



Supplementary material: Fiat Lux ... how Alessandro Volta illuminated his scripts

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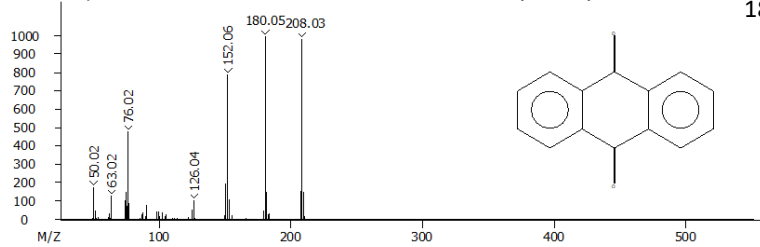
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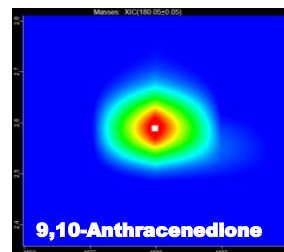
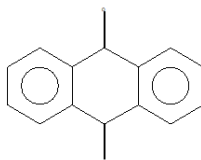
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* Corresponding author.

Peak True - sample "Volta 26032021", 9,10-Anthracenedione, at 1659.93 s, 2.590 s, Area (Abundance)

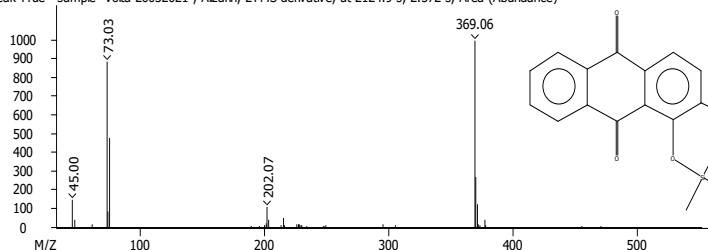


180.05

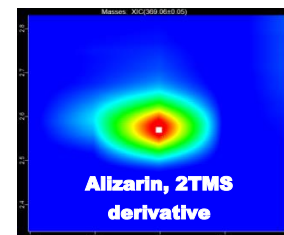
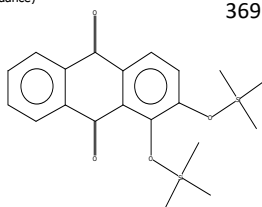


9,10-Anthracenedione

Peak True - sample "Volta 26032021", Alizarin, 2TMS derivative, at 2124.9 s, 2.572 s, Area (Abundance)

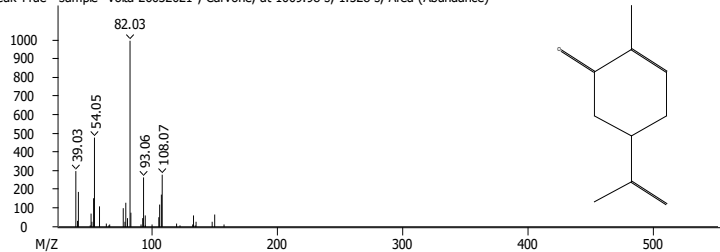


369.06

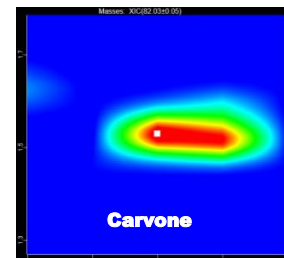
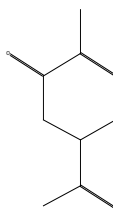


Alizarin, 2TMS
derivative

Peak True - sample "Volta 26032021", Carvone, at 1009.98 s, 1.528 s, Area (Abundance)

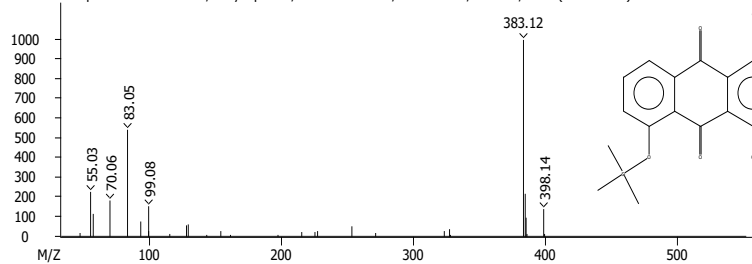


82.03

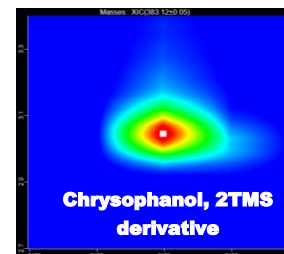
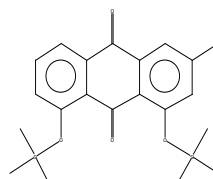


Carvone

Peak True - sample "Volta 26032021", Chrysophanol, 2TMS derivative, at 2179.9 s, 3.044 s, Area (Abundance)

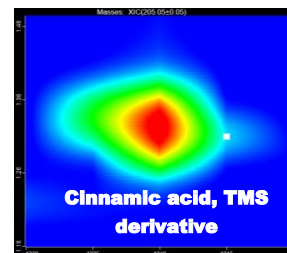
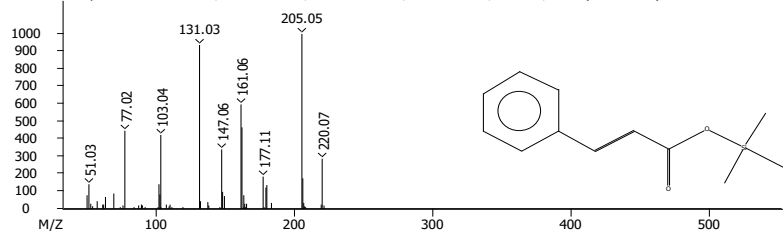


383.12

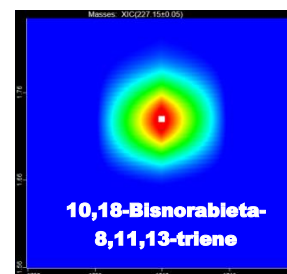
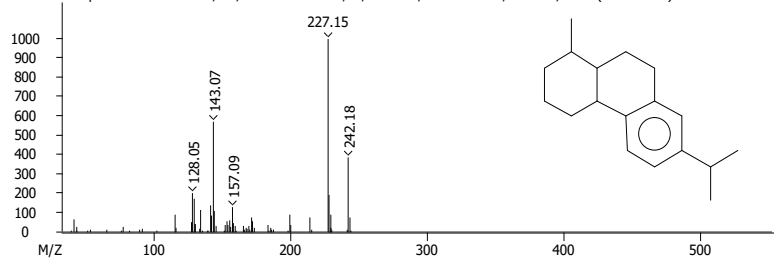


Chrysophanol, 2TMS
derivative

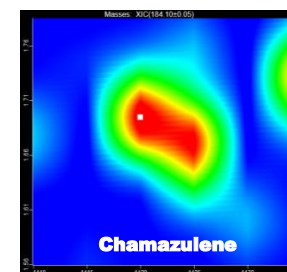
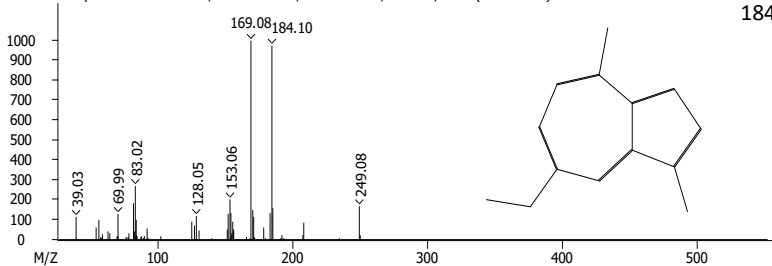
Peak True - sample "Volta 26032021", Cinnamic acid, TMS derivative, at 1244.96 s, 1.312 s, Area (Abundance) 205.05



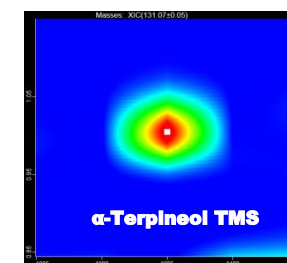
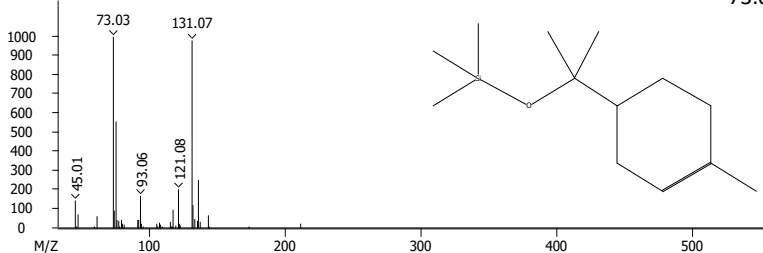
Peak True - sample "Volta 26032021", 10,18-Bisnorabieta-8,11,13-triene, at 1709.93 s, 1.728 s, Area (Abundance) 227.15



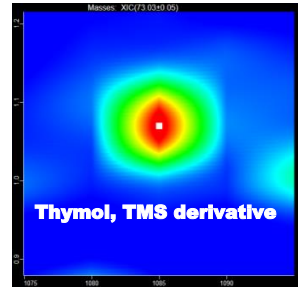
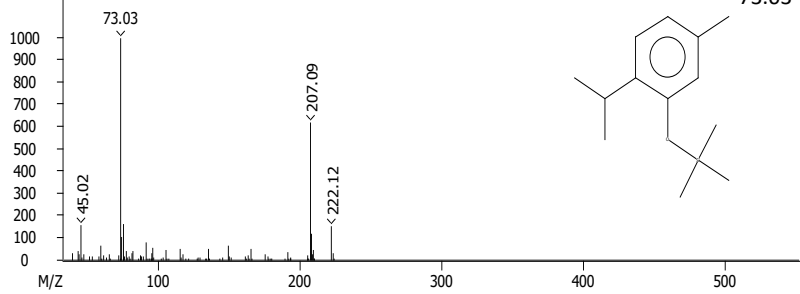
Peak True - sample "Volta 26032021", Chamazulene, at 1419.95 s, 1.696 s, Area (Abundance) 184.10



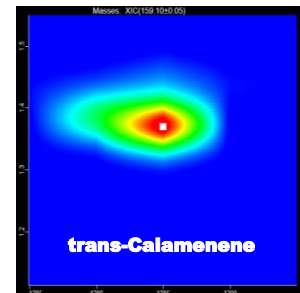
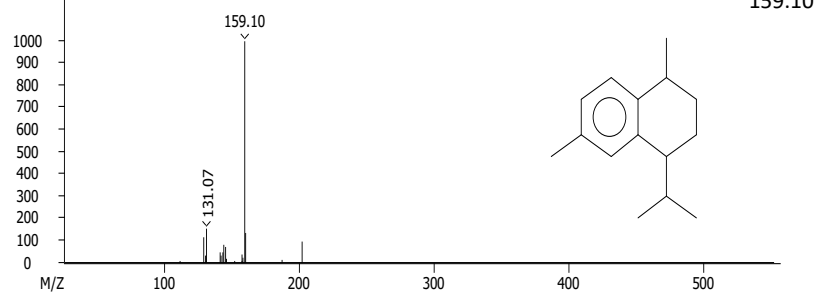
Peak True - sample "Volta 26032021", α -Terpineol TMS, at 1094.97 s, 1.006 s, Area (Abundance) 73.03



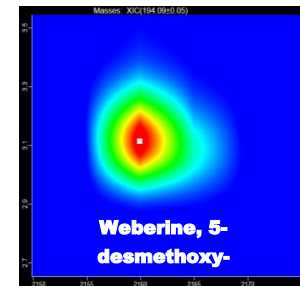
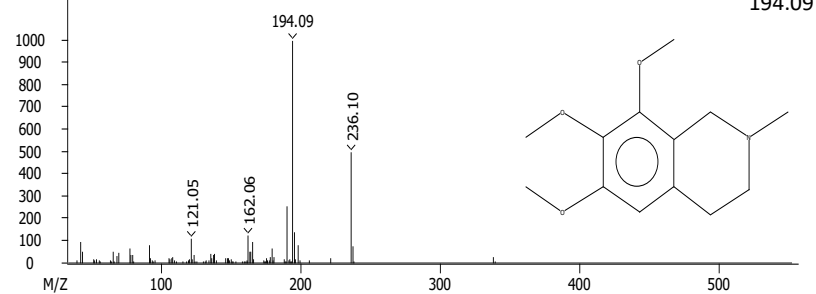
Peak True - sample "Volta 26032021", Thymol, TMS derivative, at 1084.97 s, 1.069 s, Area (Abundance)



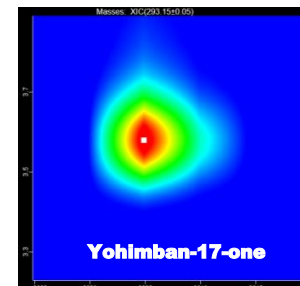
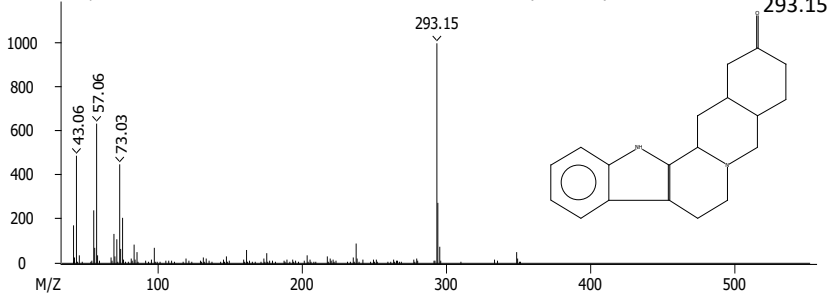
Peak True - sample "Volta 26032021", trans-Calamenene, at 1294.96 s, 1.372 s, Area (Abundance)



Peak True - sample "Volta 26032021", Weberine, 5-desmethoxy-, at 2159.9 s, 3.116 s, Area (Abundance)



Peak True - sample "Volta 26032021", Yohimban-17-one, at 2634.87 s, 3.580 s, Area (Abundance)



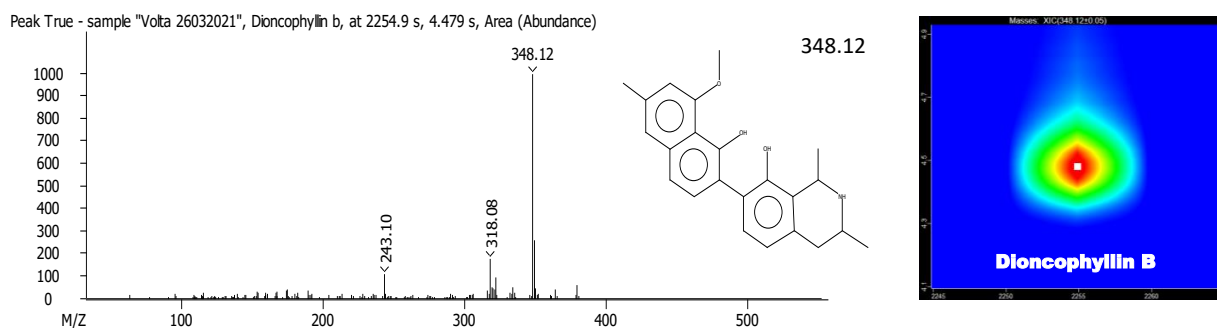
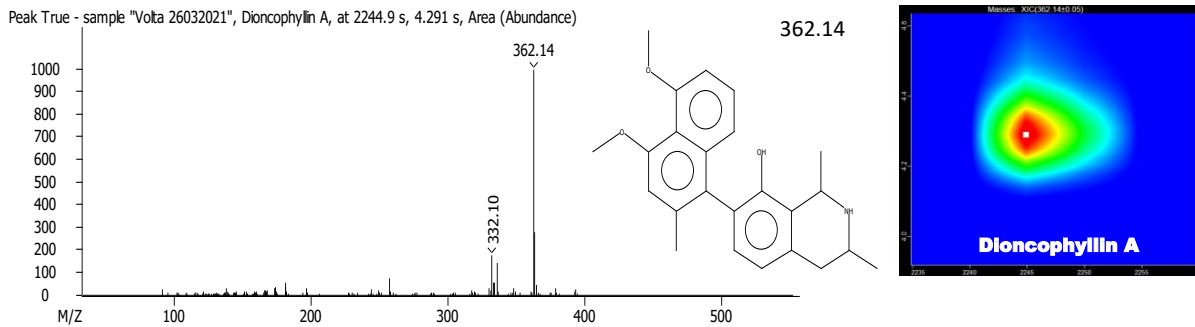


Figure 1S. In the supplementary figure are reported the peak true with the spectra, the quant masses (m/z assignment), the structure and the magnifications of contour 3d plot of the main molecules discussed in the paper.

VOLTA'S INK (FROM EVA DISKS)	R.T. 1st, 2nd Dim. (s)	Area	Similarity	Base Mass	Retentio Index	Peak S/N	Quant Masses
(+)-N-Benzyl-alpha-methyl-N-nitrosobenzylamine	1429.95, 1.635	41029618	760	105.06	1694.1	1897	XIC(105.06±500ppm)
(s)-1-Phenyl-propan-2-ol, N-(trimethylsilyl)	1004.98, 1.079	43849951	709	73.03	1245.5	829	XIC(73.03±500ppm)
(s)-2,5-Dimethoxy-4-Iodoamphetamine, N-trimethylsilyl-	1489.95 s, 1.214 s	504772929	737	116.07	1489.95	16682	XIC(116.07±500ppm)
(1-Propoxy-pentyl)-cyclopropane	1744.93 s, 1.002 s	274186367	739	71.08	1744.93	732	XIC(71.08±500ppm)
(1R,2R,5R,E)-7-Ethylidene-1,2,8,8-tetramethylbicyclo[3.2.1]octane	954.98, 1.080	21852340	758	57.07	1200	2682	XIC(57.07±500ppm)
(2,3-Dimethylbutan-2-yloxy)trimethylsilane	924.982 s, 1.497 s	4567417	768	131	924.982	579	XIC(131.00±500ppm)
(2,3-Diphenylcyclopropyl)methyl phenyl sulfoxide, trans-	2029.91, 2.327	35259536	709	91.04	2486.7	586	XIC(91.04±500ppm)
(2,4-Dimethylheptyloxy)trimethylsilane	889.984 s, 0.819 s	79007035	728	57.06	889.984	6248	XIC(57.06±500ppm)
(2,5-Dimethoxyphenyl)acetone	1329.96 s, 1.916 s	1014543316	903	151.05	1329.96	9045	XIC(151.05±500ppm)
(2-Aziridinylethyl)amine	1499.94, 2.024	123844808	796	43.99	1781.3	1573	XIC(43.99±500ppm)
(2R,3S,5S,6R)-2,5-bis(4-Methoxyphenyl)-3,6-dimethyl-1,4-dioxane-rel-	1934.92 s, 1.752 s	25794155	753	148.09	1934.92	1601	XIC(148.09±500ppm)
(3-Methylphenyl) methanol, 1-methylpropyl ether	1664.93, 1.300	24316533	749	105.06	2000	1014	XIC(105.06±500ppm)
(3-Methylphenyl) methanol, 2-methylpropyl ether	1334.96 s, 1.243 s	24094264	747	105.05	1334.96	823	XIC(105.05±500ppm)
(4-Methoxybenzyl)trimethylsilane	1364.95 s, 1.242	41446388	727	73.03	1617.7	629	XIC(73.03±500ppm)
(7a-Isopropenyl-4,5-dimethyloctahydroindeno-4-yl)methanol	1419.95 s, 1.426 s	116460721	741	191.15	1419.95	3074	XIC(191.15±500ppm)
(9H-fluoren-9-yl)methanol, O-methoxycarbonyl-	1614.94 s, 1.999 s	608867918	749	178.07	1614.94	6011	XIC(178.07±500ppm)
(Methoxymethyl)trimethylsilane	949.98 s, 1.197 s	6663383	741	73.02	949.98	591	XIC(73.02±500ppm)
(Z)-(Z)-Hex-3-en-1-yl-2-methylbut-2-enoate	1399.95 s, 1.088	155920657	720	83.06	1658.8	1222	XIC(83.06±500ppm)
(Z)-2-Heptene	1924.92, 1.136	164356256	727	41.04	2346.7	1089	XIC(41.04±500ppm)
(Z)-4-(but-1-en-1-yl)-1,2-dimethoxybenzene	1224.96, 1.549	6458845	746	192.09	1463.2	1193	XIC(192.09±500ppm)
(Z)-5-Methoxy-3,5-dimethyl-2-hexenyltrimethylsilane	3424.82, 0.497	103243589	745	73.03	4346.8	699	XIC(73.03±500ppm)
(Z)-Docos-9-enenitrile	1984.91 s, 1.540 s	53440810	821	55.05	1984.91	875	XIC(55.05±500ppm)
[1,1'-Biphenyl]-4,4'-diamine, 3,3',5,5'-tetramethyl-	2059.91, 0.692	36880602	706	240.08	2526.7	863	XIC(240.08±500ppm)
[1,1'-Biphenyl]-4-carboxaldehyde	1404.95 s, 1.907 s	30367314	841	182.05	1404.95	1114	XIC(182.05±500ppm)
[2-(2-Ethoxyethoxy)ethoxy]acetic acid, TBDMS derivative	1179.97, 0.870	35448574	727	73.04	1415.8	600	XIC(73.04±500ppm)
[(2-(Trichloromethyl)-1,3-dioxane-5,5-diy)bis(methanediyl)oxy]bis(trimethylsilane)	1194.96 s, 0.967 s	222645779	759	73.03	1194.96	2020	XIC(73.03±500ppm)
4-(Octyloxy)-2-[[trimethylsilyloxy]phenyl][phenyl]methanone	2134.9 s, 2.063 s	14232703	746	271.05	2134.9	2564	XIC(271.05±500ppm)
4-Methoxy-2-[[trimethylsilyloxy]phenyl][2-[[trimethylsilyloxy]phenyl]methanone	2034.91 s, 2.224 s	39003783	759	373.09	2034.91	1522	XIC(373.09±500ppm)
1-(1-Butoxy-2-propoxy)-2-propanol, TMS derivative	889.984 s, 0.942 s	53390859	737	117.05	889.984	1054	XIC(117.05±500ppm)
1-(1-Hydroxybutyl)-2,5-dimethoxybenzene	1734.93, 2.635	54222475	734	167.05	2093.3	1537	XIC(167.05±500ppm)
1-(2,4-Dimethyl-furan-3-yl)-ethanone	839.987, 1.417	29357602	840	123.03	1100	2526	XIC(123.03±500ppm)
1-(2,5-Dimethoxyphenyl)-1-[[trimethylsilyloxy]propan-2-amine	1434.95 s, 1.431 s	587542124	735	239.08	1434.95	4921	XIC(239.08±500ppm)
1-(2-Ethyl-[1,3]dithian-2-yl)-3-methyl-butan-1-ol	709.966, 0.815	1081606302	755	147.17	1003.7	4797	XIC(147.17±500ppm)
1(2H)-Naphthalenone, 3,4-dihydro-	1149.97, 2.027	3047795	903	118.03	1385	568	XIC(118.03±500ppm)
1(2H)-Naphthalenone, 3,4-dihydro-3-phenyl-	1724.93 s, 2.458 s	25695969	884	118.02	1724.93	953	XIC(118.02±500ppm)
1-(2-Hydroxymethylpyrrolidin-1-yl)ethanone	964.979, 0.875	38203938	750	70.07	1209.1	1704	XIC(70.07±500ppm)
1-(2-Methoxy-1-methylethoxy)-2-propanol, TMS derivative	909.983 s, 0.960 s	95975628	838	73.04	909.983	1484	XIC(73.04±500ppm)
1-(2-Methoxyethoxy)-2-methyl-2-propanol, methyl ether	929.981, 1.040	219340577	759	73.03	1178.3	1710	XIC(73.03±500ppm)
1(3H)-Isobenzofuranone	1124.97 s, 2.324 s	23624617	937	105.02	1124.97	2812	XIC(105.02±500ppm)
1(3H)-Isobenzofuranone, 3,3-dimethyl-	1134.97 s, 1.924 s	4775305	815	147.03	1134.97	601	XIC(147.03±500ppm)
1(3H)-Isobenzofuranone, 5-methyl-	1239.96 s, 2.290 s	22555668	899	119.03	1239.96	2187	XIC(119.03±500ppm)
1-(3-Methylbutyl)-2,3,4,6-tetramethylbenzene	854.986 s, 0.971 s	33559563	749	147.05	854.986	4091	XIC(147.05±500ppm)
1-(benzo[d][1,3]dioxol-5-yl)hexan-1-one	1229.96, 1.225	21095358	745	149.08	1468.4	4636	XIC(149.08±500ppm)
1-(benzo[d][1,3]dioxol-5-yl)pentan-1-one	1254.96, 1.283	31489231	713	149.07	1494.7	599	XIC(149.07±500ppm)
1-(Dimethyldodecylsilyloxy)butane	1776.96 s, 0.877 s	349865166	736	131.07	1339.96	10196	XIC(131.07±500ppm)
1-(Dimethyldodecylsilyloxy)heptane	984.978 s, 0.781 s	5971342	738	173.11	984.978	1919	XIC(173.11±500ppm)
1-(Trimethylsilyloxy)cyclopentene	664.998 s, 0.921 s	59720737	781	75.01	664.998	503	XIC(75.01±500ppm)
1,1,1,2-Tetramethyldisilane	1759.93, 1.130	36975093	715	73.03	2126.7	606	XIC(73.03±500ppm)
1,1,3,3-Tetramethyl-1,3-disilaphenolane	1729.93 s, 1.685 s	15324655	737	241.17	1729.93	1060	XIC(241.17±500ppm)
1,1,4-Trimethylcyclohexane	1019.98, 0.929	78476955	741	69.06	1259.1	2525	XIC(69.06±500ppm)
1,1':3,1''-Terphenyl, 4,4''-dimethyl-5'-(4-methylphenyl)-	2479.88 s, 1.679 s	52150592	858	348.15	2479.88	905	XIC(348.15±500ppm)
1,10-Decanediol, 2TMS derivative	819.988, 2.280	143762213	745	73.04	1085.2	567	XIC(73.04±500ppm)
1,12-Tridecadiene	1664.93, 1.390	78869847	753	55.05	2000	597	XIC(55.05±500ppm)
1,13-Tetradecadiene	1694.93, 1.476	124156286	754	55.05	2040	686	XIC(55.05±500ppm)
1,15-Pentadecanediol	1664.93, 1.385	124138535	763	55.05	2000	645	XIC(55.05±500ppm)
1,1'-Biphenyl, 2,2',3,4'-tetrachloro-	1649.94 s, 1.909 s	2836893	820	291.9	1649.94	1696	XIC(291.90±500ppm)
1,1'-Biphenyl, 2,2',4,4'-tetrachloro-	1649.94, 1.912	3729349	797	291.9	1980	2423	XIC(291.90±500ppm)
1,1'-Biphenyl, 2,2',5,5'-tetramethyl-	1414.95 s, 1.646 s	51577185	736	195.09	1414.95	2254	XIC(195.09±500ppm)
1,1'-Biphenyl, 2,3,3'-trichloro-	1589.94, 1.897	1643702	742	255.93	1900	627	XIC(255.93±500ppm)
1,1'-Biphenyl, 2-methyl-	1264.96 s, 1.707 s	37946127	734	84.03	1264.96	3537	XIC(84.03±500ppm)
1,1'-Biphenyl, 3-methyl-	1254.96, 1.702	89348314	782	168.07	1494.7	10210	XIC(168.07±500ppm)
1,1'-Biphenyl, 4-(1-methylethyl)-	1354.95, 1.683	12145789	726	181.08	1605.9	630	XIC(181.08±500ppm)
1,1'-Biphenyl, 4,4'-dichloro-	1504.94 s, 1.841 s	51262245	739	69.04	1504.94	1669	XIC(69.04±500ppm)
1,1'-Biphenyl, 4-methyl-	1264.96, 1.716	37809045	873	168.07	1505.6	2675	XIC(168.07±500ppm)
1,1-Dimethyl-3-(3-nitrophenyl)urea	1494.95, 1.323	853710874	706	72.07	1775	7430	XIC(72.07±500ppm)
1,1-Dimethyl-3-(4-nitrophenyl)urea	1539.94 s, 1.373 s	55377629	766	72.07	1539.94	1935	XIC(72.07±500ppm)
1,2,3,10,11,12-Hexahydroperylene	1939.92 s, 2.311 s	7441000	763	258.11	1939.92	899	XIC(258.11±500ppm)
1,2,3,4,5,6-Hexahydrochryseno	1789.93, 2.156	7030920	708	234.07	2166.7	528	XIC(234.07±500ppm)
1,2,3,4-Tetrahydrobenzo[a]anthracene	1679.93 s, 2.021 s	5130934	735	232.1	1679.93	664	XIC(232.10±500ppm)
1,2,3,4-Tetrahydrochryseno	1679.93, 2.025	7500619	733	232.11	2020	957	XIC(232.11±500ppm)
1,2,3,4-Tetrahydroisquinolin-6-ol, 1-[3-hydroxybenzyl]-	1934.92, 1.753	29318285	733	148.09	2360	1647	XIC(148.09±500ppm)
1,2,3-Butanetriol, 3TMS derivative	1004.98 s, 0.817 s	64581444	751	73.04	1004.98	821	XIC(73.04±500ppm)
1,2,4,5-Tetrazine, 3,6-bis(1,1-dimethylethyl)-	854.986 s, 1.871 s	16991874	740	42.04	854.986	1237	XIC(42.04±500ppm)
1,2,4,5-Tetroxane, 3,3,6,6-tetramethyl-	1959.92 s, 1.234 s	115696046	732	43.03	1959.92	887	XIC(43.03±500ppm)
1,2,5,6-Tetramethylacenaphthylene	1639.94 s, 1.867 s	16893703	741	208.11	1639.94	1268	XIC(208.11±500ppm)
1,2-Benzenedicarboxylic acid, bis(2-methylpropyl) ester	1574.94 s, 1.663 s	736563633	930	148.97	1574.94	8434	XIC(148.97±500ppm)
1,2-Benzenedicarboxylic acid, butyl 8-methylnonyl ester	1939.92 s, 1.715 s	336071815	912	149	1939.92	4983	XIC(149.00±500ppm)
1,2-Benzenedicarboxylic acid, butyl cyclohexyl ester	1574.94, 1.675	822700883	802	148.94	1880	1916	XIC(148.94±500ppm)
1,2-Benzenediol, O-(4-butylbenzoyl)-O'-(isobutoxycarbonyl)-	1139.97, 1.688	62755218	725	161.02	1375	769	XIC(161.02±500ppm)
1,2-Benzenediol, O-(4-ethylbenzoyl)-O'-propargyloxycarbonyl-	1054.97 s, 1.610 s	8766141	732	133.05	1054.97	741	XIC(133.05±500ppm)

1,2-Benzenediol, O-(4-methylbenzoyl)-O'-propoxycarbonyl-	1314.96, 1.243	19835676	716	119.07	1561.1	873	XiC(119.07±500ppm)
1,2-Benzenediol, O-(5-bromovaleryl)-O'-(1-naphthoyl)-	894.984 s, 1.343 s	30845471	734	155.03	894.984	3151	XiC(155.03±500ppm)
1,2-Butanediol, 2TMS derivative	839.987, 0.761	7998800	756	73.04	1100	1944	XiC(73.04±500ppm)
1,2-Cyclohexanedicarboxylic acid, 2-ethylhexyl nonyl ester	2119.91 s, 1.699 s	18230349	749	155.05	2119.91	1096	XiC(155.05±500ppm)
1,2-Cyclohexanedicarboxylic acid, 2-methylpent-3-yl nonyl ester	2104.91, 1.669	19103325	718	155.05	2586.7	1223	XiC(155.05±500ppm)
1,2-Cyclohexanedicarboxylic acid, dinonyl ester	2144.9, 1.774	10322970	722	155.05	2640.1	541	XiC(155.05±500ppm)
1,2-Di-n-butyl-3-methylthiaziridine	1089.97 s, 0.878 s	216114060	745	71.12	1089.97	1016	XiC(71.12±500ppm)
1,2-Ethenediol, 2TMS derivative	1869.92 s, 0.847 s	57552646	733	73.06	2273.4	701	XiC(73.06±500ppm)
1,3,5-Triazine-2,4,6-(1H,3H,5H)-trione, 1,3,5-tri-2-propenyl-	1414.95 s, 1.716 s	5914797	793	83.02	1414.95	1358	XiC(83.02±500ppm)
1,3,5-Tri-O-benzoyl- α -D-ribofuranose	1444.95 s, 1.226 s	310862516	772	105.05	1444.95	2531	XiC(105.05±500ppm)
1,3,5-Trisiloxane, 1,1,3,3,5,5-hexamethyl-1,5-di(tert.butyl)-	684.997, 0.718	805724955	769	221.05	985.2	2353	XiC(221.05±500ppm)
1,3-2H-Isobenzofuranone, 3,3,7-trimethyl-	1284.96 s, 1.750 s	1545487	751	161.08	1527.8	645	XiC(161.08±500ppm)
1,3-Benzenedicarboxylic acid, 5-(1,1-dimethylethyl)-	1474.95 s, 1.466 s	25713519	737	207.08	1474.95	892	XiC(207.08±500ppm)
1,3-Benzenedicarboxylic acid, bis(2-ethylhexyl) ester	2099.91 s, 1.631 s	211829841	914	70.06	2099.91	2354	XiC(70.06±500ppm)
1,3-Benzenediol, 4-ethyl-	839.987 s, 1.399 s	22781333	818	123.03	839.987	1948	XiC(123.03±500ppm)
1,3-Benzenediol, monobenzoate	1474.95, 1.671	31057139	732	105.06	1750	611	XiC(105.06±500ppm)
1,3-Benzenediol, o-(2-bromopropionyl)-o'-(3-methylbenzoyl)-	1654.94 s, 2.109 s	12085276	818	119.04	1654.94	708	XiC(119.04±500ppm)
1,3-Benzenediol, o-(2-furyl)-o'-(4-methylbenzoyl)-	2169.9, 3.270	16710549	737	119.04	2673.4	974	XiC(119.04±500ppm)
1,3-Benzenediol, o-cyclopropanecarbonyl-o'-(3-methylbut-2-enoyl)-	1439.95, 1.045	114766063	748	83.07	1706.2	1771	XiC(83.07±500ppm)
1,3-Benzenediol, O-ethoxycarbonyl-O'-(3-methylbenzoyl)-	1664.93, 1.340	58349279	709	119.07	2000	1306	XiC(119.07±500ppm)
1,3-Bis(trimethylsilyloxy)pentane	1114.97, 0.793	80560336	825	131.07	1350	4373	XiC(131.07±500ppm)
1,3-Butanediol, 2TMS derivative	824.988 s, 2.121 s	214493309	907	147.05	824.988	2165	XiC(147.05±500ppm)
1,3-Cyclohexadiene, 1-methyl-4-(1-methylethyl)-	829.988 s, 1.097 s	28695381	787	75.04	829.988	549	XiC(75.04±500ppm)
1,3-Cyclopentadiene, 1,2-dimethyl-5,5-diphenyl-	1909.91 s, 2.260 s	48242502	803	246.11	1909.92	1273	XiC(246.11±500ppm)
1,3-Dihydroxyanthraquinone, O,O'-bis(trimethylsilyl)-	2289.89 s, 1.672 s	223965832	749	369.29	2833.4	1291	XiC(369.29±500ppm)
1,3-di-iso-propylnaphthalene	1429.95 s, 1.517 s	6144030	797	197.15	1694.1	1209	XiC(197.15±500ppm)
1,3-Dioxane, 2,2-dimethyl-5-trimethylsilyloxy-	834.988 s, 1.197 s	12248604	755	101.03	834.988	848	XiC(101.03±500ppm)
1,3-dioxane-5,5-dimethanol, 2-hexyl-	714.995, 0.868	228157004	736	147.02	1007.4	1164	XiC(147.02±500ppm)
1,3-Dioxolane, 2-(bromomethyl)-2-(2-methylphenyl)-	1119.97 s, 1.782 s	11791155	741	163.05	1119.97	914	XiC(163.05±500ppm)
1,3-Dioxolane, 2-(phenylmethyl)-	1004.98 s, 1.073 s	29217266	748	73.03	1004.98	686	XiC(73.03±500ppm)
1,3-Dioxolane, 2,2-diethyl-	1194.96, 1.493	24950769	729	101.01	1431.6	2092	XiC(101.01±500ppm)
1,3-Dioxolane, 2-butyl-	1674.93, 1.159	33972405	735	73.03	2013.3	548	XiC(73.03±500ppm)
1,3-Dioxolane, 2-heptyl-	779.991 s, 0.745 s	172873228	792	73.03	779.991	1220	XiC(73.03±500ppm)
1,3-Dioxolane, 2-pentadecyl-	2769.86 s, 0.499 s	38649322	742	73.03	2769.86	722	XiC(73.03±500ppm)
1,3-Dioxolane, 2-phenyl-	1004.98 s, 1.778 s	2429299	802	149.04	1004.98	537	XiC(149.04±500ppm)
1,3-Dioxolane-2-methanol	1124.97 s, 1.030 s	39387676	752	73.03	1124.97	599	XiC(73.03±500ppm)
1,3-Diphenyl-4H-1,2,4-triazoline-5-thione	1644.94 s, 1.036 s	10322297	742	253.27	1644.94	1695	XiC(253.27±500ppm)
1,3-Oxazolidine, 2,5-diphenyl-4-methyl-, trans-	1924.92, 2.471	14153028	706	132.06	2346.7	1051	XiC(132.06±500ppm)
1,3-Oxazolidine, 4-methyl-2-(4-methylphenyl)-St-phenyl-	1994.91, 2.551	21852539	748	146.08	2440	1273	XiC(146.08±500ppm)
1,3-Propanediol, 2TMS derivative	794.99 s, 0.826 s	186139194	848	147.04	794.99	5625	XiC(147.04±500ppm)
1,3-Propanediol, TMS derivative	824.988, 0.970	92869177	755	75.01	1088.9	1197	XiC(75.01±500ppm)
1,4,5,8-Tetramethylnaphthalene	1384.95 s, 1.637 s	35745872	753	169.08	1384.95	2321	XiC(169.08±500ppm)
1,4,7,10,13,16-Hexaoxacyclooctadecane	1594.94 s, 2.113 s	24806287	943	45.04	1594.94	736	XiC(45.04±500ppm)
1,4-Benzenedicarboxylic acid, bis(2-ethylhexyl) ester	2124.9 s, 1.647 s	144247676	764	112.11	2124.9	587	XiC(112.11±500ppm)
1,4-Benzenedicarboxylic acid, diethyl ester	1399.95 s, 1.609 s	202344472	897	177.03	1399.95	4568	XiC(177.03±500ppm)
1,4-Benzenedicarboxylic acid, dimethyl ester	1264.96 s, 1.760 s	56294939	884	163.02	1264.96	3060	XiC(163.02±500ppm)
1,4-Benzenedicarboxylic acid, ethyl methyl ester	1334.96 s, 1.674 s	19945950	851	163.02	1334.96	1046	XiC(163.02±500ppm)
1,4-Bis(trimethylsilyl)-1,3-butadiene	1004.98, 1.122	12927836	791	179.07	1245.5	2318	XiC(179.07±500ppm)
1,4-Butanediol, 2TMS derivative	924.982 s, 0.846 s	443459157	879	147.04	924.982	26865	XiC(147.04±500ppm)
1,4-Dimethoxy-3-butylbenzene	1389.95 s, 1.608 s	7605513	755	151.06	1389.95	578	XiC(151.06±500ppm)
1,4-Dimethoxy-6,7,8,9-tetrahydro-5-benzocycloheptenone	2159.9, 3.238	335936630	748	220.11	2660.1	1312	XiC(220.11±500ppm)
1,4-Dimethyl-2-phenyl-naphthalene	1714.93 s, 2.144 s	4483321	740	232.1	1714.93	713	XiC(232.10±500ppm)
1,4-Methano-1H-indene, octahydro-1,7a-dimethyl-4-(1-methylethenyl)-, [1S-(1 α ,3 α β,4 α ,7 α β)]-	1179.97 s, 1.222 s	73778153	889	95.07	1179.97	2306	XiC(95.07±500ppm)
1,4-Methanoazulen-9-one, decahydro-1,5,5,8a-tetramethyl-, [1R-(1 α ,3 α β,4 α ,8 α β)]-	1374.95 s, 1.267 s	49329277	725	81.05	1629.4	1513	XiC(81.05±500ppm)
1,4-Methanobenzocyclodecene, 1,2,3,4,4a,5,8,9,12,12a-decahydro-	1389.95 s, 1.515 s	15806085	794	67.04	1389.95	1000	XiC(67.04±500ppm)
1,5-Anhydroglucitol, 4TMS derivative	1589.94, 0.856	69568707	726	73.04	1900	1567	XiC(73.04±500ppm)
1,5-Dihydroxy-6-methoxyanthone	1689.93, 1.627	17085136	747	258.21	2033.3	1067	XiC(258.21±500ppm)
1,5-Dimethoxy-4-methylnaphthalene	1529.94, 2.008	28098067	761	187.06	1820	5235	XiC(187.06±500ppm)
1,5-Diphenyl-2H-1,2,4-triazoline-3-thione	1489.95, 1.350	143907040	746	253.1	1768.8	4348	XiC(253.10±500ppm)
1,6-Dimethyl-4-ethylnaphthalene (Norcadalene)	1394.95, 1.666	17926828	763	169.09	1652.9	1120	XiC(169.09±500ppm)
1,6-Dioxacyclododecane-7,12-dione	1309.96 s, 2.067 s	189520707	923	55.03	1309.96	4609	XiC(55.03±500ppm)
1,7,7-Trimethyl-3-phenethylidenebicyclo[2.2.1]heptan-2-one	1719.93, 1.906	4346390	714	254.14	2073.3	528	XiC(254.14±500ppm)
1,7-Dimethyl-4-(1-methylethyl)cyclododecane	1469.95, 1.030	395478799	746	57.06	1743.8	1228	XiC(57.06±500ppm)
1,7-Dimethyldibenzothiophene	1649.94 s, 2.128 s	12125282	742	212.05	1649.94	1401	XiC(212.05±500ppm)
1-[(1-Oxo-2-propenyl)oxy]-2,5-pyrroli-dione	1189.96, 0.911	58927776	746	55.06	1426.3	727	XiC(55.06±500ppm)
1-[(2-Bromo-phenyl)-(2,2-dimethyl-propionyl)-methyl]-3,4-dihydro-1H-isoquinoline-2-carboxylic a	1954.92, 2.242	5995892	705	204.01	2386.7	1254	XiC(204.01±500ppm)
1-[2,4-Bis(trimethylsilyloxy)phenyl]-2-[[4-(trimethylsilyloxy)phenyl]propan-1-one	904.983 s, 0.768 s	7393219	785	281.02	904.983	1128	XiC(281.02±500ppm)
10,18-Bisnorabieta-5,7,9(10),11,13-pentaene	1749.93 s, 1.864 s	8876864	801	223.12	1749.93	856	XiC(223.12±500ppm)
10,18-Bisnorabieta-8,11,13-triene	1709.93 s, 1.728 s	56894226	797	227.15	1709.93	4016	XiC(227.15±500ppm)
10H-Phenoxaphosphine, 2-chloro-8-ethyl-10-hydroxy-, 10-oxide	1429.95 s, 1.222 s	20038549	744	279.15	1429.95	1804	XiC(279.15±500ppm)
11-Bromo-1-undecanol, TMS derivative	1774.93 s, 1.140 s	109177226	741	43.02	1774.93	641	XiC(43.02±500ppm)
11-Hexadecen-1-ol, (Z)-	1664.93 s, 1.389 s	124152928	735	55.05	1664.93	657	XiC(55.05±500ppm)
11-Tricosene	1834.92, 1.020	390456667	734	57.07	2226.7	2134	XiC(57.07±500ppm)
12-Crown-4	1079.97, 1.800	11154746	889	45.04	1315	527	XiC(45.04±500ppm)
13-Docosamide, (Z)-	2144.9 s, 2.029 s	203734204	848	59.03	2144.9	3641	XiC(59.03±500ppm)
15-Crown-5	1369.95 s, 1.938 s	48686018	755	45.04	1369.95	1258	XiC(45.04±500ppm)
15-Octadecenoic acid, methyl ester	1734.93 s, 1.298 s	117843526	739	55.05	1734.93	953	XiC(55.05±500ppm)
16-Methyl-heptadecane-1,2-diol, trimethylsilyl ether	1679.93, 0.895	13688712	740	327.28	2020	1707	XiC(327.28±500ppm)
17-Octadecynoic acid	1709.93, 1.484	120782321	739	55.05	2060	629	XiC(55.05±500ppm)
1-Acetyl-4,6,8-trimethylazulene	1439.95 s, 1.495 s	18407186	737	197.11	1439.95	520	XiC(197.11±500ppm)
1-benzyl-3-methylnaphthalene	1834.92 s, 2.284 s	17562528	820	232.1	1834.92	667	XiC(232.10±500ppm)

1-Benzoyloxy-1-ethyl-1-silacyclopentane	1279.96, 0.766	97794014	734	191.08	1522.2	593	XIC(191.08±500ppm)
1-Bromo-3-butene-2-ol	2184.9, 1.164	511532705	749	57.07	2693.4	1448	XIC(57.07±500ppm)
1-Butanamine, N,N-diethyl-	819.988 s, 1.423 s	7378482	744	86.04	819.988	689	XIC(86.04±500ppm)
1-Butanol, 3-methyl-, benzoate	1514.94, 1.411	46490001	759	105.02	1800	1199	XIC(105.02±500ppm)
1-Butanol, 4-(hexyloxy)-	1729.93 s, 1.755 s	33011022	736	71.04	1729.93	1307	XIC(71.04±500ppm)
1-Butanol, TMS derivative	904.983 s, 0.841 s	287487142	733	131.07	904.983	12372	XIC(131.07±500ppm)
1-Butoxy-2-propanol, TMS derivative	804.989, 0.874	1455415909	750	73.04	1074.1	3123	XIC(73.04±500ppm)
1-Butyl(dimethyl)silyloxy-2-methylpropane	1284.96, 0.889	36312619	753	131.07	1527.8	745	XIC(131.07±500ppm)
1-Butyl(dimethyl)silyloxy-4-methylpentane	1039.97, 0.814	27513049	738	159.1	1277.3	2574	XIC(159.10±500ppm)
1-Chloro-3-methoxy-2-propanol, TMS derivative	784.991, 0.968	18073887	731	45.03	1059.3	604	XIC(45.03±500ppm)
1-Chloroundecane	1234.96, 1.113	59345511	878	43.04	1473.7	1140	XIC(43.04±500ppm)
1-Cyclohexyldimethylsilyloxy-3-phenylpropane	1314.96 s, 1.355 s	5747280	745	193.08	1314.96	500	XIC(193.08±500ppm)
1-Cyclohexyldimethylsilyloxy-4-methylpentane	694.996 s, 0.913 s	32308704	746	159.06	694.996	2182	XIC(159.06±500ppm)
1-Cyclohexyldimethylsilyloxybutane	1699.93, 0.938	13397382	731	131.07	2046.7	983	XIC(131.07±500ppm)
1-Cyclohexylethanol, TMS derivative	1279.96, 1.021	635955328	773	117.06	1522.2	2249	XIC(117.06±500ppm)
1-Decanol	1874.92, 1.111	313378052	745	55.05	2280	3445	XIC(55.05±500ppm)
1-Decanol, 2-ethyl-	1479.95, 0.970	339068874	822	57.05	1756.3	3444	XIC(57.05±500ppm)
1-Decanol, 2-hexyl-	1494.95, 0.962	607483166	816	69.06	1775	2534	XIC(69.06±500ppm)
1-Decanol, TMS derivative	1034.97 s, 0.853 s	387262726	762	75.01	1034.97	10340	XIC(75.01±500ppm)
1-Decene, 2-methyl-	989.978 s, 1.408 s	6730501	745	56.02	989.978	686	XIC(56.02±500ppm)
1-Decene, 4-methyl-	724.995, 0.826	92777568	814	43.05	1014.8	1899	XIC(43.05±500ppm)
1-Decene, 8-methyl-	814.989 s, 2.265 s	341708923	808	43.06	814.989	603	XIC(43.06±500ppm)
1-Dimethyl(isopropyl)silyloxyoctane	939.981, 0.873	147676040	830	75.01	1187	13180	XIC(75.01±500ppm)
1-Docosene	1919.92, 1.173	736222251	844	57.06	2340	1626	XIC(57.06±500ppm)
1-Dodecanol, 2-hexyl-	1494.95 s, 0.961 s	914747583	815	57.04	1494.95	2391	XIC(57.04±500ppm)
1-Dodecanol, TMS derivative	1324.96 s, 0.944 s	160314554	859	243.27	1324.96	2906	XIC(243.27±500ppm)
1-Dodecene	949.98 s, 0.913 s	87467826	905	43.06	949.98	3584	XIC(43.06±500ppm)
1-Eicosanol	1864.92 s, 1.284 s	126051240	743	55.03	1864.92	1244	XIC(55.03±500ppm)
1-Eicosanol, TMS derivative	1899.92 s, 1.081 s	60318049	865	75.01	1899.92	1656	XIC(75.01±500ppm)
1-Ethoxy-2-propanol, TMS derivative	1759.93 s, 1.125 s	45048883	743	73.03	1759.93	629	XIC(73.03±500ppm)
1-Ethyl-2,2,6-trimethylcyclohexane	1039.97 s, 0.923 s	80267496	761	69.06	1039.97	652	XIC(69.06±500ppm)
1-Ethyl-2-pyrrolidinone	854.986 s, 1.849 s	30205681	811	98.04	854.986	2831	XIC(98.04±500ppm)
1H-1,2,3-Triazole	1589.94 s, 1.061 s	159083747	762	69.06	1589.94	595	XIC(69.06±500ppm)
1H-Cyclopropa[1]phenanthrene,1a,9b-dihydro-	1624.94 s, 2.244 s	91432317	750	192.07	1624.94	3217	XIC(192.07±500ppm)
1-Heneicosanol	1869.92, 1.110	156833187	728	55.05	2273.4	657	XIC(55.05±500ppm)
1-Heneicosanol, TMS derivative	1939.92, 1.112	6196555	718	75.01	2366.7	567	XIC(75.01±500ppm)
1-Heptadecanol, TMS derivative	1704.93 s, 1.025 s	25869969	775	313.26	1704.93	612	XIC(313.26±500ppm)
1-Heptadecene	1509.94, 1.068	102699811	896	43.04	1793.8	2567	XIC(43.04±500ppm)
1-Heptatriacotanol	2079.91 s, 1.480 s	135948722	743	73.08	2553.4	765	XIC(73.08±500ppm)
1-Hepten-3-one	1654.94, 1.077	220389106	773	70.07	1986.7	2034	XIC(70.07±500ppm)
1-Hexacosene	2409.89 s, 1.737 s	384061301	748	69.06	2409.89	1857	XIC(69.06±500ppm)
1-Hexadecanol	1979.91, 1.354	52291884	748	43.05	2420	552	XIC(43.05±500ppm)
1-Hexadecanol, acetate	1809.93 s, 1.239 s	121432171	774	43.04	1809.93	1036	XIC(43.04±500ppm)
1-Hexadecanol, TBDMS derivative	1639.94 s, 1.024 s	200765760	802	299.25	1639.94	866	XIC(299.25±500ppm)
1-Hexadecanol, TMS derivative	1639.94 s, 1.009 s	343818014	858	75.01	1639.94	2379	XIC(75.01±500ppm)
1-Hexanol, 2-ethyl-	709.996 s, 0.855 s	13710609	792	57.07	709.996	575	XIC(57.07±500ppm)
1-Hexanol, 4-methyl-	1804.93, 1.547	133146460	706	56.07	2186.7	763	XIC(56.07±500ppm)
1-Hexanol, 5-methyl-2-(1-methylethyl)-	1049.97 s, 2.206 s	25982594	835	43.06	1049.97	511	XIC(43.06±500ppm)
1-Hexanol, TMS derivative	694.996 s, 0.826 s	73897698	868	75.04	992.6	2980	XIC(75.04±500ppm)
1-Hexene, 3,3,5-trimethyl-	1609.94, 1.014	192072339	749	69.06	1926.7	1868	XIC(69.06±500ppm)
1-Hexene, 3,4,5-trimethyl-	2299.89 s, 1.648 s	94539901	735	43.06	2299.89	673	XIC(43.06±500ppm)
1-Hexene, 3-methyl-	1499.94, 1.019	270446925	731	69.06	1781.3	990	XIC(69.06±500ppm)
1-Hexene, 3-methyl-6-phenyl-4-(1-phenylethoxy)-	1679.93 s, 1.267 s	76694098	832	105.05	1679.93	2572	XIC(105.05±500ppm)
1H-Inden-1-one, 2,3-dihydro-3,3,4,5-tetramethyl-	1204.96 s, 1.398 s	5708752	763	173.08	1204.96	668	XIC(173.08±500ppm)
1H-Indene, 1-(phenylmethylene)-	1579.94 s, 2.114 s	17640534	916	204.07	1579.94	1189	XIC(204.07±500ppm)
1H-Indene, 2,3-dihydro-5-methyl-	1709.93 s, 1.875 s	27279924	767	131.06	1709.93	940	XIC(131.06±500ppm)
1H-Indole, 1,3-dimethyl-	1289.96, 1.222	21539043	733	144.08	1533.3	2181	XIC(144.08±500ppm)
1H-Indole, 1-butyl-3-methyl-	1429.95, 1.959	5432137	739	187.08	1694.1	744	XIC(187.08±500ppm)
1H-Indole, 5-methoxy-2-methyl-	1414.95, 2.170	5493242	904	161.07	1676.5	660	XIC(161.07±500ppm)
1H-Pyrazole, 4,5-dihydro-5-propyl-	1889.92, 1.051	220892043	769	69.06	2300	891	XIC(69.06±500ppm)
1H-Pyrazolo[2,3-b]pyridine, 4-methyl-2-phenyl-	1614.94, 2.110	16770028	739	208.07	1933.3	723	XIC(208.07±500ppm)
1H-Tetrazol-5-amine	1814.92 s, 1.005 s	305385445	741	57.04	1814.92	548	XIC(57.04±500ppm)
1-Iodoundecane	1214.96 s, 0.921 s	463191022	808	57.06	1214.96	2737	XIC(57.06±500ppm)
1-Isopropoxy-2-trihexylsilyloxybenzene	1619.94, 1.107	12906226	712	307.18	1940	3878	XIC(307.18±500ppm)
1-Methoxy-2-propanol, TMS derivative	979.978 s, 1.473 s	27290990	758	117.02	979.978	1237	XIC(117.02±500ppm)
1-Methyl-10,18-bisnorabieta-8,11,13-triene	1794.93 s, 1.772 s	14415030	732	241.17	1794.93	794	XIC(241.17±500ppm)
1-Methyl-1H-1,2,4-triazole	1054.97, 0.919	77651255	733	83.07	1290.9	815	XIC(83.07±500ppm)
1-Methyl-4-p-tolynaphthalene	1824.92 s, 2.234 s	69390268	871	232.1	1824.92	1471	XIC(232.10±500ppm)
1-Methyl-5-mercaptopotetrazole	1524.94 s, 1.564 s	2025378129	798	116.13	1524.94	1175	XIC(116.13±500ppm)
1-Mono-cis-vaccenonylglycerol bis-trimethylsilyl ether	2134.9, 1.307	19966678	772	73.03	2626.7	832	XIC(73.03±500ppm)
1-Monomyrustin, 2TMS derivative	1929.92 s, 1.121 s	637135214	863	343.35	1929.92	10066	XIC(343.35±500ppm)
1-Monopalmitin, 2TMS derivative	2039.91 s, 1.185 s	924232031	840	73.01	2039.91	3479	XIC(73.01±500ppm)
1-Naphthalenecarbonitrile	1269.96 s, 2.120 s	5764898	746	153.04	1269.96	947	XIC(153.04±500ppm)
1-Naphthalenemethanol, 1,2,3,4-tetrahydro-8-methyl-	1789.93 s, 1.891 s	16491667	755	145.08	1789.93	1114	XIC(145.08±500ppm)
1-Nonadecene	2349.89, 1.563	55536998	703	69.05	2913.4	716	XIC(69.05±500ppm)
1-Nonene, 4,6,8-trimethyl-	869.985 s, 0.865 s	108374216	838	57.06	869.985	7388	XIC(57.06±500ppm)
1-Octacosanol, TMS derivative	2324.89, 1.681	15607654	753	75.01	2880.1	531	XIC(75.01±500ppm)
1-Octadecanol	1724.93, 1.256	546594812	948	43.05	2080	5118	XIC(43.05±500ppm)
1-Octadecanol, TBDMS derivative	1774.93, 1.011	64232308	795	327.39	2146.7	684	XIC(327.39±500ppm)
1-Octadecanol, TMS derivative	1769.93 s, 1.046 s	251484274	854	75.01	1769.93	2738	XIC(75.01±500ppm)
1-Octanol, 2,2-dimethyl-	784.991 s, 2.179 s	237898072	861	43.06	784.991	716	XIC(43.06±500ppm)

1-Octanol, 2-butyl-	934.981 s, 0.851 s	17319481	783	57.06	934.981	2774	XIC(57.06±500ppm)
1-Octanol, TMS derivative	939.981 s, 0.864 s	160675373	813	75.01	939.981	2113	XIC(75.01±500ppm)
1-Octene, 3,7-dimethyl-	1014.98, 0.891	117200627	736	55.05	1254.5	916	XIC(55.05±500ppm)
1-Oxa-3,4-diazacyclopentadiene	2184.9, 0.670	123392580	738	42.03	2693.4	509	XIC(42.03±500ppm)
1-Pentadecanol, TBDMS derivative	1539.94 s, 0.866 s	34276282	733	285.23	1539.94	7323	XIC(285.23±500ppm)
1-Pentadecanol, TMS derivative	1564.94 s, 0.987 s	43855807	786	75.01	1564.94	1703	XIC(75.01±500ppm)
1-Pentanol, 2,2,4-trimethyl-	2054.91, 1.284	273160855	742	43.06	2520	548	XIC(43.06±500ppm)
1-Pentanol, 3-methyl-	1799.93, 1.094	161794844	741	41.04	2180	1135	XIC(41.04±500ppm)
1-Pentene, 2,3,3-trimethyl-	1884.92 s, 1.124 s	241265063	745	55.05	1884.92	1508	XIC(55.05±500ppm)
1-Pentene, 2,4,4-trimethyl-	1389.95 s, 0.964 s	749947566	747	57.07	1389.95	1045	XIC(57.07±500ppm)
1-Pentene, 3-ethyl-2-methyl-	1069.97 s, 0.916 s	179920406	784	55.05	1069.97	4042	XIC(55.05±500ppm)
1-Pentyn-1-ol, 4-methyl-	849.987, 0.883	86344844	707	69.05	1108.7	952	XIC(69.05±500ppm)
1-Phenanthrenecarboxylic acid, 1,2,3,4,4a,9,10,10a-octahydro-1,4a-dimethyl-, methyl ester	1804.93 s, 2.135 s	71720748	744	257.12	1804.93	3945	XIC(257.12±500ppm)
1-Phenanthrenecarboxylic acid, 1,2,3,4,4a,9,10,10a-octahydro-1,4a-dimethyl-, methyl ester, [1S-(1α,2α,3α,4α,9α,10α,10aα)]	1804.93, 2.137	101359491	729	257.12	2186.7	4241	XIC(257.12±500ppm)
1-Phenyl-1,2-ethanediol, 2TMS derivative	1204.96 s, 1.021 s	69621044	875	73.03	1204.96	4728	XIC(73.03±500ppm)
1-Phenyl-2-butanone	989.978 s, 1.643 s	16614354	927	57.03	989.978	858	XIC(57.03±500ppm)
1-Phenyl-3-buten-1-ol, TMS derivative	1554.94, 1.351	111452341	762	73.04	1853.3	700	XIC(73.04±500ppm)
1-Phenylbicyclo(4.1.0)heptane	1374.95, 1.822	49605775	736	119.03	1629.4	1968	XIC(119.03±500ppm)
1-Phenylethanol, TBDMS derivative	894.984 s, 1.024 s	22090465	746	75.01	894.984	3073	XIC(75.01±500ppm)
1-Propanamine, N,N-diethyl-	759.992 s, 1.472 s	13278385	786	58.06	759.992	1237	XIC(58.06±500ppm)
1-Propanol, 2-(2-hydroxypropoxy)-	1734.93, 1.980	30547781	746	59.04	2093.3	823	XIC(59.04±500ppm)
1-Propanol, TMS derivative	1499.94 s, 1.146 s	1221604276	749	73.04	1499.94	5542	XIC(73.04±500ppm)
1-Propene, 3-(2-cyclopentenyl)-2-methyl-1,1-diphenyl-	2034.91, 2.304	161781701	763	207.1	2493.4	651	XIC(207.10±500ppm)
1-Propene-1-thiol	889.984 s, 0.970 s	93581371	773	73.03	889.984	1219	XIC(73.03±500ppm)
1-Tetracosanol, TBDMS derivative	2124.9, 1.235	57393804	755	43.06	2613.4	1134	XIC(43.06±500ppm)
1-Tetracosene	2524.88 s, 2.113 s	81953699	741	69.06	2524.88	932	XIC(69.06±500ppm)
1-Tetradecanol, TMS derivative	1489.95 s, 0.982 s	75528984	842	75	1489.95	1193	XIC(75.00±500ppm)
1-Tetradecene	1159.97 s, 0.961 s	432834336	937	55.05	1159.97	4904	XIC(55.05±500ppm)
1-Tetradecyl acetate	1804.93, 1.251	395753260	794	43.05	2186.7	2207	XIC(43.05±500ppm)
1-Tridecanol, TMS derivative	1409.95, 0.961	89148687	714	70.09	1670.6	1053	XIC(70.09±500ppm)
1-Tridecene	1829.92, 1.090	138802012	732	55.06	2220	728	XIC(55.06±500ppm)
1-Undecanol, TMS derivative	1129.97, 0.881	19686568	744	75.02	1365	832	XIC(75.02±500ppm)
1-Undecene, 4-methyl-	1484.95 s, 0.955 s	613320660	832	71.05	1484.95	4788	XIC(71.05±500ppm)
1-Undecene, 7-methyl-	1069.97, 0.924 s	354220833	783	69.06	1305	5646	XIC(69.06±500ppm)
2-(1,1-Dimethylethyl)-6-(1-methylethyl)phenol	1214.96, 1.460	3566255	715	177.07	1452.6	500	XIC(177.07±500ppm)
2(1H)-Naphthalenone, 3,4,4a,5,6,7-hexahydro-1,1,4a-trimethyl-	954.98 s, 1.068 s	19174211	798	41.05	954.98	2736	XIC(41.05±500ppm)
2(1H)-Pyridinone	769.992, 3.492	20675613	891	95.02	1048.1	1025	XIC(95.02±500ppm)
2-(2-(2-Ethoxyethoxy)ethoxy)ethyl benzoate	1539.94 s, 1.509 s	367904330	764	149.04	1539.94	6142	XIC(149.04±500ppm)
2-(2-Methoxyethoxy)ethanol, TMS derivative	849.987 s, 1.068 s	61855319	841	59.04	849.987	1740	XIC(59.04±500ppm)
2-(2-Naphthyl)-1,2-propanediol	1514.94, 1.438	42435385	752	171.09	1800	2161	XIC(171.09±500ppm)
2-(2-Trimethylsilyloxy-5-methylphenyl)benzotriazole	1754.93 s, 1.876 s	13802507	817	282.08	1754.93	2550	XIC(282.08±500ppm)
2(3H)-Furanone, 5-butylidihydro-	1024.98 s, 1.753 s	8678039	813	85.01	1024.98	571	XIC(85.01±500ppm)
2(3H)-Furanone, 5-dodecylidihydro-	1739.93 s, 1.638 s	55943019	828	85.01	1739.93	1244	XIC(85.01±500ppm)
2(3H)-Furanone, 5-heptyldihydro-	1334.96 s, 1.619 s	15443084	752	85.02	1334.96	1591	XIC(85.02±500ppm)
2(3H)-Furanone, 5-hexylidihydro-	1234.96 s, 1.670 s	10725909	768	85.01	1234.96	928	XIC(85.01±500ppm)
2(3H)-Furanone, dihydro-3-hydroxy-4,4-dimethyl-, (±)-	1524.94, 0.972	523957249	748	71.06	1813.3	3272	XIC(71.06±500ppm)
2(3H)-Furanone, dihydro-5-pentyl-	1134.97 s, 1.695 s	18482581	903	85.01	1134.97	1667	XIC(85.01±500ppm)
2(3H)-Furanone, dihydro-5-tetradecyl-	1879.92 s, 1.675 s	529023625	856	84.99	1879.92	818	XIC(84.99±500ppm)
2-(4-Methoxyphenyl)-2-(3'-methyl-4'-methoxyphenyl)propane	1739.93 s, 2.005 s	5422911	727	255.11	1739.93	1017	XIC(255.11±500ppm)
2(5H)-Furanone, 3,5,5-trimethyl-	744.993, 1.542	6212866	762	43.02	1029.6	645	XIC(43.02±500ppm)
2(5H)-Furanone, 5-(acetyloxy)-	1719.93, 1.153	141772330	711	83.06	2073.3	1574	XIC(83.06±500ppm)
2-(Methylmercapto)benzothiazole	1364.95 s, 2.162 s	13088378	916	180.98	1364.95	2525	XIC(180.98±500ppm)
2-(p-Tolylmethyl)-p-xylene	1504.94 s, 1.747 s	21059371	768	104.05	1504.94	942	XIC(104.05±500ppm)
2'-(Tert.-butyldimethylsilyloxy)-2,3,6'-trimethoxychalcone	2314.89, 4.039	393908800	716	371.16	2866.7	3893	XIC(371.16±500ppm)
2'-(Tert.-butyldimethylsilyloxy)-3,4,5'-trimethoxychalcone	2314.89 s, 4.030 s	251414948	754	371.16	2314.89	13431	XIC(371.16±500ppm)
2,2',4,5'-Tetrachloro-1,1'-biphenyl	1649.94, 1.911	2777473	812	291.89	1980	1532	XIC(291.89±500ppm)
2,2,5,5-Tetramethyl-3,4-diphenyl-1-oxa-2,5-disilacyclopent-3-ene	1754.93, 1.602	5135833	734	295.13	2120	900	XIC(295.13±500ppm)
2,2'-Bi-1,3-oxathiolane, 2-methyl-	1099.97, 1.393	22378834	759	103.06	1335	879	XIC(103.06±500ppm)
2,2'-Bifuran, octahydro-	849.987, 0.830	181301161	716	41.03	1108.7	2169	XIC(41.03±500ppm)
2,2'-Biphenylphenolphosphoric acid	2169.9, 2.036	414654365	741	248.17	2673.4	4189	XIC(248.17±500ppm)
2,2'-Bipyridine	1214.96 s, 2.024 s	13747699	911	156.05	1214.96	987	XIC(156.05±500ppm)
2,2'-Bipyrrolidine	1019.98 s, 0.908 s	57061560	793	70.06	1019.98	884	XIC(70.06±500ppm)
2,2-Diallylpyrrolidine	974.979 s, 2.032 s	13294135	758	110.04	974.979	2189	XIC(110.04±500ppm)
2,2-Diisopropyl-1,3-dioxolane	2229.9 s, 1.789 s	139788287	731	115.02	2229.9	4152	XIC(115.02±500ppm)
2,2'-Dimethylbiphenyl	1339.96 s, 1.665 s	11725217	789	167.07	1339.96	1195	XIC(167.07±500ppm)
2,2-Dimethylpropane-1,3-diol, O,O'-bis(trimethylsilyl)-	834.988 s, 0.762 s	36861806	730	75.01	834.988	1410	XIC(75.01±500ppm)
2,2-Dimethylpropanoic anhydride	1104.97 s, 1.935 s	6984644	805	57.07	1104.97	648	XIC(57.07±500ppm)
2,2-Dimethylpropionic acid, 4-methylpentyl ester	814.989, 2.205	148523662	754	57.07	1081.5	2436	XIC(57.07±500ppm)
2,2-Dimethyl-propyl 2,2-dimethyl-propanesulfonfyl sulfone	789.99, 2.217	113637411	715	57.03	1063	1084	XIC(57.03±500ppm)
2,2'-Isopropylidenebis(5-methylfuran)	1199.96 s, 1.369 s	20046423	768	189.11	1199.96	2168	XIC(189.11±500ppm)
2,2'-Isopropylidenebis(6-methoxy-3-methylbenzofuran)	2189.9 s, 2.857 s	2329853	742	364.11	2189.9	525	XIC(364.11±500ppm)
2,3,3-Trimethyl-1-hexene	864.986, 0.889	117685964	741	55.05	1121.7	1312	XIC(55.05±500ppm)
2,3,4,6-Tetramethoxystyrene	1189.96, 1.224	2329263	758	224.1	1426.3	534	XIC(224.10±500ppm)
2,3,4-Trifluorobenzoic acid, 4-nitrophenyl ester	1049.97 s, 0.955 s	27317882	728	159.1	1049.97	1043	XIC(159.10±500ppm)
2,3-Butanediol, 2TMS derivative	779.991 s, 0.771 s	102872093	836	117.05	779.991	4927	XIC(117.05±500ppm)
2,3-Dihydroxy-2-methylpropanoic acid, 3TMS derivative	1169.97, 0.826	507819547	740	73.04	1405.3	5409	XIC(73.04±500ppm)
2,3-Dihydroxypropyl icosanoate, 2TMS derivative	2244.9 s, 1.413 s	129573635	761	73.03	2244.9	3280	XIC(73.03±500ppm)
2,3-Dimethyl-1-hexene	1654.94 s, 1.074 s	140455682	771	70.07	1654.94	2711	XIC(70.07±500ppm)
2,3-Dimethylenetricyclo[9.2.2.2(4,7)]heptadeca-1(14),4(17),5,7(16),11(15),12-hexaene	1874.92 s, 2.073 s	3416341	747	246.11	1874.92	6413	XIC(246.11±500ppm)
2,3'-Dipyridyl	1304.96, 2.180	15436964	848	156.05	1550	1877	XIC(156.05±500ppm)
2,3-Naphthalenediamine, 2TMS derivative	1324.96 s, 1.087 s	17330627	741	73.06	1572.2	862	XIC(73.06±500ppm)

2,3-Octanedione	684.997 s, 1.528 s	10776424	733	43.04	985.2	839	XIC(43.04±500ppm)
2,3-Pentanedione	1494.95 s, 0.964 s	379395449	747	43.06	1494.95	886	XIC(43.06±500ppm)
2,4,4-Trimethyl-1-pentanol, TMS derivative	769.992 s, 0.804 s	86835171	783	103.04	769.992	2471	XIC(103.04±500ppm)
2,4,4-Trimethyl-3-(3-methylbutyl)cyclohex-2-enone	1114.97 s, 1.328 s	35632348	735	138.05	1114.97	2528	XIC(138.05±500ppm)
2',4',5'-Trimethoxyacetophenone	1139.97, 1.259	74664224	748	210.09	1375	2552	XIC(210.09±500ppm)
2,4,6(1H,3H,5H)-Pyrimidinotriene, 5-ethyl-1,3-dimethyl-5-(1-methylpropyl)-	1439.95 s, 1.736 s	21051815	734	184.1	1439.95	1419	XIC(184.10±500ppm)
2,4,6,8-Tetramethyl-1-undecene	1659.93, 1.213	294425231	739	43.04	1993.3	2002	XIC(43.04±500ppm)
2,4,6-Tris(1,1-dimethylethyl)-4-methylcyclohexa-2,5-dien-1-one	1749.93 s, 2.016 s	14789988	736	220.08	1749.93	835	XIC(220.08±500ppm)
2,4,7,9-Tetramethyl-5-decyne-4,7-diol, 2TMS derivative	1334.96 s, 0.849 s	94258034	791	73.03	1334.96	4014	XIC(73.03±500ppm)
2,4,8-Trimethyl-1,2,3,4-tetrahydroquinoline	1189.96 s, 1.597 s	7050569	745	160.1	1189.96	863	XIC(160.10±500ppm)
2,4-Diamino-8-hydroxy-5-propyl-5H-chromeno[2,3-b]pyridine-3-carbonitrile	1609.94, 1.016	6558193	716	253.27	1926.7	864	XIC(253.27±500ppm)
2,4-Dichlorobenzyl alcohol, TBDMS derivative	1234.96 s, 1.202 s	5080902	756	232.97	1234.96	1733	XIC(232.97±500ppm)
2,4-Dicyanopyrrole	774.991, 0.761	106366469	725	117.05	1051.9	1453	XIC(117.05±500ppm)
2,4'-Dihydroxydiphenyl sulfone, 2TMS derivative	1894.92, 1.401	1925621	762	379.27	2306.7	879	XIC(379.27±500ppm)
2,4-Diphenyl-4-methyl-1-pentene	1524.94, 1.684	36779615	737	119.07	1813.3	1281	XIC(119.07±500ppm)
2,4-Diphenyl-4-methyl-2[E]-pentene	1554.94 s, 1.666 s	44537989	737	105.05	1554.94	1308	XIC(105.05±500ppm)
2,4-Disilapentane, 2,4-dimethyl-	889.984, 0.949	64582169	741	117.06	1143.5	877	XIC(117.06±500ppm)
2,4-Di-tert-butylphenol	1294.96 s, 1.319 s	222686151	902	191.12	1294.96	7548	XIC(191.12±500ppm)
2,4-Di-tert-butylphenoxytrimethylsilane	1304.96 s, 1.084 s	324478883	875	263.16	1304.96	6543	XIC(263.16±500ppm)
2,4-Thiazolidinedione	1679.93, 1.936	379316120	752	117.05	2020	2847	XIC(117.05±500ppm)
2,5,8,11,14-Pentaoxaheptadecan-16-ol	1754.93, 2.005	152392031	811	45.04	2120	1310	XIC(45.04±500ppm)
2,5,8,11-Tetraoxadodecane	1739.93, 1.959	153215651	752	59.04	2100	535	XIC(59.04±500ppm)
2,5-Cyclohexadiene-1,4-dione, 2,6-bis(1,1-dimethylethyl)-	1239.96 s, 1.319 s	191426543	922	177.1	1239.96	3829	XIC(177.10±500ppm)
2,5-Dichlorophenol, trimethylsilyl ether	1139.97 s, 1.204 s	5352634	784	92.98	1139.97	879	XIC(92.98±500ppm)
2,5-Dihydroxybenzaldehyde, 2TMS derivative	854.986 s, 0.802 s	4024583	734	267	1113	727	XIC(267.00±500ppm)
2,5-Dimethoxy-4-methylamphetamine, N-(trimethylsilyl)-	1519.94 s, 1.113 s	224032333	754	116.15	1519.94	2051	XIC(116.15±500ppm)
2,5-Dimethoxy-4-methylbenzonitrile	1334.96 s, 2.028 s	12442099	773	162.04	1334.96	1075	XIC(162.04±500ppm)
2,5-Dimethoxybenzonitrile	1264.96 s, 2.050 s	5566992	892	148.02	1264.96	786	XIC(148.02±500ppm)
2,5-Dimethoxyethylbenzene	1089.97 s, 1.532 s	50392024	833	151.05	1089.97	5201	XIC(151.05±500ppm)
2,5-Dimethoxymandelic acid, di-TMS	1784.93 s, 0.870 s	27643513	744	239.08	1784.93	1293	XIC(239.08±500ppm)
2,5-Dimethoxyphenol, TMS	1209.96 s, 1.381 s	13222578	753	196.03	1209.96	3211	XIC(196.03±500ppm)
2',5'-Dimethyl-p-terphenyl	1939.92, 2.312	8983809	732	258.12	2366.7	1090	XIC(258.12±500ppm)
2,5-Diphenyl-2,4-hexadiene	1689.93 s, 2.016 s	10177279	767	219.1	1689.93	596	XIC(219.10±500ppm)
2,5-di-tert-Butyl-1,4-benzoquinone	1684.93 s, 1.899 s	54877206	761	57.06	1684.93	2168	XIC(57.06±500ppm)
2,5-Di-tert-butylhydroquinone, O-pentafluoropropionyl-	2089.91 s, 2.797 s	31317505	756	83.03	2089.91	1034	XIC(83.03±500ppm)
2,5-Hexanediol, 2TMS derivative	979.978 s, 0.816 s	28510848	737	117.05	979.978	1649	XIC(117.05±500ppm)
2,6,10-Trimethyltridecane	1109.97, 0.906	1502147130	858	71.07	1345	9731	XIC(71.07±500ppm)
2,6,8-Trimethyl-4-nonyl acetate	1999.91, 1.066	317807849	719	43.06	2446.7	1343	XIC(43.06±500ppm)
2,6-Bis(1,1-dimethylethyl)-4-cyanomethylphenol	1414.95 s, 1.382 s	24590925	744	230.13	1414.95	1138	XIC(230.13±500ppm)
2,6-Bis(tert-butyl)phenol, TMS derivative	1309.96, 1.078	625343790	818	73	1555.6	2825	XIC(73.00±500ppm)
2,6-Di(2-furylmethylidene)cyclohexan-1-one	1814.92 s, 1.882 s	22399169	734	254.24	2200	1958	XIC(254.24±500ppm)
2,6-Dihydroxyacetophenone, 2TMS derivative	1284.96 s, 1.042 s	35354528	768	73.06	1527.8	3305	XIC(73.06±500ppm)
2,6-Diisopropylinaphthalene	1429.95 s, 1.516 s	475195612	881	197.11	1429.95	12598	XIC(197.11±500ppm)
2,6-Dimethyl-6-nitro-2-hepten-4-one	1489.95 s, 1.095	134111021	732	83.07	1768.8	2265	XIC(83.07±500ppm)
2,6-Dimethyl-6-trifluoroacetoxyoctane	809.989 s, 0.838 s	97654675	750	43.06	809.989	1627	XIC(43.06±500ppm)
2,6-Dimethyldecan-1-one	1274.96, 0.940	614998295	827	57.07	1516.7	5621	XIC(57.07±500ppm)
2,7-Dimethyldibenzothiophene	1664.93 s, 2.143 s	11660872	810	212.05	1664.93	1210	XIC(212.05±500ppm)
2,8-Dimethyldibenzo[b,d]thiophene	1664.93, 2.137	139548001	762	212.05	2000	1226	XIC(212.05±500ppm)
2-[[Trimethylsilyloxy]propan-1-ol	1409.95 s, 1.320	95286555	743	73.03	1670.6	1266	XIC(73.03±500ppm)
2-[1-(4-Cyano-1,2,3,4-tetrahydro-naphthyl)]propanenitrile	1659.93, 1.780	10892243	801	129.06	1993.3	568	XIC(129.06±500ppm)
2-[2-[2-[2-[2-[2-(2-Hydroxyethoxy)ethoxy]ethoxy]ethoxy]ethoxy]ethoxy]ethanol	2214.9, 3.511	339257842	921	45.04	2733.4	2436	XIC(45.04±500ppm)
2-[2-[2-[2-[2-[2-(2-Methoxyethoxy)ethoxy]ethoxy]ethoxy]ethoxy]ethoxy]ethanol	1924.92, 2.042	59496532	728	45.03	2346.7	791	XIC(45.03±500ppm)
2-[2-[2-[2-[2-[2-(2-Hydroxyethoxy)ethoxy]ethoxy]ethoxy]ethoxy]ethoxy]ethoxy]ethanol	2579.88 s, 1.662 s	27325345	820	45.04	2579.88	666	XIC(45.04±500ppm)
2-[[tert-Butyl(dimethyl)silyloxy]ethanol	809.989, 0.966	64110176	802	75.01	1077.8	569	XIC(75.01±500ppm)
2-Acetyl-3,5-dimethylbenzo(b)thiophene	1199.96, 1.374	24041890	732	189.1	1436.8	1938	XIC(189.10±500ppm)
2-Acetyl-5-methylthiophene	1014.98 s, 1.222 s	10601624	749	125.05	1014.98	1043	XIC(125.05±500ppm)
2-Allyl-1,4-dimethoxy-3-methyl-benzene	1224.96, 1.549	9992830	775	192.1	1463.2	1810	XIC(192.10±500ppm)
2-Allyl-1,4-dimethoxy-3-vinyloxymethylbenzene	2224.9, 3.640	136429088	741	151.06	2746.7	2967	XIC(151.06±500ppm)
2-Allyl-1,4-dimethoxybenzene	1204.96 s, 1.642 s	6361430	799	178.08	1204.96	1312	XIC(178.08±500ppm)
2-Aminoethanol, N-acetyl-, O-TMS	974.979, 1.386	9505823	770	73.04	1218.2	674	XIC(73.04±500ppm)
2-Benzyloxyphenylacetic acid	1669.93 s, 1.927 s	44770282	744	91.04	1669.93	1353	XIC(91.04±500ppm)
2-Bromoamphetamine, N-TMS	1909.92 s, 1.287 s	34762625	727	116.05	1909.92	1740	XIC(116.05±500ppm)
2-Bromotetradecane	959.98 s, 0.837 s	85309059	805	57.15	959.98	675	XIC(57.15±500ppm)
2-Butanol, TMS derivative	1294.96 s, 0.868 s	82701618	771	131.07	1294.96	1203	XIC(131.07±500ppm)
2-Butanone, 1,1,1-trifluoro-	2044.91 s, 1.113 s	155268432	789	57.06	2044.91	1212	XIC(57.06±500ppm)
2-Butanone, 4-[2-methyl-1,3-dioxolan-2-yl]-	909.983 s, 1.578 s	7257790	844	43.03	909.983	722	XIC(43.03±500ppm)
2-Buten-1-one, 1,3-diphenyl-	1764.93, 2.244	8650914	733	207.06	2133.3	603	XIC(207.06±500ppm)
2-Butenedioic acid (E)-, dibutyl ester	1334.96 s, 1.283 s	32486047	828	117	1334.96	1406	XIC(117.00±500ppm)
2-Butenedioic acid (Z)-, dibutyl ester	1294.96 s, 1.496 s	126828835	926	98.99	1294.96	5941	XIC(98.99±500ppm)
2-Butyl-3,4,5,6-tetrahydropyridine	1614.94 s, 1.111 s	164692465	742	97.09	1614.94	1025	XIC(97.09±500ppm)
2-Chlorohydrocinnamonitrile	1569.94, 1.828	446000901	743	125.01	1873.3	1243	XIC(125.01±500ppm)
2-Cyano-2-O-fluorosulfatofluoropropane	1209.96, 0.941	90214750	746	69.06	1447.4	627	XIC(69.06±500ppm)
2-Cyano-4-phenylpentane	1599.94, 1.265	53404783	705	105.05	1913.3	4188	XIC(105.05±500ppm)
2-Cyclohexen-1-one, 3,5-dimethyl-	849.987 s, 1.611 s	22983135	899	82.03	849.987	1154	XIC(82.03±500ppm)
2-Cyclohexen-1-one, 3-methyl-	799.99, 1.681	4513330	828	82.03	1070.4	523	XIC(82.03±500ppm)
2-Cyclohexene-1,4-dione, 5,6-dichloro-2,3-dimethyl-, 1-oxime, o-benzoyl-	1524.94, 1.243	392940914	793	105.06	1813.3	2082	XIC(105.06±500ppm)
2-Cyclopenten-1-one, 2,3,4,5-tetramethyl-	1049.97 s, 1.228 s	40638281	757	123.06	1049.97	3381	XIC(123.06±500ppm)
2-Cyclopenten-1-one, 3-methyl-	1084.97 s, 1.953 s	3502211	749	96.04	1084.97	553	XIC(96.04±500ppm)
2-Decanone	949.98 s, 1.167 s	12438166	772	58.03	949.98	1010	XIC(58.03±500ppm)
2-Decanone, 5,9-dimethyl-	1064.97 s, 1.124 s	131599691	846	43.03	1064.97	1527	XIC(43.03±500ppm)
2-Dodecane, (Z)-	814.989, 2.197	187135227	769	43.06	1081.5	2147	XIC(43.06±500ppm)

2-Dodecene, 4-methyl-	1279.96 s, 0.947 s	110039695	745	41.04	1279.96	982	XIC(41.04±500ppm)
2-Ethyl-1-cyclohexyldimethylsilyloxyhexane	1174.97 s, 0.860 s	10382437	758	187.13	1174.97	2202	XIC(187.13±500ppm)
2-Ethyl-5-methyl-3,3-diphenylpyrrolidine	1434.95, 1.759	11996087	725	130.06	1700	1745	XIC(130.06±500ppm)
2-Ethylbutyric acid, tetrahydrofurfuryl ester	1339.96 s, 1.185 s	40717675	738	71.05	1339.96	561	XIC(71.05±500ppm)
2-Ethylhexanal ethylene glycol acetal	884.984 s, 0.850 s	58478308	731	73.03	884.984	846	XIC(73.03±500ppm)
2-Ethylhexanoic acid, TBDMS derivative	1149.97 s, 0.817 s	249350648	734	201.14	1149.97	23854	XIC(201.14±500ppm)
2-Ethylhexanol, TMS derivative	849.987 s, 2.158 s	1393079760	896	75.01	849.987	1367	XIC(75.01±500ppm)
2-Ethylhexyl 2-ethylhexanoate	1354.95 s, 1.095 s	173219271	756	57.06	1354.95	4754	XIC(57.06±500ppm)
2-Ethylhexyl acrylate	1559.94, 1.101	315439985	738	55.06	1860	854	XIC(55.06±500ppm)
2-Ethylhexyl methyl isophthalate	1759.93, 1.565	10941858	752	70.07	2126.7	568	XIC(70.07±500ppm)
2-Ethylhexyl salicylate	1529.94, 1.400	16053320	750	120.01	1820	552	XIC(120.01±500ppm)
2-Fluoro-6-trifluoromethylbenzoic acid, 2,3,4,6-tetrachlorophenyl ester	1284.96 s, 0.866 s	208797875	747	191.06	1284.96	761	XIC(191.06±500ppm)
2-Fluorobenzylamine, diundecyl	2284.89, 2.695	3917937	755	292.2	2826.7	1602	XIC(292.20±500ppm)
2-Furaldehyde diethyl acetal	819.988 s, 1.217 s	8806060	877	97.01	819.988	769	XIC(97.01±500ppm)
2-Furoic acid, TMS derivative	884.984 s, 1.286 s	19488903	759	125.06	1139.1	6273	XIC(125.06±500ppm)
2H-1-Benzopyran-2-one, 7-(diethylamino)-	1604.94 s, 2.054 s	211328980	756	202.07	1604.94	6950	XIC(202.07±500ppm)
2H-2,4a-Methanonaphthalene, 1,3,4,5,6,7-hexahydro-1,1,5,5-tetramethyl-, (2S)-	1169.97 s, 1.178 s	14033708	833	161.11	1169.97	2160	XIC(161.11±500ppm)
2-Heptanol, TBDMS derivative	1719.93 s, 1.342 s	22535965	749	173.05	1719.93	1507	XIC(173.05±500ppm)
2-Heptanol, TMS derivative	689.997, 0.878	15783311	752	73.03	988.9	1503	XIC(73.03±500ppm)
2-Heptanone, 4,6-dimethyl-	714.995, 1.038	53469646	887	43.03	1007.4	1042	XIC(43.03±500ppm)
2-Heptanone, 4-methyl-	939.981 s, 1.095 s	150694946	735	43.03	939.981	2322	XIC(43.03±500ppm)
2-Heptenoic acid, tridec-2-yn-1-yl ester	959.98 s, 1.497 s	28543380	737	111.04	959.98	1529	XIC(111.04±500ppm)
2-Hexene, 3,5-dimethyl-	1244.96, 0.938	188210854	755	55.06	1484.2	1613	XIC(55.06±500ppm)
2-Hexenoic acid, (E)-, TMS derivative	969.979 s, 1.396 s	1856720	757	75.01	969.979	566	XIC(75.01±500ppm)
2-Hexyl-1-octanol	1294.96, 0.937	1911253873	843	57.06	1538.9	3686	XIC(57.06±500ppm)
2-Hexyldodecanol, TMS derivative	1774.93, 1.026	104231959	728	74.97	2146.7	1164	XIC(74.97±500ppm)
2H-Pyran-2-one, 5,6-dihydro-4,6,6-trimethyl-	979.978 s, 1.871 s	5179682	733	82.03	979.978	597	XIC(82.03±500ppm)
2H-Pyran-2-one, tetrahydro-6-undecyl-	1764.93 s, 1.710 s	9826649	737	99.03	1764.93	584	XIC(99.03±500ppm)
2-Hydroxy-2-methyl-1-phenylpropan-1-one, TMS derivative	1189.96 s, 1.261 s	544515971	901	73.04	1189.96	11798	XIC(73.04±500ppm)
2-Hydroxy-2-methylbutyric acid, 2TMS derivative	889.984 s, 0.834 s	3692398	740	145.12	1143.5	1556	XIC(145.12±500ppm)
2-Hydroxy-5-methoxybenzaldehyde, TBDMS derivative	1389.95, 1.469	12011087	707	209.04	1647.1	1270	XIC(209.04±500ppm)
2-Hydroxyanthraquinone, trimethylsilyl ether	1959.92 s, 2.499 s	10281938	750	281.09	1959.92	1761	XIC(281.09±500ppm)
2-Hydroxy-iso-butylphenone	1054.97 s, 1.644 s	25296529	850	59.04	1054.97	1594	XIC(59.04±500ppm)
2-Hydroxyphenethyl alcohol, 2TMS derivative	1364.95 s, 1.117 s	39082393	752	73.03	1364.95	2895	XIC(73.03±500ppm)
2-Imino-6-mercapto-4,4-dimethyl-1,2,3,4-tetrahydro-pyridine-3,5-dicarbonitrile	1284.96 s, 0.741 s	163914021	743	191.07	1284.96	961	XIC(191.07±500ppm)
2-Isopropyl-5-methyl-1-heptanol	1069.97 s, 2.165 s	53835276	826	43.06	1069.97	1452	XIC(43.06±500ppm)
2-Ketobutyric acid eo-tms	934.981, 1.000	120174369	741	73.03	1182.6	2028	XIC(73.03±500ppm)
2-Mercapto-4,6-dimethylnicotinonitrile, TBDMS derivative	919.982 s, 0.787 s	8328819	746	221.06	919.982	576	XIC(221.06±500ppm)
2-Methoxy-1,3-dioxolane	1484.95, 1.347	1036082683	742	73.03	1762.5	936	XIC(73.03±500ppm)
2-Methoxy-5-methylphenol, 2-methylpropyl ether	1079.97 s, 1.217 s	12232642	744	123.06	1079.97	845	XIC(123.06±500ppm)
2-Methoxybenzoic acid, 2,4,6-trichlorophenyl ester	2379.89, 0.669	12612187	732	135.05	2953.4	506	XIC(135.05±500ppm)
2-Methyl-1,2-bis(trimethylsilyloxy)butane	864.986, 0.763	80438562	886	73.04	1121.7	2922	XIC(73.04±500ppm)
2-Methyl-1,3-butanediol, 2TMS derivative	859.986 s, 0.768 s	68238384	754	73.03	859.986	1999	XIC(73.03±500ppm)
2-Methyl-1,4-bis(trimethylsilyloxy)butane	954.98 s, 0.837 s	37213741	745	147.04	954.98	1037	XIC(147.04±500ppm)
2-Methyl-1-dimethyl(octyl)silyloxypropane	1074.97, 0.844	13424728	711	131.07	1310	1099	XIC(131.07±500ppm)
2-Methyl-1-pentanol, TMS derivative	989.978, 0.833	130046607	737	73.04	1231.8	5375	XIC(73.04±500ppm)
2-Methyl-1-undecanol	1049.97 s, 0.946 s	84017215	830	43.06	1049.97	3286	XIC(43.06±500ppm)
2-methyl-3-((trimethylsilyl)ethynyl)cyclopent-2-en-1-one	1214.96, 1.460	4642760	734	177.07	1452.6	695	XIC(177.07±500ppm)
2-Methyl-3-buten-2-ol, TMS derivative	1159.97 s, 0.910 s	21926001	745	73.03	1159.97	1397	XIC(73.03±500ppm)
2-Methylbenzoic acid, 2,3-dichlorophenyl ester	1984.91 s, 2.249 s	14957249	772	119.03	1984.91	680	XIC(119.03±500ppm)
2-Methylbenzoic acid, 2-fluorophenyl ester	1439.95, 2.126	5857383	757	119.04	1706.2	546	XIC(119.04±500ppm)
2-Methylbenzyl alcohol, TMS derivative	1009.98 s, 1.149 s	19930536	765	105.05	1009.98	1148	XIC(105.05±500ppm)
2-Methylbutanoic acid, TMS derivative	1264.96, 0.854	43416720	718	73.03	1505.6	845	XIC(73.03±500ppm)
2-Methyldibenzothiophene	1589.94 s, 2.163 s	17656045	739	198.03	1589.94	2201	XIC(198.03±500ppm)
2-Methylheptanoic acid	1609.94, 1.211	498648360	743	74.02	1926.7	3154	XIC(74.02±500ppm)
2-Methylpentan-2-ol, trimethylsilyl ether	1184.97, 0.970	26907533	714	131.07	1421	1393	XIC(131.07±500ppm)
2-Methylthiolane, S,S-dioxide	1719.93 s, 1.065 s	204208068	731	69.06	1719.93	1151	XIC(69.06±500ppm)
2-Mono-isobutyryn, 2TMS derivative	2124.9 s, 1.254 s	72063658	755	73.03	2124.9	1231	XIC(73.03±500ppm)
2-Monomyrustin, 2TMS derivative	1909.92 s, 1.110 s	67743549	837	73.03	1909.92	2575	XIC(73.03±500ppm)
2-Monostearin, 2TMS derivative	2129.9 s, 1.304 s	488065650	834	129.01	2129.9	1154	XIC(129.01±500ppm)
2-Naphthalenecarbonitrile	1269.96, 2.123	10230637	782	153.04	1511.1	837	XIC(153.04±500ppm)
2-Naphthyl methyl ketone	1374.95 s, 2.089 s	5977352	868	127.04	1374.95	733	XIC(127.04±500ppm)
2-n-Hexylthiolane, S,S-dioxide	1124.97 s, 0.938 s	69113655	745	55.05	1124.97	857	XIC(55.05±500ppm)
2-Nonen-4-one	2009.91, 1.198	113713383	732	69.06	2460	564	XIC(69.06±500ppm)
2-Nonene, (E)-	1539.94, 1.429	29298635	717	55.05	1833.3	512	XIC(55.05±500ppm)
2-n-Propylthiolane, S,S-dioxide	969.979 s, 0.883 s	15959596	741	56.06	969.979	1239	XIC(56.06±500ppm)
2-Octanol, TMS derivative	1024.98, 0.922	698567811	768	117.06	1263.6	2510	XIC(117.06±500ppm)
2-Octen-4-one, 2-methoxy-	1819.92, 1.581	22535096	739	99.03	2206.7	966	XIC(99.03±500ppm)
2-Octene, 4-ethyl-, (E)-	1429.95, 1.031	180269693	746	55.05	1694.1	949	XIC(55.05±500ppm)
2-Oxo-6-phenyl-4-(4-hydroxyphenyl)-1,2-dihydropyrimidine	1304.96, 1.137	380308460	789	263.14	1550	640	XIC(263.14±500ppm)
2-Oxobicyclo(3.2.2)nona-3,6-dien-1-yl benzoate	1524.94, 1.235	314950558	718	105.03	1813.3	1559	XIC(105.03±500ppm)
2-Oxoctanoic acid, TMS derivative	1119.97 s, 1.445 s	14770340	747	73.03	1119.97	1016	XIC(73.03±500ppm)
2-Oxopentanoic acid, TMS derivative	1379.95, 0.884	29875670	748	73.04	1635.3	633	XIC(73.04±500ppm)
2-Palmitoylglycerol, 2TMS derivative	2024.91 s, 1.136 s	197433427	758	129.04	2024.91	967	XIC(129.04±500ppm)
2-Pentamethyldisilyloxybutane	1499.94 s, 0.881 s	225517469	739	73.03	1499.94	1256	XIC(73.03±500ppm)
2-Pentanol, TMS derivative	1264.96 s, 0.855 s	36210797	743	73.03	1264.96	702	XIC(73.03±500ppm)
2-Pentanone, 4-hydroxy-4-methyl-	1349.95 s, 1.197 s	136390602	755	43.03	1349.95	1294	XIC(43.03±500ppm)
2-Pentanone, 5,5-diethoxy-	909.983 s, 1.298 s	9995926	731	43.03	909.983	521	XIC(43.03±500ppm)
2-Pentene, 3,4,4-trimethyl-	1114.97 s, 0.928 s	125123578	717	55.05	1114.97	3031	XIC(55.05±500ppm)
2-Pentene, 3-methyl-	1054.97 s, 0.910 s	89587104	769	55.05	1054.97	3411	XIC(55.05±500ppm)
2-Phenazincarbonitrile, 7-amino-	2134.9, 2.246	714751788	734	220.37	2626.7	618	XIC(220.37±500ppm)

2-Phenylisopropanol, TMS derivative	984.978 s, 1.059 s	164081072	914	75.01	984.978	7333	XiC(75.01±500ppm)
2-Piperidinone, N-[4-bromo-n-butyl]-	1509.94 s, 1.169 s	77792089	730	55.05	1509.94	600	XiC(55.05±500ppm)
2-Propanol, 1-chloro-, phosphate (3:1)	1524.94, 1.762	22845994	824	124.99	1813.3	1690	XiC(124.99±500ppm)
2-Propanol, 1-hexyloxy-(1-piperidinyl)-	684.997, 1.149	17166179	755	98.03	985.2	1278	XiC(98.03±500ppm)
2-Propanone, 1-(4-hydroxy-3-methoxyphenyl)-	1429.95, 1.939	38369218	752	137.04	1694.1	1996	XiC(137.04±500ppm)
2-Propanone, 1,1,1-trifluoro-	2014.91, 1.270	61352172	734	43.03	2466.7	896	XiC(43.03±500ppm)
2-Propen-1-one, 1-(4-methylphenyl)-3-phenyl-	1764.93, 2.243	9197221	748	207.05	2133.3	622	XiC(207.05±500ppm)
2-Propen-1-one, 2-methyl-1-phenyl-	969.979 s, 1.559 s	12910843	826	105.02	969.979	861	XiC(105.02±500ppm)
2-Propenamamide, N,N-dimethyl-3-phenyl-	1364.95 s, 2.075 s	12102239	818	131.03	1364.95	856	XiC(131.03±500ppm)
2-Propenoic acid, 2,2,3,3,4,4,5,5,6,6,7,7,8,8,8-pentadecafluorooctyl ester	1784.93, 1.042	104004208	757	55.03	2160	611	XiC(55.03±500ppm)
2-Propenoic acid, 2-methyl-, 2,3-bis[[trimethylsilyloxy]propyl ester	1149.97, 0.821	290261638	741	201.15	1385	30330	XiC(201.15±500ppm)
2-Propenoic acid, 2-methyl-, 3,3,5-trimethylcyclohexyl ester	1099.97 s, 1.238 s	22883300	820	69.04	1099.97	791	XiC(69.04±500ppm)
2-Propenoic acid, 3-(2-hydroxyphenyl)-, (E)-	1214.96 s, 2.318 s	3308911	917	118.03	1214.96	910	XiC(118.03±500ppm)
2-Propenoic acid, 3-(4-methoxyphenyl)-, 2-ethylhexyl ester	1784.93 s, 1.777 s	33702283	757	178.04	1784.93	1611	XiC(178.04±500ppm)
2-Propenoic acid, 3-phenyl-, ethyl ester	1174.97 s, 1.574 s	15409721	829	131.03	1174.97	951	XiC(131.03±500ppm)
2-Propenoic acid, 3-phenyl-, phenyl ester, (E)-	1194.96, 1.225	77944343	720	131.06	1431.6	1451	XiC(131.06±500ppm)
2-Propenoic acid, anhydride	1664.93, 1.069	97680085	747	55.05	2000	701	XiC(55.05±500ppm)
2-Propenoic acid, ethenyl ester	1749.93, 1.081	112883347	744	55.04	2113.3	540	XiC(55.04±500ppm)
2-Propyl-1-pentanol, TMS derivative	849.987, 2.173	904637945	819	75.01	1108.7	2482	XiC(75.01±500ppm)
2-Propyl-1-pentanol, triethylsilyl ether	1029.98, 0.872	10353180	746	103.04	1268.2	909	XiC(103.04±500ppm)
2-Propyn-1-amine, N,N-diethyl-	854.986, 1.952	8375021	759	96.03	1113	982	XiC(96.03±500ppm)
2-Propynitrile, 3-fluoro-	1204.96 s, 0.926 s	80074495	845	69.06	1204.96	889	XiC(69.06±500ppm)
2-Pyrazoline, 1-isobutyl-3-methyl-	1424.95 s, 1.044 s	112728756	742	97.08	1424.95	1528	XiC(97.08±500ppm)
2-Pyrazoline, 1-isopropyl-3,4-dimethyl-	1014.98, 1.228	12808591	719	125.04	1254.5	1247	XiC(125.04±500ppm)
2-Pyrazoline-1-carboxaldehyde, 5-tert-butyl-5-hydroxy-3-methyl-	1124.97 s, 1.511 s	8525976	746	98.99	1124.97	944	XiC(98.99±500ppm)
2-Pyridinemethanol, TBDMS derivative	939.981, 1.238	2962600	732	166.05	1187	630	XiC(166.05±500ppm)
2-Pyrrolidinone	829.988 s, 2.073 s	27161323	936	85.03	829.988	759	XiC(85.03±500ppm)
2-Pyrrolidinone, 5,5-dimethyl-	869.985, 1.900	7941649	754	98.05	1126.1	658	XiC(98.05±500ppm)
2-Pyrrolidinone, TMS derivative	899.983 s, 1.406 s	494656517	931	142.05	899.983	6518	XiC(142.05±500ppm)
2-t-Butyl-1-methyl-3-phenyl-imidazolidin-4-one	1019.98 s, 1.073 s	324623918	806	175.13	1019.98	1687	XiC(175.13±500ppm)
2-t-Butyl-thiazolidine-3,4-dicarboxylic acid, dimethyl ester	1529.94, 0.839	3866879	737	204.07	1820	925	XiC(204.07±500ppm)
2-tert-Butoxytetrahydrofuran	684.997 s, 1.149 s	65018588	768	43.02	684.997	1108	XiC(43.02±500ppm)
2-tert-Butyl-4-ethylphenol, trimethylsilyl ether	1344.95 s, 1.226 s	13614005	728	235.09	1344.95	2444	XiC(235.09±500ppm)
2-Thiopheneacetic acid, oct-3-en-2-yl ester	1544.94, 1.069	143149539	725	97.08	1840	1375	XiC(97.08±500ppm)
2-Tridecanone	1154.97, 1.136	47734803	730	43.03	1390	1398	XiC(43.03±500ppm)
2-Trifluoromethylbenzoic acid, 2,3,4,6-tetrachlorophenyl ester	1084.97, 0.821	4298047	707	173.11	1320	914	XiC(173.11±500ppm)
2-Undecanethiol, 2-methyl-	1359.95, 0.996	219087222	739	41.04	1611.8	2030	XiC(41.04±500ppm)
2-Undecanone, 6,10-dimethyl-	1154.97 s, 1.127 s	38681162	766	43.03	1154.97	946	XiC(43.03±500ppm)
2-Undecen-4-ol	1664.93 s, 1.247 s	100618224	785	71.05	1664.93	806	XiC(71.05±500ppm)
2-Undecene, (E)-	1364.95, 0.993	262927331	710	55.05	1617.7	1758	XiC(55.05±500ppm)
2-Undecene, 5-methyl-	2809.86, 3.067	72607640	744	57.07	3526.8	629	XiC(57.07±500ppm)
3-(Acetyl)oxy-7,8,3'-trimethoxyflavone	1769.93, 1.055	171138667	751	327.51	2140	757	XiC(327.51±500ppm)
3,26-Dioxo-2,27-disilaocacosane, 2,2,4,25,27,27-hexamethyl-	1724.93, 1.004	36077967	740	117.05	2080	2017	XiC(117.05±500ppm)
3,3,5-Trimethylcyclohexan-1-ol, trimethylsilyl ether	894.984 s, 0.842 s	111242296	838	75.01	894.984	3668	XiC(75.01±500ppm)
3,3-Diethoxy-1-propanol	1329.96 s, 1.058 s	56029389	755	103.06	1329.96	3059	XiC(103.06±500ppm)
3,3'-Dimethylbiphenyl	1349.95 s, 1.678 s	56113067	836	182.08	1349.95	4179	XiC(182.08±500ppm)
3,4,5-Trifluorobenzyl alcohol, 1-methylpropyl ether	879.985, 0.782	6725394	718	145.08	1134.8	1620	XiC(145.08±500ppm)
3,4-Dichloroaniline, N-trimethylsilyl-	1219.96, 1.277	15672558	746	92.98	1457.9	1072	XiC(92.98±500ppm)
3,4-Difluorobenzoic acid, 4-cyanophenyl ester	1054.97, 1.327	9696679	735	113.09	1290.9	672	XiC(113.09±500ppm)
3,4-Dihydrocoumarin, 4,4-dimethyl-6-dimethylamino-	1479.95 s, 2.003 s	2884110	737	219.1	1756.3	695	XiC(219.10±500ppm)
3,4'-Diisopropylbiphenyl	1604.94 s, 1.588 s	17591692	765	223.13	1604.94	1836	XiC(223.13±500ppm)
3,4-Dimethylmandelic acid, di-TMS	1324.96 s, 1.287 s	12083903	746	239.08	1324.96	1174	XiC(239.08±500ppm)
3,4-Diphenyl(1H)anthra[1,2-d]-1,3-diazepine-2(3H),8,13-trione	2539.88, 4.008	1239672974	716	57.14	3166.8	2526	XiC(57.14±500ppm)
3,4-Hexanedione, 2,2,5-trimethyl-	1414.95 s, 1.143 s	106419576	734	57.06	1414.95	956	XiC(57.06±500ppm)
3,5-Diamino-1,2,4-triazole	1819.92, 1.579	24391071	813	99.02	2206.7	963	XiC(99.02±500ppm)
3,5-Dimethyl-2-furyl methyl ketone	839.987, 1.419	32530152	848	123.02	1100	3736	XiC(123.02±500ppm)
3,5-Dimethyl-3-phenyl-3H-pyrazole	1374.95 s, 1.812 s	44974154	741	119.03	1374.95	2967	XiC(119.03±500ppm)
3,5-Dimethyl-4-octanone	1909.92, 1.126	536085137	752	57.06	2326.7	620	XiC(57.06±500ppm)
3,5-Dimethylphenol, TBDMS derivative	989.978, 1.112	73806731	750	179.06	1231.8	4124	XiC(179.06±500ppm)
3,5-di-tert-Butyl-4-hydroxyacetophenone	1539.94, 1.616	70480614	820	233.13	1833.3	2862	XiC(233.13±500ppm)
3,5-di-tert-Butyl-4-hydroxyphenylpropionic acid	1664.93, 1.674	76597100	781	263.14	2000	2909	XiC(263.14±500ppm)
3,5-Heptanedione, 2,2,4,6,6-pentamethyl-	1854.92, 1.028	349270802	752	57.06	2253.4	1374	XiC(57.06±500ppm)
3,6,10,13-Tetraoxa-2,14-disilapentadecane, 2,2,14,14-tetramethyl-	1279.96 s, 1.015 s	1342046647	800	117.05	1279.96	3026	XiC(117.05±500ppm)
3,6,10-Trioxa-2,11-disiladodecane, 2,2,11,11-tetramethyl-	1034.97 s, 0.925 s	373029477	764	73.01	1034.97	6632	XiC(73.01±500ppm)
3,6,9,12,15,18,21,24-Octaoxapentacosan-1-ol, TMS derivative	1814.92, 1.546	93780303	758	59.04	2200	840	XiC(59.04±500ppm)
3,6,9,12,15,18-Hexaoxanonadecan-1-ol, TMS derivative	1784.93 s, 1.589 s	20248651	768	59.04	1784.93	842	XiC(59.04±500ppm)
3,6,9,12,15-Pentaoxahexadecan-1-ol, TMS derivative	1389.95, 1.336	41300696	829	59.04	1647.1	2351	XiC(59.04±500ppm)
3,6,9,12,15-Pentaoxonadecan-1-ol	2274.9, 2.544	17894516	752	45.04	2813.4	540	XiC(45.04±500ppm)
3,6,9,12-Tetraoxatridecan-1-ol, TMS derivative	1599.94 s, 1.450 s	34302460	830	59.05	1599.94	1615	XiC(59.05±500ppm)
3,6-Bis(trimethylsilyl)-1,4-cyclohexadiene	1194.96, 1.242	101682161	725	73.03	1431.6	979	XiC(73.03±500ppm)
3,7-Decadiene, 2,9-dimethyl-	1294.96 s, 1.040 s	50524476	756	41.04	1294.96	553	XiC(41.04±500ppm)
3,7-Dimethylidbenzothiophene	1649.94, 2.130	13042280	779	212.05	1980	1287	XiC(212.05±500ppm)
3,7-dioxo-2,8-disilanonane, 2,2,5,5,8,8-hexamethyl-4-(1-methylethyl)-	1079.97 s, 0.817 s	188739953	811	73.03	1079.97	11053	XiC(73.03±500ppm)
3,7-dioxo-2,8-disilanonane, 2,2,8,8-tetramethyl-5,5-bis[[trimethylsilyloxy]methyl]-	1279.96 s, 0.790 s	251679606	884	73.04	1279.96	15785	XiC(73.04±500ppm)
3,7-dioxo-2,8-disilanonane, 5-(chloromethyl)-2,2,8,8-tetramethyl-5-[[trimethylsilyloxy]methyl]-	1269.96 s, 0.849 s	45243824	759	73.03	1269.96	802	XiC(73.03±500ppm)
3-[1-(4-Cyano-1,2,3,4-tetrahydronaphthyl)]propanenitrile	1659.93, 2.783	12120125	777	129.06	1993.3	670	XiC(129.06±500ppm)
3-[4-Methylsulphonylbenzoyl]propionic acid	1604.94 s, 2.385 s	11658905	753	182.99	1604.94	1402	XiC(182.99±500ppm)
3-Acetonilyclopentanone	1089.97, 1.973	20153736	754	43.03	1325	545	XiC(43.03±500ppm)
3-Amino-5-t-butylisoxazole	1089.97, 1.350	86385443	743	125.05	1325	2218	XiC(125.05±500ppm)
3-Buten-1-one, 1,4-diphenyl-	1569.94, 1.765	53097285	740	105.06	1873.3	1397	XiC(105.06±500ppm)
3-Buten-2-ol	1354.95 s, 0.948 s	305095725	737	57.06	1354.95	1115	XiC(57.06±500ppm)

3-Buten-2-one, 4-(2,5,6,6-tetramethyl-1-cyclohexen-1-yl)-	1419.95, 1.426	110169349	744	191.16	1682.4	2194	XiC(191.16±500ppm)
3-Buten-2-one, 4-phenyl-	1074.97 s, 1.751 s	5740249	793	131.03	1074.97	838	XiC(131.03±500ppm)
3-Buten-2-one, 4-phenyl-, (E)-	1074.97, 1.756	7125565	733	131.04	1310	941	XiC(131.04±500ppm)
3-Butene-1,2-diol, 1-(2-furanyl)-	1464.95, 1.018	80911844	739	97.08	1737.5	742	XiC(97.08±500ppm)
3-Butenoic acid, 2-oxo-4-phenyl-	1174.97, 1.581	13566340	810	131.04	1410.5	1143	XiC(131.04±500ppm)
3-Carene	729.994, 1.013	29743047	837	93.06	1018.5	1202	XiC(93.06±500ppm)
3-Chloro-1-(methoxymethyl)-1,2,4-triazole	1794.93, 1.724	341744700	749	45.04	2173.4	3500	XiC(45.04±500ppm)
3-Cyano-5,5-dimethoxycarbonyl-N-methylisoxazolidine	1089.97, 0.866	12722436	818	169.17	1325	517	XiC(169.17±500ppm)
3-Decanol, TMS derivative	864.986 s, 2.210 s	160083114	784	131.07	864.986	819	XiC(131.07±500ppm)
3-Dimethyl(octyl)silyloxy-1-propene	699.996, 0.987	14789738	763	115.04	996.3	847	XiC(115.04±500ppm)
3-Dodecanol, 3,7,11-trimethyl-	769.992 s, 1.248 s	56377461	744	73.05	769.992	769	XiC(73.05±500ppm)
3-Dodecene, (Z)-	949.98, 0.928	104078184	902	43.06	1195.7	3473	XiC(43.06±500ppm)
3-Eicosene, (E)-	1809.93, 1.021	492755630	754	69.06	2193.4	3428	XiC(69.06±500ppm)
3-Ethoxy-1,1,1,5,5,5-hexamethyl-3-(trimethylsilyloxy)trisiloxane	884.984 s, 0.747 s	49315151	809	281.02	884.984	2457	XiC(281.02±500ppm)
3-Ethyl-3-hexene	1234.96 s, 0.937 s	139350517	749	55.06	1234.96	788	XiC(55.06±500ppm)
3-Ethyl-3-methylheptane	1224.96, 0.917	1629202449	846	57.07	1463.2	7583	XiC(57.07±500ppm)
3-Ethylpentan-3-ol, trimethylsilyl ether	1044.97 s, 1.000 s	130165108	823	73.03	1044.97	1733	XiC(73.03±500ppm)
3-Ethylphenol, TMS derivative	1004.98 s, 1.116 s	13023379	801	179.07	1004.98	3456	XiC(179.07±500ppm)
3-Heptadecanone	1589.94 s, 1.161 s	87054757	754	72.04	1589.94	2426	XiC(72.04±500ppm)
3-Heptanol, TMS derivative	739.994 s, 0.768 s	73399339	770	73.03	739.994	1528	XiC(73.03±500ppm)
3-Heptanone, 4-methyl-	1464.95, 0.957	354841960	759	57.05	1737.5	1446	XiC(57.05±500ppm)
3-Heptyne-2,6-dione, 5-methyl-5-(1-methylethyl)-	1049.97, 1.234	47171227	770	123.07	1286.4	2861	XiC(123.07±500ppm)
3-Hexanone	1044.97 s, 0.866 s	342406843	740	57.06	1044.97	2306	XiC(57.06±500ppm)
3-Hexanone, 2,5-dimethyl-4-nitro-	1354.95 s, 1.187 s	197434239	749	43.06	1354.95	764	XiC(43.06±500ppm)
3-Hexene, 3-ethyl-2,5-dimethyl-	1394.95 s, 1.033 s	240367115	760	55.05	1394.95	713	XiC(55.05±500ppm)
3H-Pyrazol-3-one, 1,2-dihydro-5-methyl-	909.983, 1.621	16827714	791	98.02	1160.9	1746	XiC(98.02±500ppm)
3-Hydroxy-2-((trimethylsilyloxy)propyl) palmitate	2029.91, 1.409	1669983903	732	73.03	2486.7	1264	XiC(73.03±500ppm)
3-Hydroxy-7-methoxy-3-phenyl-4-chromanone	1954.92, 2.859	8455541	732	151.01	2386.7	695	XiC(151.01±500ppm)
3-Hydroxybenzoic acid, 2TMS derivative	1324.96 s, 1.161 s	22664874	858	73.06	1572.2	2223	XiC(73.06±500ppm)
3-Hydroxybutyric acid, 2TMS derivative	919.982 s, 0.885 s	51445391	805	147.09	1169.6	3966	XiC(147.09±500ppm)
3-Isopropyl-1-methylnaphthalene	1344.95, 1.624	8021593	743	169.09	1594.4	656	XiC(169.09±500ppm)
3-Methoxyamphetamine, 4-Trimethylsilyloxy, N,N-bis(Trimethylsilyloxy)-	1739.93 s, 1.221 s	128594847	748	188.1	1739.93	5622	XiC(188.10±500ppm)
3-Methoxyamphetamine, 4-trimethylsilyloxy, N-trimethylsilyl-	1544.94 s, 1.100 s	139141022	749	116.07	1544.94	6676	XiC(116.07±500ppm)
3-Methyl-1,2-bis(trimethylsilyl)butane	909.983, 0.793	13516816	737	145.09	1160.9	716	XiC(145.09±500ppm)
3-Methyl-1,3-bis(trimethylsilyloxy)butane	899.983 s, 0.822 s	625009113	901	73.04	899.983	2194	XiC(73.04±500ppm)
3-Methyl-2-butanol, TMS derivative	1289.96, 1.020	268689733	745	73.04	1533.3	1489	XiC(73.04±500ppm)
3-Methyl-2-oxovaleric acid, TMS derivative	879.985, 0.830	58938224	702	73.03	1134.8	809	XiC(73.03±500ppm)
3-Methyl-3-hexene	1364.95 s, 1.013 s	242298171	752	55.07	1364.95	1079	XiC(55.07±500ppm)
3-Methyl-9H-carbazol-2-ol	1294.96, 0.966	21797014	746	197.21	1538.9	749	XiC(197.21±500ppm)
3-Methylbenzidine	1609.94 s, 2.257 s	21344403	745	198.06	1609.94	1710	XiC(198.06±500ppm)
3-Methyl-p-anisaldehyde	1129.97 s, 1.878 s	8963447	862	149.04	1129.97	1122	XiC(149.04±500ppm)
3-Methylpentan-2-ol, O-trimethylsilyl ether	1724.93 s, 0.999 s	31568021	803	117.05	1724.93	1842	XiC(117.05±500ppm)
3-Methylvaleric acid, TMS	764.992 s, 0.893 s	57603270	838	75.01	764.992	1448	XiC(75.01±500ppm)
3-Octene, (Z)-	1299.96, 0.968	238374980	726	41.03	1544.4	3878	XiC(41.03±500ppm)
3-Pentadecanone	1429.95 s, 1.194 s	97374373	811	57.05	1429.95	2437	XiC(57.05±500ppm)
3-Pentanone	934.981 s, 1.070 s	50476416	784	57.06	934.981	1679	XiC(57.06±500ppm)
3-Phenyl-1-propanol, acetate	1824.92 s, 2.302 s	15334153	763	117.05	1824.92	765	XiC(117.05±500ppm)
3-Phenyl-1-p-tolylimino-3-trifluoromethyl-2,3,6,7,8,9-hexahydro-1H,5H,2,4b,10,10a-tetraaza-benzol	2194.9 s, 1.503 s	3173845	743	395.35	2194.9	599	XiC(395.35±500ppm)
3-Phenyl-2-butanol, TMS derivative	1499.94, 1.144	593268164	809	117.04	1781.3	15603	XiC(117.04±500ppm)
3-Phenylbutyropheneone	1579.94 s, 1.993 s	47287237	781	105.02	1579.94	1794	XiC(105.02±500ppm)
3-Phenylpropyl benzoate	1774.93 s, 2.053 s	16475294	777	118.06	1774.93	965	XiC(118.06±500ppm)
3-Piperidino-1,2-propanediol	674.998 s, 1.190 s	23577982	742	98.02	674.998	2377	XiC(98.02±500ppm)
3-Pyridinecarbonitrile, 1,4-dihydro-1-methyl-	1599.94, 1.271	41193277	738	119.07	1913.3	507	XiC(119.07±500ppm)
3-Pyridinol, TMS derivative	764.992 s, 2.390 s	172003343	762	152.03	764.992	651	XiC(152.03±500ppm)
3-tert-Butyl-2-pyrazolin-5-one	1089.97 s, 1.344 s	73403051	753	125.04	1089.97	3627	XiC(125.04±500ppm)
3-Tridecanone	1254.96 s, 1.171 s	29415847	774	57.05	1254.96	3464	XiC(57.05±500ppm)
3-Trimethylsilyl-2-trimethylsilyloxypropene	884.984, 0.909	17642032	734	147.05	1139.1	922	XiC(147.05±500ppm)
4-((5-Ethenyl-1-azabicyclo(2,2,2)octan-2-yl)oxymethyl)-6-methoxy-quinoline	2014.91, 1.455	13437827	746	136.04	2466.7	774	XiC(136.04±500ppm)
4(1H)-Pyridinone, 2,3-dihydro-1-methyl-	1499.94 s, 2.302 s	9105499	745	111.03	1499.94	541	XiC(111.03±500ppm)
4(1H)-Pyrimidinone, 2-methyl-	974.979, 2.041	14370208	729	110.05	1218.2	1308	XiC(110.05±500ppm)
4-(2-Methyl-cyclohex-1-enyl)-but-3-en-2-one	1254.96 s, 1.279 s	27180626	747	149.08	1254.96	1017	XiC(149.08±500ppm)
4-(3-Hydroxyphenyl)-4-oxobutyric acid	1399.95, 1.583	84415538	754	121.04	1658.8	2673	XiC(121.04±500ppm)
4-(Allylthio)-2-(4-methoxyphenyl)quinazoline	1619.94 s, 1.104 s	15791900	734	307.19	1619.94	3908	XiC(307.19±500ppm)
4-(Trifluoromethyl)benzyl alcohol, 1-methylpropyl ether	1019.98, 1.217	548998500	832	175.12	1259.1	878	XiC(175.12±500ppm)
4-(Trifluoromethyl)benzyl alcohol, 2-methylpropyl ether	1019.98 s, 1.199 s	528096719	759	175.13	1019.98	1063	XiC(175.13±500ppm)
4,4'-Bipyridine	1304.96 s, 2.177 s	22059943	799	156.05	1304.96	2044	XiC(156.05±500ppm)
4,4'-Diisopropylbiphenyl	1634.94, 1.627	7133931	743	223.13	1960	724	XiC(223.13±500ppm)
4,4'-Dimethoxydiphenylamine	1564.94 s, 2.080 s	19866325	738	229.08	1564.94	2161	XiC(229.08±500ppm)
4,4-Dimethyl octane	1359.95 s, 0.923 s	462079505	755	57.08	1359.95	798	XiC(57.08±500ppm)
4,4-Dimethyl-2-pentanol, TMS derivative	689.997, 0.860	38337991	748	75.01	988.9	565	XiC(75.01±500ppm)
4,4-Dimethyl-3-oxopentanenitrile	759.992, 0.854	63085504	748	57.07	1040.7	565	XiC(57.07±500ppm)
4,4'-Dimethylbiphenyl	1274.96 s, 1.633 s	5378173	740	167.07	1274.96	567	XiC(167.07±500ppm)
4,4-Dipropylheptane	2169.9 s, 1.867 s	429431245	754	57.06	2169.9	829	XiC(57.06±500ppm)
4,6-Dimethyl-3-(4-hydroxyphenyl)coumarin, trimethylsilyl ether	2219.9 s, 3.407 s	15300409	746	338.11	2219.9	1052	XiC(338.11±500ppm)
4,6-Dimethylheptan-2-one	1189.96 s, 1.097 s	73293630	731	43.03	1189.96	1878	XiC(43.03±500ppm)
4,7-Dimethoxy-2-methyl-1H-indene	1384.95, 1.817	7028323	734	175.06	1641.2	533	XiC(175.06±500ppm)
4-[4-(1,1,3,3-Tetramethylbutyl)phenoxy]-2,3,5,6-tetrafluoropyridine	1779.93, 1.396	288816474	740	284.27	2153.3	555	XiC(284.27±500ppm)
4-Anilinoquinazoline	2134.9 s, 2.135 s	235841705	746	220.12	2134.9	1042	XiC(220.12±500ppm)
4b,8-Dimethyl-2-isopropylphenanthrene, 4b,5,6,7,8a,9,10-octahydro-	1664.93 s, 1.649 s	34106450	788	159.1	1664.93	2403	XiC(159.10±500ppm)
4-Bromoheptane	1324.96, 0.959	333228005	748	57.04	1572.2	2845	XiC(57.04±500ppm)
4-Chloro-3-methylphenol, trimethylsilyl ether	1094.97 s, 1.179 s	3979330	767	199.01	1094.97	1117	XiC(199.01±500ppm)

4-Cumylphenol, TMS derivative	1599.94 s, 1.489 s	4732513	779	269.11	1599.94	1064	XiC(269.11±500ppm)
4-Decene, 2,2-dimethyl-, (E)-	1699.93, 1.021	190863899	746	57.07	2046.7	628	XiC(57.07±500ppm)
4'-Dimethylamino-2'-(trimethylsilyl)acetanilide	1344.95, 1.230	12781551	715	235.09	1594.4	2438	XiC(235.09±500ppm)
4-Ethylbenzoic acid, 2,6-dimethylnon-1-en-3-yn-5-yl ester	959.98, 1.259	3952373	731	133.08	1204.5	626	XiC(133.08±500ppm)
4-Ethylbenzoic acid, cyclobutyl ester	1194.96, 0.876	33004470	770	133.04	1431.6	806	XiC(133.04±500ppm)
4-Ethylbiphenyl	1259.96 s, 1.694 s	6233758	744	167.07	1259.96	696	XiC(167.07±500ppm)
4-Fluorobenzylamine, N-decyl-N-methyl-	829.988, 0.939	4196078	712	152.03	1092.6	588	XiC(152.03±500ppm)
4H-1,2,4-Triazole, 4-methyl-	1149.97 s, 0.969 s	75469564	764	83.07	1149.97	664	XiC(83.07±500ppm)
4H-1,3-Dioxin-4-one, 2-(1,1-dimethylethyl)-6-methyl-, (R)-	1244.96 s, 0.892 s	169701583	730	85.08	1244.96	1094	XiC(85.08±500ppm)
4H-Benz[de]anthracene, 5,6-dihydro-	1659.93 s, 2.107 s	13051061	756	218.09	1659.93	1439	XiC(218.09±500ppm)
4H-Cyclopenta[def]phenanthrene	1624.94 s, 2.304 s	13736310	777	190.06	1624.94	1203	XiC(190.06±500ppm)
4-Heptanone, 2,6-dimethyl-	1859.92, 1.037	168024147	727	43.05	2260	1594	XiC(43.05±500ppm)
4-Heptanone, 2-methyl-	1514.94 s, 0.952 s	434517054	760	71.07	1514.94	1127	XiC(71.07±500ppm)
4-Hepten-2-one, (E)-	1884.92, 1.038	147763853	747	43.05	2293.4	1094	XiC(43.05±500ppm)
4-Hexylanisole	1334.96, 1.220	37587109	748	121.05	1583.3	2183	XiC(121.05±500ppm)
4H-Pyran-4-one, 2-methoxy-6-methyl-	1004.98 s, 0.584 s	3304446	736	69.01	1245.5	755	XiC(69.01±500ppm)
4H-thiopyran-3-carboxaldehyde, 4-oxo-2,6-diphenyl-	1309.96, 1.156	893832229	730	263.14	1555.6	1053	XiC(263.14±500ppm)
4-Hydroxy-3,4,6-trimethylhept-5-enoic acid lactone	844.987, 0.910	388737448	717	43.01	1104.3	1159	XiC(43.01±500ppm)
4-Hydroxybenzaldehyde, TMS derivative	1144.97 s, 1.392 s	4496690	808	179.03	1144.97	6306	XiC(179.03±500ppm)
4-Hydroxybutanoic acid, 2TMS derivative	904.983 s, 0.785 s	14381331	765	147.05	904.983	783	XiC(147.05±500ppm)
4-Methoxybenzyl alcohol, 2-methylpropyl ether	1424.95 s, 1.458	49453010	734	121.05	1688.2	1103	XiC(121.05±500ppm)
4-Methoxybenzyl alcohol, TMS derivative	1169.97 s, 1.297 s	6435435	752	121.05	1169.97	715	XiC(121.05±500ppm)
4-Methoxyphenol, TMS derivative	1059.97 s, 1.267 s	49930598	856	181.04	1059.97	6306	XiC(181.04±500ppm)
4-Methyl-1-(dimethyl(prop-2-enyl)silyloxy)pentane	799.99, 1.075	50220166	750	75.01	1070.4	735	XiC(75.01±500ppm)
4-Methyl-1,2-bis(trimethylsilyloxy)pentane	999.977, 0.817	43084655	750	73.03	1240.9	3617	XiC(73.03±500ppm)
4-Methylbenzoic acid, 2-methylbutyl ester	1549.94, 1.422	122802836	793	119.03	1846.7	1240	XiC(119.03±500ppm)
4-Methylpentyl benzoate	1549.94 s, 1.462 s	105221177	748	105.02	1549.94	1094	XiC(105.02±500ppm)
4-Methylphthalaldehyde	1249.96 s, 2.268 s	4918306	899	119.03	1249.96	511	XiC(119.03±500ppm)
4-Methylvaleric acid, TMS derivative	839.987, 1.035	119512213	737	75.01	1100	2090	XiC(75.01±500ppm)
4-Octanol, TMS derivative	834.988 s, 0.784 s	34337261	744	73.03	834.988	1607	XiC(73.03±500ppm)
4-Octene, 2,3,6-trimethyl-	1089.97 s, 0.926 s	548740146	767	69.08	1089.97	2401	XiC(69.08±500ppm)
4-Octene, 2,3,7-trimethyl-, [5-(E)]-	1919.92, 1.053	626430560	755	69.06	2340	1458	XiC(69.06±500ppm)
4-Oxazolecarboxylic acid, 4,5-dihydro-2-phenyl-, 1-methylethyl ester	1704.93 s, 2.282 s	59865513	810	146.04	1704.93	2627	XiC(146.04±500ppm)
4-Penten-2-ol, TMS derivative	929.981 s, 1.030 s	75097480	730	73.03	929.981	1994	XiC(73.03±500ppm)
4-Pentalen, 2-ethyl-	1284.96 s, 0.953 s	112055950	740	41.03	1284.96	2366	XiC(41.03±500ppm)
4-Pentenoic acid, 2,2-diethyl-3-oxo-5-phenyl-, ethyl ester	1194.96, 1.221	72210670	749	131.07	1431.6	1751	XiC(131.07±500ppm)
4-Phenyl-2,3-dihydro-1H-1,5-benzodiazepin-2-one	2159.9, 3.124	794734828	734	194.09	2660.1	2495	XiC(194.09±500ppm)
4-Phenylphenol, TMS derivative	1359.95 s, 1.431 s	37817298	763	211.04	1359.95	5043	XiC(211.04±500ppm)
4-Propylbenzaldehyde diethyl acetal	1384.95 s, 1.603 s	56855105	735	177.07	1384.95	6627	XiC(177.07±500ppm)
4-tert-Amylphenol, TMS derivative	1219.96 s, 1.131 s	5570466	742	207.1	1219.96	759	XiC(207.10±500ppm)
4'-tert-Butyl-2',6'-dimethylacetophenone	1174.97 s, 1.323 s	123435799	826	189.1	1174.97	11684	XiC(189.10±500ppm)
4-tert-Butylphenol, TMS derivative	1099.97 s, 1.099 s	18861970	745	207.1	1099.97	1461	XiC(207.10±500ppm)
4-tert-Octylphenol, TMS derivative	1349.95, 1.069	5416376	764	207.1	1600	774	XiC(207.10±500ppm)
4-Trifluoromethylbenzoic acid, cyclobutyl ester	1034.97, 1.176	8945332	739	173.12	1272.7	635	XiC(173.12±500ppm)
4-Trimethylsilyloxy(trimethylsilyl)valerate	1194.96, 0.815	60991186	736	73.02	1431.6	522	XiC(73.02±500ppm)
4-Trimethylsilylphenol	779.991 s, 1.073 s	3433979	844	151.06	1055.6	1179	XiC(151.06±500ppm)
4-Undecene, 5-methyl-	839.987 s, 0.833 s	43200935	765	55.05	839.987	1090	XiC(55.05±500ppm)
5-(1-Naphthyl)tricyclo[4.1.0.0(2,7)]hept-3-ene	1744.93, 2.212	69252187	793	218.09	2106.7	2818	XiC(218.09±500ppm)
5,6-Dimethyl-4-phenyl-3-cyanopyridine-2(1H)-thione	1444.95 s, 1.522 s	962861988	744	239.22	1444.95	1132	XiC(239.22±500ppm)
5,7-Dihydroxy-3-[2,3-dihydro-4-hydroxy-2-(2-hydroxyisopropyl)benzofuran-7-yl]chromone	1844.92, 1.211	3857100	730	311.27	2240	1122	XiC(311.27±500ppm)
5,9,14,18-anthrazinetetrone, 6,15-dihydro-	2544.88 s, 4.030 s	534968924	744	441.82	2544.88	1411	XiC(441.82±500ppm)
5,9-Undecadien-2-one, 6,10-dimethyl-	1219.96 s, 1.304 s	43583603	862	43.02	1219.96	1570	XiC(43.02±500ppm)
5-Eicosene, (E)-	1484.95, 1.019	401009121	783	57.05	1762.5	3385	XiC(57.05±500ppm)
5-hydroxy-7-methoxyflavanone, tert-butyl(dimethylsilyl) ether	1774.93 s, 1.394 s	1829899719	754	327.38	1774.93	551	XiC(327.38±500ppm)
5-Iodopentan-2-one	819.988, 1.547	62945189	767	43.02	1085.2	791	XiC(43.02±500ppm)
5-Methoxy-2,3-dimethylindole	1964.92, 1.629	6415087	701	174.99	2400	589	XiC(174.99±500ppm)
5-methoxy- α -ethyltryptamine	1044.97 s, 1.431 s	12967364	738	58.06	1044.97	689	XiC(58.06±500ppm)
5-Methyl-1-phenyloctane	1329.96, 1.234	19417896	717	92.04	1577.8	1907	XiC(92.04±500ppm)
5-Methyl-2-(2-methyl-2-tetrahydrofuryl)tetrahydrofuran	844.987 s, 0.802 s	317840793	750	85.08	844.987	1273	XiC(85.08±500ppm)
5-Nonanol, TMS derivative	1274.96, 0.846	37954400	733	73.03	1516.7	693	XiC(73.03±500ppm)
5-Nonen-4-one, 6-methyl-	959.98, 1.502	30062346	754	111.04	1204.5	1998	XiC(111.04±500ppm)
5-Octadecene, (E)-	1864.92, 1.287	190252782	729	55.03	2266.7	1866	XiC(55.03±500ppm)
5-Oxotetrahydrofuran-2-carboxylic acid, ethyl ester	2989.85, 3.688	96808490	806	85.1	3766.8	587	XiC(85.10±500ppm)
5-Phenylvaleric acid, tert-butyl(dimethylsilyl) ester	1209.96 s, 1.102 s	20723915	728	235.13	1209.96	6585	XiC(235.13±500ppm)
5-Trimethylsilyluracil	984.978, 1.447	4254000	750	169.02	1227.3	559	XiC(169.02±500ppm)
6-(4-Methoxyphenyl)hex-3-en-2-one	1334.96 s, 1.218 s	37503660	747	121.04	1334.96	2006	XiC(121.04±500ppm)
6,6,8,8,10,10-Hexamethyl-2,5,7,9,11,14-hexaoxa-6,8,10-trisilapentadecane	669.998, 0.722	242717526	747	237.05	974.1	4813	XiC(237.05±500ppm)
6,7-Dihydro-5H-benzo[1,2,5]oxadiazol-4-one o-(6-chloro-benzo[1,3]dioxol-5-ylmethyl)-oxime	1799.93 s, 1.991 s	6735779	745	169.02	1799.93	564	XiC(169.02±500ppm)
6-Dodecanone	1514.94, 0.960	383211932	757	71.07	1800	1430	XiC(71.07±500ppm)
6-Ethyl-3-octanol, TMS derivative	864.986, 2.201	29247495	754	57.06	1121.7	641	XiC(57.06±500ppm)
6H-Cyclobuta[jk]phenanthrene	1624.94, 2.308	17801499	855	190.06	1946.7	891	XiC(190.06±500ppm)
6H-Dibenzo[b,d]pyran-1-ol, 3-hexyl-7,8,9,10-tetrahydro-6,6,9-trimethyl-	1694.93 s, 1.123 s	78212662	737	313.19	1694.93	2030	XiC(313.19±500ppm)
6H-Dibenzo[b,d]-pyran	1379.95, 1.855	56995190	884	182.05	1635.3	4403	XiC(182.05±500ppm)
6-Methoxy-3-methylbenzofuran	1139.97 s, 1.711 s	584803033	820	162.04	1139.97	8366	XiC(162.04±500ppm)
6-Methyl-3,5-heptadiene-2-one	854.986, 1.420	4147816	843	109.05	1113	522	XiC(109.05±500ppm)
7,7,9,9,11,11-Hexamethyl-3,6,8,10,12,15-hexaoxa-7,9,11-trisilaheptadecane	739.994, 0.740	11836100	743	207.01	1025.9	1261	XiC(207.01±500ppm)
7,9-Di-tert-butyl-1-oxaspiro[4,5]deca-6,9-diene-2,8-dione	1614.94 s, 1.664 s	180648471	921	57.07	1614.94	5170	XiC(57.07±500ppm)
7-Acetyl-6-ethyl-1,1,4,4-tetramethyltetralin	1579.94 s, 1.527 s	68344585	861	43.02	1579.94	3038	XiC(43.02±500ppm)
7-Butyl-3,4,5,6(2H)-tetrahydroazepine	2069.91, 1.361	206048623	716	111.09	2540	681	XiC(111.09±500ppm)
7-Isopropyl-1,1,4a-trimethyl-1,2,3,4,4a,9,10,10a-octahydrophenanthrene	1719.93 s, 1.677 s	2892855	735	69.06	1719.93	774	XiC(69.06±500ppm)
7-Oxodehydroabietic acid, trimethylsilyl ester	2054.91 s, 2.130 s	507580925	782	268.32	2520	2050	XiC(268.32±500ppm)

7-Tetradecene	1039.97, 0.930	95001043	759	69.06	1277.3	1186	XIC(69.06±500ppm)
8-(4-Hydroxyphenyl)-1-methyl-3H,6H,7H-imidazo[1,2-g]purine-2,4-dione	1634.94 s, 1.097 s	248640124	753	299.25	1634.94	547	XIC(299.25±500ppm)
8,8,9-Trimethyl-deca-3,5-diene-2,7-dione	1229.96 s, 1.417 s	25505914	742	165.09	1229.96	1454	XIC(165.09±500ppm)
8-Amino-5-dimethylamino-6-methoxyquinoline	1549.94 s, 1.985	9705886	718	217.08	1846.7	1155	XIC(217.08±500ppm)
8-Amino-6-quinolinol, 2TMS derivative	2139.9 s, 0.979 s	7061613	786	289.14	2633.4	1366	XIC(289.14±500ppm)
8-Chloro-1-octanol, TMS derivative	759.992 s, 0.892 s	41279102	745	69.06	759.992	1890	XIC(69.06±500ppm)
8-Dodecen-1-ol, acetate, (Z)-	2019.91, 1.272	42332483	749	43.05	2473.4	672	XIC(43.05±500ppm)
8-Ethyl-4,6,6,8-tetramethyl-3,4,6,7-tetrahydro-1H-cyclopenta(G)-2-benzopyran	1539.94, 1.484	21778641	756	229.13	1833.3	1549	XIC(229.13±500ppm)
8-Isopropyl-1,3-dimethylphenanthrene	1629.94 s, 1.787 s	15145961	746	233.12	1629.94	1391	XIC(233.12±500ppm)
9(10H)-Acridinone	1509.94 s, 1.666 s	26797820	735	195.1	1509.94	987	XIC(195.10±500ppm)
9,10-Anthracenedione	1659.93 s, 2.590 s	16403933	909	180.05	1659.93	1826	XIC(180.05±500ppm)
9,10-Anthracenedione, 1,2,4-trihydroxy-	1999.91 s, 2.438 s	1020840	764	256.04	2446.7	584	XIC(256.04±500ppm)
9,10-Anthracenedione, 1,4-diamino-2,3-dihydro-	1459.95 s, 0.686 s	118805826	744	240.08	1459.95	533	XIC(240.08±500ppm)
9,10-Anthracenedione, 2-methyl-	1754.93 s, 2.574 s	5012296	901	165.08	2120	2478	XIC(165.08±500ppm)
9,10-Dimethylanthracene	1704.93, 2.203	39151307	862	206.09	2053.3	2088	XIC(206.09±500ppm)
9,9-Dimethyl-9-silafluorene	1134.97, 1.233	65193304	731	195.05	1370	1734	XIC(195.05±500ppm)
9-Eicosene, (E)-	1794.93, 1.120	456921507	867	55.05	2173.4	6781	XIC(55.05±500ppm)
9H-Carbazole-9-methanol	1559.94, 2.513	7239691	891	167.05	1860	546	XIC(167.05±500ppm)
9-Hexadecenoic acid, hexadecyl ester, (Z)-	2459.88 s, 2.913 s	38053907	853	43.05	2459.88	596	XIC(43.05±500ppm)
9-Hexadecenoic acid, octadecyl ester, (Z)-	2644.87 s, 4.160 s	38940406	872	43.05	2644.87	509	XIC(43.05±500ppm)
9H-Fluoren-9-one	1484.95 s, 2.235 s	155810620	932	180.03	1484.95	4716	XIC(180.03±500ppm)
9H-Fluorene, 9-methylene-	1519.94 s, 2.210 s	584938160	939	178.05	1519.94	13722	XIC(178.05±500ppm)
9H-Purine	1324.96, 1.534	10962564	735	120.04	1572.2	570	XIC(120.04±500ppm)
9H-Pyrido[3,4-b]indol-7-ol, 1-methyl-	1609.94, 2.265	26383723	761	198.07	1926.7	2911	XIC(198.07±500ppm)
9H-Xanthene	1379.95 s, 1.848 s	56593201	882	182.05	1379.95	4547	XIC(182.05±500ppm)
9-Methyl-10-vinylnanthracene	1634.94, 2.115	5602824	789	218.09	1960	755	XIC(218.09±500ppm)
9-Octadecenamide, (Z)-	1904.92 s, 1.775 s	7677997	749	59.03	1904.92	507	XIC(59.03±500ppm)
9-Octadecenoic acid	2329.89 s, 2.128 s	131562448	820	43.05	2329.89	586	XIC(43.05±500ppm)
9-Octadecenoic acid (Z)-, methyl ester	1739.93, 2.195	116355290	716	69.06	2100	704	XIC(69.06±500ppm)
9-Phenyl-5H-benzocycloheptene	1634.94 s, 2.115 s	5502504	801	218.09	1634.94	817	XIC(218.09±500ppm)
Abietic acid	1959.92 s, 2.354 s	70814900	796	105.08	2393.4	1510	XIC(105.08±500ppm)
Abietic acid, TMS derivative	1949.92 s, 1.629 s	38465902	863	256.24	2380	4751	XIC(256.24±500ppm)
Acenaphthene	1259.96 s, 1.900 s	28443443	946	153.05	1259.96	4038	XIC(153.05±500ppm)
Acetaldehyde, tetramer	1909.92, 2.316	646475989	739	45.04	2326.7	4565	XIC(45.04±500ppm)
Acetamide, 2,2,2-trifluoro-	694.996, 0.667	420748625	850	44.02	992.6	1017	XIC(44.02±500ppm)
Acetamide, N-(2-butyl)-N-methyl-	834.988, 1.445	22204371	746	58.06	1096.3	900	XIC(58.06±500ppm)
acetamide, N-(4-hydroxy-1-naphthalenyl)-	1039.97 s, 0.810 s	25545628	737	159.1	1039.97	2395	XIC(159.10±500ppm)
Acetamide, N,N'-ethylenebis(N-nitro-	2269.9, 1.680	64589961	748	43.03	2806.7	634	XIC(43.03±500ppm)
Acetamide, N-2-propenyl-	1064.97, 0.892	180169381	743	57.06	1300	1915	XIC(57.06±500ppm)
Acetamide, N-bicyclo[2.2.1]hept-2-ylmethyl-2-oxo-2-(2-phenyl-1H-indol-3-yl)-	2134.9 s, 2.150 s	232728457	789	220.19	2134.9	1189	XIC(220.19±500ppm)
Acetic acid n-octadecyl ester	1804.93, 1.254	394274399	815	43.04	2186.7	1492	XIC(43.04±500ppm)
Acetic acid, [(1,1-dimethylethyl)thio]-	2054.91, 1.088	604131626	766	57.06	2520	1983	XIC(57.06±500ppm)
Acetic acid, bis(trimethylsilyloxy)-, trimethylsilyl ester	1394.95, 0.781	47823141	737	73.04	1652.9	940	XIC(73.04±500ppm)
Acetic acid, diethoxy-, ethyl ester	1019.98, 0.983	35062146	731	103.06	1259.1	1487	XIC(103.06±500ppm)
Acetic acid, TBDMS derivative	769.992, 0.783	148991891	752	117.05	1048.1	1804	XIC(117.05±500ppm)
Acetic anhydride	1709.93, 1.145	81496318	712	43.01	2060	679	XIC(43.01±500ppm)
Acetin, bis-1,3-trimethylsilyl ether	2074.91, 1.198	42300309	737	73.04	2546.7	668	XIC(73.04±500ppm)
Acetophenone	809.989 s, 1.638 s	63460233	863	105.02	809.989	2844	XIC(105.02±500ppm)
Alanine, N-methyl-N-isobutoxycarbonyl-, nonyl ester	1309.96 s, 1.731 s	37264744	749	57.06	1309.96	1323	XIC(57.06±500ppm)
Alanine, N-methyl-N-methoxycarbonyl-, undecyl ester	1519.94 s, 1.087 s	225381865	733	116.1	1519.94	1631	XIC(116.10±500ppm)
Alanylglycine, 2TMS derivative	1524.94 s, 1.077 s	199241945	825	116.11	1524.94	2363	XIC(116.11±500ppm)
Alizarin, 2TMS derivative	2124.9 s, 2.572 s	3445145	787	369.06	2124.9	1559	XIC(369.06±500ppm)
Allylescaline	1794.93 s, 2.829 s	28788728	748	167.05	1794.93	1362	XIC(167.05±500ppm)
Alpha, alpha, 2,3-tetrachlorotoluene	1244.96 s, 1.741 s	2629729	866	192.92	1244.96	1074	XIC(192.92±500ppm)
Ammonium Chloride	1589.94, 0.622	5876189	803	35.98	1900	1084	XIC(35.98±500ppm)
Anthra[1,9-cd]pyrazol-6(2H)-one	2134.9 s, 2.514 s	3196706036	851	220.28	2134.9	921	XIC(220.28±500ppm)
Anthracene	1529.94 s, 2.166 s	31433362	938	178.05	1529.94	965	XIC(178.05±500ppm)
Anthracene, 2-ethyl-	1684.93, 2.143	13641160	798	206.09	2026.7	942	XIC(206.09±500ppm)
Anthracene, 9,10-dihydro-2-methyl-	1549.94 s, 1.868 s	53706828	805	179.06	1549.94	1292	XIC(179.06±500ppm)
Anthracene, 9,10-dihydro-9,10-dimethyl-	1629.94, 1.853	9773356	736	208.11	1953.3	550	XIC(208.11±500ppm)
Anthracene, 9-ethyl-	1684.93, 2.143	19096449	753	206.09	2026.7	859	XIC(206.09±500ppm)
Anthraquinone, 1-(o-chlorophenyl)-	1744.93 s, 1.191 s	7250304	737	283.23	1744.93	904	XIC(283.23±500ppm)
Anthrone	1549.94 s, 2.174 s	51967617	888	194.05	1549.94	1443	XIC(194.05±500ppm)
anti-2-Acetoxyacetaldoxime	1824.92 s, 1.022 s	939297184	743	57.06	1824.92	3562	XIC(57.06±500ppm)
Arabinitol, 5TMS derivative	1474.95 s, 0.810 s	537737123	887	73.03	1474.95	6091	XIC(73.03±500ppm)
Arabinofuranose, 1,2,3,5-tetrakis-O-(trimethylsilyl)-	1554.94, 0.908	37178033	766	73.05	1853.3	602	XIC(73.05±500ppm)
Arachidic acid, TMS derivative	1949.92 s, 1.189 s	110405690	879	73.03	1949.92	2703	XIC(73.03±500ppm)
Artedouglasia oxide A	994.977 s, 1.175 s	31634702	751	125.05	994.977	2903	XIC(125.05±500ppm)
Azelaic acid, 2TMS derivative	1519.94 s, 1.129 s	10014856	824	73.05	1806.7	663	XIC(73.05±500ppm)
Azetidine, 1-acetyl-2-methyl-	659.999 s, 2.713 s	125273872	743	56.04	659.999	702	XIC(56.04±500ppm)
Azulene, 4,8-dimethyl-6-phenyl-	1844.92, 2.145	22533007	794	232.1	2240	2069	XIC(232.10±500ppm)
Batyl alcohol, 2TMS derivative	2089.91 s, 1.148 s	2850048	748	73.03	2089.91	501	XIC(73.03±500ppm)
Behenic acid, TMS derivative	2064.91 s, 1.260 s	30436427	790	117.04	2533.4	776	XIC(117.04±500ppm)
Behenic alcohol	1849.92, 1.184	121369978	761	43.05	2246.7	976	XIC(43.05±500ppm)
Benzaldehyde	674.998 s, 1.589 s	9507065	932	77.02	674.998	632	XIC(77.02±500ppm)
Benzaldehyde diethylacetal	994.977 s, 1.307 s	124265264	941	135.06	994.977	8990	XIC(135.06±500ppm)
Benzaldehyde, 2,4-dimethyl-	979.978 s, 1.675 s	10507827	882	133.05	979.978	1843	XIC(133.05±500ppm)
Benzaldehyde, 2,5-dimethoxy-	1229.96 s, 1.909 s	141295047	930	166.04	1229.96	6544	XIC(166.04±500ppm)
Benzaldehyde, 2,5-dimethyl-	979.978, 1.681	11025329	913	133.04	1222.7	1604	XIC(133.04±500ppm)
Benzaldehyde, 2-methyl-	824.988 s, 1.628 s	41957120	955	91.04	824.988	3034	XIC(91.04±500ppm)
Benzaldehyde, 4-(1-phenyl-2-propenyloxy)-	1824.92, 2.302	13764414	731	117.06	2213.4	536	XIC(117.06±500ppm)

Benzaldehyde, 4-methoxy-	1024.98 s, 1.907 s	8452689	928	135.03	1024.98	723	XiC(135.03±500ppm)
Benzaldehyde, 4-methoxy-3-(2,6-dimethylphenoxyethyl)-	1099.97 s, 1.332 s	216090768	755	149.07	1099.97	15390	XiC(149.07±500ppm)
benzamide, N-(2,6-dihydroxyphenyl)-4-heptyl-	2034.91, 1.243	21815477	736	203.09	2493.4	2297	XiC(203.09±500ppm)
Benzamide, N,N,3-trimethyl-	1254.96 s, 1.977 s	70281466	810	119.03	1254.96	767	XiC(119.03±500ppm)
Benzamide, N-benzoyl-N-(3-propylthio-1,2,4-thiadiazol-5-yl)-	1384.95, 2.062	549869847	845	105.01	1641.2	3375	XiC(105.01±500ppm)
Benzamide, N-propyl-	1974.91 s, 2.288 s	8445736	775	105.02	1974.91	768	XiC(105.02±500ppm)
Benzamide, o-(β-hydroxyphenethyl)-	1679.93 s, 2.310 s	45895496	743	135.03	1679.93	3069	XiC(135.03±500ppm)
Benzen, 2-acetate-1,3-dimethoxy-5-(1-propenyl)-	2159.9, 3.124	878787376	711	194.08	2660.1	2740	XiC(194.08±500ppm)
Benzenamine, 2,6-bis(1-methylethyl)-	2064.91 s, 2.065 s	13123548	728	177.13	2064.91	902	XiC(177.13±500ppm)
Benzenamine, 2-ethoxy-	1004.98, 1.731	5375167	779	108.03	1245.5	604	XiC(108.03±500ppm)
Benzenamine, 2-ethyl-	914.982 s, 1.672 s	5305003	892	106.05	914.982	1100	XiC(106.05±500ppm)
benzenamine, 4-methyl-N-(4-methylphenyl)-N-[4-[2-(4-nitrophenyl)ethenyl]phenyl]-	2284.89, 3.811	4648910	754	420.17	2826.7	668	XiC(420.17±500ppm)
Benzenamine, N,N'-1,2-ethanediylienebis[4-methyl-	1854.92 s, 2.266 s	8172942	745	221.07	1854.92	715	XiC(221.07±500ppm)
benzenamine, N,N-diethyl-3,5-dimethyl-	1334.96, 2.032	23297093	754	162.03	1583.3	1226	XiC(162.03±500ppm)
Benzenamine, N,N-diethyl-4-[2-(4-nitrophenyl)ethenyl]-	1959.92, 2.501	13261503	746	281.09	2393.4	1193	XiC(281.09±500ppm)
Benzenamine, N-methyl-N-phenyl-	1229.96 s, 0.949 s	13716446	792	183.19	1229.96	728	XiC(183.19±500ppm)
Benzene, (1,2-dicyclopropyl-2-phenylethyl)-	1694.93, 1.854	22031284	730	131.07	2040	898	XiC(131.07±500ppm)
Benzene, (1,3-dimethylbutyl)-	1429.95, 1.632	46482864	707	105.05	1694.1	2296	XiC(105.05±500ppm)
Benzene, (1-bromoethyl)-	1369.95 s, 1.664 s	12258064	729	105.05	1369.95	712	XiC(105.05±500ppm)
Benzene, (1-butylheptyl)-	1384.95 s, 1.173 s	263445520	886	91.04	1384.95	8711	XiC(91.04±500ppm)
Benzene, (1-butylhexyl)-	1299.96, 1.173	84910982	728	91.04	1544.4	2046	XiC(91.04±500ppm)
Benzene, (1-ethyldecyl)-	1499.94, 1.210	61381656	750	91.04	1781.3	2356	XiC(91.04±500ppm)
Benzene, (1-ethylnonyl)-	1409.95 s, 1.206 s	192922863	859	91.04	1409.95	9875	XiC(91.04±500ppm)
Benzene, (1-ethylloctyl)-	1324.96 s, 1.187 s	75315290	836	91.04	1324.96	712	XiC(91.04±500ppm)
Benzene, (1-ethylundecyl)-	1574.94 s, 1.226 s	143321803	823	91.04	1574.94	4863	XiC(91.04±500ppm)
Benzene, (1-hexylheptyl)-	1539.94 s, 1.195 s	240902714	787	91.04	1539.94	3700	XiC(91.04±500ppm)
Benzene, (1-methyldecyl)-	1444.95 s, 1.219 s	155902582	908	105.16	1444.95	1187	XiC(105.16±500ppm)
Benzene, (1-methylnonyl)-	1354.95 s, 1.214 s	261210760	839	105.05	1354.95	14831	XiC(105.05±500ppm)
Benzene, (1-methylrdecyl)-	1679.93, 1.272	95752060	748	105.05	2020	3287	XiC(105.05±500ppm)
Benzene, (1-methylundecyl)-	1529.94 s, 1.225 s	150603984	840	105.05	1529.94	6995	XiC(105.05±500ppm)
Benzene, (1-pentylheptyl)-	1469.95 s, 1.172 s	193662836	852	91.04	1469.95	4337	XiC(91.04±500ppm)
Benzene, (1-pentylloctyl)-	1539.94, 1.197	263543836	766	91.04	1833.3	4831	XiC(91.04±500ppm)
Benzene, (1-propyldecyl)-	1554.94 s, 1.215 s	172723897	764	91.04	1554.94	3936	XiC(91.04±500ppm)
Benzene, (1-propylheptyl)-	1304.96 s, 1.179 s	52555680	833	91.04	1304.96	1893	XiC(91.04±500ppm)
Benzene, (1-propylnonyl)-	1479.95 s, 1.205 s	86544393	784	91.04	1479.95	3753	XiC(91.04±500ppm)
Benzene, (1-propylloctyl)-	1394.95 s, 1.182 s	187769898	778	91.04	1394.95	6256	XiC(91.04±500ppm)
Benzene, (3-chloro-1-propenyl)-	1014.98, 1.652	31136057	768	117.06	1254.5	1131	XiC(117.06±500ppm)
Benzene, (propoxymethyl)-	1584.94, 1.273	33178166	748	91.04	1893.3	1317	XiC(91.04±500ppm)
Benzene, [1-[(1-(1-methylethyl)-3-butenyl)oxy]ethyl]-, [5-(R*,R*)]-	1604.94 s, 1.250 s	424996134	775	105.06	1604.94	2751	XiC(105.06±500ppm)
Benzene, [1-chloro-2-(chloromethyl)-3-methoxypropyl]-	1344.95 s, 1.634 s	52619123	825	117.05	1344.95	1783	XiC(117.05±500ppm)
Benzene, 1-(1,5-dimethyl-4-hexenyl)-4-methyl-	1249.96, 1.265	9816214	751	119.07	1489.5	527	XiC(119.07±500ppm)
Benzene, 1-(1,5-dimethylhexyl)-4-methyl-	1214.96 s, 1.182 s	26622362	743	119.07	1214.96	1343	XiC(119.07±500ppm)
Benzene, 1-(chloromethyl)-3,5-dimethoxy-	1244.96, 1.813	5558496	745	151.06	1484.2	882	XiC(151.06±500ppm)
Benzene, 1,1'-(1,2-cyclobutanediyl)bis-, cis-	1494.95 s, 1.756 s	170259061	753	104.04	1494.95	4477	XiC(104.04±500ppm)
Benzene, 1,1'-(1,2-cyclobutanediyl)bis-, trans-	1489.95, 1.769	63293085	719	104.04	1768.8	1365	XiC(104.04±500ppm)
Benzene, 1,1'-(1,2-dimethyl-1,2-ethanediyl)bis-	1319.96, 1.630	12645338	751	105.06	1566.7	600	XiC(105.06±500ppm)
Benzene, 1,1'-(1,2-dimethyl-1,2-ethanediyl)bis-, (R*,S*)-	1319.96 s, 1.626 s	10583212	728	105.05	1319.96	731	XiC(105.05±500ppm)
Benzene, 1,1'-(1,2-dimethyl-1,2-ethenediyl)bis-, (Z)-	1564.94, 1.822	19748920	752	115.04	1866.7	556	XiC(115.04±500ppm)
Benzene, 1,1'-(1,3-propanediyl)bis-	1404.95 s, 1.677 s	48680517	905	92.04	1404.95	2645	XiC(92.04±500ppm)
Benzene, 1,1'-(1,5-hexadiene-1,6-diyl)bis-	1659.93 s, 1.885 s	23676640	796	117.06	1659.93	1098	XiC(117.06±500ppm)
Benzene, 1,1'-(1-butene-1,4-diyl)bis-, (Z)-	1544.94 s, 1.820 s	17937185	738	57.05	1544.94	689	XiC(57.05±500ppm)
Benzene, 1,1'-(1-methyl-1,3-propanediyl)bis-	1429.95 s, 1.628 s	38100351	750	105.05	1429.95	2326	XiC(105.05±500ppm)
benzene, 1,1'-(1-methylethylidene)bis[4-methyl-	1514.94 s, 1.703 s	64798869	743	209.11	1514.94	1019	XiC(209.11±500ppm)
Benzene, 1,1'-(3-methyl-1-propene-1,3-diyl)bis-	1564.94, 1.821	16979871	730	115.05	1866.7	553	XiC(115.05±500ppm)
Benzene, 1,1'-(1-(2-propenyl)-1,2-ethanediyl)bis-	1439.95 s, 1.644 s	149306620	899	181.08	1439.95	5072	XiC(181.08±500ppm)
Benzene, 1,1'-(1,2-ethanediylbis(oxy))bis-	1529.94 s, 1.953 s	67855891	954	77.02	1529.94	2454	XiC(77.02±500ppm)
Benzene, 1,1'-[oxybis(methylene)]bis-	1404.95, 1.836	14652069	744	92.04	1664.7	612	XiC(92.04±500ppm)
Benzene, 1,1'-dodecylidenebis[4-methyl-	1509.94, 1.667	30080400	736	195.1	1793.8	1132	XiC(195.10±500ppm)
Benzene, 1,1'-ethenylidenebis[4-methyl-	1639.94, 1.877	15666826	753	208.11	1966.7	1221	XiC(208.11±500ppm)
Benzene, 1,1'-methylenebis[3-methyl-	1389.95, 1.702	17374338	796	181.08	1647.1	1566	XiC(181.08±500ppm)
Benzene, 1,2,4,5-tetrachloro-	1104.97 s, 1.510 s	7909352	765	104.05	1104.97	1470	XiC(104.05±500ppm)
Benzene, 1,2,4,5-tetramethyl-	869.985 s, 1.221 s	7993935	889	119.07	869.985	677	XiC(119.07±500ppm)
Benzene, 1,2-dichloro-3-nitro-	1164.97, 1.862	3433804	913	144.95	1400	790	XiC(144.95±500ppm)
Benzene, 1,2-dichloro-4-nitro-	1164.97 s, 1.860 s	3833302	912	144.94	1164.97	899	XiC(144.94±500ppm)
Benzene, 1,3,5-trimethoxy-	1504.94, 1.977	638587737	747	168.09	1787.5	623	XiC(168.09±500ppm)
Benzene, 1,3,5-tris(1-methylethyl)-	1104.97, 1.116	4653429	749	189.15	1340	614	XiC(189.15±500ppm)
Benzene, 1,3-bis(1,1-dimethylethyl)-	1019.98 s, 1.117 s	303943002	871	175.24	1019.98	3029	XiC(175.24±500ppm)
Benzene, 1,3-dibromo-	954.98 s, 1.623 s	1972696	861	235.84	954.98	1370	XiC(235.84±500ppm)
Benzene, 1,4-dibromo-	954.98, 1.626	1989793	817	235.84	1200	861	XiC(235.84±500ppm)
Benzene, 1,4-diethyl-2,3,5,6-tetramethyl-	1329.96 s, 1.462 s	9629883	755	175.13	1329.96	886	XiC(175.13±500ppm)
Benzene, 1,4-dimethoxy-	919.982 s, 1.617 s	38569093	927	123.02	919.982	4048	XiC(123.02±500ppm)
Benzene, 1,4-dimethoxy-2-methyl-	1014.98 s, 1.574 s	181099027	926	137.04	1014.98	13045	XiC(137.04±500ppm)
Benzene, 1-chloro-2-(trichloromethyl)-	1244.96, 1.749	2911045	853	192.92	1484.2	1115	XiC(192.92±500ppm)
Benzene, 1-ethenyl-2-methyl-	1774.93, 2.065	26024293	772	117.05	2146.7	887	XiC(117.05±500ppm)
Benzene, 1-ethyl-4-methyl-	1264.96 s, 1.197 s	12519649	735	105.05	1264.96	754	XiC(105.05±500ppm)
Benzene, 1-isociano-3-methyl-	1859.92 s, 1.422 s	523806151	750	116.03	1859.92	792	XiC(116.03±500ppm)
Benzene, 1-methyl-2-[(3-methylphenyl)methyl]-	1374.95, 1.728	10350058	772	181.09	1629.4	563	XiC(181.09±500ppm)
Benzene, 1-methyl-3-(1-methylethenyl)-	834.988, 1.261	4300697	871	117.05	1096.3	634	XiC(117.05±500ppm)
Benzene, 1-methyl-3-(2-phenylethenyl)-, (E)-	1549.94, 1.872	84543812	827	179.06	1846.7	1828	XiC(179.06±500ppm)
Benzene, 1-methyl-3-(phenylmethyl)-	1304.96 s, 1.706 s	13372160	869	167.07	1304.96	1728	XiC(167.07±500ppm)
Benzene, 1-methyl-3-[(4-methylphenyl)methyl]-	1374.95 s, 1.706 s	16551758	851	181.08	1374.95	1480	XiC(181.08±500ppm)

Benzene, 1-methyl-4-(phenylmethyl)-	1294.96 s, 1.709 s	22775871	820	167.07	1294.96	1845	XIC(167.07±500ppm)
Benzene, 1-tert-butyl-4-cyclopropylmethyl-	1069.97 s, 1.198 s	6984928	748	173.11	1069.97	1328	XIC(173.11±500ppm)
Benzene, 2,4-dichloro-1-methoxy-	1059.97 s, 1.631 s	7077700	927	175.96	1059.97	2216	XIC(175.96±500ppm)
Benzene, 2-methoxy-4-methyl-1-(1-methylethyl)-	999.977 s, 1.293 s	27950687	882	149.08	999.977	3262	XIC(149.08±500ppm)
Benzene, 4-butyl-1,2-dimethoxy-	2084.91 s, 2.186 s	13139227	741	151.06	2084.91	676	XIC(151.06±500ppm)
Benzene, 4-ethenyl-1,2-dimethoxy-	1134.97 s, 1.661 s	19302617	780	164.06	1134.97	3043	XIC(164.06±500ppm)
Benzene, decyl-	1419.95 s, 1.239 s	30177044	782	92.04	1419.95	2089	XIC(92.04±500ppm)
Benzene, nonyl-	1329.96 s, 1.231 s	17278128	731	92.04	1329.96	1522	XIC(92.04±500ppm)
Benzene, octyl-	1234.96 s, 1.219 s	8138579	758	92.05	1234.96	776	XIC(92.05±500ppm)
Benzene, pentachloro-	1289.96, 1.664	216800	765	43.03	1533.3	1306	XIC(43.03±500ppm)
Benzene, pentamethyl-	959.98, 1.259	3575778	777	133.09	1204.5	513	XIC(133.09±500ppm)
Benzenoacetic acid, α-cyano-, ethyl ester	1269.96, 1.138	703022527	734	117.06	1511.1	502	XIC(117.06±500ppm)
Benzenoacetic acid, α-methoxy-, methyl ester, (±)-	1499.94, 1.610	41985050	744	121.05	1781.3	1324	XIC(121.05±500ppm)
Benzenoacetic acid, α-methyl-, methyl ester	1899.92, 2.826	46782054	753	105.01	2313.4	1327	XIC(105.01±500ppm)
Benzenoacetic acid, α-oxo-, methyl ester	1399.95, 1.973	25274647	798	105.01	1658.8	1031	XIC(105.01±500ppm)
Benzenoacetoneitrile, 3,4-dimethoxy-α-(1-methylethyl)-	1484.95, 1.972	4467475	735	219.07	1762.5	698	XIC(219.07±500ppm)
Benzenoacetoneitrile, α-(β-D-glucopyranosyloxy)-, (R)-	1269.96 s, 1.134 s	617860469	738	117.05	1269.96	649	XIC(117.05±500ppm)
Benzenobutanol, γ,4-dimethyl-	1729.93, 1.884	13609471	749	132.08	2086.7	642	XIC(132.08±500ppm)
Benzenocarbothioic acid, 2,4,6-triethyl-, S-(2-phenylethyl) ester	2024.91, 2.591	15728864	760	189.08	2480	1335	XIC(189.08±500ppm)
Benzenoethanol, β-(1-methylethyl)-β-phenyl-	1534.94 s, 1.705 s	21545973	736	129.05	1534.94	1166	XIC(129.05±500ppm)
Benzenoethanol, β-methyl-	1264.96, 1.202	12354141	783	105.06	1505.6	631	XIC(105.06±500ppm)
Benzenemethanol, α-2-cyclohexen-1-yl-	1439.95, 1.847	9973845	732	107.04	1706.2	665	XIC(107.04±500ppm)
Benzenepropanenitrile, 3,4-dimethoxy-	2224.9 s, 3.625 s	14891027	743	151.06	2224.9	1364	XIC(151.06±500ppm)
Benzenepropanoic acid, 3,5-bis(1,1-dimethylethyl)-4-hydroxy-, 2-ethylhexyl ester	1989.91, 1.625	1872982	707	375.24	2433.4	896	XIC(375.24±500ppm)
Benzenepropanoic acid, 3,5-bis(1,1-dimethylethyl)-4-hydroxy-, ethyl ester	1674.93 s, 1.548 s	150980401	789	291.17	1674.93	3374	XIC(291.17±500ppm)
Benzenepropanoic acid, 3,5-bis(1,1-dimethylethyl)-4-hydroxy-, methyl ester	1629.94 s, 1.566 s	89299576	844	277.16	1629.94	2226	XIC(277.16±500ppm)
Benzenepropanoic acid, 3,5-bis(1,1-dimethylethyl)-4-hydroxy-, octadecyl ester	2729.87 s, 1.000 s	666490356	889	57.06	2729.87	5054	XIC(57.06±500ppm)
Benzenesulfonamide, N-butyl-	1514.94 s, 2.191 s	43985825	878	77.02	1514.94	2376	XIC(77.02±500ppm)
Benzenimidazo[2,1-a]isoquinoline	2129.9 s, 1.411	506574879	704	218.08	2620	694	XIC(218.08±500ppm)
Benzenimidazo[5-a]amine, 1-(4-ethoxyphenyl)-	1599.94, 1.020	5303637	757	253.27	1913.3	651	XIC(253.27±500ppm)
Benzo[2,1-b:3,4-b']bis[1]benzothioephene	1429.95 s, 0.856 s	5514917	746	290.16	1429.95	1921	XIC(290.16±500ppm)
Benzo[b]dihydropyran, 6-hydroxy-4,4,5,7,8-pentamethyl-	1254.96, 1.351	320330383	749	205.05	1494.7	12474	XIC(205.05±500ppm)
Benzo[b]naphtho[2,3-d]furan	1769.93 s, 2.384 s	7634517	801	218.05	1769.93	1123	XIC(218.05±500ppm)
Benzo[b]thiophene, 2-ethyl-	1189.96, 1.499	4596982	712	162.05	1426.3	538	XIC(162.05±500ppm)
Benzo[c]cinnoline, 4,7-dimethyl-	1649.94, 2.151	15551661	833	208.07	1980	924	XIC(208.07±500ppm)
Benzo[c]phenanthridin-6(5H)-one, 11,12-dihydro-2,3,8,9-tetramethoxy	2124.9 s, 3.583 s	10895564	760	367.14	2124.9	10819	XIC(367.14±500ppm)
Benzo[f]naphtho[2,1-c]cinnoline	2254.9 s, 1.815 s	9340294	761	280.27	2254.9	1196	XIC(280.27±500ppm)
Benzocaine, N-methyl-	1434.95 s, 2.056 s	11730701	840	134.04	1434.95	1442	XIC(134.04±500ppm)
Benzocycloheptene, 3-hydroxy-, TMS derivative	1289.96 s, 1.219 s	19482005	740	144.07	1289.96	2625	XIC(144.07±500ppm)
Benzoic acid, 2,4,5-trichlorophenyl ester	1474.95 s, 1.665 s	33589917	782	105.05	1474.95	700	XIC(105.05±500ppm)
Benzoic acid, 2,4,6-trimethyl-, 2,4,6-trimethylphenyl ester	1074.97 s, 1.565 s	12337908	811	147.06	1074.97	515	XIC(147.06±500ppm)
Benzoic acid, 2,4-dichloro-, ethyl ester	1249.96 s, 1.614 s	5439319	881	172.94	1249.96	1307	XIC(172.94±500ppm)
Benzoic acid, 2,4-dichloro-, methyl ester	1179.97, 1.685	3827576	884	172.94	1415.8	1147	XIC(172.94±500ppm)
Benzoic acid, 2,5-dichloro-, methyl ester	1179.97, 1.680 s	3775809	895	172.94	1179.97	1255	XIC(172.94±500ppm)
Benzoic acid, 2-hydroxy-, 2-methylbutyl ester	1334.96, 1.462	18898377	785	120	1583.3	1644	XIC(120.00±500ppm)
Benzoic acid, 2-hydroxy-, pentyl ester	1334.96, 1.459	19581004	813	120.01	1583.3	1486	XIC(120.01±500ppm)
Benzoic acid, 2-hydroxy-3-[(2-hydroxy-4-methoxy-6-propylbenzoyloxy)-4-methoxy-6-propyl-, methyl	1374.95 s, 1.989 s	8165239	735	162.07	1374.95	995	XIC(162.07±500ppm)
Benzoic acid, 2-methylbutyl ester	1514.94 s, 1.412 s	46149416	729	105.02	1514.94	1116	XIC(105.02±500ppm)
Benzoic acid, 2-methylpropyl ester	1589.94, 1.463	34570469	715	105.01	1900	697	XIC(105.01±500ppm)
Benzoic acid, 3,5-bis(1,1-dimethylethyl)-4-hydroxy-, methyl ester	1819.92 s, 1.974 s	5118248	745	249.1	1819.92	576	XIC(249.10±500ppm)
Benzoic acid, 3-methyl-, methyl ester	974.979, 1.563	81265841	918	119.03	1218.2	2103	XIC(119.03±500ppm)
Benzoic acid, 4-(4-ethylcyclohexyl)-, 2,3-dicyano-4-ethoxyphenyl ester	1659.93, 1.501	18391477	717	215.16	1993.3	661	XIC(215.16±500ppm)
Benzoic acid, 4-ethenyl-, 4-[[[methylsulfonyl]amino]methyl]phenyl ester	924.982 s, 0.793 s	23323451	760	131.07	924.982	543	XIC(131.07±500ppm)
Benzoic acid, 4-ethoxy-, ethyl ester	1289.96 s, 1.629 s	17382314	830	121.01	1289.96	1821	XIC(121.01±500ppm)
Benzoic acid, 4-methyl-, 1-methylethyl ester	1159.97, 1.500	8537027	874	119.04	1395	792	XIC(119.04±500ppm)
Benzoic acid, 4-methyl-, 2-methylpropyl ester	1194.96 s, 1.414 s	16134261	897	119.03	1194.96	1207	XIC(119.03±500ppm)
Benzoic acid, 4-methyl-, 2-oxo-2-phenylethyl ester	1614.94 s, 2.035 s	10145546	760	105.02	1614.94	570	XIC(105.02±500ppm)
Benzoic acid, 4-methyl-, methyl ester	979.978 s, 1.530 s	20134313	876	119.03	979.978	1079	XIC(119.03±500ppm)
Benzoic acid, 4-methyl-, phenyl ester	1644.94 s, 2.133 s	69453301	736	119.03	1644.94	2601	XIC(119.03±500ppm)
Benzoic acid, 4-methyl-, propyl ester	1159.97 s, 1.493 s	7730311	881	119.03	1159.97	850	XIC(119.03±500ppm)
Benzoic acid, 4-methyl-2-trimethylsilyloxy-, trimethylsilyl ester	1339.96 s, 1.074 s	86917422	730	73.03	1339.96	2778	XIC(73.03±500ppm)
Benzoic acid, dec-2-yl ester	1584.94 s, 1.402 s	51856740	750	105.02	1584.94	703	XIC(105.02±500ppm)
Benzoic acid, ethyl ester	929.981 s, 1.482 s	56510762	912	105.02	929.981	5705	XIC(105.02±500ppm)
Benzoic acid, hept-3-yl ester	1324.96 s, 1.591 s	77135624	777	105.01	1324.96	1784	XIC(105.01±500ppm)
Benzoic acid, heptyl ester	1564.94 s, 1.466 s	52959230	755	105.02	1564.94	1269	XIC(105.02±500ppm)
Benzoic acid, hexyl ester	1549.94, 1.465	76198304	759	105.02	1846.7	1353	XIC(105.02±500ppm)
Benzoic acid, methyl ester	839.987 s, 1.536 s	42350865	904	105.01	839.987	3427	XIC(105.01±500ppm)
Benzoic acid, octyl ester	1934.92 s, 1.584 s	20890109	738	123.02	1934.92	647	XIC(123.02±500ppm)
Benzoic acid, pentyl ester	1589.94, 1.469	30305191	743	123.03	1900	900	XIC(123.03±500ppm)
Benzoic Acid, TBDS derivative	989.978 s, 1.105 s	63931479	815	179.06	989.978	3170	XIC(179.06±500ppm)
Benzoic acid, tetradecyl ester	1564.94, 1.472	58889719	745	105.01	1866.7	1434	XIC(105.01±500ppm)
Benzoic Acid, TMS derivative	1014.98 s, 1.258 s	240700819	882	179.03	1014.98	5188	XIC(179.03±500ppm)
Benzoic acid, undecyl ester	1564.94, 1.472	56039939	792	105.02	1866.7	1431	XIC(105.02±500ppm)
Benzophenone	1384.95 s, 2.057 s	849330734	832	105.01	1384.95	3548	XIC(105.01±500ppm)
Benzophenone, 2,4,6-trimethyl-	1539.94 s, 1.910 s	9908256	755	223.09	1539.94	838	XIC(223.09±500ppm)
Benzosuberol, TMS derivative	1289.96, 1.223	23006080	712	144.07	1533.3	2376	XIC(144.07±500ppm)
Benzothiazole	994.977 s, 1.960 s	239518586	953	134.99	994.977	12298	XIC(134.99±500ppm)
Benzothiazole, 2-(o-aminophenyl)-4-methyl-	1469.95, 1.718	5914651370	748	240.09	1743.8	1430	XIC(240.09±500ppm)
Benzothiazole, 2-methyl-	1069.97 s, 1.834 s	9454008	925	149.01	1069.97	1217	XIC(149.01±500ppm)
Benzothiazole, 2-phenyl-	1664.93, 2.363	7245130	823	211.02	2000	514	XIC(211.02±500ppm)
Benzyl alcohol, TMS derivative	909.983 s, 1.122 s	362760125	860	91.04	909.983	6835	XIC(91.04±500ppm)

Benzyl butyl phthalate	1904.92 s, 2.334 s	31977715	931	149.01	1904.92	1931	XiC(149.01±500ppm)
Benzyl sulfone	1289.96, 1.696	31694820	861	91.04	1533.3	1633	XiC(91.04±500ppm)
Bibenzyl	1289.96 s, 1.692 s	26629744	877	91.04	1289.96	1393	XiC(91.04±500ppm)
Bicyclo[3.1.1]heptane, 2,6,6-trimethyl-, [1R-(1a,2a,5a)]-	1674.93, 1.419	44208546	733	55.05	2013.3	686	XiC(55.05±500ppm)
Biphenyl	1154.97 s, 1.716 s	66289707	927	154.05	1154.97	8817	XiC(154.05±500ppm)
Bis(2-chloroethyl) ether	709.996 s, 1.466 s	87414883	890	92.99	709.996	813	XiC(92.99±500ppm)
Bis(2-ethylhexyl) phthalate	1989.91 s, 1.692 s	15973559	825	149	1989.91	1247	XiC(149.00±500ppm)
Bis(4-tert-butylidimethylsiloxy)benzyl ether	919.982, 0.791	10203949	730	221.07	1169.6	528	XiC(221.07±500ppm)
Bisphenol A monomethyl ether, TMS derivative	1084.97 s, 0.970 s	6501337	814	299.04	1084.97	535	XiC(299.04±500ppm)
Bisphenol AF, bis(trimethylsilyl) ether	1684.93, 1.064	3132067	739	411.12	2026.7	513	XiC(411.12±500ppm)
Borane, diethyl(decyloxy)-	1979.91 s, 1.080 s	255367445	757	57.06	1979.91	1215	XiC(57.06±500ppm)
Borane, ethylisopropylmethyl-	1109.97, 0.904	122224582	719	41.03	1345	8330	XiC(41.03±500ppm)
Boric acid, 3TMS derivative	699.996 s, 0.714 s	643448166	896	73.03	699.996	5148	XiC(73.03±500ppm)
Boric acid, diethyl-	1529.94 s, 1.898 s	91176163	731	57.05	1529.94	794	XiC(57.05±500ppm)
Butanal, 2,3,4-tris(trimethylsilyloxy)-3-[[trimethylsilyloxy]methyl]-, O-methyloxime, (S)-	1254.96, 0.785	80286614	801	73.04	1494.7	2344	XiC(73.04±500ppm)
Butane, 1-chloro-2-methyl-	1969.91, 1.072	308276621	729	57.07	2406.7	1729	XiC(57.07±500ppm)
Butane, 2,2-dimethyl-	2199.9, 1.341	141152527	747	43.06	2713.4	613	XiC(43.06±500ppm)
Butane-1,3-diol, 1-methylene-3-methyl-, bis(trimethylsilyl)ether	1189.96, 1.264	418793369	731	73.03	1426.3	2171	XiC(73.03±500ppm)
Butanedioic acid, 2TMS derivative	1089.97 s, 1.055 s	15144718	733	147.05	1089.97	2226	XiC(147.05±500ppm)
Butanedioic acid, diethyl ester	934.981 s, 1.417 s	13584248	886	101.01	934.981	1760	XiC(101.01±500ppm)
Butanenitrile, 2-hydroxy-3-methyl-	1054.97 s, 0.868 s	234949957	733	43.06	1054.97	2685	XiC(43.06±500ppm)
Butanoic acid, (tetrahydro-2-furanyl)methyl ester	1339.96, 1.186	64817070	736	71.06	1588.9	510	XiC(71.06±500ppm)
Butanoic acid, 2-hydroxy-2-methyl-, methyl ester	2129.9 s, 1.282 s	572064969	746	73.03	2129.9	1669	XiC(73.03±500ppm)
Butanoic acid, 2-oxo-, ethyl ester	1714.93 s, 1.015 s	344313665	739	57.06	1714.93	881	XiC(57.06±500ppm)
Butanoic acid, tributylsilyl ester	1129.97 s, 0.882 s	25126143	746	103.04	1129.97	2020	XiC(103.04±500ppm)
Butoxytriglycol, TMS derivative	1969.91 s, 1.320 s	128229306	783	73.03	1969.91	3707	XiC(73.03±500ppm)
Butyl benzoate	1144.97 s, 1.474 s	8066606	912	105.02	1144.97	705	XiC(105.02±500ppm)
Butyl meta toluate	1259.96, 1.493	70732795	916	119.03	1500	3180	XiC(119.03±500ppm)
Butylated Hydroxytoluene	1279.96 s, 1.324 s	36260828	766	205.13	1279.96	1436	XiC(205.13±500ppm)
Butyric acid, neopentyl ester	1399.95, 0.994	427691928	737	43.06	1658.8	1431	XiC(43.06±500ppm)
Caffeine	1564.94 s, 2.658 s	8530430	913	194.06	1564.94	518	XiC(194.06±500ppm)
Campesterol, TMS derivative	2419.89, 2.793	8659942	826	129.05	3006.7	900	XiC(129.05±500ppm)
Caprolactam	1019.98, 2.216	12997605	906	55.02	1259.1	835	XiC(55.02±500ppm)
Carbamic acid, methyl ester	1259.96 s, 0.632 s	21748175	751	44	1259.96	707	XiC(44.00±500ppm)
Carbamic acid, N,N-dimethyl-, TBDMS ester	679.997, 1.018	10966966	760	146.04	981.5	840	XiC(146.04±500ppm)
Carbazole, TMS derivative	1959.92 s, 1.562 s	22263109	735	73.06	2393.4	708	XiC(73.06±500ppm)
Carbazolo[3,4-c]carbazole, 5,10-dihydro-2,13-dimethyl-	2384.89 s, 0.289 s	9376081	767	334.14	2384.89	1192	XiC(334.14±500ppm)
Carbitol, TMS derivative	1739.93, 1.163	43296959	758	73.04	2100	913	XiC(73.04±500ppm)
Carbon dioxide	1439.95 s, 1.472 s	100929379	760	44.05	1439.95	3089	XiC(44.05±500ppm)
Carbonic acid, dodecyl undecyl ester	1869.92, 1.104	285038681	741	43.06	2273.4	1564	XiC(43.06±500ppm)
Carbonic acid, decyl vinyl ester	1284.96, 0.924	285514832	803	57.03	1527.8	1628	XiC(57.03±500ppm)
Carbonic acid, eicosyl vinyl ester	1294.96 s, 0.934 s	894153059	837	57.06	1294.96	3384	XiC(57.06±500ppm)
Carbonic acid, ethyl octadecyl ester	2004.91, 1.539	58495439	744	91.02	2453.4	2348	XiC(91.02±500ppm)
Carbonic acid, O(1)-benzyl-O(2)-1,2-dihydroxyethyl(ester)	1624.94 s, 2.155 s	78843814	798	91.04	1624.94	1192	XiC(91.04±500ppm)
Carbonic acid, O(1)-benzyl-O(2)-ethyl(ester)	1104.97 s, 1.686 s	4045230	897	91.04	1104.97	691	XiC(91.04±500ppm)
Carbonic acid, octadecyl vinyl ester	1309.96 s, 0.947 s	488581684	814	57.03	1309.96	10265	XiC(57.03±500ppm)
Carvacrol, TMS derivative	1084.97, 1.071	292347843	815	73.04	1320	2251	XiC(73.04±500ppm)
Carvone	1009.98 s, 1.528 s	6734443	820	82.03	1009.98	722	XiC(82.03±500ppm)
Catechol, 2TMS derivative	1299.96 s, 1.152 s	42651035	752	73.05	1544.4	2971	XiC(73.05±500ppm)
Cetene	1344.95 s, 1.045 s	596386225	867	43.05	1344.95	4958	XiC(43.05±500ppm)
Chalcone	1674.93, 2.222	7629462	940	77.03	2013.3	560	XiC(77.03±500ppm)
Chamazulene	1419.95 s, 1.696 s	12567457	747	169.08	1419.95	2599	XiC(169.08±500ppm)
Cholesta-3,5-diene	2214.9, 2.103	2692256	741	368.31	2733.4	598	XiC(368.31±500ppm)
Cholesterol, TMS derivative	2349.89 s, 2.360 s	175072892	932	129.05	2349.89	7202	XiC(129.05±500ppm)
Chrysene	1984.91 s, 3.084 s	2123122	849	228.1	2426.7	592	XiC(228.10±500ppm)
Chrysophanol, 2TMS derivative	2179.9 s, 3.044 s	5836307	742	383.12	2179.9	1019	XiC(383.12±500ppm)
Cinnamic acid, TMS derivative	1244.96 s, 1.312 s	3825834	730	205.05	1244.96	620	XiC(205.05±500ppm)
Cinnamyl alcohol, trimethylsilyl ether	1149.97 s, 1.215 s	134844226	816	117.05	1149.97	6078	XiC(117.05±500ppm)
Cinnamyl cinnamate	1709.93, 1.871	37217107	706	131.06	2060	1132	XiC(131.06±500ppm)
cis-2-Nonene	1539.94, 1.431	14304022	744	84.08	1833.3	979	XiC(84.08±500ppm)
Coumarin	1214.96, 2.318	2623843	903	118.03	1452.6	534	XiC(118.03±500ppm)
Cumyl alcohol, trimethylsilyl ether	1324.96 s, 1.422 s	46032302	751	133.04	1324.96	1798	XiC(133.04±500ppm)
Cyanic acid, butyl ester	1354.95, 1.040	359411557	717	41.04	1605.9	1658	XiC(41.04±500ppm)
Cyanic acid, ethyl ester	1514.94 s, 1.872 s	253891323	759	71.06	1514.94	1683	XiC(71.06±500ppm)
Cyclobutane, 1,2:3,4-di-O-ethylboranediyl-	909.983, 1.621	14411833	779	98.02	1160.9	1588	XiC(98.02±500ppm)
Cyclobutane, ethyl-	1569.94, 1.010	91760891	740	56.06	1873.3	2795	XiC(56.06±500ppm)
Cyclobutane-1,2-dicarboxylic acid peroxide t-butyl ester	1309.96 s, 0.911 s	297931521	753	57.06	1309.96	901	XiC(57.06±500ppm)
Cyclobutanecarboxylic acid chloride	1634.94, 1.042	182468880	752	55.04	1960	734	XiC(55.04±500ppm)
Cyclobutanecarboxylic acid, 2-propenyl ester	1874.92 s, 1.101 s	104212369	735	55.05	1874.92	1353	XiC(55.05±500ppm)
Cyclobutanecarboxylic acid, 3-methylbutyl ester	1019.98 s, 0.908 s	58026966	733	55.05	1019.98	779	XiC(55.05±500ppm)
Cyclodecacyclotetradecene, 14,15-didehydro-1,4,5,8,9,10,11,12,13,16,17,18,19,20-tetradecahydro-	1844.92, 1.888	4924417	732	67.04	2240	514	XiC(67.04±500ppm)
Cyclododecanone	1279.96 s, 1.615 s	29711283	922	55.05	1279.96	824	XiC(55.05±500ppm)
Cycloicosane	1659.93 s, 1.062 s	356393334	845	55.05	1659.93	2064	XiC(55.05±500ppm)
Cycloheptane, bromo-	1784.93, 1.109	290378894	747	55.04	2160	542	XiC(55.04±500ppm)
Cycloheptasiloxane, tetradecamethyl-	1239.96 s, 0.751 s	13082289	868	73.04	1239.96	912	XiC(73.04±500ppm)
Cyclohexadecane	1344.95, 1.050	385945625	880	83.11	1594.4	3481	XiC(83.11±500ppm)
cyclohexane, [1,1'-biphenyl]-4-yl-	1729.93 s, 1.934 s	11328740	817	236.13	1729.93	954	XiC(236.13±500ppm)
Cyclohexane, 1,2,3,4,5,6-hexamethyl-	2614.87, 2.458	142499124	730	69.06	3266.8	1250	XiC(69.06±500ppm)
Cyclohexane, 1,2-diethyl-3-methyl-	984.978, 0.889	85773542	759	69.06	1227.3	1533	XiC(69.06±500ppm)
Cyclohexane, 1-bromo-4-methyl-	1489.95, 1.048	316750122	730	55.05	1768.8	943	XiC(55.05±500ppm)
Cyclohexane, 1-ethyl-1,3-dimethyl-, cis-	1859.92, 1.106	207717206	751	55.05	2260	2336	XiC(55.05±500ppm)

Cyclohexane, 1-ethyl-2,4-dimethyl-	999.977, 0.894	84226425	755	69.06	1240.9	3873	XIC(69.06±500ppm)
Cyclohexane, 1-ethyl-2-propyl-	1814.92 s, 1.014 s	1994181496	763	69.06	1814.92	5801	XIC(69.06±500ppm)
Cyclohexane, 2-propenyl-	1214.96, 1.036	51985563	751	83.07	1452.6	1457	XIC(83.07±500ppm)
Cyclohexane, decyl-	1399.95 s, 1.082 s	156939109	743	83.07	1399.95	2092	XIC(83.07±500ppm)
Cyclohexane, methyl-	1754.93, 1.076	94177026	755	41.05	2120	2591	XIC(41.05±500ppm)
Cyclohexane, octadecyl-	1644.94 s, 1.140 s	176307334	734	83.07	1644.94	1060	XIC(83.07±500ppm)
Cyclohexane, octyl-	1164.97 s, 0.992 s	201830106	731	55.05	1164.97	2907	XIC(55.05±500ppm)
Cyclohexane, pentyl-	1489.95, 1.098	141375831	743	83.06	1768.8	2364	XIC(83.06±500ppm)
Cyclohexane, tetradecyl-	1674.93 s, 1.099 s	144105568	730	83.07	1674.93	827	XIC(83.07±500ppm)
Cyclohexane, undecyl-	1489.95 s, 1.093 s	130651500	753	83.06	1489.95	1631	XIC(83.06±500ppm)
Cyclohexanepropanol-	1744.93 s, 1.184 s	86171648	734	67.04	1744.93	500	XIC(67.04±500ppm)
Cyclohexanone, 2-propyl-	904.983 s, 1.642 s	4411322	767	98.02	904.983	786	XIC(98.02±500ppm)
Cyclohexanone, 3,3,5-trimethyl-	1629.94, 1.050	219608561	734	41.05	1953.3	1108	XIC(41.05±500ppm)
Cyclohexanone, 3-butyl-	1479.95 s, 0.998 s	219962373	757	41.03	1479.95	8219	XIC(41.03±500ppm)
Cyclohexasiloxane, dodecamethyl-	1074.97 s, 0.744 s	5618239	834	340.98	1074.97	1488	XIC(340.98±500ppm)
Cyclohexene, 1-methyl-4-(1-methylethenyl)-, (S)-	759.992, 1.011	16866407	893	68.05	1040.7	1155	XIC(68.05±500ppm)
Cyclohexene, 3-methyl-6-(1-methylethyl)-	1394.95, 1.102	50891754	751	81.06	1652.9	955	XIC(81.06±500ppm)
Cyclooctane, 1,2-diethyl-	1199.96, 0.929	75053015	727	55.05	1436.8	553	XIC(55.05±500ppm)
Cyclooctane, 1,4-dimethyl-, trans-	1244.96 s, 0.949 s	483128038	738	69.06	1244.96	3210	XIC(69.06±500ppm)
Cyclooctane, methyl-	1179.97, 0.981	22607666	735	55.05	1415.8	799	XIC(55.05±500ppm)
Cyclooctane, tetradecyl-	2794.86 s, 3.022 s	37422013	737	69.06	2794.86	1027	XIC(69.06±500ppm)
Cyclopent-2-enone, 2-methyl-3,4-diphenyl-	1869.92 s, 2.179 s	80341921	740	248.09	1869.92	2588	XIC(248.09±500ppm)
Cyclopenta(def)phenanthrene	1714.93 s, 2.627 s	6225022	877	204.03	1714.93	921	XIC(204.03±500ppm)
Cyclopenta[g]-2-benzopyran, 1,3,4,6,7,8-hexahydro-4,6,6,7,8-hexamethyl-	1569.94 s, 1.579 s	136847864	874	243.15	1569.94	8218	XIC(243.15±500ppm)
Cyclopentane, (1-methylbutyl)-	1549.94 s, 1.163 s	338663138	756	55.05	1549.94	6675	XIC(55.05±500ppm)
Cyclopentane, 1,2,3-trimethyl-	1579.94, 1.008	84446928	749	70.08	1886.7	936	XIC(70.08±500ppm)
Cyclopentane, 1-hexyl-3-methyl-	1354.95 s, 1.027 s	544250362	751	55.05	1354.95	3139	XIC(55.05±500ppm)
Cyclopentane, 1-butyl-2-propyl-	1274.96 s, 0.965 s	125620431	735	55.05	1274.96	6427	XIC(55.05±500ppm)
Cyclopentane, butyl-	1564.94 s, 1.096 s	94881770	744	68.05	1564.94	2960	XIC(68.05±500ppm)
Cyclopentane, heneicosyl-	2089.91 s, 1.315 s	41738135	759	43.05	2089.91	568	XIC(43.05±500ppm)
Cyclopentane, hexyl-	2144.9 s, 1.159 s	52264952	748	69.06	2144.9	873	XIC(69.06±500ppm)
Cyclopentane, nonyl-	1214.96, 1.025	71596846	729	55.05	1452.6	1808	XIC(55.05±500ppm)
Cyclopentane, pentyl-	1714.93 s, 1.134 s	86386116	733	55.03	1714.93	2183	XIC(55.03±500ppm)
Cyclopentane-1-carbonitrile, 1-(4-hydroxy-3-methoxyphenyl)-	1524.94 s, 2.060 s	17918896	729	217.09	1524.94	2858	XIC(217.09±500ppm)
Cyclopentanecarboxamide, N-(1-naphthyl)-	1364.95, 0.919	6851474	718	143.07	1617.7	901	XIC(143.07±500ppm)
Cyclopentanone	2004.91 s, 1.176 s	116785564	731	55.04	2004.91	795	XIC(55.04±500ppm)
Cyclopentasiloxane, decamethyl-	874.985 s, 0.751 s	4166986	818	266.97	874.985	863	XIC(266.97±500ppm)
Cyclopropane, 1,1-diethyl-	1514.94 s, 1.019 s	193326330	755	41.04	1514.94	745	XIC(41.04±500ppm)
Cyclopropane, 1,2-dimethyl-3-pentyl-	1039.97, 0.928	89719290	738	69.06	1277.3	1128	XIC(69.06±500ppm)
Cyclopropane, 1-butyl-1-methyl-2-propyl-	1239.96, 0.943	394392046	730	69.06	1478.9	1812	XIC(69.06±500ppm)
Cyclopropane, 1-methyl-2-(3-methylpentyl)-	1089.97, 0.951	428104753	816	43.04	1325.9	5096	XIC(43.04±500ppm)
Cyclopropane, 2-bromo-1-methyl-1-phenyl-	1694.93, 1.858	21477152	737	131.07	2040	842	XIC(131.07±500ppm)
Cyclotetacosane	1974.91, 1.245	91994318	778	43.05	2413.4	914	XIC(43.05±500ppm)
Cyclotetradecane	1314.96 s, 0.977 s	240793439	739	41.04	1314.96	926	XIC(41.04±500ppm)
Cyclotetrasiloxane, (iodomethyl)heptamethyl-	1994.91 s, 0.481 s	1587472	745	45	1994.91	722	XIC(45.00±500ppm)
Cyclotetrasiloxane, octamethyl-	719.995 s, 0.713 s	75011304	867	281.02	719.995	4530	XIC(281.02±500ppm)
Cyclotrisiloxane, 2,4-dimethyl-2,4,6,6-tetrahenyl-	2139.9 s, 2.506 s	1088473	745	377.01	2139.9	1087	XIC(377.01±500ppm)
Cyclotrisiloxane, hexamethyl-	694.996 s, 0.952	78745106	790	207.01	694.996	3619	XIC(207.01±500ppm)
Cycloundecane, 1,1,2-trimethyl-	1049.97, 0.952	85420937	833	43.05	1286.4	2860	XIC(43.05±500ppm)
D-(-)-Fructofuranose, pentakis(trimethylsilyl) ether (isomer 1)	1544.94, 0.835	301282563	925	73.04	1840	1809	XIC(73.04±500ppm)
D-(-)-Fructofuranose, pentakis(trimethylsilyl) ether (isomer 2)	2064.91 s, 0.969 s	17441914	760	73.03	2064.91	576	XIC(73.03±500ppm)
D-(-)-Ribofuranose, tetrakis(trimethylsilyl) ether (isomer 1)	1959.92, 1.157	29978146	756	73.04	2393.4	3547	XIC(73.04±500ppm)
D-(-)-Ribofuranose, tetrakis(trimethylsilyl) ether (isomer 2)	1959.92 s, 1.156 s	92865861	774	73.03	1959.92	3420	XIC(73.03±500ppm)
D-(-)-Tagatofuranose, pentakis(trimethylsilyl) ether (isomer 1)	1599.94 s, 0.786 s	8129238	731	73.04	1599.94	520	XIC(73.04±500ppm)
D-(-)-Tagatofuranose, pentakis(trimethylsilyl) ether (isomer 2)	1539.94 s, 0.878 s	366460192	745	73.03	1539.94	289	XIC(73.03±500ppm)
D-(+)-Talofuranose, pentakis(trimethylsilyl) ether (isomer 1)	1559.94 s, 0.904 s	37569228	770	73.04	1559.94	1689	XIC(73.04±500ppm)
D-(+)-Xylose, tetrakis(trimethylsilyl) ether, trimethylsilyloxime (isomer 1)	1254.96 s, 0.791 s	52730132	794	73.03	1254.96	1693	XIC(73.03±500ppm)
Dantron, 2TMS derivative	2039.91 s, 2.038 s	23422622	856	73.05	2500	1941	XIC(73.05±500ppm)
d-Arabinal	1039.97, 0.874	373284388	729	73.03	1277.3	1154	XIC(73.03±500ppm)
Decaethylene glycol, TMS derivative	2414.89, 0.178	235021329	928	45.04	3000.1	1411	XIC(45.04±500ppm)
Decane	744.993, 0.811	693186806	868	57.06	1029.6	3182	XIC(57.06±500ppm)
Decane, 1,1-diethoxy-	1244.96 s, 1.036 s	158012861	777	103.06	1244.96	5492	XIC(103.06±500ppm)
Decane, 1-iodo-	1224.96 s, 0.913 s	305990548	788	57.06	1224.96	4687	XIC(57.06±500ppm)
Decane, 2,3,6-trimethyl-	1704.93 s, 0.993 s	289464138	732	57.06	1704.93	3112	XIC(57.06±500ppm)
Decane, 2,3,8-trimethyl-	1454.95, 0.961	425470439	747	57.1	1725	668	XIC(57.10±500ppm)
Decane, 2,4,6-trimethyl-	844.987 s, 2.185 s	33087243	849	43.06	844.987	759	XIC(43.06±500ppm)
Decane, 2,4-dimethyl-	1089.97 s, 0.903 s	348782263	780	43.05	1089.97	4334	XIC(43.05±500ppm)
Decane, 2-cyclohexyl-	1499.94, 2.331	13847492	743	111.03	1781.3	751	XIC(111.03±500ppm)
Decane, 3,3,5-trimethyl-	1464.95 s, 0.929 s	250017989	733	85.08	1464.95	3566	XIC(85.08±500ppm)
Decane, 3,6-dimethyl-	1044.97 s, 0.869 s	281430740	839	43.05	1044.97	1805	XIC(43.05±500ppm)
Decane, 3,7-dimethyl-	749.993 s, 2.219 s	60810174	889	57.06	749.993	811	XIC(57.06±500ppm)
Decane, 3,8-dimethyl-	1069.97 s, 0.856 s	259433851	734	71.07	1069.97	8527	XIC(71.07±500ppm)
Decane, 5,6-dimethyl-	774.991 s, 0.804 s	110281061	893	43.06	774.991	7291	XIC(43.06±500ppm)
Decane, 6-ethyl-2-methyl-	2309.89, 1.610	638213621	738	57.07	2860.1	2031	XIC(57.07±500ppm)
Decanoic acid, ethyl ester	1159.97 s, 1.141 s	7345594	750	88.04	1159.97	1113	XIC(88.04±500ppm)
Decanoic acid, methyl ester	1609.94 s, 1.209 s	346617362	759	74.02	1609.94	2263	XIC(74.02±500ppm)
Decanoic acid, TMS derivative	1224.96 s, 1.015 s	98179654	899	75.01	1224.96	4271	XIC(75.01±500ppm)
Dehydroabietic acid	1944.92 s, 2.379 s	9256886	809	239.21	2373.4	587	XIC(239.21±500ppm)
Dehydroabietic acid, TMS derivative	1929.92 s, 1.697 s	56170925	808	239.2	2353.4	1533	XIC(239.20±500ppm)
Dehydrothio-p-toluidine-3-sulfonic acid	1459.95, 1.800	283577581	725	239.75	1731.3	714	XIC(239.75±500ppm)
Desmethoxyencecalin	1529.94 s, 1.998 s	24551857	759	187.05	1529.94	3291	XIC(187.05±500ppm)

D-Fucitol, 5TMS derivative	1524.94 s, 0.803 s	14632459	744	147.05	1524.94	888	XIC(147.05±500ppm)
D-Glucopyranose, 5TMS derivative	2164.9 s, 0.963 s	6807790	756	204.08	2164.9	579	XIC(204.08±500ppm)
D-Glucose, 5TMS derivative	1609.94, 0.882	43072049	858	73.04	1926.7	1419	XIC(73.04±500ppm)
Di(1,2,5-oxadiazolo)[3,4-b:3',4'-E]pyrazine, 4,8-diacetyl-	1959.92, 1.233	114342090	727	43.02	2393.4	888	XIC(43.02±500ppm)
Di-3,7-dimethyl-1-octyl phthalate	2134.9 s, 1.772 s	485738646	820	149	2134.9	3434	XIC(149.00±500ppm)
Diacetone alcohol, TMS derivative	774.991 s, 0.951 s	50608077	851	115.04	774.991	3053	XIC(115.04±500ppm)
Diacetyl sulphide	1959.92, 1.234	130119465	730	43.03	2393.4	931	XIC(43.03±500ppm)
Diazene, bis(1,1-dimethylethyl)-	1344.95 s, 1.050 s	415188550	729	57.06	1344.95	604	XIC(57.06±500ppm)
Diazene-carboximidoyl bromide	1569.94, 1.004	112929839	724	41.05	1873.3	727	XIC(41.05±500ppm)
Dibenzo[a,b]biphenylene, 5,6,6a,6b,7,8,12b,12c-octahydro-2,11-dimethoxy-	1084.97 s, 1.476 s	2832899	743	160.07	1084.97	531	XIC(160.07±500ppm)
Dibenzofuran	1289.96 s, 1.864 s	245920770	900	168.03	1289.96	13196	XIC(168.03±500ppm)
Dibenzofuran, 4-methyl-	1394.95 s, 1.843 s	79139521	876	182.05	1394.95	4577	XIC(182.05±500ppm)
Dibenzothiophene	1499.94 s, 2.170 s	65515373	940	184.01	1499.94	2841	XIC(184.01±500ppm)
Dibenzothiophene, 4,6-dimethyl-	1664.93, 2.142	16101067	787	212.05	2000	1138	XIC(212.05±500ppm)
Dibenzothiophene, 4-methyl-	1574.94, 2.155	31232215	738	198.04	1880	3113	XIC(198.04±500ppm)
Dibutyl phthalate	1609.94 s, 1.698 s	122504395	902	149.01	1609.94	3562	XIC(149.01±500ppm)
Dibutyl-dodecylamine	1639.94 s, 1.045 s	20075242	761	142.14	1639.94	1592	XIC(142.14±500ppm)
Dichloroacetic acid, 6-ethyl-3-octyl ester	1799.93, 1.018	132795048	725	43.05	2180	655	XIC(43.05±500ppm)
Dicyclohexyl phthalate	2179.9, 2.118	5579646365	837	149	2686.7	2595	XIC(149.00±500ppm)
Didecan-2-yl phthalate	2174.9 s, 1.827 s	162419276	781	167.13	2174.9	807	XIC(167.13±500ppm)
Dienestrol, 2TMS derivative	2194.9 s, 2.939 s	174869444	759	73.03	2194.9	4683	XIC(73.03±500ppm)
Diethyl adipate	1149.97, 1.434	4349582	858	111.03	1385	500	XIC(111.03±500ppm)
Diethyl Phthalate	1349.95 s, 1.845 s	393618577	899	149	1349.95	7062	XIC(149.00±500ppm)
Diethylene glycol dibenzoate	1979.91 s, 2.644 s	93635461	935	105.01	1979.91	2688	XIC(105.01±500ppm)
Diethylene glycol, 2TMS derivative	1014.98 s, 0.962 s	406862756	901	117.11	1014.98	21623	XIC(117.11±500ppm)
Diethylene glycol, n-butyl ether, trimethylsilyl ether	1109.97 s, 1.080 s	265808280	916	73.03	1109.97	3155	XIC(73.03±500ppm)
Diethylmalonic acid, di(3-phenylpropyl) ester	1734.93 s, 2.010 s	50073279	813	118.06	1734.93	1807	XIC(118.06±500ppm)
Diflalone	1814.92 s, 2.427 s	10254996	746	132.04	1814.92	799	XIC(132.04±500ppm)
Dihydromyrcenol, trimethylsilyl ether	1309.96 s, 0.874 s	159133646	829	131.07	1309.96	4935	XIC(131.07±500ppm)
Dihydroxyacetone, 2TMS derivative	1254.96, 0.786	82902331	754	73.03	1494.7	2042	XIC(73.03±500ppm)
Diisodecyl phthalate	2109.91 s, 1.704 s	51445339	738	149.01	2109.91	1115	XIC(149.01±500ppm)
Di-isononyl phthalate	2139.9, 1.914	57301752	730	148.98	2633.4	2332	XIC(148.98±500ppm)
Dimethyl 3,6,9,12,15,18,21-hepta-oxatricosane-1,23-dioate	2294.89, 2.379	180935624	746	117.06	2840.1	521	XIC(117.06±500ppm)
Dimethyl phthalate	1224.96 s, 1.951 s	71513620	824	163.02	1224.96	4179	XIC(163.02±500ppm)
Dimethyl-(isopropyl)-silyloxybenzene	2069.91 s, 2.279 s	70364665	759	151.06	2069.91	633	XIC(151.06±500ppm)
Dimetilan	1534.94 s, 1.391 s	57026720	757	72.07	1534.94	2116	XIC(72.07±500ppm)
Di-n-octyl phenyl phosphate	1964.92, 1.631	5945117	751	175	2400	606	XIC(175.00±500ppm)
Dioncophyllin A	2244.9 s, 4.291 s	23297926	732	362.14	2244.9	1989	XIC(362.14±500ppm)
Dioncophyllin B	2254.9 s, 4.479 s	42899591	752	348.12	2254.9	2862	XIC(348.12±500ppm)
Diphenyl ether	1174.97 s, 1.723 s	70497305	935	170.05	1174.97	6351	XIC(170.05±500ppm)
Diphenyl sulfone	1624.94 s, 2.685 s	26423890	925	124.99	1624.94	4504	XIC(124.99±500ppm)
Diphenylamine	1379.95 s, 2.024 s	15478271	857	169.07	1379.95	1964	XIC(169.07±500ppm)
Diphenylmethane	1204.96 s, 1.727 s	9715858	868	168.07	1204.96	2608	XIC(168.07±500ppm)
Disilane, pentamethyl-	1704.93 s, 1.164 s	368377846	789	73.04	1704.93	1803	XIC(73.04±500ppm)
Disilathiane, hexamethyl-	659.999, 0.876	122242214	867	73.03	966.7	567	XIC(73.03±500ppm)
Disiloxane, hexamethyl-	884.984 s, 0.884 s	13474809	780	147.05	884.984	737	XIC(147.05±500ppm)
Disulfide, diphenyl	1554.94 s, 2.172 s	7910218	881	109	1554.94	1849	XIC(109.00±500ppm)
di-tert-butyl dicarbonate	1514.94 s, 1.995 s	354138087	757	57.05	1514.94	1646	XIC(57.05±500ppm)
dl-7-Azatryptophan	1159.97 s, 0.843 s	27683275	798	131.07	1159.97	772	XIC(131.07±500ppm)
D-Limonene	754.993, 1.024	21706007	922	68.05	1037	896	XIC(68.05±500ppm)
DL-Proline, 5-oxo-	1424.95, 2.995	24085144	836	84.03	1688.2	4173	XIC(84.03±500ppm)
Docosane	1714.93, 1.001	1107513733	838	57.07	2066.7	6800	XIC(57.07±500ppm)
Docosanoic acid, ethyl ester	2354.89 s, 2.212 s	28127417	765	88.04	2354.89	2042	XIC(88.04±500ppm)
Docosanoic acid, methyl ester	2004.91 s, 1.339 s	34054059	757	74.02	2004.91	1127	XIC(74.02±500ppm)
Docosanol, TBMS derivative	2014.91, 1.140	23003204	798	75.01	2466.7	1301	XIC(75.01±500ppm)
Docosanol, TMS derivative	2014.91 s, 1.132 s	31215259	844	75.01	2014.91	1070	XIC(75.01±500ppm)
Docosyl nonyl ether	2984.85 s, 3.736 s	53065225	756	71.07	2984.85	622	XIC(71.07±500ppm)
Docosyl octyl ether	1519.94 s, 0.961 s	246979646	734	69.06	1519.94	2216	XIC(69.06±500ppm)
Dodecanamide	1919.92, 1.692	34361539	811	59.03	2340	1647	XIC(59.03±500ppm)
Dodecane	794.99 s, 2.139 s	723125579	872	43.06	794.99	2711	XIC(43.06±500ppm)
Dodecane, 1-chloro-	1234.96, 1.111	76132458	822	43.06	1473.7	1065	XIC(43.06±500ppm)
Dodecane, 1-iodo-	1054.97 s, 0.861 s	432560547	806	71.07	1054.97	5809	XIC(71.07±500ppm)
Dodecane, 2,6,10-trimethyl-	1134.97, 0.918	713347620	880	57.06	1370	6121	XIC(57.06±500ppm)
Dodecane, 2,6,11-trimethyl-	919.982 s, 0.821 s	30925469	769	43.06	919.982	3696	XIC(43.06±500ppm)
Dodecane, 2,7,10-trimethyl-	1244.96 s, 0.907 s	311321733	836	71.06	1244.96	5224	XIC(71.06±500ppm)
Dodecane, 4,6-dimethyl-	994.977 s, 2.220 s	86497494	886	71.07	994.977	911	XIC(71.07±500ppm)
Dodecanoic acid, 1-methylethyl ester	1374.95 s, 1.112 s	55308703	760	60.01	1374.95	3085	XIC(60.01±500ppm)
Dodecanoic acid, ethyl ester	1344.95 s, 1.161 s	17255288	811	88.04	1344.95	2034	XIC(88.04±500ppm)
Dodecanoic acid, TMS derivative	1394.95 s, 1.052 s	107298094	766	73.03	1394.95	2242	XIC(73.03±500ppm)
Dodecylcyclohexane	1524.94, 1.064	458955621	759	55.05	1813.3	3172	XIC(55.05±500ppm)
Dopamine, 4TMS derivative	1714.93 s, 1.197 s	46839401	785	174.09	1714.93	5326	XIC(174.09±500ppm)
Dotriacontyl propyl ether	2384.89 s, 2.211 s	32811679	830	43.02	2384.89	688	XIC(43.02±500ppm)
Eicosane	1424.95, 0.974	191682914	755	57.03	1688.2	2242	XIC(57.03±500ppm)
Eicosanoic acid, ethyl ester	1924.92 s, 1.284 s	23085353	732	88.04	1924.92	2042	XIC(88.04±500ppm)
Eicosanoic acid, methyl ester	1884.92 s, 1.279 s	74985815	810	74.02	1884.92	1861	XIC(74.02±500ppm)
Eicosyl octyl ether	1854.92, 1.017	230830047	731	69.06	2253.4	7187	XIC(69.06±500ppm)
Estra-1,3,5(10),7-tetraen-17-one, 3-hydroxy-, O-methylxime, TMS derivative	2089.91 s, 3.228 s	38025733	733	338.14	2089.91	3999	XIC(338.14±500ppm)
Estragole	959.98 s, 1.447 s	5157494	893	148.07	959.98	844	XIC(148.07±500ppm)
Ethanamine, 2TMS derivative	6029.11795	602911795	904	100.04	966.7	1914	XIC(100.04±500ppm)
Ethanamine, N-ethyl-N-[(trimethylsilyl)methyl]-	979.978, 1.238	4985215	747	86.06	1222.7	568	XIC(86.06±500ppm)
Ethandione, bis(p-tolyl)-	1739.93 s, 2.184 s	34356236	889	119.03	1739.93	1534	XIC(119.03±500ppm)

Ethane, 1,1-diethoxy-	849.987 s, 1.013 s	249419314	747	73.05	849.987	4519	XiC(73.05±500ppm)
Ethane, 1,2-diphenyl-1,2-bis(azetidiny-1)-	1704.93, 2.297	90489401	790	146.04	2053.3	2723	XiC(146.04±500ppm)
Ethane, isocyanato-	1514.94, 1.844	385756389	769	71.05	1800	2842	XiC(71.05±500ppm)
Ethanedioic acid, dibutyl ester	1519.94, 0.968	453074784	736	57.07	1806.7	3075	XiC(57.07±500ppm)
Ethanedione, diphenyl-	1539.94, 2.188	65912832	934	105.02	1833.3	2255	XiC(105.02±500ppm)
Ethaneperoxoic acid, 1-cyano-1-[2-(2-phenyl-1,3-dioxolan-2-yl)ethyl]pentyl ester	1574.94, 1.658	852098407	815	148.97	1880	2250	XiC(148.97±500ppm)
Ethanol, 2-(1,2,3,4-tetrahydro-6,7-dimethoxy-1-methylisoquinolin-2-yl)-1-(3-nitrophenyl)-	2199.9, 3.382	1546834398	741	220.11	2713.4	3182	XiC(220.11±500ppm)
Ethanol, 2-(2-butoxyethoxy)-, acetate	1129.97 s, 1.402 s	156071434	960	43.02	1129.97	4177	XiC(43.02±500ppm)
Ethanol, 2-(trimethylsilyl)-	1474.95 s, 1.067 s	237297204	732	73.03	1474.95	2062	XiC(73.03±500ppm)
Ethanol, 2,2'-oxybis-, diacetate	1034.97, 1.210	11592509	766	87.03	1272.7	935	XiC(87.03±500ppm)
Ethanol, 2-((triethylsilyloxy)-	949.98, 0.851	26240947	744	75.02	1195.7	725	XiC(75.02±500ppm)
Ethanol, 2-[(2-methoxyethoxy)ethoxy]-	1524.94, 1.953	112725999	753	45.04	1813.3	762	XiC(45.04±500ppm)
Ethanol, tert-butyl(dimethylsilyl) ether	1844.92 s, 1.161 s	26413197	764	103.05	1844.92	2058	XiC(103.05±500ppm)
Ethanol, TMS derivative	989.978 s, 0.825 s	183575291	742	73.03	989.978	897	XiC(73.03±500ppm)
Ethanone, 1-(2,3,4-trimethylphenyl)-	1074.97, 1.567	12002491	819	147.07	1310	976	XiC(147.07±500ppm)
Ethanone, 1-(2,4,6-trimethylphenyl)-	1074.97, 1.568	14044198	789	147.06	1310	794	XiC(147.06±500ppm)
Ethanone, 1-(2,5-dimethoxyphenyl)-	1274.96 s, 1.883 s	12738175	870	165.03	1274.96	1267	XiC(165.03±500ppm)
Ethanone, 1-(3,4-dimethylphenyl)-	1139.97 s, 2.126 s	6163050	754	105.02	1139.97	1215	XiC(105.02±500ppm)
Ethanone, 1-(3-methyloxiranyl)-	819.988 s, 1.540 s	50066454	735	43.02	819.988	1036	XiC(43.02±500ppm)
Ethanone, 1-(4-ethylphenyl)-	1049.97, 1.653	13544105	836	133.05	1286.4	544	XiC(133.05±500ppm)
Ethanone, 1-(4-methyl-2-thienyl)-	1089.97, 1.352	90347639	740	125.04	1325	3677	XiC(125.04±500ppm)
Ethanone, 1-(4-methylphenyl)-	944.98 s, 1.653 s	65871888	933	119.03	944.98	3575	XiC(119.03±500ppm)
Ethanone, 1-(5-chloro-2-hydroxy-4-methylphenyl)-	1374.95, 1.623	27010198	747	169.08	1629.4	1028	XiC(169.08±500ppm)
Ethanone, 1-(5-methoxy-2-methyl-3(1H)-indolyl)-	1569.94 s, 2.085 s	66154437	759	188.05	1569.94	3054	XiC(188.05±500ppm)
Ethanone, 1,1'-(1,3-phenylene)bis-	1204.96, 2.046	64879975	896	147.03	1442.1	4461	XiC(147.03±500ppm)
Ethanone, 1,1'-(1,4-phenylene)bis-	1204.96 s, 2.037 s	57144609	890	147.02	1204.96	4142	XiC(147.02±500ppm)
Ethanone, 1,1',1''-(1,3,5-benzenetriyl)tris-	1104.97 s, 1.102 s	5225412	752	189.14	1104.97	542	XiC(189.14±500ppm)
Ethanone, 1-[4-(1,1-dimethylethyl)phenyl]-	1184.97 s, 1.547 s	27085752	866	161.08	1184.97	2635	XiC(161.08±500ppm)
Ethanone, 1-[4-(methoxymethyl)phenyl]-	1174.97 s, 1.791 s	12273977	838	149.04	1174.97	1603	XiC(149.04±500ppm)
Ethanone, 2-(formyloxy)-1-phenyl-	1539.94 s, 2.184 s	57357626	929	105.01	1539.94	2069	XiC(105.01±500ppm)
Ether, 6-methylheptyl vinyl	849.987, 0.842	375201649	826	43.05	1108.7	1646	XiC(43.05±500ppm)
Ethoxy(dimethyl)isopropylsilane	1099.97 s, 1.388 s	22654692	742	103.07	1099.97	790	XiC(103.07±500ppm)
Ethoxyacetylene	1064.97, 0.905	81121911	755	41.05	1300	2592	XiC(41.05±500ppm)
Ethyl (2-hydroxyphenyl)acetate, TMS derivative	1409.95 s, 1.336 s	25808652	734	163.05	1409.95	2248	XiC(163.05±500ppm)
Ethyl 23-hydroxy-3,6,9,12,15,18,21-heptaooxatricosan-1-olate	789.99 s, 0.975 s	20908600	736	73.03	789.99	863	XiC(73.03±500ppm)
Ethyl 2-benzoylheptanoate	1339.96 s, 1.583 s	30457580	750	105.02	1339.96	902	XiC(105.02±500ppm)
Ethyl 3-((tert-butyl)dimethylsilyloxy)but-2-enoate	909.983, 0.816	12765307	713	75.01	1160.9	735	XiC(75.01±500ppm)
Ethyl 4-methylbenzoate	1059.97 s, 1.493 s	100692577	948	119.03	1059.97	5707	XiC(119.03±500ppm)
Ethyl cis-2-trimethylsilyl-cyclopropane-1-carboxylate	944.98, 1.338	5136482	771	143.05	1191.3	6209	XiC(143.05±500ppm)
Ethyl glycolate, TMS	729.994 s, 1.018 s	22036172	729	133.02	729.994	740	XiC(133.02±500ppm)
Ethyl m-methylbenzoate	1059.97, 1.497	109940036	938	119.03	1295.5	6399	XiC(119.03±500ppm)
Ethyl orthoformate	1569.94 s, 1.091 s	33955756	748	103.06	1569.94	1280	XiC(103.06±500ppm)
Ethyl triacontanate	2499.88, 3.090	8300597	757	88.04	3113.4	793	XiC(88.04±500ppm)
Ethyl α-D-glucopyranoside, 4TMS derivative	2109.91 s, 1.084 s	11280379	766	204.07	2109.91	866	XiC(204.07±500ppm)
Ethylene glycol - Adipate - Diethylene glycol	1394.95 s, 2.171 s	16741064	751	173.06	1394.95	1541	XiC(173.06±500ppm)
Ethylene glycol butyl ether, trimethylsilyl ether	809.989 s, 0.918 s	88519961	862	75.01	809.989	1144	XiC(75.01±500ppm)
Ethylene glycol, 2TMS derivative	704.996 s, 0.821 s	505657557	932	147.16	704.996	884	XiC(147.16±500ppm)
Ethylene glycol, TMS derivative	989.978, 0.835	130651483	739	73.03	1231.8	1112	XiC(73.03±500ppm)
Ethylene, 1,1-bis(trimethylsilyl)-	839.987 s, 1.140 s	16237117	742	73.04	839.987	518	XiC(73.04±500ppm)
Ethylmalonate, ethyltrimethylsilyl ester	1069.97, 1.068	33062922	757	75.01	1305	1130	XiC(75.01±500ppm)
Ethylmalonic acid, 2TMS derivative	1099.97, 1.027	38695422	707	147.04	1335	1394	XiC(147.04±500ppm)
Ethyltriethylene glycol, TBDMS derivative	949.98 s, 0.843 s	49822522	735	73.03	949.98	1011	XiC(73.03±500ppm)
Ethyltriethylene glycol, TMS derivative	1924.92 s, 1.267 s	83902485	808	73.03	1924.92	8493	XiC(73.03±500ppm)
Ethyne, fluoro-	1334.96, 1.782	35257161	851	44.05	1583.3	1256	XiC(44.05±500ppm)
Ferrocene, 1,1',3,3'-tetrakis(1,1-dimethylethyl)-	2219.9, 2.985	8891755	734	410.16	2740.1	659	XiC(410.16±500ppm)
Fluoranthene	1724.93 s, 2.502 s	115514873	950	202.05	1724.93	3554	XiC(202.05±500ppm)
Fluorene	1349.95 s, 1.935 s	100336726	904	166.05	1349.95	3974	XiC(166.05±500ppm)
Formamide, N,N-dibutyl-	1069.97 s, 1.422 s	460866531	904	72.03	1069.97	2294	XiC(72.03±500ppm)
Formamide, N,N-diethyl-	640 s, 4.192 s	216708428	928	58.05	640	995	XiC(58.05±500ppm)
Formic acid, (3-methyl-2-nitrophenyl)methyl ester	1074.97, 1.327	12206389	745	149.08	1310	1120	XiC(149.08±500ppm)
Formic acid, TMS derivative	1154.97 s, 0.877 s	47614451	736	75.01	1154.97	2451	XiC(75.01±500ppm)
Fumaric acid, di(3-phenylpropyl) ester	1734.93, 2.012	48923538	784	118.06	2093.3	2331	XiC(118.06±500ppm)
Fumaric acid, ethyl tetrahydrofurfuryl ester	2069.91, 1.091	383097793	753	71.07	2540	1343	XiC(71.07±500ppm)
Furan, 2,5-diphenyl-	1704.93, 2.147	6641208	785	220.07	2053.3	655	XiC(220.07±500ppm)
Furan, 2-butyltetrahydro-	1259.96 s, 0.985 s	546034244	755	71.07	1259.96	672	XiC(71.07±500ppm)
Furan, tetrahydro-2,5-dimethyl-, trans-(±)-	1689.93, 1.040	188914781	743	85.08	2033.3	2324	XiC(85.08±500ppm)
Furfuryl alcohol, TMS derivative	719.995 s, 1.006 s	22875662	836	81.02	719.995	1263	XiC(81.02±500ppm)
Galactopyranose, 3,4-di-O-methyl-1,2,6-tris-O-(trimethylsilyl)-	1584.94 s, 1.094 s	181428598	741	73.05	1893.3	1875	XiC(73.05±500ppm)
Galactopyranose, 5TMS derivative	2144.9 s, 1.623 s	4926574507	754	204.22	2640.1	630	XiC(204.22±500ppm)
Galic acid, 4TMS derivative	1644.93 s, 0.995 s	18430479	757	281.11	1689.93	659	XiC(281.11±500ppm)
Glucopyranose, 5TMS derivative	1619.94 s, 0.859 s	17268156	811	73.04	1619.94	2779	XiC(73.04±500ppm)
Glucose, 5TMS derivative	2109.91, 1.087	11270259	764	204.08	2593.4	771	XiC(204.08±500ppm)
Glutaric acid, 3-fluorophenyl octadecyl ester	2229.9, 1.795	202722310	701	115.02	2753.4	5448	XiC(115.02±500ppm)
Glycerol 1-palmitate	1994.91, 1.788	490402268	752	43.03	2440	5316	XiC(43.03±500ppm)
Glycerol monostearate, 2TMS derivative	2144.9 s, 1.315 s	540088647	782	73	2144.9	1316	XiC(73.00±500ppm)
Glycerol, 1,2-di(TMS)-	959.98 s, 0.936 s	14114913	863	73.05	1204.5	643	XiC(73.05±500ppm)
Glycerol, 1-tert-butyl-3-trimethylsilyl ether	1904.92, 1.304	107787463	731	103.04	2320	2430	XiC(103.04±500ppm)
Glycerol, 3TMS derivative	1049.97 s, 0.839 s	336214607	922	72.97	1049.97	1874	XiC(72.97±500ppm)
Glycolaldehyde dimethyl acetal	1079.97 s, 1.109 s	96824897	803	75.02	1079.97	621	XiC(75.02±500ppm)
Glycolic acid, 2TBDMS derivative	1199.96 s, 0.796 s	6902557	730	73.03	1199.96	577	XiC(73.03±500ppm)
Glycolic acid, 2TMS derivative	819.988 s, 0.928 s	610209059	903	73.03	819.988	3291	XiC(73.03±500ppm)

Glycolic acid, TMS derivative	1069.97, 0.838	46660453	711	73.03	1305	635	XIC(73.03±500ppm)
Glyoxylic acid, phenyl-, 2'-cyanophenyl ester	1299.96 s, 1.378 s	273781465	743	105.01	1299.96	8444	XIC(105.01±500ppm)
Guanidine, N,N-dimethyl-	689.997 s, 1.669 s	147373270	739	43.02	689.997	3099	XIC(43.02±500ppm)
Heicicosane	1509.94 s, 0.970 s	270839154	747	57.07	1509.94	842	XIC(57.07±500ppm)
Henicos-1-ene	1949.92 s, 1.056 s	774305162	750	69.06	1949.92	2640	XIC(69.06±500ppm)
Hentriacontane	2089.91 s, 1.100 s	1745532477	830	57.06	2089.91	24533	XIC(57.06±500ppm)
Heptacosane	1929.92 s, 1.031 s	1244629266	808	71.07	1929.92	3854	XIC(71.07±500ppm)
Heptadecane	1184.97 s, 0.893 s	529759931	868	57.06	1184.97	2694	XIC(57.06±500ppm)
Heptadecane, 2,6,10,14-tetramethyl-	1274.96 s, 0.942 s	1071821237	878	71.07	1274.96	4366	XIC(71.07±500ppm)
Heptadecane, 2,6-dimethyl-	1549.94, 0.992	980996717	788	57.06	1846.7	9357	XIC(57.06±500ppm)
Heptadecane, 2-methyl-	1789.93, 1.001	1452604325	807	57.06	2166.7	4145	XIC(57.06±500ppm)
Heptadecane, 3-methyl-	1494.95, 1.006	157643676	767	41.03	1775	1510	XIC(41.03±500ppm)
Heptadecane, 7-methyl-	1444.95, 0.969	246029485	744	57.03	1712.5	1444	XIC(57.03±500ppm)
Heptadecanoic acid, ethyl ester	1729.93, 1.214	30955258	742	88.04	2086.7	1909	XIC(88.04±500ppm)
Heptadecanoic acid, glycerine-(1)-monoester, bis-O-trimethylsilyl-	2074.91 s, 1.193 s	42372169	757	73.03	2074.91	976	XIC(73.03±500ppm)
Heptadecanoic acid, TMS derivative	1709.93, 1.236	19871358	732	44.05	2060	609	XIC(44.05±500ppm)
Heptaethylene glycol	2064.91, 2.830	337968443	926	45.04	2533.4	3018	XIC(45.04±500ppm)
Heptaethylene glycol, 2TMS derivative	2014.91 s, 1.584 s	2944055214	954	73.03	2014.91	11796	XIC(73.03±500ppm)
Heptaethylene glycol, TMS derivative	2334.89 s, 2.550 s	15075045	768	73.04	2334.89	630	XIC(73.04±500ppm)
Heptane	1934.92, 1.040	266631723	746	57.03	2360	1247	XIC(57.03±500ppm)
Heptane, 1,1-diethoxy-	944.98 s, 0.994 s	31698876	855	103.06	944.98	1214	XIC(103.06±500ppm)
Heptane, 1,1'-oxybis-	954.98 s, 0.864 s	103544307	744	57.06	954.98	5372	XIC(57.06±500ppm)
Heptane, 2,2,4,6,6-pentamethyl-	704.996, 0.768	107746690	884	57.06	1000	1203	XIC(57.06±500ppm)
Heptane, 2,3-dimethyl-	884.984, 0.843	110819291	797	43.06	1139.1	8599	XIC(43.06±500ppm)
Heptane, 2,5-dimethyl-	1204.96, 0.910	192489724	764	57.06	1442.1	3145	XIC(57.06±500ppm)
Heptane, 3,3-dimethyl-	684.997, 3.364	79147977	751	57.04	985.2	811	XIC(57.04±500ppm)
Heptane, 3-ethyl-4-methyl-	844.987 s, 0.900 s	473614360	764	43.09	844.987	724	XIC(43.09±500ppm)
Heptane, 4-methylene-	1164.97, 0.989	177864482	726	55.05	1400	1575	XIC(55.05±500ppm)
Heptane, 5-ethyl-2-methyl-	719.995 s, 0.833 s	119574158	875	43.06	719.995	1855	XIC(43.06±500ppm)
Heptanoic acid, 4-octyl ester	974.979 s, 1.513 s	24545018	737	43.02	974.979	1402	XIC(43.02±500ppm)
Heptanoic acid, TMS derivative	924.982 s, 0.963 s	39955636	809	73.03	924.982	1500	XIC(73.03±500ppm)
Heptasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13-tetradecamethyl-	1539.94 s, 0.771 s	35084597	729	73.04	1539.94	855	XIC(73.04±500ppm)
Heptasiloxane, hexadecamethyl-	1274.96 s, 0.736 s	65691348	878	73.03	1274.96	6268	XIC(73.03±500ppm)
Hexacosane, 1-iodo-	3059.85, 3.999	121716633	798	57.07	3860.1	697	XIC(57.07±500ppm)
Hexacosanoic acid, 2-methyl-, methyl ester	2249.9 s, 1.677 s	40628565	735	88.03	2249.9	3195	XIC(88.03±500ppm)
Hexadecahydro-benzo[de]anthracene	1489.95, 1.432	22657501	707	232.19	1768.8	1812	XIC(232.19±500ppm)
Hexadecanamide	1789.93, 1.638	56903984	816	59.03	2166.7	1424	XIC(59.03±500ppm)
Hexadecane	1139.97 s, 0.903 s	315238204	870	43.06	1139.97	4875	XIC(43.06±500ppm)
Hexadecane, 1-iodo-	1259.96, 0.898	1284593796	723	71.08	1500	1797	XIC(71.08±500ppm)
Hexadecane, 2,6,10,14-tetramethyl-	1394.95 s, 0.938 s	229829978	758	57.13	1394.95	902	XIC(57.13±500ppm)
Hexadecane, 2,6,11,15-tetramethyl-	1994.91, 1.065	199628498	736	71.07	2440	1359	XIC(71.07±500ppm)
Hexadecane, 2-methyl-	1589.94 s, 0.954 s	516361316	788	71.06	1589.94	1741	XIC(71.06±500ppm)
Hexadecane, 3-methyl-	1339.96 s, 0.944 s	266543741	737	57.04	1339.96	561	XIC(57.04±500ppm)
Hexadecanoic acid, 2-hydroxy-1-(hydroxymethyl)ethyl ester	1999.91, 1.748	1237511160	754	43.06	2446.7	2779	XIC(43.06±500ppm)
Hexadecanoic acid, 4-[(trimethylsilyloxy)butyl] ester	2024.91, 1.352	230660550	717	73.01	2480	1102	XIC(73.01±500ppm)
Hexadecanoic acid, dodecyl ester	2234.9 s, 1.603 s	106247236	737	57.06	2234.9	774	XIC(57.06±500ppm)
Hexadecanoic acid, ethyl ester	1659.93 s, 1.213 s	918417859	901	88.08	1659.93	4398	XIC(88.08±500ppm)
Hexadecanoic acid, hexadecyl ester	2474.88 s, 2.881 s	37109482	805	57.06	2474.88	959	XIC(57.06±500ppm)
Hexadecanoic acid, methyl ester	1614.94, 1.161 s	119888374	781	74.02	1933.3	3743	XIC(74.02±500ppm)
Hexadecanoic acid, octadecyl ester	2339.89, 2.106	25805556	763	57.06	2900.1	537	XIC(57.06±500ppm)
Hexaethoxydisiloxane	1119.97 s, 1.008 s	23941383	788	75.01	1119.97	1704	XIC(75.01±500ppm)
Hexaethylene glycol	1729.93, 2.093	443317159	876	45.04	2086.7	3724	XIC(45.04±500ppm)
Hexaethylene glycol monododecyl ether	2359.89 s, 3.652 s	16588079	844	45.04	2359.89	661	XIC(45.04±500ppm)
Hexaethylene glycol, 2TMS derivative	1704.93 s, 1.161 s	231538065	754	73.1	1704.93	838	XIC(73.1±500ppm)
Hexaethylene glycol, TMS derivative	2074.91 s, 1.451 s	129743634	812	73.03	2074.91	1430	XIC(73.03±500ppm)
Hexamethylene diacrylate	1339.96 s, 1.526 s	38906732	804	55.02	1339.96	1309	XIC(55.02±500ppm)
Hexan-3-ol, trimethylsilyl ether	1219.96 s, 0.857 s	60890028	760	73.03	1219.96	1249	XIC(73.03±500ppm)
Hexanal, 2,2-dimethyl-	1279.96 s, 0.932 s	236098263	754	57.06	1279.96	1961	XIC(57.06±500ppm)
Hexane, 1-(ethenyl-oxy)-	749.993, 1.533	15807157	721	43.02	1033.3	667	XIC(43.02±500ppm)
Hexane, 1-(hexyl-oxy)-5-methyl-	759.992 s, 0.858 s	10493787	756	57.06	759.992	525	XIC(57.06±500ppm)
Hexane, 1,1-diethoxy-	834.988 s, 0.942 s	56383136	843	103.06	834.988	1556	XIC(103.06±500ppm)
Hexane, 2,3,5-trimethyl-	1394.95, 0.984	258619210	737	85.09	1652.9	2955	XIC(85.09±500ppm)
Hexane, 2,4,4-trimethyl-	1649.94, 0.980	396788155	732	57.07	1980	1417	XIC(57.07±500ppm)
Hexane, 2,4-dimethyl-	849.987, 0.824	297632364	774	43.09	1108.7	2488	XIC(43.09±500ppm)
Hexane, 2,5-dimethoxy-2,5-dimethyl-	774.991, 1.263	60696582	732	73.05	1051.9	877	XIC(73.05±500ppm)
Hexane, 2,5-dimethyl-2,5-bis(trimethylsilyloxy)-	1059.97 s, 0.815 s	472137955	901	131.07	1059.97	11272	XIC(131.07±500ppm)
Hexane, 2-bromo-	954.98 s, 0.869 s	79190737	794	43.06	954.98	2896	XIC(43.06±500ppm)
Hexane, 3,3-dimethyl-	1654.94, 0.979	255388966	730	57.03	1986.7	2360	XIC(57.03±500ppm)
Hexane, 3,4-bis(1,1-dimethylethyl)-2,2,5,5-tetramethyl-	1439.95, 0.948	461096645	731	57.08	1706.2	2921	XIC(57.08±500ppm)
Hexanedioic acid, bis(2-ethylhexyl) ester	1924.92 s, 1.417 s	32233764	804	129.03	1924.92	1121	XIC(129.03±500ppm)
Hexanoic acid, 2-[(trimethylsilyloxy)-, trimethylsilyl] ester	934.981 s, 0.776 s	171244606	804	73.03	934.981	4453	XIC(73.03±500ppm)
Hexanoic acid, anhydride	1819.92 s, 1.576 s	16084986	754	99.03	1819.92	732	XIC(99.03±500ppm)
Hexanoic acid, TMS derivative	1049.97 s, 1.578 s	46991119	754	75.01	1049.97	2012	XIC(75.01±500ppm)
Hexasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11-dodecamethyl-	1009.98 s, 0.772 s	2652620	734	266.98	1009.98	905	XIC(266.98±500ppm)
Hexasiloxane, tetradecamethyl-	1124.97 s, 0.724 s	64495810	897	73.03	1124.97	1787	XIC(73.03±500ppm)
Hexatriacontane	2229.9 s, 1.353 s	105085237	813	57.06	2229.9	581	XIC(57.06±500ppm)
Hexenyl angelate, 4z-	1449.95, 1.076	291135152	750	55.05	1718.8	788	XIC(55.05±500ppm)
Hexestrol dimethyl ether	1074.97 s, 1.324 s	15247469	736	149.08	1074.97	893	XIC(149.08±500ppm)
Hexethyl-permethylated	1434.95, 1.738	25160309	728	169.09	1700	1408	XIC(169.09±500ppm)
Hippuric acid, TBDMS derivative	1879.92 s, 1.906 s	123189462	748	105.01	1879.92	3057	XIC(105.01±500ppm)
Homosalate, TMS derivative	1554.94 s, 1.355 s	89379018	765	195.02	1554.94	4842	XIC(195.02±500ppm)

Humulene epoxide I	1364.95 s, 1.473 s	15940821	806	93.09	1617.7	627	XIC(93.09±500ppm)
Hydracrylic acid, 2TMS derivative	899.983 s, 0.934 s	38779590	911	147.09	1152.2	3001	XIC(147.09±500ppm)
Hydrazinecarboxylic acid, (4-methoxyphenyl)methyl ester	1354.95 s, 1.790 s	32804160	728	121.02	1354.95	706	XIC(121.02±500ppm)
Hydrobenzoin, 2TMS derivative	1554.94 s, 1.336 s	60408363	748	179.06	1554.94	2510	XIC(179.06±500ppm)
Hydrogen azide	1709.93 s, 1.149 s	115052731	756	43.01	1709.93	549	XIC(43.01±500ppm)
Hydrogen chloride	1244.96, 0.601	8817584	757	35.98	1484.2	1047	XIC(35.98±500ppm)
Hydrogen isocyanate	844.987 s, 0.897 s	303429335	741	43.01	844.987	1437	XIC(43.01±500ppm)
Hydroquinone, 2TMS derivative	1174.97 s, 1.035 s	10790283	807	239.06	1174.97	2896	XIC(239.06±500ppm)
Hydroxylamine, O-(3-methylbutyl)-	689.997, 1.181	146424882	752	43.02	988.9	4773	XIC(43.02±500ppm)
Hydroxymethyl 2-hydroxy-2-methylpropionate	1984.91, 1.606	22309227	844	59.05	2426.7	779	XIC(59.05±500ppm)
Imidazole, 2,3-dihydro-1-methyl-2-acetylimino-3-acetyl-4-acetyloxy-	1229.96, 0.892	42808058	732	113.12	1468.4	2687	XIC(113.12±500ppm)
Imidazole, 2,5-dimethyl-4-trifluoromethyl-	1044.97 s, 1.639 s	6104377	743	43.02	1044.97	1723	XIC(43.02±500ppm)
Iminodiacetic acid, N-[[5-fluorenyloxy]carbonyl]-	1614.94, 1.994	633193398	747	178.06	1933.3	5139	XIC(178.06±500ppm)
Iminostilbene-10,11-dihydro-10-ol,1TMS derivative	1824.92 s, 1.740 s	21716567	730	193.08	1824.92	980	XIC(193.08±500ppm)
Indolizine, 5-methyl-	1274.96, 1.019	12294999	749	131.07	1516.7	532	XIC(131.07±500ppm)
Inosose, 2-desoxy-, O-methylxime, tetrakis-O-(trimethylsilyl)-	1209.96 s, 0.833 s	195211167	734	73.03	1209.96	9005	XIC(73.03±500ppm)
Isophthalic acid, 2-fluorophenyl pentyl ester	2199.9 s, 2.115 s	25034084	765	219.15	2199.9	1436	XIC(219.15±500ppm)
Isophthalic acid, 4-chloro-3-methylphenyl hexyl ester	2329.89, 4.509	8862574	747	233.08	2886.7	789	XIC(233.08±500ppm)
Isophthalic acid, 4-chlorophenyl hexyl ester	2489.88, 4.464	4619729	744	233.09	3100.1	576	XIC(233.09±500ppm)
Isophthalic acid, 4-formylphenyl hexyl ester	2339.89, 4.511	6471820	707	233.07	2900.1	650	XIC(233.07±500ppm)
Isophthalic acid, butyl 2-methylprop-2-en-1-yl ester	1524.94, 1.102	6666472	711	205.09	1813.3	777	XIC(205.09±500ppm)
Isophthalic acid, di(2-fluorophenyl) ester	1639.94 s, 1.457 s	17833978	747	243.2	1639.94	1545	XIC(243.20±500ppm)
Isophthalic acid, di(2-methylphenyl) ester	1449.95, 1.355	86607533	861	239.09	1718.8	658	XIC(239.09±500ppm)
Isophthalic acid, octyl 1-propylbutyl ester	2039.91, 1.555	40158970	795	149	2500	2320	XIC(149.00±500ppm)
Isopimaric acid, TMS	1899.92 s, 1.540 s	17965335	852	73.06	2313.4	2023	XIC(73.06±500ppm)
Isopropyl myristate	1534.94 s, 1.142 s	277921799	888	43.05	1534.94	5703	XIC(43.05±500ppm)
Isopropyl palmitate	1679.93 s, 1.168 s	153281446	733	43.06	1679.93	618	XIC(43.06±500ppm)
Isopropylamine, N-trimethylsilyl-	1519.94 s, 1.228 s	235422981	828	116.16	1519.94	950	XIC(116.16±500ppm)
Isoquinolin-6-ol, 1-[4-hydroxybenzyl]-1,2,3,4-tetrahydro-7-methoxy-	1969.91 s, 2.199 s	4760603	801	178.12	2406.7	560	XIC(178.12±500ppm)
Kaur-16-en-18-oic acid, (4α)-, O-TMS	1914.92 s, 1.517 s	86164115	731	241.3	2333.4	1149	XIC(241.30±500ppm)
Kaur-16-ene, 18-[[trimethylsilyloxy]-, (4α)-	1829.92 s, 1.353 s	132401513	739	257.32	2220	517	XIC(257.32±500ppm)
Kauren-19-oic acid	1949.92 s, 2.214 s	1260366	794	43.06	1949.92	1028	XIC(43.06±500ppm)
L-(-)-Arabitol, 5TMS derivative	1454.95 s, 0.788 s	50896762	867	73.06	1725	3214	XIC(73.06±500ppm)
Labda-8(20),14-dien-13-ol, (13S)-, O-TMS	1784.93 s, 1.256 s	244490395	749	73.06	2160	13736	XIC(73.06±500ppm)
Lactic Acid, 2TMS derivative	804.989 s, 0.868 s	662535174	923	73.04	804.989	10702	XIC(73.04±500ppm)
Lactic acid, monoanhydride with 1-butanboronic acid, cyclic ester	999.977 s, 1.629 s	26684079	747	112.06	999.977	2631	XIC(112.06±500ppm)
L-Alanine ethylamide, (S)-	1329.96, 1.806	53781975	816	44.05	1577.8	933	XIC(44.05±500ppm)
L-Alanine, 2TMS derivative	2159.9 s, 1.868 s	375091432	737	116.1	2159.9	717	XIC(116.10±500ppm)
Lanost-8-en-3-ol, (3β)-, TMS derivative	2449.88, 2.858	5157203	731	395.34	3046.7	1319	XIC(395.34±500ppm)
Levoglucofan, 3TMS derivative	1454.95 s, 1.057 s	61396261	923	73.05	1725	4494	XIC(73.05±500ppm)
Levulinic acid, TMS derivative	884.984 s, 1.275 s	36789622	758	75.01	884.984	511	XIC(75.01±500ppm)
Lignoceric acid, TMS derivative	2174.9, 1.381	27658922	743	73.04	2680.1	735	XIC(73.04±500ppm)
l-Norvaline, n-propargyloxycarbonyl-, isohexyl ester	834.988 s, 1.380 s	74977674	742	154.01	834.988	3130	XIC(154.01±500ppm)
L-Rhamnose, 4TMS derivative	1529.94 s, 0.839 s	5894053	750	204.08	1529.94	2035	XIC(204.08±500ppm)
Lumiflavine	1634.94, 1.338	73337818	728	256.24	1960	1129	XIC(256.24±500ppm)
m,p-Quaterphenyl	2234.9 s, 3.510 s	2109406	770	306.11	2234.9	614	XIC(306.11±500ppm)
Malic acid, 3TMS derivative	1264.96 s, 0.960 s	8164456	802	147.09	1505.6	610	XIC(147.09±500ppm)
m-Aminophenylacetylene	1499.94 s, 1.127 s	342629485	739	117.03	1499.94	4277	XIC(117.03±500ppm)
m-Cresol, TMS derivative	894.984 s, 1.060 s	11567774	849	165.05	894.984	2488	XIC(165.05±500ppm)
Mepronil, n-heptafluorobutyl-yl-	2279.9, 2.650	83573472	739	119.04	2820.1	1845	XIC(119.04±500ppm)
Mepronil, n-pentafluoropropionyl-	1644.94, 2.134	70201147	752	119.03	1973.3	2504	XIC(119.03±500ppm)
Mepronil, N-trifluoroacetyl-	2169.9 s, 3.256 s	13624529	760	119.03	2169.9	763	XIC(119.03±500ppm)
Mercaptoacetic acid, 2TMS derivative	1124.97, 0.728	82950902	743	73.04	1360	2121	XIC(73.04±500ppm)
Mercaptoethanol, 2TMS derivative	3019.85 s, 0.513 s	77470272	730	73.06	3806.8	1401	XIC(73.06±500ppm)
Methacrylic acid, TMS derivative	804.989 s, 1.176 s	8053948	744	143.03	804.989	827	XIC(143.03±500ppm)
Methane, di-p-tolyl-	1399.95, 1.698	10542234	726	181.08	1658.8	763	XIC(181.08±500ppm)
Methanone, (2-methylphenyl)phenyl-	1419.95 s, 1.970 s	3657418	765	195.06	1419.95	555	XIC(195.06±500ppm)
Methanone, (4-chlorophenyl)phenyl-	1534.94 s, 2.065 s	6835942	904	105.02	1534.94	568	XIC(105.02±500ppm)
Methanone, (4-methylphenyl)phenyl-	1499.94 s, 1.989 s	50162077	765	119.03	1499.94	1730	XIC(119.03±500ppm)
Methanone, [1,1'-biphenyl]-4-ylphenyl-	1974.91, 2.775	2209575	825	181.05	2413.4	1845	XIC(181.05±500ppm)
Methanone, bis(3-methylphenyl)-	1594.94 s, 2.025 s	20765915	787	119.03	1594.94	1324	XIC(119.03±500ppm)
Methanone, bis(4-methylphenyl)-	1594.94, 2.026	20991323	808	119.04	1906.7	1306	XIC(119.04±500ppm)
Methoxamine	2019.91, 0.835	1340067570	733	44.05	2473.4	876	XIC(44.05±500ppm)
Methoxamine acetate	1734.93, 2.432	18275378	762	87.05	2093.3	1229	XIC(87.05±500ppm)
Methoxynonaethylene glycol, TMS derivative	2259.9, 2.569	55035039	781	45.04	2793.4	631	XIC(45.04±500ppm)
Methyl (3,4-dimethoxyphenyl)(hydroxy)acetate, TMS derivative	1444.95 s, 1.396 s	113293429	746	238.98	1444.95	1046	XIC(238.98±500ppm)
Methyl 15-hydroxyabieta-9(11),8(14),12-trien-18-olate, TMS derivative	2014.91 s, 1.751 s	43107241	736	327.25	2466.7	1191	XIC(327.25±500ppm)
Methyl 2,2-dimethyl-3,6,9,12,15,18,21-heptaoxa-2-silatricosan-23-olate	1864.92 s, 1.358 s	1500733258	796	117	1864.92	2559	XIC(117.00±500ppm)
Methyl 2,2-dimethyl-3,6,9,12,15-pentaaxa-2-silaheptadecan-17-olate	1274.96, 1.079	312528333	749	116.06	1516.7	3512	XIC(116.06±500ppm)
Methyl 2,2-dimethyl-3,6,9,12-tetraoxa-2-silatetradecan-14-olate	2289.89 s, 2.608 s	614196372	737	73.09	2289.89	1012	XIC(73.09±500ppm)
Methyl 2,5,8,11,14,17,20,23,26,29-decaoxahentriacontan-31-olate	1974.91, 1.735	211235576	753	45.04	2413.4	1120	XIC(45.04±500ppm)
Methyl 2,5,8,11,14,17-hexaoxonadecan-19-olate	1784.93, 1.599	18233581	724	59.04	2160	581	XIC(59.04±500ppm)
Methyl 20-methyl-heneicosanoate	2004.91, 1.344	39549656	759	74.02	2453.4	1310	XIC(74.02±500ppm)
Methyl abietate	1959.92 s, 1.763 s	1717201623	761	256.28	2393.4	1229	XIC(256.28±500ppm)
Methyl dehydroabietate	1904.92 s, 2.008 s	51886089	902	239.16	1904.92	1628	XIC(239.16±500ppm)
Methyl galactoside, 4TMS derivative	2949.85 s, 3.843 s	389684146	756	73.05	3713.5	7337	XIC(73.05±500ppm)
Methyl nicotinate	894.984, 1.679	5143591	919	106.02	1147.8	975	XIC(106.02±500ppm)
Methyl p-(2-phenyl-1-benzimidazolyl)benzoate	1774.93, 1.212	95261237	734	328.11	2146.7	1093	XIC(328.11±500ppm)
Methyl stearate	1754.93 s, 1.234 s	396427936	895	74.02	1754.93	2836	XIC(74.02±500ppm)
Methyl vanillate, TMS derivative	1424.95, 1.557	72637971	745	224.03	1688.2	3515	XIC(224.03±500ppm)
Methyl α-D-glucufuranoside, 4TMS derivative	2639.87 s, 2.573 s	176778317	749	73.05	3300.1	7873	XIC(73.05±500ppm)

Methyl α -Lyxofuranoside, 3TMS derivative	2294.89 s, 0.638 s	106747162	747	217.12	2840.1	691	XIC(217.12±500ppm)
Methyl β -Arabinofuranoside, 3TMS derivative	2449.88 s, 0.626 s	129569054	741	73.05	3046.7	563	XIC(73.05±500ppm)
Methyl(methyl 2,3,4-tri-O-methyl- α -D-glucopyranoside)uronate	1794.93 s, 1.251	436589721	737	88.03	2173.4	3011	XIC(88.03±500ppm)
Methyl-6-deoxy-6-fluoro-2,3,4-tri-O-methyl β -D-galactopyranoside	1794.93 s, 1.241 s	685347312	752	88.03	1794.93	3734	XIC(88.03±500ppm)
Methylamine, N,N-dimethyl-	1259.96 s, 1.186 s	20703237	729	58.03	1259.96	871	XIC(58.03±500ppm)
Methylhydroquinone, 2TMS derivative	1234.96 s, 1.043	34755097	806	73.03	1473.7	4508	XIC(73.03±500ppm)
Methyltrioxitol, TMS derivative	1139.97 s, 1.218 s	59043311	836	59.04	1139.97	2557	XIC(59.04±500ppm)
Methyltris(trimethylsilyloxy)silane	804.989 s, 0.713 s	211550115	890	207.01	804.989	136016	XIC(207.01±500ppm)
mono-Ethyl malonate, TMS derivative	924.982 s, 1.067 s	99931148	782	75.01	924.982	2292	XIC(75.01±500ppm)
Monolaurin, 2TMS derivative	1809.93 s, 1.083 s	20216495	762	73.03	1809.93	694	XIC(73.03±500ppm)
Monomethyl succinate, trimethylsilyl ester	939.981 s, 1.208 s	11988708	787	89.03	939.981	1005	XIC(89.03±500ppm)
m-Terphenyl	1779.93 s, 2.264 s	7861591	889	230.08	1779.93	959	XIC(230.08±500ppm)
m-Toluic acid, TBDMS derivative	999.977 s, 1.080 s	22623284	736	193.08	999.977	566	XIC(193.08±500ppm)
Myristic acid, TMS derivative	1554.94 s, 1.070 s	223863592	904	73.03	1554.94	5167	XIC(73.03±500ppm)
N-(2-Methyl-5-trimethylsilylphenyl)acetamide	1479.95 s, 1.687	20898793	749	221.16	1756.3	1852	XIC(221.16±500ppm)
N-(7-Dimethyl-2-oxobicyclo[2.2.1]hept-1-yl)methanesulfonamide #	2414.89 s, 1.766	221348551	711	83.07	3000.1	1805	XIC(83.07±500ppm)
N-(α -Toluoyl)-glycine	1094.97 s, 1.157 s	22216268	743	119.07	1094.97	595	XIC(119.07±500ppm)
N-(p-Vinylbenzoyl)-l-alanine	1364.95 s, 2.082	8323223	790	131.03	1617.7	776	XIC(131.03±500ppm)
N,N,O-Triacetylhydroxylamine	1899.92 s, 1.204	67621353	743	43.03	2313.4	746	XIC(43.03±500ppm)
N,N-Dimethyl-2,2-diphenyl-2-phenylhydrazinoacetamide	1754.93 s, 1.672	33349068	743	239.09	2120	657	XIC(239.09±500ppm)
N,N'-Ethylenebis(N-ethylbenzamide)	814.989 s, 1.041 s	11644835	738	105.02	814.989	809	XIC(105.02±500ppm)
N,O-Bis(trimethylsilyl)carbamate	804.989 s, 0.929	433545321	734	146.98	1074.1	698	XIC(146.98±500ppm)
N-[2-(Trimethylsilyloxy)ethyl]succinimide	1234.96 s, 1.723	2307026	735	200.06	1473.7	710	XIC(200.06±500ppm)
Naphthalene	949.98 s, 1.649 s	53940996	931	128.04	949.98	4439	XIC(128.04±500ppm)
Naphthalene, 1-(phenylmethoxy)-	1784.93 s, 2.385 s	687081523	891	91.04	1784.93	15326	XIC(91.04±500ppm)
Naphthalene, 1,2,3,4-tetrahydro-1,6-dimethyl-4-(1-methylethyl)-, (1S-cis)-	1294.96 s, 1.371	52941033	772	159.1	1538.9	1603	XIC(159.10±500ppm)
Naphthalene, 1,2,3,4-tetrahydro-2,5,8-trimethyl-	1314.96 s, 1.880 s	4134015	737	159.11	1561.1	1142	XIC(159.11±500ppm)
Naphthalene, 1,2,3,4-tetramethyl-	1374.95 s, 1.621 s	23704549	748	169.08	1374.95	925	XIC(169.08±500ppm)
Naphthalene, 1,2-dihydro-7-methoxy-	1084.97 s, 1.478	3036128	742	160.07	1320	593	XIC(160.07±500ppm)
Naphthalene, 1,4,3-dimethyl-	1214.96 s, 1.713	31125280	753	158.08	1452.6	4538	XIC(158.08±500ppm)
Naphthalene, 1,4-dichloro-	1324.96 s, 1.876	6093230	886	195.97	1572.2	1099	XIC(195.97±500ppm)
Naphthalene, 1,4-dimethyl-	1214.96 s, 1.714	32952256	738	158.08	1452.6	5296	XIC(158.08±500ppm)
Naphthalene, 1,6,7-trimethyl-	1329.96 s, 1.718 s	50953007	900	170.08	1329.96	3851	XIC(170.08±500ppm)
Naphthalene, 1,6-dimethyl-	1219.96 s, 1.740	7776902	755	156.08	1457.9	570	XIC(156.08±500ppm)
Naphthalene, 1,7-dimethyl-	1179.97 s, 1.630	43023777	913	156.07	1179.97	6032	XIC(156.07±500ppm)
Naphthalene, 1,8-dimethyl-	1229.96 s, 1.760	14455933	891	141.06	1468.4	1900	XIC(141.06±500ppm)
Naphthalene, 1-bromo-	1254.96 s, 1.921 s	16843034	905	127.04	1254.96	2202	XIC(127.04±500ppm)
Naphthalene, 1-chloro-	1149.97 s, 1.779 s	40776533	931	162	1149.97	969	XIC(162.00±500ppm)
Naphthalene, 1-ethyl-	1169.97 s, 1.621	18787854	785	141.06	1405.3	1841	XIC(141.06±500ppm)
Naphthalene, 1-heptyl-1,2,3,4-tetrahydro-4-methyl-	1789.93 s, 1.899	28860057	714	145.08	2166.7	1138	XIC(145.08±500ppm)
Naphthalene, 1-methyl-	1069.97 s, 1.639 s	44426930	919	142.06	1069.97	3278	XIC(142.06±500ppm)
Naphthalene, 1-methyl-7-(1-methylethyl)-	1394.95 s, 1.660 s	21238210	791	169.08	1394.95	1255	XIC(169.08±500ppm)
Naphthalene, 1-propyl-	1259.96 s, 1.614 s	19906704	794	141.05	1259.96	1420	XIC(141.05±500ppm)
Naphthalene, 2-(1-methylethyl)-	1229.96 s, 1.578 s	7392928	849	155.07	1229.96	794	XIC(155.07±500ppm)
Naphthalene, 2-(phenylmethyl)-	1744.93 s, 2.203 s	34718162	773	218.08	1744.93	1969	XIC(218.08±500ppm)
Naphthalene, 2,3,6-trimethyl-	1299.96 s, 1.651 s	95757447	897	170.08	1299.96	5142	XIC(170.08±500ppm)
Naphthalene, 2,3-dimethyl-	1214.96 s, 1.716 s	35006099	816	156.07	1214.96	3474	XIC(156.07±500ppm)
Naphthalene, 2,7-dichloro-	1324.96 s, 1.875 s	5991441	882	195.96	1324.96	1416	XIC(195.96±500ppm)
Naphthalene, 2-chloro-	1149.97 s, 1.782	30837038	934	162.01	1385	905	XIC(162.01±500ppm)
Naphthalene, 2-ethoxy-	1294.96 s, 1.773 s	22662061	826	144.04	1294.96	2047	XIC(144.04±500ppm)
Naphthalene, 2-ethyl-	1169.97 s, 1.628 s	18376302	784	141.05	1169.97	2217	XIC(141.05±500ppm)
Naphthalene, 2-methoxy-	1224.96 s, 1.870 s	34183342	863	115.04	1224.96	3236	XIC(115.04±500ppm)
Naphthalene, 2-methyl-	1084.97 s, 1.720 s	42638621	928	142.06	1084.97	4501	XIC(142.06±500ppm)
Naphthalene, 2-methyl-1-propyl-	1359.95 s, 1.595 s	28894566	791	155.06	1359.95	1607	XIC(155.06±500ppm)
Naphthalene, 2-phenyl-	1659.93 s, 2.237 s	42103327	778	204.07	1659.93	627	XIC(204.07±500ppm)
Naphthalene, 6-(1,1-dimethylethyl)-1,2,3,4-tetrahydro-	1179.97 s, 1.336	5305843	824	173.11	1415.8	1626	XIC(173.11±500ppm)
Naphtho[2,1-b]furan, 1,2-dimethyl-	1484.95 s, 1.802 s	25851351	732	196.07	1484.95	910	XIC(196.07±500ppm)
Naphtho[2,1-b]furan-2(1H)-one, decahydro-3a,6,9a-tetramethyl-, [3a-(3aa,5aa,9a β ,9ba)]-	1694.93 s, 2.118	7356519	798	136.11	2040	551	XIC(136.11±500ppm)
Naphtho[2,3-b]thiophene, 4,9-dimethyl-	1694.93 s, 2.251	9159724	748	212.06	2040	794	XIC(212.06±500ppm)
Nb,Nb-Dibenzyltryptamine product	1569.94 s, 2.073	22059272	742	77.04	1873.3	727	XIC(77.04±500ppm)
n-Butyl- α -bromobenziminium bromide	1219.96 s, 2.015	3655886	704	104.03	1457.9	625	XIC(104.03±500ppm)
n-Butyric acid tetrahydrofurfuryl ester	1234.96 s, 0.897 s	358569233	743	71.07	1234.96	5279	XIC(71.07±500ppm)
N-carbobenzoyloxy-hydroxyproline, benzyl ester	1624.94 s, 2.160	86677109	819	91.04	1946.7	1492	XIC(91.04±500ppm)
n-Decanoic acid	1779.93 s, 1.340	588963080	787	55.04	2153.3	1437	XIC(55.04±500ppm)
n-Heptadecanol-1	1519.94 s, 0.963	164906408	734	69.09	1806.7	1055	XIC(69.09±500ppm)
n-Hexadecanoic acid	1639.94 s, 1.323	852676897	863	60.01	1966.7	3969	XIC(60.01±500ppm)
Nitrosothymol	1279.96 s, 1.956	18726897	749	179.08	1522.2	1760	XIC(179.08±500ppm)
Nitrous oxide	1499.94 s, 1.273 s	513954293	928	44.05	1499.94	1845	XIC(44.05±500ppm)
N-Methylbenzamide, N-heptafluorobutryl-	964.979 s, 1.515	7219942	760	105.02	1209.1	705	XIC(105.02±500ppm)
n-Nonadecanol-1	2424.89 s, 1.794 s	458079377	738	69.05	2424.89	1315	XIC(69.05±500ppm)
Nonadecane	1309.96 s, 0.942	354177529	834	57.03	1555.6	1510	XIC(57.03±500ppm)
Nonadecanoic acid-glycerine(1)-monoester, bis-O-trimethylsilyl-	2194.9 s, 1.318 s	13932968	760	73.03	2194.9	2244	XIC(73.03±500ppm)
Nonaethylene glycol, TMS derivative	2199.9 s, 1.707 s	49900740	824	73.03	2199.9	5449	XIC(73.03±500ppm)
Nonanamide	1789.93 s, 1.629 s	30724259	811	59.03	1789.93	1333	XIC(59.03±500ppm)
Nonane, 1,1-diethoxy-	1149.97 s, 1.023 s	180863974	795	103.06	1149.97	8905	XIC(103.06±500ppm)
Nonane, 1-chloro-	2004.91 s, 1.542	70338944	720	91.02	2453.4	2731	XIC(91.02±500ppm)
Nonane, 2,2,4,4,6,8-heptamethyl-	1404.95 s, 0.957 s	670294589	748	57.08	1404.95	2148	XIC(57.08±500ppm)
Nonane, 2,6-dimethyl-	734.994 s, 0.805 s	743416486	869	43.06	734.994	1673	XIC(43.06±500ppm)
Nonane, 2-methyl-3-methylene-	1089.97 s, 0.957	325747005	779	69.06	1325	1865	XIC(69.06±500ppm)
Nonane, 2-methyl-5-propyl-	1459.95 s, 0.967	429631069	742	71.07	1731.3	830	XIC(71.07±500ppm)
Nonane, 3-methyl-	699.996 s, 0.819	19552627	708	43.06	996.3	647	XIC(43.06±500ppm)

Nonane, 5-methyl-5-propyl-	1709.93 s, 0.983 s	293758857	744	71.07	1709.93	976	XIC(71.07±500ppm)
Nonanoic acid, TMS derivative	1129.97 s, 0.999 s	132553806	893	73.03	1129.97	5015	XIC(73.03±500ppm)
Noscapine	2139.9 s, 2.220 s	3076955290	732	220.11	2139.9	2733	XIC(220.11±500ppm)
n-Pentadecanol	2104.91 s, 1.120 s	68052969	751	69.06	2104.91	1783	XIC(69.06±500ppm)
n-Tetacosanol-1	1974.91 s, 1.243 s	81083786	781	43.05	1974.91	573	XIC(43.05±500ppm)
n-Tridecylcyclohexane	1644.94, 1.142	115813904	740	83.07	1973.3	1221	XIC(83.07±500ppm)
o-Cresol, TMS derivative	884.984, 1.053	4571800	755	165.06	1139.1	615	XIC(165.06±500ppm)
Octabenzene	2144.9, 2.396	30533807	906	213.04	2640.1	1719	XIC(213.04±500ppm)
Octacosanoic acid, ethyl ester	2354.89, 2.217	26457433	739	88.04	2920.1	2105	XIC(88.04±500ppm)
Octacosanol	1659.93 s, 1.109 s	517845715	730	57.07	1659.93	1007	XIC(57.07±500ppm)
Octadecanamide	1919.92, 1.695	29094378	774	59.03	2340	1504	XIC(59.03±500ppm)
Octadecane	1349.95 s, 0.934 s	857752118	900	57.06	1349.95	2971	XIC(57.06±500ppm)
Octadecane, 1-iodo-	1499.94, 0.946	319257322	730	71.07	1781.3	3748	XIC(71.07±500ppm)
Octadecane, 2-methyl-	1564.94 s, 0.983 s	352429957	752	57.06	1564.94	3371	XIC(57.06±500ppm)
Octadecanoic acid	1779.93, 1.373	744162258	797	43.03	2153.3	722	XIC(43.03±500ppm)
Octadecanoic acid, 2,3-dihydroxypropyl ester	2109.91, 1.854	67108240	870	43.06	2593.4	2237	XIC(43.06±500ppm)
Octadecanoic acid, ethyl ester	1799.93 s, 1.232 s	965199971	860	101.04	1799.93	4103	XIC(101.04±500ppm)
Octadecanoic acid, octadecyl ester	2339.89 s, 2.097 s	32096476	762	57.06	2339.89	749	XIC(57.06±500ppm)
Octadecyl octyl ether	2994.85, 3.800	50887018	759	71.08	3773.5	865	XIC(71.08±500ppm)
Octaethylene glycol monododecyl ether	2524.88, 4.404	11469414	756	73.03	3146.8	524	XIC(73.03±500ppm)
Octaethylene glycol, 2TMS derivative	1699.93 s, 1.249 s	197610703	749	161.08	1699.93	10475	XIC(161.08±500ppm)
Octaethylene glycol, TMS derivative	2114.91 s, 2.249 s	112322344	907	45.04	2114.91	1753	XIC(45.04±500ppm)
Octan-3-ol, O-TMS	804.989 s, 0.786 s	25504861	750	75.01	804.989	720	XIC(75.01±500ppm)
Octane	1309.96, 0.985	271533428	746	43.07	1555.6	1238	XIC(43.07±500ppm)
Octane, 1,1-diethoxy-	1049.97 s, 1.026 s	132354019	850	103.06	1049.97	1150	XIC(103.06±500ppm)
Octane, 1,1'-oxybis-	1404.95, 1.068	192263113	825	57.06	1664.7	1189	XIC(57.06±500ppm)
Octane, 1-chloro-	1029.98 s, 1.086 s	17457093	749	43.05	1029.98	841	XIC(43.05±500ppm)
Octane, 2,3,6,7-tetramethyl-	834.988 s, 0.834 s	303030610	848	71.07	834.988	38726	XIC(71.07±500ppm)
Octane, 2,3,6-trimethyl-	1109.97 s, 0.897 s	630269192	822	43.06	1109.97	2919	XIC(43.06±500ppm)
Octane, 2,3-dimethyl-	1474.95, 1.003	345128366	737	57.08	1750	705	XIC(57.08±500ppm)
Octane, 2,4,6-trimethyl-	684.997 s, 0.798 s	287392232	882	57.09	684.997	665	XIC(57.09±500ppm)
Octane, 2,6,6-trimethyl-	1439.95 s, 0.956 s	353929359	768	71.06	1439.95	1457	XIC(71.06±500ppm)
Octane, 2,6-dimethyl-	1019.98 s, 2.206 s	10850270	782	55.02	1019.98	859	XIC(55.02±500ppm)
Octane, 2,7-dimethyl-	1324.96 s, 0.958 s	356779038	765	57.04	1324.96	3367	XIC(57.04±500ppm)
Octane, 3-ethyl-2,7-dimethyl-	959.98 s, 0.840 s	537305883	871	57.06	959.98	3764	XIC(57.06±500ppm)
Octane, 5-ethyl-2-methyl-	1804.93, 1.010	1379080859	815	71.07	2186.7	4290	XIC(71.07±500ppm)
Octane, 6-ethyl-2-methyl-	859.986 s, 0.846 s	747075334	876	43.06	859.986	2125	XIC(43.06±500ppm)
Octanoic acid, methyl ester	874.985, 1.115	10217973	809	74.02	1130.4	717	XIC(74.02±500ppm)
Octanoic acid, TMS derivative	1029.98 s, 0.987 s	95032362	896	75.01	1029.98	2649	XIC(75.01±500ppm)
Octanoic acid, triethylsilyl ester	1129.97, 0.874	17966372	725	103.04	1365	587	XIC(103.04±500ppm)
Octicizer	1954.92 s, 2.038 s	54815174	880	251.02	1954.92	3560	XIC(251.02±500ppm)
Octocrylene	2094.91, 2.367	6019498	829	249.06	2573.4	1013	XIC(249.06±500ppm)
Octyl tetracosyl ether	1969.91, 1.113	159852390	735	43.05	2406.7	1256	XIC(43.05±500ppm)
o-Cymene	754.993, 1.106	10148136	793	119.07	1037	587	XIC(119.07±500ppm)
Oleic Acid	1709.93 s, 1.483 s	120940976	745	55.05	1709.93	795	XIC(55.05±500ppm)
ortho tert-Butyl cyclohexyl acetate	1064.97, 1.214	11602180	704	57.06	1300	530	XIC(57.06±500ppm)
Orthoformic acid, triisobutyl ester	724.995 s, 0.939 s	135548499	791	57.06	724.995	1913	XIC(57.06±500ppm)
o-Toluic acid, 4-nitrophenyl ester	1654.94, 2.108	18468961	840	119.04	1986.7	893	XIC(119.04±500ppm)
o-Toluic acid, TMS derivative	1109.97 s, 1.169 s	21305631	728	119.07	1109.97	1281	XIC(119.07±500ppm)
Oxacycloheptadecan-2-one	2324.89, 2.118	90351320	709	43.03	2880.1	657	XIC(43.03±500ppm)
Oxalic acid, 2TMS derivative	1649.94, 0.801	104627736	731	73.04	1980	1372	XIC(73.04±500ppm)
Oxalic acid, 6-ethyloct-3-yl isoheptyl ester	1169.97 s, 1.098 s	76145336	739	43.03	1169.97	2317	XIC(43.03±500ppm)
Oxalic acid, allyl hexyl ester	2129.9, 1.244	514180175	714	43.06	2620	1327	XIC(43.06±500ppm)
Oxalic acid, allyl octyl ester	1344.95, 0.985	126418643	797	41.03	1594.4	693	XIC(41.03±500ppm)
Oxalic acid, bis(isobutyl) ester	1589.94, 1.011	297252270	752	57.11	1900	1067	XIC(57.11±500ppm)
Oxalic acid, butyl propyl ester	1039.97 s, 0.905 s	162103541	756	57.06	1039.97	5399	XIC(57.06±500ppm)
Oxalic acid, cyclobutyl heptyl ester	1894.92 s, 1.076 s	285286018	748	43.06	1894.92	2124	XIC(43.06±500ppm)
Oxalic acid, dicyclobutyl ester	1489.95 s, 1.059 s	287925296	804	55.05	1489.95	1752	XIC(55.05±500ppm)
Oxalic acid, diisohexyl ester	859.986, 0.847	848437586	751	43.06	1117.4	1752	XIC(43.06±500ppm)
Oxalic acid, heptyl propyl ester	1039.97, 0.913	183873105	719	57.06	1277.3	2428	XIC(57.06±500ppm)
Oxalic acid, isobutyl hexyl ester	1254.96 s, 0.915 s	625823007	794	57.07	1254.96	10250	XIC(57.07±500ppm)
Oxalic acid, isobutyl pentyl ester	1054.97, 0.868	413506679	836	43.06	1290.9	3736	XIC(43.06±500ppm)
Oxalic acid, isobutyl propyl ester	2289.89, 1.547	407645209	754	57.07	2833.4	734	XIC(57.07±500ppm)
Oxalic acid, isoheptyl pentyl ester	774.991, 0.811	54237953	721	43.06	1051.9	1254	XIC(43.06±500ppm)
Oxalic acid, octyl propyl ester	1444.95 s, 0.946 s	453701538	766	71.04	1444.95	15302	XIC(71.04±500ppm)
Oxazolidin-2-one	1789.93 s, 1.399 s	61315013	743	87.06	1789.93	2012	XIC(87.06±500ppm)
Oxirane, hexadecyl-	2224.9, 1.642	82661087	781	43.03	2746.7	781	XIC(43.03±500ppm)
Palmitic Acid, TMS derivative	1679.93 s, 1.133 s	26703079	753	117.02	1679.93	938	XIC(117.02±500ppm)
Pantolactone, (3R)-, TMS derivative	904.983 s, 1.206 s	36387140	733	73.03	904.983	1288	XIC(73.03±500ppm)
p-Cymene	749.993, 1.122	7076976	741	119.07	1033.3	942	XIC(119.07±500ppm)
p-Dicyclohexylbenzene	1669.93 s, 1.655 s	24922651	763	159.1	1669.93	840	XIC(159.10±500ppm)
Pentacosane	2724.87 s, 2.831 s	110320488	839	57.07	2724.87	638	XIC(57.07±500ppm)
Pentadecane	969.979 s, 2.232 s	38322885	895	57.06	969.979	764	XIC(57.06±500ppm)
Pentadecane, 2,6,10-trimethyl-	1149.97 s, 0.899 s	97637839	743	57.06	1149.97	1701	XIC(57.06±500ppm)
Pentadecane, 2-methyl-	1319.96 s, 0.944 s	1622560759	885	43.05	1319.96	4419	XIC(43.05±500ppm)
Pentadecane, 3-methyl-	1324.96 s, 0.991 s	242083872	735	41.04	1324.96	532	XIC(41.04±500ppm)
Pentadecane, 4-methyl-	1309.96, 0.991	221656721	716	71.06	1555.6	2001	XIC(71.06±500ppm)
Pentadecanoic acid, glycerine-(1)-monoester, bis-O-trimethylsilyl-	1964.92 s, 1.125 s	7916771	750	73.04	1964.92	863	XIC(73.04±500ppm)
Pentadecanoic acid, TMS derivative	1629.94 s, 1.078 s	37223411	867	73.04	1629.94	1562	XIC(73.04±500ppm)
Pentaethylene glycol	1714.93, 2.246	649707077	849	45.04	2066.7	4295	XIC(45.04±500ppm)
Pentaethylene glycol, 2TMS derivative	1504.94 s, 1.108 s	932849853	812	117.08	1504.94	4448	XIC(117.08±500ppm)

Pentaethylene glycol, TMS derivative	1794.93 s, 1.713 s	27876353	787	45.04	1794.93	756	XIC(45.04±500ppm)
Pentan-3-ol, trimethylsilyl ether	869.985 s, 0.785 s	196207055	799	131.07	869.985	8658	XIC(131.07±500ppm)
Pentanamide, 2-(dimethylamino)-3-methyl-N-[3-(1-methylethyl)-7-(2-methylpropyl)-5,8-dioxo-2-oxa-	1729.93 s, 1.613 s	8010212	767	114.07	1729.93	718	XIC(114.07±500ppm)
Pentane, 2,2,4,4-tetramethyl-	2189.9, 1.297	75377765	721	57.06	2700.1	810	XIC(57.06±500ppm)
Pentane, 2,2,4,4-tetramethyl-3-methoxy-	1194.96 s, 1.489 s	27563705	749	101.01	1194.96	6728	XIC(101.01±500ppm)
Pentane, 2,2,4-trimethyl-	2139.9, 1.251	293047794	741	57.07	2633.4	229	XIC(57.07±500ppm)
Pentane, 2-methoxy-2,4,4-trimethyl-	2024.91, 1.335	126837881	755	73.03	2480	598	XIC(73.03±500ppm)
Pentane, 3,3-dimethyl-	1584.94 s, 0.973 s	340653733	748	71.07	1584.94	2040	XIC(71.07±500ppm)
Pentane, 3-bromo-	1814.92, 1.011	354474330	761	71.06	2200	1312	XIC(71.06±500ppm)
Pentane, 3-ethyl-	1399.95 s, 0.978 s	409706237	731	71.07	1399.95	2814	XIC(71.07±500ppm)
Pentanedioic acid, (2,4-di-t-butylphenyl) mono-ester	1134.97, 1.360	5254670	763	191.08	1370	905	XIC(191.08±500ppm)
Pentanoic acid, 5-hydroxy-, 2,4-di-t-butylphenyl esters	1134.97 s, 1.353 s	4444868	729	191.09	1134.97	716	XIC(191.09±500ppm)
Pentanoic acid, TMS derivative	699.996, 0.904	56134209	802	75.01	996.3	537	XIC(75.01±500ppm)
Pentanoic acid, triisopropylsilyl ester	1344.95, 0.889	9269061	709	215.15	1594.4	1355	XIC(215.15±500ppm)
Pentasiloxane, dodecamethyl-	939.981 s, 0.717 s	648810556	906	73.03	939.981	13039	XIC(73.03±500ppm)
Pentitol, 3-desoxy-tetakis-O-(trimethylsilyl)-	1374.95 s, 0.832 s	14831899	833	73.04	1374.95	3934	XIC(73.04±500ppm)
Phenalenol[1,9-bc]thiophene	1754.93, 2.627	3737661	765	208.01	2120	559	XIC(208.01±500ppm)
Phenanthrene	1519.94, 2.205	745925373	942	178.06	1806.7	6534	XIC(178.06±500ppm)
Phenanthrene, 1,2,3,4,4a,9,10,10a-octahydro-1,1,4a-trimethyl-7-(1-methylethyl)-, (4aS-trans)-	1829.92 s, 2.072 s	7939374	735	173.08	1829.92	5000	XIC(173.08±500ppm)
Phenanthrene, 1-methyl-	1609.94 s, 2.182 s	156657240	938	192.07	1609.94	4122	XIC(192.07±500ppm)
Phenanthrene, 2,3,5-trimethyl-	1789.93 s, 2.176 s	4337906	746	220.1	1789.93	564	XIC(220.1±500ppm)
Phenanthrene, 2,7-dimethyl-	1704.93 s, 2.194 s	53684126	864	206.09	1704.93	1752	XIC(206.09±500ppm)
Phenanthrene, 3,6-dimethyl-	1684.93 s, 2.137 s	10110921	749	206.09	1684.93	752	XIC(206.09±500ppm)
Phenol, 2-(2H-benzotriazol-2-yl)-4,6-bis(1,1-dimethylpropyl)-	2084.91, 2.075	6417180	821	322.17	2560	1041	XIC(322.17±500ppm)
Phenol, 2,4,6-tris(1-methylethyl)-	1254.96 s, 1.346 s	204804889	748	205.04	1254.96	16067	XIC(205.04±500ppm)
Phenol, 2-amino-6-(1,1-dimethylethyl)-4-methyl-	1279.96 s, 1.947 s	7923875	730	179.07	1279.96	1646	XIC(179.07±500ppm)
Phenol, 3-(ethylamino)-4-methyl-	754.993 s, 1.126 s	24711605	733	136.04	754.993	2317	XIC(136.04±500ppm)
Phenol, 4,6-di(1,1-dimethylethyl)-2-methyl-	1209.96 s, 1.219 s	12534858	731	205.13	1209.96	1599	XIC(205.13±500ppm)
Phenol, TMS derivative	784.991 s, 2.444 s	59941122	893	151.04	784.991	529	XIC(151.04±500ppm)
Phenoxazine	1204.96, 0.930	9480058	716	183.18	1442.1	597	XIC(183.18±500ppm)
Phenyl cyclohexyl ketone	1364.95 s, 1.768 s	12087000	749	105.02	1364.95	958	XIC(105.02±500ppm)
Phenylpropanolamine, 2TMS derivative	1524.94 s, 1.381 s	531981692	729	73.01	1524.94	958	XIC(73.01±500ppm)
Phloroglucinol, O,O'-bis(trimethylsilyl)-	1144.97, 0.956	19717447	744	255.08	1380	5185	XIC(255.08±500ppm)
Phosphine, 1,2-ethanediybis[dicyclohexyl]-	1984.91, 1.291	6482547	727	339.28	2426.7	2338	XIC(339.28±500ppm)
Phosphorocyanidous difluoride	1179.97 s, 0.969 s	51914211	756	69.06	1179.97	532	XIC(69.06±500ppm)
Phthalic acid, 2-pentyl 2-propyl ester	1749.93 s, 1.633 s	16510845	836	149	1749.93	955	XIC(149.00±500ppm)
Phthalic acid, bis(2-pentyl) ester	2104.91 s, 1.740 s	21103654	826	149.01	2104.91	668	XIC(149.01±500ppm)
Phthalic acid, butyl 4-methylpent-2-yl ester	1914.92, 1.684	38809398	807	149	2333.4	1776	XIC(149.00±500ppm)
Phthalic acid, cyclobutyl decyl ester	2174.9, 2.261	5289087101	712	149.11	2680.1	1041	XIC(149.11±500ppm)
Phthalic acid, cyclobutyl hexyl ester	1574.94, 1.660	1349691407	803	149	1880	2171	XIC(149.00±500ppm)
Phthalic acid, cyclobutyl isobutyl ester	2179.9, 2.245	7426081213	844	149	2686.7	1042	XIC(149.00±500ppm)
Phthalic acid, cyclobutyl tridecyl ester	2179.9, 2.062	5404935972	747	149.09	2686.7	2478	XIC(149.09±500ppm)
Phthalic acid, cyclohexyl 2-propyl ester	1749.93, 1.638	24262760	755	149	2113.3	1092	XIC(149.00±500ppm)
Phthalic acid, dec-2-yl ethyl ester	1834.92, 1.691	150608651	859	149.01	2226.7	3363	XIC(149.01±500ppm)
Phthalic acid, dec-2-yl isobutyl ester	1939.92, 1.717	432614203	909	149	2366.7	5755	XIC(149.00±500ppm)
Phthalic acid, di(2,3-dimethylphenyl) ester	1704.93, 1.036	3597648	748	253.26	2053.3	516	XIC(253.26±500ppm)
Phthalic acid, di(3-methylphenyl) ester	1449.95 s, 1.769 s	1818672584	752	239.27	1449.95	605	XIC(239.27±500ppm)
Phthalic acid, di(hept-4-yl) ester	2174.9, 2.377	7354989634	790	149.08	2680.1	1312	XIC(149.08±500ppm)
Phthalic acid, di(hex-3-yl) ester	1179.9, 1.806	166566083	791	148.94	2686.7	1046	XIC(148.94±500ppm)
Phthalic acid, di(oct-3-yl) ester	1989.91, 1.683	93707293	746	149.01	2433.4	616	XIC(149.01±500ppm)
Phthalic acid, ethyl 2-ethylbutyl ester	1834.92 s, 1.695 s	126843759	882	149	1834.92	2821	XIC(149.00±500ppm)
Phthalic acid, ethyl hept-2-yl ester	1834.92, 1.694	158220030	836	149	2226.7	3047	XIC(149.00±500ppm)
Phthalic acid, hept-2-yl isohexyl ester	2174.9 s, 1.812 s	1525217108	829	149.05	2174.9	1679	XIC(149.05±500ppm)
Phthalic acid, hept-4-yl isobutyl ester	1569.94, 1.698	83207763	703	149	1873.3	971	XIC(149.00±500ppm)
Phthalic acid, isobutyl 4-methylpent-2-yl ester	1914.92 s, 1.681 s	29085998	835	149	1914.92	1444	XIC(149.00±500ppm)
Phthalic acid, nonyl 2-propylpentyl ester	2119.91, 1.857	27391650	744	149.01	2606.7	550	XIC(149.01±500ppm)
p-Hydroxydiisopropylbenzene, TMS derivative	1179.97 s, 1.047 s	47353567	824	73.03	1179.97	1135	XIC(73.03±500ppm)
Pinacol, 2TMS derivative	1009.98, 0.801	20324496	816	131.07	1250	2379	XIC(131.07±500ppm)
Pipicolylpiperonic acid, N-ethoxycarbonyl-, dodecyl ester	1174.97, 1.676	4573217	811	156.07	1410.5	583	XIC(156.07±500ppm)
Pivalic acid vinyl ester	979.978 s, 1.292 s	53348553	810	57.06	979.978	1646	XIC(57.06±500ppm)
Pivalic acid, 2-tetrahydrofurylmethyl ester	1444.95, 0.955	275153892	778	71.04	1712.5	2462	XIC(71.04±500ppm)
Pregn-1,4,6-triene-3,20-dione, 6,16-dimethyl-, (16α)-	2129.9 s, 3.188 s	31756911	733	338.12	2129.9	3338	XIC(338.12±500ppm)
Pregna-3,5-dien-20α-ol, O-trimethylsilyl	1024.98, 0.919	638176916	784	117.06	1263.6	1838	XIC(117.06±500ppm)
Propan-2-ol, O-tert-butylidimethylsilyl ether	1079.97 s, 0.836 s	43077738	751	117.05	1079.97	1046	XIC(117.05±500ppm)
Propane, 1,1,3,3-tetraethoxy-	1019.98 s, 0.977 s	35247826	738	103.06	1019.98	1647	XIC(103.06±500ppm)
Propane, 1,1,3-triethoxy-	819.988, 1.065	17814700	745	59.04	1085.2	565	XIC(59.04±500ppm)
Propane, 1-[1-(difluoro(trifluoroethenyl)oxy)methyl]-1,2,2,2-tetrafluoroethoxy]-1,1,2,2,3,3,3-heptafluoro-	989.978 s, 1.866 s	27001591	751	168.97	989.978	940	XIC(168.97±500ppm)
Propane, 2-methyl-1,2-bis(trimethylsiloxy)-	764.992 s, 0.775 s	297491708	896	131.07	764.992	5881	XIC(131.07±500ppm)
Propanedinitrile, (2,3-dihydro-1-methyl-1H-inden-1-yl)-	1694.93 s, 1.851 s	14931673	738	131.07	1694.93	616	XIC(131.07±500ppm)
Propanedinitrile, cyclohexyl(2-methylcyclohexyl)-	1834.92, 1.077	152764409	724	41.04	2226.7	1050	XIC(41.04±500ppm)
Propanedioic acid, 2TMS derivative	969.979, 1.033	13389342	741	147.05	1213.6	926	XIC(147.05±500ppm)
Propanoic acid, 2,2-dimethyl-, butyl ester	729.994, 0.942	135317567	787	57.06	1018.5	1940	XIC(57.06±500ppm)
Propanoic acid, 2-hydroxy-, ethyl ester	1899.92, 2.464	345573257	768	45.04	2313.4	4476	XIC(45.04±500ppm)
Propanoic acid, 2-hydroxy-, methyl ester, (±)-	929.981, 2.212	23264177	792	45.04	1178.3	991	XIC(45.04±500ppm)
Propanoic acid, 2-methyl-, anhydride	1639.94 s, 0.951 s	293763908	756	71.07	1639.94	1126	XIC(71.07±500ppm)
Propanoic acid, 2-methyl-3-[(trimethylsilyl)oxy]-, trimethylsilyl ester	904.983, 0.790	482633681	745	73.04	1156.5	4466	XIC(73.04±500ppm)
Propanoic acid, 2-methylpropyl ester	2064.91, 1.099	766130077	736	57.06	2533.4	1389	XIC(57.06±500ppm)
Propanoic acid, 2-oxo-3-(trimethylsilyl)-, trimethylsilyl ester	994.977 s, 0.994 s	20462190	805	73.06	1236.4	161	XIC(73.06±500ppm)
Propanoic acid, 3-(trimethylsilyl)-, ethyl ester	944.98 s, 1.206 s	21118784	746	73.06	1191.3	1206	XIC(73.06±500ppm)
Propanoic acid, 3-phenyl-2-(benzoylamino)-, ethyl ester	1899.92 s, 2.397 s	48483880	823	105.01	1899.92	2167	XIC(105.01±500ppm)
Propanoic acid, anhydride	1354.95 s, 0.934 s	88885347	746	57.16	1354.95	501	XIC(57.16±500ppm)

Propanoic acid, ethenyl ester	1859.92, 1.028	338524511	750	57.07	2260	739	XIC(57.07±500ppm)
Propanoic acid, TBDMS derivative	984.978, 1.418	5602951	722	131.03	1227.3	737	XIC(131.03±500ppm)
Propanoic acid, TMS derivative	1449.95, 0.864	66426280	726	73.04	1718.8	696	XIC(73.04±500ppm)
Propanoic acid, trimethylsilyl ester	1344.95 s, 0.886 s	8295558	746	215.16	1344.95	1823	XIC(215.16±500ppm)
Propanoic acid, 2,3,3,3-tetrafluoro-2-[1,1,1,2,3,3,3-hexafluoro-2-(heptafluoropropoxy)propoxy]-	754.993 s, 1.506 s	3665699	752	168.97	754.993	565	XIC(168.97±500ppm)
Propyl pyruvate	1219.96, 0.938	240209870	702	43.06	1457.9	889	XIC(43.06±500ppm)
Propyl triacontyl ether	2384.89, 2.214	45828268	730	43.03	2960.1	722	XIC(43.03±500ppm)
Propylamine, 2TMS derivative	884.984 s, 1.022 s	323094592	740	73.03	884.984	3194	XIC(73.03±500ppm)
Propylene glycol, 2TMS derivative	724.995 s, 2.150 s	981140776	904	73.03	724.995	5790	XIC(73.03±500ppm)
p-Toluic acid, 2-ethylhexyl ester	1549.94 s, 1.420 s	73014338	781	119.03	1549.94	1356	XIC(119.03±500ppm)
p-Toluic acid, 3,5-difluorophenyl ester	1399.95 s, 1.398 s	23149313	751	119.03	1399.95	730	XIC(119.03±500ppm)
p-Toluic acid, butyl ester	1259.96 s, 1.487 s	67898820	908	119.03	1259.96	3312	XIC(119.03±500ppm)
p-Toluic acid, TMS derivative	1134.97 s, 1.248 s	279598754	877	119.03	1134.97	4918	XIC(119.03±500ppm)
Pyrene	1764.93 s, 2.654 s	63497484	936	202.05	1764.93	4101	XIC(202.05±500ppm)
Pyrene, 1,2,3,6,7,8-hexahydro-	1639.94, 1.874	18433180	736	208.11	1966.7	610	XIC(208.11±500ppm)
Pyridine	749.993 s, 0.707 s	9572109	933	79.02	749.993	675	XIC(79.02±500ppm)
Pyridine, 2,3,5-trimethyl-	764.992, 1.135	4715481	820	121.07	1044.4	597	XIC(121.07±500ppm)
Pyridine, 2,4,6-trimethyl-	714.995 s, 1.258 s	109972990	945	121.07	714.995	784	XIC(121.07±500ppm)
Pyridine, 2,4-dimethyl-	645, 3.943	35577204	924	107.06	955.6	916	XIC(107.06±500ppm)
Pyroglutamic acid, TMS derivative	1264.96, 1.707	15988552	732	84.03	1505.6	541	XIC(84.03±500ppm)
Pyrollidine, 2,5-bis(imino)-	1054.97, 0.932	26155338	746	97.09	1290.9	548	XIC(97.09±500ppm)
Pyrrolidine, 1-[2-(4-bromophenoxy)ethyl]-	1554.94, 1.000	71406373	756	84.09	1853.3	1611	XIC(84.09±500ppm)
Pyrrolo(2,3-b)pyrazine	1569.94 s, 1.036 s	11464172	746	119.04	1569.94	1375	XIC(119.04±500ppm)
Pyruvic acid, butyl ester	1164.97 s, 0.935 s	233299887	766	43.06	1164.97	4101	XIC(43.06±500ppm)
Pyruvic acid, TMS derivative	1509.94 s, 0.888 s	140358621	739	73.05	1509.94	865	XIC(73.05±500ppm)
Quinoline, 1,2-dihydro-2,4-trimethyl-	1219.96 s, 1.688 s	29831897	828	158.08	1219.96	3791	XIC(158.08±500ppm)
Quinoline, 2,4-dimethyl-	1214.96 s, 1.888 s	11581001	854	157.07	1214.96	526	XIC(157.07±500ppm)
Quinoline, 6-methoxy-2-methyl-	1369.95, 2.001	11900443	756	173.07	1623.5	1090	XIC(173.07±500ppm)
Quinoline, 6-methoxy-4-methyl-	1369.95, 2.003	12339689	732	173.06	1623.5	1148	XIC(173.06±500ppm)
Quinoxaline, 6-methyl-2-phenyl-	2134.9, 2.440	3069449988	740	220.26	2626.7	625	XIC(220.26±500ppm)
Resorcinol, 2TMS derivative	1174.97 s, 1.035 s	6139769	855	239.13	1410.5	1619	XIC(239.13±500ppm)
Retene	1829.92 s, 2.157 s	11365980	762	219.09	1829.92	1211	XIC(219.09±500ppm)
Retinoic acid, TMS derivative	2019.91 s, 1.829 s	276609786	744	254.45	2473.4	1919	XIC(254.45±500ppm)
Ribitol, 5TMS derivative	1644.94 s, 0.813 s	272088105	853	73.04	1644.94	3334	XIC(73.04±500ppm)
Salsoline	1384.95 s, 1.944 s	40792870	756	178.07	1384.95	1259	XIC(178.07±500ppm)
Sebacic acid, 2TBDMS derivative	2104.91, 2.485	12359295	766	373.1	2586.7	653	XIC(373.10±500ppm)
Sedoheptulose anhydride, tetrakis(trimethylsilyl) ether	1464.95, 1.054	34452487	746	204.09	1737.5	503	XIC(204.09±500ppm)
Silanamine, N,N'-methanetetraylbis(1,1,1-trimethyl-	674.998 s, 2.254 s	537447641	907	171.05	674.998	2097	XIC(171.05±500ppm)
Silane, [(dimethylsilyl)methyl]trimethyl-	1964.92 s, 0.994 s	4511382	738	131.07	1964.92	5148	XIC(131.07±500ppm)
Silane, diethyl(2-ethylbutoxy)hexadecyloxy-	2134.9, 1.524	79794107	750	399.44	2626.7	5759	XIC(399.44±500ppm)
Silane, diethylbutoxypentyl-oxo-	1554.94, 0.906	37339772	726	217.09	1853.3	5252	XIC(217.09±500ppm)
Silane, diethyldecyloxy(3-methylbutoxy)-	2139.9 s, 3.498 s	5136238	742	301.06	2139.9	1410	XIC(301.06±500ppm)
Silane, diethyldecyloxyoctyloxy-	1929.92 s, 1.161 s	692413202	788	343.27	1929.92	857	XIC(343.27±500ppm)
Silane, diethyldecyloxyxypentyl-oxo-	2139.9 s, 3.511	9009019	714	301.05	2633.4	2178	XIC(301.05±500ppm)
Silane, diethyldodecyloxyoctyloxy-	2039.91 s, 1.328 s	1051805928	749	371.26	2039.91	787	XIC(371.26±500ppm)
Silane, diethylheptadecyloxy(2-methylbutoxy)-	2149.9, 1.709	415624159	851	399.33	2646.7	6419	XIC(399.33±500ppm)
Silane, diethylheptadecyloxy(2-phenylethoxy)-	1419.95, 0.770	4476915	749	433.03	1682.4	950	XIC(433.03±500ppm)
Silane, diethylheptyloxyoctadecyloxy-	2539.88 s, 3.989 s	2257148970	751	57.08	2539.88	5006	XIC(57.08±500ppm)
Silane, diethylheptyloxyxypentadecyloxy-	2144.9, 1.387	20264885	715	399.38	2640.1	1012	XIC(399.38±500ppm)
Silane, diethylnonyloxytridecyloxy-	2149.9 s, 1.723 s	355820822	855	399.38	2149.9	634	XIC(399.38±500ppm)
Silane, diethyloctyloxytetradecyloxy-	2134.9, 1.558	64906876	886	399.26	2626.7	502	XIC(399.26±500ppm)
Silane, dimethyl(2,6-dimethoxyphenoxy)tridecyloxy-	2219.9 s, 2.972 s	3697076	741	410.15	2219.9	626	XIC(410.15±500ppm)
Silane, dimethyl(2-hexyloxy)ethoxy-	2054.91 s, 1.309 s	330937308	733	147.02	2054.91	3003	XIC(147.02±500ppm)
Silane, dimethyl(2-naphthoxy)heptadecyloxy-	2409.89, 2.328	2068485	737	456.34	2993.4	513	XIC(456.34±500ppm)
Silane, dimethyl(3-methylphenoxy)ethoxy-	1139.97 s, 1.254 s	11489380	739	210.08	1139.97	1036	XIC(210.08±500ppm)
Silane, dimethyl(4-(2-phenylprop-2-yl)phenoxy)butoxy-	1769.93 s, 1.049 s	228053145	786	327.43	1769.93	5030	XIC(327.43±500ppm)
Silane, dimethyl-2-propenyl(tetradecyloxy)-	1429.95 s, 0.839 s	879896	745	271.22	1429.95	637	XIC(271.22±500ppm)
Silane, dimethyloctyloxyheptadecyloxy-	2244.9 s, 1.423 s	109622299	743	427.32	2244.9	2256	XIC(427.32±500ppm)
Silane, methoxytripropyl-	1229.96, 0.869	3987968	751	145.08	1468.4	621	XIC(145.08±500ppm)
Silane, methyl-diisopropoxyethoxy-	1284.96, 0.856	226953378	745	191.07	1527.8	1291	XIC(191.07±500ppm)
Silane, tetramethyl-	839.987 s, 0.942 s	92749095	734	73.04	839.987	1077	XIC(73.04±500ppm)
Silane, trimethyl(3-methylbutyl)-	2164.9, 1.685	156387317	723	73.01	2666.7	587	XIC(73.01±500ppm)
Silane, trimethylphenyl-	1249.96, 1.316	18885246	746	135.07	1489.5	1126	XIC(135.07±500ppm)
Silanol, trimethyl-	704.996 s, 0.573 s	346370303	876	75.01	704.996	597	XIC(75.01±500ppm)
Silanol, trimethyl-, carbonate (2:1)	709.996, 0.868	1245444455	853	147.04	1003.7	1064	XIC(147.04±500ppm)
Silanol, trimethyl-, phosphate (3:1)	1049.97 s, 1.017 s	129478966	832	299.04	1049.97	2392	XIC(299.04±500ppm)
Silicic acid, diethyl bis(trimethylsilyl) ester	829.988 s, 0.746 s	32988973	844	207.01	829.988	2305	XIC(207.01±500ppm)
Silicon tetrafluoride	1644.94 s, 1.231 s	74060719	752	85.07	1644.94	510	XIC(85.07±500ppm)
s-Indacen-1(2H)-one, 3,5,6,7-tetrahydro-3,3,4,4,5,5,8-hexamethyl-	1729.93, 1.689	16898073	746	241.18	2086.7	1101	XIC(241.18±500ppm)
Squalene	2169.9 s, 1.720 s	147455863	728	81.07	2169.9	558	XIC(81.07±500ppm)
Stearic acid, TMS derivative	1829.92 s, 1.171 s	68711772	781	42.98	1829.92	1094	XIC(42.98±500ppm)
Stigmast-5-ene, 3β-(trimethylsilyloxy)-, (24S)-	2489.88, 3.190	14557096	846	129.06	3100.1	1128	XIC(129.06±500ppm)
Stigmasterol, TMS derivative	2444.88 s, 2.891 s	26757789	875	83.07	2444.88	610	XIC(83.07±500ppm)
Suberic acid, 2TBDMS derivative	1969.91 s, 2.263 s	531905	748	73.04	1969.91	502	XIC(73.04±500ppm)
Succinic acid, 2-chloro-6-fluorophenyl 4-methoxybenzyl ester	1499.94, 1.609	45829078	799	121.04	1781.3	1372	XIC(121.04±500ppm)
Succinic acid, 2-methylpent-3-yl 2-fluoro-3-(trifluoromethyl)phenyl ester	1304.96, 1.052	181627449	759	263.16	1550	1028	XIC(263.16±500ppm)
Succinic acid, 3-chlorophenyl 3-phenylprop-2-en-1-yl ester	1014.98 s, 1.644 s	16597409	761	117.05	1014.98	640	XIC(117.05±500ppm)
Succinic acid, 3-chlorophenyl 4-methoxybenzyl ester	1419.95, 1.446	45309851	841	121.04	1682.4	848	XIC(121.04±500ppm)
Succinic acid, 3-methylbut-2-yl 2,2,3,3,3-pentafluoropropyl ester	2519.88, 4.457	3978851	736	233.08	3140.1	590	XIC(233.08±500ppm)
Succinic acid, cyclohexylmethyl 2,4-dimethylpent-3-yl ester	1294.96, 1.066	71738169	754	97.08	1538.9	579	XIC(97.08±500ppm)
Succinic acid, ethyl 3-hexyl ester	1684.93 s, 1.520 s	16793981	804	101.01	1684.93	1030	XIC(101.01±500ppm)

Succinic acid, phenethyl 2,3-dichlorophenyl ester	1369.95, 1.665	14940761	753	105.05	1623.5	623	XIC(105.05±500ppm)
Sulfone, 2-hydroxypropyl t-butyl	1849.92 s, 1.066 s	334328885	734	57.06	1849.92	1174	XIC(57.06±500ppm)
Sulfurous acid, 2-ethylhexyl hexyl ester	1349.95 s, 0.999 s	837211397	826	57.07	1349.95	926	XIC(57.07±500ppm)
Sulfurous acid, di(cyclohexylmethyl) ester	1599.94, 1.082	154112077	812	97.09	1913.3	1872	XIC(97.09±500ppm)
Sulfurous acid, dodecyl pentyl ester	1324.96, 0.957	207821346	718	71.03	1572.2	1164	XIC(71.03±500ppm)
Sulfurous acid, hexyl nonyl ester	844.987, 0.822	237629493	765	85.08	1104.3	801	XIC(85.08±500ppm)
Sulfurous acid, isobutyl pentyl ester	1569.94, 0.986	152059470	759	71.05	1873.3	893	XIC(71.05±500ppm)
Supraene	2169.9 s, 1.591 s	568046269	929	69.03	2169.9	3331	XIC(69.03±500ppm)
Syringaldehyde, TMS derivative	1414.95 s, 1.583 s	89176655	729	224.02	1414.95	4032	XIC(224.02±500ppm)
Terephthalic acid, 5-methylhex-2-yl octyl ester	2039.91, 1.566	40596147	746	149.02	2500	1031	XIC(149.02±500ppm)
Terephthalic acid, di(4-methylhept-3-yl) ester	2074.91, 1.590	26983713	846	261.13	2546.7	1918	XIC(261.13±500ppm)
Terephthalic acid, di(4-octyl) ester	2124.9 s, 1.826 s	1008123281	781	112.04	2124.9	1277	XIC(112.04±500ppm)
Terephthalic acid, ethyl 2-ethylhexyl ester	1804.93 s, 1.553 s	685374957	852	70.08	1804.93	937	XIC(70.08±500ppm)
Terephthalic acid, octyl 2,3,4-trifluorophenyl ester	2074.91 s, 1.582 s	20444465	839	261.12	2074.91	1498	XIC(261.12±500ppm)
Terephthalic acid, pentyl 2-phenoxyethyl ester	1309.96, 1.156	1074582430	779	263.19	1555.6	2063	XIC(263.19±500ppm)
Terpinen-4-ol	934.981 s, 1.288 s	14855425	914	71.06	1182.6	1831	XIC(71.06±500ppm)
tert-Butyl[4-(tert-butylimino-oxo- ¹ (5)-azanylidene)-1,2,5-oxadiazol-3-yl-oxo- ¹ (5)-azanylidene]amine	1704.93, 1.010	208646027	720	57.04	2053.3	1550	XIC(57.04±500ppm)
tert-Butylpentamethylidisloxane	2334.89 s, 0.513 s	5787682	759	147.05	2334.89	844	XIC(147.05±500ppm)
Tetracosane	1554.94, 0.980	138262052	775	71.05	1853.3	772	XIC(71.05±500ppm)
Tetracosanoic acid, methyl ester	2114.91 s, 1.441 s	19383115	741	74.02	2114.91	1095	XIC(74.02±500ppm)
Tetradecane	1164.97 s, 0.934 s	491129908	915	71.07	1164.97	1578	XIC(71.07±500ppm)
Tetradecane, 1-iodo-	1014.98 s, 0.862 s	52600336	748	57.14	1014.98	576	XIC(57.14±500ppm)
Tetradecane, 4,11-dimethyl-	1314.96 s, 0.961 s	549293250	849	57.04	1314.96	1390	XIC(57.04±500ppm)
Tetradecanoic acid, 2-hydroxy-1-(hydroxymethyl)ethyl ester	1869.92, 1.653	109958414	899	43.05	2273.4	2809	XIC(43.05±500ppm)
Tetradecanoic acid, ethyl ester	1514.94 s, 1.168 s	187297210	751	88.03	1514.94	3196	XIC(88.03±500ppm)
Tetraethyl silicate	709.996 s, 0.919 s	40775776	875	149.04	709.996	755	XIC(149.04±500ppm)
Tetraethylene glycol	1864.92, 1.513	41377196	781	45.03	2266.7	908	XIC(45.03±500ppm)
Tetraethylene glycol, 2TMS derivative	1494.95 s, 1.180 s	222998426	898	117.05	1494.95	2182	XIC(117.05±500ppm)
Tetraethylene glycol, TMS derivative	1889.92, 1.653	31014549	795	73.03	1889.92	781	XIC(73.03±500ppm)
Tetrahydro[2,2']bifuranyl-5-one	1409.95, 0.955	412181526	729	71.07	1670.6	2239	XIC(71.07±500ppm)
Tetrahydrogeranyl formate	824.988 s, 0.833 s	381821266	838	43.06	824.988	2954	XIC(43.06±500ppm)
Tetrahydropyran Z-10-dodecenoate	1299.96, 0.895	353519535	777	85.08	1544.4	796	XIC(85.08±500ppm)
Tetrasiloxane, decamethyl-	784.991 s, 0.706 s	533044614	904	207.01	784.991	20101	XIC(207.01±500ppm)
Thieno[2,3-b]pyridine, 3-chloro-	1799.93, 1.994	7870134	729	169.02	2180	548	XIC(169.02±500ppm)
Thiophene, 2-ethynyl-5-[(trimethylsilyl)ethynyl]-	1199.96, 1.377	20398705	734	189.11	1436.8	1409	XIC(189.11±500ppm)
Thiophene, tetrahydro-3-phenyl-, 1-oxide	1709.93, 1.878	34025009	756	131.06	2060	949	XIC(131.06±500ppm)
Thiophene-2-carboxylic acid, 2,4,6-trichlorophenyl ester	1744.93, 1.092	113523424	735	111.1	2106.7	921	XIC(111.10±500ppm)
Thioxanthone	1749.93 s, 2.720 s	3019175	859	212	1749.93	635	XIC(212.00±500ppm)
Thymol	1249.96 s, 1.311 s	13570234	747	135.06	1249.96	775	XIC(135.06±500ppm)
Thymol, TMS derivative	1084.97 s, 1.069 s	315144013	834	73.03	1084.97	4157	XIC(73.03±500ppm)
trans-(2-Chlorovinyl)dimethylethoxysilane	664.998, 0.720	3858659	742	149.03	970.4	671	XIC(149.03±500ppm)
trans-13-Octadecenoic acid, methyl ester	1739.93, 1.293	230445543	774	55.05	2100	606	XIC(55.05±500ppm)
trans-2-Nonenyl acetate	2539.88 s, 3.066 s	20639983	731	43.02	2539.88	554	XIC(43.02±500ppm)
trans-4-Methoxy-3-buten-2-one	1664.93, 1.002	278252266	710	85.07	2000	1013	XIC(85.07±500ppm)
trans-Calamenene	1294.96 s, 1.372 s	51151028	766	159.1	1294.96	1969	XIC(159.10±500ppm)
Tri(2-chloroethyl) phosphate	1494.95 s, 2.100 s	13949264	813	62.99	1494.95	901	XIC(62.99±500ppm)
Triacetin	1114.97 s, 1.565 s	18872127	757	43.02	1114.97	685	XIC(43.02±500ppm)
Triacotane	2249.9 s, 1.438 s	128197550	872	57.06	2249.9	815	XIC(57.06±500ppm)
Tributyl acetylacrylate	1844.92, 1.582	24872796	734	43.03	2240	1009	XIC(43.03±500ppm)
Tricarbomethoxyethylene	1514.94, 1.444	19861072	731	171.11	1800	570	XIC(171.11±500ppm)
Tricyclo[9.2.2.2(4,7)]heptadeca-(1(14),2(4(17),5(7(16),11(15),12-heptaene	1624.94 s, 1.884 s	30879460	816	220.11	1624.94	1572	XIC(220.11±500ppm)
Tridecane	909.983 s, 0.823 s	77942127	829	43.06	909.983	6907	XIC(43.06±500ppm)
Tridecane, 1-iodo-	1409.95, 0.965	110685351	742	43.03	1670.6	928	XIC(43.03±500ppm)
Tridecane, 2,2,4,10,12,12-hexamethyl-7-(3,5,5-trimethylhexyl)-	764.992 s, 0.830 s	13912887	732	57.07	764.992	557	XIC(57.07±500ppm)
Tridecane, 3-methylene-	1149.97 s, 0.968 s	74240276	756	70.06	1149.97	2084	XIC(70.06±500ppm)
Tridecanoic acid	1449.95, 1.318	69880326	875	60.01	1718.8	1988	XIC(60.01±500ppm)
Tridecanoic acid, methyl ester	1369.95 s, 1.179 s	398899747	854	74.02	1369.95	2487	XIC(74.02±500ppm)
Tridecanoic acid, TMS derivative	1479.95 s, 1.032 s	83254029	837	73.02	1479.95	1660	XIC(73.02±500ppm)
Triethanolamine, 3TMS derivative	1384.95, 0.900	19693564	805	73.04	1641.2	5013	XIC(73.04±500ppm)
Triethyl phosphate	874.985 s, 1.514 s	5333145	914	98.97	874.985	949	XIC(98.97±500ppm)
Triethylene glycol monododecyl ether	1909.92, 1.590	108590065	802	45.04	2326.7	2278	XIC(45.04±500ppm)
Triethylene glycol, 2TMS derivative	1014.98 s, 1.020 s	616335516	749	73.07	1014.98	1273	XIC(73.07±500ppm)
Trifluoroacetamide, N-trimethylsilyloxymethyl	664.998, 0.909	4646820	788	170	970.4	745	XIC(170.00±500ppm)
Trifluoroacetoxy hexadecane	1784.93 s, 1.009 s	1004896135	757	69.06	1784.93	6289	XIC(69.06±500ppm)
trimethyl((2-((2S,4aS)-4a-methyl-8-methylenedecahydronaphthalen-2-yl)propan-2-yl)oxy)silane	2394.89 s, 2.052 s	25776319	740	131.07	2394.89	1249	XIC(131.07±500ppm)
Trimethyl(3,3-difluoro-2-propenyl)silane	1009.98 s, 0.963 s	469411554	760	73.03	1009.98	1622	XIC(73.03±500ppm)
Trimethylolpropane, 3TMS derivative	1174.97 s, 0.809 s	441763807	753	73.03	1174.97	7407	XIC(73.03±500ppm)
Trimethylsilyl 3,5-bis(trimethylsilyloxy)-3-methylvalerate	1169.97, 0.829	207714147	705	73.03	1405.3	3476	XIC(73.03±500ppm)
Triphenylene, 1,2,3,4-tetrahydro-	1844.92 s, 2.145 s	16265304	788	232.1	1844.92	1451	XIC(232.10±500ppm)
Tripropylene glycol monomethyl ether, TMS derivative	1869.92 s, 1.303 s	1726662843	796	73.06	1869.92	2509	XIC(73.06±500ppm)
Tripropylene glycol monopropyl ether, TMS derivative	2299.89 s, 2.150 s	78349682	739	73.03	2299.89	780	XIC(73.03±500ppm)
Tris(trimethylsilyl)carbamate	774.991 s, 0.710 s	184576687	739	73.03	774.991	8222	XIC(73.03±500ppm)
Trisiloxane, octamethyl-	814.989 s, 0.767 s	220978936	867	221.06	814.989	17761	XIC(221.06±500ppm)
Tuaminoheptane	1514.94, 1.921	1550569987	748	44.02	1800	737	XIC(44.02±500ppm)
Undecane	754.993 s, 0.809 s	157221361	893	57.06	754.993	4269	XIC(57.06±500ppm)
Undecane, 2,3-dimethyl-	2174.9, 1.813	295488409	715	57.06	2680.1	891	XIC(57.06±500ppm)
Undecane, 2,4-dimethyl-	1654.94, 0.980	656677537	754	43.05	1986.7	4357	XIC(43.05±500ppm)
Undecane, 2,5-dimethyl-	1584.94, 0.979	375233885	748	57.07	1893.3	2642	XIC(57.07±500ppm)
Undecane, 2,6-dimethyl-	739.994 s, 2.210 s	28903728	882	57.06	739.994	737	XIC(57.06±500ppm)
Undecane, 3,7-dimethyl-	909.983, 0.835	82960753	868	43.06	1160.9	5670	XIC(43.06±500ppm)
Undecane, 3,8-dimethyl-	1494.95 s, 0.933 s	681091079	747	71.07	1494.95	1100	XIC(71.07±500ppm)

Undecane, 3-methyl-	1529.94 s, 0.968 s	642959939	766	71.07	1529.94	5440	XIC(71.07±500ppm)
Undecane, 4,7-dimethyl-	844.987 s, 0.848 s	804519497	839	57.04	844.987	3091	XIC(57.04±500ppm)
Undecane, 4,8-dimethyl-	1454.95, 0.937	386175501	728	43.06	1725	3010	XIC(43.06±500ppm)
Undecane, 4-methyl-	859.986 s, 0.848 s	222887022	884	43.12	859.986	2120	XIC(43.12±500ppm)
Undecane, 5,7-dimethyl-	844.987, 1.061	384572775	790	57.07	1104.3	533	XIC(57.07±500ppm)
Undecane, 6,6-dimethyl-	1514.94, 0.966	635005596	721	57.05	1800	3774	XIC(57.05±500ppm)
Undecanenitrile	1544.94 s, 1.260 s	58619732	760	55.05	1544.94	602	XIC(55.05±500ppm)
Vinyl caprylate	1804.93, 1.086	358654060	755	57.06	2186.7	773	XIC(57.06±500ppm)
Weberine, 5-desmethoxy-	2159.9 s, 3.116 s	288569878	740	194.09	2159.9	2325	XIC(194.09±500ppm)
Yohimban-17-one	2634.87 s, 3.580 s	185684370	742	293.15	2634.87	8556	XIC(293.15±500ppm)
α-Amino-γ-butyrolactone	1069.97 s, 0.879 s	239985454	737	43.05	1069.97	2162	XIC(43.05±500ppm)
α-D-Arabinopyranose, 4TMS derivative	1469.95, 1.051	26216923	722	204.08	1743.8	781	XIC(204.08±500ppm)
α-D-Mannopyranose, 5TMS derivative	1674.93 s, 0.871 s	37430461	917	73.04	1674.93	5956	XIC(73.04±500ppm)
α-D-Xylofuranoside, methyl 5-O-methyl-	1039.97 s, 0.871 s	366849594	751	73.04	1039.97	4079	XIC(73.04±500ppm)
α-Hydroxyisobutyric acid, 2TMS derivative	879.985 s, 0.872 s	8051281	733	73.06	1134.8	586	XIC(73.06±500ppm)
α-l-Galactofuranoside, methyl 6-deoxy-2,3,5-tris-O-(trimethylsilyl)-	2009.91, 1.218	4528873	721	217.08	2460	606	XIC(217.08±500ppm)
α-Methylstilbene	1549.94, 1.870	51886541	817	179.07	1846.7	1721	XIC(179.07±500ppm)
α-Muurolene	1269.96 s, 1.246 s	34189050	879	105.09	1511.1	3383	XIC(105.09±500ppm)
α-Terpineol TMS	1094.97 s, 1.006 s	84292904	866	73.03	1094.97	1463	XIC(73.03±500ppm)
α-Tocopheryl acetate	2364.89 s, 2.939 s	13868104	891	165.07	2364.89	1218	XIC(165.07±500ppm)
β-Arabinopyranose, 4MS derivative	1574.94 s, 0.958 s	124240540	803	73.05	1880	1270	XIC(73.05±500ppm)
β-D-(+)-Talopyranose, 5TMS derivative	1609.94 s, 0.879 s	41135738	843	73.04	1609.94	2246	XIC(73.04±500ppm)
β-D-Glucopyranose, 5TMS derivative	1674.93 s, 0.869 s	225981505	942	73.05	2013.3	53586	XIC(73.05±500ppm)
β-Eudesmol, TMS derivative	1679.93, 0.928	87235257	740	131.07	2020	2264	XIC(131.07±500ppm)
β-Lyxopyranose, 4TMS derivative	1934.92 s, 0.978 s	14378265	762	73.05	2360	519	XIC(73.05±500ppm)
β-Phenylpropiofenone	1569.94 s, 2.062 s	46830369	823	105.01	1569.94	827	XIC(105.01±500ppm)
β-Pimaric acid	1949.92, 2.216	4150924	790	105.05	2380	836	XIC(105.05±500ppm)
β-Sitosterol, TMS derivative	2484.88 s, 3.175 s	9759749	754	129.05	2484.88	546	XIC(129.05±500ppm)
γ-Dodecalactone	1879.92 s, 1.670 s	349998024	746	43.05	1879.92	4327	XIC(43.05±500ppm)
γ-Tetradecalactone	1589.94 s, 1.619 s	15029886	749	85.01	1589.94	664	XIC(85.01±500ppm)

RUBIA	R.T. (s)	Area	Similarity	Retention Index	Base Mass	Peak S/N	Quant Masses
(2,3-Dimethylbutan-2-yloxy)trimethylsilane	924.982 s, 1.500 s	1729408	747	1173.9	131.02	633	XIC(131.02±500ppm)
(2,4,6-Tri-tert-butylphenyl)(difluoro)methylsilane	1974.91 s, 2.171 s	15630093	777	2413.4	255.05	1626	XIC(255.05±500ppm)
(2,5-Dimethoxyphenyl)acetone	1329.96 s, 1.916 s	8789825	899	1577.8	151.08	1925	XIC(151.08±500ppm)
(2S,3R)-3-[(4E,7E)-Nona-4,7-dienyl]-N,N-bis(trimethylsilyl)oxirane-2-carboxamide	1234.96 s, 2.240 s	15736239	707	1473.7	73.05	1267	XIC(73.05±500ppm)
(3-Hydroxy-4-methoxyphenyl)ethylene glycol tris(trimethylsilyl) ether	1699.93 s, 1.446 s	85202023	775	2046.7	73.05	832	XIC(73.05±500ppm)
(4-Methoxy-2,5-dimethyl-phenoxy)-trimethyl-silane	1334.96 s, 1.476 s	1295299	700	1583.3	73.05	649	XIC(73.05±500ppm)
(9H-fluoren-9-yl)methanol, O-methoxycarbonyl-	1614.94 s, 2.008 s	39017761	739	1933.3	178.08	3696	XIC(178.08±500ppm)
(2)-5-Methoxy-3,5-dimethyl-2-hexenyltrimethylsilane	2569.88 s, 0.499 s	236562857	830	3206.8	73.05	2501	XIC(73.05±500ppm)
[1,1'-Biphenyl]-2-ol, 5-(1,1-dimethylethyl)-	1849.92 s, 1.618 s	16732975	728	2246.7	211.08	755	XIC(211.08±500ppm)
1-(1-Hydroxybutyl)-2,5-dimethoxybenzene	1464.95 s, 1.898 s	67516523	712	1737.5	167.07	1815	XIC(167.07±500ppm)
1-(2,5-Dimethoxyphenyl)-1-[[trimethylsilyloxy]propan-2-amine	1454.95 s, 1.418 s	206739326	899	1725	44.06	2907	XIC(44.06±500ppm)
1-(2-Methoxyethoxy)-2-methyl-2-propanol, methyl ether	2449.88 s, 0.500 s	208789022	753	3046.7	73.05	1456	XIC(73.05±500ppm)
1-(5-Bicyclo[2.2.1]heptyl)ethylamine	744.993 s, 0.422 s	19495261	709	1029.6	44	776	XIC(44.00±500ppm)
1-(t-Butyldimethylsilyl)-4-(2,2-dimethyl-6-methylene-cyclohexyl)-butan-1-ol	1944.92 s, 1.223 s	16735490	710	2373.4	73.05	629	XIC(73.05±500ppm)
1,2,3,4-Tetrahydro-1-naphthylamine, N-tert-butylidimethylsilyl-	1899.92 s, 0.897 s	3875473	712	2313.4	204.11	552	XIC(204.11±500ppm)
1,2,3,4-Tetrahydroisoquinoline, 7-hydroxy-6-methoxy-1-(5-hydroxy-4-methoxy-2-methylbenzyl)-	2124.9 s, 0.487 s	8025605	728	2613.4	178.11	615	XIC(178.11±500ppm)
1,2,3-Butanetriol, 3TMS derivative	1074.97 s, 0.791 s	45445355	929	1310	73.05	3814	XIC(73.05±500ppm)
1,2-Benzenedicarboxylic acid, bis(2-methylpropyl) ester	1569.94 s, 1.688 s	31198704	762	1873.3	149.03	2605	XIC(149.03±500ppm)
1,2-Benzenediol, o-(4-methoxybenzoyl)-o'-(2,2,3,3,4,4,4-heptafluorobutyl)-	2754.86 s, 0.677 s	12066721	817	3453.4	135.07	502	XIC(135.07±500ppm)
1,2-Diphenyltetramethylsilane	2544.88 s, 0.672 s	25175526	712	3173.4	135.07	594	XIC(135.07±500ppm)
1,2-Ethenediol, 2TMS derivative	679.997 s, 0.875 s	20879878	906	981.5	73.05	2230	XIC(73.05±500ppm)
1,3-Benzenediol, o-(2-methoxybenzoyl)-o'-ethoxycarbonyl-	3124.84 s, 0.672 s	10936664	711	3946.8	135.07	532	XIC(135.07±500ppm)
1,3-Benzenediol, O-methoxycarbonyl-O'-(2-trifluoromethylbenzoyl)-	1944.92 s, 1.244 s	2542495	738	2373.4	173.14	774	XIC(173.14±500ppm)
1,3-Butanediol, 2TMS derivative	824.988 s, 0.826 s	5527196	716	1088.9	73.05	780	XIC(73.05±500ppm)
1,3-Dihydroxyacetone dimer, 4TMS derivative	1494.95 s, 0.904 s	39037788	731	1775	73.05	2661	XIC(73.05±500ppm)
1,3-di-iso-propylnaphthalene	1424.95 s, 1.516 s	1779984	728	1688.2	197.14	622	XIC(197.14±500ppm)
1,3-Dioxane, 2,2-dimethyl-5-trimethylsilyloxy-	1039.97 s, 1.286 s	2571596	746	1277.3	101.04	576	XIC(101.04±500ppm)
1,3-Dioxolane, 2,2-dimethyl-	669.998 s, 1.845 s	10069628	730	974.1	43.03	629	XIC(43.03±500ppm)
1,3-Dioxolane, 2-heptyl-	2984.85 s, 0.496 s	62695817	729	3760.1	73.02	637	XIC(73.02±500ppm)
1,3-Dioxolane-2-methanol	2909.85 s, 0.496 s	111742741	809	3660.1	73.05	1059	XIC(73.05±500ppm)
1,3-Propanediol, ethyl octadecyl ether	2299.89 s, 1.394 s	26455318	726	2846.7	57.08	1533	XIC(57.08±500ppm)
1,3-Propanediol, TMS derivative	774.991 s, 1.123 s	14920766	790	1051.9	75.03	692	XIC(75.03±500ppm)
1,4-Benzenedicarboxylic acid, bis(2-ethylhexyl) ester	2124.9 s, 1.689 s	24108766	911	2613.4	70.08	2038	XIC(70.08±500ppm)
1,5-Anhydroglucitol, 4TMS derivative	2324.89 s, 0.912 s	1.088E+10	755	2880.1	73.05	2733	XIC(73.05±500ppm)
1,6-Dioxacyclododecane-7,12-dione	1309.96 s, 2.076 s	3741987446	932	1555.6	55.05	6548	XIC(55.05±500ppm)
11H-Benzo[b]fluorene	1839.92 s, 2.610 s	908705	731	2233.4	216.1	726	XIC(216.10±500ppm)
13-Docosenamide, (Z)-	2144.9 s, 2.012 s	22647424	890	2640.1	59.04	976	XIC(59.04±500ppm)
18-Methyl-nonadecanol, trimethylsilyl ether	1899.92 s, 1.077 s	9645058	794	2313.4	75.03	547	XIC(75.03±500ppm)
19-Norandrosterone, 2TMS derivative	1939.92 s, 1.183 s	42488042	702	2366.7	73.05	546	XIC(73.05±500ppm)
1-Aminocyclopentanecarboxylic acid, 3-chloropropoxycarbonyl-, tridecyl ester	1889.92 s, 0.904 s	7635312	729	2300	204.11	919	XIC(204.11±500ppm)
1-Decene, 2,4-dimethyl-	809.989 s, 0.868 s	38832599	820	1077.8	43.07	1469	XIC(43.07±500ppm)
1-Deoxyepititol, 4TMS derivative	1314.96 s, 0.817 s	24182190	829	1561.1	73.05	1891	XIC(73.05±500ppm)
1-Docosene	1794.93 s, 1.104 s	3741314	865	2173.4	43.07	708	XIC(43.07±500ppm)
1-Hexadecanol, TMS derivative	1634.94 s, 1.010 s	22058514	852	1960	75.03	4146	XIC(75.03±500ppm)
1-Hexanol, 2-ethyl-	1484.95 s, 0.968 s	102524697	731	1762.5	57.08	4875	XIC(57.08±500ppm)
1-Hexanol, TMS derivative	694.996 s, 0.831 s	17108833	864	992.6	75.02	2804	XIC(75.02±500ppm)
1-Hydroxy-3-methylanthraquinone	1819.92 s, 2.552 s	18816344	868	2206.7	238.07	2276	XIC(238.07±500ppm)
1-Hydroxy-3-methylanthraquinone tms	1929.92 s, 2.194 s	22240089	859	2353.4	295.09	5042	XIC(295.09±500ppm)
1-Methyladenosine, tris(trimethylsilyl) ether	2054.91 s, 1.715 s	17917842	727	2520	73.05	736	XIC(73.05±500ppm)
1-Monoacetin, 2O-TMS	1089.97 s, 0.972 s	15615406	930	1325	175.08	1516	XIC(175.08±500ppm)
1-Monomyrstin, 2TMS derivative	1929.92 s, 1.118 s	14189721	854	2353.4	73.05	1149	XIC(73.05±500ppm)
1-Monopalmitin, 2TMS derivative	2039.91 s, 1.174 s	203651749	886	2500	73.05	1497	XIC(73.05±500ppm)
1-Nonene, 4,6,8-trimethyl-	1074.97 s, 0.899 s	33452158	842	1310	43.07	2573	XIC(43.07±500ppm)
1-Octadecanol, TMS derivative	1774.93 s, 1.037 s	48599377	897	2146.7	75.03	1704	XIC(75.03±500ppm)
1-Octanamine, N-methyl-	894.984 s, 0.378 s	12889241	721	1147.8	44	576	XIC(44.00±500ppm)
1-Pentyne, 3-methyl-3-(1-methylethoxy)-	1114.97 s, 0.906 s	9292888	700	1350	69.07	880	XIC(69.07±500ppm)
1-Tetradecene	1159.97 s, 0.960 s	13763578	953	1395	43.07	740	XIC(43.07±500ppm)
2-(2,5-Dimethoxy-phenyl)-propionaldehyde	1309.96 s, 1.815 s	9212065	836	1555.6	165.1	1994	XIC(165.10±500ppm)
2(3H)-Furanone, 5-dodecyldihydro-	1739.93 s, 1.643 s	11670452	927	2100	85.03	1789	XIC(85.03±500ppm)
2(3H)-Furanone, dihydro-5-tetraedcyl-	1879.92 s, 1.675 s	10109375	901	2286.7	85.03	1554	XIC(85.03±500ppm)
2,2'-Bipyridine	1214.96 s, 2.031 s	9582268	923	1452.6	156.07	1190	XIC(156.07±500ppm)
2,3,4,5-Tetrahydroxypentanoic acid, 1,4-lactone, tris(trimethylsilyl)-	1394.95 s, 1.039 s	101266202	922	1652.9	73.05	1744	XIC(73.05±500ppm)
2,3,4-Trihydroxybutyric acid tetrakis(trimethylsilyl) deriv., (R*,R*)	1334.96 s, 0.876 s	60827068	945	1583.3	73.05	1473	XIC(73.05±500ppm)
2,3-Butanediol, 2TMS derivative	759.992 s, 0.797 s	72758473	925	1040.7	117.07	6266	XIC(117.07±500ppm)
2,3'-Dipyridyl	1314.96 s, 2.127 s	2608692	748	1561.1	156.07	591	XIC(156.07±500ppm)
2,4-Dihydroxybenzaldehyde, 2TMS derivative	1629.94 s, 0.929 s	2870818	745	1953.3	267.13	584	XIC(267.13±500ppm)
2,4-Dimethyl-6-phenylpyridine	1389.95 s, 0.944 s	1523665	715	1647.1	183.22	508	XIC(183.22±500ppm)
2,4-Di-tert-butylphenol	1274.96 s, 1.369 s	7602417	893	1516.7	191.15	1990	XIC(191.15±500ppm)
2,4-Di-tert-butylphenoxytrimethylsilane	1309.96 s, 1.059 s	23010557	806	1555.6	73.05	902	XIC(73.05±500ppm)
2,5-Cyclohexadiene-1,4-dione, 2,6-bis(1,1-dimethylethyl)-	1239.96 s, 1.317 s	7871100	916	1478.9	41.06	5054	XIC(41.06±500ppm)
2,5-Dihydroxybenzaldehyde, 2TMS derivative	854.986 s, 0.802 s	4024583	729	1113	267	727	XIC(267.00±500ppm)
2,5-Dimethoxybenzhydrazide	1384.95 s, 1.996 s	39118182	818	1641.2	165.06	4265	XIC(165.06±500ppm)
2,5-Dimethoxymandelic acid, di-TMS	1999.91 s, 2.299 s	9346439	750	2446.7	239.12	1236	XIC(239.12±500ppm)
2,5-Dimethoxyphenol, TMS	1209.96 s, 1.383 s	3182372	757	1447.4	196.06	1353	XIC(196.06±500ppm)
2,5-Hexanediol, 2TMS derivative	974.979 s, 0.826 s	19354135	826	1218.2	117.07	2493	XIC(117.07±500ppm)
2,6-Diisopropylnaphthalene	1459.95 s, 1.536 s	10975797	782	1731.3	197.14	664	XIC(197.14±500ppm)
2-Allyl-1,4-dimethoxybenzene	1204.96 s, 1.653 s	9160701	900	1442.1	178.1	1977	XIC(178.10±500ppm)
2-Amino-7,10-dimethylidene[b,f][1,4]oxazepin-11(10H)-one, TMS derivative	2024.91 s, 2.209 s	8521733	743	2480	311.08	2381	XIC(311.08±500ppm)
2-Aminobenzophenone, N-trimethylsilyl-	1299.96 s, 1.143 s	10238382	742	1544.4	73.05	1123	XIC(73.05±500ppm)
2-Amino-oxazole	1384.95 s, 0.951 s	11858573	709	1641.2	56.07	1228	XIC(56.07±500ppm)
2-Aminopyridine, N-trifluoroacetyl-	769.992 s, 1.253 s	3675312	905	1048.1	78.03	1123	XIC(78.03±500ppm)
2-Butanamine, N,N-dimethyl-	994.977 s, 2.626 s	55047300	706	1236.4	72.05	1097	XIC(72.05±500ppm)
2-Butene, 1-butoxy-3-methyl-	854.986 s, 1.228 s	39098587	709	1113	71.09	519	XIC(71.09±500ppm)
2-Butenedioic acid, (E)-, 2TMS derivative	1119.97 s, 0.976 s	3147992	850	1355	73.05	855	XIC(73.05±500ppm)
2-Ethylhexanal ethylene glycol acetal	2704.87 s, 0.496 s	103728065	854	3386.8	73.04	641	XIC(73.04±500ppm)
2H,8H-Benzo[1,2-b:5,4-b']dipyran-2-one, 5-methoxy-8,8-dimethyl-10-(3-methyl-2-butenyl)-	1919.92 s, 2.326 s	999396	744	2340	311.08	795	XIC(311.08±500ppm)
2-Hexadecanone	1869.92 s, 1.308 s	2162299	828	2273.4	58.05	554	XIC(58.05±500ppm)
2-Hexanamine, 4-methyl-	909.983 s, 0.388 s	10901755	714	1160.9	44	568	XIC(44.00±500ppm)
2-Hexenedioic acid, 2-[[trimethylsilyloxy]-, bis(trimethylsilyl) ester	1439.95 s, 1.045 s	68696738	730	1706.2	73.05	3618	XIC(73.05±500ppm)

2H-Pyran-2-one, tetrahydro-6-undecyl-	1764.93 s, 1.713 s	3209321	889	2133.3	99.05	906	XiC(99.05±500ppm)
2-Hydroxy-4-methylanthraquinone, O-trimethylsilyl	1999.91 s, 2.194 s	2606742	725	2446.7	295.09	1029	XiC(295.09±500ppm)
2'-Hydroxy-5'-methoxyacetophenone, TBDMS derivative	1689.93 s, 1.938 s	1703340	730	2033.3	223.08	671	XiC(223.08±500ppm)
2-Hydroxy-5-methoxybenzaldehyde, TMS derivative	1319.96 s, 1.474 s	6033266	800	1566.7	209.07	1856	XiC(209.07±500ppm)
2-Ketohexanoic acid, trimethylsilyl ester	1119.97 s, 1.465 s	19611538	756	1355	73.05	1133	XiC(73.05±500ppm)
2-Mercapto-4,6-dimethylnicotinonitrile, TBDMS derivative	1099.97 s, 0.812 s	1316401	721	1335	221.09	656	XiC(221.09±500ppm)
2-Methoxybenzoic acid, 2,4,6-trichlorophenyl ester	2389.89 s, 0.672 s	12458592	735	2966.7	135.07	530	XiC(135.07±500ppm)
2-Methoxybenzoic acid, 4-isopropylphenyl ester	2734.87 s, 0.671 s	11814974	803	3426.8	135.07	525	XiC(135.07±500ppm)
2-Methyl-1,3-butanediol, 2TMS derivative	999.977 s, 0.971 s	6850260	748	1240.9	73.05	549	XiC(73.05±500ppm)
2-Nonadecanone	1994.91 s, 1.360 s	14865017	883	2440	43.05	2313	XiC(43.05±500ppm)
2-Palmitoylglycerol, 2TMS derivative	2024.91 s, 1.155 s	25671936	883	2480	73.05	2164	XiC(73.05±500ppm)
2-Propenoic acid, 2-methyl-, 3,3,5-trimethylcyclohexyl ester	1119.97 s, 1.183 s	425234789	913	1355	69.05	2943	XiC(69.05±500ppm)
2-Pyrrolidinone, TMS derivative	894.984 s, 1.425 s	34530252	936	1147.8	142.07	2197	XiC(142.07±500ppm)
2-Trimethylsilyloxyheptanoic acid, trimethylsilyl ester	1139.97 s, 0.918 s	3930612	744	1375	73.05	647	XiC(73.05±500ppm)
2-Undecene, 5-methyl-	864.986 s, 0.876 s	4124504	807	1121.7	57.08	626	XiC(57.08±500ppm)
3-(Benzyloxy)-1,2,4-butanetriol, 3TMS derivative	1354.95 s, 1.268 s	16577851	700	1605.9	91.06	835	XiC(91.06±500ppm)
3-(Methylthio)benzoic acid, TMS derivative	1394.95 s, 1.547 s	2149936	751	1652.9	225.06	1052	XiC(225.06±500ppm)
3,4-Dihydrocoumarin, 4,4-dimethyl-6-dimethylamino-	1479.95 s, 2.003 s	2884110	713	1756.3	219.1	695	XiC(219.10±500ppm)
3,4-Dimethoxymandelic acid, di-TMS	2054.91 s, 1.465 s	12048534	746	2520	73.05	728	XiC(73.05±500ppm)
3,5-(2H)-Dihydroindazol-5-one, 2-acetyl-3-methyl-3-phenyl-	1834.92 s, 1.925 s	6523446	716	2226.7	224.09	1150	XiC(224.09±500ppm)
3H-Indole, 3,3-dimethyl-2-[[4-dimethylaminophenyl]ethenyl]-	1694.93 s, 1.073 s	4143930	730	2040	289.17	1339	XiC(289.17±500ppm)
3-Hydroxybutyric acid, 2TMS derivative	919.982 s, 0.897 s	49476067	887	1169.6	73.05	2883	XiC(73.05±500ppm)
3-Methylpentan-2-ol, O-trimethylsilyl ether	979.978 s, 1.477 s	33081722	755	1222.7	117.04	3618	XiC(117.04±500ppm)
3-Pyridinol	884.984 s, 1.520 s	8340273	926	1139.1	95.04	716	XiC(95.04±500ppm)
3-Pyridinol, TMS derivative	884.984 s, 1.253 s	95223286	932	1139.1	152.05	6755	XiC(152.05±500ppm)
4-(2-Amino-1-hydroxyethyl)-2-methoxyphenol, di-TMS	2189.9 s, 1.497 s	4758788	728	2700.1	297.07	554	XiC(297.07±500ppm)
4-(Trimethylsilyloxy)-3-penten-2-one	874.985 s, 1.375 s	25217132	721	1130.4	73.05	1073	XiC(73.05±500ppm)
4,4'-[Hexafluoroisopropylidene]diphenol	1699.93 s, 1.995 s	9865834	840	2046.7	267.07	2159	XiC(267.07±500ppm)
4-Hydroxybenzaldehyde, TMS derivative	1144.97 s, 1.395 s	1382092	855	1380	179.05	670	XiC(179.05±500ppm)
4-Methyl-1-hexanol, 5-(t-butylidimethylsilyloxy)-	749.993 s, 0.962 s	13647175	734	1033.3	73.05	1729	XiC(73.05±500ppm)
4-Methylvaleric acid, TMS derivative	834.988 s, 1.060 s	132355181	775	1096.3	75.03	3245	XiC(75.03±500ppm)
4-Oxopentanoic acid	684.997 s, 1.541 s	32222590	738	985.2	43.03	931	XiC(43.03±500ppm)
4-tert-Amylphenol, TMS derivative	2964.85 s, 0.526 s	43205741	700	3733.5	207.04	711	XiC(207.04±500ppm)
4-Trimethylsilylphenol	779.991 s, 1.073 s	3433979	844	1055.6	151.06	1179	XiC(151.06±500ppm)
5-(Methylthio)salicylic acid, 2TMS derivative	2039.91 s, 2.340 s	44989050	710	2500	313.06	2910	XiC(313.06±500ppm)
5,6-Dimethyl-4-phenyl-3-cyanopyridine-2(1H)-thione	1449.95 s, 1.375 s	97763023	777	1718.8	239.1	713	XiC(239.10±500ppm)
5,7-Bis(trimethylsilyloxy)-3-[[4-[(trimethylsilyloxy)phenyl]-4H-chromen-4-one	2169.9 s, 1.874 s	21873986	703	2673.4	73.05	1314	XiC(73.05±500ppm)
5-Hydroxy-2-methylpyridine, TMS derivative	944.98 s, 1.208 s	10943504	854	1191.3	166.07	1657	XiC(166.07±500ppm)
5-Hydroxyisophthalic acid, TBDMS derivative	1509.94 s, 1.265 s	23425399	716	1793.8	239.12	1646	XiC(239.12±500ppm)
5-Methyluridine, 3TMS derivative	2084.91 s, 1.174 s	46368574	757	2560	73.05	595	XiC(73.05±500ppm)
7,9-Di-tert-butyl-1-oxaspiro[4,5]deca-6,9-diene-2,8-dione	1614.94 s, 1.668 s	16676323	931	1933.3	57.08	2059	XiC(57.08±500ppm)
8-Amino-6-quinolinol, 2TMS derivative	2139.9 s, 0.979 s	7061613	786	2633.4	289.14	1366	XiC(289.14±500ppm)
9,10-Anthracenedione, 1,2,4-trihydroxy-	2009.91 s, 2.377 s	1132213	801	2460	256.04	638	XiC(256.04±500ppm)
9,10-Anthracenedione, 2-methyl-	1754.93 s, 2.574 s	5012296	901	2120	165.08	478	XiC(165.08±500ppm)
9,10-Anthracenedione, 2-methyl-1,6-bis(trimethylsilyloxy)-	2129.9 s, 2.023 s	6050618	712	2620	73.04	2485	XiC(73.04±500ppm)
9,12-Octadecadienoic acid (Z,Z)-	1754.93 s, 1.422 s	26144508	933	2120	67.06	1331	XiC(67.06±500ppm)
9,12-Octadecadienoic acid (Z,Z)-, TMS derivative	1809.93 s, 1.237 s	238608260	931	2193.4	75.03	3253	XiC(75.03±500ppm)
Acetin, bis-1,3-trimethylsilyl ether	939.981 s, 0.915 s	17801816	811	1187	73.05	1069	XiC(73.05±500ppm)
Acetoin, TMS derivative	1084.97 s, 1.443 s	12363986	729	1320	73.05	997	XiC(73.05±500ppm)
Adonitol, 5TMS derivative	1639.94 s, 0.804 s	301617078	845	1966.7	73.05	7281	XiC(73.05±500ppm)
Alizarin	1849.92 s, 2.809 s	80410228	893	2246.7	240.05	3609	XiC(240.05±500ppm)
Allonic acid, γ-lactone, 4TMS derivativative	2094.91 s, 0.941 s	710221756	733	2573.4	73.04	10361	XiC(73.04±500ppm)
Anthracene	1514.94 s, 2.239 s	4471596	939	1800	178.08	594	XiC(178.08±500ppm)
Arabinofuranose, 1,2,3,5-tetrakis-O-(trimethylsilyl)-	1509.94 s, 0.927 s	237012062	808	1793.8	73.05	7342	XiC(73.05±500ppm)
Arachidic acid, TMS derivative	1949.92 s, 1.187 s	23881797	915	2380	73.05	1959	XiC(73.05±500ppm)
Azelaic acid, 2TMS derivative	1519.94 s, 1.129 s	10014856	824	1806.7	73.05	667	XiC(73.05±500ppm)
Behenic acid, TMS derivative	2064.91 s, 1.260 s	30436427	790	2533.4	117.04	776	XiC(117.04±500ppm)
Benzaldehyde, 2,5-dimethoxy-	1229.96 s, 1.921 s	195172127	930	1468.4	166.06	672	XiC(166.06±500ppm)
Benzaldehyde, 2-hydroxy-5-methoxy-	1064.97 s, 1.788 s	5650112	936	1300	152.05	1521	XiC(152.05±500ppm)
Benzene, (1-butylheptyl)-	1379.95 s, 1.197 s	63118673	855	1635.3	91.06	929	XiC(91.06±500ppm)
Benzene, (1-butylonyl)-	1539.94 s, 1.208 s	31100224	882	1833.3	91.06	1363	XiC(91.06±500ppm)
Benzene, (1-ethylundecyl)-	1569.94 s, 1.242 s	20298798	854	1873.3	91.06	1605	XiC(91.06±500ppm)
Benzene, (1-methylododecyl)-	1599.94 s, 1.265 s	97243508	895	1913.3	105.07	8083	XiC(105.07±500ppm)
Benzene, (1-methyltridecyl)-	1674.93 s, 1.279 s	8463789	808	2013.3	105.07	703	XiC(105.07±500ppm)
Benzene, (1-methylundecyl)-	1519.94 s, 1.255 s	18108180	754	1806.7	105.07	1015	XiC(105.07±500ppm)
Benzene, (1-pentyldecyl)-	1614.94 s, 1.213 s	39931813	809	1933.3	91.06	2006	XiC(91.06±500ppm)
Benzene, (1-propyldecyl)-	1549.94 s, 1.227 s	20370064	850	1846.7	91.06	1096	XiC(91.06±500ppm)
Benzene, (1-propyldecyl)-	1629.94 s, 1.230 s	6009681	729	1953.3	91.06	766	XiC(91.06±500ppm)
Benzene, 1,1'-(1,2-cyclobutanediyl)bis-, cis-	1394.95 s, 2.153 s	2598052	807	1652.9	104.06	598	XiC(104.06±500ppm)
Benzene, 1,1'-(1,2-cyclobutanediyl)bis-, trans-	1434.95 s, 1.918 s	25724049	893	1700	104.07	1002	XiC(104.07±500ppm)
Benzene, 1,3-bis(1,1-dimethylethyl)-	1019.98 s, 1.118 s	1673294	836	1259.1	175.15	792	XiC(175.15±500ppm)
Benzene, 1,4-dimethoxy-	919.982 s, 1.622 s	3859145	797	1169.6	123.05	1444	XiC(123.05±500ppm)
Benzeneopropanoic acid, 3,5-bis(1,1-dimethylethyl)-4-hydroxy-, methyl ester	1629.94 s, 1.568 s	4991149	820	1953.3	277.19	1753	XiC(277.19±500ppm)
Benzeneopropanoic acid, 3,5-bis(1,1-dimethylethyl)-4-hydroxy-, octadecyl ester	2729.87 s, 0.975 s	61749485	858	3420.1	57.08	1109	XiC(57.08±500ppm)
Benzenesulfonamide, N-butyl-	1509.94 s, 2.232 s	3876572	913	1793.8	77.04	563	XiC(77.04±500ppm)
benzo[g]quinolin-4-ol, 3-amino-	1754.93 s, 2.255 s	2251349	713	2120	210.04	726	XiC(210.04±500ppm)
benzoic acid, 4-ethenyl-, 4-[[methylsulfonyl]amino]methyl]phenyl ester	1634.94 s, 0.938 s	7745701	744	1960	131.08	914	XiC(131.08±500ppm)
Benzoic acid, 4-methoxy-, phenyl ester	3149.84 s, 0.707 s	24463849	718	3980.1	135.07	620	XiC(135.07±500ppm)
Benzoic Acid, TMS derivative	1009.98 s, 1.253 s	26145084	928	1250	179.05	3814	XiC(179.05±500ppm)
Benzyl alcohol, TMS derivative	904.983 s, 1.144 s	10792100	867	1156.5	91.05	1276	XiC(91.05±500ppm)
Biphenyl, 4,4'-bis(trimethylsilyl)-	1684.93 s, 1.597 s	3061346	741	2026.7	283.13	1243	XiC(283.13±500ppm)
Bisphenol A, 2TMS derivative	2019.91 s, 1.809 s	3496235	739	2473.4	73.05	540	XiC(73.05±500ppm)
Bisphenol AF, bis(trimethylsilyl) ether	1684.93 s, 1.059 s	58670379	823	2026.7	73.05	444	XiC(73.05±500ppm)
Bisphenol C, bis(trimethylsilyl) ether	2114.91 s, 2.095 s	8989700	736	2600	73.05	752	XiC(73.05±500ppm)
Butanedioic acid, 2TMS derivative	1084.97 s, 1.057 s	84273580	941	1320	147.06	7948	XiC(147.06±500ppm)
Butanoic acid, 2,4-bis(trimethylsilyloxy)-, trimethylsilyl ester	1189.96 s, 0.906 s	9632360	881	1426.3	103.06	2021	XiC(103.06±500ppm)
Butanoic acid, 3,4-bis(trimethylsilyloxy)-, trimethylsilyl ester	1209.96 s, 0.897 s	48776016	920	1447.4	73.05	1603	XiC(73.05±500ppm)
Chrysen	1984.91 s, 3.084 s	2123122	849	2426.7	228.1	592	XiC(228.10±500ppm)
Chrysin, 2TMS derivative	2079.91 s, 1.946 s	13995076	777	2553.4	73.05	1899	XiC(73.05±500ppm)
cyclobutanecarboxylic acid, trimethylsilyl ester	944.98 s, 1.549 s	2558602	747	1191.3	157.03	1102	XiC(157.03±500ppm)

Cycloleicosane	1659.93 s, 1.063 s	8700811	926	1993.3	57.08	532	XiC(57.08±500ppm)
Cycloheptasiloxane, tetradecamethyl-	1259.96 s, 0.745 s	31791133	895	1500	73.05	3652	XiC(73.05±500ppm)
Cyclohexane, 1-ethyl-2-propyl-	1089.97 s, 0.904 s	20409505	755	1325	69.07	2365	XiC(69.07±500ppm)
Cyclohexasiloxane, dodecamethyl-	2034.91 s, 0.509 s	419993082	896	2493.4	73.05	1106	XiC(73.05±500ppm)
Cyclopentasiloxane, decamethyl-	904.983 s, 0.723 s	99201431	900	1156.5	73.05	13161	XiC(73.05±500ppm)
Cyclotetrasiloxane, octamethyl-	704.996 s, 0.731 s	50110893	912	1000	281.05	10890	XiC(281.05±500ppm)
Cyclotrisiloxane, 2,4-dimethyl-2,4,6,6-tetrahenyl-	2144.9 s, 2.471 s	40978569	859	2640.1	377.06	1005	XiC(377.06±500ppm)
Cyclotrisiloxane, hexamethyl-	679.997 s, 0.807 s	13224856	781	981.5	207.03	2381	XiC(207.03±500ppm)
D-(-)-Fructofuranose, pentakis(trimethylsilyl) ether (isomer 1)	1549.94 s, 0.838 s	1181538936	938	1846.7	73.05	2604	XiC(73.05±500ppm)
D-(-)-Fructofuranose, pentakis(trimethylsilyl) ether (isomer 2)	2004.91 s, 0.925 s	23868234	726	2453.4	73.05	1495	XiC(73.05±500ppm)
D-(-)-Ribofuranose, tetrakis(trimethylsilyl) ether (isomer 1)	1654.94 s, 1.024 s	45162160	820	1986.7	73.05	2744	XiC(73.05±500ppm)
D-(-)-Ribofuranose, tetrakis(trimethylsilyl) ether (isomer 2)	2269.9 s, 0.587 s	129495268	813	2806.7	73.05	1220	XiC(73.05±500ppm)
D-(-)-Tagatofuranose, pentakis(trimethylsilyl) ether (isomer 2)	2419.89 s, 0.582 s	79346911	792	3006.7	73.05	803	XiC(73.05±500ppm)
D-(+)-Galactopyranose, 5TMS derivative (isomer 2)	1609.94 s, 0.897 s	167687403	733	1926.7	204.1	1095	XiC(204.10±500ppm)
D-(+)-Glucosamine, 4TMS derivative	1594.94 s, 0.950 s	17288900	754	1906.7	131.08	1711	XiC(131.08±500ppm)
D-(+)-Talofuranose, pentakis(trimethylsilyl) ether (isomer 1)	1969.91 s, 0.894 s	4432332	790	2406.7	73.05	629	XiC(73.05±500ppm)
D-Allofuranose, pentakis(trimethylsilyl) ether	1664.93 s, 0.875 s	122658550	816	2000	73.05	4414	XiC(73.05±500ppm)
Danthron, 2TMS derivative	2039.91 s, 2.038 s	23422622	856	2500	73.05	1941	XiC(73.05±500ppm)
Decane, 2,4,6-trimethyl-	829.988 s, 0.846 s	33545645	869	1092.6	43.07	1461	XiC(43.07±500ppm)
Decane, 3,7-dimethyl-	744.993 s, 0.822 s	13488692	899	1029.6	57.08	2017	XiC(57.08±500ppm)
Decanoic acid, TMS derivative	1224.96 s, 1.014 s	38609216	887	1463.2	73.05	1594	XiC(73.05±500ppm)
Decyl oleate	2224.9 s, 1.653 s	16398237	882	2746.7	43.07	1162	XiC(43.07±500ppm)
Dextroamphetamine	774.991 s, 0.380 s	28375302	747	1051.9	44	696	XiC(44.00±500ppm)
Diamide	1489.95 s, 1.342 s	15279173	819	1768.8	72.08	2101	XiC(72.08±500ppm)
Dibutyl phthalate	1644.94 s, 1.746 s	16791930	932	1973.3	149.03	1864	XiC(149.03±500ppm)
Dibutyldodecylamine	1639.94 s, 1.048 s	3223326	718	1966.7	142.16	551	XiC(142.16±500ppm)
Diethylene glycol, 2TMS derivative	1014.98 s, 0.947 s	26147911	902	1254.5	73.05	848	XiC(73.05±500ppm)
Diethylene glycol, n-butyl ether, trimethylsilyl ether	1109.97 s, 1.074 s	14071456	899	1345	73.05	678	XiC(73.05±500ppm)
Dimethyl hexopyranosiduronate, α-D-, 3TMS derivative	2644.87 s, 1.832 s	23395937	732	3306.8	73.05	631	XiC(73.05±500ppm)
Dimethyl phthalate	994.977 s, 4.890 s	4063322	900	1236.4	163.04	835	XiC(163.04±500ppm)
Disiloxane, hexamethyl-	2224.9 s, 0.516 s	19256431	702	2746.7	147.07	603	XiC(147.07±500ppm)
Docosane	1559.94 s, 0.992 s	24165482	867	1860	57.08	1263	XiC(57.08±500ppm)
Dodecane, 1-iodo-	1069.97 s, 0.865 s	39536648	826	1305	57.08	3241	XiC(57.08±500ppm)
Dodecane, 2,6,11-trimethyl-	1094.97 s, 0.881 s	241131357	909	1330	57.08	8194	XiC(57.08±500ppm)
Dodecane, 2,7,10-trimethyl-	1044.97 s, 0.860 s	78767849	878	1281.8	57.08	832	XiC(57.08±500ppm)
D-Psicofuranose, pentakis(trimethylsilyl) ether (isomer 1)	2104.91 s, 0.962 s	107088123	753	2586.7	73.05	667	XiC(73.05±500ppm)
D-Ribose, 4TMS derivative	1379.95 s, 0.857 s	7727878	825	1635.3	73.05	1260	XiC(73.05±500ppm)
D-Xylopyranose, 4TMS derivative	1459.95 s, 0.915 s	11577641	831	1731.3	73.05	863	XiC(73.05±500ppm)
Eicosane, 7-hexyl-	2659.87 s, 2.570 s	7548681	799	3326.8	57.08	519	XiC(57.08±500ppm)
Erucic acid	1759.93 s, 1.384 s	23172252	764	2126.7	55.06	832	XiC(55.06±500ppm)
Erythrono-1,4-lactone, (E)-, 2TMS derivative	1149.97 s, 1.132 s	14506795	897	1385	73.05	2211	XiC(73.05±500ppm)
Erythrono-1,4-lactone, 2TMS derivative	1204.96 s, 1.275 s	186409399	932	1442.1	73.05	5753	XiC(73.05±500ppm)
Ethamivan	1604.94 s, 2.389 s	5016565	755	1920	151.04	628	XiC(151.04±500ppm)
Ethane, isocyanato-	1509.94 s, 1.879 s	22186845	725	1793.8	71.08	1716	XiC(71.08±500ppm)
Ethanol, 2-(trimethylsilyl)-	2294.89 s, 1.457 s	1128062623	805	2840.1	75.03	898	XiC(75.03±500ppm)
Ethanone, 1-(5-methoxy-2-methyl-3(1H)-indolyl)-	1569.94 s, 2.093 s	1563982	737	1873.3	188.08	715	XiC(188.08±500ppm)
Ethyl 4-oxo-2-phenylpentanoate	1279.96 s, 1.323 s	2999731	792	1522.2	205.17	1219	XiC(205.17±500ppm)
Ethyl α-D-glucopyranoside, 4TMS derivative	2014.91 s, 0.891 s	15766860	843	2466.7	73.05	1973	XiC(73.05±500ppm)
Ethylene glycol - Adipate - Diethylene glycol	1389.95 s, 2.213 s	3390727	714	1647.1	173.09	1418	XiC(173.09±500ppm)
Ethylene glycol, 2TMS derivative	689.997 s, 0.855 s	32574875	895	988.9	147.06	3059	XiC(147.06±500ppm)
Ethylene glycol, TMS derivative	799.99 s, 0.991 s	138015073	858	1070.4	75.02	1210	XiC(75.02±500ppm)
Ethyltriethylene glycol, TBDMS derivative	989.978 s, 0.992 s	12498123	766	1231.8	73.05	575	XiC(73.05±500ppm)
Farnesol isomer a	2234.9 s, 1.856 s	7337689	797	2760.1	69.07	690	XiC(69.07±500ppm)
Ferulic acid, trimethylsiloxy, trimethylsilyl ester	1734.93 s, 1.389 s	22094208	854	2093.3	73.05	2082	XiC(73.05±500ppm)
Fluoranthene	1724.93 s, 2.500 s	12813848	926	2080	202.09	1580	XiC(202.09±500ppm)
Gallacetophenone-4'-methylether, bis(trimethylsilyl) ether	2054.91 s, 2.304 s	5480040	709	2520	311.08	794	XiC(311.08±500ppm)
Gluconolactone (3R,4S,5R,6R)-, 4TMS derivative	1599.94 s, 1.002 s	58965696	875	1913.3	73.05	1217	XiC(73.05±500ppm)
Glucopyranose, 5TMS derivative	1619.94 s, 0.856 s	17967870	915	1940	73.05	815	XiC(73.05±500ppm)
Gluonic acid, γ-lactone, 4TMS derivavative	1609.94 s, 0.988 s	83523236	842	1926.7	73.05	828	XiC(73.05±500ppm)
Glyceric acid, 3TMS derivative	1109.97 s, 0.906 s	169918728	885	1345	73.05	810	XiC(73.05±500ppm)
Glycerol monoacetate, 2TMS derivative	2144.9 s, 1.259 s	194877995	848	2640.1	73.05	1696	XiC(73.05±500ppm)
Glycerol, 1,2-di(TMS)-	959.98 s, 0.936 s	14114913	863	1204.5	73.05	643	XiC(73.05±500ppm)
Glycerol, 3TMS derivative	1049.97 s, 0.832 s	447470202	942	1286.4	73.05	6794	XiC(73.05±500ppm)
Glycolic acid, 2TMS derivative	814.989 s, 0.948 s	62584402	887	1081.5	73.05	2839	XiC(73.05±500ppm)
Gulonic acid, γ-lactone, 4TMS derivavative	2404.89 s, 2.332 s	23566248	709	2986.7	73.05	724	XiC(73.05±500ppm)
Heneicosane	1519.94 s, 0.977 s	395570419	926	1806.7	57.08	4584	XiC(57.08±500ppm)
Hentriacontane	2069.91 s, 1.089 s	47785689	871	2540	57.08	1288	XiC(57.08±500ppm)
Heptacosane	2354.89 s, 1.870 s	13122118	942	2920.1	57.08	826	XiC(57.08±500ppm)
Heptadecane	1389.95 s, 1.963 s	283788665	897	1647.1	57.08	19814	XiC(57.08±500ppm)
Heptadecane, 2,6,10,15-tetramethyl-	1299.96 s, 0.918 s	443759415	882	1544.4	57.08	7938	XiC(57.08±500ppm)
Heptadecane, 2-methyl-	2334.89 s, 1.490 s	7216820	785	2893.4	57.08	637	XiC(57.08±500ppm)
Heptadecanoic acid, TMS derivative	1764.93 s, 1.117 s	11709769	914	2133.3	73.05	1939	XiC(73.05±500ppm)
Heptane, 2,2,4,6,6-pentamethyl-	689.997 s, 0.815 s	23864801	747	988.9	57.08	1017	XiC(57.08±500ppm)
Heptanoic acid, TMS derivative	924.982 s, 0.970 s	6464262	837	1173.9	75.03	1654	XiC(75.03±500ppm)
Heptasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13-tetradecamethyl-	1394.95 s, 0.771 s	25134844	750	1652.9	73.05	696	XiC(73.05±500ppm)
Heptasiloxane, hexadecamethyl-	2019.91 s, 0.797 s	10281689	799	2473.4	73.05	779	XiC(73.05±500ppm)
Hexadecane	1269.96 s, 0.929 s	235559723	922	1511.1	57.08	5993	XiC(57.08±500ppm)
Hexadecane, 2,6,10,14-tetramethyl-	1639.94 s, 0.967 s	158465913	850	1966.7	57.08	5822	XiC(57.08±500ppm)
Hexadecane, 2,6,11,15-tetramethyl-	1119.97 s, 0.891 s	58006848	881	1355	71.09	6705	XiC(71.09±500ppm)
Hexadecanoic acid, 4-[[trimethylsilyloxy]butyl] ester	2024.91 s, 1.089 s	40128905	742	2480	73.05	2598	XiC(73.05±500ppm)
Hexadecanoic acid, dodecyl ester	2234.9 s, 1.605 s	6117770	859	2760.1	43.07	507	XiC(43.07±500ppm)
Hexadecanoic acid, octadecyl ester	2664.87 s, 4.108 s	9769035	910	3333.4	57.08	1051	XiC(57.08±500ppm)
Hexane, 1-(ethoxymethoxy)-	714.995 s, 0.877 s	11707102	705	1007.4	43.07	1188	XiC(43.07±500ppm)
Hexanoic acid, TMS derivative	899.983 s, 1.152 s	38488176	729	1152.2	73.05	925	XiC(73.05±500ppm)
Hexasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11-dodecamethyl-	1249.96 s, 0.774 s	8803655	798	1489.5	73.05	1049	XiC(73.05±500ppm)
Hexatriacontane	2299.89 s, 1.632 s	23364971	925	2846.7	57.08	1303	XiC(57.08±500ppm)
Hexonic acid, 3-deoxy-, γ-lactone, 2,5,6-tris-O-TMS	1509.94 s, 1.072 s	37295776	840	1793.8	73.05	623	XiC(73.05±500ppm)
Hexopyranose, 5TMS derivative	2684.87 s, 1.871 s	98340304	738	3360.1	73.05	1317	XiC(73.05±500ppm)
Hydracrylic acid, 2TMS derivative	899.983 s, 0.935 s	86874611	896	1152.2	147.06	11492	XiC(147.06±500ppm)
Hydroquinone, 2TMS derivative	1174.97 s, 1.037 s	2252376	821	1410.5	239.1	954	XiC(239.10±500ppm)

Hydroxylamine, O-(2-methylpropyl)-	1434.95 s, 0.984 s	99435652	747	1700	43.07	524	XIC(43.07±500ppm)
Kojic acid, 2TMS derivative	1339.96 s, 1.321 s	17330408	839	1588.9	73.05	1778	XIC(73.05±500ppm)
L-(-)-Arahitol, 5TMS derivative	1474.95 s, 0.809 s	197817230	948	1750	73.05	7931	XIC(73.05±500ppm)
L-(+)-Rhamnopyranose, 4TMS derivative	2169.9 s, 1.056 s	61276402	735	2673.4	204.1	909	XIC(204.10±500ppm)
L-5-Oxoproline, , 2TMS derivative	1289.96 s, 1.308 s	87863488	919	1533.3	156.08	11716	XIC(156.08±500ppm)
Lactic Acid, 2TMS derivative	799.99 s, 0.872 s	107480819	928	1070.4	73.05	2052	XIC(73.05±500ppm)
Levoglucosan, 3TMS derivative	1454.95 s, 1.057 s	61396261	923	1725	73.05	4494	XIC(73.05±500ppm)
Lignoceric acid, TMS derivative	2169.9 s, 1.360 s	31585580	893	2673.4	73.05	808	XIC(73.05±500ppm)
L-Proline, 2TMS derivative	1344.95 s, 1.294 s	10430068	708	1594.4	73.05	2499	XIC(73.05±500ppm)
L-Rhamnose, 4TMS derivative	1529.94 s, 0.843 s	6372703	827	1820	73.05	699	XIC(73.05±500ppm)
Malic acid, 2TMS derivative	1174.97 s, 1.083 s	46938125	771	1410.5	73.05	1582	XIC(73.05±500ppm)
Malic acid, 3TMS derivative	1259.96 s, 0.986 s	231347526	947	1500	73.05	7519	XIC(73.05±500ppm)
Maltol, TMS derivative	1054.97 s, 1.425 s	1840910	799	1290.9	183.05	588	XIC(183.05±500ppm)
meso-Erythritol, 4TMS derivative	1284.96 s, 1.007 s	55836003	946	1527.8	73.05	694	XIC(73.05±500ppm)
Metanephrine, 2TMS derivative	1499.94 s, 1.198 s	15568389	727	1781.3	73.05	694	XIC(73.05±500ppm)
Methane, isocyanato-	1509.94 s, 2.002 s	29223836	710	1793.8	57.07	1622	XIC(57.07±500ppm)
Methyl (3,4-dimethoxyphenyl)(hydroxy)acetate, TMS derivative	1449.95 s, 1.515 s	999675890	784	1718.8	239.15	1851	XIC(239.15±500ppm)
Methyl 2,5-dihydroxybenzoate, 2TMS derivative	2539.88 s, 1.386 s	3160995	763	3166.8	297.07	505	XIC(297.07±500ppm)
Methyl 2,6-dihydroxybenzoate, 2TMS derivative	2054.91 s, 1.234 s	1883105	787	2520	297.15	709	XIC(297.15±500ppm)
Methyl 2α,3β-dihydroxyolean-12-en-28-oate	2839.86 s, 2.730 s	48609222	740	3566.8	203.19	544	XIC(203.19±500ppm)
Methyl galactoside, 4TMS derivative	1889.92 s, 1.007 s	28087338	736	2300	73.05	786	XIC(73.05±500ppm)
Methyl α-Arabinofuranoside, 3TMS derivative	1484.95 s, 1.067 s	25229912	702	1762.5	217.11	1435	XIC(217.11±500ppm)
Mollugin, trimethylsilyl ether	1884.92 s, 1.908 s	168245269	901	2293.4	237.06	9651	XIC(237.06±500ppm)
Myristic acid, TMS derivative	1554.94 s, 1.068 s	102430124	901	1853.3	73.05	3697	XIC(73.05±500ppm)
N-(Trimethylsilyl)-5-((trimethylsilyl)amino)-1H-imidazole-4-carboxamide	1239.96 s, 1.042 s	4875024	721	1478.9	73.05	540	XIC(73.05±500ppm)
n-Hexadecanoic acid	1634.94 s, 1.280 s	75078874	936	1960	43.07	7004	XIC(43.07±500ppm)
Nonadecane	1214.96 s, 0.924 s	26836304	908	1452.6	57.08	2116	XIC(57.08±500ppm)
Nonanoic acid, TMS derivative	1129.97 s, 1.001 s	31181828	927	1365	73.05	3957	XIC(73.05±500ppm)
Octacosane, 2-methyl-	2879.86 s, 3.319 s	3364324	804	3620.1	57.08	692	XIC(57.08±500ppm)
Octadecanoic acid	1774.93 s, 1.315 s	37338145	918	2146.7	43.07	4996	XIC(43.07±500ppm)
Octanoic acid, TMS derivative	1029.98 s, 0.988 s	46149366	942	1268.2	73.05	3806	XIC(73.05±500ppm)
Oxalic acid, 2TMS derivative	1519.94 s, 1.796 s	29282281	794	1806.7	73.05	1503	XIC(73.05±500ppm)
Palmitic acid, TMS derivative	1694.93 s, 1.108 s	644986382	936	2040	73.05	5278	XIC(73.05±500ppm)
Pentadecane	1259.96 s, 0.950 s	319372935	888	1500	57.08	1330	XIC(57.08±500ppm)
Pentadecanoic acid, TMS derivative	1624.94 s, 1.089 s	39524278	925	1946.7	73.05	2230	XIC(73.05±500ppm)
Pentane, 2,2,4,4-tetramethyl-	1304.96 s, 0.942 s	141283378	755	1550	57.08	2524	XIC(57.08±500ppm)
Pentanedioic acid, 2-((trimethylsilyloxy)-, bis(trimethylsilyl) ester	1339.96 s, 0.994 s	5072981	877	1588.9	73.05	704	XIC(73.05±500ppm)
Pentasiloxane, dodecamethyl-	939.981 s, 0.720 s	27702626	918	1187	73.05	3448	XIC(73.05±500ppm)
Phenol, 2-[[[4-methylphenyl]imino]methyl]-	1404.95 s, 0.979 s	2636165	725	1664.7	211.25	704	XIC(211.25±500ppm)
Phenol, p-1-indanyl-	1724.93 s, 1.659 s	1671540	732	2080	195.09	512	XIC(195.09±500ppm)
Phloroglucinol, trimethylsilyl ether	969.979 s, 1.264 s	1644000	745	1213.6	183.05	679	XIC(183.05±500ppm)
Phthalic acid, 2TMS derivative	1439.95 s, 1.351 s	14126346	897	1706.2	147.07	873	XIC(147.07±500ppm)
Phthalic acid, di(3-methylphenyl) ester	1449.95 s, 1.544 s	914187981	739	1718.8	239.1	643	XIC(239.10±500ppm)
Propanoyl fluoride, 2,3,3,3-tetrafluoro-2-[1,1,2,3,3,3-hexafluoro-2-(heptafluoropropoxy)propoxy]-	809.989 s, 1.606 s	2941845	727	1077.8	168.99	513	XIC(168.99±500ppm)
Propylamine, 2TMS derivative	884.984 s, 1.032 s	20740784	714	1139.1	73.05	1572	XIC(73.05±500ppm)
Propylene glycol, 2TMS derivative	714.995 s, 0.816 s	31738427	874	1007.4	73.04	2794	XIC(73.04±500ppm)
Pyrene	1759.93 s, 2.692 s	45396841	937	2126.7	202.09	3349	XIC(202.09±500ppm)
Pyrene, 1,3-dimethyl-	1904.92 s, 2.570 s	2633726	845	2320	230.12	789	XIC(230.12±500ppm)
Pyridine	814.989 s, 0.723 s	11284508	903	1081.5	79.04	1138	XIC(79.04±500ppm)
Pyridine, 2,4,6-trimethyl-	699.996 s, 1.395 s	8442754	828	996.3	121.09	728	XIC(121.09±500ppm)
Pyroglutamic acid, TMS derivative	1264.96 s, 1.718 s	62919558	887	1505.6	84.04	5447	XIC(84.04±500ppm)
Pyrrrole-2-carboxylic acid, 2TMS derivative	1129.97 s, 1.091 s	1101555	733	1365	240.09	955	XIC(240.09±500ppm)
Quinizarin, O-(trimethylsilyl)-	1974.91 s, 2.254 s	155504430	791	2413.4	297.06	1119	XIC(297.06±500ppm)
Quinoline, 1,2-dihydro-2,4-trimethyl-	1214.96 s, 1.717 s	56769019	837	1452.6	158.1	938	XIC(158.10±500ppm)
Ribitol, 5TMS derivative	1609.94 s, 0.882 s	329476745	807	1926.7	73.05	3145	XIC(73.05±500ppm)
Ribonic acid, 2,3,4,5-tetrakis-O-(trimethylsilyl)-, trimethylsilyl ester	1694.93 s, 0.856 s	31321898	817	2040	73.05	1843	XIC(73.05±500ppm)
Scopoletin, TMS derivative	1704.93 s, 1.956 s	2841613	810	2053.3	234.04	1380	XIC(234.04±500ppm)
Silane, 1,8-octanediybis(trimethyl-	929.981 s, 0.825 s	2378802	752	1178.3	147.07	775	XIC(147.07±500ppm)
Silane, diethylethoxytridecyloxy-	2024.91 s, 1.402 s	1131200	852	2480	371.31	502	XIC(371.31±500ppm)
Silane, dimethyldi(4-acetylphenoxy)-	1994.91 s, 2.599 s	1437663	720	2440	313.06	663	XIC(313.06±500ppm)
Silane, methylvinylid(hept-4-yloxy)-	1204.96 s, 1.148 s	1974622	725	1442.1	257.07	917	XIC(257.07±500ppm)
Silane, tetramethyl-	2864.86 s, 0.496 s	101322028	882	3600.1	73.04	818	XIC(73.04±500ppm)
Silanol, trimethyl-	814.989 s, 0.558 s	28230935	934	1081.5	75.02	1333	XIC(75.02±500ppm)
Silanol, trimethyl-, phosphate (3:1)	1049.97 s, 0.999 s	183015880	909	1286.4	299.08	2027	XIC(299.08±500ppm)
Stearic acid, TMS derivative	1829.92 s, 1.140 s	301110651	884	2220	73.04	4780	XIC(73.04±500ppm)
Stigmast-4-en-3-one	2589.88 s, 1.047 s	7286760	799	3233.4	124.09	978	XIC(124.09±500ppm)
Stigmast-5-ene, 3β-(trimethylsilyloxy)-, (24S)-	2489.88 s, 3.182 s	129213276	925	3100.1	129.08	2754	XIC(129.08±500ppm)
Stigmasterol, TMS derivative	2444.88 s, 2.896 s	22348976	922	3040.1	83.09	1216	XIC(83.09±500ppm)
Supraene	2169.9 s, 1.589 s	109172769	949	2673.4	69.07	5571	XIC(69.07±500ppm)
Syringaldehyde, TMS derivative	1414.95 s, 1.586 s	11955038	743	1676.5	224.06	4018	XIC(224.06±500ppm)
Terephthalic acid, 2TMS derivative	1514.94 s, 1.173 s	4931079	849	1800	295.09	1486	XIC(295.09±500ppm)
tert-Butylpentamethylsiloxane	849.987 s, 0.948 s	3946607	780	1108.7	147.06	338	XIC(147.06±500ppm)
Tetracosane	1984.91 s, 1.148 s	56236243	942	2426.7	57.08	5350	XIC(57.08±500ppm)
Tetradecane	1139.97 s, 0.907 s	16766064	878	1375	43.07	742	XIC(43.07±500ppm)
Tetradecane, 2-methyl-	1224.96 s, 0.929 s	45803540	913	1463.2	57.08	1792	XIC(57.08±500ppm)
Tetrasiloxane, decamethyl-	774.991 s, 0.719 s	16327288	818	1051.9	207.03	3107	XIC(207.03±500ppm)
Tridecanoic acid	1404.95 s, 1.220 s	4627710	760	1664.7	73.03	747	XIC(73.03±500ppm)
Tridecanoic acid, TMS derivative	1474.95 s, 1.066 s	307654589	915	1750	73.05	5354	XIC(73.05±500ppm)
Trisiloxane, octamethyl-	809.989 s, 0.783 s	11784275	833	1077.8	73.05	1400	XIC(73.05±500ppm)
Undecane	839.987 s, 0.833 s	244292675	900	1100	43.07	30038	XIC(43.07±500ppm)
Undecane, 4-methyl-	854.986 s, 0.841 s	115110690	910	1113	43.07	7371	XIC(43.07±500ppm)
Uridine, 3TMS derivative	1969.91 s, 1.448 s	27397967	908	2406.7	73.05	1933	XIC(73.05±500ppm)
Ursolic aldehyde TMS ether	2714.87 s, 1.837 s	38956262	726	3400.1	73.05	975	XIC(73.05±500ppm)
Vanillic Acid, 2TMS derivative	1494.95 s, 1.267 s	15612120	850	1775	73.05	724	XIC(73.05±500ppm)
Vanillin, TMS derivative	1299.96 s, 1.539 s	8257189	850	1544.4	194.04	2867	XIC(194.04±500ppm)
Xylonic acid, 2,3,4-tris-O-(trimethylsilyl)-, δ-lactone, D-	1424.95 s, 1.073 s	34412481	883	1688.2	73.05	1918	XIC(73.05±500ppm)
α-D-Glucopyranose, 5TMS derivative	2039.91 s, 0.967 s	87095156	712	2500	73.06	992	XIC(73.06±500ppm)
α-Linolenic acid, TMS derivative	1814.92 s, 1.262 s	42510038	880	2200	75.03	1649	XIC(75.03±500ppm)
β-Arabinopyranose, 4MS derivative	1574.94 s, 0.958 s	124240540	803	1880	73.05	1270	XIC(73.05±500ppm)
β-Carboline, 7-(tert.-butyldimethylsilyloxy)-1-methyl-	2059.91 s, 1.811 s	13018341	713	2526.7	255.05	650	XIC(255.05±500ppm)

β -D-(+)-Talopyranose, 5TMS derivative	2404.89 s, 1.937 s	21921784	753	2986.7	73.05	960 XIC(73.05 \pm 500ppm)
β -D-Glucopyranose, 5TMS derivative	1674.93 s, 0.869 s	225981505	942	2013.3	73.05	53586 XIC(73.05 \pm 500ppm)
β -Lyxopyranose, 4TMS derivative	1934.92 s, 0.978 s	14378265	762	2360	73.05	519 XIC(73.05 \pm 500ppm)

LOGWOOD INK	R.T. (s)	Area	Similarity	Retention	Base Mass	Peak S/N	Quant Masses
Norleucine, N-trimethylsilyl-, trimethylsilyl ester	2319.89 s, 0.711 s	7.31E+09	730	2873.4	158.11	2552	XIC(158.11±500ppm)
Galactopyranose, 5TMS derivative	2144.9 s, 1.623 s	4.93E+09	731	2640.1	204.22	630	XIC(204.22±500ppm)
[1,1'-Biphenyl-3-ol], 6-chloro-	2724.87 s, 2.325 s	3.94E+09	757	3413.4	204.09	1728	XIC(204.09±500ppm)
D-Glucopyranose, 5TMS derivative	2119.91 s, 1.166 s	3.56E+09	830	2606.7	204.2	2606	XIC(204.20±500ppm)
6-Cyanophenanthridine	2574.88 s, 1.999 s	2.4E+09	723	3213.4	204.09	623	XIC(204.09±500ppm)
Tetracyano-p-quinodimethane	2714.87 s, 2.158 s	2.21E+09	728	3400.1	204.07	540	XIC(204.07±500ppm)
α-D-Arabinopyranose, 4TMS derivative	2104.91 s, 1.160 s	1.75E+09	718	2586.7	73.02	865	XIC(73.02±500ppm)
2,3-Butanediol, 2TMS derivative	759.992 s, 0.836 s	1.24E+09	934	1040.7	117.08	5009	XIC(117.08±500ppm)
l-Norleucine, N-ethoxycarbonyl-, decyl ester	2054.91 s, 0.808 s	1.15E+09	719	2520	158.11	2825	XIC(158.11±500ppm)
Glucose, 5TMS derivative	1999.91 s, 1.001 s	1.06E+09	732	2446.7	73.05	2485	XIC(73.05±500ppm)
1,3-Propanediol, 2TMS derivative	789.99 s, 0.858 s	9.22E+08	922	1063	147.16	9579	XIC(147.16±500ppm)
Oxalic acid, 2TMS derivative	1054.97 s, 0.816 s	9.15E+08	708	1290.9	73.06	2498	XIC(73.06±500ppm)
β-D-(+)-Mannopyranose, 5TMS derivative	1619.94 s, 0.848 s	8.83E+08	939	1940	73.04	4367	XIC(73.04±500ppm)
Heneicosane	1314.96 s, 0.932 s	7.74E+08	836	1561.1	57.08	6049	XIC(57.08±500ppm)
Talose, 5TMS derivative	2089.91 s, 0.929 s	7.67E+08	803	2566.7	204.22	1879	XIC(204.22±500ppm)
meso-Erythritol, 4TMS derivative	1289.96 s, 0.803 s	7.55E+08	948	1533.3	73.05	20127	XIC(73.05±500ppm)
β-D-Allopyranose, 5TMS derivative	2564.88 s, 1.798 s	7.33E+08	786	3200.1	204.11	2524	XIC(204.11±500ppm)
Butanedioic acid, 2TMS derivative	1084.97 s, 1.072 s	7.01E+08	881	1320	147.08	2471	XIC(147.08±500ppm)
Lactic Acid, 2TMS derivative	794.99 s, 2.229 s	6.96E+08	953	1066.7	73.05	3180	XIC(73.05±500ppm)
1-Hexanol, 2-ethyl-	1444.95 s, 0.970 s	6.87E+08	776	1712.5	57.08	1425	XIC(57.08±500ppm)
Galactonic acid, γ-lactone, 4TMS derivavative	1604.94 s, 0.958 s	6.38E+08	712	1920	73.06	823	XIC(73.06±500ppm)
D-Allofuranose, pentakis(trimethylsilyl) ether	1564.94 s, 0.900 s	5.69E+08	709	1866.7	73.05	1134	XIC(73.05±500ppm)
Ribonic acid, 2,3,4,5-tetrakis-O-(trimethylsilyl)-, trimethylsilyl ester	2154.94 s, 0.857 s	5.27E+08	832	1813.3	73.06	5068	XIC(73.06±500ppm)
3-Phenyl-2-butanol, TMS derivative	774.991 s, 0.772 s	5.23E+08	798	1051.9	117.08	3362	XIC(117.08±500ppm)
Silane, methylidynetris(trimethyl-)	1544.94 s, 0.835 s	4.88E+08	792	1840	73.04	2138	XIC(73.04±500ppm)
Benzaldehyde, 1,5-dimethoxy-	1229.96 s, 1.920 s	4.6E+08	924	1468.4	166.08	7588	XIC(166.08±500ppm)
Stearic acid, TMS derivative	1829.92 s, 1.141 s	4.57E+08	934	2220	73.05	4110	XIC(73.05±500ppm)
D-(+)-Talofuranose, pentakis(trimethylsilyl) ether (isomer 1)	2349.89 s, 0.586 s	4.5E+08	752	2913.4	73.05	768	XIC(73.05±500ppm)
Methyl galactoside (1S,2R,3S,4R,5R)-, 4TMS derivative	2484.88 s, 1.310 s	4.5E+08	774	3093.4	73.05	1446	XIC(73.05±500ppm)
β-D-(-)-Ribopyranose, 4TMS derivative	1589.94 s, 0.840 s	4.39E+08	731	1900	73.11	1551	XIC(73.11±500ppm)
Gallic acid, 4TMS derivative	1649.94 s, 1.025 s	4.24E+08	841	1980	73.07	780	XIC(73.07±500ppm)
3,5-Dihydroxybenzoic acid, 3TMS derivative	2289.89 s, 1.679 s	4.24E+08	711	2833.4	73.01	1243	XIC(73.01±500ppm)
Octadecane, 2-methyl-	1404.95 s, 0.961 s	4.23E+08	901	1664.7	57.08	6131	XIC(57.08±500ppm)
Protocatechoic acid, 3TMS derivative	1539.94 s, 1.112 s	4.23E+08	863	1833.3	73.05	1783	XIC(73.05±500ppm)
Hydracrylic acid, 2TMS derivative	899.983 s, 0.943 s	4.2E+08	902	1152.2	147.08	6625	XIC(147.08±500ppm)
Methyl (3,4-dimethoxyphenyl)(hydroxy)acetate, TMS derivative	1574.94 s, 1.133 s	4.1E+08	843	1880	239.13	1439	XIC(239.13±500ppm)
2-[[tert-Butyl(dimethyl)silyloxy]ethanol	799.99 s, 1.019 s	4.01E+08	789	1070.4	75.03	2412	XIC(75.03±500ppm)
4-Chloro-3-methylphenol, trimethylsilyl ether	1090.97 s, 1.175 s	3.99E+08	749	1330	199.05	1518	XIC(199.05±500ppm)
1,2-Ethenediol, 2TMS derivative	679.997 s, 0.867 s	3.95E+08	907	981.5	73.05	3818	XIC(73.05±500ppm)
Glycolic acid, 2TMS derivative	814.989 s, 0.934 s	3.9E+08	886	1081.5	73.05	6390	XIC(73.05±500ppm)
D-Mannopyranose, 5TMS derivative	2069.91 s, 0.979 s	3.75E+08	793	2540	204.11	2640	XIC(204.11±500ppm)
3,4-Dimethoxymandelic acid, di-TMS	1984.91 s, 1.687 s	3.71E+08	745	2426.7	239.13	1993	XIC(239.13±500ppm)
2-Ethylhexanal ethylene glycol acetal	1589.94 s, 0.845 s	3.67E+08	729	1900	73.06	2107	XIC(73.06±500ppm)
Shikimic acid, 4TMS derivative	1534.94 s, 0.970 s	3.58E+08	895	1826.7	204.12	2061	XIC(204.12±500ppm)
β-D-Glucopyranose, 5TMS derivative	1584.94 s, 0.884 s	3.51E+08	741	1893.3	73.03	1936	XIC(73.03±500ppm)
6-Fluoro-2-trifluoromethylbenzoic acid, 2,3-dichlorophenyl ester	2574.88 s, 1.820 s	3.45E+08	767	3213.4	190.99	529	XIC(190.99±500ppm)
Undecane, 4,7-dimethyl-	839.987 s, 0.830 s	3.41E+08	888	1100	43.08	8978	XIC(43.08±500ppm)
Ethyl gallate, 3TMS derivative	1634.94 s, 1.159 s	3.37E+08	839	1960	73.05	8799	XIC(73.05±500ppm)
1-Octanol, 2-butyl-	1389.95 s, 0.959 s	3.37E+08	837	1647.1	57.08	6330	XIC(57.08±500ppm)
1-Monopalmitin, 2TMS derivative	2044.91 s, 1.171 s	3.36E+08	832	2506.7	73.04	1878	XIC(73.04±500ppm)
α-D-Mannopyranose, 5TMS derivative	1609.94 s, 0.897 s	3.32E+08	738	1926.7	191.09	1663	XIC(191.09±500ppm)
2-Palmitoylglycerol, 2TMS derivative	2024.91 s, 1.163 s	3.26E+08	854	2480	73.05	1969	XIC(73.05±500ppm)
β-Hydroxypruvic acid, trimethylsilyl ether, trimethylsilyl ester	2094.91 s, 0.601 s	3.26E+08	727	2573.4	73.05	1307	XIC(73.05±500ppm)
N,9-bis(trimethylsilyl)-6-[[trimethylsilyloxy]-9H-purin-2-amine	1554.94 s, 1.107 s	3.2E+08	761	1853.3	73.14	2135	XIC(73.14±500ppm)
Methyl 2,4-dihydroxybenzoate, 2TMS derivative	2304.89 s, 1.953 s	3.13E+08	719	2853.4	297.12	911	XIC(297.12±500ppm)
β-Lyxopyranose, 4TMS derivative	1554.94 s, 0.835 s	3.07E+08	818	1853.3	73.05	1214	XIC(73.05±500ppm)
D-Xylopyranose, 4TMS derivative	1494.95 s, 0.900 s	3E+08	758	1775	73.06	3494	XIC(73.06±500ppm)
Ethyl α-D-glucopyranoside, 4TMS derivative	1644.94 s, 0.920 s	2.99E+08	915	1973.3	204.12	4713	XIC(204.12±500ppm)
2-Monostearin, 2TMS derivative	2129.9 s, 1.251 s	2.99E+08	704	2620	129.07	607	XIC(129.07±500ppm)
Hexasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11-dodecamethyl-	1849.92 s, 0.944 s	2.96E+08	719	2246.7	73.06	4955	XIC(73.06±500ppm)
Heptacosane	1479.95 s, 0.941 s	2.93E+08	878	1756.3	57.08	8395	XIC(57.08±500ppm)
Pyrogallol, 3TMS derivative	1314.96 s, 1.016 s	2.91E+08	864	1561.1	73.05	1820	XIC(73.05±500ppm)
Hexopyranose, 5TMS derivative	1984.91 s, 0.956 s	2.9E+08	754	2426.7	73.05	726	XIC(73.05±500ppm)
1-Monoacetin, 2O-TMS	1089.97 s, 0.980 s	2.8E+08	791	1325	43.04	1792	XIC(43.04±500ppm)
(Methoxymethyl)trimethylsilane	1479.95 s, 1.052 s	2.77E+08	743	1756.3	73.06	2110	XIC(73.06±500ppm)
D-(+)-Talofuranose, pentakis(trimethylsilyl) ether (isomer 2)	1569.94 s, 0.863 s	2.73E+08	872	1873.3	217.12	3456	XIC(217.12±500ppm)
D-(-)-Fructofuranose, pentakis(trimethylsilyl) ether (isomer 1)	1479.95 s, 0.840 s	2.72E+08	945	1846.7	73.01	2256	XIC(73.01±500ppm)
Ethanol, 2-(2-ethoxyethoxy)-, acetate	939.981 s, 1.446 s	2.72E+08	948	1187	43.04	5802	XIC(43.04±500ppm)
1,2,3-Butanetriol, 3TMS derivative	1074.97 s, 0.790 s	2.69E+08	942	1310	73.05	22301	XIC(73.05±500ppm)
Dihydroxyacetone, 2TMS derivative	884.984 s, 0.914 s	2.64E+08	773	1139.1	73.05	3867	XIC(73.05±500ppm)
Phthalic acid, di(3-methylphenyl) ester	1449.95 s, 1.395 s	2.6E+08	729	1718.8	239.13	1866	XIC(239.13±500ppm)
Octadecane	1269.96 s, 0.926 s	2.6E+08	919	1511.1	57.08	6881	XIC(57.08±500ppm)
Gulonic acid, γ-lactone, 4TMS derivavative	1624.94 s, 0.982 s	2.59E+08	830	1946.7	73.05	2305	XIC(73.05±500ppm)

Vanillylmandelic acid, 3TMS derivative	2264.9 s, 1.451 s	2.57E+08	761	2800.1	73.06	838	XIC(73.06±500ppm)
1,3-Dioxolane-2-methanol	1979.91 s, 1.108 s	2.53E+08	747	2420	73.05	1369	XIC(73.05±500ppm)
β-Arabinopyranose, 4MS derivative	1704.93 s, 0.944 s	2.53E+08	808	2053.3	73.05	1621	XIC(73.05±500ppm)
1-Butanamine	2564.88 s, 0.498 s	2.5E+08	743	3200.1	73.06	1161	XIC(73.06±500ppm)
1-Deoxypentitol, 4TMS derivative	1314.96 s, 0.808 s	2.48E+08	893	1561.1	73.05	19857	XIC(73.05±500ppm)
Butanoic acid, 3,4-bis[(trimethylsilyloxy)-, trimethylsilyl ester	1209.96 s, 0.899 s	2.48E+08	824	1447.4	73.05	2766	XIC(73.05±500ppm)
Glucopyranose, 5TMS derivative	2169.9 s, 1.061 s	2.45E+08	757	2673.4	73.02	935	XIC(73.02±500ppm)
Acetoxyacetic acid, TBDMS derivative	829.988 s, 1.043 s	2.44E+08	795	1092.6	75.03	6787	XIC(75.03±500ppm)
2,2,6,6-Tetramethyl-2,6-disilapiperidine	2094.91 s, 0.781 s	2.4E+08	742	2573.4	158.11	3390	XIC(158.11±500ppm)
Ethyl tartrate, tris(trimethylsilyl)-	1369.95 s, 1.020 s	2.34E+08	891	1623.5	73.05	4095	XIC(73.05±500ppm)
Malonic acid, bis(2-trimethylsilylethyl ester	1159.97 s, 0.840 s	2.32E+08	733	1395	73.06	3954	XIC(73.06±500ppm)
1,6-Dioxacyclododecane-7,12-dione	1309.96 s, 2.070 s	2.31E+08	932	1555.6	55.05	5602	XIC(55.05±500ppm)
2-Undecene, 5-methyl-	1484.92 s, 0.964 s	2.31E+08	740	1762.5	57.08	3777	XIC(57.08±500ppm)
Inosose-2, 1,3,4,5,6-pentakis-O-(trimethylsilyl)-, myo-	1709.93 s, 0.852 s	2.26E+08	745	2060	73.05	1880	XIC(73.05±500ppm)
1,3-Dihydroxyanthraquinone, O,O'-bis(trimethylsilyl)-	2289.89 s, 1.672 s	2.24E+08	756	2833.4	369.29	1291	XIC(369.29±500ppm)
D-(+)-Galactopyranose, 5TMS derivative (isomer 1)	2124.9 s, 0.981 s	2.24E+08	799	2613.4	204.23	3792	XIC(204.23±500ppm)
Levoglucofan, 3TMS derivative	1454.95 s, 1.052 s	2.24E+08	933	1725	73.05	3140	XIC(73.05±500ppm)
Silane, diethylbutoxypropyl-oxo-	2349.89 s, 0.631 s	2.23E+08	731	2913.4	217.12	903	XIC(217.12±500ppm)
Succinic acid, monoethyl ester-, (TMS)	1014.98 s, 1.199 s	2.13E+08	892	1254.5	75.03	8506	XIC(75.03±500ppm)
Uridine, 5-chloro-2'-desoxytris-O-(trimethylsilyl)-	1279.96 s, 1.169 s	2.11E+08	746	1522.2	73.05	5906	XIC(73.05±500ppm)
2,3,4-Trihydroxybutyric acid tetrakis(trimethylsilyl) deriv., (, (R*,R*))	1319.96 s, 0.854 s	2.09E+08	869	1566.7	73.05	6470	XIC(73.05±500ppm)
Propylene glycol, 2TMS derivative	714.995 s, 0.805 s	2.09E+08	914	1007.4	73.05	20011	XIC(73.05±500ppm)
Gluconolactone (3R,4S,5R,6R)-, 4TMS derivative	1964.92 s, 1.071 s	2.06E+08	707	2400	73.05	2395	XIC(73.05±500ppm)
Hexonic acid, 3-deoxy-, γ-lactone, 2,5,6-tris-O-TMS	1439.95 s, 1.016 s	2.06E+08	711	1706.2	73.05	981	XIC(73.05±500ppm)
Propane, 2-methyl-1,2-bis(trimethylsilyloxy)-	1174.97 s, 0.862 s	2.05E+08	730	1410.5	73.05	7910	XIC(73.05±500ppm)
Methane, trimethoxy-	1449.95 s, 1.475 s	1.93E+08	754	1718.8	75.03	818	XIC(75.03±500ppm)
Methyl 4-methoxysalicylate, TBDMS derivative	1534.94 s, 1.080 s	1.87E+08	755	1826.7	239.13	3601	XIC(239.13±500ppm)
1,3-Bis(trimethylsilyloxy)pentane	1034.97 s, 0.900 s	1.86E+08	714	1272.7	73.05	5467	XIC(73.05±500ppm)
Isopropyl alcohol, TMS derivative	714.995 s, 1.004 s	1.84E+08	745	1007.4	73.05	541	XIC(73.05±500ppm)
Eicosane	1289.96 s, 0.937 s	1.83E+08	907	1533.3	57.08	4778	XIC(57.08±500ppm)
D-Erythro-Pentitol, 2-deoxy-1,3,4,5-tetrakis-O-(trimethylsilyl)-	1364.95 s, 0.839 s	1.83E+08	798	1617.7	73.05	3958	XIC(73.05±500ppm)
Galactopyranose, 3,4-di-O-methyl-1,2,6-tris-O-(trimethylsilyl)-	1584.94 s, 1.094 s	1.81E+08	705	1893.3	73.05	1875	XIC(73.05±500ppm)
Glyceric acid, 3TMS derivative	1109.97 s, 0.913 s	1.81E+08	922	1345	73.06	4380	XIC(73.06±500ppm)
Methyltartronic acid	799.99 s, 0.814 s	1.81E+08	748	1070.4	45.06	657	XIC(45.06±500ppm)
(Z)-5-Methoxy-3,5-dimethyl-2-hexenyltrimethylsilane	2254.9 s, 0.739 s	1.8E+08	712	2786.7	73.05	624	XIC(73.05±500ppm)
Xyonic acid, 2,3,4-tris-O-(trimethylsilyl)-, δ-lactone, D-	1424.95 s, 1.070 s	1.75E+08	884	1688.2	73.05	4284	XIC(73.05±500ppm)
Hentriacontane	1799.93 s, 0.994 s	1.71E+08	880	2180	57.08	2208	XIC(57.08±500ppm)
2,3,4,5-Tetrahydroxypentanoic acid-1,4-lactone, tris(trimethylsilyl)-	1484.95 s, 1.072 s	1.69E+08	790	1762.5	73.05	1746	XIC(73.05±500ppm)
Deoxyglucose, 4TMS derivative	2309.89 s, 0.738 s	1.68E+08	763	2860.1	73.02	730	XIC(73.02±500ppm)
1,3-Propanediol, TMS derivative	814.989 s, 0.968 s	1.65E+08	782	1081.5	75.03	3436	XIC(75.03±500ppm)
L-Rhamnose, 4TMS derivative	1394.95 s, 0.861 s	1.65E+08	943	1652.9	73.05	5370	XIC(73.05±500ppm)
Tridecanoic acid, TMS derivative	1474.95 s, 1.061 s	1.65E+08	907	1750	73.05	2588	XIC(73.05±500ppm)
1-Trisopropylsilyloxyheptadecane	2289.89 s, 1.601 s	1.6E+08	767	2833.4	369.16	874	XIC(369.16±500ppm)
D-(-)-Ribofuranose, tetrakis(trimethylsilyl) ether (isomer 2)	1379.95 s, 0.859 s	1.58E+08	931	1635.3	73.05	4607	XIC(73.05±500ppm)
2-Allyl-1,4-dimethoxybenzene	1204.96 s, 1.648 s	1.58E+08	881	1442.1	178.11	27504	XIC(178.11±500ppm)
α-D-(+)-Talopyranose, 5TMS derivative	2109.91 s, 0.984 s	1.57E+08	767	2593.4	72.99	999	XIC(72.99±500ppm)
2,5,9-Dihydroxyacetophenone, 2TMS derivative	1559.94 s, 1.166 s	1.57E+08	706	1913.3	73.05	6742	XIC(73.05±500ppm)
Palmitic Acid, TMS derivative	1694.93 s, 1.106 s	1.56E+08	931	2040	73.05	3446	XIC(73.05±500ppm)
Methyl α-D-glucofuranoside, 4TMS derivative	1659.93 s, 0.881 s	1.54E+08	743	1993.3	217.12	696	XIC(217.12±500ppm)
Methyl galactoside, 3TMS derivative	2629.87 s, 2.154 s	1.52E+08	729	3286.8	73.05	595	XIC(73.05±500ppm)
3-Hydroxy-2,3-dihydromaltol, 2-O-TMS	1224.96 s, 1.127 s	1.49E+08	912	1463.2	73.05	4010	XIC(73.05±500ppm)
3-Methylpentan-2-ol, O-trimethylsilyl ether	979.978 s, 1.473 s	1.45E+08	756	1222.7	117.05	11058	XIC(117.05±500ppm)
3,4-Dihydroxy-5-methyl-dihydrofuran-2-one, (D)-, 2TMS derivative	1174.97 s, 1.084 s	1.44E+08	786	1410.5	73.05	4762	XIC(73.05±500ppm)
2',5'-Dimethoxypropiofenone	1349.95 s, 1.821 s	1.44E+08	886	1600	165.07	10179	XIC(165.07±500ppm)
Xylose, 4TMS derivative	1439.95 s, 0.892 s	1.42E+08	897	1706.2	73.05	3053	XIC(73.05±500ppm)
1,4-Butanediol, 2TMS derivative	919.982 s, 0.864 s	1.41E+08	792	1169.6	147.08	10012	XIC(147.08±500ppm)
D-(-)-Tagatofuranose, pentakis(trimethylsilyl) ether (isomer 2)	1604.94 s, 0.787 s	1.4E+08	714	1920	73.05	1114	XIC(73.05±500ppm)
L-5-Oxoproline, , 2TMS derivative	1289.96 s, 1.305 s	1.36E+08	881	1533.3	156.1	7204	XIC(156.10±500ppm)
D-Glucose, 5TMS derivative	1544.94 s, 0.879 s	1.3E+08	735	1840	204.11	907	XIC(204.11±500ppm)
Methyl β-Arabinofuranoside, 3TMS derivative	2449.88 s, 0.626 s	1.3E+08	748	3046.7	73.05	563	XIC(73.05±500ppm)
Trimethyl(3,3-difluoro-2-propenyl)silane	2029.91 s, 0.857 s	1.28E+08	732	2486.7	73.05	535	XIC(73.05±500ppm)
Carbonic acid, eicosyl vinyl ester	2149.9 s, 1.277 s	1.27E+08	713	2646.7	57.08	1155	XIC(57.08±500ppm)
Hexadecane, 2,6,10,14-tetramethyl-	2049.91 s, 1.077 s	1.23E+08	846	2513.4	57.08	1898	XIC(57.08±500ppm)
4,6-Dioxoheptanoic acid, tris-(O-trimethylsilyl)-	2424.89 s, 1.154 s	1.22E+08	746	3013.4	257.13	979	XIC(257.13±500ppm)
1,2,4,5-Cyclohexanetetrol, 4TMS derivative	2224.9 s, 0.638 s	1.2E+08	737	2746.7	217.12	1128	XIC(217.12±500ppm)
1,3-Dioxolane, 2-pentadecyl-	2599.87 s, 0.497 s	1.17E+08	724	3246.8	73.05	988	XIC(73.05±500ppm)
1-Propene-1-thiol	2294.89 s, 0.501 s	1.17E+08	705	2840.1	73.05	710	XIC(73.05±500ppm)
1,3-Dioxolane, 2-heptyl-	2444.88 s, 0.498 s	1.14E+08	735	3040.1	73.05	504	XIC(73.05±500ppm)
Carbitol, TMS derivative	919.982 s, 1.067 s	1.13E+08	939	1169.6	73.06	3613	XIC(73.06±500ppm)
Dimethyl hexopyranosiduronate, α-D-, 3TMS derivative	2174.9 s, 0.778 s	1.12E+08	758	2680.1	204.11	912	XIC(204.11±500ppm)
Silane, tetramethyl-	1309.96 s, 1.031 s	1.11E+08	728	1555.6	73.06	989	XIC(73.06±500ppm)
D-Glucrono-γ-lactone (isomer 1), 3TMS derivative	1134.97 s, 0.998 s	1.1E+08	712	1370	73.05	3401	XIC(73.05±500ppm)
β-L-Mannofuranose, 6-deoxy-1,2,3,5-tetrakis-O-(trimethylsilyl)-	2629.87 s, 0.615 s	1.09E+08	713	3286.8	73.05	674	XIC(73.05±500ppm)
(9H-fluoren-9-yl)methanol, O-methoxycarbonyl-	1614.94 s, 2.002 s	1.09E+08	746	1933.3	178.1	8290	XIC(178.10±500ppm)

Methyl α -Lyxofuranoside, 3TMS derivative	2294.89 s, 0.638 s	1.07E+08	754	2840.1	217.12	691	XIC(217.12±500ppm)
Ethylene glycol, 2TMS derivative	694.996 s, 0.822 s	1.06E+08	881	992.6	147.08	1998	XIC(147.08±500ppm)
Ribitol, 5TMS derivative	1184.97 s, 0.868 s	1.03E+08	784	1421	73.05	6938	XIC(73.05±500ppm)
Heptane, 4-azido-	1259.96 s, 0.907 s	1.02E+08	757	1500	43.06	719	XIC(43.06±500ppm)
Tyrosol, 2TMS derivative	1334.96 s, 1.092 s	1.02E+08	909	1583.3	179.1	8850	XIC(179.10±500ppm)
2-Isopropyl-5-methyl-1-heptanol	1074.97 s, 0.898 s	1.01E+08	849	1310	43.08	3382	XIC(43.08±500ppm)
Kojic acid, 2TMS derivative	1254.96 s, 1.136 s	98983181	793	1494.7	73.06	872	XIC(73.06±500ppm)
2-Methoxy-1,3-dioxolane	2134.9 s, 0.531 s	98771361	821	2626.7	73.07	576	XIC(73.07±500ppm)
3-Methylglutaconic acid, O,O',O''-tris(trimethylsilyl)-	1339.96 s, 0.998 s	94200917	706	1588.9	73.05	3152	XIC(73.05±500ppm)
1-Aminocyclopentanecarboxylic acid, 3-chloropropoxycarbonyl-, tridecyl ester	1534.94 s, 0.887 s	91609682	735	1826.7	204.12	735	XIC(204.12±500ppm)
Hexane, 1,1'-oxybis-	1394.95 s, 0.963 s	91061454	752	1652.9	43.08	1323	XIC(43.08±500ppm)
Malic acid, 3TMS derivative	1264.96 s, 0.961 s	89492514	940	1505.6	73.05	2892	XIC(73.05±500ppm)
Phenylethyl Alcohol, TMS derivative	989.978 s, 1.134 s	88628949	920	1231.8	73.05	3802	XIC(73.05±500ppm)
O,O',O''-Tris-trimethylsilylmalonate	1689.93 s, 0.878 s	88073336	739	2033.3	73.05	900	XIC(73.05±500ppm)
2',3',4',-Tri(trimethylsilyl)oxyacetophenone	2159.9 s, 1.485 s	84906796	794	2660.1	369.17	4107	XIC(369.17±500ppm)
2-Hydroxymethylcyclopentanol, (E)-, 2TMS derivative	1259.96 s, 1.136 s	84314951	728	1500	73.05	2578	XIC(73.05±500ppm)
Hexadecane, 2,6,11,15-tetramethyl-	1119.97 s, 0.889 s	83378634	882	1355	71.09	14043	XIC(71.09±500ppm)
D-(+)-Ribono-1,4-lactone (R,S,R)-, 3TMS derivative	1284.96 s, 1.256 s	80363511	749	1527.8	73.05	1563	XIC(73.05±500ppm)
4-Hydroxybutanoic acid, 2TMS derivative	1004.98 s, 0.947 s	80108278	926	1245.5	147.08	1807	XIC(147.08±500ppm)
Ethylene glycol butyl ether, trimethylsilyl ether	804.989 s, 0.945 s	72392972	796	1074.1	75.03	2699	XIC(75.03±500ppm)
2,6-Dimethyldecane	844.987 s, 2.179 s	72385029	878	1104.3	57.09	948	XIC(57.09±500ppm)
L-Proline, 2TMS derivative	1344.95 s, 1.291 s	71885421	752	1594.4	73.05	4985	XIC(73.05±500ppm)
2,2,4-Trimethyl-1,3-pentanediol diisobutylate	1354.95 s, 1.207 s	71400322	885	1605.9	71.06	3588	XIC(71.06±500ppm)
1-Trisopropylsilyloxynonane	2089.91 s, 1.004 s	70707800	731	2566.7	257.13	2461	XIC(257.13±500ppm)
1,5-Anhydroglucitol, 4TMS derivative	1949.92 s, 1.060 s	69587168	728	2380	73.05	2295	XIC(73.05±500ppm)
5-Methylhydantoin, bis-N-TMS	1044.97 s, 0.993 s	69145216	740	1281.8	73.05	2954	XIC(73.05±500ppm)
Propanoyl fluoride, 2,3,3,3-tetrafluoro-2-[1,1,2,2,3,3,3-hexafluoro-2-(heptafluoro)]	794.99 s, 1.733 s	68595411	743	1066.7	169.01	2934	XIC(169.01±500ppm)
l-Norvaline, n-propoxycarbonyl-, undecyl ester	2234.9 s, 0.714 s	68578455	757	2760.1	158.1	1140	XIC(158.10±500ppm)
Acetin, bis-1,3-trimethylsilyl ether	939.981 s, 0.915 s	67346210	797	1187	73.05	2599	XIC(73.05±500ppm)
Heptadecane	1584.94 s, 0.987 s	61582682	834	1893.3	57.08	1694	XIC(57.08±500ppm)
Decane, 3,7-dimethyl-	959.98 s, 0.837 s	61218895	863	1204.5	57.08	4246	XIC(57.08±500ppm)
Diacetone alcohol, TMS derivative	764.992 s, 0.992 s	60868728	835	1044.4	115.07	1678	XIC(115.07±500ppm)
Methyl galactoside, 4TMS derivative	1909.92 s, 1.025 s	60737951	785	2326.7	73.05	907	XIC(73.05±500ppm)
3,4,5-Trihydroxypentanoic acid, tetrakis(trimethylsilyl)-	1349.95 s, 0.838 s	60632896	764	1600	73.05	2623	XIC(73.05±500ppm)
l-Norleucine, N-ethoxycarbonyl-, hexyl ester	2079.91 s, 0.793 s	58025204	717	2553.4	158.11	1680	XIC(158.11±500ppm)
dl-2-Benzylaminooctanol	1944.92 s, 1.131 s	57831445	761	2373.4	204.12	1357	XIC(204.12±500ppm)
Pentadecane	1009.98 s, 0.863 s	57409948	897	1250	57.08	1916	XIC(57.08±500ppm)
Cicosane, 2-methyl-	1899.92 s, 1.008 s	57270590	786	2313.4	57.08	1839	XIC(57.08±500ppm)
Cyclopentasiloxane, decamethyl-	904.983 s, 0.725 s	56787739	884	1156.5	73.05	2175	XIC(73.05±500ppm)
Chloricromen	2109.91 s, 0.779 s	56770627	746	2593.4	86.07	1510	XIC(86.07±500ppm)
Pyroglutamic acid, TMS derivative	1264.96 s, 1.711 s	56523488	911	1505.6	84.05	4174	XIC(84.05±500ppm)
Dehydroabietic acid, TMS derivative	1929.92 s, 1.697 s	56170925	808	2353.4	239.2	1533	XIC(239.2±500ppm)
Tricarballic acid, 3TMS derivative	1469.95 s, 1.069 s	56106913	836	1743.8	73.05	1068	XIC(73.05±500ppm)
Octanoic acid, TMS derivative	1029.98 s, 0.982 s	55819127	913	1268.2	73.05	2967	XIC(73.05±500ppm)
Acetoacetic acid, bis(trimethylsilyl)- deriv.	1064.97 s, 1.043 s	55667151	709	1300	73.05	1975	XIC(73.05±500ppm)
Dodecane, 2,6,11-trimethyl-	1024.98 s, 0.871 s	54174443	890	1263.6	57.08	2469	XIC(57.08±500ppm)
Phthalic acid, 2TMS derivative	1439.95 s, 1.345 s	53950963	928	1706.2	147.08	3699	XIC(147.08±500ppm)
L-(-)-Fucose, tetrakis(trimethylsilyl) ether, trimethylsilyloxime (isomer 2)	1329.96 s, 0.793 s	53864319	752	1577.8	73.05	8416	XIC(73.05±500ppm)
Butane, 2,3-dimethoxy-2-methyl-	1004.98 s, 0.944 s	53658433	716	1245.5	73.06	1207	XIC(73.06±500ppm)
2-Pentamethylsilylanyloxybutane	1194.96 s, 1.029 s	53568954	721	1431.6	73.06	785	XIC(73.06±500ppm)
Ethanone, 1-(2-hydroxy-5-methoxyphenyl)-	1259.96 s, 1.754 s	53239072	789	1500	166.08	1257	XIC(166.08±500ppm)
Tetracosane	1864.92 s, 1.092 s	52743238	939	2266.7	57.08	2698	XIC(57.08±500ppm)
Malic acid 1-ethyl ester, 2TMS	1209.96 s, 1.050 s	51473891	909	1447.4	73.05	950	XIC(73.05±500ppm)
2-Ketoisocaproic acid, TMS derivative	1084.97 s, 1.450 s	51374408	731	1320	73.06	1568	XIC(73.06±500ppm)
L-(-)-Arabitol, 5TMS derivative	1454.95 s, 0.788 s	50890672	867	1725	73.06	3214	XIC(73.06±500ppm)
β -D-(+)-Talopyranose, 5TMS derivative	1714.93 s, 0.830 s	50655647	758	2066.7	73.05	918	XIC(73.05±500ppm)
Tetrahydrogeranyl formate	814.989 s, 0.836 s	48805950	802	1081.5	43.07	1947	XIC(43.07±500ppm)
Hexanoic acid, TMS derivative	794.99 s, 1.008 s	48682911	766	1066.7	75.04	796	XIC(75.04±500ppm)
Benzoic Acid, TMS derivative	1009.98 s, 1.250 s	48208847	895	1250	179.07	5879	XIC(179.07±500ppm)
4-Hydroxybenzeneacetic acid, 2TMS derivative	1389.95 s, 1.218 s	47964608	909	1647.1	73.05	1393	XIC(73.05±500ppm)
1-Octadecanol, TMS derivative	1774.93 s, 1.035 s	47520696	894	2146.7	75.03	2372	XIC(75.03±500ppm)
2-Propanoic acid, 2-methyl-, 3,3,5-trimethylcyclohexyl ester	1114.97 s, 1.193 s	47416270	916	1350	69.06	4606	XIC(69.06±500ppm)
Ethyltriethylene glycol, TBDMS derivative	1104.97 s, 1.024 s	47371258	722	1340	73.06	1740	XIC(73.06±500ppm)
Butanoic acid, 2-methyl-3-[[trimethylsilyloxy]-, trimethylsilyl ester	1229.96 s, 1.077 s	47230407	732	1468.4	73.05	2023	XIC(73.05±500ppm)
D-(-)-Fructofuranose, pentakis(trimethylsilyl) ether (isomer 2)	1859.92 s, 0.956 s	45203301	720	2260	73.05	874	XIC(73.05±500ppm)
2-Ketohexanoic acid, trimethylsilyl ester	1119.97 s, 1.460 s	44874109	756	1355	73.05	2194	XIC(73.05±500ppm)
Benzyl alcohol, α -(1-(dimethylamino)ethyl)-	1489.95 s, 1.329 s	44347294	808	1768.8	72.09	2927	XIC(72.09±500ppm)
2,4-Di-tert-butylphenoxymethyltrimethylsilane	1009.98 s, 1.065 s	44052761	846	1555.6	263.21	5276	XIC(263.21±500ppm)
Nonanoic acid, TMS derivative	1129.97 s, 0.998 s	43397023	910	1365	73.05	12968	XIC(73.05±500ppm)
Cyclohexanemethanol, TMS derivative	1044.97 s, 1.512 s	43156914	739	1281.8	73.05	3380	XIC(73.05±500ppm)
Catechol, 2TMS derivative	1299.96 s, 1.152 s	42651035	705	1544.4	73.05	1437	XIC(73.05±500ppm)
Benzoic acid, 4-(4-pentylcyclohexyl)-, 4'-cyano[1,1'-biphenyl]-4-yl ester	2319.89 s, 1.166 s	42234737	713	2873.4	257.13	691	XIC(257.13±500ppm)
Octane, 2,6,6-trimethyl-	844.987 s, 2.240 s	41964269	819	1104.3	43.08	655	XIC(43.08±500ppm)
2,5-Dimethoxybenzoic acid, TMS derivative	1414.95 s, 1.586 s	41512538	718	1676.5	224.07	4691	XIC(224.07±500ppm)

Eicosane, 1-iodo-	1704.93 s, 0.982 s	41079914	760	2053.3	57.08	1870	XIC(57.08±500ppm)
Malic acid, 4-ethyl ester, 2TMS	1219.96 s, 1.063 s	40815229	771	1457.9	73.06	1307	XIC(73.06±500ppm)
Anthracene-9,10-bimine-11,12-dicarboxylic acid, 9,10-dihydro-, diethyl ester	2839.86 s, 3.731 s	40579860	710	3566.8	178.12	875	XIC(178.12±500ppm)
Undecane, 3,5-dimethyl-	729.994 s, 0.823 s	39970685	783	1018.5	57.08	1028	XIC(57.08±500ppm)
2-Butanamine, N,N-dimethyl-	1089.97 s, 1.880 s	39834415	706	1325	72.05	2094	XIC(72.05±500ppm)
Pentanedioic acid, 2-[(trimethylsilyloxy)-, bis(trimethylsilyl) ester	1339.96 s, 0.985 s	39704630	761	1588.9	129.09	728	XIC(129.09±500ppm)
Abietic acid, TMS derivative	1949.92 s, 1.629 s	38465902	863	2380	256.24	4751	XIC(256.24±500ppm)
3-Methoxymethcathinone, N-trimethylsilyl-	1739.93 s, 1.556 s	37888458	724	2100	130.1	2470	XIC(130.10±500ppm)
Trisiloxane, octamethyl-	809.989 s, 0.779 s	37383179	872	1077.8	73.05	5299	XIC(73.05±500ppm)
Cyclotrisiloxane, hexamethyl-	679.997 s, 0.792 s	36489245	763	981.5	207.06	1032	XIC(207.06±500ppm)
Diethylene glycol, n-butyl ether, trimethylsilyl ether	1109.97 s, 1.072 s	36444580	919	1345	73.05	2129	XIC(73.05±500ppm)
Ethanol, (2-(3,4-dihydroxyphenyl)-, tris(trimethylsilyl)-	1499.94 s, 1.045 s	36404398	851	1781.3	73.05	2585	XIC(73.05±500ppm)
Methylsuccinic acid, 2TMS derivative	1099.97 s, 1.011 s	36005941	895	1335	147.08	2685	XIC(147.08±500ppm)
1,2-Butanediol, 2TMS derivative	869.985 s, 0.781 s	35708851	818	1126.1	73.05	2832	XIC(73.05±500ppm)
1,2-Benzenedicarboxylic acid, bis(2-methylpropyl) ester	1574.94 s, 1.659 s	35695130	902	1880	149.04	1658	XIC(149.04±500ppm)
Isophthalic acid, di(2-methylpropyl) ester	1734.93 s, 0.864 s	35490296	748	2093.3	239.14	1327	XIC(239.14±500ppm)
2-Ketobutyric acid, TMS derivative	1129.97 s, 1.661 s	35292969	760	1365	73.06	4081	XIC(73.06±500ppm)
2,2,8,8-Tetramethyl-3,7-dioxo-4-aza-2,8-disilanon-4-ene	849.987 s, 0.942 s	34981883	763	1108.7	147.08	3723	XIC(147.08±500ppm)
Cyclohexasiloxane, dodecamethyl-	1094.97 s, 0.732 s	34944458	894	1330	73.06	3088	XIC(73.06±500ppm)
Octadecanoic acid	1774.93 s, 1.312 s	34421429	927	2146.7	43.07	2896	XIC(43.07±500ppm)
Pentasiloxane, dodecamethyl-	939.981 s, 0.719 s	34249008	918	1187	73.06	16302	XIC(73.06±500ppm)
7,9-Di-tert-butyl-1-oxaspiro(4,5)deca-6,9-diene-2,8-dione	1614.94 s, 1.662 s	33937075	929	1933.3	57.08	2858	XIC(57.08±500ppm)
Arachidic acid, TMS derivative	1949.92 s, 1.182 s	33838572	852	2380	73.05	1155	XIC(73.05±500ppm)
Nonadecane	1214.96 s, 0.923 s	33702196	899	1452.6	57.08	2847	XIC(57.08±500ppm)
2-Aminoethanol, N-acetyl-, O-TMS	969.979 s, 1.380 s	33454703	926	1213.6	73.06	751	XIC(73.06±500ppm)
3-Phenylacetic acid, 2TMS derivative	1349.95 s, 1.138 s	33134163	717	1600	73.05	885	XIC(73.05±500ppm)
Arabinofuranose, 1,2,3,5-tetrakis-O-(trimethylsilyl)-	1019.98 s, 1.089 s	32880156	725	1259.1	73.06	715	XIC(73.06±500ppm)
Terephthalic acid, octyl 2-phenoxyethyl ester	1479.95 s, 0.825 s	32748121	742	1756.3	305.17	4656	XIC(305.17±500ppm)
Dibutyl phthalate	1644.94 s, 1.746 s	32380846	935	1973.3	149.04	1773	XIC(149.04±500ppm)
2,5-Dimethoxymandelic acid, di-TMS	1704.93 s, 1.302 s	32307844	728	2053.3	73.05	1457	XIC(73.05±500ppm)
Glycerol, 1,2-di(TMS)-	959.98 s, 0.936 s	32170062	876	1204.5	73.05	1370	XIC(73.05±500ppm)
3,8-Dioxa-2,9-disiladecane, 2,2,4,9,9-pentamethyl-5-[(trimethylsilyloxy)-	1169.97 s, 0.823 s	32151793	824	1405.3	73.05	2341	XIC(73.05±500ppm)
α-L-Mannofuranose, 6-deoxy-1,2,3,5-tetrakis-O-(trimethylsilyl)-	1814.92 s, 0.827 s	31478296	761	2200	217.12	1030	XIC(217.12±500ppm)
2-(2,5-Dimethoxy-phenyl)-propionaldehyde	1309.96 s, 1.809 s	31305855	853	1555.6	165.11	4032	XIC(165.11±500ppm)
Disiloxane, hexamethyl-	3099.84 s, 0.514 s	31071432	731	3913.5	147.08	1577	XIC(147.08±500ppm)
Danthron, 2TMS derivative	2099.91 s, 1.378 s	31042190	812	2580	369.17	1783	XIC(369.17±500ppm)
D-(-)-Ribofuranose, tetrakis(trimethylsilyl) ether (isomer 1)	1084.97 s, 0.833 s	30882358	776	1320	73.06	4813	XIC(73.06±500ppm)
2-Methyl-1,3-butanediol, 2TMS derivative	1269.96 s, 1.213 s	30307295	765	1511.1	73.06	1966	XIC(73.06±500ppm)
2-Methoxyethanol, triisobutylsilyl ether	1489.95 s, 0.870 s	30294632	784	1768.8	217.13	1279	XIC(217.13±500ppm)
tert-Butylpentamethyldisiloxane	2649.87 s, 0.516 s	29775473	760	3313.4	147.08	633	XIC(147.08±500ppm)
Silanol, trimethyl-, phosphate (3:1)	1049.97 s, 1.033 s	29626974	840	1286.4	299.1	1349	XIC(299.10±500ppm)
Butanoic acid, 2,4-bis[(trimethylsilyloxy)-, trimethylsilyl ester	1114.97 s, 0.904 s	29623326	861	1426.3	73.05	1014	XIC(73.05±500ppm)
Glycine	884.984 s, 0.378 s	29583254	722	1139.1	44.01	689	XIC(44.01±500ppm)
Dimethyl(trimethylsilyl)ethoxysilane	1024.98 s, 0.938 s	29179479	775	1263.6	73.06	1049	XIC(73.06±500ppm)
Benzo[1,2-c:3,4-c':5,6-c'']tris[1,2,5]oxadiazole	1929.92 s, 0.901 s	28832827	753	2353.4	204.12	578	XIC(204.12±500ppm)
4-Coumaric acid, 2TMS derivative	1629.94 s, 1.282 s	28698670	823	1953.3	73.05	3530	XIC(73.05±500ppm)
Phloroglucinol, trimethylsilyl ether	969.979 s, 1.259 s	28327748	777	1213.6	183.07	7819	XIC(183.07±500ppm)
Tuaminoheptane	904.983 s, 0.375 s	28176991	755	1156.5	44.01	539	XIC(44.01±500ppm)
Erythrono-1,4-lactone, 2TMS derivative	1149.97 s, 1.129 s	27803913	889	1385	73.06	2754	XIC(73.06±500ppm)
3-Hydroxybenzoic acid, 2TMS derivative	1324.96 s, 1.163 s	27778922	880	1572.2	73.06	2847	XIC(73.06±500ppm)
L-Proline, ethyl ester	1449.95 s, 1.365 s	27376664	731	1718.8	70.08	2840	XIC(70.08±500ppm)
D-(-)-Citramalic acid, 3TMS derivative	1249.96 s, 0.941 s	27153705	839	1489.5	147.08	742	XIC(147.08±500ppm)
Benzene, (1-methyldodecyl)-	1604.94 s, 1.246 s	26990211	886	1920	105.08	2607	XIC(105.08±500ppm)
3-Aminopropanephosphonic acid, 3TBDMS derivative	2344.89 s, 2.774 s	26801799	707	2906.7	73.05	1341	XIC(73.05±500ppm)
Trimethylsilyl 5-acetyl-(2-trimethylsilyloxy)benzoic acid	1709.93 s, 1.186 s	26798579	707	2060	73.05	1026	XIC(73.05±500ppm)
Itaconic acid, 2TMS derivative	1114.97 s, 1.084 s	26195988	907	1350	73.06	755	XIC(73.06±500ppm)
(R*,S*)-2,3-Dihydroxybutanoic acid, tris(trimethylsilyl) deriv.	1124.97 s, 0.862 s	25942836	923	1360	73.06	2404	XIC(73.06±500ppm)
Docosane	1799.93 s, 1.071 s	25833756	933	2180	57.08	846	XIC(57.08±500ppm)
Heptadecanoic acid, TMS derivative	1184.97 s, 1.113 s	25654513	874	2133.3	73.06	904	XIC(73.06±500ppm)
4-[β-Diethylaminoethylamino]-2,6-di[p-chlorophenyl]pyridine	2089.91 s, 0.795 s	24841103	727	2566.7	86.07	1763	XIC(86.07±500ppm)
Glycerol, 3TMS derivative	949.98 s, 0.928 s	24642728	768	1195.7	73.06	1179	XIC(73.06±500ppm)
5-Ethyl-2-hepten-4-one	1509.94 s, 1.025 s	24618895	732	1793.8	69.08	852	XIC(69.08±500ppm)
Tetrasiloxane, decamethyl-	774.991 s, 0.700 s	24451363	837	1051.9	207.05	2165	XIC(207.05±500ppm)
5-Nitro-3-phenyl-1H-indazole	1704.93 s, 0.897 s	24385410	705	2053.3	239.14	1060	XIC(239.14±500ppm)
Hexadecane	974.979 s, 0.838 s	24325401	886	1218.2	57.08	2119	XIC(57.08±500ppm)
Dextroamphetamine	754.993 s, 0.408 s	24222614	737	1037	44.01	727	XIC(44.01±500ppm)
4-Hydroxybenzoic acid, 2TMS derivative	1379.95 s, 1.157 s	23669148	841	1635.3	73.05	715	XIC(73.05±500ppm)
Hexanoic acid, 3-trimethylsilyloxy, trimethylsilyl ester	1184.97 s, 1.147 s	23651323	735	1421	73.06	716	XIC(73.06±500ppm)
N-(Trimethylsilyl)-5-[(trimethylsilyl)amino]-1H-imidazole-4-carboxamide	1239.96 s, 1.137 s	23263661	757	1478.9	73.06	1148	XIC(73.06±500ppm)
Heptane, 2,2,4,6,6-pentamethyl-	689.997 s, 0.821 s	22549382	870	988.9	57.08	1182	XIC(57.08±500ppm)
Pyridine, 2,4,6-trimethyl-	699.996 s, 1.382 s	22357111	909	996.3	121.1	1654	XIC(121.10±500ppm)
1,2,3,6-Tetrahydropyridin-2-carboxylic acid	1054.97 s, 1.297 s	22349110	726	1290.9	82.07	1885	XIC(82.07±500ppm)
Carbazole, TMS derivative	1959.92 s, 1.562 s	22263109	742	2393.4	73.06	708	XIC(73.06±500ppm)
4-Hydroxyphenylacetic acid, 3TMS derivative	1604.94 s, 1.096 s	22238872	836	1920	179.11	3282	XIC(179.11±500ppm)

Hexadecanoic acid, 4-[(trimethylsilyloxy)butyl ester	2024.91 s, 1.364 s	22202741	733	2480	43.07	926	XIC(43.07±500ppm)
D-(+)-Galactopyranose, 5TMS derivative (isomer 2)	1729.93 s, 0.827 s	21290876	729	2086.7	73.06	570	XIC(73.06±500ppm)
2-Oxo-4-phenyl-6-(4-chlorophenyl)-1,2-dihydropyrimidine	2484.88 s, 0.517 s	21240723	737	3093.4	281.08	734	XIC(281.08±500ppm)
Pipecolic acid, 2TMS derivative	1249.96 s, 1.153 s	21108472	727	1489.5	73.05	693	XIC(73.05±500ppm)
Hydroquinone, 2TMS derivative	1174.97 s, 1.034 s	21005458	835	1410.5	239.12	5791	XIC(239.12±500ppm)
Pantolactone, (3R)-, TMS derivative	949.98 s, 1.265 s	20953240	928	1195.7	75.03	1473	XIC(75.03±500ppm)
Heptadecane, 9-octyl-	2094.91 s, 1.111 s	20812227	747	2573.4	57.08	661	XIC(57.08±500ppm)
Phenol, 4-chloro-3-methyl-	1094.97 s, 1.150 s	20722968	718	1330	107.06	1484	XIC(107.06±500ppm)
1-Monomyristin, 2TMS derivative	1929.92 s, 1.115 s	20639209	883	2353.4	73.05	874	XIC(73.05±500ppm)
Resorcinol, 2TMS derivative	1154.97 s, 1.063 s	20637986	722	1390	73.04	2058	XIC(73.04±500ppm)
Cinnamic acid, TMS derivative	1304.96 s, 1.405 s	20561101	906	1550	131.06	3893	XIC(131.06±500ppm)
1-Methyldodecylamine	699.996 s, 0.398 s	20449415	729	996.3	44.01	838	XIC(44.01±500ppm)
Bicyclo[2.2.2]oct-5-en-2-yl-dimethylamine	1509.94 s, 1.869 s	20222478	710	1793.8	71.08	1186	XIC(71.08±500ppm)
Diethylene glycol, 2TMS derivative	1009.98 s, 0.906 s	19938966	747	1250	73.06	911	XIC(73.06±500ppm)
Heptadecane, 2,6,10,15-tetramethyl-	1189.96 s, 0.880 s	19900130	856	1426.3	57.08	2146	XIC(57.08±500ppm)
Salicylic acid, 2TMS derivative	1279.96 s, 1.195 s	19602948	782	1522.2	267.11	5426	XIC(267.11±500ppm)
Myristic acid, TMS derivative	1554.94 s, 1.055 s	19590836	806	1853.3	117.05	1302	XIC(117.05±500ppm)
2-Furoic acid, TMS derivative	884.984 s, 1.286 s	19488903	759	1139.1	125.06	6273	XIC(125.06±500ppm)
Benzenepropanoic acid, 3,5-bis(1,1-dimethylethyl)-4-hydroxy-, methyl ester	1629.94 s, 1.568 s	18775730	842	1953.3	277.21	2554	XIC(277.21±500ppm)
Undecane, 3,8-dimethyl-	1609.94 s, 0.966 s	18165523	734	1926.7	57.08	708	XIC(57.08±500ppm)
Benzenemethanol, α -(1-phenylaminoethyl)-	2279.9 s, 0.959 s	17993179	729	2820.1	120.09	560	XIC(120.09±500ppm)
Isopimaric acid, TMS	1899.92 s, 1.540 s	17965335	852	2313.4	73.06	2023	XIC(73.06±500ppm)
Estra-1,3,5(10)-trien-6-one, 3,17-bis(acetyloxy)-2-methoxy-, (17 β)-	2124.9 s, 2.085 s	17453179	743	2613.4	358.19	1851	XIC(358.19±500ppm)
Undecane	744.993 s, 0.824 s	17357783	881	1029.6	57.08	1744	XIC(57.08±500ppm)
2,3-Naphthalenediamine, 2TMS derivative	1324.96 s, 1.087 s	17330627	705	1572.2	73.06	862	XIC(73.06±500ppm)
Octane, 2,4,6-trimethyl-	669.998 s, 0.809 s	17188078	883	974.1	57.08	683	XIC(57.08±500ppm)
2-Hydroxy-3-methylbutyric acid, 2TMS derivative	924.982 s, 0.863 s	16784657	742	1173.9	145.12	3109	XIC(145.12±500ppm)
5-methoxy DET	2249.9 s, 0.724 s	16768896	722	2780.1	86.07	736	XIC(86.07±500ppm)
2-Furanmethanol, tetrahydro-, acetate	1219.96 s, 0.925 s	16622971	728	1457.9	43.07	1283	XIC(43.07±500ppm)
Acrylic acid, 2,3-bis[(trimethylsilyloxy)-, trimethylsilyl ester	1179.97 s, 0.957 s	16429594	911	1415.8	73.06	1984	XIC(73.06±500ppm)
Boric acid, 3TMS derivative	704.996 s, 0.712 s	16338641	785	1000	73.06	947	XIC(73.06±500ppm)
Propanoic acid, 2-oxo-3-(trimethylsilyl)-, trimethylsilyl ester	1299.96 s, 0.851 s	15926053	751	1544.4	73.06	618	XIC(73.06±500ppm)
Methyl 2,6-dihydroxybenzoate, 2TMS derivative	2444.88 s, 4.340 s	15567141	758	3040.1	297.12	770	XIC(297.12±500ppm)
Acetamide, 2,2,2-trifluoro-	684.997 s, 0.678 s	15371384	773	985.2	44.03	582	XIC(44.03±500ppm)
Hydroquinone, TMS derivative	1119.97 s, 1.376 s	15079676	795	1355	167.07	1103	XIC(167.07±500ppm)
N-Methoxy-N-methylamino-N,N-diethylaminomethane	2164.9 s, 0.750 s	14983973	712	2666.7	86.07	918	XIC(86.07±500ppm)
2,5-Dimethoxy-4-(n)-propylthiophenethylamine, N,N-bis(trimethylsilyl)-	1769.93 s, 1.372 s	14943620	742	2140	174.11	1421	XIC(174.11±500ppm)
3-Methyl-5-keto-3-hexenoic acid, O ¹⁶ - bis(trimethylsilyl) deriv.	1404.95 s, 1.262 s	14868216	748	1664.7	73.06	1148	XIC(73.06±500ppm)
Ethanol, 2-(2-butoxyethoxy)-, acetate	1134.97 s, 1.386 s	14694193	950	1370	43.04	2219	XIC(43.04±500ppm)
Cyclohexane, 1-ethyl-2-propyl-	1784.93 s, 1.004 s	14598758	731	2160	69.08	1305	XIC(69.08±500ppm)
Benzyl alcohol, TMS derivative	909.983 s, 1.105 s	14506102	728	1160.9	57.05	1468	XIC(57.05±500ppm)
1H-1,2,4-Triazole	1499.94 s, 1.872 s	14404550	706	1781.3	69.07	1162	XIC(69.07±500ppm)
Pyridine, 4-propyl-	1989.91 s, 2.865 s	14352035	719	2433.4	121.06	1752	XIC(121.06±500ppm)
Silane, trimethylphenyl-	3094.84 s, 0.666 s	14319603	751	3906.8	135.08	555	XIC(135.08±500ppm)
Ethanamine, N-ethyl-N-[(trimethylsilyl)methyl]-	2059.91 s, 1.808 s	14080929	709	2526.7	86.07	508	XIC(86.07±500ppm)
2,6-Dimethoxybenzoyl chloride	1384.95 s, 1.988 s	13960554	796	1641.2	165.07	2313	XIC(165.07±500ppm)
1,2-Benzenediol, o-(4-methoxybenzoyl)-o'-(2,2,3,3,4,4,4-heptafluorobutyl)-	3149.84 s, 0.671 s	13936610	733	3980.1	135.08	586	XIC(135.08±500ppm)
Allonic acid, γ -lactone, 4TMS derivativae	1879.92 s, 1.029 s	13858689	725	2286.7	73.06	591	XIC(73.06±500ppm)
Cycloheptasiloxane, tetradecamethyl-	1259.96 s, 0.745 s	13750795	893	1500	73.06	2642	XIC(73.06±500ppm)
Benzene, 1,2-dimethoxy-4-(1-propenyl)-	2034.91 s, 2.294 s	13581034	714	2493.4	178.12	935	XIC(178.12±500ppm)
Silane, ethyldimethylphenyl-	3209.84 s, 0.677 s	13509706	715	4060.1	135.08	565	XIC(135.08±500ppm)
Terephthalic acid, 2TMS derivative	1514.94 s, 1.170 s	13048697	852	1800	295.11	2363	XIC(295.11±500ppm)
Furfuryl alcohol, TMS derivative	704.996 s, 1.062 s	12806924	920	1000	81.04	920	XIC(81.04±500ppm)
Decane, 4-methyl-	724.995 s, 0.811 s	12778805	892	1014.8	43.07	1230	XIC(43.07±500ppm)
3-Methylsalicylic acid, 2TMS derivative	1359.95 s, 1.182 s	12297868	830	1611.8	73.06	691	XIC(73.06±500ppm)
D-(-)- Erythrofuranoose, tris(trimethylsilyl) ether (isomer 1)	1029.98 s, 0.961 s	11909016	717	1268.2	147.08	2038	XIC(147.08±500ppm)
Phenol, TMS derivative	779.991 s, 1.069 s	11868867	853	1055.6	151.07	3124	XIC(151.07±500ppm)
Benzene, 1,4-dimethoxy-	919.982 s, 1.619 s	11606890	922	1169.6	123.06	3587	XIC(123.06±500ppm)
Pimaric acid, TMS derivative	1884.97 s, 1.471 s	11519181	866	2293.4	73.06	2036	XIC(73.06±500ppm)
Silanol, trimethyl-	689.997 s, 0.582 s	11213962	914	988.9	75.03	534	XIC(75.03±500ppm)
Ethanoen, 1-(5-methoxy-2-methyl-3(1H)-indolyl)-	1569.94 s, 2.091 s	11151849	793	1873.3	188.09	1560	XIC(188.09±500ppm)
2-Hydroxy-5-methoxybenzaldehyde, TMS derivative	1389.95 s, 1.465 s	10939432	743	1647.1	209.09	1100	XIC(209.09±500ppm)
2,3-Octanedione	684.997 s, 1.528 s	10776424	733	985.2	43.04	839	XIC(43.04±500ppm)
Acetamide, N-ethyl-	669.998 s, 1.805 s	10579997	735	974.1	43.04	730	XIC(43.04±500ppm)
(2,5-Dimethoxyphenyl)acetone	1329.96 s, 1.913 s	10424265	909	1577.8	151.09	1354	XIC(151.09±500ppm)
3,4-Dihydrocoumarin, 4,4-dimethyl-6-dimethylamino-	1479.95 s, 1.994 s	10097057	753	1756.3	219.11	1887	XIC(219.11±500ppm)
1,2,4-Butanetriol, 3TMS derivative	1139.97 s, 0.837 s	10013016	876	1375	103.07	2268	XIC(103.07±500ppm)
3-Methyl-2-furoic acid, TMS derivative	1084.97 s, 1.397 s	10011435	709	1320	183.07	1127	XIC(183.07±500ppm)
1-(2,5-Dimethoxyphenyl)-1-[(trimethylsilyloxy)propan-2-amine	1324.96 s, 1.280 s	9848256	749	1572.2	73.06	522	XIC(73.06±500ppm)
1-Tetradecene	1159.97 s, 0.959 s	9526162	930	1395	55.07	547	XIC(55.07±500ppm)
Octacosane, 2-methyl-	2379.89 s, 1.590 s	9384417	736	2953.4	57.09	743	XIC(57.09±500ppm)
1-Adamantylamine, N-tert-butyl-dimethylsilyl-	2029.91 s, 1.679 s	9351366	767	2486.7	208.14	619	XIC(208.14±500ppm)
Benzene, (1-pentyloctyl)-	1539.94 s, 1.197 s	9311927	750	1833.3	91.07	560	XIC(91.07±500ppm)
Sedoheptulose anhydride, tetrakis(trimethylsilyl) ether	1634.94 s, 1.049 s	9178420	762	1960	204.12	639	XIC(204.12±500ppm)

2-Propenoic acid, 2-[[trimethylsilyloxy]-, trimethylsilyl ester	829.988 s, 0.912 s	9118287	792	1092.6	147.08	602	XIC(147.08±500ppm)
Isophthalic acid, 2TMS derivative	1489.95 s, 1.230 s	9050763	729	1768.8	179.11	1399	XIC(179.11±500ppm)
Propanedioic acid, 2TMS derivative	969.979 s, 1.036 s	8965498	928	1213.6	147.08	1001	XIC(147.08±500ppm)
1,4-Dioxin, 2,3-dihydro-	2134.9 s, 0.769 s	8866954	718	2626.7	86.07	1119	XIC(86.07±500ppm)
2-Propanol, 1-(2-methoxy-1-methylethoxy)-	1079.97 s, 1.319 s	8551298	841	1315	59.06	630	XIC(59.06±500ppm)
Dodecanoic acid, 1-methylethyl ester	1374.95 s, 1.112 s	8523251	889	1629.4	43.08	831	XIC(43.08±500ppm)
Silane, [[dimethylsilyl)methyl]trimethyl-	819.988 s, 0.806 s	8503078	761	1085.2	73.06	602	XIC(73.06±500ppm)
1-Diphenyl(tert-butyl)silyloxy-4-methoxybenzene	1559.94 s, 0.862 s	8476318	704	1860	305.17	1289	XIC(305.17±500ppm)
Mono-TMS of (pyridoxine-H ₂ O)	1989.91 s, 2.115 s	8372401	711	2433.4	223.12	3059	XIC(223.12±500ppm)
tert-Butyldimethylsilyl methacrylate	1159.97 s, 1.117 s	8260160	755	1395	143.07	979	XIC(143.07±500ppm)
Pentylone, N-trimethylsilyl-	2844.86 s, 0.712 s	7694589	731	3573.4	158.12	630	XIC(158.12±500ppm)
Butylated Hydroxytoluene	1279.96 s, 1.324 s	7597527	859	1522.2	205.18	1115	XIC(205.18±500ppm)
Heptadecane, 2-methyl-	2364.89 s, 1.555 s	7529173	705	2933.4	57.08	948	XIC(57.08±500ppm)
Dimethyl phthalate	1224.96 s, 1.953 s	7405480	907	1463.2	163.06	2217	XIC(163.06±500ppm)
1-Nonene, 4,6,8-trimethyl-	864.986 s, 0.863 s	7358914	777	1121.7	57.09	726	XIC(57.09±500ppm)
2,6-Diisopropylphthalene	1464.95 s, 1.553 s	7253248	732	1737.5	197.15	1122	XIC(197.15±500ppm)
Glyoxylic acid, phenyl-, 2'-cyanophenyl ester	1299.96 s, 1.382 s	7205040	722	1544.4	105.05	963	XIC(105.05±500ppm)
Tetradecanoic acid, ethyl ester	1509.94 s, 1.174 s	7176405	768	1793.8	88.06	879	XIC(88.06±500ppm)
Communic Acid, TMS Derivative	1914.92 s, 1.546 s	7089177	757	2333.4	73.06	687	XIC(73.06±500ppm)
2,4-Di-tert-butylphenol	1274.96 s, 1.367 s	6969994	890	1516.7	191.16	2169	XIC(191.16±500ppm)
1-Iodo-2-methylundecane	994.977 s, 0.874 s	6812524	845	1236.4	57.09	721	XIC(57.09±500ppm)
15-Trimethylsilyloxydehydroabiatic acid, trimethylsilyl ester	2049.91 s, 1.583 s	6563374	714	2513.4	445.31	1300	XIC(445.31±500ppm)
phenoxyethanol, TMS derivative	1134.97 s, 1.258 s	6553634	744	1370	73.06	953	XIC(73.06±500ppm)
L-Proline, trimethylsilyl ester	954.98 s, 1.201 s	6512372	747	1200	70.08	701	XIC(70.08±500ppm)
2-Hydroxy-4-methoxybenzaldehyde, TMS derivative	1319.96 s, 1.466 s	6432510	741	1566.7	209.09	1842	XIC(209.09±500ppm)
Butanedioic acid, diethyl ester	934.981 s, 1.418 s	6416690	913	1182.6	101.04	1076	XIC(101.04±500ppm)
Benzene, (1-methylundecyl)-	1524.94 s, 1.236 s	6402149	834	1813.3	105.08	780	XIC(105.08±500ppm)
Anthracene	1514.94 s, 2.230 s	6402064	935	1800	178.1	909	XIC(178.10±500ppm)
Conhydrin	1034.97 s, 1.247 s	6288019	778	1272.7	84.09	860	XIC(84.09±500ppm)
Mevalonolactone, TMS derivative	1139.97 s, 1.547 s	6209432	880	1375	75.03	685	XIC(75.03±500ppm)
1,3-di-iso-propylphthalene	1429.95 s, 1.517 s	6144030	797	1694.1	197.15	1209	XIC(197.15±500ppm)
1-Dodecanol, 3,7,11-trimethyl-	804.989 s, 0.846 s	6078385	803	1074.1	69.08	741	XIC(69.08±500ppm)
4,4'-Ethylenedi-m-toluidine	2189.9 s, 1.005 s	5973552	741	2700.1	120.09	527	XIC(120.09±500ppm)
Quinoline, 1,2-dihydro-2,2,4-trimethyl-	1214.96 s, 1.711 s	5921141	855	1452.6	158.11	1381	XIC(158.11±500ppm)
Pyridine	689.997 s, 0.758 s	5819644	747	988.9	79.05	518	XIC(79.05±500ppm)
5-Benzimidazolecarbonitrile	799.99 s, 1.226 s	5737779	720	1070.4	143.07	807	XIC(143.07±500ppm)
1-(1-Hydroxybutyl)-2,5-dimethoxybenzene	1564.94 s, 1.679 s	5730655	729	1866.7	167.09	931	XIC(167.09±500ppm)
3-Heptanol, TMS derivative	924.982 s, 1.497 s	5725240	743	1173.9	131.03	1695	XIC(131.03±500ppm)
Trimethylsilyl 14-acetoxy-3,6,9,12-tetraoxatetradecan-1-olate	1034.97 s, 1.200 s	5703103	768	1272.7	87.05	1170	XIC(87.05±500ppm)
Decane, 5,6-dimethyl-	879.985 s, 0.841 s	5509226	866	1134.8	43.07	645	XIC(43.07±500ppm)
Ethylene glycol - Adipate - Diethylene glycol	1389.95 s, 2.205 s	5393574	731	1647.1	173.1	707	XIC(173.10±500ppm)
Benzene, (1-butylheptyl)-	1384.95 s, 1.174 s	5025466	824	1641.2	91.07	507	XIC(91.07±500ppm)
2H-1,4-Benzoxazine, 3,4-dihydro-	1969.91 s, 2.740 s	5004600	750	2406.7	135.08	594	XIC(135.08±500ppm)
Isoquinolin-6-ol, 1-[4-hydroxybenzyl]-1,2,3,4-tetrahydro-7-methoxy-	1969.91 s, 2.199 s	4760603	801	2406.7	178.12	560	XIC(178.12±500ppm)
2,3,4-Trifluorobenzoic acid, 4-nitrophenyl ester	799.997 s, 0.930 s	4675831	768	981.5	159.1	580	XIC(159.10±500ppm)
3,9-Dioxa-2,10-disilaundecane, 2,2,10,10-tetramethyl-5-[[trimethylsilyloxy]-	1239.96 s, 0.851 s	4425419	757	1478.9	143.1	1360	XIC(143.10±500ppm)
2-Pyrrolidinone, TMS derivative	904.984 s, 1.423 s	4370967	832	1147.8	142.08	624	XIC(142.08±500ppm)
2,5-Cyclohexadiene-1,4-dione, 2,6-bis(1,1-dimethylethyl)-	1239.96 s, 1.314 s	4355313	897	1478.9	41.06	1464	XIC(41.06±500ppm)
Deprenyl	1034.97 s, 1.218 s	4339908	723	1272.7	96.09	1082	XIC(96.09±500ppm)
Benzothiazole, 2-(m-tolyl)-	1489.95 s, 0.999 s	4307702	718	1768.8	225.28	1061	XIC(225.28±500ppm)
Terbutaline, N-trifluoroacetyl-O,O,o-tris(trimethylsilyl)deriv.	2729.87 s, 0.538 s	4286529	708	3420.1	355.1	732	XIC(355.10±500ppm)
Hexanedioic acid, 2TMS derivative	1269.96 s, 1.094 s	4206017	753	1511.1	111.06	538	XIC(111.06±500ppm)
Homosalate, TMS derivative	1554.94 s, 1.354 s	4166310	710	1853.3	195.07	576	XIC(195.07±500ppm)
N-Ethylamphetamine, N-trimethylsilyl-	1724.93 s, 1.442 s	4082626	720	2080	144.12	779	XIC(144.12±500ppm)
Malto, TMS derivative	1024.98 s, 1.391 s	4048449	791	1263.6	183.07	987	XIC(183.07±500ppm)
Cycluron	1284.96 s, 1.851 s	3904591	735	1527.8	72.05	730	XIC(72.05±500ppm)
2-(2-(2-Ethoxyethoxy)ethoxy)ethyl benzoate	1534.94 s, 1.522 s	3868330	726	1826.7	73.06	637	XIC(73.06±500ppm)
2,5-Dichlorophenol, trimethylsilyl ether	1139.97 s, 1.207 s	3771602	827	1375	93	1775	XIC(93.00±500ppm)
Cycloctetrasiloxane, octamethyl-	709.996 s, 0.722 s	3756911	834	1003.7	281.07	1015	XIC(281.07±500ppm)
2-Hydroxy-2-methylbutyric acid, 2TMS derivative	889.984 s, 0.834 s	3692398	717	1143.5	145.12	1556	XIC(145.12±500ppm)
Bisphenol AF, bis(trimethylsilyl) ether	1684.93 s, 1.054 s	3681883	734	2026.7	411.19	2395	XIC(411.19±500ppm)
Benzene, 1,1'-(1,2-cyclobutanediyl)bis-, cis-	1444.95 s, 1.859 s	3674947	750	1712.5	104.07	704	XIC(104.07±500ppm)
3,7-dioxa-2,8-disilaonane, 2,2,5,5,8,8-hexamethyl-4-(1-methylethyl)-	1079.97 s, 0.811 s	3647327	714	1315	145.12	742	XIC(145.12±500ppm)
Triethanolamine, 3TMS derivative	1384.95 s, 0.907 s	3587873	793	1641.2	262.19	1796	XIC(262.19±500ppm)
1-Triethylsilyloxyundecane	1204.96 s, 1.145 s	3403638	723	1442.1	257.09	1237	XIC(257.09±500ppm)
4H-Pyran-4-one, 2-methoxy-6-methyl-	1004.98 s, 0.584 s	3304446	713	1245.5	69.01	755	XIC(69.01±500ppm)
Monomethyl succinate, trimethylsilyl ester	934.981 s, 1.227 s	3294543	726	1182.6	89.05	541	XIC(89.05±500ppm)
4,8-Dimethyl-2-hydroxyquinoline, tert-butylidimethylsilyl ether	989.978 s, 0.976 s	3107421	742	1231.8	230.14	1492	XIC(230.14±500ppm)
Phosphine, [2-(6-methyl-2-pyridyl)ethyl]-(phenyl)-[3-(di-t-butylphosphino)propyl]-	2224.9 s, 1.723 s	3073933	715	2746.7	358.18	517	XIC(358.18±500ppm)
1,2-Epoxy-3-propyl trifluoroacetate	1014.98 s, 0.582 s	2917807	705	1254.5	69.01	676	XIC(69.01±500ppm)
1-Isopropoxy-2-trihexylsilyloxybenzene	1619.94 s, 1.098 s	2887053	713	1940	307.24	518	XIC(307.24±500ppm)
Pyrene	1764.93 s, 2.651 s	2822690	924	2133.3	202.1	798	XIC(202.10±500ppm)
Benzene, 1,4-dimethoxy-2-methyl-	1014.98 s, 1.563 s	2767704	849	1254.5	137.08	1031	XIC(137.08±500ppm)
2,5-Pyrrolidinedione, 3-(1-chloroethyl)-4-methyl-	1044.97 s, 0.583 s	2708290	704	1281.8	69.01	556	XIC(69.01±500ppm)

2-Mercapto-4,6-dimethylnicotinonitrile, TBDMS derivative	1099.97 s, 0.813 s	2599890	710	1335	221.11	835	XIC(221.11±500ppm)
1,3-Dioxane, 2,2-dimethyl-5-trimethylsilyloxy-	999.977 s, 1.325 s	2592845	752	1240.9	131.07	593	XIC(131.07±500ppm)
Alizarin, 2TMS derivative	1699.93 s, 1.044 s	2558336	763	2046.7	369.14	668	XIC(369.14±500ppm)
Isophthalic acid, 2-isopropylphenyl propyl ester	814.989 s, 0.873 s	2480320	728	1081.5	191.11	525	XIC(191.11±500ppm)
3,5-di-tert-Butyl-4-hydroxyacetophenone	1539.94 s, 1.614 s	2460463	779	1833.3	233.18	510	XIC(233.18±500ppm)
Syringic acid, 2TMS derivative	1599.94 s, 1.358 s	2416157	763	1913.3	327.14	693	XIC(327.14±500ppm)
2-Pyrrolidone-5-carboxylic acid, TBDMS derivative	1174.97 s, 1.620 s	2101538	710	1410.5	186.08	789	XIC(186.08±500ppm)
2,5-Dimethoxyphenol, TMS	1209.96 s, 1.384 s	2044168	722	1447.4	196.08	929	XIC(196.08±500ppm)
2,5-cyclohexadiene-1,4-dione, 2-(1,1-dimethylethyl)-5-(2-methyl-2-propen-1-yl)-	1249.96 s, 1.281 s	1964385	761	1489.5	161.11	722	XIC(161.11±500ppm)
3,5-di-tert-Butyl-4-hydroxybenzaldehyde	1499.94 s, 1.628 s	1960198	789	1781.3	219.16	564	XIC(219.16±500ppm)
Cyclohexene, 3,3-dimethyl-1-(trimethylsilyloxy)-	1069.97 s, 1.380 s	1959275	709	1305	73.06	542	XIC(73.06±500ppm)
4-Mercaptophenol, 2TMS derivative	1929.92 s, 1.358 s	1901512	714	2353.4	270.16	667	XIC(270.16±500ppm)
Benzothiazole	994.977 s, 1.962 s	1876770	897	1236.4	135.03	611	XIC(135.03±500ppm)
1,3-Benzodioxole, 4-methoxy-6-(2-propenyl)-	1339.96 s, 1.949 s	1775023	715	1588.9	165.07	646	XIC(165.07±500ppm)
2H-1-Benzopyran-3-carbonitrile, 2-oxo-	939.981 s, 1.294 s	1624695	755	1187	171.07	542	XIC(171.07±500ppm)
2,3-Dimethoxyphenol, TMS	1224.96 s, 1.403 s	1546610	795	1463.2	196.08	646	XIC(196.08±500ppm)
1,3-2H-Isobenzofuranone, 3,3,7-trimethyl-	1284.96 s, 1.750 s	1545487	758	1527.8	161.08	645	XIC(161.08±500ppm)
1,3-bis[(Trimethylsilyl)ethynyl]benzene	1144.97 s, 0.944 s	1264808	733	1380	255.12	555	XIC(255.12±500ppm)
Cyclotrisiloxane, 2,4-dimethyl-2,4,6,6-tetrahenyl-	1984.91 s, 3.750 s	991991	789	2426.7	377.09	724	XIC(377.09±500ppm)

IRON GALL INK	R.T. (s)	Area	Similarity	Retention	Base Mass	Peak S/N	Quant Masses
(2,5-Dimethoxyphenyl)acetone	1329.96 s, 1.909 s	58672662	901	1577.8	151.1	3354	XIC(151.10±500ppm)
(3-Hydroxy-4-methoxyphenyl)ethylene glycol tris(trimethylsilyl) ether	2414.89 s, 3.049 s	46032672	735	3000.1	297.13	1585	XIC(297.13±500ppm)
(5S,8R,8aS)-8-Ethyl-5-((Z)-penta-2,4-dien-1-yl)octahydroindolizine	1984.91 s, 2.659 s	28478538	737	2426.7	152.09	2959	XIC(152.09±500ppm)
(9H-fluoren-9-yl)methanol, O-methoxycarbonyl-	1614.94 s, 1.996 s	79050021	747	1933.3	178.1	6278	XIC(178.10±500ppm)
(Methoxymethyl)trimethylsilane	919.982 s, 0.853 s	64210283	745	1169.6	73.06	1562	XIC(73.06±500ppm)
(R*,S*)-2,3-Dihydroxybutanoic acid, tris(trimethylsilyl) deriv.	1124.97 s, 0.862 s	15380771	911	1360	73.06	686	XIC(73.06±500ppm)
(S)-(-)-1,1'-Bi-2-naphthol, O,O'-bis(trimethylsilyl)-	1469.95 s, 0.931 s	771408	702	1743.8	430.25	695	XIC(430.25±500ppm)
(Z)-5-Methoxy-3,5-dimethyl-2-hexenyltrimethylsilane	2314.89 s, 0.490 s	63331392	824	2866.7	73.06	855	XIC(73.06±500ppm)
1-(2,5-Dimethoxyphenyl)-1-[(trimethylsilyl)oxy]propan-2-amine	1434.95 s, 1.434 s	36755849	748	1700	73.06	4479	XIC(73.06±500ppm)
1-(2-Methoxyethoxy)-2-methyl-2-propanol, methyl ether	2954.85 s, 0.488 s	48471856	807	3720.1	73.06	905	XIC(73.06±500ppm)
1-(5-Bicyclo[2.2.1]heptyl)ethylamine	769.992 s, 0.403 s	44778619	700	1048.1	44.01	1058	XIC(44.01±500ppm)
1,2,3,4-Butanetetrol, [S-(R*,R*)]-	1289.96 s, 1.053 s	10000713	876	1533.3	44.05	529	XIC(44.05±500ppm)
1,2,3-Benzenetriol	2444.88 s, 0.605 s	4093074	705	3040.1	126.05	573	XIC(126.05±500ppm)
1,2,3-Butanetriol, 3TMS derivative	1074.97 s, 0.790 s	63600256	938	1310	73.06	3904	XIC(73.06±500ppm)
1,2-Butanediol, 2TMS derivative	854.986 s, 0.786 s	6658628	750	1113	73.06	895	XIC(73.06±500ppm)
1,2-Ethenediol, 2TMS derivative	679.997 s, 0.867 s	25393112	727	981.5	73.06	2665	XIC(73.06±500ppm)
1,3-Butanediol, 2TMS derivative	824.988 s, 0.812 s	11599627	876	1088.9	73.06	1235	XIC(73.06±500ppm)
1,3-Dioxolane-2-methanol	1544.94 s, 0.834 s	4.6E+08	776	1840	73.06	3093	XIC(73.06±500ppm)
1,3-Dipentyl-heptabarbital	2099.91 s, 0.920 s	14397649	749	2580	361.21	2369	XIC(361.21±500ppm)
1,3-Propanediol, 2TMS derivative	789.99 s, 0.826 s	2.58E+08	895	1063	147.09	14856	XIC(147.09±500ppm)
1,3-Propanediol, TMS derivative	779.991 s, 1.108 s	1.19E+08	743	1055.6	75.03	621	XIC(75.03±500ppm)
1,4-Butanediol, 2TMS derivative	919.982 s, 0.862 s	48106368	766	1169.6	147.09	2160	XIC(147.09±500ppm)
1,5-Anhydroglucitol, 4TMS derivative	1654.94 s, 0.885 s	2.77E+08	784	1986.7	73.06	1307	XIC(73.06±500ppm)
1,6-Dioxacyclododecane-7,12-dione	1309.96 s, 2.072 s	2.05E+08	929	1555.6	55.06	4409	XIC(55.06±500ppm)
1,7,7-Trimethyl-3-phenethylidenebicyclo[2.2.1]heptan-2-one	2019.91 s, 1.800 s	2873100	700	2473.4	254.24	584	XIC(254.24±500ppm)
11-Methyldodecanol	814.989 s, 0.836 s	43714154	792	1081.5	43.08	1418	XIC(43.08±500ppm)
1-Aminocyclopentanecarboxylic acid, 3-chloropropoxycarbonyl-, tridecyl ester	2119.91 s, 0.897 s	2.71E+08	762	2606.7	204.11	682	XIC(204.11±500ppm)
1-Hexadecanol, TMS derivative	1634.94 s, 1.009 s	17482193	812	1960	75.04	2710	XIC(75.04±500ppm)
1-Hexanol, 2-ethyl-	1444.95 s, 0.962 s	1.24E+08	769	1712.5	57.09	5457	XIC(57.09±500ppm)
1-Methoxy-2-propanol, TMS derivative	979.978 s, 1.476 s	76000708	756	1222.7	117.05	7233	XIC(117.05±500ppm)
1-Monocetin, 2O-TMS	1094.97 s, 0.969 s	2.54E+08	933	1330	43.04	3951	XIC(43.04±500ppm)
1-Monomyrstin, 2TMS derivative	1929.92 s, 1.110 s	14343842	875	2353.4	73.06	5572	XIC(73.06±500ppm)
1-Monopalmitin, 2TMS derivative	2044.91 s, 1.166 s	2.4E+08	889	2506.7	73.06	1521	XIC(73.06±500ppm)
1-Nonene, 4,6,8-trimethyl-	994.977 s, 0.874 s	5944133	843	1236.4	57.09	625	XIC(57.09±500ppm)
1-Octadecanol, TMS derivative	1774.93 s, 1.031 s	41781589	824	2146.7	75.04	960	XIC(75.04±500ppm)
1-Octanol, 2-butyl-	864.986 s, 0.859 s	6325061	764	1121.7	43.08	751	XIC(43.08±500ppm)
1-Tetradecene	949.98 s, 0.919 s	16190440	924	1195.7	43.08	1095	XIC(43.08±500ppm)
2-(2,5-Dimethoxy-phenyl)-propionaldehyde	1309.96 s, 1.811 s	39221296	857	1555.6	165.12	4215	XIC(165.12±500ppm)
2,2'-Bipyridine	1214.96 s, 2.018 s	16819761	941	1452.6	156.09	2204	XIC(156.09±500ppm)
2,2-Dimethyl-5-[2-(2-trimethylsilyloxyethoxy)-propyl]-[1,3]dioxolane-4-carboxaldehyde	2034.91 s, 1.461 s	23410938	704	2493.4	73.06	1052	XIC(73.06±500ppm)
2,3,4,5-Tetrahydroxypentanoic acid-1,4-lactone, tris(trimethylsilyl)-	1394.95 s, 1.035 s	2.03E+08	911	1652.9	73.06	3636	XIC(73.06±500ppm)
2,3,4-Trihydroxybutyric acid tetrakis(trimethylsilyl) deriv., (, (R*,R*)-)	1319.96 s, 0.858 s	97496379	931	1566.7	73.06	4787	XIC(73.06±500ppm)
2,3-Butanediol, 2TMS derivative	759.992 s, 0.791 s	4.09E+08	938	1040.7	117.09	16078	XIC(117.09±500ppm)
2,4'-Bipyridine	1304.96 s, 2.173 s	36576757	916	1550	156.09	2194	XIC(156.09±500ppm)
2,4-Di-tert-butylphenol	1274.96 s, 1.362 s	7301224	882	1516.7	191.17	1954	XIC(191.17±500ppm)
2,4-Di-tert-butylphenoxymethyltrimethylsilane	1209.96 s, 1.064 s	42989695	818	1555.6	263.22	10177	XIC(263.22±500ppm)
2,5-Cyclohexadiene-1,4-dione, 2,6-bis(1,1-dimethylethyl)-	1239.96 s, 1.315 s	4669749	882	1478.9	41.06	1263	XIC(41.06±500ppm)
2,5-Dichlorophenol, trimethylsilyl ether	1139.97 s, 1.209 s	3966533	833	1375	93.01	1326	XIC(93.01±500ppm)
2,5-Dimethoxybenzhydrazide	1384.95 s, 1.988 s	1.06E+08	827	1641.2	165.08	13083	XIC(165.08±500ppm)
2,5-Dimethoxymandelic acid, di-TMS	1719.93 s, 1.822 s	5699814	752	2073.3	239.14	810	XIC(239.14±500ppm)
2,5-Dimethoxyphenol, TMS	1209.96 s, 1.380 s	5068495	798	1447.4	196.09	1620	XIC(196.09±500ppm)
2-[[tert-Butyl(dimethylsilyl)oxy]ethanol	799.99 s, 0.989 s	2.81E+08	805	1070.4	75.04	1397	XIC(75.04±500ppm)
2-Allyl-1,4-dimethoxybenzene	1204.96 s, 1.649 s	26520086	876	1442.1	178.13	6782	XIC(178.13±500ppm)
2-Decene, 7-methyl-, (Z)-	1089.97 s, 0.900 s	34530542	769	1325	43.07	2772	XIC(43.07±500ppm)
2-Ethylhexanal ethylene glycol acetal	1584.94 s, 0.859 s	3E+08	721	1893.3	73.07	1009	XIC(73.07±500ppm)
2-Furoic acid, TMS derivative	884.984 s, 1.280 s	5706431	700	1139.1	125.06	795	XIC(125.06±500ppm)
2-Hydroxy-4-methoxybenzaldehyde, TBDMS derivative	1664.93 s, 1.987 s	16610019	746	2000	209.09	1369	XIC(209.09±500ppm)
2-Hydroxyglutaric acid, 5 ethyl ester, 2TMS	1294.96 s, 1.083 s	6770251	805	1538.9	85.05	1047	XIC(85.05±500ppm)
2-Isopropyl-5-methyl-1-heptanol	1074.97 s, 0.897 s	43029256	848	1310	43.08	2916	XIC(43.08±500ppm)
2-Methyl-6-propylpyridine	989.978 s, 1.285 s	3478656	747	1231.8	107.09	677	XIC(107.09±500ppm)
2-Palmitoylglycerol, 2TMS derivative	2024.91 s, 1.154 s	90631622	859	2480	73.06	1362	XIC(73.06±500ppm)
2-Pentamethylsilyloxybutane	929.981 s, 0.824 s	31959865	718	1178.3	75.06	816	XIC(75.06±500ppm)
2-Propenoic acid, 2-methyl-, 3,3,5-trimethylcyclohexyl ester	1114.97 s, 1.194 s	36918424	906	1350	69.07	3691	XIC(69.07±500ppm)
2-Pyridinemethanol, TBDMS derivative	939.981 s, 1.233 s	15210923	801	1187	166.1	4408	XIC(166.10±500ppm)
2-Pyrrolidinone, 5-(cyclohexylmethyl)-	1214.96 s, 2.097 s	5892726	893	1452.6	84.06	1167	XIC(84.06±500ppm)
2-Tributylsilyloxybut-3-yne	894.984 s, 1.352 s	1891010	746	1147.8	155.08	589	XIC(155.08±500ppm)
3,4-Dimethoxymandelic acid, di-TMS	2069.91 s, 2.236 s	45369577	702	2540	239.14	1626	XIC(239.14±500ppm)
3,5-di-tert-Butyl-4-hydroxybenzaldehyde	1499.94 s, 1.629 s	2177637	757	1781.3	219.17	504	XIC(219.17±500ppm)
3,9-Dioxo-2,10-disilaundecane, 2,2,10,10-tetramethyl-5-[[trimethylsilyl]oxy]-	1239.96 s, 0.855 s	925113	735	1478.9	73.05	1126	XIC(73.05±500ppm)
3-Aminopropanephosphonic acid, 3TBDMS derivative	2344.89 s, 2.774 s	1516829	777	2906.7	424.24	589	XIC(424.24±500ppm)
3-Ethylphenol, TMS derivative	1004.98 s, 1.116 s	1596868	742	1245.5	179.12	719	XIC(179.12±500ppm)
3-Heptanol, TMS derivative	924.982 s, 1.496 s	7664579	736	1173.9	131.04	1676	XIC(131.04±500ppm)
3-Hydroxybenzoic acid, 2TMS derivative	1324.96 s, 1.163 s	31267195	881	1572.2	73.06	975	XIC(73.06±500ppm)
3-Methyl-2-furoic acid, TMS derivative	1084.97 s, 1.390 s	46957960	738	1320	183.08	5505	XIC(183.08±500ppm)
3-Pyridinecarboxylic acid, 1,4,5,6-tetrahydro-4-[[[4-methoxyphenyl]amino]carbonyl]-2-methyl-	1829.92 s, 2.319 s	39867575	700	2220	123.09	1993	XIC(123.09±500ppm)
3-Pyridinol	884.984 s, 1.499 s	22669047	954	1139.1	95.05	1518	XIC(95.05±500ppm)
3-Pyridinol, TMS derivative	759.992 s, 1.078 s	64224830	778	1040.7	152.07	3563	XIC(152.07±500ppm)
3-Pyridylcarbinol, trimethylsilyl ether	1019.98 s, 1.246 s	3192051	808	1259.1	166.1	921	XIC(166.10±500ppm)
3-Ureidopropionic acid, tert.-butyldimethylsilyl ester	1189.96 s, 0.953 s	59307748	700	1426.3	73.06	2410	XIC(73.06±500ppm)

4-Chloro-3-methylphenol, trimethylsilyl ether	1094.97 s, 1.176 s	2.86E+08	900	1330	199.06	5466	XIC(199.06±500ppm)
4-Hydroxybenzaldehyde, TMS derivative	1144.97 s, 1.391 s	1627536	767	1380	179.08	591	XIC(179.08±500ppm)
4-Hydroxybenzeneacetic acid, 2TMS derivative	1389.95 s, 1.213 s	19973889	814	1647.1	73.06	820	XIC(73.06±500ppm)
4-Hydroxybenzoic acid, 2TMS derivative	1369.95 s, 1.067 s	3318123	780	1623.5	267.13	1133	XIC(267.13±500ppm)
4-Hydroxybutanoic acid, 2TMS derivative	1269.96 s, 1.213 s	10917162	700	1511.1	117.06	1146	XIC(117.06±500ppm)
4-Methoxymandelic acid, ethyl ester, TMS	1319.96 s, 1.463 s	3352127	743	1566.7	209.09	1199	XIC(209.09±500ppm)
4-Methyl-1,2-bis(trimethylsilyloxy)pentane	694.996 s, 0.825 s	38401530	787	992.6	73.06	1117	XIC(73.06±500ppm)
4-Methylvaleric acid, TMS derivative	834.988 s, 1.054 s	83746553	773	1096.3	73.06	4587	XIC(73.06±500ppm)
5-Hydroxymethylfurfural	1079.97 s, 1.600 s	1887551	863	1315	97.05	512	XIC(97.05±500ppm)
5-Oxotetrahydrofuran-2-carboxylic acid, ethyl ester	1069.97 s, 2.104 s	31262916	913	1305	85.04	1524	XIC(85.04±500ppm)
6-Methoxy-3-methylbenzofuran	1139.97 s, 1.712 s	13342580	815	1375	162.09	3583	XIC(162.09±500ppm)
6-Methylisoeugenol	1884.92 s, 0.686 s	1893770	703	2293.4	178.13	563	XIC(178.13±500ppm)
7,9-Diethyl-2,4-bis(dimethylamino)-10-imino-8-thio-1,7,9-triazaspiro[4.5]-1,3-decadiene-6,8	1959.92 s, 1.951 s	11401775	701	2393.4	73.06	515	XIC(73.06±500ppm)
7,9-Di-tert-butyl-1-oxaspiro[4.5]deca-6,9-diene-2,8-dione	1614.94 s, 1.659 s	29704821	920	1933.3	57.09	2084	XIC(57.09±500ppm)
9,9-Dimethyl-9-sila-9,10-dihydrophenanthrene	1334.96 s, 1.475 s	1293514	700	1583.3	73.06	810	XIC(73.06±500ppm)
Abietic acid, TMS derivative	1949.92 s, 1.634 s	17004165	865	2380	256.25	2125	XIC(256.25±500ppm)
Acetamide, 2,2,2-trifluoro-	684.997 s, 0.682 s	17546222	726	985.2	44.03	619	XIC(44.03±500ppm)
Acetic acid, 2-phenylethyl ester	1024.98 s, 1.552 s	2497794	953	1263.6	104.08	702	XIC(104.08±500ppm)
Acetin, bis-1,3-trimethylsilyl ether	1079.97 s, 0.970 s	71540142	924	1315	73.06	2589	XIC(73.06±500ppm)
Acetoxycetic acid, TBDMS derivative	824.988 s, 1.071 s	8258046	763	1088.9	43.04	657	XIC(43.04±500ppm)
Arabinofuranose, 1,2,3,5-tetrakis-O-(trimethylsilyl)-	1369.95 s, 0.860 s	6347161	767	1623.5	73.06	828	XIC(73.06±500ppm)
Arachidic acid, TMS derivative	1949.92 s, 1.186 s	4427562	895	2380	73.06	874	XIC(73.06±500ppm)
Benzaldehyde, 2,4-dimethyl-	979.978 s, 1.678 s	2497035	927	1222.7	133.09	600	XIC(133.09±500ppm)
Benzaldehyde, 2,5-dimethoxy-	1229.96 s, 0.921 s	9.01E+08	924	1468.4	166.08	14347	XIC(166.08±500ppm)
Benzaldehyde, 2-hydroxy-5-methoxy-	1064.97 s, 1.784 s	1993772	894	1300	152.07	668	XIC(152.07±500ppm)
Benzene, (1-methyldecyl)-	1439.95 s, 1.229 s	5892888	801	1706.2	105.09	788	XIC(105.09±500ppm)
Benzene, 1,4-dimethoxy-	919.982 s, 1.619 s	3537899	872	1169.6	123.07	1380	XIC(123.07±500ppm)
Benzene, 1,4-dimethoxy-2-methyl-	1014.98 s, 1.560 s	2059968	857	1254.5	137.08	984	XIC(137.08±500ppm)
Benzene, 4-ethenyl-1,2-dimethoxy-	1134.97 s, 1.665 s	1603204	783	1370	164.11	701	XIC(164.11±500ppm)
Benzenethanamine, N-[(pentafluorophenyl)methylene]-4-[(trimethylsilyloxy)-	1329.96 s, 1.106 s	10844176	741	1577.8	179.12	2797	XIC(179.12±500ppm)
Benzenepropanoic acid, 3,5-bis(1,1-dimethylethyl)-4-hydroxy-, methyl ester	1629.94 s, 1.563 s	10056483	845	1953.3	277.22	2519	XIC(277.22±500ppm)
Benzenepropanoic acid, 3,5-bis(1,1-dimethylethyl)-4-hydroxy-, octadecyl ester	2734.87 s, 0.970 s	38267856	726	3426.8	57.09	921	XIC(57.09±500ppm)
Benzoic acid, 4-(4-pentylcyclohexyl)-, 4'-cyano[1,1'-biphenyl]-4-yl ester	2079.91 s, 0.988 s	16098019	746	2553.4	257.14	1954	XIC(257.14±500ppm)
Benzoic acid, TMS derivative	1009.98 s, 1.250 s	30048769	903	1250	105.05	6808	XIC(105.05±500ppm)
Benzothiazole	994.977 s, 1.962 s	7496001	937	1236.4	135.04	1809	XIC(135.04±500ppm)
Benzyl alcohol, TMS derivative	904.983 s, 1.143 s	11905150	860	1156.5	91.07	821	XIC(91.07±500ppm)
Butane, 2-nitro-	1259.96 s, 0.951 s	1.57E+08	748	1500	57.08	728	XIC(57.08±500ppm)
Butanedioic acid, 2TMS derivative	1084.97 s, 1.059 s	2.77E+08	941	1320	147.09	15897	XIC(147.09±500ppm)
Butanedioic acid, diethyl ester	934.981 s, 1.417 s	7848970	919	1182.6	101.04	1340	XIC(101.04±500ppm)
Butanoic acid, 3,4-bis[(trimethylsilyloxy)-, trimethylsilyl ester	1209.96 s, 0.895 s	14606224	888	1447.4	73.06	747	XIC(73.06±500ppm)
Butylated Hydroxytoluene	1279.96 s, 1.318 s	4309363	817	1522.2	205.19	1049	XIC(205.19±500ppm)
Cetene	1344.95 s, 0.994 s	34466807	863	1594.4	43.08	1549	XIC(43.08±500ppm)
Cinnamic acid, TMS derivative	1304.96 s, 1.402 s	18810108	884	1550	131.07	3424	XIC(131.07±500ppm)
Citric acid 3TMS	1519.94 s, 1.086 s	5.6E+08	837	1806.7	73.06	4139	XIC(73.06±500ppm)
Citric acid, 4TMS derivative	1519.94 s, 1.028 s	1.86E+08	844	1806.7	147.09	3334	XIC(147.09±500ppm)
Cyanoic acid, ethyl ester	1544.94 s, 1.700 s	6.45E+08	756	1840	71.09	4128	XIC(71.09±500ppm)
Cycloheptasiloxane, tetradecamethyl-	1259.96 s, 0.745 s	20264500	895	1500	73.06	1374	XIC(73.06±500ppm)
Cyclohexane, nonadecyl-	2254.9 s, 1.629 s	5423144	850	2786.7	82.09	624	XIC(82.09±500ppm)
Cyclohexasiloxane, dodecamethyl-	1094.97 s, 0.731 s	51205685	887	1330	73.06	3941	XIC(73.06±500ppm)
Cyclohexene, 3-butyl-3-methyl-1-trimethylsilyloxy-	2049.91 s, 2.164 s	1085586	738	2513.4	73.06	506	XIC(73.06±500ppm)
Cyclopentasiloxane, decamethyl-	889.984 s, 0.735 s	3677152	869	1143.5	73.06	501	XIC(73.06±500ppm)
Cyclotetrasiloxane, octamethyl-	704.996 s, 0.728 s	7367802	909	1000	281.09	1721	XIC(281.09±500ppm)
Cyclotrisiloxane, 2,4-dimethyl-2,4,6,6-tetrahenyl-	2454.88 s, 2.022 s	1102663	766	3053.4	377.1	526	XIC(377.10±500ppm)
Cyclotrisiloxane, hexamethyl-	679.997 s, 0.801 s	19769778	772	981.5	207.06	4623	XIC(207.06±500ppm)
Cytosine	1854.92 s, 2.596 s	16116336	748	2253.4	111.08	2182	XIC(111.08±500ppm)
D-(-)-Erythroranose, tris(trimethylsilyl) ether (isomer 1)	1394.95 s, 0.859 s	66085838	744	1652.9	73.06	2496	XIC(73.06±500ppm)
D-(-)-Fructofuranose, pentakis(trimethylsilyl) ether (isomer 1)	1539.94 s, 0.834 s	1.94E+08	938	1833.3	73.06	13989	XIC(73.06±500ppm)
D-(-)-Lactic acid, trimethylsilyl ether	714.995 s, 1.000 s	3.59E+08	833	1007.4	73.06	2731	XIC(73.06±500ppm)
D-(-)-Ribofuranose, tetrakis(trimethylsilyl) ether (isomer 1)	1654.94 s, 1.026 s	1.13E+09	830	1986.7	73.06	2480	XIC(73.06±500ppm)
D-(-)-Ribofuranose, tetrakis(trimethylsilyl) ether (isomer 2)	1084.97 s, 0.833 s	2271984	738	1320	217.14	898	XIC(217.14±500ppm)
D-(-)-Tagatofuranose, pentakis(trimethylsilyl) ether (isomer 2)	1904.92 s, 0.655 s	20666087	758	2320	73.06	1031	XIC(73.06±500ppm)
D-(+)-Galactopyranose, 5TMS derivative (isomer 2)	1609.94 s, 0.870 s	2.87E+08	929	1926.7	73.05	2169	XIC(73.05±500ppm)
D-(+)-Ribono-1,4-lactone (R,S,R)-, 3TMS derivative	1409.95 s, 1.058 s	59596393	884	1670.6	73.06	1167	XIC(73.06±500ppm)
D-Allofuranose, pentakis(trimethylsilyl) ether	1709.93 s, 0.849 s	76725652	732	2060	73.06	1640	XIC(73.06±500ppm)
Danthron, 2TMS derivative	2144.9 s, 1.710 s	7079382	842	2640.1	369.18	849	XIC(369.18±500ppm)
Decane	729.994 s, 0.821 s	40654447	877	1018.5	57.09	995	XIC(57.09±500ppm)
Decane, 2,4,6-trimethyl-	899.983 s, 0.820 s	5610741	895	1152.2	43.08	587	XIC(43.08±500ppm)
Decane, 3,7-dimethyl-	959.98 s, 0.837 s	53247514	868	1204.5	57.09	3035	XIC(57.09±500ppm)
Decane, 5,6-dimethyl-	824.988 s, 0.823 s	25759683	909	1088.9	43.08	2663	XIC(43.08±500ppm)
Decyl oleate	2224.9 s, 1.648 s	13651577	859	2746.7	43.08	1110	XIC(43.08±500ppm)
Dehydroabietic acid, TMS derivative	1929.92 s, 1.692 s	15187062	808	2353.4	239.21	1154	XIC(239.21±500ppm)
Deoxyglucose, 4TMS derivative	1524.94 s, 0.908 s	48218150	780	1813.3	73.06	873	XIC(73.06±500ppm)
D-Fucitol, 5TMS derivative	1509.94 s, 0.802 s	11893671	907	1793.8	73.06	961	XIC(73.06±500ppm)
D-Galactose, 5TMS derivative	1869.92 s, 0.848 s	51045230	802	2273.4	73.06	1171	XIC(73.06±500ppm)
D-Glucose, 5TMS derivative	1674.93 s, 0.877 s	2.97E+08	945	2013.3	73.01	2605	XIC(73.01±500ppm)
Diacetin, 2-trimethylsilyl ether	1109.97 s, 1.196 s	8941660	872	1345	43.04	687	XIC(43.04±500ppm)
Diacetone alcohol, TMS derivative	764.992 s, 0.992 s	68200261	907	1044.4	115.07	4892	XIC(115.07±500ppm)
Dibenzofuran	1289.96 s, 1.865 s	1903739	831	1533.3	168.08	643	XIC(168.08±500ppm)
Dibutyl phthalate	1644.94 s, 1.748 s	16206662	911	1973.3	149.05	959	XIC(149.05±500ppm)
Diethylene glycol, 2TMS derivative	1014.98 s, 0.945 s	24410276	943	1254.5	73.06	1468	XIC(73.06±500ppm)

Diethylene glycol, n-butyl ether, trimethylsilyl ether	1109.97 s, 1.070 s	23654244	875	1345	73.06	1121	XIC(73.06±500ppm)
Dimethyl hexopyranosiduronate, α-D-, 3TMS derivative	2139.9 s, 1.034 s	8.53E+08	730	2633.4	217.24	2630	XIC(217.24±500ppm)
Dimethyl phthalate	1224.96 s, 1.951 s	10429307	867	1463.2	163.07	2915	XIC(163.07±500ppm)
Disilane, pentamethyl-	1174.97 s, 1.069 s	1.14E+08	700	1410.5	73.06	1888	XIC(73.06±500ppm)
Disiloxane, hexamethyl-	849.987 s, 0.945 s	12696408	750	1108.7	147.09	1599	XIC(147.09±500ppm)
DL-Arabinopyranose, 4TMS derivative	1409.95 s, 0.899 s	48848898	894	1670.6	73.06	770	XIC(73.06±500ppm)
D-Mannopyranose, 5TMS derivative	2119.91 s, 0.981 s	7.67E+08	755	2606.7	73	2731	XIC(73.00±500ppm)
D-Mannose, 5TMS derivative	1674.93 s, 0.929 s	3.54E+08	758	2013.3	204.12	572	XIC(204.12±500ppm)
Dodecane, 2,6,11-trimethyl-	1009.98 s, 0.864 s	54414666	853	1250	57.09	1714	XIC(57.09±500ppm)
Dodecane, 2,7,10-trimethyl-	1199.96 s, 0.886 s	26405906	867	1436.8	57.09	1346	XIC(57.09±500ppm)
D-Psicofuranose, pentakis(trimethylsilyl) ether (isomer 2)	1484.95 s, 0.889 s	70421609	810	1762.5	73.06	1509	XIC(73.06±500ppm)
D-Xylose, 4TMS derivative	2164.9 s, 1.055 s	5.03E+08	721	2666.7	73.04	3282	XIC(73.04±500ppm)
Eicosane, 1-iodo-	2829.86 s, 3.111 s	4940386	816	3553.4	57.09	531	XIC(57.09±500ppm)
Eicosane, 2-methyl-	2229.9 s, 1.366 s	13632295	882	2753.4	57.09	959	XIC(57.09±500ppm)
Erythro-1,4-lactone, (E)-, 2TMS derivative	1149.97 s, 1.132 s	24888608	895	1385	73.06	1485	XIC(73.06±500ppm)
Erythro-1,4-lactone, 2TMS derivative	1209.96 s, 1.251 s	1.38E+08	928	1447.4	73.06	3488	XIC(73.06±500ppm)
Ethanone, 1-(5-methoxy-2-methyl-3(1H)-indolyl)-	1569.94 s, 2.086 s	31408186	775	1873.3	188.1	3390	XIC(188.10±500ppm)
Ethyl gallate, 3TMS derivative	1634.94 s, 1.169 s	1.51E+08	702	1960	73.06	1593	XIC(73.06±500ppm)
Ethyl glycolate, TBDMS derivative	719.995 s, 1.060 s	7524969	746	1011.1	133.06	722	XIC(133.06±500ppm)
Ethyl α-D-glucopyranoside, 4TMS derivative	1604.94 s, 0.934 s	1.08E+08	754	1920	204.13	2228	XIC(204.13±500ppm)
Fluoranthene	1764.93 s, 2.646 s	2450409	917	2133.3	202.11	714	XIC(202.11±500ppm)
Galactopyranose, 5TMS derivative	2124.9 s, 0.977 s	1.51E+09	741	2613.4	204.16	1410	XIC(204.16±500ppm)
Gallacetophenone-4'-methylether	2334.89 s, 0.556 s	6.09E+08	700	2893.4	167.04	887	XIC(167.04±500ppm)
Gallic acid, 4TMS derivative	1644.94 s, 1.075 s	4.84E+08	863	1973.3	73.05	7167	XIC(73.05±500ppm)
Glyceric acid, 3TMS derivative	1109.97 s, 0.907 s	1.29E+08	907	1345	73.06	4141	XIC(73.06±500ppm)
Glycerol monostearate, 2TMS derivative	2144.9 s, 1.266 s	58069805	779	2640.1	43.08	1325	XIC(43.08±500ppm)
Glycerol, 1,2-di(TMS)-	959.98 s, 0.935 s	20451721	878	1204.5	73.06	1581	XIC(73.06±500ppm)
Glycerol, 3TMS derivative	1049.97 s, 0.793 s	2.44E+08	934	1286.4	73.05	1723	XIC(73.05±500ppm)
Glycine	699.996 s, 0.770 s	30999768	738	996.3	75.03	611	XIC(75.03±500ppm)
Glycolic acid, 2TBDMS derivative	1164.97 s, 1.174 s	16546163	739	1400	73.06	699	XIC(73.06±500ppm)
Glycolic acid, 2TMS derivative	814.989 s, 0.945 s	64872174	872	1081.5	73.06	4069	XIC(73.06±500ppm)
Glyoxime, 2TMS derivative	994.977 s, 1.003 s	17915551	725	1236.4	73.06	627	XIC(73.06±500ppm)
Glyoxylic acid, phenyl-, 2'-cyanophenyl ester	1299.96 s, 1.380 s	3896982	701	1544.4	105.05	661	XIC(105.05±500ppm)
Gulonic acid, γ-lactone, 4TMS derivavative	1599.94 s, 0.980 s	2.25E+08	727	1913.3	73.06	1756	XIC(73.06±500ppm)
Heneicosane	1359.95 s, 0.945 s	9.64E+08	920	1611.8	57.09	9660	XIC(57.09±500ppm)
Hentriacontane	1799.93 s, 0.994 s	35479663	781	2180	57.09	1124	XIC(57.09±500ppm)
Heptacosane	1299.96 s, 0.914 s	4.74E+08	873	1544.4	57.09	12628	XIC(57.09±500ppm)
Heptadecane	1374.95 s, 0.952 s	1.76E+08	897	1629.4	57.09	1970	XIC(57.09±500ppm)
Heptadecane, 2,6,10,15-tetramethyl-	1189.96 s, 0.880 s	40822304	872	1426.3	57.09	2013	XIC(57.09±500ppm)
Heptane, 2,2,4,6,6-pentamethyl-	689.997 s, 0.818 s	24201312	829	988.9	57.09	866	XIC(57.09±500ppm)
Heptanoic acid, TMS derivative	924.982 s, 0.962 s	6360582	818	1173.9	73.06	812	XIC(73.06±500ppm)
Heptasiloxane, hexadecamethyl-	1329.96 s, 0.732 s	7091857	872	1577.8	73.06	1235	XIC(73.06±500ppm)
Hexadecane	1139.97 s, 0.906 s	23119889	862	1375	43.08	2036	XIC(43.08±500ppm)
Hexadecane, 2,6,10,14-tetramethyl-	1809.93 s, 0.994 s	1.53E+08	843	2193.4	57.09	2286	XIC(57.09±500ppm)
Hexadecane, 2,6,11,15-tetramethyl-	1119.97 s, 0.890 s	75836748	883	1355	43.08	8656	XIC(43.08±500ppm)
Hexadecanoic acid, 2-hydroxy-1-(hydroxymethyl)ethyl ester	1994.91 s, 1.717 s	4660791	775	2440	43.08	870	XIC(43.08±500ppm)
Hexaethylene glycol, 2TMS derivative	1024.98 s, 0.943 s	18089196	769	1263.6	73.06	917	XIC(73.06±500ppm)
Hexanoic acid, TMS derivative	804.989 s, 0.952 s	20659380	805	1074.1	73.06	1651	XIC(73.06±500ppm)
Hexasiloxane, tetradecamethyl-	1179.97 s, 0.728 s	4552135	893	1415.8	73.06	553	XIC(73.06±500ppm)
Hexatriacontane	2249.9 s, 1.446 s	1.2E+08	939	2780.1	57.09	5295	XIC(57.09±500ppm)
Hexopyranose, 5TMS derivative	2649.87 s, 1.755 s	7.73E+08	745	3313.4	73.06	7505	XIC(73.06±500ppm)
Hydracrylic acid, 2TMS derivative	899.983 s, 0.933 s	57043130	897	1152.2	147.09	3383	XIC(147.09±500ppm)
Hydroquinone, 2TMS derivative	1174.97 s, 1.033 s	47286151	830	1410.5	239.12	8560	XIC(239.12±500ppm)
Hydroquinone, TMS derivative	1119.97 s, 1.375 s	18322450	823	1355	167.08	2330	XIC(167.08±500ppm)
Ionic acid, γ-lactone, 4TMS derivavative	1624.94 s, 0.975 s	2.55E+08	860	1946.7	73.06	1966	XIC(73.06±500ppm)
Inosose-2, 1,3,4,5,6-pentakis-O-(trimethylsilyl)-, myo-	1754.93 s, 0.852 s	2.92E+08	744	2120	73.06	5776	XIC(73.06±500ppm)
Isopimaric acid, TMS	1899.92 s, 1.538 s	11138042	860	2313.4	73.06	984	XIC(73.06±500ppm)
Isoquinolinium, 2-methyl-1-phenyl-, iodide	2729.87 s, 1.956 s	1.3E+09	772	3420.1	204.09	512	XIC(204.09±500ppm)
Itaconic acid, 2TMS derivative	1114.97 s, 1.088 s	10579887	920	1350	147.09	536	XIC(147.09±500ppm)
L-(-)-Arabitol, 5TMS derivative	1474.95 s, 0.804 s	1.87E+08	914	1750	73.06	3478	XIC(73.06±500ppm)
L-(-)-Sorbofuranose, pentakis(trimethylsilyl) ether	2229.9 s, 1.132 s	57744866	729	2753.4	73.06	896	XIC(73.06±500ppm)
L-(+)-Threose, tris(trimethylsilyl) ether, ethyloxime (isomer 1)	1064.97 s, 0.980 s	23211974	722	1300	73.06	1306	XIC(73.06±500ppm)
L-5-Oxoprolone, , 2TMS derivative	1249.96 s, 1.150 s	68290216	736	1489.5	73.06	1453	XIC(73.06±500ppm)
Lactic Acid, 2TMS derivative	794.99 s, 2.219 s	2.64E+08	951	1066.7	73.06	1924	XIC(73.06±500ppm)
Lapachol, trimethylsilyl ether	1609.94 s, 1.386 s	8.52E+08	700	1926.7	73.05	1400	XIC(73.05±500ppm)
Levoglucofan, 3TMS derivative	1454.95 s, 1.050 s	1.61E+08	921	1725	73.06	3316	XIC(73.06±500ppm)
L-Norvaline, n-propargyloxycarbonyl-, isohexyl ester	829.988 s, 1.411 s	23410164	727	1092.6	154.06	3767	XIC(154.06±500ppm)
L-Rhamnose, 4TMS derivative	1394.95 s, 0.867 s	67886950	746	1652.9	204.12	654	XIC(204.12±500ppm)
Malic acid 1-ethyl ester, 2TMS	1209.96 s, 1.046 s	47031893	907	1447.4	73.06	1425	XIC(73.06±500ppm)
Malic acid, 3TMS derivative	1264.96 s, 0.960 s	3.06E+08	764	1505.6	73.06	2835	XIC(73.06±500ppm)
Malic acid, 4-ethyl ester, 2TMS	1219.96 s, 1.062 s	2.02E+08	896	1457.9	73.06	4885	XIC(73.06±500ppm)
Maltol, TBDMS derivative	1989.91 s, 1.587 s	31589881	750	2433.4	183.11	1659	XIC(183.11±500ppm)
Maltol, TMS derivative	969.979 s, 1.260 s	1339432	734	1213.6	183.08	531	XIC(183.08±500ppm)
Menthol, TMS derivative	1024.98 s, 0.902 s	1947497	708	1263.6	143.11	513	XIC(143.11±500ppm)
meso-Erythritol, 4TMS derivative	1284.96 s, 0.805 s	3.47E+08	948	1527.8	73.06	6596	XIC(73.06±500ppm)
Metanephrine, 2TMS derivative	1699.93 s, 1.438 s	1.02E+08	752	2046.7	73.06	874	XIC(73.06±500ppm)
Methoxamine	1494.95 s, 2.027 s	3.2E+08	811	1775	44.07	2100	XIC(44.07±500ppm)
Methyl (3,4-dimethoxyphenyl)(hydroxy)acetate, TMS derivative	1809.93 s, 1.752 s	9207867	745	2193.4	239.14	1191	XIC(239.14±500ppm)
Methyl 2,4-dihydroxybenzoate, 2TMS derivative	2164.9 s, 1.641 s	13156771	700	2666.7	73.06	813	XIC(73.06±500ppm)
Methyl galactoside, 3TMS derivative	2054.91 s, 1.456 s	55727230	789	2520	73.06	1032	XIC(73.06±500ppm)

Methyl galactoside, 4TMS derivative	1974.91 s, 1.057 s	1.33E+08	814	2413.4	73.06	3435	XIC(73.06±500ppm)
Methyl α-Lyxofuranoside, 3TMS derivative	1354.95 s, 0.931 s	11095139	702	1605.9	217.13	766	XIC(217.13±500ppm)
Methylsuccinic acid, 2TMS derivative	1099.97 s, 1.011 s	25399646	877	1335	147.09	3535	XIC(147.09±500ppm)
Mevalonolactone, TMS derivative	1139.97 s, 1.545 s	16726883	878	1375	75.04	583	XIC(75.04±500ppm)
Myristic acid, TMS derivative	1554.94 s, 1.062 s	21134102	789	1853.3	117.05	1080	XIC(117.05±500ppm)
N8-(3-Chloro-4-fluorophenyl)-N2-(1-methylpiperidin-4-yl)pyrimido[5,4-d]pyrimidine-2,8-dia	1034.97 s, 1.216 s	2367817	705	1272.7	96.1	583	XIC(96.10±500ppm)
n-Heptadecylcyclohexane	2309.89 s, 1.849 s	4214313	833	2860.1	82.09	527	XIC(82.09±500ppm)
Nonadecane	1214.96 s, 0.921 s	32232257	904	1452.6	57.09	2633	XIC(57.09±500ppm)
Nonadecane, 2-methyl-	2074.91 s, 1.196 s	11611644	868	2546.7	57.09	674	XIC(57.09±500ppm)
Nonanoic acid, TMS derivative	1129.97 s, 0.997 s	24107312	899	1365	73.06	3524	XIC(73.06±500ppm)
Octacosane, 2-methyl-	2869.86 s, 3.261 s	4347132	828	3606.8	57.09	517	XIC(57.09±500ppm)
Octadecane	1269.96 s, 0.925 s	2.95E+08	921	1511.1	57.09	7891	XIC(57.09±500ppm)
Octadecane, 2-methyl-	1644.94 s, 0.966 s	1.91E+08	866	1973.3	57.09	3782	XIC(57.09±500ppm)
Octadecanoic acid	1774.93 s, 1.310 s	98243696	925	2146.7	43.08	5734	XIC(43.08±500ppm)
Octane, 2,4,6-trimethyl-	669.998 s, 0.809 s	10941015	880	974.1	57.09	505	XIC(57.09±500ppm)
Octanoic acid, TMS derivative	1029.98 s, 0.985 s	41086274	942	1268.2	73.06	4672	XIC(73.06±500ppm)
Oxalic acid, heptyl isohexyl ester	1309.96 s, 0.934 s	2.39E+08	807	1555.6	43.08	4648	XIC(43.08±500ppm)
Palmitic acid, TMS derivative	1634.94 s, 1.239 s	26804600	772	1960	117.05	897	XIC(117.05±500ppm)
Pantolactone, (3R)-, TMS derivative	949.98 s, 1.267 s	3605509	782	1195.7	73.06	614	XIC(73.06±500ppm)
Pentacosane	2479.88 s, 1.947 s	14485156	761	3086.7	57.09	661	XIC(57.09±500ppm)
Pentadecane	1024.98 s, 0.873 s	51805834	885	1263.6	57.09	2313	XIC(57.09±500ppm)
Pentadecane, 2-methyl-	1854.92 s, 1.003 s	25872842	755	2253.4	57.09	1227	XIC(57.09±500ppm)
Pentanoic acid, 2,2,4-trimethyl-3-carboxyisopropyl, isobutyl ester	1354.95 s, 1.202 s	26161172	777	1605.9	71.06	1969	XIC(71.06±500ppm)
Pentasiloxane, dodecamethyl-	939.981 s, 0.719 s	38465712	918	1187	73.06	8801	XIC(73.06±500ppm)
Phenol, TMS derivative	779.991 s, 1.066 s	19292857	871	1055.6	151.08	3857	XIC(151.08±500ppm)
Phenylethyl Alcohol, TMS derivative	989.978 s, 1.135 s	41947839	912	1231.8	73.06	2789	XIC(73.06±500ppm)
Phthalic acid, di(3-methylphenyl) ester	1449.95 s, 1.369 s	1.37E+08	735	1718.8	239.14	1219	XIC(239.14±500ppm)
Pimaric acid, TMS derivative	1884.92 s, 1.472 s	6924351	870	2293.4	73.06	1098	XIC(73.06±500ppm)
Propanamide, 2,2-dimethyl-N-(2'-t-butylcarbonylphenyl)-	2119.91 s, 1.088 s	1.47E+09	813	2606.7	204.06	2080	XIC(204.06±500ppm)
Propanoic acid, anhydride	1569.94 s, 1.701 s	10708911	742	1873.3	57.08	605	XIC(57.08±500ppm)
Propanoyl fluoride, 2,3,3,3-tetrafluoro-2-(1,1,2,3,3,3-hexafluoro-2-(heptafluoropropoxy)pro	794.99 s, 1.730 s	30588918	764	1066.7	169.02	1412	XIC(169.02±500ppm)
Propiophenone, 3',4'-dimethoxy-	1349.95 s, 1.818 s	12500572	700	1600	165.08	1260	XIC(165.08±500ppm)
Propylene glycol, 2TMS derivative	714.995 s, 0.805 s	55206517	904	1007.4	73.06	1880	XIC(73.06±500ppm)
Protocatechoic acid, 3TMS derivative	1539.94 s, 1.105 s	63480591	879	1833.3	73.06	2731	XIC(73.06±500ppm)
Pyridine	709.996 s, 0.744 s	18733030	912	1003.7	79.06	1443	XIC(79.06±500ppm)
Pyridine, 2,4,6-trimethyl-	704.996 s, 1.364 s	9733550	897	1000	121.11	1550	XIC(121.11±500ppm)
Pyridine, 2-chloro-6-(2-furanylmethoxy)-4-(trichloromethyl)-	1919.92 s, 2.354 s	3596251	700	2340	81.05	504	XIC(81.05±500ppm)
Pyrogallol, 3TMS derivative	1314.96 s, 1.011 s	1.65E+08	900	1561.1	73.06	5162	XIC(73.06±500ppm)
Pyrrrolidine, 4-((N,N-dimethylcarbamoyl)benzyl)triphenylacetyl-	2084.91 s, 1.223 s	2168669	742	2560	404.26	1000	XIC(404.26±500ppm)
Pyruvic acid, TMS derivative	1559.94 s, 0.915 s	2605338	700	1860	75.04	2158	XIC(75.04±500ppm)
Quinoline, 1,2-dihydro-2,2,4-trimethyl-	1214.96 s, 1.706 s	3694433	805	1452.6	158.12	1005	XIC(158.12±500ppm)
Resorcinol, TMS derivative	2744.87 s, 0.554 s	4625349	705	3440.1	167.04	541	XIC(167.04±500ppm)
Ribitol, 5TMS derivative	1464.95 s, 0.812 s	38140728	837	1737.5	73.06	803	XIC(73.06±500ppm)
Shikimic acid, 4TMS derivative	1534.94 s, 0.951 s	2.73E+08	824	1826.7	73.06	1777	XIC(73.06±500ppm)
Silane, methylidynetris(trimethyl-	1584.94 s, 0.820 s	70610575	755	1893.3	217.13	1638	XIC(217.13±500ppm)
Silane, tetramethyl-	2289.89 s, 0.490 s	31007655	859	2833.4	73.06	545	XIC(73.06±500ppm)
Silanol, trimethyl-	799.99 s, 0.456 s	22226500	792	1070.4	75.04	973	XIC(75.04±500ppm)
Silanol, trimethyl-, phosphate (3:1)	1049.97 s, 1.022 s	62307940	846	1286.4	299.12	10462	XIC(299.12±500ppm)
Silanol, trimethyl-, triester with arsenic acid	1134.97 s, 1.024 s	3354578	701	1370	207.06	556	XIC(207.06±500ppm)
Stearic acid, TMS derivative	1774.93 s, 1.248 s	37988629	770	2146.7	75.04	1320	XIC(75.04±500ppm)
Succinic acid, monoethyl ester-, (TMS)	1014.98 s, 1.194 s	56798021	891	1254.5	73.06	3830	XIC(73.06±500ppm)
Sulfuric acid, 2TMS derivative	1319.96 s, 0.693 s	16864637	910	1566.7	147.09	797	XIC(147.09±500ppm)
Syringaldehyde, TMS derivative	1414.95 s, 1.584 s	53056476	735	1676.5	224.08	6289	XIC(224.08±500ppm)
Talose, 5TMS derivative	1619.94 s, 0.853 s	63331293	889	1940	73.06	2369	XIC(73.06±500ppm)
Tartaric acid (2R,3R)-, 3TMS derivative	1349.95 s, 1.026 s	1.9E+08	875	1600	73.06	2835	XIC(73.06±500ppm)
Tartaric acid, 4TMS derivative	1404.95 s, 0.930 s	2.17E+08	920	1664.7	73.06	5719	XIC(73.06±500ppm)
Tartaric acid, ethyl ester, 3TMS	1369.95 s, 1.019 s	1.46E+08	901	1623.5	73.06	2498	XIC(73.06±500ppm)
Terephthalic acid, 2TMS derivative	1514.94 s, 1.166 s	18531031	837	1800	295.13	6626	XIC(295.13±500ppm)
Tetracosane	1864.92 s, 1.088 s	76675065	949	2266.7	57.09	3664	XIC(57.09±500ppm)
Tetracyano-p-quinodimethane	1609.94 s, 0.848 s	3.79E+08	778	1926.7	204.11	618	XIC(204.11±500ppm)
Tetradecane	1164.97 s, 0.930 s	13959296	924	1400	57.09	1140	XIC(57.09±500ppm)
Tetradecane, 2-methyl-	1224.96 s, 0.922 s	49636917	913	1463.2	57.09	2772	XIC(57.09±500ppm)
Tetradecane, 3-methyl-	1234.96 s, 0.924 s	99279795	894	1473.7	57.09	6308	XIC(57.09±500ppm)
Tetrasiloxane, decamethyl-	774.991 s, 0.711 s	20574597	851	1051.9	207.07	4543	XIC(207.07±500ppm)
Tiglic acid, TMS derivative	944.98 s, 1.547 s	2662152	733	1191.3	157.06	837	XIC(157.06±500ppm)
Tricarballic acid, 3TMS derivative	1469.95 s, 1.065 s	1.33E+08	898	1743.8	73.06	3872	XIC(73.06±500ppm)
Tridecane	1069.97 s, 0.861 s	51031816	839	1305	57.09	3827	XIC(57.09±500ppm)
Tridecanoic acid, TMS derivative	1479.95 s, 1.051 s	3.8E+08	918	1756.3	73.06	5605	XIC(73.06±500ppm)
Trimethylsilyl 4-methyl-1,3-oxazole-5-carboxylate	1059.97 s, 1.468 s	15807198	700	1295.5	184.07	4464	XIC(184.07±500ppm)
Trisiloxane, octamethyl-	809.989 s, 0.779 s	16843382	867	1077.8	73.06	1636	XIC(73.06±500ppm)
Tuaminoheptane	969.979 s, 0.383 s	10411904	700	1213.6	44.01	522	XIC(44.01±500ppm)
Undecane	744.993 s, 0.821 s	13334578	876	1029.6	57.09	1582	XIC(57.09±500ppm)
Undecane, 4-methyl-	854.986 s, 0.840 s	2.15E+08	903	1113	43.08	6969	XIC(43.08±500ppm)
α-D-(+)-Talopyranose, 5TMS derivative	2069.91 s, 0.964 s	49081278	798	2540	73.06	1216	XIC(73.06±500ppm)
α-D-Glactopyranose, 5TMS derivative	2054.91 s, 0.882 s	16215586	839	2520	204.13	728	XIC(204.13±500ppm)
β-Arabinopyranose, 4MS derivative	1734.93 s, 0.909 s	60524180	770	2093.3	73.06	518	XIC(73.06±500ppm)
β-D-(+)-Mannopyranose, 5TMS derivative	2874.86 s, 2.736 s	2.2E+08	783	3613.5	204.13	1831	XIC(204.13±500ppm)
β-D-(+)-Talopyranose, 5TMS derivative	2079.91 s, 0.958 s	1.2E+08	813	2553.4	73.06	1806	XIC(73.06±500ppm)
β-D-Allopyranose, 5TMS derivative	1944.92 s, 0.919 s	21799814	792	2373.4	73.06	601	XIC(73.06±500ppm)
β-Hydroxypruvic acid, trimethylsilyl ether, trimethylsilyl ester	884.984 s, 0.917 s	33516927	720	1139.1	73.06	958	XIC(73.06±500ppm)

β -L-(-)-Fucopyranose, 4TMS derivative	1449.95 s, 0.866 s	1.11E+08	925	1718.8	73.06	5271 XIC(73.06 \pm 500ppm)
β -L-Mannofuranose, 6-deoxy-1,2,3,5-tetrakis-O-(trimethylsilyl)-	1494.95 s, 0.897 s	63060704	732	1775	73.06	1446 XIC(73.06 \pm 500ppm)

COLOPHONY

	R.T. (s)	Area	Similarity	Retention	Base Mass	Peak S/N	Quant	Masses
(((1R,4S,4aS,8aS)-4-isopropyl-1,6-dimethyl-1,2,3,4,4a,7,8,8a-octahydronaphthalen-1-yl)oxy)trimethylsilane	1489.95 s, 1.095 s	38000376	832	1768.8	161.16	3070	XIC(161.16±500ppm)	
(((3S,3aS,3bS,4R,7S,7aS)-4-isopropyl-3,7-dimethylcloctahydro-1H-cyclopenta[1,3]cyclopropa[1,2]benzen-3-yl)oxy)trimethylsilane	1599.94 s, 1.009 s	7003175	752	1913.3	279.26	2419	XIC(279.26±500ppm)	
((1S,4aR,4bR,10aR)-7-isopropyl-1,4a-dimethyl-1,2,3,4,4a,4b,5,6,10,10a-decahydrophenanthren-1-yl)methyl acetate	1929.92 s, 1.878 s	1.37E+08	721	2353.4	43.04	724	XIC(43.04±500ppm)	
((4-isopropyl-1-methylcyclohex-3-en-1-yl)oxy)trimethylsilane	1024.98 s, 0.944 s	50299295	854	1263.6	143.11	5202	XIC(143.11±500ppm)	
(-)-Isolongifolol, TMS derivative	1544.94 s, 1.309 s	1.06E+08	733	1840	73.06	3543	XIC(73.06±500ppm)	
(+)-cis-Verbenol, trimethylsilyl ether	999.977 s, 0.941 s	24271491	892	1240.9	73.06	1203	XIC(73.06±500ppm)	
(+)-Longicamphenylene	1334.96 s, 1.636 s	18449039	910	1583.3	41.06	1558	XIC(41.06±500ppm)	
(1R,3E,7E,11R)-1,5,5,8-Tetramethyl-12-oxabicyclo[9.1.0]dodeca-3,7-diene	1374.95 s, 1.489 s	37817900	850	1629.4	43.05	2468	XIC(43.05±500ppm)	
(1R,4aR,4bR,10aR)-7-isopropyl-1,4a-dimethyl-1,2,3,4,4a,4b,5,6,10,10a-decahydrophenanthrene-1-carbaldehyde	1889.92 s, 1.992 s	1.7E+08	909	2300	187.17	2666	XIC(187.17±500ppm)	
(1R,4aR,4bS,10aR)-1,4a-Dimethyl-7-(propan-2-ylidene)-1,2,3,4,4a,4b,5,6,7,9,10,10a-dodecahydrophenanthrene-1-carbaldehyde	1934.92 s, 2.164 s	33415496	731	2360	135.14	732	XIC(135.14±500ppm)	
(1R,4aR,4bS,7R,10aR)-1,4a,7-Trimethyl-7-vinyl-1,2,3,4,4a,4b,5,6,7,9,10,10a-dodecahydrophenanthrene-1-carbaldehyde	1799.93 s, 1.821 s	1.44E+08	856	2180	41.06	1548	XIC(41.06±500ppm)	
(1R,4aR,4bS,7S,10aR)-1,4a,7-Trimethyl-7-vinyl-1,2,3,4,4a,4b,5,6,7,9,10,10a-dodecahydrophenanthrene-1-carbaldehyde	1834.92 s, 1.896 s	1.84E+08	933	2226.7	187.17	8740	XIC(187.17±500ppm)	
(1S,4aR,5S)-trimethylsilyl 1,4a-dimethyl-5-(3-methyl-5-oxopentyl)-6-methylenedecahydrophenanthrene-1-carboxylate (2,5-Dimethoxyphenyl)acetone	1759.93 s, 1.251 s	1.22E+08	710	2126.7	73.06	1829	XIC(73.06±500ppm)	
(2,5-Dimethoxyphenyl)acetone	1329.96 s, 1.909 s	19865145	913	1577.8	151.1	2417	XIC(151.10±500ppm)	
(4aS,4bR,10aS)-7-isopropyl-1,1,4a-trimethyl-1,2,3,4,4a,4b,5,6,10,10a-decahydrophenanthrene	1739.93 s, 1.578 s	23944017	898	2100	105.09	4187	XIC(105.09±500ppm)	
(7a-Isopropenyl-4,5-dimethylcyclohex-4-en-yl)methanol	1589.94 s, 1.585 s	10712866	776	1900	43.05	649	XIC(43.05±500ppm)	
(S)-(-)-α-Terpineol, TMS derivative	1094.97 s, 0.995 s	3.78E+08	767	1330	73.06	2759	XIC(73.06±500ppm)	
(S,E)-8,12,15,15-Tetramethyl-4-methylenebicyclo[9.3.1]pentadeca-7,11-diene	1909.92 s, 1.769 s	1.89E+08	735	2326.7	135.13	1361	XIC(135.13±500ppm)	
(Z)-((1,11-dimethyl-8-methylenebicyclo[7.2.1]dodec-4-en-4-yl)oxy)trimethylsilane	1389.95 s, 1.070 s	3.17E+08	828	1647.1	73.06	6377	XIC(73.06±500ppm)	
(Z)-5-Methoxy-3,5-dimethyl-2-hexenyltrimethylsilane	2674.87 s, 0.492 s	82623499	760	3346.8	73.07	551	XIC(73.07±500ppm)	
1-(1-Hydroxybutyl)-2,5-dimethoxybenzene	1404.95 s, 1.998 s	5380909	812	1664.7	167.1	1178	XIC(167.10±500ppm)	
1-(2,5-Dimethoxyphenyl)-1-((trimethylsilyloxy)propan-2-amine	1324.96 s, 1.286 s	38903408	749	1572.2	73.06	1090	XIC(73.06±500ppm)	
1-(2-Methoxyethoxy)-2-methyl-2-propanol, methyl ether	1039.97 s, 0.871 s	74101975	755	1277.3	73.05	625	XIC(73.05±500ppm)	
1-(3-Methylbutyl)-2,3,4,6-tetramethylbenzene	849.987 s, 0.947 s	16581489	751	1108.7	147.09	1435	XIC(147.09±500ppm)	
1-(p-Cumenyl)adamantane	1679.93 s, 1.745 s	43611500	706	2020	197.16	3022	XIC(197.16±500ppm)	
1,2,3,1',2',3'-Hexamethyl-bicyclopentyl-2,2'-diene	959.98 s, 0.923 s	12386811	710	1204.5	109.12	2985	XIC(109.12±500ppm)	
1,2,4-Benzenetriol, tris(trimethylsilyl) ether	1364.95 s, 1.002 s	1894675	753	1617.7	342.2	2621	XIC(342.20±500ppm)	
1,2,4-Methenoazulene, decahydro-1,5,5,8a-tetramethyl-, [1S-(1α,2α,3αβ,4α,8aβ,9R*)]-	1149.97 s, 1.160 s	65262760	920	1385	94.09	6026	XIC(94.09±500ppm)	
1,2-Benzenedicarboxylic acid, bis(2-methylpropyl) ester	1574.94 s, 1.656 s	18379802	886	1880	149.05	2046	XIC(149.05±500ppm)	
1,2-Benzisothiazole	994.977 s, 1.962 s	2217374	873	1236.4	135.04	556	XIC(135.04±500ppm)	
1,2-Dimethylcyclopentanol	794.99 s, 1.463 s	6615037	784	1066.7	71.06	558	XIC(71.06±500ppm)	
1,2-Ethenediol, 2TMS derivative	679.997 s, 0.866 s	27321221	754	981.5	73.06	1849	XIC(73.06±500ppm)	
1,3,5-Trimethyl-2-cyclopentylbenzene	1564.94 s, 1.338 s	9877866	705	1866.7	173.16	1465	XIC(173.16±500ppm)	
1,3,6,10-Cyclotetradecatetraene, 3,7,11-trimethyl-14-(1-methylethyl)-, [S-(E,Z,E,E)]-	1584.94 s, 1.422 s	41565074	774	1893.3	123.13	4984	XIC(123.13±500ppm)	
1,3-Benzenediol, O,O'-di(2-methoxybenzoyl)-	3409.82 s, 0.666 s	23720971	776	4326.8	135.08	649	XIC(135.08±500ppm)	
1,3-Cyclohexadiene, 5,6-dimethyl-	1269.96 s, 2.018 s	5275569	766	1511.1	93.09	764	XIC(93.09±500ppm)	
1,3-Dioxolane, 2,2-dimethyl-	669.998 s, 1.828 s	13259988	715	974.1	43.04	793	XIC(43.04±500ppm)	
1,3-Dioxolane-2-methanol	2809.86 s, 0.491 s	77670004	854	3526.8	73.06	1858	XIC(73.06±500ppm)	
1,3-Propanediol, 2TMS derivative	789.99 s, 0.843 s	3467206	870	1063	147.09	587	XIC(147.09±500ppm)	
1,3-Propanediol, TMS derivative	779.991 s, 1.110 s	51998405	761	1055.6	75.04	1033	XIC(75.04±500ppm)	
1,4-Methano-1H-indene, octahydro-4-methyl-8-methylene-7-(1-methylethyl)-, [1S-(1α,3αβ,4α,7α,7aβ)]-	1169.97 s, 1.149 s	21583735	880	1405.3	108.11	2950	XIC(108.11±500ppm)	
1,6,10,14-Hexadecatetraen-3-ol, 3,7,11,15-tetramethyl-, (E,E)-	1689.93 s, 1.463 s	20660258	784	2033.3	81.08	879	XIC(81.08±500ppm)	
1,6-Dioxacyclododecane-7,12-dione	1309.96 s, 2.072 s	2.1E+08	933	1555.6	55.06	5851	XIC(55.06±500ppm)	
10,12-Docosadiynoic acid, 2TMS derivative	1629.94 s, 1.067 s	47962237	712	1953.3	73.06	1018	XIC(73.06±500ppm)	
10,12-Tricosadiynoic acid, TMS derivative	1519.94 s, 1.275 s	69843260	739	1806.7	73.06	731	XIC(73.06±500ppm)	
11-Hexadecyn-1-ol	1434.95 s, 1.770 s	16887113	798	1700	96.08	2905	XIC(96.08±500ppm)	
15-Hydroxy-7-oxodehydroabietic acid, trimethylsilyl ester, 15-trimethylsilyl ether	2154.9 s, 2.006 s	5.77E+08	705	2653.4	73.1	2053	XIC(73.10±500ppm)	
17α-Methyl-5β-androstane-3α,17β-diol	1809.93 s, 1.502 s	82077707	715	2193.4	73.06	3183	XIC(73.06±500ppm)	
1-Cyclohexene-1-acetaldehyde, 2,6,6-trimethyl-	2119.91 s, 2.875 s	4.07E+08	771	2606.7	151.13	3488	XIC(151.13±500ppm)	
1-Cyclohexene-1-carboxaldehyde, 4-(1-methylethyl)-	964.979 s, 1.501 s	5270333	830	1209.1	68.08	660	XIC(68.08±500ppm)	
1-Dodecene	949.98 s, 0.917 s	40493800	934	1195.7	43.08	2216	XIC(43.08±500ppm)	
1-Heptatriacotanol	2079.91 s, 1.480 s	1.36E+08	703	2553.4	73.08	765	XIC(73.08±500ppm)	
1-Hexanol, TMS derivative	694.996 s, 0.826 s	73897698	868	992.6	75.04	2980	XIC(75.04±500ppm)	
1H-Naphtho[2,1-b]pyran, 3-ethenyldodecahydro-3,4a,7,7,10a-pentamethyl-, [3R-(3α,4αβ,6aa,10aβ,10ba)]-	1694.93 s, 1.523 s	66868359	890	2040	43.04	2519	XIC(43.04±500ppm)	
1H-Naphtho[2,1-b]pyran-8(4aH)-one, 3-ethenyldodecahydro-3,4a,7,7,10a-pentamethyl-	1844.92 s, 1.956 s	57561407	769	2240	43.05	928	XIC(43.05±500ppm)	
1-Monoacetin, 2O-TMS	1089.97 s, 0.969 s	2807068	840	1325	175.11	1056	XIC(175.11±500ppm)	
1-Monomyrstin, 2TMS derivative	1934.92 s, 1.133 s	13633446	754	2360	343.31	1610	XIC(343.31±500ppm)	
1-Naphthalenepropanol, α-ethenyldodecahydro-2-hydroxy-α,2,5,8a-pentamethyl-, [1R-(1α(R*),2β,4aβ,8aβ)]-	1759.93 s, 1.575 s	25165452	782	2126.7	43.05	1626	XIC(43.05±500ppm)	
1-Nonadecene	1659.93 s, 1.062 s	16236749	918	1993.3	43.08	1070	XIC(43.08±500ppm)	
1-Octadecanol, TMS derivative	1774.93 s, 1.032 s	25217611	891	2146.7	75.04	2369	XIC(75.04±500ppm)	
1-Octanol, 2-butyl-	994.977 s, 0.881 s	10492258	753	1236.4	43.08	511	XIC(43.08±500ppm)	
1-Phenanthrenecarboxaldehyde, 1,2,3,4,4a,9,10,10a-octahydro-1,4a-dimethyl-7-(1-methylethyl)-, [1R-(1α,4aβ,10aα)]-	1864.92 s, 2.093 s	85796332	921	2266.7	43.06	1669	XIC(43.06±500ppm)	
1-Phenanthrenecarboxylic acid, 1,2,3,4,4a,10a-hexahydro-1,4a-dimethyl-7-(1-methylethyl)-, methyl ester, [1R-(1α,4aβ,10aα)]-	1904.92 s, 2.092 s	55070810	783	2320	237.21	2773	XIC(237.21±500ppm)	
1-Phenanthrenecarboxylic acid, 1,2,3,4,4a,4b,5,6,7,9,10,10a-decahydro-1,4a-dimethyl-7-(1-methylethyl)-, methyl ester, [1R-(1α,4aβ,10aα)]-	1755.92 s, 2.139 s	42567868	765	2453.4	121.12	618	XIC(121.12±500ppm)	
1-Phenanthrenecarboxylic acid, 1,2,3,4,4a,4b,5,6,7,9,10,10a-decahydro-1,4a-dimethyl-7-(1-methylethylidene)-, [1R-(1α,4aβ,4ba),1C 2009.91 s, 2.422 s]	1749.93 s, 2.004 s	17589693	801	2113.3	197.16	2109	XIC(197.16±500ppm)	
1-Phenanthrenecarboxylic acid, 1,2,3,4,4a,9,10,10a-octahydro-1,4a-dimethyl-, methyl ester, [1R-(1α,4aβ,10aα)]-	1749.93 s, 2.004 s	17589693	801	2113.3	197.16	2109	XIC(197.16±500ppm)	
1-Phenanthrenecarboxylic acid, 7-ethenyl-1,2,3,4,4a,4b,5,6,7,8,10,10a-decahydro-1,4a,7-trimethyl-, methyl ester, [1R-(1α,4aβ,4ba),1879.92 s, 1.843 s]	1879.92 s, 1.843 s	35427359	876	2286.7	241.23	1302	XIC(241.23±500ppm)	
1-Phenanthrenemethanol, 1,2,3,4,4a,9,10,10a-octahydro-1,4a-dimethyl-7-(1-methylethyl)-, 1-acetate, [1R,4aS,10aR]-	1959.92 s, 2.092 s	45719366	802	2393.4	253.24	1450	XIC(253.24±500ppm)	
1R,3Z,9S,4,11,11-Trimethyl-8-methylenebicyclo[7.2.0]undec-3-ene	1224.96 s, 1.205 s	40613354	933	1463.2	91.07	2018	XIC(91.07±500ppm)	
1-Tetradecene	1159.97 s, 0.959 s	62397369	958	1395	43.08	4878	XIC(43.08±500ppm)	
2-(2-(2-Ethoxyethoxy)ethoxy)ethyl benzoate	1534.94 s, 1.524 s	8377755	701	1826.7	73.06	562	XIC(73.06±500ppm)	
2-(2,5-Dimethoxy-phenyl)-propionaldehyde	1309.96 s, 1.812 s	23139261	853	1555.6	165.12	3408	XIC(165.12±500ppm)	
2-(3-Pentyl)pyridine	959.98 s, 1.273 s	15001771	783	1204.5	106.09	1532	XIC(106.09±500ppm)	
2,2,6,8-Tetramethyl-7-oxatricyclo[6.1.0.0(1,6)]nonane	2254.9 s, 4.310 s	9004751	753	2786.7	137.12	671	XIC(137.12±500ppm)	
2,2'-Bipyridine	1214.96 s, 2.020 s	3974912	931	1452.6	156.09	838	XIC(156.09±500ppm)	
2,2'-Bipyrrolidine	1449.95 s, 1.354 s	17662360	731	1718.8	70.08	1331	XIC(70.08±500ppm)	
2',3',4',-Tri(trimethylsilyloxy)acetophenone	1464.95 s, 0.999 s	14165640	764	1737.5	73.06	901	XIC(73.06±500ppm)	
2,3'-Dipyrilidyl	1309.96 s, 2.151 s	2365286	780	1555.6	156.09	808	XIC(156.09±500ppm)	
2,4,4'-Trihydroxybenzophenone, tris(trimethylsilyl) ether	2004.91 s, 1.428 s	6860952	708	2453.4	431.35	1564	XIC(431.35±500ppm)	
2,4a,8,8-Tetramethyldodecahydrocyclopropa[d]naphthalene	1729.93 s, 1.580 s	19200111	786	2086.7	191.21	1310	XIC(191.21±500ppm)	
2,4-Dimethyldodecane	1259.96 s, 0.896 s	1.51E+08	814	1500	43.08	1607	XIC(43.08±500ppm)	
2,4-Di-tert-butylphenol	1274.96 s, 1.362 s	5844876	754	1516.7	191.17	789	XIC(191.17±500ppm)	
2,4-Di-tert-butylphenoxytrimethylsilane	1309.96 s, 1.064 s	46154248	839	1555.6	263.22	9837	XIC(263.22±500ppm)	
2,5-Cyclohexadiene-1,4-dione, 2,6-bis(1,1-dimethylethyl)-	1239.96 s, 1.312 s	22595882	919	1478.9	41.06			

2-Amino-4-(1-ethylpropyl)-4H-benzo[h]chromene-3-carbonitrile	1869.92 s, 1.238 s	1.23E+08	706	2273.4	221.17	1106	XIC(221.17±500ppm)
2-Butanamine, 3,3-dimethyl-	1504.94 s, 1.270 s	22344760	715	1787.5	44.07	667	XIC(44.07±500ppm)
2-Butene-1,4-diol, 2TBDMs derivative	1124.97 s, 1.122 s	10604182	706	1360	147.09	1156	XIC(147.09±500ppm)
2-Cyclohexen-1-one, 3-methyl-	784.991 s, 1.775 s	14336229	930	1059.3	82.06	2129	XIC(82.06±500ppm)
2-Cyclohexen-1-one, 4-(1-methylethyl)-	949.98 s, 1.558 s	8697698	907	1195.7	96.08	1177	XIC(96.08±500ppm)
2-Decene, 5-methyl-, (Z)-	1259.96 s, 0.952 s	2.49E+08	806	1500	57.09	1454	XIC(57.09±500ppm)
2-Ethyl-2-phenyl-1,3-benzodioxole	2164.9 s, 2.197 s	34734479	739	2666.7	197.13	601	XIC(197.13±500ppm)
2-Furancarboxylic acid, tetrahydro-2-methyl-5-oxo-, trimethylsilyl ester	1094.97 s, 1.513 s	2716803	744	1330	99.06	564	XIC(99.06±500ppm)
2-Hexenoic acid, (E)-, TMS derivative	969.979 s, 1.391 s	5766358	711	1213.6	143.08	1166	XIC(143.08±500ppm)
2-Hexenoic acid, 5-(1-ethoxyethoxy)-, (2-trimethylsilyl)ethyl ester	1159.97 s, 1.388 s	15859840	728	1395	73.06	1320	XIC(73.06±500ppm)
2-Hydroxy-2-methylbutyric acid, 2TMS derivative	889.984 s, 0.834 s	6406048	826	1143.5	145.13	784	XIC(145.13±500ppm)
2-Hydroxy-3-methylbutyric acid, 2TMS derivative	924.982 s, 0.865 s	27028936	862	1173.9	73.06	2502	XIC(73.06±500ppm)
2-Hydroxy-4-methoxybenzaldehyde, TMS derivative	1319.96 s, 1.466 s	7522544	733	1566.7	209.1	1703	XIC(209.10±500ppm)
2-Isopropyl-5-methyl-1-heptanol	1074.97 s, 0.897 s	39335172	856	1310	43.08	3531	XIC(43.08±500ppm)
2-Mercapto-4,6-dimethylnicotinonitrile, TBDMs derivative	1099.97 s, 0.817 s	2159301	741	1335	221.12	720	XIC(221.12±500ppm)
2-Methyl-3,5-heptadiene, 7-trimethylsilyl-2,3-bis(trimethylsilyloxy)-	1454.95 s, 0.898 s	63806881	706	1725	131.11	3839	XIC(131.11±500ppm)
2-Methyl-3-trimethylsilyloxy-2-pentene	854.986 s, 1.111 s	1.38E+08	762	1113	75.04	1527	XIC(75.04±500ppm)
2-Methyl-5-octyn-4-ol, TMS derivative	894.984 s, 1.351 s	2944289	746	1147.8	155.08	906	XIC(155.08±500ppm)
2-Oxabicyclo[2.2.2]octan-6-one, 1,3,3-trimethyl-	999.977 s, 1.800 s	33510258	711	1240.9	82.06	5796	XIC(82.06±500ppm)
2-Oxo-4-phenyl-6-(4-chlorophenyl)-1,2-dihydropyrimidine	2399.89 s, 0.522 s	20834483	793	2980.1	281.09	2321	XIC(281.09±500ppm)
2-Palmitoylglycerol, 2TMS derivative	2024.91 s, 1.175 s	29756366	773	2480	129.09	1186	XIC(129.09±500ppm)
2-Pentamethylsilylalloxybutane	699.996 s, 0.813 s	25625101	738	996.3	75.04	1075	XIC(75.04±500ppm)
2-Phenylbutyric acid, TBDMs derivative	1264.96 s, 1.300 s	63072823	767	1505.6	75.04	3722	XIC(75.04±500ppm)
2-Propenoic acid, 2-methyl-, 3,3,5-trimethylcyclohexyl ester	1114.97 s, 1.193 s	32304272	908	1350	69.07	1757	XIC(69.07±500ppm)
2-Propylphenol, TMS derivative	1094.97 s, 1.127 s	72221239	771	1330	179.11	9580	XIC(179.11±500ppm)
2-Pyridinemethanol, TBDMs derivative	939.981 s, 1.234 s	42314887	798	1187	166.09	6219	XIC(166.09±500ppm)
2-Pyridinepropanol, TBDMs derivative	1094.97 s, 1.215 s	41515462	778	1330	194.13	1138	XIC(194.13±500ppm)
2-Pyrrolo[tert-butyl(dimethylsilyl)oxymorphopropan-1-ol	684.997 s, 0.856 s	26177098	741	985.2	75.04	605	XIC(75.04±500ppm)
3-Hydroxy-2,3-dihydrosebacic acid, tris(trimethylsilyl) derivative	1229.96 s, 1.020 s	50070831	707	1468.4	73.06	1691	XIC(73.06±500ppm)
3-(2,5-Dimethylfuran-3-yl)-2-phenylcyclopent-2-en-1-one	1719.93 s, 1.809 s	1.01E+08	721	2073.3	237.2	12578	XIC(237.20±500ppm)
3-(Trimethylsilyl)methyl-1-hepten-4-one	1024.98 s, 1.235 s	19637386	746	1263.6	73.06	1695	XIC(73.06±500ppm)
3,26-Dioxo-2,27-disilaooctacosane, 2,2,4,25,27-hexamethyl-	974.979 s, 0.822 s	28396289	709	1218.2	117.09	2556	XIC(117.09±500ppm)
3,4-Dimethoxymandelic acid, di-TMS	2069.91 s, 2.250 s	1.18E+08	733	2540	239.14	1620	XIC(239.14±500ppm)
3,5-Dimethylphenol, TMS derivative	1189.96 s, 1.407 s	2847667	794	1426.3	179.14	604	XIC(179.14±500ppm)
3,6-Bis(2-methylphenyl)-2,5-dihydropyrrolo[3,4-c]pyrrole-1,4-dione	2114.91 s, 2.047 s	2.04E+08	705	2600	316.28	614	XIC(316.28±500ppm)
3,7-dioxo-2,8-disilanonane, 2,2,8,8-tetramethyl-5,5-bis[[[trimethylsilyl]oxy]methyl]-	1284.96 s, 0.780 s	2723940	876	1527.8	73.06	754	XIC(73.06±500ppm)
3-Buten-2-one, 3-trimethylsilyloxy-	954.98 s, 1.144 s	7849083	747	1200	73.06	1150	XIC(73.06±500ppm)
3-Buten-2-one, 4-(4-methoxyphenyl)-	1284.96 s, 1.747 s	28508157	780	1527.8	161.09	5187	XIC(161.09±500ppm)
3-Cyclohexene-1-methanol, α,α,4-trimethyl-, (R)-	949.98 s, 1.324 s	57847516	927	1195.7	59.07	4141	XIC(59.07±500ppm)
3-Ethyl-1-p-tolyltriazene	989.978 s, 1.291 s	24087543	708	1231.8	107.09	2300	XIC(107.09±500ppm)
3-Hydroxybenzoic acid, 2TMS derivative	1324.96 s, 1.161 s	22664874	858	1572.2	73.06	2223	XIC(73.06±500ppm)
3-Hydroxybutyric acid, 2TMS derivative	919.982 s, 0.885 s	51445391	805	1169.6	147.09	3968	XIC(147.09±500ppm)
3-Methylene-1,4-bis(trimethylsilyloxy)butane	864.986 s, 0.813 s	15222090	772	1121.7	73.06	7569	XIC(73.06±500ppm)
3-Octen-2-ol, TMS derivative	1004.98 s, 1.131 s	9301373	754	1245.5	73.06	988	XIC(73.06±500ppm)
3-Pyridinol	884.984 s, 1.503 s	39706736	945	1139.1	95.05	1753	XIC(95.05±500ppm)
3-Pyridinol, TMS derivative	759.992 s, 1.080 s	23290443	737	1040.7	152.08	2827	XIC(152.08±500ppm)
3-Pyridylcarbinol, trimethylsilyl ether	1014.98 s, 1.267 s	19228391	763	1254.5	166.1	2806	XIC(166.10±500ppm)
3-Trimethylsilylmethyl-4-hydroxy-2-methyl-1-hexene	2174.9 s, 1.528 s	5.72E+08	734	2680.1	73.04	867	XIC(73.04±500ppm)
3β-(Methoxymethoxy)androst-5-en-17-one	2074.91 s, 1.995 s	2.84E+08	741	2546.7	270.37	1873	XIC(270.37±500ppm)
3β,16α,17α-Tris(trimethylsilyloxy)androst-5-ene	1869.92 s, 1.208 s	74852697	755	2273.4	73.06	1709	XIC(73.06±500ppm)
4a(2H)-Naphthalenol, 1,3,4,5,6,8a-hexahydro-4,7-dimethyl-1-(1-methylethyl)-, (1S,4R,4aS,8aR)-	1399.95 s, 1.406 s	11191357	775	1658.8	161.16	1170	XIC(161.16±500ppm)
4a(2H)-Naphthalenol, 1,3,4,5,6,8a-hexahydro-4,7-dimethyl-1-(1-methylethyl)-, (1S,4S,4aS,8aR)-	1389.95 s, 1.395 s	19835796	819	1647.1	119.11	722	XIC(119.11±500ppm)
4-Acetyl-1-methylcyclohexene	2199.9 s, 3.382 s	83096545	802	2713.4	138.12	1646	XIC(138.12±500ppm)
4b,8-Dimethyl-2-isopropylphenanthrene, 4b,5,6,7,8a,9,10-octahydro-	1664.93 s, 1.642 s	28926921	843	2000	159.14	1691	XIC(159.14±500ppm)
4-Cyclopentene-1,3-dione, 4-propyl-	984.978 s, 1.600 s	12719637	756	1227.3	43.04	663	XIC(43.04±500ppm)
4H-1,2,4-Triazole, 4-ethyl-	1584.94 s, 1.729 s	5684264	711	1893.3	97.11	599	XIC(97.11±500ppm)
4-Hydroxybenzoic acid, 2TMS derivative	1379.95 s, 1.152 s	4631721	808	1635.3	267.13	1481	XIC(267.13±500ppm)
4-Isopropylphenol, TMS derivative	1039.97 s, 1.085 s	27253046	794	1277.3	193.14	4045	XIC(193.14±500ppm)
4-Isopropylpyridine	749.993 s, 1.427 s	3.2E+08	938	1033.3	106.08	3377	XIC(106.08±500ppm)
4-Methoxymandelic acid, 2TMS derivative	1574.94 s, 1.045 s	16519985	716	1880	209.13	1457	XIC(209.13±500ppm)
4-Methoxy-o-phenylenediamine	2184.9 s, 3.330 s	9832193	740	2693.4	138.13	697	XIC(138.13±500ppm)
4-Methyl-4-vinylbutyrolactone	764.992 s, 1.817 s	2458583	827	1044.4	111.06	608	XIC(111.06±500ppm)
4-Methylvaleric acid, TMS derivative	834.988 s, 1.057 s	1.16E+08	765	1096.3	75.04	2929	XIC(75.04±500ppm)
4-Oxopentanoic acid	684.997 s, 1.537 s	78653866	736	985.2	43.04	3300	XIC(43.04±500ppm)
4-Thujanol, trimethylsilyl ether	1054.97 s, 0.963 s	25509641	708	1290.9	73.06	1480	XIC(73.06±500ppm)
5-Cyano-2-methyl-4-methylthio-6-phenylpyrimidine	1924.92 s, 1.499 s	50693316	706	2346.7	241.22	1006	XIC(241.22±500ppm)
5-Methyl-1-phenylbicyclo[3.2.0]heptane	1229.96 s, 1.481 s	8534356	762	1468.4	118.1	1082	XIC(118.10±500ppm)
5-Methyl-4-hexene-1-yl acetate	1729.93 s, 1.814 s	8188173	740	2086.7	96.11	852	XIC(96.11±500ppm)
5-Oxohexanoic Acid, TMS derivative	1004.98 s, 1.258 s	8320015	773	1245.5	75.04	673	XIC(75.04±500ppm)
6,7-Dihydroxy-1-tetralone, 2TMS derivative	2069.91 s, 1.281 s	42137673	743	2540	322.22	3690	XIC(322.22±500ppm)
7,7,9,9-Tetramethyl-3,6,8,10,13-pentaoxa-7,9-disilapentadecane	744.993 s, 0.876 s	5630543	757	1029.6	133.06	1212	XIC(133.06±500ppm)
7,8-Dimethoxy-3,3-dimethyl-1-methylene-1,2,3,4-tetrahydrodibenzofuran	1574.94 s, 1.431 s	6705098	706	1880	272.2	1858	XIC(272.20±500ppm)
7,9-Di-tert-butyl-1-oxaspiro[4.5]deca-6,9-diene-2,8-dione	1614.94 s, 1.660 s	31155604	926	1933.3	57.09	2539	XIC(57.09±500ppm)
7-Isopropyl-1,1,4a-trimethyl-1,2,3,4,4a,9,10,10a-octahydrophenanthrene	1719.93 s, 1.677 s	28277293	873	2073.3	255.25	3899	XIC(255.25±500ppm)
7-Oxodehydroabietic acid, methyl ester	2049.91 s, 2.529 s	1.07E+08	843	2513.4	253.19	2285	XIC(253.19±500ppm)
7-Oxodehydroabietic acid, trimethylsilyl ester	2054.91 s, 2.130 s	5.08E+08	782	2520	268.32	2050	XIC(268.32±500ppm)
7-Oxoctanoic acid, 2-trimethylsilyl ethyl ester	1134.97 s, 1.240 s	30125532	754	1370	73.06	1995	XIC(73.06±500ppm)
7-Phenyl-7H-triazolo[e]benzofuran	1914.92 s, 1.814 s	3.61E+08	718	2333.4	237.19	607	XIC(237.19±500ppm)
9H-xanthen-9-one, 1-(1,1-dimethylethyl)-	1914.92 s, 1.772 s	4.78E+08	707	2333.4	237.23	1835	XIC(237.23±500ppm)
Abietic acid	1959.92 s, 2.354 s	70814900	796	2393.4	105.08	750	XIC(105.08±500ppm)
Abietic acid, TMS derivative	1949.92 s, 1.609 s	1.53E+08	820	2380	256.42	933	XIC(256.42±500ppm)
Acetamide, 2,2,2-trifluoro-	764.992 s, 0.662 s	53250283	775	1044.4	44.03	504	XIC(44.03±500ppm)
Acetate, 4-hydroxy-3-methyl-2-butenyl-	694.996 s, 1.168 s	9934050	745	992.6	43.08	590	XIC(43.08±500ppm)
Acetic acid, 1,7,7-trimethyl-bicyclo[2.2.1]hept-2-yl ester	1054.97 s, 1.271 s	91539673	952	1290.9	95.1	4062	XIC(95.10±500ppm)
Actin, bis-1,3-trimethylsilyl ether	939.981 s, 0.916 s	45334971	807	1187	73.06	1775	XIC(73.06±500ppm)
Androstan-17-one, 3-ethyl-3-hydroxy-, (5α)-	1714.93 s, 1.693 s	48814844	718	2066.7	43.04	1726	XIC(43.04±500ppm)
Anthracene	1514.94 s, 2.226 s	8243852	945	1800	178.11	909	XIC(178.11±500ppm)
Anthracene, 9-ethyl-9,10-dihydro-9-methyl-	1714.93 s, 1.842 s	17138857	728	2066.7	193.13	2246	XIC(193.13±500ppm)
Benzaldehyde, 2,5-dimethoxy-	1229.96 s, 1.923 s	7.8E+08	930	1468.4	166.09	4793	XIC(166.09±500ppm)
Benzaldehyde, 4-(1-methylethyl)-	984.978 s, 1.527 s	33717627	910	1227.3	133.09	3094	XIC(133.09±500ppm)
Benzaldehyde, 4-methoxy-	1024.98 s, 1.908 s	11474846	931	1263.6	135.07	1203	XIC(135.07±500ppm)
Benzene, (1-methyldecyl)-	1439.95 s, 1.228 s	9017451	868	1762.2	105.09	623	XIC(105.09±500ppm)
Benzene, (1-methyldodecyl)-	1604.94 s, 1.246 s	15562419	903	1906	105.09	1068	XIC(105.09±500ppm)
Benzene, 1,3-dimethoxy-5-[(1E)-2-phenylethenyl]-	1659.93 s, 2.132 s	9452651	741	1993.3	166.09	1589	XIC(166.09±500ppm)
Benzene, 1,4-dimethoxy-	919.982 s, 1.618 s	21867050	926	1169.6	123.07	3129	XIC(123.07±500ppm)
benzene, 1,4-dimethoxy-2-(2-phenylethynyl)-	1889.92 s, 2.681 s	12038359	814	2300	238.13	655	XIC(238.13±500ppm)
Benzene, 1,4-dimethoxy-2-methyl-	1014.98 s, 1.560 s	5052138	838	1254.5	137.08	1260	XIC(137.08±500ppm)
Benzene, 2-methoxy-4-methyl-1-(1-methylethyl)-	999.977 s, 1.293 s	6754142	846	1240.9	149.12	1252	XIC(149.12±500ppm)

Benzene, 4-ethenyl-1,2-dimethoxy-	1134.97 s, 1.665 s	1486795	719	1370	164.11	553	XIC(164.11±500ppm)
Benzenecarbothioic acid, 2,4,6-triethyl-, S-(2-phenylethyl) ester	1699.93 s, 1.579 s	11808317	815	2046.7	189.19	587	XIC(189.19±500ppm)
Benzenepropanoic acid, 3,5-bis(1,1-dimethylethyl)-4-hydroxy-, octadecyl ester	2734.87 s, 0.970 s	46845595	743	3426.8	57.09	1207	XIC(57.09±500ppm)
Benzenepropanoic acid, TBDMS derivative	1079.97 s, 1.083 s	1.23E+08	718	1315	73.06	2672	XIC(73.06±500ppm)
benzoic acid, 4-ethenyl-, 4-[[[(methylsulfonyl)amino]methyl]phenyl] ester	1039.97 s, 0.927 s	41293404	728	1277.3	131.11	1392	XIC(131.11±500ppm)
Benzoic acid, TMS derivative	1009.98 s, 1.252 s	34989590	803	1250	105.05	9259	XIC(105.05±500ppm)
Benzyl alcohol, TMS derivative	904.983 s, 1.141 s	15793400	817	1156.5	91.07	891	XIC(91.07±500ppm)
Bicyclo[2.2.1]heptan-2-ol, 1,7,7-trimethyl-, formate, endo-	994.977 s, 1.286 s	6763667	858	1236.4	95.1	520	XIC(95.10±500ppm)
Bicyclo[2.2.1]heptan-2-one, 1,7,7-trimethyl-, (1S)-	899.983 s, 1.414 s	52583474	950	1152.2	95.1	3515	XIC(95.10±500ppm)
Bicyclo[3.1.0]hexane, 4-methylene-1-(1-methylethyl)-	744.993 s, 1.089 s	54117394	892	1029.6	93.08	1633	XIC(93.08±500ppm)
Bicyclo[3.1.1]hept-2-ene-2-carboxaldehyde, 6,6-dimethyl-	959.98 s, 1.466 s	12057982	747	1204.5	79.07	658	XIC(79.07±500ppm)
Bicyclo[3.1.1]hept-3-en-2-one, 4,6,6-trimethyl-	974.979 s, 1.562 s	20943916	860	1218.2	107.1	944	XIC(107.10±500ppm)
Bicyclo[3.1.1]heptan-2-one, 6,6-dimethyl-, (1R)-	889.984 s, 1.596 s	8781199	736	1143.5	83.06	1005	XIC(83.06±500ppm)
Bicyclo[3.1.1]heptan-3-one, 2,6,6-trimethyl-	919.982 s, 1.392 s	18199766	870	1169.6	83.1	975	XIC(83.10±500ppm)
Biphenyl	1154.97 s, 1.718 s	1836438	902	1390	154.1	556	XIC(154.10±500ppm)
Bisphenol AF, bis(trimethylsilyl) ether	1684.93 s, 1.056 s	16313250	816	2026.7	73.06	1694	XIC(73.06±500ppm)
Butanedioic acid, 2TMS derivative	1084.97 s, 1.055 s	80235312	840	1320	73.06	5968	XIC(73.06±500ppm)
Carvacrol, TMS derivative	1104.97 s, 1.066 s	8825837	714	1340	207.15	522	XIC(207.15±500ppm)
Carvone	1014.98 s, 1.488 s	4672721	812	1254.5	82.06	748	XIC(82.06±500ppm)
Caryophyllene	1199.96 s, 1.193 s	87515858	957	1436.8	41.06	1710	XIC(41.06±500ppm)
Caryophyllene oxide	1324.96 s, 1.394 s	13732104	779	1572.2	41.06	510	XIC(41.06±500ppm)
Cetene	1344.95 s, 0.996 s	55171738	897	1594.4	43.08	2195	XIC(43.08±500ppm)
Chrysanthemyl alcohol, trimethylsilyl ether (stereoisomer 1)	1119.97 s, 1.098 s	1.41E+08	745	1355	123.14	6024	XIC(123.14±500ppm)
cis-Carveol, trimethylsilyl ether	1104.97 s, 1.035 s	27407328	739	1340	73.06	985	XIC(73.06±500ppm)
Communic Acid, TMS Derivative	1884.92 s, 1.521 s	52437988	719	2293.4	72.85	1019	XIC(72.85±500ppm)
Cuminy alcohol, trimethylsilyl ether	1164.97 s, 1.149 s	8329196	834	1400	133.12	1140	XIC(133.12±500ppm)
Cycloheptasiloxane, tetradecamethyl-	1259.96 s, 0.744 s	25502063	885	1500	73.06	2883	XIC(73.06±500ppm)
Cyclohexane, 1-ethyl-2-propyl-	1089.97 s, 0.904 s	23598439	712	1325	69.08	2241	XIC(69.08±500ppm)
Cyclohexanemethanol, α,α,4-trimethyl-	894.984 s, 1.218 s	1.21E+08	864	1147.8	59.07	9639	XIC(59.07±500ppm)
Cyclohexasiloxane, dodecamethyl-	1094.97 s, 0.732 s	62647736	885	1330	73.06	4924	XIC(73.06±500ppm)
Cyclopentane, 1-pentyl-2-propyl-	1664.93 s, 0.975 s	11240896	741	2000	69.08	1020	XIC(69.08±500ppm)
Cyclopentasiloxane, decamethyl-	904.983 s, 0.720 s	79796134	898	1156.5	73.06	6547	XIC(73.06±500ppm)
Cyclopentene, 4,4-dimethyl-	1019.98 s, 1.820 s	9399017	911	1259.1	81.09	1001	XIC(81.09±500ppm)
Cyclotetrasiloxane, octamethyl-	704.996 s, 0.729 s	41049886	894	1000	281.09	3739	XIC(281.09±500ppm)
Cyclotrisiloxane, 2,4-dimethyl-2,4,6,6-tetrahenyl-	2304.89 s, 2.053 s	9589935	834	2853.4	377.1	718	XIC(377.10±500ppm)
Cyclotrisiloxane, hexamethyl-	679.997 s, 0.802 s	15780514	767	981.5	207.06	4081	XIC(207.06±500ppm)
Cytosine	1854.92 s, 2.599 s	6682851	738	2253.4	111.09	678	XIC(111.09±500ppm)
Decane, 2,4,6-trimethyl-	784.991 s, 0.446 s	16786127	732	1059.3	44.01	587	XIC(44.01±500ppm)
Decane, 3,7-dimethyl-	1024.98 s, 0.872 s	54683040	881	1263.6	57.09	2261	XIC(57.09±500ppm)
Decane, 5,6-dimethyl-	879.985 s, 0.839 s	5275463	837	1134.8	43.08	650	XIC(43.08±500ppm)
Decanoic acid, TMS derivative	1224.96 s, 1.009 s	23494270	898	1463.2	73.06	1982	XIC(73.06±500ppm)
Dehydroabietic acid	1944.92 s, 2.379 s	9256886	809	2373.4	239.21	587	XIC(239.21±500ppm)
Dehydroabietol benzoate	1704.93 s, 1.851 s	1958939	701	2053.3	253.2	507	XIC(253.20±500ppm)
Dibenzofuran	1289.96 s, 1.863 s	2350672	872	1533.3	168.08	713	XIC(168.08±500ppm)
Dibutyl phthalate	1644.94 s, 1.737 s	26315332	930	1973.3	149.05	2398	XIC(149.05±500ppm)
Diethylene glycol, 2TMS derivative	1014.98 s, 0.946 s	59166055	838	1254.5	73.06	2303	XIC(73.06±500ppm)
Dihydromyrcenol, trimethylsilyl ether	1039.97 s, 2.264 s	2.73E+08	902	1277.3	131.11	3302	XIC(131.11±500ppm)
Dimethyl phthalate	1224.96 s, 1.950 s	7494659	840	1463.2	163.07	1686	XIC(163.07±500ppm)
Dimethyl(trimethylsilyl)ethoxysilane	674.998 s, 0.830 s	13011511	728	977.8	73.06	2306	XIC(73.06±500ppm)
Disiloxane, hexamethyl-	3224.83 s, 0.513 s	16593516	837	4080.2	147.08	1290	XIC(147.08±500ppm)
Doconexent, TBDMS derivative	1594.94 s, 1.015 s	26373534	723	1906.7	73.06	512	XIC(73.06±500ppm)
Doconexent, TMS derivative	1709.93 s, 1.276 s	35567051	742	2060	75.04	530	XIC(75.04±500ppm)
Docosane	1729.93 s, 0.980 s	7690130	750	2086.7	57.09	1007	XIC(57.09±500ppm)
Dodecane	744.993 s, 0.819 s	12712382	871	1029.6	57.09	1095	XIC(57.09±500ppm)
Dodecane, 2,6,11-trimethyl-	1054.97 s, 0.859 s	69908219	890	1290.9	57.09	3148	XIC(57.09±500ppm)
Estragole	959.98 s, 1.445 s	30710133	912	1204.5	148.11	3182	XIC(148.11±500ppm)
Ethanol, 2-(2-butoxyethoxy)-, acetate	1134.97 s, 1.385 s	3248932	894	1370	43.04	815	XIC(43.04±500ppm)
Ethanone, 1-(1,3-dimethyl-3-cyclohexen-1-yl)-	1159.97 s, 2.071 s	7599784	805	1395	109.12	1207	XIC(109.12±500ppm)
Ethanone, 1-(3-methylphenyl)-	944.98 s, 1.653 s	11118800	813	1191.3	119.07	1635	XIC(119.07±500ppm)
Ethanone, 1-(4-pyridinyl)-	839.987 s, 1.861 s	3274597	902	1100	78.05	642	XIC(78.05±500ppm)
Ethanone, 1-(5-methoxy-2-methyl-3(1H)-indolyl)-	1569.94 s, 2.083 s	9770415	776	1873.3	188.1	1315	XIC(188.10±500ppm)
Ethanone, 1-[4-(1-methylethyl)phenyl]-	1089.97 s, 1.529 s	7303476	790	1325	147.11	1175	XIC(147.11±500ppm)
Ethyl cis-2-trimethylsilyl-cyclopropane-1-carboxylate	939.981 s, 1.357 s	12092883	755	1187	143.08	2322	XIC(143.08±500ppm)
Ethylamine, N,N-diocetyl-2-phenylthio	2039.91 s, 1.829 s	1.98E+08	783	2500	254.23	1065	XIC(254.23±500ppm)
Ethylene glycol, 2TMS derivative	3054.85 s, 0.513 s	81890641	734	3853.5	73.07	701	XIC(73.07±500ppm)
Eucalyptol	749.993 s, 1.126 s	19537904	752	1033.3	43.05	532	XIC(43.05±500ppm)
exo-7-(trans-1-Propenyl)bicyclo[4.2.0]oct-1(2)-ene	1674.93 s, 1.430 s	9281056	733	2013.3	148.15	869	XIC(148.15±500ppm)
exo-Borneol, TMS derivative	989.978 s, 0.918 s	3.35E+08	946	1231.8	95.1	9880	XIC(95.10±500ppm)
Fenchone	824.988 s, 1.331 s	79810872	846	1088.9	81.08	3158	XIC(81.08±500ppm)
Ferulic acid, 2TMS derivative	1734.93 s, 1.391 s	2361258	742	2093.3	338.19	815	XIC(338.19±500ppm)
Glycerol monostearate, 2TMS derivative	2144.9 s, 1.271 s	43024142	825	2640.1	43.08	1777	XIC(43.08±500ppm)
Glycerol, 3TMS derivative	949.98 s, 0.935 s	59238316	793	1195.7	73.06	1809	XIC(73.06±500ppm)
Glycine	729.994 s, 0.411 s	18764931	722	1018.5	44.01	715	XIC(44.01±500ppm)
Harmol, bis(ethyl)-	1734.93 s, 1.717 s	17728598	707	2093.3	254.24	1043	XIC(254.24±500ppm)
Heneicosane	1684.93 s, 0.970 s	1.4E+08	877	2026.7	57.09	1584	XIC(57.09±500ppm)
Hentriacontane	1799.93 s, 0.994 s	1.7E+08	875	2180	57.09	1821	XIC(57.09±500ppm)
Heptacosane	1479.95 s, 0.942 s	2.85E+09	871	1756.3	57.09	5698	XIC(57.09±500ppm)
Heptadecane, 2,6,10,14-tetramethyl-	1284.96 s, 0.931 s	81185660	846	1527.8	57.09	4899	XIC(57.09±500ppm)
Heptadecane, 2,6,10,15-tetramethyl-	1189.96 s, 0.880 s	49829616	859	1426.3	57.09	1881	XIC(57.09±500ppm)
Heptadecane, 2-methyl-	2159.9 s, 1.138 s	37515691	750	2660.1	57.09	1172	XIC(57.09±500ppm)
Heptadecanoic acid, TMS derivative	1764.93 s, 1.109 s	4980581	866	2133.3	117.06	668	XIC(117.06±500ppm)
Heptane, 2,2,4,6,6-pentamethyl-	689.997 s, 0.817 s	24307618	745	988.9	57.09	1256	XIC(57.09±500ppm)
Heptasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13-tetradecamethyl-	1249.96 s, 0.773 s	4065941	832	1489.5	73.06	525	XIC(73.06±500ppm)
Heptasiloxane, hexadecamethyl-	1464.95 s, 0.736 s	6079993	791	1737.5	73.06	764	XIC(73.06±500ppm)
Hexadecane	959.98 s, 0.836 s	53965728	829	1204.5	57.09	3792	XIC(57.09±500ppm)
Hexadecane, 2,6,11,15-tetramethyl-	1119.97 s, 0.890 s	67892197	879	1355	43.08	10410	XIC(43.08±500ppm)
Hexanoic acid, TMS derivative	904.983 s, 1.098 s	45173801	725	1156.5	75.04	1264	XIC(75.04±500ppm)
Hentriacontane	2354.89 s, 1.869 s	99595709	934	2920.1	57.09	3871	XIC(57.09±500ppm)
Humulene epoxide I	1364.95 s, 1.473 s	15940821	806	1617.7	93.09	627	XIC(93.09±500ppm)
Hydracrylic acid, 2TMS derivative	899.983 s, 0.934 s	38779590	911	1152.2	147.09	3001	XIC(147.09±500ppm)
Hydroquinone, TMS derivative	1114.97 s, 1.393 s	3119957	775	1350	167.08	701	XIC(167.08±500ppm)
Iminodiacetic acid, N-[[5-fluorenyloxy]carbonyl]-	1614.94 s, 1.998 s	58427660	735	1933.3	178.1	5924	XIC(178.10±500ppm)
Isonicotinic Acid, TMS derivative	929.981 s, 1.144 s	40603299	739	1178.3	180.11	7421	XIC(180.11±500ppm)
Isophthalic acid, 2,4-dichlorophenyl pentyl ester	1179.97 s, 1.131 s	1469720	706	1415.8	219.16	771	XIC(219.16±500ppm)
Isophthalic acid, 2TMS derivative	1339.96 s, 1.029 s	7890339	727	1588.9	295.2	2564	XIC(295.20±500ppm)
Isopimaric acid, TMS	1864.92 s, 1.486 s	1.09E+08	773	2266.7	241.22	3189	XIC(241.22±500ppm)
Isospathulenol	1334.96 s, 1.370 s	13035067	730	1583.3	43.05	1827	XIC(43.05±500ppm)
Kaur-16-en-18-olc acid, (4α)-, O-TMS	1914.92 s, 1.517 s	86164115	731	2333.4	241.3	1149	XIC(241.30±500ppm)

Kaur-16-ene, 18-[[trimethylsilyloxy]-, (4a)-	1829.92 s, 1.353 s	1.32E+08	749	2220	257.32	517	XIC(257.32±500ppm)
Kolavenol, O-TMS	1739.93 s, 1.206 s	1.22E+08	728	2100	73.06	1232	XIC(73.06±500ppm)
L-(+)-Lactic acid, trimethylsilyl ether	799.99 s, 0.987 s	2.34E+08	862	1070.4	75.04	838	XIC(75.04±500ppm)
Labda-8(20),14-dien-13-ol, (13S)-, O-TMS	1784.93 s, 1.256 s	2.44E+08	729	2160	73.06	13736	XIC(73.06±500ppm)
Lactic Acid, TMS derivative	794.99 s, 2.223 s	46139408	943	1066.7	73.06	908	XIC(73.06±500ppm)
Levulinic acid, TMS derivative	884.984 s, 1.282 s	28490792	905	1139.1	75.04	1435	XIC(75.04±500ppm)
Linolool oxide, [E]-, TMS derivative	1264.96 s, 1.201 s	26916148	715	1505.6	131.11	2110	XIC(131.11±500ppm)
Linolool oxide, [Z]-, TMS derivative	1409.95 s, 1.292 s	18282584	762	1670.6	131.11	1229	XIC(131.11±500ppm)
Linolool oxide, TMS derivative	1359.95 s, 1.248 s	40472861	751	1611.8	131.11	2612	XIC(131.11±500ppm)
Longifolene	1184.97 s, 1.227 s	1.65E+08	944	1421	41.06	4075	XIC(41.06±500ppm)
Malic acid, 3TMS derivative	1264.96 s, 0.960 s	8164456	802	1505.6	147.09	610	XIC(147.09±500ppm)
m-Cresol, TMS derivative	889.984 s, 1.096 s	3097677	841	1143.5	165.1	867	XIC(165.10±500ppm)
Mercaptoethanol, TMS derivative	3019.85 s, 0.513 s	77470272	730	3806.8	73.06	1401	XIC(73.06±500ppm)
Methyl 15-hydroxyabieta-9(11),8(14),12-trien-18-ate, TMS derivative	2014.91 s, 1.751 s	43107241	716	2466.7	327.25	1191	XIC(327.25±500ppm)
Methyl 2,6-dihydroxybenzoate, 2TMS derivative	1699.93 s, 1.440 s	5848148	748	2046.7	297.18	1256	XIC(297.18±500ppm)
Methyl abietate	1699.93 s, 1.644 s	35105224	746	2046.7	256.26	2483	XIC(256.26±500ppm)
Methyl dehydroabietate	1804.93 s, 2.050 s	22898103	746	2186.7	239.21	1075	XIC(239.21±500ppm)
Methyleugenol	1174.97 s, 1.626 s	22141297	919	1410.5	178.13	3691	XIC(178.13±500ppm)
Myristic acid, TMS derivative	1554.94 s, 1.061 s	33427335	919	1853.3	73.06	8647	XIC(73.06±500ppm)
Naphthalene	944.98 s, 1.674 s	4160689	857	1191.3	128.08	849	XIC(128.08±500ppm)
Naphthalene, 1,2,3,4-tetrahydro-1,6-dimethyl-4-[(1-methylethyl)-, (1S)-cis-	1294.96 s, 1.358 s	2.07E+08	905	1538.9	159.14	12008	XIC(159.14±500ppm)
Naphthalene, 1,2,3,4-tetrahydro-2,5,8-trimethyl-	1314.96 s, 1.880 s	4134015	737	1561.1	159.11	1142	XIC(159.11±500ppm)
Naphthalene, 1,2,4a,5,8a-hexahydro-4,7-dimethyl-1-(1-methylethyl)-, [1S-(1a,4a,8a)]-	1289.96 s, 1.269 s	89000458	906	1533.3	161.16	5402	XIC(161.16±500ppm)
Naphthalene, 1,6-dimethyl-4-[(1-methylethyl)-	1424.95 s, 1.632 s	6846495	779	1688.2	183.15	835	XIC(183.15±500ppm)
Naphthalene, 1-methyl-7-[(1-methylethyl)-	1344.95 s, 1.614 s	20700106	889	1594.4	169.13	3621	XIC(169.13±500ppm)
Naphthalene, 3-[1,1-dimethylethyl]-1,2-dihydro-	1304.96 s, 1.503 s	29049501	810	1550	171.14	2657	XIC(171.14±500ppm)
Naphthalene, decahydro-1,1,4a-trimethyl-6-methylene-5-(3-methyl-2,4-pentadienyl)-, [4aS-(4a,5a,8a)]-	1769.93 s, 1.879 s	66335346	826	2140	133.12	1943	XIC(133.12±500ppm)
Naphthalene, decahydro-1,1,4a-trimethyl-6-methylene-5-(3-methylene-4-pentenyl)-, [4aS-(4a,5a,8a)]-	1754.93 s, 1.926 s	8492441	718	2120	257.23	789	XIC(257.23±500ppm)
n-Hexadecanoic acid	1634.94 s, 1.269 s	63708162	914	1960	73.04	2049	XIC(73.04±500ppm)
Niacin, TMS derivative	1039.97 s, 1.279 s	9368589	823	1277.3	180.08	1772	XIC(180.08±500ppm)
Nonadecane, 2-methyl-	2124.9 s, 1.120 s	20622579	741	2613.4	57.09	644	XIC(57.09±500ppm)
Nonanal	844.987 s, 1.170 s	13473895	944	1104.3	57.08	595	XIC(57.08±500ppm)
Nonanoic acid, TMS derivative	1129.97 s, 0.996 s	47564872	894	1365	73.06	1458	XIC(73.06±500ppm)
Octacosane, 2-methyl-	2844.86 s, 3.173 s	11289290	816	3573.4	57.09	693	XIC(57.09±500ppm)
Octadecane	1944.92 s, 1.025 s	1.19E+08	833	2373.4	57.09	2610	XIC(57.09±500ppm)
Octanoic acid, TMS derivative	1029.98 s, 0.985 s	64601009	938	1268.2	73.06	5218	XIC(73.06±500ppm)
Oxalic acid, 2TMS derivative	2989.85 s, 0.513 s	77294767	750	3766.8	73.06	1186	XIC(73.06±500ppm)
p-(Benzylideneamino)phenol	1319.96 s, 0.960 s	4451304	753	1566.7	197.26	745	XIC(197.26±500ppm)
Palmitic Acid, TMS derivative	1634.94 s, 1.232 s	10462480	775	1960	117.06	1056	XIC(117.06±500ppm)
p-Anisic acid, TMS derivative	1284.96 s, 1.425 s	16589408	869	1527.8	135.07	1532	XIC(135.07±500ppm)
p-Cymene	739.994 s, 1.144 s	45119979	941	1025.9	119.1	2055	XIC(119.10±500ppm)
Pentan-3-ol, trimethylsilyl ether	1269.96 s, 0.881 s	87754627	830	1511.1	131.11	2515	XIC(131.11±500ppm)
Pentanoic acid, 4-oxo-	884.984 s, 1.216 s	29548672	788	1139.1	43.04	748	XIC(43.04±500ppm)
Pentanoic acid, TMS derivative	789.99 s, 1.122 s	34059606	706	1063	75.04	780	XIC(75.04±500ppm)
Pentasiloxane, dodecamethyl-	939.981 s, 0.719 s	43791763	918	1187	73.06	8046	XIC(73.06±500ppm)
Phenanthrene, 7-ethenyl-1,2,3,4,4a,4b,5,6,7,8,10,10a-dodecahydro-4a,7-dimethyl-1-methylene-, [4aS-(4a,4a,7,7,10a)]-	1594.94 s, 1.439 s	16910478	842	1906.7	145.12	1483	XIC(145.12±500ppm)
Phenanthrene, 7-ethenyl-1,2,3,4,4a,4b,5,6,7,9,10,10a-dodecahydro-1,1,4a,7-tetramethyl-, [4aS-(4a,4a,7,7,10a)]-	1644.94 s, 1.439 s	82739866	921	1973.3	137.15	7548	XIC(137.15±500ppm)
Phenol, TMS derivative	779.991 s, 1.063 s	10463630	875	1055.6	151.08	2356	XIC(151.08±500ppm)
Phthalic acid, di(3-methylphenyl) ester	1909.92 s, 1.983 s	5.97E+08	840	2326.7	239.2	2222	XIC(239.20±500ppm)
Picolinic acid, TMS derivative	1094.97 s, 1.598 s	2795562	864	1330	180.08	764	XIC(180.08±500ppm)
Pimaric acid, TMS derivative	1884.92 s, 1.582 s	1.43E+08	798	2293.4	72.99	513	XIC(72.99±500ppm)
Pinacol, 2TMS derivative	1184.97 s, 1.046 s	33149573	727	1421	73.06	3244	XIC(73.06±500ppm)
p-Menthane, 3-allylperoxy-	2229.9 s, 3.401 s	11617857	743	2753.4	138.13	933	XIC(138.13±500ppm)
p-Propionolactide	1084.97 s, 1.337 s	8438107	721	1320	106.08	752	XIC(106.08±500ppm)
Pregnane-3,20-diol, (3a,5b,20S)-, 2TMS derivative	1949.92 s, 1.194 s	1.16E+08	716	2380	73.06	1056	XIC(73.06±500ppm)
Propanedioic acid, 2TMS derivative	969.979 s, 1.035 s	7422882	850	1213.6	147.09	1056	XIC(147.09±500ppm)
Propanoic acid, 2-oxo-3-(trimethylsilyl)-, trimethylsilyl ester	994.977 s, 0.994 s	20462190	805	1236.4	73.06	1601	XIC(73.06±500ppm)
Propanoic acid, 3-(trimethylsilyl)-, ethyl ester	944.98 s, 1.206 s	21118784	756	1191.3	73.06	1216	XIC(73.06±500ppm)
Propanoic acid, TBDMS derivative	944.98 s, 0.794 s	5665837	713	1191.3	131.11	1080	XIC(131.11±500ppm)
Propanoyl fluoride, 2,3,3,3-tetrafluoro-2-[1,1,2,3,3-hexafluoro-2-(heptafluoropropoxy)propoxy]-	774.991 s, 1.585 s	1380256	732	1051.9	169.02	509	XIC(169.02±500ppm)
Propylene glycol, 2TMS derivative	714.995 s, 0.805 s	82632843	872	1007.4	73.06	2000	XIC(73.06±500ppm)
Pyrene	1764.93 s, 2.645 s	2697475	915	2133.3	202.11	607	XIC(202.11±500ppm)
Pyridine	699.996 s, 0.760 s	30401049	891	996.3	79.05	1621	XIC(79.05±500ppm)
Pyridine, 2-hexyl-	1069.97 s, 1.352 s	7151191	767	1305	93.07	541	XIC(93.07±500ppm)
Pyrido[2,3-b]isoquinolino[3,4-d]furan-5(6H)-one, 7,9-dimethyl-	2014.91 s, 1.327 s	34180107	705	2466.7	280.17	5172	XIC(280.17±500ppm)
Quinoline, 1,2-dihydro-2,2,4-trimethyl-	1214.96 s, 1.706 s	2504714	805	1452.6	158.12	860	XIC(158.12±500ppm)
Resorcinol, 2TMS derivative	1174.97 s, 1.035 s	6139769	855	1410.5	239.13	1619	XIC(239.13±500ppm)
Retinoic acid, TMS derivative	2019.91 s, 1.829 s	2.77E+08	724	2473.4	254.45	1919	XIC(254.45±500ppm)
S-(+)-S-(1-Hydroxy-1-methylethyl)-2-methyl-2-cyclohexen-1-one	1199.96 s, 1.835 s	19017403	913	1436.8	59.07	2336	XIC(59.07±500ppm)
Sclareolide	1734.93 s, 2.169 s	5496733	856	2093.3	43.05	675	XIC(43.05±500ppm)
Silane, [[dimethylsilyl]methyl]trimethyl-	1044.97 s, 0.924 s	4.97E+08	855	1281.8	131.1	2563	XIC(131.10±500ppm)
Silane, diethylheptadecyloxy(2-methoxyethoxy)-	2034.91 s, 1.856 s	48680275	752	2493.4	387.29	917	XIC(387.29±500ppm)
Silane, diethylhexyloxytridecyloxy-	2004.91 s, 1.909 s	50744211	785	2453.4	357.27	2145	XIC(357.27±500ppm)
Silane, dimethyl[(2-methoxyethoxy)heptadecyloxy-	2049.91 s, 2.339 s	18614246	708	2513.4	373.27	658	XIC(373.27±500ppm)
Silane, tetramethyl-	814.989 s, 0.945 s	1.98E+08	846	1081.5	73.06	2514	XIC(73.06±500ppm)
Silane, trimethylphenyl-	3399.82 s, 0.663 s	33251890	730	4313.5	135.08	991	XIC(135.08±500ppm)
Silanol, trimethyl-	814.989 s, 0.557 s	9.52E+08	935	1081.5	75.04	1274	XIC(75.04±500ppm)
Silanol, trimethyl-, carbonate (2:1)	669.998 s, 0.946 s	19877978	856	974.1	147.09	644	XIC(147.09±500ppm)
Silanol, trimethyl-, phosphate (3:1)	1049.97 s, 0.974 s	50439034	786	1286.4	73.06	649	XIC(73.06±500ppm)
Stearic acid, TMS derivative	1829.92 s, 1.139 s	1.78E+08	921	2220	117.02	744	XIC(117.02±500ppm)
Syringaldehyde, TMS derivative	1414.95 s, 1.580 s	87537717	751	1676.5	224.08	5643	XIC(224.08±500ppm)
Terpin, 2TMS derivative	1289.96 s, 0.907 s	2.67E+08	860	1533.3	131.11	20861	XIC(131.11±500ppm)
Terpinen-4-ol	934.981 s, 1.288 s	14855425	914	1182.6	71.06	1831	XIC(71.06±500ppm)
tert-Butyl[4-(tert-butylimino-oxo-1{5}-azanylidene)-1,2,5-oxadiazol-3-yl-oxo-1{5}-azanylidene]amine	1324.96 s, 0.957 s	1.71E+08	753	1572.2	57.1	1103	XIC(57.10±500ppm)
tert-Butyldimethylsilyl methacrylate	1499.94 s, 1.158 s	18648208	713	1781.3	143.11	1326	XIC(143.11±500ppm)
Tetracosane	1864.92 s, 1.091 s	61713541	938	2266.7	57.09	2591	XIC(57.09±500ppm)
Tetradecane	1009.98 s, 0.863 s	55897943	896	1250	57.09	1945	XIC(57.09±500ppm)
Tetradecane, 3-methyl-	1234.96 s, 0.928 s	1.44E+08	876	1473.7	57.09	3698	XIC(57.09±500ppm)
Tetrahydrogeranyl formate	814.989 s, 0.835 s	61984345	799	1081.5	43.08	1221	XIC(43.08±500ppm)
Tetrasiloxane, decamethyl-	774.991 s, 0.716 s	17801381	870	1051.9	73.06	1066	XIC(73.06±500ppm)
Tiglic acid, TMS derivative	724.995 s, 1.009 s	11704466	841	1014.8	157.09	1565	XIC(157.09±500ppm)
Trachyloban-18-ol, (4a)-	1829.92 s, 1.819 s	1.04E+08	806	2220	81.08	1668	XIC(81.08±500ppm)
trans-Carveol, trimethylsilyl ether	1214.96 s, 1.163 s	32641532	725	1452.6	75.04	1128	XIC(75.04±500ppm)
trans-Geranylgerniol	1629.94 s, 1.420 s	26116152	759	1953.3	41.06	591	XIC(41.06±500ppm)
Tricyclo[5.4.0.0(2,8)]undec-9-ene, 2,6,6,9-tetramethyl-, (1R,2S,7R,8R)-	1129.97 s, 1.114 s	35312635	810	1365	119.1	2275	XIC(119.10±500ppm)
Tricyclo[7.2.2.0(3,8)]trideca-5,12-dien-2-one, 1-methoxy-4-methyl-	2014.91 s, 3.277 s	22859906	734	2466.7	110.09	514	XIC(110.09±500ppm)
Tridecane	974.979 s, 0.835 s	28386758	827	1218.2	57.09	1291	XIC(57.09±500ppm)
Tridecanoic acid, TMS derivative	1479.95 s, 1.049 s	3.14E+08	923	1756.3	73.06	15209	XIC(73.06±500ppm)

Trifluoroacetamide, N-trimethylsilyloxymethyl	814.989 s, 0.750 s	7831572	823	1081.5	77.04	995	XIC(77.04±500ppm)
trimethyl(((1s,4s)-1-methyl-4-(prop-1-en-2-yl)cyclohexyl)oxy)silane	1034.97 s, 0.947 s	17341038	825	1272.7	75.04	863	XIC(75.04±500ppm)
trimethyl(((2R,4S)-1,3,3-trimethylbicyclo[2.2.1]heptan-2-yl)oxy)silane	979.978 s, 0.885 s	2.07E+08	877	1222.7	73.06	1389	XIC(73.06±500ppm)
trimethyl(((2-(2S,4aS)-4a-methyl-8-methylenedecahydronaphthalen-2-yl)propan-2-yl)oxy)silane	2139.9 s, 1.441 s	2.5E+08	731	2633.4	131.1	1640	XIC(131.10±500ppm)
Trimethyl(3,3-difluoro-2-propenyl)silane	3079.84 s, 0.491 s	1.41E+08	829	3886.8	73.05	1690	XIC(73.05±500ppm)
Trimethylsilyl 4-propylbenzoate	1244.96 s, 1.240 s	88019164	805	1484.2	221.13	16563	XIC(221.13±500ppm)
Trimethylsilyl propaneperoxoate	724.995 s, 0.869 s	19785108	706	1014.8	89.06	3027	XIC(89.06±500ppm)
Tris(trimethylsilyl)carbamate	764.992 s, 0.718 s	97664944	755	1044.4	73.06	4508	XIC(73.06±500ppm)
Trisiloxane, octamethyl-	809.989 s, 0.777 s	77083494	868	1077.8	73.06	8957	XIC(73.06±500ppm)
Undecane	784.991 s, 0.798 s	1.86E+08	889	1059.3	43.08	3976	XIC(43.08±500ppm)
Undecane, 4,6-dimethyl-	724.995 s, 0.810 s	9271738	840	1014.8	43.08	520	XIC(43.08±500ppm)
Undecane, 4,7-dimethyl-	839.987 s, 0.830 s	2.52E+08	891	1100	43.08	4373	XIC(43.08±500ppm)
Undecane, 4-methyl-	854.986 s, 0.839 s	2.17E+08	902	1113	43.08	5125	XIC(43.08±500ppm)
Vanillic Acid, 2TMS derivative	1494.95 s, 1.253 s	2936723	768	1775	297.14	842	XIC(297.14±500ppm)
Vanillin, TMS derivative	1299.96 s, 1.533 s	11890330	823	1544.4	194.07	1970	XIC(194.07±500ppm)
α-Calacorene	1309.96 s, 1.449 s	14089469	745	1555.6	157.13	981	XIC(157.13±500ppm)
α-Campholenal	874.985 s, 1.294 s	3630926	796	1130.4	108.11	670	XIC(108.11±500ppm)
α-Corocalene	1819.92 s, 2.148 s	10378803	741	2206.7	43.05	807	XIC(43.05±500ppm)
α-FENCHYL ACETATE	984.978 s, 1.161 s	18020042	905	1227.3	81.08	1276	XIC(81.08±500ppm)
α-Guaiene	1984.91 s, 2.388 s	51497335	753	2426.7	109.12	545	XIC(109.12±500ppm)
α-Hydroxyisobutyric acid, 2TMS derivative	799.99 s, 0.855 s	1.09E+08	830	1070.4	73.06	2473	XIC(73.06±500ppm)
α-Murolene	1269.96 s, 1.246 s	34189050	879	1511.1	105.09	3383	XIC(105.09±500ppm)
β-Eudesmol, TMS derivative	1299.96 s, 0.936 s	1.36E+08	817	1544.4	131.11	8350	XIC(131.11±500ppm)
β-Thujaplicin, tert-butylidimethylsilyl ether	1329.96 s, 1.317 s	2451966	735	1577.8	221.13	588	XIC(221.13±500ppm)

	R.T. 1st, 2nd Dim. (s Area	Similarity	Base Mass	Peak S/N	Quant Masses
BLANK					
(±)-2,5-Dimethoxy-4-Iodoamphetamine, N-trimethylsilyl-	1514.94 s, 1.150 s	2.3E+08	769	116.18	1393 XIC(116.18±500ppm)
(±)-N-Ethylcathinone ephedrine, N-trimethylsilyl-, trimethylsilyl ether	1589.94 s, 1.138 s	4.03E+08	810	144.11	9888 XIC(144.11±500ppm)
(S)-(+)-1-Cyclohexylethylamine, N-trimethylsilyl-	1574.94 s, 1.030 s	3.25E+08	765	116.08	3419 XIC(116.08±500ppm)
(Z)-5-Methoxy-3,5-dimethyl-2-hexenyltrimethylsilane	1034.97 s, 0.820 s	18011633	765	73.04	650 XIC(73.04±500ppm)
1-(2,5-Dimethoxyphenyl)-1-[(trimethylsilyloxy)propan-2-amine	1444.95 s, 1.395 s	1.56E+09	900	73.04	2309 XIC(73.04±500ppm)
1-(2-Methoxy-1-methylethoxy)-2-propanol, TMS derivative	909.983 s, 0.964 s	28524501	887	117.06	1716 XIC(117.06±500ppm)
1,2-Benzenedicarboxylic acid, bis(2-methylpropyl) ester	1194.96 s, 1.661 s	1.17E+08	923	149.01	5130 XIC(149.01±500ppm)
1,2-Cyclohexanedicarboxylic acid, dinonyl ester	2129.9 s, 1.730 s	39788631	770	155.05	1605 XIC(155.05±500ppm)
1,3-Benzenedicarboxylic acid, bis(2-ethylhexyl) ester	2124.9 s, 1.687 s	51421062	922	70.07	2249 XIC(70.07±500ppm)
1,3-Dibutyl-1,1,3,3-tetramethyldisiloxane	1194.96 s, 0.888 s	35174229	803	133.04	4279 XIC(133.04±500ppm)
1,4-Butanediol, 2TMS derivative	924.982 s, 0.848 s	1.13E+08	851	147.05	2783 XIC(147.05±500ppm)
1,6-Dioxacyclododecane-7,12-dione	1309.96 s, 2.072 s	98151503	931	55.04	3966 XIC(55.04±500ppm)
13-Docosanamide, (Z)-	2139.9 s, 2.030 s	60627100	897	59.03	3519 XIC(59.03±500ppm)
1-Butanol, 2-methyl-, propanoate	789.99 s, 0.807 s	1.72E+08	758	43.06	1960 XIC(43.06±500ppm)
1-Butanol, 2-methyl-, trifluoroacetate	1104.97 s, 0.945 s	3.4E+08	790	57.05	3746 XIC(57.05±500ppm)
1-Decanol, 2-ethyl-	984.978 s, 2.167 s	23437970	850	57.07	520 XIC(57.07±500ppm)
1H-Indole-3-ethanamine, 6-fluoro- α -methyl-N,1-bis(trimethylsilyl)-	1494.95 s, 1.203 s	1.27E+08	818	115.96	713 XIC(115.96±500ppm)
1-Monomyristin, 2TMS derivative	1929.92 s, 1.117 s	32883723	843	73.04	1754 XIC(73.04±500ppm)
1-Nonanol, 4,8-dimethyl-	719.995 s, 1.136 s	2.67E+08	813	57.07	564 XIC(57.07±500ppm)
1-Octadecanol, TMS derivative	1774.93 s, 1.035 s	30624162	831	75.02	891 XIC(75.02±500ppm)
1-Octanol, 2-methyl-	1499.94 s, 0.979 s	3.87E+08	766	57.07	2613 XIC(57.07±500ppm)
1-Phenyl-1,2-ethanediol, 2TMS derivative	1204.96 s, 1.030 s	63847769	866	73.04	1787 XIC(73.04±500ppm)
1-Propanamine, N,N-diethyl-	764.992 s, 1.460 s	25022065	820	58.06	1930 XIC(58.06±500ppm)
2(1H)-Naphthalenone, 3,4,4a,5,6,7-hexahydro-1,1,4a-trimethyl-	954.98 s, 1.082 s	20039260	811	41.05	2392 XIC(41.05±500ppm)
2-(Methylamino)ethanol, N,O-bis(trimethylsilyl)-	1499.94 s, 1.230 s	1.8E+08	828	116.16	2561 XIC(116.16±500ppm)
2,2'-Bipyridine	1214.96 s, 2.024 s	10073194	940	156.06	2226 XIC(156.06±500ppm)
2,2-Dimethylpropanoic anhydride	934.981 s, 1.072 s	1.07E+08	800	57.07	5200 XIC(57.07±500ppm)
2,3-Pentanedione	834.988 s, 0.806 s	3.45E+08	806	43.06	2551 XIC(43.06±500ppm)
2,4'-Bipyridine	1304.96 s, 2.175 s	13112906	886	156.06	2096 XIC(156.06±500ppm)
2,4-Di-tert-butylphenoxytrimethylsilane	1309.96 s, 1.082 s	2.05E+08	874	263.17	14058 XIC(263.17±500ppm)
2,5-Cyclohexadiene-1,4-dione, 2,6-bis(1,1-dimethylethyl)-	1239.96 s, 1.317 s	53418036	928	177.12	14456 XIC(177.12±500ppm)
2,5-Dimethoxyphenol, TMS	1209.96 s, 1.385 s	19676841	858	196.04	6001 XIC(196.04±500ppm)
2,5-di-tert-Butyl-1,4-benzoquinone	1579.94 s, 1.708 s	17322949	787	57.07	1835 XIC(57.07±500ppm)
2,6,10-Trimethyltridecane	1109.97 s, 0.905 s	1.34E+09	864	71.07	8443 XIC(71.07±500ppm)
2,6-Diisopropyl-naphthalene	1429.95 s, 1.517 s	2.13E+08	890	197.12	12392 XIC(197.12±500ppm)
2,6-Dimethyldecane	1089.97 s, 0.936 s	1.69E+09	852	43.06	7568 XIC(43.06±500ppm)
2-Butyl-3-(4- β -diethylaminoethoxybenzoyl)benzofuran	1549.94 s, 1.306 s	77297373	813	86.08	3297 XIC(86.08±500ppm)
2-Butylamine, N-tetradecyl-	1479.95 s, 1.412 s	3.84E+09	775	240.13	1147 XIC(240.13±500ppm)
2-Cyclohexen-1-one, 3,5-dimethyl-	854.986 s, 1.591 s	45423245	900	82.03	2934 XIC(82.03±500ppm)
2-Cyclopenten-1-one, 2,3,4,5-tetramethyl-	1049.97 s, 1.211 s	89084104	780	123.07	4741 XIC(123.07±500ppm)
2-Ethylhexyl acrylate	989.978 s, 1.127 s	17379554	841	55.03	1062 XIC(55.03±500ppm)
2-Furanmethanamine, tetrahydro-	1309.96 s, 0.991 s	2.01E+08	782	71.07	732 XIC(71.07±500ppm)
2-Heptanone, 4,6-dimethyl-	719.995 s, 1.011 s	62099763	886	43.03	1555 XIC(43.03±500ppm)
2-Hydroxy-5-methoxybenzaldehyde, TMS derivative	1389.95 s, 1.469 s	10571021	752	209.05	2679 XIC(209.05±500ppm)
2-Isopropyl-5-methyl-1-heptanol	1074.97 s, 0.915 s	9E+08	835	69.06	3874 XIC(69.06±500ppm)
2-Palmitoylglycerol, 2TMS derivative	2024.91 s, 1.152 s	13143305	845	73.04	3408 XIC(73.04±500ppm)
2-Propanoic acid, 2-methyl-, 3,3,5-trimethylcyclohexyl ester	1119.97 s, 1.194 s	10698393	769	109.09	615 XIC(109.09±500ppm)
3,7-dioxo-2,8-disilanonane, 2,2,8,8-tetramethyl-5,5-bis[(trimethylsilyloxy)methyl]-	1284.96 s, 0.789 s	51044052	870	73.04	3726 XIC(73.04±500ppm)
3-Ethyl-3-methylheptane	1244.96 s, 0.916 s	8.76E+08	800	57.07	2544 XIC(57.07±500ppm)
3-Methylvaleric acid, TMS	769.992 s, 0.896 s	79545674	861	73.04	2903 XIC(73.04±500ppm)
3-Pyridinol, TMS derivative	894.984 s, 1.217 s	22352869	882	152.04	3259 XIC(152.04±500ppm)
7,9-Di-tert-butyl-1-oxaspiro(4,5)deca-6,9-diene-2,8-dione	1614.94 s, 1.667 s	1.79E+08	931	57.07	6089 XIC(57.07±500ppm)
8-Methylnonanoic acid, trimethylsilyl ester	1224.96 s, 1.017 s	72336840	857	75.02	2311 XIC(75.02±500ppm)
Acetophenone	814.989 s, 1.619 s	12832026	883	105.02	2155 XIC(105.02±500ppm)
Adrenaline, 4TMS derivative	1544.94 s, 1.098 s	7.72E+08	767	116.08	1693 XIC(116.08±500ppm)
Behenic acid, TMS derivative	2064.91 s, 1.248 s	16271570	864	73.04	2827 XIC(73.04±500ppm)
Benzaldehyde	689.997 s, 1.510 s	12572988	905	77.03	625 XIC(77.03±500ppm)
Benzaldehyde, 2,4-dimethyl-	984.978 s, 1.651 s	13365309	943	133.05	1956 XIC(133.05±500ppm)
Benzaldehyde, 2,5-dimethoxy-	1229.96 s, 1.911 s	46230018	920	166.05	4683 XIC(166.05±500ppm)
Benzenamine, N-methyl-N-phenyl-	1199.96 s, 0.931 s	14826411	753	183.2	963 XIC(183.20±500ppm)
Benzene, (1-butylheptyl)-	1384.95 s, 1.178 s	30677588	806	91.04	1404 XIC(91.04±500ppm)
Benzene, (1-ethylnonyl)-	1409.95 s, 1.209 s	10498790	789	91.05	850 XIC(91.05±500ppm)
Benzene, (1-methyldodecyl)-	1604.94 s, 1.254 s	21031918	819	105.06	1064 XIC(105.06±500ppm)
Benzene, 1,1'-(1,2-cyclobutanediyl)bis-, trans-	1494.95 s, 1.802 s	25443987	871	104.05	1119 XIC(104.05±500ppm)
Benzene, 1,3-bis(1,1-dimethylethyl)-	1019.98 s, 1.122 s	1.24E+08	931	175.13	22492 XIC(175.13±500ppm)
Benzene, 1,4-dimethoxy-	924.982 s, 1.593 s	19862772	902	123.04	3181 XIC(123.04±500ppm)
Benzene, 2-[(ethenyl)oxy)methyl]-1,4-dimethoxy-	2084.91 s, 2.196 s	13269620	758	151.06	1006 XIC(151.06±500ppm)
Benzenepropanoic acid, 3,5-bis(1,1-dimethylethyl)-4-hydroxy-, methyl ester	1629.94 s, 1.568 s	1.07E+08	846	277.16	3609 XIC(277.16±500ppm)
Benzoic acid, methyl ester	844.987 s, 1.518 s	13796172	914	105.02	2795 XIC(105.02±500ppm)
Benzoic Acid, TMS derivative	1014.98 s, 1.239 s	57401389	895	179.04	8027 XIC(179.04±500ppm)
Benzophenone	1389.95 s, 2.027 s	25656931	787	105.03	594 XIC(105.03±500ppm)

Benzothiazole, 2-(4-amino-3-methylphenyl)-	1514.94 s, 1.292 s	1.99E+09	781	240.1	1004	XIC(240.10±500ppm)
Benzyl alcohol, TMS derivative	909.983 s, 1.124 s	28470165	871	91.05	2388	XIC(91.05±500ppm)
Bis(2-chloroethyl) ether	719.995 s, 1.421 s	16807120	889	93	911	XIC(93.00±500ppm)
Bisphenol AF, bis(trimethylsilyl) ether	1684.93 s, 1.062 s	10413290	801	73.04	741	XIC(73.04±500ppm)
Borane, diethyl(decyloxy)-	1264.96 s, 0.918 s	1.32E+09	768	57.08	6899	XIC(57.08±500ppm)
Boric acid, 3TMS derivative	704.996 s, 0.710 s	1.76E+09	861	73.04	3954	XIC(73.04±500ppm)
Butane, 1-chloro-2-methyl-	754.993 s, 0.813 s	96452063	806	57.07	1703	XIC(57.07±500ppm)
Butane, 2,2-dimethyl-	1069.97 s, 0.871 s	2.86E+08	798	43.06	2876	XIC(43.06±500ppm)
Butylated Hydroxytoluene	1279.96 s, 1.327 s	19497270	848	205.15	2854	XIC(205.15±500ppm)
Cycloheptasiloxane, tetradecamethyl-	1259.96 s, 0.752 s	74587121	898	73.04	8668	XIC(73.04±500ppm)
Cyclohexane, tetracosyl-	2309.89 s, 1.853 s	20886229	910	82.07	1417	XIC(82.07±500ppm)
Cyclohexane, tricosyl-	2254.9 s, 1.626 s	22460534	917	82.06	1564	XIC(82.06±500ppm)
Cyclohexane, undecyl-	2204.9 s, 1.486 s	16502846	857	82.07	923	XIC(82.07±500ppm)
Cyclohexanone, 3,3,5-trimethyl-	779.991 s, 1.233 s	38632377	899	83.04	1861	XIC(83.04±500ppm)
Cyclopentane, 1-pentyl-2-propyl-	1159.97 s, 0.963 s	1.52E+08	765	55.06	1326	XIC(55.06±500ppm)
Cyclopentane, nonyl-	1214.96 s, 1.032 s	40240200	836	55.05	2018	XIC(55.05±500ppm)
Cyclopentasiloxane, decamethyl-	889.984 s, 0.744 s	20610100	816	73.04	552	XIC(73.04±500ppm)
Cyclotetrasiloxane, octamethyl-	724.995 s, 0.714 s	2.16E+08	881	281.03	1912	XIC(281.03±500ppm)
Cyclotrisiloxane, hexamethyl-	704.996 s, 0.774 s	59114932	781	207.02	3425	XIC(207.02±500ppm)
Decane	794.99 s, 0.808 s	4.66E+08	873	43.05	2440	XIC(43.05±500ppm)
Decane, 2,4-dimethyl-	1099.97 s, 0.898 s	3.58E+08	796	57.07	2771	XIC(57.07±500ppm)
Decane, 2,6,6-trimethyl-	959.98 s, 0.850 s	3.82E+08	855	57.07	3143	XIC(57.07±500ppm)
Decane, 2-methyl-	994.977 s, 0.879 s	3.68E+08	836	43.06	6327	XIC(43.06±500ppm)
Decane, 3,8-dimethyl-	1254.96 s, 0.916 s	4.19E+08	792	57.09	3005	XIC(57.09±500ppm)
Decane, 5,6-dimethyl-	779.991 s, 0.803 s	1.58E+08	883	43.06	2234	XIC(43.06±500ppm)
Dibutyl phthalate	1644.94 s, 1.744 s	49349092	940	149.01	2714	XIC(149.01±500ppm)
Diethyl Phthalate	1354.95 s, 1.812 s	33002349	875	149.01	3201	XIC(149.01±500ppm)
Diethylene glycol, 2TMS derivative	1014.98 s, 0.956 s	79878621	871	73.04	3762	XIC(73.04±500ppm)
Diethylene glycol, n-butyl ether, trimethylsilyl ether	1109.97 s, 1.083 s	39701241	848	73.04	1561	XIC(73.04±500ppm)
Disiloxane, 1,3-diethyl-1,1,3,3,-tetramethyl-	1044.97 s, 0.941 s	26537507	803	133.04	670	XIC(133.04±500ppm)
D-Mannopyranose, 5TMS derivative	1609.94 s, 0.884 s	13187535	770	73.04	792	XIC(73.04±500ppm)
Docosane	1864.92 s, 1.093 s	1.43E+08	874	57.07	1461	XIC(57.07±500ppm)
Dodecane	804.989 s, 0.790 s	5.51E+08	872	43.06	4255	XIC(43.06±500ppm)
Dodecane, 1-iodo-	1069.97 s, 0.867 s	4.26E+08	779	71.08	2110	XIC(71.08±500ppm)
Dodecane, 2,6,10-trimethyl-	1284.96 s, 0.931 s	4.37E+08	843	57.06	9539	XIC(57.06±500ppm)
Dodecane, 2,6,11-trimethyl-	1029.98 s, 0.883 s	7.65E+08	856	57.07	3440	XIC(57.07±500ppm)
Dodecane, 2,7,10-trimethyl-	1054.97 s, 0.867 s	6.54E+08	870	71.08	6683	XIC(71.08±500ppm)
Dodecane, 4,6-dimethyl-	1009.98 s, 0.874 s	8.99E+08	875	57.07	5314	XIC(57.07±500ppm)
Ephedrine, 2TMS derivative	1569.94 s, 1.167 s	1.54E+08	860	130.09	13032	XIC(130.09±500ppm)
Ethanone, 1-(3-methyloxiranyl)-	824.988 s, 1.520 s	1.29E+08	801	43.03	731	XIC(43.03±500ppm)
Formamide, N,N-diethyl-	659.999 s, 1.423 s	1.36E+08	893	58.06	1577	XIC(58.06±500ppm)
Glycerol, 3TMS derivative	1049.97 s, 0.817 s	2.91E+08	935	73.04	12633	XIC(73.04±500ppm)
Glycolic acid, 2TMS derivative	824.988 s, 0.923 s	1.16E+08	918	73.04	1230	XIC(73.04±500ppm)
Heptacosane	1484.95 s, 0.952 s	1.23E+09	872	71.06	8528	XIC(71.06±500ppm)
Heptadecane, 2,6,10,14-tetramethyl-	1209.96 s, 0.932 s	1.66E+08	855	57.07	3652	XIC(57.07±500ppm)
Heptadecane, 4-methyl-	1379.95 s, 0.961 s	2.6E+09	838	57.07	3148	XIC(57.07±500ppm)
Heptadecanoic acid, TMS derivative	1764.93 s, 1.114 s	83568946	907	73.04	2968	XIC(73.04±500ppm)
Heptasiloxane, hexadecamethyl-	1274.96 s, 0.737 s	64146327	881	73.04	13504	XIC(73.04±500ppm)
Hexadecane	1189.96 s, 0.885 s	5.55E+08	855	57.07	3959	XIC(57.07±500ppm)
Hexadecane, 1-iodo-	1444.95 s, 0.923 s	3.82E+08	776	85.09	1464	XIC(85.09±500ppm)
Hexadecane, 2,6,10,14-tetramethyl-	1669.93 s, 0.967 s	3.61E+08	819	71.07	2616	XIC(71.07±500ppm)
Hexadecane, 2-methyl-	1404.95 s, 0.971 s	8.6E+08	907	71.05	2182	XIC(71.05±500ppm)
Hexadecane, 7-methyl-	1389.95 s, 0.969 s	6.08E+08	881	57.04	3400	XIC(57.04±500ppm)
Hexadecanoic acid, dodecyl ester	2234.9 s, 1.605 s	12882867	793	43.06	772	XIC(43.06±500ppm)
Hexane, 3,3-dimethyl-	1234.96 s, 0.935 s	1.67E+08	809	43.05	3293	XIC(43.05±500ppm)
Hexasiloxane, tetradecamethyl-	1124.97 s, 0.733 s	40179225	902	73.04	3158	XIC(73.04±500ppm)
Hexatriacontane	2334.89 s, 1.745 s	76401899	881	57.07	1328	XIC(57.07±500ppm)
Hydracrylic acid, 2TMS derivative	904.983 s, 0.925 s	19205690	864	147.06	937	XIC(147.06±500ppm)
Isopropylamine, N-trimethylsilyl-	1559.94 s, 1.534 s	86061452	778	116.08	876	XIC(116.08±500ppm)
L-Leucine, 2TMS derivative	1614.94 s, 1.125 s	17667351	788	158.12	3853	XIC(158.12±500ppm)
Methyl (3,4-dimethoxyphenyl)(hydroxy)acetate, TMS derivative	1459.95 s, 1.313 s	2.19E+08	780	239.09	629	XIC(239.09±500ppm)
Methyltris(trimethylsiloxy)silane	789.99 s, 0.704 s	5.88E+08	900	207.02	13630	XIC(207.02±500ppm)
N,O-Bis(trimethylsilyl)carbamate	804.989 s, 0.968 s	1.98E+08	879	147.05	3074	XIC(147.05±500ppm)
Naphthalene	949.98 s, 1.650 s	17362112	919	128.05	3730	XIC(128.05±500ppm)
Nonadecane	969.979 s, 2.184 s	33927029	866	57.07	778	XIC(57.07±500ppm)
Nonane, 2,6-dimethyl-	739.994 s, 2.208 s	4.97E+08	865	43.06	1648	XIC(43.06±500ppm)
Nonanoic acid, TMS derivative	1129.97 s, 1.000 s	83995664	906	75.02	3747	XIC(75.02±500ppm)
Norflurane	1034.97 s, 0.912 s	40511909	864	69.07	1868	XIC(69.07±500ppm)
Octadecane	1354.95 s, 0.943 s	2.33E+09	877	57.06	15614	XIC(57.06±500ppm)
Octane, 2,3,6,7-tetramethyl-	844.987 s, 0.832 s	5.49E+08	841	71.08	2350	XIC(71.08±500ppm)
Octane, 2,3,7-trimethyl-	869.985 s, 0.860 s	3.82E+08	843	57.07	5188	XIC(57.07±500ppm)
Octane, 2,4,6-trimethyl-	694.996 s, 2.207 s	4.71E+08	897	57.07	960	XIC(57.07±500ppm)

Octane, 5-ethyl-2-methyl-	1134.97 s, 0.904 s	4.76E+08	847	43.06	5133	XIC(43.06±500ppm)
Octane, 6-ethyl-2-methyl-	789.99 s, 2.235 s	3.58E+08	873	43.06	619	XIC(43.06±500ppm)
Octanoic acid, TMS derivative	1029.98 s, 0.989 s	1.22E+08	899	75.02	6603	XIC(75.02±500ppm)
Oxalic acid, butyl propyl ester	2149.9 s, 1.271 s	4.98E+08	759	57.07	2217	XIC(57.07±500ppm)
Palmitelaidic acid, TMS derivative	1679.93 s, 1.136 s	58088588	828	73.04	6242	XIC(73.04±500ppm)
Pentadecane	1174.97 s, 0.912 s	1.47E+08	927	57.07	7278	XIC(57.07±500ppm)
Pentadecanoic acid, TMS derivative	1629.94 s, 1.077 s	77020501	904	73.03	10657	XIC(73.03±500ppm)
Pentasiloxane, dodecamethyl-phenoxyethanol, TMS derivative	944.98 s, 0.717 s	1.87E+08	912	73.04	9559	XIC(73.04±500ppm)
Phenylpropanolamine, 2TMS derivative	1134.97 s, 1.259 s	12402663	841	73.04	894	XIC(73.04±500ppm)
Pivalic acid vinyl ester	1519.94 s, 1.081 s	2.06E+08	806	116.08	1128	XIC(116.08±500ppm)
Propanoic acid, 2-propenyl ester	979.978 s, 1.296 s	16249121	778	57.07	815	XIC(57.07±500ppm)
Propanoic acid, anhydride	1569.94 s, 0.994 s	3.04E+08	754	57.06	5944	XIC(57.06±500ppm)
Pyridine	1514.94 s, 2.004 s	1.84E+08	835	57.06	734	XIC(57.06±500ppm)
Pyridine, 2,4,6-trimethyl-	689.997 s, 3.460 s	38368224	868	79.03	528	XIC(79.03±500ppm)
Pyridine, 2,4-dimethyl-	729.994 s, 1.200 s	95156472	947	121.08	1759	XIC(121.08±500ppm)
Silane, 1,8-octanediybis(trimethyl-	654.999 s, 3.996 s	56049170	883	107.06	564	XIC(107.06±500ppm)
Silanol, trimethyl-	934.981 s, 0.814 s	51074816	815	147.05	1806	XIC(147.05±500ppm)
Sulfurous acid, 2-ethylhexyl hexyl ester	694.996 s, 0.551 s	2.81E+08	858	75.02	648	XIC(75.02±500ppm)
Sulfurous acid, 2-ethylhexyl pentyl ester	1264.96 s, 0.901 s	4.25E+08	798	57.06	1222	XIC(57.06±500ppm)
Sulfurous acid, cyclohexylmethyl heptadecyl ester	729.994 s, 0.820 s	3.15E+08	837	57.07	2262	XIC(57.07±500ppm)
Supraene	2389.89 s, 2.176 s	11370169	824	97.09	656	XIC(97.09±500ppm)
Tetracosane	2169.9 s, 1.587 s	39839050	931	69.06	966	XIC(69.06±500ppm)
Tetradecane	1924.92 s, 1.115 s	1.67E+08	920	43.06	1093	XIC(43.06±500ppm)
Tetradecane, 1-iodo-	974.979 s, 0.848 s	1.51E+08	864	57.15	1027	XIC(57.15±500ppm)
Tetradecane, 2-methyl-	1014.98 s, 0.871 s	1.68E+08	762	57.15	696	XIC(57.15±500ppm)
Tetradecane, 4-ethyl-	1224.96 s, 0.936 s	6.04E+08	841	57.07	1173	XIC(57.07±500ppm)
Tetrahydrogeranyl formate	1394.95 s, 0.999 s	1.48E+09	851	57.06	2651	XIC(57.06±500ppm)
Tetrasiloxane, decamethyl-	819.988 s, 2.179 s	1.2E+09	826	43.06	2875	XIC(43.06±500ppm)
Triacetin	809.989 s, 0.710 s	3.05E+08	889	207.02	11313	XIC(207.02±500ppm)
Triacantane	1114.97 s, 1.564 s	15861278	882	43.03	688	XIC(43.03±500ppm)
Tridecane	2249.9 s, 1.449 s	3.07E+08	888	71.07	660	XIC(71.07±500ppm)
Tridecane, 6-methyl-	919.982 s, 0.839 s	1.29E+08	873	43.06	4880	XIC(43.06±500ppm)
Trimethyl(3,3-difluoro-2-propenyl)silane	2279.9 s, 1.542 s	1.54E+08	847	57.06	678	XIC(57.06±500ppm)
Trimethylaluminum	3314.83 s, 0.495 s	28148880	824	73.03	561	XIC(73.03±500ppm)
Tripropylene glycol monomethyl ether, TMS derivative	1219.96 s, 0.915 s	2.78E+08	753	57.07	2235	XIC(57.07±500ppm)
Trisiloxane, octamethyl-	894.984 s, 0.946 s	56565367	764	73.04	800	XIC(73.04±500ppm)
Undecane	819.988 s, 0.763 s	2.6E+08	868	221.07	13003	XIC(221.07±500ppm)
Undecane, 4-methyl-	699.996 s, 0.778 s	3.74E+08	896	57.07	2159	XIC(57.07±500ppm)
Undecane, 5,7-dimethyl-	859.986 s, 2.179 s	1.6E+09	905	43.06	3283	XIC(43.06±500ppm)
	849.987 s, 0.802 s	1.11E+08	770	43.14	621	XIC(43.14±500ppm)

R1		R2		R3		R4	
palmitic acid	stearic acid	palmitic acid	stearic acid	palmitic acid	stearic acid	palmitic acid	stearic acid
68711772	92090476	27813174	29055808	560005264	552351434	3278665	2874322
722348989	35732696	4960992	56685204			646549813	704102313
996185728	238885520	442500550	479033643				
1787246489	1412821502	142313432	128411410				
	1779530194	24330755	3836007				

P/S ratio* 1.004336142

0.920944872

1.013856812

0.919165423

*from all signals (slices) of each samples