

EQQuan User Manual

For detailed information about EQQuan, please refer to our published paper titled “EQQuan: A Stacked Ensemble Learning-Based Predictor for Quantification of Nontarget Chemicals in GC-HRMS Analysis.” EQQuan and its example data are available for download on GitHub at the following link:

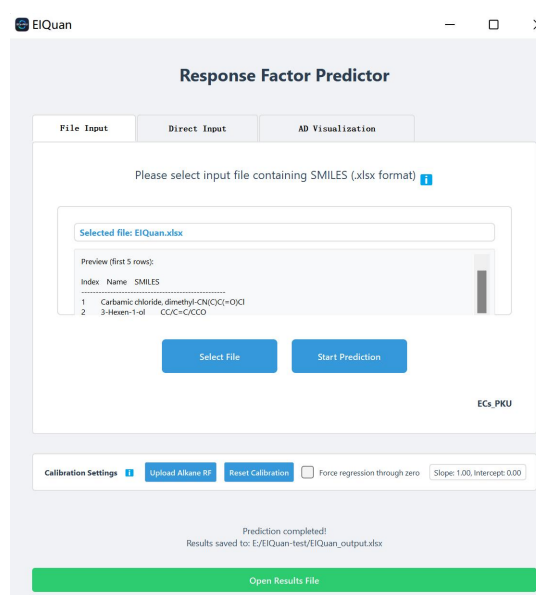
<https://github.com/ECsPKU-LY/EQQuan.git>. If you are unable to access GitHub, you may need a VPN to access the international internet.

EQQuan is only compatible with the Windows operating system and does not require the installation of any additional programming environments. If the current user account name contains non-English characters (e.g., Chinese), the model may fail to load properly. The simplest solution is to create a new user account with an English name and then re-download and run the software under that account.

The input Excel file should follow the specified format: the first column (optional, can be left empty) contains the molecule name, and the second column must contain the SMILES string (required). Column headers should not be included. Please refer to the input format shown in the figure below.

	A	B	C	D
1	Carbamic chloride	<chem>CN(C)C(=O)Cl</chem>		
2	3-Hexen-1-ol	<chem>CC/C=C/CCO</chem>		
3	1-Pentanol	<chem>CC(C)CCCO</chem>		
4	2-Butoxy-1-propanol	<chem>CCCCOCCO</chem>		
5	2-Propanol	<chem>CC(COC(C)COC)O</chem>		
6	1-Octanol	<chem>CC(C)CCCC(C)CCO</chem>		
7	Ethanol, 2-methyl-1-octadecyl-	<chem>C(COCCOCCS)O</chem>		
8	3,5-Nonadiene	<chem>CC#C/C=C/C=C/C(C)O</chem>		
9	1,4,7-Trimethyl-2-octanol	<chem>CC(CO)OCC(C)OCC(C)O</chem>		
10	2,7-Octadiene	<chem>C/C(=C\CCC(C)(C=C)O)/CO</chem>		

The software interface after completing the prediction of the input Excel file is shown below.



The example of the output Excel result file is as follows.

	A	B	C	D	E
1	Name	SMILES	RF (Area-Under the Curve)	AD Status	
2	Carbamic	<chem>CN(C)C(=O)C</chem>	12.14616	Within AD	
3	3-Hexen-1	<chem>CC/C=C/CC</chem>	11.715863	Within AD	
4	1-Pentan	<chem>CCCCC</chem>	11.794058	Within AD	
5	2-Butoxy-	<chem>CCCCOCC</chem>	12.591647	Within AD	
6	2-Propan	<chem>CCC(C)C</chem>	12.568144	Within AD	
7	1-Octanol	<chem>CCCCCCCCO</chem>	12.360122	Within AD	
8	Ethanol,	<chem>CCO</chem>	12.257974	Within AD	
9	3,5-Nona	<chem>CC(C)C(=O)C</chem>	12.276489	Within AD	
10	1,4,7-Tri	<chem>CC(CO)CC</chem>	12.28719	Within AD	
11	2,7-Octa	<chem>C/C(=C)CCCC</chem>	12.137988	Within AD	
12	Pentanal,	<chem>CCCC=O</chem>	12.267535	Within AD	
13	Hexanal,	<chem>CCCCCC=O</chem>	12.284542	Within AD	
14	Nonanal	<chem>CCCCCCC=O</chem>	12.571475	Out of AD	
15	Dodecanal	<chem>CCCCCCCCC=O</chem>	12.734766	Within AD	
16	Urea, for	<chem>CN(C)C(=O)N</chem>	12.267535	Within AD	
17	Urea, N-e	<chem>CCN(C(=O)O)</chem>	12.486567	Within AD	
18	2-Propan	<chem>CC(C)N</chem>	12.257974	Within AD	
19	tert-Buty	<chem>CC(C)(C)C</chem>	12.262152	Within AD	
20	Butanami	<chem>CCCC(N)</chem>	12.53575	Within AD	
21	Isobutyra	<chem>CC(C)CC</chem>	12.714836	Within AD	
22	Formamida	<chem>CCCN(C=O)</chem>	12.713875	Within AD	
23	acetamida	<chem>CC(C)CC(N)C(=O)C</chem>	12.753436	Within AD	
24	2-Amino-N	<chem>CC(C)CC(N)C</chem>	13.436543	Within AD	

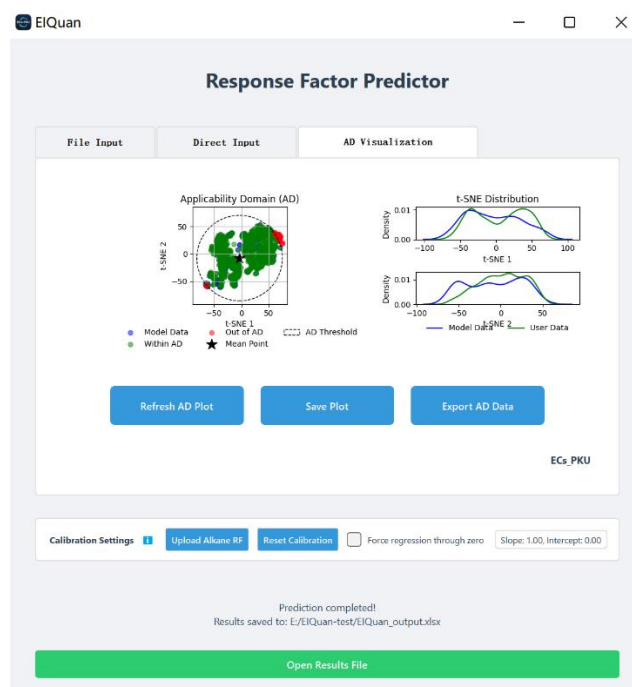
In addition to making predictions by inputting an Excel file, users can also directly input the SMILES of substances to be predicted to obtain the output results directly. See the figure below.

Uploading user-defined n-alkane response factors is not mandatory. However, it is recommended that users provide laboratory-specific n-alkane response factors

(covering carbon numbers 8-39, log₁₀-transformed, in .xlsx format) to calibrate the predicted response factors. The required file format includes: the first column with carbon numbers (integers from 8 to 39), and the second column with log₁₀RF values (numeric), also without column headers. In mass spectra, the most abundant ion is selected as the quantification ion for calculating the n-alkane response factors. Please refer to the input format shown in the figure below. Click “Upload Alkane RF” to select the Excel file of n-alkane response factors for calibration setting.

	A	B
1	17	16.01384467
2	19	16.09276296
3	21	16.15723549
4	25	16.21438675
5	27	16.24373271
6	28	16.26989245
7	29	16.23095869
8		

The prediction results automatically include a label indicating whether each compound falls within the applicability domain of EIQuan. In the applicability domain visualization interface, the user must click the “refresh AD plot” button to display the plot. The plot supports zooming via the mouse scroll wheel. Both the visualization and the underlying data used for plotting can be downloaded. The font size displayed in the software interface depends on the user’s screen scaling settings and monitor resolution, so the interface font size may vary due to differences in the devices used. The results interface of the applicable domain was shown in the figure below.



The information on the 278 reference standards used in this model is shown in the table below:

Number	Name	Compound Identifier Number (CID)	CAS	Retention time (min)	Molecular weight (Da)	Molecular formula
1	2,5-Dimethylfuran	12266	625-86-5	3.024	96.13	C ₆ H ₈ O
2	2-Methylthiophene	11126	554-14-3	3.039	98.17	C ₅ H ₆ S
3	5-Hexen-1-one	7989	109-49-9	3.126	98.14	C ₆ H ₁₀ O
4	3-Methylthiophene	12024	616-44-4	3.148	98.17	C ₅ H ₆ S
5	2-Hexanone	11583	591-78-6	3.298	100.16	C ₆ H ₁₂ O
6	Ethyl methacrylate	7343	97-63-2	3.3	114.14	C ₆ H ₁₀ O ₂
7	n-Octane	356	111-65-9	3.37	114.23	C ₈ H ₁₈
8	4-Hydroxy-2-butanone	111509	590-90-9	3.375	88.11	C ₄ H ₈ O ₂
9	4-Methylmorpholine	7972	109-02-4	3.393	101.15	C ₅ H ₁₁ NO
10	4-Methyl-3-penten-2-one	8858	141-79-7	3.43	98.14	C ₆ H ₁₀ O

11	N,N-Dimethyl formamide	6228	68-12-2	3.39	73.09	C3H7NO
12	Tetrahydrothio phene	1127	110-01-0	3.567	88.17	C4H8S
13	Ethyl lactate	7344	97-64-3	3.708	118.13	C5H10O3
14	2-Methylpyraz ine	7976	109-08-0	3.843	94.11	C5H6N2
15	3-Chloro-1-pr opanol	12313	627-30-5	3.854	94.54	C3H7ClO
16	2-Methyl-2-pe ntenal	5319754	623-36-9	3.938	98.14	C6H10O
17	2-Furaldehyde	7362	98-01-1	3.967	96.08	C5H4O2
18	2,4-Dimethyl- 3-pentanol	11752	600-36-2	4.152	116.2	C7H16O
19	2-Ethyl-1-buta nol	7358	97-95-0	4.11	102.17	C6H14O
20	Ethyl (E)-crotonate	429065	623-70-1	4.253	114.14	C6H10O2
21	(E)-2-Hexenal	5281168	6728-26-3	4.419	98.14	C6H10O
22	Methyl isoamyl ketone	8034	110-12-3	4.485	114.19	C7H14O
23	Leaf alcohol	5281167	928-96-1	4.505	100.16	C6H12O
24	2-Ethylthiophe ne	13388	872-55-9	4.576	112.19	C6H8S
25	2,5-Dimethylt hiophene	12514	638-02-8	4.673	112.19	C6H8S
26	Cyclohexanol	7966	108-93-0	4.688	100.16	C6H12O
27	N,N-Dimethyl acetamide	31374	127-19-5	4.81	87.12	C4H9NO
28	n-Hexanol	8103	111-27-3	4.755	102.17	C6H14O
29	4-Heptanone	31246	123-19-3	4.777	114.19	C7H14O
30	3-Ethylthiophe ne	74530	1795-01-3	4.823	112.19	C6H8S
31	3-Heptanone	7802	106-35-4	4.993	114.19	C7H14O
32	Isopropyl crotonate	5354359	18060-77- 0	5.07	128.169	C7H12O2
33	2-Heptanone	8051	110-43-0	5.136	114.19	C7H14O
34	4-Heptanol	11513	589-55-9	5.209	116.2	C7H16O
35	Cyclohexanon e	7967	108-94-1	5.275	98.14	C6H10O
36	n-Nonane	8141	111-84-2	5.34	128.25	C9H20
37	Heptaldehyde	8130	111-71-7	5.392	114.19	C7H14O
38	Ethylene	8095	111-15-9	5.439	132.16	C6H12O3

	glycol					
	monoethyl					
	ether acetate					
	3-(Methylthio)					
39	propionaldehyde	18635	3268-49-3	5.514	104.17	C4H8OS
40	2-Acetylfuran	14505	1192-62-7	5.584	110.11	C6H6O2
41	2,5-Dimethylpyrazine	31252	123-32-0	5.578	108.14	C6H8N2
42	(E,E)-2,4-Hexadienal	637564	142-83-6	5.6	96.13	C6H8O
43	2,6-Dimethylpyrazine	7938	108-50-9	5.629	108.14	C6H8N2
44	2,3-Dimethylpyrazine	22201	5910-89-4	5.697	108.14	C6H8N2
45	2-Ethylpyrazine	26331	13925-00-3	5.704	108.14	C6H8N2
46	3-Methoxy-3-methylbutanol	62118	56539-66-3	5.739	118.17	C6H14O2
47	2,3,4-Trimethyl-3-pentanol	520484	3054-92-0	5.889	130.229	C8H18O
48	2,5-Hexanedione	8035	110-13-4	5.931	114.14	C6H10O2
49	2-Vinylpyridine	7521	100-69-6	6.112	105.14	C7H7N
50	N,N-Diethylformamide	12051	617-84-5	6.127	101.15	C5H11NO
51	N,N-Dimethylacrylamide	17587	2680-03-7	6.45	99.13	C5H9NO
52	Diethylphosphite	6327654	762-04-9	6.545	137.09	C4H10O3 P+
53	trans-2-Heptenal	5283316	18829-55-5	6.686	112.17	C7H12O
54	4-Methylcyclohexanone	11525	589-92-4	6.75	112.17	C7H12O
55	5-Methylfurfural	12097	620-02-0	6.787	110.11	C6H6O2
56	2-Hydroxypropyl acrylate	61249	999-61-1	6.794	130.139	C6H10O3
57	Diisobutyl ketone	7958	108-83-8	7.024	142.24	C9H18O
58	1-Octen-3-one	61346		7.202	126.2	C8H14O

			4312-99-6			
59	3-Methylthiop ropanol	10448	505-10-2	7.35	106.19	C4H10OS
60	n-Butyl methacrylate	7354	97-88-1	7.251	142.2	C8H14O2
61	Phenol	996	108-95-2	7.28	94.11	C6H6O
62	1-Octen-3-ol	18827	3391-86-4	7.291	128.21	C8H16O
63	Ethyl 3-ethoxypropi onate	12989	763-69-9	7.368	146.18	C7H14O3
64	Methyl heptenone	9862	110-93-0	7.399	126.2	C8H14O
65	3-Octanone	246728	106-68-3	7.419	128.21	C8H16O
66	2-Chloropheno l	7245	95-57-8	7.51	128.55	C6H5ClO
67	2-Octanone	8093	111-13-7	7.529	128.21	C8H16O
68	2-Pentylfuran	19602	3777-69-3	7.553	138.21	C9H14O
69	2-Propylpyridi ne	69320	622-39-9	7.633	121.18	C8H11N
70	3-Octanol	11527	589-98-0	7.734	130.229	C8H18O
71	1,2-Cyclohexa nedione	13006	765-87-7	7.75	112.13	C6H8O2
72	n-Decane	15600	124-18-5	7.82	142.28	C10H22
73	Octanal	454	124-13-0	7.889	128.21	C8H16O
74	Butyl lactate	8738	138-22-7	7.975	146.18	C7H14O3
75	(E,E)-2,4-Hept andienal	5283321	4313-03-5	8.107	110.15	C7H10O
76	Dimethyl maleate	5271565	624-48-6	8.291	144.12	C6H8O4
77	Cycloheptanol	10399	502-41-0	8.386	114.19	C7H14O
78	5-Ethyl-2-met hylpyridine	7728	104-90-5	8.443	121.18	C8H11N
79	2-Ethylhexano l	7720	104-76-7	8.578	130.229	C8H18O
80	Dimethyl succinate	7820	106-65-0	8.617	146.14	C6H10O4
81	1-Methyl-2-py rrolidon	13387	872-50-4	8.726	99.13	C5H9NO
82	Benzylalcohol	244	100-51-6	8.739	108.14	C7H8O
83	Phenylacetalde hyde	998	122-78-1	8.993	120.15	C8H8O
84	Salicylaldehyd	6998	90-02-8	9.006	122.12	C7H6O2

	e					
85	o-Cresol	335	95-48-7	9.22	108.14	C7H8O
86	Furaneol	19309	3658-77-3	9.299	128.13	C6H8O3
87	trans-2-Octenal	5283324	2548-87-0	9.388	126.2	C8H14O
88	1-Phenylethanol	7409	98-85-1	9.472	122.16	C8H10O
89	Diethyl malonate	7761	105-53-3	9.617	160.17	C7H12O4
90	2-Bromophenol	7244	95-56-7	9.63	173.01	C6H5BrO
91	n-Octanol	957	111-87-5	9.752	130.229	C8H18O
92	5-Nonanone	10405	502-56-7	9.781	142.24	C9H18O
93	p-Cresol	2879	106-44-5	9.84	108.14	C7H8O
94	Benzyl formate	7708	104-57-4	9.915	136.15	C8H8O2
95	2-chloro-4-methylphenol	14851	6640-27-3	9.95	142.58	C7H7ClO
96	Allyl hexylate	31266	123-68-2	10.026	156.22	C9H16O2
97	Benzylthiol	7509	100-53-8	10.028	124.21	C7H8S
98	Guaiacol	460	90-05-1	10.15	124.14	C7H8O2
99	2-Isopropyl-3-methoxypyrazine	33166	25773-40-4	10.238	152.19	C8H12N2O
100	2-Nonanone	13187	821-55-6	10.299	142.24	C9H18O
101	2-Chloro-5-methylphenol	12008	615-74-7	10.46	142.58	C7H7ClO
102	Ethyl sorbate	1550470	2396-84-1	10.505	140.18	C8H12O2
103	N-Ethyl-2-pyrrolidone	17595	2687-91-4	10.536	113.16	C6H11NO
104	N-Vinyl-2-pyrrolidone	6917	88-12-0	10.564	111.14	C6H9NO
105	Linalool	6549	78-70-6	10.569	154.25	C10H18O
106	n-Undecane	14257	1120-21-4	10.6	156.31	C11H24
107	2-Nonanol	12367	628-99-9	10.624	144.25	C9H20O
108	1,3-Dimethyl-2-imidazolidinone	6661	80-73-9	10.688	114.15	C5H10N2O
109	Aldehyde C9	31289	124-19-6	10.697	142.24	C9H18O
110	Phenethyl alcohol	6054	60-12-8	10.915	122.16	C8H10O

111	Fenchyl alcohol	15406	1632-73-1	11.134	154.25	C10H18O
112	Isophorone	6544	78-59-1	11.156	138.21	C9H14O
113	Dimethyl malate	12674	1587-15-1	11.233	162.14	C6H10O5
114	2-Nitrophenol	6947	88-75-5	11.41	139.11	C6H5NO3
115	2-Ethylphenol	6997	90-00-6	11.55	122.16	C8H10O
116	S-(-)-cis-Verbenol	87839	18881-04-4	11.778	152.23	C10H16O
117	Cyclooctanol	12766	696-71-9	11.882	128.21	C8H16O
118	2-Ethylhexyl acetate	7635	103-09-3	11.889	172.26	C10H20O2
119	2-Ethoxyphenol	66755	94-71-3	11.93	138.16	C8H10O2
120	Citronellal	7794	106-23-0	12.032	154.25	C10H18O
121	m-Tolyl acetate	67406	122-46-3	12.211	150.17	C9H10O2
122	trans-2-Nonenal	5283335	18829-56-6	12.251	140.22	C9H16O
123	Isoborneol	6321405	124-76-5	12.379	154.25	C10H18O
124	4-Ethylphenol	31242	123-07-9	12.39	122.16	C8H10O
125	2,6-Dimethylaniline	6896	87-62-7	12.385	121.18	C8H11N
126	2,6-Dichlorophenol	6899	87-65-0	12.45	163	C6H4Cl2O
127	4-Ethylaniline	11504	589-16-2	12.491	121.18	C8H11N
128	2,6-Dimethylphenol	11335	576-26-1	12.5	122.16	C8H10O
129	2-Isobutyl-3-methoxypyrazine	32594	24683-00-9	12.701	166.22	C9H14N2O
130	p-Ethylbenzaldehyde	20861	4748-78-1	12.827	134.17	C9H10O
131	Diethyl fumarate	638144	623-91-6	12.959	172.18	C8H12O4
132	P-methyl acetophenone	8500	122-00-9	12.964	134.17	C9H10O
133	Naphthalene	931	91-20-3	12.98	128.169	C10H8
134	2-(4-Methylphenyl)-2-propanol	14529	1197-01-9	13.028	150.22	C10H14O
135	2-Methylisobornol	11062802		13.109	168.28	C11H20O

	rneol		2371-42-8			
136	2-Decanone	12741	693-54-9	13.138	156.26	C10H20O
137	2,3-Dimethylphenol	10687	526-75-0	13.15	122.16	C8H10O
138	Thianaphthene	7221	95-15-8	13.178	134.2	C8H6S
139	Methyl salicylate	4133	119-36-8	13.18	152.15	C8H8O3
140	(E,E)-2,4-Nonadienal	5283339	5910-87-2	13.235	138.21	C9H14O
141	Tertrahydrogeraniol	7792	106-21-8	13.253	158.28	C10H22O
142	α -Terpineol	17100	98-55-5	13.268	154.25	C10H18O
143	2-Isopropylphenol	6943	88-69-7	13.31	136.19	C9H12O
144	Ethyl maltol	21059	4940-11-8	13.35	140.14	C7H8O3
145	n-Dodecane	8182	112-40-3	13.42	170.33	C12H26
146	Isopropyl benzoate	13654	939-48-0	13.529	164.2	C10H12O2
147	n-Decanal	8175	112-31-2	13.553	156.26	C10H20O
148	(-)-Verbenone	92874	1196-01-6	13.597	150.22	C10H14O
149	2-Acetylcyclohexanone	13400	874-23-7	13.652	140.18	C8H12O2
150	Methyl p-toluate	7455	99-75-2	13.734	150.17	C9H10O2
151	2-Phenoxyethanol	31236	122-99-6	13.873	138.16	C8H10O2
152	2-Propylphenol	12570	644-35-9	13.9	136.19	C9H12O
153	L-Carveol	7438	99-48-9	13.93	152.23	C10H16O
154	N,N-Diethylaniline	7061	91-66-7	13.959	149.23	C10H15N
155	p-Isopropylphenol	7465	99-89-8	14.07	136.19	C9H12O
156	Benzothiazole	7222	95-16-9	14.076	135.19	C7H5NS
157	2-Ethylhexyl acrylate	7636	103-11-7	14.118	184.27	C11H20O2
158	(\pm)-beta-Citronellol	8842	106-22-9	14.125	156.26	C10H20O
159	Phenyl propyl alcohol	31234	122-97-4	14.211	136.19	C9H12O
160	Benzylacetone	17355	2550-26-7	14.531	148.2	C10H12O

161	(-)-Carvone	439570	6485-40-1	14.612	150.22	C10H14O
162	Geraniol	637566	106-24-1	14.774	154.25	C10H18O
163	γ -Octalactone	7704	104-50-7	14.855	142.2	C8H14O2
164	Anisic aldehyde	31244	123-11-5	14.891	136.15	C8H8O2
165	4,6-Dichloro-o-cresol	15292	1570-65-6	14.91	177.02	C7H6Cl2O
166	4-Propylphenol	12580	645-56-7	14.94	136.19	C9H12O
167	Isoquinoline	8405	119-65-3	15.027	129.16	C9H7N
168	trans-2-Decenal	5283345	3913-81-3	15.1	154.25	C10H18O
169	Ethyl salicylate	8365	118-61-6	15.272	166.17	C9H10O3
170	2-Chloro-6-methylphenol	6898	87-64-9	15.29	142.58	C7H7ClO
171	(+)-Carvone	16724	2244-16-8	15.292	150.22	C10H14O
172	6-Undecanone	13561	927-49-1	15.321	170.29	C11H22O
173	1-Decanol	8174	112-30-1	15.374	158.28	C10H22O
174	trans-Cinnamaldehyde	637511	14371-10-9	15.396	132.16	C9H8O
175	4-Chloro-2-methoxyphenol	28050	16766-30-6	15.41	158.58	C7H7ClO2
176	4-Ethylguaiaicol	62465	2785-89-9	15.42	152.19	C9H12O2
177	Perillaldehyde	16441	2111-75-3	15.487	150.22	C10H14O
178	(-)-Bornyl acetate	93009	5655-61-8	15.712	196.29	C12H20O2
179	4-Bromophenol	7808	106-41-2	15.72	173.01	C6H5BrO
180	3-Undecanone	75189	2216-87-7	15.771	170.29	C11H22O
181	Isobornyl acetate	6950273	125-12-2	15.776	196.29	C12H20O2
182	Carvacrol	10364	499-75-2	15.88	150.22	C10H14O
183	Indole	798	120-72-9	15.902	117.15	C8H7N
184	2-Undecanone	8163	112-12-9	15.915	170.29	C11H22O
185	3-Methylbenzothiophene	73817	1455-18-1	16.023	148.23	C9H8S
186	Tridecane	12388	629-50-5	16.16	184.36	C13H28
187	Methacrylic	12713	688-84-6	16.239	198.3	C12H22O

	acid, 2-ethylhexyl ester					2
188	N,N-Diethyl- m-toluidine	66679	91-67-8	16.279	163.26	C11H17N
189	2,6-Dichloro-4- -methylphenol	17077	194649	16.36	177.02	C7H6Cl2 O
190	2-Methoxy-4- vinylphenol	332	7786-61-0	16.4	150.17	C9H10O2
191	(E,E)-2,4-Dec adienal	5283349	25152-84- 5	16.61	152.23	C10H16O
192	2,6-Diethylanil ine	11369	579-66-8	16.712	149.23	C10H15N
193	Piperonal	8438	120-57-0	17.065	150.13	C8H6O3
194	2-n-Hexylcycl opentanone	114454	13074-65- 2	17.312	168.28	C11H20O
195	Benzyl butyrate	7650	103-37-7	17.305	178.23	C11H14O 2
196	Terpinyl acetate	111037	80-26-2	17.358	196.29	C12H20O 2
197	2,4,6-Trichlor ophenol	6914	88-06-2	17.45	197.4	C6H3Cl3 O
198	2-Undecenal	5283356	2463-77-6	17.82	168.28	C11H20O
199	1-Undecanol	8184	112-42-5	18.054	172.31	C11H24O
200	2,4-Dibromop henol	12005	615-58-7	18.07	251.9	C6H4Br2 O
201	2-Phenoxyethy l acetate	22568	6192-44-5	18.277	180.2	C10H12O 3
202	Methyl cinnamate	637520	103-26-4	18.327	162.18	C10H10O 2
203	3-Methylindol e	6736	83-34-1	18.356	131.17	C9H9N
204	2,2' -Bithioph ene	68120	492-97-7	18.599	166.3	C8H6S2
205	Methyl eugenol	7127	93-15-2	18.74	178.23	C11H14O 2
206	n-Tetradecane	12389	629-59-4	18.78	198.39	C14H30
207	2,4,6-Trichlor oaniline	12471	634-93-5	18.86	196.5	C6H4Cl3 N
208	4-Bromo-2,6-d imethylphenol	16919	2374-05-2	18.98	201.06	C8H9BrO
209	Aldehyde C12	8194	112-54-9	18.983	184.32	C12H24O
210	2,6-Di-tert-but	31405	128-39-2	19.58	206.32	C14H22O

	ylphenol					
211	Eugenol	3314	97-53-0	19.93	164.2	C10H12O 2
212	Acenaphthylene	9161	208-96-8	19.98	152.19	C12H8
213	4-Pentylphenol	26975	14938-35-3	20.19	164.24	C11H16O
214	γ -Decalactone	12813	706-14-9	20.349	170.25	C10H18O 2
215	Ethyl cinnamate	637758	103-36-6	20.411	176.21	C11H12O 2
216	1-Dodecanol	8193	112-53-8	20.612	186.33	C12H26O
217	Acenaphthene	6734	83-32-9	20.82	154.21	C12H10
218	2,6-Dibromo-4-cresol	31404	2432-14-6	20.88	220.35	C15H24O
219	n-Pentadecane	12391	629-62-9	21.28	212.41	C15H32
220	2,6-Di-tert-butyl-4-methylphenol	31404	128-37-0	21.32	220.35	C15H24O
221	2,4-Di-tert-butylphenol	7311	96-76-4	21.39	206.32	C14H22O
222	Eugenol acetate	7136	93-28-7	21.559	206.24	C12H14O 3
223	Lilestralis	228987	80-54-6	21.866	204.31	C14H20O
224	Ethyl p-hydroxybenzoate	8434	120-47-8	21.923	166.17	C9H10O3
225	4-Hydroxybenzoic acid isopropyl ester	20161	4191-73-5	22.546	180.2	C10H12O 3
226	N,N-Dibutylaniline	61154	613-29-6	22.674	205.34	C14H23N
227	2-Acetonaphthalene	7122	34184	23.082	170.21	C12H10O
228	Fluorene	6853	86-73-7	23.22	166.22	C13H10
229	2,2,4-Trimethyl-1,3-pentanediol diisobutyrate	23284	6846-50-0	23.303	286.41	C16H30O 4
230	n-Hexadecane	11006	544-76-3	23.64	226.44	C16H34
231	Tetradecanal	31291	124-25-4	23.908	212.37	C14H28O
232	Benzophenone	3102	119-61-9	24.239	182.22	C13H10O
233	2,4,6-Tribrom	1483	118-79-6	24.36	330.8	C6H3Br3

	phenol					O
234	α -Amylcinnamal	1712058	122-40-7	24.627	202.29	C14H18O
235	Dihydrojasmonic Acid Methyl Ester (cis- and trans-mixture)	102861	24851-98-7	24.691	226.31	C13H22O3
236	sec-Butyl 4-hydroxybenzoate	86607	17696-61-6	24.786	194.23	C11H14O3
237	γ -Dodecalactone	16821	2305-05-7	25.316	198.3	C12H22O2
238	Tetradecyl alcohol	8209	112-72-1	25.353	214.39	C14H30O
239	n-Heptadecane	12398	629-78-7	25.89	240.5	C17H36
240	n-Butyl p-hydroxybenzoate	7184	94-26-8	26.514	194.23	C11H14O3
241	Dibenzothiophene	3023	132-65-0	27.004	184.26	C12H8S
242	Benzyl benzoate	2345	120-51-4	27.285	212.24	C14H12O2
243	Phenanthrene	995	31055	27.59	178.23	C14H10
244	Anthracene	8418	120-12-7	27.83	178.23	C14H10
245	n-Octadecane	11635	593-45-3	28.03	254.5	C18H38
246	Nootkatone	1268142	4674-50-4	28.082	218.33	C15H22O
247	Benzyl phenyllacetate	60999	102-16-9	28.148	226.27	C15H14O2
248	n-Nonadecane	12401	629-92-5	30.07	268.5	C19H40
249	n-Eicosane	8222	112-95-8	32.01	282.5	C20H42
250	Fluoranthene	9154	206-44-0	33.11	202.25	C16H10
251	n-Heneicosane	12403	629-94-7	33.87	296.6	C21H44
252	Pyrene	31423	129-00-0	34.09	202.25	C16H10
253	n-Docosane	12405	629-97-0	35.65	310.6	C22H46
254	n-Tricosane	12534	638-67-5	37.35	324.6	C23H48
255	n-Tetracosane	12592	646-31-1	38.99	338.7	C24H50
256	Benzo(a)anthracene	5954	56-55-3	39.77	228.3	C18H12
257	Chrysene	9171	218-01-9	39.92	228.3	C18H12
258	n-Pentacosane	12406	629-99-2	40.57	352.7	C25H52
259	n-Hexacosane	12407	630-01-3	42.09	366.7	C26H54
260	n-Heptacosane	11636	593-49-7	43.53	380.7	C27H56

261	Benzo(b)fluoranthene	9153	205-99-2	44.33	252.3	C20H12
262	Benzo(k)fluoranthene	9158	207-08-9	44.42	252.3	C20H12
263	n-Octacosane	12408	630-02-4	44.74	394.8	C28H58
264	benzo[a]pyrene	2336	50-32-8	45.35	252.3	C20H12
265	n-Nonacosane	12409	630-03-5	45.86	408.8	C29H60
266	n-Triacontane	12535	638-68-6	47.13	422.8	C30H62
267	n-Hentriacontane	12410	630-04-6	48.61	436.8	C31H64
268	indeno(1,2,3-cd)pyrene	9131	193-39-5	49.76	276.3	C22H12
269	dibenz(a,h)anthracene	5889	53-70-3	49.98	278.3	C22H14
270	n-Dotriacontane	11008	544-85-4	50.4	450.9	C32H66
271	benzo(g,h,i)perylene	9117	191-24-2	50.97	276.3	C22H12
272	n-Tritriacontane	12411	630-05-7	52.58	464.9	C33H68
273	n-Tetratriacontane	26519	14167-59-0	55.25	478.9	C34H70
274	n-Pentatriacontane	12413	630-07-9	58.55	492.9	C35H72
275	n-Hexatriacontane	12412	630-06-8	62.64	507	C36H74
276	n-Heptatriacontane	23598	7194-84-5	67.75	521	C37H76
277	n-Octatriacontane	23599	7194-85-6	74.09	535	C38H78
278	n-Nonatriacontane	114842	7194-86-7	82.03	549.1	C39H80
