rornalized Randic-like eigenvector-based index from Barysz matrix / weighted by atomic number Cogarithmic Randic-like eigenvector-based index from Barysz matrix / weighted by atomic number Graph energy from Barysz matrix / weighted by mass Leading eigenvalue from Barysz matrix / weighted by mass Leading eigenvalue from Barysz matrix / weighted by mass Spectral diameter from Barysz matrix / weighted by mass Spectral mean absolute deviation from Barysz matrix / weighted by mass Coefficient sum of the last eigenvector from Barysz matrix / weighted by mass Estrada-like index from Barysz matrix / weighted by mass Coefficient sum of the last eigenvector from Barysz matrix / weighted by mass Logarithmic coefficient sum of the last eigenvector from Barysz matrix / weighted by mass Normalized Randic-like eigenvector-based index from Barysz matrix / weighted by mass Randic-like eigenvector-based index from Barysz matrix / weighted by mass

396	SpDiam_Dzv	Spectral diameter from Barysz matrix / weighted by van der Waals volumes
397	SpAD_Dzv	Spectral absolute deviation from Barysz matrix / weighted by valder Waals volumes
398	SpMAD_Dzv	Spectral mean absolute deviation from Barysz matrix / weighted by van der Waals volumes
399	EE_Dzv	Estrada-like index from Barysz matrix / weighted by van der Waals volumes (ln(1+x))
400	SM1_Dzv	Spectral moment of order 1 from Barysz matrix / weighted by
401	VE1_Dzv	van der Waals volumes Coefficient sum of the last eigenvector from Barysz matrix /
402	VE2_Dzv	weighted by van der Waals volumes Average coefficient sum of the last eigenvector from Barysz
403	VE3_Dzv	matrix / weighted by van der Waals volumes Logarithmic coefficient sum of the last eigenvector from Barysz
404	VR1_Dzv	matrix / weighted by van der Waals volumes Randic-like eigenvector-based index from Barysz matrix /
	VR2_Dzv	weighted by van der Waals volumes Normalized Randic-like eigenvector-based index from Barysz
		matrix / weighted by van der Waals volumes
	VR3_Dzv	Logarithmic Randic-like eigenvector-based index from Barysz matrix / weighted by van der Waals volumes
407	SpAbs_Dze	Graph energy from Barysz matrix / weighted by Sanderson electronegativities
408	SpMax_Dze	Leading eigenvalue from Barysz matrix / weighted by Sanderson electronegativities
409	SpDiam_Dze	Spectral diameter from Barysz matrix / weighted by Sanderson electronegativities
410	SpAD_Dze	Spectral absolute deviation from Barysz matrix / weighted by
411	SpMAD_Dze	Sanderson electronegativities Spectral mean absolute deviation from Barysz matrix / weighted
412	EE_Dze	by Sanderson electronegativities Estrada-like index from Barysz matrix / weighted by Sanderson
413	SM1_Dze	electronegativities (ln(1+x)) Spectral moment of order 1 from Barysz matrix / weighted by
	VE1_Dze	Sanderson electronegativities Coefficient sum of the last eigenvector from Barysz matrix /
	VE2_Dze	weighted by Sanderson electronegativities Average coefficient sum of the last eigenvector from Barysz
		matrix / weighted by Sanderson electronegativities
	VE3_Dze	Logarithmic coefficient sum of the last eigenvector from Barysz matrix / weighted by Sanderson electronegativities
417	VR1_Dze	Randic-like eigenvector-based index from Barysz matrix / weighted by Sanderson electronegativities
418	VR2_Dze	Normalized Randic-like eigenvector-based index from Barysz matrix / weighted by Sanderson electronegativities
419	VR3_Dze	Logarithmic Randic-like eigenvector-based index from Barysz matrix / weighted by Sanderson electronegativities
420	SpAbs_Dzp	Graph energy from Barysz matrix / weighted by polarizabilities
421	SpMax_Dzp	Leading eigenvalue from Barysz matrix / weighted by
422	SpDiam_Dzp	polarizabilities Spectral diameter from Barysz matrix / weighted by
423	SpAD_Dzp	polarizabilities Spectral absolute deviation from Barysz matrix / weighted by
424	SpMAD_Dzp	polarizabilities Spectral mean absolute deviation from Barysz matrix / weighted
	EE_Dzp	by polarizabilities Estrada-like index from Barysz matrix / weighted by
	•	polarizabilities (ln(1+x))
	SM1_Dzp	Spectral moment of order 1 from Barysz matrix / weighted by polarizabilities
	VE1_Dzp	Coefficient sum of the last eigenvector from Barysz matrix / weighted by polarizabilities
428	VE2_Dzp	Average coefficient sum of the last eigenvector from Barysz matrix / weighted by polarizabilities
429	VE3_Dzp	Logarithmic coefficient sum of the last eigenvector from Barysz matrix / weighted by polarizabilities
430	VR1_Dzp	Randic-like eigenvector-based index from Barysz matrix / weighted by polarizabilities
431	VR2_Dzp	Normalized Randic-like eigenvector-based index from Barysz
432	VR3_Dzp	matrix / weighted by polarizabilities Logarithmic Randic-like eigenvector-based index from Barysz
433	SpAbs_Dzi	matrix / weighted by polarizabilities Graph energy from Barysz matrix / weighted by first ionization
	SpMax_Dzi	potential Leading eigenvalue from Barysz matrix / weighted by first
	SpDiam_Dzi	ionization potential Spectral diameter from Barysz matrix / weighted by first
	SpAD_Dzi	ionization potential
		Spectral absolute deviation from Barysz matrix / weighted by first ionization potential
	SpMAD_Dzi	Spectral mean absolute deviation from Barysz matrix / weighted by first ionization potential
	EE_Dzi	Estrada-like index from Barysz matrix / weighted by first ionization potential $(ln(1+x))$
439	SM1_Dzi	Spectral moment of order 1 from Barysz matrix / weighted by first ionization potential
440	VE1_Dzi	Coefficient sum of the last eigenvector from Barysz matrix / weighted by first ionization potential
441	VE2_Dzi	Average coefficient sum of the last eigenvector from Barysz
442	VE3_Dzi	matrix / weighted by first ionization potential Logarithmic coefficient sum of the last eigenvector from Barysz
443	VR1_Dzi	matrix / weighted by first ionization potential Randic-like eigenvector-based index from Barysz matrix /
444	VR2_Dzi	weighted by first ionization potential Normalized Randic-like eigenvector-based index from Barysz
	VR3_Dzi	matrix / weighted by first ionization potential Logarithmic Randic-like eigenvector-based index from Barysz
		matrix / weighted by first ionization potential
	SpAbs_Dzs SpMax_Dzs	Graph energy from Barysz matrix / weighted by I-state Leading eigenvalue from Barysz matrix / weighted by I-state
448	SpDiam_Dzs	Spectral diameter from Barysz matrix / weighted by I-state
	SpAD_Dzs	Spectral absolute deviation from Barysz matrix / weighted by I-
	SpMAD_Dzs	state Spectral mean absolute deviation from Barysz matrix / weighted
	_	by I-state
451	EE_Dzs	Estrada-like index from Barysz matrix / weighted by I-state (ln(1+x)) Spectral moment of order 1 from Barysz matrix / weighted by I-
	SM1_Dzs	

453	VE1_Dzs	Coefficient sum of the last eigenvector from Barysz matrix / weighted by I-state
454	VE2_Dzs	Average coefficient sum of the last eigenvector from Barysz matrix / weighted by I-state
455	VE3_Dzs	Logarithmic coefficient sum of the last eigenvector from Barysz
456	VR1_Dzs	matrix / weighted by I-state Randic-like eigenvector-based index from Barysz matrix /
457	VR2_Dzs	weighted by I-state Normalized Randic-like eigenvector-based index from Barysz
		matrix / weighted by I-state
	VR3_Dzs	Logarithmic Randic-like eigenvector-based index from Barysz matrix / weighted by I-state
459	nBase	Number of basic groups. The list of basic groups is defined by this SMARTS "[\$([NH2]-[CX4])]", "[\$([NH](-[CX4])-[CX4])]",
		"[\$(N(-[CX4])(-[CX4])-[CX4])]", "[\$([*;+;!\$(*~[*;-])])]", "[\$(N=C-N)]", and "[\$(N-C=N)]" originally presented in JOELib
4.50	D.C.L.T. 11	
	BCUTw-11 BCUTw-1h	nhigh lowest atom weighted BCUTS nlow highest atom weighted BCUTS
	BCUTc-11 BCUTc-1h	nhigh lowest partial charge weighted BCUTS nlow highest partial charge weighted BCUTS
	BCUTp-11 BCUTp-1h	nhigh lowest polarizability weighted BCUTS nlow highest polarizability weighted BCUTS
466	nBonds	Number of bonds (excluding bonds with hydrogen)
	nBonds2 nBondsS	Total number of bonds (including bonds to hydrogens) Number of single bonds (including bonds with hydrogen)
469	nBondsS2	Total number of single bonds (including bonds to hydrogens, excluding aromatic bonds)
470	nBondsS3	Total number of single bonds (excluding bonds to hydrogens and aromatic bonds)
	nBondsD	Number of double bonds
	nBondsD2	Total number of double bonds (excluding bonds to aromatic bonds)
	nBondsT nBondsQ	Number of triple bonds Number of quadruple bonds
	nBondsM	Total number of bonds that have bond order greater than one (aromatic bonds have bond order 1.5).
476	bpol	Sum of the absolute value of the difference between atomic
		polarizabilities of all bonded atoms in the molecule (including implicit hydrogens)
477	SpMax1_Bhm	Largest absolute eigenvalue of Burden modified matrix - n 1 / weighted by relative mass
478	SpMax2_Bhm	Largest absolute eigenvalue of Burden modified matrix - n 2 /
479	SpMax3_Bhm	weighted by relative mass Largest absolute eigenvalue of Burden modified matrix - n 3 /
480	SpMax4_Bhm	weighted by relative mass Largest absolute eigenvalue of Burden modified matrix - n 4 /
481	SpMax5_Bhm	weighted by relative mass Largest absolute eigenvalue of Burden modified matrix - n 5 /
	-	weighted by relative mass
	SpMax6_Bhm	Largest absolute eigenvalue of Burden modified matrix - n 6 / weighted by relative mass
483	SpMax7_Bhm	Largest absolute eigenvalue of Burden modified matrix - n 7 / weighted by relative mass
484	SpMax8_Bhm	Largest absolute eigenvalue of Burden modified matrix - n 8 / weighted by relative mass
485	SpMin1_Bhm	Smallest absolute eigenvalue of Burden modified matrix - n 1 /
486	SpMin2_Bhm	weighted by relative mass Smallest absolute eigenvalue of Burden modified matrix - n 2 /
487	SpMin3_Bhm	weighted by relative mass Smallest absolute eigenvalue of Burden modified matrix - n 3 /
488	SpMin4_Bhm	weighted by relative mass Smallest absolute eigenvalue of Burden modified matrix - n 4 /
	•	weighted by relative mass
	SpMin5_Bhm	Smallest absolute eigenvalue of Burden modified matrix - n 5 / weighted by relative mass
490	SpMin6_Bhm	Smallest absolute eigenvalue of Burden modified matrix - n 6 / weighted by relative mass
491	SpMin7_Bhm	Smallest absolute eigenvalue of Burden modified matrix - n 7 / weighted by relative mass
492	SpMin8_Bhm	Smallest absolute eigenvalue of Burden modified matrix - n 8 /
493	SpMax1_Bhv	weighted by relative mass Largest absolute eigenvalue of Burden modified matrix - n 1 /
494	SpMax2_Bhv	weighted by relative van der Waals volumes Largest absolute eigenvalue of Burden modified matrix - n 2 /
	SpMax3_Bhv	weighted by relative van der Waals volumes Largest absolute eigenvalue of Burden modified matrix - n 3 /
	_	weighted by relative van der Waals volumes
	SpMax4_Bhv	Largest absolute eigenvalue of Burden modified matrix - n 4 / weighted by relative van der Waals volumes
497	SpMax5_Bhv	Largest absolute eigenvalue of Burden modified matrix - n 5 / weighted by relative van der Waals volumes
498	SpMax6_Bhv	Largest absolute eigenvalue of Burden modified matrix - n 6 / weighted by relative van der Waals volumes
499	SpMax7_Bhv	Largest absolute eigenvalue of Burden modified matrix - n 7 /
500	SpMax8_Bhv	weighted by relative van der Waals volumes Largest absolute eigenvalue of Burden modified matrix - n 8 /
501	SpMin1_Bhv	weighted by relative van der Waals volumes Smallest absolute eigenvalue of Burden modified matrix - n 1 /
	SpMin2_Bhv	weighted by relative van der Waals volumes Smallest absolute eigenvalue of Burden modified matrix - n 2 /
		weighted by relative van der Waals volumes
	SpMin3_Bhv	Smallest absolute eigenvalue of Burden modified matrix - n 3 / weighted by relative van der Waals volumes
504	SpMin4_Bhv	Smallest absolute eigenvalue of Burden modified matrix - n 4 / weighted by relative van der Waals volumes
505	SpMin5_Bhv	Smallest absolute eigenvalue of Burden modified matrix - n 5 / weighted by relative van der Waals volumes
506	SpMin6_Bhv	Smallest absolute eigenvalue of Burden modified matrix - n 6 /
507	SpMin7_Bhv	weighted by relative van der Waals volumes Smallest absolute eigenvalue of Burden modified matrix - n 7 /
508	SpMin8_Bhv	weighted by relative van der Waals volumes Smallest absolute eigenvalue of Burden modified matrix - n 8 /
	SpMax1_Bhe	weighted by relative van der Waals volumes Largest absolute eigenvalue of Burden modified matrix - n 1 /
	•	weighted by relative Sanderson electronegativities
510	SpMax2_Bhe	Largest absolute eigenvalue of Burden modified matrix - n 2 / weighted by relative Sanderson electronegativities
511	SpMax3_Bhe	Largest absolute eigenvalue of Burden modified matrix - n 3 / weighted by relative Sanderson electronegativities
512	SpMax4_Bhe	Largest absolute eigenvalue of Burden modified matrix - n 4 /
	L	weighted by relative Sanderson electronegativities

513	SpMax5_Bhe	Largest absolute eigenvalue of Burden modified matrix - n 5 / weighted by relative Sanderson electronegativities
514	SpMax6_Bhe	Largest absolute eigenvalue of Burden modified matrix - n 6 / weighted by relative Sanderson electronegativities
515	SpMax7_Bhe	Largest absolute eigenvalue of Burden modified matrix - n 7 / weighted by relative Sanderson electronegativities
516	SpMax8_Bhe	Largest absolute eigenvalue of Burden modified matrix - n 8 / weighted by relative Sanderson electronegativities
517	SpMin1_Bhe	Smallest absolute eigenvalue of Burden modified matrix - n 1 /
518	SpMin2_Bhe	weighted by relative Sanderson electronegativities Smallest absolute eigenvalue of Burden modified matrix - n 2 /
519	SpMin3_Bhe	weighted by relative Sanderson electronegativities Smallest absolute eigenvalue of Burden modified matrix - n 3 /
520	SpMin4_Bhe	weighted by relative Sanderson electronegativities Smallest absolute eigenvalue of Burden modified matrix - n 4 /
521	SpMin5_Bhe	weighted by relative Sanderson electronegativities Smallest absolute eigenvalue of Burden modified matrix - n 5 /
	SpMin6_Bhe	weighted by relative Sanderson electronegativities Smallest absolute eigenvalue of Burden modified matrix - n 6 /
	SpMin7_Bhe	weighted by relative Sanderson electronegativities Smallest absolute eigenvalue of Burden modified matrix - n 7 /
	-	weighted by relative Sanderson electronegativities
	SpMin8_Bhe	Smallest absolute eigenvalue of Burden modified matrix - n 8 / weighted by relative Sanderson electronegativities
	SpMax1_Bhp	Largest absolute eigenvalue of Burden modified matrix - n 1 / weighted by relative polarizabilities
	SpMax2_Bhp	Largest absolute eigenvalue of Burden modified matrix - n 2 / weighted by relative polarizabilities
527	SpMax3_Bhp	Largest absolute eigenvalue of Burden modified matrix - n 3 / weighted by relative polarizabilities
528	SpMax4_Bhp	Largest absolute eigenvalue of Burden modified matrix - n 4 / weighted by relative polarizabilities
529	SpMax5_Bhp	Largest absolute eigenvalue of Burden modified matrix - n 5 / weighted by relative polarizabilities
530	SpMax6_Bhp	Largest absolute eigenvalue of Burden modified matrix - n 6 / weighted by relative polarizabilities
531	SpMax7_Bhp	Largest absolute eigenvalue of Burden modified matrix - n 7 / weighted by relative polarizabilities
532	SpMax8_Bhp	Largest absolute eigenvalue of Burden modified matrix - n 8 / weighted by relative polarizabilities
533	SpMin1_Bhp	Smallest absolute eigenvalue of Burden modified matrix - n 1 / weighted by relative polarizabilities
534	SpMin2_Bhp	Smallest absolute eigenvalue of Burden modified matrix - n 2 /
535	SpMin3_Bhp	weighted by relative polarizabilities Smallest absolute eigenvalue of Burden modified matrix - n 3 /
536	SpMin4_Bhp	weighted by relative polarizabilities Smallest absolute eigenvalue of Burden modified matrix - n 4 /
537	SpMin5_Bhp	weighted by relative polarizabilities Smallest absolute eigenvalue of Burden modified matrix - n 5 /
538	SpMin6_Bhp	weighted by relative polarizabilities Smallest absolute eigenvalue of Burden modified matrix - n 6 /
539	SpMin7_Bhp	weighted by relative polarizabilities Smallest absolute eigenvalue of Burden modified matrix - n 7 /
540	SpMin8_Bhp	weighted by relative polarizabilities Smallest absolute eigenvalue of Burden modified matrix - n 8 /
541	SpMax1_Bhi	weighted by relative polarizabilities Largest absolute eigenvalue of Burden modified matrix - n 1 /
542	SpMax2_Bhi	weighted by relative first ionization potential Largest absolute eigenvalue of Burden modified matrix - n 2 /
543	SpMax3_Bhi	weighted by relative first ionization potential Largest absolute eigenvalue of Burden modified matrix - n 3 /
544	SpMax4_Bhi	weighted by relative first ionization potential Largest absolute eigenvalue of Burden modified matrix - n 4 /
545	SpMax5_Bhi	weighted by relative first ionization potential Largest absolute eigenvalue of Burden modified matrix - n 5 /
546	SpMax6_Bhi	weighted by relative first ionization potential Largest absolute eigenvalue of Burden modified matrix - n 6 /
547	SpMax7_Bhi	weighted by relative first ionization potential Largest absolute eigenvalue of Burden modified matrix - n 7 /
548	SpMax8_Bhi	weighted by relative first ionization potential Largest absolute eigenvalue of Burden modified matrix - n 8 /
549	SpMin1_Bhi	weighted by relative first ionization potential Smallest absolute eigenvalue of Burden modified matrix - n 1 /
550	SpMin2_Bhi	weighted by relative first ionization potential Smallest absolute eigenvalue of Burden modified matrix - n 2 /
551	SpMin3_Bhi	weighted by relative first ionization potential Smallest absolute eigenvalue of Burden modified matrix - n 3 /
	SpMin4_Bhi	weighted by relative first ionization potential Smallest absolute eigenvalue of Burden modified matrix - n 4 /
553	SpMin5_Bhi	weighted by relative first ionization potential Smallest absolute eigenvalue of Burden modified matrix - n 5 /
	SpMin6_Bhi	weighted by relative first ionization potential Smallest absolute eigenvalue of Burden modified matrix - n 6 /
	SpMin7_Bhi	weighted by relative first ionization potential Smallest absolute eigenvalue of Burden modified matrix - n 7 /
	SpMin8_Bhi	weighted by relative first ionization potential Smallest absolute eigenvalue of Burden modified matrix - n 8 /
	SpMax1_Bhs	weighted by relative first ionization potential Largest absolute eigenvalue of Burden modified matrix - n 1 /
	SpMax2_Bhs	weighted by relative I-state Largest absolute eigenvalue of Burden modified matrix - n 2 /
		weighted by relative I-state
	SpMax3_Bhs	Largest absolute eigenvalue of Burden modified matrix - n 3 / weighted by relative I-state
	SpMax4_Bhs	Largest absolute eigenvalue of Burden modified matrix - n 4 / weighted by relative I-state
	SpMax5_Bhs	Largest absolute eigenvalue of Burden modified matrix - n 5 / weighted by relative I-state
	SpMax6_Bhs	Largest absolute eigenvalue of Burden modified matrix - n 6 / weighted by relative I-state
	SpMax7_Bhs	Largest absolute eigenvalue of Burden modified matrix - n 7 / weighted by relative I-state
	SpMax8_Bhs	Largest absolute eigenvalue of Burden modified matrix - n 8 / weighted by relative I-state
	SpMin1_Bhs	Smallest absolute eigenvalue of Burden modified matrix - n 1 / weighted by relative I-state
	SpMin2_Bhs	Smallest absolute eigenvalue of Burden modified matrix - n 2 / weighted by relative I-state
	SpMin3_Bhs	Smallest absolute eigenvalue of Burden modified matrix - n 3 / weighted by relative I-state
568	SpMin4_Bhs	Smallest absolute eigenvalue of Burden modified matrix - n 4 / weighted by relative I-state

569	SpMin5_Bhs	Smallest absolute eigenvalue of Burden modified matrix - n 5 /
570	SpMin6_Bhs	weighted by relative I-state Smallest absolute eigenvalue of Burden modified matrix - n 6 /
		weighted by relative I-state
571	SpMin7_Bhs	Smallest absolute eigenvalue of Burden modified matrix - n 7 / weighted by relative I-state
572	SpMin8_Bhs	Smallest absolute eigenvalue of Burden modified matrix - n 8 /
573	C1SP1	weighted by relative I-state Triply bound carbon bound to one other carbon
574	C2SP1	Triply bound carbon bound to two other carbons
	C1SP2 C2SP2	Doubly bound carbon bound to one other carbon Doubly bound carbon bound to two other carbons
577	C3SP2	Doubly bound carbon bound to three other carbons
	C1SP3 C2SP3	Singly bound carbon bound to one other carbon Singly bound carbon bound to two other carbons
580	C3SP3	Singly bound carbon bound to three other carbons
	C4SP3 SCH-3	Singly bound carbon bound to four other carbons Simple chain, order 3
583	SCH-4	Simple chain, order 4
	SCH-5 SCH-6	Simple chain, order 5 Simple chain, order 6
586	SCH-7	Simple chain, order 7
	VCH-3 VCH-4	Valence chain, order 3 Valence chain, order 4
	VCH-5 VCH-6	Valence chain, order 5
	VCH-6 VCH-7	Valence chain, order 6 Valence chain, order 7
	2 SC-3	Simple cluster, order 3
	SC-4 SC-5	Simple cluster, order 4 Simple cluster, order 5
	SC-6 VC-3	Simple cluster, order 6
597	VC-4	Valence cluster, order 3 Valence cluster, order 4
	VC-5 VC-6	Valence cluster, order 5 Valence cluster, order 6
600	SPC-4	Simple path cluster, order 4
	SPC-5 SPC-6	Simple path cluster, order 5 Simple path cluster, order 6
603	VPC-4	Valence path cluster, order 4
	VPC-5 VPC-6	Valence path cluster, order 5 Valence path cluster, order 6
606	SP-0	Simple path, order 0
	SP-1 SP-2	Simple path, order 1 Simple path, order 2
609	SP-3	Simple path, order 3
	SP-4 SP-5	Simple path, order 4 Simple path, order 5
612	SP-6	Simple path, order 6
	SP-7 ASP-0	Simple path, order 7 Average simple path, order 0
615	S ASP-1	Average simple path, order 1
	ASP-2 ASP-3	Average simple path, order 2 Average simple path, order 3
618	ASP-4	Average simple path, order 4
	ASP-5 ASP-6	Average simple path, order 5 Average simple path, order 6
621	ASP-7	Average simple path, order 7
	VP-0 VP-1	Valence path, order 0 Valence path, order 1
	VP-2	Valence path, order 2
	VP-3 VP-4	Valence path, order 3 Valence path, order 4
	VP-5	Valence path, order 5
	VP-6 VP-7	Valence path, order 6 Valence path, order 7
	AVP-0	Average valence path, order 0
	AVP-1 2 AVP-2	Average valence path, order 1 Average valence path, order 2
	AVP-3 AVP-4	Average valence path, order 3
	AVP-4 AVP-5	Average valence path, order 4 Average valence path, order 5
	AVP-6 AVP-7	Average valence path, order 6 Average valence path, order 7
	S Sv	Sum of atomic van der Waals volumes (scaled on carbon atom)
630	Sse	Sum of atomic Sanderson electronegativities (scaled on carbon
		atom)
640	Spe	Sum of atomic Pauling electronegativities (scaled on carbon atom)
641	Sare	Sum of atomic Allred-Rochow electronegativities (scaled on
642	2 Sp	carbon atom) Sum of atomic polarizabilities (scaled on carbon atom)
643		Sum of first first ionization potentials (scaled on carbon atom)
644	Mv	Mean atomic van der Waals volumes (scaled on carbon atom)
645	Mse	Mean atomic Sanderson electronegativities (scaled on carbon atom)
646	Мре	Mean atomic Pauling electronegativities (scaled on carbon atom)
647	' Mare	Mean atomic Allred-Rochow electronegativities (scaled on
		carbon atom)
	IMID	Mean atomic polarizabilities (scaled on carbon atom)
648	Mi	Mean first first ionization potentials (scaled on carbon atom)
649	Mi	•
649		Mean first first ionization potentials (scaled on carbon atom) Crippen's LogP Crippen's molar refractivity
650 651 652	Mi CrippenLogP CrippenMR SpMax_Dt	Crippen's LogP Crippen's molar refractivity Leading eigenvalue from detour matrix
649 650 651 652 653	Mi CrippenLogP CrippenMR	Crippen's LogP Crippen's molar refractivity
649 650 651 652 653 654 655	Mi CrippenLogP CrippenMR SpMax_Dt SpDiam_Dt SpAD_Dt SpMAD_Dt	Crippen's LogP Crippen's molar refractivity Leading eigenvalue from detour matrix Spectral diameter from detour matrix Spectral absolute deviation from detour matrix Spectral mean absolute deviation from detour matrix
649 650 651 652 653 654 655	Mi CrippenLogP CrippenMR SpMax_Dt SpDiam_Dt SpAD_Dt	Crippen's LogP Crippen's molar refractivity Leading eigenvalue from detour matrix Spectral diameter from detour matrix Spectral absolute deviation from detour matrix
649 650 651 652 653 654 655 656	Mi CrippenLogP CrippenMR SpMax_Dt SpDiam_Dt SpAD_Dt SpMAD_Dt EE_Dt	Crippen's LogP Crippen's molar refractivity Leading eigenvalue from detour matrix Spectral diameter from detour matrix Spectral absolute deviation from detour matrix Spectral mean absolute deviation from detour matrix Estrada-like index from detour matrix Coefficient sum of the last eigenvector from detour matrix Average coefficient sum of the last eigenvector from detour
649 650 651 652 653 654 655 656 657	Mi CrippenLogP CrippenMR SpMax_Dt SpDiam_Dt SpAD_Dt SpMAD_Dt EE_Dt VE1_Dt	Crippen's LogP Crippen's molar refractivity Leading eigenvalue from detour matrix Spectral diameter from detour matrix Spectral absolute deviation from detour matrix Spectral mean absolute deviation from detour matrix Estrada-like index from detour matrix Coefficient sum of the last eigenvector from detour matrix
649 650 651 652 653 654 655 656 657 658	Mi CrippenLogP CrippenMR SpMax_Dt SpDiam_Dt SpAD_Dt SpMAD_Dt EE_Dt VE1_Dt VE2_Dt VE3_Dt	Crippen's LogP Crippen's molar refractivity Leading eigenvalue from detour matrix Spectral diameter from detour matrix Spectral absolute deviation from detour matrix Spectral mean absolute deviation from detour matrix Estrada-like index from detour matrix Coefficient sum of the last eigenvector from detour matrix Average coefficient sum of the last eigenvector from detour matrix Logarithmic coefficient sum of the last eigenvector from detour matrix
649 650 651 652 653 654 655 656 657 658	Mi CrippenLogP CrippenMR SpMax_Dt SpDiam_Dt SpAD_Dt SpMAD_Dt EE_Dt VE1_Dt VE2_Dt	Crippen's LogP Crippen's molar refractivity Leading eigenvalue from detour matrix Spectral diameter from detour matrix Spectral absolute deviation from detour matrix Spectral mean absolute deviation from detour matrix Estrada-like index from detour matrix Coefficient sum of the last eigenvector from detour matrix Average coefficient sum of the last eigenvector from detour matrix Logarithmic coefficient sum of the last eigenvector from detour matrix Randic-like eigenvector-based index from detour matrix Normalized Randic-like eigenvector-based index from detour
649 650 651 652 653 654 655 656 657 658	Mi CrippenLogP CrippenMR SpMax_Dt SpDiam_Dt SpAD_Dt SpMAD_Dt EE_Dt VE1_Dt VE2_Dt VE3_Dt VR1_Dt	Crippen's LogP Crippen's molar refractivity Leading eigenvalue from detour matrix Spectral diameter from detour matrix Spectral absolute deviation from detour matrix Spectral mean absolute deviation from detour matrix Estrada-like index from detour matrix Coefficient sum of the last eigenvector from detour matrix Average coefficient sum of the last eigenvector from detour matrix Logarithmic coefficient sum of the last eigenvector from detour matrix Randic-like eigenvector-based index from detour matrix

663	ECCEN	A topological descriptor combining distance and adjacency information
664	nHBd	Count of E-States for (strong) Hydrogen Bond donors
	nwHBd nHBa	Count of E-States for weak Hydrogen Bond donors Count of E-States for (strong) Hydrogen Bond accentors
	пнва nwHBa	Count of E-States for (strong) Hydrogen Bond acceptors Count of E-States for weak Hydrogen Bond acceptors
668	nHBint2	Count of E-State descriptors of strength for potential Hydrogen Bonds of path length 2
669	nHBint3	Count of E-State descriptors of strength for potential Hydrogen
670	nHBint4	Bonds of path length 3 Count of E-State descriptors of strength for potential Hydrogen
671	nHBint5	Bonds of path length 4
0/1	nhBini3	Count of E-State descriptors of strength for potential Hydrogen Bonds of path length 5
672	nHBint6	Count of E-State descriptors of strength for potential Hydrogen Bonds of path length 6
673	nHBint7	Count of E-State descriptors of strength for potential Hydrogen
674	nHBint8	Bonds of path length 7 Count of E-State descriptors of strength for potential Hydrogen
675	nHBint9	Bonds of path length 8 Count of E-State descriptors of strength for potential Hydrogen
		Bonds of path length 9
676	nHBint10	Count of E-State descriptors of strength for potential Hydrogen Bonds of path length 10
	nHsOH	Count of atom-type H E-State: -OH
	nHdNH nHsSH	Count of atom-type H E-State: =NH Count of atom-type H E-State: -SH
	nHsNH2	Count of atom-type H E-State: -NH2
	nHssNH nHaaNH	Count of atom-type H E-State: -NH- Count of atom-type H E-State: :NH:
	nHsNH3p	Count of atom-type H E-State: -NH3+
	nHssNH2p nHsssNHp	Count of atom-type H E-State: -NH2-+ Count of atom-type H E-State: >NH-+
	nHtCH nHdCH2	Count of atom-type H E-State: #CH Count of atom-type H E-State: =CH2
688	nHdsCH	Count of atom-type H E-State: =CH-
	nHaaCH nHCHnX	Count of atom-type H E-State: :CH: Count of atom-type H E-State: CHnX
	nHCsats	Count of atom-type H E-State: H bonded to B, Si, P, Ge, As, Se,
692	nHCsatu	Sn or Pb Count of atom-type H E-State: H on C sp3 bonded to unsaturate
		С
693	nHAvin	Count of atom-type H E-State: H on C vinyl bonded to C aromatic
694	nHother	Count of atom-type H E-State: H on aaCH, dCH2 or dsCH
695	nHmisc	Count of atom-type H E-State: H bonded to B, Si, P, Ge, As, Se,
606		Sn or Pb
	nsLi nssBe	Count of atom-type E-State: -Li Count of atom-type E-State: -Be-
	nssssBem nsBH2	Count of atom-type E-State: >Be<-2 Count of atom-type E-State: -BH2
	nssBH	Count of atom-type E-State: -BH-
	nsssB nssssBm	Count of atom-type E-State: -B< Count of atom-type E-State: >B<-
703	nsCH3	Count of atom-type E-State: -CH3
	ndCH2 nssCH2	Count of atom-type E-State: =CH2 Count of atom-type E-State: -CH2-
706	ntCH	Count of atom-type E-State: #CH
	ndsCH naaCH	Count of atom-type E-State: =CH- Count of atom-type E-State: :CH:
709	nsssCH	Count of atom-type E-State: >CH-
	nddC ntsC	Count of atom-type E-State: =C= Count of atom-type E-State: #C-
	ndssC naasC	Count of atom-type E-State: =C< Count of atom-type E-State: :C:-
714	naaaC	Count of atom-type E-State: ::C:
	nssssC nsNH3p	Count of atom-type E-State: >C< Count of atom-type E-State: -NH3+
717	nsNH2	Count of atom-type E-State: -NH2
	nssNH2p ndNH	Count of atom-type E-State: -NH2-+ Count of atom-type E-State: =NH
720	nssNH	Count of atom-type E-State: -NH-
	naaNH ntN	Count of atom-type E-State: :NH: Count of atom-type E-State: #N
723	nsssNHp	Count of atom-type E-State: >NH-+
	ndsN naaN	Count of atom-type E-State: =N- Count of atom-type E-State: :N:
726	nsssN nddsN	Count of atom-type E-State: >N-
728	naasN	Count of atom-type E-State: -N<< Count of atom-type E-State: :N:-
	nssssNp nsOH	Count of atom-type E-State: >N<+ Count of atom-type E-State: -OH
731	ndO	Count of atom-type E-State: =O
	nssO naaO	Count of atom-type E-State: -O-Count of atom-type E-State: :O:
734	naOm	Count of atom-type E-State: :O-0.5
	nsOm nsF	Count of atom-type E-State: -O- Count of atom-type E-State: -F
737	nsSiH3	Count of atom-type E-State: -SiH3
739	nssSiH2 nsssSiH	Count of atom-type E-State: -SiH2- Count of atom-type E-State: >SiH-
	nssssSi nsPH2	Count of atom-type E-State: >Si< Count of atom-type E-State: -PH2
742	nssPH	Count of atom-type E-State: -PH-
	nsssP ndsssP	Count of atom-type E-State: >P- Count of atom-type E-State: ->P=
	nddsP	Count of atom-type E-State: -=P=
	nsssssP nsSH	Count of atom-type E-State: ->P< Count of atom-type E-State: -SH
746	ndS	Count of atom-type E-State: =S
746 747 748	~	Count of atom-type E-State: -S-
746 747 748 749	nssS naaS	Count of atom-type E-State: aSa
746 747 748 749 750 751	naaS ndssS	Count of atom-type E-State: >S=
746 747 748 749 750 751 752	naaS	* *
746 747 748 749 750 751 752 753 754	naaS ndssS nddssS nssssssS nSm	Count of atom-type E-State: >S= Count of atom-type E-State: >S== Count of atom-type E-State: >S<< Count of atom-type E-State: -S-
746 747 748 749 750 751 752 753 754 755	naaS ndssS nddssS nssssssS	Count of atom-type E-State: >S= Count of atom-type E-State: >S== Count of atom-type E-State: >S<<
746 747 748 749 750 751 752 753 754 755 756 757	naaS ndssS nddssS nssssssS nSm	Count of atom-type E-State: >S= Count of atom-type E-State: >S== Count of atom-type E-State: >S<< Count of atom-type E-State: -S- Count of atom-type E-State: -Cl

	nssAsH	Count of atom-type E-State: -AsH-
	nsssAs ndsssAs	Count of atom-type E-State: >As- Count of atom-type E-State: ->As=
764	nddsAs	Count of atom-type E-State: -=As=
	nsssssAs nsSeH	Count of atom-type E-State: ->As< Count of atom-type E-State: -SeH
767	ndSe	Count of atom-type E-State: =Se
	nssSe naaSe	Count of atom-type E-State: -Se- Count of atom-type E-State: aSea
770	ndssSe	Count of atom-type E-State: >Se=
	nssssssSe nddssSe	Count of atom-type E-State: >Se<< Count of atom-type E-State: -=Se=-
773	nsBr	Count of atom-type E-State: -Br
	nsSnH3 nssSnH2	Count of atom-type E-State: -SnH3 Count of atom-type E-State: -SnH2-
776	nsssSnH	Count of atom-type E-State: >SnH-
777	nssssSn nsI	Count of atom-type E-State: >Sn< Count of atom-type E-State: -I
	nsPbH3	Count of atom-type E-State: -PbH3
	nssPbH2 nsssPbH	Count of atom-type E-State: -PbH2- Count of atom-type E-State: >PbH-
	nssssPb	Count of atom-type E-State: >Pb<
	SHBd SwHBd	Sum of E-States for (strong) hydrogen bond donors Sum of E-States for weak hydrogen bond donors
	SHBa SwHBa	Sum of E-States for (strong) hydrogen bond acceptors Sum of E-States for weak hydrogen bond acceptors
	SHBint2	Sum of E-State descriptors of strength for potential hydrogen
788	SHBint3	bonds of path length 2 Sum of E-State descriptors of strength for potential hydrogen
700	SHBIIIIS	bonds of path length 3
789	SHBint4	Sum of E-State descriptors of strength for potential hydrogen bonds of path length 4
790	SHBint5	Sum of E-State descriptors of strength for potential hydrogen
701	SHBint6	bonds of path length 5 Sum of E-State descriptors of strength for potential hydrogen
		bonds of path length 6
792	SHBint7	Sum of E-State descriptors of strength for potential hydrogen bonds of path length 7
793	SHBint8	Sum of E-State descriptors of strength for potential hydrogen
794	SHBint9	bonds of path length 8 Sum of E-State descriptors of strength for potential hydrogen
		bonds of path length 9
795	SHBint10	Sum of E-State descriptors of strength for potential hydrogen bonds of path length 10
	SHsOH	Sum of atom-type H E-State: -OH
	SHdNH SHsSH	Sum of atom-type H E-State: =NH Sum of atom-type H E-State: -SH
799	SHsNH2	Sum of atom-type H E-State: -NH2
	SHssNH SHaaNH	Sum of atom-type H E-State: -NH- Sum of atom-type H E-State: :NH:
802	SHsNH3p	Sum of atom-type H E-State: -NH3+
	SHssNH2p SHsssNHp	Sum of atom-type H E-State: -NH2-+ Sum of atom-type H E-State: >NH-+
805	SHtCH	Sum of atom-type H E-State: #CH
	SHdCH2 SHdsCH	Sum of atom-type H E-State: =CH2 Sum of atom-type H E-State: =CH-
	SHaaCH	Sum of atom-type H E-State: :CH:
	SHCHnX	Sum of atom-type H E-State: CHnX
810	SHCsats	Sum of atom-type H E-State: H on C sp3 bonded to saturated C
	SHCsats SHCsatu	Sum of atom-type H E-State: H on C sp3 bonded to unsaturated C
811		Sum of atom-type H E-State: H on C sp3 bonded to unsaturated
811 812 813	SHCsatu SHAvin SHother	Sum of atom-type H E-State: H on C sp3 bonded to unsaturated C Sum of atom-type H E-State: H on C vinyl bonded to C aromatic Sum of atom-type H E-State: H on aaCH, dCH2 or dsCH
811 812 813	SHCsatu SHAvin	Sum of atom-type H E-State: H on C sp3 bonded to unsaturated C Sum of atom-type H E-State: H on C vinyl bonded to C aromatic Sum of atom-type H E-State: H on aaCH, dCH2 or dsCH Sum of atom-type H E-State: H bonded to B, Si, P, Ge, As, Se,
811 812 813 814 815	SHCsatu SHAvin SHother SHmisc SsLi	Sum of atom-type H E-State: H on C sp3 bonded to unsaturated C Sum of atom-type H E-State: H on C vinyl bonded to C aromatic Sum of atom-type H E-State: H on aaCH, dCH2 or dsCH Sum of atom-type H E-State: H bonded to B, Si, P, Ge, As, Se, Sn or Pb Sum of atom-type E-State: -Li
811 812 813 814 815 816	SHCsatu SHAvin SHother SHmisc SsLi SssBe	Sum of atom-type H E-State: H on C sp3 bonded to unsaturated C Sum of atom-type H E-State: H on C vinyl bonded to C aromatic Sum of atom-type H E-State: H on aaCH, dCH2 or dsCH Sum of atom-type H E-State: H bonded to B, Si, P, Ge, As, Se, Sn or Pb Sum of atom-type E-State: -Li Sum of atom-type E-State: -Be-
811 812 813 814 815 816 817 818	SHCsatu SHAvin SHother SHmisc SsLi SssBe SsssBem SsBH2	Sum of atom-type H E-State: H on C sp3 bonded to unsaturated C Sum of atom-type H E-State: H on C vinyl bonded to C aromatic Sum of atom-type H E-State: H on aaCH, dCH2 or dsCH Sum of atom-type H E-State: H bonded to B, Si, P, Ge, As, Se, Sn or Pb Sum of atom-type E-State: -Li Sum of atom-type E-State: -Be- Sum of atom-type E-State: >Be<-2 Sum of atom-type E-State: -BH2
811 812 813 814 815 816 817 818 819	SHCsatu SHAvin SHother SHmisc SsLi SssBe SssssBem	Sum of atom-type H E-State: H on C sp3 bonded to unsaturated C Sum of atom-type H E-State: H on C vinyl bonded to C aromatic Sum of atom-type H E-State: H on aaCH, dCH2 or dsCH Sum of atom-type H E-State: H bonded to B, Si, P, Ge, As, Se, Sn or Pb Sum of atom-type E-State: -Li Sum of atom-type E-State: -Be- Sum of atom-type E-State: >Be<-2
811 812 813 814 815 816 817 818 819 820 821	SHCsatu SHAvin SHother SHmisc SsLi SssBe SsssBem SsBH2 SssBH SsssB SsssBm	Sum of atom-type H E-State: H on C sp3 bonded to unsaturated C Sum of atom-type H E-State: H on C vinyl bonded to C aromatic Sum of atom-type H E-State: H on aaCH, dCH2 or dsCH Sum of atom-type H E-State: H bonded to B, Si, P, Ge, As, Se, Sn or Pb Sum of atom-type E-State: -Li Sum of atom-type E-State: -Be- Sum of atom-type E-State: -BH2 Sum of atom-type E-State: -BH- Sum of atom-type E-State: -B< Sum of atom-type E-State: -B< Sum of atom-type E-State: -B< Sum of atom-type E-State: -B< Sum of atom-type E-State: -B< Sum of atom-type E-State: -B< Sum of atom-type E-State: -B<
811 812 813 814 815 816 817 818 819 820 821 822	SHCsatu SHAvin SHother SHmisc SsLi SssBe SsssBem SsBH2 SssBH SsssB	Sum of atom-type H E-State: H on C sp3 bonded to unsaturated C Sum of atom-type H E-State: H on C vinyl bonded to C aromatic Sum of atom-type H E-State: H on aaCH, dCH2 or dsCH Sum of atom-type H E-State: H bonded to B, Si, P, Ge, As, Se, Sn or Pb Sum of atom-type E-State: -Li Sum of atom-type E-State: -Be- Sum of atom-type E-State: >Be<-2 Sum of atom-type E-State: -BH2 Sum of atom-type E-State: -BH- Sum of atom-type E-State: -B<
811 812 813 814 815 816 817 818 819 820 821 822 823 824	SHCsatu SHAvin SHother SHmisc SsLi SssBe SsssBem SsBH2 SssBH SsssB SsssBm SsCH3 SdCH2 SssCH2	Sum of atom-type H E-State: H on C sp3 bonded to unsaturated C Sum of atom-type H E-State: H on C vinyl bonded to C aromatic Sum of atom-type H E-State: H on aaCH, dCH2 or dsCH Sum of atom-type H E-State: H bonded to B, Si, P, Ge, As, Se, Sn or Pb Sum of atom-type E-State: -Li Sum of atom-type E-State: -Be- Sum of atom-type E-State: >Be<-2 Sum of atom-type E-State: -BH2 Sum of atom-type E-State: -BH- Sum of atom-type E-State: -B<- Sum of atom-type E-State: -B<- Sum of atom-type E-State: >CH3 Sum of atom-type E-State: =CH2 Sum of atom-type E-State: -CH2-
811 812 813 814 815 816 817 818 819 820 821 822 823 824 825 826	SHCsatu SHAvin SHother SHmisc SsLi SssBe SsssBem SsBH2 SssBH SsssB SsssBm SsCH3 SdCH2 StCH SdsCH	Sum of atom-type H E-State: H on C sp3 bonded to unsaturated C Sum of atom-type H E-State: H on C vinyl bonded to C aromatic Sum of atom-type H E-State: H on aaCH, dCH2 or dsCH Sum of atom-type H E-State: H bonded to B, Si, P, Ge, As, Se, Sn or Pb Sum of atom-type E-State: -Li Sum of atom-type E-State: -Be- Sum of atom-type E-State: -BH2 Sum of atom-type E-State: -BH- Sum of atom-type E-State: -B< Sum of atom-type E-State: -B< Sum of atom-type E-State: -B< Sum of atom-type E-State: -B< Sum of atom-type E-State: -B< Sum of atom-type E-State: -CH3 Sum of atom-type E-State: -CH3
811 812 813 814 815 816 817 818 819 820 821 822 823 824 825 826 827	SHCsatu SHAvin SHother SHmisc SsLi SssBe SsssBem SsBH2 SssBH SsssB SsssBm SsCH3 SdCH2 SssCH2 StCH SdsCH SdsCH SaaCH	Sum of atom-type H E-State: H on C sp3 bonded to unsaturated C Sum of atom-type H E-State: H on C vinyl bonded to C aromatic Sum of atom-type H E-State: H on aaCH, dCH2 or dsCH Sum of atom-type H E-State: H bonded to B, Si, P, Ge, As, Se, Sn or Pb Sum of atom-type E-State: -Li Sum of atom-type E-State: -Be- Sum of atom-type E-State: -Be- Sum of atom-type E-State: -BH2 Sum of atom-type E-State: -BH- Sum of atom-type E-State: -B< Sum of atom-type E-State: -B< Sum of atom-type E-State: -CH3 Sum of atom-type E-State: -CH2 Sum of atom-type E-State: +CH2- Sum of atom-type E-State: #CH Sum of atom-type E-State: -CH- Sum of atom-type E-State: -CH- Sum of atom-type E-State: -CH- Sum of atom-type E-State: -CH- Sum of atom-type E-State: -CH:
811 812 813 814 815 816 817 818 819 820 821 822 823 824 825 826 827 828 829	SHCsatu SHAvin SHother SHmisc SsLi SssBe SsssBem SsBH2 SssBH SsssB SsssBm SsCH3 SdCH2 StCH SdsCH SaaCH SssSCH SdsCH SddC	Sum of atom-type H E-State: H on C sp3 bonded to unsaturated C Sum of atom-type H E-State: H on C vinyl bonded to C aromatic Sum of atom-type H E-State: H on aaCH, dCH2 or dsCH Sum of atom-type H E-State: H bonded to B, Si, P, Ge, As, Se, Sn or Pb Sum of atom-type E-State: -Li Sum of atom-type E-State: -Be- Sum of atom-type E-State: -BH2 Sum of atom-type E-State: -BH- Sum of atom-type E-State: -B- Sum of atom-type E-State: -B- Sum of atom-type E-State: -B- Sum of atom-type E-State: -CH3 Sum of atom-type E-State: -CH2 Sum of atom-type E-State: #CH Sum of atom-type E-State: -CH- Sum of atom-type E-State: -CH- Sum of atom-type E-State: -CH- Sum of atom-type E-State: -CH- Sum of atom-type E-State: -CH- Sum of atom-type E-State: -CH- Sum of atom-type E-State: -CH- Sum of atom-type E-State: -CH- Sum of atom-type E-State: -CH- Sum of atom-type E-State: -CH- Sum of atom-type E-State: -CH- Sum of atom-type E-State: -CH- Sum of atom-type E-State: -CH- Sum of atom-type E-State: -CH- Sum of atom-type E-State: -CH- Sum of atom-type E-State: -CH- Sum of atom-type E-State: -CH-
811 812 813 814 815 816 817 818 819 820 821 822 823 824 825 826 827 828 829 830	SHCsatu SHAvin SHother SHmisc SsLi SssBe SsssBem SsBH2 SssBH SsssB SssssBm SsCH3 SdCH2 SssCH2 StCH SdsCH SdsCH SaaCH SssSCH SddC StsC	Sum of atom-type H E-State: H on C sp3 bonded to unsaturated C Sum of atom-type H E-State: H on C vinyl bonded to C aromatic Sum of atom-type H E-State: H on aaCH, dCH2 or dsCH Sum of atom-type H E-State: H bonded to B, Si, P, Ge, As, Se, Sn or Pb Sum of atom-type E-State: -Li Sum of atom-type E-State: -Be- Sum of atom-type E-State: -BH2 Sum of atom-type E-State: -BH2 Sum of atom-type E-State: -B- Sum of atom-type E-State: -B- Sum of atom-type E-State: -CH3 Sum of atom-type E-State: -CH2 Sum of atom-type E-State: +CH2 Sum of atom-type E-State: +CH2 Sum of atom-type E-State: -CH2 Sum of atom-type E-State: -CH2 Sum of atom-type E-State: -CH3 Sum of atom-type E-State: -CH2 Sum of atom-type E-State: -CH2 Sum of atom-type E-State: -CH3 Sum of atom-type E-State: -CH3 Sum of atom-type E-State: -CH3 Sum of atom-type E-State: -CH3 Sum of atom-type E-State: -CH3 Sum of atom-type E-State: -CH3 Sum of atom-type E-State: -CH3 Sum of atom-type E-State: -CH3 Sum of atom-type E-State: -CH3 Sum of atom-type E-State: -CH3 Sum of atom-type E-State: -CH3 Sum of atom-type E-State: -CH3 Sum of atom-type E-State: -CH3 Sum of atom-type E-State: -CH3 Sum of atom-type E-State: -CH3 Sum of atom-type E-State: -CH3 Sum of atom-type E-State: -CH3
811 812 813 814 815 816 817 818 819 820 821 822 823 824 825 826 827 828 829 830 831 832	SHCsatu SHAvin SHother SHmisc SsLi SssBe SsssBem SsBH2 SssBH SsssB SsssBm SsCH3 SdCH2 StSCH2 StCH SdsCH SdaCH SasCH SdsC SdssC SdssC SaasC	Sum of atom-type H E-State: H on C sp3 bonded to unsaturated C Sum of atom-type H E-State: H on C vinyl bonded to C aromatic Sum of atom-type H E-State: H on aaCH, dCH2 or dsCH Sum of atom-type H E-State: H bonded to B, Si, P, Ge, As, Se, Sn or Pb Sum of atom-type E-State: -Li Sum of atom-type E-State: -Be- Sum of atom-type E-State: -BH2 Sum of atom-type E-State: -BH- Sum of atom-type E-State: -B- Sum of atom-type E-State: -B- Sum of atom-type E-State: -B- Sum of atom-type E-State: -CH3 Sum of atom-type E-State: -CH2 Sum of atom-type E-State: -CH2- Sum of atom-type E-State: -CH- Sum of atom-type E-State: -CH- Sum of atom-type E-State: -CH- Sum of atom-type E-State: -CH- Sum of atom-type E-State: -CH- Sum of atom-type E-State: -CH- Sum of atom-type E-State: -CC- Sum of atom-type E-State: -CC- Sum of atom-type E-State: -CC- Sum of atom-type E-State: -CC- Sum of atom-type E-State: -CC- Sum of atom-type E-State: -CC- Sum of atom-type E-State: -CC- Sum of atom-type E-State: -CC- Sum of atom-type E-State: -CC- Sum of atom-type E-State: -CC- Sum of atom-type E-State: -CC- Sum of atom-type E-State: -CC- Sum of atom-type E-State: -CC-
811 812 813 814 815 816 817 818 819 820 821 822 823 824 825 826 827 828 829 830 831 832 833	SHCsatu SHAvin SHother SHmisc SsLi SssBe SsssBem SsBH2 SssBH SsssB SssssBm SsCH3 SdCH2 StCH SdsCH SaaCH SasCH SdSC SdssC SaasC SaaaC	Sum of atom-type H E-State: H on C sp3 bonded to unsaturated C Sum of atom-type H E-State: H on C vinyl bonded to C aromatic Sum of atom-type H E-State: H on aaCH, dCH2 or dsCH Sum of atom-type H E-State: H bonded to B, Si, P, Ge, As, Se, Sn or Pb Sum of atom-type E-State: -Li Sum of atom-type E-State: -Be- Sum of atom-type E-State: -Be- Sum of atom-type E-State: -BH2 Sum of atom-type E-State: -BH- Sum of atom-type E-State: -B- Sum of atom-type E-State: -B- Sum of atom-type E-State: -CH3 Sum of atom-type E-State: -CH2 Sum of atom-type E-State: -CH2- Sum of atom-type E-State: -CH- Sum of atom-type E-State: -CH- Sum of atom-type E-State: -CH- Sum of atom-type E-State: -CH- Sum of atom-type E-State: -CH- Sum of atom-type E-State: -C- Sum of atom-type E-State: -C- Sum of atom-type E-State: -C- Sum of atom-type E-State: -C- Sum of atom-type E-State: -C- Sum of atom-type E-State: -C- Sum of atom-type E-State: -C- Sum of atom-type E-State: -C- Sum of atom-type E-State: -C- Sum of atom-type E-State: -C- Sum of atom-type E-State: -C- Sum of atom-type E-State: -C- Sum of atom-type E-State: -C- Sum of atom-type E-State: -C- Sum of atom-type E-State: -C- Sum of atom-type E-State: -C- Sum of atom-type E-State: -C- Sum of atom-type E-State: -C- Sum of atom-type E-State: -C- Sum of atom-type E-State: -C- Sum of atom-type E-State: -C-
811 812 813 814 815 816 817 818 819 820 821 822 823 824 825 826 827 828 829 830 831 832 833	SHCsatu SHAvin SHother SHmisc SsLi SssBe SsssBe SssssBem SsBH2 SssBH SsssB SssssBm SsCH3 SdCH2 StsCH2 StCH SdsCH SaaCH SssCH SdsC SdssC SaasC SaaaC SssSSC SsNH3p	Sum of atom-type H E-State: H on C sp3 bonded to unsaturated C Sum of atom-type H E-State: H on aaCH, dCH2 or dsCH Sum of atom-type H E-State: H bonded to B, Si, P, Ge, As, Se, Sn or Pb Sum of atom-type E-State: -Li Sum of atom-type E-State: -Be- Sum of atom-type E-State: -Be- Sum of atom-type E-State: -BH2 Sum of atom-type E-State: -BH2 Sum of atom-type E-State: -B< Sum of atom-type E-State: -B< Sum of atom-type E-State: -B< Sum of atom-type E-State: -CH3 Sum of atom-type E-State: -CH2 Sum of atom-type E-State: +CH2 Sum of atom-type E-State: +CH2 Sum of atom-type E-State: +CH2 Sum of atom-type E-State: -CH2 Sum of atom-type E-State: -CH3 Sum of atom-type E-State: -CH3 Sum of atom-type E-State: -CH3 Sum of atom-type E-State: -CH3 Sum of atom-type E-State: -CH3 Sum of atom-type E-State: -CH3 Sum of atom-type E-State: -CH3 Sum of atom-type E-State: -CH3 Sum of atom-type E-State: -CH3 Sum of atom-type E-State: -CH3 Sum of atom-type E-State: -CH3 Sum of atom-type E-State: -CH3 Sum of atom-type E-State: -CH3 Sum of atom-type E-State: -CH3 Sum of atom-type E-State: -CH3 Sum of atom-type E-State: -CH3 Sum of atom-type E-State: -CH3 Sum of atom-type E-State: -CH3 Sum of atom-type E-State: -CH3 Sum of atom-type E-State: -CH3 Sum of atom-type E-State: -CH3
811 812 813 814 815 816 817 818 819 820 821 822 823 824 825 826 827 828 829 830 831 832 833 834 835 836	SHCsatu SHAvin SHother SHmisc SsLi SssBe SsssBe SssssBem SsBH2 SssBH SsssB SssssBm SsCH3 SdCH2 StCH SdCH SdsCH SaaCH SasCH SdCC StsC SdssC SaasC SaaaC SsssSC SsNH3p SsNH2	Sum of atom-type H E-State: H on C sp3 bonded to unsaturated C Sum of atom-type H E-State: H on aaCH, dCH2 or dsCH Sum of atom-type H E-State: H bonded to B, Si, P, Ge, As, Se, Sn or Pb Sum of atom-type E-State: -Li Sum of atom-type E-State: -Be- Sum of atom-type E-State: -Be- Sum of atom-type E-State: -BH2 Sum of atom-type E-State: -BH2 Sum of atom-type E-State: -B<- Sum of atom-type E-State: -B<- Sum of atom-type E-State: -B<- Sum of atom-type E-State: -CH3 Sum of atom-type E-State: -CH2 Sum of atom-type E-State: +CH2 Sum of atom-type E-State: +CH2 Sum of atom-type E-State: +CH5 Sum of atom-type E-State: -CH2 Sum of atom-type E-State: -CH2 Sum of atom-type E-State: -CH3 Sum of atom-type E-State: -CH3 Sum of atom-type E-State: -CH3 Sum of atom-type E-State: -CH3 Sum of atom-type E-State: -CH3 Sum of atom-type E-State: -CH3 Sum of atom-type E-State: -CH3 Sum of atom-type E-State: -CH3 Sum of atom-type E-State: -CH3 Sum of atom-type E-State: -CC Sum of atom-type E-State: -CC Sum of atom-type E-State: -CC Sum of atom-type E-State: -CC Sum of atom-type E-State: -CC Sum of atom-type E-State: -NH3+ Sum of atom-type E-State: -NH2
811 812 813 814 815 816 817 818 819 820 821 822 823 824 825 826 827 828 829 830 831 832 833 834 835 836	SHCsatu SHAvin SHother SHmisc SsLi SssBe SsssBe SsssBe SsssBH SssBH SsssB SsssBM SsCH3 SdCH2 StCH SdsCH SdsCH SaaCH SssCH SdSC SdsC SaasC SaaaC SssSSC SsNH3p SsNH2 SsNH2p SdNH	Sum of atom-type H E-State: H on C sp3 bonded to unsaturated C Sum of atom-type H E-State: H on C vinyl bonded to C aromatic Sum of atom-type H E-State: H on aaCH, dCH2 or dsCH Sum of atom-type H E-State: H bonded to B, Si, P, Ge, As, Se, Sn or Pb Sum of atom-type E-State: -Li Sum of atom-type E-State: -Be- Sum of atom-type E-State: -Be- Sum of atom-type E-State: -BH2 Sum of atom-type E-State: -BH- Sum of atom-type E-State: -B<- Sum of atom-type E-State: -B<- Sum of atom-type E-State: -CH3 Sum of atom-type E-State: -CH2 Sum of atom-type E-State: -CH2 Sum of atom-type E-State: #CH Sum of atom-type E-State: +CH Sum of atom-type E-State: -CH- Sum of atom-type E-State: -CH- Sum of atom-type E-State: -CH- Sum of atom-type E-State: -CC- Sum of atom-type E-State: -CC- Sum of atom-type E-State: -CC- Sum of atom-type E-State: -CC- Sum of atom-type E-State: -CC- Sum of atom-type E-State: -CC- Sum of atom-type E-State: -CC- Sum of atom-type E-State: -CC- Sum of atom-type E-State: -CC- Sum of atom-type E-State: -CC- Sum of atom-type E-State: -CC- Sum of atom-type E-State: -CC- Sum of atom-type E-State: -CC- Sum of atom-type E-State: -CC- Sum of atom-type E-State: -CC- Sum of atom-type E-State: -NH3+ Sum of atom-type E-State: -NH2- Sum of atom-type E-State: -NH2- Sum of atom-type E-State: -NH2- Sum of atom-type E-State: -NH2-
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811 812 813 814 815 816 817 818 819 820 821 822 823 824 825 826 827 828 829 830 831 832 833 834 835 836 837 838 839 840 841 842 843 844 845 846 847 848 849 850 851 852 853 856 857 858	SHCsatu SHAvin SHother SHmisc SsLi SssBe SsssBe SssssBem SsBH2 SsssBH SsssB SssssBm SsCH3 SdCH2 StCH SdsCH SaaCH SasCH SasCH SdsC SasSC SasSC SasSC SasSC SasSC SsNH3p SsNH2 SsSNH2 SSSNH2 SSSNH2 SdNH StN SssNH StN SaaNH StN SssSN SddsN SaasN SsssSN SddsN SaasN SssSO SaaC SssSC SsSSO SaaC SssSC SsSSSSSSSSSSSSSSSSSSSSSSSSSS	Sum of atom-type H E-State: H on C sp3 bonded to unsaturated C Sum of atom-type H E-State: H on C vinyl bonded to C aromatic Sum of atom-type H E-State: H on aaCH, dCH2 or dsCH Sum of atom-type H E-State: H bonded to B, Si, P, Ge, As, Se, Sn or Pb Sum of atom-type E-State: -Li Sum of atom-type E-State: -Be- Sum of atom-type E-State: -BH- Sum of atom-type E-State: -BH2 Sum of atom-type E-State: -BH2 Sum of atom-type E-State: -BH- Sum of atom-type E-State: -BS- Sum of atom-type E-State: -CH3 Sum of atom-type E-State: -CH2 Sum of atom-type E-State: -CH2 Sum of atom-type E-State: -CH2 Sum of atom-type E-State: -CH2 Sum of atom-type E-State: -CH- Sum of atom-type E-State: -CH- Sum of atom-type E-State: -CH- Sum of atom-type E-State: -C- Sum of atom-type E-State: -C- Sum of atom-type E-State: -C- Sum of atom-type E-State: -C- Sum of atom-type E-State: -C- Sum of atom-type E-State: -C- Sum of atom-type E-State: -C- Sum of atom-type E-State: -C- Sum of atom-type E-State: -C- Sum of atom-type E-State: -C- Sum of atom-type E-State: -C- Sum of atom-type E-State: -N- Sum of atom-type E-State: -NH2 Sum of atom-type E-State: -NH- Sum of atom-type E-State: -NH- Sum of atom-type E-State: -NH- Sum of atom-type E-State: -N- Sum of atom-type E-State: -N- Sum of atom-type E-State: -N- Sum of atom-type E-State: -N- Sum of atom-type E-State: -N- Sum of atom-type E-State: -N- Sum of atom-type E-State: -N- Sum of atom-type E-State: -N- Sum of atom-type E-State: -N- Sum of atom-type E-State: -N- Sum of atom-type E-State: -N- Sum of atom-type E-State: -N- Sum of atom-type E-State: -N- Sum of atom-type E-State: -N- Sum of atom-type E-State: -N- Sum of atom-type E-State: -N- Sum of atom-type E-State: -N- Sum of atom-type E-State: -N- Sum of atom-type E-State: -N- Sum of atom-type E-State: -N- Sum of atom-type E-State: -N- Sum of atom-type E-State: -N- Sum of atom-type E-State: -N- Sum of atom-type E-State: -N- Sum of atom-type E-State: -N- Sum of atom-type E-State: -N- Sum of atom-type E-State: -N- Sum of atom-type E-State: -N- Sum of ato
811 812 813 814 815 816 817 818 819 820 821 822 823 824 825 826 827 828 829 830 831 832 833 834 835 836 837 838 839 840 841 842 843 844 845 846 847 848 849 850 851 852 853 854 855 856	SHCsatu SHAvin SHother SHmisc SsLi SssBe SsssBe SssssBem SsBH2 SsssBH SsssB SssssBm SsCH3 SdCH2 StCH SdsCH SdsCH SaaCH SssCH SddC StsC SaasC SaasC SassC SassC SashH3p SsNH2 SssNH2p SdNH StN SssNH2 StN SssNHp SdsN SaaN SsssN SddsN SaaN SsssN SddsN SaasN SsssSC SaaC SssSC SaaC SsssSC SsSSNH3p SsSNH2 SsSNH2 SSSNH2 SSSNH2 SdSNH SaaN SssSNH SaaN SssSNH SaaN SsssN SddsN SaaSN SasSN SddsN SaaSN SssSSSSSSSSSSSSSSSSSSSSSSSSSSSS	Sum of atom-type H E-State: H on C sp3 bonded to unsaturated C Sum of atom-type H E-State: H on C vinyl bonded to C aromatic Sum of atom-type H E-State: H on aaCH, dCH2 or dsCH Sum of atom-type H E-State: H bonded to B, Si, P, Ge, As, Se, Sn or Pb Sum of atom-type E-State: -Li Sum of atom-type E-State: -Be- Sum of atom-type E-State: -Be- Sum of atom-type E-State: -BH2 Sum of atom-type E-State: -BH2 Sum of atom-type E-State: -BH- Sum of atom-type E-State: -B- Sum of atom-type E-State: -CH3 Sum of atom-type E-State: -CH2 Sum of atom-type E-State: -CH2 Sum of atom-type E-State: -CH2 Sum of atom-type E-State: -CH- Sum of atom-type E-State: -CH- Sum of atom-type E-State: -CH- Sum of atom-type E-State: -CH- Sum of atom-type E-State: -C- Sum of atom-type E-State: -C- Sum of atom-type E-State: -C- Sum of atom-type E-State: -C- Sum of atom-type E-State: -C- Sum of atom-type E-State: -C- Sum of atom-type E-State: -C- Sum of atom-type E-State: -C- Sum of atom-type E-State: -C- Sum of atom-type E-State: -C- Sum of atom-type E-State: -C- Sum of atom-type E-State: -C- Sum of atom-type E-State: -C- Sum of atom-type E-State: -NH3+ Sum of atom-type E-State: -NH2- Sum of atom-type E-State: -NH2- Sum of atom-type E-State: -NH- Sum of atom-type E-State: -NH- Sum of atom-type E-State: -NH- Sum of atom-type E-State: -NH- Sum of atom-type E-State: -N- Sum of atom-type E-State: -N- Sum of atom-type E-State: -N- Sum of atom-type E-State: -N- Sum of atom-type E-State: -N- Sum of atom-type E-State: -N- Sum of atom-type E-State: -N- Sum of atom-type E-State: -N- Sum of atom-type E-State: -N- Sum of atom-type E-State: -N- Sum of atom-type E-State: -N- Sum of atom-type E-State: -N- Sum of atom-type E-State: -N- Sum of atom-type E-State: -N- Sum of atom-type E-State: -N- Sum of atom-type E-State: -N- Sum of atom-type E-State: -N- Sum of atom-type E-State: -N- Sum of atom-type E-State: -N- Sum of atom-type E-State: -N- Sum of atom-type E-State: -N- Sum of atom-type E-State: -N- Sum of atom-type E-State: -N- Sum of atom-type E-State: -N- Sum o

	SssPH	Sum of atom-type E-State: -PH-
	SsssP SdsssP	Sum of atom-type E-State: >P- Sum of atom-type E-State: ->P=
864	SddsP	Sum of atom-type E-State: -=P=
	SsssssP SsSH	Sum of atom-type E-State: ->P< Sum of atom-type E-State: -SH
867	SdS	Sum of atom-type E-State: =S
	SssS SaaS	Sum of atom-type E-State: -S- Sum of atom-type E-State: aSa
870	SdssS	Sum of atom-type E-State: >S=
	SddssS SsssssS	Sum of atom-type E-State: >S== Sum of atom-type E-State: >S<<
873	SSm	Sum of atom-type E-State: -S-
	SsCl SsGeH3	Sum of atom-type E-State: -Cl Sum of atom-type E-State: -GeH3
876	SssGeH2	Sum of atom-type E-State: -GeH2-
	SsssGeH SssssGe	Sum of atom-type E-State: >GeH- Sum of atom-type E-State: >Ge<
	SsAsH2	Sum of atom-type E-State: -AsH2
	SssAsH SsssAs	Sum of atom-type E-State: -AsH- Sum of atom-type E-State: >As-
	SdsssAs	Sum of atom-type E-State: ->As=
	SddsAs SsssssAs	Sum of atom-type E-State: -=As= Sum of atom-type E-State: ->As<
	SsSeH SdSe	Sum of atom-type E-State: -SeH Sum of atom-type E-State: =Se
	SssSe	Sum of atom-type E-State: –Se-
	SaaSe SdssSe	Sum of atom-type E-State: aSea Sum of atom-type E-State: >Se=
890	SsssssSe	Sum of atom-type E-State: >Se<<
	SddssSe SsBr	Sum of atom-type E-State: -=Se=- Sum of atom-type E-State: -Br
893	SsSnH3	Sum of atom-type E-State: -SnH3
	SssSnH2 SsssSnH	Sum of atom-type E-State: -SnH2- Sum of atom-type E-State: >SnH-
896	SssssSn	Sum of atom-type E-State: >Sn<
897 898	SsI SsPbH3	Sum of atom-type E-State: -I Sum of atom-type E-State: -PbH3
899	SssPbH2	Sum of atom-type E-State: -PbH2-
	SsssPbH SssssPb	Sum of atom-type E-State: >PbH- Sum of atom-type E-State: >Pb<
902	minHBd	Minimum E-States for (strong) Hydrogen Bond donors
	minwHBd minHBa	Minimum E-States for weak Hydrogen Bond donors Minimum E-States for (strong) Hydrogen Bond acceptors
905	minwHBa	Minimum E-States for weak Hydrogen Bond acceptors
906	minHBint2	Minimum E-State descriptors of strength for potential Hydrogen Bonds of path length 2
907	minHBint3	Minimum E-State descriptors of strength for potential Hydrogen Bonds of path length 3
908	minHBint4	Minimum E-State descriptors of strength for potential Hydrogen
909	minHBint5	Bonds of path length 4 Minimum E-State descriptors of strength for potential Hydrogen
		Bonds of path length 5
910	minHBint6	Minimum E-State descriptors of strength for potential Hydrogen Bonds of path length 6
911	minHBint7	Minimum E-State descriptors of strength for potential Hydrogen
912	minHBint8	Bonds of path length 7 Minimum E-State descriptors of strength for potential Hydrogen
		Bonds of path length 8
913	minHBint9	Minimum E-State descriptors of strength for potential Hydrogen Bonds of path length 9
914	minHBint10	Minimum E-State descriptors of strength for potential Hydrogen
915	minHsOH	Bonds of path length 10 Minimum atom-type H E-State: -OH
	minHdNH minHsSH	Minimum atom-type H E-State: =NH Minimum atom-type H E-State: -SH
	minHsNH2	Minimum atom-type H E-State: -SH Minimum atom-type H E-State: -NH2
	minHssNH minHaaNH	Minimum atom-type H E-State: -NH- Minimum atom-type H E-State: :NH:
921	minHsNH3p	Minimum atom-type H E-State: -NH3+
	minHssNH2p minHsssNHp	Minimum atom-type H E-State: -NH2-+ Minimum atom-type H E-State: >NH-+
924	minHtCH	Minimum atom-type H E-State: #CH
	minHdCH2 minHdsCH	Minimum atom-type H E-State: =CH2 Minimum atom-type H E-State: =CH-
927	minHaaCH	Minimum atom-type H E-State: :CH:
	minHCHnX minHCsats	Minimum atom-type H E-State: CHnX Minimum atom-type H E-State: H bonded to B, Si, P, Ge, As,
		Se, Sn or Pb
930	minHCsatu	Minimum atom-type H E-State: H on C sp3 bonded to unsaturated C
931	minHAvin	Minimum atom-type H E-State: H on C vinyl bonded to C
932	minHother	aromatic Minimum atom-type H E-State: H on aaCH, dCH2 or dsCH
022	main I Imai o o	Minimum stom tyme HE State, Hhandad to D. Si. D. Co. As
	minHmisc	Minimum atom-type H E-State: H bonded to B, Si, P, Ge, As, Se, Sn or Pb
	minsLi minssBe	Minimum atom-type E-State: -Li Minimum atom-type E-State: -Be-
	minssssBem	Minimum atom-type E-State: >Be<-2
	minsBH2 minssBH	Minimum atom-type E-State: -BH2 Minimum atom-type E-State: -BH-
939	minsssB	Minimum atom-type E-State: -B<
	minssssBm minsCH3	Minimum atom-type E-State: >B<- Minimum atom-type E-State: -CH3
942	mindCH2	Minimum atom-type E-State: =CH2
	minssCH2 mintCH	Minimum atom-type E-State: -CH2- Minimum atom-type E-State: #CH
945	mindsCH	Minimum atom-type E-State: =CH-
	minaaCH minsssCH	Minimum atom-type E-State: :CH: Minimum atom-type E-State: >CH-
948	minddC	Minimum atom-type E-State: =C=
	mintsC mindssC	Minimum atom-type E-State: #C- Minimum atom-type E-State: =C<
951	minaasC	Minimum atom-type E-State: :C:-
	minaaaC minssssC	Minimum atom-type E-State: ::C: Minimum atom-type E-State: >C<
954	minsNH3p	Minimum atom-type E-State: -NH3+
	minsNH2 minssNH2p	Minimum atom-type E-State: -NH2 Minimum atom-type E-State: -NH2-+
957	mindNH	Minimum atom-type E-State: =NH
	minssNH minaaNH	Minimum atom-type E-State: -NH- Minimum atom-type E-State: :NH:

	mintN	Minimum atom-type E-State: #N
	minsssNHp mindsN	Minimum atom-type E-State: >NH-+ Minimum atom-type E-State: =N-
	minaaN minsssN	Minimum atom-type E-State: :N: Minimum atom-type E-State: >N-
965	minddsN	Minimum atom-type E-State: -N<<
	minaasN minssssNp	Minimum atom-type E-State: :N:- Minimum atom-type E-State: >N<+
968	minsOH	Minimum atom-type E-State: -OH
	mindO minssO	Minimum atom-type E-State: =O Minimum atom-type E-State: -O-
	minaaO minaOm	Minimum atom-type E-State: :O: Minimum atom-type E-State: :O-0.5
973	minsOm	Minimum atom-type E-State: -O-
	minsF minsSiH3	Minimum atom-type E-State: -F Minimum atom-type E-State: -SiH3
	minssSiH2	Minimum atom-type E-State: -SiH2-
	minsssSiH minssssSi	Minimum atom-type E-State: >SiH- Minimum atom-type E-State: >Si<
	minsPH2 minssPH	Minimum atom-type E-State: -PH2 Minimum atom-type E-State: -PH-
981	minsssP	Minimum atom-type E-State: >P-
	mindsssP minddsP	Minimum atom-type E-State: ->P= Minimum atom-type E-State: -=P=
	minsssssP minsSH	Minimum atom-type E-State: ->P<
	mindS	Minimum atom-type E-State: -SH Minimum atom-type E-State: =S
	minssS minaaS	Minimum atom-type E-State: -S- Minimum atom-type E-State: aSa
989	mindssS	Minimum atom-type E-State: >S=
	minddssS minssssssS	Minimum atom-type E-State: >S== Minimum atom-type E-State: >S<<
	minSm minsCl	Minimum atom-type E-State: -S-
	minsCi minsGeH3	Minimum atom-type E-State: -Cl Minimum atom-type E-State: -GeH3
	minssGeH2 minsssGeH	Minimum atom-type E-State: -GeH2- Minimum atom-type E-State: >GeH-
997	minssssGe	Minimum atom-type E-State: >Ge<
	minsAsH2 minssAsH	Minimum atom-type E-State: -AsH2 Minimum atom-type E-State: -AsH-
1000	minsssAs	Minimum atom-type E-State: >As-
	mindsssAs minddsAs	Minimum atom-type E-State: ->As= Minimum atom-type E-State: -=As=
	minsssssAs minsSeH	Minimum atom-type E-State: ->As< Minimum atom-type E-State: -SeH
1005	mindSe	Minimum atom-type E-State: =Se
	minssSe minaaSe	Minimum atom-type E-State: -Se- Minimum atom-type E-State: aSea
1008	mindssSe	Minimum atom-type E-State: >Se=
	minssssssSe minddssSe	Minimum atom-type E-State: >Se<< Minimum atom-type E-State: -=Se=-
	minsBr minsSnH3	Minimum atom-type E-State: -Br Minimum atom-type E-State: -SnH3
1013	minssSnH2	Minimum atom-type E-State: -SnH2-
	minsssSnH minssssSn	Minimum atom-type E-State: >SnH- Minimum atom-type E-State: >Sn<
1016	minsI	Minimum atom-type E-State: -I
	minsPbH3 minssPbH2	Minimum atom-type E-State: -PbH3 Minimum atom-type E-State: -PbH2-
	minsssPbH minssssPb	Minimum atom-type E-State: >PbH-
1021	maxHBd	Minimum atom-type E-State: >Pb< Maximum E-States for (strong) Hydrogen Bond donors
	maxwHBd maxHBa	Maximum E-States for weak Hydrogen Bond donors Maximum E-States for (strong) Hydrogen Bond acceptors
1024	maxwHBa	Maximum E-States for weak Hydrogen Bond acceptors
1025	maxHBint2	Maximum E-State descriptors of strength for potential Hydrogen Bonds of path length 2
1026	maxHBint3	Maximum E-State descriptors of strength for potential Hydrogen Bonds of path length 3
1027	maxHBint4	Maximum E-State descriptors of strength for potential Hydrogen
1028	maxHBint5	Bonds of path length 4 Maximum E-State descriptors of strength for potential Hydrogen
		Bonds of path length 5
1029	maxHBint6	Maximum E-State descriptors of strength for potential Hydrogen Bonds of path length 6
1030	maxHBint7	Maximum E-State descriptors of strength for potential Hydrogen
1031	maxHBint8	Bonds of path length 7 Maximum E-State descriptors of strength for potential Hydrogen
1022	maxHBint9	Bonds of path length 8 Maximum E-State descriptors of strength for potential Hydrogen
		Bonds of path length 9
1033	maxHBint10	Maximum E-State descriptors of strength for potential Hydrogen Bonds of path length 10
	maxHsOH	Maximum atom-type H E-State: -OH
	maxHdNH maxHsSH	Maximum atom-type H E-State: =NH Maximum atom-type H E-State: -SH
1037	maxHsNH2 maxHssNH	Maximum atom-type H E-State: -NH2 Maximum atom-type H E-State: -NH-
1039	maxHaaNH	Maximum atom-type H E-State: :NH:
	maxHsNH3p maxHssNH2p	Maximum atom-type H E-State: -NH3+ Maximum atom-type H E-State: -NH2-+
1042	maxHsssNHp	Maximum atom-type H E-State: >NH-+
	maxHtCH maxHdCH2	Maximum atom-type H E-State: #CH Maximum atom-type H E-State: =CH2
	maxHdsCH maxHaaCH	Maximum atom-type H E-State: =CH- Maximum atom-type H E-State: :CH:
1047	maxHCHnX	Maximum atom-type H E-State: CHnX
1048	maxHCsats	Maximum atom-type H E-State: H bonded to B, Si, P, Ge, As, Se, Sn or Pb
1049	maxHCsatu	Maximum atom-type H E-State: H on C sp3 bonded to
1050	maxHAvin	unsaturated C Maximum atom-type H E-State: H on C vinyl bonded to C
		aromatic
	maxHother	Maximum atom-type H E-State: H on aaCH, dCH2 or dsCH
1052	maxHmisc	Maximum atom-type H E-State: H bonded to B, Si, P, Ge, As, Se, Sn or Pb
	maxsLi	Maximum atom-type E-State: -Li
	maxssBe maxssssBem	Maximum atom-type E-State: -Be- Maximum atom-type E-State: >Be<-2
1056	maxsBH2	Maximum atom-type E-State: -BH2
	maxssBH maxsssB	Maximum atom-type E-State: -BH- Maximum atom-type E-State: -B<
-		

	maxssssBm	Maximum atom-type E-State: >B<-
	maxsCH3 maxdCH2	Maximum atom-type E-State: -CH3 Maximum atom-type E-State: =CH2
	maxssCH2	Maximum atom-type E-State: -CH2-
	maxtCH	Maximum atom-type E-State: #CH
	maxdsCH maxaaCH	Maximum atom-type E-State: =CH- Maximum atom-type E-State: :CH:
	maxsssCH	Maximum atom-type E-State: >CH-
	maxddC	Maximum atom-type E-State: =C=
	maxtsC	Maximum atom-type E-State: #C-
	maxdssC maxaasC	Maximum atom-type E-State: =C< Maximum atom-type E-State: :C:-
	maxaaaC	Maximum atom-type E-State: ::C:
	maxssssC	Maximum atom-type E-State: >C<
	maxsNH3p maxsNH2	Maximum atom-type E-State: -NH3+ Maximum atom-type E-State: -NH2
	maxssNH2p	Maximum atom-type E-State: -NH2-+
1076	maxdNH	Maximum atom-type E-State: =NH
	maxssNH	Maximum atom-type E-State: -NH-
	maxaaNH maxtN	Maximum atom-type E-State: :NH: Maximum atom-type E-State: #N
	maxsssNHp	Maximum atom-type E-State: >NH-+
	maxdsN	Maximum atom-type E-State: =N-
	maxaaN maxsssN	Maximum atom-type E-State: :N: Maximum atom-type E-State: >N-
	maxddsN	Maximum atom-type E-State: -N<<
1085	maxaasN	Maximum atom-type E-State: :N:-
	maxssssNp	Maximum atom-type E-State: >N<+
	maxsOH maxdO	Maximum atom-type E-State: -OH Maximum atom-type E-State: =O
	maxso	Maximum atom-type E-State: =O Maximum atom-type E-State: -O-
1090	maxaaO	Maximum atom-type E-State: :O:
	maxaOm	Maximum atom-type E-State: :O-0.5
	maxsOm maxsF	Maximum atom-type E-State: -O- Maximum atom-type E-State: -F
	maxsSiH3	Maximum atom-type E-State: -SiH3
	maxssSiH2	Maximum atom-type E-State: -SiH2-
	maxsssSiH	Maximum atom-type E-State: >SiH-
	maxssssSi maxsPH2	Maximum atom-type E-State: >Si< Maximum atom-type E-State: -PH2
	maxssPH	Maximum atom-type E-State: -PH-
	maxsssP	Maximum atom-type E-State: >P-
	maxdsssP maxddsP	Maximum atom-type E-State: ->P= Maximum atom-type E-State: -=P=
	maxsssssP	Maximum atom-type E-State: ->P<
	maxsSH	Maximum atom-type E-State: -SH
	maxdS	Maximum atom-type E-State: =S
	maxssS maxaaS	Maximum atom-type E-State: -S- Maximum atom-type E-State: aSa
	maxdssS	Maximum atom-type E-State: >S=
	maxddssS	Maximum atom-type E-State: >S==
	maxssssssS maxSm	Maximum atom-type E-State: >S<< Maximum atom-type E-State: -S-
	maxsCl	Maximum atom-type E-State: -S-
	maxsGeH3	Maximum atom-type E-State: -GeH3
	maxssGeH2	Maximum atom-type E-State: -GeH2-
	maxssssGeH maxssssGe	Maximum atom-type E-State: >GeH- Maximum atom-type E-State: >Ge<
	maxsAsH2	Maximum atom-type E-State: -AsH2
	maxssAsH	Maximum atom-type E-State: -AsH-
	maxsssAs maxdsssAs	Maximum atom-type E-State: >As- Maximum atom-type E-State: ->As=
	maxddsAs	Maximum atom-type E-State: -=As=
	maxsssssAs	Maximum atom-type E-State: ->As<
	maxsSeH	Maximum atom-type E-State: -SeH
	maxdSe maxssSe	Maximum atom-type E-State: =Se Maximum atom-type E-State: -Se-
	maxaaSe	Maximum atom-type E-State: aSea
	maxdssSe	Maximum atom-type E-State: >Se=
	maxssssssSe maxddssSe	Maximum atom-type E-State: >Se<< Maximum atom-type E-State: -=Se=-
	maxsBr	Maximum atom-type E-State: -=Se=- Maximum atom-type E-State: -Br
1131	maxsSnH3	Maximum atom-type E-State: -SnH3
	maxssSnH2 maxsssSnH	Maximum atom-type E-State: -SnH2-
	maxssssSnH maxssssSn	Maximum atom-type E-State: >SnH- Maximum atom-type E-State: >Sn<
1135	maxsI	Maximum atom-type E-State: -I
	maxsPbH3	Maximum atom-type E-State: -PbH3
	maxssPbH2 maxsssPbH	Maximum atom-type E-State: -PbH2- Maximum atom-type E-State: >PbH-
	maxssssPb	Maximum atom-type E-State: >Pb<
	sumI	Sum of the intrinsic state values I
	meanI hmax	Mean intrinsic state values I Maximum H E-State
	gmax	Maximum E-State
1144	hmin	Minimum H E-State
	gmin	Minimum E-State
	LipoaffinityIndex MAXDN	Lipoaffinity index Maximum negative intrinsic state difference in the molecule
	MAXDP	(related to the nucleophilicity of the molecule). Using deltaV = (Zv-maxBondedHydrogens) /(atomicNumber-Zv-1). Gramatica, P., Corradi, M., and Consonni, V. (2000). Modelling and prediction of soil sorption coefficients of non-ionic organic pesticides by molecular descriptors. Chemosphere 41, 763-777. Maximum positive intrinsic state difference in the molecule (related to the electrophilicity of the molecule). Using deltaV =
1149	DELS	(Zv-maxBondedHydrogens) /(atomicNumber-Zv-1). Gramatica, P., Corradi, M., and Consonni, V. (2000). Modelling and prediction of soil sorption coefficients of non-ionic organic pesticides by molecular descriptors. Chemosphere 41, 763-777. Sum of all atoms intrinsic state differences (measure of total
1149	DELA	charge transfer in the molecule). Using deltaV = (Zv-maxBondedHydrogens) /(atomicNumber-Zv-1). Gramatica, P., Corradi, M., and Consonni, V. (2000). Modelling and prediction of soil sorption coefficients of non-ionic organic pesticides by molecular descriptors. Chemosphere 41, 763-777.

1150 MAXDN2	Maximum negative intrinsic state difference in the molecule (related to the nucleophilicity of the molecule). Using deltaV =
	Zv-maxBondedHydrogens. Gramatica, P., Corradi, M., and
	Consonni, V. (2000). Modelling and prediction of soil sorption coefficients of non-ionic organic pesticides by molecular
	descriptors. Chemosphere 41, 763-777.
1151 MAXDP2	Maximum positive intrinsic state difference in the molecule
	(related to the electrophilicity of the molecule). Using deltaV = Zv-maxBondedHydrogens. Gramatica, P., Corradi, M., and
	Consonni, V. (2000). Modelling and prediction of soil sorption
	coefficients of non-ionic organic pesticides by molecular descriptors. Chemosphere 41, 763-777.
1152 DELS2	Sum of all atoms intrinsic state differences (measure of total
1132 DEL32	charge transfer in the molecule). Using deltaV = Zv-
	maxBondedHydrogens. Gramatica, P., Corradi, M., and Consonni, V. (2000). Modelling and prediction of soil sorption
	coefficients of non-ionic organic pesticides by molecular descriptors. Chemosphere 41, 763-777.
1153 ETA_Alpha	Sum of alpha values of all non-hydrogen vertices of a molecule
1154 ETA_AlphaP	Sum of alpha values of all non-hydrogen vertices of a molecule
1155 ETA_dAlpha_A	relative to molecular size A measure of count of non-hydrogen heteroatoms
1156 ETA_dAlpha_B	A measure of count of hydrogen bond acceptor atoms and/or
1157 ETA_Epsilon_1	polar surface area A measure of electronegative atom count
1158 ETA_Epsilon_2 1159 ETA_Epsilon_3	A measure of electronegative atom count A measure of electronegative atom count
1160 ETA_Epsilon_4	A measure of electronegative atom count
1161 ETA_Epsilon_5 1162 ETA_dEpsilon_A	A measure of electronegative atom count A measure of contribution of unsaturation and electronegative
	atom count
1163 ETA_dEpsilon_B 1164 ETA_dEpsilon_C	A measure of contribution of unsaturation A measure of contribution of electronegativity
1165 ETA_dEpsilon_D 1166 ETA_Psi_1	A measure of contribution of hydrogen bond donor atoms A measure of hydrogen bonding propensity of the molecules
	and/or polar surface area
1167 ETA_dPsi_A	A measure of hydrogen bonding propensity of the molecules
1168 ETA_dPsi_B	A measure of hydrogen bonding propensity of the molecules
1169 ETA_Shape_P	Shape index P
1170 ETA_Shape_Y 1171 ETA_Shape_X	Shape index Y Shape index X
1172 ETA_Beta	A measure of electronic features of the molecule
1173 ETA_BetaP	A measure of electronic features of the molecule relative to molecular size
1174 ETA_Beta_s 1175 ETA_BetaP_s	A measure of electronegative atom count of the molecule A measure of electronegative atom count of the molecule relative
	to molecular size
1176 ETA_Beta_ns 1177 ETA_BetaP_ns	A measure of electron-richness of the molecule A measure of electron-richness of the molecule relative to
	molecular size A measure of relative unsaturation content
1178 ETA_dBeta	A measure of ferative unsaturation content
1179 ETA_dBetaP	A measure of relative unsaturation content relative to molecular
1179 ETA_dBetaP 1180 ETA_Beta_ns_d	size
	A measure of lone electrons entering into resonance A measure of lone electrons entering into resonance relative to
1180 ETA_Beta_ns_d 1181 ETA_BetaP_ns_d 1182 ETA_Eta	A measure of lone electrons entering into resonance A measure of lone electrons entering into resonance relative to molecular size Composite index Eta
1180 ETA_Beta_ns_d 1181 ETA_BetaP_ns_d	A measure of lone electrons entering into resonance A measure of lone electrons entering into resonance relative to molecular size
1180 ETA_Beta_ns_d 1181 ETA_BetaP_ns_d 1182 ETA_Eta 1183 ETA_EtaP 1184 ETA_Eta_R 1185 ETA_Eta_F	A measure of lone electrons entering into resonance A measure of lone electrons entering into resonance relative to molecular size Composite index Eta Composite index Eta relative to molecular size Composite index Eta for reference alkane Functionality index EtaF
1180 ETA_Beta_ns_d 1181 ETA_BetaP_ns_d 1182 ETA_Eta 1183 ETA_EtaP 1184 ETA_Eta_R 1185 ETA_Eta_F 1186 ETA_EtaP_F 1187 ETA_Eta_L	A measure of lone electrons entering into resonance A measure of lone electrons entering into resonance relative to molecular size Composite index Eta Composite index Eta relative to molecular size Composite index Eta for reference alkane Functionality index EtaF Functionality index EtaF relative to molecular size Local index Eta_local
1180 ETA_Beta_ns_d 1181 ETA_BetaP_ns_d 1182 ETA_Eta 1183 ETA_EtaP 1184 ETA_Eta_R 1185 ETA_Eta_F 1186 ETA_EtaP_F 1187 ETA_Eta_L 1188 ETA_EtaP_L	A measure of lone electrons entering into resonance A measure of lone electrons entering into resonance relative to molecular size Composite index Eta Composite index Eta relative to molecular size Composite index Eta for reference alkane Functionality index EtaF Functionality index EtaF relative to molecular size Local index Eta_local Local index Eta_local relative to molecular size
1180 ETA_Beta_ns_d 1181 ETA_BetaP_ns_d 1182 ETA_Eta 1183 ETA_EtaP 1184 ETA_Eta_R 1185 ETA_Eta_F 1186 ETA_Eta_F 1187 ETA_Eta_L 1188 ETA_Eta_L 1189 ETA_Eta_L 1190 ETA_Eta_F_L	A measure of lone electrons entering into resonance A measure of lone electrons entering into resonance relative to molecular size Composite index Eta Composite index Eta relative to molecular size Composite index Eta for reference alkane Functionality index EtaF Functionality index EtaF relative to molecular size Local index Eta_local Local index Eta_local relative to molecular size Local index Eta_local for reference alkane Local functionality contribution EtaF_local
1180 ETA_Beta_ns_d 1181 ETA_BetaP_ns_d 1182 ETA_Eta 1183 ETA_EtaP 1184 ETA_Eta_R 1185 ETA_Eta_F 1186 ETA_EtaP_F 1187 ETA_Eta_L 1188 ETA_EtaP_L 1189 ETA_Eta_R	A measure of lone electrons entering into resonance A measure of lone electrons entering into resonance relative to molecular size Composite index Eta Composite index Eta relative to molecular size Composite index Eta for reference alkane Functionality index EtaF Functionality index EtaF Functionality index EtaF relative to molecular size Local index Eta_local Local index Eta_local relative to molecular size Local index Eta_local for reference alkane Local functionality contribution EtaF_local Local functionality contribution EtaF_local relative to molecular size
1180 ETA_Beta_ns_d 1181 ETA_BetaP_ns_d 1182 ETA_Eta 1183 ETA_EtaP 1184 ETA_Eta_R 1185 ETA_Eta_F 1186 ETA_Eta_F 1187 ETA_Eta_L 1188 ETA_Eta_L 1189 ETA_Eta_L 1190 ETA_Eta_F_L 1191 ETA_Eta_F_L	A measure of lone electrons entering into resonance A measure of lone electrons entering into resonance relative to molecular size Composite index Eta Composite index Eta relative to molecular size Composite index Eta for reference alkane Functionality index EtaF Functionality index EtaF Functionality index EtaF relative to molecular size Local index Eta_local Local index Eta_local relative to molecular size Local index Eta_local for reference alkane Local functionality contribution EtaF_local Local functionality contribution EtaF_local relative to molecular size Branching index EtaB
1180 ETA_Beta_ns_d 1181 ETA_BetaP_ns_d 1182 ETA_Eta 1183 ETA_EtaP 1184 ETA_Eta_R 1185 ETA_Eta_F 1186 ETA_EtaP_F 1187 ETA_Eta_L 1188 ETA_EtaP_L 1190 ETA_Eta_R_L 1190 ETA_Eta_F_L 1191 ETA_EtaP_F	A measure of lone electrons entering into resonance A measure of lone electrons entering into resonance relative to molecular size Composite index Eta Composite index Eta relative to molecular size Composite index Eta for reference alkane Functionality index EtaF Functionality index EtaF Functionality index EtaF relative to molecular size Local index Eta_local Local index Eta_local relative to molecular size Local index Eta_local for reference alkane Local functionality contribution EtaF_local Local functionality contribution EtaF_local relative to molecular size Branching index EtaB Branching index EtaB (with ring correction)
1180 ETA_Beta_ns_d 1181 ETA_BetaP_ns_d 1182 ETA_Eta 1183 ETA_EtaP 1184 ETA_Eta_R 1185 ETA_Eta_F 1186 ETA_Eta_F 1187 ETA_Eta_L 1188 ETA_Eta_L 1190 ETA_Eta_R_L 1190 ETA_Eta_F_L 1191 ETA_Eta_P_L 1192 ETA_Eta_B 1193 ETA_Eta_B	A measure of lone electrons entering into resonance A measure of lone electrons entering into resonance relative to molecular size Composite index Eta Composite index Eta relative to molecular size Composite index Eta for reference alkane Functionality index EtaF Functionality index EtaF Functionality index EtaF relative to molecular size Local index Eta_local Local index Eta_local relative to molecular size Local index Eta_local for reference alkane Local functionality contribution EtaF_local Local functionality contribution EtaF_local relative to molecular size Branching index EtaB Branching index EtaB relative to molecular size
1180 ETA_Beta_ns_d 1181 ETA_BetaP_ns_d 1182 ETA_Eta 1183 ETA_EtaP 1184 ETA_Eta_R 1185 ETA_Eta_F 1186 ETA_Eta_F 1187 ETA_Eta_L 1188 ETA_Eta_L 1190 ETA_Eta_R 1191 ETA_Eta_P_L 1191 ETA_Eta_P_L 1192 ETA_Eta_B 1193 ETA_Eta_B 1194 ETA_Eta_B_RC 1195 ETA_EtaP_B_RC	A measure of lone electrons entering into resonance A measure of lone electrons entering into resonance relative to molecular size Composite index Eta Composite index Eta relative to molecular size Composite index Eta for reference alkane Functionality index EtaF Functionality index EtaF Functionality index EtaF relative to molecular size Local index Eta_local Local index Eta_local relative to molecular size Local index Eta_local for reference alkane Local functionality contribution EtaF_local Local functionality contribution EtaF_local Functionality contribution EtaF_local Coal functionality contribution EtaF_local relative to molecular size Branching index EtaB Branching index EtaB (with ring correction) Branching index EtaB (with ring correction) relative to molecular size Complexity of a molecule
1180 ETA_Beta_ns_d 1181 ETA_BetaP_ns_d 1182 ETA_Eta 1183 ETA_EtaP 1184 ETA_Eta_R 1185 ETA_Eta_F 1186 ETA_EtaP_F 1187 ETA_Eta_L 1188 ETA_EtaP_L 1190 ETA_Eta_F_L 1191 ETA_Eta_F_L 1191 ETA_EtaP_F_L 1192 ETA_Eta_B 1193 ETA_Eta_B 1194 ETA_Eta_B_RC 1195 ETA_EtaP_B_RC	A measure of lone electrons entering into resonance A measure of lone electrons entering into resonance relative to molecular size Composite index Eta Composite index Eta relative to molecular size Composite index Eta for reference alkane Functionality index EtaF Functionality index EtaF Functionality index EtaF relative to molecular size Local index Eta_local Local index Eta_local relative to molecular size Local index Eta_local for reference alkane Local functionality contribution EtaF_local Local functionality contribution EtaF_local relative to molecular size Branching index EtaB Branching index EtaB (with ring correction) Branching index EtaB (with ring correction) relative to molecular size Complexity of a molecule Complexity of a system Number of hydrogen bond acceptors (using CDK
1180 ETA_Beta_ns_d 1181 ETA_BetaP_ns_d 1182 ETA_Eta 1183 ETA_EtaP 1184 ETA_Eta_R 1185 ETA_Eta_F 1186 ETA_Eta_F 1187 ETA_Eta_L 1188 ETA_EtaP_L 1190 ETA_Eta_F_L 1191 ETA_Eta_F_L 1192 ETA_Eta_B 1193 ETA_Eta_B 1194 ETA_Eta_B 1195 ETA_Eta_B_RC 1196 FMF 1197 fragC	A measure of lone electrons entering into resonance A measure of lone electrons entering into resonance relative to molecular size Composite index Eta Composite index Eta relative to molecular size Composite index Eta for reference alkane Functionality index EtaF Functionality index EtaF Functionality index EtaF relative to molecular size Local index Eta_local Local index Eta_local relative to molecular size Local index Eta_local for reference alkane Local functionality contribution EtaF_local Local functionality contribution EtaF_local relative to molecular size Branching index EtaB Branching index EtaB (with ring correction) Branching index EtaB (with ring correction) Complexity of a molecule Complexity of a system
1180 ETA_Beta_ns_d 1181 ETA_BetaP_ns_d 1182 ETA_Eta 1183 ETA_EtaP 1184 ETA_Eta_R 1185 ETA_Eta_F 1186 ETA_Eta_F 1187 ETA_Eta_L 1188 ETA_Eta_L 1190 ETA_Eta_R 1191 ETA_Eta_F 1192 ETA_Eta_B 1193 ETA_Eta_B 1194 ETA_Eta_B 1195 ETA_Eta_B 1196 FMF 1197 fragC 1198 nHBAcc	A measure of lone electrons entering into resonance A measure of lone electrons entering into resonance relative to molecular size Composite index Eta Composite index Eta relative to molecular size Composite index Eta for reference alkane Functionality index EtaF Functionality index EtaF Functionality index EtaF relative to molecular size Local index Eta_local Local index Eta_local relative to molecular size Local index Eta_local for reference alkane Local functionality contribution EtaF_local Local functionality contribution EtaF_local relative to molecular size Branching index EtaB Branching index EtaB (with ring correction) Branching index EtaB (with ring correction) Complexity of a molecule Complexity of a system Number of hydrogen bond acceptors (using CDK HBondAcceptorCountDescriptor algorithm) Number of hydrogen bond acceptors (any oxygen; any nitrogen where the formal charge of the nitrogen is non-positive (i.e.
1180 ETA_Beta_ns_d 1181 ETA_BetaP_ns_d 1182 ETA_Eta 1183 ETA_EtaP 1184 ETA_Eta_R 1185 ETA_Eta_F 1186 ETA_Eta_F 1187 ETA_Eta_L 1188 ETA_Eta_L 1190 ETA_Eta_R 1191 ETA_Eta_F 1192 ETA_Eta_B 1193 ETA_Eta_B 1194 ETA_Eta_B 1195 ETA_Eta_B 1196 FMF 1197 fragC 1198 nHBAcc	A measure of lone electrons entering into resonance A measure of lone electrons entering into resonance relative to molecular size Composite index Eta Composite index Eta relative to molecular size Composite index Eta for reference alkane Functionality index EtaF Functionality index EtaF relative to molecular size Local index Eta_local Local index Eta_local relative to molecular size Local index Eta_local relative to molecular size Local index Eta_local for reference alkane Local functionality contribution EtaF_local Local functionality contribution EtaF_local relative to molecular size Branching index EtaB Branching index EtaB (with ring correction) Branching index EtaB (with ring correction) relative to molecular size Complexity of a molecule Complexity of a system Number of hydrogen bond acceptors (using CDK HBondAcceptorCountDescriptor algorithm) Number of hydrogen bond acceptors (any oxygen; any nitrogen where the formal charge of the nitrogen is non-positive (i.e. formal charge <= 0) except a non-aromatic nitrogen that is adjacent to an oxygen and aromatic ring, or an aromatic nitrogen
1180 ETA_Beta_ns_d 1181 ETA_BetaP_ns_d 1182 ETA_Eta 1183 ETA_EtaP 1184 ETA_Eta_R 1185 ETA_Eta_F 1186 ETA_Eta_F 1187 ETA_Eta_L 1188 ETA_Eta_L 1190 ETA_Eta_R 1191 ETA_Eta_F 1192 ETA_Eta_B 1193 ETA_Eta_B 1194 ETA_Eta_B 1195 ETA_Eta_B 1196 FMF 1197 fragC 1198 nHBAcc	A measure of lone electrons entering into resonance A measure of lone electrons entering into resonance relative to molecular size Composite index Eta Composite index Eta relative to molecular size Composite index Eta for reference alkane Functionality index EtaF Functionality index EtaF Functionality index EtaF relative to molecular size Local index Eta_local Local index Eta_local relative to molecular size Local index Eta_local for reference alkane Local functionality contribution EtaF_local Local functionality contribution EtaF_local Local functionality contribution EtaF_local relative to molecular size Branching index EtaB Branching index EtaB (with ring correction) Branching index EtaB (with ring correction) Complexity of a molecule Complexity of a molecule Complexity of a system Number of hydrogen bond acceptors (using CDK HBondAcceptorCountDescriptor algorithm) Number of hydrogen bond acceptors (any oxygen; any nitrogen where the formal charge of the nitrogen is non-positive (i.e. formal charge <= 0) except a non-aromatic nitrogen that is
1180 ETA_Beta_ns_d 1181 ETA_BetaP_ns_d 1182 ETA_Eta 1183 ETA_EtaP 1184 ETA_Eta_R 1185 ETA_Eta_F 1186 ETA_Eta_F 1187 ETA_Eta_L 1189 ETA_Eta_L 1190 ETA_Eta_F_L 1191 ETA_Eta_F_L 1192 ETA_Eta_B 1193 ETA_Eta_B 1194 ETA_Eta_B 1195 ETA_Eta_B_RC 1196 FMF 1197 fragC 1198 nHBAcc	A measure of lone electrons entering into resonance A measure of lone electrons entering into resonance relative to molecular size Composite index Eta Composite index Eta relative to molecular size Composite index Eta for reference alkane Functionality index EtaF Functionality index EtaF Functionality index EtaF relative to molecular size Local index Eta_local Local index Eta_local relative to molecular size Local index Eta_local for reference alkane Local functionality contribution EtaF_local Local functionality contribution EtaF_local relative to molecular size Branching index EtaB Branching index EtaB (with ring correction) Branching index EtaB (with ring correction) Branching index EtaB (with ring correction) relative to molecular size Complexity of a molecule Complexity of a molecule Complexity of a system Number of hydrogen bond acceptors (using CDK HBondAcceptorCountDescriptor algorithm) Number of hydrogen bond acceptors (any oxygen; any nitrogen where the formal charge of the nitrogen is non-positive (i.e. formal charge <= 0) except a non-aromatic nitrogen that is adjacent to an oxygen and aromatic ring, or an aromatic nitrogen with 3 neighouring atoms in a ring, or a nitrogen with total bond order >=4; any fluorine)
1180 ETA_Beta_ns_d 1181 ETA_BetaP_ns_d 1182 ETA_Eta 1183 ETA_EtaP 1184 ETA_Eta_R 1185 ETA_Eta_F 1186 ETA_Eta_F 1187 ETA_Eta_L 1188 ETA_Eta_L 1190 ETA_Eta_R 1191 ETA_Eta_F 1192 ETA_Eta_B 1193 ETA_Eta_B 1194 ETA_Eta_B 1195 ETA_Eta_B 1196 FMF 1197 fragC 1198 nHBAcc	A measure of lone electrons entering into resonance A measure of lone electrons entering into resonance relative to molecular size Composite index Eta Composite index Eta relative to molecular size Composite index Eta for reference alkane Functionality index EtaF Functionality index EtaF relative to molecular size Local index Eta_local Local index Eta_local relative to molecular size Local index Eta_local for reference alkane Local functionality contribution EtaF_local Local functionality contribution EtaF_local relative to molecular size Branching index EtaB Branching index EtaB (with ring correction) Branching index EtaB (with ring correction) Branching index EtaB (with ring correction) Branching index EtaB (with ring correction) Branching index EtaB (with ring correction) relative to molecular size Complexity of a molecule Complexity of a molecule Complexity of a molecule Complexity of a system Number of hydrogen bond acceptors (using CDK HBondAcceptorCountDescriptor algorithm) Number of hydrogen bond acceptors (any oxygen; any nitrogen where the formal charge of the nitrogen is non-positive (i.e. formal charge <= 0) except a non-aromatic nitrogen that is adjacent to an oxygen and aromatic ring, or an aromatic nitrogen with 3 neighouring atoms in a ring, or an airomatic nitrogen with 3 neighouring atoms in a ring, or an airomatic nitrogen with 5 neighouring atoms in a ring, or an airomatic nitrogen where the formal charge of the nitrogen is non-positive (i.e.
1180 ETA_Beta_ns_d 1181 ETA_BetaP_ns_d 1182 ETA_Eta 1183 ETA_EtaP 1184 ETA_Eta_R 1185 ETA_Eta_F 1186 ETA_Eta_F 1187 ETA_Eta_L 1189 ETA_Eta_L 1190 ETA_Eta_F_L 1191 ETA_Eta_F_L 1192 ETA_Eta_B 1193 ETA_Eta_B 1194 ETA_Eta_B 1195 ETA_Eta_B_RC 1196 FMF 1197 fragC 1198 nHBAcc	A measure of lone electrons entering into resonance A measure of lone electrons entering into resonance relative to molecular size Composite index Eta Composite index Eta relative to molecular size Composite index Eta for reference alkane Functionality index EtaF Functionality index EtaF relative to molecular size Local index Eta_local Local index Eta_local relative to molecular size Local index Eta_local for reference alkane Local functionality contribution EtaF_local Local functionality contribution EtaF_local Local functionality contribution EtaF_local relative to molecular size Branching index EtaB Branching index EtaB (with ring correction) Branching index EtaB (with ring correction) Branching index EtaB (with ring correction) Branching index EtaB (with ring correction) relative to molecular size Complexity of a molecule Complexity of a system Number of hydrogen bond acceptors (using CDK HBondAcceptorCountDescriptor algorithm) Number of hydrogen bond acceptors (any oxygen; any nitrogen where the formal charge of the nitrogen is non-positive (i.e. formal charge <= 0) except a non-aromatic nitrogen that is adjacent to an oxygen and aromatic ring, or an aromatic nitrogen with 3 neighouring atoms in a ring, or a nitrogen with total bond order >=4; any fluorine) Number of hydrogen bond acceptors (any oxygen; any nitrogen with of hydrogen bond acceptors (any oxygen; any nitrogen with of hydrogen bond acceptors (any oxygen; any nitrogen with of hydrogen bond acceptors (any oxygen; any nitrogen with of hydrogen bond acceptors (any oxygen; any nitrogen with of hydrogen bond acceptors (any oxygen; any nitrogen with of hydrogen bond acceptors (any oxygen; any nitrogen with of hydrogen bond acceptors (any oxygen; any nitrogen with of hydrogen bond acceptors (any oxygen; any nitrogen with of hydrogen bond acceptors (any oxygen; any nitrogen with of hydrogen bond acceptors (any oxygen; any nitrogen with of hydrogen bond acceptors (any oxygen; any nitrogen with of hydrogen bond acceptors (any oxygen; any nitrogen with of
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order) 1212 TIC1 Total information content index (neighborhood)	d symmetry of 1-
order) 1213 TIC2 Total information content index (neighborhood)	d symmetry of 2-
order)	
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1216 TIC5 Total information content index (neighborhood	d symmetry of 5-
order) 1217 SIC0 Structural information content index (neighbored)	rhood symmetry of
0-order) 1218 SIC1 Structural information content index (neighbored)	rhood symmetry of
1-order) 1219 SIC2 Structural information content index (neighbored)	rhood symmetry of
2-order) 1220 SIC3 Structural information content index (neighbored)	
3-order)	
4-order)	
1222 SIC5 Structural information content index (neighbor 5-order)	rhood symmetry of
1223 CIC0 Complementary information content index (ne symmetry of 0-order)	ighborhood
1224 CIC1 Complementary information content index (ne symmetry of 1-order)	ighborhood
1225 CIC2 Complementary information content index (ne	ighborhood
symmetry of 2-order) 1226 CIC3 Complementary information content index (ne	ighborhood
symmetry of 3-order) 1227 CIC4 Complementary information content index (ne	
symmetry of 4-order) 1228 CIC5 Complementary information content index (ne	
symmetry of 5-order)	
BICO Bond information content index (neighborhoo order)	
Bond information content index (neighborhoo order)	d symmetry of 1-
Bond information content index (neighborhoo order)	d symmetry of 2-
1232 BIC3 Bond information content index (neighborhoo order)	d symmetry of 3-
1233 BIC4 Bond information content index (neighborhoo	d symmetry of 4-
order) 1234 BIC5 Bond information content index (neighborhoo	d symmetry of 5-
order) 1235 MIC0 Modified information content index (neighbor	hood symmetry of
0-order) 1236 MIC1 Modified information content index (neighbor	
1-order)	
2-order)	
Modified information content index (neighbor 3-order)	hood symmetry of
Modified information content index (neighbor 4-order)	hood symmetry of
1240 MIC5 Modified information content index (neighbor 5-order)	hood symmetry of
1241 ZMIC0 Z-modified information content index (neighbor of 0-order)	orhood symmetry
1242 ZMIC1 Z-modified information content index (neighb	orhood symmetry
of 1-order) 1243 ZMIC2 Z-modified information content index (neighbor)	orhood symmetry
of 2-order) 1244 ZMIC3 Z-modified information content index (neighbor)	orhood symmetry
of 3-order) 1245 ZMIC4 Z-modified information content index (neighbor)	
of 4-order)	
1246 ZMIC5 Z-modified information content index (neighbor of 5-order)	ornood symmetry
1247 Kier1 First kappa shape index 1248 Kier2 Second kappa shape index	
1249 Kier3 Third kappa (κ) shape index 1250 nAtomLC Number of atoms in the largest chain	
1251 nAtomP Number of atoms in the largest pi system	1
1253 MLogP Mannhold LogP	1
1254 McGowan_Volume McGowan characteristic volume 1255 MDEC-11 Molecular distance edge between all primary of	
1256 MDEC-12 Molecular distance edge between all primary a carbons	
1257 MDEC-13 Molecular distance edge between all primary a	and tertiary carbons
1258 MDEC-14 Molecular distance edge between all primary a	and quaternary
carbons 1259 MDEC-22 Molecular distance edge between all secondar	
1260 MDEC-23 Molecular distance edge between all secondar carbons	
1261 MDEC-24 Molecular distance edge between all secondar carbons	y and quaternary
1262 MDEC-33 Molecular distance edge between all tertiary c 1263 MDEC-34 Molecular distance edge between all tertiary a	
carbons	
1264 MDEC-44 Molecular distance edge between all quaternal 1265 MDEO-11 Molecular distance edge between all primary of the control of the control of the control of the control of the control of the control of the control of the control of the control of the control of the control of the control of the control of the control of the control of the control of the control of the control of the control of the control of the control of the control of the control of the control of the control of the control of the control of the control of the control of the control of the control of the control of the control of the control of the control of the control of the control of the control of the control of the control of the control of the control of the control of the control of the control of the control of the control of the control of the control of the control of the control of the control of the control of the control of the control of the control of the control of the control of the control of the control of the control of the control of the control of the control of the control of the control of the control of the control of the control of the control of the control of the control of the control of the control of the control of the control of the control of the control of the control of the control of the control of the control of the control of the control of the control of the control of the control of the control of the control of the control of the control of the control of the control of the control of the control of the control of the control of the control of the control of the control of the control of the control of the control of the control of the control of the control of the control of the control of the control of the control of the control of the control of the control of the control of the control of the control of the control of the control of the control of the control of the control of the control of the control of the control of the control of the control of the control of the control of the con	oxygens
1266 MDEO-12 Molecular distance edge between all primary a oxygens	•
1267 MDEO-22 Molecular distance edge between all secondar 1268 MDEN-11 Molecular distance edge between all primary r	
1269 MDEN-12 Molecular distance edge between all primary a nitrogens	
	and tertiary
Molecular distance edge between all primary a	
niroqens 1271 MDEN-22 Molecular distance edge between all secondar	
niroqens	

	MLFER_A	Overall or summation solute hydrogen bond acidity
	MLFER_BH MLFER_BO	Overall or summation solute hydrogen bond basicity Overall or summation solute hydrogen bond basicity
	MLFER_S	Combined dipolarity/polarizability
	MLFER_E MLFER_L	Excessive molar refraction Solute gas-hexadecane partition coefficient
	MPC2	Molecular path count of order 2
	MPC3 MPC4	Molecular path count of order 3 Molecular path count of order 4
	MPC5 MPC6	Molecular path count of order 5 Molecular path count of order 6
	MPC7	Molecular path count of order 7
	MPC8 MPC9	Molecular path count of order 8 Molecular path count of order 9
1288	MPC10	Molecular path count of order 10
	TPC piPC1	Total path count (up to order 10) Conventional bond order ID number of order 1 (ln(1+x)
1291	piPC2	Conventional bond order ID number of order 2 (ln(1+x)
	piPC3 piPC4	Conventional bond order ID number of order 3 (ln(1+x) Conventional bond order ID number of order 4 (ln(1+x)
1294	piPC5	Conventional bond order ID number of order 5 (ln(1+x)
	piPC6 piPC7	Conventional bond order ID number of order 6 (ln(1+x) Conventional bond order ID number of order 7 (ln(1+x)
	piPC8 piPC9	Conventional bond order ID number of order 8 (ln(1+x) Conventional bond order ID number of order 9 (ln(1+x)
	piPC9	Conventional bond order ID number of order 10 (ln(1+x)
	TpiPC R_TpiPCTPC	Total conventional bond order (up to order 10) (ln(1+x)) Ratio of total conventional bond order (up to order 10) with total
	-	path count (up to order 10)
	PetitjeanNumber nRing	Petitjean number Number of rings
1304	n3Ring	Number of 3-membered rings
	n4Ring n5Ring	Number of 4-membered rings Number of 5-membered rings
1307	n6Ring	Number of 6-membered rings
	n7Ring n8Ring	Number of 7-membered rings Number of 8-membered rings
1310	n9Ring	Number of 9-membered rings
	n10Ring n11Ring	Number of 10-membered rings Number of 11-membered rings
	n12Ring	Number of 12-membered rings Number of >12-membered rings
	nG12Ring nFRing	Number of fused rings
	nF4Ring nF5Ring	Number of 4-membered fused rings Number of 5-membered fused rings
1318	nF6Ring	Number of 6-membered fused rings
	nF7Ring nF8Ring	Number of 7-membered fused rings Number of 8-membered fused rings
1321	nF9Ring	Number of 9-membered fused rings
	nF10Ring nF11Ring	Number of 10-membered fused rings Number of 11-membered fused rings
	nF12Ring	Number of 12-membered fused rings Number of >12-membered fused rings
	nFG12Ring nTRing	Number of rings (includes counts from fused rings)
1327	nT4Ring	Number of 4-membered rings (includes counts from fused rings)
1328	nT5Ring	Number of 5-membered rings (includes counts from fused rings)
1329	nT6Ring	Number of 6-membered rings (includes counts from fused rings)
1330	nT7Ping	Number of 7-membered rings (includes counts from fused rings)
	nT7Ring	Number of 7-membered rings (includes counts from fused rings)
	nT7Ring nT8Ring	Number of 7-membered rings (includes counts from fused rings) Number of 8-membered rings (includes counts from fused rings)
1331		
1331	nT8Ring	Number of 8-membered rings (includes counts from fused rings)
1331 1332 1333	nT8Ring nT9Ring nT10Ring	Number of 8-membered rings (includes counts from fused rings) Number of 9-membered rings (includes counts from fused rings) Number of 10-membered rings (includes counts from fused rings)
1331 1332 1333 1334	nT8Ring nT9Ring nT10Ring nT11Ring	Number of 8-membered rings (includes counts from fused rings) Number of 9-membered rings (includes counts from fused rings) Number of 10-membered rings (includes counts from fused rings) Number of 11-membered rings (includes counts from fused rings)
1331 1332 1333 1334	nT8Ring nT9Ring nT10Ring	Number of 8-membered rings (includes counts from fused rings) Number of 9-membered rings (includes counts from fused rings) Number of 10-membered rings (includes counts from fused rings) Number of 11-membered rings (includes counts from fused rings) Number of 12-membered rings (includes counts from fused rings)
1331 1332 1333 1334 1335	nT8Ring nT9Ring nT10Ring nT11Ring	Number of 8-membered rings (includes counts from fused rings) Number of 9-membered rings (includes counts from fused rings) Number of 10-membered rings (includes counts from fused rings) Number of 11-membered rings (includes counts from fused rings) Number of 12-membered rings (includes counts from fused rings) Number of >12-membered rings (includes counts from fused rings)
1331 1332 1333 1334 1335	nT8Ring nT9Ring nT10Ring nT11Ring nT12Ring	Number of 8-membered rings (includes counts from fused rings) Number of 9-membered rings (includes counts from fused rings) Number of 10-membered rings (includes counts from fused rings) Number of 11-membered rings (includes counts from fused rings) Number of 12-membered rings (includes counts from fused rings) Number of >12-membered rings (includes counts from fused rings)
1331 1332 1333 1334 1335 1336	nT8Ring nT9Ring nT10Ring nT11Ring nT12Ring nTG12Ring nHeteroRing	Number of 8-membered rings (includes counts from fused rings) Number of 9-membered rings (includes counts from fused rings) Number of 10-membered rings (includes counts from fused rings) Number of 11-membered rings (includes counts from fused rings) Number of 12-membered rings (includes counts from fused rings) Number of >12-membered rings (includes counts from fused rings) Number of rings containing heteroatoms (N, O, P, S, or halogens)
1331 1332 1333 1334 1335 1336 1337	nT8Ring nT9Ring nT10Ring nT11Ring nT12Ring nTG12Ring nHeteroRing	Number of 8-membered rings (includes counts from fused rings) Number of 9-membered rings (includes counts from fused rings) Number of 10-membered rings (includes counts from fused rings) Number of 11-membered rings (includes counts from fused rings) Number of 12-membered rings (includes counts from fused rings) Number of >12-membered rings (includes counts from fused rings) Number of rings containing heteroatoms (N, O, P, S, or halogens) Number of 3-membered rings containing heteroatoms (N, O, P, S, or halogens)
1331 1332 1333 1334 1335 1336 1337	nT8Ring nT9Ring nT10Ring nT11Ring nT12Ring nTG12Ring nHeteroRing	Number of 8-membered rings (includes counts from fused rings) Number of 9-membered rings (includes counts from fused rings) Number of 10-membered rings (includes counts from fused rings) Number of 11-membered rings (includes counts from fused rings) Number of 12-membered rings (includes counts from fused rings) Number of >12-membered rings (includes counts from fused rings) Number of rings containing heteroatoms (N, O, P, S, or halogens) Number of 3-membered rings containing heteroatoms (N, O, P,
1331 1332 1333 1334 1335 1336 1337 1338	nT8Ring nT9Ring nT10Ring nT11Ring nT12Ring nTG12Ring nHeteroRing	Number of 8-membered rings (includes counts from fused rings) Number of 9-membered rings (includes counts from fused rings) Number of 10-membered rings (includes counts from fused rings) Number of 11-membered rings (includes counts from fused rings) Number of 12-membered rings (includes counts from fused rings) Number of >12-membered rings (includes counts from fused rings) Number of rings containing heteroatoms (N, O, P, S, or halogens) Number of 3-membered rings containing heteroatoms (N, O, P, S, or halogens) Number of 4-membered rings containing heteroatoms (N, O, P, S, or halogens) Number of 5-membered rings containing heteroatoms (N, O, P, S, or halogens)
1331 1332 1333 1334 1335 1336 1337 1338 1339	nT8Ring nT9Ring nT10Ring nT11Ring nT12Ring nTG12Ring nHeteroRing n3HeteroRing	Number of 8-membered rings (includes counts from fused rings) Number of 9-membered rings (includes counts from fused rings) Number of 10-membered rings (includes counts from fused rings) Number of 11-membered rings (includes counts from fused rings) Number of 12-membered rings (includes counts from fused rings) Number of >12-membered rings (includes counts from fused rings) Number of rings containing heteroatoms (N, O, P, S, or halogens) Number of 3-membered rings containing heteroatoms (N, O, P, S, or halogens) Number of 4-membered rings containing heteroatoms (N, O, P, S, or halogens)
1331 1332 1333 1334 1335 1336 1337 1338 1339 1340 1341	nT8Ring nT9Ring nT10Ring nT11Ring nT12Ring nTG12Ring nHeteroRing n3HeteroRing n4HeteroRing n5HeteroRing	Number of 8-membered rings (includes counts from fused rings) Number of 9-membered rings (includes counts from fused rings) Number of 10-membered rings (includes counts from fused rings) Number of 11-membered rings (includes counts from fused rings) Number of 12-membered rings (includes counts from fused rings) Number of >12-membered rings (includes counts from fused rings) Number of rings containing heteroatoms (N, O, P, S, or halogens) Number of 3-membered rings containing heteroatoms (N, O, P, S, or halogens) Number of 4-membered rings containing heteroatoms (N, O, P, S, or halogens) Number of 5-membered rings containing heteroatoms (N, O, P, S, or halogens) Number of 6-membered rings containing heteroatoms (N, O, P, S, or halogens)
1331 1332 1333 1334 1335 1336 1337 1338 1339 1340 1341	nT8Ring nT9Ring nT10Ring nT11Ring nT12Ring nTG12Ring nHeteroRing n3HeteroRing n4HeteroRing	Number of 8-membered rings (includes counts from fused rings) Number of 9-membered rings (includes counts from fused rings) Number of 10-membered rings (includes counts from fused rings) Number of 11-membered rings (includes counts from fused rings) Number of 12-membered rings (includes counts from fused rings) Number of >12-membered rings (includes counts from fused rings) Number of rings containing heteroatoms (N, O, P, S, or halogens) Number of 3-membered rings containing heteroatoms (N, O, P, S, or halogens) Number of 4-membered rings containing heteroatoms (N, O, P, S, or halogens) Number of 5-membered rings containing heteroatoms (N, O, P, S, or halogens) Number of 6-membered rings containing heteroatoms (N, O, P, S, or halogens) Number of 7-membered rings containing heteroatoms (N, O, P, S, or halogens)
1331 1332 1333 1334 1335 1336 1337 1338 1339 1340 1341 1342	nT8Ring nT9Ring nT10Ring nT11Ring nT12Ring nTG12Ring nHeteroRing n3HeteroRing n4HeteroRing n5HeteroRing	Number of 8-membered rings (includes counts from fused rings) Number of 9-membered rings (includes counts from fused rings) Number of 10-membered rings (includes counts from fused rings) Number of 11-membered rings (includes counts from fused rings) Number of 12-membered rings (includes counts from fused rings) Number of >12-membered rings (includes counts from fused rings) Number of rings containing heteroatoms (N, O, P, S, or halogens) Number of 3-membered rings containing heteroatoms (N, O, P, S, or halogens) Number of 4-membered rings containing heteroatoms (N, O, P, S, or halogens) Number of 5-membered rings containing heteroatoms (N, O, P, S, or halogens) Number of 6-membered rings containing heteroatoms (N, O, P, S, or halogens) Number of 7-membered rings containing heteroatoms (N, O, P, S, or halogens) Number of 8-membered rings containing heteroatoms (N, O, P, S, or halogens)
1331 1332 1333 1334 1335 1336 1337 1338 1339 1340 1341 1342 1343	nT8Ring nT9Ring nT10Ring nT11Ring nT12Ring nTG12Ring nHeteroRing n3HeteroRing n4HeteroRing n5HeteroRing n6HeteroRing	Number of 8-membered rings (includes counts from fused rings) Number of 9-membered rings (includes counts from fused rings) Number of 10-membered rings (includes counts from fused rings) Number of 11-membered rings (includes counts from fused rings) Number of 12-membered rings (includes counts from fused rings) Number of >12-membered rings (includes counts from fused rings) Number of rings containing heteroatoms (N, O, P, S, or halogens) Number of 3-membered rings containing heteroatoms (N, O, P, S, or halogens) Number of 4-membered rings containing heteroatoms (N, O, P, S, or halogens) Number of 5-membered rings containing heteroatoms (N, O, P, S, or halogens) Number of 6-membered rings containing heteroatoms (N, O, P, S, or halogens) Number of 7-membered rings containing heteroatoms (N, O, P, S, or halogens) Number of 8-membered rings containing heteroatoms (N, O, P, S, or halogens) Number of 9-membered rings containing heteroatoms (N, O, P, S, or halogens)
1331 1332 1333 1334 1335 1336 1337 1338 1339 1340 1341 1342 1343 1344	nT8Ring nT9Ring nT10Ring nT11Ring nT11Ring nT12Ring nTG12Ring nHeteroRing n3HeteroRing n4HeteroRing n5HeteroRing n6HeteroRing n7HeteroRing n8HeteroRing	Number of 8-membered rings (includes counts from fused rings) Number of 9-membered rings (includes counts from fused rings) Number of 10-membered rings (includes counts from fused rings) Number of 11-membered rings (includes counts from fused rings) Number of 12-membered rings (includes counts from fused rings) Number of >12-membered rings (includes counts from fused rings) Number of rings containing heteroatoms (N, O, P, S, or halogens) Number of 3-membered rings containing heteroatoms (N, O, P, S, or halogens) Number of 4-membered rings containing heteroatoms (N, O, P, S, or halogens) Number of 5-membered rings containing heteroatoms (N, O, P, S, or halogens) Number of 6-membered rings containing heteroatoms (N, O, P, S, or halogens) Number of 7-membered rings containing heteroatoms (N, O, P, S, or halogens) Number of 8-membered rings containing heteroatoms (N, O, P, S, or halogens) Number of 9-membered rings containing heteroatoms (N, O, P, S, or halogens)
1331 1332 1333 1334 1335 1336 1337 1338 1339 1340 1341 1342 1343 1344 1345	nT8Ring nT9Ring nT10Ring nT11Ring nT11Ring nT12Ring nTG12Ring nHeteroRing n3HeteroRing n4HeteroRing n5HeteroRing n6HeteroRing n7HeteroRing n7HeteroRing n8HeteroRing	Number of 8-membered rings (includes counts from fused rings) Number of 9-membered rings (includes counts from fused rings) Number of 10-membered rings (includes counts from fused rings) Number of 11-membered rings (includes counts from fused rings) Number of 12-membered rings (includes counts from fused rings) Number of >12-membered rings (includes counts from fused rings) Number of rings containing heteroatoms (N, O, P, S, or halogens) Number of 3-membered rings containing heteroatoms (N, O, P, S, or halogens) Number of 4-membered rings containing heteroatoms (N, O, P, S, or halogens) Number of 5-membered rings containing heteroatoms (N, O, P, S, or halogens) Number of 6-membered rings containing heteroatoms (N, O, P, S, or halogens) Number of 7-membered rings containing heteroatoms (N, O, P, S, or halogens) Number of 8-membered rings containing heteroatoms (N, O, P, S, or halogens) Number of 9-membered rings containing heteroatoms (N, O, P, S, or halogens) Number of 9-membered rings containing heteroatoms (N, O, P, S, or halogens)
1331 1332 1333 1334 1335 1336 1337 1338 1339 1340 1341 1342 1343 1344 1345	nT8Ring nT9Ring nT10Ring nT11Ring nT11Ring nT12Ring nTG12Ring nHeteroRing n3HeteroRing n4HeteroRing n5HeteroRing n6HeteroRing n7HeteroRing n8HeteroRing	Number of 8-membered rings (includes counts from fused rings) Number of 9-membered rings (includes counts from fused rings) Number of 10-membered rings (includes counts from fused rings) Number of 11-membered rings (includes counts from fused rings) Number of 12-membered rings (includes counts from fused rings) Number of >12-membered rings (includes counts from fused rings) Number of rings containing heteroatoms (N, O, P, S, or halogens) Number of 3-membered rings containing heteroatoms (N, O, P, S, or halogens) Number of 4-membered rings containing heteroatoms (N, O, P, S, or halogens) Number of 5-membered rings containing heteroatoms (N, O, P, S, or halogens) Number of 6-membered rings containing heteroatoms (N, O, P, S, or halogens) Number of 7-membered rings containing heteroatoms (N, O, P, S, or halogens) Number of 8-membered rings containing heteroatoms (N, O, P, S, or halogens) Number of 9-membered rings containing heteroatoms (N, O, P, S, or halogens) Number of 10-membered rings containing heteroatoms (N, O, P, S, or halogens) Number of 11-membered rings containing heteroatoms (N, O, P, S, or halogens)
1331 1332 1333 1334 1335 1336 1337 1338 1339 1340 1341 1342 1343 1344 1345 1346	nT8Ring nT9Ring nT10Ring nT11Ring nT11Ring nT12Ring nTG12Ring nHeteroRing n3HeteroRing n4HeteroRing n5HeteroRing n6HeteroRing n7HeteroRing n7HeteroRing n8HeteroRing	Number of 8-membered rings (includes counts from fused rings) Number of 9-membered rings (includes counts from fused rings) Number of 10-membered rings (includes counts from fused rings) Number of 11-membered rings (includes counts from fused rings) Number of 12-membered rings (includes counts from fused rings) Number of >12-membered rings (includes counts from fused rings) Number of rings containing heteroatoms (N, O, P, S, or halogens) Number of 3-membered rings containing heteroatoms (N, O, P, S, or halogens) Number of 4-membered rings containing heteroatoms (N, O, P, S, or halogens) Number of 5-membered rings containing heteroatoms (N, O, P, S, or halogens) Number of 6-membered rings containing heteroatoms (N, O, P, S, or halogens) Number of 7-membered rings containing heteroatoms (N, O, P, S, or halogens) Number of 8-membered rings containing heteroatoms (N, O, P, S, or halogens) Number of 9-membered rings containing heteroatoms (N, O, P, S, or halogens) Number of 10-membered rings containing heteroatoms (N, O, P, S, or halogens) Number of 11-membered rings containing heteroatoms (N, O, P, S, or halogens) Number of 11-membered rings containing heteroatoms (N, O, P, S, or halogens)
1331 1332 1333 1334 1335 1336 1337 1338 1339 1340 1341 1342 1343 1344 1345 1346 1347	nT8Ring nT9Ring nT10Ring nT11Ring nT11Ring nT12Ring nTG12Ring nHeteroRing n3HeteroRing n4HeteroRing n5HeteroRing n6HeteroRing n7HeteroRing n7HeteroRing n8HeteroRing n9HeteroRing	Number of 8-membered rings (includes counts from fused rings) Number of 10-membered rings (includes counts from fused rings) Number of 11-membered rings (includes counts from fused rings) Number of 11-membered rings (includes counts from fused rings) Number of 12-membered rings (includes counts from fused rings) Number of >12-membered rings (includes counts from fused rings) Number of rings containing heteroatoms (N, O, P, S, or halogens) Number of 3-membered rings containing heteroatoms (N, O, P, S, or halogens) Number of 4-membered rings containing heteroatoms (N, O, P, S, or halogens) Number of 5-membered rings containing heteroatoms (N, O, P, S, or halogens) Number of 6-membered rings containing heteroatoms (N, O, P, S, or halogens) Number of 7-membered rings containing heteroatoms (N, O, P, S, or halogens) Number of 8-membered rings containing heteroatoms (N, O, P, S, or halogens) Number of 9-membered rings containing heteroatoms (N, O, P, S, or halogens) Number of 10-membered rings containing heteroatoms (N, O, P, S, or halogens) Number of 11-membered rings containing heteroatoms (N, O, P, S, or halogens) Number of 12-membered rings containing heteroatoms (N, O, P, S, or halogens) Number of 12-membered rings containing heteroatoms (N, O, P, S, or halogens)
1331 1332 1333 1334 1335 1336 1337 1338 1339 1340 1341 1342 1343 1344 1345 1344 1345 1346 1347	nT8Ring nT9Ring nT10Ring nT11Ring nT11Ring nT12Ring nTG12Ring nHeteroRing n3HeteroRing n4HeteroRing n5HeteroRing n6HeteroRing n7HeteroRing n8HeteroRing n9HeteroRing n10HeteroRing n11HeteroRing	Number of 8-membered rings (includes counts from fused rings) Number of 10-membered rings (includes counts from fused rings) Number of 11-membered rings (includes counts from fused rings) Number of 11-membered rings (includes counts from fused rings) Number of 12-membered rings (includes counts from fused rings) Number of >12-membered rings (includes counts from fused rings) Number of rings containing heteroatoms (N, O, P, S, or halogens) Number of 3-membered rings containing heteroatoms (N, O, P, S, or halogens) Number of 4-membered rings containing heteroatoms (N, O, P, S, or halogens) Number of 5-membered rings containing heteroatoms (N, O, P, S, or halogens) Number of 6-membered rings containing heteroatoms (N, O, P, S, or halogens) Number of 7-membered rings containing heteroatoms (N, O, P, S, or halogens) Number of 8-membered rings containing heteroatoms (N, O, P, S, or halogens) Number of 9-membered rings containing heteroatoms (N, O, P, S, or halogens) Number of 10-membered rings containing heteroatoms (N, O, P, S, or halogens) Number of 11-membered rings containing heteroatoms (N, O, P, S, or halogens) Number of 11-membered rings containing heteroatoms (N, O, P, S, or halogens) Number of 12-membered rings containing heteroatoms (N, O, P, S, or halogens)
1331 1332 1333 1334 1335 1336 1337 1338 1339 1340 1341 1342 1343 1344 1345 1346 1347 1348	nT8Ring nT9Ring nT10Ring nT11Ring nT11Ring nT12Ring nTG12Ring nHeteroRing n3HeteroRing n4HeteroRing n5HeteroRing n6HeteroRing n7HeteroRing n8HeteroRing n9HeteroRing n11HeteroRing n11HeteroRing n12HeteroRing nG12HeteroRing	Number of 8-membered rings (includes counts from fused rings) Number of 10-membered rings (includes counts from fused rings) Number of 11-membered rings (includes counts from fused rings) Number of 11-membered rings (includes counts from fused rings) Number of 12-membered rings (includes counts from fused rings) Number of >12-membered rings (includes counts from fused rings) Number of rings containing heteroatoms (N, O, P, S, or halogens) Number of 3-membered rings containing heteroatoms (N, O, P, S, or halogens) Number of 4-membered rings containing heteroatoms (N, O, P, S, or halogens) Number of 5-membered rings containing heteroatoms (N, O, P, S, or halogens) Number of 6-membered rings containing heteroatoms (N, O, P, S, or halogens) Number of 7-membered rings containing heteroatoms (N, O, P, S, or halogens) Number of 8-membered rings containing heteroatoms (N, O, P, S, or halogens) Number of 9-membered rings containing heteroatoms (N, O, P, S, or halogens) Number of 10-membered rings containing heteroatoms (N, O, P, S, or halogens) Number of 11-membered rings containing heteroatoms (N, O, P, S, or halogens) Number of 12-membered rings containing heteroatoms (N, O, P, S, or halogens) Number of >12-membered rings containing heteroatoms (N, O, P, S, or halogens) Number of 5-12-membered rings containing heteroatoms (N, O, P, S, or halogens) Number of fused rings containing heteroatoms (N, O, P, S, or halogens)
1331 1332 1333 1334 1335 1336 1337 1338 1339 1340 1341 1342 1343 1344 1345 1346 1347 1348	nT8Ring nT9Ring nT10Ring nT11Ring nT11Ring nT12Ring nTG12Ring nHeteroRing n3HeteroRing n4HeteroRing n5HeteroRing n6HeteroRing n7HeteroRing n8HeteroRing n9HeteroRing n11HeteroRing n11HeteroRing n12HeteroRing	Number of 8-membered rings (includes counts from fused rings) Number of 9-membered rings (includes counts from fused rings) Number of 10-membered rings (includes counts from fused rings) Number of 11-membered rings (includes counts from fused rings) Number of 12-membered rings (includes counts from fused rings) Number of >12-membered rings (includes counts from fused rings) Number of rings containing heteroatoms (N, O, P, S, or halogens) Number of 3-membered rings containing heteroatoms (N, O, P, S, or halogens) Number of 4-membered rings containing heteroatoms (N, O, P, S, or halogens) Number of 5-membered rings containing heteroatoms (N, O, P, S, or halogens) Number of 6-membered rings containing heteroatoms (N, O, P, S, or halogens) Number of 7-membered rings containing heteroatoms (N, O, P, S, or halogens) Number of 8-membered rings containing heteroatoms (N, O, P, S, or halogens) Number of 9-membered rings containing heteroatoms (N, O, P, S, or halogens) Number of 10-membered rings containing heteroatoms (N, O, P, S, or halogens) Number of 11-membered rings containing heteroatoms (N, O, P, S, or halogens) Number of 11-membered rings containing heteroatoms (N, O, P, S, or halogens) Number of 12-membered rings containing heteroatoms (N, O, P, S, or halogens) Number of >12-membered rings containing heteroatoms (N, O, P, S, or halogens)
1331 1332 1333 1334 1335 1336 1337 1338 1339 1340 1341 1342 1343 1344 1345 1346 1347 1348 1349	nT8Ring nT9Ring nT10Ring nT11Ring nT11Ring nT12Ring nTG12Ring nHeteroRing n3HeteroRing n4HeteroRing n5HeteroRing n6HeteroRing n7HeteroRing n8HeteroRing n9HeteroRing n11HeteroRing n11HeteroRing n12HeteroRing nG12HeteroRing	Number of 8-membered rings (includes counts from fused rings) Number of 10-membered rings (includes counts from fused rings) Number of 11-membered rings (includes counts from fused rings) Number of 11-membered rings (includes counts from fused rings) Number of 12-membered rings (includes counts from fused rings) Number of >12-membered rings (includes counts from fused rings) Number of rings containing heteroatoms (N, O, P, S, or halogens) Number of 3-membered rings containing heteroatoms (N, O, P, S, or halogens) Number of 4-membered rings containing heteroatoms (N, O, P, S, or halogens) Number of 5-membered rings containing heteroatoms (N, O, P, S, or halogens) Number of 6-membered rings containing heteroatoms (N, O, P, S, or halogens) Number of 7-membered rings containing heteroatoms (N, O, P, S, or halogens) Number of 8-membered rings containing heteroatoms (N, O, P, S, or halogens) Number of 9-membered rings containing heteroatoms (N, O, P, S, or halogens) Number of 10-membered rings containing heteroatoms (N, O, P, S, or halogens) Number of 11-membered rings containing heteroatoms (N, O, P, S, or halogens) Number of 11-membered rings containing heteroatoms (N, O, P, S, or halogens) Number of 12-membered rings containing heteroatoms (N, O, P, S, or halogens) Number of 5-12-membered rings containing heteroatoms (N, O, P, S, or halogens) Number of fused rings containing heteroatoms (N, O, P, S, or halogens) Number of 4-membered fused rings containing heteroatoms (N, O, P, S, or halogens)
1331 1332 1333 1334 1335 1336 1337 1338 1339 1340 1341 1342 1343 1344 1345 1346 1347 1348 1349 1350 1351	nT8Ring nT9Ring nT10Ring nT11Ring nT11Ring nT12Ring nTG12Ring nHeteroRing n3HeteroRing n4HeteroRing n5HeteroRing n6HeteroRing n7HeteroRing n7HeteroRing n8HeteroRing n1HeteroRing n11HeteroRing n11HeteroRing n12HeteroRing nF4HeteroRing	Number of 8-membered rings (includes counts from fused rings) Number of 9-membered rings (includes counts from fused rings) Number of 10-membered rings (includes counts from fused rings) Number of 11-membered rings (includes counts from fused rings) Number of 12-membered rings (includes counts from fused rings) Number of >12-membered rings (includes counts from fused rings) Number of rings containing heteroatoms (N, O, P, S, or halogens) Number of 3-membered rings containing heteroatoms (N, O, P, S, or halogens) Number of 4-membered rings containing heteroatoms (N, O, P, S, or halogens) Number of 5-membered rings containing heteroatoms (N, O, P, S, or halogens) Number of 6-membered rings containing heteroatoms (N, O, P, S, or halogens) Number of 7-membered rings containing heteroatoms (N, O, P, S, or halogens) Number of 8-membered rings containing heteroatoms (N, O, P, S, or halogens) Number of 9-membered rings containing heteroatoms (N, O, P, S, or halogens) Number of 10-membered rings containing heteroatoms (N, O, P, S, or halogens) Number of 11-membered rings containing heteroatoms (N, O, P, S, or halogens) Number of 11-membered rings containing heteroatoms (N, O, P, S, or halogens) Number of 12-membered rings containing heteroatoms (N, O, P, S, or halogens) Number of 12-membered rings containing heteroatoms (N, O, P, S, or halogens) Number of 12-membered rings containing heteroatoms (N, O, P, S, or halogens) Number of 4-membered fused rings containing heteroatoms (N, O, P, S, or halogens) Number of 5-membered fused rings containing heteroatoms (N, O, P, S, or halogens)
1331 1332 1333 1334 1335 1336 1337 1338 1339 1340 1341 1342 1343 1344 1345 1346 1347 1348 1349 1350 1351	nT8Ring nT9Ring nT10Ring nT11Ring nT11Ring nT12Ring nTG12Ring nHeteroRing n3HeteroRing n4HeteroRing n5HeteroRing n6HeteroRing n7HeteroRing n8HeteroRing n9HeteroRing n10HeteroRing n11HeteroRing n11HeteroRing n12HeteroRing nF4HeteroRing nF4HeteroRing	Number of 8-membered rings (includes counts from fused rings) Number of 9-membered rings (includes counts from fused rings) Number of 10-membered rings (includes counts from fused rings) Number of 11-membered rings (includes counts from fused rings) Number of 12-membered rings (includes counts from fused rings) Number of >12-membered rings (includes counts from fused rings) Number of rings containing heteroatoms (N, O, P, S, or halogens) Number of 3-membered rings containing heteroatoms (N, O, P, S, or halogens) Number of 4-membered rings containing heteroatoms (N, O, P, S, or halogens) Number of 5-membered rings containing heteroatoms (N, O, P, S, or halogens) Number of 6-membered rings containing heteroatoms (N, O, P, S, or halogens) Number of 7-membered rings containing heteroatoms (N, O, P, S, or halogens) Number of 8-membered rings containing heteroatoms (N, O, P, S, or halogens) Number of 9-membered rings containing heteroatoms (N, O, P, S, or halogens) Number of 10-membered rings containing heteroatoms (N, O, P, S, or halogens) Number of 11-membered rings containing heteroatoms (N, O, P, S, or halogens) Number of 12-membered rings containing heteroatoms (N, O, P, S, or halogens) Number of 12-membered rings containing heteroatoms (N, O, P, S, or halogens) Number of 12-membered rings containing heteroatoms (N, O, P, S, or halogens) Number of 12-membered rings containing heteroatoms (N, O, P, S, or halogens) Number of 5-12-membered rings containing heteroatoms (N, O, P, S, or halogens) Number of 5-12-membered rings containing heteroatoms (N, O, P, S, or halogens) Number of 5-12-membered rings containing heteroatoms (N, O, P, S, or halogens)
1331 1332 1333 1334 1335 1336 1337 1338 1339 1340 1341 1342 1343 1344 1345 1346 1347 1348 1349 1350 1351	nT8Ring nT9Ring nT10Ring nT11Ring nT11Ring nT12Ring nTG12Ring nHeteroRing n3HeteroRing n4HeteroRing n5HeteroRing n6HeteroRing n7HeteroRing n8HeteroRing n9HeteroRing n10HeteroRing n11HeteroRing n11HeteroRing n12HeteroRing nF4HeteroRing nF5HeteroRing	Number of 8-membered rings (includes counts from fused rings) Number of 10-membered rings (includes counts from fused rings) Number of 11-membered rings (includes counts from fused rings) Number of 11-membered rings (includes counts from fused rings) Number of 12-membered rings (includes counts from fused rings) Number of >12-membered rings (includes counts from fused rings) Number of rings containing heteroatoms (N, O, P, S, or halogens) Number of 3-membered rings containing heteroatoms (N, O, P, S, or halogens) Number of 4-membered rings containing heteroatoms (N, O, P, S, or halogens) Number of 5-membered rings containing heteroatoms (N, O, P, S, or halogens) Number of 6-membered rings containing heteroatoms (N, O, P, S, or halogens) Number of 7-membered rings containing heteroatoms (N, O, P, S, or halogens) Number of 8-membered rings containing heteroatoms (N, O, P, S, or halogens) Number of 9-membered rings containing heteroatoms (N, O, P, S, or halogens) Number of 10-membered rings containing heteroatoms (N, O, P, S, or halogens) Number of 11-membered rings containing heteroatoms (N, O, P, S, or halogens) Number of 12-membered rings containing heteroatoms (N, O, P, S, or halogens) Number of 12-membered rings containing heteroatoms (N, O, P, S, or halogens) Number of fused rings containing heteroatoms (N, O, P, S, or halogens) Number of 12-membered rings containing heteroatoms (N, O, P, S, or halogens) Number of 14-membered fused rings containing heteroatoms (N, O, P, S, or halogens) Number of 5-membered fused rings containing heteroatoms (N, O, P, S, or halogens) Number of 6-membered fused rings containing heteroatoms (N, O, P, S, or halogens)
1331 1332 1333 1334 1335 1336 1337 1338 1339 1340 1341 1342 1343 1344 1345 1346 1347 1348 1349 1350 1351 1352 1353	nT8Ring nT9Ring nT10Ring nT11Ring nT11Ring nT12Ring nTG12Ring nHeteroRing n3HeteroRing n4HeteroRing n5HeteroRing n6HeteroRing n7HeteroRing n8HeteroRing n9HeteroRing n10HeteroRing n11HeteroRing n12HeteroRing nF4HeteroRing nF5HeteroRing nF5HeteroRing nF6HeteroRing	Number of 8-membered rings (includes counts from fused rings) Number of 10-membered rings (includes counts from fused rings) Number of 11-membered rings (includes counts from fused rings) Number of 11-membered rings (includes counts from fused rings) Number of 12-membered rings (includes counts from fused rings) Number of >12-membered rings (includes counts from fused rings) Number of rings containing heteroatoms (N, O, P, S, or halogens) Number of 3-membered rings containing heteroatoms (N, O, P, S, or halogens) Number of 4-membered rings containing heteroatoms (N, O, P, S, or halogens) Number of 5-membered rings containing heteroatoms (N, O, P, S, or halogens) Number of 6-membered rings containing heteroatoms (N, O, P, S, or halogens) Number of 7-membered rings containing heteroatoms (N, O, P, S, or halogens) Number of 8-membered rings containing heteroatoms (N, O, P, S, or halogens) Number of 9-membered rings containing heteroatoms (N, O, P, S, or halogens) Number of 10-membered rings containing heteroatoms (N, O, P, S, or halogens) Number of 11-membered rings containing heteroatoms (N, O, P, S, or halogens) Number of 11-membered rings containing heteroatoms (N, O, P, S, or halogens) Number of 11-membered rings containing heteroatoms (N, O, P, S, or halogens) Number of 12-membered rings containing heteroatoms (N, O, P, S, or halogens) Number of 12-membered rings containing heteroatoms (N, O, P, S, or halogens) Number of 4-membered rings containing heteroatoms (N, O, P, S, or halogens) Number of 5-membered fused rings containing heteroatoms (N, O, P, S, or halogens) Number of 6-membered fused rings containing heteroatoms (N, O, P, S, or halogens) Number of 5-membered fused rings containing heteroatoms (N, O, P, S, or halogens)
1331 1332 1333 1334 1335 1336 1337 1338 1339 1340 1341 1342 1343 1344 1345 1346 1347 1348 1349 1350 1351 1352	nT8Ring nT9Ring nT10Ring nT11Ring nT11Ring nT12Ring nTG12Ring nHeteroRing n3HeteroRing n4HeteroRing n5HeteroRing n6HeteroRing n7HeteroRing n8HeteroRing n9HeteroRing n10HeteroRing n11HeteroRing n11HeteroRing n12HeteroRing nF4HeteroRing nF5HeteroRing	Number of 8-membered rings (includes counts from fused rings) Number of 10-membered rings (includes counts from fused rings) Number of 11-membered rings (includes counts from fused rings) Number of 11-membered rings (includes counts from fused rings) Number of >12-membered rings (includes counts from fused rings) Number of >12-membered rings (includes counts from fused rings) Number of rings containing heteroatoms (N, O, P, S, or halogens) Number of 3-membered rings containing heteroatoms (N, O, P, S, or halogens) Number of 4-membered rings containing heteroatoms (N, O, P, S, or halogens) Number of 5-membered rings containing heteroatoms (N, O, P, S, or halogens) Number of 6-membered rings containing heteroatoms (N, O, P, S, or halogens) Number of 7-membered rings containing heteroatoms (N, O, P, S, or halogens) Number of 8-membered rings containing heteroatoms (N, O, P, S, or halogens) Number of 9-membered rings containing heteroatoms (N, O, P, S, or halogens) Number of 10-membered rings containing heteroatoms (N, O, P, S, or halogens) Number of 11-membered rings containing heteroatoms (N, O, P, S, or halogens) Number of 11-membered rings containing heteroatoms (N, O, P, S, or halogens) Number of 11-membered rings containing heteroatoms (N, O, P, S, or halogens) Number of 11-membered rings containing heteroatoms (N, O, P, S, or halogens) Number of 12-membered rings containing heteroatoms (N, O, P, S, or halogens) Number of 5-membered rings containing heteroatoms (N, O, P, S, or halogens) Number of 4-membered fused rings containing heteroatoms (N, O, P, S, or halogens) Number of 5-membered fused rings containing heteroatoms (N, O, P, S, or halogens) Number of 5-membered fused rings containing heteroatoms (N, O, P, S, or halogens)

	nF10HeteroRing	Number of 10-membered fused rings containing heteroatoms (NO, P, S, or halogens)
1357	nF11HeteroRing	Number of 11-membered fused rings containing heteroatoms (NO, P, S, or halogens)
1358	nF12HeteroRing	Number of 12-membered fused rings containing heteroatoms (N
1359	nFG12HeteroRing	O, P, S, or halogens) Number of >12-membered fused rings containing heteroatoms
		(N, O, P, S, or halogens)
1360	nTHeteroRing	Number of rings (includes counts from fused rings) containing heteroatoms (N, O, P, S, or halogens)
1361	nT4HeteroRing	Number of 4-membered rings (includes counts from fused rings
1262	nT5HatanaDin a	containing heteroatoms (N, O, P, S, or halogens)
1302	nT5HeteroRing	Number of 5-membered rings (includes counts from fused rings containing heteroatoms (N, O, P, S, or halogens)
1363	nT6HeteroRing	Number of 6-membered rings (includes counts from fused rings
1364	nT7HeteroRing	containing heteroatoms (N, O, P, S, or halogens) Number of 7-membered rings (includes counts from fused rings
		containing heteroatoms (N, O, P, S, or halogens)
1365	nT8HeteroRing	Number of 8-membered rings (includes counts from fused rings containing heteroatoms (N, O, P, S, or halogens)
1366	nT9HeteroRing	Number of 9-membered rings (includes counts from fused rings
1367	nT10HeteroRing	containing heteroatoms (N, O, P, S, or halogens) Number of 10-membered rings (includes counts from fused rings) containing heteroatoms (N, O, P, S, or halogens)
1368	nT11HeteroRing	Number of 11-membered rings (includes counts from fused rings) containing heteroatoms (N, O, P, S, or halogens)
1369	nT12HeteroRing	Number of 12-membered rings (includes counts from fused
1370	nTG12HeteroRing	rings) containing heteroatoms (N, O, P, S, or halogens) Number of >12-membered rings (includes counts from fused
		rings) containing heteroatoms (N, O, P, S, or halogens)
	nRotB RotBFrac	Number of rotatable bonds, excluding terminal bonds Fraction of rotatable bonds, excluding terminal bonds
1373	nRotBt	Number of rotatable bonds, including terminal bonds
	RotBtFrac LipinskiFailures	Fraction of rotatable bonds, including terminal bonds Number failures of the Lipinski's Rule Of 5
1376	topoRadius	Topological radius (minimum atom eccentricity)
	topoDiameter	Topological diameter (maximum atom eccentricity) Petitiean topological shape index
	topoShape GGI1	Petitjean topological shape index Topological charge index of order 1
1380	GGI2	Topological charge index of order 2
	GGI3 GGI4	Topological charge index of order 3
	GGI4 GGI5	Topological charge index of order 4 Topological charge index of order 5
1384	GGI6	Topological charge index of order 6
	GGI7 GGI8	Topological charge index of order 7 Topological charge index of order 8
	GGI9	Topological charge index of order 9
	GGI10	Topological charge index of order 10
	JGI1 JGI2	Mean topological charge index of order 1 Mean topological charge index of order 2
	JGI3	Mean topological charge index of order 2
	JGI4	Mean topological charge index of order 4
	JGI5 JGI6	Mean topological charge index of order 5 Mean topological charge index of order 6
	JGI7	Mean topological charge index of order 7
	JGI8	Mean topological charge index of order 8
	JGI9 JGI10	Mean topological charge index of order 9 Mean topological charge index of order 10
1399	JGT	Global topological charge index
	SpMax_D SpDiam_D	Leading eigenvalue from topological distance matrix Spectral diameter from topological distance matrix
1402	SpAD_D	Spectral absolute deviation from topological distance matrix
	SpMAD_D EE_D	Spectral mean absolute deviation from topological distance matrix Estrada-like index from topological distance matrix
	VE1_D VE2_D	Coefficient sum of the last eigenvector from topological distance matrix
	_	Average coefficient sum of the last eigenvector from topologica distance matrix
1407	VE3_D	Logarithmic coefficient sum of the last eigenvector from
1408	VR1_D	topological distance matrix Randic-like eigenvector-based index from topological distance
	VR2_D	matrix Normalized Randic-like eigenvector-based index from topological distance matrix
1410	VR3_D	Logarithmic Randic-like eigenvector-based index from
1 / 1 1	Tono DC A	topological distance matrix
	TopoPSA VABC	Topological polar surface area Van der Waals volume calculated using the method proposed in
		[Zhao, Yuan H. and Abraham, Michael H. and Zissimos, Andreas M., Fast Calculation of van der Waals Volume as a Su of Atomic and Bond Contributions and Its Application to Drug Compounds, The Journal of Organic Chemistry, 2003, 68:7368
		7373]
	vAdjMat MWC2	Vertex adjacency information (magnitude) Molecular walk count of order 2 (ln(1+x)
1415	MWC3	Molecular walk count of order 3 (ln(1+x)
	MWC4 MWC5	Molecular walk count of order 4 (ln(1+x) Molecular walk count of order 5 (ln(1+x)
	MWC6	Molecular walk count of order 5 (ln(1+x) Molecular walk count of order 6 (ln(1+x)
1419	MWC7	Molecular walk count of order 7 (ln(1+x)
	MWC8 MWC9	Molecular walk count of order 8 (ln(1+x) Molecular walk count of order 9 (ln(1+x)
1422	MWC10	Molecular walk count of order 10 (ln(1+x)
	TWC	Total walk count (up to order 10) Self returning walk count of order 2 (ln(1+x))
	SRW2 SRW3	Self-returning walk count of order 2 (ln(1+x) Self-returning walk count of order 3 (ln(1+x)
1426	SRW4	Self-returning walk count of order 4 (ln(1+x)
	SRW5 SRW6	Self-returning walk count of order 5 (ln(1+x) Self-returning walk count of order 6 (ln(1+x)
	SRW7	Self-returning walk count of order 7 (ln(1+x)
1430	SRW8	Self-returning walk count of order 8 (ln(1+x)
1/131	SRW9 SRW10	Self-returning walk count of order 9 (ln(1+x) Self-returning walk count of order 10 (ln(1+x)
	DICTO	
1432 1433	TSRW	Total self-return walk count (up to order 10) (ln(1+x))
1432 1433 1434		Total self-return walk count (up to order 10) (ln(1+x)) Molecular weight Average molecular weight (Molecular weight / Total number o

1436	WTPT-1	Molecular ID
1437	WTPT-2	Molecular ID / number of atoms
1438	WTPT-3	Sum of path lengths starting from heteroatoms
1439	WTPT-4	Sum of path lengths starting from oxygens
1440	WTPT-5	Sum of path lengths starting from nitrogens
1441	WPATH	Weiner path number
1442	WPOL	Weiner polarity number
1443	XLogP	XLogP
1444	Zagreb	Sum of the squares of atom degree over all heavy atoms i

Sr.	Distribution of Smell 1		ina test set	Sr.		Т	
No	Smells	Training set	Test set	No	Smells	Training set	Test set
1	aldehydic	102	25	53	lactonic	43	11
2	alliaceous	66	16	54	leafy	90	22
3	almond	70	17	55	lemon	53	13
4	amber	76	19	56	lily	50	12
5	animal	109	27	57	meaty	186	46
6	anisic	60	15	58	medicinal	60	15
7	apple	273	68	59	melon	91	23
8	apricot	67	16	60	metallic	100	25
9	balsamic	209	52	61	milky	54	13
10	banana	96	24	62	minty	171	43
11	berry	182	46	63	mushroom	67	17
12	brown	42	10	64	musky	70	18
13	burnt	66	17	65	musty	164	41
14	buttery	94	24	66	natural	54	13
15	camphor	114	29	67	nutty	237	59
16	caramellic	138	34	68	odorless	982	246
17	cedar	40	10	69	oily	223	56
18	cheese	101	25	70	onion	104	26
19	cherry	65	16	71		74	18
20	chocolate	70	17	72	orange peach	79	20
21					•		
	cinnamon	53 274	13	73	pear	101	25
22	citrus		69	74	phenolic	106	27
23	clean	73	18	75	pine	209	52
24	cocoa	57	14	76	pineapple	146	37
25	coconut	80	20	77	plum	50	13
26	coffee	88	22	78	potato	41	10
27	cooling	63	16	79	powdery	140	35
28	cortex	42	10	80	powerful	52	13
29	coumarinic	42	10	81	pungent	120	30
30	creamy	148	37	82	raspberry	42	11
31	cucumber	44	11	83	roasted	134	33
32	dairy	58	14	84	rose	263	66
33	dry	107	27	85	rummy	49	12
34	earthy	225	56	86	savory	52	13
35	estery	43	11	87	sharp	42	10
36	ethereal	125	31	88	smoky	45	11
37	fatty	358	89	89	soapy	53	13
38	fermented	46	12	90	spicy	322	81
39	fishy	51	13	91	strawberry	44	11
40	floral	754	189	92	sulfurous	222	56
41	fresh	319	80	93	sweet	887	222
42	fruity	1053	263	94	terpenic	44	11
43	garlic	70	17	95	tobacco	68	17
44	geranium	43	11	96	tropical	204	51
45	grape	111	28	97	vanilla	90	22
46	grapefruit	49	12	98	vegetbale	178	45
47	grassy	46	11	99	violet	61	15
48	green	872	218	100	warm	53	13
49	herbaceous	466	116	101	waxy	326	82
50	honey	110	27	102	winey	132	33
51	hyacinth	49	12	103	woody	522	131
52	jasmine	88	21	104	orris	39	10

Table S4:	Ontimal set of	f features for RF model features
	Feature	Description Description
	ATS0m	Broto-Moreau autocorrelation - lag 0 / weighted by mass
	ATS5m	Broto-Moreau autocorrelation - lag 5 / weighted by mass
		Average centered Broto-Moreau autocorrelation - lag 0 / weighted by van der
3	AATSC0v	Waals volumes
		Average centered Broto-Moreau autocorrelation - lag 4 / weighted by
4	ATSC4p	polarizabilities
	Постр	Average centered Broto-Moreau autocorrelation - lag 2 / weighted by first
5	ATSC2i	ionization potential
	1112021	Average centered Broto-Moreau autocorrelation - lag 8 / weighted by first
6	ATSC8i	ionization potential
		Average centered Broto-Moreau autocorrelation - lag 3 / weighted by van der
7	AATSC3v	Waals volumes
		Average centered Broto-Moreau autocorrelation - lag 1 / weighted by first
8	AATSC1i	ionization potential
	GATS7s	Geary autocorrelation - lag 7 / weighted by I-state
		Normalized Randic-like eigenvector-based index from Barysz matrix /
10	VR2_Dze	weighted by Sanderson electronegativities
	BCUTw-1h	nlow highest atom weighted BCUTS
		Smallest absolute eigenvalue of Burden modified matrix - n 8 / weighted by
12	SpMin8_Bhe	relative Sanderson electronegativities
	C4SP3	Singly bound carbon bound to four other carbons
14	VCH-5	Valence chain, order 5
15	VC-6	Valence cluster, order 6
16	mindsCH	Minimum atom-type E-State: =CH-
17	maxHdCH2	Maximum atom-type H E-State: =CH2
18	maxdCH2	Maximum atom-type E-State: =CH2
19	maxssssC	Maximum atom-type E-State: >C<
		Number of basic groups. The list of basic groups is defined by this SMARTS
		"[\$([NH2]-[CX4])]", "[\$([NH](-[CX4])-[CX4])]", "[\$(N(-[CX4])(-[CX4])-
		[CX4])]", "[\$([*;+;!\$(*~[*;-])])]", "[\$(N=C-N)]", and "[\$(N-C=N)]" originally
20	nBase	presented in JOELib
21	Mse	Mean atomic Sanderson electronegativities (scaled on carbon atom)
22	nsssN	Count of atom-type E-State: >NH-+
	ETA_EtaP	Composite index Eta relative to molecular size
24	FMF	Complexity of a molecule
	MIC0	Modified information content index (neighborhood symmetry of 0-order)
	MIC3	Modified information content index (neighborhood symmetry of 3-order)
	MDEC-11	Molecular distance edge between all primary carbons
	MDEC-14	Molecular distance edge between all primary and quaternary carbons
	MDEC-24	Molecular distance edge between all secondary and quaternary carbons
	n12Ring	Number of 12-membered rings
	nF6Ring	Number of 6-membered fused rings
	WTPT-3	Sum of path lengths starting from heteroatoms
	JGI5	Mean topological charge index of order 5
		MACCS Fingerprint
	SubFPC1	Substructure Fingerprint
41	SubFPC296	Substructure Fingerprint

Table S5: Smell-w Smell Percepts Pr aldehydic alliaceous almond amber animal anisic apple apricot balsamic banana berry brown burnt buttery camphor caramellic cedar cheese cherry chocolate cinnamon citrus clean cocoa coconut coffee cooling cortex coumarinic creamy cucumber dairy dry earthy	ecision (P) 1.00 0.96 1.00 0.99 0.97 0.98 1.00 0.99 1.00 0.98 1.00 0.97 0.97 0.97 0.97 0.97 0.97 0.97 0	CNN+IMG (Recall (R) 0.39 0.78 0.39 0.52 0.71 0.43 0.65 0.14 0.87 0.55 0.60 0.64 0.52 0.60 0.73 0.83 0.42 0.43 0.41 0.28 0.30 0.82 0.47 0.31 0.50 0.64 0.42 0.43	Name	0.89 0.89 0.84 0.76 0.86 0.71 0.82 0.57 0.94 0.78 0.80 0.52 0.76 0.80 0.71 0.60 0.71 0.70 0.64 0.65 0.91 0.74 0.66	PR_AUC 0.40 0.75 0.30 0.53 0.71 0.42 0.65 0.16 0.87 0.56 0.60 0.65 0.72 0.81 0.21 0.43 0.39 0.26 0.31 0.82 0.48	Precision (P) 0.93 0.83 0.83 0.78 0.86 1.00 0.66 0.82 0.89 0.89 0.88 0.82 1.00 0.76 0.75 0.85 0.75 0.90 0.81 0.86		PMF model F1-Score 0.28 0.38 0.52 0.25 0.24 0.35 0.45 0.71 0.39 0.42 0.18 0.85 0.62 0.29 0.55 0.48 0.29 0.26 0.27 0.13 0.57	0.87 0.89 0.87 0.77 0.74 0.84 0.66 0.76 0.85 0.77 0.72 0.63 0.76 0.75 0.78 0.85 0.79	0.49 0.51 0.48 0.49 0.56 0.69 0.59 0.46 0.35 0.61 0.34 0.45 0.62 0.61 0.51 0.56 0.50
aldehydic alliaceous almond amber animal anisic apple apricot balsamic banana berry brown burnt buttery camphor caramellic cedar cheese cherry chocolate cinnamon citrus clean cocoa coconut coffee cooling cortex coumarinic creamy cucumber dairy dry	1.00 0.96 1.00 1.00 0.99 0.97 0.98 1.00 0.99 1.00 1.00 0.97 0.97 0.97 0.97 0.98 1.00 0.99 1.00 0.99 1.00 0.99 1.00 0.99	0.39 0.78 0.39 0.52 0.71 0.43 0.65 0.14 0.87 0.55 0.60 0.64 0.52 0.60 0.73 0.83 0.42 0.43 0.41 0.28 0.30 0.82 0.47 0.50 0.64	0.56 0.86 0.45 0.68 0.83 0.59 0.78 0.25 0.93 0.71 0.74 0.77 0.68 0.74 0.84 0.90 0.63 0.59 0.57 0.42 0.47 0.90 0.64 0.47 0.67 0.67	0.89 0.89 0.84 0.76 0.86 0.71 0.82 0.57 0.94 0.78 0.80 0.52 0.76 0.80 0.87 0.91 0.60 0.71 0.70 0.64 0.65 0.91 0.74 0.66	0.40 0.75 0.30 0.53 0.71 0.42 0.65 0.16 0.87 0.56 0.60 0.65 0.53 0.59 0.72 0.81 0.21 0.43 0.39 0.26 0.31 0.82 0.48	0.93 0.83 0.83 0.78 0.86 1.00 0.66 0.82 0.82 0.89 0.89 0.88 0.75 0.75 0.85 0.75 0.90 0.81 0.86	0.51 0.24 0.41 0.15 0.14 0.68 0.33 0.81 0.25 0.37 0.54 0.79 0.51 0.41 0.38 0.33 0.18 0.15	0.28 0.38 0.52 0.25 0.24 0.35 0.45 0.71 0.39 0.42 0.18 0.85 0.62 0.29 0.55 0.48 0.29 0.26 0.27 0.13	0.87 0.89 0.87 0.77 0.74 0.84 0.66 0.76 0.85 0.77 0.72 0.63 0.76 0.75 0.78 0.85 0.76 0.75 0.76 0.75 0.76 0.85	0.56 0.64 0.49 0.51 0.48 0.49 0.56 0.69 0.59 0.46 0.34 0.45 0.62 0.61 0.56 0.50 0.50
alliaceous almond amber animal anisic apple apricot balsamic banana berry brown burnt buttery camphor caramellic cedar cheese cherry chocolate cinnamon citrus clean cocoa coconut coffee cooling cortex coumarinic creamy cucumber dairy dry	0.96 1.00 1.00 0.99 0.97 0.98 1.00 0.99 1.00 0.98 1.00 1.00 0.97 0.97 0.97 0.98 1.00 0.97 0.97 1.00 0.96 0.94 0.91 1.00 0.99 1.00 1.00 1.00 1.00 1.00	0.78 0.39 0.52 0.71 0.43 0.65 0.14 0.87 0.55 0.60 0.64 0.52 0.60 0.73 0.83 0.42 0.43 0.41 0.28 0.30 0.82 0.47 0.31 0.50 0.64 0.42 0.43	0.86 0.45 0.68 0.83 0.59 0.78 0.25 0.93 0.71 0.74 0.77 0.68 0.74 0.84 0.90 0.63 0.57 0.42 0.47 0.90 0.64 0.47 0.67 0.77	0.89 0.84 0.76 0.86 0.71 0.82 0.57 0.94 0.78 0.80 0.52 0.76 0.80 0.87 0.91 0.60 0.71 0.70 0.64 0.65 0.91 0.74 0.66	0.75 0.30 0.53 0.71 0.42 0.65 0.16 0.87 0.56 0.60 0.65 0.53 0.59 0.72 0.81 0.21 0.43 0.39 0.26 0.31 0.82 0.48	0.83 0.83 0.78 0.86 1.00 0.66 0.82 0.82 0.89 0.88 0.82 1.00 0.76 0.75 0.85 0.75 0.90 0.81 0.86	0.24 0.41 0.15 0.14 0.68 0.33 0.81 0.25 0.37 0.54 0.79 0.51 0.41 0.38 0.33 0.18 0.15 0.16	0.38 0.52 0.25 0.24 0.35 0.45 0.71 0.39 0.42 0.18 0.85 0.62 0.29 0.55 0.48 0.29 0.29 0.26 0.27 0.13	0.89 0.87 0.77 0.74 0.84 0.66 0.76 0.85 0.77 0.72 0.63 0.76 0.75 0.78 0.85 0.79 0.76 0.76	0.64 0.49 0.51 0.48 0.49 0.56 0.69 0.59 0.46 0.35 0.61 0.34 0.45 0.62 0.51 0.56
almond amber animal anisic apple apricot balsamic banana berry brown burnt buttery camphor caramellic cedar cheese cherry chocolate cinnamon citrus clean cocoa coconut coffee cooling cortex coumarinic creamy cucumber dairy dry	1.00 1.00 0.99 0.97 0.98 1.00 0.99 1.00 0.98 1.00 1.00 0.97 0.97 0.97 0.98 1.00 0.96 0.94 0.91 1.00 0.99 1.00 1.00 1.00 1.00 1.00	0.39 0.52 0.71 0.43 0.65 0.14 0.87 0.55 0.60 0.64 0.52 0.60 0.73 0.83 0.42 0.43 0.41 0.28 0.30 0.82 0.47 0.31 0.50 0.64 0.42 0.43	0.45 0.68 0.83 0.59 0.78 0.25 0.93 0.71 0.74 0.77 0.68 0.74 0.84 0.90 0.63 0.59 0.57 0.42 0.47 0.90 0.64 0.47 0.67 0.77	0.84 0.76 0.86 0.71 0.82 0.57 0.94 0.78 0.80 0.52 0.76 0.80 0.87 0.91 0.60 0.71 0.70 0.64 0.65 0.91 0.74	0.30 0.53 0.71 0.42 0.65 0.16 0.87 0.56 0.60 0.65 0.53 0.59 0.72 0.81 0.21 0.43 0.39 0.26 0.31 0.82 0.48	0.83 0.78 0.86 1.00 0.66 0.82 0.82 0.89 0.88 0.82 1.00 0.76 0.75 0.85 0.75 0.90 0.81 0.86	0.41 0.15 0.14 0.68 0.33 0.81 0.25 0.37 0.54 0.79 0.51 0.41 0.38 0.33 0.18 0.15 0.16	0.52 0.25 0.24 0.35 0.45 0.71 0.39 0.42 0.18 0.85 0.62 0.29 0.55 0.48 0.29 0.26 0.27 0.13	0.87 0.77 0.74 0.84 0.66 0.76 0.85 0.77 0.72 0.63 0.76 0.75 0.78 0.85 0.79 0.76 0.76	0.49 0.51 0.48 0.49 0.56 0.69 0.59 0.46 0.34 0.45 0.61 0.51 0.50 0.50
animal anisic apple apricot balsamic banana berry brown burnt buttery camphor caramellic cedar cheese cherry chocolate cinnamon citrus clean cocoa coconut coffee cooling cortex coumarinic creamy cucumber dairy dry	1.00 0.99 0.97 0.98 1.00 0.99 1.00 1.00 1.00 0.97 0.97 0.98 1.00 0.96 0.94 0.91 1.00 0.99 1.00 1.00 1.00 1.00 0.99	0.52 0.71 0.43 0.65 0.14 0.87 0.55 0.60 0.64 0.52 0.60 0.73 0.83 0.42 0.43 0.41 0.28 0.30 0.82 0.47 0.31 0.50 0.64 0.42 0.43	0.68 0.83 0.59 0.78 0.25 0.93 0.71 0.74 0.77 0.68 0.74 0.84 0.90 0.63 0.59 0.57 0.42 0.47 0.90 0.64 0.47 0.67 0.77	0.76 0.86 0.71 0.82 0.57 0.94 0.78 0.80 0.52 0.76 0.80 0.87 0.91 0.60 0.71 0.70 0.64 0.65 0.91 0.74 0.66	0.53 0.71 0.42 0.65 0.16 0.87 0.56 0.60 0.65 0.53 0.59 0.72 0.81 0.21 0.43 0.39 0.26 0.31 0.82 0.48	0.78 0.86 1.00 0.66 0.82 0.89 0.88 0.82 1.00 0.76 0.75 0.85 0.75 0.90 0.81 0.86	0.15 0.14 0.68 0.33 0.81 0.25 0.37 0.54 0.79 0.51 0.41 0.38 0.33 0.18 0.15 0.16 0.27 0.44	0.25 0.24 0.35 0.45 0.71 0.39 0.42 0.18 0.85 0.62 0.29 0.55 0.48 0.29 0.26 0.27 0.13 0.57	0.77 0.74 0.84 0.66 0.76 0.85 0.77 0.72 0.63 0.76 0.75 0.78 0.85 0.76 0.75 0.76 0.75	0.51 0.48 0.49 0.56 0.69 0.59 0.46 0.35 0.61 0.34 0.45 0.62 0.61 0.56 0.50
anisic apple apricot balsamic banana berry brown burnt buttery camphor caramellic cedar cheese cherry chocolate cinnamon citrus clean cocoa coconut coffee cooling cortex coumarinic creamy cucumber dairy dry	0.97 0.98 1.00 0.99 1.00 0.98 1.00 1.00 0.97 0.97 0.97 0.98 1.00 0.96 0.94 0.91 1.00 1.00 1.00 1.00 1.00 1.00 1.00	0.43 0.65 0.14 0.87 0.55 0.60 0.64 0.52 0.60 0.73 0.83 0.42 0.43 0.41 0.28 0.30 0.82 0.47 0.31 0.50 0.64	0.59 0.78 0.25 0.93 0.71 0.74 0.77 0.68 0.74 0.84 0.90 0.63 0.59 0.57 0.42 0.47 0.90 0.64 0.47 0.67	0.71 0.82 0.57 0.94 0.78 0.80 0.52 0.76 0.80 0.87 0.91 0.60 0.71 0.70 0.64 0.65 0.91 0.74	0.42 0.65 0.16 0.87 0.56 0.60 0.65 0.53 0.59 0.72 0.81 0.21 0.43 0.39 0.26 0.31 0.82 0.48	1.00 0.66 0.82 0.89 0.88 0.82 1.00 0.76 0.75 0.85 0.75 0.90 0.81 0.86	0.68 0.33 0.81 0.25 0.37 0.54 0.79 0.51 0.41 0.38 0.33 0.18 0.15 0.16 0.27	0.35 0.45 0.71 0.39 0.42 0.18 0.85 0.62 0.29 0.55 0.48 0.29 0.26 0.27 0.13	0.84 0.66 0.76 0.85 0.77 0.72 0.63 0.76 0.75 0.78 0.85 0.79 0.76 0.76	0.49 0.56 0.69 0.46 0.35 0.61 0.34 0.45 0.62 0.51 0.56 0.50 0.51
apple apricot balsamic banana berry brown burnt buttery camphor caramellic cedar cheese cherry chocolate cinnamon citrus clean cocoa coconut coffee cooling cortex coumarinic creamy cucumber dairy dry	0.98 1.00 0.99 1.00 0.98 1.00 1.00 0.97 0.97 0.97 0.98 1.00 0.94 0.94 0.91 1.00 1.00 1.00 1.00 1.00 1.00 1.00	0.65 0.14 0.87 0.55 0.60 0.64 0.52 0.60 0.73 0.83 0.42 0.43 0.41 0.28 0.30 0.82 0.47 0.31 0.50 0.64 0.42 0.21 0.31	0.78 0.25 0.93 0.71 0.74 0.77 0.68 0.74 0.84 0.90 0.63 0.59 0.57 0.42 0.47 0.90 0.64 0.47 0.67	0.82 0.57 0.94 0.78 0.80 0.52 0.76 0.80 0.87 0.91 0.60 0.71 0.70 0.64 0.65 0.91 0.74 0.66	0.65 0.16 0.87 0.56 0.60 0.65 0.53 0.59 0.72 0.81 0.21 0.43 0.39 0.26 0.31 0.82 0.48	0.66 0.82 0.82 0.89 0.88 0.82 1.00 0.76 0.75 0.85 0.75 0.90 0.81 0.86 0.83	0.33 0.81 0.25 0.37 0.54 0.79 0.51 0.41 0.38 0.33 0.18 0.15 0.16 0.27	0.45 0.71 0.39 0.42 0.18 0.85 0.62 0.29 0.55 0.48 0.29 0.26 0.27 0.13	0.66 0.76 0.85 0.77 0.72 0.63 0.76 0.75 0.78 0.85 0.79 0.76 0.76 0.76	0.56 0.69 0.59 0.46 0.35 0.61 0.34 0.45 0.62 0.51 0.56 0.50 0.51
apricot balsamic banana berry brown burnt buttery camphor caramellic cedar cheese cherry chocolate cinnamon citrus clean cocoa coconut coffee cooling cortex coumarinic creamy cucumber dairy dry	1.00 0.99 1.00 0.98 1.00 1.00 0.97 0.97 0.98 1.00 0.96 0.94 0.91 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00	0.14 0.87 0.55 0.60 0.64 0.52 0.60 0.73 0.83 0.42 0.43 0.41 0.28 0.30 0.82 0.47 0.31 0.50 0.64 0.42 0.43	0.25 0.93 0.71 0.74 0.77 0.68 0.74 0.84 0.90 0.63 0.59 0.57 0.42 0.47 0.90 0.64 0.47 0.67	0.57 0.94 0.78 0.80 0.52 0.76 0.80 0.87 0.91 0.60 0.71 0.70 0.64 0.65 0.91 0.74 0.66	0.16 0.87 0.56 0.60 0.65 0.53 0.59 0.72 0.81 0.21 0.43 0.39 0.26 0.31 0.82 0.48	0.82 0.82 0.89 0.88 0.82 1.00 0.76 0.75 0.85 0.75 0.90 0.81 0.86	0.81 0.25 0.37 0.54 0.79 0.51 0.41 0.38 0.33 0.18 0.15 0.16 0.27	0.71 0.39 0.42 0.18 0.85 0.62 0.29 0.55 0.48 0.29 0.26 0.27 0.13	0.76 0.85 0.77 0.72 0.63 0.76 0.75 0.78 0.85 0.79 0.76 0.76 0.76	0.69 0.59 0.46 0.35 0.61 0.34 0.45 0.62 0.61 0.51 0.50 0.50
balsamic banana berry brown burnt buttery camphor caramellic cedar cheese cherry chocolate cinnamon citrus clean cocoa coconut coffee cooling cortex coumarinic creamy cucumber dairy dry	0.99 1.00 0.98 1.00 1.00 0.97 0.97 0.98 1.00 0.96 0.94 0.91 1.00 1.00 1.00 1.00 1.00 1.00 1.00	0.87 0.55 0.60 0.64 0.52 0.60 0.73 0.83 0.42 0.43 0.41 0.28 0.30 0.82 0.47 0.31 0.50 0.64 0.42 0.43	0.93 0.71 0.74 0.77 0.68 0.74 0.84 0.90 0.63 0.59 0.57 0.42 0.47 0.90 0.64 0.47	0.94 0.78 0.80 0.52 0.76 0.80 0.87 0.91 0.60 0.71 0.70 0.64 0.65 0.91 0.74 0.66	0.87 0.56 0.60 0.65 0.53 0.59 0.72 0.81 0.21 0.43 0.39 0.26 0.31 0.82 0.48	0.82 0.89 0.88 0.82 1.00 0.76 0.75 0.85 0.75 0.90 0.81 0.86	0.25 0.37 0.54 0.79 0.51 0.41 0.38 0.33 0.18 0.15 0.16 0.27 0.44	0.39 0.42 0.18 0.85 0.62 0.29 0.55 0.48 0.29 0.26 0.27 0.13	0.85 0.77 0.72 0.63 0.76 0.75 0.78 0.85 0.79 0.76 0.76 0.65	0.59 0.46 0.35 0.61 0.34 0.45 0.62 0.61 0.51 0.56 0.50 0.51
banana berry brown burnt buttery camphor caramellic cedar cheese cherry chocolate cinnamon citrus clean cocoa coconut coffee cooling cortex coumarinic creamy cucumber dairy dry	1.00 0.98 1.00 1.00 0.97 0.97 0.98 1.00 0.96 0.94 0.91 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00	0.55 0.60 0.64 0.52 0.60 0.73 0.83 0.42 0.43 0.41 0.28 0.30 0.82 0.47 0.31 0.50 0.64 0.42 0.21	0.71 0.74 0.77 0.68 0.74 0.84 0.90 0.63 0.59 0.57 0.42 0.47 0.90 0.64 0.47	0.78 0.80 0.52 0.76 0.80 0.87 0.91 0.60 0.71 0.70 0.64 0.65 0.91 0.74	0.56 0.60 0.65 0.53 0.59 0.72 0.81 0.21 0.43 0.39 0.26 0.31 0.82 0.48	0.89 0.88 0.82 1.00 0.76 0.75 0.85 0.75 0.90 0.81 0.86 0.83	0.37 0.54 0.79 0.51 0.41 0.38 0.33 0.18 0.15 0.16 0.27 0.44	0.42 0.18 0.85 0.62 0.29 0.55 0.48 0.29 0.26 0.27 0.13 0.57	0.77 0.72 0.63 0.76 0.75 0.78 0.85 0.79 0.76 0.76 0.65	0.46 0.35 0.61 0.34 0.45 0.62 0.51 0.56 0.50
brown burnt buttery camphor caramellic cedar cheese cherry chocolate cinnamon citrus clean cocoa coconut coffee cooling cortex coumarinic creamy cucumber dairy dry	1.00 1.00 0.97 0.98 1.00 0.96 0.94 0.91 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00	0.64 0.52 0.60 0.73 0.83 0.42 0.43 0.41 0.28 0.30 0.82 0.47 0.31 0.50 0.64 0.42 0.21	0.77 0.68 0.74 0.84 0.90 0.63 0.59 0.57 0.42 0.47 0.90 0.64 0.47 0.67	0.52 0.76 0.80 0.87 0.91 0.60 0.71 0.70 0.64 0.65 0.91 0.74 0.66	0.65 0.53 0.59 0.72 0.81 0.21 0.43 0.39 0.26 0.31 0.82 0.48	0.82 1.00 0.76 0.75 0.85 0.75 0.90 0.81 0.86	0.79 0.51 0.41 0.38 0.33 0.18 0.15 0.16 0.27 0.44	0.85 0.62 0.29 0.55 0.48 0.29 0.26 0.27 0.13 0.57	0.63 0.76 0.75 0.78 0.85 0.79 0.76 0.76 0.65	0.61 0.34 0.45 0.62 0.61 0.51 0.56 0.50 0.51
burnt buttery camphor caramellic cedar cheese cherry chocolate cinnamon citrus clean cocoa coconut coffee cooling cortex coumarinic creamy cucumber dairy dry	1.00 0.97 0.98 1.00 0.96 0.94 0.91 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00	0.52 0.60 0.73 0.83 0.42 0.43 0.41 0.28 0.30 0.82 0.47 0.31 0.50 0.64 0.42 0.21	0.68 0.74 0.84 0.90 0.63 0.59 0.57 0.42 0.47 0.90 0.64 0.47 0.67	0.76 0.80 0.87 0.91 0.60 0.71 0.70 0.64 0.65 0.91 0.74 0.66	0.53 0.59 0.72 0.81 0.21 0.43 0.39 0.26 0.31 0.82 0.48	1.00 0.76 0.75 0.85 0.75 0.90 0.81 0.86	0.51 0.41 0.38 0.33 0.18 0.15 0.16 0.27 0.44	0.62 0.29 0.55 0.48 0.29 0.26 0.27 0.13	0.76 0.75 0.78 0.85 0.79 0.76 0.76	0.34 0.45 0.62 0.61 0.51 0.56 0.50 0.51
buttery camphor caramellic cedar cheese cherry chocolate cinnamon citrus clean cocoa coconut coffee cooling cortex coumarinic creamy cucumber dairy dry	0.97 0.98 1.00 0.96 0.94 0.91 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00	0.60 0.73 0.83 0.42 0.43 0.41 0.28 0.30 0.82 0.47 0.31 0.50 0.64 0.42 0.21	0.74 0.84 0.90 0.63 0.59 0.57 0.42 0.47 0.90 0.64 0.47 0.67	0.80 0.87 0.91 0.60 0.71 0.70 0.64 0.65 0.91 0.74 0.66	0.59 0.72 0.81 0.21 0.43 0.39 0.26 0.31 0.82 0.48	0.76 0.75 0.85 0.75 0.90 0.81 0.86 0.83	0.41 0.38 0.33 0.18 0.15 0.16 0.27	0.29 0.55 0.48 0.29 0.26 0.27 0.13 0.57	0.75 0.78 0.85 0.79 0.76 0.76	0.45 0.62 0.61 0.51 0.56 0.50 0.51
camphor caramellic cedar cheese cherry chocolate cinnamon citrus clean cocoa coconut coffee cooling cortex coumarinic creamy cucumber dairy dry	0.97 0.98 1.00 0.96 0.94 0.91 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00	0.73 0.83 0.42 0.43 0.41 0.28 0.30 0.82 0.47 0.31 0.50 0.64 0.42 0.21	0.84 0.90 0.63 0.59 0.57 0.42 0.47 0.90 0.64 0.47 0.67	0.87 0.91 0.60 0.71 0.70 0.64 0.65 0.91 0.74 0.66	0.72 0.81 0.21 0.43 0.39 0.26 0.31 0.82 0.48	0.75 0.85 0.75 0.90 0.81 0.86 0.83	0.38 0.33 0.18 0.15 0.16 0.27 0.44	0.55 0.48 0.29 0.26 0.27 0.13	0.78 0.85 0.79 0.76 0.76	0.62 0.61 0.51 0.56 0.50 0.50
caramellic cedar cheese cherry chocolate cinnamon citrus clean cocoa coconut coffee cooling cortex coumarinic creamy cucumber dairy dry	0.98 1.00 0.96 0.94 0.91 1.00 0.99 1.00 1.00 1.00 1.00 1.00	0.83 0.42 0.43 0.41 0.28 0.30 0.82 0.47 0.31 0.50 0.64 0.42 0.21	0.90 0.63 0.59 0.57 0.42 0.47 0.90 0.64 0.47 0.67	0.91 0.60 0.71 0.70 0.64 0.65 0.91 0.74 0.66	0.81 0.21 0.43 0.39 0.26 0.31 0.82 0.48	0.85 0.75 0.90 0.81 0.86 0.83	0.33 0.18 0.15 0.16 0.27 0.44	0.48 0.29 0.26 0.27 0.13 0.57	0.85 0.79 0.76 0.76 0.65	0.61 0.51 0.56 0.50 0.51
cheese cherry chocolate cinnamon citrus clean cocoa coconut coffee cooling cortex coumarinic creamy cucumber dairy dry	0.96 0.94 0.91 1.00 0.99 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00	0.43 0.41 0.28 0.30 0.82 0.47 0.31 0.50 0.64 0.42 0.21 0.31	0.59 0.57 0.42 0.47 0.90 0.64 0.47 0.67	0.71 0.70 0.64 0.65 0.91 0.74	0.43 0.39 0.26 0.31 0.82 0.48	0.90 0.81 0.86 0.83	0.15 0.16 0.27 0.44	0.26 0.27 0.13 0.57	0.76 0.76 0.65	0.56 0.50 0.51
cherry chocolate cinnamon citrus clean cocoa coconut coffee cooling cortex coumarinic creamy cucumber dairy dry	0.94 0.91 1.00 0.99 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00	0.41 0.28 0.30 0.82 0.47 0.31 0.50 0.64 0.42 0.21 0.31	0.57 0.42 0.47 0.90 0.64 0.47 0.67 0.77	0.70 0.64 0.65 0.91 0.74 0.66	0.39 0.26 0.31 0.82 0.48	0.81 0.86 0.83	0.16 0.27 0.44	0.27 0.13 0.57	0.76 0.65	0.50 0.51
chocolate cinnamon citrus clean cocoa coconut coffee cooling cortex coumarinic creamy cucumber dairy dry	0.91 1.00 0.99 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00	0.28 0.30 0.82 0.47 0.31 0.50 0.64 0.42 0.21 0.31	0.42 0.47 0.90 0.64 0.47 0.67	0.64 0.65 0.91 0.74 0.66	0.26 0.31 0.82 0.48	0.86 0.83	0.27 0.44	0.13 0.57	0.65	0.51
cinnamon citrus clean cocoa coconut coffee cooling cortex coumarinic creamy cucumber dairy dry	1.00 0.99 1.00 1.00 1.00 0.99 1.00 1.00	0.30 0.82 0.47 0.31 0.50 0.64 0.42 0.21 0.31	0.47 0.90 0.64 0.47 0.67	0.65 0.91 0.74 0.66	0.31 0.82 0.48	0.83	0.44	0.57		
citrus clean cocoa coconut coffee cooling cortex coumarinic creamy cucumber dairy dry	1.00 1.00 1.00 0.99 1.00 1.00 1.00 1.00	0.82 0.47 0.31 0.50 0.64 0.42 0.21 0.31	0.90 0.64 0.47 0.67 0.77	0.91 0.74 0.66	0.82 0.48					
cocoa coconut coffee cooling cortex coumarinic creamy cucumber dairy dry	1.00 1.00 0.99 1.00 1.00 1.00 1.00 1.00	0.31 0.50 0.64 0.42 0.21 0.31	0.47 0.67 0.77	0.66		0.74	0.57	0.48	0.64	0.62
coconut coffee cooling cortex coumarinic creamy cucumber dairy dry	1.00 0.99 1.00 1.00 1.00 1.00 1.00 0.95	0.50 0.64 0.42 0.21 0.31	0.67 0.77			0.89	0.79	0.75	0.70	
coffee cooling cortex coumarinic creamy cucumber dairy dry	0.99 1.00 1.00 1.00 1.00 1.00 1.00 0.95	0.64 0.42 0.21 0.31	0.77		0.32	0.92	0.15	0.27	0.78	
cooling cortex coumarinic creamy cucumber dairy dry	1.00 1.00 1.00 1.00 1.00 1.00 0.95	0.42 0.21 0.31		0.75 0.82	0.51 0.64	0.75	0.51 0.36	0.61 0.48	0.69 0.88	0.70 0.62
cortex coumarinic creamy cucumber dairy dry	1.00 1.00 1.00 1.00 1.00 0.95	0.21 0.31	0.59	0.82	0.04	1.00	0.39	0.46	0.87	0.62
creamy cucumber dairy dry	1.00 1.00 1.00 0.95		0.35	0.61	0.22	0.91	0.44	0.56	0.68	0.60
cucumber dairy dry	1.00 1.00 0.95		0.47	0.65	0.32	0.81	0.40	0.54	0.69	
dairy dry	1.00 0.95	0.59	0.75 0.78	0.80 0.82	0.61	0.76	0.29 0.52	0.32 0.36	0.63 0.79	0.49 0.50
dry	0.95	0.64 0.14	0.78	0.82	0.64 0.15	1.00	0.52	0.36	0.79	
_		0.57	0.24	0.78	0.15	0.91	0.33	0.34	0.43	
_ <u>* </u>	1.00	0.83	0.91	0.92	0.84	0.88	0.71	0.79	0.86	0.76
estery	1.00	0.24	0.39	0.62	0.25	0.69	0.76	0.34	0.44	0.64
ethereal fatty	1.00 0.97	0.72 0.93	0.84 0.95	0.86 0.97	0.73 0.91	0.71 0.70	0.19 0.38	0.29 0.49	0.74 0.83	0.46 0.60
fermented	1.00	0.93	0.95	0.97	0.91	1.00	0.38	0.49	0.83	
fishy	1.00	0.32	0.46	0.61	0.23	0.81	0.57	0.40	0.77	0.36
floral	0.99	0.96	0.98	0.98	0.96	0.74	0.63	0.68	0.88	0.75
fresh	0.99	0.68	0.81	0.84	0.70	1.00	0.32	0.34	0.88	0.39
fruity garlic	1.00 0.99	0.96 0.90	0.98 0.94	0.98 0.95	0.97 0.89	0.76 0.86	0.66 0.43	0.71 0.57	0.72 0.90	0.80
geranium	1.00	0.59	0.74	0.80	0.60	1.00	0.49	0.37	0.77	0.55
grape	1.00	0.38	0.51	0.59	0.19	0.76	0.29	0.31	0.66	0.47
grapefruit	1.00	0.41	0.58	0.71	0.42	0.75	0.15	0.25	0.68	0.37
grassy	0.96 0.99	0.47 0.99	0.64 0.99	0.74 0.99	0.46 0.98	0.50 0.75	0.21 0.39	0.16 0.52	0.26 0.79	
green herbaceous	0.99	0.99	0.99	0.99	0.98	0.73	0.39	0.48	0.79	
honey	0.93	0.62	0.75	0.81	0.59	0.78	0.43	0.33	0.74	0.48
hyacinth	1.00	0.52	0.69	0.76	0.53	0.93	0.61	0.35	0.79	
jasmine	1.00	0.60	0.75	0.80	0.61	0.87	0.55	0.39	0.57	0.42
lactonic leafy	0.91 1.00	0.26 0.46		0.63 0.73	0.24 0.48	0.62 1.00	0.29 0.53	0.29 0.45	0.59 0.84	
lemon	1.00	0.14	0.24	0.57	0.15	0.90	0.14	0.24	0.67	0.50
lily	1.00	0.65	0.78	0.82	0.65	1.00	0.48	0.39	0.87	0.51
meaty	0.96	0.87	0.92	0.94	0.85	0.82	0.44	0.57	0.77	0.69
medicinal melon	1.00 0.92	0.51 0.73	0.67 0.81	0.75 0.86	0.51 0.68	0.85 0.86	0.15 0.45	0.25 0.51	0.76 0.85	
metallic	0.92	0.73	0.76		0.62	1.00	0.43	0.22	0.83	0.42
milky	0.90	0.43	0.58	0.72	0.39	1.00	0.33	0.50	0.86	0.40
minty	1.00	0.63	0.77	0.82	0.65	0.79	0.33	0.47	0.66	
mushroom	1.00 1.00	0.69 0.82	0.82 0.90	0.85 0.91	0.70 0.82	0.82 0.98	0.21 0.64	0.29 0.77	0.78 0.89	
musky musty	0.98	0.82	0.90	0.91	0.82	1.00	0.64	0.77	0.89	
natural	1.00	0.43	0.54	0.57	0.15	1.00	0.21	0.13	0.34	0.35
nutty	0.99	0.80	0.88	0.90	0.80	0.76	0.34	0.47	0.64	0.60
odorless	1.00 0.96	0.97 0.71	0.98	0.99	0.97	0.98 1.00	0.94	0.96 0.71	1.00 0.89	0.99 0.37
oily onion	0.96	0.71	0.81 0.90	0.85 0.93	0.69 0.82	0.83	0.60 0.44	0.71	0.89	
orange	1.00	0.39	0.56		0.40	0.78	0.44	0.39	0.66	
orris	1.00	0.31	0.47	0.65	0.31	0.82	0.26	0.37	0.81	0.44
peach	1.00	0.28		0.64	0.30	1.00	0.03	0.06	0.50	
pear phenolic	0.98 0.99	0.37 0.62	0.54 0.76	0.69 0.81	0.38 0.62	0.63 0.77	0.23 0.36	0.34 0.49	0.47 0.71	0.30 0.62
pine	1.00	0.62	0.76	0.81	0.62	0.78	0.30	0.49	0.71	
pineapple	1.00	0.56		0.78	0.58	0.74	0.27	0.39	0.67	0.56
plum	1.00	0.17	0.30	0.59	0.19	1.00	0.06	0.12	0.66	
potato	1.00 0.97	0.16 0.54		0.58	0.17	0.86	0.12	0.21	0.49	
powdery powerful	0.97	0.54		0.77 0.53	0.54 0.05	0.93 0.73	0.48 0.43	0.55 0.41	0.56 0.61	0.52 0.54
pungent	0.07	0.39			0.03	0.73	0.43	0.35	0.85	
raspberry	1.00	0.15	0.26	0.58	0.16	0.67	0.04	0.07	0.39	0.37
roasted	0.94	0.92	0.93	0.96	0.87	0.83	0.39	0.48	0.80	
rose	0.99	0.82	0.90		0.82	0.78	0.36		0.76	
rummy savory	1.00 0.94	0.39 0.72	0.46 0.82	0.65 0.86	0.30 0.68	1.00 1.00	0.28 0.58	0.27 0.56	0.34 0.57	
sharp	0.74									
smoky	1.00	0.45	0.62	0.72	0.45	0.77	0.58	0.49	0.65	0.50
soapy	1.00	0.38		0.59	0.19	1.00	0.13	0.26	0.44	
spicy	1.00	0.82			0.84	0.80	0.42	0.54	0.81	0.52
strawberry sulfurious	1.00 0.96	0.36 0.94	0.53 0.95	0.68 0.97	0.37 0.90	0.80 0.82	0.15 0.87	0.25 0.85	0.68 0.80	
sweet	0.90	0.94		0.97	0.90	0.82	0.87	0.46	0.59	

terpenic	1.00	0.53	0.61	0.56	0.14	0.76	0.35	0.47	0.53	0.46
tobacco	1.00	0.41	0.59	0.55	0.12	0.70	0.28	0.35	0.67	0.10
tropical	0.96	0.79	0.87	0.89	0.77	0.88	0.43	0.50	0.71	0.41
vanilla	0.96	0.63	0.76	0.82	0.62	0.92	0.40	0.56	0.87	0.59
vegetable	0.96	0.79	0.86	0.89	0.76	0.87	0.62	0.68	0.84	0.48
violet	1.00	0.62	0.76	0.81	0.62	0.81	0.34	0.48	0.77	0.64
warm	1.00	0.44	0.61	0.72	0.45	0.83	0.49	0.58	0.81	0.64
waxy	0.98	0.82	0.89	0.91	0.82	0.66	0.31	0.42	0.43	0.45
winey	0.96	0.59	0.73	0.80	0.58	0.74	0.55	0.61	0.68	0.52
woody	0.98	0.96	0.97	0.98	0.94	0.77	0.47	0.58	0.73	0.71