

Open, high-resolution EI+ spectral library of anthropogenic compounds

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Supplementary Tables

Supplementary Table 1. Match scores, retention index comparisons, presence on HBM4EU CECscreen and other openly available libraries.

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Name	NIST Match	HBM4EU CECscreen	Experimental RI	NIST consensus semi non-polar RI	Common with open libraries
1,1-Dibromo-2,3,3,4,4,5-hexachloro-2-cyclopenta-2,4-dien-1-ylcyclooctane			2836.80		
1,2,3,4,6,7,8-Heptachlorodibenzofuran		Y	2904.35	2898	
1,2,3,4,6,7,8-Heptachlorodibenzo-p-dioxin			2956.73	2994	
1,2,3,4,7,8-Hexachlorodibenzofuran		Y	2705.67		
1,2,3,4,7,8-Hexachlorodibenzo-p-dioxin	774	Y	2796.54	2781	
1,2,3,7,8-Pentachlorodibenzofuran	878	Y	2496.11	2507	
1,2,3,7,8-Pentachlorodibenzo-p-dioxin	890	Y	2561.60	2587	
1,2,5,6-Tetrabromocyclooctane	862	Y	2074.80		
1,2,7,9-Tetrachlorodibenzofuran	835	Y	2336.90		
1,2,7,9-Tetrachlorodibenzo-p-dioxin	737		2339.30		
1,2-Benzanthraquinone	929	Y	2588.46	2500	
1,2-Dimethylnaphthalene	882		1432.00	1452	Y
1,3-Dimethylnaphthalene	924	Y	1395.40	1417	
1,4-Chrysenequinone	520	Y	2717.18		
1,4-Dimethylnaphthalene	815	Y	1414.30	1436	
1,4-Naphthoquinone	705	Y	1371.54	1404	
1,5-Dimethylnaphthalene	632	Y	1418.00	1440	
1,8-Dimethylnaphthalene	925	Y	1452.80	1472	
17-alpha-Ethynylestradiol	884	Y	2792.70	2783	
17-beta-Estradiol	769	Y	2723.00	2717	
1-Fluoronaphthalene	891	Y	1196.42	1207	
1-Methylnaphthalene	974		1286.60	1307	Y
1-Methylphenanthrene	932	Y	1967.30	1900	
1-Nitronaphthalene	843	Y	1569.52	1612	Y
2,2',3,3',4,4',5,5',6-Nonachlorobiphenyl	867	Y	2778.40		

Name	NIST Match	HBM4EU CECscreen	Experimental RI	NIST consensus semi non-polar RI	Common with open libraries
2,2',3,3',4,4',5-Heptachlorobiphenyl	928	Y	2566.50	2532	
2,2',3,3',4,5',6,6'-Octachlorobiphenyl	659	Y	2473.00	2518	
2,2',3,4,4',5,5'-Heptachlorobiphenyl	862	Y	2504.78	2484	
2,2',3,4,4',5',6-Heptabromodiphenyl ether	523	Y	3206.14		
2,2',3,4,4',5',6-Heptachlorobiphenyl	927	Y	2386.00	2392	
2,2',3',4,4',5-Hexachloro-3-methoxybiphenyl			2492.51		
2,2',3,4,4',5'-Hexachlorobiphenyl		Y	2356.30	2345	
2,2',3,4',5,5',6-Heptachloro-4-methoxybiphenyl			2592.52		
2,2',3,4,5,5',6-Heptachlorobiphenyl	879	Y	2425.21	2389	
2,2',3,4',5,5',6-Heptachlorobiphenyl	931	Y	2394.20	2378	
2,2',3,4',5,5'-Hexachloro-4-methoxybiphenyl			2554.15		
2,2',3,4,5,5'-Hexachlorobiphenyl	919	Y	2321.77	2315	
2,2',3,4,5'-Pentachlorobiphenyl	864	Y	2162.46	2162	
2,2',3,4',5-Pentachlorobiphenyl	905	Y	2134.21	2074	
2,2',3,5,5',6-Hexachlorobiphenyl	854	Y	2211.16	2198	
2,2',3,5'-Tetrachlorobiphenyl	941	Y	1962.88	1965	
2,2',4,4',5,5'-Hexachlorobiphenyl		Y	2293.50	2300	
2,2',4,5,5'-Pentachlorobiphenyl	820	Y	2135.00	2117	
2,2',5,5'-Tetrachlorobiphenyl	912	Y	1967.40	1933	
2,2',5-Trichlorobiphenyl	892	Y	1753.31	1774	
2,3,3',4',5,5',6-Heptachlorobiphenyl		Y	2504.60	2482	
2,3,3',4,5,6-Hexachlorobiphenyl	897	Y	2357.83	2362	
2,3,3',4',5,6-Hexachlorobiphenyl	866		2360.80	2350	
2,3,3',4',5',6-Hexachlorobiphenyl	900	Y	2356.10	2317	
2,3,3',4,5-Pentachlorobiphenyl	908	Y	2258.70	2207	
2,3,3',4',6-Pentachlorobiphenyl	932	Y	2183.98	2185	

Name	NIST Match	HBM4EU CECscreen	Experimental RI	NIST consensus semi non-polar RI	Common with open libraries
2,3',4,4',5',6-Hexachlorobiphenyl	887	Y	2305.40	2447	
2,3',4,4',5-Pentachlorobiphenyl	926	Y	2262.45	2194	
2,3',4,4'-Tetrachlorobiphenyl	867	Y	2053.00	2056	
2,3,4,5,6-Pentabromobenzyl alcohol			2726.00		
2,3,4,5,6-Pentabromoethylbenzene	913	Y	2323.70		
2,3,4,5,6-Pentabromotoluene	895		2270.30		
2,3,4,5-Tetrabromo-6-chlorotoluene	826	Y	2139.40		
2,3',4,6-Tetrachlorobiphenyl	829	Y	1958.00	1932	
2,3,5,6-Tetrabromo-p-xylene	926	Y	2051.40		
2,3',5',6-Tetrachlorobiphenyl	903	Y	1964.70	1959	
2,3,7,8-Tetrachlorodibenzofuran	835	Y	2314.81	2338	
2,3,7,8-Tetrachlorodibenzo-p-dioxin	868	Y	2347.66	2385	
2,3-Benzofluorene	914	Y	2257.49	2190	
2,3-Dichlorobiphenyl	887	Y	1668.15	1692	
2,4,4'-Trichlorobiphenyl	882	Y	1905.18	1861	
2,4',5-Trichlorobiphenyl	845	Y	1846.20	1859	
2,4,6-Tribromophenol	838	Y	1677.90	1624	Y
2,4,6-Trichlorobiphenyl	888	Y	1796.69		
2,4-D	761		1696.60	1671	
2,4'-Dichlorodiphenyldichloroethane	850	Y	2185.62	2170	
2,4'-Dichlorodiphenyldichloroethylene	895	Y	2107.71	2097	
2,4'-Dichlorodiphenyltrichloroethane	894	Y	2336.20	2261	
2,4-Di-tert-butyl-6-(5-chloro-2H-benzotriazol-2-yl)phenol	752	Y	2652.80		
2,6-Dichloro-4-nitroaniline	696		1755.75	1732	
2,6-Dimethylnaphthalene	855	Y	1381.90	1401	Y
2-Bromoallyl(2,4,6-tribromophenyl) ether			2060.10		

Name	NIST Match	HBM4EU CECscreen	Experimental RI	NIST consensus semi non-polar RI	Common with open libraries
2-Chlorobiphenyl	901	Y	1463.02	1492	
2-Ethylhexyl 2,3,4,5-Tetrabromobenzoate		Y	2834.10		
2-Methylnaphthalene	959	Y	1270.17	1298	Y
2-tert-Butyl-4-methoxyphenol	899	Y	1497.77	1497	
3,3',4,5,5'-Pentachlorobiphenyl	919	Y	2316.20	2266	
4,4'-Dichlorodiphenyldichloroethane	907	Y	2264.41	2257	
4,4'-Dichlorodiphenyldichloroethylene	908	Y	2171.68	2168	
4,4'-Dichlorodiphenyltrichloroethane	911	Y	2348.06	2334	
4-Methoxybenzyl alcohol	908	Y	1285.70	1290	Y
4-Methylbenzophenone	768	Y	1786.55		Y
4-tert-Octylphenol	829	Y	1601.60	1601	
7,12-Dimethylbenz[a]anthracene	855	Y	2819.70	2712	
Acenaphthene	898	Y	1528.33	1486	Y
Acenaphthylene	781	Y	1500.98	1454	Y
Acephate	143	Y	1464.27	1420	Y
Acibenzolar-S-methyl	861	Y	1900.60		
Alachlor	689	Y	1889.49	1894	
Aldrin	903	Y	1940.09	1955	
Allyl 2,4,6-tribromophenyl ether	773	Y	1753.50		
alpha-1,2,3,4,5,6-Hexachlorocyclohexane	822	Y	1732.42	1693	
alpha-1,2-Dibromo-4-(1,2-dibromoethyl)cyclohexane	865	Y	1992.50		
alpha-Amylcinnamaldehyde	951	Y	1651.24	1659	Y
alpha-Amylcinnamyl alcohol	898		1688.80	1675	
alpha-Hexylcinnamaldehyde	951		1751.05	1750	Y
Ametryn	867	Y	1892.00	1898	
Aminocarb	925	Y	1743.20	1770	

Name	NIST Match	HBM4EU CECscreen	Experimental RI	NIST consensus semi non-polar RI	Common with open libraries
Amitraz	946		2563.60	2559	
Anthanthrene	590	Y	3283.45	3185	
Anthracene	903	Y	1844.37	1775	Y
anti-Dechlorane plus		Y	3412.90		
Atrazine	604	Y	1730.38	1746	
Azoxystrobin		Y	3076.10	3076	
Benalaxyl	831	Y	2388.60	2313	
Bendiocarb	886	Y	1647.10	1667	
Benzanthracene/Benzophenanthrene		Y	2469.98	2441	
Benzo(a)pyrene	945	Y	2858.04	2790	Y
Benzo(g,h,i)perylene	954	Y	3243.52	3150	
Benzo(k)fluoranthene	943	Y	2777.20	2748	Y
Benzo[b]naphtho[2,1-d]thiophene	882	Y	2419.34	2359	
Benzo[e]pyrene	953		2843.99	2771	
Benzo[ghi]fluoranthene	902	Y	2407.20		
Benzofluoranthene		Y	2769.96		
Benzophenone	846	Y	1659.58	1666	Y
Benzoximate		Y	1925.60		
Benzyl alcohol	868	Y	1033.20	1036	Y
Benzyl benzoate	895	Y	1776.60	1762	Y
Benzyl cinnamate	882	Y	2110.20	2135	
Benzyl salicylate	929	Y	1882.40	1869	Y
beta-1,2-Dibromo-4-(1,2-dibromoethyl)cyclohexane	843	Y (alpha above)	2006.10		
beta-Hexachlorocyclohexane	911	Y	1775.60	1741	
Bifenazate	869	Y	2450.20	2515	
Bifenthrin	870		2464.20	2470	

Name	NIST Match	HBM4EU CECscreen	Experimental RI	NIST consensus semi non-polar RI	Common with open libraries
Bisphenol A	805		2195.20	2108	
Bitertanol_isomer1	860	Y	2714.60	2637	
Bitertanol_isomer2	841	(as above)	2725.00	2648	
Boscalid	774	Y	2830.20		
Bromuconazole_isomer1	848	Y	2485.50	2487	
Bromuconazole_isomer2	796	(as above)	2527.80	2487	
Bumetrizole		Y	2541.48		
Bupirimate	816	Y	2206.20	2202	
Buprofezin	902	Y	2197.80	2195	
Butafenacil	848	Y	2741.70		
Butylated hydroxytoluene	754	Y	1516.07	1513	
Camphor	890	Y	1156.46	1142	Y
Carbaryl	892	Y	1908.00	1901	Y
Carbetamide	853	Y	2009.30	1974	
Carbofuran	939	Y	1703.80	1735	
Carbofuran phenol	941	Y	1292.20	1286	
Carboxin	854	Y	2221.00	2189	
Carfentrazone-ethyl		Y	2335.60	2327	
Cashmeran	905	Y	1493.70	1508	
Celestolide	907	Y	1696.07	1707	
Chlorferone		Y	2275.41		
Chlorpyrifos	750	Y	1977.26	1973	
Chlorpyrifos oxon	822	Y	1968.14	1973	
Cinnamaldehyde	971		1278.08	1274	Y
Cinnamyl alcohol	920		1309.50	1313	Y
cis-Allethrin	846		2071.80		

Name	NIST Match	HBM4EU CECscreen	Experimental RI	NIST consensus semi non-polar RI	Common with open libraries
cis-Chlordane	895	Y	2112.09	2111	
cis-Cyfluthrin_isomer1	650	Y	2764.18		
cis-Cyfluthrin_isomer2		(as above)	2787.22		
cis-Cypermethrin_isomer1		Y	2809.30	2574	
cis-Cypermethrin_isomer2	730	(as above)	2831.80	2774	
cis-Cyphenothrin		Y	2652.77		
cis-Fenvalerate	819	Y	2945.03	2847	
cis-Heptachlor epoxide	872		2026.06	2059	
cis-Permethrin	825		2686.26	2648	
cis-Phenothrin	863	Y	2517.10	2524	
cis-Prallethrin	823	Y	2096.98	2136	
cis-Resmethrin	810		2394.50	2394	
cis-Tetramethrin	716		2448.80		
Coronene	688	Y	3652.60	3498	Y
Coumarin	957	Y	1446.80	1441	Y
Cyazofamid	528	Y	2429.80	2388	
Cycluron	856	Y	1752.20	1760	
Cyproconazole_isomer1	868	Y	2235.30	2236	
Cyproconazole_isomer2	860	(as above)	2239.80	2339	
delta-Hexachlorocyclohexane	829	Y	1842.60	1801	
delta-Iraldeine	802		1500.30	1506	
Deltamethrin	620	Y	3045.50	3059	
Diazinone	650	Y	1791.02	1791	
Dibenzanthracene		Y	3190.46		
Diclobutrazol	818		2205.20	2191	
Dicofol		Y	2379.70	2467	

Name	NIST Match	HBM4EU CECscreen	Experimental RI	NIST consensus semi non-polar RI	Common with open libraries
Dicrotophos	777	Y	1656.09	1656	
Diethofencarb	794	Y	1966.60	1964	
Difenoconazole_isomer1	757	Y	3010.30	3017	
Difenoconazole_isomer2	756	(as above)	3016.20	3025	
Diflubenzuron		Y	1298.90		
Dimethachlor	876	Y	1854.55	1863	
Dimethoate	819	Y	1702.17	1720	Y
Dimethomorph_isomer1		Y	3076.97	3080	
Dimethomorph_isomer2		(as above)	3111.30	3159	
Diniconazole	734		2263.70	2370	
Dioxacarb	870	Y	1872.81	1850	
Drometrizole	850		2085.60		
Endosulfan	785	Y	2024.49	2114	
Endosulfan sulphate	825	Y	2328.83	2328	
Endrin	905		2205.33	2211	
Endrin aldehyde	855		2275.78	2261	
Endrin ketone	914		2430.05	2426	
Enilconazole	747		2158.30	2161	
Enzacamene			2079.00		
Epoxiconazole	855	Y	2463.90	2425	
epsilon-Hexachlorocyclohexane		Y	1865.93		
Estragole	934	Y	1202.15	1196	Y
Estrone	929	Y	2701.20	2694	Y
Ethiofencarb	842	Y	1850.20	1837	
Ethiprole		Y	2434.50		
Ethofumesate	866	Y	1954.40	1938	

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Etoazole	881	Y	2491.50	2489	
Eucalyptol		Y	1037.80	1032	Y
Eugenol	957	Y	1355.58	1357	Y
Fenamidone	812	Y	2516.10	2499	
Fenarimol	820	Y	2638.90	2579	
Fenazaquin	918	Y	2559.00	2506	
Fenhexamid	887	Y	2416.60		
Fenobucarb	945	Y	1582.00	1608	
Fenoxaprop-ethyl	779	Y	2684.27		
Fenoxycarb	789	Y	2487.80	2459	
Fenpropathrin	824	Y	2481.19	2495	
Fenpropimorph_isomer1	823	Y	1911.80		
Fenpropimorph_isomer2	833	(as above)	1954.80		
Fipronil	774	Y	2045.70	2052	
Flucythrinate_isomer1	834		2833.70	2844	
Flucythrinate_isomer2	731		2862.27	2844	
Fludioxonil	863	Y	2240.80	2169	
Flufenacet	893	Y	1983.70		
Fluoranthene	970	Y	2102.69	2054	Y
Fluquinconazole	905	Y	2744.90	2729	
Flusilazole	750	Y	2204.80	2192	
Flutolanil	933	Y	2130.00	2147	
Flutriafol	919	Y	2126.70	2155	
Fuberidazole	906	Y	1921.20	1891	
Furalaxyl	844	Y	2065.00	2074	
Furathiocarb	778	Y	2521.00	2508	

Name	NIST Match	HBM4EU CECscreen	Experimental RI	NIST consensus semi non-polar RI	Common with open libraries
Galaxolide	891	Y	1830.61	1851	
Geranial	872	Y	1268.00	1270	
Heptachlor	909	Y	1871.08	1887	
Hexabromobenzene	703	Y	2475.30	2473	
Hexachlorobenzene	930	Y	1744.46	1707	Y
Hexaconazole	843	Y	2125.50	2150	
Hydroxychrysene	890	Y	2864.21		
Hydroxyfluorenone	901	Y	1751.11		
Indeno[1,2,3-cd]pyrene	826	Y	3177.05	3095	
Indoxacarb	756	Y	3019.30		
Ipconazole	874	Y	2595.00		
Iprovalicarb isomer 1	842	Y	2168.30		
Iprovalicarb isomer 2	837	(as above)	2205.10		
Isocarbophos	683	Y	2005.30		
Isodecyl diphenyl phosphate	835		2427.00		
Isoeugenol	849	Y	1452.11	1450	Y
Isomethyl-alpha-ionone	929		1479.90	1480	
Isoproc carb	898	Y	1511.80	1532	
Kresoxim-methyl	931	Y	2211.30	2202	
lambda-Cyhalothrin	764	Y	2585.27	2565	
Lilial	927	Y	1532.00	1534	
Limonene	879	Y	1032.90	1030	Y
Lindane	889	Y	1798.00	1754	Y
Linuron	689	Y	1954.10	1946	
Malathion	877	Y	1964.44	1959	Y
Mefenacet	885	Y	2584.70	2566	

Name	NIST Match	HBM4EU CECscreen	Experimental RI	NIST consensus semi non-polar RI	Common with open libraries
Mepanipyrim	837	Y	2096.60	2134	
Mepronil	716	Y	2296.40	2298	Y
Metalaxyl	842	Y	1906.80	1903	
Metazachlor	685	Y	2036.81	2043	
Metconazole	869	Y	2520.10		
Methabenzthiazuron		Y	1648.30		
Methiocarb	720	Y	1946.60	1932	
Methomyl		Y	1568.50	1532	
Methoprotryne	750	Y	2207.70	2193	
Methoxychlor	904	Y	2475.70	2453	
Methyl parathion	818	Y	1890.00	1876	Y
Methyleugenol	943	Y	1398.78	1402	
Metobromuron	869	Y	1843.90	1837	
Metolachlor	873	Y	1956.20		
Metribuzin	769	Y	1876.10	1864	
Mevinphos	774	Y	1445.50	1419	
Mexacarbate	929	Y	1812.30		
Mirex	933	Y	2586.68	2530	
Monocrotophos	870	Y	1723.10	1662	
Monolinuron	920	Y	1705.30	1740	
Myclobutanil	923	Y	2197.70	2198	Y
Nuarimol	843	Y	2440.10	2374	
Octachlorodibenzofuran		Y	3099.39	3147	
Octachlorodibenzo-p-dioxin		Y	3097.63	3197	
Octrizole	757	Y	2571.94		
Oxadixyl	743	Y	2295.70	2268	

Name	NIST Match	HBM4EU CECscreen	Experimental RI	NIST consensus semi non-polar RI	Common with open libraries
Paclobutrazol	852		2084.00	2109	
para-Terphenyl	897		2207.51	2152	
Penconazole	844	Y	2037.70	2045	
Pendimethalin	804	Y	2044.58	2038	
Pentabromobenzene		Y	2083.60		
Pentachlorobenzene	864	Y	1554.64	1511	
Perylene	935	Y	2886.93	2815	Y
Perylene_2H12	818		2875.96		
Phantolide	869	Y	1737.42		
Phenanthrene	916	Y	1832.86	1775	Y
Phenanthrene_2H10	866	Y	1827.10	1784	
Phosmet	915		2460.21	2445	
Picoxystrobin	937	Y	2105.40		
Piperonyl butoxide	874	Y	2431.90	2396	
Pirimicarb	778	Y	1829.60	1837	
Praziquantel	916	Y	2970.57		
Progesterone	906	Y	2892.70		Y
Promecarb	916	Y	1652.70	1687	
Prometon	867	Y	1691.20	1727	
Prometryn	875	Y	1894.10	1905	
Propargite_isomer1	821	Y	2426.80	2387	
Propargite_isomer2	860	(as above)	2429.50	2387	
Propham	912	Y	1428.80	1453	
Propiconazole_isomer1	726	Y	2404.40	2336	
Propiconazole_isomer2	831	(as above)	2412.00	2351	
Propoxur	909	Y	1588.60	1606	

Name	NIST Match	HBM4EU CECscreen	Experimental RI	NIST consensus semi non-polar RI	Common with open libraries
Pyracarbolid	858	Y	2019.90		
Pyraclostrobin	819	Y	2964.19	2967	
Pyrene	969	Y	2154.49	2091	Y
Pyridaben	892	Y	2723.80	2648	
Pyrimethanil	765	Y	1769.70	1793	
Pyriproxyfen	848	Y	2557.70	2574	
Quinoxyfen	762	Y	2403.20	2347	
Retene	852	Y	2236.17	2198	
Rotenone	644	Y	3213.70	3242	
Safrole	910	Y	1296.00	1287	Y
Secbumeton	847	Y	1805.00	1804	
Siduron	666	Y	2153.50	2132	
Simetryn		Y	1890.90	1902	
Spirodiclofen		Y	2708.90	2690	
Spiromesifen	732	Y	2456.30		
Spirotetramat			2767.80		
Spiroxamine_isomer1	843	Y	1859.10	1896	
Spiroxamine_isomer2	811	(as above)	1907.20	1949	
Sulfentrazone	867	Y	2507.80		
syn-Dechlorane plus		Y (anti above)	3373.90		
Tebuconazole	830	Y	2434.30	2391	
Tebufenpyrad	899	Y	2493.50	2501	
Tebuthiuron	857	Y	1523.20	1504	
Tefluthrin	812	Y	1811.79		
Temephos	600	Y	3218.50	3097	
Terbufos	896	Y	1748.90	1768	

Name	NIST Match	HBM4EU CECscreen	Experimental RI	NIST consensus semi non-polar RI	Common with open libraries
Terbumeton	876	Y	1721.00	1738	
Terbutylazine	839	Y	1758.80	1771	
Terbutryn		Y	1927.70	1928	
Testosterone	926	Y	2733.00		Y
Tetraconazole	782	Y	2000.40	1998	
Thiabendazole	869	Y	2074.20	2052	Y
Thiobencarb	882	Y	1957.00	1974	
Thiofanox		Y	1214.20	1277	
Tonalide	807	Y	1845.27	1843	
trans-Allethrin	896		2075.10	2062	
trans-Chlordane	856		2079.00	2078	
trans-Cyfluthrin_isomer1	763	Y	2779.20		
trans-Cyfluthrin_Isomer2	726	(as above)	2793.60		
trans-Cypermethrin_isomer1	797	Y	2817.29	2766	
trans-Cypermethrin_isomer2	699	(as above)	2841.71	2777	
trans-Cyphenothrin		Y (cis above)	2656.66		
trans-Fenvalerate	707	Y (cis above)	2965.30	2847	
Transfluthrin	881	Y	1902.49	1910	
trans-Permethrin	841	Y	2701.88	2657	
trans-Phenothrin	831	Y	2532.40	2524	
trans-Prallethrin	844	Y (cis above)	2102.15	2136	
trans-Resmethrin	831		2407.62	2394	
trans-Tetramethrin	895	Y	2468.00		
Traseolide	788	Y	1830.96	1830	
Triadimefon	771	Y	1987.90	1986	
Triadimenol_isomer1	885	Y	2056.90	2076	

Name	NIST Match	HBM4EU CECscreen	Experimental RI	NIST consensus semi non-polar RI	Common with open libraries
Triadimenol_isomer2	708	(as above)	2070.70	2083	
Triclosan	784	Y	2122.80	2114	
Tricyclazole	762	Y	2214.60	2158	
Trifloxystrobin	863		2399.00	2339	
Triflumizole	755		2061.50	2080	
Trifluralin	811	Y	1666.18	1669	Y
Tri-m-cresyl phosphate	840	Y	2686.60	2664	
Tri-n-butyl-phosphate	890	Y	1628.13	1655	
Tri-o-cresyl phosphate	945	Y	2611.20	2555	
Tri-p-cresyl-phosphate	892		2784.00		
Triphenyl phosphate	833	Y	2400.00	2387	Y
Triphenylene	917	Y	2463.80	2416	Y
Tris(1,3-dichloro-2-propyl)phosphate	825	Y	2338.54	2251	
Tris(1-chloro-2-propyl) phosphate	679	Y	1783.15	1816	
Tris(2-butoxyethyl) phosphate	842	Y	2407.00	2421	
Tris(2-chloroethyl) phosphate	912	Y	1756.00	1777	
Tris(2-ethylhexyl) phosphate	836	Y	2465.00	2463	
Tris(3,5-xylenyl)phosphate			2906.40		
Tris(4-tert-butylphenyl) phosphate	800	Y	3270.93		
Tris(isopropylphenyl)phosphate	868		2815.13		
Triticonazole	828		2553.00		
Vamidotion	724	Y	2125.30	2109	
Zoxamide	633	Y	2453.90	2428	