Supplementary Material

Development of a Hierarchical Support Vector Regression-Based *In Silico* Model for the Prediction of the Cysteine Depletion in DPRA

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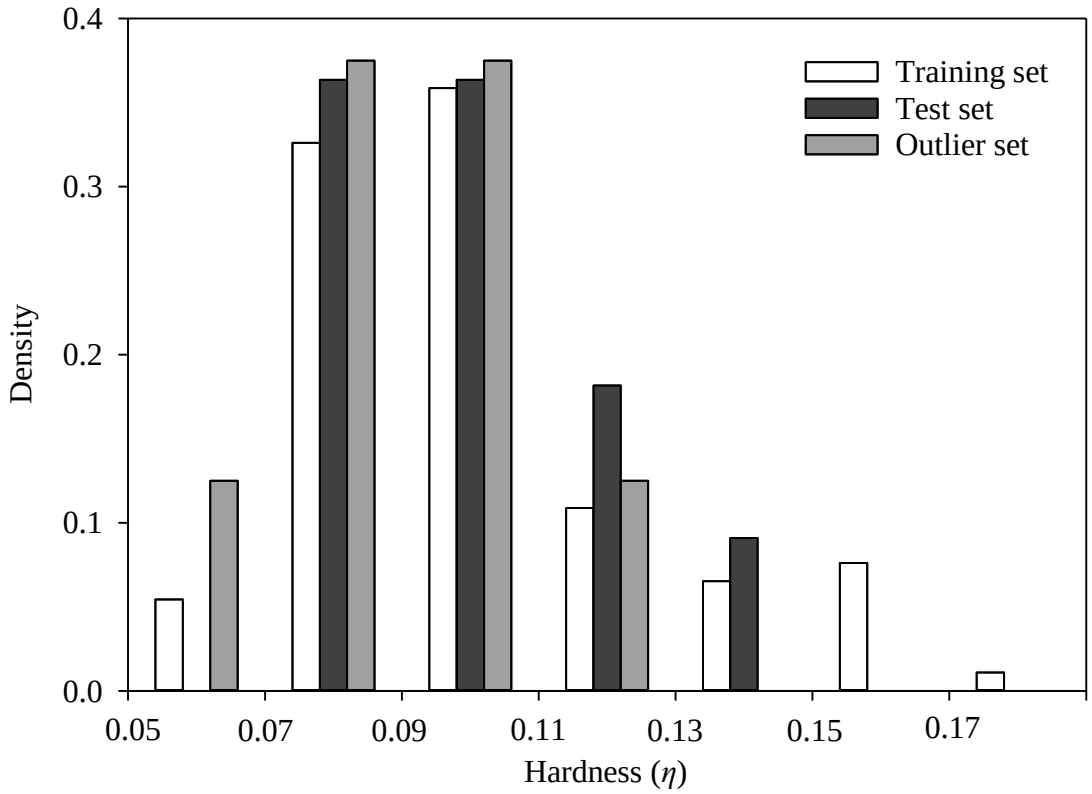
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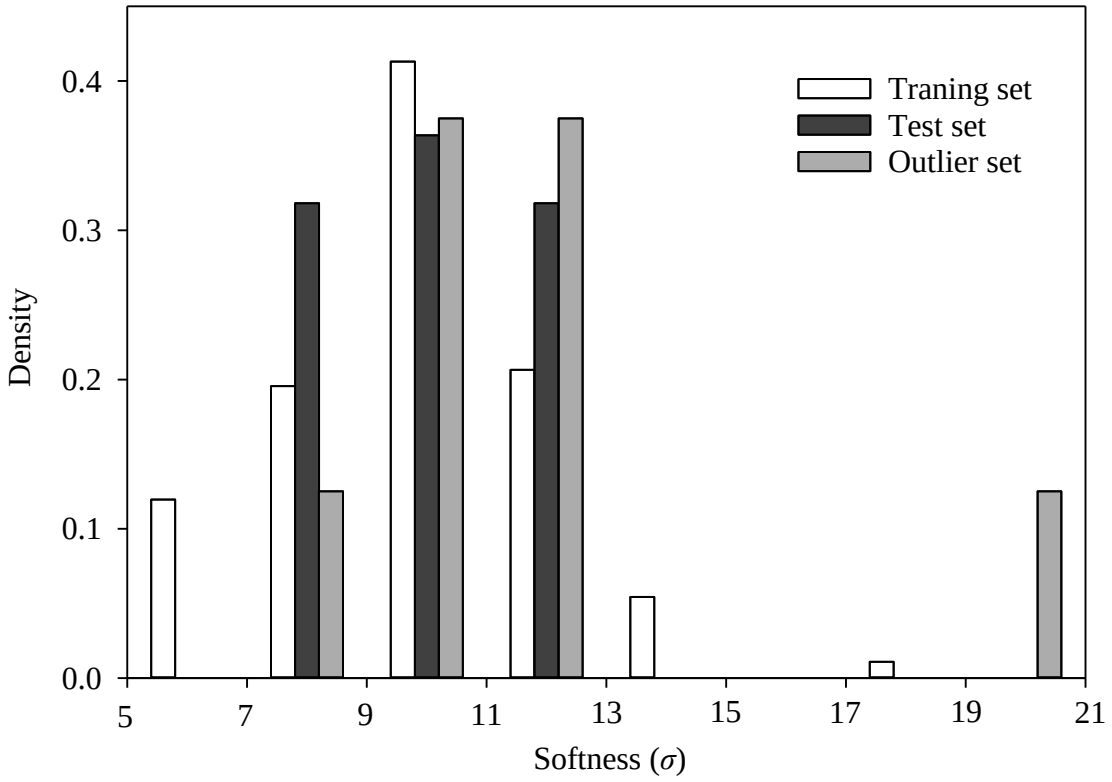
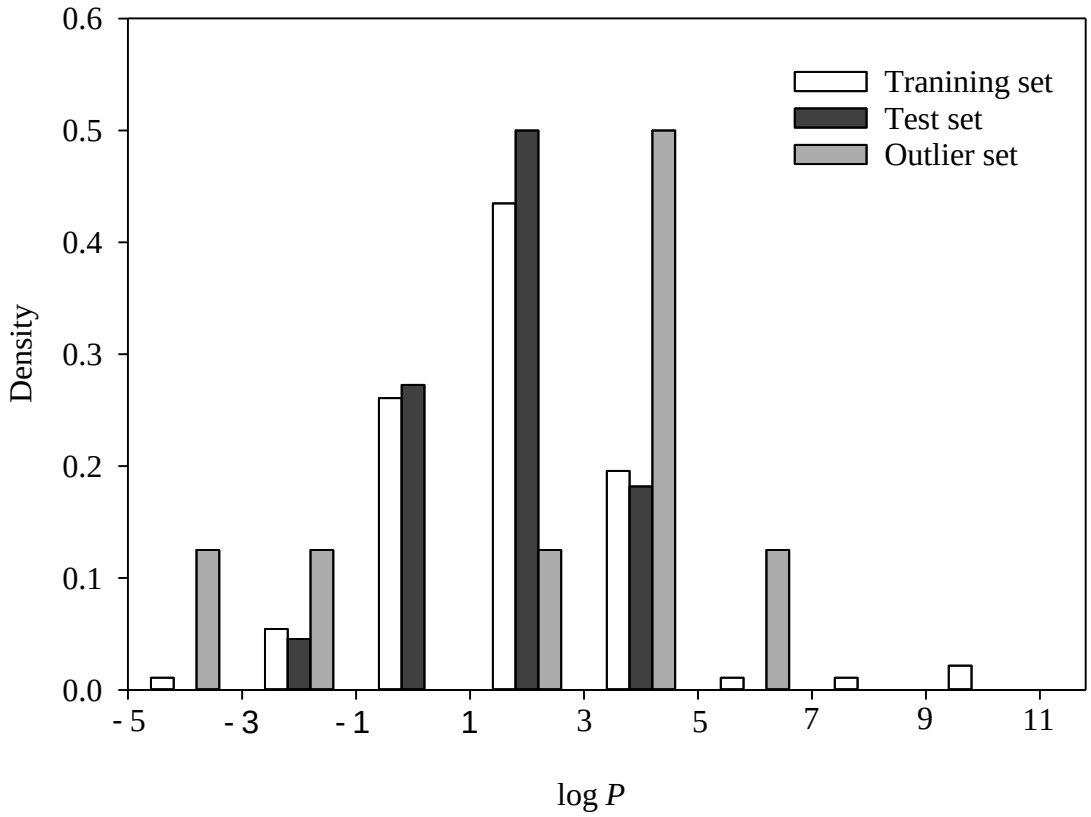
0.3
0.2
0.1
0.0
Density
0.05
0.07
0.09
0.11
0.13
0.15
0.17
Hardness (η)
Training set
Test set
Outlier set

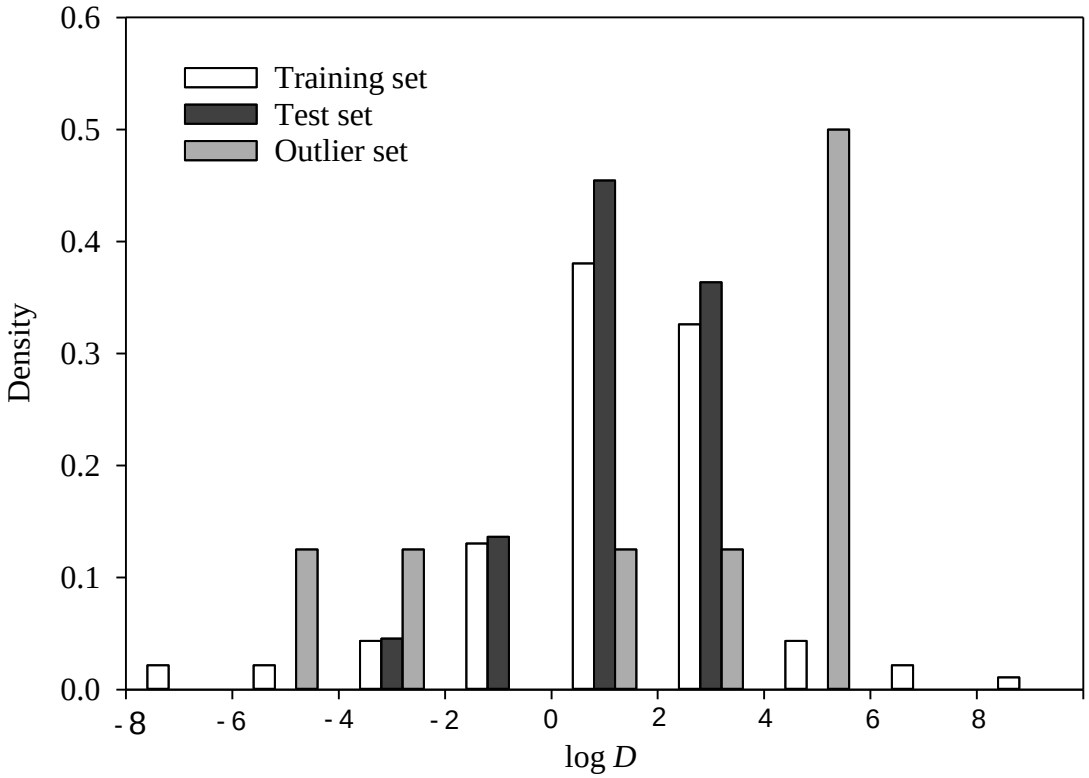
(A)


Density
0.0
0.1
0.2
0.3
0.4
5
7
9
11
13
15
17
19
21
Softness (σ)
Traning set
Test set
Outlier set

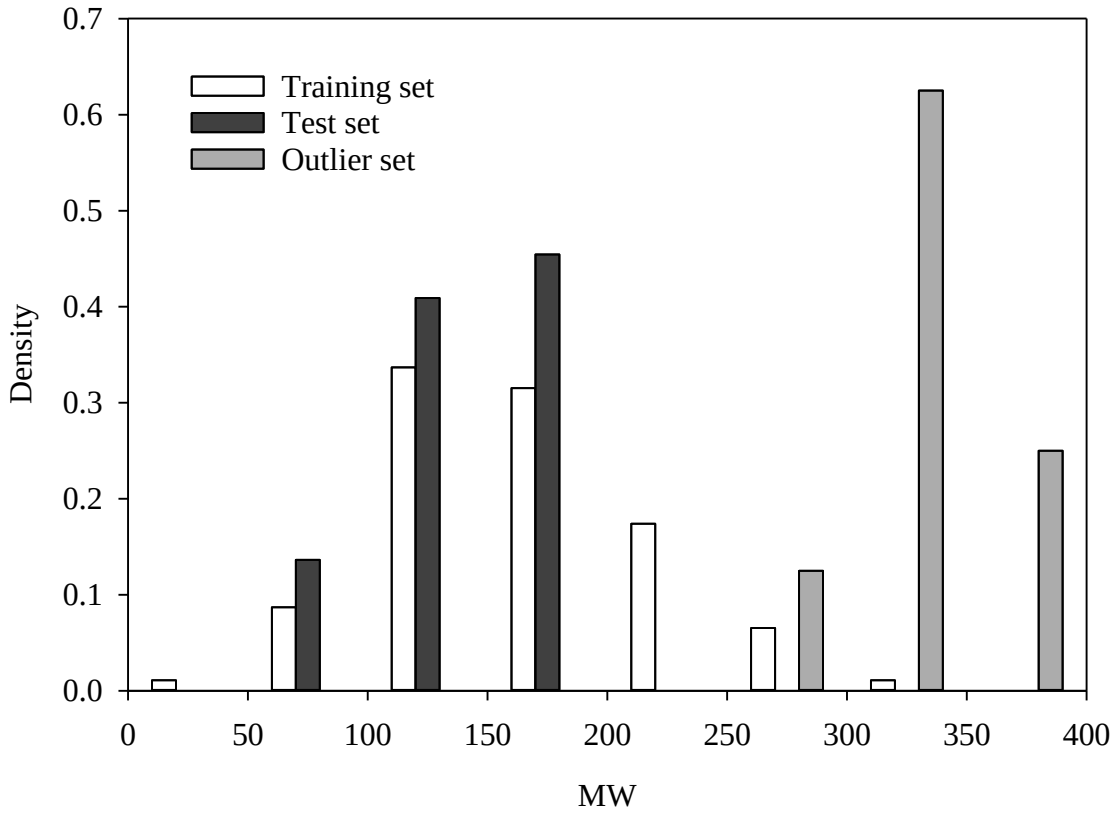
(B)


0.6
0.5
0.4
0.3
0.2
0.1
0.0
Density
Tranining set
Test set
Outlier set
- 5
- 3
- 1
1
3
5
7
9
11
log P

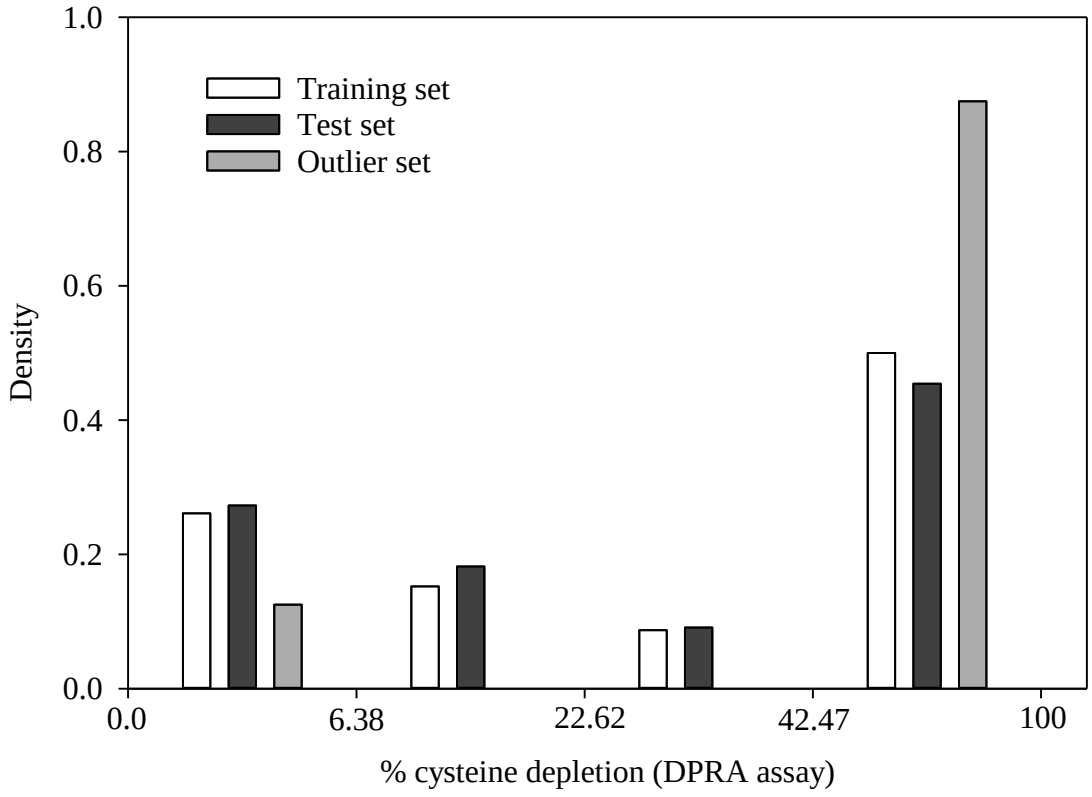
(C)


Training set
Test set
Outlier set
Density
0.6
0.5
0.4
0.3
0.2
0.1
0.0
-8
-6
-4
-2
0
2
4
6
8
log D

(D)


Training set
Test set
Outlier set
Density
MW
0.0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0
50
100
150
200
250
300
350
400

(E)



(F)

Supplementary Figure S1. Histogram representation of the distributions of various descriptors for all molecules in the training set, test set, and outlier set. (A) Hardness (η), (B) Softness (σ), (C) log *P*, (D) log *D*, (E) molecular weight (MW), and (F) % cysteine depletion (DPRA assay) in the training set, test set, and outlier set.

Table S1. A. Compound source for this study, their names, Pubchem SID/CID, CAS numbers, , SMILES strings, observed log cysteine depletion values, and predicted values by SVR A, SVR B, SVC, and HSVR, data partition, and references.

No.	Compounds	CAS No	SMILES	Obs. Cystein depletion	Obs. log %cys	SVR A	|Δ|	SVR B	|Δ|	SVR C	|Δ|	HSVR	|Δ|	Set†
1	1-(p-Methoxyphenyl)-1-penten-3-one	104-27-8	O=C(C([H])=C([H])C1=C([H])C([H])=C(OC([H])([H])[H])C([H])=C1[H])C([H])([H])C([H])([H])[H]	29.90	1.48	1.36	0.12	1.99	0.52	1.45	0.02	1.59	0.12	T
2	Methyl salicylate	119-36-8	O=C(OC([H])([H])[H])C1=C(O[H])C([H])=C([H])C([H])=C1[H]	0.43	-0.37	0.64	1.01	0.19	0.56	1.00	1.37	0.40	0.77	T
3	1,2-Dibromo-2,4-dicyanobutane (Methyldibromo glutaronitrile)	35691-65-7	[Br][C@@](C#N)(C([H])([H])C([H])([H])C#N)C([Br])([H])[H]	93.48	1.97	1.85	0.12	1.41	0.56	1.64	0.33	1.91	0.06	T
4	1,4-Dihydroquinone (1,4-Dihydroxybenzene) (Hydroquinone)	123-31-9	[H]/C1=C(\O[H])C([H])=C([H])C(O[H])=C1[H]	87.38	1.94	1.48	0.47	1.49	0.45	0.56	1.38	0.95	0.99	T
5	1, 4-Phenylenediamine	106-50-3	[H]/C1=C(\N([H])[H])C([H])=C([H])C(N([H])[H])=C1[H]	89.08	1.95	2.07	0.12	1.84	0.11	1.62	0.33	1.98	0.03	T
6	1-Bromobutane	109-65-9	[Br]C([H])([H])C([H])([H])C([H])([H])C([H])([H])[H]	12.04	1.08	1.20	0.12	0.82	0.26	1.26	0.18	1.10	0.02	T

7	1-Bromohexadecane	112-82-3	[Br]C([H])([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])[H]	22.90	1.36	1.24	0.12	0.80	0.56	1.03	0.33	0.92	0.44	T
8	1-Butanol	71-36-3	[H]C([H])(C([H])([H])C([H])([H])[H])C([H])([H])O[H]	0.40	-0.40	0.15	0.55	-0.22	0.17	-0.06	0.33	-0.28	0.11	T
9	1-Chloro-2,4-dinitrobenzene	97-00-7	[Cl]C=1C(N(O[H])O[H])=C([H])C(N(O[H])O[H])=C([H])C=1[H]	99.95	2.00	1.88	0.12	1.44	0.56	1.67	0.33	1.93	0.07	T
10	1-Chlorooctadecane	3386-33-2	[Cl]C([H])([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])[H]	3.80	0.58	0.70	0.12	0.88	0.30	0.91	0.33	0.57	0.01	T
11	1-methoxy-4-methyl-2-nitrobenzene	119-10-8	[H]/C1=C(/C([H])=C([H])C(OC([H])([H])[H])=C1N(O[H])O[H])C([H])([H])[H]	1.65	0.22	0.84	0.62	0.78	0.56	0.55	0.33	0.30	0.08	T

12	1-Phenyl-1,2-propanedione	579-07-7	O=C(/C1=C(\[H])C([H])=C([H])C([H])=C1[H])C(=O)C([H])([H])[H]	53.23	1.73	1.84	0.12	1.60	0.13	0.55	1.18	1.98	0.26	T
13	2,3-Butanedione	431-03-8	O=C(C(=O)C([H])([H])[H])C([H])([H])[H]	80.97	1.91	2.03	0.12	1.35	0.56	2.24	0.33	2.01	0.10	T
14	2,4,6-Trichloro-1,3,5-triazine (cyanuric chloride)	108-77-0	[Cl]C=1/N=C(/[Cl])N=C([Cl])N=1	56.00	1.75	1.72	0.03	1.75	0.00	1.95	0.20	1.95	0.20	T
15	2,4-Heptadienal	4313-03-5	O=C([H])C([H])=C([H])C([H])=C([H])C([H])([H])C([H])([H])[H]	97.30	1.99	1.84	0.14	1.43	0.56	1.60	0.38	1.89	0.10	T
16	2-Acetylcyclohexanone	874-23-7	O=C1[C@@]([H])(C(=O)C([H])([H])[H])C([H])([H])C([H])([H])C([H])([H])C1([H])[H]	15.24	1.18	1.30	0.12	1.43	0.24	0.90	0.28	1.12	0.07	T
17	2-Benzylideneheptanal (Amyl cinnamic aldehyde)	122-40-7	O=C([H])C(=C([H])C1=C([H])C([H])=C([H])C([H])=C1[H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])[H]	0.60	-0.22	0.62	0.84	1.31	1.53	0.11	0.33	0.14	0.36	T
18	Ethanol-2-butoxy-, acetate (2-Butoxyethyl Acetate)	112-07-2	O=C(OC([H])([H])C([H])([H])OC([H])([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])[H]	13.10	1.12	1.00	0.12	1.31	0.20	0.78	0.33	0.79	0.33	T

19	2-Ethylhexyl acrylate	103-11-7	O=C(OC([H])([H])[C@]([H])(C([H])([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])[H])C([H])=C([H])[H]	99.40	2.00	1.97	0.03	1.44	0.56	1.86	0.13	2.01	0.01	T
20	2-Hydroxyethyl acrylate	818-61-1	O=C(OC([H])([H])C([H])([H])O[H])C([H])=C([H])[H]	94.09	1.97	1.85	0.12	1.41	0.56	1.92	0.05	1.98	0.01	T
21	2-Nitro-1,4-phenylenediamine	5307-14-2	O=N(O)C=1C(N([H])[H])=C([H])C([H])=C(N([H])[H])C=1[H]	95.27	1.98	1.86	0.12	1.98	0.00	2.31	0.33	1.92	0.06	T
22	2-Phenylpropionaldehyde	93-53-8	O=C([H])[C@@]([H])(C1=C([H])C([H])=C([H])C([H])=C1[H])C([H])([H])[H]	42.79	1.63	1.51	0.12	1.20	0.43	1.30	0.33	1.48	0.15	T
23	3,5,5-Trimethylhexanoyl chloride	36727-29-4	[Cl]C(=O)C([H])([H])[C@]([H])(C([H])([H])C(C([H])([H])[H])([H])C([H])([H])C([H])([H])[H])C([H])([H])[H]	29.30	1.47	1.59	0.12	2.03	0.56	1.80	0.33	1.83	0.36	T
24	3-Chloro-4-methoxybenzaldehyde (3-Chloro-p-anisaldehyde)	4903-09-7	[Cl]C=1C(OC([H])([H])[H])=C([H])C([H])=C(C=1[H])C(=O)[H]	6.50	0.81	1.48	0.67	0.91	0.10	1.15	0.33	1.22	0.41	T
25	3-Methylcatechol	488-17-5	[H]/C1=C(/C(O[H])=C(O[H])C([H])=C1[H])C([H])([H])[H]	87.20	1.94	1.29	0.65	1.38	0.56	1.52	0.42	1.54	0.40	T

26	3-Propylidenephthalide	17369-59-4	O=C1OC(C=2/C1=C(/[H])C([H])=C([H])C=2[H])=C([H])C([H])([H])C([H])([H])[H]	10.90	1.04	1.36	0.32	1.14	0.10	1.37	0.33	1.42	0.38	T
27	4-Amino-2-hydroxytoluene (5-Amino-2-methylphenol)	2835-95-2	[H]C=1/C(=C(/O[H])C([H])=C(N([H])[H])C=1[H])C([H])([H])[H]	89.20	1.95	1.83	0.12	1.54	0.41	2.10	0.15	2.00	0.04	T
28	4-Amino-3-methylphenol (4-Aminocresol) (SCCP/0898/05)	2835-99-6	[H]C=1/C(=C(/N([H])[H])C([H])=C([H])C=1O[H])C([H])([H])[H]	67.05	1.83	1.70	0.12	1.63	0.20	2.16	0.33	1.95	0.12	T
29	4-Carboxyphenylacetate	2345-34-8	O=C(O[H])C=1C([H])=C([H])C(OC(=O)C([H])([H])[H])=C([H])C=1[H]	90.60	1.96	1.51	0.45	1.45	0.51	1.51	0.45	1.69	0.27	T
30	4-Ethoxymethylene-2-phenyl-2-oxazolin-5-one (oxazolone)	15646-46-5	O=C1OC(=N/C1=C(/[H])OC([H])([H])C([H])([H])[H])C2=C([H])C([H])=C([H])C([H])=C2[H]	74.73	1.87	1.34	0.54	1.36	0.52	1.54	0.33	1.58	0.30	T
31	4-Nitrobenzyl bromide	100-11-8	[Br]C([H])([H])C=1C([H])=C([H])C(N(=O)O)=C([H])C=1[H]	99.93	2.00	1.88	0.12	1.44	0.56	2.07	0.07	2.00	0.00	T
32	5-Chloro-2-methyl-4-isothiazolin-3-one (MCI/MI)	26172-55-4	[Cl]C=1[S]N(C(=O)C=1[H])C([H])([H])[H]	94.53	1.98	1.86	0.12	1.41	0.56	1.64	0.33	1.91	0.07	T
33	5-Methyl-2,3-hexanedione	13706-86-0	O=C(C(=O)C([H])([H])[H])C([H])([H])C([H])(C([H])([H])[H])C([H])([H])[H]	25.80	1.41	1.53	0.12	1.40	0.01	1.74	0.33	1.79	0.38	T

34	Alpha-isomethylionone	127-51-5	O=C(/C(=C(\[H])[C@@]1([H])C(=C([H])C([H])([H])C([H])([H])C1(C([H])([H])[H])C([H])([H])[H])C([H])([H])[H])C([H])([H])[H])C([H])([H])[H]	4.95	0.69	1.15	0.45	1.26	0.56	0.90	0.20	0.95	0.26	T
35	Aniline	62-53-3	[H]/C1=C(\N([H])[H])C([H])=C([H])C([H])=C1[H]	0.15	-0.82	1.66	2.48	-0.26	0.56	0.15	0.97	0.02	0.85	T
36	Benzoic-acid	65-85-0	O=C(O[H])C1=C([H])C([H])=C([H])C([H])=C1[H]	19.40	1.29	1.33	0.05	1.10	0.18	1.62	0.33	1.54	0.25	T
37	Benzoyl peroxide	94-36-0	O=C(OOC(=O)C=1C([H])=C([H])C([H])=C([H])C=1[H])C2=C([H])C([H])=C([H])C([H])=C2[H]	100.00	2.00	1.88	0.12	1.44	0.56	2.33	0.33	1.97	0.03	T
38	Benzyl benzoate	120-51-4	O=C(OC([H])([H])C=1C([H])=C([H])C([H])=C([H])C=1[H])C=2C([H])=C([H])C([H])=C([H])C=2[H]	0.20	-0.70	1.01	1.71	1.11	1.81	1.06	1.75	0.94	1.64	T
39	Benzyl bromide	100-39-0	[Br]C([H])([H])C1=C([H])C([H])=C([H])C([H])=C1[H]	99.97	2.00	1.86	0.14	1.44	0.56	1.67	0.33	1.92	0.08	T
40	beta-Propiolactone	57-57-8	O=C1OC([H])([H])C1([H])[H]	21.90	1.34	1.46	0.12	1.60	0.26	1.40	0.06	1.62	0.28	T
41	Butyl acrylate	141-32-2	O=C(OC([H])([H])C([H])([H])C([H])([H])C([H])([H])[H])C([H])=C([H])[H]	100.00	2.00	2.04	0.04	1.44	0.56	1.67	0.33	1.98	0.02	T

42	Butyl glycidyl ether	2426-08-6	[H][C@]1(OC1([H])[H])C([H])([H])OC([H])([H])C([H])([H])C([H])([H])C([H])([H])[H]	64.97	1.81	1.69	0.12	1.25	0.56	1.48	0.33	1.72	0.09	T
43	4-(N-Ethyl-N-2-methan-sulphonamido-ethyl)-2-methyl-1,4-phenylenediamine (CD3)	25646-71-3	O=[S](=O)(N([H])C([H])([H])C([H])([H])N(/C1=C(\[H])C(=C(N([H])[H])C([H])=C1[H])C([H])([H])[H])C([H])([H])[H])C([H])([H])[H]	90.09	1.95	2.07	0.12	1.39	0.56	1.62	0.33	1.96	0.00	T
44	Chloramine T (Tosylchloramide sodium)	127-65-1; 149358-73-7	[Cl]N[S](=O)(=O)C=1C([H])=C([H])C(=C([H])C=1[H])C([H])([H])[H]	100.00	2.00	2.12	0.12	1.44	0.56	2.33	0.33	2.00	0.00	T
45	Chlorobenzene	108-90-7	[Cl]/C1=C(\[H])C([H])=C([H])C([H])=C1[H]	0.40	-0.40	1.43	1.82	0.17	0.56	-0.06	0.33	-0.10	0.30	T
46	Chlorothalonil	1897-45-6	[Cl]/C1=C(\C#N)C([Cl])=C([Cl])C([Cl])=C1C#N	100.00	2.00	2.12	0.12	1.55	0.45	2.33	0.33	2.01	0.01	T
47	Cinnamaldehyde (Cinnamic aldehyde)	104-55-2	O=C([H])C([H])=C([H])C1=C([H])C([H])=C([H])C([H])=C1[H]	71.27	1.85	1.73	0.12	1.57	0.28	2.19	0.33	1.96	0.10	T
48	cis-6-nonenal	2277-19-2	O=C([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C([H])=C([H])C([H])([H])C([H])([H])[H]	8.00	0.90	1.37	0.47	1.03	0.12	1.18	0.28	1.24	0.33	T

49	Citral	5392-40-5	O=C([H])C([H])=C(C([H])([H])C([H])([H])C([H])=C(C([H])([H])[H])C([H])([H])[H])C([H])([H])[H]	83.93	1.92	1.45	0.47	1.25	0.67	1.59	0.33	1.65	0.28	T
50	Clofibrate (Ethyl (2-(4-chlorophenoxy)-2-methylpropanoate)	637-07-0	[Cl]C=1C([H])=C([H])C(OC(C(=O)OC([H])([H])C([H])([H])[H])(C([H])([H])[H])C([H])([H])[H])=C([H])C=1[H]	4.08	0.61	0.73	0.12	1.17	0.56	0.94	0.33	0.71	0.10	T
51	Glucose (D-Glucose)	492-62-6	[H][C@]1(O[H])[C@]([H])(O[H])[C@@]([H])(O[H])[C@@]([H])(O[C@]1([H])C([H])([H])O[H])O[H]	0.10	-1.00	-0.88	0.12	-0.44	0.56	-0.67	0.33	-0.12	0.88	T
52	Diethyl acetaldehyde	97-96-1	O=C([H])C([H])(C([H])([H])C([H])([H])[H])C([H])([H])C([H])([H])[H]	54.50	1.74	1.62	0.12	1.10	0.64	1.40	0.33	1.58	0.16	T
53	Diethyl sulfate	64-67-5	O=[S](=O)(OC([H])([H])C([H])([H])[H])OC([H])([H])C([H])([H])[H]	34.07	1.53	1.41	0.12	1.80	0.26	1.29	0.24	1.55	0.01	T
54	Dimethyl sulfate	77-78-1	O=[S](=O)(OC([H])([H])[H])OC([H])([H])[H]	97.70	1.99	1.87	0.12	1.79	0.20	1.66	0.33	1.94	0.05	T
55	Dimethylsulfoxide	67-68-5	O[S](C([H])([H])[H])C([H])([H])[H]	0.40	-0.40	-0.28	0.12	0.09	0.49	-0.73	0.33	-0.33	0.07	T
56	Diphenylcyclopropenone	886-38-4	O=C1/C(=C1\C=2C([H])=C([H])C([H])=C([H])C=2[H])C=3C([H])=C([H])C([H])=C([H])C=3[H]	98.95	2.00	1.88	0.12	1.43	0.56	1.66	0.33	1.93	0.07	T

57	Ethyl benzoylacetate	94-02-0	O=C(/C1=C(\[H])C([H])=C([H])C([H])=C1[H])C([H])([H])C(=O)OC([H])([H])C([H])([H])[H]	2.30	0.36	1.09	0.73	0.20	0.17	1.16	0.80	0.68	0.32	T
58	Ethylenediamine	107-15-3	[H]C([H])(N([H])[H])C([H])([H])N([H])[H]	3.40	0.53	0.41	0.12	0.17	0.37	0.20	0.33	-0.19	0.72	T
59	Ethyleneglycol dimethacrylate	97-90-5	O=C(OC([H])([H])C([H])([H])OC(=O)C(=C([H])[H])C([H])([H])[H])C(=C([H])[H])C([H])([H])[H]	87.53	1.94	1.82	0.12	1.82	0.13	1.94	0.00	1.98	0.04	T
60	Farnesal	502-67-0	O=C([H])C([H])=C(C([H])([H])C([H])([H])C([H])=C(C([H])([H])C([H])([H])C([H])=C([H])[H])C([H])([H])[H]	21.63	1.33	1.22	0.12	1.23	0.10	1.47	0.14	1.42	0.09	T
61	Formaldehyde	50-00-0	O=C([H])[H]	56.04	1.75	1.73	0.02	1.50	0.25	1.42	0.33	1.76	0.01	T
62	Fumaric acid	110-17-8	O=C(O[H])C([H])=C([H])C(=O)O[H]	10.80	1.03	1.15	0.12	1.60	0.56	1.37	0.33	1.40	0.36	T
63	Furil	492-94-4	O=C(C=1OC([H])=C([H])C=1[H])C(=O)C=2OC([H])=C([H])C=2[H]	97.90	1.99	1.87	0.12	1.98	0.01	2.32	0.33	1.92	0.07	T
64	Glyoxal	107-22-2	O=C([H])C(=O)[H]	59.43	1.77	1.69	0.08	2.34	0.56	1.70	0.08	1.76	0.01	T

65	Hexadecyltrimethyl ammonium bromide	57-09-0	[H]C([H])([N+](C([H])([H])[H])(C([H])([H])[H])C([H])([H])[H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])[H]	2.40	0.38	0.42	0.04	-0.18	0.56	0.40	0.02	-0.09	0.47	T
66	Hexyl salicylate	6259-76-3	O=C(OC([H])([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])[H])C=1C(O[H])=C([H])C([H])=C([H])C=1[H]	1.95	0.29	0.54	0.25	0.20	0.09	0.41	0.12	-0.05	0.34	T
67	Hydroxycitronellal	107-75-5	O=C([H])C([H])([H])[C@]([H])(C([H])([H])C([H])([H])C([H])([H])C(O[H])(C([H])([H])[H])C([H])([H])[H])C([H])([H])[H]	18.29	1.26	1.34	0.08	1.09	0.17	1.60	0.33	1.53	0.27	T
68	Lilial (p-tert-Butyl-.alpha.-methylhydrocinnamaldehyde)	80-54-6	O=C([H])[C@@]([H])(C([H])([H])C=1C([H])=C([H])C(=C([H])C=1[H])C(C([H])([H])[H])(C([H])([H])[H])C([H])([H])[H])C([H])([H])[H]	14.00	1.15	0.65	0.50	1.03	0.12	0.81	0.33	0.52	0.63	T
69	Tartaric acid (L-tartaric acid)	87-69-4	O=C(O[H])[C@]([H])(O[H])[C@@]([H])(O[H])C(=O)O[H]	4.73	0.68	0.79	0.12	0.65	0.03	1.01	0.33	0.60	0.07	T

70	Lyral (3 and 4-(4-Hydroxy-4-methylpentyl)-3-cyclohexene-1-carboxaldehyde)	31906-04-4	O=C([H])[C@]1([H])C([H])([H])C([H])([H])C(=C([H])C1([H])[H])C([H])([H])C([H])([H])C([H])([H])C(O[H])(C([H])([H])[H])C([H])([H])[H]	40.50	1.61	1.49	0.12	1.05	0.56	1.27	0.33	1.39	0.22	T
71	Maleic anhydride	108-31-6	O=C1OC(=O)C([H])=C1[H]	100.00	2.00	1.88	0.12	1.44	0.56	1.67	0.33	1.93	0.07	T
72	Methyl 2-nonynoate	111-80-8	O=C(OC([H])([H])[H])C#CC([H])([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])[H]	99.93	2.00	1.63	0.37	1.44	0.56	1.67	0.33	1.83	0.17	T
73	Methyl methanesulfonate	66-27-3	O=[S](=O)(OC([H])([H])[H])C([H])([H])[H]	93.00	1.97	1.85	0.12	1.41	0.56	1.64	0.33	1.90	0.06	T
74	N-Ethyl-N-nitrosourea	759-73-9	O=C(N(NO)C([H])([H])C([H])([H])[H])N([H])[H]	42.70	1.63	1.75	0.12	1.07	0.56	1.30	0.33	1.56	0.08	T
75	N-Methyl-P-Aminophenol Sulfate (Metol)	55-55-0	[H]/C1=C(\N([H])C([H])([H])[H])C([H])=C([H])C(O[H])=C1[H]	100.00	2.00	2.12	0.12	1.67	0.33	2.33	0.33	2.01	0.01	T
76	N,N-Diethyl-m-toluamide	134-62-3	O=C(N(C([H])([H])C([H])([H])[H])C([H])([H])C([H])([H])[H])C1=C([H])C(=C([H])C([H])=C1[H])C([H])([H])[H]	6.70	0.83	0.71	0.12	1.04	0.21	1.16	0.33	0.81	0.01	T

77	Palmitoyl chloride	112-67-4	[Cl]C(=O)C([H])([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])[H]	25.50	1.41	1.53	0.12	1.93	0.52	1.30	0.10	1.62	0.21	T
78	p-Aminobenzoic acid	150-13-0	O=C(O[H])C1=C([H])C([H])=C(N([H])[H])C([H])=C1[H]	5.90	0.77	0.89	0.12	0.29	0.48	1.10	0.33	0.59	0.18	T
79	p-Benzoquinone (1,4-Benzoquinone)	106-51-4	O=C1C([H])=C([H])C(=O)C([H])=C1[H]	98.57	1.99	1.88	0.12	2.56	0.56	1.66	0.33	1.72	0.27	T
80	Perillaldehyde	2111-75-3	O=C([H])C1=C([H])C([H])([H])[C@]([H])(C(=C([H])[H])C([H])([H])[H])C([H])([H])C1([H])[H]	31.89	1.50	1.62	0.12	1.40	0.10	1.17	0.33	1.52	0.02	T
81	Phenylacetaldehyde	122-78-1	O=C([H])C([H])([H])C1=C([H])C([H])=C([H])C([H])=C1[H]	55.76	1.75	1.63	0.12	1.18	0.56	1.41	0.33	1.62	0.12	T
82	Phthalic anhydride	85-44-9	O=C1OC(=O)C2=C1C([H])=C([H])C([H])=C2[H]	0.95	-0.02	1.43	1.45	0.54	0.56	0.31	0.33	0.26	0.29	T

83	Propyl gallate	121-79-9	O=C(OC([H])([H])C([H])([H])C([H])([H])[H])C=1C([H])=C(O[H])C(O[H])=C(O[H])C=1[H]	52.75	1.72	1.24	0.48	2.28	0.56	1.39	0.33	1.45	0.27	T
84	Propyl paraben (Propyl 4-hydroxybenzoate)	94-13-3	O=C(OC([H])([H])C([H])([H])C([H])([H])[H])C=1C([H])=C([H])C(O[H])=C([H])C=1[H]	8.20	0.91	0.80	0.12	0.35	0.56	1.14	0.23	0.61	0.31	T
85	Octanoic acid	124-07-2	O=C(O[H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])[H]	0.63	-0.20	0.78	0.98	0.36	0.56	0.13	0.33	-0.15	0.05	T
86	Squaric acid	2892-51-5	O=C1C(O[H])=C(O[H])C1=O	46.90	1.67	1.55	0.12	1.11	0.56	1.64	0.03	1.68	0.01	T
87	Squaric acid diethyl ester	5231-87-8	O=C1C(OC([H])([H])C([H])([H])[H])=C(OC([H])([H])C([H])([H])[H])C1=O	2.40	0.38	1.43	1.05	0.94	0.56	0.71	0.33	0.81	0.43	T
88	Sulfanilamide	63-74-1	O=[S](=O)(N([H])[H])C1=C([H])C([H])=C(N([H])[H])C([H])=C1[H]	1.30	0.11	0.88	0.77	0.68	0.56	0.45	0.33	0.19	0.08	T
89	Sulphanilic acid (Sulfanic acid)	121-57-3	O=[S](=O)(O[H])C=1C([H])=C([H])C(N([H])[H])=C([H])C=1[H]	5.30	0.72	1.01	0.29	0.87	0.15	0.39	0.33	0.28	0.44	T
90	Tetramethylthiuram disulfide	137-26-8	[S]=C([S][S]C(=[S])N(C([H])([H])[H])C([H])([H])[H])N(C([H])([H])[H])C([H])([H])[H]	99.67	2.00	1.96	0.04	1.44	0.56	2.33	0.33	1.99	0.01	T

91	trans-2-Decenal	3913-71-1; 3913-81-4	O=C([H])C([H])=C([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])[H]	94.90	1.98	1.50	0.48	1.47	0.50	2.31	0.33	1.84	0.14	T
92	Undec-10-enal	112-45-8	O=C([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C([H])=C([H])[H]	2.70	0.43	1.14	0.71	1.07	0.64	0.77	0.33	0.76	0.32	T
93	1-Bromohexane	111-25-1	[Br]C([H])([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])[H]	12.05	1.08	0.88	0.20	0.81	0.27	1.14	0.06	0.82	0.26	t
94	2,5-Diaminotoluene sulfate	615-50-9	[H]C=1/C(=C(/N([H])[H])C([H])=C([H])C=1N([H])[H])C([H])([H])[H]	85.60	1.93	2.16	0.23	1.82	0.12	1.80	0.14	2.03	0.10	t
95	2-Aminophenol	95-55-6	[H]C=1C(N([H])[H])=C(O[H])C([H])=C([H])C=1[H]	92.97	1.97	1.43	0.54	1.57	0.40	2.11	0.14	1.82	0.15	t
96	4-Hydroxybenzoic acid	99-96-7	O=C(O[H])C1=C([H])C([H])=C(O[H])C([H])=C1[H]	1.18	0.07	1.08	1.01	0.55	0.48	0.90	0.83	0.61	0.54	t
97	4-Methoxyacetophenone (Acetanisole)	100-06-1	O=C(C=1C([H])=C([H])C(OC([H])([H])[H])=C([H])C=1[H])C([H])([H])[H]	4.01	0.60	1.33	0.72	1.25	0.65	0.16	0.45	0.43	0.17	t
98	6-Methyl coumarin	92-48-8	O=C2OC=1/C(=C(/[H])C(=C([H])C=1[H])C([H])([H])[H])C([H])=C2[H]	1.58	0.20	1.58	1.38	1.06	0.86	0.42	0.23	0.69	0.49	t

99	alpha-Methyl cinnamaldehyde (α-methyl-trans-cinnamaldehyde)	101-39-3	O=C([H])C(=C([H])C=1C([H])=C([H])C([H])=C([H])C=1[H])C([H])([H])[H]	10.73	1.03	1.65	0.62	1.59	0.56	0.85	0.18	1.33	0.30	t
100	Benzylidene acetone (4-phenyl-3-buten-2-one)	122-57-6	O=C(C([H])=C([H])C1=C([H])C([H])=C([H])C([H])=C1[H])C([H])([H])[H]	93.84	1.97	1.84	0.13	1.42	0.55	0.61	1.37	1.15	0.82	t
101	Cyclamen aldehyde	103-95-7	O=C([H])[C@@]([H])(C([H])([H])C1=C([H])C([H])=C(C([H])=C1[H])C([H])(C([H])([H])[H])C([H])([H])[H])C([H])([H])[H]	17.55	1.24	0.81	0.44	1.03	0.22	0.49	0.75	0.34	0.91	t
102	Diethyl maleate	141-05-9	O=C(OC([H])([H])C([H])([H])[H])C([H])=C([H])C(=O)OC([H])([H])C([H])([H])[H]	99.93	2.00	2.29	0.29	1.85	0.15	2.04	0.04	2.03	0.03	t
103	DL-lactic acid (Lactic acid)	50-21-5	O=C(O[H])[C@]([H])(O[H])C([H])([H])[H]	1.20	0.08	0.09	0.01	0.59	0.51	1.36	1.28	0.57	0.49	t
104	Ethyl acrylate	140-88-5	O=C(OC([H])([H])C([H])([H])[H])C([H])=C([H])[H]	97.30	1.99	2.36	0.37	1.44	0.55	1.73	0.26	2.02	0.03	t
105	Ethyl vanillin	121-32-4	O=C([H])C=1C([H])=C(OC([H])([H])C([H])([H])[H])C(O[H])=C([H])C=1[H]	1.09	0.04	1.05	1.01	-0.26	0.30	0.57	0.54	0.10	0.07	t

106	Isoeugenol	97-54-1	[H]C=1/C(=C(/[H])C([H])=C(O[H])C=1OC([H])([H])[H])C([H])=C([H])C([H])([H])[H]	83.38	1.92	1.29	0.63	1.45	0.47	1.21	0.71	1.36	0.56	t
107	Linalool	78-70-6	[H]C([H])([C@@](O[H])(C([H])=C([H])[H])C([H])([H])[H])C([H])([H])C([H])=C(C([H])([H])[H])C([H])([H])[H]	0.65	-0.19	1.24	1.43	-0.56	0.37	-0.08	0.11	-0.17	0.02	t
108	Methyl acrylate	96-33-3	O=C(OC([H])([H])[H])C([H])=C([H])[H]	99.53	2.00	2.36	0.37	1.47	0.53	1.76	0.24	2.03	0.03	t
109	Methyl methacrylate	(80-62-6)	O=C(OC([H])([H])[H])C(=C([H])[H])C([H])([H])[H]	55.30	1.74	2.10	0.35	1.37	0.37	1.68	0.07	1.98	0.24	t
110	1,2-cyclohexanedicarboxylic anhydride	85-42-7	O=C1OC(=O)[C@]2([H])[C@]1([H])C([H])([H])C([H])([H])C([H])([H])C2([H])[H]	15.70	1.20	1.77	0.57	1.70	0.50	2.53	1.33	1.88	0.69	t
111	N-Methyl-N-nitrosourea	684-93-5	O=C(N(NO)C([H])([H])[H])N([H])[H]	32.40	1.51	1.62	0.11	1.10	0.41	1.24	0.27	1.46	0.05	t
112	Glutaraldehyde	111-30-8	O=C([H])C([H])([H])C([H])([H])C([H])([H])C(=O)[H]	29.20	1.47	1.71	0.25	1.43	0.04	1.39	0.08	1.72	0.26	t
113	Phenyl benzoate	93-99-2	O=C(OC=1C([H])=C([H])C([H])=C([H])C=1[H])C=2C([H])=C([H])C([H])=C([H])C=2[H]	45.30	1.66	1.28	0.38	0.92	0.74	1.27	0.38	1.20	0.45	t
114	trans-2-Hexenal	6728-26-4	O=C([H])C([H])=C([H])C([H])([H])C([H])([H])C([H])([H])[H]	97.90	1.99	2.18	0.19	1.47	0.52	1.75	0.24	2.03	0.04	t

115	2,4,6-Trinitrobenzenesulfonic acid	2508-19-2	O=[S](=O)(O[H])C=1C(N(=O)O)=C([H])C(N(=O)O)=C([H])C=1N(=O)O	99.70	2.00	2.04	0.04	2.48	0.49	2.34	0.34	1.94	0.06	o
116	Fluorescein-5-isothiocyanate	3326-32-7	[S]=C=NC=1C([H])=C2/C(=C(/[H])C=1[H])[C@]3(OC2=O)C5=C(OC4=C3C([H])=C([H])C(O[H])=C4[H])C([H])=C(O[H])C([H])=C5[H]	100.00	2.00	2.43	0.43	3.82	1.82	1.74	0.26	1.83	0.17	o
117	Imidazolidinyl urea	39236-46-9	O=C1N([H])C(=O)N([C@@]1([H])N([H])C(=O)N([H])C([H])([H])N([H])C(=O)N([H])[C@]2([H])N(C(=O)N([H])C2=O)C([H])([H])O[H])C([H])([H])O[H]	52.90	1.72	2.75	1.03	2.57	0.85	1.71	0.01	1.91	0.19	o
118	Bandrowski’s Base (1,4-Cyclohexadiene-1,4-diamine)	20048-27-6	[H]C=3C(N/C1=C(\[H])C([H])=C(N([H])[H])C([H])=C1[H])=C(N([H])[H])C([H])=C(N/C2=C(\[H])C([H])=C(N([H])[H])C([H])=C2[H])C=3N([H])[H]	87.50	1.94	2.11	0.17	2.29	0.35	1.63	0.31	1.96	0.02	o

119	Bisphenol A-diglycidyl ether	1675-54-3	[H][C@@]1(OC1([H])[H])C([H])([H])O/C2=C(\[H])C([H])=C(C([H])=C2[H])C(C=4C([H])=C([H])C(OC([H])([H])[C@]3([H])OC3([H])[H])=C([H])C=4[H])(C([H])([H])[H])C([H])([H])[H]	53.27	1.73	1.32	0.40	1.29	0.43	1.41	0.32	1.37	0.36	o
120	Lauryl gallate	1166-52-5	O=C(OC([H])([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C1=C([H])C(O[H])=C(O[H])C(O[H])=C1[H]	90.90	1.96	1.61	0.35	1.75	0.21	3.00	1.04	1.51	0.45	o
121	Abietic acid	514-10-3	O=C(O[H])[C@]3([C@@]1([H])[C@@]([C@]2([H])C(=C([H])C1([H])[H])C([H])=C(C([H])([H])C2([H])[H])C([H])(C([H])([H])[H])C([H])([H])[H])(C([H])([H])C([H])([H])C3([H])[H])C([H])([H])[H])C([H])([H])[H]	99.90	2.00	1.94	0.06	2.20	0.20	2.26	0.26	1.98	0.02	o

122	Butylbenzylphthalate	85-68-7	O=C(OC([H])([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])[H])C=1/C(=C(/[H])C([H])=C([H])C=1[H])C(=O)OC([H])([H])C2=C([H])C([H])=C([H])C([H])=C2[H]	3.60	0.56	0.33	0.22	1.27	0.72	1.07	0.52	0.61	0.05	o

Table S1. B. Qualitative predictions by QSAR Toolbox 4.4 (QT), PredSkin 3.0 (PS), ToxTree online (TT), Danish (Q)SAR database, and VEGAHUB (VH)

No.	Compounds	CAS No	SMILES	Sensitizer[+/-*]		Qualitative prediction							References
				6.38%	13.89%	QT[A]	QT[B]	PS	TT	Danish	VH[C]	VH[D]	
1	1-(p-Methoxyphenyl)-1-penten-3-one	104-27-8	O=C(C([H])=C([H])C1=C([H])C([H])=C(OC([H])([H])[H])C([H])=C1[H])C([H])([H])C([H])([H])[H]	+	+	+	+	+	+	-	+	+	Natsch13aa; Gerberick04aa; Jaworska11ab; Gerberick07a;
2	Methyl salicylate	119-36-8	O=C(OC([H])([H])[H])C1=C(O[H])C([H])=C([H])C([H])=C1[H]	+	+	-	-	-	-	-	-	-	Takenouchi15a; Natsch13aa; Gerberick04aa; Jaworska11ab; Gerberick07a;
3	1,2-Dibromo-2,4-dicyanobutane (Methyldibromo glutaronitrile)	35691-65-7	[Br][C@@](C#N)(C([H])([H])C([H])([H])C#N)C([Br])([H])[H]	+	+	+	-	+	+	-	+	+	Takenouchi15a; Natsch13aa; Jaworska11ab; Bauch12aa;
4	1,4-Dihydroquinone (1,4-Dihydroxybenzene) (Hydroquinone)	123-31-9	[H]/C1=C(\O[H])C([H])=C([H])C(O[H])=C1[H]	+	+	+	+	+	+	+	+	+	Takenouchi15a; Natsch13aa; Gerberick04aa; Jaworska11ab;
5	1, 4-Phenylenediamine	106-50-3	[H]/C1=C(\N([H])[H])C([H])=C([H])C(N([H])[H])=C1[H]	+	+	+	+	+	+	+	+	+	Takenouchi15a; Natsch13aa; Jaworska11ab; Bauch12aa;
6	1-Bromobutane	109-65-9	[Br]C([H])([H])C([H])([H])C([H])([H])C([H])([H])[H]	+	+	-	-	-	+	-	-	-	Takenouchi15a; Natsch13aa; Jaworska11ab; Gerberick07a;

7	1-Bromohexadecane	112-82-3	[Br]C([H])([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])[H]	+	+	+	+	-	+	-	+	+	Jaworska11ab;
8	1-Butanol	71-36-3	[H]C([H])(C([H])([H])C([H])([H])[H])C([H])([H])O[H]	+	+	-	-	-	-	-	-	-	Takenouchi15a; Natsch13aa; Jaworska11ab; Bauch12aa;
9	1-Chloro-2,4-dinitrobenzene	97-00-7	[Cl]C=1C(N(O[H])O[H])=C([H])C(N(O[H])O[H])=C([H])C=1[H]	+	+	N/A[‡]	+	+	N/A	N/A	+	-	Takenouchi15a; Natsch13aa; Gerberick04aa; Jaworska11ab; Bauch12aa; Gerberick07a;
10	1-Chlorooctadecane	3386-33-2	[Cl]C([H])([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])[H]	+	+	+	+	-	+	-	+	+	Jaworska11ab;
11	1-methoxy-4-methyl-2-nitrobenzene	119-10-8	[H]/C1=C(/C([H])=C([H])C(OC([H])([H])[H])=C1N(O[H])O[H])C([H])([H])[H]	+	+	-	-	-	N/A	N/A	+	-	Takenouchi15a; Urbisch15aa;

12	1-Phenyl-1,2-propanedione	579-07-7	O=C(/C1=C(\[H])C([H])=C([H])C([H])=C1[H])C(=O)C([H])([H])[H]	+	+	+	+	-	+	-	+	+	Takenouchi15a; Natsch13aa; Jaworska11ab;
13	2,3-Butanedione	431-03-8	O=C(C(=O)C([H])([H])[H])C([H])([H])[H]	+	+	+	+	-	+	-	+	+	Takenouchi15a; Natsch13aa; Jaworska11ab; Bauch12aa; Gerberick07a;
14	2,4,6-Trichloro-1,3,5-triazine (cyanuric chloride)	108-77-0	[Cl]C=1/N=C(/[Cl])N=C([Cl])N=1	+	+	+	+	-	N/A	N/A	+	-	Jaworska11ab;
15	2,4-Heptadienal	4313-03-5	O=C([H])C([H])=C([H])C([H])=C([H])C([H])([H])C([H])([H])[H]	+	+	+	+	+	N/A	-	+	+	Natsch13aa; Jaworska11ab; Gerberick07a;
16	2-Acetylcyclohexanone	874-23-7	O=C1[C@@]([H])(C(=O)C([H])([H])[H])C([H])([H])C([H])([H])C([H])([H])C1([H])[H]	+	+	-	-	+	N/A	-	-	+	Takenouchi15a; Natsch13aa; Jaworska11ab; Gerberick07a;
17	2-Benzylideneheptanal (Amyl cinnamic aldehyde)	122-40-7	O=C([H])C(=C([H])C1=C([H])C([H])=C([H])C([H])=C1[H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])[H]	+	+	+	+	+	+	N/A	+	+	Natsch13aa; Gerberick04aa; Jaworska11ab; Gerberick07a;
18	Ethanol-2-butoxy-, acetate (2-Butoxyethyl Acetate)	112-07-2	O=C(OC([H])([H])C([H])([H])OC([H])([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])[H]	+	+	-	-	-	-	-	+	-	Natsch13aa;

19	2-Ethylhexyl acrylate	103-11-7	O=C(OC([H])([H])[C@]([H])(C([H])([H])C([H])([H])C([H])([H])C([H])([H])[H])C([H])([H])C([H])([H])C([H])([H])[H])C([H])=C([H])[H]	+	+	+	+	+	+	N/A	+	+	Takenouchi15a; Natsch13aa; Jaworska11ab; Urbisch15aa;
20	2-Hydroxyethyl acrylate	818-61-1	O=C(OC([H])([H])C([H])([H])O[H])C([H])=C([H])[H]	+	+	-	-	+	+	+	+	+	Takenouchi15a; Natsch13aa; Gerberick04aa; Jaworska11ab; Gerberick07a;
21	2-Nitro-1,4-phenylenediamine	5307-14-2	O=N(O)C=1C(N([H])[H])=C([H])C([H])=C(N([H])[H])C=1[H]	+	+	+	+	N/A	+	+	+	-	Takenouchi15a; Natsch13aa; Jaworska11ab;
22	2-Phenylpropionaldehyde	93-53-8	O=C([H])[C@@]([H])(C1=C([H])C([H])=C([H])C([H])=C1[H])C([H])([H])[H]	+	+	+	+	-	N/A	N/A	+	+	Natsch13aa; Jaworska11ab; Bauch12aa; Gerberick07a;
23	3,5,5-Trimethylhexanoyl chloride	36727-29-4	[Cl]C(=O)C([H])([H])[C@]([H])(C([H])([H])C(C([H])([H])[H])([H])C([H])([H])C([H])([H])[H])C([H])([H])[H]	+	+	+	+	-	N/A	N/A	+	+	Jaworska11ab;
24	3-Chloro-4-methoxybenzaldehyde (3-Chloro-p-anisaldehyde)	4903-09-7	[Cl]C=1C(OC([H])([H])[H])=C([H])C([H])=C(C=1[H])C(=O)[H]	+	+	+	+	-	+	-	-	-	Natsch13aa;
25	3-Methylcatechol	488-17-5	[H]/C1=C(/C(O[H])=C(O[H])C([H])=C1[H])C([H])([H])[H]	+	+	+	+	-	+	+	+	-	Natsch13aa; Jaworska11ab;

26	3-Propylidenephthalide	17369-59-4	O=C1OC(C=2/C1=C(/[H])C([H])=C([H])C=2[H])=C([H])C([H])([H])C([H])([H])[H]	+	+	+	+	+	N/A	N/A	-	-	Natsch13aa; Jaworska11ab;
27	4-Amino-2-hydroxytoluene (5-Amino-2-methylphenol)	2835-95-2	[H]C=1/C(=C(/O[H])C([H])=C(N([H])[H])C=1[H])C([H])([H])[H]	+	+	+	+	+	+	+	+	+	Natsch13aa;
28	4-Amino-3-methylphenol (4-Aminocresol) (SCCP/0898/05)	2835-99-6	[H]C=1/C(=C(/N([H])[H])C([H])=C([H])C=1O[H])C([H])([H])[H]	+	+	+	+	+	+	+	+	+	Natsch13aa; Jaworska11ab;
29	4-Carboxyphenylacetate	2345-34-8	O=C(O[H])C=1C([H])=C([H])C(OC(=O)C([H])([H])[H])=C([H])C=1[H]	+	+	+	+	-	+	+	-	+	Natsch13aa; Jaworska11ab;
30	4-Ethoxymethylene-2-phenyl-2-oxazolin-5-one (oxazolone)	15646-46-5	O=C1OC(=N/C1=C(/[H])OC([H])([H])C([H])([H])[H])C2=C([H])C([H])=C([H])C([H])=C2[H]	+	+	+	+	+	N/A	+	+	+	Takenouchi15a; Natsch13aa; Gerberick04aa; Jaworska11ab; Bauch12aa; Gerberick07a;
31	4-Nitrobenzyl bromide	100-11-8	[Br]C([H])([H])C=1C([H])=C([H])C(N(=O)O)=C([H])C=1[H]	+	+	+	+	N/A	+	N/A	+	+	Takenouchi15a; Natsch13aa; Jaworska11ab;
32	5-Chloro-2-methyl-4-isothiazolin-3-one (MCI/MI)	26172-55-4	[Cl]C=1[S]N(C(=O)C=1[H])C([H])([H])[H]	+	+	+	+	+	+	N/A	+	+	Takenouchi15a; Natsch13aa; Bauch12aa; Gerberick07a;
33	5-Methyl-2,3-hexanedione	13706-86-0	O=C(C(=O)C([H])([H])[H])C([H])([H])C([H])(C([H])([H])[H])C([H])([H])[H]	+	+	+	+	-	+	-	+	+	Natsch13aa; Gerberick04aa; Jaworska11ab; Gerberick07a;

34	Alpha-isomethylionone	127-51-5	O=C(/C(=C(\[H])[C@@]1([H])C(=C([H])C([H])([H])C([H])([H])C1(C([H])([H])[H])C([H])([H])C([H])([H])[H])C([H])([H])[H])C([H])([H])[H])C([H])([H])[H]	+	+	+	+	-	N/A	-	+	+	Hoffman18aa; Urbisch15aa;
35	Aniline	62-53-3	[H]/C1=C(\N([H])[H])C([H])=C([H])C([H])=C1[H]	+	+	-	-	+	-	+	+	+	Natsch13aa; Jaworska11ab;
36	Benzoic-acid	65-85-0	O=C(O[H])C1=C([H])C([H])=C([H])C([H])=C1[H]	+	+	+	+	-	-	+	-	-	Natsch13aa; Jaworska11ab;
37	Benzoyl peroxide	94-36-0	O=C(OOC(=O)C=1C([H])=C([H])C([H])=C([H])C=1[H])C2=C([H])C([H])=C([H])C([H])=C2[H]	+	+	+	+	+	+	N/A	+	+	Takenouchi15a; Natsch13aa; Jaworska11ab; Gerberick07a;
38	Benzyl benzoate	120-51-4	O=C(OC([H])([H])C=1C([H])=C([H])C([H])=C([H])C=1[H])C=2C([H])=C([H])C([H])=C([H])C=2[H]	+	+	+	+	-	+	-	+	+	Natsch13aa; Gerberick04aa; Jaworska11ab; Gerberick07a;
39	Benzyl bromide	100-39-0	[Br]C([H])([H])C1=C([H])C([H])=C([H])C([H])=C1[H]	+	+	+	+	+	+	-	+	+	Takenouchi15a; Natsch13aa; Jaworska11ab;
40	beta-Propiolactone	57-57-8	O=C1OC([H])([H])C1([H])[H]	+	+	+	+	+	+	N/A	+	+	Jaworska11ab;
41	Butyl acrylate	141-32-2	O=C(OC([H])([H])C([H])([H])C([H])([H])C([H])([H])[H])C([H])=C([H])[H]	+	+	+	+	+	+	+	+	+	Takenouchi15a; Natsch13aa; Jaworska11ab; Urbisch15aa;

42	Butyl glycidyl ether	2426-08-6	[H][C@]1(OC1([H])[H])C([H])([H])OC([H])([H])C([H])([H])C([H])([H])C([H])([H])[H]	+	+	+	+	+	+	+	+	-	Takenouchi15a; Natsch13aa; Jaworska11ab;
43	4-(N-Ethyl-N-2-methan-sulphonamido-ethyl)-2-methyl-1,4-phenylenediamine (CD3)	25646-71-3	O=[S](=O)(N([H])C([H])([H])C([H])([H])N(/C1=C(\[H])C(=C(N([H])[H])C([H])=C1[H])C([H])([H])[H])C([H])([H])C([H])([H])[H])C([H])([H])[H]	+	+	+	+	+	N/A	+	+	+	Takenouchi15a; Natsch13aa; Gerberick04aa; Jaworska11ab; Gerberick07a;
44	Chloramine T (Tosylchloramide sodium)	127-65-1; 149358-73-7	[Cl]N[S](=O)(=O)C=1C([H])=C([H])C(=C([H])C=1[H])C([H])([H])[H]	+	+	N/A	N/A	+	N/A	N/A	+	-	Takenouchi15a; Urbisch15aa;
45	Chlorobenzene	108-90-7	[Cl]/C1=C(\[H])C([H])=C([H])C([H])=C1[H]	+	+	+	+	-	-	-	+	-	Natsch13aa; Gerberick04aa; Jaworska11ab; Gerberick07a;
46	Chlorothalonil	1897-45-6	[Cl]/C1=C(\C#N)C([Cl])=C([Cl])C([Cl])=C1C#N	+	+	+	+	-	+	-	+	-	Takenouchi15a; Urbisch15aa;
47	Cinnamaldehyde (Cinnamic aldehyde)	104-55-2	O=C([H])C([H])=C([H])C1=C([H])C([H])=C([H])C([H])=C1[H]	+	+	+	+	+	+	+	+	+	Takenouchi15a; Natsch13aa; Gerberick04aa; Jaworska11ab; Gerberick07a;
48	cis-6-nonenal	2277-19-2	O=C([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C([H])=C([H])C([H])([H])C([H])([H])[H]	+	+	+	+	+	+	-	+	+	Natsch13aa; Jaworska11ab;

49	Citral	5392-40-5	O=C([H])C([H])=C(C([H])([H])C([H])([H])C([H])=C(C([H])([H])[H])C([H])([H])[H])C([H])([H])[H]	+	+	+	+	+	+	N/A	+	+	Natsch13aa; Gerberick04aa; Jaworska11ab; Bauch12aa;
50	Clofibrate (Ethyl (2-(4-chlorophenoxy)-2-methylpropanoate)	637-07-0	[Cl]C=1C([H])=C([H])C(OC(C(=O)OC([H])([H])C([H])([H])[H])(C([H])([H])[H])C([H])([H])[H])=C([H])C=1[H]	+	+	-	-	+	-	-	+	-	Natsch13aa; Jaworska11ab;
51	Glucose (D-Glucose)	492-62-6	[H][C@]1(O[H])[C@]([H])(O[H])[C@@]([H])(O[H])[C@@]([H])(O[C@]1([H])C([H])([H])O[H])O[H]	+	+	-	-	+	-	+	+	-	Bauch12aa;
52	Diethyl acetaldehyde	97-96-1	O=C([H])C([H])(C([H])([H])C([H])([H])C([H])([H])C([H])([H])[H])[H]	+	+	+	+	-	+	-	+	+	Takenouchi15a; Natsch13aa; Jaworska11ab;
53	Diethyl sulfate	64-67-5	O=[S](=O)(OC([H])([H])C([H])([H])[H])OC([H])([H])C([H])([H])[H]	+	+	+	+	-	+	N/A	+	+	Takenouchi15a; Jaworska11ab; Urbisch15aa;
54	Dimethyl sulfate	77-78-1	O=[S](=O)(OC([H])([H])[H])OC([H])([H])[H]	+	+	+	+	-	+	N/A	+	+	Jaworska11ab;
55	Dimethylsulfoxide	67-68-5	O[S](C([H])([H])[H])C([H])([H])[H]	+	+	-	-	-	-	-	-	+	Jaworska11ab;
56	Diphenylcyclopropenone	886-38-4	O=C1/C(=C1\C=2C([H])=C([H])C([H])=C([H])C=2[H])C=3C([H])=C([H])C([H])=C([H])C=3[H]	+	+	+	+	+	+	-	+	+	Takenouchi15a; Natsch13aa; Gerberick04aa; Jaworska11ab; Gerberick07a;

57	Ethyl benzoylacetate	94-02-0	O=C(/C1=C(\[H])C([H])=C([H])C([H])=C1[H])C([H])([H])C(=O)OC([H])([H])C([H])([H])[H]	+	+	-	-	-	-	-	-	-	Jaworska11ab; Gerberick07a;
58	Ethylenediamine	107-15-3	[H]C([H])(N([H])[H])C([H])([H])N([H])[H]	+	+	+	+	+	+	+	-	+	Natsch13aa; Jaworska11ab;
59	Ethyleneglycol dimethacrylate	97-90-5	O=C(OC([H])([H])C([H])([H])OC(=O)C(=C([H])[H])C([H])([H])[H])C(=C([H])[H])C([H])([H])[H]	+	+	+	+	+	+	+	+	+	Takenouchi15a; Natsch13aa; Gerberick04aa; Jaworska11ab; Bauch12aa; Gerberick07a;
60	Farnesal	502-67-0	O=C([H])C([H])=C(C([H])([H])C([H])([H])C([H])=C(C([H])([H])C([H])=C(C([H])([H])[H])C([H])([H])[H])C([H])([H])C([H])([H])[H]	+	+	+	+	+	+	N/A	+	+	Natsch13aa; Jaworska11ab; Bauch12aa; Gerberick07a;
61	Formaldehyde	50-00-0	O=C([H])[H]	+	+	+	+	+	+	N/A	-	-	Takenouchi15a; Natsch13aa; Jaworska11ab; Bauch12aa; Gerberick07a;
62	Fumaric acid	110-17-8	O=C(O[H])C([H])=C([H])C(=O)O[H]	+	+	+	+	-	+	-	+	+	Bauch12aa;
63	Furil	492-94-4	O=C(C=1OC([H])=C([H])C=1[H])C(=O)C=2OC([H])=C([H])C=2[H]	+	+	+	+	+	+	-	-	+	Jaworska11ab; Urbisch15aa;
64	Glyoxal	107-22-2	O=C([H])C(=O)[H]	+	+	+	+	+	-	+	+	+	Takenouchi15a; Natsch13aa; Jaworska11ab; Gerberick07a;

65	Hexadecyltrimethyl ammonium bromide	57-09-0	[H]C([H])([N+](C([H])([H])[H])(C([H])([H])[H])C([H])([H])[H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])[H]	+	+	N/A	N/A	-	N/A	-	-	-	Bauch12aa;
66	Hexyl salicylate	6259-76-3	O=C(OC([H])([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])[H])C=1C(O[H])=C([H])C([H])=C([H])C=1[H]	+	+	-	-	+	-	-	+	-	Takenouchi15a; Urbisch15aa;
67	Hydroxycitronellal	107-75-5	O=C([H])C([H])([H])[C@]([H])(C([H])([H])C([H])([H])C([H])([H])C([H])([H])C(O[H])(C([H])([H])[H])C([H])([H])[H])C([H])([H])[H]	+	+	+	+	+	+	N/A	+	+	Takenouchi15a; Natsch13aa; Gerberick04aa; Jaworska11ab; Gerberick07a;
68	Lilial (p-tert-Butyl-.alpha.-methylhydrocinnamaldehyde)	80-54-6	O=C([H])[C@@]([H])(C([H])([H])C=1C([H])=C([H])C(=C([H])C=1[H])C(C([H])([H])[H])(C([H])([H])[H])C([H])([H])[H])C([H])([H])[H])[H]	+	+	+	+	-	+	N/A	+	+	Natsch13aa; Gerberick04aa; Jaworska11ab; Gerberick07a;
69	Tartaric acid (L-tartaric acid)	87-69-4	O=C(O[H])[C@]([H])(O[H])[C@@]([H])(O[H])C(=O)O[H]	+	+	-	-	-	-	N/A	+	+	Natsch13aa; Jaworska11ab; Bauch12aa;

70	Lyral (3 and 4-(4-Hydroxy-4-methylpentyl)-3-cyclohexene-1-carboxaldehyde)	31906-04-4	O=C([H])[C@]1([H])C([H])([H])C([H])([H])C(=C([H])C1([H])[H])C([H])([H])C([H])([H])C([H])([H])C(O[H])(C([H])([H])[H])C([H])([H])[H]	+	+	+	+	+	+	-	+	+	Natsch13aa; Jaworska11ab;
71	Maleic anhydride	108-31-6	O=C1OC(=O)C([H])=C1[H]	+	+	+	+	+	+	+	+	+	Takenouchi15a; Natsch13aa; Jaworska11ab;
72	Methyl 2-nonynoate	111-80-8	O=C(OC([H])([H])[H])C#CC([H])([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])[H]	+	+	+	+	+	+	-	+	-	Takenouchi15a; Natsch13aa; Jaworska11ab; Gerberick07a;
73	Methyl methanesulfonate	66-27-3	O=[S](=O)(OC([H])([H])[H])C([H])([H])[H]	+	+	+	+	-	+	N/A	+	+	Takenouchi15a; Natsch13aa; Jaworska11ab;
74	N-Ethyl-N-nitrosourea	759-73-9	O=C(N(NO)C([H])([H])C([H])([H])[H])N([H])[H]	+	+	+	+	-	+	+	+	+	Jaworska11ab;
75	N-Methyl-P-Aminophenol Sulfate (Metol)	55-55-0	[H]/C1=C(\N([H])C([H])([H])[H])C([H])=C([H])C(O[H])=C1[H]	+	+	+	+	+	+	N/A	+	-	Natsch13aa; Jaworska11ab; Gerberick07a;
76	N,N-Diethyl-m-toluamide	134-62-3	O=C(N(C([H])([H])C([H])([H])[H])C([H])([H])C([H])([H])[H])C1=C([H])C(=C([H])C([H])=C1[H])C([H])([H])[H]	+	+	-	-	-	-	+	+	-	Urbisch15aa;

77	Palmitoyl chloride	112-67-4	[Cl]C(=O)C([H])([H])[H]	+	+	+	+	-	+	N/A	+	+	Jaworska11ab; Gerberick07a;
78	p-Aminobenzoic acid	150-13-0	O=C(O[H])C1=C([H])C([H])=C(N([H])[H])C([H])=C1[H]	+	+	+	+	-	-	+	-	-	Bauch12aa;
79	p-Benzoquinone (1,4-Benzoquinone)	106-51-4	O=C1C([H])=C([H])C(=O)C([H])=C1[H]	+	+	+	+	+	+	+	+	+	Takenouchi15a; Natsch13aa; Gerberick04aa; Jaworska11ab; Bauch12aa; Gerberick07a;
80	Perillaldehyde	2111-75-3	O=C([H])C1=C([H])C([H])([H])[C@]([H])(C(=C([H])[H])C([H])([H])[H])C([H])([H])C1([H])[H]	+	+	+	+	+	+	-	+	+	Natsch13aa; Jaworska11ab; Gerberick07a;
81	Phenylacetaldehyde	122-78-1	O=C([H])C([H])([H])C1=C([H])C([H])=C([H])C([H])=C1[H]	+	+	+	+	+	+	N/A	+	+	Takenouchi15a; Natsch13aa; Gerberick04aa; Jaworska11ab; Gerberick07a;
82	Phthalic anhydride	85-44-9	O=C1OC(=O)C2=C1C([H])=C([H])C([H])=C2[H]	+	+	+	+	+	+	+	-	+	Natsch13aa; Jaworska11ab;

83	Propyl gallate	121-79-9	O=C(OC([H])([H])C([H])([H])C([H])([H])C=1C([H])=C(O[H])C(O[H])=C(O[H])C=1[H]	+	+	+	+	+	+	+	+	+	Takenouchi15a; Natsch13aa; Jaworska11ab; Bauch12aa; Gerberick07a;
84	Propyl paraben (Propyl 4-hydroxybenzoate)	94-13-3	O=C(OC([H])([H])C([H])([H])C([H])([H])C=1C([H])=C([H])C(O[H])=C([H])C=1[H]	+	+	-	-	-	-	+	-	-	Natsch13aa; Jaworska11ab; Gerberick07a;
85	Octanoic acid	124-07-2	O=C(O[H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])[H]	+	+	-	-	-	-	-	+	-	Takenouchi15a; Natsch13aa; Jaworska11ab;
86	Squaric acid	2892-51-5	O=C1C(O[H])=C(O[H])C1=O	+	+	+	+	+	+	N/A	+	+	Natsch13aa; Gerberick04aa; Jaworska11ab; Gerberick07a;
87	Squaric acid diethyl ester	5231-87-8	O=C1C(OC([H])([H])C([H])([H])[H])=C(OC([H])([H])C([H])([H])[H])C1=O	+	+	+	+	+	N/A	N/A	+	+	Natsch13aa;
88	Sulfanilamide	63-74-1	O=[S](=O)(N([H])[H])C1=C([H])C([H])=C(N([H])[H])C([H])=C1[H]	+	+	-	-	+	-	+	-	-	Takenouchi15a; Natsch13aa; Jaworska11ab; Bauch12aa;
89	Sulphanilic acid (Sulfanic acid)	121-57-3	O=[S](=O)(O[H])C=1C([H])=C([H])C(N([H])[H])=C([H])C=1[H]	+	+	-	-	-	-	+	-	-	Takenouchi15a; Natsch13aa; Jaworska11ab; Gerberick07a;
90	Tetramethylthiuram disulfide	137-26-8	[S]=C([S][S]C(=[S])N(C([H])([H])[H])C([H])([H])[H])N(C([H])([H])[H])C([H])([H])[H]	+	+	-	-	+	-	+	+	+	Takenouchi15a; Natsch13aa; Jaworska11ab;

91	trans-2-Decenal	3913-71-1; 3913-81-4	O=C([H])C([H])=C([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])[H]	+	+	+	+	+	+	-	+	+	Natsch13aa; Jaworska11ab;
92	Undec-10-enal	112-45-8	O=C([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C([H])=C([H])[H]	+	+	+	+	+	N/A	-	+	+	Jaworska11ab; Urbisch15aa;
93	1-Bromohexane	111-25-1	[Br]C([H])([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])[H]	+	+	+	+	-	+	-	-	-	Takenouchi15a; Natsch13aa;
94	2,5-Diaminotoluene sulfate	615-50-9	[H]C=1/C(=C(/N([H])[H])C([H])=C([H])C=1N([H])[H])C([H])([H])[H]	+	+	+	+	+	+	+	+	-	Takenouchi15a; Natsch13aa; Jaworska11ab;
95	2-Aminophenol	95-55-6	[H]C=1C(N([H])[H])=C(O[H])C([H])=C([H])C=1[H]	+	+	+	+	+	+	+	+	-	Takenouchi15a; Natsch13aa; Jaworska11ab;
96	4-Hydroxybenzoic acid	99-96-7	O=C(O[H])C1=C([H])C([H])=C(O[H])C([H])=C1[H]	+	+	+	+	-	-	+	-	-	Takenouchi15a; Natsch13aa; Jaworska11ab; Bauch12aa;
97	4-Methoxyacetophenone (Acetanisole)	100-06-1	O=C(C=1C([H])=C([H])C(OC([H])([H])[H])=C([H])C=1[H])C([H])([H])[H]	+	+	-	-	-	-	-	-	-	Takenouchi15a; Natsch13aa; Jaworska11ab; Gerberick07a;
98	6-Methyl coumarin	92-48-8	O=C2OC=1/C(=C(/[H])C(=C([H])C=1[H])C([H])([H])[H])C([H])=C2[H]	+	+	+	+	-	+	-	-	-	Takenouchi15a; Natsch13aa; Gerberick04aa; Jaworska11ab; Gerberick07a;

99	alpha-Methyl cinnamaldehyde (α-methyl-trans-cinnamaldehyde)	101-39-3	O=C([H])C(=C([H])C=1C([H])=C([H])C([H])=C([H])C=1[H])C([H])([H])[H]	+	+	+	+	-	N/A	N/A	+	+	Takenouchi15a; Natsch13aa; Jaworska11ab;
100	Benzylidene acetone (4-phenyl-3-buten-2-one)	122-57-6	O=C(C([H])=C([H])C1=C([H])C([H])=C([H])C([H])=C1[H])C([H])([H])[H]	+	+	+	+	+	+	-	+	+	Takenouchi15a; Natsch13aa; Jaworska11ab; Bauch12aa; Gerberick07a;
101	Cyclamen aldehyde	103-95-7	O=C([H])[C@@]([H])(C([H])([H])C1=C([H])C([H])=C(C([H])=C1[H])C([H])(C([H])([H])[H])C([H])([H])[H])C([H])([H])[H]	+	+	+	+	-	N/A	-	+	+	Takenouchi15a; Natsch13aa; Jaworska11ab; Gerberick07a;
102	Diethyl maleate	141-05-9	O=C(OC([H])([H])C([H])([H])[H])C([H])=C([H])C(=O)OC([H])([H])C([H])([H])[H]	+	+	+	+	+	+	+	+	-	Takenouchi15a; Natsch13aa; Gerberick04aa; Jaworska11ab; Bauch12aa; Gerberick07a;
103	DL-lactic acid (Lactic acid)	50-21-5	O=C(O[H])[C@]([H])(O[H])C([H])([H])[H]	+	+	-	-	-	-	-	-	+	Takenouchi15a; Natsch13aa; Jaworska11ab; Bauch12aa;
104	Ethyl acrylate	140-88-5	O=C(OC([H])([H])C([H])([H])[H])C([H])=C([H])[H]	+	+	+	+	+	+	+	+	+	Natsch13aa; Jaworska11ab; Gerberick07a; Urbisch15aa;
105	Ethyl vanillin	121-32-4	O=C([H])C=1C([H])=C(OC([H])([H])C([H])([H])[H])C(O[H])=C([H])C=1[H]	+	+	+	+	-	+	N/A	-	+	Natsch13aa; Jaworska11ab; Gerberick07a;

106	Isoeugenol	97-54-1	[H]C=1/C(=C(/[H])C([H])=C(O[H])C=1OC([H])([H])[H])C([H])=C([H])C([H])([H])[H]	+	+	+	+	+	+	+	+	+	Takenouchi15a; Natsch13aa; Jaworska11ab; Bauch12aa;
107	Linalool	78-70-6	[H]C([H])([C@@](O[H])(C([H])=C([H])[H])C([H])([H])[H])C([H])([H])C([H])=C(C([H])([H])[H])C([H])([H])[H]	+	+	+	+	+	-	-	+	+	Takenouchi15a; Natsch13aa;
108	Methyl acrylate	96-33-3	O=C(OC([H])([H])[H])C([H])=C([H])[H]	+	+	+	+	+	+	N/A	+	+	Natsch13aa; Jaworska11ab; Urbisch15aa;
109	Methyl methacrylate	(80-62-6)	O=C(OC([H])([H])[H])C(=C([H])[H])C([H])([H])[H]	+	+	-	-	+	+	+	+	+	Bauch12aa;
110	1,2-cyclohexanedicarboxylic anhydride	85-42-7	O=C1OC(=O)[C@]2([H])[C@]1([H])C([H])([H])C([H])([H])C([H])([H])C2([H])[H]	+	+	+	+	+	+	+	-	+	Natsch13aa; Jaworska11ab;
111	N-Methyl-N-nitrosourea	684-93-5	O=C(N(NO)C([H])([H])[H])N([H])[H]	+	+	+	+	+	N/A	+	+	+	Jaworska11ab;
112	Glutaraldehyde	111-30-8	O=C([H])C([H])([H])C([H])([H])C([H])([H])C(=O)[H]	+	+	+	+	+	+	N/A	+	+	Takenouchi15a; Natsch13aa; Gerberick04aa; Jaworska11ab; Gerberick07a;
113	Phenyl benzoate	93-99-2	O=C(OC=1C([H])=C([H])C([H])=C([H])C=1[H])C=2C([H])=C([H])C([H])=C([H])C=2[H]	+	+	+	+	+	+	-	+	+	Takenouchi15a; Bauch12aa; Hoffman18aa;
114	trans-2-Hexenal	6728-26-4	O=C([H])C([H])=C([H])C([H])([H])C([H])([H])C([H])([H])[H]	+	+	+	+	+	+	-	+	+	Natsch13aa; Jaworska11ab; Gerberick07a;

115	2,4,6-Trinitrobenzenesulfonic acid	2508-19-2	O=[S](=O)(O[H])C=1C(N(=O)O)=C([H])C(N(=O)O)=C([H])C=1N(=O)O	+	+	+	+	N/A	N/A	N/A	+	+	Bauch12aa;
116	Fluorescein-5-isothiocyanate	3326-32-7	[S]=C=NC=1C([H])=C2/C(=C(/[H])C=1[H])[C@]3(OC2=O)C5=C(OC4=C3C([H])=C([H])C(O[H])=C4[H])C([H])=C(O[H])C([H])=C5[H]	+	+	+	+	+	-	N/A	+	+	Natsch13aa; Jaworska11ab; Gerberick07a;
117	Imidazolidinyl urea	39236-46-9	O=C1N([H])C(=O)N([C@@]1([H])N([H])C(=O)N([H])C([H])([H])N([H])C(=O)N([H])[C@]2([H])N(C(=O)N([H])C2=O)C([H])([H])O[H])C([H])([H])O[H]	+	+	+	+	+	+	+	+	+	Takenouchi15a; Jaworska11ab; Bauch12aa; Gerberick07a;
118	Bandrowski’s Base (1,4-Cyclohexadiene-1,4-diamine)	20048-27-6	[H]C=3C(N/C1=C(\[H])C([H])=C(N([H])[H])C([H])=C1[H])=C(N([H])[H])C([H])=C(N/C2=C(\[H])C([H])=C(N([H])[H])C([H])=C2[H])C=3N([H])[H]	+	+	+	+	+	N/A	N/A	+	+	Takenouchi15a; Natsch13aa; Jaworska11ab; Gerberick07a;

119	Bisphenol A-diglycidyl ether	1675-54-3	[H][C@@]1(OC1([H])[H])C([H])([H])O/C2=C(\[H])C([H])=C(C([H])=C2[H])C(C=4C([H])=C([H])C(OC([H])([H])[C@]3([H])OC3([H])[H])=C([H])C=4[H])(C([H])([H])[H])C([H])([H])[H]	+	+	+	+	+	+	+	+	+	Takenouchi15a; Natsch13aa; Jaworska11ab;
120	Lauryl gallate	1166-52-5	O=C(OC([H])([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C1=C([H])C(O[H])=C(O[H])C(O[H])=C1[H]	+	+	-	-	+	+	+	+	+	Takenouchi15a; Natsch13aa; Gerberick04aa; Jaworska11ab; Gerberick07a;
121	Abietic acid	514-10-3	O=C(O[H])[C@]3([C@@]1([H])[C@@]([C@]2([H])C(=C([H])C1([H])[H])C([H])=C(C([H])([H])C2([H])[H])C([H])(C([H])([H])[H])C([H])([H])[H])(C([H])([H])C([H])([H])C3([H])[H])C([H])([H])[H])C([H])([H])[H]	+	+	+	+	+	-	-	+	-	Takenouchi15a; Natsch13aa; Jaworska11ab;

122	Butylbenzylphthalate	85-68-7	O=C(OC([H])([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])[H])C=1/C(=C(/[H])C([H])=C([H])C=1[H])C(=O)OC([H])([H])C2=C([H])C([H])=C([H])C([H])=C2[H]	+	+	-	-	-	+	-	+	+	Urbisch15aa;

[†]T, t, and o stand for the traning set, test set and outlier set, respectively.

[‡]N/A: not available

*defined based on 2 thresholds suggesting by OECD; +: sensitizer; -: non sensitizer

A: QSAR Toolbox (automated option); B: QSAR Toolbox (standardized option); C: VEGAHUB (CAESAR 2.1.6); D: VEGAHUB (IRFMN/JRC 1.0.0)

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Takenouchi15a Takenouchi, O., et al., *Test battery with the human cell line activation test, direct peptide reactivity assay and DEREK based on a 139 chemical data set for predicting skin sensitizing potential and potency of chemicals.* J. Appl. Toxicol., 2015. **35**(11): p. 1318-1332

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Gerberick04aa Gerberick, G.F., et al., *Development of a peptide reactivity assay for screening contact allergens.* Toxicol. Sci., 2004. **81**(2): p. 332-343

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Table S2. Optimal runtime parameters for the SVR models.

Parameter	SVR A	SVR B	SVR C	HSVR
SVM type	ε-SVR	ε-SVR	ε-SVR	ε-SVR
Kernal type	Radial basis function	Radial basis function	Radial basis function	Radial basis function
γ	0.175582990397805	0.222222222222222	0.225254058837891	0.25
Cost	9.48148148148148	115.330078125	76.88671875	0.32
ε	0.11865234375	0.5625	0.333333333333333	0.0125

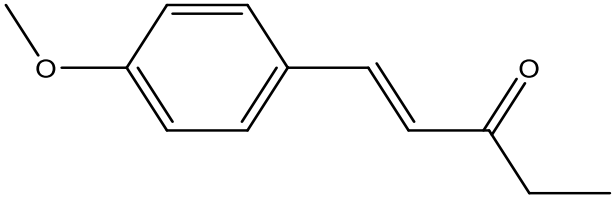
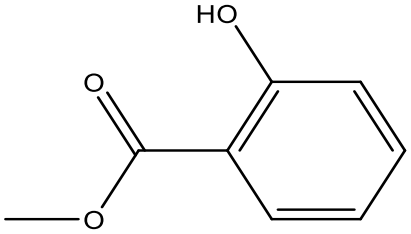
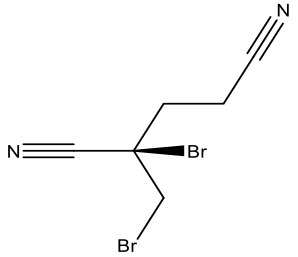
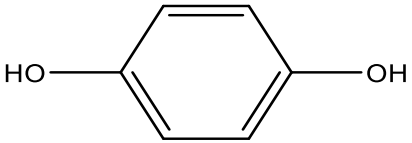
Table S3. Confusion matrix for the qualitative predictive model

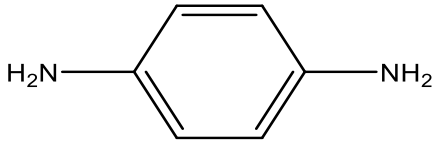
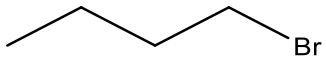
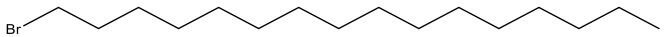
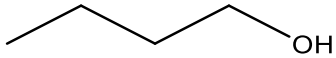
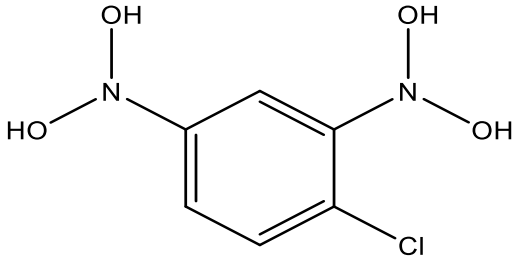
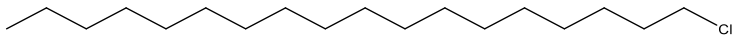
		Observed	
		+	−
Predicted	+	true positive (TP)	false positive (FP)
	−	false negative (FN)	true negative (TN)

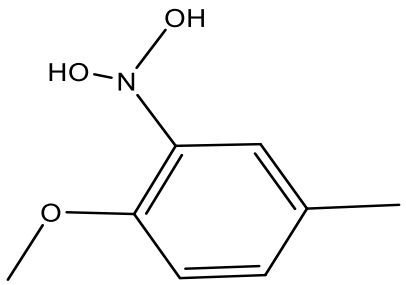
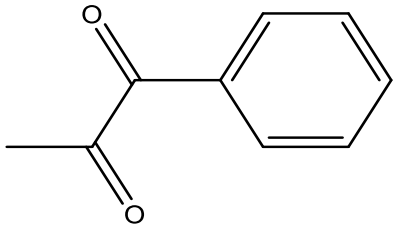
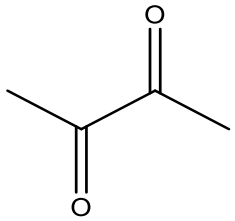
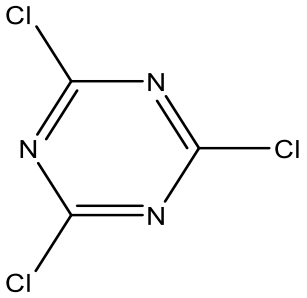
Table S4. The Cooper statistics and Kubat's G-mean calculated from the confusion matrix

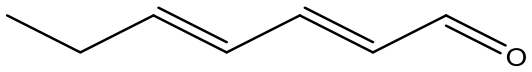
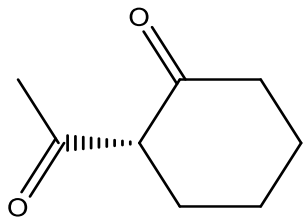
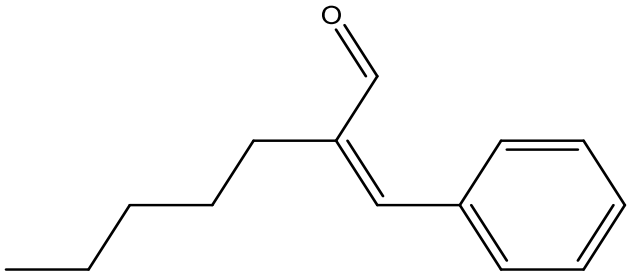
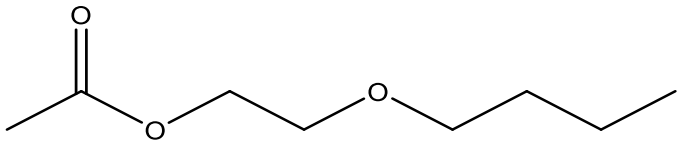
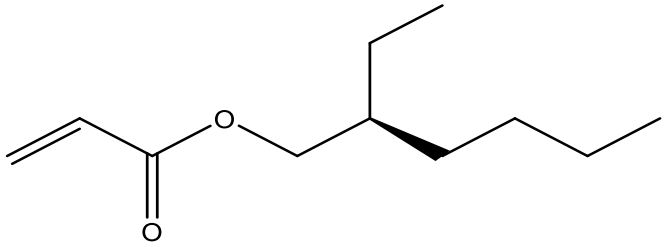
Parameter	Definition
Sensitivity (Se)	TP / (TP + FN)
Specificity (Sp)	TN / (FP +TN)
Accuracy (Acc)	(TP + TN) / (TP + TN + FP + FN)
Positive predictivity (PP)	TP / (TP + FP)
Negative predictivity (NP)	TN / (TN + FN)
Matthews Correlation Coefficient (MCC)	$\frac{\mathrm{TP}\times\mathrm{TN}-\mathrm{FP}\times\mathrm{FN}}{\sqrt{(\mathrm{TP}+\mathrm{FP})\times(\mathrm{TP}+\mathrm{FN})\times(\mathrm{TN}+\mathrm{FP})\times(\mathrm{TN}+\mathrm{FN})}}$
Geometric mean (*g*- mean)	(Sensitivity × Specificity)^{½}
Harmonic mean of sensitivity and positive predictivity (*F-measure*)	$F-measure=\frac{2}{PP^{-1}+Se^{-1}}$
Cohen's kappa	κ = (Accuracy – p_e) / (1 – p_e) $p_{\mathrm{True}}=\frac{\mathrm{TP}+\mathrm{FN}}{\mathrm{TP}+\mathrm{TN}+\mathrm{FP}+\mathrm{FN}}\cdot\frac{\mathrm{TP}+\mathrm{FP}}{\mathrm{TP}+\mathrm{TN}+\mathrm{FP}+\mathrm{FN}}$ $p_{\mathrm{False}}=\frac{\mathrm{TN}+\mathrm{FN}}{\mathrm{TP}+\mathrm{TN}+\mathrm{FP}+\mathrm{FN}}\cdot\frac{\mathrm{TN}+\mathrm{FP}}{\mathrm{TP}+\mathrm{TN}+\mathrm{FP}+\mathrm{FN}}$
The proportion of chance agreement	$p_e = p_{\mathrm{True}} + p_{\mathrm{False}}$

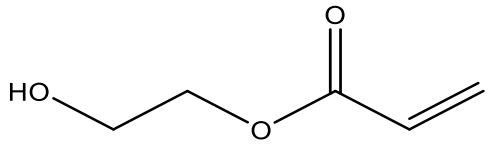
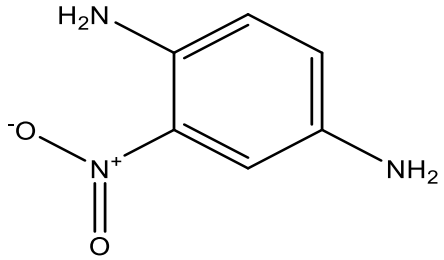
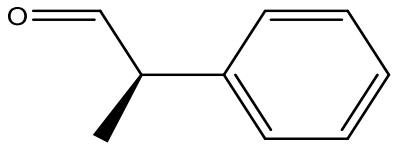
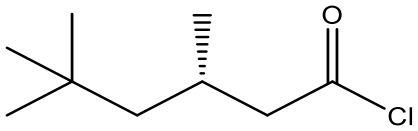
Table S5. Compound source for this study, their names, Pubchem SID/CID, CAS numbers, , SMILES strings, chemical structures and descriptor values

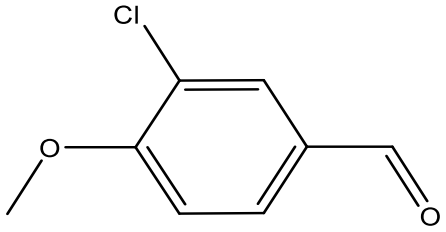
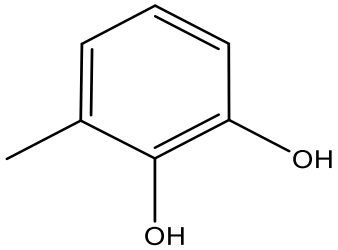
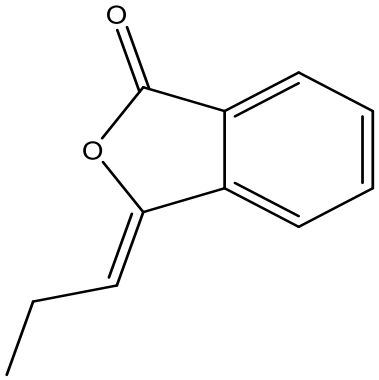
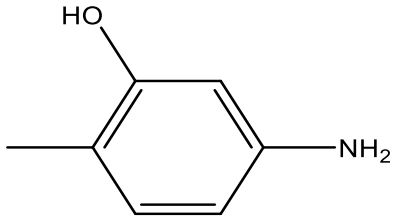
No.	Compounds	Structures	ω	E_{HOMO}	E_{LUMO}	μ	σ	SA	Jurs_DPSA_1	n_{Ar}	HBA	HBD	Jurs_FPSA_3	$\lvert\mu\rvert_{max}$
1	1-(p-Methoxyphenyl)-1-penten-3-one		0.13	-0.22	-0.07	-0.14	13.37	204.9	174.7	1	2	0	0.03	0.18
2	Methyl salicylate		0.1	-0.23	-0.05	-0.14	10.66	154.8	108.58	1	3	1	0.06	0.37
3	1,2-Dibromo-2,4-dicyanobutane (Methyldibromo glutaronitrile)		0.15	-0.3	-0.07	-0.18	8.93	205.7	-107.1	0	2	0	0.01	0.17
4	1,4-Dihydroquinone (1,4-Dihydroxybenzene) (Hydroquinone)		0.06	-0.2	-0.01	-0.11	10.17	110.6	36.9	1	2	2	0.06	0

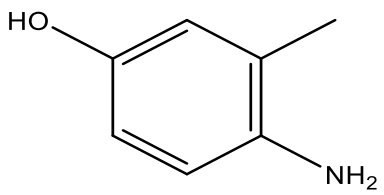
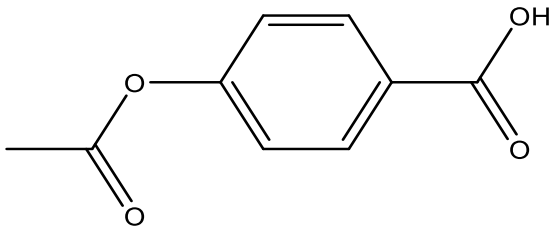
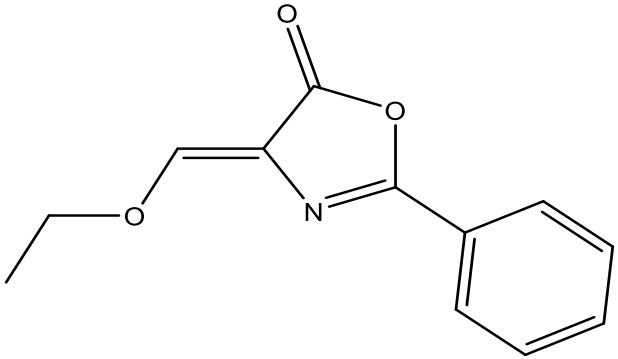
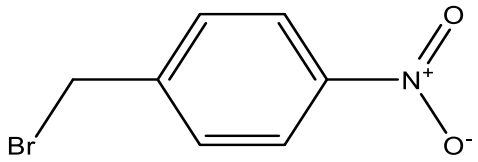
5	1, 4-Phenylenediamine		0.04	-0.18	0	-0.09	11.11	120.6	116.02	1	2	2	0.06	0
6	1-Bromobutane		0.07	-0.28	0	-0.14	7.29	114.4	104.53	0	0	0	0.02	0.47
7	1-Bromohexadecane		0.07	-0.27	0	-0.14	7.32	306	474.64	0	0	0	0.02	0.44
8	1-Butanol		0.02	-0.26	0.09	-0.09	5.68	96.72	185.46	0	1	1	0.05	0.67
9	1-Chloro-2,4-dinitrobenzene		0.08	-0.23	-0.03	-0.13	9.9	180.9	-57.65	1	6	4	0.07	0.69
10	1-Chlorooctadecane		0.06	-0.28	0.02	-0.13	6.61	327.9	553.17	0	0	0	0.02	0.3

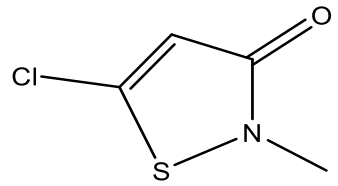
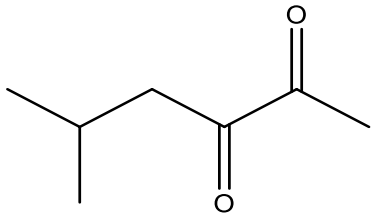
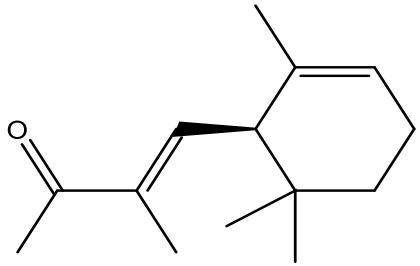
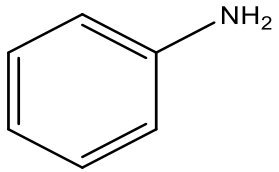
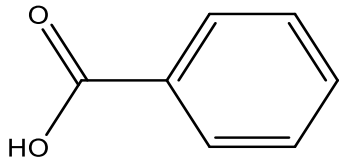
11	1-methoxy-4-methyl-2-nitrobenzene		0.06	-0.21	-0.01	-0.11	9.85	172.8	140.36	1	4	2	0.06	0.48
12	1-Phenyl-1,2-propanedione		0.18	-0.24	-0.09	-0.17	12.77	153.5	75.67	1	2	0	0.03	0.82
13	2,3-Butanedione		0.17	-0.25	-0.09	-0.17	12.56	103.5	98.91	0	2	0	0.03	0
14	2,4,6-Trichloro-1,3,5-triazine (cyanuric chloride)		0.17	-0.32	-0.08	-0.2	8.53	155.9	-248.4	1	3	0	0.02	0

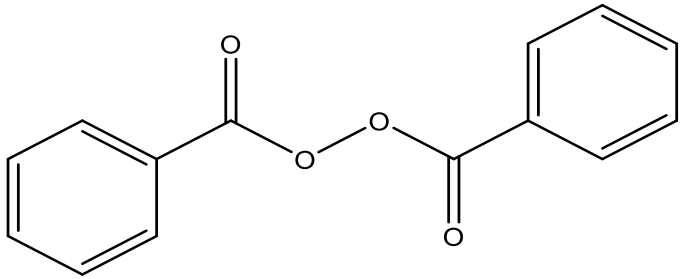
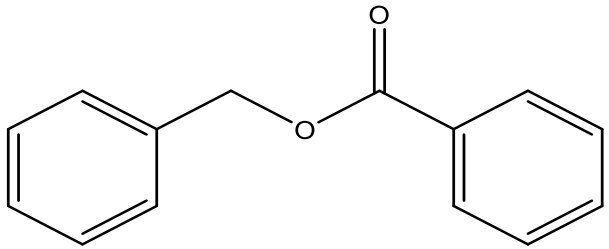
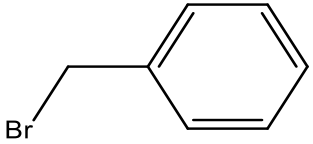
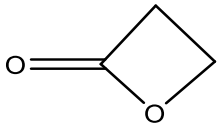
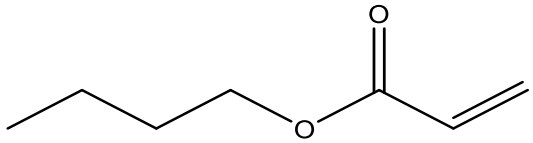
15	2,4-Heptadienal		0.15	-0.24	-0.07	-0.16	12.12	131.4	119.75	0	1	0	0.04	0.38
16	2-Acetylcyclohexanone		0.09	-0.25	-0.03	-0.14	9.15	148.2	165.63	0	2	0	0.02	0.89
17	2-Benzylidenehept anal (Amyl cinnamic aldehyde)		0.14	-0.23	-0.07	-0.15	12.25	220.8	226.55	1	1	0	0.03	0.51
18	Ethanol-2-butoxy-, acetate (2-Butoxyethyl Acetate)		0.06	-0.26	0.01	-0.13	7.48	185.3	291.91	0	3	0	0.04	1.42
19	2-Ethylhexyl acrylate		0.12	-0.28	-0.05	-0.16	8.65	214.4	302.52	0	2	0	0.03	0.31

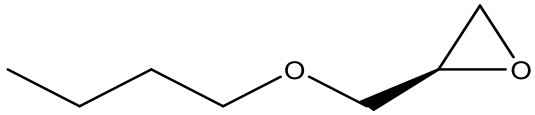
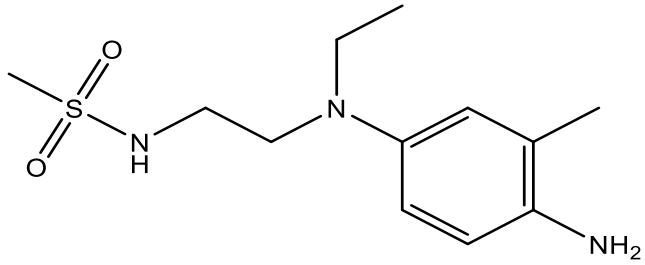
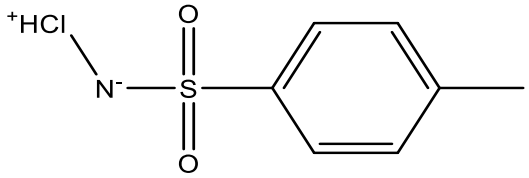
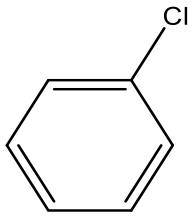
20	2-Hydroxyethyl acrylate		0.12	-0.28	-0.05	-0.16	8.85	128.9	112.8	0	3	1	0.06	1.51
21	2-Nitro-1,4-phenylenediamine		0.18	-0.19	-0.08	-0.14	18.41	158.6	41.12	1	4	4	0.06	0.28
22	2-Phenylpropionaldehyde		0.09	-0.25	-0.03	-0.14	9.39	143.3	116.39	1	1	0	0.04	0.32
23	3,5,5-Trimethylhexanoyl chloride		0.11	-0.3	-0.04	-0.17	7.87	206.4	133.67	0	1	0	0.02	0.67

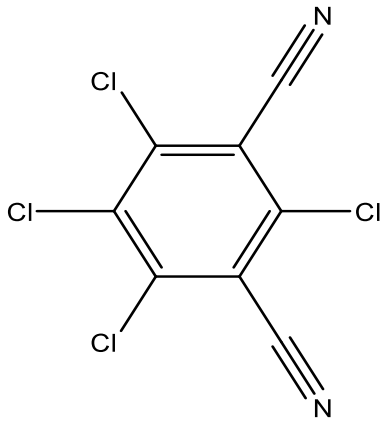
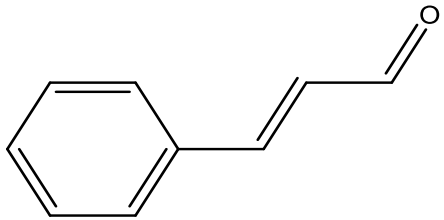
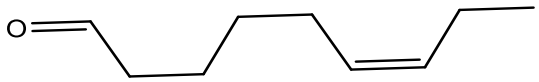
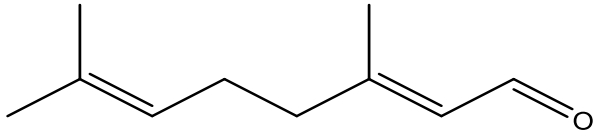
24	3-Chloro-4-methoxybenzaldehyde (3-Chloro-p-anisaldehyde)		0.13	-0.24	-0.06	-0.15	11.45	165.2	33.47	1	2	0	0.04	0.62
25	3-Methylcatechol		0.05	-0.21	0.01	-0.1	9.35	129.9	81.49	1	2	2	0.05	0.45
26	3-Propylidenephthalide		0.13	-0.23	-0.07	-0.15	11.97	168.4	120.09	1	2	0	0.04	1.82
27	4-Amino-2-hydroxytoluene (5-Amino-2-methylphenol)		0.04	-0.19	0.01	-0.09	9.74	135	124.86	1	2	2	0.06	0.59

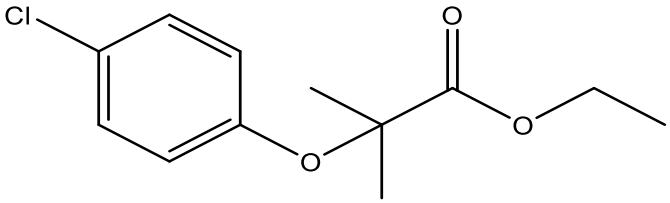
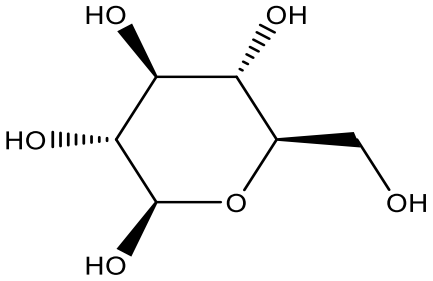
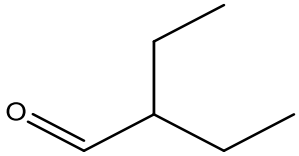
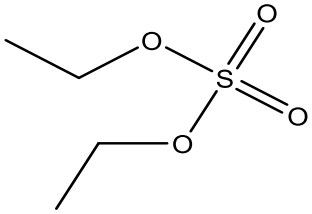
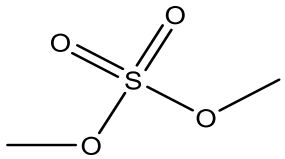
28	4-Amino-3-methylphenol (4-Aminocresol) (SCCP/0898/05)		0.05	-0.19	0	-0.09	10.54	135	106.31	1	2	2	0.06	0.44
29	4-Carboxyphenylacetate		0.12	-0.26	-0.05	-0.16	9.82	177.7	60.03	1	4	1	0.05	0.77
30	4-Ethoxymethylene-2-phenyl-2-oxazolin-5-one (oxazolone)		0.15	-0.22	-0.07	-0.15	13.53	210	141.24	1	4	0	0.04	0.29
31	4-Nitrobenzyl bromide		0.2	-0.27	-0.1	-0.19	11.75	170.9	-84.23	1	2	2	0.03	0.23

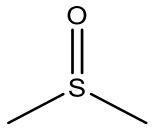
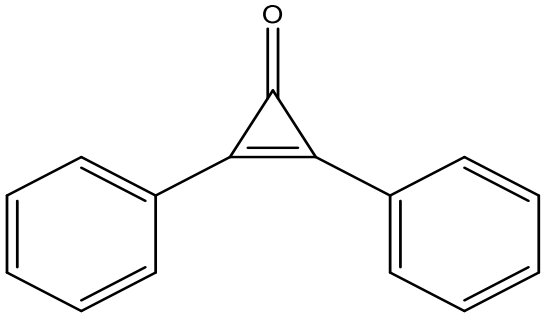
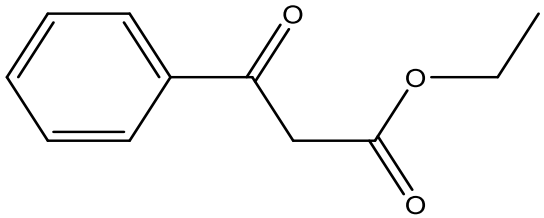
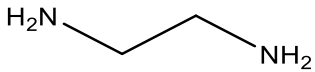
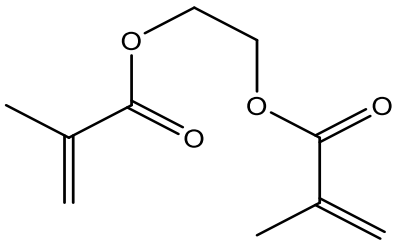
32	5-Chloro-2-methyl-4-isothiazolin-3-one (MCI/MI)		0.1	-0.23	-0.04	-0.14	10.71	134.2	-26.72	0	2	0	0.03	1.43
33	5-Methyl-2,3-hexanedione		0.17	-0.24	-0.09	-0.16	12.66	153	185.24	0	2	0	0.03	0.04
34	Alpha-isomethylionone		0.11	-0.23	-0.05	-0.14	10.96	243.5	281.52	0	1	0	0.03	0.38
35	Aniline		0.05	-0.2	0	-0.1	9.75	102.3	98.79	1	1	1	0.05	0
36	Benzoic-acid		0.12	-0.26	-0.05	-0.16	9.5	122.3	27.63	1	2	1	0.06	0.69

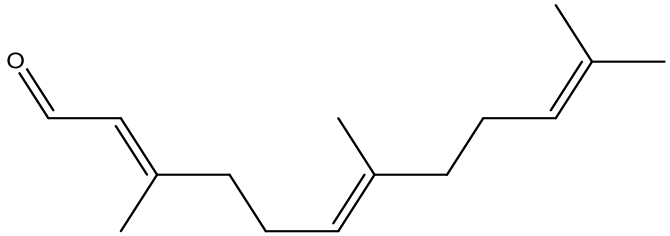
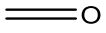
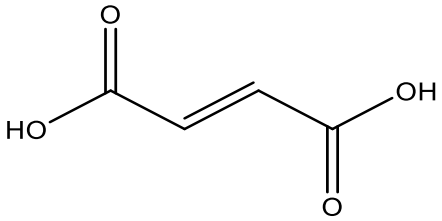
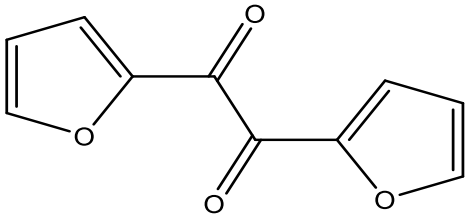
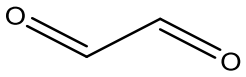
37	Benzoyl peroxide		0.14	-0.27	-0.06	-0.17	9.9	223.6	48.43	2	4	0	0.04	0
38	Benzyl benzoate		0.11	-0.25	-0.05	-0.15	9.8	207.3	119.49	2	2	0	0.04	1.02
39	Benzyl bromide		0.1	-0.25	-0.04	-0.15	9.59	133	23.45	1	0	0	0.03	0.21
40	beta-Propiolactone		0.07	-0.29	0	-0.14	6.91	69.9	46.79	0	2	0	0.04	0.05
41	Butyl acrylate		0.12	-0.28	-0.05	-0.16	8.65	148.9	202.8	0	2	0	0.03	0.79

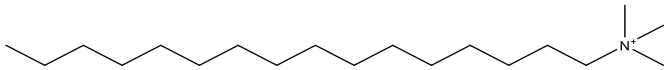
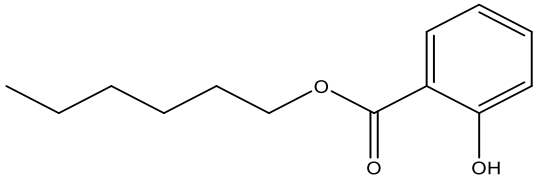
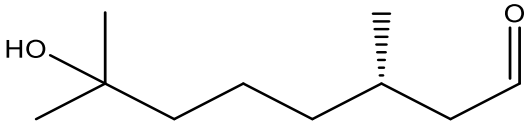
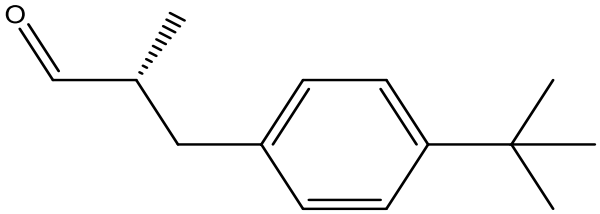
42	Butyl glycidyl ether		0.02	-0.26	0.08	-0.09	5.9	145.3	254.92	0	2	0	0.04	0.79
43	4-(N-Ethyl-N-2-methan-sulphonamido-ethyl)-2-methyl-1,4-phenylenediamine (CD3)		0.04	-0.18	0	-0.09	10.85	280.8	220.08	1	4	2	0.03	1.25
44	Chloramine T (Tosylchloramide sodium)		0.08	-0.19	-0.03	-0.11	12.53	181.4	-73.51	1	2	1	0.02	0.43
45	Chlorobenzene		0.07	-0.25	-0.01	-0.13	8.47	107	-15.92	1	0	0	0.03	0

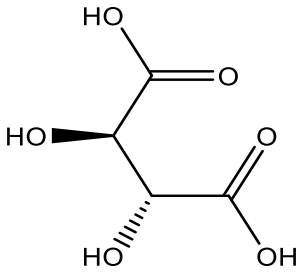
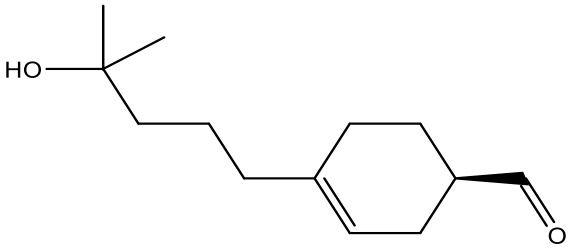
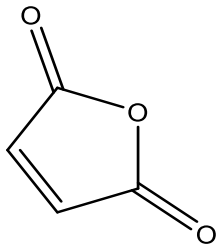
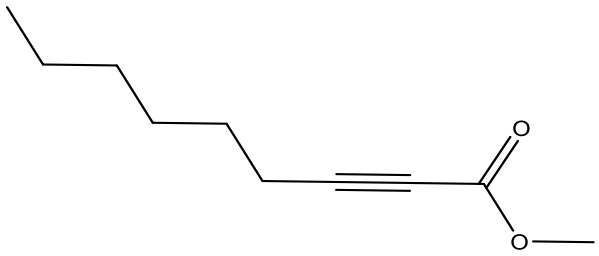
46	Chlorothalonil		0.2	-0.28	-0.1	-0.19	11.19	235.3	-268.5	1	2	0	0.01	1.28
47	Cinnamaldehyde (Cinnamic aldehyde)		0.16	-0.24	-0.08	-0.16	12.4	137.6	35.55	1	1	0	0.04	0
48	cis-6-nonenal		0.08	-0.24	-0.03	-0.13	9.39	167.4	242.52	0	1	0	0.03	0.14
49	Citral		0.12	-0.23	-0.06	-0.14	11.4	186.6	199.8	0	1	0	0.03	1.95

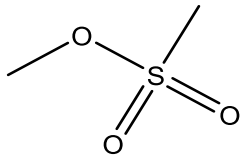
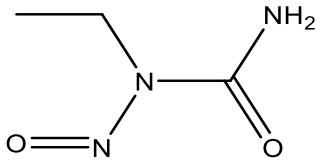
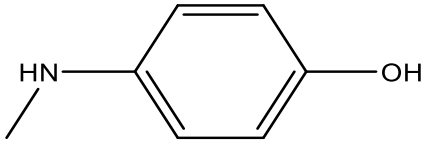
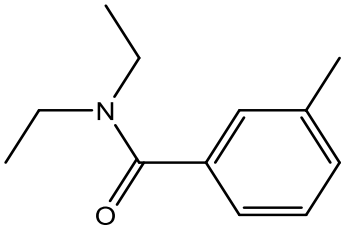
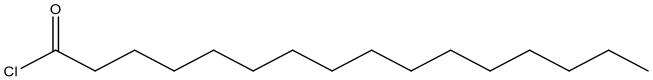
50	Clofibrate (Ethyl (2-(4-chlorophenoxy)-2-methylpropanoate)		0.07	-0.23	-0.02	-0.12	9.59	245.6	144.19	1	3	0	0.03	1.77
51	Glucose (D-Glucose)		0.03	-0.26	0.06	-0.1	6.17	174.5	86.1	0	6	5	0.09	1.55
52	Diethyl acetaldehyde		0.08	-0.25	-0.02	-0.14	8.65	124.9	174.28	0	1	0	0.03	1.22
53	Diethyl sulfate		0.06	-0.3	0.03	-0.14	6.06	151.1	122.43	0	4	0	0.02	0.88
54	Dimethyl sulfate		0.06	-0.31	0.02	-0.14	6.09	120.5	9.91	0	4	0	0.03	0

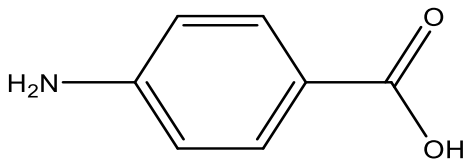
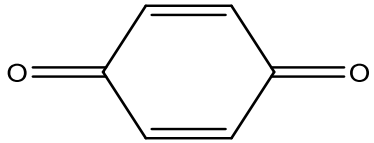
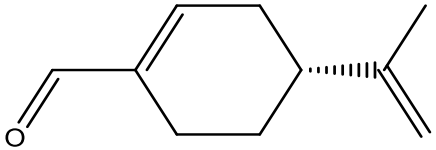
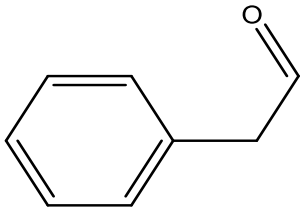
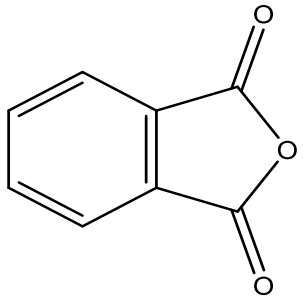
55	Dimethylsulfoxide		0.03	-0.23	0.04	-0.09	7.32	76.71	98.58	0	1	2	0.07	0.09
56	Diphenylcyclopropenone		0.15	-0.23	-0.07	-0.15	12.84	191.8	48.29	2	1	0	0.04	2.29
57	Ethyl benzoylacetate		0.14	-0.26	-0.07	-0.16	10.15	198.2	135.12	1	3	0	0.04	1.06
58	Ethylenediamine		0.02	-0.24	0.09	-0.07	6.2	86.57	165.13	0	2	2	0.07	0
59	Ethyleneglycol dimethacrylate		0.11	-0.27	-0.05	-0.16	9.03	219.9	183.97	0	4	0	0.04	1.31

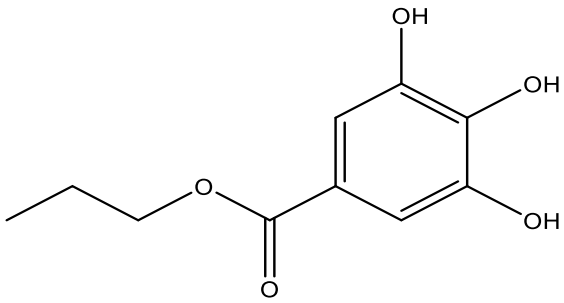
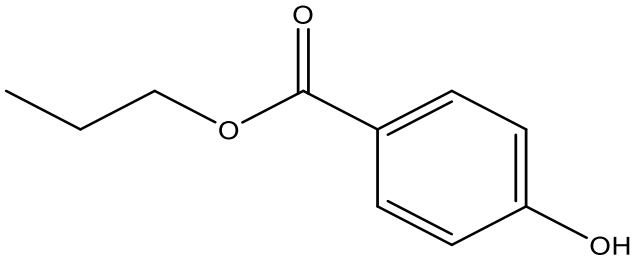
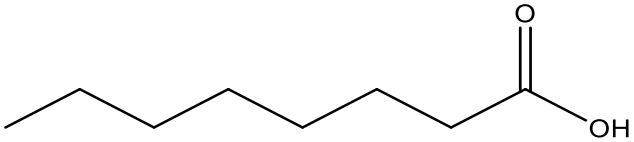
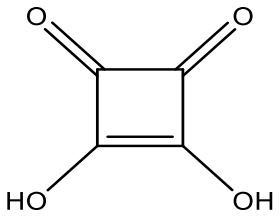
60	Farnesal		0.12	-0.22	-0.06	-0.14	11.87	266.2	298.88	0	1	0	0.03	1.63
61	Formaldehyde		0.1	-0.27	-0.04	-0.15	8.82	42.32	30.36	0	1	0	0.06	0.9
62	Fumaric acid		0.18	-0.29	-0.09	-0.19	10	119.3	-14.82	0	4	2	0.07	0
63	Furil		0.19	-0.24	-0.09	-0.17	13.18	180.1	62.42	2	2	0	0.05	0.51
64	Glyoxal		0.22	-0.26	-0.11	-0.19	12.8	65.87	-15.17	0	2	0	0.06	0

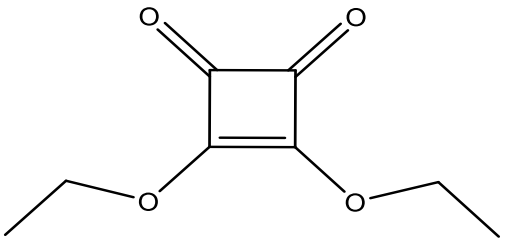
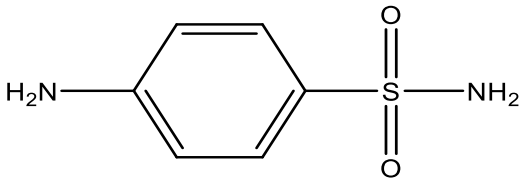
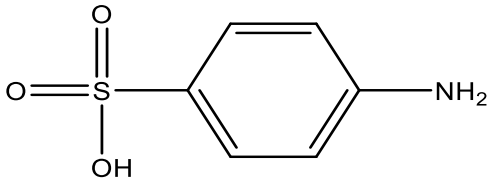
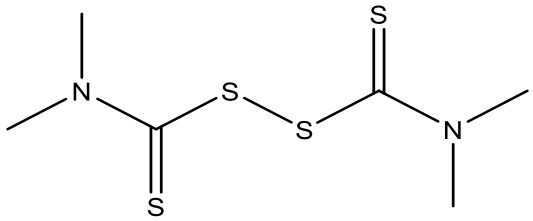
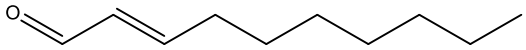
65	Hexadecyltrimethylammonium bromide		0.05	-0.29	0.03	-0.13	6.26	354.3	651.08	0	0	1	0.03	0.35
66	Hexyl salicylate		0.1	-0.23	-0.05	-0.14	10.65	234	264.45	1	3	1	0.04	0.6
67	Hydroxycitronellal		0.09	-0.25	-0.03	-0.14	8.78	208	242.39	0	2	1	0.04	0.11
68	Lilial (p-tert-Butyl-.alpha.-methylhydrocinnamaldehyde)		0.08	-0.23	-0.03	-0.13	9.71	235.8	248.24	1	1	0	0.03	1.3

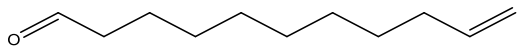
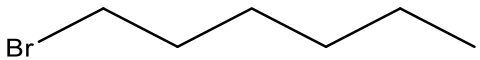
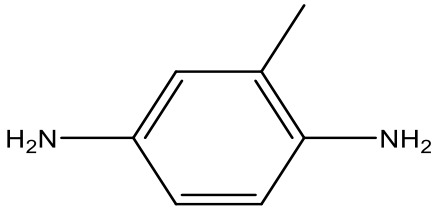
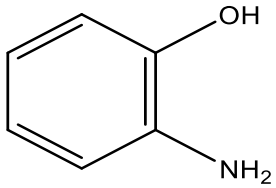
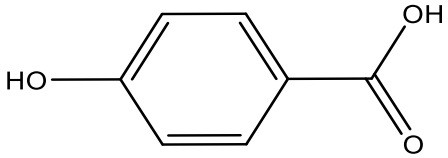
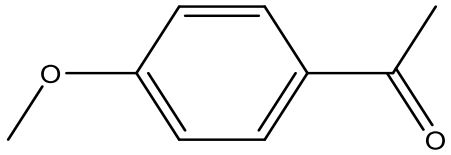
69	Tartaric acid (L-tartaric acid)		0.08	-0.27	-0.02	-0.14	7.89	149.3	-46.82	0	6	4	0.08	0.81
70	Lyral (3 and 4-(4-Hydroxy-4-methylpentyl)-3-cyclohexene-1-carboxaldehyde)		0.08	-0.23	-0.03	-0.13	9.78	234.5	289.8	0	2	1	0.04	0.33
71	Maleic anhydride		0.22	-0.3	-0.11	-0.21	10.61	88.98	-27.05	0	3	0	0.04	1.97
72	Methyl 2-nonynoate		0.1	-0.27	-0.04	-0.16	8.69	195.8	280.3	0	2	0	0.03	1.1

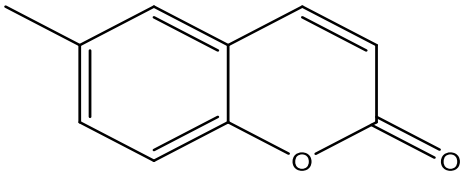
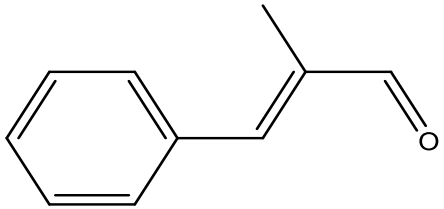
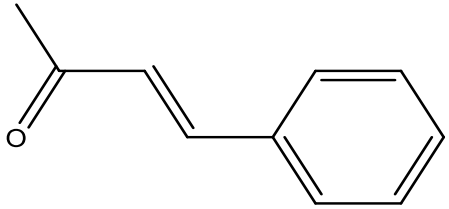
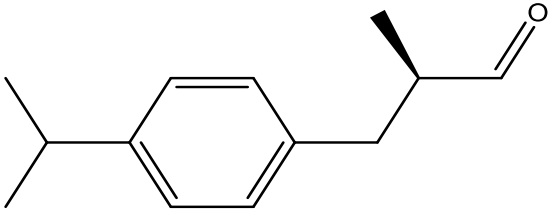
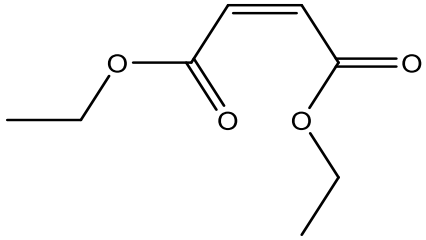
73	Methyl methanesulfonate		0.05	-0.3	0.04	-0.13	5.89	108.2	27.73	0	3	0	0.02	1.45
74	N-Ethyl-N-nitrosourea		0.14	-0.25	-0.07	-0.16	11.22	133	27.47	0	3	3	0.04	1.56
75	N-Methyl-P-Aminophenol Sulfate (Metol)		0.05	-0.18	0	-0.09	11	131	104.84	1	2	2	0.05	0.82
76	N,N-Diethyl-m-toluamide		0.08	-0.24	-0.02	-0.13	9.19	215.9	244.22	1	1	0	0.03	1.61
77	Palmitoyl chloride		0.11	-0.28	-0.04	-0.16	8.15	305.5	412.19	0	1	0	0.02	1.45

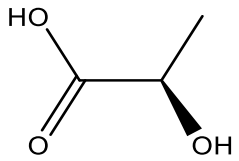
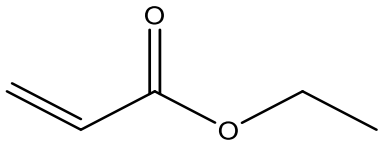
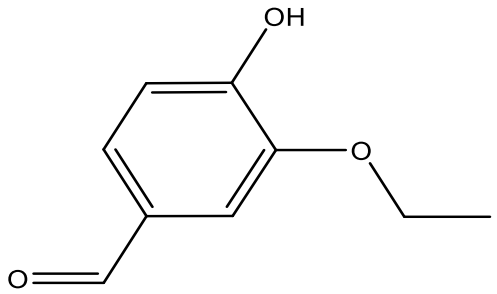
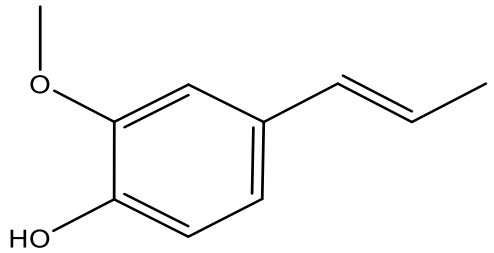
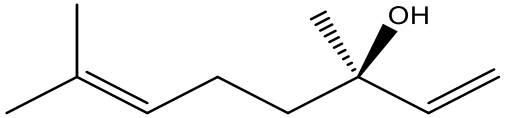
78	p-Aminobenzoic acid		0.09	-0.21	-0.04	-0.12	11.28	140.7	50.05	1	3	2	0.07	1.92
79	p-Benzoquinone (1,4-Benzoquinone)		0.28	-0.27	-0.13	-0.2	14.04	106.1	-31.24	0	2	0	0.04	0
80	Perillaldehyde		0.12	-0.25	-0.05	-0.15	10.4	165.3	179.65	0	1	0	0.04	1.38
81	Phenylacetaldehyde		0.09	-0.24	-0.03	-0.14	9.55	125.9	78.67	1	1	0	0.04	0.06
82	Phthalic anhydride		0.19	-0.28	-0.09	-0.19	10.54	130.3	-39.92	1	3	0	0.04	2.28

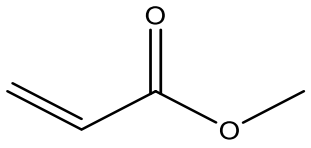
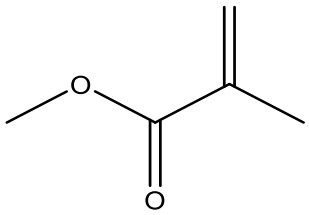
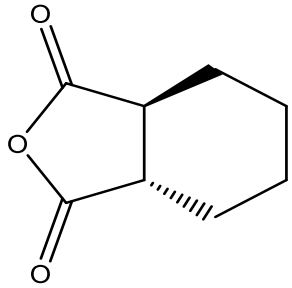
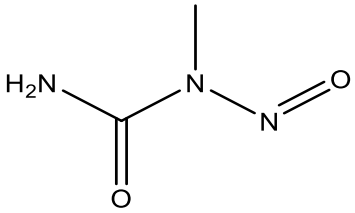
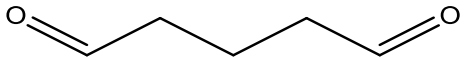
83	Propyl gallate		0.09	-0.22	-0.04	-0.13	11.32	212.7	123.36	1	5	3	0.06	0.01
84	Propyl paraben (Propyl 4-hydroxybenzoate)		0.1	-0.23	-0.04	-0.14	10.27	186.1	144.12	1	3	1	0.05	0.32
85	Octanoic acid		0.06	-0.28	0.01	-0.13	6.95	168	231.09	0	2	1	0.04	0.72
86	Squaric acid		0.11	-0.24	-0.05	-0.15	10.35	104.6	-78.41	0	4	2	0.07	1.82

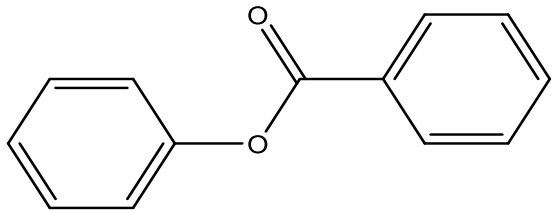
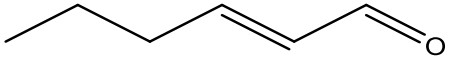
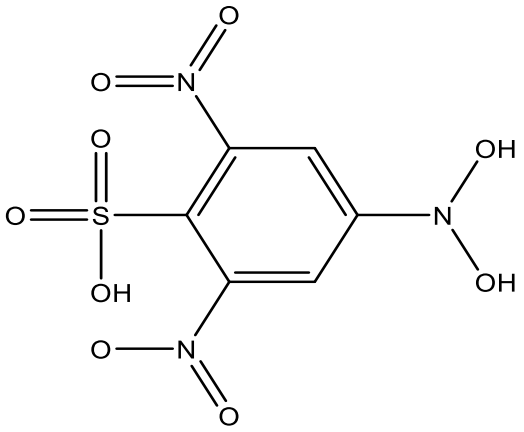
87	Squaric acid diethyl ester		0.11	-0.24	-0.05	-0.14	10.71	173.7	134.62	0	4	0	0.04	2.37
88	Sulfanilamide		0.07	-0.22	-0.02	-0.12	10.19	162.1	33.82	1	3	2	0.05	0.01
89	Sulphanilic acid (Sulfanic acid)		0.08	-0.22	-0.03	-0.13	10.33	156.3	-7.71	1	4	2	0.05	2.92
90	Tetramethylthiuram disulfide		0.14	-0.21	-0.07	-0.14	13.69	251.8	86.93	0	4	0	0.03	0
91	trans-2-Decenal		0.12	-0.25	-0.06	-0.16	10.1	183.2	266.05	0	1	0	0.03	1.84

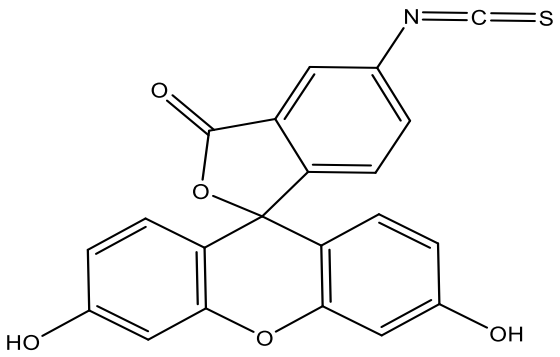
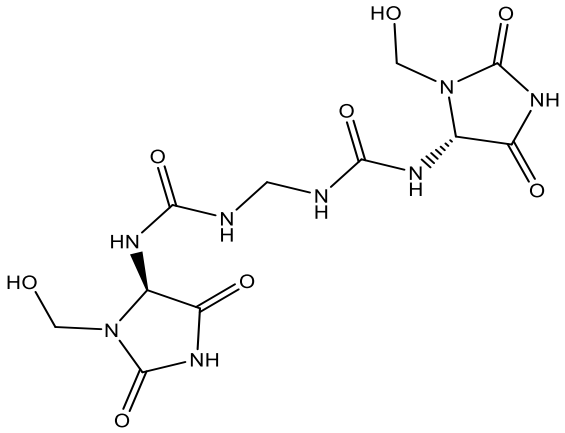
92	Undec-10-enal		0.08	-0.25	-0.02	-0.14	8.83	197.6	287.52	0	1	0	0.03	1
93	1-Bromohexane		0.07	-0.27	0	-0.14	7.3	146.3	160.08	0	0	0	0.02	0.21
94	2,5-Diaminotoluene sulfate		0.04	-0.18	0.01	-0.09	10.92	140	146.17	1	2	2	0.06	1.11
95	2-Aminophenol		0.04	-0.2	0.01	-0.09	9.83	115.6	88.06	1	2	2	0.07	0.37
96	4-Hydroxybenzoic acid		0.1	-0.24	-0.04	-0.14	10.31	135.6	-2.32	1	3	2	0.07	0.01
97	4-Methoxyacetophenone (Acetanisole)		0.11	-0.23	-0.05	-0.14	11.09	161	126.38	1	2	0	0.04	0.72

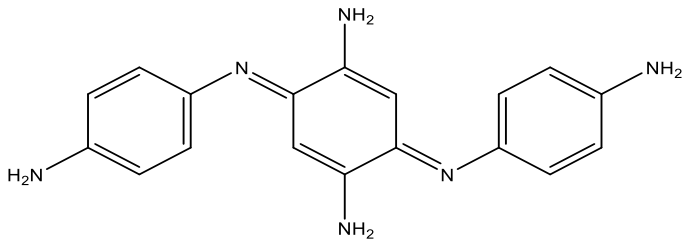
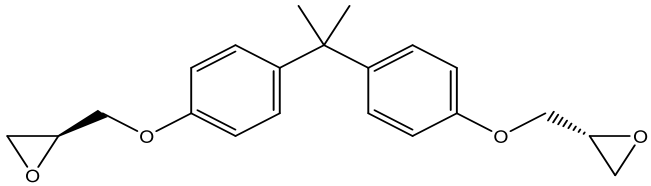
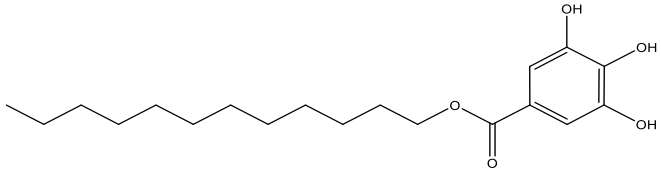
98	6-Methyl coumarin		0.14	-0.23	-0.07	-0.15	12.1	152.7	89.52	1	2	0	0.04	1.15
99	alpha-Methyl cinnamaldehyde (α-methyl-trans-cinnamaldehyde)		0.16	-0.23	-0.08	-0.15	13	157	74.01	1	1	0	0.04	0.72
100	Benzylidene acetone (4-phenyl-3-buten-2-one)		0.15	-0.24	-0.07	-0.15	12.34	156.5	78.58	1	1	0	0.03	1.27
101	Cyclamen aldehyde		0.08	-0.23	-0.03	-0.13	9.7	212.3	241.09	1	1	0	0.03	0.59
102	Diethyl maleate		0.13	-0.28	-0.06	-0.17	9.27	188.3	226.97	0	4	0	0.04	0.31

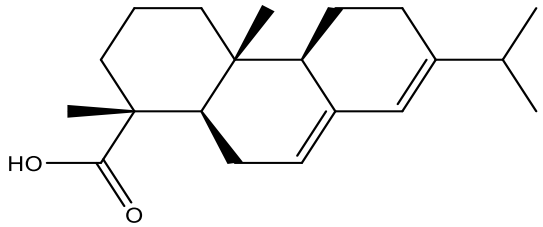
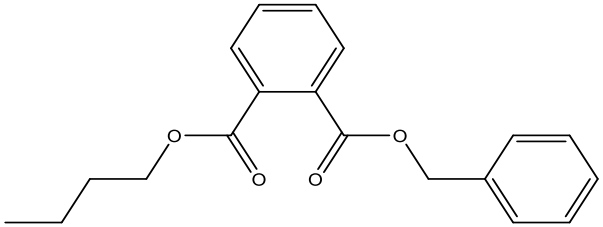
103	DL-lactic acid (Lactic acid)		0.07	-0.28	0	-0.14	7.07	101.1	49.09	0	3	2	0.07	0.08
104	Ethyl acrylate		0.12	-0.28	-0.05	-0.16	8.64	116.9	138.51	0	2	0	0.04	0.8
105	Ethyl vanillin		0.12	-0.22	-0.06	-0.14	12.37	170.7	119.3	1	3	1	0.05	1.51
106	Isoeugenol		0.07	-0.2	-0.02	-0.11	11.45	177.1	156.84	1	2	1	0.05	0
107	Linalool		0.05	-0.23	0.01	-0.11	8.24	192.2	250.98	0	1	1	0.04	0.02

108	Methyl acrylate		0.12	-0.28	-0.05	-0.16	8.59	101.7	107.28	0	2	0	0.04	0.75
109	Methyl methacrylate		0.11	-0.27	-0.04	-0.16	8.81	121.1	138.05	0	2	0	0.04	0.84
110	1,2-cyclohexanedicarboxylic anhydride		0.1	-0.29	-0.03	-0.16	7.93	139.3	76.94	0	3	0	0.03	0.14
111	N-Methyl-N-nitrosourea		0.14	-0.25	-0.07	-0.16	11.1	117.7	2.39	0	3	3	0.05	1.89
112	Glutaraldehyde		0.09	-0.25	-0.03	-0.14	9.18	114	78.51	0	2	0	0.04	0

113	Phenyl benzoate		0.12	-0.25	-0.05	-0.15	10.19	189.3	96.62	2	2	0	0.04	0.57
114	trans-2-Hexenal		0.12	-0.26	-0.06	-0.16	10.1	119.3	146.29	0	1	0	0.04	1.89
115	2,4,6-Trinitrobenzenesulfonic acid		0.31	-0.31	-0.14	-0.23	11.84	251.9	-254	1	9	7	0.03	0.92

116	Fluorescein-5-isothiocyanate		0.13	-0.23	-0.07	-0.15	12.36	331.5	-36.61	3	7	2	0.04	2.19
117	Imidazolidinyl urea		0.09	-0.26	-0.03	-0.14	8.67	361.4	20.24	0	8	8	0.07	1.3

118	Bandrowski's Base (1,4-Cyclohexadiene-1,4-diamine)		0.17	-0.18	-0.08	-0.13	20.85	320.4	233.99	3	6	6	0.06	0
119	Bisphenol A-diglycidyl ether		0.06	-0.21	-0.01	-0.11	9.83	332.1	311.01	2	4	0	0.04	1.15
120	Lauryl gallate		0.09	-0.22	-0.04	-0.13	11.31	356.4	406.49	1	5	3	0.05	0.01

121	Abietic acid		0.06	-0.2	-0.01	-0.11	10.36	316.9	353.77	0	2	1	0.03	0.58
122	Butylbenzylphthalate		0.12	-0.25	-0.06	-0.16	10.17	312.1	246.34	2	4	0	0.04	0.64