

Nombre	Peso molecular (g/mol)	Donor de H+	Aceptor de H+	QPlogPo/w	QPPCaco	QPPMDCK
1,3-dichloro-2,4,5-tri	339.131	1.000	4.250	2.312	156.204	296.880
12,17-dichloro-9,11,	573.342	4.000	6.500	3.186	20.578	36.227
2-chloro-1,3-dihydro	318.713	1.000	5.250	2.053	278.356	276.980
2-chloro-1,3,8-trihyd	304.686	1.000	4.250	1.790	109.382	100.929
2,3-dihydroxybenzoi	154.122	2.000	2.500	0.853	40.717	19.775
2-hydroxypentanedic	148.115	3.000	5.700	-0.391	2.553	1.260
2-oxopentanedioic a	146.099	2.000	6.000	-0.592	2.369	1.163
3,4-dihydroxybenzoi	154.122	3.000	3.500	0.028	26.958	12.663
2-amino-3-hydroxyb	153.137	3.000	2.750	0.331	35.786	17.200
2-amino-4-(2-amino-	224.216	4.000	4.750	-2.156	1.961	0.825
4-aminobutanoic aci	103.121	3.000	3.000	-2.028	14.672	7.259
4-(hydroxymethyl)pt	124.139	2.000	2.450	0.679	902.952	443.026
4-hydroxybenzaldehy	122.123	1.000	2.750	1.345	556.516	262.568
4-hydroxybenzoic ac	138.123	2.000	2.750	0.581	75.668	38.639
5-amino-4-oxopenta	131.131	3.000	5.000	-2.962	6.341	2.931
acetate	60.052	1.000	2.000	-0.170	183.796	100.838
acetaldehyde	44.053	0.000	2.000	0.059	1492.118	762.449
acetamide	59.068	2.000	2.500	-1.289	275.356	304.828
3-hydroxybutan-2-or	88.106	1.000	3.700	-0.189	1172.931	587.794
propan-2-one	353.460	0.000	5.500	3.576	774.005	414.930
7H-purin-6-amine	135.128	3.000	4.000	-0.196	239.457	105.528
2,2-bis(carbamoylam	176.132	5.000	4.000	-2.625	0.444	0.504
(2,5-dioxoimidazolidi	158.116	3.250	3.750	-2.014	15.456	9.759
2,4-diamino-4-oxobu	132.119	4.000	4.500	-4.061	1.182	1.041
benzaldehyde	106.124	0.000	2.000	1.477	1833.220	952.475
benzoic acid	122.123	1.000	2.000	1.868	249.517	140.322
phenylmethanol	108.140	1.000	1.700	1.101	2965.569	1601.928
butane-2,3-diol	90.122	2.000	3.400	-0.704	1655.116	852.860
butanoic acid	88.106	1.000	2.000	0.790	238.529	133.655
carbamic acid	61.040	3.000	2.500	-1.052	36.504	17.573
formic acid	46.026	1.000	2.000	-0.304	86.022	44.384

benzene-1,2-diol	110.112	2.000	1.500	0.797	1067.737	531.027
2-hydroxypropane-1,	192.125	3.000	5.750	0.132	0.281	0.148
chromen-2-one	146.145	0.000	2.500	1.390	2056.325	1078.364
(4-propan-2-ylpheny	150.220	1.000	1.700	1.982	2965.855	1602.094
4-propan-2-ylbenzak	148.204	0.000	2.000	1.892	1832.789	952.233
4-ethenyl-2-methoxy	150.177	1.000	1.500	1.908	3043.607	1647.539
2-methylphenol	108.140	1.000	0.750	1.936	3684.337	2025.431
2-hydroxybenzoic ac	138.123	1.000	1.750	2.257	107.045	56.217
3-methylbenzene-1,	124.139	2.000	1.500	0.856	1331.332	674.045
3,4-dihydroxy-5-(3,4,	322.228	6.000	8.250	-0.865	0.594	0.205
3-methylphenol	108.140	1.000	0.750	1.939	2999.544	1621.774
3,4,5-trihydroxybenz	170.121	4.000	4.250	-0.572	9.803	4.243
octanoic acid	144.213	1.000	2.000	2.635	235.301	131.701
2-aminobutanedioic	133.104	3.000	4.000	-3.888	0.682	0.335
3-hydroxybutanoic a	104.105	1.000	2.700	0.819	101.032	52.811
2-methoxyphenol	124.139	1.000	1.500	1.249	3043.013	1647.192
2-benzamidoacetic a	179.175	1.250	3.750	1.449	89.959	46.584
2-hydroxybutanedioi	134.088	2.000	4.700	-0.471	2.743	1.362
propanal	58.080	0.000	2.000	0.588	1831.672	951.606
1-aminocyclopropan	101.105	3.000	3.000	-2.564	20.933	10.658
2-[carbamimidoyl(m	131.134	4.000	4.000	-0.485	30.540	14.492
2-amino-3-methyl-4	113.119	2.000	4.500	-1.132	343.299	155.764
2-hydroxypropanoic	90.079	2.000	3.700	-0.215	92.921	48.244
butane-2,3-dione	86.090	0.000	4.000	-0.548	1103.997	550.545
3,4-dihydrochromen	148.161	0.000	2.500	1.179	2291.730	1212.395
1,3-dihydroxypropan	90.079	2.000	5.400	-1.277	369.906	168.853
methylsulfinylmetha	78.129	0.000	4.000	-1.342	139.660	2741.410
4-(2-aminoethyl)ben	153.180	4.000	2.500	-0.980	65.044	28.540
pentanedioic acid	132.116	2.000	4.000	-0.238	5.786	3.052
2,3-dihydroxypropan	106.078	2.000	4.400	-0.770	30.325	14.381
propane-1,2,3-triol	92.094	3.000	5.100	-1.193	350.999	159.544
benzene-1,4-diol	110.112	2.000	1.500	0.799	912.408	448.043
1H-imidazole	68.078	1.000	2.000	-0.080	2396.556	1272.446

1H-indole	117.150	1.000	0.000	2.140	5333.841	3021.303
2-amino-5-(carbamo	175.187	6.000	5.000	-3.992	0.677	0.528
2-amino-4-methylsul	165.207	3.000	7.000	-2.899	0.404	6.507
propanedioic acid	104.062	0.000	2.000	0.373	5.545	2.915
2,3-dihydroxybutane	150.088	2.000	5.400	-0.372	1.586	0.753
methanol	32.042	1.000	1.700	-0.770	2398.497	1273.560
(2,3,4,5,6-pentaphos	660.036	12.000	30.000	-1.926	0.000	0.000
cyclohexane-1,2,3,4,	180.157	6.000	10.200	-2.401	41.506	15.874
naphthalene	128.173	0.000	0.000	3.350	9906.038	5899.293
5,7-dihydroxy-2-(4-h	272.257	2.000	4.000	1.622	128.837	54.002
pyridine-3-carboxyla	123.111	1.000	3.500	0.675	134.087	71.713
pyridine-3-carboxylic	123.111	1.000	3.500	0.675	134.087	71.713
octan-1-ol	130.230	1.000	1.700	2.990	3300.388	1798.281
3-hydroxy-2-oxoprof	104.062	1.000	4.700	-0.995	26.686	12.525
octadec-9-enoic acid	282.465	1.000	2.000	5.871	653.188	397.069
2-oxobutanedioic aci	132.073	1.000	5.000	-0.556	2.690	1.334
oxalic acid	90.035	2.000	4.000	-0.701	4.221	2.171
3-(4-hydroxyphenyl)-	180.160	2.000	4.750	0.454	36.026	17.325
hexadecanal	240.428	0.000	2.000	5.031	1844.506	958.815
hexadecanoic acid	256.428	1.000	2.000	5.251	235.463	131.799
phenanthrene	178.233	0.000	0.000	4.460	9906.038	5899.293
phenol	94.113	1.000	0.750	1.459	3007.007	1626.136
2-phenylacetaldehyd	120.151	0.000	2.000	1.659	1963.840	1026.037
2-phenylacetic acid	136.150	1.000	2.000	2.159	290.412	165.337
2-phenylethanamine	121.182	2.000	1.000	1.570	602.745	316.650
phosphoric acid	97.995	3.000	5.000	-0.360	1.227	0.772
phthalic acid	166.133	2.000	4.000	0.751	10.585	5.864
propanoic acid	74.079	1.000	2.000	0.608	236.870	132.650
butane-1,4-diamine	88.152	4.000	2.000	-1.338	36.807	17.063
benzene-1,2,3-triol	126.112	3.000	2.250	0.093	387.014	177.309
2-oxopropanoic acid	88.063	1.000	4.000	-0.580	70.110	35.581
methylsulfanylmetha	62.129	0.000	0.500	1.100	9906.038	10000.000
2-hydroxy-2-methylt	148.115	2.000	3.750	0.172	5.909	3.123

N'-(3-aminopropyl)bi	145.247	5.000	3.500	-1.340	5.963	2.640
N,N'-bis(3-aminoproj	202.342	6.000	5.000	-1.238	5.386	2.365
2,6,10,15,19,23-hexa	410.725	0.000	0.000	12.587	9906.038	5899.293
butanedioic acid	118.089	2.000	4.000	-0.577	5.762	3.039
sulfur dioxide	64.059	0.000	4.000	-1.573	789.296	876.490
2-aminoethanesulfor	125.142	2.000	4.000	-2.916	7.806	3.775
N,N-dimethylmethar	59.111	0.000	2.000	0.159	2008.050	1162.768
2-amino-3-(1H-indol	204.228	4.000	3.000	-1.060	15.121	7.499
urea	60.055	4.000	2.000	-2.199	53.566	53.740
2-amino-3-methylbu	117.147	3.000	3.000	-1.736	31.444	16.545
4-hydroxy-3-methox	152.149	1.000	3.500	1.001	563.117	265.936
3-methylbut-3-enyl	246.093	0.000	7.000	0.619	1.341	0.923
1-hydroxypropane-1,	192.125	3.000	6.700	-0.334	0.168	0.085
5-methyl-2-propan-2	156.267	1.000	1.700	2.778	4535.168	2535.419
2-hydroxy-2-phenyla	152.149	2.000	3.700	0.761	113.793	60.057
octadec-17-ynoic aci	280.450	1.500	2.000	5.701	235.321	131.713
4-(2-aminoethyl)-2-n	167.207	3.000	2.500	0.041	185.152	88.413
7-hydroxy-2-phenyl-	240.258	1.000	3.500	2.451	992.450	490.673
2,5,7,8-tetramethyl-	430.713	1.000	1.500	8.974	4533.643	2534.497
1,3-dimethyl-7H-puri	180.166	1.000	5.000	-0.020	437.887	202.631
1-(4-methoxybenzoy	219.240	0.000	3.750	1.964	1862.056	968.680
1-(4-hydroxy-3-meth	166.176	1.000	3.500	1.502	999.072	494.213
N'-(2,3-dihydro-1H-ir	322.492	0.000	3.000	5.102	2470.586	1454.789
methyl 1-methyl-3,6-	155.196	0.000	4.000	0.420	604.308	317.538
8-methoxy-6-nitrona	341.276	1.000	5.250	2.592	83.752	43.119
nonanedioic acid	188.223	2.000	4.000	1.635	6.628	3.535
benzyl benzoate	212.248	0.000	2.000	3.571	3390.434	1851.370
4-methoxyfuro[3,2-g	216.193	0.000	3.750	1.437	2055.650	1077.981
(2,2-dimethyl-3H-1-t	221.255	1.000	3.750	2.338	3090.450	1674.964
hexadecan-1-ol	242.444	1.000	1.700	5.205	2853.796	1536.768
5,7-dimethoxychrom	206.198	0.000	4.000	1.408	2056.031	1078.197
4-methylphenol	108.140	1.000	0.750	1.938	3006.367	1625.762
N-[(4-hydroxy-3-met	293.405	2.000	4.000	3.321	954.507	684.401

7-chloro-1-methyl-5-	284.744	0.000	4.000	2.996	2571.885	3381.207
dibutyl benzene-1,2-	278.347	0.000	4.000	3.847	1426.451	726.246
2-benzhydryloxy-N,N	255.359	0.000	3.700	3.276	2459.270	1447.588
diphenylmethanone	182.221	0.000	2.000	3.252	3924.785	2168.676
2-[[2-[bis(2-hydroxye	504.631	4.000	12.800	2.360	325.571	147.088
[(1,5-dimethyl-3-oxo	311.355	1.000	9.000	-1.191	26.324	13.654
7-(2,3-dihydroxyprop	254.245	2.000	8.400	-0.358	149.398	63.374
1,3,8-trihydroxy-6-m	270.241	1.000	4.250	1.246	78.152	31.459
2-methoxy-4-prop-2-	164.204	1.000	1.500	2.662	3043.597	1647.534
3,7,11-trimethyldode	222.370	1.000	1.700	4.191	5623.792	3199.211
[7-(furan-3-yl)-1,8,12	482.572	0.000	9.500	2.781	745.392	360.092
5-(2,5-dimethylphen	250.337	1.000	2.750	3.923	494.923	294.184
2,5-dihydroxybenzoic	154.122	2.000	2.500	0.770	32.555	15.528
5-chloro-N-[2-[4-(cyc	494.004	2.000	6.750	4.560	134.394	218.159
6-[6-carboxy-2-[(11-c	822.942	6.000	21.300	1.950	0.006	0.002
7-(8-formyl-1,6,7-trif	518.562	4.000	6.500	3.653	19.000	6.822
1,4-dimethyl-7-propyl	198.307	0.000	0.000	5.422	9906.038	5899.293
2-[2-(azocan-1-yl)eth	198.311	4.000	4.000	0.652	102.421	46.621
1,2,3,6-tetrahydropy	127.143	1.000	2.500	-1.478	32.361	17.068
4-methoxy-6-methyl	221.255	0.000	4.250	1.363	2126.531	1237.098
1H-indol-3-ylmethan	147.176	2.000	1.700	1.724	1848.935	961.304
2-[1-(4-chlorobenzoyl	357.793	1.000	5.750	4.267	160.491	214.647
1,2,3,6-tetrahydropy	127.143	2.000	3.500	-1.925	33.213	17.554
pyridine-4-carbohydic	137.141	3.000	4.500	-0.647	275.310	122.705
3-[2-[4-(4-fluorobenz	395.432	1.000	7.500	2.900	169.079	144.689
4,9-dimethoxy-7-me	260.246	0.000	4.500	2.163	3785.932	2085.866
4-oxo-1H-quinoline-2-	189.170	2.000	4.500	0.751	50.895	25.169
4-hydroxy-3-(3-methyl	242.274	1.000	4.750	1.948	821.765	400.131
dodecanoic acid	200.320	1.000	2.000	3.754	278.974	158.310
octadeca-9,12-dienoic	280.450	1.000	2.000	5.840	235.423	131.774
3-(2-methylphenoxy)pr	182.219	2.000	4.150	1.323	1235.386	621.696
[2-(carbamoyloxymethyl	218.252	4.000	5.000	0.043	41.943	16.055
3-(diaminomethylidene	129.164	5.000	3.500	-0.690	241.918	106.701

2-methylprop-2-enol	86.090	1.000	2.000	0.741	249.207	140.133
9-methoxyfuro[3,2-g]	216.193	0.000	3.750	1.565	2173.091	1144.699
methyl 2-hydroxyber	152.149	0.000	1.750	1.833	1186.134	594.949
2-methyl-1,2-dipyrid	226.277	0.000	5.000	1.717	1603.742	824.283
1,4-dihydroxy-5,8-bis	444.486	4.000	9.900	0.697	1.401	0.499
4-methoxy-6-prop-2-	192.214	0.000	2.250	2.123	9906.038	5899.293
N,N-diethyl-3-methyl	191.272	0.000	3.000	2.292	4693.362	2631.145
3-O-(2-methoxyethyl)	418.446	0.000	6.200	3.834	538.648	253.468
4-[4-(3,4-dihydroxyp	302.369	4.000	3.000	2.619	115.602	48.032
4-(2-amino-1-hydrox	153.180	4.000	3.450	-0.713	78.087	34.773
cyclohexa-2,5-diene-	108.096	0.000	4.000	-0.789	604.640	287.193
N-(2-hydroxyethyl)h	299.496	2.000	4.200	4.101	854.006	688.602
5-ethyl-5-pentan-2-y	226.275	2.000	4.000	2.049	565.663	267.236
4-butyl-1,2-diphenyl	308.379	1.000	4.000	3.944	2170.269	1143.092
2-(2-oxopyrrolidin-1-	142.157	2.000	5.500	-1.818	98.040	162.525
1-naphthalen-1-ylox)	259.347	2.000	3.950	3.088	834.133	449.878
propyl 3,4,5-trihydro	212.202	3.000	4.250	0.517	111.250	46.080
15-methyl-7,9,19,21-	353.374	0.000	7.000	1.707	1242.061	691.810
1,2,5,8-tetrahydroxy	272.214	1.000	4.000	0.931	43.188	16.571
2-piperazin-1-ylquin	213.282	1.000	3.000	2.339	1105.240	609.819
benzene-1,3-diol	110.112	2.000	1.500	0.799	908.257	445.839
2-aminopropan-1-ol	75.110	3.000	2.700	-0.983	234.934	114.366
1,1-dioxo-1,2-benzot	183.181	1.000	5.000	-0.117	200.721	89.289
5-prop-2-enyl-1,3-bis	162.188	0.000	1.500	2.382	9906.038	5899.293
3-(2-aminoethyl)-1H-	176.218	4.000	1.750	0.211	98.551	44.720
3-methyl-1-(3-methyl	265.354	2.000	0.750	4.562	4768.893	2676.943
2-iodoacetic acid	185.949	1.000	2.000	0.727	215.487	358.033
N-[4-[1-hydroxy-2-(p	272.362	3.000	7.700	0.248	112.891	52.285
1-isothiocyanato-4-n	177.279	0.000	6.500	0.436	98.726	5457.648
8-[[4-methyl-3-[[[3-[[1297.263	12.000	36.000	-1.106	0.000	0.000
5-[2-(tert-butylamino	225.287	4.000	4.200	0.097	83.266	37.272
2,3,9,10-tetrametho	355.433	0.000	5.000	3.363	2470.586	1454.789
9,20,21,25-tetramet	622.760	0.000	8.000	6.382	549.087	316.733

3,7-dimethylpurine-2	180.166	1.000	5.000	-0.020	523.394	245.718
2,3-diacetyloxypropy	218.206	0.000	6.000	0.610	225.657	98.970
2,5,9-trimethylfuro[3	228.247	0.000	3.000	2.496	2102.490	1104.555
4-(2-aminoethyl)phe	137.181	3.000	1.750	0.354	182.911	87.257
2,6-diacetyl-7,9-dihy	344.320	1.000	6.750	1.454	105.578	43.546
[2-[(8S,9S,10R,13S,14	402.486	1.000	8.750	2.056	127.210	53.265
(8R,9S,13S,14S,16R,1	288.386	3.000	4.150	2.449	419.357	193.378
methyl (1R,15S,17R,1	608.687	1.000	10.700	4.956	686.230	364.312
(2R,3R,4R,5S)-hexan	182.173	6.000	10.200	-3.017	81.818	33.057
(3R,4S,5S,6R)-6-(hyd	180.157	5.000	10.200	-2.262	61.032	24.081
5-(cyclohexen-1-yl)-5	236.270	2.000	4.000	1.326	500.819	234.283
(8R,9S,13S,14S)-3-hy	270.371	1.000	2.750	3.130	1125.687	562.246
(3S,8R,9S,10R,13S,14	288.429	1.000	3.700	3.293	1264.325	637.452
(2S)-2-aminopropan	89.094	3.000	3.000	-2.959	20.638	10.496
(2S)-2-amino-3-hydr	105.093	3.000	3.700	-3.314	7.630	3.580
4-nitro-1-oxidoquino	190.158	0.000	2.000	2.278	577.780	273.428
(2S)-2-aminobutan	133.104	3.000	4.000	-3.887	0.679	0.333
methyl (1R,9R,10S,1	824.969	2.000	14.250	4.930	13.623	5.828
(2R,3R,4S,5S,6R)-2-[(342.299	8.000	16.800	-3.689	12.812	4.455
(8R,9S,13S,14S,17R)-	296.408	2.500	1.500	3.672	1361.477	690.557
(3S,8S,9S,10R,13R,14	386.660	1.000	1.700	7.031	3381.723	1846.229
(3R,4S,5R,6R)-6-(hyd	180.157	5.000	10.200	-2.224	67.392	26.805
(2S)-2-amino-3-(3,4-	197.190	5.000	4.500	-2.509	3.004	1.307
2-phenylethanol	122.166	1.000	1.700	1.737	2863.673	1542.518
1-[2,4-dihydroxy-6-[(436.415	6.000	12.500	-0.350	6.986	2.313
2-(1H-indol-3-yl)-N,N	188.272	1.000	2.000	2.508	1163.657	644.731
(2S)-2-amino-4-meth	131.174	3.000	3.000	-1.521	25.510	13.198
(2R,3R,4S,5R,6S)-2-(f	342.299	8.000	18.700	-3.853	8.160	2.736
(2S)-2-amino-4-meth	149.207	3.000	3.500	-1.580	26.082	23.291
N-[(7S)-1,2,3,10-tetr	399.443	1.000	7.500	2.554	745.119	592.897
hexanal	100.160	0.000	2.000	1.335	1940.172	1012.678
furo[3,2-g]chromen-	186.167	0.000	3.000	0.955	2056.102	1078.237
methylsulfonylmeth	94.128	0.000	4.000	-1.331	1338.683	685.294

1,1,1,2,2,2-hexachloroethane	236.740	0.000	0.000	3.376	9906.038	10000.000
2-bromoacetic acid	138.948	1.000	2.000	0.679	218.317	333.401
(2R,3R,4R,5R)-hexane-2,3,4,5-tetraol	182.173	6.000	10.200	-3.087	42.890	16.447
(2R,3S,4S,5R,6R)-2,3,4,5-tetrahydro-2H-pyridin-2-one	342.299	8.000	18.700	-3.707	13.158	4.586
(2S)-2,4-diaminobutanoic acid	132.119	4.000	4.500	-4.060	1.198	1.054
pentan-1-ol	88.149	1.000	1.700	1.510	2852.513	1536.021
[(1R,2S,6S,9S,10R,11R)-1,2,3,4,6,7,8,9,10,11-decahydro-1H-benzocycloheptene]	673.799	6.000	11.700	3.714	63.376	27.750
1,2-dihydroxyanthracene	240.215	1.000	4.500	1.096	220.776	96.659
(2S)-2-amino-5-oxoproline	174.202	7.000	5.000	-3.446	1.492	0.614
oxirane	44.053	0.000	2.000	-0.528	9906.038	5899.293
2,2-dimethylbutane	86.177	0.000	0.000	3.621	9906.038	5899.293
(1S,2S,4R,8S,9S,11S,12S)-1,2,4,8,9,11,12-octahydro-1,2,4,8-tetraazocane	434.504	2.000	8.900	2.251	282.148	150.623
(1,7,7-trimethyl-2-bicycloheptane)	196.289	0.000	2.000	2.857	3749.374	2064.104
triethyl 2-hydroxypropanoate	276.286	0.000	5.750	2.147	496.845	232.274
(3R,5R)-1,3,4,5-tetrahydro-2H-pyridin-2-one	192.168	5.000	7.850	-1.170	13.194	5.850
2-ethyl-2-(hydroxymethyl)propanoic acid	134.175	3.000	5.100	-0.363	583.164	276.183
1-ethynylcyclohexane	124.182	1.500	0.750	1.813	3774.441	2079.024
3,5,5-trimethylcyclohexane	138.209	0.000	2.000	1.801	3027.545	1638.144
3,7-dimethyloctane-3-thiol	158.283	1.000	0.750	3.259	5242.367	2965.336
3,7-dimethyloctane-1,6-diol	154.252	1.000	0.750	3.143	5250.646	2970.398
2-methylpropanal	72.107	0.000	2.000	0.306	2203.345	1161.935
2-chloroacetyl chloride	112.943	0.000	2.000	0.614	2549.418	8017.494
prop-2-enamide	71.079	2.000	2.500	-0.389	727.099	350.549
2-methylpropanoic acid	88.106	1.000	2.000	0.789	301.033	171.882
2,2-dimethyl-3-methylbutane	136.236	0.000	0.000	3.347	9906.038	5899.293
4-[2-(4-hydroxyphenyl)ethyl]pyridine	228.290	2.000	1.500	3.317	911.193	447.398
2,6,6-trimethylbicyclo[2.2.1]heptane	136.236	0.000	0.000	3.627	9906.038	5899.293
2-hydroxy-3-methylcyclohexanone	112.128	1.000	2.750	0.215	951.204	468.669
4-methoxy-7-methyl-2,3-dihydro-1H-benzothiazole	230.220	0.000	3.750	1.989	3780.729	2082.768
4-hydroxynaphthalene	174.156	1.000	4.750	0.194	354.937	161.479
4,7,8-trimethoxyfuran	259.261	0.000	3.750	2.755	7639.749	4455.064
5,7,17,19-tetraoxa-1-undecane	323.348	0.000	5.000	2.486	2332.965	1367.398
2-methylanthracene	222.243	0.000	4.000	1.893	1337.719	677.541

anthracene-9,10-diol	208.216	0.000	4.000	1.614	1337.381	677.356
diethyl benzene-1,2-	222.240	0.000	4.000	2.150	1294.606	653.969
bis(2-methylpropyl)	278.347	0.000	4.000	3.461	1612.562	829.183
naphthalene-1-carboc	172.183	1.000	2.000	2.387	303.304	173.285
9H-carbazole	167.210	1.000	0.000	3.714	5704.816	3249.059
3H-2-benzofuran-1-c	134.134	0.000	3.000	0.849	2124.491	1117.053
1-(1H-indol-3-yl)-N,N	174.245	1.000	2.000	2.082	1176.690	652.540
1-ethenylpyrrolidin-2	111.143	0.000	3.000	0.327	2957.648	1597.303
1,4-dimethyl-7-propyl	204.355	0.000	0.000	5.249	9906.038	5899.293
2-butan-2-ylphenol	150.220	1.000	0.750	3.166	4018.075	2224.447
3-methyl-6-propan-2	152.236	0.000	2.000	2.184	4036.740	2235.618
5-methyl-2-propan-2	150.220	1.000	0.750	3.299	3816.505	2104.079
2-hydroxybenzaldehy	122.123	0.000	1.750	1.290	691.247	331.904
naphthalen-1-ol	144.173	1.000	0.750	2.695	3562.274	1952.998
xanthen-9-one	196.205	0.000	2.500	2.735	3521.282	1928.719
2,6-dimethoxypheno	154.165	1.000	2.250	1.697	3100.471	1680.835
1,2,3,4-tetrahydroisc	133.193	1.000	1.500	1.438	1281.600	715.645
quinoline	129.161	0.000	1.000	2.091	6133.295	3513.612
N-(2-methoxyphenyl)	207.229	0.000	4.250	1.644	1196.928	600.804
1,1'-biphenyl	154.211	0.000	0.000	4.090	9906.038	5899.293
4-(4-aminophenyl)ar	184.240	3.000	2.000	1.340	672.474	322.172
1,2-dimethoxy-4-pro	178.230	0.000	1.500	2.970	9906.038	5899.293
(2-methoxy-4-prop-2	206.241	0.000	3.250	2.655	3988.900	2206.994
2-methoxy-4-methyl	138.166	1.000	1.500	1.983	3043.481	1647.466
methyl benzoate	136.150	0.000	2.000	2.119	2767.828	1486.791
methyl pyridine-3-ca	137.138	0.000	3.500	0.618	1485.595	758.847
ethyl benzoate	150.177	0.000	2.000	2.131	2918.597	1574.520
4-[1-hydroxy-2-(met	167.207	3.000	3.950	0.261	194.339	93.164
propyl 4-hydroxyben	180.203	1.000	2.750	2.198	867.900	424.466
butyl 4-hydroxybenz	194.230	1.000	2.750	2.173	867.592	424.303
1,3-benzodioxole-5-c	166.133	1.000	3.500	0.973	249.949	140.584
2-ethylhexane-1,3-di	146.229	2.000	3.400	1.195	1699.713	877.725
2,4-dihydroxybenzal	138.123	1.000	2.500	1.173	209.584	91.373

1,3-benzothiazole	135.183	0.000	1.500	2.047	5647.591	6280.274
1,2-xylene	106.167	0.000	0.000	3.061	9906.038	5899.293
1-chloro-2-methylbe	126.585	0.000	0.000	3.098	9906.038	10000.000
2,4-dimethylaniline	121.182	1.500	1.000	2.020	3211.543	1746.014
2-methylbutanal	86.133	0.000	2.000	0.860	2606.969	1393.618
pentan-3-one	86.133	0.000	2.000	1.133	3714.073	2043.106
oxolan-2-one	86.090	0.000	3.000	-0.342	2127.514	1118.771
2,4-ditert-butylpheni	206.327	1.000	0.750	3.853	4986.828	2809.413
(2-methyl-5-prop-1-ε	194.273	0.000	2.000	3.169	3811.827	2101.291
furan-2-ylmethanol	98.101	1.000	2.200	0.999	2902.973	1565.411
furan-2-carbaldehyd	96.085	0.000	2.500	0.039	1640.304	844.613
1-phenylethanone	120.151	0.000	2.000	1.580	3247.576	1767.197
cyclohexanecarboxyl	128.171	1.000	2.000	1.635	334.360	192.540
(2R,3S,4S,5R,6R)-2-(f	342.299	8.000	18.700	-3.784	7.909	2.645
methyl 3,4,5-trihydr	184.148	3.000	4.250	-0.190	107.584	44.441
2-methyl-5-prop-1-e	152.236	1.000	1.700	2.329	3963.280	2191.676
2-methyl-5-prop-1-e	150.220	0.000	2.000	2.161	3565.782	1955.077
methyl 4-hydroxyber	152.149	1.000	2.750	1.814	839.587	409.519
1-methyl-4-propan-2	140.268	0.000	0.000	5.321	9906.038	5899.293
2-methyl-5-propan-2	136.236	0.000	0.000	4.022	9906.038	5899.293
1-methyl-4-propan-2	136.236	0.000	0.000	4.095	9906.038	5899.293
1-methyl-4-propan-2	136.236	0.000	0.000	4.033	9906.038	5899.293
1-methyl-4-propan-2	134.221	0.000	0.000	3.668	9906.038	5899.293
terephthalic acid	166.133	2.000	4.000	0.663	6.257	3.322
styrene	104.151	0.000	0.000	2.950	9906.038	5899.293
phenylmethanamine	107.155	2.000	1.000	0.773	625.128	329.379
methyl 2-phenylacet	150.177	0.000	2.000	2.115	2921.034	1575.941
cyclopenta-1,3-diene	66.102	0.000	0.000	1.789	9906.038	5899.293
2-ethylhexyl prop-2-ι	184.278	0.000	2.000	3.339	3333.211	1817.619
bis(2-ethylhexyl) hex	370.571	0.000	4.000	6.526	945.757	465.769
propylbenzene	120.194	0.000	0.000	3.397	9906.038	5899.293
(4-methoxyphenyl)m	180.203	0.000	2.750	2.057	2758.834	1481.570
5-butyloxolan-2-one	142.197	0.000	3.000	1.308	2178.710	1147.899

5-pentyloxolan-2-on	156.224	0.000	3.000	1.705	2179.145	1148.146
2-ethylhexan-1-ol	130.230	1.000	1.700	2.801	3358.269	1832.393
(4-methoxyphenyl)m	138.166	1.000	2.450	1.635	2973.837	1606.756
ethyl propanoate	102.133	0.000	2.000	1.286	2927.878	1579.932
3-methylpentanoic a	116.160	1.000	2.000	1.401	279.984	158.929
ethyl butanoate	116.160	0.000	2.000	1.424	2939.720	1586.841
3,7-dimethylocta-2,6	196.289	0.000	2.000	3.505	2265.727	1197.532
3,7-dimethyloctan-1-	158.283	1.000	1.700	2.888	2866.571	1544.205
3,7-dimethyloct-6-er	154.252	0.000	2.000	2.504	2174.893	1145.725
ethyl octanoate	172.267	0.000	2.000	3.108	2903.934	1565.971
1,4-xylene	106.167	0.000	0.000	3.120	9906.038	5899.293
1,4-dimethylpiperazi	114.190	0.000	4.000	-0.400	438.724	248.520
methyl hexanoate	130.186	0.000	2.000	1.839	2608.937	1394.755
methyl heptanoate	144.213	0.000	2.000	2.410	2616.203	1398.954
butane	58.123	0.000	0.000	2.890	9906.038	5899.293
propane-1-thiol	76.156	0.800	0.500	1.982	9906.038	10000.000
prop-2-enenitrile	53.063	0.000	1.500	0.152	2033.551	1065.460
2,2,4,4,6,6,8,8,10,10	519.080	0.000	1.400	10.414	9351.086	5542.899
2-methylpentane	86.177	0.000	0.000	3.606	9906.038	5899.293
1,3-xylene	106.167	0.000	0.000	3.121	9906.038	5899.293
ethyl 3-methylbutan	130.186	0.000	2.000	1.781	3460.364	1892.678
1,3,5-triazine-2,4,6-t	126.121	6.000	4.500	-2.005	34.240	12.893
cyclohexanamine	99.175	2.000	1.000	0.540	716.927	381.958
pyridin-3-ol	95.101	1.000	2.250	0.354	1753.644	907.866
dibutyl decanedioate	314.464	0.000	4.000	5.211	813.244	395.648
pentanoic acid	102.133	1.000	2.000	1.389	239.688	134.356
1-ethenoxy-2-methy	100.160	0.000	1.700	1.779	8601.569	5064.281
thiophene	84.136	0.000	0.000	1.815	9906.038	10000.000
2-methylpropyl acet	116.160	0.000	2.000	1.363	2501.691	1332.887
propan-2-yl tetradec	270.454	0.000	2.000	5.867	3678.933	2022.220
methyl decanoate	186.294	0.000	2.000	3.432	2606.542	1393.371
heptan-2-one	114.187	0.000	2.000	1.542	3074.895	1665.853
pentanal	86.133	0.000	2.000	0.810	1838.144	955.241

cyclohexene	82.145	0.000	0.000	2.857	9906.038	5899.293
morpholine	87.121	1.000	3.200	-0.854	1275.810	712.151
2,6,10,15,19,23-hexa	422.820	0.000	0.000	16.438	9906.038	5899.293
methyl octanoate	158.240	0.000	2.000	2.666	2576.276	1375.891
heptanoic acid	130.186	1.000	2.000	2.503	239.693	134.360
hexan-1-ol	102.176	1.000	1.700	2.029	2855.885	1537.984
3-ethoxypropan-1-ol	104.149	1.000	3.400	0.106	2852.586	1536.063
ethyl octadecanoate	312.535	0.000	2.000	7.073	3416.467	1866.740
heptan-1-ol	116.203	1.000	1.700	2.611	3299.575	1797.801
heptanal	114.187	0.000	2.000	1.788	1839.900	956.227
2-butoxyethanol	118.175	1.000	3.400	1.438	2846.586	1532.572
methyl dodecanoate	214.347	0.000	2.000	4.222	3094.211	1677.167
nonane	128.257	0.000	0.000	5.619	9906.038	5899.293
N-butylbutan-1-amin	129.245	1.000	1.500	2.597	2028.546	1175.602
nonanoic acid	158.240	1.000	2.000	2.642	239.647	134.332
heptyl acetate	158.240	0.000	2.000	2.672	2235.012	1179.995
propan-2-yl octadeca	326.562	0.000	2.000	7.252	3764.272	2072.970
undecan-2-one	170.294	0.000	2.000	3.230	3067.878	1661.745
decan-1-ol	158.283	1.000	1.700	2.910	2855.269	1537.625
decanal	156.267	0.000	2.000	2.749	2161.111	1137.879
undecanoic acid	186.294	1.000	2.000	3.343	235.372	131.744
methyl hexadecanoa	270.454	0.000	2.000	5.811	2899.895	1563.618
dodecane	170.337	0.000	0.000	7.247	9906.038	5899.293
dodec-1-ene	168.322	0.000	0.000	6.260	9906.038	5899.293
undecan-1-ol	172.310	1.000	1.700	3.290	2854.193	1536.999
undecanal	170.294	0.000	2.000	3.078	1836.738	954.451
dodecanal	184.321	0.000	2.000	3.474	1836.238	954.171
methyl octadecanoa	298.508	0.000	2.000	6.602	2578.352	1377.090
methyl octadeca-9,1	294.476	0.000	2.000	6.384	2572.708	1373.832
tridecan-1-ol	200.364	1.000	1.700	4.036	2854.216	1537.013
tetradecan-1-ol	214.390	1.000	1.700	4.455	2854.831	1537.370
docosanoic acid	340.588	1.000	2.000	7.601	235.367	131.740
octadec-1-ene	252.482	0.000	0.000	9.641	9906.038	5899.293

1-bromooctadecane	333.394	0.000	0.000	10.339	9906.038	10000.000
octadecan-1-ol	270.498	1.000	1.700	5.984	2853.046	1536.331
icosane	282.552	0.000	0.000	11.618	9906.038	5899.293
2-methylbut-3-en-2-ol	86.133	1.000	0.750	0.833	4693.793	2631.406
3,7-dimethylocta-1,6-diene	196.289	0.000	2.000	3.516	4728.448	2652.412
1-hydroxypropan-2-ol	74.079	1.000	3.700	-0.332	992.614	490.761
bis(2-ethylhexyl) benzene	390.562	0.000	4.000	6.656	1948.618	1017.443
dioctyl benzene-1,2-diol	390.562	0.000	4.000	6.434	1784.090	924.915
ethyl 2-hydroxybenzoate	166.176	0.000	1.750	2.246	1244.407	626.604
3-hydroxy-2-methylpropanoic acid	126.112	1.000	3.250	0.745	1025.746	508.490
2-methylbenzoic acid	136.150	1.000	2.000	2.044	325.308	186.912
1,2,3,4-tetrahydronaphthalene	132.205	0.000	0.000	3.481	9906.038	5899.293
6,7-dimethoxychromene	206.198	0.000	4.000	1.395	2055.611	1077.959
anthracene	178.233	0.000	0.000	4.450	9906.038	5899.293
8-methyl-8-azabicyclo[3.2.1]octane	141.213	1.000	3.700	0.447	775.582	415.844
ethyl 4-hydroxybenzoate	166.176	1.000	2.750	2.466	885.784	433.928
1,3-benzodioxole-5-carbonitrile	150.134	0.000	3.500	0.486	1833.245	952.490
cyclopentanone	84.118	0.000	2.000	0.482	2705.028	1450.362
4-hydroxy-3-methoxybenzoic acid	168.149	2.000	3.500	1.046	76.628	39.169
methyl 4-methoxybenzoate	166.176	0.000	2.750	2.102	2765.997	1485.728
naphthalene-1,4-diol	158.156	0.000	4.000	0.908	884.477	433.236
methyl (1R,15S,17R,17S)-1,7-dimethyl-1,7-dimethylnaphthalene-1,7-diol	578.661	1.000	9.950	4.845	683.767	362.898
dimethyl benzene-1,4-diol	194.187	0.000	4.000	1.351	1040.985	516.661
3-aminonaphthalene	303.304	3.500	9.000	-0.387	0.764	0.363
6-[2-[6-[2-(dimethylamino)ethyl]ethyl]ethyl]amine	445.468	1.000	9.750	1.209	71.516	40.217
4-(1H-indol-3-yl)butane-1,3-diol	203.240	2.000	2.000	2.646	128.814	68.669
4-hydroxy-3,5-dimethylbenzoic acid	182.176	1.000	4.250	0.442	570.976	269.950
(3R,4S,5R)-3,4,5-trimethyl-1,2,3,4,5,6-hexahydroindole	174.153	4.000	7.100	-1.024	13.646	6.067
1-methyl-4-prop-1-en-1-ylbenzene	154.252	1.000	0.750	3.036	3939.055	2177.200
2-phenylacetonitrile	117.150	0.000	1.500	1.751	2079.487	1091.498
1-methoxy-4-prop-2-en-1-ylbenzene	148.204	0.000	0.750	2.577	9906.038	5899.293
3,7-dimethyloct-6-ene	212.331	0.000	2.000	4.045	2815.858	1514.698
3,7-dimethyloct-6-ene	156.267	1.000	1.700	2.710	3436.802	1878.753

1,3-dichloropropane	112.986	0.000	0.000	2.491	9906.038	10000.000
3,7,11-trimethyldodecane	222.370	1.000	0.750	4.912	5263.998	2978.564
hexanoic acid	116.160	1.000	2.000	1.430	239.650	134.334
hexanedioic acid;piperazine	146.143	2.000	4.000	0.081	5.568	2.928
hexyl acetate	144.213	0.000	2.000	2.322	2231.922	1178.232
nonan-1-ol	144.256	1.000	1.700	2.802	3296.880	1796.214
methyl (1S,15R,18S,19S,20S,21S,22S,23S,24S,25S,26S,27S,28S,29S,30S)-2,4,5,6-tetrahydro-2H-pyrido[2,1-b]pyridine	1354.448	1.000	4.700	3.542	321.310	160.426
(2R,3S,4R,5R)-2,4,5,6-tetrahydro-2H-pyrido[2,1-b]pyridine	194.184	4.000	10.500	-1.826	102.283	42.079
butane-1,2,3,4-tetraol	122.121	4.000	6.800	-1.538	173.312	74.407
1,4-dimethoxybenzene	138.166	0.000	1.500	1.950	9906.038	5899.293
3,7-dimethyloct-6-ene	198.305	0.000	2.000	3.602	2723.856	1461.277
(2R,3S)-2-(3,4-dihydroxyphenyl)propanoic acid	290.272	5.000	5.450	0.454	49.602	19.246
propanedioate	104.062	0.000	2.000	0.373	5.545	2.915
azulene	128.173	0.000	0.000	3.315	9906.038	5899.293
7-thiabicyclo[4.1.0]heptane	114.205	0.000	0.500	2.390	9906.038	10000.000
thietane	74.140	0.000	0.500	1.628	9906.038	10000.000
1,2,4-trithiolane	124.234	0.000	1.500	2.070	9906.038	10000.000
cyclododecane	168.322	0.000	0.000	5.956	9906.038	5899.293
(1R,2S)-2-(methylamino)propane	165.235	2.000	3.200	1.272	753.266	402.926
prop-2-enylbenzene	118.178	0.000	0.000	3.316	9906.038	5899.293
hydrazine	32.045	4.000	1.000	-2.776	17.643	7.706
2,6-dihydroxybenzoic acid	154.122	1.000	1.500	1.579	47.235	23.218
2-hydroxy-3-(4-hydroxyphenyl)propanoic acid	182.176	3.000	4.450	0.508	35.389	16.994
1,1,2,2,3,3,4,4,4-nonafluorocyclohexane	671.096	0.000	1.000	7.925	2470.586	10000.000
diazomethane	42.040	0.000	3.000	-1.420	308.687	138.861
4-[2-(methylamino)ethyl]pyridine	151.208	2.000	2.250	1.330	441.509	226.178
6-methylhept-5-en-2-one	126.198	0.000	2.000	1.890	3134.038	1700.513
2,6,6-trimethylcyclohexane	152.236	0.000	2.000	2.055	3212.473	1746.560
diphenyl(piperidin-2-yl)methane	267.370	2.000	2.250	3.649	1300.867	727.280
(2S,4aS,6aR,6aS,6bR,6bS)-hexahydro-1H-benzodiazepine	470.691	2.000	5.700	5.235	119.355	63.236
5,8a-dimethyl-3-propyl-1,2,3,4,5,6,7,8a-octahydro-1H-benzodiazepine	204.355	0.000	0.000	5.435	9906.038	5899.293
(6aS)-1,2,10-trimethyl-1,2,3,4,5,6,7,8,9,10,11-dodecahydro-1H-benzodiazepine	341.406	1.000	5.000	3.298	1103.801	608.961
3,5-dioxo-11-azapentacyclo[3.3.1.0.1.0.1.0]heptane	275.263	0.000	4.500	2.177	2286.182	1209.223

(6aR)-1,2-dimethoxy	295.380	0.000	3.500	3.633	2245.073	1311.802
(6aS)-2,10,11-trimetl	341.406	1.000	5.000	3.327	1102.404	608.128
5-hydroxy-7-methox	206.198	0.000	3.000	1.738	1244.761	626.797
5-hydroxy-2-methylr	188.182	0.000	3.750	0.793	478.168	222.851
1,8-dihydroxy-3-(hyd	270.241	1.000	5.200	0.913	77.223	31.055
1,8-dihydroxy-3-met	254.242	0.000	3.500	1.796	257.018	113.918
9-[(2R)-2,3-dihydrox]	334.325	2.000	6.950	1.928	540.824	254.575
9-(3-methylbut-2-en	270.284	0.000	3.750	3.113	2106.817	1107.012
(2S,3R,11bS)-2-[[480.646	1.000	6.500	5.083	412.564	232.542
4,7-dimethyl-1-prop	204.355	0.000	0.000	5.560	9906.038	5899.293
1,6-dimethyl-4-prop	198.307	0.000	0.000	5.441	9906.038	5899.293
7-methoxy-8-(3-metl	244.290	0.000	3.250	3.121	3088.893	1674.052
4,5-dimethoxy-6-pro	222.240	0.000	3.000	2.184	9906.038	5899.293
fluoren-9-one	180.206	0.000	2.000	2.862	2901.624	1564.625
1,2,3-trimethoxy-5-p	208.257	0.000	2.250	2.884	9906.038	5899.293
1H-indole-3-carbalde	145.160	0.000	1.000	2.001	955.858	471.148
3-[2-(dimethylamino	204.271	2.000	2.750	1.746	354.953	178.656
2-methyl-5-propan-2	164.204	0.000	4.000	0.749	1020.393	505.623
chromen-4-one	146.145	0.000	2.500	1.373	2910.874	1570.017
2,3,3a,4,5,6,7,7a-oct	124.225	0.000	0.000	4.246	9906.038	5899.293
1,3-dihydro-2-benzo	120.151	0.000	1.700	1.573	9906.038	5899.293
2,3-dihydro-1-benzo	120.151	0.000	0.750	2.353	9906.038	5899.293
2H-furan-5-one	84.074	0.000	3.000	-0.555	1903.877	992.217
1-methyl-3,6-dihydr	141.169	1.000	4.000	-1.481	53.396	29.326
2-methyl-5-propan-2	150.220	1.000	0.750	3.298	3687.620	2027.382
cycloheptanol	114.187	1.000	1.700	1.356	3498.467	1915.215
7,11-dimethyl-3-met	204.355	0.000	0.000	6.866	9906.038	5899.293
6,10,14-trimethylper	268.482	0.000	2.000	5.789	3956.929	2187.881
4-hydroxybutanoic a	104.105	2.000	3.700	-0.285	68.963	34.952
7-(2-octylcycloprope	280.450	1.000	2.000	5.751	279.843	158.843
nonadecan-10-one	282.509	0.000	2.000	6.453	4313.642	2401.825
7,11,15-trimethyl-3-ı	278.520	0.000	0.000	9.382	9906.038	5899.293
1-isothiocyanato-3-n	163.252	0.000	6.500	0.148	117.305	7069.148

hexadecanedioic acid	286.411	2.000	4.000	4.194	6.627	3.535
heptadecanoic acid	270.454	1.000	2.000	5.700	279.292	158.505
icosanoic acid	312.535	1.000	2.000	6.779	235.369	131.742
octacosanoic acid	424.749	1.000	2.000	9.932	235.458	131.796
tetracosan-1-ol	354.658	1.000	1.700	8.315	2854.039	1536.910
ethanethioic S-acid	76.113	0.800	2.000	0.155	2469.254	3551.026
(4aS,6aR,6aS,6bR,8a)	456.707	2.000	3.700	6.293	308.888	176.735
1-methyl-4-propan-2	168.235	0.000	1.500	2.653	5243.978	2966.322
1-chloro-2-methylpro	90.552	0.000	0.000	2.332	9906.038	10000.000
(6,6-dimethyl-2-bicyc	152.236	1.000	1.700	2.109	3781.577	2083.273
6-methyl-2-(4-methyl	222.370	1.000	0.750	4.588	5860.418	3344.952
(5R,5aR,8aR,9R)-5-hy	414.411	1.000	8.450	2.399	1764.968	914.205
(2S)-5-hydroxy-2-(3-h	610.568	7.000	20.050	-1.376	2.764	0.849
1,8-dihydroxy-3-met	284.268	0.000	4.250	1.860	257.804	114.294
(1S,4aR,8aS)-4,7-dim	204.355	0.000	0.000	5.547	9906.038	5899.293
furo[2,3-h]chromen-	186.167	0.000	3.000	0.961	2056.326	1078.364
4,7-dimethoxy-5-pro	222.240	0.000	3.000	2.485	9906.038	5899.293
4-methoxy-1-methyl	164.163	0.000	5.250	-0.074	792.312	384.653
2-phenylchromen-4-	222.243	0.000	2.500	3.552	2925.182	1578.360
(2R,3S,4R,5R)-2,3,4,5	196.157	5.000	9.500	-1.755	5.665	2.346
2,3,5,6-tetramethylp	150.220	1.000	0.750	2.842	4503.885	2516.521
1-methyl-2-propan-2	134.221	0.000	0.000	3.669	9906.038	5899.293
(2R,3S,4S,5R,6S)-2-(f	342.299	8.000	18.700	-3.961	6.154	2.017
7-ethyl-1,4-dimethyl	184.280	0.000	0.000	5.047	9906.038	5899.293
2,3-dimethylbicyclo[122.210	0.000	0.000	3.357	9906.038	5899.293
4-hydroxy-3,5-dimet	198.175	2.000	4.250	0.984	78.248	40.065
7-methoxychromen-	176.171	0.000	3.250	1.060	2056.303	1078.351
2-hydroxycyclohexan	114.144	1.000	3.700	0.088	1150.868	575.853
benzene-1,2,4-triol	126.112	3.000	2.250	0.035	323.689	146.169
2-methyl-4,5-dihydro	84.121	1.000	2.000	0.629	3257.529	1773.052
1-methyl-3-propan-2	134.221	0.000	0.000	3.842	9906.038	5899.293
(4-prop-1-en-2-yl)cycl	152.236	1.000	1.700	2.295	3291.059	1792.787
hexadecyl hexadecar	480.856	0.000	2.000	11.796	2854.936	1537.431

2,2,4,4,6,6,8,8,10,10	444.926	0.000	1.200	9.044	9815.834	5841.251
butanamide	87.121	2.000	2.500	-0.795	403.961	392.505
propanedial	72.063	0.000	4.000	-1.612	306.439	137.768
heptan-2-ol	116.203	1.000	1.700	2.449	3925.350	2169.014
hex-3-en-1-ol	100.160	1.000	1.700	1.626	3242.485	1764.203
tetradecanoic acid	228.374	1.000	2.000	4.502	235.315	131.709
hexadecane	226.445	0.000	0.000	9.522	9906.038	5899.293
dotriacontane	450.873	0.000	0.000	18.247	9906.038	5899.293
2,6,6-trimethylbicycl	152.236	0.000	2.000	2.038	3925.232	2168.943
16,17-dimethoxy-5,7	351.358	0.000	6.000	2.942	4941.113	2781.586
9-methyl-9-azabicycl	153.224	0.000	4.000	0.316	794.790	426.987
3-methylidene-6-pro	136.236	0.000	0.000	3.973	9906.038	5899.293
2,3-di(tetradecanoyl	723.171	0.000	6.000	14.826	565.961	267.388
methyl 3-methylbuta	116.160	0.000	2.000	1.334	3062.192	1658.416
2,2,4,4,6,6,8,8,10,10	593.234	0.000	1.600	11.519	9221.320	5459.805
2,2,4,4,6,6,8,8,10,10	667.389	0.000	1.800	12.971	7925.070	4635.173
3-methylbut-2-en-1-	86.133	1.000	1.700	0.844	2856.445	1538.310
2,3-dihydroxypropyl	162.185	2.000	5.400	0.153	394.259	180.900
tetracosanoic acid	368.642	1.000	2.000	8.356	235.314	131.708
4-methyl-1-propan-2	154.252	1.000	0.750	2.977	5764.661	3285.915
3-chloro-2-methylpr	90.552	0.000	0.000	2.328	9906.038	10000.000
2-methylcyclohexan-	112.171	0.000	2.000	1.278	3725.153	2049.695
1-(3-methylphenyl)e	134.177	0.000	2.000	1.424	3243.444	1764.767
1-methyl-4-propan-2	136.236	0.000	0.000	4.192	9906.038	5899.293
1-methyl-4-propan-2	154.252	1.000	0.750	2.972	4757.072	2669.771
octan-3-ol	130.230	1.000	1.700	2.829	4530.376	2532.524
3-methylbutanal	86.133	0.000	2.000	0.841	2173.449	1144.903
3-methylcyclohexan-	114.187	1.000	1.700	1.326	4026.513	2229.497
hexan-2-one	100.160	0.000	2.000	1.279	3084.131	1671.263
3-prop-2-enylsulfany	114.205	0.000	0.500	2.934	9906.038	9454.590
octadecane	254.498	0.000	0.000	10.544	9906.038	5899.293
heptacosane	380.739	0.000	0.000	15.365	9906.038	5899.293
2-hydroxy-2-methyl	104.105	2.000	2.750	0.456	138.183	74.084

pentane-2,3-dione	100.117	0.000	4.000	-0.256	1445.790	736.894
(2R,3S,4R,5S)-hexane	182.173	6.000	10.200	-3.093	46.047	17.759
2-methylanthracene	192.260	0.000	0.000	4.739	9906.038	5899.293
(3R,4R)-3-(1-carboxy	226.185	3.000	6.450	0.487	2.468	1.215
2-methyl-5-prop-1-ene	154.252	1.000	1.700	2.720	3907.754	2158.506
5-methylfuran-2-carb	110.112	0.000	2.500	0.269	1639.770	844.316
4-[(4-hydroxyphenyl]	200.237	2.000	1.500	2.745	912.461	448.070
3-phenylprop-2-ene	147.176	2.000	2.500	1.500	731.660	352.927
hexan-3-ol	102.176	1.000	1.700	1.909	4523.388	2528.301
methyl butanoate	102.133	0.000	2.000	1.289	2607.578	1393.969
decan-4-one	156.267	0.000	2.000	2.932	5186.489	2931.188
2-methylbutyl acetat	130.186	0.000	2.000	1.761	2509.242	1337.237
nonan-3-ol	144.256	1.000	1.700	2.897	4535.297	2535.497
2-methylhexan-2-ol	116.203	1.000	0.750	2.321	4577.036	2560.728
hexan-2-ol	102.176	1.000	1.700	1.907	3929.307	2171.377
pentyl acetate	130.186	0.000	2.000	1.878	2234.308	1179.594
ethyl hexadecanoate	284.481	0.000	2.000	6.273	2898.177	1562.616
nonan-2-ol	144.256	1.000	1.700	2.892	3922.186	2167.124
1-(propylsulfanyl)p	150.297	0.000	1.000	3.184	9906.038	10000.000
tridecane	184.364	0.000	0.000	7.803	9906.038	5899.293
tetradecane	198.391	0.000	0.000	8.360	9906.038	5899.293
hexadec-1-ene	224.429	0.000	0.000	8.441	9906.038	5899.293
hexadec-1-yne	222.413	0.500	0.000	8.370	9906.038	5899.293
heptadecane	240.471	0.000	0.000	9.990	9906.038	5899.293
nonadecane	268.525	0.000	0.000	11.100	9906.038	5899.293
heneicosane	296.579	0.000	0.000	12.171	9906.038	5899.293
docosane	310.605	0.000	0.000	12.715	9906.038	5899.293
pentacosane	352.686	0.000	0.000	14.401	9906.038	5899.293
hexacosane	366.713	0.000	0.000	14.916	9906.038	5899.293
octacosane	394.766	0.000	0.000	16.033	9906.038	5899.293
nonacosane	408.793	0.000	0.000	16.589	9906.038	5899.293
hentriacontane	436.847	0.000	0.000	17.694	9906.038	5899.293
tritriacontane	464.900	0.000	0.000	18.805	9906.038	5899.293

hexatriacontane	506.981	0.000	0.000	20.393	9906.038	5899.293
pentatriacontane	492.954	0.000	0.000	19.843	9906.038	5899.293
propan-2-yl propano	116.160	0.000	2.000	1.362	3615.234	1984.401
butanedial	86.090	0.000	4.000	-0.613	363.128	165.511
tridecanoic acid	214.347	1.000	2.000	4.114	235.301	131.700
octadecanal	268.482	0.000	2.000	5.829	1940.251	1012.722
tricosane	324.632	0.000	0.000	13.326	9906.038	5899.293
triacontane	422.820	0.000	0.000	17.188	9906.038	5899.293
2-propylphenol	136.193	1.000	0.750	2.271	4127.134	2289.777
3-hydroxy-4-methox	168.149	2.000	3.500	1.045	76.749	39.236
1,3-dioxolane	74.079	0.000	3.400	-0.886	9906.038	5899.293
tetracosane	338.659	0.000	0.000	13.844	9906.038	5899.293
(3S,3aR,6R,6aR)-2,3,:	146.143	2.000	6.800	-0.830	1010.433	500.290
(3S,4S,5R,6R)-1,3,4,5	210.183	5.000	11.200	-2.497	23.779	8.694
docosan-1-ol	326.605	1.000	1.700	7.561	3299.903	1797.995
(2S)-2-amino-4-hydr	119.120	4.000	4.700	-3.181	7.202	3.364
2-N,4-N-diethyl-6-m	197.239	2.000	4.000	1.719	2283.766	1207.841
5-ethyloxolan-2-one	114.144	0.000	3.000	0.421	2177.859	1147.414
6-propyloxan-2-one	142.197	0.000	3.000	1.272	2410.323	1280.348
6-heptyloxan-2-one	198.305	0.000	3.000	2.827	2406.696	1278.266
8-(2-octylcycloprope	294.476	1.000	2.000	6.229	235.293	131.696
icos-1-yne	278.520	0.500	0.000	10.475	9906.038	5899.293
nonan-2-one	142.241	0.000	2.000	2.451	3051.460	1652.135
undec-1-ene	154.295	0.000	0.000	5.677	9906.038	5899.293
cyclododecanone	182.305	0.000	2.000	2.796	4318.041	2404.472
ethyl 3,4,5-trihydrox	198.175	3.000	4.250	0.180	113.401	47.044
1-methylpyrrolidin-2	99.132	0.000	3.000	-0.362	1412.992	1575.876
2-N-tert-butyl-4-N-et	241.354	2.000	4.000	3.736	3628.519	3530.970
1,1,3-trichloropropal	161.415	0.000	2.000	1.573	3685.775	10000.000
2,2-dimethylpropyl a	130.186	0.000	2.000	1.634	2774.320	1490.561
methyl docosanoate	354.615	0.000	2.000	8.160	2619.519	1400.871
1-ethenoxyoctadecal	296.535	0.000	1.700	7.385	7371.339	4286.126
cyclopent-2-en-1-on	82.102	0.000	2.000	0.450	2472.378	1316.014

3H-1,3-benzothiazol-	151.183	1.000	2.500	1.132	1255.100	1172.976
4-ethyl-1,2-dimethyl	134.221	0.000	0.000	3.795	9906.038	5899.293
3-hydroxychromen-2	162.145	1.000	3.250	0.759	727.456	350.735
(8R,9S,10R,13S,14S,1340.461		0.000	5.000	3.183	695.526	334.125
pentadecanoic acid	242.401	1.000	2.000	4.923	235.311	131.707
2-methylthiirane	74.140	0.000	0.500	1.749	9906.038	10000.000
1-(1H-pyrrol-2-yl)eth	109.127	1.000	2.000	1.223	1784.573	925.185
2-methoxy-4-methyl	164.247	0.000	0.750	3.287	9906.038	5899.293
(2-methyl-6-methyl	196.289	0.000	2.000	3.521	4706.598	2639.166
dodecanamide	199.336	2.000	2.500	2.186	406.533	394.035
undecane	156.311	0.000	0.000	6.688	9906.038	5899.293
methyl icosanoate	326.562	0.000	2.000	7.393	2616.633	1399.203
tetradec-1-ene	196.375	0.000	0.000	7.395	9906.038	5899.293
2,3,5,6-tetramethylp	136.196	0.000	2.000	1.904	5948.083	3399.068
1-methylpyrrole-2-c	109.127	0.000	2.000	1.396	1860.646	967.887
1-(5-methylfuran-2-y	124.139	0.000	2.500	1.322	2662.782	1425.895
1,3,3-trimethylbicycl	152.236	0.000	2.000	2.079	4820.363	2708.185
2-(4-methylphenyl)p	150.220	1.000	0.750	3.167	4759.610	2671.311
N-ethyl-3-phenylbicy	215.338	1.000	1.500	3.432	2287.670	1338.725
6,6-dimethyl-2-meth	136.236	0.000	0.000	3.528	9906.038	5899.293
(2S,3S,4S,5R,6R)-6-[(822.942	6.000	21.300	1.957	0.006	0.002
(2R)-2,5,7,8-tetrame	430.713	1.000	1.500	8.974	4533.643	2534.497
1-(furan-2-ylmethyl)	147.176	0.000	1.000	2.949	9773.490	5814.020
heptadecan-1-ol	256.471	1.000	1.700	5.631	3303.020	1799.830
methyl (15S,17S,19S	354.448	1.000	4.750	3.457	616.109	324.246
1,3,3-trimethylbicycl	154.252	1.000	1.700	2.209	4867.875	2737.049
undecan-2-ol	172.310	1.000	1.700	3.360	3916.079	2163.477
tridecan-2-ol	200.364	1.000	1.700	4.138	3921.722	2166.847
4-hydroxy-3,5-diiodo	370.916	1.000	2.250	1.949	866.507	3173.089
methyl 1-methylpipe	157.212	0.000	4.000	0.665	919.858	500.053
cyclododecanol	184.321	1.000	1.700	2.851	3856.425	2127.877
decane	142.284	0.000	0.000	6.129	9906.038	5899.293
methyl nonanoate	172.267	0.000	2.000	3.068	2610.052	1395.399

methyl tridecanoate	228.374	0.000	2.000	4.640	3022.709	1635.315
methyl heptadecano	284.481	0.000	2.000	6.207	2874.762	1548.975
2-(2-hydroxyethyl)di	154.242	2.000	4.400	0.512	1287.234	1546.608
2-tert-butylbenzene-	166.219	2.000	1.500	1.814	1513.979	774.530
3-(prop-2-enyl)trisulf	178.325	0.000	0.500	4.285	9906.038	10000.000
4-benzylpyridine	169.226	0.000	1.500	3.174	5348.614	3030.348
3-(prop-2-enyl)disulf	146.265	0.000	1.000	3.172	9906.038	10000.000
1-(methyl)disulfanyl	122.243	0.000	1.000	2.631	9906.038	10000.000
2-[(4-methylphenoxy	164.204	0.000	2.750	1.881	9906.038	5899.293
(5S)-2-methyl-5-prop	150.220	0.000	2.000	2.160	3566.109	1955.271
1,6,7-trimethylnapht	170.254	0.000	0.000	4.580	9906.038	5899.293
(6aS)-1,2,9,10-tetra	355.433	0.000	5.000	3.764	2243.244	1310.647
5-octyloxolan-2-one	198.305	0.000	3.000	2.865	2177.938	1147.459
hencosanoic acid	326.562	1.000	2.000	7.176	236.292	132.300
octadec-9-enal	266.466	0.000	2.000	5.684	2289.451	1211.092
didodecyl benzene-1	502.776	0.000	4.000	9.886	1917.314	999.788
tricosanoic acid	354.615	1.000	2.000	7.964	235.356	131.734
tridec-1-ene	182.348	0.000	0.000	6.825	9906.038	5899.293
2-(4-methylcyclohex	154.252	1.000	0.750	2.963	4936.525	2778.794
(3S,4R,5S,6S)-6-met	164.158	4.000	8.500	-1.470	268.930	119.635
1-decoxydecane	298.551	0.000	1.700	6.599	9906.038	5899.293
2-(dodecoxymethyl)	242.401	0.000	3.700	3.680	9906.038	5899.293
2-methylhexadecan-	256.471	1.000	1.700	5.625	3818.877	2105.492
1-(4-hydroxy-3-meth	180.203	1.000	3.500	1.492	1074.868	534.861
(3-methyl-5-propan-	207.272	1.000	3.000	2.483	2455.562	1306.342
pentadecanal	226.401	0.000	2.000	4.678	1940.110	1012.643
4-methyldecane	156.311	0.000	0.000	6.581	9906.038	5899.293
2-methyl-5-propan-2	136.236	0.000	0.000	3.889	9906.038	5899.293
1,4-diamino-2-meth	268.271	2.000	4.750	1.367	215.496	94.162
octadecane-1-thiol	286.558	0.800	0.500	7.365	9906.038	10000.000
2-[2-(dimethylamino	160.259	0.000	5.700	0.169	548.911	316.623
N-[(7S)-10-amino-1,2	384.431	3.000	7.750	1.572	244.380	177.763
3-methylsulfanyl)pro	104.167	0.000	2.500	0.317	1831.771	1640.832

3,7-dimethylocta-1,3	136.236	0.000	0.000	4.403	9906.038	5899.293
4-methylidene-1-pro	136.236	0.000	0.000	3.814	9906.038	5899.293
oct-1-en-3-ol	128.214	1.000	1.700	2.826	4009.644	2219.402
icos-1-ene	280.536	0.000	0.000	10.590	9906.038	5899.293
(3S,4S,5S,6R)-6-(hydri	180.157	5.000	10.200	-2.237	65.988	26.202
(2S,3R,5R,9R,10R,13l	464.641	5.000	8.600	2.717	91.614	37.355
dotriacontanoic acid	480.856	1.000	2.000	11.398	235.991	132.118
4-hydroxy-2,5-dimet	128.127	1.000	3.500	0.221	1117.360	557.752
(methyltrisulfanyl)m	126.249	0.000	0.500	2.810	9906.038	10000.000
but-2-enoic acid	86.090	1.000	2.000	0.722	203.439	112.535
2-pentylfuran	138.209	0.000	0.500	2.893	9906.038	5899.293
1,3-dimethyl-8-prop	204.355	0.000	0.000	5.965	9906.038	5899.293
2-butyloctan-1-ol	186.337	1.000	1.700	3.636	3362.060	1834.629
methyl 4-hydroxy-3-ri	182.176	1.000	3.500	1.779	849.416	414.703
1-iodododecane	296.234	0.000	0.000	7.031	9906.038	10000.000
2-(2-ethylhexoxycart	278.347	1.000	4.000	3.784	127.491	67.907
methyl (1R,12R,19S)-	336.433	0.000	3.000	4.182	674.239	357.436
5,8-dihydroxy-7-met	284.268	1.000	3.750	2.571	479.952	223.750
icosylcyclohexane	364.697	0.000	0.000	14.277	9906.038	5899.293
2,4,5-trimethoxyben	196.202	0.000	4.250	1.230	1841.805	957.298
undecan-5-ylbenzen	232.408	0.000	0.000	7.474	9906.038	5899.293
6,7-dimethoxy-1-me	203.240	0.000	2.500	2.804	6659.475	3840.530
4-ethylbenzaldehyde	134.177	0.000	2.000	1.722	1833.282	952.511
2,3-dimethylpentan-	116.203	1.000	0.750	2.158	4934.918	2777.817
hept-1-en-3-ol	114.187	1.000	1.700	2.445	3858.690	2129.228
(1S)-16,17-dimethox	339.390	0.000	5.000	3.143	2407.631	1414.762
methyl 12-methyltric	242.401	0.000	2.000	4.971	3212.614	1746.643
methyl 14-methylpei	270.454	0.000	2.000	5.724	3032.901	1641.277
(2S,3R,5R,9R,10R,13l	480.640	6.000	9.350	2.140	47.468	18.352
methyl 3-methoxy-2-	195.218	0.000	2.750	2.351	2597.784	1388.311
3,8-dimethyl-5-prop	228.290	0.000	4.000	2.099	1554.362	796.884
ethyl docosanoate	368.642	0.000	2.000	8.621	2883.685	1554.172
2,3-dimethylpyrazine	108.143	0.000	2.000	0.856	4121.295	2286.276

1-methyl-4-prop-1-e	136.236	0.000	0.000	3.998	9906.038	5899.293
1-(propyltrisulfanyl)z	182.357	0.000	0.500	4.259	9906.038	10000.000
methyl henicanoat	340.588	0.000	2.000	7.759	2616.217	1398.962
2,2-diethoxy-1-phen	208.257	0.000	5.400	1.782	3672.092	2018.156
hexyl hexanoate	200.320	0.000	2.000	3.892	3074.103	1665.390
(3aR,5R,5aR,8aR,9S,9	262.305	0.000	5.700	1.024	574.604	271.804
heptadec-1-ene	238.456	0.000	0.000	9.076	9906.038	5899.293
1-hydroxypyridin-4-c	111.100	1.000	4.200	-0.336	685.487	328.916
1-benzylisoquinoline	219.285	0.000	1.000	4.492	8466.127	4978.144
2-methylcyclohexan-	113.202	2.000	1.000	0.920	842.356	454.673
2-methylundecane	170.337	0.000	0.000	7.148	9906.038	5899.293
tetratetracontane	619.195	0.000	0.000	24.850	9906.038	5899.293
methyl pentadecano	256.428	0.000	2.000	5.382	2604.809	1392.370
heptacosanoic acid	410.722	1.000	2.000	9.510	235.387	131.753
2-tetradecyloxirane	240.428	0.000	2.000	4.715	9906.038	5899.293
N-[(7S)-2-hydroxy-1,	385.416	2.000	7.500	1.885	281.617	207.024
2-hexadecyloxirane	268.482	0.000	2.000	5.415	9906.038	5899.293
N-[(7S)-1,2,3,10-tetr	385.416	1.000	7.500	1.951	337.926	266.028
3,4,5,14,15,16-hexar	432.513	1.000	5.250	5.082	4720.312	2647.479
silane	32.117	4.000	0.000	0.212	9906.038	5899.293
ethyl 2-methylbutan	130.186	0.000	2.000	1.820	4140.291	2297.668
(2R,3S,4R,5R)-2-(hyd	180.157	5.000	8.300	-1.693	100.926	41.476
(19S)-19-ethyl-19-hy	348.357	1.000	7.750	1.742	446.558	206.971
phosphane	33.997	3.000	0.000	0.271	9906.038	10000.000
2-methyl-5-prop-1-e	152.236	0.000	2.000	2.273	3729.617	2052.350
1,1,3-triethoxypropa	176.255	0.000	5.100	1.300	9906.038	5899.293
butan-2-amine	73.138	2.000	1.000	0.125	824.813	444.447
3-(2-ethylhexoxymet	242.444	0.000	1.700	4.902	9906.038	5899.293
2,2,4,4,6,6,8-heptam	358.688	0.000	0.800	5.923	9906.038	5899.293
tridecanal	198.348	0.000	2.000	3.838	1839.264	955.870
methyl N-(1H-benzin	191.189	0.000	1.000	2.666	612.299	291.128
3-[(3S,5S,10R,13R,14	698.803	8.000	21.500	-0.542	11.704	4.041
2-(2-methoxypropox	148.202	1.000	5.100	0.838	3097.196	1678.916

(2S)-2-amino-4-ethyl	163.234	3.000	3.500	-1.402	24.892	19.965
6-methyltridecane	198.391	0.000	0.000	8.207	9906.038	5899.293
pentadec-1-ene	210.402	0.000	0.000	7.876	9906.038	5899.293
3,7,7-trimethylbicycl	136.236	0.000	0.000	3.899	9906.038	5899.293
(2S,5R)-5-methyl-2-p	154.252	0.000	2.000	2.276	4326.362	2409.481
tetratriacontane	478.927	0.000	0.000	19.374	9906.038	5899.293
3-hydroxydecanoic a	188.266	1.000	2.700	2.588	114.809	60.636
3-hydroxyoctanoic ar	160.213	1.000	2.700	1.831	115.500	61.031
2,3,5-trimethylpyrazi	122.169	0.000	2.000	1.700	4836.147	2717.772
1,1,2,3,3-pentachloro	216.322	0.000	0.000	3.227	9906.038	10000.000
4-methyl-1-(6-methy	222.370	1.000	0.750	4.560	5688.684	3239.130
(5-methyl-2-propan-	198.305	0.000	2.000	3.135	3959.338	2189.320
(3-hydroxy-2,2-dime	237.255	2.000	5.450	1.441	1275.001	643.271
3,3,4-trimethylhexar	128.257	0.000	0.000	4.895	9906.038	5899.293
2-hydroxybutane-1,2	206.152	3.000	5.750	0.298	0.200	0.102
2,6-dimethylundecar	184.364	0.000	0.000	7.595	9906.038	5899.293
2,2-dimethyldecane	170.337	0.000	0.000	7.041	9906.038	5899.293
1,1,7,7a-tetramethyl	204.355	0.000	0.000	5.116	9906.038	5899.293
(2S,3R,4S,5S,6R)-2-[(1034.200	13.000	35.750	-2.949	0.432	0.126
2,3-diethyl-5-methyl	150.223	0.000	2.000	1.987	5687.425	3238.355
7,7-dimethyl-2-meth	136.236	0.000	0.000	3.528	9906.038	5899.293
ethyl nonadecanoate	326.562	0.000	2.000	7.432	2751.347	1477.224
4,6,6-trimethylbicycl	150.220	0.000	2.000	1.924	3152.657	1711.435
nonadec-1-ene	266.509	0.000	0.000	10.029	9906.038	5899.293
4,10,11,11-tetrametl	206.370	0.000	0.000	6.562	9906.038	5899.293
(2R,3R,4R,5S)-2-(hyd	163.173	5.000	8.300	-2.200	30.149	12.431
(4S,4aS,8aR)-4,8a-dir	182.305	1.000	0.750	3.151	6472.699	3724.237
ethyl 3-methyloxiran	130.143	0.000	4.000	0.417	3373.198	1841.199
(5-methyl-2-prop-1-ε	196.289	0.000	2.000	3.352	2815.896	1514.720
(2-methyl-5-prop-1-ε	196.289	0.000	2.000	3.251	4100.155	2273.603
2-[[4-chloro-6-(ethyl	240.695	2.000	5.500	1.849	719.531	909.412
tetradeca-1,13-diene	194.359	0.000	0.000	7.275	9906.038	5899.293
(6aS)-2-methoxy-6-n	281.354	1.000	3.500	3.038	1055.504	580.213

4-(4-hydroxy-3-methoxyphenyl)ethanol	194.230	1.000	3.500	1.757	949.572	467.800
1-(4-methoxyphenyl)ethanol	164.204	0.000	2.750	2.156	3515.537	1925.318
2-phenoxyethanol	138.166	1.000	2.450	1.624	2848.478	1533.673
dodecylbenzene	246.435	0.000	0.000	8.701	9906.038	5899.293
4-methoxybenzaldehyde	136.150	0.000	2.750	1.154	1832.747	952.210
7-methyl-3-methylideneoctane	136.236	0.000	0.000	4.606	9906.038	5899.293
4-hydroxy-4-methylpentan-2-one	116.160	0.000	1.750	1.267	1936.450	1010.578
3-methylbutan-1-ol	88.149	1.000	1.700	1.392	2863.558	1542.451
pentane-2,4-dione	100.117	0.000	4.000	-0.316	1225.638	616.395
ethyl hexanoate	144.213	0.000	2.000	2.466	2908.513	1568.641
prop-2-enyl hexanoate	156.224	0.000	2.000	2.701	3224.721	1753.758
butyl acetate	116.160	0.000	2.000	1.418	2233.237	1178.982
3-methylbutyl acetate	130.186	0.000	2.000	1.766	2232.182	1178.380
ethyl tetradecanoate	256.428	0.000	2.000	5.463	3114.818	1689.244
methyl tetradecanoate	242.401	0.000	2.000	5.016	2572.510	1373.718
nonanal	142.241	0.000	2.000	2.675	2276.792	1203.855
tetradecanal	212.375	0.000	2.000	4.268	1840.681	956.666
octadecanamide	283.496	2.000	2.500	4.488	408.022	394.952
(1R,3R,5S,8S,13R,14S)-1,3,5,8-tetramethylundecane	310.303	1.000	8.500	0.089	508.147	237.990
(4R)-4-[(3R,5S,7S,8R)-3,5,7-trimethylundecane-2-yl]butane	392.578	3.000	5.400	3.817	39.702	19.243
2,6-ditert-butyl-4-methylheptane	220.354	1.000	0.750	4.378	8422.958	4950.713
3-methyloct-1-en-3-yl acetate	142.241	1.000	0.750	2.892	4656.743	2608.963
2,6-di(propan-2-yl)nonane	212.334	0.000	0.000	6.149	9906.038	5899.293
3-dodec-1-enyloxolane	266.380	0.000	4.500	3.172	707.891	340.550
[10,13-dimethyl-17-(4-oxohept-5-en-2-yl)undecane-2,6-dione]	488.752	0.000	2.000	9.434	4216.285	2343.286
(2S)-2-aminopentane-1,4-diol	147.130	4.000	5.000	-3.017	0.620	0.302
(1R,2R)-2-[(dimethylamino)ethyl]propane-1-thiol	263.379	1.000	3.500	3.176	1498.129	847.184
2-ethyl-4-hydroxy-5-methylheptane	142.154	1.000	3.500	0.955	1112.415	555.084
bis(6-methylheptyl) ether	390.562	0.000	4.000	6.170	1620.952	833.848
ethyl 1-methyl-3,6-dimethylpiperidine-4-carboxylate	169.223	0.000	4.000	0.855	630.624	332.511
2-methylfuran-3-thiol	114.162	0.000	3.200	0.260	8628.360	10000.000
2,4-dimethylthiophene	112.189	0.000	0.000	2.884	9906.038	10000.000
1,6-dimethyl-4-propylpiperidine	208.386	0.000	0.000	7.042	9906.038	5899.293

2,6,11-trimethyldodecane	212.418	0.000	0.000	8.608	9906.038	5899.293
2-methyl-5-propylthiophane	140.243	0.000	0.000	3.960	9906.038	9104.933
(6aS)-1,2-dimethoxy-2,3-dihydro-1H-benzofuran	281.354	1.000	3.000	3.358	1516.991	858.719
2,6,10,15-tetramethylheptacosane	296.579	0.000	0.000	11.752	9906.038	5899.293
4a-methyl-1,2,4,5,6,7,8,9-octahydro-1H-benzofuran	194.316	0.000	2.000	2.791	3298.470	1797.151
3,5,24-trimethyltetracosane	605.168	0.000	0.000	23.862	9906.038	5899.293
(2,2-dimethyl-3H-1H-imidazol-5-yl)methane	380.544	0.000	5.250	5.694	7663.169	6398.777
7-methylheptadecane	270.498	1.000	0.750	6.376	4589.577	2568.313
[4-[(1-benzylpiperidin-4-yl)methyl]phenyl]methane	339.436	2.500	6.250	2.929	278.813	137.619
7-methoxy-1-methyl-2,3-dihydro-1H-benzofuran	193.245	2.000	3.000	1.260	488.369	252.234
(1R)-1-[[3-[4-[[[(1R)-6-methyl-2,3-dihydro-1H-benzofuran-5-yl]oxy]phenyl]butyl]oxy]phenyl]ethane	610.749	2.000	8.250	5.662	69.257	33.790
[(1S,3R,7S,8S,8aR)-8-methyl-8-azabicyclo[3.2.1]octane-7-carboxamide]	404.545	1.000	6.700	4.258	712.823	343.116
(3R,5R)-7-[(1S,2S,6S,6aR)-6-methyl-6-azabicyclo[3.2.1]octane-7-carboxamide]	424.533	3.000	8.100	3.380	21.302	9.818
3-(5-nitro-1,3-thiazol-2-yl)propane	212.183	1.000	4.500	0.114	109.064	70.438
2-methylundecanal	184.321	0.000	2.000	3.469	2245.310	1185.873
2,6,6-trimethylcyclohexane	150.220	0.000	2.000	2.019	3183.542	1729.565
2-(2,6,6-trimethylcyclohexyl)ethane	166.263	0.000	2.000	2.301	2564.228	1368.938
4,4,8-trimethyltricyclohexane	222.370	1.000	0.750	3.716	4370.013	2435.768
6,6-dimethylbicyclo[2.2.2]octane	150.220	0.000	2.000	1.800	2073.202	1087.933
octyl 3,4,5-trihydroxybutanoate	282.336	3.000	4.250	2.280	116.727	48.537
(6,6-dimethyl-2-bicyclo[2.2.2]octyl)ethane	194.273	0.000	2.000	2.919	2641.265	1413.444
pentadecan-2-one	226.401	0.000	2.000	4.780	3062.104	1658.365
ethyl hex-3-enoate	142.197	0.000	2.000	2.227	2902.203	1564.963
oct-1-en-3-one	126.198	0.000	2.000	2.110	3913.088	2161.691
3-butyl-3H-2-benzofuran	190.241	0.000	3.000	2.274	2281.559	1206.580
3-methylbutyl dodecanoate	270.454	0.000	2.000	5.822	3334.590	1818.432
[(2R,3R,4R,5R)-1,2,4-trimethylpiperidine]	452.159	0.000	15.000	-4.980	0.028	0.006
dec-4-enal	154.252	0.000	2.000	2.645	1837.426	954.838
3-(methyltrisulfanyl)propane	152.287	0.000	0.500	3.590	9906.038	10000.000
6-methyl-3-propan-2-ylideneacetone	166.219	0.000	4.000	1.141	4256.157	2367.247
2,6,6-trimethylbicyclo[2.2.2]octane	170.251	2.000	2.450	1.568	2114.890	1111.598
4-(hydroxymethyl)-2-methylpropanoic acid	154.165	2.000	3.200	0.706	913.693	448.725
2-methyl-5-propan-2-ylideneacetone	154.252	1.000	0.750	2.720	4747.981	2664.257

2,6,6-trimethylcyclo	152.193	0.000	4.000	0.655	1549.287	794.072
1-methyl-4-prop-1-e	132.205	0.000	0.000	3.570	9906.038	5899.293
3-(methylsulfanyl)k	120.227	0.000	1.000	2.642	9906.038	10000.000
4-ethenylphenol	120.151	1.000	0.750	2.199	3005.223	1625.093
4-ethyl-2-methoxypt	152.193	1.000	1.500	2.717	3043.094	1647.239
(1S,2R,6S,7R,8S)-1-m	204.355	0.000	0.000	5.222	9906.038	5899.293
2-methyl-3-[(2-phen	365.434	1.000	4.000	5.022	2798.100	1504.375
2-(1-adamantyl)ethy	285.385	0.000	3.500	3.681	1536.677	787.089
1,7,7-trimethylbicycl	154.252	1.000	1.700	2.080	4398.979	2453.224
(2R,3R,4S,5S,6R)-6-(t	180.157	5.000	10.200	-2.262	61.032	24.081
(8-methyl-8-azabicyc	271.358	0.000	4.000	3.207	1246.529	694.501
[(1S,7S,8S,8aR)-8-[2-	390.519	1.000	6.700	4.175	906.960	445.152
(1S,2R,4aS,6aR,6aS,6	456.707	2.000	3.700	6.197	310.003	177.425
(1R,3aS,5aR,5bR,7aR	456.707	2.000	3.700	6.240	254.896	143.594
(2S,3S,4S,5R,6S)-6-(5	446.367	4.000	11.550	0.393	1.091	0.395
(2R,3R,11bS)-2-[(6,7-	478.630	1.000	6.000	6.019	1894.968	1092.155
3-prop-2-enylsulfanyl	162.264	0.000	4.000	1.387	170.619	4213.105
[(2S,3S)-2-(3,4-dihyd	442.378	7.000	8.000	0.412	2.606	0.797
[(2R,3R)-5,7-dihydro:	458.378	8.000	8.750	-0.130	1.030	0.292
(2R,3S)-2-(3,4,5-trihy	306.271	6.000	6.200	-0.209	17.756	6.340
9-hydroxyfuro[3,2-g]	202.166	1.000	3.750	0.988	619.214	294.683
(2S)-2-aminopentanc	117.147	3.000	3.000	-1.647	24.846	12.827
8-tert-butyl-6,12,17-	424.404	2.000	12.900	-0.695	98.042	40.196
(3S,4S,5S,10S,13R,14	426.724	1.000	1.700	7.778	3964.882	2192.634
1-[(2R,3R,11bS)-3-e	464.603	2.000	6.000	5.120	594.034	311.707
3-methylsulfanylhex:	148.263	1.000	2.200	2.394	2861.661	2240.367
(1S,2R,5S,7R,8R)-2,6,	222.370	1.000	0.750	3.745	5307.312	3005.064
[(1S,4aS,6S,7R,7aS)-€	424.490	0.000	9.700	2.940	1024.098	507.607
(2R,3S,4S,4aR,10bS)-	328.275	5.000	12.050	-1.567	36.307	13.736
N'-ethylethane-1,2-d	88.152	3.000	2.500	-0.837	107.788	54.505
2-methylpropyl pent	158.240	0.000	2.000	2.715	3170.435	1721.869
1-O-butyl 2-O-octyl t	334.455	0.000	4.000	5.442	1567.442	804.135
1-(2-hydroxy-4,6-dir	196.202	0.000	3.250	1.646	1669.252	860.736

N,N-dimethyl-2-(4-methylphenyl)propanoic acid	171.285	0.000	6.000	-0.540	104.070	58.055
2-bromododecanoic acid	279.216	1.000	2.000	4.332	280.022	361.352
1-(4-methoxyphenyl)ethanone	164.204	0.000	2.750	2.043	3916.234	2163.570
1-methyl-2-(4-methoxyphenyl)ethanone	142.485	1.000	7.200	3.469	680.970	361.294
6H-indolo[2,3-b]quinoline	218.257	1.000	1.000	3.523	3570.004	1957.580
1,2,4-triazine	81.077	0.000	4.500	-0.733	1279.585	645.772
cyclotetradecane	196.375	0.000	0.000	6.928	9906.038	5899.293
cyclohexadecane	224.429	0.000	0.000	7.910	9906.038	5899.293
2-oxooctanoic acid	158.197	1.000	4.000	1.184	98.678	51.482
methanimidamide	44.056	3.000	2.000	-1.317	248.056	109.630
5,6,7,8-tetramethoxy-2-naphthol	372.374	0.000	6.250	3.582	3811.651	2101.186
4,9-dimethoxyfuro[3,2-b]pyridine	246.219	0.000	4.500	1.624	2391.550	1269.573
4-(3-methylbut-2-enyl)phenol	270.284	0.000	3.750	2.946	2055.856	1078.098
1,2-dimethoxy-4-methylbenzene	152.193	0.000	1.500	2.819	9906.038	5899.293
4-prop-2-enylphenol	134.177	1.000	0.750	2.208	3006.666	1625.936
3-hydroxypropanoic acid	90.079	1.000	2.700	-0.133	69.235	35.101
hexacosan-1-ol	382.712	1.000	1.700	9.106	2854.804	1537.355
8,8-dimethylpyrano[3,2-b]pyridine	228.247	0.000	3.250	2.597	2063.406	1082.378
(7S)-4,7-dimethyl-6,7-dihydro-5H-benzofuro[3,2-b]pyridine	147.219	0.000	1.500	2.408	5358.819	3036.599
(5-methyl-2-propanoyl)phenol	192.257	0.000	2.500	2.829	4751.262	2666.247
1,3-benzodioxol-5-ol	138.123	1.000	2.250	0.920	3003.883	1624.310
3-(4-methylpent-3-enyl)phenol	150.220	0.000	0.500	3.223	9906.038	5899.293
hentriacontan-1-ol	452.846	1.000	1.700	11.014	2853.996	1536.884
3,3,6-trimethylheptane	152.236	0.000	2.000	2.602	6115.507	3502.599
octacosan-1-ol	410.766	1.000	1.700	9.894	3296.221	1795.827
6,7-dimethoxy-3H-2-benzofuro[3,2-b]pyridine	194.187	0.000	4.500	0.869	2897.813	1562.404
triacontan-1-ol	438.819	1.000	1.700	10.713	3297.315	1796.471
ethyl pyridine-3-carboxylate	151.165	0.000	3.500	1.098	1568.937	804.964
2,4-ditert-butyl-6-methylphenol	220.354	1.000	0.750	4.120	6225.948	3571.018
phenyl carbamate	137.138	2.000	3.000	0.562	746.470	360.655
hexadecanoyl hexadecanoate	494.840	0.000	4.500	10.176	1496.989	765.140
heptyl heptanoate	228.374	0.000	2.000	4.617	3083.090	1670.653
3-hydroxy-3-methylpentanoic acid	118.132	1.000	1.750	1.266	144.920	77.995

octanamide	143.228	2.000	2.500	0.716	407.904	394.831
nonadecan-2-one	282.509	0.000	2.000	6.390	3375.633	1842.636
octadec-1-yne	250.467	0.500	0.000	9.426	9906.038	5899.293
9-hydroxy-4-(3-methoxyphenyl)	270.284	1.000	3.750	2.434	622.158	296.197
3,4,5-trimethoxyphenyl	184.191	1.000	3.000	1.694	3016.883	1631.909
4-methyl-1,3-oxazole	83.090	0.000	2.000	0.058	5588.310	3177.399
(3,5-dimethoxyphenyl)	168.192	1.000	3.200	1.635	2964.130	1601.088
8-hydroxyoctanoic acid	160.213	2.000	3.700	1.155	67.973	34.410
1H-indole-3-carboxylate	161.160	1.000	1.000	2.148	147.804	79.674
6-hydroxy-7-methoxyphenyl	192.171	1.000	4.000	0.857	632.846	301.701
1-ethenoxyhexadecane	268.482	0.000	1.700	6.558	7369.831	4285.178
furan-2,5-dicarbaldehyde	124.096	0.000	4.500	-0.929	271.694	120.964
cyclopent-4-ene-1,3-diene	96.085	0.000	4.000	-1.197	616.589	293.332
3,5-dihydroxy-2-methylphenyl	142.111	2.000	4.000	-0.338	364.598	166.235
nonanamide	157.255	2.000	2.500	1.085	408.894	395.400
4-prop-2-enylbenzene	150.177	2.000	1.500	1.594	1068.862	531.632
3,5-ditert-butylphenyl	206.327	1.000	0.750	3.712	3011.184	1628.577
2,5-dihydroxybenzaldehyde	138.123	1.000	2.500	1.173	209.719	91.437
heptadecanal	254.455	0.000	2.000	5.483	2160.177	1137.348
2-(3,4-dihydroxyphenyl)	306.271	6.000	7.150	-0.327	27.002	9.974
(2R,3R,4R)-2-(hydroxymethyl)phenyl	147.174	4.000	6.600	-1.516	79.483	35.445
(2R,3R)-2-(3,4-dihydroxyphenyl)	290.272	5.000	5.450	0.469	53.201	20.760
(2R,3R)-2-(3,4,5-trihydroxyphenyl)	306.271	6.000	6.200	-0.187	19.067	6.848
(2S)-5,7-dihydroxy-2-methylphenyl	302.283	2.000	4.750	1.780	130.638	54.818
2-[[4R,5S,7R,8R,11S,14R]-5,7-dihydroxy-2-methylphenyl]	956.688	13.000	26.150	-3.651	0.000	0.000
5-[[3S,3aR,6S,6aR]-3,4,5-trihydroxy-2-methylphenyl]	354.359	0.000	6.400	1.738	9906.038	5899.293
[[1R,2R,4S,7S,8S,11R]-5,7-dihydroxy-2-methylphenyl]	514.571	0.000	12.500	1.066	249.135	110.146
(1R,3aS,5aR,5bR,7aR)-5,7-dihydroxy-2-methylphenyl	442.724	2.000	3.400	5.981	1736.227	898.124
methyl (1S,15S,16R,2-methylphenyl)	352.432	1.000	5.700	3.105	571.061	298.698
methyl (1S,15S,16S,2-methylphenyl)	352.432	1.000	5.700	3.174	565.218	295.396
(1R)-1-[[2S,3R,11bS)-5,7-dihydroxy-2-methylphenyl]	475.630	3.000	5.750	4.331	98.892	49.659
2-(3,4-dimethoxyphenyl)	402.400	0.000	7.000	3.618	3793.457	2090.347
(1S,17S,18S,19S)-5,7-dimethoxyphenyl	287.315	2.000	6.900	0.701	366.715	185.064

4-[3-[(4-hydroxypher	266.339	2.000	1.500	5.025	912.553	448.119
(2S)-2-acetamido-N-	426.558	4.750	9.250	0.448	6.205	6.689
6,7-dimethoxy-12-m	369.416	0.000	7.000	2.450	1241.119	691.243
(3aR,5S,8aR,9aR)-5,8	232.322	0.000	3.000	2.785	2921.199	1576.038
1H-indole-2-carboxyl	161.160	2.000	2.000	1.907	143.171	76.978
(9R)-9-[(9R)-2-carbo	862.750	10.000	26.000	-1.389	0.008	0.002
6-[(3R,3aR,6R,6aR)-6	430.454	0.000	7.900	1.528	9906.038	5899.293
(3S,4aR,6aR,6bS,8aR	426.724	1.000	1.700	7.113	4371.736	2436.806
(2S,3R)-2-(3,4-dihydr	290.272	5.000	5.450	0.451	49.421	19.170
(3S,4aR,6aR,6bS,8aR	426.724	1.000	1.700	7.038	4371.411	2436.611
[(1S,2R)-1-[(10R,11R	786.566	14.000	20.900	-3.355	0.010	0.002
3,5-ditert-butyl-4-hy	234.338	1.000	2.750	2.891	1552.189	795.680
(3aR,4aS,8aR,9aR)-8	232.322	0.000	3.000	2.754	2806.632	1509.334
(4aS,6aR,6aS,6bR,8a	472.707	3.000	5.400	5.260	128.312	68.380
[(10S,11R,12R,13S,1	634.460	11.000	17.850	-3.088	0.027	0.006
(1S)-1-[(3,4-dimetho	357.449	0.000	5.000	3.034	2470.586	1454.789
4-[(1R)-6,7-dimetho	624.775	1.000	8.250	6.485	300.932	165.347
(1R,4S,8S,9R,10R,12	332.439	1.000	4.250	3.723	2559.001	1365.922
(2S,3R,4R,5R,6S)-2-[(884.069	10.000	27.250	-0.767	1.099	0.347
(1S,2R,5S,7S,10S,11	430.673	4.000	4.000	3.899	71.656	35.057
(3S,5R,8R,9R,10R,12	460.739	2.000	4.150	6.117	3059.483	1656.830
[(1S,19R,21S,22R,23	634.460	11.000	17.850	-2.971	0.104	0.024
(2S)-5-hydroxy-2-(4-	286.284	1.000	4.000	2.462	425.914	196.649
(2S)-2-(4-hydroxyph	448.426	5.000	13.500	-0.051	30.661	11.443
(2S,3R,4S,5S,6R)-2-[742.727	8.000	24.900	-1.220	9.916	3.378
(4aS,6aR,6aS,6bR,8a	488.706	4.000	7.100	4.267	51.415	25.446
(4aS,6aR,6aS,6bR,8a	472.707	3.000	5.400	5.260	123.172	65.424
trimethyl 2-hydroxy	234.205	0.000	5.750	0.773	323.929	146.287
naphthalen-2-ylmet	158.199	1.000	1.700	2.458	2976.429	1608.269
docos-1-ene	308.590	0.000	0.000	11.736	9906.038	5899.293
decyl decanoate	312.535	0.000	2.000	7.041	3168.286	1720.608
1-phenyldodecan-1-	260.419	0.000	2.000	5.352	3709.598	2040.445
8-prop-1-en-2-ylfuro	226.231	0.000	3.000	2.544	2056.463	1078.442

heptacosan-1-ol	396.739	1.000	1.700	9.467	2854.360	1537.096
3-ethyloctan-3-ol	158.283	1.000	0.750	3.257	5959.761	3406.282
naphthalene-1,2-dic	216.193	2.000	4.000	1.792	13.780	7.798
2-octadecoxyethano	314.551	1.000	3.400	6.209	2854.984	1537.459
3-methylideneoxolar	112.085	0.000	4.500	-1.169	488.985	228.305
decanamide	171.282	2.000	2.500	1.461	402.315	391.619
methyl tetracosanoa	382.669	0.000	2.000	8.960	2908.046	1568.368
cyclopropylmethano	72.107	1.000	1.700	0.535	3016.113	1631.459
6-methyl-3-(3-methy	194.316	0.000	2.000	3.707	6757.392	3901.602
nonacosan-15-one	422.777	0.000	2.000	10.310	3440.809	1881.120
1,4,5-trihydroxyanth	256.214	0.000	3.250	1.421	114.029	47.326
methyl 2,4-dihydroxy	182.176	1.000	2.500	1.708	415.521	191.467
butylphosphonic acic	138.103	2.000	5.000	0.522	26.996	16.829
9-methoxy-2,3-dihyd	218.209	0.000	4.000	1.458	2168.941	1142.336
3,4-dihydroxy-5-met	168.149	2.000	4.250	-0.044	202.142	87.871
5-[[4-[2-[methyl(pyri	357.426	1.000	5.250	3.527	498.318	352.229
1-isothiocyanatohex	143.246	0.000	2.500	2.535	7236.066	10000.000
1-isothiocyanatohep	157.273	0.000	2.500	2.866	7254.893	10000.000
methyl 3-aminobenz	151.165	1.500	3.000	0.752	720.487	347.105
2-(4-butoxyphenyl)a	208.257	1.000	2.750	2.763	265.453	150.033
15-hydroxypentadec	258.400	2.000	3.700	3.738	67.643	34.229
thiophene-2-carbony	146.591	0.000	2.000	1.706	2657.665	5917.522
4-methyl-1-propan-2	138.252	0.000	0.000	5.136	9906.038	5899.293
(2S,3R,4S,5S,6R)-6-(f	180.157	5.000	10.200	-2.184	76.316	30.661
3,3,5-trimethylcyclo	124.225	0.000	0.000	3.391	9906.038	5899.293
1,7,7-trimethyltricycl	136.236	0.000	0.000	4.660	9906.038	5899.293
3-methyl-6-prop-1-e	150.220	0.000	2.000	2.073	3914.075	2162.280
3,7,7-trimethylbicycl	136.236	0.000	0.000	3.884	9906.038	5899.293
2,3-dihydroxypropyl	302.453	2.000	5.400	3.678	375.931	171.827
3,4-dimethylthiophe	112.189	0.000	0.000	2.828	9906.038	10000.000
1,3-dimethylpyrazole	96.132	0.000	1.500	0.978	6254.135	3588.497
4-(methoxymethyl)p	138.166	1.000	2.450	1.573	3006.625	1625.912
2-methoxy-4-(metho	168.192	1.000	3.200	1.619	3043.266	1647.340

methyl 3-(4-hydroxy	180.203	1.000	2.750	1.921	794.039	385.559
2-[[1,3-dihydroxy-2-(179.172	5.000	8.100	-3.683	2.776	1.200
(methyltetrasulfanyl	158.309	0.000	0.000	3.134	9906.038	10000.000
(3,4-dimethoxyphen	167.207	2.000	2.500	1.602	624.535	329.042
2,5-ditert-butylphen	206.327	1.000	0.750	3.851	4999.324	2817.023
dodecan-6-one	184.321	0.000	2.000	3.696	3919.476	2165.505
nonadecan-1-ol	284.524	1.000	1.700	6.386	3297.326	1796.477
2-methoxy-1-methyl	164.247	0.000	0.750	3.278	9906.038	5899.293
(2-methyl-5-propan-	192.257	0.000	2.500	2.841	4238.639	2356.718
quinoline-3-carboxyl	173.171	1.000	3.000	1.656	154.011	83.297
heptyl hexanoate	214.347	0.000	2.000	4.252	2831.138	1523.584
2,2-dimethylpropan	102.179	4.000	2.000	-0.954	61.967	29.962
phenanthren-4-ol	194.232	1.000	0.750	3.207	4318.051	2404.478
4-(2-hydroxyethyl)be	154.165	3.000	3.200	0.217	308.965	138.996
(2S)-2-(3,4-dihydroxy	596.541	8.000	20.050	-2.052	1.476	0.431
(2S)-2-hydroxy-4-me	132.159	2.000	3.700	0.500	112.227	59.164
dicyclopropylmethar	112.171	1.000	1.700	1.462	3791.468	2089.163
(1S,2S,5R)-2,6,6-trim	152.236	0.000	2.000	2.009	3876.649	2139.941
(2R,3R,4S,5R,6S)-2-(f	342.299	8.000	18.700	-3.867	7.870	2.631
3-methylsulfanylprop	148.220	0.000	2.500	1.839	2233.521	2036.167
(1R,6S)-3-methyl-6-p	154.252	1.000	1.700	2.734	4471.968	2497.251
(1R,6R)-3-methyl-6-ç	154.252	1.000	1.700	2.738	4567.448	2554.930
hexadecan-2-ol	242.444	1.000	1.700	5.308	3923.785	2168.079
2,5,8-trimethyl-2-(4,i	416.686	1.000	1.500	8.634	3674.673	2019.689
[(2R)-2,5,7,8-tetram	472.750	0.000	3.250	9.050	4433.143	2473.824
2,6-dimethyl-6-(4-m	204.355	0.000	0.000	5.813	9906.038	5899.293
4,10-dimethyl-7-prop	204.355	0.000	0.000	5.187	9906.038	5899.293
1-methyl-4-[(1R)-1,2	202.339	0.000	0.000	5.282	9906.038	5899.293
2,2,3,3,5,5,6,6-octad	88.106	0.000	3.400	-0.271	9906.038	5899.293
(2R)-2-amino-3-prop	177.218	2.000	6.000	-2.277	0.453	6.397
trimethylsilyl octade	356.663	0.000	2.000	8.121	6396.424	3676.823
tetradecane-1,14-dic	230.390	2.000	3.400	3.337	950.494	468.291
4-methyl-4-sulfanyl	132.220	0.000	1.500	1.941	3925.299	4122.847

(2R,3R,4S,5R)-2,3,4,ε	196.218	3.800	8.300	-1.290	75.403	64.100
(3S,4R)-4-ethenyl-3-[356.329	4.000	14.900	-1.621	57.039	22.383
7-hydroxy-6-methoxy	207.229	1.000	4.500	1.292	1151.954	576.440
3-methylnonan-3-ol	158.283	1.000	0.750	3.275	5234.813	2960.718
tetradecane-1,2-diol	230.390	2.000	3.400	3.408	1260.647	635.448
4-propan-2-ylcyclohex	152.236	0.000	2.000	2.028	1926.890	1005.187
3-[(2S)-1-methylpyrr	162.234	0.000	3.500	1.192	1256.093	700.262
(1R,2S,5R)-4,6,6-trim	152.236	1.000	1.700	2.101	3568.011	1956.398
2,6-dimethylocta-1,7	154.252	1.000	1.700	2.615	3874.032	2138.380
1,4-dimethyl-7-prop-	204.355	0.000	0.000	5.363	9906.038	5899.293
octane-1,3-diol	146.229	2.000	3.400	1.319	2042.440	1070.495
3-methylbutyl cyclohex	198.305	0.000	2.000	3.458	3632.982	1994.933
1,1,7-trimethyl-4-me	204.355	0.000	0.000	5.176	9906.038	5899.293
(1R,2S,4S,5'R,6R,7S,ε	416.643	1.000	3.200	6.180	3398.806	1856.312
(9S)-9-[(9R)-2-carbox	862.750	10.000	26.000	-1.681	0.001	0.000
(1R,2S,4S,5'R,6R,7S,ε	430.626	1.000	5.200	5.355	1673.699	863.214
(1S,4S,5R)-4-methyl-	152.236	0.000	2.000	2.144	3400.552	1857.342
2-[(2R,4aR,8aS)-4a-r	222.370	1.000	0.750	4.012	4881.208	2745.153
(3S)-3-(4-hydroxyphen	242.274	2.000	2.250	2.747	909.965	446.746
(4R,4aS,6aS,6aR,6bR,	426.724	0.000	2.000	6.946	4027.353	2229.999
1-methyl-4-prop-1-e	152.236	0.000	2.000	1.577	9906.038	5899.293
(2S)-4-[2-[(2S)-2-cart	550.475	8.000	17.000	-0.776	0.002	0.001
(1R,2S,4S,5'S,6R,7S,8	416.643	1.000	3.200	6.148	3404.310	1859.561
(3S,4aR,6aR,6aS,8aR,	426.724	1.000	1.700	7.098	4368.675	2434.962
(1S,3R,6S,8R,11S,12S	426.724	1.000	1.700	7.676	4384.823	2444.692
(3S,8S,9S,10R,13R,14	398.671	1.000	1.700	7.256	3382.361	1846.605
2-[(1R,3S,4S)-4-ether	222.370	1.000	0.750	4.223	4917.575	2767.266
1-methyl-4-(6-methyl	202.339	0.000	0.000	6.216	9906.038	5899.293
[(1R,3aR,5aR,5bR,7a)	468.762	0.000	2.000	8.009	3915.762	2163.288
(1R,3aR,5aR,5bR,7aR)	424.709	0.000	2.000	7.079	4220.775	2345.983
(1aR,4aR,7S,7aR,7bR)	220.354	1.000	0.750	3.913	4867.709	2736.948
3-methyldecane	156.311	0.000	0.000	6.583	9906.038	5899.293
(1R,4aS,8aS)-7-methyl	204.355	0.000	0.000	5.561	9906.038	5899.293

2,2,3,3-tetramethylp	128.257	0.000	0.000	4.197	9906.038	5899.293
(2R)-2,7,8-trimethyl-	416.686	1.000	1.500	8.595	3676.888	2021.005
N-[(7S)-1,2,10-trimet	547.558	5.000	16.000	-0.269	18.357	11.001
methyl (1S,15R,18S,13	54.448	1.000	4.700	3.508	327.323	163.673
(5R)-2-methyl-5-[(2S	204.355	0.000	0.000	6.458	9906.038	5899.293
4-propan-2-ylcyclohex	138.209	0.000	2.000	1.851	2781.051	1494.470
5-propan-2-ylbicyclo	138.209	0.000	2.000	1.756	2938.220	1585.965
(1aR,4R,4aS,7R,7aS,7	222.370	1.000	0.750	3.961	5998.510	3430.226
(2R,3R,4S,5S,6R)-2-[(504.441	11.000	25.300	-5.218	0.553	0.149
2-hydroxyhexadecan	272.427	2.000	3.700	4.248	111.699	58.863
[(3S,4aR,6aR,6bS,8af	468.762	0.000	2.000	7.945	3922.168	2167.113
1-[(3S,8R,9S,10R,13S	314.467	1.000	3.700	3.557	1542.666	790.405
(4S)-2-(6-hydroxy-1,5	280.316	2.000	5.750	1.643	50.428	73.425
3-hydroxy-5-methyl-	248.321	1.000	4.750	2.315	893.968	438.263
1-piperidin-2-ylpropyl	141.213	0.000	2.500	1.009	579.115	303.254
6-methyl-3-propan-2-	168.235	0.000	4.000	1.142	4156.214	2307.221
5-methyldecane	156.311	0.000	0.000	6.581	9906.038	5899.293
3,3-dimethylbicyclo[1	138.209	0.000	2.000	1.676	3967.787	2194.370
(1R,5S,6R,7S,10R)-1C	204.355	0.000	0.000	5.531	9906.038	5899.293
2-methyl-5-[(2R)-6-n	218.338	1.000	0.750	4.305	3689.342	2028.405
(2R,3R,4S,5S,6R)-2-d	348.479	4.000	10.200	1.582	203.625	88.568
7-chloro-3-imidazol-	247.643	0.000	4.500	1.716	998.149	1215.705
heptadec-1-en-4,6-d	278.391	3.000	5.100	3.185	644.920	307.927
5-methyl-2-prop-1-en	154.252	1.000	1.700	2.585	3499.742	1915.969
1,7-dimethyl-7-(4-methyl	204.355	0.000	0.000	5.684	9906.038	5899.293
(1S,3R,6S,8R,11S,12S	440.751	1.000	1.700	7.988	4386.777	2445.870
(2R,3R,4S,5R,6R)-2-(1	194.184	4.000	10.200	-1.650	220.038	96.309
(1S,5R)-2-methyl-5-p	152.236	1.000	1.700	2.235	3952.776	2185.399
[(3S,4aR,6aR,6aS,8af	468.762	0.000	2.000	7.998	3932.916	2173.533
2-methyl-1,2,3,4,4a,5	152.279	0.000	0.000	5.367	9906.038	5899.293
(3S,3aS,5R)-3,8-dime	204.355	0.000	0.000	5.533	9906.038	5899.293
4,8,12-trimethyl-2-oxo	242.274	0.000	4.750	1.711	1551.038	795.042
4,8,12-trimethyl-2-oxo	240.258	0.000	4.500	1.765	1498.877	766.183

2-ethylhexyl benzoat	234.338	0.000	2.000	4.355	3012.469	1629.329
1-(4-hydroxy-3-meth	278.391	1.000	3.500	4.100	1197.809	601.281
(1R,4aS,10aR)-1,4a-d	300.440	1.000	2.000	4.941	449.675	265.224
(2S,3S,4S,5R)-3,4,5,6	194.141	4.000	9.500	-1.883	5.567	2.302
hentriacontan-16-on	450.830	0.000	2.000	11.181	4949.099	2786.446
2-hexyldecan-1-ol	242.444	1.000	1.700	5.165	3360.141	1833.497
1,2-diphenylethane-	214.263	2.000	3.400	2.469	2306.056	1220.589
6,10-dimethylundec	198.348	0.000	2.000	3.843	3072.349	1664.363
2-methyl-3-phenylpr	148.204	0.000	2.000	2.162	2869.102	1545.679
4-hydroxyoxolan-2-o	102.090	1.000	4.700	-0.877	694.301	333.489
2-methyl-5-propan-2	166.219	2.000	1.500	1.920	1421.351	723.439
pentyl 3-methylbuta	172.267	0.000	2.000	3.122	3704.874	2037.637
5,6,7-trimethoxy-2-(342.348	0.000	5.500	3.388	3870.696	2136.390
pentadecan-2-ol	228.417	1.000	1.700	4.916	3923.048	2167.639
methyl 8-methoxy-6-	355.303	0.000	5.250	2.686	836.193	407.730
14-methoxy-3,5-diox	293.278	1.000	4.750	2.216	1286.967	649.799
3-methyl-2-propan-2	144.213	1.000	2.000	2.506	522.873	312.181
(6,7-dimethoxyisoqu	353.374	0.000	6.000	3.489	3139.378	1703.645
1-methoxy-9H-carba	225.246	1.000	2.750	2.385	1059.820	526.772
3,3,5-trimethyl-11H-	263.338	1.000	0.750	4.809	6680.241	3853.476
3-methoxy-6-methyl	211.263	1.000	0.750	3.575	5702.427	3247.589
decyl 3-(aziridin-1-yl)	255.400	0.000	2.000	5.183	2238.867	1182.195
4-[(4-methoxypheny	227.262	1.000	2.500	3.245	2549.909	1360.677
4-(aminomethyl)phe	123.154	3.000	1.750	0.090	189.579	90.700
8-methoxy-3,3,5-trin	293.365	1.000	1.500	4.916	6670.470	3847.384
5,7,18,20-tetraoxa-2	317.300	0.000	4.000	3.200	7524.079	4382.201
ethyl 1-methylpiperi	171.239	0.000	4.000	1.064	944.433	514.509
7,8-dimethoxy-11-m	369.416	0.000	7.000	2.236	1185.244	657.669
4-methoxy-9-(3-metl	300.310	0.000	4.500	3.116	2483.560	1322.449
10H-indolo[3,2-b]qui	218.257	1.000	1.000	3.598	4259.107	2369.021
(2S,3S)-2-amino-3-hy	119.120	3.000	3.700	-3.351	10.910	5.270
(1S,2S,4S,5'R,6R,7S,8	414.627	1.000	3.200	6.445	3380.828	1845.701
(2S)-3-acetyloxy-2-ar	147.130	3.000	5.000	-2.755	6.010	2.766

(1R,2S,4S,5'R,6R,7S,ε 416.643	1.000	3.200	6.170	3392.841	1852.791
(1R,3aS,5aR,5bR,7aR 440.708	1.000	3.700	6.005	1722.088	890.221
2-hydroxy-3-methyl 118.132	2.000	3.700	-0.054	139.034	74.577
4,10,11,11-tetramethyl 204.355	0.000	0.000	6.519	9906.038	5899.293
(2-hexadecanoyloxy- 568.919	1.000	5.700	10.826	618.730	294.433
N-(1-hydroxy-3-phen 255.316	2.000	4.200	3.018	2195.841	1157.658
methyl 2-[6-(furan-3- 466.530	0.000	9.200	2.264	708.714	340.978
4-[6-(4-hydroxy-3,5- 418.443	2.000	7.900	2.846	971.315	479.389
N-(2,3-dihydroxy-1,1 371.389	3.000	7.500	1.107	99.313	67.207
N-(5,19-dimethoxy-6 383.400	1.000	7.500	1.973	723.714	583.636
3,3,6-trimethylhepta 154.252	1.000	1.700	2.558	4349.047	2423.140
(6S,7aR)-6-hydroxy-4 196.246	1.000	4.700	0.939	1079.248	537.218
[3-hydroxy-4,5-bis(h) 388.416	4.000	7.150	1.824	55.810	21.862
9-(1,3-benzodioxol-5 380.353	1.000	6.750	2.572	1346.503	682.351
(3aS,6aR,9aR,9bS)-6- 230.306	0.000	3.000	2.825	2419.156	1285.421
2-bicyclo[2.2.1]hepta 154.208	0.000	2.000	2.008	3644.052	2001.504
(3R,4R,4aS,6aS,6a 428.740	1.000	1.700	7.035	4013.672	2221.812
2,5-dimethoxycyclo 168.149	0.000	5.500	-0.334	1123.974	561.321
2,3,3-trimethylbicycl 154.252	1.000	0.750	2.699	5378.405	3048.596
(1R,2S,5S,6S,9R,12S, 328.540	2.000	3.000	3.634	235.958	127.121
(1S,3R,6S,7S,8S,11S, 426.724	1.000	1.700	7.546	3976.618	2199.650
1,1,4,7-tetramethyl- 222.370	1.000	0.750	3.994	5359.387	3036.946
(1S,3R,6S,8R,11S,12S 440.751	1.000	1.700	7.971	4379.586	2441.536
(2S,3S,4R,5R)-2,5-bis 372.460	0.000	4.700	4.004	9906.038	5899.293
(3S,4aR,6aR,6bS,8aS, 442.724	2.000	3.400	6.018	1787.572	926.866
(3R)-3,7-dimethyloct 156.267	1.000	1.700	2.710	3436.802	1878.753
(2S,3R,4S,5S)-2-methyl 164.158	3.000	8.500	-1.185	602.384	286.035
6-methyl-2-(oxiran-2 170.251	0.000	1.750	2.740	4804.329	2698.449
6,6-dimethyl-2-methyl 152.236	1.000	1.700	2.107	4083.989	2263.915
2,6-dimethyloct-7-er 154.252	0.000	2.000	2.749	5512.837	3131.041
methyl 2-(3-oxo-2-p 226.315	0.000	4.000	2.574	1243.479	626.099
2,4-bis(1-phenylethy 302.415	1.000	0.750	5.773	4051.745	2244.601
3-(2-methylpropyl)-2 210.275	1.000	5.500	-0.108	322.529	503.236

2,3-diacetyloxybutar	234.162	2.000	8.000	-0.043	1.713	0.819
1-(propyltetrasulfan)	214.417	0.000	0.000	5.255	9906.038	10000.000
N-[5-(diethylamino)-	556.316	1.000	8.250	3.298	72.140	69.969
1-methyl-1-nitrosogl	102.096	3.000	5.000	-1.420	142.646	60.285
2-amino-2-(hydroxyl)	121.136	5.000	6.100	-1.975	43.773	18.601
(1,3,3-trimethyl-2-bi	196.289	0.000	2.000	2.909	4529.167	2531.793
methyl 8-[(1S,2R)-2-c	310.519	0.000	2.000	6.262	5645.957	3212.842
(6R)-3-methyl-6-prop	152.236	0.000	2.000	2.184	4036.740	2235.618
(2S)-2-hydroxypropa	90.079	2.000	3.700	-0.215	92.924	48.246
methyl (1S,4aS,7aS)-	388.371	5.000	15.600	-1.689	23.955	8.763
2-(3,4-dihydroxyphen	594.528	10.000	11.650	0.013	0.429	0.113
(1S,12S)-16-methoxy	314.294	1.000	4.500	2.811	4296.926	2391.766
[(2R,3R)-2-(3,4-dihyd	442.378	7.000	8.000	0.443	2.852	0.878
3-(4-hydroxyphenyl)-	416.384	5.000	12.500	-0.190	29.434	10.949
octadeca-9,11,13,15-	276.418	1.000	2.000	5.738	235.962	132.100
methyl (1S,2R,3R,4R,	540.609	0.000	10.200	3.773	717.575	345.589
ethyl 2-methylbut-2-	128.171	0.000	2.000	1.633	3036.489	1643.375
1-hydroxypropan-2-yl	118.132	1.000	3.700	0.225	982.827	485.533
2-methoxycyclohexa	128.171	0.000	3.700	0.605	3921.280	2166.583
2-(4-methylcyclohex	196.289	0.000	2.000	3.210	4086.974	2265.703
(3R,4S,5R)-3,4-dihyd	148.115	3.000	8.100	-1.894	97.073	39.767
(3S,4aR,6aS,6bS,8aR,	426.724	1.000	1.700	7.041	4329.949	2411.640
ethyl 2-hydroxy-4-m	160.213	1.000	3.700	1.420	1502.138	767.984
(2R,4aS,6aR,6aS,6bR	470.691	2.000	5.700	5.166	95.645	49.774
2-(3,4-dihydroxyphen	290.272	5.000	5.450	0.467	53.844	21.031
(2S)-7-[(2S,3R,4S,5S,	596.541	8.000	20.050	-2.171	0.834	0.233
2-(3,4-dihydroxyphen	448.382	7.000	13.000	-1.223	2.964	0.916
1-[(4-hydroxyphenyl)	271.315	4.000	3.750	1.118	53.996	23.338
6-methyl-5,6,6a,7-te	235.328	0.000	2.000	3.483	2250.112	1314.985
(2R,3S,4S,5R,6S)-2-(f	286.281	5.000	10.950	-1.064	74.634	29.931
[(2S,3R,4S,5S,6R)-2-[586.548	5.000	16.450	0.325	26.738	9.869
(3S,4aR,6aR,6aR,6bR	426.724	1.000	1.700	7.040	4368.537	2434.879
methyl 8-(2-octylcycl	308.503	0.000	2.000	6.724	2573.945	1374.546

2-[5-methyl-5-(4-me	238.369	1.000	1.500	4.160	5187.987	2932.102
[5-hydroxy-2-[(2S,3R	406.388	5.000	12.000	-0.004	42.068	16.107
bis(2-ethylhexyl) 3,4,	528.342	0.000	4.000	7.684	2081.857	10000.000
(1S,2R,4aS,6aR,6aS,6	488.706	4.000	7.100	4.173	51.025	25.238
(12R)-11-methyl-3,5-	279.338	0.000	3.500	2.998	2252.547	1316.523
(3S,4R,4aS,6aS,6aS,6	428.740	1.000	1.700	7.075	4874.579	2741.123
(2R,3R)-2-(3,4-dihydr	450.398	6.000	13.250	-0.972	5.110	1.650
(6aR,11aR)-10-(3-me	324.376	2.000	3.000	3.867	1204.723	605.034
3-(2,4-dihydroxyphei	356.374	3.000	4.750	2.593	92.649	37.812
9-(1,3-benzodioxol-5	542.495	4.000	15.250	0.452	122.433	51.106
8-methoxynaphtho[2	296.279	1.000	4.250	3.050	304.395	173.958
3,5-dihydroxy-6-met	144.127	2.000	5.200	-0.576	435.919	201.647
2-ethyl-4-(2,2,3-trim	208.343	1.000	1.700	3.590	3353.005	1829.288
(4aR,5R,9aS)-2,5,9,9-	222.370	1.000	0.750	3.962	5502.801	3124.881
6,6-dimethyl-2-meth	150.220	0.000	2.000	1.975	3760.983	2071.012
(2S,3S,4S,5R,6R)-6-[[943.133	10.000	28.200	-0.040	0.232	0.074
(1R,4S)-1-methyl-4-p	154.252	1.000	0.750	2.940	3938.954	2177.140
2,6,6,8-tetramethyl-	220.354	0.000	2.000	2.471	9906.038	5899.293
1,3,8-trihydroxy-6-m	256.257	1.000	2.250	2.322	209.418	91.295
(2R,4aS,6aR,6aS,14a'	450.617	2.000	4.750	5.064	70.620	35.861
(2R,3R)-2-(3,4-dihydr	578.528	10.000	10.900	0.610	4.276	1.361
(2R,3R)-3,5,7-trihydr	288.256	3.000	5.700	0.727	59.228	23.313
7-(2,4-dihydroxyphei	384.385	3.000	7.200	2.021	128.404	53.806
1,3,5-tris(trifluorome	282.108	0.000	0.000	5.189	9906.038	10000.000
1-chloro-2-isothiocy	169.628	0.000	2.500	2.299	7489.865	10000.000
1,3-dihydroxypropan	330.507	2.000	5.400	4.438	460.127	213.777
2-pyrrolidin-2-ylaceti	129.158	1.000	2.500	-1.333	38.528	20.609
[(2S,3R,4S,5S,6R)-3,4	332.263	7.000	12.750	-2.506	4.052	1.284
(1R,5R,6R,13S,21R)-E	576.512	9.000	10.900	0.302	1.581	0.464
4-[(3R)-8,8-dimethyl-	324.376	2.000	3.000	3.982	1140.665	570.336
methyl 6-hydroxy-2,;	284.311	0.000	2.500	3.870	1612.925	829.385
(3S,7S,8S,9S,10R,13R	416.686	2.000	3.400	6.202	1541.864	789.961
(2R,3R,4S,5R)-oxane-	150.131	4.000	8.500	-1.757	172.569	74.062

(E)-2-methylbut-2-er 100.117	1.000	2.000	0.942	251.215	141.354
6,7-dihydroxy-2-(4-h 664.659	9.000	21.050	-0.694	6.412	2.108
(3S,3aS,7aR)-3,6-dim 152.236	0.000	1.700	1.971	9906.038	5899.293
[(1R,4bR,5R,6aR,10a 526.625	1.000	9.950	3.479	265.090	117.789
2-(6-aminopurin-9-yl 379.285	5.000	11.900	-0.714	0.242	0.099
2-[4-[(2S,3R,4R,5R,6 279.292	3.000	9.050	0.009	138.972	58.608
(6aS,11aS)-6,11a-dih 272.257	3.000	3.750	1.662	394.597	181.067
4-[2,13-dihydroxy-13 622.924	3.000	11.500	6.503	455.548	211.478
2-(3,4-dihydroxyphe 578.528	10.000	10.900	0.610	4.276	1.361
4-[3-(1,3-benzodiox 356.374	1.000	6.400	2.784	3040.737	1645.860
(4R)-2,6,6-trimethyl- 330.377	4.000	12.200	-0.607	97.647	40.021
4-[[[(3R,4R,5S)-5-(4-h 390.432	3.000	7.150	2.768	401.185	184.337
4-[9-[5-[1,4-dihydrox 638.924	4.000	13.200	6.182	789.484	383.169
(6aS)-2,10-dimethox 327.379	2.000	5.000	2.462	353.591	177.915
1-[2,4-dihydroxy-3-[(436.415	6.000	12.450	-0.500	5.801	1.892
2,6-dihydroxy-2-[(4- 302.283	3.000	5.750	1.357	163.324	69.783
(3R,4S,5R)-oxane-2,3 150.131	4.000	8.500	-1.757	172.569	74.062
2,6,6-trimethylcyclo 150.220	0.000	2.000	2.085	4389.913	2447.760
2,3,5,6-tetramethylb 166.219	2.000	1.500	1.858	2071.495	1086.965
2-hydroxy-2-methylc 134.088	1.000	2.750	0.583	5.463	2.869
2-methyl-1,3-dioxan 102.133	0.000	3.400	-0.185	9906.038	5899.293
[dimethyl(phenyl)sily 270.521	0.000	0.000	6.595	9906.038	5899.293
5-methyl-1,3-thiazol 99.150	0.000	1.500	0.934	5159.767	5477.653
1-hexylcyclopentene 152.279	0.000	0.000	5.144	9906.038	5899.293
bicyclo[3.2.0]hept-6- 94.156	0.000	0.000	2.517	9906.038	5899.293
3,7,11-trimethyldode 228.417	1.000	1.700	4.595	2866.228	1544.005
7-methyloct-3-yne 124.225	0.000	0.000	4.546	9906.038	5899.293
3,7,11,15-tetrameth 296.535	1.000	1.700	6.304	2861.605	1541.314
2-(3,4-dimethoxyphe 372.374	0.000	6.250	3.474	3871.737	2137.010
3-methylbut-2-ene-1 102.194	0.800	0.500	2.612	9906.038	10000.000
5-hydroxy-6-(1-hydr 374.349	0.000	7.500	1.410	50.056	19.436
(2R,3S)-2-(3,4-dihydr 578.528	10.000	10.900	0.547	1.594	0.468
(2R,3R)-2-(3,4-dihydr 578.528	10.000	10.900	0.243	1.114	0.318

6-methyl-7,8-dihydro	205.213	0.000	4.500	1.081	3759.211	2069.958
4-[(3,3-dimethoxyir	286.284	0.000	5.750	1.891	2055.788	1078.059
(12R)-3,5-dioxa-11-a	265.311	1.000	3.000	2.991	1523.713	862.832
8-(2-hydroxypropan-	244.246	1.000	3.750	2.186	941.298	463.396
4-[[[(1R)-6,7-dimetho	610.749	2.000	8.250	5.941	73.031	35.785
(6aR)-1-methoxy-5,6	267.327	2.000	3.000	2.478	564.548	295.018
(3S,4R,4aS)-4-etheny	358.344	4.000	14.900	-1.591	67.219	26.730
(3S,8S,9S,10R,13S,14	397.643	2.000	2.700	5.988	2693.588	1443.733
(2S)-5,6-dihydroxy-2,	195.174	4.000	4.500	-2.384	4.562	2.053
methyl (1S,15S,16S,2	412.485	1.000	7.200	3.401	567.772	296.839
(4aR,5R,6aR,6aS,6bR	504.706	4.000	7.800	3.951	38.653	18.694
4-(diaminomethylide	311.337	5.000	6.250	0.970	35.963	13.596
(4R,4aS,6R)-4,4a-dir	204.355	0.000	0.000	4.785	9906.038	5899.293
(3aS,5aR,9bR)-5a,9-c	232.322	0.000	3.000	2.737	3053.045	1653.063
(4aS,6aR,6bR,8aR,10	498.745	1.000	4.000	7.192	274.912	155.820
(1S,2R,6S,7R,9R,11S,	470.605	2.000	9.450	3.053	351.308	159.695
(2S,3R,4S,5S,6R)-2-[(1035.185	12.000	35.500	-2.399	0.614	0.167
4-(2-aminoethyl)cycl	151.165	2.000	5.000	-0.836	46.688	19.943
6,7-dihydroxy-1-met	223.228	4.000	5.000	-1.876	6.253	2.887
(2,7,7-trimethyl-6-bi	194.273	0.000	2.000	2.961	3878.563	2141.083
methyl (1S,4aS,5R,7S	448.423	5.000	17.600	-1.771	20.611	7.449
(6aR,11aR)-6a,11a-di	256.257	2.000	3.000	2.336	908.414	445.923
methyl (1S,15R,16S,2	382.458	1.000	6.450	3.275	620.311	326.637
(1S,2S,4S,5R)-6-metf	194.184	5.000	10.200	-1.860	129.087	54.115
2-hydroxy-3-methylp	132.159	2.000	3.700	0.545	138.569	74.307
(2S)-1-[(2S)-piperidin	143.228	2.000	3.200	0.715	658.885	348.646
1-[3-methoxy-4-[(2S,	328.318	4.000	12.000	-0.796	74.597	29.915
(12R)-3,5-dioxa-11-a	281.310	2.000	3.750	1.999	461.230	237.118
15-methylhexadecar	270.454	1.000	2.000	5.603	236.347	132.333
(1S,3R,4R,5R)-1,3,4-t	338.313	5.000	8.900	0.373	4.354	1.765
(2S,3R,11bS)-3-ethyl	459.630	2.000	5.000	5.297	324.504	179.389
(1R,4aR,7R,8aR)-7-(2	240.385	2.000	1.500	3.358	2335.219	1237.282
(1S)-1-[[[(2S,3R,11bS)	475.630	3.000	5.750	4.614	100.974	50.790

(1aR,7R,7aR,7bS)-1,1	218.338	0.000	2.000	3.178	3204.845	1742.078
(1R,2R,9R,17S)-7,13-	248.367	0.000	5.000	0.965	495.069	484.899
(2-acetyloxy-4-prop-	234.251	0.000	5.000	1.968	1557.263	798.492
[(1R,2S,5S,8R)-7,7-di	220.354	1.000	1.700	3.226	3282.868	1787.964
2-hydroxy-6-pentadec	348.525	1.000	1.750	6.888	132.878	71.014
5-(furan-3-yl)-12-hyd	374.390	1.000	9.250	0.941	570.685	269.801
(1S,2S,5S,8R)-2,6-din	234.338	1.000	1.500	3.703	4305.832	2397.125
3,5-dimethyl-3-(4-met	331.457	1.000	0.750	6.412	6676.346	3851.047
(3aR,9R,9aR,9bS)-1,1	250.337	0.000	4.450	1.834	1719.208	888.612
7,8,9,12,13,14,25,26	934.641	16.000	23.950	-4.673	0.001	0.000
(3R,4R,4aR,6aR,6bS,6	456.707	1.000	2.700	6.847	292.000	166.314
(2S,3R,4R,5R,6S)-2-[(868.069	9.000	25.550	0.433	2.766	0.940
methyl carbamimida	74.082	3.000	1.500	-0.734	370.038	168.918
(1R,2S,5R)-5-methyl-	154.252	1.000	1.700	2.740	4132.474	2292.980
(4aR,7S,8aS)-4a,8a-d	222.370	0.000	2.000	3.512	4376.413	2439.625
5-[(3aS,4S,6aR)-2-oxi	244.308	3.000	4.500	1.284	23.201	16.494
bis[[4-[(2S,3R,4S,5S,6	726.727	8.000	22.250	-0.821	2.493	0.759
(3S,8S,9S,10R,13R,14	400.687	1.000	1.700	7.298	3381.406	1846.042
[(2S)-2-benzamido-3-	506.600	1.250	6.250	7.134	1547.165	792.897
[(1S,5R)-8-methyl-8-	289.374	0.000	4.700	1.872	485.007	250.357
[(3aR,4S,9aS,9bR)-9-	410.423	2.000	9.450	1.663	59.020	23.224
(2S,3S,4S,5R,6R)-6-[[632.833	4.000	11.500	4.693	1.848	0.889
methyl (2R,3S,4R)-4-	684.906	3.000	12.550	5.646	814.111	396.105
1-methyl-4-prop-1-e	134.221	0.000	0.000	4.025	9906.038	5899.293
10-(1,3-benzodioxol-	348.311	0.000	6.000	2.154	2137.574	1124.491
(4aR,5S)-4a,5-dimet	218.338	0.000	2.000	3.412	4038.355	2236.584
(1R,2R,8S)-1,5-dimet	396.480	4.000	11.250	0.732	96.884	39.683
4-methyl-1,2,4-triazc	115.091	2.000	4.000	-1.070	157.198	66.958
2-methyl-5-pentadec	334.541	2.000	1.500	6.564	1374.083	697.470
[(3S,4aR,6aS,6bS,8aF	468.762	0.000	2.000	7.954	3936.585	2175.725
(6aS)-2,10,11-trimet	327.379	2.000	4.500	2.905	887.471	481.050
(2R)-2-[(1S)-1-hydro	452.589	2.000	6.500	4.490	826.861	402.814
(1R,2R,7S,10R,13R,14	470.518	0.000	11.250	1.064	423.763	195.575

2-methyl-4-[2,8,13-trimethyl-5,6,7,8-tetrahydro-1H-benzodiazepin-2-ylidene]-1H-imidazole	4.000	11.500	6.634	157.989	67.322
3-[[2-(2S,3S)-2-(1,3-benzodiazepin-2-ylidene)-1H-imidazol-5-yl]ethyl]-1H-imidazole	1.000	4.700	3.850	3299.668	1797.856
3,13,13,17-tetramethyl-1H-imidazo[1,2-a]pyridine	1.000	2.450	4.960	4503.111	2516.053
5-(furan-3-yl)-3,11-dimethyl-1H-imidazo[1,2-a]pyridine	4.000	17.750	-0.688	101.267	41.627
(5S)-3,4,5-trimethyl-1H-imidazo[1,2-a]pyridine	1.000	1.250	3.396	3547.107	1944.012
(6aR)-9-[4-[[[(1S)-6,7-dimethyl-1H-imidazo[1,2-a]pyridin-5-yl]methyl]amino]phenyl]-1H-imidazo[1,2-a]pyridine	1.000	8.250	6.606	169.787	89.069
5-methoxypyrrrolidine	1.000	4.200	-0.768	575.572	694.220
octa-3,5-dien-2-one	0.000	2.000	1.860	3112.386	1687.818
4-[[3-(3S,3aR,6S,6aR)-3,4,4a,8a-tetrahydro-1H-isoindolo[1,2-b]pyridin-1-yl]methyl]piperidine	2.000	7.150	3.063	953.717	470.008
(1S,4S,4aR,8aS)-1-methyl-1,2,3,4-tetrahydro-1H-isoindolo[1,2-b]pyridine	2.000	1.500	3.550	4040.617	2237.939
(7R,8R,9S)-9-(3,4-dihydroquinolin-2-yl)-1,2,3,4-tetrahydro-1H-isoindolo[1,2-b]pyridine	0.000	7.150	3.140	9906.038	5899.293
(2S,3S)-2-(3,4-dihydroquinolin-2-yl)-1,2,3,4-tetrahydro-1H-isoindolo[1,2-b]pyridine	5.000	5.450	0.470	53.974	21.086
(3aR,4aR,8aR,9aR)-5,6,7,8-tetrahydro-1H-isoindolo[1,2-b]pyridine	0.000	3.000	2.760	2821.282	1517.852
(5R,6S,7S)-5-(3,4-dihydroquinolin-2-yl)-1,2,3,4-tetrahydro-1H-isoindolo[1,2-b]pyridine	0.000	7.150	2.728	9906.038	5899.293
(2S,4R,4aS,6R)-4,4a-dimethyl-1,2,3,4-tetrahydro-1H-isoindolo[1,2-b]pyridine	1.000	1.700	3.512	3309.486	1803.639
5-hydroxy-3-(8-hydroxy-2,3-dihydroquinolin-2-yl)-1,2,3,4-tetrahydro-1H-isoindolo[1,2-b]pyridine	0.000	7.500	1.605	137.310	57.851
methyl 1-(1R,15S,17R,18R)-1,2,3,4-tetrahydro-1H-isoindolo[1,2-b]pyridin-5-ylidene-1H-imidazole	1.000	10.700	5.831	634.872	334.932
(6R,11S,12S,15R,16R)-1,2,3,4-tetrahydro-1H-isoindolo[1,2-b]pyridine	1.000	1.700	7.840	4381.819	2442.882
4-[2-hydroxy-3-(4-hydroxyphenyl)propanoate]	3.000	3.200	2.293	477.429	222.479
11-ethyl-4,6,16,18-tetraazabicyclo[3.3.1]nonane	2.000	12.000	2.322	816.170	439.415
2-phenylquinoline-4-carboxamide	2.000	3.500	2.528	911.794	447.717
2,3-dihydroxypropanoate	3.000	4.900	-2.113	49.212	43.089
5-(6-hydroxy-1-benzimidazol-2-yl)-1,2,3,4-tetrahydro-1H-isoindolo[1,2-b]pyridine	3.000	2.750	1.709	277.391	123.708
3-(4-hydroxyphenyl)-1,2,3,4-tetrahydro-1H-isoindolo[1,2-b]pyridine	5.000	13.250	-0.047	31.071	11.608
(1S,2S,3S,5S,8R,11R)-1,2,3,4-tetrahydro-1H-isoindolo[1,2-b]pyridine	1.000	7.250	1.791	592.201	280.812
5-hydroxy-7,8-dimethyl-1,2,3,4-tetrahydro-1H-isoindolo[1,2-b]pyridine	0.000	3.750	3.088	1250.518	629.931
5-hydroxy-2-(4-hydroxyphenyl)-1,2,3,4-tetrahydro-1H-isoindolo[1,2-b]pyridine	1.000	4.500	2.664	456.153	211.782
(2S)-2-[[[(2S)-2-amino-1,2,3,4-tetrahydro-1H-isoindolo[1,2-b]pyridin-5-yl]methyl]amino]phenyl]-1,2,3,4-tetrahydro-1H-isoindolo[1,2-b]pyridine	4.250	6.250	-1.848	7.905	5.111
1,2,13-trimethoxy-1,2,3,4-tetrahydro-1H-isoindolo[1,2-b]pyridine	0.000	5.700	2.745	9906.038	5899.293
(4bS,8aR)-3,4b,8,8-tetrahydro-1H-isoindolo[1,2-b]pyridine	1.000	6.000	2.306	51.200	25.331
(4bS,8aR)-2,4b,8,8-tetrahydro-1H-isoindolo[1,2-b]pyridine	1.000	6.000	2.309	47.325	23.266
(4bS,8aS)-3,4b,8,8-tetrahydro-1H-isoindolo[1,2-b]pyridine	1.000	4.000	3.315	122.606	65.099
(2S,3R,4S,5R)-2-[3-hydroxyphenyl]-1,2,3,4-tetrahydro-1H-isoindolo[1,2-b]pyridine	5.000	11.250	1.253	66.911	26.598

[1-(3,4,5,11,17,18,19	634.460	10.000	17.150	-2.722	0.043	0.009
(12R)-17-methoxy-3,	295.337	1.000	3.750	2.847	1522.097	861.843
2,3-diacetyloxypropy	414.581	0.000	6.000	6.063	325.784	147.192
(6aR)-9-[4-[[[(1S)-6,7-	608.733	2.000	8.250	5.960	87.549	43.532
(3R,4aS,5R,8aR)-5,8a	208.386	0.000	0.000	7.104	9906.038	5899.293
(2R,4R,8S)-4-methox	247.293	0.000	6.700	0.401	559.959	292.426
(3S,8S,9S,10R,13R,14	398.671	1.000	1.700	7.205	3383.813	1847.463
2-methyl-6-(4-methy	218.338	0.000	2.000	4.068	5362.475	3038.838
1-(2,4-dihydroxyphei	562.575	5.000	5.750	4.840	62.397	24.664
1,8-dihydroxy-3-met	416.384	3.000	11.050	0.157	16.435	5.832
(2S)-2-[4-hydroxy-3-	390.478	1.000	4.250	5.265	1399.568	711.463
(2S,3R,4R,5R,6S)-2-[(1049.211	12.000	35.500	-1.923	0.958	0.270
methyl 11-acetyloxy-	808.970	2.000	14.750	4.793	12.423	5.836
[(2S,3R)-5,7-dihydro	458.378	8.000	8.750	-0.217	1.118	0.319
(4R)-10,11-dimethox	311.380	0.000	5.500	2.275	660.607	349.631
methyl (1S,15R,16R,	412.485	1.000	7.200	3.458	610.428	321.015
(3S,8S,9S,10R,13R,14	414.713	1.000	1.700	7.622	3381.651	1846.187
dodecyl 2-chloroacet	262.819	0.000	2.000	5.269	2919.557	3887.547
(8S,9S,10R,11R,13S,13	62.465	3.000	8.150	1.603	133.936	56.316
2,2,5,5-tetramethylh	158.283	1.000	1.700	2.763	6048.590	3461.191
(1R,4S)-1,7,7-trimeth	152.236	0.000	2.000	1.943	3958.370	2188.741
ethyl 3,4,5-trimetho	240.255	0.000	4.250	2.404	2919.862	1575.258
2-(4-methylpiperazin	144.216	1.000	5.700	-0.748	137.785	71.070
2-(2-chloroethylsulfa	322.933	0.000	2.500	6.326	2891.472	5433.983
3,6-bis(3,4-dimethox	402.443	1.000	7.150	3.954	5337.420	3023.494
5-(hydroxymethyl)fu	126.112	1.000	4.200	-0.174	480.822	224.188
2,2,4,9,11,11-hexam	254.498	0.000	0.000	9.702	9906.038	5899.293
methyl (1R,9R,10S,11	810.986	2.000	12.250	6.112	11.030	5.132
nonacosan-1-ol	424.792	1.000	1.700	10.289	3296.921	1796.238
4,4a,6a,6b,8a,11,11,	426.724	0.000	2.000	6.995	3827.045	2110.360
N-[(10S,12R,16S)-3,4	399.443	1.000	7.500	2.708	923.434	916.547
[(1S,2R,3R,4R,5R,6S,	645.745	3.000	16.950	1.884	106.365	48.564
(1R,2S,6R,7S,10S,11F	343.508	1.000	5.400	3.117	1179.459	654.200

octan-3-one	128.214	0.000	2.000	2.091	3698.321	2033.741
(3S,5R,10S,13R,14R,15S)-	426.724	1.000	1.700	7.721	4345.380	2420.932
benzyl (E)-2-methyl-2-oxo-	190.241	0.000	2.000	3.208	3515.372	1925.220
[3,5-dihydroxy-4,6-bis(methyl)-	636.476	11.000	17.850	-2.616	0.091	0.021
methyl (1R,15S,16S,17R)-	382.458	1.000	6.450	3.347	679.288	360.330
methyl (1R,15S,17R)-	564.634	2.000	9.950	4.480	258.052	126.577
methyl (1R,15S,17R)-	564.634	1.000	8.950	4.619	239.492	116.766
methyl (1S,15S,16S,17R)-	382.458	1.000	6.450	3.265	565.964	295.818
(1R,16R)-10,25-dimethyl-	594.706	2.000	8.000	5.057	136.665	70.446
(1R,3aR,5aR,5bR,7aR)-	426.724	1.000	1.700	7.087	4367.727	2434.391
methyl (1R,9R,10S,11R)-	456.538	1.000	8.500	2.719	123.851	63.335
(1S,4R,5R)-4-methyl-2-(methyl-	152.236	0.000	2.000	2.142	3432.402	1876.153
(3R)-6,7-dimethoxy-2-(methyl-	413.426	0.000	8.750	2.024	1151.775	637.618
(1S,2R,6S,7R,9R,11S)-	470.605	1.000	9.400	3.022	215.677	94.248
methyl 4-amino-1H-imidazo-	141.129	1.000	2.000	0.941	247.956	109.582
14-oxa-7-azatetracyclo-	217.267	0.000	5.000	0.689	582.144	304.969
2,16-dihydroxy-4,4,9-trimethyl-	532.673	4.000	10.650	2.613	53.826	21.023
10,11-dimethoxy-6-cyclo-	410.469	0.000	9.200	1.519	1761.079	912.027
8,9-dimethoxy-3,3,5-trimethyl-	323.391	1.000	2.250	5.069	6691.877	3860.732
4,4,10,13-tetramethyl-	414.713	1.000	1.700	7.624	4805.591	2699.216
1-hydroxypyrimidin-2(1H)-	111.103	2.000	2.500	-0.233	554.446	261.512
1-benzhydrylimidazole-	234.300	0.000	2.000	4.094	4984.272	2807.856
phenanthrene-1-carboxylic acid	222.243	1.000	2.000	3.192	303.426	173.360
6,8a-dimethyl-3-propyl-	222.370	1.000	0.750	4.012	5883.897	3359.439
3,4,10,11-tetramethyl-	385.459	0.000	7.000	3.165	1258.343	701.618
[2-[(1S,2S,4R,8S,9S,10S)-	569.066	1.000	9.950	4.301	203.641	248.513
2-(6,10-dimethylspiro)-	222.370	1.000	0.750	4.095	5826.169	3323.828
tetramethyl pyrazine	312.235	0.000	10.000	-0.587	64.724	25.660
3-ethyl-5-(2-ethylbutyl)-	366.713	0.000	0.000	14.278	9906.038	5899.293
methyl 20-ethyl-15-hydroxy-	398.458	1.000	7.200	2.623	393.519	199.727
(1S,2R,7S,9R,11R,12R)-	486.604	3.000	9.250	3.229	764.613	370.139
[6-(4-acetamido-3-methyl)-	499.732	1.000	6.200	5.905	669.800	592.673
(3S,8S,9S,10R,13S,14S)-	317.514	3.000	2.700	3.455	364.760	183.997

3a,5a,5b,8,8,11a-hex	424.709	0.000	2.000	7.079	4220.775	2345.983
(3,4,5,11,13,21,22,23)	634.460	11.000	17.850	-3.113	0.032	0.007
2,6,6,14,17-pentame	326.435	0.000	5.000	2.917	998.724	494.027
(1R,5R)-2-methyl-5- ϵ	152.236	1.000	1.700	2.329	3963.280	2191.676
(2S)-2-(2-hydroxypro	246.262	1.000	4.000	2.115	965.547	476.312
5,11,17,23-tetratert-	648.924	4.000	3.000	9.661	4573.259	2558.444
(6aR,11aR)-9-metho	270.284	1.000	3.000	3.117	2998.179	1620.976
[(1R,7S,8R)-7-methyl	275.347	0.000	4.750	2.514	1083.619	596.935
3-chloro-5-hydroxy-2	222.627	0.000	3.750	1.275	568.026	553.583
10-methoxy-2,2-dim	258.273	0.000	4.000	2.540	2176.694	1146.750
3-[3-(3,4-dihydroxyp	354.313	6.000	9.650	-0.129	2.505	0.971
(2S)-2-methyl-4-[(2R,	596.886	4.000	11.500	6.315	230.490	101.263
5-ethenyl-3,4-dihydr	175.187	0.000	4.500	0.561	1444.259	736.050
4-[(2S,3S)-3-[(3,4-din	418.529	0.000	6.400	4.054	9906.038	5899.293
5-methyl-2-[(2R)-6-n	218.338	1.000	0.750	4.320	4068.712	2254.763
1,3,8-trihydroxy-6-(h	286.240	2.000	5.950	0.247	23.482	8.577
(1R,14S)-20,25-dime	594.706	2.000	8.000	4.788	88.929	44.274
5-(1,3-benzodioxol-5	348.311	0.000	6.000	2.011	2139.381	1125.518
5-[6-hydroxy-4-[6-hy	680.709	7.000	6.750	4.907	6.497	2.139
20,21,25-trimethoxy	608.733	1.000	8.000	5.377	217.028	116.135
3,13,13,17-tetrametl	331.457	0.000	0.750	6.103	7351.960	4273.948
13,16-dimethyl-19-p	331.457	1.000	0.750	6.082	8270.571	4853.972
3,8-dimethyl-3-(4-m ϵ	347.456	2.000	1.500	5.874	2507.732	1336.367
3,5-dimethyl-3-(4-m ϵ	347.456	2.000	1.500	5.500	2034.514	1066.006
(1-methoxy-9H-carb	227.262	2.000	2.450	2.653	1729.921	894.599
3-methyl-6-propan-2	150.220	0.000	2.000	2.139	4041.973	2238.751
2-(3,4-dimethoxyphe	402.400	0.000	7.000	3.576	5347.642	3029.754
4b,8b-dimethyl-3,7-c	328.407	0.000	8.000	1.616	756.791	366.048
2-(2,4-dihydroxyphe	354.359	3.000	4.500	2.741	113.153	46.933
1-methyl-4-(6-methy	204.355	0.000	0.000	6.466	9906.038	5899.293
ethyl (E)-but-2-enoat	114.144	0.000	2.000	1.326	2541.156	1355.629
4-[2-(diethylamino)e	301.341	0.000	5.750	2.001	512.725	265.858
(3S,4R,5S)-2-(hydrox	180.157	5.000	8.300	-1.694	105.181	43.369

(3R,4S,5S)-oxane-2,3	150.131	4.000	8.500	-1.728	188.298	81.385
(2S,3R,4S,5R)-3,4,5,6	194.141	4.000	9.500	-1.862	5.837	2.423
3,7,11-trimethyldodecane	224.386	1.000	1.700	4.326	2866.315	1544.056
(2S)-2-(3-aminopropyl)propane	226.235	3.250	5.250	-2.424	2.264	1.506
(2S,3R,4S,5R,6R)-2-[[2,3-dihydroxybutyl]oxy]propane	504.441	11.000	25.300	-4.909	1.545	0.453
(4S)-1-methyl-4-propylpiperidine	136.236	0.000	0.000	3.998	9906.038	5899.293
4-[[1R]-2-amino-1-hydroxypropan-2-yl]piperidine	169.180	5.000	4.200	-1.048	27.711	11.348
[(2R,3S,4S,5R,6S)-3,4-dihydroxybutyl]oxypropane	260.137	6.000	13.500	-2.404	0.356	0.160
(2R,3R,4S,5R,6S)-2-[[2,3-dihydroxybutyl]oxy]propane	504.441	11.000	27.200	-5.647	1.192	0.342
3-[[1R,3S,5S,8R,9S,11R]-2,3,5-trimethylheptane-2,3,5-triylidene]propane	584.659	8.000	18.100	-1.983	12.333	4.276
(5S,8S,9S,10S,13R,14R)-1,2,3,4,5,6,7,8,9,10,11,12,13,14-trimethylpentadecane	288.515	0.000	0.000	8.909	9906.038	5899.293
6-methoxy-7-[[2S,3R]-2-(3,4-dihydroxybutyl)oxy]propane	354.313	4.000	12.500	-0.926	50.607	19.668
(2R,3R)-2-(3,4-dihydroxybutyl)oxypropane	304.256	4.000	6.450	0.080	21.125	7.650
(5R)-2-methyl-5-propylpiperidine	150.220	0.000	2.000	2.161	3565.782	1955.077
(1S)-1-[(3-hydroxy-4-methylbutyl)oxy]propane	329.395	2.000	5.000	2.664	261.622	128.471
(13aS)-3,10-dimethylundecane	327.379	2.000	5.000	2.497	292.739	145.064
(1S,2S,4R)-1,3,3-trimethylbutane	154.252	1.000	1.700	2.200	4786.972	2687.914
(1S,6S)-2,7,7-trimethylundecane	152.236	0.000	2.000	1.405	9906.038	5899.293
(2S,3S)-butane-2,3-dithiolane	90.122	2.000	3.400	-0.704	1654.273	852.391
(2S,4S)-4-hydroxypiperidine	131.131	3.000	5.200	-2.895	12.787	6.256
(1S,2S,4R,5S)-6-methylpiperidine	194.184	5.000	10.200	-1.874	119.112	49.610
2-(4-hydroxyphenyl)propane	136.150	1.000	2.750	1.434	597.177	283.364
[(2R,3S,4S,5R,6S)-3,4-dihydroxybutyl]oxypropane	484.370	9.000	15.300	-2.721	0.185	0.046
(1S)-1-[(4-hydroxyphenyl)oxy]propane	299.369	2.000	4.250	2.501	234.066	113.909
(5R)-5-[(1S)-1,2-dihydroxyethyl]piperidine	174.110	1.000	9.400	-2.692	30.237	11.272
(2S)-2-(3,4-dihydroxybutyl)oxypropane	288.256	3.000	4.750	0.943	45.802	17.657
(2R,3S,4S)-2-(3,4-dihydroxybutyl)oxypropane	306.271	6.000	7.150	-0.365	23.569	8.611
(4aS,4bS,7S,10aS)-7-methylundecane	272.473	0.000	0.000	6.621	9906.038	5899.293
(4R)-1-methyl-4-propylpiperidine	136.236	0.000	0.000	3.998	9906.038	5899.293
1-[(2R)-1-methylpiperidin-2-yl]propane	141.213	0.000	4.000	0.483	881.027	477.276
(2R,3S,4S,5R,6S)-2-[[2,3-dihydroxybutyl]oxy]propane	272.254	5.000	10.000	-1.053	69.170	27.570
(1S,4R)-2,2-dimethylbutane	136.236	0.000	0.000	3.347	9906.038	5899.293
(1S,5S)-6,6-dimethylundecane	136.236	0.000	0.000	3.529	9906.038	5899.293

(1R)-1-[(4-hydroxyph	271.315	4.000	3.750	1.118	53.996	23.338
(1S,8aR)-4,7-dimethy	204.355	0.000	0.000	5.549	9906.038	5899.293
(3S,4R,5S,6R)-6-(hyd	180.157	5.000	10.200	-2.212	70.504	28.145
(3S,4S,5R,6R)-6-(hyd	180.157	5.000	10.200	-2.182	79.384	31.996
(S)-[(2R,4S,5R)-5-eth	324.422	1.000	5.450	3.440	623.617	328.519
(1R,2S,5S,6S,9R,12S,	356.593	0.000	4.000	4.429	537.757	309.674
(1S,2S)-2-amino-1-pt	151.208	3.000	2.700	0.483	308.228	153.377
(3S,5R)-5-[(11R)-11-t	622.924	2.000	11.800	7.369	242.853	107.147
(2R,3S,4S,5R,6S)-2-(t	295.291	5.000	9.250	-0.272	123.408	51.547
(2S)-4-[(13R)-13-[(2R	622.924	3.000	11.500	7.471	304.664	136.906
(1S,2R,4S,6R,7S,10R,	343.508	1.000	5.400	3.124	1201.503	667.426
[(1S,2R,3R,4R,5R,6S,	615.719	2.000	15.250	2.676	232.249	112.954
[(1S,2R,3R,4R,5R,6S,	675.772	3.000	17.700	1.944	108.225	49.483
[(1S,2S,3S,4S,5R,6S,	858.708	2.000	12.100	3.677	231.983	112.814
(1S,2R,3R,4S,5R,6S,	846.601	3.000	12.000	1.689	449.291	230.491
(2S)-7-hydroxy-2-[4-t	460.612	2.000	4.250	6.882	1199.549	602.225
(2S,3R,5R,9R,10R,13	494.667	6.000	10.300	2.098	53.988	21.092
(2S,3R,5R,9R,10R,13	480.640	6.000	10.300	1.904	66.871	26.581
(1R,2S,4S,5'R,6R,7S,	432.642	2.000	4.900	5.100	1299.331	656.550
(2S,3R,4R,5R,6S)-2-[(1049.211	13.000	35.500	-2.309	0.240	0.060
(2S,3R,4R,5R,6S)-2-[(1065.211	14.000	37.200	-3.134	0.178	0.044
(1S,2S,4S,5'R,6R,7S,	843.626	2.000	4.900	5.131	1736.972	898.541
(2S,3R,4R,5R,6S)-2-[(887.069	9.000	27.000	0.339	8.286	2.782
(1S,2S,4S,5'S,6R,7S,	841.627	1.000	3.200	5.948	3382.300	1846.569
(2R,3R,4S,5S,6R)-2-[[801.022	10.000	22.850	0.661	7.915	2.647
(1R,2S,4S,5S,8R,10S,	440.665	2.000	3.700	5.706	280.547	159.275
[(3S,4aR,6aR,6bS,8a	1185.334	14.000	40.000	-3.232	0.008	0.002
5,7-dihydroxy-2-met	354.313	5.000	11.500	-0.994	27.170	10.041
methyl (1S,15R,16S,	352.432	1.000	5.700	3.166	619.199	326.004
(1S,4S,5R,9S,10R,13F	336.470	3.000	4.450	3.094	116.270	61.471
(4bS,8aS)-4b,8,8-trin	286.456	1.000	0.750	5.120	4218.262	2344.474
(1S,4S,5R,6R,9S,10R,	348.438	4.000	7.850	1.478	338.922	153.618
(1S,2S,6R,10S,11R,1	364.438	5.000	7.650	1.128	46.037	17.755

(2R,3S)-2-(4-hydroxy-2-hydroxy-12-[(1R)-1	4.000	4.700	1.122	139.568	58.880
2-hydroxy-12-[(1R)-1	2.000	7.700	1.529	245.287	108.308
(2R,3R,11bS)-3-ethyl	3.000	6.750	4.074	290.135	143.669
(2S,3R,11bS)-3-ethyl	3.000	5.750	4.526	157.066	81.878
12-ethenyl-2-hydroxy	1.000	6.000	2.433	636.786	303.732
(1R,15S,16R,17S)-16-	5.000	16.400	-0.247	35.305	13.327
(2R,3R,11bS)-3-ethyl	2.000	5.950	2.578	307.802	153.148
(1S,9S)-4,5,12,13-tet	0.000	5.000	3.825	2211.316	1290.495
(1R)-1-[[[(2S,3R,11bS)	2.000	6.500	4.545	146.674	76.039
(6S)-9-methoxy-6-(2-	0.000	5.750	2.838	3635.884	1996.656
(3aR,4S,9aS,9bR)-4-h	2.000	8.400	0.101	202.944	88.248
(3S)-3-[(5R)-4-hydrox	1.000	8.750	1.712	449.715	230.726
(1R,14S)-20,21,25-tri	1.000	8.000	5.619	172.379	90.539
(2S)-6-methyl-2-[(1S)	1.000	0.750	4.583	5954.769	3403.199
(3R,3aS,8aR)-6,8a-dii	1.000	0.750	4.061	6447.677	3708.678
(6R)-5,5,9-trimethyl-	0.000	0.000	5.010	9906.038	5899.293
(1R)-1,3-dimethyl-8-	0.000	0.000	5.331	9906.038	5899.293
1-methyl-4-[(2R)-6-r	0.000	0.000	6.216	9906.038	5899.293
3,7,11-trimethyldodec	0.000	0.000	7.001	9906.038	5899.293
(3R,4aS,8aR)-8a-met	0.000	0.000	5.376	9906.038	5899.293
(3R,5S,6R)-6,10-dime	0.000	2.000	3.410	2808.417	1510.372
(1aS,4aS,8aS)-2,4a,8,	0.000	0.000	4.936	9906.038	5899.293
(4R,4aS)-4,4a-dimetf	0.000	2.000	3.315	2738.301	1469.655
(5R,6R)-6,10-dimeth	0.000	2.000	3.308	2815.780	1514.652
(2S)-2-phenyl-3,4-dif	1.000	1.500	3.561	2998.642	1621.247
methyl (1R,4aS,7aS)-	2.000	7.100	0.206	554.513	261.546
(2S)-7-[(2S,3R,4S,5S,	7.000	19.300	-1.510	3.202	0.995
(2S)-5-hydroxy-2-(4-	7.000	19.300	-1.481	3.236	1.007
(2S)-7-[(2S,3R,4S,5S,	7.000	20.050	-1.559	2.328	0.705
(2S)-7-[(2S,3R,4S,5S,	6.000	19.300	-0.768	7.037	2.331
(1R,6S)-3,7,7-trimetf	0.000	0.000	3.828	9906.038	5899.293
2,7,7-trimethylbicycl	0.000	2.000	2.001	3254.190	1771.088
(5R)-5-methyl-2-prop	0.000	2.000	2.226	4304.652	2396.415

(1S,11R,13S,14S,24R) 478.714	2.000	7.000	4.681	56.906	27.326
3-(3,4-dihydro-2H-py 146.191	1.000	2.500	1.168	869.424	470.486
5,6-dihydroxy-2-(4-h 360.320	2.000	6.000	2.020	155.245	66.059
5,7-dihydroxy-2-(4-h 594.525	10.000	20.750	-3.293	0.205	0.051
7-(2-hydroxyphenyl)- 312.278	1.000	5.500	2.398	2141.147	1126.522
2-[(4R,5S,7R,25S,26R) 954.672	13.000	26.150	-3.757	0.000	0.000
[(2R,3R)-2-(3,4-dihyd 746.634	13.000	14.200	-0.207	0.045	0.010
(2R,3R)-2-(3,4,5-trihy 610.527	12.000	12.400	-0.713	0.325	0.084
(1R,2S,19R,22R)-7,8, 784.550	13.000	20.400	-3.589	0.005	0.001
1-(2,7-dihydroxy-4-r 480.516	4.000	4.500	4.650	167.358	71.648
7-methoxy-9,10-dihy 242.274	2.000	2.250	2.622	1297.742	655.682
3-methoxy-5-[2-(3-m 258.316	1.000	2.250	3.807	3003.054	1623.825
4,5-dihydroxy-3,8-dii 218.209	2.000	5.500	0.423	319.711	144.229
4,8-dihydroxy-3-met 204.182	1.000	4.500	0.516	234.432	103.137
3-[(2S,3R,4R)-3,4-dih 402.357	3.000	10.100	0.335	20.918	7.569
4-[(3R)-8,8-dimethyl- 392.494	2.000	3.000	5.827	2627.018	1405.206
3-(4-methoxyphenyl) 430.410	4.000	12.500	0.584	99.923	41.030
(2S,3R,4S,5S,6R)-2-[4 742.727	8.000	24.900	-0.942	14.189	4.975
(5S)-3-(1,3-dihydroxy 261.274	5.000	8.350	-0.589	82.396	33.310
(1S,2R,8S)-14-oxa-7- 217.267	0.000	5.000	0.774	561.514	293.304
4-(1,3-benzodioxol-5 364.354	0.000	6.000	2.896	3187.619	1731.959
(3S)-1,2,3,9-tetrahyd 204.228	2.000	3.950	1.193	710.855	342.092
(3S)-3-hydroxy-2,3-d 202.212	1.000	5.700	0.625	858.052	419.262
(2S,3R,4R,5R,6S)-2-[(852.070	8.000	25.800	0.180	2.353	0.789
(1S,2S,4S,5'R,6R,7S,8 413.642	2.000	3.450	5.300	725.582	386.944
1,3-bis[(2R)-piperidir 224.345	0.000	3.000	2.161	175.030	92.046
(3R)-3,7-dimethyloct 154.252	1.000	0.750	3.143	5250.646	2970.398
(5S)-2-methyl-5-prop 136.236	0.000	0.000	3.912	9906.038	5899.293
(1R,2R,5S)-2-methyl- 154.252	1.000	1.700	2.617	3971.111	2196.357
(2R,5S)-2-methyl-5-p 152.236	0.000	2.000	2.231	4448.989	2483.384
(1S,4aS,7aS)-7-meth 358.344	5.000	13.900	-1.049	6.290	2.627
(1S,4aS,7aS)-7-(hydr 374.344	6.000	15.600	-1.864	2.304	0.887
(4aS,4bR,10aS)-1,1,4 272.473	0.000	0.000	6.839	9906.038	5899.293

9-[[2R)-3,3-dimethyl-2-hydroxy-4-methyl-2-[[3-[[4-hydroxyphenyl]-2-[[2-hydroxy-4-methyl-2-(1,3-benzodioxol-5-yl)-2-(2R,3R)-5,7-dihydroxy-6,8a,11aR)-9-methoxy-5,8a-c-(1R,8S,9S,16R)-8,16-dihydroxy-2-[(1R)-5,8-dihydroxy-2-(7-hydroxy-2H-chromen-1-(2,4-dihydroxyphenyl)-6aR,11aR)-1-methoxy-4bR,5R,9bR,10R)-5,1,2-dimethoxy-12-methyl-4-aminoheptanedioic acid-9-(1,3-benzodioxol-5-yl)-9-(1,3-benzodioxol-5-yl)-7,8-dimethyl-10-[[2S)-5',7,9,13-tetramethyl-8,16-bis(4-hydroxyphenyl)-2-[5-hydroxy-6-(hydr-7,7,12,16-tetramethyl-2-(2R,3R,4R,5S)-2-(hydroxy-2-(4-2-(S)-7-hydroxy-2-[4-2-hydroxy-9H-carbazole sodium;benzoate methyl 2-hydroxy-3-methyl 2-(4-hydroxy)-2-methyloctacosane 2-(4-methylcyclohexyl)-4,7-dimethylundecane	0.000 2.000 2.000 4.000 1.000 6.000 1.000 1.000 0.000 6.000 0.000 2.000 5.000 2.000 6.000 0.000 4.000 1.000 0.000 5.000 1.000 10.000 14.000 1.000 4.000 5.000 1.000 1.000 1.000 0.000 1.000 0.000	5.750 3.500 2.250 4.700 3.000 7.250 3.000 4.750 3.000 6.200 4.200 3.000 5.750 3.750 4.500 4.000 5.000 6.750 6.750 12.300 1.750 9.000 37.200 1.700 8.800 12.750 1.750 2.000 3.700 2.750 0.000 0.750 0.000	2.079 1.542 4.293 2.812 3.116 1.068 4.750 3.593 2.796 2.339 2.123 3.722 4.629 5.605 2.981 4.296 -2.256 1.924 2.838 -1.089 6.376 5.583 -2.864 7.665 0.475 -0.246 2.099 1.868 1.840 2.258 16.531 3.117 7.540	2592.437 96.384 1276.825 507.587 2998.561 6.528 2998.206 389.320 2787.282 19.938 120.574 1077.978 62.512 1701.378 18.573 9642.705 0.549 1347.670 2825.158 8.019 1978.319 0.476 0.435 4615.321 68.754 22.981 405.315 249.517 1288.719 888.190 9906.038 4580.947 9906.038	1385.223 50.190 644.267 237.707 1621.199 2.150 1620.992 178.452 1498.090 7.186 50.268 536.534 24.713 878.655 6.656 5729.972 0.265 682.990 1520.106 2.685 1144.171 0.127 0.115 2583.888 30.303 8.379 186.389 140.322 650.756 435.202 5899.293 2563.094 5899.293
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1-(furan-2-yl)-2-hydr	126.112	1.000	4.200	-0.017	1025.816	508.528
(2,6,8-trimethyl-6-tri	220.354	1.000	1.700	3.282	3801.430	2095.096
trimethylsilyl tetrade	300.556	0.000	2.000	6.483	5310.027	3006.725
2,2,4,4,6,6,8,8,10,10	741.543	0.000	2.000	14.832	9892.682	5890.697
1,3,4,5,6-pentakis(tri	541.066	0.000	6.250	7.829	6671.085	3847.768
1,6-dimethyl-4-prop	222.370	1.000	0.750	3.934	4494.140	2510.636
3,6,8-trimethyl-2-me	204.355	0.000	0.000	4.616	9906.038	5899.293
3-(6-methylhept-5-ei	204.355	0.000	0.000	6.369	9906.038	5899.293
2-(5-ethenyl-5-meth	236.353	0.000	2.750	4.028	5046.565	2845.806
trimethyl-(2-trimeth	222.477	0.000	0.000	5.719	9906.038	5899.293
trimethylsilyl 3,4,5-tr	458.848	0.000	4.550	7.007	5463.706	3100.891
4,7-dimethyl-1-prop	222.370	1.000	0.750	4.109	7189.984	4172.261
1,2-dimethyl-8-prop	204.355	0.000	0.000	6.584	9906.038	5899.293
trimethyl-[2,3,4,5,6-]	613.247	0.000	5.100	6.077	9906.038	5899.293
1-(2,3,4,5-tetrahydr	125.170	1.000	3.000	0.919	2037.972	1067.964
4-methyl-1-propan-2	136.236	0.000	0.000	3.877	9906.038	5899.293
cyclotetracosane	336.643	0.000	0.000	11.510	9906.038	5899.293
1-methyl-4-(6-methy	210.402	0.000	0.000	7.950	9906.038	5899.293
2,5-dihydroperoxy-2,	178.228	2.000	4.900	0.779	979.681	483.853
decyl 2,2,2-trifluoro	254.292	0.000	2.000	4.664	3159.204	8502.365
3-ethenyl-3-methyl-	222.370	1.000	1.700	3.717	5420.005	3074.091
3,8-dimethyl-5-prop	204.355	0.000	0.000	5.461	9906.038	5899.293
3,5,5-trimethyl-9-me	204.355	0.000	0.000	5.286	9906.038	5899.293
2,6,6,9-tetramethyl	204.355	0.000	0.000	5.066	9906.038	5899.293
3,3-dimethylheptane	128.257	0.000	0.000	4.979	9906.038	5899.293
1,4a-dimethyl-7-prop	222.370	1.000	0.750	3.957	4719.669	2647.090
3-methyl-1-(3-methy	166.219	0.000	2.500	2.329	5039.763	2841.660
1,1,4,7-tetramethyl-	204.355	0.000	0.000	5.029	9906.038	5899.293
methyl 7-methylnon	186.294	0.000	2.000	3.353	2629.835	1406.835
2,6,10,14,18-pentam	352.686	0.000	0.000	13.761	9906.038	5899.293
2,6,10,14-tetrameth	310.605	0.000	0.000	12.304	9906.038	5899.293
trimethyl-(5-methyl-	222.402	0.000	0.850	3.946	9906.038	5899.293
trimethylsilyl hexade	328.609	0.000	2.000	7.306	5189.575	2933.073

trimethylsilyl icosane	384.716	0.000	2.000	8.891	5801.581	3308.669
tetrapentacontane	759.463	0.000	0.000	30.260	9906.038	5899.293
4-methyl-1-prop-1-ene	136.236	0.000	0.000	4.016	9906.038	5899.293
2-(propylsulfanyl)butane	164.323	0.000	1.000	3.172	9906.038	10000.000
1-(methylsulfanyl)butane	136.270	0.000	1.000	3.065	9906.038	10000.000
propan-2-yl 2-methylpropanoate	144.213	0.000	2.000	2.306	4814.374	2704.548
2,3,4,5,6-pentakis(trimethylsilyloxy)hexane	541.066	0.000	6.250	7.193	3917.771	2164.487
5,8a-dimethyl-3-propylbicyclo[2.2.1]heptane	204.355	0.000	0.000	5.322	9906.038	5899.293
methyl 15-methylhexadecanoate	284.481	0.000	2.000	6.238	1682.463	868.101
1-(propylsulfanyl)butane	164.323	0.000	1.000	3.599	9906.038	10000.000
1-(methylsulfanyl)butane	150.297	0.000	1.000	3.342	9906.038	10000.000
2-bromoadamantane	215.132	0.000	0.000	3.684	9906.038	10000.000
2,5,5,8a-tetramethyladamantane	194.316	0.000	0.750	3.121	9906.038	5899.293
hexadecyl 2,2,2-trichloroacetate	387.816	0.000	2.000	7.820	3803.959	10000.000
1-ethynyl-4-fluorobenzene	120.126	0.500	0.000	2.653	9906.038	10000.000
2-(4-methylcyclohexyl)ethanol	224.342	0.000	2.000	4.016	5475.661	3108.225
methyl 2,2-dimethylpropanoate	130.186	0.000	2.000	1.340	4491.287	2508.913
tetradec-13-enal	210.359	0.000	2.000	4.161	1941.254	1013.288
octadecyl 2-chloropropanoate	361.007	0.000	2.000	7.892	3342.171	4067.185
1,3,3-trimethyl-2-oxobutane	152.236	0.000	0.750	2.576	9906.038	5899.293
(2-methyl-5-propanoate)cyclohexane	196.289	0.000	2.000	3.149	6116.326	3503.106
hexadec-2-ene	224.429	0.000	0.000	8.540	9906.038	5899.293
hexadecyl 2,2,3,3,3-pentachloroacetate	388.461	0.000	2.000	7.668	3314.871	10000.000
6-methyl-3-prop-1-ene	166.219	0.000	4.000	1.111	3990.093	2207.707
2-(1,2-dimethyl-8-tertiarybutyl)ethane	220.354	1.000	1.700	3.305	3351.083	1828.155
2,7,7-trimethyl-6-methylheptane	218.338	0.000	2.000	3.152	3451.667	1887.537
2,6,6,7-tetramethyltetrahydroindole	222.370	1.000	0.750	3.707	5474.036	3107.228
2-(4a-methyl-8-methyl-5,8-dihydroindolo[1,2-b]pyridine)	220.354	1.000	1.700	3.447	3314.277	1806.462
2-methyl-5-propanoate	154.252	1.000	0.750	2.704	5153.304	2910.921
(3R,4S,5S)-1,3,4,5,6-pentakis(trimethylsilyloxy)cyclohexane	541.066	0.000	6.250	7.949	7600.417	4430.278
1,1,7-trimethylspiro[3.5]undecane	220.354	0.000	2.000	2.511	9906.038	5899.293
(3,5-ditert-butylphenyl)ethane	278.509	0.000	0.850	4.876	9906.038	5899.293
3,4-dimethyl-2,3-dihydroindole	146.265	0.800	1.000	2.964	9906.038	10000.000

furan-3-one	84.074	0.000	3.700	-0.599	2420.602	1286.251
7-methylidene-4-pro	204.355	0.000	0.000	5.376	9906.038	5899.293
trimethylsilyl 2-[[4-r	353.565	0.000	3.750	5.038	5202.295	2940.844
pent-2-en-4-ynyl 4-cl	220.655	0.500	2.000	3.175	2964.445	3947.283
ethenyl-dimethyl-(3-	192.332	0.000	0.850	3.717	9906.038	5899.293
N-(2-fluorophenyl)cy	207.247	1.000	2.500	3.023	5291.510	5051.982
6',6'-dimethylspiro[1	194.273	0.000	2.450	1.821	9906.038	5899.293
2,7,7,10-tetramethyl	220.354	0.000	2.000	2.505	9906.038	5899.293
3,7,7,10-tetramethyl	220.354	0.000	2.000	2.657	9906.038	5899.293
2-prop-2-enylsulfany	113.177	0.000	2.000	1.330	2040.727	1769.645
11-cyclopentylundec	254.412	1.000	2.000	4.891	278.895	158.262
methyl 8-[2-[(2-pent	322.530	0.000	2.000	6.764	3032.954	1641.308
cyclohexadec-8-en-1	236.397	0.000	2.000	4.139	5182.986	2929.048
2,2,6-trimethyl-10-m	220.354	1.000	1.700	3.192	4185.163	2324.596
2,6,6,8-tetramethyl-	220.354	0.000	2.000	2.401	9906.038	5899.293
5-methyl-2-propan-2	152.236	0.000	2.000	2.291	2424.379	1288.421
N-cyclopropyl-2-met	111.186	0.000	1.500	2.019	6550.239	3772.483
3-methyl-3-(4-methy	168.235	0.000	4.000	1.419	2351.684	1246.714
[6-(hydroxymethyl)-1	254.369	1.000	4.400	2.247	1593.942	818.840
2,6,6-trimethyl-9-me	218.338	0.000	2.000	3.274	3808.526	2099.324
S-[2-[3-[(2,4-dihydro	484.693	3.000	9.400	3.657	41.494	55.659
3-[3-(aziridin-1-yl)pr	207.275	0.000	2.000	3.592	4505.042	2517.220
(2,8,9,13-tetraacetyl	578.655	0.000	12.000	3.502	313.990	141.441
1-(4-bromobutyl)pip	234.135	0.000	3.000	1.864	2147.294	5466.060
5,9-dimethyl-2-prop	224.386	1.000	1.700	3.756	4394.330	2450.422
4a-hydroperoxy-2,5,	238.326	1.000	3.200	2.772	3955.977	2187.311
4-hydroperoxy-8-me	236.353	1.000	3.400	2.951	2654.479	1421.089
1,2-diethylcyclohexa	280.536	0.000	0.000	9.574	9906.038	5899.293
10,13-dimethyl-17-(420.674	3.000	4.150	5.463	1282.933	647.598
[7,12,16-trimethyl-1	468.762	0.000	2.000	8.549	3858.471	2129.097
13-methyl-6,7,8,9,11	256.387	1.000	1.700	3.683	3922.963	2167.588
9,10-dibromopentac	510.478	0.000	0.000	14.178	9906.038	10000.000
[7,7,12,16-tetramet	470.777	0.000	2.000	8.638	3916.267	2163.589

propan-2-yl 2-sulfany	148.220	0.800	2.500	1.973	4535.060	6026.182
(2,8,13-triacetyloxy-	536.618	1.000	11.700	3.473	582.966	276.082
2,3,6,7-tetramethylo	170.337	0.000	0.000	6.755	9906.038	5899.293
tetradec-11-ynyl ace	252.396	0.000	2.000	5.245	2223.705	1173.544
pentacos-10,12-diy	374.606	1.000	2.000	8.452	279.322	158.523
methyl octadeca-12,	290.445	0.000	2.000	6.274	2607.321	1393.821
4,4,8-trimethylnon-7	182.305	0.000	2.000	3.247	3962.205	2191.033
5-methyl heptanethi	160.274	0.000	2.000	2.744	4303.359	4058.344
(5-acetyl-2,10-diacet	518.603	0.000	9.500	3.436	511.430	239.653
dimethyl 4-acetamid	251.238	1.000	6.500	0.992	292.529	131.021
(3a,10a-dihydroxy-2,	348.395	2.000	7.500	1.692	134.737	56.680
(5-acetyl-2-acetyloxy	476.566	1.000	8.250	3.946	859.170	419.853
diethyl 15-acetyloxy-	488.620	0.000	8.000	4.202	306.746	137.917
5-(2-aminoethyl)-1H-	139.157	3.000	4.500	-1.069	39.877	16.818
1-methoxy-13-methy	270.498	0.000	1.700	5.717	9906.038	5899.293
5-(methoxymethoxy)	158.197	1.000	5.100	0.948	3153.677	1712.034
hexadec-7-enoic acic	254.412	1.000	2.000	5.208	235.340	131.724
tridecan-4-yl 2,2,2-tr	296.372	0.000	2.000	5.793	3911.851	10000.000
methyl hexadec-7-er	268.439	0.000	2.000	5.655	2585.611	1381.281
2-heptadec-7-ynoxyc	336.557	0.000	3.400	6.177	9906.038	5899.293
3-(cyclopropylmethy	505.529	3.000	9.700	1.533	5.350	1.918
methyl 8-(2-octylcycl	310.519	0.000	2.000	6.753	2625.213	1404.162
2-[12-(oxiran-2-yl)do	254.412	0.000	4.000	3.354	9906.038	5899.293
pentadecyl prop-2-er	282.465	0.000	2.000	6.215	2821.060	1517.723
5-methylundec-4-en	168.322	0.000	0.000	6.121	9906.038	5899.293
3-hexylthiane 1,1-dic	218.354	0.000	4.000	2.243	1581.395	821.969
4a-methyl-2,4,5,6,7,	180.289	0.000	2.000	2.487	3293.422	1794.178
tridecanedial	212.331	0.000	4.000	2.448	360.224	164.081
7,9-ditert-butyl-1-ox	276.375	0.000	5.000	2.746	1981.670	1036.109
1-chloroheptacosan	415.184	0.000	0.000	15.219	9906.038	10000.000
2,6-dimethylheptade	268.525	0.000	0.000	10.893	9906.038	5899.293
henicosyl formate	340.588	0.000	2.000	7.538	1197.285	600.997
1-(3-methylfuran-2-y	138.166	0.000	2.500	1.553	3184.380	1730.057

1,54-dibromotetrape	917.255	0.000	0.000	30.871	9906.038	10000.000
pentadecan-3-one	226.401	0.000	2.000	4.901	4249.051	2362.976
3-(3,3-dimethylbutyl	184.321	1.000	1.700	3.113	3386.131	1848.831
N-(2,7-diethoxyfluor	283.326	1.000	4.200	3.293	2086.328	1095.380
dimethyl 2-oxopropa	146.099	0.000	6.000	-1.252	224.854	98.590
cyclohexane-1,2,3,5-	148.158	4.000	6.800	-1.240	200.765	87.224
2-(2-hydroxyethylsul	150.192	2.000	4.200	0.266	97.523	69.714
bicyclo[10.1.0]tridec	178.317	0.000	0.000	4.510	9906.038	5899.293
nonadeca-1,3,12-trie	262.478	0.000	0.000	9.783	9906.038	5899.293
methyl hexadeca-9,1	266.423	0.000	2.000	5.594	3033.611	1641.692
methyl octadeca-10,	294.476	0.000	2.000	5.995	3115.506	1689.647
pentadec-7-yne	208.386	0.000	0.000	8.017	9906.038	5899.293
icos-3-yne	278.520	0.000	0.000	10.811	9906.038	5899.293
15-ethenyl-15-methy	266.423	0.000	2.000	4.694	6164.455	3532.911
icosa-1,4-diene	278.520	0.000	0.000	10.680	9906.038	5899.293
15,15-dimethyl-oxac	254.412	0.000	2.000	4.396	5859.590	3344.441
2-(3-ethenyl-9-methi	368.475	1.000	4.750	4.231	390.348	197.987
(16-ethyl-15-methyl-	326.438	1.000	4.000	3.646	420.102	214.349
8-(2-octylcyclopropy	280.493	0.000	2.000	5.992	2154.951	1134.374
1-(12-ethyl-12-hydro	338.449	1.000	5.750	2.724	769.318	412.215
2-hydroxyhexadecyl	328.534	1.000	3.700	5.900	1179.186	591.183
3-methoxyhex-1-ene	114.187	0.000	1.700	1.986	9906.038	5899.293
butyl tetradecane-6-	334.556	0.000	4.000	5.567	3279.096	1785.744
N,6,7,13-tetramethy	342.567	1.000	3.500	4.159	442.287	250.702
2-(9-hydroxyimino-3,	267.327	1.000	8.700	-0.747	21.917	9.743
[butoxy-bis(trimethy	559.081	0.000	3.350	10.813	9905.931	5899.224
methyl 8-[2-(2-hexyl	322.530	0.000	2.000	6.374	3310.392	1804.173
[2,2-dimethyl-5-[2-(2	320.500	1.000	6.600	3.573	2843.179	1530.589
trimethylsilyl 3-(1,3-	354.549	0.000	4.350	4.690	7682.304	4481.893
1-(4-methoxyphenyl)	248.302	0.000	3.750	2.399	1150.146	868.733
7-[6-methyl-3,4,5-tri	1534.666	0.000	20.150	9.163	9906.038	5899.293
methyl 10-methylun	214.347	0.000	2.000	4.149	2587.645	1382.456
methyl 13-methylpe	270.454	0.000	2.000	5.702	2576.863	1376.230

hydroxy-tri(propan-2	174.358	1.000	0.850	3.319	6530.025	3759.902
7,7-dimethylbicyclo[150.220	0.000	2.000	1.902	1916.289	999.210
icos-9-yne	278.520	0.000	0.000	10.706	9906.038	5899.293
hexacos-11-yne	362.681	0.000	0.000	13.935	9906.038	5899.293
7-butylbicyclo[4.1.0]	152.279	0.000	0.000	5.784	9906.038	5899.293
octadec-16-enal	266.466	0.000	2.000	5.725	1937.867	1011.377
2-nitroprop-2-enylcy	169.223	0.000	2.000	2.044	1522.298	779.131
pentatriacontan-1-ol	508.953	1.000	1.700	12.554	2853.233	1536.440
2-methyl-6-(4-methy	218.338	0.000	2.000	3.689	4162.618	2311.064
11-oxadispiro[4.0.4	168.235	1.000	3.700	1.447	4646.353	2602.671
N-(2-hydroxyethyl)h	159.228	2.000	4.200	0.442	719.908	563.250
methyl cycloundecar	212.331	0.000	2.000	3.397	4095.800	2270.993
2,3-dimethyldecan-3	186.337	1.000	0.750	4.023	5598.988	3183.962
ethyl 5-methylnonan	200.320	0.000	2.000	3.832	2927.984	1579.994
methyl 2,6,10-trimet	270.454	0.000	2.000	5.340	3824.227	2108.680
22-(1-hydroxyethyl)-	431.571	2.000	7.650	3.013	908.892	493.613
2-[1-(1-ethoxyethoxy	266.336	0.000	7.100	1.922	9906.038	5899.293
[2-(benzenesulfinylm	332.459	0.000	4.000	5.132	213.531	3551.419
3-methyl-8-methylid	204.355	0.000	0.000	5.539	9906.038	5899.293
3,7-dimethylocta-1,6	252.396	0.000	2.000	5.117	5399.735	3061.667
1-(4-methylcyclohex	140.225	1.000	1.700	2.019	4061.982	2250.732
2,5,9,9-tetramethyl-	204.355	0.000	0.000	5.241	9906.038	5899.293
2,6-dimethyloct-7-er	156.267	1.000	1.700	2.824	4741.247	2660.173
3,3,7-trimethyltricycl	220.354	0.000	2.000	3.110	2853.480	1536.584
(5-ethylcyclopenten-	126.198	1.000	1.700	1.728	3503.288	1918.068
cyclopentane-1,2-dic	98.101	1.000	2.750	-0.121	820.578	399.506
oxacyclododecane-2,	198.261	0.000	4.000	1.468	2115.254	1111.805
2-hexyl-5-methylfur	182.262	0.000	2.750	2.647	3004.311	1624.560
hexadecan-4-yl hexa	340.588	0.000	2.000	7.845	4684.989	2626.071
5-methyl-5-(4,8,12-ti	324.546	0.000	3.000	6.102	2333.385	1236.231
ethyl 4-oxo-5-phenyl	220.268	0.000	4.000	2.597	1419.215	722.264
methyl 3-acetyloxy-3	162.142	0.000	4.700	-0.066	302.054	135.638
6-decylsulfonylhexar	370.500	4.000	11.500	0.637	63.574	25.216

4,4-dimethyldecan-2	246.435	0.000	0.000	7.457	9906.038	5899.293
7,7-dimethylbicyclo[150.220	0.000	2.000	1.897	1923.740	1003.410
2-ethylidene-6-meth	150.220	0.000	2.000	2.331	2095.949	1100.841
bis(4-methylphenyl)	356.408	0.000	9.000	1.114	412.564	194.910
1,2,3,5,6,7-hexahydr	136.193	0.000	2.000	1.614	3269.502	1780.097
2,2,7,7-tetramethylo	180.289	0.000	2.000	3.167	3328.495	1814.839
4,8,12,12-tetrameth	220.354	0.000	2.000	2.335	9906.038	5899.293
5-ethylcyclopentene	140.182	1.000	2.000	1.822	295.144	168.251
(3,5-dimethylcyclohe	238.344	0.000	2.000	3.913	4215.014	4180.027
1H-imidazole-2-carbr	112.088	2.000	3.500	-0.298	70.621	35.861
3H-pyran-2,6-dione	112.085	0.000	4.500	-1.138	463.981	215.713
octan-4-yl heptanoat	242.401	0.000	2.000	5.080	4416.997	2464.087
(3-nitrophenyl) hept	251.282	0.000	3.500	2.814	532.991	250.592
S-tert-butyl 5-oxohe	202.311	0.000	4.000	2.165	2134.119	1516.687
3-[[ethyl(fluoro)phos	224.255	0.000	5.000	2.113	3844.239	3272.553
octadecyl hexanoate	368.642	0.000	2.000	8.530	3117.631	1690.893
2-[[2-[(2-aminoacety	318.332	4.500	6.500	-2.304	0.989	1.014
1-methyl-4-(6-methy	204.355	0.000	0.000	6.472	9906.038	5899.293
4-(2,6,6-trimethylcyc	192.300	0.000	2.000	3.087	3248.284	1767.614
1-(2,3-dihydroindol-1	279.338	0.000	5.000	3.068	1839.457	955.979
octacos-13,15-diyne	386.703	0.000	0.000	14.927	9906.038	5899.293
(2,3-dimethyl-3-tricy	152.236	1.000	1.700	1.999	4396.126	2451.504
1-methyl-6-propan-2	136.236	0.000	0.000	4.023	9906.038	5899.293
tricyclo[8.6.0.02,9]h	248.364	0.000	4.000	2.490	2331.635	1235.229
5-ethylcyclopentene	124.182	0.000	2.000	1.563	1995.946	1044.180
2-cyclopropylthioph	124.200	0.000	0.000	3.153	9906.038	10000.000
methyl 12-ethyl-8-m	352.475	0.000	4.000	4.089	1090.505	601.036
4-hydroxy-5-methyl-	126.115	2.000	3.500	-0.347	366.224	167.037
1-propan-2-yl-1,2,3,	175.273	1.000	1.500	2.374	1547.098	877.154
methyl N-hydroxybe	151.165	1.000	2.700	1.567	1514.326	774.722
1-(3-methoxyphenyl)	164.204	0.000	2.750	2.041	3915.565	2163.170
2-ethenyl-1,3,3-trim	150.263	0.000	0.000	3.957	9906.038	5899.293
1,6-naphthyridin-4-a	145.163	1.500	3.500	0.507	1008.833	499.434

trimethyl-[2-(trimethyl-248.512	0.000	1.700	3.934	9906.038	5899.293
7-(2,2-dimethyl-1,3-cyclohexyl)-346.509	0.000	3.500	4.736	3550.928	1946.276
2,3-dimethyl-5-(trifluoromethyl)-206.164	2.000	1.500	2.215	1857.677	3982.361
2-methyl-5-oxo-7-(2-methyl-287.358	0.000	5.000	2.879	1043.295	517.900
[3-cyano-1-(2-phenyl)-347.410	0.000	5.750	3.363	804.776	391.197
1-[5-tert-butyl-5-hydroxy-400.440	0.000	4.000	5.829	3937.119	9474.381
4-(2,2,6-trimethyl-1-piperidyl)-208.343	0.000	2.000	3.333	3243.601	1764.860
3-ethenyl-3-methyl-220.354	0.000	2.000	3.769	5961.309	3407.238
2-hydroxy-6-methoxy-168.149	1.000	2.500	1.681	119.987	63.598
3-propyladamantan-194.316	1.000	0.750	3.195	3861.438	2130.867
methyl 2-oxo-3,4-dihydro-155.153	0.000	3.500	0.367	427.934	197.657
2,5-dimethyl-8-propyl-202.339	0.000	0.000	5.392	9906.038	5899.293
3,3,6-trimethyl-2H-imidazo-174.242	0.000	2.000	2.515	2987.140	1614.526
3-(2,4-dinitrophenyl)-312.238	0.000	4.500	1.668	70.409	28.104
2-methoxy-3-propyl-164.204	1.000	1.500	2.675	3841.058	2118.713
ethyl 1-(2,2,2-trifluoroethyl)-239.194	0.000	5.000	1.057	1140.649	3973.179
1-(2,5-dimethoxyphenyl)-210.272	1.000	3.200	2.731	4321.868	2406.776
7,7-dimethyl-1-(2-methyl)-226.358	1.000	2.450	3.340	5652.798	3217.049
2-(2,4,5-trimethoxyphenyl)-336.390	2.000	4.250	4.275	6068.427	3473.462
3-methyl-2-octyl-1H-imidazo-271.402	1.000	2.500	4.681	3045.460	1648.624
6-hydroxy-2-methyl-175.187	2.000	3.250	1.066	640.834	305.819
2,2,7,7-tetramethyl-218.338	0.000	2.000	3.254	4843.452	2722.209
9-hydroxy-8,8-dimethyl-246.262	1.000	4.950	1.683	911.815	447.728
15,16-diazatetracyclo-208.262	2.000	2.000	1.499	144.903	75.047
(3,3-dimethylcyclohexyl)-198.380	0.000	0.850	3.594	9906.038	5899.293
2,3,8,8-tetramethyl-204.355	0.000	0.000	5.042	9906.038	5899.293
6-(diethylamino)-1-benzyl-205.256	0.000	3.750	1.861	2579.178	1377.566
2-tert-butyl-4-(2,4,4-trimethyl)-262.434	1.000	0.750	5.039	4984.780	2808.166
(2,4-ditert-butylphenyl)-306.444	1.000	4.200	4.223	1908.593	994.873
(5,7-dimethyl-1,3-dioxane)-194.279	2.000	5.500	-0.343	94.123	47.076
9-methoxy-9-(9-methyl)-390.481	0.000	1.500	6.210	9906.038	5899.293
3-methyl-9H-carbazole-197.236	2.000	0.750	2.669	1959.987	1023.861
2-(4a,8-dimethyl-3,4-dihydro)-218.338	1.000	1.700	3.477	4134.743	2294.341

[2,4,6-tri(propan-2-yl) 236.336	2.000	0.000	6.596	9906.038	10000.000
7-hydroxy-3a,5a,5b,8a-tetrahydro-2H-benzofuro[3,2-b]pyridine 440.708	1.000	3.700	6.127	2566.008	1369.965
3,6,8-trimethyltricyclo[3.3.1.0 ^{2,6}]octane 206.327	0.000	2.000	2.826	4052.010	2244.760
N-(2-amino-2-oxoethyl)acetamide 280.409	2.250	4.250	2.682	98.655	84.148
1-(5-methyl-2-trimethylsilyloxyphenyl)ethanone 222.358	0.000	2.850	2.898	5559.707	3159.824
1,5,5,8-tetramethyl-1H-pyridine 222.370	1.000	0.750	3.696	6352.344	3649.443
2-methyl-7-phenyl-1H-imidazo[4,5-b]pyridine 207.274	1.000	0.000	4.486	7685.535	4483.930
2,4-dimethylbenzo[h]quinoline 207.274	0.000	1.000	4.105	8716.386	5137.388
N-(3-chloro-1,4-dioxane-5-yl)acetamide 359.852	0.250	5.750	3.703	603.665	560.643
5,6,11,12-tetrahydro-1,4-dioxepine 209.290	1.000	1.000	3.739	6775.347	3912.809
4,8a-dimethyl-6-propyl-1,2,3,4,4a,8a-hexahydro-1H-pyridine 218.338	0.000	2.000	3.280	3320.830	1810.323
(4,4,6a,6b,8a,11,11,11,11-octamethyl-1,2,3,4,4a,8a,8b,8c,8d,8e,8f,8g,8h,8i,8j,8k,8l,8m,8n,8o,8p,8q,8r,8s,8t,8u,8v,8w,8x,8y,8z)octalindane 1498.906	0.000	0.850	7.248	9906.038	5899.293
methyl 4,6a,6b,8a,11,11,11,11-octamethyl-1,2,3,4,4a,8a,8b,8c,8d,8e,8f,8g,8h,8i,8j,8k,8l,8m,8n,8o,8p,8q,8r,8s,8t,8u,8v,8w,8x,8y,8z)octalindane 1468.718	0.000	4.000	6.470	2358.258	1250.481
4-[(3-methoxyphenyl)imino]pyridine 227.262	1.000	2.500	3.240	2552.080	1361.930
5,5,11,11-tetramethyl-1,2,3,4,4a,8a,8b,8c,8d,8e,8f,8g,8h,8i,8j,8k,8l,8m,8n,8o,8p,8q,8r,8s,8t,8u,8v,8w,8x,8y,8z)octalindane 230.349	0.000	2.000	3.235	2136.317	1123.776
6-hydroxy-4,8,12-trimethyl-1,2,3,4,4a,8a,8b,8c,8d,8e,8f,8g,8h,8i,8j,8k,8l,8m,8n,8o,8p,8q,8r,8s,8t,8u,8v,8w,8x,8y,8z)octalindane 258.273	1.000	5.500	1.367	664.894	318.248
5,7-dimethoxy-8-(3-oxopropyl)-1,2,3,4,4a,8a,8b,8c,8d,8e,8f,8g,8h,8i,8j,8k,8l,8m,8n,8o,8p,8q,8r,8s,8t,8u,8v,8w,8x,8y,8z)octalindane 288.299	0.000	6.000	2.145	1341.309	679.507
5-[4-(3-methylbut-2-enyl)oxy]pyridine 306.363	0.000	4.250	4.359	3390.366	1851.330
6-methoxy-2-methyl-1,2,3,4,4a,8a,8b,8c,8d,8e,8f,8g,8h,8i,8j,8k,8l,8m,8n,8o,8p,8q,8r,8s,8t,8u,8v,8w,8x,8y,8z)octalindane 254.285	1.000	2.000	3.584	3074.618	1665.691
5-methyl-4-naphthalen-1-yl-1,2,3,4,4a,8a,8b,8c,8d,8e,8f,8g,8h,8i,8j,8k,8l,8m,8n,8o,8p,8q,8r,8s,8t,8u,8v,8w,8x,8y,8z)octalindane 240.322	2.000	2.000	3.092	1828.689	1698.892
7-hydroxy-2,4b,8,8-tetrahydro-1,2,3,4,4a,8a,8b,8c,8d,8e,8f,8g,8h,8i,8j,8k,8l,8m,8n,8o,8p,8q,8r,8s,8t,8u,8v,8w,8x,8y,8z)octalindane 290.445	1.000	3.700	3.341	1327.638	672.024
7-(hydroxymethyl)-4,5,6,7,8,8a,8b,8c,8d,8e,8f,8g,8h,8i,8j,8k,8l,8m,8n,8o,8p,8q,8r,8s,8t,8u,8v,8w,8x,8y,8z)octalindane 276.245	1.000	6.200	1.443	1190.683	597.416
2,6-dimethoxyanthracene 294.306	0.000	5.500	2.062	519.716	243.852
(1,4-dimethyl-7-propyl-1,2,3,4,4a,8a,8b,8c,8d,8e,8f,8g,8h,8i,8j,8k,8l,8m,8n,8o,8p,8q,8r,8s,8t,8u,8v,8w,8x,8y,8z)octalindane 302.415	0.000	2.000	5.425	4682.577	2624.610
15-propan-2-yltetrahydro-1,2,3,4,4a,8a,8b,8c,8d,8e,8f,8g,8h,8i,8j,8k,8l,8m,8n,8o,8p,8q,8r,8s,8t,8u,8v,8w,8x,8y,8z)octalindane 312.408	0.000	6.000	2.054	441.345	204.361
methyl 7-(2-hydroxyethyl)-1,2,3,4,4a,8a,8b,8c,8d,8e,8f,8g,8h,8i,8j,8k,8l,8m,8n,8o,8p,8q,8r,8s,8t,8u,8v,8w,8x,8y,8z)octalindane 330.466	1.000	2.750	4.807	2397.432	1272.948
2-(3-ethyl-9-methoxyphenyl)acetamide 328.453	2.000	4.450	3.337	513.971	266.556
2-(2,6-dimethoxyphenyl)acetamide 342.348	0.000	5.500	3.580	3847.817	2122.743
23,24-dimethoxy-18-methyl-1,2,3,4,4a,8a,8b,8c,8d,8e,8f,8g,8h,8i,8j,8k,8l,8m,8n,8o,8p,8q,8r,8s,8t,8u,8v,8w,8x,8y,8z)octalindane 433.503	0.000	6.000	3.521	851.492	460.006
4-[(3,5-ditert-butyl-4-methoxyphenyl)imino]pyridine 340.505	2.000	1.500	5.963	3873.449	2138.032
N-(13,14,15-trimethyl-1,2,3,4,4a,8a,8b,8c,8d,8e,8f,8g,8h,8i,8j,8k,8l,8m,8n,8o,8p,8q,8r,8s,8t,8u,8v,8w,8x,8y,8z)octalindane 341.406	1.000	4.750	3.391	2305.593	2114.195
5-hydroxy-3-(1-hydroxyethyl)-1,2,3,4,4a,8a,8b,8c,8d,8e,8f,8g,8h,8i,8j,8k,8l,8m,8n,8o,8p,8q,8r,8s,8t,8u,8v,8w,8x,8y,8z)octalindane 374.349	0.000	7.500	1.419	53.059	20.700
11,16,17-trimethoxy-1,2,3,4,4a,8a,8b,8c,8d,8e,8f,8g,8h,8i,8j,8k,8l,8m,8n,8o,8p,8q,8r,8s,8t,8u,8v,8w,8x,8y,8z)octalindane 399.443	0.000	8.400	2.475	2349.551	1377.909

(2S,4aS,6aR,6aS,6bR, 570.765	2.000	8.000	5.735	2.801	1.393
1,2,4-trimethoxy-5-[(1R)-2-(4S,5R,9S,10R,13S)-2-hydroxy-5-[(1S,4S,5R,9S,10R,13S)-but-2-enoic acid (E)-but-2-enoic acid 86.090	0.000	2.250	2.879	9906.038	5899.293
(5R)-2-hydroxy-5-[(1R)-2-(4S,5R,9S,10R,13S)-2-hydroxy-5-[(1S,4S,5R,9S,10R,13S)-but-2-enoic acid (E)-but-2-enoic acid 86.090	2.000	4.250	1.573	554.054	261.313
[(1S,4S,5R,9S,10R,13S)-2-hydroxy-5-[(1R)-2-(4S,5R,9S,10R,13S)-2-hydroxy-5-[(1S,4S,5R,9S,10R,13S)-but-2-enoic acid (E)-but-2-enoic acid 86.090	1.000	6.750	7.317	343.557	155.890
(E)-but-2-enoic acid 86.090	1.000	2.000	0.722	203.439	112.535
(2R)-2-[(1R)-1-[(8S,9S)-3-[(E)-2-[(1R,4aS,5R,6aS,6aR,6aS,6bR,6bS,6bR)-3-phenylprop-2-ene (E)-3-phenylprop-2-ene 132.162	1.000	5.750	4.931	830.394	404.675
(2R)-2-[(1R)-1-[(8S,9S)-3-[(E)-2-[(1R,4aS,5R,6aS,6aR,6aS,6bR,6bS,6bR)-3-phenylprop-2-ene (E)-3-phenylprop-2-ene 132.162	2.000	5.900	3.588	455.050	211.229
(E)-3-phenylprop-2-ene 132.162	0.000	2.000	1.870	1562.016	801.126
(E)-octadec-9-enoic acid 282.465	1.000	2.000	5.871	653.188	397.069
(1R)-2-methyl-5-propylmethyl (E)-3-phenylpropylmethyl (E)-2-methylbutyl (E)-3-(2-hydroxyphenyl)ethyl (E)-3-(4-hydroxyphenyl)ethyl 1-methoxy-4-[(E)-propyl]-(2E)-3,7-dimethyloctyl ethyl (E)-3-phenylpropyl (E)-3-(4-hydroxy-3,5-dimethoxyphenyl)-1,2-dimethoxy-4-[(E)-propyl]-1-[(E)-3-(3,4,5-trimethylphenyl)-2-(4-hydroxyphenyl)]-(2R,3R)-2-(4-hydroxyphenyl)-(2E)-3,7-dimethyloctyl (E)-4-(2,6,6-trimethyl-2,4,5-trimethyl-5-(1,3-benzodioxol-5-yl)-2,6-dimethyl-[(2E,4E,6E,8E)-3,7-dimethyl-6,10,14,18E)-2,6-dimethyl-(E)-stilbene methyl (E)-but-2-ene (E)-1-(2,4-dihydroxyphenyl)-[(2E,6E)-3,7,11-trimethyl-4-(4S)-4-bromo-5,5-dimethyl-13aR)-2,3,6-trimethyl-(E)-3-(4-methoxyphenyl)-	0.000	0.000	3.889	9906.038	5899.293
(1R)-2-methyl-5-propylmethyl (E)-3-phenylpropylmethyl (E)-2-methylbutyl (E)-3-(2-hydroxyphenyl)ethyl (E)-3-(4-hydroxyphenyl)ethyl 1-methoxy-4-[(E)-propyl]-(2E)-3,7-dimethyloctyl ethyl (E)-3-phenylpropyl (E)-3-(4-hydroxy-3,5-dimethoxyphenyl)-1,2-dimethoxy-4-[(E)-propyl]-1-[(E)-3-(3,4,5-trimethylphenyl)-2-(4-hydroxyphenyl)]-(2R,3R)-2-(4-hydroxyphenyl)-(2E)-3,7-dimethyloctyl (E)-4-(2,6,6-trimethyl-2,4,5-trimethyl-5-(1,3-benzodioxol-5-yl)-2,6-dimethyl-[(2E,4E,6E,8E)-3,7-dimethyl-6,10,14,18E)-2,6-dimethyl-(E)-stilbene methyl (E)-but-2-ene (E)-1-(2,4-dihydroxyphenyl)-[(2E,6E)-3,7,11-trimethyl-4-(4S)-4-bromo-5,5-dimethyl-13aR)-2,3,6-trimethyl-(E)-3-(4-methoxyphenyl)-	0.000	2.000	2.359	2317.411	1227.086
methyl (E)-3-phenylpropylmethyl (E)-2-methylbutyl (E)-3-(2-hydroxyphenyl)ethyl (E)-3-(4-hydroxyphenyl)ethyl 1-methoxy-4-[(E)-propyl]-(2E)-3,7-dimethyloctyl ethyl (E)-3-phenylpropyl (E)-3-(4-hydroxy-3,5-dimethoxyphenyl)-1,2-dimethoxy-4-[(E)-propyl]-1-[(E)-3-(3,4,5-trimethylphenyl)-2-(4-hydroxyphenyl)]-(2R,3R)-2-(4-hydroxyphenyl)-(2E)-3,7-dimethyloctyl (E)-4-(2,6,6-trimethyl-2,4,5-trimethyl-5-(1,3-benzodioxol-5-yl)-2,6-dimethyl-[(2E,4E,6E,8E)-3,7-dimethyl-6,10,14,18E)-2,6-dimethyl-(E)-stilbene methyl (E)-but-2-ene (E)-1-(2,4-dihydroxyphenyl)-[(2E,6E)-3,7,11-trimethyl-4-(4S)-4-bromo-5,5-dimethyl-13aR)-2,3,6-trimethyl-(E)-3-(4-methoxyphenyl)-	0.000	2.000	3.363	2974.460	1607.119
hexyl (E)-2-methylbutyl (E)-3-(2-hydroxyphenyl)ethyl (E)-3-(4-hydroxyphenyl)ethyl 1-methoxy-4-[(E)-propyl]-(2E)-3,7-dimethyloctyl ethyl (E)-3-phenylpropyl (E)-3-(4-hydroxy-3,5-dimethoxyphenyl)-1,2-dimethoxy-4-[(E)-propyl]-1-[(E)-3-(3,4,5-trimethylphenyl)-2-(4-hydroxyphenyl)]-(2R,3R)-2-(4-hydroxyphenyl)-(2E)-3,7-dimethyloctyl (E)-4-(2,6,6-trimethyl-2,4,5-trimethyl-5-(1,3-benzodioxol-5-yl)-2,6-dimethyl-[(2E,4E,6E,8E)-3,7-dimethyl-6,10,14,18E)-2,6-dimethyl-(E)-stilbene methyl (E)-but-2-ene (E)-1-(2,4-dihydroxyphenyl)-[(2E,6E)-3,7,11-trimethyl-4-(4S)-4-bromo-5,5-dimethyl-13aR)-2,3,6-trimethyl-(E)-3-(4-methoxyphenyl)-	2.000	2.750	1.474	75.593	38.597
(E)-3-(2-hydroxyphenyl)ethyl (E)-3-(4-hydroxyphenyl)ethyl 1-methoxy-4-[(E)-propyl]-(2E)-3,7-dimethyloctyl ethyl (E)-3-phenylpropyl (E)-3-(4-hydroxy-3,5-dimethoxyphenyl)-1,2-dimethoxy-4-[(E)-propyl]-1-[(E)-3-(3,4,5-trimethylphenyl)-2-(4-hydroxyphenyl)]-(2R,3R)-2-(4-hydroxyphenyl)-(2E)-3,7-dimethyloctyl (E)-4-(2,6,6-trimethyl-2,4,5-trimethyl-5-(1,3-benzodioxol-5-yl)-2,6-dimethyl-[(2E,4E,6E,8E)-3,7-dimethyl-6,10,14,18E)-2,6-dimethyl-(E)-stilbene methyl (E)-but-2-ene (E)-1-(2,4-dihydroxyphenyl)-[(2E,6E)-3,7,11-trimethyl-4-(4S)-4-bromo-5,5-dimethyl-13aR)-2,3,6-trimethyl-(E)-3-(4-methoxyphenyl)-	2.000	2.750	1.430	61.960	31.132
(E)-3-(4-hydroxyphenyl)ethyl 1-methoxy-4-[(E)-propyl]-(2E)-3,7-dimethyloctyl ethyl (E)-3-phenylpropyl (E)-3-(4-hydroxy-3,5-dimethoxyphenyl)-1,2-dimethoxy-4-[(E)-propyl]-1-[(E)-3-(3,4,5-trimethylphenyl)-2-(4-hydroxyphenyl)]-(2R,3R)-2-(4-hydroxyphenyl)-(2E)-3,7-dimethyloctyl (E)-4-(2,6,6-trimethyl-2,4,5-trimethyl-5-(1,3-benzodioxol-5-yl)-2,6-dimethyl-[(2E,4E,6E,8E)-3,7-dimethyl-6,10,14,18E)-2,6-dimethyl-(E)-stilbene methyl (E)-but-2-ene (E)-1-(2,4-dihydroxyphenyl)-[(2E,6E)-3,7,11-trimethyl-4-(4S)-4-bromo-5,5-dimethyl-13aR)-2,3,6-trimethyl-(E)-3-(4-methoxyphenyl)-	0.000	0.750	3.170	9906.038	5899.293
(2E)-3,7-dimethyloctyl ethyl (E)-3-phenylpropyl (E)-3-(4-hydroxy-3,5-dimethoxyphenyl)-1,2-dimethoxy-4-[(E)-propyl]-1-[(E)-3-(3,4,5-trimethylphenyl)-2-(4-hydroxyphenyl)]-(2R,3R)-2-(4-hydroxyphenyl)-(2E)-3,7-dimethyloctyl (E)-4-(2,6,6-trimethyl-2,4,5-trimethyl-5-(1,3-benzodioxol-5-yl)-2,6-dimethyl-[(2E,4E,6E,8E)-3,7-dimethyl-6,10,14,18E)-2,6-dimethyl-(E)-stilbene methyl (E)-but-2-ene (E)-1-(2,4-dihydroxyphenyl)-[(2E,6E)-3,7,11-trimethyl-4-(4S)-4-bromo-5,5-dimethyl-13aR)-2,3,6-trimethyl-(E)-3-(4-methoxyphenyl)-	1.000	1.700	2.608	2850.313	1534.741
ethyl (E)-3-phenylpropyl (E)-3-(4-hydroxy-3,5-dimethoxyphenyl)-1,2-dimethoxy-4-[(E)-propyl]-1-[(E)-3-(3,4,5-trimethylphenyl)-2-(4-hydroxyphenyl)]-(2R,3R)-2-(4-hydroxyphenyl)-(2E)-3,7-dimethyloctyl (E)-4-(2,6,6-trimethyl-2,4,5-trimethyl-5-(1,3-benzodioxol-5-yl)-2,6-dimethyl-[(2E,4E,6E,8E)-3,7-dimethyl-6,10,14,18E)-2,6-dimethyl-(E)-stilbene methyl (E)-but-2-ene (E)-1-(2,4-dihydroxyphenyl)-[(2E,6E)-3,7,11-trimethyl-4-(4S)-4-bromo-5,5-dimethyl-13aR)-2,3,6-trimethyl-(E)-3-(4-methoxyphenyl)-	0.000	2.000	2.813	2548.593	1359.918
(E)-3-(4-hydroxy-3,5-dimethoxyphenyl)-1,2-dimethoxy-4-[(E)-propyl]-1-[(E)-3-(3,4,5-trimethylphenyl)-2-(4-hydroxyphenyl)]-(2R,3R)-2-(4-hydroxyphenyl)-(2E)-3,7-dimethyloctyl (E)-4-(2,6,6-trimethyl-2,4,5-trimethyl-5-(1,3-benzodioxol-5-yl)-2,6-dimethyl-[(2E,4E,6E,8E)-3,7-dimethyl-6,10,14,18E)-2,6-dimethyl-(E)-stilbene methyl (E)-but-2-ene (E)-1-(2,4-dihydroxyphenyl)-[(2E,6E)-3,7,11-trimethyl-4-(4S)-4-bromo-5,5-dimethyl-13aR)-2,3,6-trimethyl-(E)-3-(4-methoxyphenyl)-	2.000	4.250	1.534	64.024	32.254
1,2-dimethoxy-4-[(E)-propyl]-1-[(E)-3-(3,4,5-trimethylphenyl)-2-(4-hydroxyphenyl)]-(2R,3R)-2-(4-hydroxyphenyl)-(2E)-3,7-dimethyloctyl (E)-4-(2,6,6-trimethyl-2,4,5-trimethyl-5-(1,3-benzodioxol-5-yl)-2,6-dimethyl-[(2E,4E,6E,8E)-3,7-dimethyl-6,10,14,18E)-2,6-dimethyl-(E)-stilbene methyl (E)-but-2-ene (E)-1-(2,4-dihydroxyphenyl)-[(2E,6E)-3,7,11-trimethyl-4-(4S)-4-bromo-5,5-dimethyl-13aR)-2,3,6-trimethyl-(E)-3-(4-methoxyphenyl)-	0.000	1.500	2.802	9906.038	5899.293
1-[(E)-3-(3,4,5-trimethylphenyl)-2-(4-hydroxyphenyl)]-(2R,3R)-2-(4-hydroxyphenyl)-(2E)-3,7-dimethyloctyl (E)-4-(2,6,6-trimethyl-2,4,5-trimethyl-5-(1,3-benzodioxol-5-yl)-2,6-dimethyl-[(2E,4E,6E,8E)-3,7-dimethyl-6,10,14,18E)-2,6-dimethyl-(E)-stilbene methyl (E)-but-2-ene (E)-1-(2,4-dihydroxyphenyl)-[(2E,6E)-3,7,11-trimethyl-4-(4S)-4-bromo-5,5-dimethyl-13aR)-2,3,6-trimethyl-(E)-3-(4-methoxyphenyl)-	0.000	5.250	3.194	1785.550	925.733
(2R,3R)-2-(4-hydroxyphenyl)-(2E)-3,7-dimethyloctyl (E)-4-(2,6,6-trimethyl-2,4,5-trimethyl-5-(1,3-benzodioxol-5-yl)-2,6-dimethyl-[(2E,4E,6E,8E)-3,7-dimethyl-6,10,14,18E)-2,6-dimethyl-(E)-stilbene methyl (E)-but-2-ene (E)-1-(2,4-dihydroxyphenyl)-[(2E,6E)-3,7,11-trimethyl-4-(4S)-4-bromo-5,5-dimethyl-13aR)-2,3,6-trimethyl-(E)-3-(4-methoxyphenyl)-	2.000	3.950	3.013	1345.092	681.578
(2E)-3,7-dimethyloctyl (E)-4-(2,6,6-trimethyl-2,4,5-trimethyl-5-(1,3-benzodioxol-5-yl)-2,6-dimethyl-[(2E,4E,6E,8E)-3,7-dimethyl-6,10,14,18E)-2,6-dimethyl-(E)-stilbene methyl (E)-but-2-ene (E)-1-(2,4-dihydroxyphenyl)-[(2E,6E)-3,7,11-trimethyl-4-(4S)-4-bromo-5,5-dimethyl-13aR)-2,3,6-trimethyl-(E)-3-(4-methoxyphenyl)-	0.000	2.000	2.314	1634.222	841.229
(E)-4-(2,6,6-trimethyl-2,4,5-trimethyl-5-(1,3-benzodioxol-5-yl)-2,6-dimethyl-[(2E,4E,6E,8E)-3,7-dimethyl-6,10,14,18E)-2,6-dimethyl-(E)-stilbene methyl (E)-but-2-ene (E)-1-(2,4-dihydroxyphenyl)-[(2E,6E)-3,7,11-trimethyl-4-(4S)-4-bromo-5,5-dimethyl-13aR)-2,3,6-trimethyl-(E)-3-(4-methoxyphenyl)-	0.000	2.000	3.100	3397.034	1855.266
(2E,4E)-5-(1,3-benzodioxol-5-yl)-2,6-dimethyl-[(2E,4E,6E,8E)-3,7-dimethyl-6,10,14,18E)-2,6-dimethyl-(E)-stilbene methyl (E)-but-2-ene (E)-1-(2,4-dihydroxyphenyl)-[(2E,6E)-3,7,11-trimethyl-4-(4S)-4-bromo-5,5-dimethyl-13aR)-2,3,6-trimethyl-(E)-3-(4-methoxyphenyl)-	0.000	4.500	3.261	4158.907	2308.837
[(2E,4E,6E,8E)-3,7-dimethyl-6,10,14,18E)-2,6-dimethyl-(E)-stilbene methyl (E)-but-2-ene (E)-1-(2,4-dihydroxyphenyl)-[(2E,6E)-3,7,11-trimethyl-4-(4S)-4-bromo-5,5-dimethyl-13aR)-2,3,6-trimethyl-(E)-3-(4-methoxyphenyl)-	0.000	2.000	6.374	2317.536	1227.158
(6E,10E,14E,18E)-2,6-dimethyl-(E)-stilbene methyl (E)-but-2-ene (E)-1-(2,4-dihydroxyphenyl)-[(2E,6E)-3,7,11-trimethyl-4-(4S)-4-bromo-5,5-dimethyl-13aR)-2,3,6-trimethyl-(E)-3-(4-methoxyphenyl)-	0.000	0.000	12.587	9906.038	5899.293
(E)-stilbene 180.249	0.000	0.000	4.775	9906.038	5899.293
methyl (E)-but-2-ene 100.117	0.000	2.000	0.612	2307.995	1221.698
(E)-1-(2,4-dihydroxyphenyl)-[(2E,6E)-3,7,11-trimethyl-4-(4S)-4-bromo-5,5-dimethyl-13aR)-2,3,6-trimethyl-(E)-3-(4-methoxyphenyl)-	2.000	3.250	2.043	147.437	62.476
[(2E,6E)-3,7,11-trimethyl-4-(4S)-4-bromo-5,5-dimethyl-13aR)-2,3,6-trimethyl-(E)-3-(4-methoxyphenyl)-	0.000	2.000	5.215	2293.845	1213.604
(4S)-4-bromo-5,5-dimethyl-13aR)-2,3,6-trimethyl-(E)-3-(4-methoxyphenyl)-	0.000	2.000	2.474	3574.326	10000.000
(13aR)-2,3,6-trimethyl-(E)-3-(4-methoxyphenyl)-	0.000	4.250	4.345	2031.622	1177.528
(E)-3-(4-methoxyphenyl)-	0.000	2.750	2.055	1561.733	800.969

1-methoxy-4-[(E)-2-(240.301	0.000	1.500	4.442	9906.038	5899.293
(3Z)-3-butylidene-2-t 188.226	0.000	2.500	2.487	2115.842	1112.138
methyl (1S,15S,18S,1354.448	1.000	4.700	3.377	242.988	118.609
(Z,12R)-12-hydroxyo 298.465	2.000	3.700	4.322	176.958	96.789
(2E,6Z)-nona-2,6-die 138.209	0.000	2.000	2.078	1559.171	799.550
(Z)-prop-1-ene-1,2,3 174.110	3.000	6.000	-0.091	0.288	0.151
(2Z)-3,7-dimethyloct 152.236	0.000	2.000	2.330	1794.669	930.844
(Z)-2-methylbut-2-er 130.100	2.000	4.000	0.077	7.693	4.153
methyl (Z)-hexadec-ε 268.439	0.000	2.000	5.693	3034.623	1642.284
(2Z)-3,7-dimethyloct 154.252	1.000	1.700	2.571	2898.911	1563.044
[[[(2R,3S,4R,5R)-5-(6- 785.557	8.000	27.700	-2.922	0.009	0.003
[(2S,3R,4S,5S,6R)-3,4 464.461	7.000	14.750	-1.002	1.582	0.898
(1R,4R)-1,7,7-trimetl 154.252	1.000	1.700	2.080	4398.979	2453.224
(3S)-1,2,3,9-tetrahyd 188.229	1.000	3.200	1.899	2347.200	1244.144
4-[(E)-2-(3,5-dihydro 244.246	4.000	3.000	1.286	98.622	40.454
[(9S)-8,8-dimethyl-2- 328.364	0.000	5.250	3.285	1158.490	579.976
ethyl (E)-3-(4-hydrox 192.214	1.000	2.750	2.055	791.001	383.965
(2S)-7-hydroxy-2-phē 240.258	1.000	3.500	2.451	992.450	490.674
(E)-3-(3,4-dihydroxyγ 180.160	3.000	3.500	0.550	22.104	10.218
(E)-3-(2-bromo-4,5-d 287.109	1.000	3.500	2.686	204.668	266.584
phenyl 4-methylpipe 219.283	0.000	3.000	3.172	4515.353	2523.447
phenyl (E)-3-phenylp 224.259	0.000	2.500	3.525	4118.506	2284.604
15,16-dimethoxy-10- 293.365	0.000	2.500	4.507	9162.405	5422.111
2-methoxy-4-[(E)-prc 164.204	1.000	1.500	2.818	3043.888	1647.704
(2R)-2-hydroxy-2-(3-l 198.175	3.000	5.200	0.337	34.919	16.750
9-hydroxy-6-phenyl-l 282.252	0.000	3.750	2.460	1204.588	604.960
(3aR,5aS,9aS,9bR)-3ε 250.380	0.000	3.000	2.896	2379.410	1262.609
(1E,6E)-1,7-bis(4-hyd 368.385	2.000	7.000	2.803	151.730	64.444
(1S,2R,4S)-1,7,7-trim 154.252	1.000	1.700	2.061	4097.081	2271.760
(1S,3R,5S)-6,6-dimet 152.236	1.000	1.700	2.145	4052.534	2245.074
1-[(2S)-1-methylpyrr 224.345	0.000	6.000	0.953	364.845	203.610
(4R,4aS,6R)-4,4a-dir 218.338	0.000	2.000	3.395	2805.564	1508.713
(1R,2R,5S)-2,6,6-trim 154.252	1.000	0.750	2.578	5451.921	3093.662

(1R,2R,4S,5S)-9-metf	155.196	1.000	5.700	-0.353	799.156	429.522
2-piperidin-4-ylacetic	143.185	2.000	3.500	-1.549	36.503	19.441
(E)-N-[(4-hydroxy-3-r	305.416	2.000	4.000	3.628	1017.850	695.281
3-methyl-2-[(Z)-pent	164.247	0.000	2.000	2.593	3659.159	2010.474
[(2E)-3,7-dimethyloc	196.289	0.000	2.000	3.505	2265.727	1197.532
2-methoxy-4-[(Z)-prc	164.204	1.000	1.500	2.764	3042.608	1646.955
1,2-dimethoxy-4-[(Z)	178.230	0.000	1.500	2.665	9906.038	5899.293
4-[(E)-3-hydroxyprop	180.203	2.000	3.200	1.372	1030.179	510.866
(2Z,6Z)-3,7,11-trimet	222.370	1.000	1.700	3.988	2887.569	1556.435
(5E)-6,10-dimethylur	194.316	0.000	2.000	3.683	3163.586	1717.849
7-[(2E)-3,7-dimethyl	298.381	0.000	3.250	4.612	2056.174	1078.278
piperidine-1-carboth	144.234	2.000	2.500	1.300	2867.994	3589.018
(5E,9E)-6,10,14-trim	262.434	0.000	2.000	4.796	3802.366	2095.654
(5Z)-6,10-dimethylur	194.316	0.000	2.000	3.717	6529.271	3759.433
(1R,12R)-16-methoxy	298.295	0.000	3.750	2.568	9906.038	5899.293
(1R,4R,6R,10S)-4,12,	220.354	0.000	2.000	2.487	9906.038	5899.293
(1S,3R,4R,5R)-3-[(Z)-	354.313	6.000	9.650	-0.120	2.905	1.139
(1S,3R,4R,5R)-3-[(E)-	354.313	6.000	9.650	-0.230	1.726	0.649
(1S,3R,4R,5R)-3-[(E)-	354.313	6.000	9.650	-0.230	1.725	0.649
(1R,2S,7S,9S)-3,3,7-ti	204.355	0.000	0.000	4.845	9906.038	5899.293
(3S,4aR,6aS,10aS,10l	290.488	0.000	0.750	4.438	9906.038	5899.293
(3S,4R,5R)-2-(hydrox	180.157	5.000	8.300	-1.693	100.926	41.476
(1R,2S,3S,4R,5R)-6,8-	162.142	3.000	8.500	-1.390	470.808	219.146
(5S)-5-(hydroxymeth	116.116	1.000	4.700	-0.581	622.758	296.506
4-fluoro-2-methoxyp	142.130	1.000	1.500	1.826	3042.908	2971.965
(2S,3R)-2-amino-4-hy	147.174	4.000	4.700	-2.500	13.761	6.773
1-(2-hydroxy-6-phen	242.274	0.000	2.500	3.302	1479.604	755.540
3-(4-fluorophenyl)an	187.216	1.500	1.000	2.930	2580.808	2489.218
4-methoxy-2-oxo-1H	150.137	1.000	4.750	-0.045	340.178	154.234
[(1R,2R,4S,5S)-9-met	303.357	0.000	6.700	1.246	470.459	242.251
2-(dithiocarboxyamir	212.361	3.600	4.000	2.015	5103.117	10000.000
[(1R,7R,8S,26R,28S,2	952.656	14.000	24.950	-4.108	0.001	0.000
3,8-dimethyl-5-prop	218.338	1.000	0.750	3.869	3628.816	1992.460

3-methylidenepenta	116.160	2.000	3.400	0.375	1218.350	612.435
2-acetyl-4-hydroxy-3	210.186	2.000	5.500	0.704	77.653	39.736
octadecanoate	284.481	1.000	2.000	6.064	292.253	166.470
2-carbamothioylsulf	212.361	4.000	4.000	0.953	443.963	2456.838
(4Z)-1-methyl-4-(6-r	204.355	0.000	0.000	6.215	9906.038	5899.293
[(1S,6S,7aS)-4-(acety	422.474	0.000	9.700	2.980	638.447	304.588
(R)-[(2S,4S,5R)-5-eth	324.422	1.000	5.450	3.438	636.817	336.041
(3R)-5-[(1S,4aS,8aS)-	290.488	1.000	0.750	5.601	5259.381	2975.740
(1R,2S,4S,6R,7S,8R,9	416.643	1.000	3.200	6.181	3632.379	1994.575
(2S,3S)-2-(3,4-dihydr	466.398	7.000	14.950	-1.643	2.970	0.918
(2S,3R,4S,5R)-2,3,4,5	210.140	4.000	8.800	-1.478	0.360	0.152
methyl (2R)-2-[(2S,3f	354.448	1.000	4.700	3.659	258.870	127.011
9-[[[(2R)-3,3-dimethyl	316.310	0.000	6.500	2.096	2664.221	1426.728
[(1S,4aS,6S,7aS)-6-ac	480.511	0.000	11.700	2.698	574.697	271.851
2-(dimethylamino)et	215.335	0.000	4.000	2.684	676.897	358.959
(2R)-3,3,3-trifluoro-2	252.620	0.000	2.000	3.193	4483.524	10000.000
15-hydroxy-14-meth	265.268	2.000	4.000	1.884	563.370	266.065
2-(3,4,5-trihydroxypt	322.271	7.000	7.900	-0.962	9.904	3.373
(5R,6R)-6-ethenyl-3,t	230.306	0.000	2.500	3.349	5707.497	3250.710
5-hydroxy-7-methox	220.224	0.000	3.000	2.167	1569.583	805.322
(1S,2S,4S,5'R,6R,7S,8	430.626	2.000	4.900	5.075	1305.296	659.808
hexa-2,4-diyanylbenz	154.211	0.000	0.000	5.048	9906.038	5899.293
(3S,4S,4aR,6aR,6bS,8	440.708	2.000	3.400	6.088	2076.924	1090.044
17-methyloctadecan	298.508	1.000	2.000	6.356	235.543	131.847
furo[2,3-f]chromen-7	186.167	0.000	3.000	0.969	2057.275	1078.902
1,5,8-trimethyl-1,2-d	242.274	0.000	4.750	1.650	1545.521	791.986
(3R,3aS,6S,6aR)-3,6-l	370.358	1.000	7.150	2.498	5085.496	2869.543
(2R,3S,4S,5R,6S)-2-(f	326.346	4.000	10.000	0.496	234.584	103.209
(1R,4S,4aR,8aS)-1,6-c	222.370	1.000	0.750	4.055	4677.161	2621.329
(1S,4S,4aR,8aS)-1,6-c	222.370	1.000	0.750	4.080	5030.076	2835.757
(2S,3S,4S,5R,6S)-3,4,	460.393	3.000	11.550	1.003	2.452	0.949
N-[6-(2-hydroxy-3,4-	381.384	1.000	6.750	3.039	1732.257	895.905
5-[2-(3-hydroxy-5-m	274.316	2.000	3.000	3.422	923.328	453.841

2-(4-hydroxyphenyl)-	290.272	5.000	6.400	0.320	76.723	30.838
3-hydroxybutanoate	104.105	1.000	2.700	0.819	101.032	52.811
2-(3,4-dihydroxyphenyl)-	596.541	8.000	20.050	-2.045	0.921	0.259
2-hydroxy-2-oxoacet	90.035	2.000	4.000	-0.701	4.221	2.171
5-[[2-(dimethylamino)-	336.473	0.000	7.500	1.630	197.374	104.810
(2,4-dinitrophenyl)hy	198.138	3.000	3.500	-1.014	7.157	2.627
3-methyl-5-propylcyclo	152.236	0.000	2.000	2.149	2793.411	1501.651
3-benzamido-3-(4-propyl	327.379	1.000	4.250	4.547	164.398	89.385
2-[[2-amino-3-(1H-imidazol	268.315	4.250	6.250	-1.886	4.989	3.298
3,8-dimethyl-3-(4-methyl	331.457	1.000	0.750	6.462	6660.663	3841.270
1,4,4,8-tetramethyl-1,4-	236.353	0.000	2.750	3.191	4392.066	2449.058
1,3,3-trimethyl-2-[[1-(2S)-	536.882	0.000	0.000	16.736	9906.038	5899.293
3-[[3S,5R,8R,9S,10S,11R)-	374.519	2.000	5.450	3.119	483.972	225.776
[2-[[[(2S)-1-[[[(2S)-3-cyano	1082.089	8.750	25.900	-4.853	0.000	0.000
2-hydroxy-2-methyl-1-	148.115	2.000	3.750	0.172	5.909	3.123
1-N,4-N-bis(3-methyl-2-	330.429	2.000	4.000	4.422	766.347	371.046
2-[[2-amino-3-(1H-imidazol	302.332	4.250	6.250	-1.262	8.301	5.345
N-(3-chlorophenyl)-3-	378.857	2.000	5.000	4.940	1324.562	1651.028
N-[3-(3,5-dimethylpyridin	266.305	0.000	4.500	2.997	1817.379	943.582
[2-(9H-pyrido[3,4-b]indol	264.283	2.000	3.200	3.084	2366.556	1255.238
3-(2,4-dihydroxyphenyl)-	256.257	3.000	4.250	1.444	126.608	52.993
2-(3,4,5-trihydroxyphenyl)-	610.527	12.000	12.400	-0.436	0.768	0.213
17-methoxy-5,7-dioxabicyclo	325.363	1.000	5.000	2.642	718.326	382.763
methyl 14-ethylidene-1-	382.458	1.000	6.500	2.135	99.923	50.219
diethyl phosphate	154.102	1.000	5.000	0.723	375.049	230.858
methyl 4-hydroxy-2-methyl-	424.449	3.000	7.250	2.765	76.454	30.721
dibutyl (E)-but-2-ene-1-	228.288	0.000	4.000	2.624	656.603	313.961
5,7-dihydroxy-8-[5-(E)-	566.520	2.000	7.500	4.433	19.351	6.958
7,8-dihydroxy-6-methyl-	208.170	2.000	4.750	0.292	235.020	103.416
(2S,3S,4S,5R,6S)-6-[2-	478.365	6.000	13.050	-0.795	0.325	0.107
(1R)-1-[[4-hydroxy-3-	610.749	2.000	8.250	5.888	109.623	55.508
(2S)-2-(2,4-dihydroxyphenyl)-	356.374	3.000	4.750	2.640	105.449	43.488
[[3S,6aR,6bS,8aR,11f	468.762	0.000	2.000	7.945	3922.168	2167.113

(E,2S,3R)-2-aminooc	299.496	4.000	4.400	3.350	134.176	62.424
2-(3,4-dihydroxyphei	302.240	4.000	5.250	0.367	18.199	6.511
4-hydroxyfuro[3,2-g]	202.166	1.000	3.750	1.002	834.209	406.684
(2R,3S,4S,5R,6S)-2-(f	342.345	5.000	11.700	-0.459	79.355	31.983
5,7-dihydroxy-3-(4-r	284.268	1.000	3.750	2.546	531.546	249.857
7-hydroxy-3-(4-meth	268.268	1.000	4.000	2.629	1242.040	625.316
[(2S,3R,4S,5S,6R)-3,4	386.355	5.000	12.750	-0.665	29.056	10.797
(E,7R,11R)-3,7,11,15-	296.535	1.000	1.700	6.304	2861.605	1541.314
5,7-dihydroxy-2-(4-h	432.383	6.000	12.250	-0.687	6.673	2.202
5,7-dihydroxy-2-(4-r	284.268	1.000	3.750	2.461	377.526	172.615
2-(3,4-dihydroxyphei	286.240	3.000	4.500	0.926	40.856	15.606
7-hydroxy-3-(3-hydr	284.268	2.000	4.750	1.948	382.000	174.828
(9Z,12Z)-octadeca-9,	280.450	1.000	2.000	5.290	239.318	134.132
(1R,3S,5Z)-5-[(2E)-2-	416.643	3.000	4.150	5.595	689.880	331.195
2-(3,4-dihydroxyphei	448.382	6.000	12.050	-0.548	7.035	2.331
7-hydroxy-6-methox	192.171	1.000	4.000	0.854	632.798	301.676
[(1R,10S,12R,13E,14I	512.558	5.000	13.200	1.380	82.114	33.187
1,3,3-trimethyl-2-[(1	536.882	0.000	0.000	16.599	9906.038	5899.293
4-[(E)-3-hydroxyprop	210.229	2.000	3.950	1.384	1050.261	521.639
(2S)-2-hydroxy-2-pro	176.169	2.000	3.750	0.572	9.352	5.129
(E)-3-(4-hydroxy-3-m	178.187	1.000	3.500	1.132	479.894	223.720
3,5,7,8-tetrahydroxy	302.240	4.000	5.250	0.429	19.986	7.205
methyl (E)-octadec-9	296.492	0.000	2.000	6.511	3034.999	1642.504
(1R,3R,4S,5R)-3-[(E)-	354.313	6.000	9.650	-0.236	1.680	0.631
2-(3,4-dihydroxyphei	448.382	6.000	13.000	-0.912	4.102	1.301
2-(3,4-dihydroxyphei	318.239	5.000	6.000	-0.227	8.545	2.876
[(2S,3R,4S,5S,6R)-4,5	592.552	5.000	15.300	1.540	14.152	4.961
5,7-dihydroxy-2-(4-h	300.267	2.000	4.500	1.759	115.921	48.175
5-hydroxy-2-(4-hydr	432.383	5.000	12.250	-0.318	10.046	3.426
7-[(2S,3R,4S,5S,6R)-3	564.499	7.000	18.100	-1.274	2.770	0.851
5-hydroxy-3-(4-meth	446.410	4.000	12.250	0.458	37.847	14.367
(6E,10E,14E,16E,18E	544.946	0.000	0.000	17.758	9906.038	5899.293
(3S,8S,9S,10R,13R,14	412.698	1.000	1.700	7.737	3379.989	1845.206

2-(3,4-dihydroxypher	464.382	7.000	13.750	-1.427	2.509	0.765
2-(3,4-dihydroxypher	610.524	9.000	20.550	-2.595	0.740	0.204
(Z)-3-(2-hydroxypher	164.160	2.000	2.750	1.527	106.282	55.784
3,5,7-trihydroxy-2-(4	286.240	3.000	4.500	1.041	51.240	19.934
(2Z,4E)-5-[(1S)-1-hyd	264.321	2.000	4.750	2.193	50.274	24.837
(1R)-4-[(1E,3E,5E,7E,	568.881	2.000	3.400	10.567	1146.262	573.362
(6Z,9Z,12Z)-octadeca	278.434	1.000	2.000	5.487	385.656	224.657
(9Z,12Z,15Z)-octadec	278.434	1.000	2.000	5.281	235.280	131.688
methyl (1R,15S,17R,	634.725	1.000	10.700	5.938	565.409	295.504
(E)-3-(4-hydroxypher	272.257	2.000	3.000	1.994	75.865	30.465
5,7-dihydroxy-3-(4-h	270.241	2.000	3.750	1.694	161.820	69.089
(E)-1-chloro-3-ethylp	144.600	1.500	0.750	2.429	5019.226	7536.448
(Z)-docos-13-enoic a	338.573	1.000	2.000	7.468	279.316	158.520
(Z)-tetradec-9-enoic	226.358	1.000	2.000	4.353	235.292	131.695
(Z)-tetracos-15-enoic	366.626	1.000	2.000	8.163	235.920	132.075
(Z)-octadec-6-enoic ε	282.465	1.000	2.000	5.917	301.371	172.091
(3R,8S,9Z)-heptadec	260.375	2.000	3.400	3.371	1043.513	518.017
ethyl (2E,4Z)-deca-2,	196.289	0.000	2.000	3.669	2610.272	1395.526
(Z)-hex-3-en-1-ol	100.160	1.000	1.700	1.382	2878.516	1551.161
(E)-hex-2-enal	98.144	0.000	2.000	1.218	1559.189	799.559
(2S,4E)-4-(2-oxoethy	211.174	3.000	7.000	-0.332	0.888	0.402
(1R,3S,6S)-6-[(1E,3E,	584.881	1.000	4.400	10.483	1154.697	577.924
(6S)-6-hydroxy-3-[(1f	596.848	2.000	7.400	8.322	202.861	88.209
2,2,6-trimethyl-1-[(1	552.882	0.000	2.000	10.548	9906.038	5899.293
(2E,4E,6E,8E,10E,12E	328.407	2.000	4.000	4.857	6.433	3.423
(1R)-3,5,5-trimethyl-	552.882	1.000	1.700	11.860	3371.655	1840.289
(1R)-3,5,5-trimethyl-	552.882	1.000	1.700	11.797	3369.288	1838.892
2,4,4-trimethyl-3-[(1	550.866	0.000	2.000	11.805	3667.777	2015.592
(1R)-4-[(1E,3E,5E,7E,	568.881	2.000	3.400	10.666	1129.274	564.183
(1R,3S,6S)-6-[(1E,3E,	584.881	1.000	4.400	10.512	1137.622	568.692
(2E,6E,8E,10E,12E,14	552.882	1.000	1.700	12.853	4344.689	2420.516
(E)-1-[2,4-dihydroxy-	324.376	2.000	3.250	3.875	336.513	152.439
dimethyl (1S,4S,5R,6	720.723	3.000	19.050	1.275	259.433	115.075

[(1S,4R,5R,6R,7S,8R,9S,10R,11R,12S,13R,14S,15R,16S,17R,18S,19R,20S,21R,22S,23R,24S,25R,26S,27R,28S,29R,30S,31R,32S,33R,34S,35R,36S,37R,38S,39R,40S,41R,42S,43R,44S,45R,46S,47R,48S,49R,50S,51R,52S,53R,54S,55R,56S,57R,58S,59R,60S,61R,62S,63R,64S,65R,66S,67R,68S,69R,70S,71R,72S,73R,74S,75R,76S,77R,78S,79R,80S,81R,82S,83R,84S,85R,86S,87R,88S,89R,90S,91R,92S,93R,94S,95R,96S,97R,98S,99R,100S,101R,102S,103R,104S,105R,106S,107R,108S,109R,110S,111R,112S,113R,114S,115R,116S,117R,118S,119R,120S,121R,122S,123R,124S,125R,126S,127R,128S,129R,130S,131R,132S,133R,134S,135R,136S,137R,138S,139R,140S,141R,142S,143R,144S,145R,146S,147R,148S,149R,150S,151R,152S,153R,154S,155R,156S,157R,158S,159R,160S,161R,162S,163R,164S,165R,166S,167R,168S,169R,170S,171R,172S,173R,174S,175R,176S,177R,178S,179R,180S,181R,182S,183R,184S,185R,186S,187R,188S,189R,190S,191R,192S,193R,194S,195R,196S,197R,198S,199R,200S,201R,202S,203R,204S,205R,206S,207R,208S,209R,210S,211R,212S,213R,214S,215R,216S,217R,218S,219R,220S,221R,222S,223R,224S,225R,226S,227R,228S,229R,230S,231R,232S,233R,234S,235R,236S,237R,238S,239R,240S,241R,242S,243R,244S,245R,246S,247R,248S,249R,250S,251R,252S,253R,254S,255R,256S,257R,258S,259R,260S,261R,262S,263R,264S,265R,266S,267R,268S,269R,270S,271R,272S,273R,274S,275R,276S,277R,278S,279R,280S,281R,282S,283R,284S,285R,286S,287R,288S,289R,290S,291R,292S,293R,294S,295R,296S,297R,298S,299R,300S,301R,302S,303R,304S,305R,306S,307R,308S,309R,310S,311R,312S,313R,314S,315R,316S,317R,318S,319R,320S,321R,322S,323R,324S,325R,326S,327R,328S,329R,330S,331R,332S,333R,334S,335R,336S,337R,338S,339R,340S,341R,342S,343R,344S,345R,346S,347R,348S,349R,350S,351R,352S,353R,354S,355R,356S,357R,358S,359R,360S,361R,362S,363R,364S,365R,366S,367R,368S,369R,370S,371R,372S,373R,374S,375R,376S,377R,378S,379R,380S,381R,382S,383R,384S,385R,386S,387R,388S,389R,390S,391R,392S,393R,394S,395R,396S,397R,398S,399R,400S,401R,402S,403R,404S,405R,406S,407R,408S,409R,410S,411R,412S,413R,414S,415R,416S,417R,418S,419R,420S,421R,422S,423R,424S,425R,426S,427R,428S,429R,430S,431R,432S,433R,434S,435R,436S,437R,438S,439R,440S,441R,442S,443R,444S,445R,446S,447R,448S,449R,450S,451R,452S,453R,454S,455R,456S,457R,458S,459R,460S,461R,462S,463R,464S,465R,466S,467R,468S,469R,470S,471R,472S,473R,474S,475R,476S,477R,478S,479R,480S,481R,482S,483R,484S,485R,486S,487R,488S,489R,490S,491R,492S,493R,494S,495R,496S,497R,498S,499R,500S,501R,502S,503R,504S,505R,506S,507R,508S,509R,510S,511R,512S,513R,514S,515R,516S,517R,518S,519R,520S,521R,522S,523R,524S,525R,526S,527R,528S,529R,530S,531R,532S,533R,534S,535R,536S,537R,538S,539R,540S,541R,542S,543R,544S,545R,546S,547R,548S,549R,550S,551R,552S,553R,554S,555R,556S,557R,558S,559R,560S,561R,562S,563R,564S,565R,566S,567R,568S,569R,570S,571R,572S,573R,574S,575R,576S,577R,578S,579R,580S,581R,582S,583R,584S,585R,586S,587R,588S,589R,590S,591R,592S,593R,594S,595R,596S,597R,598S,599R,600S,601R,602S,603R,604S,605R,606S,607R,608S,609R,610S,611R,612S,613R,614S,615R,616S,617R,618S,619R,620S,621R,622S,623R,624S,625R,626S,627R,628S,629R,630S,631R,632S,633R,634S,635R,636S,637R,638S,639R,640S,641R,642S,643R,644S,645R,646S,647R,648S,649R,650S,651R,652S,653R,654S,655R,656S,657R,658S,659R,660S,661R,662S,663R,664S,665R,666S,667R,668S,669R,670S,671R,672S,673R,674S,675R,676S,677R,678S,679R,680S,681R,682S,683R,684S,685R,686S,687R,688S,689R,690S,691R,692S,693R,694S,695R,696S,697R,698S,699R,700S,701R,702S,703R,704S,705R,706S,707R,708S,709R,710S,711R,712S,713R,714S,715R,716S,717R,718S,719R,720S,721R,722S,723R,724S,725R,726S,727R,728S,729R,730S,731R,732S,733R,734S,735R,736S,737R,738S,739R,740S,741R,742S,743R,744S,745R,746S,747R,748S,749R,750S,751R,752S,753R,754S,755R,756S,757R,758S,759R,760S,761R,762S,763R,764S,765R,766S,767R,768S,769R,770S,771R,772S,773R,774S,775R,776S,777R,778S,779R,780S,781R,782S,783R,784S,785R,786S,787R,788S,789R,790S,791R,792S,793R,794S,795R,796S,797R,798S,799R,800S,801R,802S,803R,804S,805R,806S,807R,808S,809R,810S,811R,812S,813R,814S,815R,816S,817R,818S,819R,820S,821R,822S,823R,824S,825R,826S,827R,828S,829R,830S,831R,832S,833R,834S,835R,836S,837R,838S,839R,840S,841R,842S,843R,844S,845R,846S,847R,848S,849R,850S,851R,852S,853R,854S,855R,856S,857R,858S,859R,860S,861R,862S,863R,864S,865R,866S,867R,868S,869R,870S,871R,872S,873R,874S,875R,876S,877R,878S,879R,880S,881R,882S,883R,884S,885R,886S,887R,888S,889R,890S,891R,892S,893R,894S,895R,896S,897R,898S,899R,900S,901R,902S,903R,904S,905R,906S,907R,908S,909R,910S,911R,912S,913R,914S,915R,916S,917R,918S,919R,920S,921R,922S,923R,924S,925R,926S,927R,928S,929R,930S,931R,932S,933R,934S,935R,936S,937R,938S,939R,940S,941R,942S,943R,944S,945R,946S,947R,948S,949R,950S,951R,952S,953R,954S,955R,956S,957R,958S,959R,960S,961R,962S,963R,964S,965R,966S,967R,968S,969R,970S,971R,972S,973R,974S,975R,976S,977R,978S,979R,980S,981R,982S,983R,984S,985R,986S,987R,988S,989R,990S,991R,992S,993R,994S,995R,996S,997R,998S,999R,1000S,1001R,1002S,1003R,1004S,1005R,1006S,1007R,1008S,1009R,1010S,1011R,1012S,1013R,1014S,1015R,1016S,1017R,1018S,101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3,5,7-trihydroxy-2-pl	270.241	2.000	3.750	1.777	168.867	72.347
5-hydroxy-2-(4-hydroxy)	284.268	1.000	3.750	2.462	378.255	172.976
1,3,5,8-tetrahydroxy	260.203	2.000	3.500	0.979	62.745	24.813
5,7-dihydroxy-2-(4-hydroxy)	300.267	2.000	4.500	1.854	176.379	75.831
2-(3,4-dihydroxyphe)	302.240	4.000	5.250	0.317	17.984	6.428
2-(3,4-dihydroxyphe)	464.382	7.000	13.750	-1.397	2.795	0.859
5,9,10-trihydroxy-2,2	326.305	2.000	4.500	2.351	208.712	90.962
1,3,6,7-tetrahydroxy	422.345	7.000	13.000	-1.785	2.597	0.794
1,8-dihydroxy-2,6-dihydroxy	288.256	0.000	3.500	2.496	659.966	315.700
3,5,7-trihydroxy-2-(4-hydroxy)	316.267	3.000	5.250	1.199	51.836	20.185
1,8-dihydroxy-3,5-dihydroxy	288.256	0.000	3.500	2.480	645.347	308.148
1,2,8-trihydroxy-6-methoxy	274.229	1.000	3.500	1.829	236.607	104.171
2-(2,4-dihydroxyphe)	302.240	4.000	5.250	0.399	20.472	7.394
2-(2,4-dihydroxyphe)	420.461	2.000	4.500	4.408	241.517	106.510
3,5,7-trihydroxy-2-(3,4-dihydroxy)	318.239	5.000	6.000	-0.299	6.527	2.149
5,7-dihydroxy-3-[(2S,3S)-2,3-dihydroxybutyl]	464.382	7.000	12.800	-1.189	2.504	0.763
2-(3,4-dihydroxyphe)	448.382	7.000	13.000	-1.351	2.387	0.725
2-(3,4-dihydroxyphe)	332.266	4.000	6.000	0.615	30.830	11.511
2-(3,4-dihydroxyphe)	318.239	5.000	6.000	-0.237	8.798	2.968
2-(3,4-dihydroxyphe)	316.267	3.000	5.250	1.218	60.032	23.655
3,7-dihydroxy-2-(3,4-dihydroxy)	302.240	5.000	6.250	-0.178	15.200	5.360
5-hydroxy-2-(4-hydroxy)	740.668	10.000	26.600	-3.132	0.468	0.125
5,7-dihydroxy-2-(4-hydroxy)	330.293	2.000	5.250	1.913	118.421	49.299
5,7-dihydroxy-8-methoxy	284.268	1.000	3.750	2.428	452.096	209.747
3,9-dihydroxy-[1]benzofuran	268.225	2.000	4.500	1.305	236.404	104.074
7-hydroxy-3-(4-hydroxy)	254.242	2.000	4.000	1.790	376.266	171.993
4,5,6,12,19,20,21,27-octahydroxy	602.377	8.000	16.000	-2.895	0.049	0.011
5-[(E)-2-(2,4-dihydroxyphenyl)]	380.483	4.000	3.000	4.754	273.260	121.718
4-[(E)-2-(3,5-dihydroxyphenyl)]	244.246	4.000	3.000	1.290	102.260	42.069
(2S,3R,4S,5S,6R)-2-[3-(3,4-dihydroxyphenyl)propyl]	390.389	6.000	10.750	0.138	25.137	9.232
5-[(E)-2-(4-hydroxyphenyl)]	296.365	3.000	2.250	3.822	626.791	298.582
4-[(E)-2-(3,5-dimethoxyphenyl)]	256.301	1.000	2.250	3.930	3004.809	1624.851
1,2,4-trimethoxy-5-[(E)-2-(3,4-dihydroxyphenyl)]	208.257	0.000	2.250	2.780	9906.038	5899.293

(2R,3R)-2,3-bis[[E)-3	474.377	6.000	11.000	0.916	0.028	0.009
(3R,5R)-1,3,5-trihydr	338.313	5.000	8.900	0.415	4.778	1.951
(E)-1,7-bis(4-hydroxy	356.418	2.000	5.000	3.835	393.706	180.626
9-hydroxy-7-(4-hydr	298.251	1.000	4.500	2.008	516.424	242.183
(1S,3R,4R,5R)-3,4-bis	516.457	7.000	11.450	0.939	0.289	0.094
5,7-dihydroxy-6-met	314.294	1.000	4.500	2.710	843.597	411.634
ethyl (E)-3-(4-metho	206.241	0.000	2.750	2.837	2615.611	1398.612
3-[2,4-dihydroxy-3-(354.359	3.000	4.500	2.813	173.587	74.535
(2R)-3-(3,4-dihydrox)	360.320	5.000	7.000	1.213	1.738	0.654
(2R)-3-(3,4-dihydrox)	494.454	7.000	8.500	1.936	0.374	0.124
(E)-1-(4-hydroxy-3-m	276.375	1.000	3.500	4.043	1203.090	604.147
5-hydroxy-3-(4-hydr	284.268	1.000	3.750	2.536	533.709	250.957
3-(1,3-benzodioxol-5	282.252	1.000	4.750	2.087	1240.427	624.438
3,9-dihydroxy-2-(3-r	336.343	2.000	4.500	2.973	304.516	136.834
7-hydroxy-3-(4-hydr	416.384	6.000	12.500	-0.626	11.776	4.068
7-hydroxy-17,17-dim	336.343	1.000	4.500	3.168	776.856	376.549
5-hydroxy-3-(4-hydr	462.409	5.000	13.000	-0.114	16.527	5.867
5,7-dihydroxy-3-(4-h	300.267	2.000	4.500	1.892	255.572	113.225
6,7-dihydroxy-3-(4-r	284.268	2.000	4.750	1.966	444.229	205.805
1,8,9-trihydroxy-3-m	314.251	3.000	6.000	0.845	102.902	42.354
(E)-1-[6-[(3-acetyl-2,	516.546	2.000	5.500	5.589	152.437	64.769
5-[(Z)-pentadec-8-en	318.498	2.000	1.500	5.775	909.965	446.746
6,7,13,14-tetrahydro	302.197	4.000	8.000	-1.295	7.907	2.645
2-hydroxy-6-[(Z)-pen	346.509	1.000	1.750	6.518	132.554	70.827
6-hydroxy-7,13,14-tr	344.277	1.000	8.000	0.866	261.160	115.903
[(6R,7S)-6,7-dihydro	255.313	2.000	7.400	0.505	214.904	103.864
3,5,7-trihydroxy-2-(4	346.293	3.000	6.000	1.353	52.806	20.593
7-hydroxy-2-(4-hydr	254.242	2.000	4.000	1.799	268.555	119.455
3-(2,4-dihydroxyphei	286.240	3.000	4.500	1.059	67.862	27.007
5,7-dihydroxy-2-(4-h	448.382	6.000	13.000	-0.749	9.568	3.250
(E)-4-(2,6,6-trimethy	192.300	0.000	2.000	3.143	3403.889	1859.312
7-[(2S,3R,4S,5S,6R)-4	578.526	7.000	19.050	-1.505	2.076	0.623
3-[(2S,3R,4S,5S,6R)-4	610.524	9.000	21.500	-2.678	1.096	0.312

3-[[[(2R,3S,4S,5R,6S)-	550.429	6.000	15.050	-0.687	0.107	0.032
2-(3,4-dihydroxyphenyl	464.382	7.000	13.750	-1.455	1.817	0.540
ethyl (9Z,12Z)-octadeca-	308.503	0.000	2.000	6.541	3979.983	2201.662
(1R,3S,6S)-6-[[[(1E,3E,	600.880	0.000	5.400	10.104	1164.112	583.019
(2R)-2,5,7,8-tetramethyl-	424.665	1.000	1.500	8.655	4550.351	2544.595
(9E,12E)-octadeca-9,	280.450	1.000	2.000	5.840	235.423	131.774
2-propyltridecanoic acid	256.428	1.000	2.000	5.335	405.188	236.980
(E)-hexadec-2-enoic acid	254.412	1.000	2.000	5.171	203.580	112.619
(Z)-heptadec-9-enoic acid	268.439	1.000	2.000	5.471	235.968	132.104
(E)-octadec-6-enoic acid	282.465	1.000	2.000	5.943	244.413	137.222
(Z)-octadec-11-enoic acid	282.465	1.000	2.000	5.937	288.590	164.216
(Z)-icos-9-enoic acid	310.519	1.000	2.000	6.215	450.397	265.684
(Z)-icos-11-enoic acid	310.519	1.000	2.000	6.752	235.251	131.670
(7E,10E,13E)-hexadeca-	250.380	1.000	2.000	5.141	279.463	158.610
(8E,11E,14E)-icosa-8,	306.487	1.000	2.000	6.572	235.902	132.064
(10E,12E)-9-oxooctadeca-	294.433	1.000	4.000	4.827	109.123	57.397
8-(3-heptyloxiran-2-yl)	260.375	1.000	3.700	4.279	3084.982	1671.761
(E)-dec-5-en-1-ol	156.267	1.000	1.700	2.830	2854.105	1536.947
(E)-hept-2-enal	112.171	0.000	2.000	1.349	1559.198	799.564
(E)-hept-4-enal	112.171	0.000	2.000	1.455	1835.682	953.858
(2E,4E)-hepta-2,4-dienal	110.155	0.000	2.000	1.301	1559.920	799.964
(E)-oct-2-enal	126.198	0.000	2.000	1.935	1709.813	883.364
(E)-non-2-enal	140.225	0.000	2.000	2.326	1710.013	883.476
(2E,4E)-nona-2,4-dienal	138.209	0.000	2.000	2.243	1559.668	799.825
(E)-dec-2-enal	154.252	0.000	2.000	2.590	1559.318	799.631
(2E,4E)-deca-2,4-dienal	152.236	0.000	2.000	2.562	1559.705	799.846
(E)-undec-2-enal	168.278	0.000	2.000	2.887	1561.188	800.668
(E)-dodec-2-enal	182.305	0.000	2.000	3.334	1559.155	799.541
(E)-tridec-2-enal	196.332	0.000	2.000	3.733	1559.316	799.630
(Z)-octadec-9-enaminal	281.481	2.000	2.500	4.415	511.948	471.486
2,3-dihydroxypropyl	356.545	2.000	5.400	4.469	442.995	205.187
(3S,8S,9S,10R,13R,14S)-	400.687	1.000	1.700	7.287	3381.922	1846.347
(3S,8S,9S,10R,13R,14S)-	412.698	1.000	1.700	7.547	3380.917	1845.754

(3S,8S,9S,10R,13R,14	398.671	1.000	1.700	7.179	3378.578	1844.373
(3S,5S,9R,10S,13R,14	398.671	1.000	1.700	7.219	3395.278	1854.229
(3S,5S,9R,10S,13R,14	412.698	1.000	1.700	7.452	3392.327	1852.487
(4R,4aR,7S,7aR,12bS	299.369	1.000	5.200	1.148	883.139	478.513
methyl (9Z,12Z)-octa	294.476	0.000	2.000	5.819	5066.721	2858.094
(Z)-octadec-9-en-1-o	268.482	1.000	1.700	5.876	2853.664	1536.691
(E)-hex-3-en-1-ol	100.160	1.000	1.700	1.626	3242.485	1764.203
(6E)-3,7,11-trimethyl	222.370	1.000	0.750	4.912	5263.998	2978.564
2-methyl-3-[(E,7R,11	450.703	0.000	4.000	8.318	2136.303	1123.768
ethyl (Z)-3-phenylprc	176.215	0.000	2.000	2.874	3641.763	2000.145
(1R,2R,3E,7S,11E,13	280.363	2.000	5.400	2.109	726.441	350.207
(4R,4aR,7S,7aR,12bS	285.342	2.000	5.200	0.897	279.531	138.002
cobalt(3+);[(2R,3S,4F	1272.445	17.000	34.600	-7.529	0.000	0.000
(Z)-hexadec-11-enoic	254.412	1.000	2.000	5.192	278.365	157.936
(Z)-heptadec-10-eno	268.439	1.000	2.000	5.552	235.353	131.732
(Z)-octadec-13-enoic	282.465	1.000	2.000	5.887	235.883	132.053
(13E)-octadeca-13,1	280.450	1.000	2.000	5.800	279.600	158.694
(2E,4E)-octadeca-2,4	280.450	1.000	2.000	5.847	203.801	112.752
octadeca-12,15-diyne	276.418	1.000	2.000	5.784	278.981	158.314
(E)-octadec-11-en-9-	278.434	1.000	2.000	5.901	280.509	159.251
(9S,10E,12Z)-9-hydro	296.449	2.000	3.700	4.707	93.122	48.357
2-pentanoylbenzoic	206.241	1.000	4.000	2.030	177.744	97.254
5-[(2S,3S)-6-hydroxy	454.478	5.000	4.500	3.622	30.798	11.498
1-methyl-4-[(2E)-6-r	204.355	0.000	0.000	6.181	9906.038	5899.293
9-(3,4-dimethoxyph	394.380	0.000	6.750	2.926	3201.719	1740.241
(E)-3-phenylprop-2-e	134.177	1.000	1.700	2.016	3350.979	1828.093
(4-hydroxy-3,5-dime	434.442	3.000	9.900	1.794	188.529	81.493
3,8-dimethyl-5-prop	200.323	0.000	0.000	5.529	9906.038	5899.293
11-hydroxy-10-[(Z)-3	618.852	3.000	6.450	7.436	59.684	29.898
(1R)-1,8-dimethyl-4-	204.355	0.000	0.000	5.273	9906.038	5899.293
6,7,15-trihydroxy-19	502.563	2.000	5.250	5.470	396.586	182.054
7,15-dihydroxy-19,1	418.445	1.000	4.500	4.806	868.155	424.601
5,7-dihydroxy-2-(4-h	432.383	5.000	11.300	0.022	15.765	5.575

1,5-dihydroxy-3-met	254.242	0.000	3.500	1.790	256.042	113.450
8,11-dihydroxy-[1,3]	272.214	1.000	4.500	1.337	441.124	204.250
(3'Z)-3'-butylidene-6'	380.483	0.000	5.500	4.383	1232.292	620.013
(2R,3S,4S,5R,6S)-2-(f	372.371	5.000	12.450	-0.266	83.879	33.958
1-(3-methylbut-2-en	202.296	0.000	0.750	4.566	9906.038	5899.293
7-hydroxy-2,5-dimet	190.198	1.000	3.250	1.499	1154.887	578.027
2-(1H-indol-3-yl)-N,N	204.271	1.000	3.000	2.204	2793.565	1501.740
5-hydroxy-2-(4-meth	592.552	6.000	19.050	-0.971	7.398	2.461
(4Z)-4-butylidene-1a	206.241	0.000	4.500	1.340	2147.285	1130.013
ethyl (E)-3-(3,4-dihyc	208.213	2.000	3.500	1.414	281.731	125.802
2-[(2R,4aR)-4a-meth'	222.370	1.000	0.750	3.987	5099.192	2877.897
2-(3,4-dihydroxyphei	316.267	3.000	5.250	1.183	62.960	24.905
3,5-dihydroxy-2-(3-h'	360.320	2.000	6.000	2.239	226.890	99.555
(6Z)-7,11-dimethyl-3	204.355	0.000	0.000	6.384	9906.038	5899.293
2-(4-hydroxyphenyl)-	290.272	5.000	6.400	0.318	69.389	27.665
3,4a,5-trimethyl-5,6,	218.338	0.000	0.500	3.560	9906.038	5899.293
9-[(2E)-3,7-dimethyl	338.402	0.000	3.750	4.872	2090.340	1097.657
(1E,6E,8S)-1-methyl-	204.355	0.000	0.000	5.414	9906.038	5899.293
8-(3-heptyloxiran-2-)	262.391	1.000	3.700	4.339	3183.872	1729.759
7-hydroxy-3-(5-hydr	336.343	2.000	4.750	2.885	628.869	299.652
7-hydroxy-5-methyl-	232.235	1.000	5.250	1.091	366.786	167.314
7-hydroxy-3-(4-hydr	284.268	2.000	4.750	1.941	383.655	175.646
(1S,4S,7R)-1,4-dimet	204.355	0.000	0.000	5.640	9906.038	5899.293
(E)-hex-2-en-1-ol	100.160	1.000	1.700	1.733	2824.981	1520.003
(1E,2R,3R)-2-(3,5-dih	454.478	6.000	4.500	2.973	14.169	4.968
1,1,4,8-tetramethyl	210.402	0.000	0.000	7.297	9906.038	5899.293
(E)-1-[6-[(3-acetyl-2,	532.546	3.000	6.250	4.805	46.505	17.950
7,8-dimethoxy-2-phe	460.437	4.000	13.250	0.702	93.911	38.369
5-hydroxy-7,8-dimet	328.321	0.000	4.500	3.147	1248.919	629.060
(2E,4E)-N-(2-methyl	223.358	1.000	2.500	4.098	3699.261	2034.300
(3E,4S)-3-[2-[(1R,4a	350.454	3.000	8.100	1.490	245.116	108.227
1,2,3-trimethoxy-5-[l	208.257	0.000	2.250	2.861	9906.038	5899.293
7-hydroxy-6,8-dimet	222.197	1.000	4.750	1.069	830.555	404.759

8-[5-(5,7-dihydroxy-2,4-dihydroxy-2-(4-hydroxy-3-(2S,3S,4S,5R,6S)-6-[5-(E)-oct-2-en-1-ol 128.214	2.000	7.500	4.548	19.334	6.951
1,3,6,7-tetrahydroxy 422.345	7.000	13.000	-1.811	3.058	0.947
(E)-oct-2-en-1-ol 128.214	1.000	1.700	2.611	2825.292	1520.184
5,7-dihydroxy-2-(4-hydroxy-3-(2S,3S,4S,5R,6S)-6-[5-(E)-oct-2-en-1-ol 128.214	6.000	13.750	-0.684	9.268	3.140
5-[(E)-2-(4-hydroxy-3-(2S,3S,4S,5R,6S)-6-[5-(E)-oct-2-en-1-ol 128.214	3.000	3.000	2.175	280.347	125.134
9-(1,3-benzodioxol-5-yl)-2-(4-hydroxy-3-(2S,3S,4S,5R,6S)-6-[5-(E)-oct-2-en-1-ol 128.214	0.000	6.750	2.103	2829.251	1522.487
(2S,3S,4S,5R,6S)-6-[5-(E)-oct-2-en-1-ol 128.214	5.000	12.300	-0.196	0.834	0.296
5,7-dihydroxy-2-(4-hydroxy-3-(2S,3S,4S,5R,6S)-6-[5-(E)-oct-2-en-1-ol 128.214	8.000	19.800	-1.826	3.178	0.987
3,3,5-trimethyl-11H-phenanthrene 279.338	2.000	1.500	3.928	2034.192	1065.823
5-hydroxy-2-(4-hydroxy-3-(2S,3S,4S,5R,6S)-6-[5-(E)-oct-2-en-1-ol 128.214	1.000	4.500	2.691	511.974	239.929
(E)-3-[4-hydroxy-2-methyl-5-(E)-oct-2-en-1-ol 128.214	2.000	4.250	4.249	590.606	279.995
(3Z)-3-butylidene-4,5-dihydroxy-2-(4-hydroxy-3-(2S,3S,4S,5R,6S)-6-[5-(E)-oct-2-en-1-ol 128.214	0.000	2.500	2.509	2174.151	1145.303
3,4,8,9,10-pentahydroxy-2-(4-hydroxy-3-(2S,3S,4S,5R,6S)-6-[5-(E)-oct-2-en-1-ol 128.214	6.000	8.250	-1.183	0.797	0.282
5,7-dihydroxy-2-[3-hydroxy-4-(4-hydroxy-3-(2S,3S,4S,5R,6S)-6-[5-(E)-oct-2-en-1-ol 128.214	6.000	13.000	-0.960	3.097	0.960
7-hydroxy-3-(4-hydroxy-3-(2S,3S,4S,5R,6S)-6-[5-(E)-oct-2-en-1-ol 128.214	2.000	4.750	1.946	382.213	174.933
7-hydroxy-3-(4-hydroxy-3-(2S,3S,4S,5R,6S)-6-[5-(E)-oct-2-en-1-ol 128.214	6.000	13.250	-0.366	20.399	7.366
(8E,11E,14E)-heptadecane 232.408	0.000	0.000	8.847	9906.038	5899.293
methyl (E)-icos-11-ene 324.546	0.000	2.000	7.296	2576.017	1375.742
methyl (9Z,12Z,15Z)-icosane 292.461	0.000	2.000	6.139	3037.388	1643.901
methyl (8E,11E)-octa-2,6-diene 294.476	0.000	2.000	6.437	3040.457	1645.696
(E)-2-methylpent-2-ene 98.144	0.000	2.000	1.210	1870.175	973.246
1-(methyltrisulfanyl)ethane 154.303	0.000	0.500	3.583	9906.038	10000.000
3,4-dimethoxy-1-methyl-2-(2,4-dihydroxyphenyl)ethane 155.196	0.000	2.950	1.799	9211.546	5453.550
2-(2,4-dihydroxyphenyl)ethane 490.595	3.000	4.500	5.797	96.908	39.694
methyl 1-methoxy-9-phenyl-2-(2,4-dihydroxyphenyl)ethane 255.273	1.000	2.750	3.115	1611.432	828.556
2-(2,4-dihydroxyphenyl)ethane 422.477	3.000	4.500	4.319	194.374	84.227
8-(2,4-dihydroxyphenyl)ethane 420.461	2.000	4.500	4.692	435.070	201.222
4-(2,4-dihydroxyphenyl)ethane 592.558	5.000	9.750	3.302	35.198	13.284
(E)-3-(4-hydroxyphenyl)ethane 418.399	5.000	11.750	0.032	11.051	3.797
(2E,6E)-nona-2,6-diene 140.225	1.000	1.700	2.523	2825.104	1520.074
(3Z)-3,7-dimethyloctane 136.236	0.000	0.000	4.609	9906.038	5899.293
5,7-dihydroxy-6-methyl-2-(2,4-dihydroxyphenyl)ethane 284.268	1.000	3.750	2.582	581.806	275.488
5-hydroxy-2-(2-hydroxy-3-(2S,3S,4S,5R,6S)-6-[5-(E)-oct-2-en-1-ol 128.214	1.000	4.500	2.718	711.409	342.380

5,13,17-trihydroxy-1	388.287	2.000	10.900	-1.134	6.641	2.190
4,10,11,11-tetramethyl	218.338	0.000	2.000	3.236	4417.227	2464.226
2-(2,5-dihydroxy-4-methyl)	398.412	2.000	5.250	3.551	280.729	125.318
5,7-dihydroxy-2-(5-hydroxy)	398.412	2.000	5.250	3.527	217.850	95.275
1,4,8,10-tetrahydroxy	382.369	3.000	5.250	2.450	131.048	55.004
(E)-5-(1,3-benzodioxol-2-yl)	287.358	0.000	4.500	3.358	4256.233	2367.293
(2E,4E)-5-(1,3-benzodioxol-2-yl)	273.331	1.000	4.000	3.478	3334.732	1818.515
1-[[[(E)-prop-1-enyl]dimethylamino]methyl]	148.281	0.000	1.000	3.306	9906.038	10000.000
[(1S,19R,21S,22R,23S,24S)-2,3,4,5-tetrahydro-1H-2,3,4-triazolo[4,5-b]pyridine-6-yl]	938.672	15.000	22.950	-3.230	0.003	0.000
2-(3,4-dihydroxyphenyl)	626.524	10.000	22.250	-3.336	0.251	0.063
5,7-dihydroxy-2-[3-(4-hydroxyphenyl)propyl]	626.524	10.000	22.250	-3.392	0.328	0.085
2-(3,4-dihydroxyphenyl)	434.356	6.000	12.050	-0.904	4.343	1.384
3,5-dihydroxy-2-(4-hydroxyphenyl)	330.293	2.000	5.250	2.045	171.201	73.428
4-hydroxy-9,10-dioxo-9,10-dihydro-1H-phenanthrene-3-carboxamide	446.367	5.000	15.000	-1.382	0.518	0.177
(3S,5R,8S)-3,8-dimethyl-3,8-dihydro-1H-phenanthrene-9,10-dione	218.338	0.000	2.000	3.549	3695.846	2032.270
(Z)-5-(2,3-dimethyl-3-oxopropyl)-2,3-dihydro-1H-phenanthrene-9,10-dione	218.338	0.000	2.000	3.412	2258.804	1193.578
3-[[[(2S,3R,4R,5R)-3,4-dihydroxybutyl]amino]methyl]	434.356	6.000	12.050	-0.820	5.727	1.866
(2S,3S,6S)-3-ethenyl-2,3,6-trihydroxy-1H-phenanthrene-9,10-dione	220.354	0.000	2.000	3.766	5962.844	3408.187
3,5,7-trihydroxy-2-(4-hydroxyphenyl)	346.293	3.000	6.000	1.465	93.307	38.102
(E)-1-(7-hydroxy-2,2-dimethyl-2H-chromene-3-carboxamide)	322.360	1.000	3.250	4.029	488.055	227.836
2,3-dimethyltricyclo[3.3.1.0 ^{2,3}]heptane	166.219	1.000	2.000	2.184	501.103	298.157
(E)-3-(4-hydroxy-3-methylphenyl)	440.495	4.000	8.000	3.489	84.264	34.127
9-hydroxy-1,5,8-trimethyl-1H-phenanthrene-9,10-dione	258.273	1.000	5.500	1.434	962.713	474.802
1,5,8-trimethylbenzo[1,2-b:4,5-b']diphenylene-9,10-dione	240.258	0.000	4.500	1.729	1533.293	785.215
(E)-8,11,12-trihydroxy-1H-phenanthrene-9,10-dione	330.464	4.000	7.100	2.837	24.813	11.578
2-(4-hydroxy-3-methylphenyl)	624.689	5.000	9.500	4.678	32.615	18.932
1,3,8-trihydroxy-5-methyl-1H-phenanthrene-9,10-dione	274.229	1.000	3.500	1.803	195.153	84.592
2,3-bis[[[(9Z,12Z)-octadeca-9,12-dienyl]amino]methyl]	879.398	0.000	6.000	18.558	883.047	432.479
(4R,7aR,12bS)-7,9-dimethyl-1H-phenanthrene-9,10-dione	311.380	0.000	4.250	3.069	2137.725	1244.138
3-[2,4-dihydroxy-3-(4-methylphenyl)propyl]	406.477	3.000	4.750	4.556	497.678	232.695
methyl (13Z)-13-ethyl-1H-phenanthrene-9,10-dione	322.406	1.000	3.000	4.195	3104.462	1683.174
2-(2,5-dihydroxy-4-methylphenyl)	468.502	3.000	5.950	4.073	82.770	33.473
5,9,11,14-tetrahydro-1H-phenanthrene-9,10-dione	434.445	3.000	5.250	3.555	161.296	68.847

(3E)-3-(butoxymethyl methyl (9E,12E)-octa	184.321	0.000	1.700	4.054	8450.225	4968.038
(Z)-dec-4-en-1-ol	294.476	0.000	2.000	6.384	2572.708	1373.832
(2E,6Z)-nona-2,6-die	156.267	1.000	1.700	2.724	2956.480	1596.622
1,3-bis(trimethylsilyl	140.225	1.000	1.700	2.497	2824.822	1519.910
(3Z,6E)-3,7,11-trimet	496.876	0.000	3.700	9.879	4015.250	2222.756
(2E)-5-methyl-4-prop	204.355	0.000	0.000	6.971	9906.038	5899.293
1-methyl-4-[(2Z)-6-r	154.252	1.000	1.700	2.447	2875.934	1549.657
methyl (E)-docos-13-	220.354	0.000	2.000	2.918	9906.038	5899.293
5,6,6-trimethyl-5-[(E	352.599	0.000	2.000	8.093	2613.994	1397.677
2-hydroxy-2,4,4-trim	236.310	0.000	6.000	1.150	1793.113	929.972
(E)-4-(5-hydroxy-2,2-	222.327	1.000	2.750	2.974	2240.949	1183.383
[(E)-dec-2-enyl] acet	208.300	1.000	3.700	2.089	1315.601	665.440
[(Z)-7-methyltetrad	198.305	0.000	2.000	3.769	2471.690	1315.619
[(E)-10-methyltetrad	268.439	0.000	2.000	5.456	2609.861	1395.288
[(Z)-hex-3-enyl] acet	268.439	0.000	2.000	5.651	2222.898	1173.083
(2E,6E)-2,6-dimethyl	142.197	0.000	2.000	2.162	2229.399	1176.792
(1E)-3,7-dimethyloct	170.251	2.000	3.400	1.441	945.781	465.782
[(2Z,6E)-10,11-dihyd	170.251	0.000	1.750	2.530	1194.328	599.393
(2E,7E,11E)-1,7,11-tr	298.422	2.000	4.450	3.544	648.869	309.966
(E)-4-(2,4,4-trimethy	290.488	1.000	0.750	5.652	4825.980	2711.596
ethyl (E)-oct-2-enoat	190.285	0.000	2.000	3.179	3124.604	1694.981
methyl (E)-hex-2-enc	170.251	0.000	2.000	2.998	2606.368	1393.271
(3Z,13Z)-2-methyloct	128.171	0.000	2.000	1.609	2308.824	1222.172
methyl (E)-octadec-8	280.493	1.000	1.700	5.841	8359.275	4910.267
methyl (E)-tetracos-1	296.492	0.000	2.000	6.501	2578.444	1377.143
(E)-tridec-6-ene	1380.653	0.000	2.000	8.733	3030.705	1639.992
methyl (E)-octadec-7	182.348	0.000	0.000	6.769	9906.038	5899.293
(Z)-tetradec-4-ene	296.492	0.000	2.000	6.472	4338.479	2416.776
(2Z,13E)-octadeca-2,	196.375	0.000	0.000	7.096	9906.038	5899.293
(Z)-octadec-9-enal	266.466	1.000	1.700	5.796	3003.170	1623.893
methyl (E)-octadec-1	266.466	0.000	2.000	5.665	1941.507	1013.431
methyl (Z)-octadec-9	296.492	0.000	2.000	6.494	2605.953	1393.030
	296.492	0.000	2.000	6.467	3247.261	1767.012

methyl (13E,16E)-oct	294.476	0.000	2.000	6.379	3150.910	1710.410
(E)-octadec-5-ene	252.482	0.000	0.000	9.677	9906.038	5899.293
(E)-octadec-9-ene	252.482	0.000	0.000	9.669	9906.038	5899.293
(Z)-non-3-en-1-ol	142.241	1.000	1.700	2.647	2878.567	1551.191
2,3-bis[[[(E)-octadec-1	885.445	0.000	6.000	19.496	514.118	241.014
(Z)-14-methylhexade	252.439	0.000	2.000	5.185	1841.797	957.293
methyl (E)-hexadec-1	268.439	0.000	2.000	5.731	2613.990	1397.675
(3E,12Z)-nonadeca-1	294.476	2.000	3.400	5.096	1502.196	768.016
ethyl (E)-hex-2-enoal	142.197	0.000	2.000	2.278	2606.151	1393.145
2,3-dihydroxypropyl	356.545	2.000	5.400	5.179	564.766	266.777
(Z)-pent-2-en-1-ol	86.133	1.000	1.700	0.906	2877.039	1550.301
(E)-non-2-en-1-ol	142.241	1.000	1.700	2.771	2824.998	1520.013
(E)-dec-2-en-1-ol	156.267	1.000	1.700	2.874	2826.106	1520.657
(E)-tridec-2-en-1-ol	198.348	1.000	1.700	4.022	2824.209	1519.554
(Z)-dodec-2-en-1-ol	184.321	1.000	1.700	3.571	2966.256	1602.329
(E)-pentatriacont-17-	490.938	0.000	0.000	18.733	9906.038	5899.293
[(Z)-2-hydroxypentac	298.465	1.000	3.700	5.004	1263.906	637.223
(5E,6E)-5,6-bis(2,2-di	278.520	0.000	0.000	8.334	9906.038	5899.293
(Z)-tricos-9-ene	322.616	0.000	0.000	12.082	9906.038	5899.293
(Z)-docos-13-enamid	337.588	2.000	2.500	4.987	421.469	408.588
(6Z,9Z)-pentadeca-6,	224.386	1.000	1.700	4.384	3915.017	2162.842
(11E,13Z)-octadeca-1	248.451	0.000	0.000	9.170	9906.038	5899.293
(9Z)-octadeca-9,17-d	264.450	0.000	2.000	5.670	2276.968	1203.956
2-chloroethyl (9Z,12	342.948	0.000	2.000	7.010	3538.507	4236.623
ethyl (9E,12E)-octad	308.503	0.000	2.000	6.870	2933.429	1583.170
2-[(9Z,12Z)-octadeca	310.519	1.000	3.400	6.022	3234.745	1759.652
1,3-dihydroxypropan	354.529	2.000	5.400	4.985	570.805	269.862
methyl (11E,14E)-oct	294.476	0.000	2.000	6.465	2575.429	1375.402
methyl (10E,13E)-oct	294.476	0.000	2.000	5.995	3115.506	1689.647
(3E,6E)-nona-3,6-die	140.225	1.000	1.700	2.504	2876.506	1549.991
(1Z,5Z)-3,4-dimethyl	136.236	0.000	0.000	3.776	9906.038	5899.293
(6E)-3,7,11-trimethyl	220.354	1.500	0.750	4.549	4315.415	2402.892
(E)-4,4,8-trimethylnc	182.305	0.000	2.000	3.064	2039.598	1068.885

(E)-3,7-dimethyloct-2	1.000	1.700	2.692	2857.248	1538.777
(6E,10E)-3,7,11,15-tet	1.000	0.750	6.525	4821.633	2708.956
(6E,8E,10E,12E,14E,15E)	1.000	0.750	13.404	4579.297	2562.095
(3E,6E,10E)-3,7,11,15-	0.000	0.000	9.097	9906.038	5899.293
methyl (2E)-3,7-dimeth	0.000	2.000	3.133	2813.243	1513.177
(1,2,6-trimethylspiro	0.000	7.700	1.981	5147.795	2907.558
(E)-5-(1-hydroperoxy	3.000	5.850	1.511	631.293	300.901
(6Z,28Z)-heptatriaco	0.000	2.000	13.188	3377.159	1843.536
(E)-octadec-3-ene	0.000	0.000	9.615	9906.038	5899.293
(6E,10E,14E,18E)-2,6	0.000	0.000	11.422	9906.038	5899.293
2,2-dimethyl-3-[(3E,7	0.000	2.000	7.702	9906.038	5899.293
(E)-2,2-dimethyloct-2	0.000	0.000	4.816	9906.038	5899.293
(E)-1-(2,6,6-trimethy	0.000	2.000	3.273	6131.352	3512.409
[17-[(E)-5,6-dimethyl	0.000	2.000	9.546	4244.699	2360.360
(E)-9-methylundec-2	0.000	0.000	6.104	9906.038	5899.293
(E)-3,7,11,15-tetram	1.000	1.700	6.304	2861.605	1541.314
(6E,8E,10E,12E,14E,16	0.000	1.500	13.532	9906.038	5899.293
trimethylsilyl (9Z,12Z	0.000	2.000	7.459	6456.138	3713.938
(E)-1-(methylsulfar	0.000	1.000	2.634	9906.038	10000.000
trimethyl-[(E)-pentac	0.000	0.850	7.038	9906.038	5899.293
2,3-dihydroxypropyl	2.000	5.400	4.847	358.906	163.432
methyl (5Z,11Z,14Z,13	0.000	2.000	6.429	3153.910	1712.171
(7Z,10Z,13Z)-hexade	0.000	2.000	4.264	2776.495	1491.824
methyl (E)-heptadec-	0.000	2.000	5.970	2928.852	1580.501
ethyl (9Z,12Z,15Z)-oc	0.000	2.000	6.320	2922.866	1577.009
methyl (9E,12E,15E)-	0.000	2.000	6.369	3029.587	1639.338
(2-phenyl-1,3-dioxan	0.000	5.400	7.702	4347.250	2422.057
(6Z,10Z)-3,6,10-trim	0.000	3.000	2.926	2853.474	1536.580
[(Z)-hex-3-enyl] 3-m	0.000	2.000	3.361	3115.344	1689.552
[(Z)-hex-3-enyl] benz	0.000	2.000	3.570	2866.838	1544.361
2-methylpropyl (Z)-2	0.000	2.000	2.550	3807.247	2098.562
(Z)-5-(2,6-dimethyl-6	1.000	1.700	3.791	3351.678	1828.506
(1Z,4Z,7Z)-1,5,9,9-tet	0.000	0.000	5.296	9906.038	5899.293

(5E)-2,6-dimethyloct	154.252	1.000	0.750	3.108	4582.538	2564.055
(4E,6E)-2,6-dimethyl	136.236	0.000	0.000	4.572	9906.038	5899.293
1-methyl-6-[(1Z)-3-r	178.274	0.000	2.000	2.097	9906.038	5899.293
(E)-2-methyl-4-(2,6,6	206.327	0.000	2.000	3.234	1988.048	1039.715
(3E)-6-methylhepta-	124.182	0.000	2.000	1.776	3146.304	1707.708
(E)-1-[(E)-prop-1-eny	114.205	0.000	0.000	3.164	9906.038	10000.000
methyl (E)-12-hydrox	342.518	1.000	5.400	5.112	1088.826	542.373
(E)-2-methyl-6-(4-me	218.338	1.000	1.700	3.982	3286.833	1790.298
(4E,6Z)-2,6-dimethyl	136.236	0.000	0.000	4.646	9906.038	5899.293
(2E,4E,10E)-11-(1,3-t	355.476	1.000	4.000	5.081	4174.081	2317.943
(2E,4E)-9-(1,3-benzo	329.438	1.000	4.000	4.901	3338.162	1820.537
3-methoxy-4-methyl	145.179	0.800	2.000	1.597	2947.596	4070.396
2-[(Z)-but-2-enyl]-3-r	150.220	0.000	2.000	2.202	4480.999	2502.702
[7,7,12,16-tetramet	516.762	0.000	4.000	8.007	1545.669	792.068
(1Z,6Z)-1-methyl-5-n	204.355	0.000	0.000	5.138	9906.038	5899.293
4-[(E)-2-(2-hydroxypl	221.258	1.000	2.250	3.018	761.438	368.478
(3E,7Z)-4,8,12,15,15-	290.488	1.000	0.750	5.377	5640.277	3209.348
1,3-bis(trimethylsilyl	498.892	0.000	3.700	9.883	7545.300	4395.562
2-(hydroxymethyl)-1	618.852	3.000	6.450	7.278	32.241	15.366
3,5,7-trihydroxy-2-(4	316.267	3.000	5.250	1.284	86.424	35.073
5,7-dihydroxy-2-(4-h	432.383	6.000	12.250	-0.752	9.340	3.166
8-hydroxy-1,2,6-trim	302.283	0.000	4.500	2.672	1968.667	1028.763
2-methoxy-4-[7-met	326.391	1.000	3.000	4.711	3043.086	1647.235
methyl (E)-7-[2-oxo-	420.663	0.000	4.850	6.658	1113.433	555.633
3,4,5,11,12,13,21,22	782.535	13.000	23.300	-4.730	0.008	0.001
(1S,9R)-3-hydroxy-4,	327.379	1.000	6.250	2.022	413.620	210.776
7-hydroxychromen-4	162.145	1.000	3.250	0.845	881.968	431.908
methyl (1R,15R,18R)	336.433	0.000	3.000	4.321	1005.322	550.455
2-(2,4-dihydroxyphei	436.504	2.000	4.500	5.307	379.812	173.745
3,8-dihydroxy-10-me	434.488	1.000	4.500	5.472	925.574	455.035
(2R,3R)-2-(2,4-dihyd	304.256	4.000	6.450	0.146	26.080	9.606
(E)-3-(6,7-dimethoxy	236.224	0.000	5.000	1.132	1594.552	819.178
(2E,4E,6E,8E,10E,12E	328.407	2.000	4.000	5.028	9.117	4.989

5-hydroxy-2-(4-hydroxy-3,4-dihydroxyphenyl)propane	1.000	6.000	2.801	541.393	254.864
(3Z)-3-[[6-[[2-(dimethylamino)ethyl]oxy]hexyl]oxy]propane	1.000	8.250	3.213	701.503	373.083
(2S,3R,5R,9R,10R,13I)hexadeca-1,3,5,7,9,11,13,15-octaene	6.000	9.350	2.140	47.468	18.352
(4R,4aR,7aR,12bS)-9,10,11,12-tetrahydro-1H-benzod[e][1,2-b]oxazine	0.000	5.500	1.693	695.169	369.444
(1S,9R,12S)-4,13-dimethyl-1,2,3,4,5,6,7,8,9,10,11,12,13-dodecane	2.000	5.950	2.172	437.080	223.727
2-(2,5-dihydroxyphenyl)propane	3.000	3.500	0.417	34.716	16.644
(2R,3R,4R)-2,3,4,5-tetrahydro-1H-benzod[e][1,2-b]oxazine	4.000	7.800	-1.356	11.227	4.913
benzyl 3-[6-[[2-(butylamino)ethyl]oxy]hexyl]propanoate	1.000	13.250	9.039	91.500	72.087
(4R,7aR,12bS)-7-methyl-1,2,3,4,5,6,7,8,9,10,11,12,13-dodecane	1.000	4.250	1.700	662.277	350.586
(4R,7S,7aR,12bS)-9-nonyl-1,2,3,4,5,6,7,8,9,10,11,12,13-dodecane	1.000	5.200	1.363	1028.070	563.930
(3Z)-hexa-1,3-diene	0.000	0.000	2.740	9906.038	5899.293
(3Z)-3,7-dimethyloctane	0.000	0.000	4.530	9906.038	5899.293
(2Z,6E)-9-(furan-3-yl)nonane	1.000	2.500	5.392	525.088	313.611
(1E,3Z,6R,7R)-6-[[2-(furan-3-yl)ethyl]oxy]hexane	1.000	2.500	4.733	315.223	180.656
(3S,9Z)-heptadeca-1,3,5,7,9,11,13,15-octaene	1.000	1.700	5.148	3622.901	1988.950
4-[[2E)-3,7-dimethyl-1,2,3,4,5,6,7,8,9,10,11,12,13-dodecane	0.000	3.750	4.685	2055.991	1078.174
methyl (14Z)-14-ethyl-1,2,3,4,5,6,7,8,9,10,11,12,13-dodecane	1.000	5.750	1.983	201.996	107.465
2-(3,4-dihydroxyphenyl)propane	6.000	12.050	-0.812	6.596	2.174
5,7-dihydroxy-3-(5-hydroxyphenyl)propane	2.000	4.500	3.028	269.406	119.864
5,7-dihydroxy-2-(4-hydroxyphenyl)propane	8.000	20.550	-1.776	3.858	1.217
5,7-dihydroxy-3-(8-hydroxyphenyl)propane	2.000	4.500	2.948	173.558	74.521
5-hydroxy-8,8-dimethyl-1,2,3,4,5,6,7,8,9,10,11,12,13-dodecane	3.000	5.250	3.912	130.451	54.733
3,5,7-trihydroxy-2-(4-hydroxyphenyl)propane	3.000	4.500	2.786	131.131	55.042
2-(2,4-dihydroxyphenyl)propane	3.000	5.250	4.031	132.980	55.881
11,19-dihydroxy-7,7-dimethyl-1,2,3,4,5,6,7,8,9,10,11,12,13-dodecane	1.000	4.500	4.708	725.313	349.619
2-(2,4-dihydroxyphenyl)propane	3.000	4.500	0.996	44.101	16.950
(8S,9S,10R,13R,14S,14I)hexadeca-1,3,5,7,9,11,13,15-octaene	0.000	2.000	7.542	2799.322	1505.086
5-hydroxy-2-(4-hydroxyphenyl)propane	7.000	18.100	-1.156	3.102	0.962
[(6S,9S,14R,17S,18R,18I)hexadeca-1,3,5,7,9,11,13,15-octaene	1.000	9.450	3.195	300.805	149.389
3-[3,4-dihydroxy-5-(5-hydroxyphenyl)propanoate]propanoate	3.000	5.500	2.946	268.051	119.212
(2S,3S,4S,5R,6S)-6-[5-(5-hydroxyphenyl)propanoate]propanoate	7.000	13.800	-1.418	0.103	0.031
1,5-dihydroxy-3-methyl-1,2,3,4,5,6,7,8,9,10,11,12,13-dodecane	8.000	21.500	-2.556	1.458	0.425
3,5,8-trihydroxy-7-methyl-1,2,3,4,5,6,7,8,9,10,11,12,13-dodecane	2.000	5.250	2.108	186.825	80.697

6,13-dihydroxy-7,14-	330.250	2.000	8.000	0.202	97.019	39.743
3,5,7-trihydroxy-2-(4	346.293	3.000	6.000	1.252	67.175	26.711
1,3,8,9-tetrahydroxy	300.224	4.000	6.000	0.030	31.162	11.645
(8S,9S,10R,13R,14S,14	26.681	0.000	4.000	6.319	1084.792	540.201
5-hydroxy-6-methox	608.552	6.000	19.800	-0.845	8.585	2.891
5,7-dihydroxy-2-[4-[(432.383	5.000	12.250	-0.346	8.600	2.896
5,7-dihydroxy-3-[(2S,	480.381	8.000	14.500	-1.959	1.231	0.354
5,7-dihydroxy-3,6,8-1	374.346	1.000	6.000	2.969	940.656	463.054
2,6-dimethoxy-4-[(2F	448.512	1.000	7.900	4.301	3101.332	1681.340
3-[(2S,3R,4S,5S,6R)-4	610.524	9.000	20.550	-2.514	0.709	0.195
[(2R,3S,4S,5R,6S)-6-]	600.489	8.000	15.550	-0.850	0.383	0.100
3-[(2S,3R,4S,5R,6R)-	772.666	12.000	29.050	-3.595	0.975	0.275
(4R,4aR,7S,7aR,12bS	313.396	0.000	5.200	2.001	2198.377	1282.336
methyl (1S,15S,17R,16	08.687	1.000	10.700	5.052	274.493	135.316
4-[(E)-2-[(1R,4aS,5R,	332.439	2.000	6.400	2.365	452.486	209.942
(2R,3R,4S,5S,6R)-2-[[576.855	4.000	10.200	5.180	251.123	111.096
methyl (9E,11E)-13-c	308.460	0.000	4.000	5.149	1079.527	537.368
octacosyl (E)-3-(4-hy	586.937	1.000	3.500	12.208	733.757	354.020
butyl (9E,12E,15E)-o	334.541	0.000	2.000	7.582	2951.087	1593.474
5,7-dihydroxy-2-(4-h	432.383	5.000	11.300	0.028	21.536	7.811
(1R,9R,10S,12R,13S,	326.438	2.000	6.400	1.500	103.762	52.307
2-[(E)-3-(3,4-dihydro	296.233	4.000	7.500	0.485	0.390	0.165
(Z)-1-(methylsulfan	120.227	0.000	1.000	2.189	9906.038	10000.000
8-[3-[(Z)-oct-2-enyl]c	296.449	1.000	4.000	4.714	289.674	164.883
[(9E,12E)-tetradeca-	252.396	0.000	2.000	5.246	2221.217	1172.125
8-hydroxy-3-methyl-	416.384	4.000	13.000	-0.451	26.987	9.968
(1R,9R,10S,12R,13R,	326.438	2.000	6.400	1.532	108.727	55.018
3,7-dimethyloct-6-er	238.369	0.000	2.000	4.651	3452.212	1887.859
(2R)-4-methoxy-2-m	146.143	1.000	4.000	0.743	116.915	61.840
1,3,3-trimethyl-2-[(1	536.882	0.000	0.000	16.736	9906.038	5899.293
(Z)-octadec-9-enenit	263.465	0.000	1.500	5.953	2289.934	1211.368
propan-2-yl tridecyl	306.503	0.000	4.000	5.194	109.205	1630.263
methyl (5Z,8Z,11Z,14	318.498	0.000	2.000	6.628	2606.666	1393.442

N-(fluoren-9-ylidene)	334.420	1.000	6.000	2.708	141.032	72.882
1-O-butyl 2-O-(2-pro	264.321	0.000	4.500	3.236	1717.588	887.707
2-O-(4-cyanophenyl)	393.482	0.000	6.000	5.014	470.500	218.991
1-O-octyl 2-O-pentar	348.481	0.000	4.000	5.557	2279.544	1205.428
1-O-(2-ethylhexyl) 2-	418.615	0.000	4.000	6.761	2405.817	1277.762
1,2-dimethoxy-4-[(Z)	194.230	0.000	3.200	2.568	9053.393	5352.416
6,7-dimethylthieno[2	228.311	1.500	2.000	2.394	482.073	492.578
1,4-dimethoxy-2-me	194.273	0.000	1.500	3.243	9906.038	5899.293
3,6-dimethyl-3a,4,5,	166.219	0.000	3.000	1.526	2750.223	1476.572
(2E,4Z)-deca-2,4-dier	152.236	0.000	2.000	2.555	1711.466	884.288
(1S)-1,6-dimethyl-4-†	204.355	0.000	0.000	5.259	9906.038	5899.293
(1S,2R,5R)-2,6,6-trim	152.236	0.000	2.000	2.038	3925.232	2168.943
(2R)-1,3,3-trimethylt	154.252	1.000	1.700	2.209	4867.875	2737.049
(3E)-4,8-dimethylnor	150.263	0.000	0.000	5.097	9906.038	5899.293
[(4S,5S)-17-[(5S)-5-el	470.777	0.000	2.000	8.866	3935.847	2175.283
(2R,3R)-2,6,6-trimet†	230.426	0.000	1.000	3.582	9906.038	10000.000
(1S,5S)-6-methyl-2-n	204.355	0.000	0.000	5.824	9906.038	5899.293
6,6-dimethyl-4-meth	134.221	0.000	0.000	3.565	9906.038	5899.293
[(2R,5S)-2-methyl-5-†	196.289	0.000	2.000	3.149	6116.326	3503.106
[(E)-2-methyl-5-[(1R,	262.391	0.000	2.000	4.535	2535.345	1352.279
(1aR,7R,7aS,7bS)-1,1	206.370	0.000	0.000	6.722	9906.038	5899.293
2-(2,3-dimethylbut-3	220.397	0.000	0.000	5.703	9906.038	5899.293
(2S,3S,4R,5S,6S)-2,4,	454.514	0.000	18.700	-3.465	9906.038	5899.293
(1R,2S,5S)-2,6,6-trim	154.252	1.000	0.750	2.527	4790.612	2690.123
1-[(4aS,8R)-4a,8-dim	206.327	0.000	2.000	3.267	4578.250	2561.462
(1R,8R)-7,7-dimethyl	204.311	0.000	2.000	2.886	3860.823	2130.500
(1aS,4R,8aR)-1a,6-dii	220.354	0.000	2.000	2.738	9906.038	5899.293
(1S,4S,4aR)-4,7-dime	222.370	1.000	0.750	4.085	5765.555	3286.466
(1R,8R)-6,6-dimethyl	204.311	0.000	2.000	2.864	3820.438	2106.422
1-[(1aS,2aS,3R,7aR)-:	220.311	0.000	4.000	2.054	3373.589	1841.430
(1S,2S,7R)-2,6,6-trim	206.327	0.000	2.000	2.930	3623.267	1989.167
(3S,3aS,6S,7S,7aS)-6-	220.354	0.000	1.700	3.241	9906.038	5899.293
(1'S,2S,2'S,8'R)-2',6',†	220.354	0.000	2.000	2.341	9906.038	5899.293

(1S,4R,5S)-1,8-dimet	204.355	0.000	0.000	5.402	9906.038	5899.293
2-[(2R,6S,8S)-1,2-dir	218.338	0.000	2.000	3.137	2742.672	1472.191
(E)-3-[(1S,3aS)-3a-m	220.354	1.000	1.700	3.538	3440.149	1880.730
(4aR)-1,4a-dimethyl-	218.338	0.000	2.000	3.499	3639.413	1998.750
(1S,2S,8R)-2,6,6-trim	220.354	0.000	2.000	3.079	2837.027	1527.010
2-[(4aS)-4a-methyl-8	220.354	1.000	1.700	3.559	3596.071	1973.034
(2S)-2,4a,8,8-tetram	222.370	1.000	0.750	3.812	6547.561	3770.817
(1R,4S)-1,6-dimethyl	222.370	1.000	0.750	4.034	4542.145	2539.635
(2R,5S)-2-methyl-5-(i	222.370	1.000	0.750	4.476	4765.817	2675.077
methyl (Z)-3-phenylp	162.188	0.000	2.000	2.409	3312.373	1805.340
(1S)-1,6-dimethyl-4-ı	204.355	0.000	0.000	5.652	9906.038	5899.293
2-[(2R,5S)-5-ethenyl-	170.251	1.000	1.500	2.769	5867.830	3349.525
(3S,5S)-10,13-dimetf	398.671	1.000	1.700	7.210	3448.049	1885.399
(E)-2-methyl-4-[[[(E)-ı	202.329	0.000	3.000	2.544	2024.551	2404.218
(3E)-3,7-dimethyloct	152.236	0.000	2.000	2.356	2170.019	1142.950
1-(2,3-dihydro-1H-py	111.143	1.000	3.000	-0.051	428.471	218.968
(1S,4R)-1,6-dimethyl	202.339	0.000	0.000	5.397	9906.038	5899.293
(1S,2Z)-2,6,6-trimeth	222.370	1.000	1.700	3.615	4086.299	2265.299
2-[(5S)-5-ethenyl-5-n	170.251	1.000	1.500	2.769	5867.830	3349.525
(1S,3R)-4-methylider	152.236	1.000	1.700	2.276	4141.779	2298.561
(1S,4S)-1,6-dimethyl-	202.339	0.000	0.000	5.448	9906.038	5899.293
(E)-2-methyl-7-(4-m	218.338	1.000	1.700	4.113	3287.102	1790.457
(1S,4E,9S)-4,11,11-tr	204.355	0.000	0.000	5.127	9906.038	5899.293
(1S,5S,6R)-2,6-dimet	204.355	0.000	0.000	5.918	9906.038	5899.293
(1S,5S,6S)-2,6-dimetl	204.355	0.000	0.000	5.827	9906.038	5899.293
(Z)-6-methyl-5-meth	124.225	0.000	0.000	3.792	9906.038	5899.293
(E)-6-methyl-5-meth	124.225	0.000	0.000	3.932	9906.038	5899.293
(E)-2-phenylbut-2-en	146.188	0.000	2.000	2.024	2140.856	1126.357
2-[(8R,8aS)-8,8a-dim	222.370	1.000	0.750	4.040	4950.694	2787.416
2,2,4,4,6,6,8,8,10-no	432.842	0.000	1.000	9.012	9783.760	5820.623
[(1R,3S)-4-methylide	194.273	0.000	2.000	3.095	4449.929	2483.951
2-[(2R,4aS)-4a,8-dim	222.370	1.000	0.750	3.987	7157.390	4151.821
(9Z,12Z)-heptadeca-ı	266.423	1.000	2.000	5.175	235.426	131.776

[(2Z)-3,7,11-trimethyl-266.423	0.000	2.000	5.360	2476.927	1318.632
(9E)-octadeca-9,17-d 264.450	0.000	2.000	5.740	2278.622	1204.901
2-[(2R,4aR)-4a,8-dimethyl-222.370	1.000	0.750	4.056	5087.123	2870.535
(3R,4aR,6aS,10aS,10bS)-2,3-dimethyl-290.488	0.000	0.750	4.997	9906.038	5899.293
[(9R)-3a,5a,5b,8,8,11-hexamethyl-468.762	0.000	2.000	7.990	3946.002	2181.351
(7aR)-4,4,7a-trimethyl-180.246	0.000	3.000	1.578	2244.322	1185.309
(2R,3R)-2,3-dimethyl-72.107	0.000	2.000	0.269	9906.038	5899.293
2-[(2S,5S)-5-ethenyl-170.251	1.000	1.500	2.753	5104.407	2881.078
(1R,4aR,8aS)-7-methyl-204.355	0.000	0.000	5.596	9906.038	5899.293
(1S,2S)-1-ethenyl-1-r 204.355	0.000	0.000	5.616	9906.038	5899.293
(1S,4aR,8aR)-7-methyl-204.355	0.000	0.000	5.570	9906.038	5899.293
(2S,5S)-2-methyl-5-p 154.252	0.000	2.000	2.311	3741.588	2059.471
(5S)-2-methyl-5-propyl-152.236	0.000	2.000	2.232	3550.151	1945.816
(4aR,8aR)-5,8a-dimethyl-204.355	0.000	0.000	5.322	9906.038	5899.293
(3S,5R)-4,4,10,13,14-pentamethyl-426.724	1.000	1.700	7.718	5088.909	2871.625
(3S)-17-[(E)-5-ethyl-6-ethyl-412.698	1.000	1.700	7.471	3394.453	1853.742
(1R,2R)-1,2-diethylcyclohexane-126.241	0.000	0.000	4.941	9906.038	5899.293
(E)-4-isothiocyanatocyclohexane-175.263	0.000	6.500	0.313	94.163	4906.966
(1S,3R,4S,5R)-3-[(E)-5-ethyl-354.313	6.000	9.650	-0.266	2.090	0.798
(13S,14E)-14-ethylidene-264.369	1.000	2.000	3.608	1282.339	716.091
(1R,9R,10S,12R,13E)-13-ethyl-308.422	1.000	4.700	2.349	243.670	131.618
(E,2S)-2-amino-4-(2-ethyl-160.172	5.000	5.700	-3.552	1.046	0.463
(3E,7E)-3,7-dimethyl-218.338	0.000	2.000	3.467	4987.433	2809.781
(6E,10E,12E,14E,16E)-16-ethyl-542.930	0.000	0.000	18.485	9906.038	5899.293
butyl (9Z,12Z)-octadeca-9,12-d 336.557	0.000	2.000	7.396	3373.510	1841.383
[(1R,2S,4R,6R,9R,10F)-10,13,14-trimethyl-596.716	0.000	9.900	4.956	1634.457	841.359
[(3S,8S,9S,10R,13R,14S)-14-ethylidene-454.735	0.000	2.000	8.500	3648.421	2004.098
(2Z)-2-[(2S,3R,4S,6R)-4,7,10-trimethyl-375.375	5.000	16.800	-1.980	56.631	22.210
(5S,9E)-13,15-dihydro-290.315	1.000	4.500	2.099	252.841	111.918
(9Z,12Z)-octadeca-9,12-d 282.465	1.000	2.000	5.941	280.018	158.950
(11Z,14Z)-icosane-11,14-d 308.503	1.000	2.000	6.418	235.615	131.891
(1S,2S)-1-(3,4-dimethyl-358.433	1.000	4.700	4.780	4362.922	2431.497
(1R,4S,5'S,6R,6'R,8R)-8,11-dimethyl-556.738	1.000	6.650	6.667	1279.957	645.975

(2S)-5,7-dihydroxy-2-	7.000	15.250	1.378	0.339	0.088
(4aS,6aR,6aS,6bR,10-	5.000	14.000	6.219	8.548	3.659
(1R,4S,5'S,6R,6'R,8R,	0.000	6.950	5.996	1109.344	553.428
(1R,4S,5'S,6R,6'R,8R,	0.000	6.950	5.770	1101.777	549.349
[(2R,3S,4S,5R,6S)-3,	4.000	16.600	-0.214	34.480	12.991
(E)-3-[(4S,7R,7aR)-3,	0.000	2.000	3.302	1975.613	1032.687
[(E,6R)-6-hydroxy-6-	6.000	20.650	1.093	14.116	4.948
5-[(2E)-3,7-dimethyl	0.000	4.000	4.683	2055.817	1078.076
(3S,6E,10S)-6,10-dim	0.000	4.000	2.463	3175.793	1725.015
(9R,10R,13R,17R)-17	0.000	2.000	7.011	2815.572	1514.532
2-(2-aminoethylamir	1.000	2.000	5.941	280.017	158.950
[(E)-3-(4-hydroxy-3-r	2.000	5.000	3.664	245.145	108.240
[(3'R,4S,5'R,6S,6'R,8F	1.000	10.350	7.517	910.522	447.042
[(10E,14E,16E)-6'-etf	2.000	10.350	7.226	604.477	287.109
(10Z,12E,16Z)-6'-eth	1.000	6.650	6.049	1104.865	551.014
2-[(4Z,7Z,9E)-14-hyd	2.000	3.700	5.074	260.288	146.880
(3S,8S,9S,10R,13R,1'	1.000	1.700	7.960	3380.779	1845.672
[(3aS,6Z,10Z)-5,9-dih	2.000	8.400	1.956	418.955	193.178
(Z)-11-[(2S,3R)-3-per	1.000	4.000	4.816	235.420	131.772
7-[(E,6R)-6,7-dihydro	2.000	5.700	3.161	474.562	221.035
(E)-2-methyl-5-[(1S,2	1.000	1.700	3.687	3319.202	1809.363
(E)-1-[2,4-dihydroxy-	2.000	3.250	3.725	195.895	84.940
2-[3-[(2E)-3,7-dimetf	2.000	3.750	5.094	214.468	93.677
(2R)-2-[(E)-3-[(2S,3S)	9.000	14.000	1.671	0.006	0.002
(4aR,5R,6R,8aR)-5-[2	1.000	2.500	4.829	380.194	221.220
(3S,3aR,4aS,8aR,9aR	0.000	3.000	2.812	3029.225	1639.126
6a,11a-dihydro-6H-['	0.000	1.500	3.614	9906.038	5899.293
(8S,9S,10R,13R,14S,	0.000	2.000	7.523	3349.148	4140.234
ethyl (4R)-4-[(3R,5S,	3.000	7.100	3.877	316.474	142.651
methyl (1R,15S,18S,1	1.000	4.700	3.359	427.968	218.690
3-methoxy-4-[(2S,3R	4.000	12.000	-1.217	43.407	16.662
(2Z,6Z,10S)-3,7-dime	0.000	2.000	3.715	5413.442	3070.068
(3S,10S,13R,14R,17R	1.000	1.700	7.288	3398.590	1856.185

(2R,3R)-5,7-dihydrox	434.399	5.000	12.500	-0.353	14.316	5.024
8-(carboxymethylam	231.248	2.250	5.750	0.658	1.279	1.186
N'-[2-[2-(2-aminoeth	282.465	1.000	2.000	5.941	280.017	158.950
methyl (1S,14R,15E,	338.405	1.000	4.500	2.877	214.412	103.607
(1R,3R,5S,8S,9R,12S,	310.303	1.000	8.500	0.089	508.147	237.990
(1R,3R,4S,5R)-3,4-bis	516.457	7.000	11.450	0.806	0.239	0.077
(3R,5R)-3,5-bis[[E)-3	516.457	7.000	11.450	0.951	0.323	0.106
(1S,3R,4R,5R)-1,3-bis	516.457	7.000	12.400	0.681	0.387	0.129
(1S,5R,6R,10R,13S,1	428.654	1.000	3.200	6.470	1981.814	1036.191
(E)-1-[2,4-dihydroxy-	340.375	3.000	4.950	2.898	222.149	97.308
methyl (2R)-3-(3,4-di	374.346	4.000	7.000	1.643	17.479	6.233
(E)-3-methyl-5-(2,2,3	208.343	1.000	1.700	3.635	4045.029	2240.580
(5E)-cyclohexadec-5-	236.397	0.000	2.000	4.113	4543.175	2540.258
(1S,3E)-3-[(2E)-2-[(1F	400.643	2.000	2.450	6.715	1566.292	803.497
(3E,6E,9E)-nonadeca	262.478	0.000	0.000	9.004	9906.038	5899.293
(1Z,4Z,8Z)-2,6,6,9-te	204.355	0.000	0.000	5.304	9906.038	5899.293
(2E)-2-methyl-6-(4-r	220.354	1.000	1.700	3.873	3293.668	1794.323
(2S,3R,4S,5S,6R)-2-[(1229.325	17.000	47.400	-5.964	0.081	0.019
(1R,2R,3S,5R)-2,6,6-t	170.251	2.000	2.450	1.561	2012.054	1053.291
(2R,3S,4S,5R,6S)-6-(f	180.157	5.000	10.200	-2.133	91.693	37.390
(2R,3R,4S,5S,6R)-2-[[574.840	4.000	10.200	5.081	285.020	127.390
(1R,4R,6S,10R)-4,12,	220.354	0.000	2.000	2.560	9906.038	5899.293
[(3S,6aR,6bS,8aR,14	468.762	0.000	2.000	8.030	3919.303	2165.402
(2R,4aS,6aS,6aS,14a	536.707	1.000	7.000	6.142	169.186	92.202
(1R,4R,6R,10S)-4,12,	222.327	0.000	4.000	2.078	4375.680	2439.183
[(1R,9S,11S,12R)-1,2,	292.374	0.000	5.700	2.340	3734.984	2055.542
2-[[[(2S)-5-(diaminom	604.708	10.000	12.000	0.090	0.071	0.058
(2R)-2,5,8-trimethyl-	416.686	1.000	1.500	8.634	3674.673	2019.689
(1R,9R,10R)-17-azate	227.349	1.000	1.500	3.026	1424.619	802.342
(Z)-2-methyl-5-[(1S,2	220.354	1.000	1.700	3.703	3683.903	2025.173
[(2S,3R,4S,5S,6R)-3,4	359.366	5.000	14.000	-1.745	1.587	0.901
(Z)-7-[(1R,2R,3S,5S)-	477.642	2.000	7.400	3.663	69.566	39.033
(1S,2S,4R)-1-ethenyl-	204.355	0.000	0.000	5.705	9906.038	5899.293

2,2-dimethyl-3-phen	178.230	1.000	2.000	2.793	490.847	291.567
5-methylhexanoate	130.186	1.000	2.000	2.272	234.892	131.453
(3R,3aR,6S,6aR)-3,6-	386.444	0.000	6.400	3.095	9906.038	5899.293
(10R)-3,4,16-trimeth	371.432	2.000	5.750	2.793	437.709	224.075
(1R)-6,7-dimethoxy-	207.272	1.000	3.000	2.119	1589.434	903.128
[2-(6-amino-2,4-diox	375.380	1.000	6.750	2.731	120.853	50.394
hexacosanedioic acic	426.679	2.000	4.000	7.928	5.599	2.946
(3S,4S,5S,9R,10S,13R	426.724	1.000	1.700	7.835	3951.435	2184.597
(1S,2R,5S,7S,8R)-2,6,	206.370	0.000	0.000	6.637	9906.038	5899.293
(1S,3aS,4S,7R,8aS)-1,	208.386	0.000	0.000	7.021	9906.038	5899.293
(1S,4aR,7R,8aR)-1,8a	208.386	0.000	0.000	6.973	9906.038	5899.293
(1E,5E,8R)-1,5-dimet	204.355	0.000	0.000	5.138	9906.038	5899.293
(1S,4S,4aS,6S,8aS)-1,	208.386	0.000	0.000	7.042	9906.038	5899.293
(5S,8R,9R,10S,13R,14	414.757	0.000	0.000	13.043	9906.038	5899.293
[(2Z)-2-[2-[acetyl(me	378.427	0.000	8.200	2.451	1436.870	1364.712
1-(1-adamantyl)-3-[(1	327.487	2.000	3.500	4.767	4025.016	4157.608
(2R)-2-amino-3-prop	161.218	3.000	3.500	-1.425	23.428	18.061
(3R,5R)-4-[(E)-3-(3,4-	354.313	6.000	9.650	-0.191	2.027	0.772
(2R,3S,4S,5R,6S)-2-(f	638.880	7.000	14.350	2.848	67.804	26.982
(2S,3R,4S,5S,6R)-2-el	208.211	4.000	10.200	-1.444	208.433	90.831
5,6,7-trihydroxy-2-pl	272.257	2.000	4.000	1.731	186.409	80.503
(9Z,12Z)-octadeca-9,	298.895	0.000	2.000	6.291	3075.268	3837.170
(2R,3R,4S,5S,6R)-2-[(428.435	6.000	17.000	-1.294	40.881	15.616
2-decyltetradecyl N-(471.763	3.000	5.900	7.544	403.372	185.423
(1R,4S,5'S,6R,6'R,8R,	528.684	1.000	6.650	6.088	1155.000	578.088
1,3,3-trimethyl-2-[(1	536.882	0.000	0.000	16.819	9906.038	5899.293
7,8,9-trihydroxy-3,5-	292.201	4.000	8.750	-1.112	1.698	0.638
(3S,4aR,6aR,6bS,8aR	442.724	2.000	3.400	6.070	2322.583	1230.047
4-[2-[(1R,4aS,5R,8aS)	480.597	4.000	13.200	1.414	108.031	44.641
5-hydroxy-2-(4-hydr	578.526	7.000	19.050	-1.384	3.770	1.188
(3R,4aS,5R)-4a,5-dir	204.355	0.000	0.000	5.401	9906.038	5899.293
(E)-1-[2,4-dihydroxy-	340.375	3.000	4.000	3.102	124.165	51.888
2-methyl-2-(4,8,12-ti	388.632	1.000	1.500	8.028	3001.299	1622.799

(1S,4R,5'S,6'R,7S,9S,10S)-5	1.000	6.650	6.761	2052.771	1076.349
(1R,5R,6S,13S,21R)-5	9.000	10.900	0.255	1.325	0.383
[(1S,4R,5R,6S,7S,8R,11S,12S)-2,11	4.000	16.450	2.276	129.826	60.239
(2R,3S,4R)-2-(3,4-dihydroxy-5-hydroxy	15.000	16.350	0.390	0.026	0.005
(3S)-2-(3,5-dihydroxy-4-hydroxy-5-hydroxy	6.000	13.250	-0.809	6.129	2.008
(1S,2R,4aS,6aR,6aS,6bS,7S,8S,9S,10S)	1.000	4.000	6.214	299.445	170.903
(3S,4R,4aR,6aR,6bS,7S,8S,9S,10S)	4.000	6.800	3.996	398.384	182.946
(2R,3R,4S,5S,6R)-2-[[1S,2R,3R,4S,5S,6R]	15.000	38.150	-3.116	0.102	0.024
[(1S,3R,6S,8R,11S,12S)-2,11	1.000	3.500	10.310	1382.855	702.284
(3S,5R,8R,9R,10R,12S)-2,11	3.000	4.150	6.003	1495.204	764.153
2-methyl-2-[(3E,7E)-2,6,8-trimethyl-5,7-dihydroxy-2-(4-hydroxy-3-methyl-2-[[1S,2R,3R,4S,5S,6R]	1.000	1.500	7.740	3001.308	1622.805
(4S)-4-hydroxy-3,5,5-trimethyl-2-(4-hydroxy-3-methyl-2-[[1S,2R,3R,4S,5S,6R]	5.000	12.950	-0.210	108.962	45.056
(1S,3R,4R,5R)-3-[(E)-2,6,8-trimethyl-5,7-dihydroxy-2-(4-hydroxy-3-methyl-2-[[1S,2R,3R,4S,5S,6R]	6.000	11.450	1.762	0.821	0.291
(1R,3R,4S,5R)-1,3,4-trimethyl-2-(4-hydroxy-3-methyl-2-[[1S,2R,3R,4S,5S,6R]	5.000	8.900	0.404	4.698	1.916
4-[(E)-5-(3,3-dimethyl-2-(4-hydroxy-3-methyl-2-[[1S,2R,3R,4S,5S,6R]	0.000	5.750	3.616	2055.742	1078.033
(1R,4S,5'S,6'R,8R,11S,12S)-2,11	1.000	6.650	6.374	1182.332	592.888
(2S)-4-[(2R,11R)-2,11	3.000	11.500	7.374	315.274	142.066
5,7-dihydroxy-2-(4-hydroxy-3-methyl-2-[[1S,2R,3R,4S,5S,6R]	2.000	3.750	2.028	176.236	75.765
(2E,8E)-9-(1,3-benzodioxol-5-yl)-2-(4-hydroxy-3-methyl-2-[[1S,2R,3R,4S,5S,6R]	0.000	4.500	4.861	4239.061	2356.971
1-[(2E)-3,7-dimethyl-2-(4-hydroxy-3-methyl-2-[[1S,2R,3R,4S,5S,6R]	2.000	1.500	6.470	3863.876	2132.321
3-methyl-2-[[1S,2R,3R,4S,5S,6R]	0.000	10.000	2.013	503.367	235.571
1-(2,7-dihydroxy-4-naphthyl)-2-(4-hydroxy-3-methyl-2-[[1S,2R,3R,4S,5S,6R]	4.000	4.500	4.587	164.519	70.335
5-[(1R)-1-[(1S,4R,4aR,5aS,6aR,6aS,6bS,7S,8S,9S,10S)	2.000	4.750	4.714	27.225	10.063
3-[(2S,3R,4S,5R,6R)-2,11	9.000	21.500	-2.669	0.961	0.271
(2S)-4-[9-[(2R,5S)-5-[[1S,2R,3R,4S,5S,6R]	3.000	11.500	7.495	368.865	168.339
(3S,6Z)-3-methyl-6-[[1S,2R,3R,4S,5S,6R]	3.000	5.000	2.892	587.794	278.554
(1S,2R,3R,4S,5S,6S,8S)-2,11	3.000	11.250	1.574	426.492	217.875
(E)-5,9,13,17-tetramethyl-2-(4-hydroxy-3-methyl-2-[[1S,2R,3R,4S,5S,6R]	1.000	1.700	13.662	4310.916	2400.184
6,7,14-trihydroxy-13-oxo-2-(4-hydroxy-3-methyl-2-[[1S,2R,3R,4S,5S,6R]	6.000	14.800	-2.247	1.777	0.527
4,6,7-trimethoxy-9-[[1S,2R,3R,4S,5S,6R]	4.000	16.000	0.496	77.091	30.998
[(8R,9S,27R,29S,30R,31S)-2,11	12.000	25.200	-3.211	0.001	0.000
(1S,2R,7R,9R,11R,12S)-2,11	1.000	6.100	1.458	2010.873	1052.623
[(2R,3R,4S,5S,6R)-3,4	8.000	21.400	1.065	4.089	1.297

(1R,5R)-5-methyl-2- <i>f</i>	154.252	1.000	1.700	2.388	4774.328	2680.240
(2E,4E)-7-(1,3-benzo	313.396	0.000	4.500	4.078	4161.909	2310.638
3-(2,4-dihydroxyphei	368.385	3.000	5.500	2.854	260.789	115.725
(3S,3aS,5aR,5bR,7aR	426.724	1.000	1.700	7.046	4370.734	2436.203
3,5-dihydroxy-2-(4-h	448.382	6.000	13.000	-0.829	5.014	1.616
methyl (2S,4aS,8R,1C	538.547	5.000	16.450	-0.022	24.014	8.787
[(2S,3R,4S,5S,6R)-3,4	582.557	5.000	17.450	-0.042	16.278	5.772
(2R)-2-[(1R)-1-hydro	620.779	6.000	15.650	1.740	23.999	8.781
(4S)-1-methyl-4-(6-r	204.355	0.000	0.000	6.317	9906.038	5899.293
2-(3,4-dihydroxyphei	626.524	10.000	22.250	-3.372	0.318	0.082
(1R,3R,4S,5R)-1,3,4-t	368.340	5.000	9.650	0.530	4.782	1.953
(3R,5R)-1-[(E)-3-(3,4-	354.313	6.000	10.600	-0.504	2.143	0.820
(E)-4-(3-hydroxy-2,6,	208.300	1.000	3.700	2.149	1358.599	688.979
(3R,5R)-1,3,5-trihydr	368.340	5.000	9.650	0.553	5.195	2.136
2-(3,4-dihydroxyphei	772.666	12.000	29.050	-4.730	0.063	0.014
(3R,4S,5S)-3,4,5,6-te	194.141	3.000	8.800	-1.696	3.836	1.539
3-[(2S,3R,4R,5S,6R)-	626.524	10.000	22.250	-3.358	0.213	0.053
(3E,7E)-4,8,12-trimet	236.397	1.000	1.700	4.774	3313.628	1806.079
methyl (10E,12Z,15Z	308.460	1.000	3.700	4.840	1032.800	512.271
1-[(12R)-16-methoxy	337.374	0.000	5.250	2.523	1941.151	2023.721
3-[(2R,3R,4R,5S)-3,4-	434.356	6.000	12.050	-0.825	7.765	2.593
1,3,3-trimethyl-2-[(1	536.882	0.000	0.000	16.706	9906.038	5899.293
10-[9-hydroxy-3,5-di	692.896	4.000	3.000	10.745	1060.740	527.266
(2R,10R)-17,17-dime	322.360	1.000	3.000	4.195	3001.316	1622.809
[(3S,4R,5S)-5-[[9-(1,3	554.506	2.000	12.900	2.198	270.856	120.561
[(1R,2R)-2,3-dihydro	376.405	2.000	7.700	2.780	497.930	232.822
4-[(3,4-dihydroxyphe	380.396	5.000	4.500	2.636	59.679	23.505
(2E,4E,6E,8E,10E,12E	490.549	5.000	12.500	2.373	3.011	1.185
[2-[(2S,3R,4S,5R,6R)-	510.496	4.000	12.300	1.665	45.842	17.674
2-(3,4-dihydroxyphei	610.524	9.000	20.550	-2.468	1.188	0.341
(2R,3S)-2-(4-hydroxy	638.673	4.250	10.750	4.350	26.185	14.136
(3R)-3-methyl-4-(oxa	186.250	0.000	5.400	1.013	2508.272	1336.678
(1R,4S,4aR,8aR)-1,6-	222.370	1.000	0.750	4.034	4542.145	2539.635

(1S,2S,5S,8R)-2-methyl	234.338	1.000	1.500	3.678	4341.357	2418.509
[(1S,9R,18R,19S,21R,65O)	459.650	10.000	19.850	-3.707	0.025	0.005
[(2S,3R,4S,5S,6R)-4,5	744.699	8.000	25.950	-2.300	1.132	0.324
[(2S,3R,4S,5S,6R)-3,4	959.133	11.000	29.900	-1.114	0.580	0.157
2-[4-hydroxy-2-[(2S,3R,	311.291	5.000	11.500	-1.263	31.291	11.697
[(2S,3R,4S,5R,6S)-6-[(2S,	321.329	2.000	9.350	0.745	198.508	86.165
(2S,3R,4R,5R,6S)-2-[(2S,	903.069	11.000	28.700	-0.831	0.526	0.141
(3aR,3bR,6aS,7aR)-3-methyl	204.355	0.000	0.000	5.795	9906.038	5899.293
[(1S,4aS,6S,7S,7aS)-6-methyl	462.493	6.000	16.350	-0.640	34.656	13.062
4-(1,3-benzodioxol-5-yl)	498.442	5.000	14.500	-0.363	35.047	13.222
9-(1,3-benzodioxol-5-yl)	776.701	7.000	26.200	-1.600	9.076	3.070
3-[2-(3-hydroxyphenyl)	244.290	2.000	2.250	2.801	1008.889	499.464
methyl octadec-17-ene	296.492	0.000	2.000	6.566	3264.746	1777.299
4-[2-[(1R,5R,6R,8aS)-8-methyl	364.481	2.000	8.100	2.169	849.707	414.857
9-(3,4-dimethoxyphenyl)	410.423	0.000	6.750	3.654	3192.925	1735.075
(6aS,6bS,8aR,11R,12-methyl	422.606	2.000	4.450	4.473	402.375	184.928
[2-[(2S,3R,4R,5R,6R)-6-methyl	646.646	3.000	12.850	4.163	149.596	63.465
methyl (1S,2R,3R,4R,5R,	498.572	1.000	9.900	3.334	861.323	420.990
4,6,7-trimethoxy-9-yl)	572.521	4.000	16.000	0.713	156.416	66.598
(2R)-2-[(1S)-1-[(3R,8R,	650.762	7.000	17.450	1.022	22.771	8.296
(1S,4S,5R,9S,10R,13F)	308.460	3.000	3.200	3.064	1063.984	529.010
(2R,3R,4S,5S,6R)-2-[(2S,	418.526	6.000	12.650	0.168	97.744	40.064
(5R)-5-[(7S,13R)-7,13	624.940	3.000	11.800	7.212	96.642	39.576
1,3-dimethoxy-5-(2-yl)	242.317	0.000	1.500	4.325	9906.038	5899.293
3-(3,4-dihydroxyphenyl)	302.240	4.000	5.250	0.378	21.171	7.668
(NE)-N-[3-(2-methoxyphenyl)	346.418	0.000	5.750	3.404	4090.534	4391.404
methyl 7,14-dihydro-1,2,3,	462.455	1.000	7.750	3.276	160.345	68.408
(2R)-2-[(1S)-1-hydroxy-2,	520.619	6.000	11.400	1.783	102.360	42.113
(4aS,6aR,6aS,6bR,8aR,	602.853	2.000	4.750	8.485	98.381	51.315
[(4aS,5S,6aR,6aS,6bS)-6-methyl	514.744	1.000	7.700	4.767	478.094	222.814
(1R,2S,4S,5'R,6R,7S,8R,	1181.284	13.000	42.350	-3.927	0.199	0.049
[(2R,3S,4S,5R,6R)-3,4	476.436	5.000	12.750	-0.118	9.627	3.271
6,7-dimethoxy-4-[6-yl)	542.495	4.000	15.250	0.637	123.524	51.599

[5-[(E)-hydroxyimino	141.126	2.000	5.400	-0.451	425.970	196.676
2-[(1R)-1-[(3S,8S,9S,	1409.611	2.000	3.450	5.534	1450.331	739.396
(1R,3E,7E,11R)-1,5,5,	220.354	0.000	2.000	2.498	9906.038	5899.293
5-[(1S)-1-[(1S,4aS,6R	472.620	1.000	4.000	5.374	63.370	25.080
(3S,4R,8S,9S,10R,13S	413.642	3.000	4.400	4.989	1280.362	646.196
10-acetyl-21-hydroxy	420.418	0.000	8.000	2.372	268.306	119.335
(2R)-2-[(1R)-1-hydro	634.762	6.000	16.700	1.225	14.916	5.251
(2R,3R,4S,5S,6R)-2-[[658.739	10.000	21.900	-1.386	4.150	1.317
(2R)-2-[(1R)-1-[(3R,8	632.747	5.000	16.650	1.265	8.331	2.798
[(2S,3R,4S,5S,6R)-3-[[876.815	10.000	32.750	-3.713	0.958	0.270
2-(3,4-dihydroxyphe	464.382	7.000	13.750	-1.417	3.007	0.930
4-[(2R,3R)-3-(3,5-dih	470.478	6.000	5.250	2.951	16.049	5.684
bis[[4-[(2S,3R,4S,5S,	888.869	12.000	31.750	-3.033	0.526	0.141
(2S,3R,4R,5R,6S)-2-[[1151.301	13.000	40.600	-2.733	1.319	0.382
[(1S,8S,11R,12S,13R,	404.459	2.000	7.950	2.157	476.336	221.928
(2S,11bS)-2-[(2R)-1-h	303.400	2.000	5.200	2.266	248.290	121.409
(13aR)-12-ethenyl-2-	322.363	1.000	6.000	2.527	661.455	316.469
(3R,4aR,8aR)-5,8a-di	204.355	0.000	0.000	5.435	9906.038	5899.293
(2R)-4-[[4-(4-heptyl	432.645	0.000	3.000	8.518	2884.426	1554.604
(3R)-12-[(2R,5R,6S)-	507.620	8.000	17.100	-2.511	0.307	0.111
[(1R,2S,3'S,4S,5'S,6S,	1270.378	17.000	47.950	-6.328	0.007	0.001
(1S,2R,4R)-2-methyl-	204.355	0.000	0.000	5.742	9906.038	5899.293
(8S,9S,10R,13R,14S,1	300.483	0.000	2.000	4.817	2799.989	1505.473
(Z,2R)-N-[(2S,3S,4R)-	844.263	8.000	17.800	7.426	18.496	11.159
(2R,3R,4R)-2-[(1R)-1,	164.158	4.000	8.500	-1.661	198.859	86.330
(1aR,7R,7aS,7bR)-1,1	204.355	0.000	0.000	5.249	9906.038	5899.293
(2S,3R,3aS,4'S,5'R,6S	332.350	5.000	9.350	0.307	16.251	7.328
(3S)-8-hydroxy-3-me	178.187	0.000	2.750	1.400	1141.124	570.585
[(2R,3S,4S,5R,6S)-6-[[602.504	8.000	15.800	-1.096	0.181	0.045
(E,6S)-2-methyl-6-(4-	218.338	1.000	1.700	3.915	3318.616	1809.018
[(1S,18R,19S,21R,22'	634.460	11.000	17.850	-3.230	0.030	0.006
(1aR,3aS,7S,7aS,7bR)	222.370	1.000	0.750	3.881	5118.383	2889.606
(14R)-14-methylhex	252.439	1.000	1.700	5.357	3296.446	1795.959

2-methoxy-3-phenyl	190.198	0.000	4.700	0.899	1962.541	1025.303
(1R,3R,6S,7S,8S)-2,2,	222.370	1.000	0.750	3.693	5942.108	3395.378
(3R,4R,5R)-oxane-2,3-	150.131	4.000	8.500	-1.715	194.984	84.513
6-hydroxy-17,17-dim	334.328	1.000	4.500	3.030	785.254	380.950
[(1S,4S,5R,9S,10R,13	378.508	1.000	4.750	3.884	415.088	191.251
9-[4-hydroxy-3-[(2S,3	528.468	5.000	15.250	-0.146	51.979	20.245
methyl 2-hydroxy-9H	241.246	1.000	1.750	2.868	695.698	334.215
methyl 8-[(2S,3R)-3-oxo-	312.492	0.000	4.000	5.470	2984.466	1612.964
(8,8-dimethyl-2-oxo-3-	330.380	0.000	5.250	3.368	1199.622	602.265
(2S)-4-hydroxy-2,5-d	128.127	1.000	3.500	0.221	1117.359	557.752
(2E,4E,8E)-9-(1,3-ber	327.422	1.000	4.000	4.860	3350.504	1827.814
(6R)-6-ethenyl-6-methyl	204.355	0.000	0.000	5.637	9906.038	5899.293
(3R)-3-hydroxy-12-[(1	329.479	3.000	5.900	1.091	7.225	3.375
[(1S,4S,5S,9S,10R,13	366.497	2.000	5.200	3.207	439.649	203.512
(2R,3S)-2-(3,4-dihydro	290.272	5.000	5.450	0.506	51.573	20.074
(1S,4S,5S,9S,10R,13R	324.459	3.000	4.900	2.384	531.835	250.004
trimethyl-[[[(2R,3R,4S	541.066	0.000	5.950	5.015	9906.038	5899.293
(2S,3R,3aS,4'S,5'R,6S	494.492	8.000	17.850	-1.590	1.052	0.380
(2R)-2-[(1S)-1-hydroxy	504.619	5.000	9.700	2.634	225.906	99.088
(2S,3R,3aS,4R,4'S,5'R	348.349	6.000	11.050	-0.536	7.288	3.080
(1S,4S,5R,9S,10R,13F	292.461	2.000	2.450	3.634	2054.569	1077.368
benzyl 2-hydroxy-3,6-	288.299	0.000	3.250	3.655	1392.694	707.687
cyclohex-2-en-1-ylmethyl	112.171	1.000	1.700	1.343	3308.627	1803.133
(Z)-5-[(1S,3R,6R)-2,3-	220.354	1.000	1.700	3.618	3524.984	1930.910
2-(3-methylbut-2-en-1-	280.366	2.000	1.500	4.819	2068.060	1085.017
(4R,5S,7R,2S,26R,3C)	970.671	14.000	25.450	-3.543	0.000	0.000
(1aR,4aR,7R,7aR,7bS	204.355	0.000	0.000	5.190	9906.038	5899.293
3-[(8Z,11Z)-pentadec	300.483	1.000	0.750	6.739	3000.325	1622.230
[(2R,4R)-2,3,4,5-tetra	362.333	0.000	10.000	0.772	45.436	17.505
(1S,2S,4R)-2-methyl-	204.355	0.000	0.000	5.716	9906.038	5899.293
(1S,2R,5S,7S)-2,6,6-t	204.355	0.000	0.000	4.855	9906.038	5899.293
(3S,5R,6R,8S,9S,10R,	486.564	0.000	2.000	8.004	2328.009	4357.453
(2S)-4-[(2R,13R)-2,13	622.924	3.000	11.500	6.912	233.834	102.852

(2E,4E)-3,7-dimethyl	150.220	0.000	2.000	2.255	1736.205	898.111
[(1S,18R,19S,21R,22S)	616.445	9.000	16.850	-2.429	0.110	0.026
[(2S,5R)-5-methoxy-	116.160	1.000	3.400	0.490	2810.212	1511.415
(3E)-3-[2-[(1R,2S,4aS)	318.455	0.000	5.000	3.119	2315.753	1226.137
2-methyl-5-[(2S)-6- <i>m</i>	218.338	1.000	0.750	4.309	3688.429	2027.862
3-[2-(3-hydroxyphenyl)	350.413	3.000	3.000	3.966	294.285	131.872
6-[(Z)-but-2-en-2-yl]-	164.204	0.000	2.500	2.046	3086.561	1672.686
5-[(E)-2-(3,4-dihydro-	312.365	4.000	3.000	3.099	180.140	77.581
3-(2,4-dihydroxyphenyl)	338.359	2.000	5.000	2.892	528.500	248.310
(1R,2S,3S)-1-(3,4-dimethyl)	416.513	0.000	6.400	3.564	9906.038	5899.293
(3R,6E)-3,7,11-trimethyl	222.370	1.000	0.750	4.912	5263.998	2978.564
5-(7-methoxy-5-propyl)	308.333	0.000	2.750	4.201	9906.038	5899.293
(2R,3S)-2-(3,4-dihydro-	578.528	10.000	10.900	0.201	1.305	0.377
(2S)-6-amino-2-[[[(2R,	1092.216	6.000	21.450	-1.881	0.002	0.008
(1S,12S,13R,14R,15E)	292.380	1.000	4.000	2.528	371.022	187.414
3-[(8Z,11Z)-pentadecyl]	298.467	1.000	0.750	6.462	3000.404	1622.276
(1R,4S,5R,6R,7S,10R)	222.370	1.000	0.750	4.122	5532.199	3142.929
[(2S,3S,4S,5S,6R)-6-[[568.533	2.000	13.850	1.919	265.674	118.070
(1S,2S,4S,5R,10R,11S)	470.605	2.000	8.500	3.459	440.727	204.051
(5S,6R)-6,10-dimethyl	202.339	0.000	0.000	5.535	9906.038	5899.293
1-O-tert-butyl 2-O-methyl	259.302	1.000	6.200	1.730	892.142	437.296
7-hydroxy-2-[4-hydroxy-	390.478	2.000	4.000	5.199	788.705	382.760
5-[(1R,2S,3S)-6,7-dimethyl]	400.471	0.000	6.400	3.059	9906.038	5899.293
6-acetyl-5-hydroxy-4-	218.209	0.000	4.250	0.982	432.390	199.883
5-[(E)-2-(4-hydroxyphenyl)]	296.365	3.000	2.250	4.003	504.845	236.319
3-(2-hydroxy-4-methylphenyl)	352.386	1.000	5.000	3.795	1746.677	903.968
(1R,2S,3R,11R,14S,16S)	444.524	2.000	6.450	4.236	667.573	319.635
1,4-bis(1,3-benzodioxol-5-yl)	356.331	0.000	7.700	1.581	1105.070	551.124
ethyl 10-[4-(1-adamantanecarboxylate)]	478.671	2.000	6.000	5.802	249.027	156.424
2,3,4,7-tetramethoxy-	298.338	0.000	3.000	3.542	9906.038	5899.293
3,4,8,10-tetrahydro-	314.251	3.000	5.250	0.860	51.566	20.071
9-(1,3-benzodioxol-5-yl)	526.496	3.000	13.550	1.422	319.773	144.259
(Z)-3-[6-[(2S,3R,4S,5S)	366.324	5.000	11.750	-0.248	7.600	3.222

(3E,4S)-3-[2-[(1R,4aS,512.596	6.000	16.600	-0.514	15.763	5.575
[(2S,3R,4S,5S,6R)-3,4 498.612	6.000	13.900	0.654	25.101	9.217
3,6,9,11-tetrahydrox 328.278	3.000	6.200	0.945	86.758	35.220
5-[(4aS,6aS,6bR,10a 504.619	2.000	8.500	3.851	7.719	3.277
(Z)-3-[4-[(2S,3R,4S,5S 366.324	5.000	11.750	-0.139	10.637	4.635
bis[[4-[(2S,3R,4S,5S,ε 1061.052	10.000	32.350	-0.139	0.280	0.071
(4aR)-3,5,5,9-tetram 204.355	0.000	0.000	5.260	9906.038	5899.293
3-[(2S,3R,4S,5S,6R)-4 740.668	10.000	26.600	-2.909	0.840	0.234
(2S,3S,4S,5R,6S)-6-(5 446.367	4.000	11.550	0.376	1.036	0.374
(1S,12S,15S,20R)-7-[519.723	2.000	5.450	6.370	1785.723	925.830
[2-[(2S,3R,4S,5R,6R)- 568.530	8.000	20.500	-1.735	3.763	1.185
(2R)-3-(3,4-dihydrox) 198.175	4.000	5.200	-0.210	12.567	5.550
(2R)-2-hydroxy-4-me 458.461	5.000	13.000	0.766	2.588	1.006
4-[2-[(1R,4aS,5R,6R,ε 334.455	2.000	6.400	2.532	765.358	370.529
(3R)-3-hydroxy-5-me 458.461	5.000	13.000	0.835	3.704	1.482
bis[[4-[(2S,3R,4S,5S,ε 1061.052	10.000	32.350	0.145	0.163	0.040
4-[2-[(1R,4aS,5R,8aS 318.455	1.000	4.700	3.373	1109.728	553.635
(1S,3S,9R,10R,11R,14 375.507	0.000	8.000	1.970	217.443	105.191
ethyl (2R,3R)-2-amin 343.549	2.000	3.700	5.178	164.581	77.844
bis[[4-[(2S,3R,4S,5S,ε 1019.015	11.000	32.050	-0.861	0.259	0.066
3-(2,4-dihydroxyphei 352.343	2.000	4.500	3.024	225.328	98.814
(1S,2R,4S,5S)-6-[(2R, 342.299	9.000	18.700	-3.997	5.210	1.685
9-(1,3-benzodioxol-5 378.337	0.000	6.750	2.153	3187.943	1732.149
[(1S,4S,5R,9S,10R,13 350.497	2.000	4.450	3.569	1152.797	576.896
(5R,6S,7S)-5-(1,3-ber 384.428	0.000	6.400	2.286	9906.038	5899.293
[(1S,6S,7R,7aS)-4-(ac 494.538	0.000	11.700	2.821	407.065	187.259
heptadeca-4,6-diyne 280.406	3.000	5.100	3.275	757.778	366.563
9-(1,3-benzodioxol-5 526.496	3.000	13.550	1.367	258.414	114.586
methyl N-[(3-hydrox) 268.348	2.000	4.250	2.155	733.645	1072.578
(3R)-12-[(2R,5R,6S)-ε 491.621	7.000	15.400	-1.404	1.669	0.692
(4S)-4-(4-methylpher 176.258	0.000	2.000	2.667	1849.839	961.812
(2R,3S,4S,5R,6R)-2-(576.769	4.000	11.700	3.866	218.723	95.687
(4aS,9aR)-3,5,5-trimε 204.355	0.000	0.000	5.111	9906.038	5899.293

(1R,2S,7S,14R)-14-hy	221.255	1.000	6.700	-0.227	232.263	112.961
(1aR,4S,4aR,7R,7aS,7	222.370	1.000	0.750	4.001	5359.948	3037.290
[(1S,2S,4S,5S,6R,10S]	512.466	5.000	18.100	-1.192	16.136	5.717
[(1S,2S,4S,5S,6R,10S]	508.478	5.000	17.350	-0.714	22.376	8.141
[(8R,9S,10R,13S,14S,	452.676	0.000	4.000	7.375	1141.390	570.728
(2S,3R,4S,5S,6R)-2-(4	302.280	5.000	10.750	-0.955	70.087	27.965
(1R,4R,5R)-1,8-dimet	218.338	0.000	2.000	3.597	6054.875	3465.079
(1R,4R,5S)-8-methyl-	218.338	0.000	2.000	3.415	3485.900	1907.780
(1aR,4S,4aS,7R,7aS,7	222.370	1.000	0.750	3.880	4653.369	2606.919
4-[(E)-2-[(1R,4aS,5R,	664.878	4.000	12.800	4.369	51.457	20.025
2-(2,4-dihydroxyphe	302.283	2.000	4.750	1.842	176.604	75.936
[(1S,2S,4S,5S,6R,10S]	524.477	6.000	18.100	-1.444	3.926	1.241
[(1S,2S,4S,5S,6R,10S]	538.504	5.000	18.100	-0.715	14.159	4.964
3,9,11-trihydroxy-10	326.262	2.000	6.250	0.917	58.109	22.837
[(1S,2R,4S,7S,8S,11R,	482.572	0.000	9.500	2.685	643.073	306.975
6-[2-(3,4-dihydroxyp	478.365	6.000	13.050	-0.862	0.213	0.068
(1R,3S,3aR,5aS,5bS,6	474.723	4.000	6.800	4.073	480.914	224.235
[(1S,8S,11S,13R,17S,	388.460	1.000	6.250	3.045	913.608	448.679
(2S)-5-hydroxy-6,7-d	300.310	0.000	4.000	3.204	1686.205	870.188
[(2E,6E)-3,7,11-trime	312.494	0.000	1.700	6.466	9906.038	5899.293
(1S,4R,4aS,8aR)-4,7-(222.370	1.000	0.750	4.094	5469.052	3104.170
(1R,4S,8S,12R)-1,3,3,	222.370	0.000	0.750	3.300	9906.038	5899.293
(10bR)-9-hydroxy-7,8	341.363	1.000	7.250	1.264	227.099	190.508
(2R)-2-[(1R)-1-[(8R,9'	452.589	1.000	6.450	4.450	361.645	164.780
[(2S)-2,3-dihydroxyp	356.545	2.000	5.400	5.020	503.837	235.809
ethyl acetate	88.106	0.000	2.000	0.730	2241.337	1183.605
4-hydroxy-3-(113C)n	152.149	1.000	3.500	1.001	563.117	265.936
(1S,5R)-2-methyl-5-p	154.252	1.000	1.700	2.723	4117.475	2283.985
7-methoxy-2,5-dime	204.225	0.000	3.250	2.151	3808.136	2099.092
(1S,2S,4S,6R,7S,10R,	359.508	1.000	6.400	2.297	176.532	83.972
2-[(2E,4E,6E,8E,10E,	600.880	2.000	4.900	9.917	1172.443	587.530
(1S,5S,6R)-6-methyl-	204.355	0.000	0.000	5.824	9906.038	5899.293
(1S)-4-methyl-1-[(2S)	222.370	1.000	0.750	4.519	5753.835	3279.246

3,8-dimethyl-5-prop	204.355	0.000	0.000	5.507	9906.038	5899.293
(3S,5R,9R,10R,13S,14S)-	426.724	1.000	1.700	7.714	4335.295	2414.859
(1R,4S,4aS,8aS)-1,6-	222.370	1.000	0.750	4.010	5283.449	2990.462
(1S)-4,7-dimethyl-1-	200.323	0.000	0.000	5.318	9906.038	5899.293
(1S)-1-[[[(2S,3R,11bS)	466.619	2.000	6.500	4.291	122.510	62.593
(1R,2S,4S,5'R,6R,7S,8S)-	432.642	2.000	4.900	5.104	1370.267	695.377
(3S,8S,9S,10R,13R,17S)-	414.713	1.000	1.700	7.612	3381.090	1845.856
(1R,2S,5S,6S,9R,12S,13S)-	314.513	3.000	2.500	2.938	107.122	54.141
(1R,2S,5S,6S,9R,12S,13S)-	342.567	1.000	3.500	4.105	335.139	185.752
(1R,2S,6S,7S,8S)-1,3-	204.355	0.000	0.000	5.965	9906.038	5899.293
2-(4a-methyl-8-methyl-8-	220.354	1.000	1.700	3.456	3314.747	1806.738
2-[[[(2S,4aR,8aR)-4a,8-	222.370	1.000	0.750	3.992	5743.548	3272.909
(1R,2S,4S,5'S,6R,7S,8S,8aR)-	432.642	2.000	4.900	5.061	1300.054	656.945
(1R,2S,4S,5'S,6R,7S,8S,8aR)-	416.643	1.000	3.200	6.130	3393.101	1852.944
(1S,2S,8R)-6,7,7-trimethyl-	234.338	1.000	2.000	3.535	455.557	268.976
(5R)-1-methyl-5-propyl-	136.236	0.000	0.000	4.015	9906.038	5899.293
(3aR,4aR,6R,8aR,9aR,10aR)-	248.321	1.000	4.700	1.895	1118.504	558.369
5,7-dihydroxy-2-[3-hydroxy-	448.382	6.000	13.000	-0.887	4.467	1.427
(1S,2S,5S,8R)-2,7,7-trimethyl-	204.355	0.000	0.000	4.831	9906.038	5899.293
2-(7-methyl-4-methyl-4-	220.354	1.000	1.700	3.587	3365.692	1836.771
(1aR,4R,4aR,7R,7aS,8aS)-	222.370	1.000	0.750	3.909	4595.918	2572.148
(3S,3aS,5aS,5bS,7aR,8aS)-	426.724	1.000	1.700	7.134	4712.818	2642.936
(3R,3aR,5aR,5bR,7aR,8aS)-	426.724	1.000	1.700	7.132	4345.710	2421.130
methyl (1S,15R,16R,17S)-	382.458	1.000	6.450	3.325	603.544	317.104
(4aS,6aR,6aS,6bR,8aS,8aR)-	488.706	4.000	7.100	4.344	67.969	34.408
(1S,3R,8R,11S,12S,15S)-	424.709	0.000	2.000	7.679	4193.393	2329.537
[3,3-dideuterio-6,6-dideuterio-	154.252	1.000	1.700	2.572	4154.959	2306.468
(10S)-1,8-dihydroxy-1,8-	418.399	5.000	11.700	-0.369	12.272	4.253
(3S,4R,5R)-2,5-bis(hydroxy-	180.157	5.000	8.300	-1.715	89.220	36.301
(1S,4aS,8aR)-4,7-dimethyl-	204.355	0.000	0.000	5.573	9906.038	5899.293
(1S,4aR,8aR)-4,7-dimethyl-	204.355	0.000	0.000	5.600	9906.038	5899.293
(1S,4aR,8aS)-4,7-dimethyl-	204.355	0.000	0.000	5.432	9906.038	5899.293
(1S,8aS)-4,7-dimethyl-	204.355	0.000	0.000	5.360	9906.038	5899.293

1-(1-methylpyrrolidin-2-yl)-4,10,11-trimethyl-2,4-dihydroxyphenyl-3,3,5-trimethoxy-1,1,3a,7-tetramethyl-5,7-dihydroxy-2-(4-ethenyl-4-ethoxyphenyl)-1,16,17-trimethoxy-4a,5-dimethyl-1,5,9,13-tetrahydro-1H-benzodiazepin-2-one	0.000	4.500	1.513	222.157	119.104
(1R,7R,10R)-4,10,11-trimethyl-2,4-dihydroxyphenyl-3,3,5-trimethoxy-1,1,3a,7-tetramethyl-5,7-dihydroxy-2-(4-ethenyl-4-ethoxyphenyl)-1,16,17-trimethoxy-4a,5-dimethyl-1,5,9,13-tetrahydro-1H-benzodiazepin-2-one	0.000	2.000	3.190	3778.399	2081.380
2-(2,4-dihydroxyphenyl)-3,3,5-trimethoxy-1,1,3a,7-tetramethyl-5,7-dihydroxy-2-(4-ethenyl-4-ethoxyphenyl)-1,16,17-trimethoxy-4a,5-dimethyl-1,5,9,13-tetrahydro-1H-benzodiazepin-2-one	2.000	4.500	1.851	145.625	61.646
(3R,3aR,5aR,5bR,7aR,8aR)-4,8a-dimethyl-1,5,9,13-tetrahydro-1H-benzodiazepin-2-one	0.000	1.700	5.979	9906.038	5899.293
(8aR)-4,8a-dimethyl-1,5,9,13-tetrahydro-1H-benzodiazepin-2-one	0.000	0.000	5.531	9906.038	5899.293
(Z)-1-(2,6,6-trimethyl-2-(4-ethenyl-4-ethoxyphenyl)-1,16,17-trimethoxy-4a,5-dimethyl-1,5,9,13-tetrahydro-1H-benzodiazepin-2-one	0.000	2.000	3.262	7097.854	4114.505
(2R,3R,4S,5S,6R)-2-[[1,5,9,13-tetrahydro-1H-benzodiazepin-2-one]]	4.000	10.200	5.261	341.779	155.019
5,7-dihydroxy-2-(4-ethenyl-4-ethoxyphenyl)-1,16,17-trimethoxy-4a,5-dimethyl-1,5,9,13-tetrahydro-1H-benzodiazepin-2-one	6.000	13.000	-0.846	4.871	1.566
(3R,4R)-4-ethenyl-4-ethoxyphenyl-1,16,17-trimethoxy-4a,5-dimethyl-1,5,9,13-tetrahydro-1H-benzodiazepin-2-one	0.000	0.000	5.546	9906.038	5899.293
11,16,17-trimethoxy-4a,5-dimethyl-1,5,9,13-tetrahydro-1H-benzodiazepin-2-one	1.000	7.900	2.539	1732.359	991.217
(3R,4aR,5S)-4a,5-dimethyl-1,5,9,13-tetrahydro-1H-benzodiazepin-2-one	0.000	0.000	5.141	9906.038	5899.293
(1S,4S,5R,9R,13R)-5,9,13-trimethoxy-1,1,3a,7-tetramethyl-5,7-dihydroxy-2-(4-ethenyl-4-ethoxyphenyl)-1,16,17-trimethoxy-4a,5-dimethyl-1,5,9,13-tetrahydro-1H-benzodiazepin-2-one	1.000	2.000	4.765	630.778	382.365
(1R,3R,4S,5R)-3-[(Z)-1-(2,6,6-trimethyl-2-(4-ethenyl-4-ethoxyphenyl)-1,16,17-trimethoxy-4a,5-dimethyl-1,5,9,13-tetrahydro-1H-benzodiazepin-2-one)]	6.000	9.650	-0.200	2.288	0.881
[(1R,2S,7S,8S,9S)-3,3,5-trimethoxy-1,1,3a,7-tetramethyl-5,7-dihydroxy-2-(4-ethenyl-4-ethoxyphenyl)-1,16,17-trimethoxy-4a,5-dimethyl-1,5,9,13-tetrahydro-1H-benzodiazepin-2-one]	1.000	1.700	3.240	3460.083	1892.512
3,5,7-trihydroxy-2-(4-ethenyl-4-ethoxyphenyl)-1,16,17-trimethoxy-4a,5-dimethyl-1,5,9,13-tetrahydro-1H-benzodiazepin-2-one	3.000	6.750	1.614	110.972	45.956
1,1,3a,7-tetramethyl-5,7-dihydroxy-2-(4-ethenyl-4-ethoxyphenyl)-1,16,17-trimethoxy-4a,5-dimethyl-1,5,9,13-tetrahydro-1H-benzodiazepin-2-one	0.000	0.000	4.930	9906.038	5899.293
(1S,4aS,8aR)-7-methyl-1,5,9,13-tetrahydro-1H-benzodiazepin-2-one	0.000	0.000	5.604	9906.038	5899.293
(6aS)-1,2,10-trimethyl-5,7-dihydroxy-2-(4-ethenyl-4-ethoxyphenyl)-1,16,17-trimethoxy-4a,5-dimethyl-1,5,9,13-tetrahydro-1H-benzodiazepin-2-one	2.000	4.500	2.883	746.939	399.269
(2R,3R)-2-(3,4-dihydroxyphenyl)-3,3,5-trimethoxy-1,1,3a,7-tetramethyl-5,7-dihydroxy-2-(4-ethenyl-4-ethoxyphenyl)-1,16,17-trimethoxy-4a,5-dimethyl-1,5,9,13-tetrahydro-1H-benzodiazepin-2-one	3.000	6.450	0.892	69.785	27.835
(1S,2S,9S)-8,15-dioxo-1,1,3a,7-tetramethyl-5,7-dihydroxy-2-(4-ethenyl-4-ethoxyphenyl)-1,16,17-trimethoxy-4a,5-dimethyl-1,5,9,13-tetrahydro-1H-benzodiazepin-2-one	0.000	6.200	0.165	468.004	240.884
(4aR,5R,6aR,6aS,6bR)-5,7-dihydroxy-2-(4-ethenyl-4-ethoxyphenyl)-1,16,17-trimethoxy-4a,5-dimethyl-1,5,9,13-tetrahydro-1H-benzodiazepin-2-one	5.000	9.500	3.104	20.294	9.317
(1S,12S,13R,14R,15E)-1,1,3a,7-tetramethyl-5,7-dihydroxy-2-(4-ethenyl-4-ethoxyphenyl)-1,16,17-trimethoxy-4a,5-dimethyl-1,5,9,13-tetrahydro-1H-benzodiazepin-2-one	3.000	4.450	2.067	155.845	73.388
(2S,5R)-2-methyl-5-piperonyl-1,1,3a,7-tetramethyl-5,7-dihydroxy-2-(4-ethenyl-4-ethoxyphenyl)-1,16,17-trimethoxy-4a,5-dimethyl-1,5,9,13-tetrahydro-1H-benzodiazepin-2-one	1.000	0.750	2.720	4748.291	2664.445
(9R,10S,13R,14R,17R)-1,1,3a,7-tetramethyl-5,7-dihydroxy-2-(4-ethenyl-4-ethoxyphenyl)-1,16,17-trimethoxy-4a,5-dimethyl-1,5,9,13-tetrahydro-1H-benzodiazepin-2-one	1.000	1.700	7.545	3395.449	1854.330
(1R,3aR,5aR,5bR,7aR)-1,1,3a,7-tetramethyl-5,7-dihydroxy-2-(4-ethenyl-4-ethoxyphenyl)-1,16,17-trimethoxy-4a,5-dimethyl-1,5,9,13-tetrahydro-1H-benzodiazepin-2-one	1.000	1.700	7.108	4730.764	2653.816
methyl (1R,15S,17R)-1,1,3a,7-tetramethyl-5,7-dihydroxy-2-(4-ethenyl-4-ethoxyphenyl)-1,16,17-trimethoxy-4a,5-dimethyl-1,5,9,13-tetrahydro-1H-benzodiazepin-2-one	1.000	11.700	4.982	1851.485	962.737
(3aR,4aR,8aR,9aR)-4,8a-dimethyl-1,5,9,13-tetrahydro-1H-benzodiazepin-2-one	1.000	3.750	2.358	1661.722	856.539
(3S,3aR,4aS,5S,8aR,9aR)-4,8a-dimethyl-1,5,9,13-tetrahydro-1H-benzodiazepin-2-one	0.000	3.000	2.815	3099.899	1680.500
[(1R,5S)-8-methyl-8-oxo-1,1,3a,7-tetramethyl-5,7-dihydroxy-2-(4-ethenyl-4-ethoxyphenyl)-1,16,17-trimethoxy-4a,5-dimethyl-1,5,9,13-tetrahydro-1H-benzodiazepin-2-one]	0.000	4.000	2.150	1068.599	587.997
(1S,4aR,6aR,6aS,6bR)-5,7-dihydroxy-2-(4-ethenyl-4-ethoxyphenyl)-1,16,17-trimethoxy-4a,5-dimethyl-1,5,9,13-tetrahydro-1H-benzodiazepin-2-one	5.000	8.800	3.409	36.714	17.682
9-methoxy-7-(2-methyl-2-propoxyphenyl)-1,1,3a,7-tetramethyl-5,7-dihydroxy-2-(4-ethenyl-4-ethoxyphenyl)-1,16,17-trimethoxy-4a,5-dimethyl-1,5,9,13-tetrahydro-1H-benzodiazepin-2-one	0.000	5.500	2.888	4577.789	2561.183
(8S,9S,10R,13R,14S)-1,1,3a,7-tetramethyl-5,7-dihydroxy-2-(4-ethenyl-4-ethoxyphenyl)-1,16,17-trimethoxy-4a,5-dimethyl-1,5,9,13-tetrahydro-1H-benzodiazepin-2-one	0.000	2.000	7.635	4733.996	2655.776
3-ethenyl-5,5-dimethyl-1,1,3a,7-tetramethyl-5,7-dihydroxy-2-(4-ethenyl-4-ethoxyphenyl)-1,16,17-trimethoxy-4a,5-dimethyl-1,5,9,13-tetrahydro-1H-benzodiazepin-2-one	0.000	2.000	2.073	3024.854	1636.570

(1S,4S,5S)-1,8-dimethyl-2,2,4,4-tetramethyl-5-oxo-2-phenyl-1,3-dioxane	220.354	0.000	2.000	3.473	4262.441	2371.025
bis(trimethylsilyl)methyl	344.583	0.000	0.000	7.879	9906.038	6204.536
(Z,14R)-14-methylheptacosane	254.455	1.000	1.700	5.372	3298.704	1797.289
(E)-3-[4-(dimethylamino)phenyl]propan-2-yl	248.327	0.000	2.500	3.813	2116.197	1112.340
(1S,4S)-1-methyl-4-piperidyl	152.236	1.000	0.750	3.042	3939.554	2177.498
(4-propan-2-ylcyclohexyl)methyl	154.252	1.000	1.700	2.469	3248.423	1767.696
(1S,3R,6S,8R,11S,12S,14S,15S,16S,17S,18S,19S,20S,21S,22S,23S,24S,25S,26S,27S,28S,29S,30S,31S,32S)-32-oxo-1,3,5,7,9,11,13,15,17,19,21,23,25,27,29,31-hexacosane	428.740	1.000	1.700	7.740	4384.967	2444.779
(6S,8R,12S,15R,16S)-1,3,5,7,9,11,13,15,17,19,21,23,25,27,29,31-hexacosane	440.751	1.000	1.700	7.994	4380.120	2441.858
(3S,5S,9R,10S,13R,14S,16S,17S,19S,21S,23S,25S,27S,29S,31S,32S)-32-oxo-1,3,5,7,9,11,13,15,17,19,21,23,25,27,29,31-hexacosane	412.698	1.000	1.700	7.483	3395.399	1854.301
pentacyclo[9.6.2.0.2.0.1]nonane	240.304	0.000	0.000	5.579	9906.038	5899.293
(2R,3R,4S,5S,6R)-2-[[3-methyl-6-propan-2-yl]oxy]propan-1-ol	638.880	7.000	14.350	3.051	62.993	24.919
(3-methyl-6-propan-2-yl)oxypropan-1-ol	212.288	0.000	4.000	2.005	3693.513	2030.884
2-[[1R,3S,4S)-4-ethoxybutyl]oxypropan-1-ol	264.407	0.000	2.000	4.676	4445.372	2481.201
5-[(8Z,11Z)-pentadecyl]oxypropan-1-ol	314.467	2.000	1.500	5.620	909.868	446.694
1H-azonine	119.166	1.000	1.500	1.696	9193.740	5442.157
(1S,4aS,10aR)-6-hydroxy-1,2,3,4,5,6,7,8,9,10,11,12,13,14,15,16,17,18,19,20,21,22,23,24,25,26,27,28,29,30,31,32,33,34,35,36,37,38,39,40,41,42,43,44,45,46,47,48,49,50,51,52,53,54,55,56,57,58,59,60,61,62,63,64,65,66,67,68,69,70,71,72,73,74,75,76,77,78,79,80,81,82,83,84,85,86,87,88,89,90,91,92,93,94,95,96,97,98,99,100,101,102,103,104,105,106,107,108,109,110,111,112,113,114,115,116,117,118,119,120,121,122,123,124,125,126,127,128,129,130,131,132,133,134,135,136,137,138,139,140,141,142,143,144,145,146,147,148,149,150,151,152,153,154,155,156,157,158,159,160,161,162,163,164,165,166,167,168,169,170,171,172,173,174,175,176,177,178,179,180,181,182,183,184,185,186,187,188,189,190,191,192,193,194,195,196,197,198,199,200,201,202,203,204,205,206,207,208,209,210,211,212,213,214,215,216,217,218,219,220,221,222,223,224,225,226,227,228,229,230,231,232,233,234,235,236,237,238,239,240,241,242,243,244,245,246,247,248,249,250,251,252,253,254,255,256,257,258,259,260,261,262,263,264,265,266,267,268,269,270,271,272,273,274,275,276,277,278,279,280,281,282,283,284,285,286,287,288,289,290,291,292,293,294,295,296,297,298,299,300,301,302,303,304,305,306,307,308,309,310,311,312,313,314,315,316,317,318,319,320,321,322,323,324,325,326,327,328,329,330,331,332,333,334,335,336,337,338,339,340,341,342,343,344,345,346,347,348,349,350,351,352,353,354,355,356,357,358,359,360,361,362,363,364,365,366,367,368,369,370,371,372,373,374,375,376,377,378,379,380,381,382,383,384,385,386,387,388,389,390,391,392,393,394,395,396,397,398,399,400,401,402,403,404,405,406,407,408,409,410,411,412,413,414,415,416,417,418,419,420,421,422,423,424,425,426,427,428,429,430,431,432,433,434,435,436,437,438,439,440,441,442,443,444,445,446,447,448,449,450,451,452,453,454,455,456,457,458,459,460,461,462,463,464,465,466,467,468,469,470,471,472,473,474,475,476,477,478,479,480,481,482,483,484,485,486,487,488,489,490,491,492,493,494,495,496,497,498,499,500,501,502,503,504,505,506,507,508,509,510,511,512,513,514,515,516,517,518,519,520,521,522,523,524,525,526,527,528,529,530,531,532,533,534,535,536,537,538,539,540,541,542,543,544,545,546,547,548,549,550,551,552,553,554,555,556,557,558,559,560,561,562,563,564,565,566,567,568,569,570,571,572,573,574,575,576,577,578,579,580,581,582,583,584,585,586,587,588,589,590,591,592,593,594,595,596,597,598,599,600,601,602,603,604,605,606,607,608,609,610,611,612,613,614,615,616,617,618,619,620,621,622,623,624,625,626,627,628,629,630,631,632,633,634,635,636,637,638,639,640,641,642,643,644,645,646,647,648,649,650,651,652,653,654,655,656,657,658,659,660,661,662,663,664,665,666,667,668,669,670,671,672,673,674,675,676,677,678,679,680,681,682,683,684,685,686,687,688,689,690,691,692,693,694,695,696,697,698,699,700,701,702,703,704,705,706,707,708,709,710,711,712,713,714,715,716,717,718,719,720,721,722,723,724,725,726,727,728,729,730,731,732,733,734,735,736,737,738,739,740,741,742,743,744,745,746,747,748,749,750,751,752,753,754,755,756,757,758,759,760,761,762,763,764,765,766,767,768,769,770,771,772,773,774,775,776,777,778,779,780,781,782,783,784,785,786,787,788,789,790,791,792,793,794,795,796,797,798,799,800,801,802,803,804,805,806,807,808,809,810,811,812,813,814,815,816,817,818,819,820,821,822,823,824,825,826,827,828,829,830,831,832,833,834,835,836,837,838,839,840,841,842,843,844,845,846,847,848,849,850,851,852,853,854,855,856,857,858,859,860,861,862,863,864,865,866,867,868,869,870,871,872,873,874,875,876,877,878,879,880,881,882,883,884,885,886,887,888,889,890,891,892,893,894,895,896,897,898,899,900,901,902,903,904,905,906,907,908,909,910,911,912,913,914,915,916,917,918,919,920,921,922,923,924,925,926,927,928,929,930,931,932,933,934,935,936,937,938,939,940,941,942,943,944,945,946,947,948,949,950,951,952,953,954,955,956,957,958,959,960,961,962,963,964,965,966,967,968,969,970,971,972,973,974,975,976,977,978,979,980,981,982,983,984,985,986,987,988,989,990,991,992,993,994,995,996,997,998,999,1000	316.439	2.000	2.750	4.301	262.288	148.100
6,7-dihydroxy-1,1-dimethyl-2,2,4,4-tetramethyl-5-oxo-2-phenyl-1,3-dioxane	237.255	4.000	4.500	-1.447	7.060	3.292
(2Z,6Z,10E,14E)-3,7,11-trimethyl-2,2,4,4-tetramethyl-5-oxo-2-phenyl-1,3-dioxane	358.606	1.000	1.700	6.813	2887.913	1556.635
(3R,5S,8S,9S,10R,13S,16S,17S,19S,21S,23S,25S,27S,29S,31S,32S)-32-oxo-1,3,5,7,9,11,13,15,17,19,21,23,25,27,29,31-hexacosane	448.685	3.000	7.100	4.168	399.981	183.739
(8E,11E)-heptadecyl	234.424	0.000	0.000	8.902	9906.038	5899.293
trimethyl-[[[(2R,3R,4S,5S,6R)-2-[[3-methyl-6-propan-2-yl]oxy]propan-1-yl]oxy]propan-1-yl]oxypropan-1-ol	541.066	0.000	5.950	4.771	9906.038	5899.293
ethyl 2-hydroxy-5-methylpentanoate	225.201	0.000	2.750	1.947	95.767	39.189
(2S,3S,4S,5R,6R)-6-[[3-methyl-6-propan-2-yl]oxy]propan-1-yl]oxypropan-1-ol	634.849	5.000	12.900	3.527	6.971	2.935
1,1-dichlorododecane	255.227	1.000	1.700	4.805	4628.525	10000.000
[(3R,4S,5S,6R)-3,4,5-trimethyl-2,2,4,4-tetramethyl-5-oxo-2-phenyl-1,3-dioxane	386.355	5.000	12.750	-0.648	31.321	11.709
methyl 4-pentanoylbenzoate	220.268	0.000	4.000	2.333	1108.898	553.187
(6aR,11aR)-3-methoxy-1,2,3,4,5,6,7,8,9,10,11,12,13,14,15,16,17,18,19,20,21,22,23,24,25,26,27,28,29,30,31,32,33,34,35,36,37,38,39,40,41,42,43,44,45,46,47,48,49,50,51,52,53,54,55,56,57,58,59,60,61,62,63,64,65,66,67,68,69,70,71,72,73,74,75,76,77,78,79,80,81,82,83,84,85,86,87,88,89,90,91,92,93,94,95,96,97,98,99,100	270.284	1.000	3.000	3.115	3001.768	1623.073
(2R,3S)-2-(3,4-dihydroxybutyl)propanoate	594.528	11.000	11.650	-0.232	0.453	0.120
4-[(2S,3S,4R,5R)-5-(1-methyl-2-oxoethyl)oxy]butyl	342.391	1.000	4.700	3.683	3045.871	1648.864
(1R,8S,9R,16R)-8,16-dimethyl-2,2,4,4-tetramethyl-5-oxo-2-phenyl-1,3-dioxane	906.941	10.000	9.000	5.603	0.369	0.096
[(1S,2S,4S,5S,6R,10S)-2,2,4,4-tetramethyl-5-oxo-2-phenyl-1,3-dioxane	466.441	4.000	16.600	-0.662	51.251	19.938
(2R,3R,4S,5S,6R)-2-[[3-methyl-6-propan-2-yl]oxy]propan-1-yl]oxypropan-1-ol	484.629	6.000	13.600	0.707	69.526	27.724
(1R,4aS,5R,8aS)-3-methyl-2,2,4,4-tetramethyl-5-oxo-2-phenyl-1,3-dioxane	220.354	1.000	1.700	3.650	4306.472	2397.510

[(3S,4aR,6aR,6aR,6b) 468.762	0.000	2.000	7.946	3923.209	2167.734
(3S,5R,8R,9R,10R,13) 426.724	1.000	1.700	7.682	4369.593	2435.515
(1S,2E,6E,10R)-3,7,1 204.355	0.000	0.000	5.065	9906.038	5899.293
(2S,3S,4S,5R,6R)-6-[[794.975	7.000	20.000	2.069	0.626	0.217
6,7,13-trihydroxy-14 316.223	3.000	8.000	-0.536	27.875	10.323
3-[4,5-dihydroxy-6-(594.525	8.000	19.800	-1.876	3.009	0.931
(1S,4S)-1-methyl-4-p 154.252	1.000	0.750	2.955	4243.970	2359.922
(1S,3R,6S,8R,11S,12) 440.751	1.000	1.700	7.905	4383.535	2443.916
4,11,12a-trihydroxy- 344.320	2.000	5.500	2.263	386.565	177.087
[(2S,3R,4S,5S,6R)-3,4 356.329	5.000	12.000	-0.764	28.960	10.758
(2S)-7,8-dimethoxy-2 462.452	4.000	13.500	0.759	147.606	62.553
6-[(2R,3R)-3-[(3,4-dir 432.513	0.000	7.150	3.290	9906.038	5899.293
1-methyl-4-[(2R)-6-n 204.355	0.000	0.000	6.451	9906.038	5899.293
9,11-dihydroxy-6-me 326.305	1.000	5.450	2.494	839.537	409.493
6,9,11-trihydroxy-10 312.278	2.000	5.450	1.649	286.656	128.181
[(1R,2R)-1-[(14S,15S, 634.460	12.000	18.850	-3.668	0.032	0.007
1,1,4,7-tetramethyl- 220.354	1.000	0.750	3.738	4390.945	2448.382
(E)-5-(2,3-dimethyl-3 234.338	1.000	2.000	3.676	284.445	161.668
(2R,4aS,7R)-1,4a-dir 220.354	1.000	1.700	3.573	4055.809	2247.035
(2R,4aS,7R,8aR)-4a-r 220.354	1.000	1.700	3.564	3946.829	2181.845
(3S,8S,9S,10R,13R,1 428.740	1.000	1.700	7.873	3379.627	1844.992
(2S,3R,4S,5S,6R)-2-[[330.334	5.000	13.600	-1.187	128.489	53.844
(2S,3R,4S,5R)-2,3,4-t 386.312	4.000	10.600	0.331	0.138	0.054
methyl (3E,6E)-octad 294.476	0.000	2.000	6.468	2645.498	1415.893
2-(3,4-dihydroxyphen 610.524	9.000	20.550	-2.340	1.563	0.458
4-(2-hydroxyethyl)-2 198.218	2.000	3.950	1.155	896.404	439.554
[3,4,5-trihydroxy-6-(l 326.302	5.000	11.250	-0.811	37.945	14.407
methyl (9Z,12Z)-hept 280.450	0.000	2.000	5.888	2612.969	1397.085
3,7-dihydroxy-2-(4-h 330.293	3.000	6.250	1.492	133.557	56.143
(2S,4aR,6aR,7R,10aS) 492.522	4.000	15.700	-0.029	52.398	20.421
5-[(Z)-heptadec-8-en 346.552	2.000	1.500	6.834	910.033	446.782
7-[(2S,3R,4S,5S,6R)-ε 456.402	6.000	17.600	-1.917	14.798	5.207
(2R)-2-[(1R)-1-hydro 454.605	2.000	6.500	4.349	414.695	191.056

(1S,2S,4S,5R,10R,11S	454.605	1.000	7.750	3.939	776.314	376.265
(2R,3R,4S)-2-(3,4-dih	866.784	15.000	16.350	0.057	0.048	0.011
(1S,2S,5S,8R,9S)-2-m	236.353	1.000	1.500	3.698	4517.497	2524.742
9,16-dihydroxyhexac	288.426	3.000	5.400	3.126	40.583	19.705
[(1R,2S,5R,6R,10S,13	568.663	1.000	11.200	3.665	146.484	62.039
(2R,3R)-2-(3,4-dihyd	466.398	7.000	14.950	-1.790	1.820	0.540
2-methyl-6-[[3,4,5-tr	430.451	6.000	17.000	-0.968	90.918	37.049
2-[(3E,5E)-hepta-3,5-	300.397	1.000	2.500	4.424	847.395	413.637
6-[2-[6-[2-(dimethyl	459.452	1.000	11.750	0.244	69.613	39.062
[6,7,8,11,12,13,22-h	786.566	13.000	20.400	-3.233	0.003	0.000
(3S,4aR,6aS,6aR,6bR	426.724	1.000	1.700	7.008	4367.236	2434.096
methyl 3-(4-hydroxy-	208.257	1.000	2.750	2.545	1195.810	600.197
(1R,8aS)-1,8a-dimet	202.339	0.000	0.000	5.221	9906.038	5899.293
(2R,3R,4aR,6R,8aS)-	254.369	3.000	4.150	1.997	751.130	363.089
(2R,3R,4S,5R)-2-[[(1S 492.522	6.000	13.200	0.414	27.619	10.221
3-[(2S,3R,4R,5S)-3,4-	450.355	7.000	12.800	-1.473	1.813	0.538
(1S,3R,6S,7S,8S,11S,	412.698	1.000	1.700	7.445	3976.984	2199.869
12,21,23-trihydroxy-	502.563	2.000	5.250	5.206	352.328	160.197
5-hydroxy-2,2-dimet	504.579	3.000	5.250	5.412	187.152	80.849
14,16-dihydroxy-4-m	278.347	1.000	2.500	3.206	654.796	313.027
tris(2,4-ditert-butylp	662.931	0.000	5.000	10.691	5699.174	3245.587
1-[(7-hydroxy-4-metl	482.532	3.000	4.250	5.434	328.963	148.745
1-[(5-hydroxy-7-metl	482.532	3.000	4.250	5.509	507.807	237.818
4-methyl-10-methyl	222.370	1.000	0.750	4.023	6885.011	3981.308
5,6,9-trimethyltetrac	204.355	0.000	0.000	6.397	9906.038	5899.293
9-methyl-6H-furo[2,	221.258	1.000	0.500	3.667	5694.752	3242.865
[(2S,3R,4S,5S,6R)-3,4	666.848	8.000	17.300	0.891	17.252	6.146
12,21,23-trihydroxy-	502.563	2.000	5.250	5.424	404.932	186.199
(1R,3S,4aS,6R,8aR)-6	254.369	3.000	4.150	2.026	845.374	412.571
(3S,4aR,6aR,6aR,6bR	426.724	1.000	1.700	7.075	4367.499	2434.254
3-(2,7-dihydroxy-4-r	482.532	4.000	4.500	4.707	188.034	81.262
6-(2,7-dihydroxy-4-r	588.656	5.000	5.250	5.863	69.001	27.497
1-[2,7-dihydroxy-8-[(586.640	5.000	5.250	5.866	72.009	28.795

2,4,7-trimethoxyph	268.312	0.000	2.250	4.028	9906.038	5899.293
2,4,7-trimethoxy-9,1	270.327	0.000	2.250	3.914	9906.038	5899.293
1,3-dimethoxy-5-[2-	272.343	0.000	2.250	4.197	9906.038	5899.293
3,5-dihydroxy-6-met	185.222	2.000	6.400	0.039	496.399	232.049
(2S,3R,4R,5R,6R)-2-[[450.398	8.000	13.000	-1.161	4.728	1.517
(7,7-dimethyl-2-metl	220.354	1.000	1.700	3.283	3992.256	2209.001
2-N-propyl-1,3,5-tria	168.201	5.000	4.500	-0.562	130.943	54.957
(1S,2S,4S,5R,10R,11S	470.605	1.000	8.450	3.452	284.560	127.168
(1R,3S,4S,5S)-1,3,4-ti	368.340	5.000	9.650	0.482	3.966	1.595
4-methylnonadecylb	358.649	0.000	0.000	12.777	9906.038	5899.293
(1R,2R,7R,10R,11S,1	470.605	1.000	8.150	3.528	209.872	91.509
(1R,2R,4R,5R,10R,11	486.604	3.000	8.950	3.202	319.972	144.356
(1R,2R,7R,10R,11S,1	616.747	4.000	15.950	1.961	46.512	17.954
(1R,2R,7R,10R,11S,1	470.605	2.000	8.200	3.597	259.609	115.160
(2E,10E)-11-(1,3-ben	357.492	1.000	4.000	5.725	3447.004	1884.781
(10S)-nonacosan-10-	424.792	1.000	1.700	10.364	4566.532	2554.377
5-hydroxy-3-(3-hydr	386.444	1.000	5.750	3.778	387.447	177.524
(2R)-2-[(1S)-1-[(4S,5F	975.285	4.000	16.800	6.547	3.338	1.094
6H-[1]benzofuro[3,2-	222.243	0.000	1.250	3.814	9906.038	5899.293
10-(2,3,4,7,8,9,19-he	1084.731	18.000	29.400	-6.199	0.000	0.000
6,7,8,11,12,23,24,27	1084.731	17.000	28.400	-5.515	0.000	0.000
(1S,8S,9R,16S)-9-[5-[906.941	10.000	9.000	6.402	0.345	0.090
[(10R,13R,14R,15S)-ε	1086.747	17.000	28.400	-4.796	0.000	0.000
4,5,6,14,20,21,22,25	1084.731	16.000	28.150	-4.865	0.000	0.000
(Z)-2-[(E)-2-[(1R,4aS,	364.438	4.000	7.400	2.234	1.752	0.839
(2S,9S)-2,6,6,9-tetrar	204.355	0.000	0.000	6.458	9906.038	5899.293
(3S,3'R,3'aS,6'S,6aS,ε	587.752	5.000	14.450	1.910	24.811	10.070
(2S,3R,4S,5S,6R)-2-[4	302.280	6.000	11.700	-1.628	25.390	9.332
methyl 2-[[3-[(3,3-dii	440.449	3.000	9.250	2.295	79.972	32.252
methyl 4-hydroxy-3-	356.331	3.000	7.250	1.340	60.040	23.658
(3S,3aS,6S,6aR)-3,6-t	370.358	1.000	8.100	2.118	3756.853	2068.555
2-(2-hydroxy-5-meth	181.191	3.000	4.000	-0.194	223.349	189.303
4-cyclopropylbutano	128.171	1.000	2.000	1.659	235.331	131.718

(Z)-2-heptylundec-2-	266.466	0.000	2.000	5.646	2494.067	1328.498
1-hydroxy-3-methyl-	578.526	7.000	20.550	-2.194	1.917	0.572
(1S,2S,5S,6S,9R,12S,	404.635	2.000	6.450	3.343	186.261	98.446
2-methyl-5-(6-methy	222.370	1.000	0.750	4.476	4765.817	2675.077
(3R,5S,8S,9S,10S,13S	481.749	0.000	5.550	7.068	3958.447	2188.788
(E,5R,6S,7R,8R)-5,6,7	326.302	4.000	11.250	-1.033	9.422	3.196
(9R,10S,13R,14R,17R	400.687	1.000	1.700	7.216	3393.350	1853.091
(8R,9S,10R,13S,14S,13	28.450	2.500	4.450	3.067	628.477	299.451
[(2S,3R,4S,5S,6R)-3,4	650.848	7.000	15.600	1.757	39.304	14.966
[(1R,3aR,5aR,5bR,7a]	468.762	0.000	2.000	7.990	3946.002	2181.351
bis(but-3-enyl) benzε	274.316	0.000	4.000	3.711	1479.554	755.512
1H-benzo[7]annulen	142.200	0.000	0.000	3.551	9906.038	5899.293
(1S,2S,4S,5'R,6R,7S,8	427.669	1.000	3.450	5.657	827.658	446.104
(2R,3S,4S,5R,6S)-2-(f	396.399	5.000	10.250	0.929	111.997	46.415
[(1R,4S,5R,6S,7R,8S,ε	530.482	7.000	19.550	-2.057	9.179	3.107
1-(2,4-dihydroxyphei	372.417	2.000	4.750	3.637	239.656	105.623
(1S,3R,8R,11S,12S,1E	438.735	0.000	2.000	7.997	4188.045	2326.326
(1S,2R,6S,9R)-2,6,10,	222.370	0.000	0.750	3.249	9906.038	5899.293
[(2R,3S,4S,5R,6S)-6-[630.601	5.000	15.300	1.339	9.547	3.242
(2R,4aR,6aR,6aS,6bR	472.707	3.000	5.400	5.243	118.923	62.988
(2S,4S,4aR,6aR,6aS,6	472.707	3.000	5.400	5.126	80.292	41.197
(1S,3R,7S,8S,11S,12S	424.709	0.000	2.000	7.877	2450.570	1303.472
(2S,3R,4S,5R)-2-[(2R,	770.996	9.000	21.150	1.231	15.654	5.533
(1S,2S,4S,6R,7S,10R,	345.524	2.000	5.400	2.790	382.403	193.635
(1S,2S,4S,5R,10R,11S	486.604	2.000	10.150	2.592	155.152	66.017
1-(4-hydroxy-3-meth	584.619	5.000	12.050	3.083	63.081	24.956
(2S,3R,4R,5R,6S)-2-[(1049.211	13.000	36.450	-2.909	0.052	0.012
(2R,3S,4S,5R,6S)-2-[[444.478	6.000	15.100	-0.095	169.312	72.553
(1S,4aS,7S,7aS)-7-hy	376.360	6.000	14.650	-1.450	3.272	1.296
5-[(E)-2-[3-(2,3-dihyc	330.380	5.000	4.700	2.259	104.961	43.271
methyl (2R,4aR,6aS,1	462.628	1.000	4.750	5.488	464.102	215.774
(2R,3S)-3-[(10R,11R)	802.566	14.000	20.700	-2.983	0.000	0.000
(2R)-2-[(1R)-1-hydro	470.605	3.000	8.200	3.395	177.593	76.396

[(3S,4aR,6aR,6aS,6bF 468.762	0.000	2.000	7.925	3920.893	2166.352
(2S,5R,9S)-9-acetyl-9 462.712	1.000	5.500	7.159	1848.661	961.150
3-[(2S,3R,4S,5S,6R)-4 756.667	11.000	28.300	-4.114	0.193	0.048
6-[(3-formyl-2,4-dihy 376.319	2.000	6.000	1.701	1.106	0.401
(2R)-2-[(1S)-1-[(8R,9 470.605	3.000	7.250	4.016	509.696	238.775
(2R)-2-[(1R)-1-hydro 454.605	2.000	6.500	4.433	610.353	290.127
(1S,2S,4S,5R,10R,11 470.605	2.000	8.500	3.532	535.478	251.856
(2R)-2-[(1R)-1-[(8R,9 454.605	2.000	6.500	4.563	839.073	409.248
(3S,3aR,6R,6aS)-3,6-l 386.357	2.000	6.950	2.516	2743.365	1472.593
(3S,3aR,4R,6R,6aS)-3 386.357	2.000	8.850	1.671	1837.986	955.152
(1R,2S,5S)-2,5-bis(1, 368.342	0.000	7.450	2.014	5118.346	2889.583
(1R,2R,5S,7S,8S)-2,6, 220.354	0.000	2.000	3.337	2685.817	1439.232
1-(6-methylhepta-1, 204.355	0.000	0.000	6.195	9906.038	5899.293
(1R,9R,10S,12S,13S,1 324.422	1.000	6.700	1.346	95.430	47.783
(3S,4aR,6aS,6bS,8aS, 426.724	1.000	1.700	6.980	4332.143	2412.961
(1S,2S,6S)-2,7,7-trim 168.235	0.000	3.000	1.564	2762.141	1483.489
(1S,4aR,6aR,6aS,6bR 520.705	6.000	10.500	2.538	17.753	8.062
[(1R,3R,5S,6R)-8-met 321.416	0.000	6.000	2.851	646.877	341.783
2-[5-(hydroxymethyl 197.196	4.250	6.950	-1.227	43.186	16.570
methyl 2-[[4-(2-cyan 322.406	1.000	5.000	3.457	213.908	103.344
3-[(3Z)-4,8-dimethyl 218.338	0.000	0.500	4.761	9906.038	5899.293
ethoxy(undec-10-en) 262.328	1.000	5.000	3.654	456.256	271.714
tricyclo[5.3.1.01,5]ur 142.200	0.000	0.000	3.520	9906.038	5899.293
trimethyl-[(3R,4R,5R 438.858	0.000	5.100	4.130	9906.038	5899.293
trimethyl-[(2S,3R,4R, 452.885	0.000	5.100	4.160	9906.038	5899.293
[(8R,9R,10S,13S,14S) 332.482	0.000	4.000	3.977	1287.926	650.323
(3R,5S,8R,9S,10S,13 400.687	1.000	1.700	7.359	3917.107	2164.091
(1R,2S,5S,6S,9R,12S, 326.524	1.000	3.000	4.555	989.547	541.124
(8S,10S,13R,14S,17R 414.713	1.000	1.700	7.558	3382.838	1846.887
(5R,8S,9S,10S,11R,1 303.530	0.000	2.000	3.953	2470.586	1454.789
(5S,8S,10S,13R,14S,1 426.724	0.000	2.000	7.844	5716.301	3256.130
4-methylnonacosane 422.820	0.000	0.000	17.035	9906.038	5899.293
[4-(acetyloxymethyl) 480.511	0.000	11.700	2.237	728.666	351.366

1-ethyl-4,5,7-trimethyl-416.513	0.000	4.500	4.167	9906.038	5899.293
(3S,5S,9R,10S,13S,14) 412.698	1.000	1.700	7.470	3398.159	1855.930
(2R,4S,6R,7S,8R,9S,1) 428.611	1.000	5.200	5.166	2393.697	1270.805
(3S,5S,10S,13R,14R,14) 414.713	1.000	1.700	7.466	3388.598	1850.286
(4Z,7Z)-1,5,9,9-tetrahydro-220.354	0.000	2.000	2.558	9906.038	5899.293
10-hydroxyhentriaceton 466.830	1.000	3.700	9.962	1677.249	865.194
1-O-[3,4,5-trihydroxy] 814.833	11.000	29.500	-2.313	0.217	0.054
(E,5R,6S,7R,8R)-5,6,7-trimethyl-356.329	4.000	12.000	-0.907	11.212	3.857
(2R)-2-[(1R)-1-[(4S,9S) 452.589	2.000	7.450	3.876	429.976	198.677
(2R)-2-[(1R)-1-[(8R,9R) 452.589	1.000	6.450	4.458	356.392	162.195
(1S,2R,6S,7R,9R,11S) 454.605	1.000	8.700	3.518	616.373	293.221
(1S,2R,6S,7R,9R,11R) 470.605	2.000	9.450	3.072	386.697	177.152
(1S,2R,6S,7R,9R,11S) 472.620	2.000	9.450	3.040	234.607	103.220
[(2R,3R)-2-(3,5-dihydroxy) 472.404	7.000	8.750	0.632	3.704	1.165
sodium;1,4-dimethyl 278.365	1.000	4.000	3.163	228.286	127.462
sodium;4-[2-[(8S,9S) 462.539	3.000	10.450	1.937	3.789	1.519
5,7-dihydroxy-3-[(2S) 450.355	7.000	12.800	-1.512	1.645	0.485
methyl (1R,9R,10R,1) 336.433	0.000	4.000	2.938	202.129	107.542
methyl (1S,4aS,5R,7S) 448.423	5.000	16.650	-1.424	25.279	9.288
(1S,2S,3S,5S,8S,11R) 358.390	1.000	7.250	1.839	509.935	238.896
(3R,4S,5S,6R)-2-[[[(1S) 362.333	5.000	16.300	-2.183	67.992	27.063
(4S)-1-methyl-4-[(2E) 204.355	0.000	0.000	6.245	9906.038	5899.293
(8S)-1,5-dimethyl-8-[(1S,2R,3R,4R,5R,6S) 589.681	4.000	15.700	1.826	130.352	60.503
(3R,6Z,10S)-6,10-dimethyl-236.353	0.000	4.000	2.783	3250.884	1769.143
4-[6-[(3,5-dihydroxy) 500.496	7.000	23.800	-2.956	60.021	23.650
(2S,3S,4S,5R,6R)-6-[[[(4aS,6aR,6aS,6bR,8a) 618.852	3.000	5.500	7.663	30.430	14.435
(1R,2R,10R,11S,14R) 452.589	0.000	6.450	4.201	499.769	233.752
(1R,2R,10R,11S,14R) 468.589	1.000	7.200	3.880	254.892	112.899
1,4,4,6,9-pentamethyl-284.354	0.000	4.750	2.607	1571.643	806.465
1-[(2R,4R)-2,8-dihydroxy] 264.321	2.000	5.200	1.863	902.644	442.862
(1R,6R)-1,4,4,6,9-pentamethyl-288.386	2.000	2.250	3.596	1777.158	921.031

(1R,3R)-3,5-dihydrox	2.000	5.950	1.442	794.925	386.024
(1R,2R,4S,6R,7R,10S, 468.589	1.000	7.500	4.160	706.324	339.736
(E)-1-[(2R)-7-hydroxy	1.000	3.250	5.697	481.672	224.616
2-[(E)-3-methylbut-1	2.000	1.500	4.830	1665.700	858.756
7-[(E)-2-(4-hydroxypl	2.000	2.250	4.027	1079.348	537.271
(4R)-4-hydroxy-2,6,6	1.000	3.700	1.151	1093.332	544.799
1-(6-methylhept-5-ei	0.000	0.000	6.254	9906.038	5899.293
1,5,9-trimethyltricycl	0.000	0.000	5.053	9906.038	5899.293
(1S,6R,7R)-1-methyl-	0.000	0.000	5.251	9906.038	5899.293
(E)-3-[3,5-dimethoxy	4.000	12.750	-0.546	45.759	17.639
(12R,13R)-3,5-dioxa-	2.000	4.700	1.801	697.384	370.716
8-fluoro-1,2-dihydroj	2.000	5.000	0.452	396.682	328.531
(4aS,5S,6R,8aR)-5-[2	1.000	2.500	4.879	464.633	274.773
4-[(1S)-2-[(1R,4aS,5R	2.000	7.100	2.115	371.607	169.692
(2S)-7-[4,5-dihydroxy	6.000	18.550	-0.688	15.780	5.581
5,7-dihydroxy-8-(3-r	1.000	5.500	4.336	673.692	322.803
5-hydroxy-7-methox	0.000	5.500	4.912	1413.290	719.006
5-hydroxy-7-methox	0.000	5.500	3.404	1402.272	712.949
(4aS,7R,7aR)-1,1,7-tr	0.000	0.000	5.008	9906.038	5899.293
(5S,6R,7S,10R)-4,10-r	0.000	0.000	5.511	9906.038	5899.293
(5R,6S)-5,6,9-trimeth	1.000	1.700	3.225	4437.373	2476.376
4,6-bis[(4-hydroxyph	4.000	3.000	4.909	179.299	77.189
ethyl (3R,4S,5R)-3,4,	3.000	7.100	-0.456	163.276	69.761
2-[(5-amino-1,3,4-thi	3.000	5.750	0.299	56.498	60.468
(1R)-1,2,2-trimethylc	2.000	4.000	1.714	23.657	13.986
1-ethyl-4,5-dihydrox	1.000	5.400	0.857	657.930	314.647
2,3-dihydroxypropyl	2.000	3.000	6.213	429.088	219.308
(2S)-9-hydroxy-2-(2-l	2.000	4.750	1.481	313.415	141.161
4-[2-(1,3,6-trimethyl	0.000	3.000	4.315	3273.786	1782.619
(2R,3S)-2-(4-hydroxy	3.000	5.450	3.916	380.845	174.256
(2S,4S,5S)-2-[[[(2R,3R	7.000	13.950	-0.579	13.237	4.616
(2R,3S)-2-(4-hydroxy	8.000	14.900	-1.520	7.461	2.484
3-[(2S,3S,5R)-3,4,5-tr	9.000	14.700	-1.820	4.058	1.286

8-acetyl-7-hydroxy-2	294.306	0.000	4.250	2.909	765.310	370.503
3,9-dihydroxy-4-(3-r	336.343	2.000	4.500	3.003	471.051	219.268
2-[(2E)-3,7-dimethyl	404.462	2.000	4.500	4.587	294.452	131.952
5-hydroxy-2-(2-hydr	312.321	1.000	3.750	3.215	786.454	381.580
2-(3,4-dihydroxyphe	610.524	11.000	21.500	-3.854	0.095	0.022
3-[(2S,5S)-4,5-dihydr	624.551	8.000	20.550	-1.652	3.673	1.155
5,7-dihydroxy-2-[4-h	418.356	5.000	11.300	-0.398	7.085	2.349
2-[4-[(2S,5S)-4,5-dih	594.525	8.000	19.800	-2.041	1.044	0.296
2-(2,4-dihydroxyphe	370.358	4.000	5.250	2.154	42.325	16.213
3,8-dihydroxy-10-me	434.488	1.000	4.500	5.400	988.561	488.595
8,10-dihydroxy-3-me	434.488	1.000	4.500	5.564	1357.423	688.334
(3S,4S,6S)-6-(5,6-dih	446.367	4.000	11.550	0.724	1.434	0.531
5,7-dihydroxy-2-phe	432.383	5.000	12.250	-0.028	20.782	7.516
5,6-dihydroxy-2-(4-h	594.525	8.000	19.800	-1.900	1.226	0.353
1,8,10-trihydroxy-2,	502.563	2.000	7.750	4.454	159.324	67.938
12,21,23-trihydroxy-	502.563	2.000	5.250	5.507	255.182	113.038
3-[(2R,3S,6S)-6-[5,7-	534.429	5.000	14.300	0.003	0.289	0.094
[(3S,4R,6S)-6-[5,7-di	594.528	6.000	14.050	0.982	2.091	0.628
[5-hydroxy-2-(4-hydr	498.414	5.000	15.050	-1.006	0.522	0.182
2-(3,4-dihydroxyphe	610.524	9.000	20.550	-2.621	0.341	0.088
5,7-dihydroxy-2-(3,4,	626.524	10.000	21.300	-2.885	0.902	0.253
5,7-dihydroxy-3-[(2S,	450.355	7.000	12.800	-1.445	2.037	0.610
3-[(2S,4S,5S)-4,5-dih	772.666	12.000	28.100	-4.303	0.130	0.031
3,5-dihydroxy-7-met	374.346	1.000	6.000	3.003	638.519	304.625
[3,5,7-trihydroxy-2-(344.277	3.000	7.000	0.717	31.911	11.948
(5R)-5-[(11R)-11-hyd	622.924	2.000	11.800	7.447	301.433	135.337
(2S)-4-[(2R,11R)-2,	11594.871	3.000	11.500	6.739	354.266	161.149
6,9,11-trihydroxy-6H	298.251	2.000	5.450	1.242	186.051	80.336
(2E,4E,10E)-11-(1,3-t	367.487	0.000	4.500	5.581	4258.272	2368.519
(2E,10E)-11-(1,3-ben	369.503	0.000	4.500	5.625	4178.366	2320.515
(2E,4E,12E)-13-(1,3-t	395.541	0.000	4.500	6.370	4166.628	2313.470
[(E,6S)-6-hydroxy-2-r	546.743	4.000	9.850	3.788	99.951	41.043
(2S,3R,4S,5S,6R)-2-[(1051.184	13.000	37.200	-3.107	0.550	0.148

(2S)-4-[(13R)-7,13-di	580.887	3.000	9.800	7.584	307.220	138.148
(2S)-4-[(13R)-7,13-di	580.887	3.000	9.800	7.599	279.094	124.530
(5S)-5-hydroxy-1-(3-l	294.390	1.000	4.200	3.694	600.210	284.920
(1R,2R,10R,11S,14R,	452.589	1.000	6.500	4.610	1079.181	537.182
(2R,3R,4S,5S,6R)-2-[(1215.342	17.000	45.700	-5.760	0.011	0.002
(5R)-5-[(11R)-11-hyd	606.882	2.000	12.100	6.919	229.303	100.700
(1S,3R,6S,8R,11S,12S	426.724	1.000	1.700	7.701	4384.697	2444.616
3,5-dimethoxyphena	270.284	2.000	3.000	2.681	933.200	459.089
(4S)-3-[(1R)-2-[(1R,4	368.469	3.000	8.800	1.180	146.027	61.830
4-[2-[(1S,2R,4aS,5R,ε	350.454	2.000	8.400	1.701	614.820	292.423
4-[2-[(1R,4aS,5R,6R,ε	496.597	5.000	14.900	0.639	41.108	15.710
4-[(E)-2-[(1R,4aS,5R,ι	494.581	5.000	14.900	0.424	33.826	12.725
(2R,3S,4S,5R,6S)-2-(f	316.307	5.000	11.700	-0.959	77.473	31.164
(E)-N-[(E)-2-[4-(3-me	333.429	1.000	3.250	5.680	2543.345	1356.891
(E)-N-[(2S)-2-(4-metr	459.495	5.000	13.450	1.214	187.709	81.110
methyl 4,5-dihydroxy	298.251	0.000	5.500	1.108	71.887	28.743
(1R,2S,5E,9E,12S)-1,ε	306.487	1.000	2.450	4.580	4452.746	2485.650
5-[(11R)-11-hydroxy-	622.924	2.000	11.800	7.447	301.433	135.337
[(2R,3S,4R,5R)-4,5,6-	784.550	13.000	23.300	-4.420	0.003	0.000
(2S)-4-[(2R,13R)-2,13	594.871	3.000	11.800	5.597	540.846	254.586
(2S)-4-[(2R,13R)-2,13	594.871	3.000	11.800	5.899	504.931	236.363
(3E,4S)-3-[2-[(1R,4aS	512.596	6.000	16.600	-0.264	19.433	6.990
(3R,5R)-1-[(Z)-3-(3,4-	354.313	6.000	10.600	-0.479	2.702	1.054
(10R)-10-hydroxy-1,ζ	456.707	2.000	3.700	6.209	289.317	164.663
(1R,6R,7R,13S,21R)-7	576.512	9.000	10.900	0.691	2.012	0.602
2-(3,5-dihydroxyphei	254.242	2.000	4.000	1.802	269.931	120.116
(9R)-4-hydroxy-9-[(9l	848.767	10.000	25.700	-1.759	0.010	0.003
(9R)-4-hydroxy-9-[(9'	848.767	10.000	25.700	-1.724	0.017	0.004
6-[(3R,4R)-3,4-dihyd	564.499	7.000	18.650	-1.765	2.955	0.913
[(2S,3R,4S,5S,6R)-3,4	375.408	5.000	14.000	-1.159	4.184	2.258
(3S,6S,7S,9S,10S)-4,1	252.353	3.000	5.100	1.416	755.711	365.483
(6S,7S,10R)-6-hydrox	234.338	1.000	3.700	2.299	1856.740	965.691
[(6S,7S,10R)-4,10,11,	276.375	0.000	4.000	2.899	1631.263	839.583

(2S)-5-hydroxy-2-ph	418.399	4.000	11.750	0.368	36.867	13.965
(2S,3S,4S,5R,6S)-6-[5	478.409	4.000	12.550	0.428	1.471	0.546
tert-butyl 4-(5-brom	380.284	1.000	3.500	4.566	1727.842	2362.329
2-[1-methyl-6-(3-me	370.574	1.000	2.000	6.789	561.402	337.118
[(1S,2R,4S,6S,7S,10R	466.573	0.000	8.500	3.154	774.403	375.264
(2R,3S,4R,5R)-2-buto	236.264	4.000	8.300	-0.389	226.932	99.575
[5-(5H-pyrido[4,3-b]i	264.283	2.000	3.200	2.839	1803.937	936.041
1-(3,4-dimethoxyphe	356.418	1.000	5.000	4.399	2133.116	1121.956
(2S,3R,4R,5R,6S)-2-[(1031.196	12.000	34.750	-1.985	0.362	0.094
(1R,4R,4aS)-4,7-dime	204.355	0.000	0.000	5.522	9906.038	5899.293
(2S)-2-(4-hydroxyph	418.399	5.000	12.750	-0.184	26.209	9.658
N-[(2-methoxypheny	405.496	1.000	5.250	4.879	783.147	597.008
(2S,3S,4S,5R,6R)-6-[(1117.243	12.000	35.600	-1.333	0.002	0.001
3,3,7-trimethyl-2,4-d	174.285	0.000	0.000	4.776	9906.038	5899.293
(1S,2S)-2-[4-[(3R,3aS	810.847	6.000	17.700	4.179	63.075	24.954
9-hydroxyoctadeca-1	294.433	2.000	3.700	4.755	111.866	58.958
octadec-5-enoic acid	282.465	1.000	2.000	5.983	278.884	158.255
1,4-dihydroxy-6,7-dii	358.304	1.000	7.000	1.729	17.227	7.804
dodecanoic acid;pro	200.320	1.000	2.000	3.754	278.974	158.310
(13-ethyl-14-hydroxy	520.624	1.000	8.950	3.871	128.159	65.719
8-methoxy-9H-carba	225.246	1.000	2.750	2.350	1058.511	526.069
(8-methoxy-9H-carb	227.262	2.000	2.450	2.659	1728.383	893.739
(3S,9S,10R,13R,14S,1	398.671	1.000	1.700	7.131	3396.822	1855.141
(8S,9S,10R,13R,14S,1	412.698	1.000	1.700	7.536	4030.582	2231.931
[(2R,3S,4R,5R)-5-(2-a	459.264	5.000	17.100	-1.102	0.095	0.134
(8S,9S,10R,13R,14S,1	384.644	1.000	1.700	7.025	3550.141	1945.810
octadeca-10,13-dien	280.450	1.000	2.000	5.839	235.179	131.627
(2R)-2-[(1S)-1,2-dihy	176.126	4.000	7.900	-1.851	35.844	13.547
(2R)-2-[(1R)-1,2-dihy	176.126	4.000	7.900	-1.851	35.832	13.542
4-carboxyphenolate	138.123	2.000	2.750	0.582	75.668	38.639
4-hydroxy-6-[(E)-2-(4	230.220	2.000	4.000	1.359	199.923	86.829
[(2S)-2-[(2R)-4-hexad	652.950	2.000	9.950	9.083	132.300	55.573
(1E,2S,3S)-2-(3,5-dih	514.531	6.000	6.000	3.238	16.349	5.799

5,7-dihydroxy-6,8-dihydro-2H-pyridin-2-one	1.000	3.000	1.511	719.140	346.404
(6R,7S)-7-methyl-6,7-dihydro-2H-pyridin-2-one	1.000	3.200	1.198	2045.786	1072.391
(1S)-2-methyl-5-[(2R,3R)-2-(3,5-dihydroxyphenyl)ethyl]pyridin-3-ylmethane	0.000	0.000	6.230	9906.038	5899.293
[(E)-hex-2-enyl] (Z)-hex-2-enyl	0.000	2.000	3.758	3759.172	2069.934
6-[(Z)-prop-1-enyl]-2-methylpyridin-3-ylmethane	1.000	1.000	2.187	7519.865	4379.548
3,5,5-trimethyl-1-(3,4-dihydroxyphenyl)pyridin-2-ylmethane	0.000	1.700	5.152	9906.038	5899.293
1-piperidin-1-ylpropylamine	0.000	4.000	1.446	873.351	472.783
(1S,6S,7S,8S)-1-methyl-2-(3,5-dihydroxyphenyl)pyridin-3-ylmethane	0.000	0.000	5.354	9906.038	5899.293
1,3,5,7,9,2,4,6,8,10-dihydro-2H-pyridin-2-one	10.000	1.000	2.565	9906.038	5899.293
4-[3-(hydroxymethyl)phenyl]pyridin-2-ylmethane	1.000	4.200	1.088	878.805	430.234
[(E)-3-(3,4-dihydroxyphenyl)propyl]pyridin-2-ylmethane	4.000	7.500	0.784	14.298	5.017
(1R,2S,3R)-2-(3,5-dihydroxyphenyl)pyridin-3-ylmethane	7.000	6.200	2.053	5.422	1.759
(1R,2S,3R)-2-(3,5-dihydroxyphenyl)pyridin-3-ylmethane	7.000	6.200	2.129	9.568	3.250
(1R,9R,10S)-6-hydroxy-2-(3,5-dihydroxyphenyl)pyridin-3-ylmethane	1.000	5.500	3.284	585.973	277.621
[(1S,4S,5R,8R,10S,13R)-1,3,5-trimethyl-2-(3,5-dihydroxyphenyl)pyridin-3-ylmethane]	0.000	5.750	8.378	1643.339	846.302
3,6-dihydroxy-5-(3-oxopropyl)pyridin-2-ylmethane	2.000	4.000	1.625	322.651	145.663
5-methoxy-3-propanoic acid	0.000	3.250	1.944	2922.591	1576.849
(4R,5S,6S,7aR)-4-hydroxy-2-(3,5-dihydroxyphenyl)pyridin-3-ylmethane	1.000	8.850	-0.150	1215.762	611.028
icosyl (E)-3-(4-hydroxyphenyl)pyridin-2-ylmethane	1.000	4.250	9.326	796.693	386.952
N-[1-(4-fluorophenyl)ethyl]pyridin-2-ylmethane	1.000	2.500	1.900	3104.088	4780.736
3-chloro-N-methyl-N-(2-(3,5-dihydroxyphenyl)pyridin-3-yl)ethanamine	0.000	3.000	2.657	2648.787	5796.337
2-ethenyl-1-methoxypropane	0.000	0.750	3.112	9906.038	5899.293
3-(2-aminoethyl)indole	3.000	3.250	0.372	148.982	69.901
(8S,9S,10R,13R,14S,14iR)-1,3,5-trimethyl-2-(3,5-dihydroxyphenyl)pyridin-3-ylmethane	1.000	1.700	7.621	3319.616	1809.607
5-fluoro-1,1,3,3-tetrahydro-2H-pyridin-2-one	0.000	0.750	3.595	9906.038	10000.000
(1S,6S,7S,8S)-1,3-dimethyl-2-(3,5-dihydroxyphenyl)pyridin-3-ylmethane	0.000	0.000	5.452	9906.038	5899.293
[(2R,3R,4S,5R,6R)-3-(3,5-dihydroxyphenyl)pyridin-3-ylmethane]	9.000	23.500	-1.971	2.244	0.678
[(2R,3R,4S,5S)-5-(acetamido)-2-(3,5-dihydroxyphenyl)pyridin-3-ylmethane]	2.000	18.600	3.302	17.150	6.107
(2R,5S)-2-[[[(3S,8S,9S)-2,3,5-trimethyl-2-(3,5-dihydroxyphenyl)pyridin-3-yl]ethyl]amino]propane	4.000	10.200	5.309	397.953	182.732
(2R,5S)-2-[[[(3S,8S,9S)-2,3,5-trimethyl-2-(3,5-dihydroxyphenyl)pyridin-3-yl]ethyl]amino]propane	4.000	10.200	5.149	281.172	125.532
(5'S,6'R,10E,12E,14R)-1,3,5-trimethyl-2-(3,5-dihydroxyphenyl)pyridin-3-ylmethane	1.000	4.250	7.154	2107.863	1107.606
[(12R,14S,15R,16R,17R)-1,3,5-trimethyl-2-(3,5-dihydroxyphenyl)pyridin-3-ylmethane]	16.000	26.700	-3.814	0.000	0.000
(2S)-2-[(3S,4S)-3-carboxyphenyl]pyridin-3-ylmethane	6.000	11.250	-1.118	0.009	0.004

(2S,3R,4R,5R,6S)-2-[(11S,12S,13S,14S,15S,16S,17S,18S,19S,20S,21S,22S,23S,24S,25S,26S,27S,28S,29S,30S)-2,3,4,5,6,7,8,9,10,11,12,13,14,15,16,17,18,19,20,21,22,23,24,25,26,27,28,29,30-dioxoheptacosanoic acid]	13.000	40.600	-2.883	1.051	0.299
(1R,3aR,5aS,5bR,7aR)-1,2,3,4,5,6,7,8,9,10,11,12,13,14,15,16,17,18,19,20,21,22,23,24,25,26,27,28,29,30-dioxoheptacosanoic acid	2.000	3.700	6.367	419.766	246.209
2-ethanimidoyloxy-1,2,3,4,5,6,7,8,9,10,11,12,13,14,15,16,17,18,19,20,21,22,23,24,25,26,27,28,29,30-dioxoheptacosanoic acid	2.000	5.000	-0.118	26.634	12.849
methyl 8-oxooctadecanoate	0.000	4.000	5.173	765.855	370.788
octadeca-13,16-diene	1.000	2.000	5.952	280.180	159.050
1,3,5,7,9,11,13,15,17,19,21,23,25,27,29,31,33,35,37,39,41,43,45,47,49,51,53,55,57,59,61,63,65,67,69,71,73,75,77,79,81,83,85,87,89,91,93,95,97,99,101,103,105,107,109,111,113,115,117,119,121,123,125,127,129,131,133,135,137,139,141,143,145,147,149,151,153,155,157,159,161,163,165,167,169,171,173,175,177,179,181,183,185,187,189,191,193,195,197,199,201,203,205,207,209,211,213,215,217,219,221,223,225,227,229,231,233,235,237,239,241,243,245,247,249,251,253,255,257,259,261,263,265,267,269,271,273,275,277,279,281,283,285,287,289,291,293,295,297,299,301,303,305,307,309,311,313,315,317,319,321,323,325,327,329,331,333,335,337,339,341,343,345,347,349,351,353,355,357,359,361,363,365,367,369,371,373,375,377,379,381,383,385,387,389,391,393,395,397,399,401,403,405,407,409,411,413,415,417,419,421,423,425,427,429,431,433,435,437,439,441,443,445,447,449,451,453,455,457,459,461,463,465,467,469,471,473,475,477,479,481,483,485,487,489,491,493,495,497,499,501,503,505,507,509,511,513,515,517,519,521,523,525,527,529,531,533,535,537,539,541,543,545,547,549,551,553,555,557,559,561,563,565,567,569,571,573,575,577,579,581,583,585,587,589,591,593,595,597,599,601,603,605,607,609,611,613,615,617,619,621,623,625,627,629,631,633,635,637,639,641,643,645,647,649,651,653,655,657,659,661,663,665,667,669,671,673,675,677,679,681,683,685,687,689,691,693,695,697,699,701,703,705,707,709,711,713,715,717,719,721,723,725,727,729,731,733,735,737,739,741,743,745,747,749,751,753,755,757,759,761,763,765,767,769,771,773,775,777,779,781,783,785,787,789,791,793,795,797,799,801,803,805,807,809,811,813,815,817,819,821,823,825,827,829,831,833,835,837,839,841,843,845,847,849,851,853,855,857,859,861,863,865,867,869,871,873,875,877,879,881,883,885,887,889,891,893,895,897,899,901,903,905,907,909,911,913,915,917,919,921,923,925,927,929,931,933,935,937,939,941,943,945,947,949,951,953,955,957,959,961,963,965,967,969,971,973,975,977,979,981,983,985,987,989,991,993,995,997,999,1001,1003,1005,1007,1009,1011,1013,1015,1017,1019,1021,1023,1025,1027,1029,1031,1033,1035,1037,1039,1041,1043,1045,1047,1049,1051,1053,1055,1057,1059,1061,1063,1065,1067,1069,1071,1073,1075,1077,1079,1081,1083,1085,1087,1089,1091,1093,1095,1097,1099,1101,1103,1105,1107,1109,1111,1113,1115,1117,1119,1121,1123,1125,1127,1129,1131,1133,1135,1137,1139,1141,1143,1145,1147,1149,1151,1153,1155,1157,1159,1161,1163,1165,1167,1169,1171,1173,1175,1177,1179,1181,1183,1185,1187,1189,1191,1193,1195,1197,1199,1201,1203,1205,1207,1209,1211,1213,1215,1217,1219,1221,1223,1225,1227,1229,1231,1233,1235,1237,1239,1241,1243,1245,1247,1249,1251,1253,1255,1257,1259,1261,1263,1265,1267,1269,1271,1273,1275,1277,1279,1281,1283,1285,1287,1289,1291,1293,1295,1297,1299,1301,1303,1305,1307,1309,1311,1313,1315,1317,1319,1321,1323,1325,1327,1329,1331,1333,1335,1337,1339,1341,1343,1345,1347,1349,1351,1353,1355,1357,1359,1361,1363,1365,1367,1369,1371,1373,1375,1377,1379,1381,1383,1385,1387,1389,1391,1393,1395,1397,1399,1401,1403,1405,1407,1409,1411,1413,1415,1417,1419,1421,1423,1425,1427,1429,1431,1433,1435,1437,1439,1441,1443,1445,1447,1449,1451,1453,1455,1457,1459,1461,1463,1465,1467,1469,1471,1473,1475,1477,1479,1481,1483,1485,1487,1489,1491,1493,1495,1497,1499,1501,1503,1505,1507,1509,1511,1513,1515,1517,1519,1521,1523,1525,1527,1529,1531,1533,1535,1537,1539,1541,1543,1545,1547,1549,1551,1553,1555,1557,1559,1561,1563,1565,1567,1569,1571,1573,1575,1577,1579,1581,1583,1585,1587,1589,1591,1593,1595,1597,1599,1601,1603,1605,1607,1609,1611,1613,1615,1617,1619,1621,1623,1625,1627,1629,1631,1633,1635,1637,1639,1641,1643,1645,1647,1649,1651,1653,1655,1657,1659,1661,1663,1665,1667,1669,1671,1673,1675,1677,1679,1681,1683,1685,1687,1689,1691,1693,1695,1697,1699,1701,1703,1705,1707,1709,1711,1713,1715,1717,1719,1721,1723,1725,1727,1729,1731,1733,1735,1737,1739,1741,1743,1745,1747,1749,1751,1753,1755,1757,1759,1761,1763,1765,1767,1769,1771,1773,1775,1777,1779,1781,1783,1785,1787,1789,1791,1793,1795,1797,1799,1801,1803,1805,1807,1809,1811,1813,1815,1817,1819,1821,1823,1825,1827,1829,1831,1833,1835,1837,1839,1841,1843,1845,1847,1849,1851,1853,1855,1857,1859,1861,1863,1865,1867,1869,1871,1873,1875,1877,1879,1881,1883,1885,1887,1889,1891,1893,1895,1897,1899,1901,1903,1905,1907,1909,1911,1913,1915,1917,1919,1921,1923,1925,1927,1929,1931,1933,1935,1937,1939,1941,1943,1945,1947,1949,1951,1953,1955,1957,1959,1961,1963,1965,1967,1969,1971,1973,1975,1977,1979,1981,1983,1985,1987,1989,1991,1993,1995,1997,1999,2001,2003,2005,2007,2009,2011,2013,2015,2017,2019,2021,2023,2025,2027,2029,2031,2033,2035,2037,2039,2041,2043,2045,2047,2049,2051,2053,2055,2057,2059,2061,2063,2065,2067,2069,2071,2073,2075,2077,2079,2081,2083,2085,2087,2089,2091,2093,2095,2097,2099,2101,2103,2105,2107,2109,2111,2113,2115,2117,2119,2121,2123,2125,2127,2129,2131,2133,2135,2137,2139,2141,2143,2145,2147,2149,2151,2153,2155,2157,2159,2161,2163,2165,2167,2169,2171,2173,2175,2177,2179,2181,2183,2185,2187,2189,2191,2193,2195,2197,2199,2201,2203,2205,2207,2209,2211,2213,2215,2217,2219,2221,2223,2225,2227,2229,2231,2233,2235,2237,2239,2241,2243,2245,2247,2249,2251,2253,2255,2257,2259,2261,2263,2265,2267,2269,2271,2273,2275,2277,2279,2281,2283,2285,2287,2289,2291,2293,2295,2297,2299,2301,2303,2305,2307,2309,2311,2313,2315,2317,2319,2321,2323,2325,2327,2329,2331,2333,2335,2337,2339,2341,2343,2345,2347,2349,2351,2353,2355,2357,2359,2361,2363,2365,2367,2369,2371,2373,2375,2377,2379,2381,2383,2385,2387,2389,2391,2393,2395,2397,2399,2401,2403,2405,2407,2409,2411,2413,2415,2417,2419,2421,2423,2425,2427,2429,2431,2433,2435,2437,2439,2441,2443,2445,2447,2449,2451,2453,2455,2457,2459,2461,2463,2465,2467,2469,2471,2473,2475,2477,2479,2481,2483,2485,2487,2489,2491,2493,2495,2497,2499,2501,2503,2505,2507,2509,2511,2513,2515,2517,2519,2521,2523,2525,2527,2529,2531,2533,2535,2537,2539,2541,2543,2545,2547,2549,2551,2553,2555,2557,2559,2561,2563,2565,2567,2569,2571,2573,2575,2577,2579,2581,2583,2585,2587,2589,2591,2593,2595,2597,2599,2601,2603,2605,2607,2609,2611,2613,2615,2617,2619,2621,2623,2625,2627,2629,2631,2633,2635,2637,2639,2641,2643,2645,2647,2649,2651,2653,2655,2657,2659,2661,2663,2665,2667,2669,2671,2673,2675,2677,2679,2681,2683,2685,2687,2689,2691,2693,2695,2697,2699,2701,2703,2705,2707,2709,2711,2713,2715,2717,2719,2721,2723,2725,2727,2729,2731,2733,2735,2737,2739,2741,2743,2745,2747,2749,2751,2753,2755,2757,2759,2761,2763,2765,2767,2769,2771,2773,2775,2777,2779,2781,2783,2785,2787,2789,2791,2793,2795,2797,2799,2801,2803,2805,2807,2809,2811,2813,2815,2817,2819,2821,2823,2825,2827,2829,2831,2833,2835,2837,2839,2841,2843,2845,2847,2849,2851,2853,2855,2857,2859,2861,2863,2865,2867,2869,2871,2873,2875,2877,2879,2881,2883,2885,2887,2889,2891,2893,2895,2897,2899,2901,2903,2905,2907,2909,2911,2913,2915,2917,2919,2921,2923,2925,2927,2929,2931,2933,2935,2937,2939,2941,2943,2945,2947,2949,2951,2953,2955,2957,2959,2961,2963,2965,2967,2969,2971,2973,2975,2977,2979,2981,2983,2985,2987,2989,2991,2993,2995,2997,2999,3001,3003,3005,3007,3009,3011,3013,3015,3017,3019,3021,3023,3025,3027,3029,3031,3033,3035,3037,3039,3041,3043,3045,3047,3049,3051,3053,3055,3057,3059,3061,3063,3065,3067,3069,3071,3073,3075,3077,3079,3081,3083,3085,3087,3089,3091,3093,3095,3097,3099,3101,3103,3105,3107,3109,3111,3113,3115,3117,3119,3121,3123,3125,3127,3129,3131,3133,3135,3137,3139,3141,3143,3145,3147,3149,3151,3153,3155,3157,3159,3161,3163,3165,3167,3169,3171,3173,3175,3177,3179,3181,3183,3185,3187,3189,3191,3193,3195,3197,3199,3201,3203,3205,3207,3209,3211,3213,3215,3217,3219,3221,3223,3225,3227,3229,3231,3233,3235,3237,3239,3241,3243,3245,3247,3249,3251,3253,3255,3257,3259,3261,3263,3265,3267,3269,3271,3273,3275,3277,3279,3281,3283,3285,3287,3289,3291,3293,3295,3297,3299,3301,3303,3305,3307,3309,3311,3313,3315,3317,3319,3321,3323,3325,3327,3329,3331,3333,3335,3337,3339,3341,3343,3345,3347,3349,3351,3353,3355,3357,3359,3361,3363,3365,3367,3369,3371,3373,3375,3377,3379,3381,3383,3385,3387,3389,3391,3393,3395,3397,3399,3401,3403,3405,3407,3409,3411,3413,3415,3417,3419,3421,3423,3425,3427,3429,3431,3433,3435,3437,3439,3441,3443,3445,3447,3449,3451,3453,3455,3457,3459,3461,3463,3465,3467,3469,3471,3473,3475,3477,3479,3481,3483,3485,3487,3489,3491,3493,3495,3497,3499,3501,3503,3505,3507,3509,3511,3513,3515,3517,3519,3521,3523,3525,3527,3529,3531,3533,3535,3537,3539,3541,3543,3545,3547,3549,3551,3553,3555,3557,3559,3561,3563,3565,3567,3569,3571,3573,3575,3577,3579,3581,3583,3585,3587,3589,3591,3593,3595,3597,3599,3601,3603,3605,3607,3609,3611,3613,3615,3617,3619,3621,3623,3625,3627,3629,3631,3633,3635,3637,3639,3641,3643,3645,3647,3649,3651,3653,3655,3657,3659,3661,3663,3665,3667,3669,3671,3673,3675,3677,3679,3681,3683,3685,3687,3689,3691,3693,3695,3697,3699,3701,3703,3705,3707,3709,3711,3713,3715,3717,3719,3721,3723,3725,3727,3729,3731,3733,3735,3737,3739,3741,3743,3745,3747,3749,3751,3753,3755,3757,3759,3761,3763,3765,3767,3769,3771,3773,3775,3777,3779,3781,3783,3785,3787,3789,3791,3793,3795,3797,3799,3801,3803,3805,3807,3809,3811,3813,3815,3817,3819,3821,3823,3825,3827,3829,3831,3833,3835,3837,3839,3841,3843,3845,3847,3849,3851,3853,3855,3857,3859,3861,3863,3865,3867,3869,3871,3873,3875,3877,3879,3881,3883,3885,3887,3889,3891,3893,3895,3897,3899,3901,3903,3905,3907,3909,3911,3913,3915,3917,3919,3921,3923,3925,3927,3929,3931,3933,3935,3937,3939,3941,3943,3945,3947,3949,3951,3953,3955,3957,3959,3961,3963,3965,3967,3969,3971,3973,3975,3977,3979,3981,3983,3985,3987,3989,3991,3993,3995,3997,3999,4001,4003,4005,4007,4009,4011,4013,4015,4017,4019,4021,4023,4025,4027,4029,4031,4033,4035,4037,4039,4041,4043,4045,4047,4049,4051,4053,4055,4057,4059,4061,4063,4065,4067,4069,4071,4073,4075,4077,4079,4081,4083,4085,4087,4089,4091,4093,4095,4097,4099,4101,4103,4105,4107,4109,4111,4113,4115,4117,4119,4121,4123,4125,4127,4129,4131,4133,4135,4137,4139,4141,4143,4145,4147,4149,4151,4153,4155,4157,4159,4161,4163,4165,4167,4169,4171,4173,4175,4177,4179,4181,4183,4185,4187,4189,4191,4193,4195,4197,4199,4201,4203,4205,4207,4209,4211,4213,4215,4217,4219,4221,4223,4225,4227,4229,4231,4233,4235,4237,4239,4241,4243,4245,4247,4249,4251,4253,4255,4257,4259,4261,4263,4265,4267,4269,4271,4273,4275,4277,4279,4281,4283,4285,4287,4289,4291,4293,4295,4297,4299,4301,4303,4305,4307,4309,4311,4313,4315,4317,4319,4321,4323,4325,4327,4329,4331,4333,4335,4337,4339,4341,4343,4345,4347,4349,4351,4353,4355,4357,4359,4361,4363,4365,4367,4369,4371,4373,4375,4377,4379,4381,4383,4385,4387,4389,4391,4393,4395,4397,4399,4401,4403,4405,4407,4409,4411,4413,4415,4417,4419,4421,4423,4425,4427,4429,4431,4433,4435,4437,4439,4441,4443,4445,4447,4449,4451,4453,4455,4457,4459,4461,4463,4465,4467,4469,4471,4473,4475,4477,4479,4481,4483,4485,4487,4489,4491,4493,4495,4497,4499,4501,4503,4505,4507,4509,4511,4513,4515,4517,4519,4521,4523,4525,4527,4529,4531,4533,4535,4537,4539,4541,4543,4545,4547,4549,4551,4553,4555,4557,4559,4561,4563,4565,4567,4569,4571,4573,4575,4577,4579,4581,4583,4585,4587,4589,4591,4593,4595,4597,4599,4601,4603,4605,4607,4609,4611,4613,4615,4617,4619,4621,4623,4625,4627,4629,4631,4633,4635,4637,4639,4641,4643,4645,4647,4649,4651,4653,4655,4657,4659,4661,4663,4665,4667,4669,4671,4673,4675,4677,4679,4681,4683,4685,4687,4689,4691,4693,4695,4697,4699,4701,4703,4705,4707,4709,4711,4713,4715,4717,4719,4721,4723,4725,4727,4729,4731,4733,4735,4737,4739,4741,4743,4745,4747,4749,4751,4753,4755,4757,4759,4761,4763,4765,4767,4769,4771,4773,4775,4777,4779,4781,4783,4785,4787,4789,4791,4793,4795,4797,4799,4801,4803,4805,4807,4809,4811,4813,4815,4817,4819,4821,4823,4825,4827,4829,4831,4833,4835,4837,4839,4841,4843,4845,4847,4849,48					

17-(2-hydroxy-6-met	412.654	2.000	2.450	6.543	2525.970	1346.875
2,3,4-trihydroxy-5-(3	362.246	6.000	11.350	-1.323	0.044	0.015
dimethyl 2,3-bis(1,3-	414.411	0.000	7.000	3.557	2218.313	1170.469
(2R)-2-[(E)-3-[2-(carb	418.356	6.000	9.000	0.996	0.079	0.030
2-[4-hydroxy-6-(hydr	1049.211	12.000	35.500	-2.004	0.649	0.177
19-[3-[(6Z,9Z)-17-car	919.416	3.000	11.100	16.159	0.158	0.079
2-(2,3-dihydroxy-3-r	330.380	5.000	4.700	2.374	156.521	66.647
2-(2,3-dihydroxy-3-r	314.380	4.000	3.950	3.093	458.446	212.933
(1R,2S,5S,6S,9R,12S,	312.497	2.000	2.500	3.694	443.550	227.309
(2S,3S,4S,5R,6S)-6-[[482.397	8.000	14.000	-1.464	0.119	0.036
[(2S,3R,4S,5S,6R)-3,4	666.848	8.000	17.300	0.816	13.054	4.547
8,16,20,20-tetrametl	331.457	1.000	0.750	5.951	8225.892	4825.635
trimethyl-[(3-trimeth	487.860	0.000	3.950	7.598	9783.137	5820.223
3-(1H-indol-3-yl)-2-r	219.240	2.000	3.700	2.185	187.366	102.956
2-(2-methyl-3-methy	164.247	0.000	2.000	2.115	2285.608	1208.895
3,5-dioxa-11-azapen	263.295	1.000	2.500	3.370	6027.399	3448.086
22-hydroxytetraatriac	508.910	1.000	3.700	11.118	2249.155	1188.068
8,10-dimethoxy-3,3,'	323.391	1.000	2.250	5.062	6719.019	3877.660
(2S,3S,4S,5R)-3,4,5-ti	448.382	4.000	11.800	0.184	0.774	0.273
[(1R)-3,5,5-trimethyl	791.294	0.000	2.000	18.351	5902.299	3370.797
3-[2-[3-hydroxy-5-[(4	562.661	5.000	4.500	6.079	56.945	22.343
1-O-ethyl 6-O-prop-2	212.245	0.500	4.000	2.391	822.331	400.429
2-methoxyethyl 2-m	176.212	0.000	3.700	1.760	1855.474	964.979
(6,6-dimethyl-2-bicy	236.353	0.000	2.000	4.117	4384.402	2444.438
(3S,3aR,5Z,9Z,11aR)-	234.338	0.000	3.000	2.899	2701.526	1448.333
(2E,4E)-5-(1,3-benzo	383.530	1.000	4.000	6.399	2966.011	1602.186
3,9-dihydroxy-6-(2-h	452.503	2.000	5.250	4.810	291.165	130.361
(1R,2S,4S,5'S,6R,7S,8	444.653	1.000	5.200	5.316	1635.828	842.122
(1R,2R,5S,6R,9R,11S,	468.675	1.000	6.700	4.390	785.041	380.839
[3-(4-hydroxy-3-metl	300.310	1.000	5.500	2.097	432.885	200.130
(1R,3R,4S,5R)-4-[(E)-	530.484	6.000	11.450	1.550	0.613	0.212
methyl 11-[(2R,3S)-3	312.492	0.000	4.000	5.472	2961.349	1599.464
butyl (Z)-pentadec-1	296.492	0.000	2.000	6.343	3233.653	1759.010

6-methyl-9-propan-2	214.307	0.000	0.500	3.695	9906.038	5899.293
[(7R,8R)-7-hydroxy-5	431.528	2.000	8.450	3.544	159.557	75.280
(1R,4R,4aR,8aS)-1,6-	222.370	1.000	0.750	4.117	6476.604	3726.666
(2R,5S,6S,8R)-1,5-di	204.355	0.000	0.000	4.969	9906.038	5899.293
(2S,3R,4S,5S,6R)-2-[(636.557	13.000	34.000	-7.376	0.159	0.039
methyl (2S,4aS,6R,6e	552.574	5.000	17.400	-0.322	21.375	7.748
(4aR,5S,6R,8aR)-5-[2	362.465	1.000	6.700	3.321	127.262	67.776
(2S,3R,4S,5S,6R)-2-[2	522.548	7.000	14.900	0.147	14.798	5.207
4-[(2R)-2-[(1R,4aS,5R	350.454	3.000	8.100	1.697	379.353	173.518
(1R,2R,4aS,6aR,6aS,ε	472.707	3.000	5.400	5.160	122.950	65.297
(E)-3-[3-[1-hydroxy-3	520.532	6.000	15.200	-0.091	7.310	2.429
(5R,8R,9S,10S,13R,1	768.980	7.000	20.450	1.836	11.780	4.069
(3R,5R)-4-[(Z)-3-(3,4-	354.313	6.000	9.650	-0.136	2.621	1.020
(1S,3R,4R,5R)-4-[(E)-	530.484	6.000	11.450	1.709	0.788	0.278
(3R)-4-(2,3-dihydrox)	224.213	2.000	4.500	1.138	29.114	13.761
1-[(1S,4aS,8aS)-7-me	204.311	0.000	2.000	3.328	4543.156	2540.246
(4aS,8R,8aS)-8-ether	202.296	0.000	2.000	3.014	1941.840	1013.619
(1R,2R,4R,5R,10R,11	488.620	2.000	8.900	3.057	162.710	69.500
(1R,2R,7R,10R,11S,1	648.746	6.000	18.400	0.524	11.542	3.980
(1aS,1bS,6aS,7S,7aR)	250.337	0.000	3.750	2.414	2429.020	1291.087
(1aS,1bS,6aS,7S,7aR)	412.479	4.000	13.250	0.104	139.377	58.792
(1S,2S,5R)-2-methyl-	222.370	1.000	0.750	4.404	4489.827	2508.032
5-hydroxy-3-[(5-hydr	374.349	0.000	7.500	1.513	72.150	28.856
(1R,11R,13R)-5,16-di	576.558	0.000	11.250	2.352	66.136	26.265
(1S,2R,5R,10R,14S,1	414.713	1.000	1.700	7.756	4050.541	2243.880
[(1S,3E,4R)-3-[2-[(1R	797.339	2.000	5.400	15.124	954.759	470.563
(1S,2R,5S,10R,14S,1E	414.713	1.000	1.700	7.729	3381.825	1846.289
(2S,5S)-2-[(1Z,2S,5R,	416.686	1.000	3.700	6.593	2434.846	1294.434
(1E,3Z,6R,7R)-6-[2-(2	360.449	1.000	6.700	3.319	134.286	71.828
(1E,3Z,6R,7R)-6-(2-cε	292.374	2.000	4.000	3.195	8.586	4.676
(2R)-2-[(1R)-1-[(8R,9	486.604	3.000	7.950	3.641	247.251	109.246
10-(1,3-benzodioxol-	364.311	1.000	7.700	1.517	926.801	455.687
(1S,8S,13R)-11-meth	233.266	0.000	6.700	-0.007	472.330	243.292

bis[[[dimethyl-[4-(1, 849.309	0.000	2.200	16.329	9894.207	10000.000
8-[(2E)-3,7-dimethyl- 724.981	4.000	3.000	11.678	2867.733	1544.882
(3S,4S)-4-[3-carboxy- 670.490	11.000	22.300	-3.315	0.001	0.000
(3S,4S)-4-[(2S)-3-carb 670.490	11.000	22.300	-3.503	0.000	0.000
(3S,4S)-4-[3-carboxy- 670.490	11.000	22.300	-3.498	0.000	0.000
(2S)-4-[(E)-2-[(2S)-2- 694.602	8.000	19.050	0.301	0.000	0.000
(4aR,5R,6aR,6aS,6bR 796.991	9.000	22.400	0.851	0.749	0.263
(1S,4aR,5S,8R,8aS)-3 238.369	2.000	2.450	3.090	2681.574	1436.775
2-[(4R,5S,7R,8R,11S, 652.475	9.000	21.050	-2.980	0.029	0.008
(2S,3S,4S,5R,6S)-3,4, 432.383	4.000	12.050	0.358	2.566	0.997
(3R,3aR,5aR,5bR,7aR 444.740	2.000	2.450	6.539	2786.880	1497.856
[(9R,12R,13Z,16S,17 502.609	0.000	7.250	4.532	263.002	142.940
(3S,3aS,6S,6aR)-3,6-t 386.357	2.000	6.950	2.500	2960.359	1598.886
(1S,2S,4S,5R,10R,11S 470.605	2.000	9.450	3.090	415.447	191.430
(2S,3S)-3-hydroxy-2- 470.605	2.000	8.150	3.569	187.655	81.085
(1R,3aR,7R,8aR)-1-m 222.370	1.000	0.750	4.101	4553.830	2546.698
(1S,2R,3S,6S,9R,10S, 375.507	1.000	7.450	2.098	386.755	196.019
(3aR,5Z,9Z,11aR)-6,1 232.322	0.000	3.000	2.843	2815.550	1514.519
(1S,2R,5S,6S,7R,8S)-2 222.370	1.000	1.700	3.438	4339.021	2417.102
(1S,3R,6S,8R,11S,12S 454.778	1.000	1.700	8.167	4383.866	2444.115
(1S,3R,8R,11S,12S,1E 452.762	0.000	2.000	8.195	4187.936	2326.261
(1R,4aR,8aR)-1-ethyl 190.328	0.000	0.000	5.266	9906.038	5899.293
[5-hydroxy-2-[(2S,3R 582.557	7.000	20.500	-1.191	9.465	3.212
(2S,3R,4S,5S,6R)-2-[(799.007	10.000	23.800	-0.148	5.956	1.947
(2S,3R,4S,5S,6R)-2-[(961.149	13.000	32.300	-2.409	0.678	0.186
(2S,3R,4S,5S,6R)-2-[(813.033	9.000	23.800	0.209	9.032	3.054
(2S,3R,4S,5S,6R)-2-[(975.175	12.000	32.300	-1.810	1.364	0.396
(E)-2-methyl-5-[(1S,2 234.338	1.000	2.000	3.816	311.831	178.556
3-(hydroxymethylid 126.112	0.000	3.450	0.001	751.426	363.244
(2S,3R,4R,5R,6S)-2-[(1067.227	14.000	37.200	-3.148	0.087	0.020
7-methyl-7-(3-methy 190.328	0.000	0.000	5.296	9906.038	5899.293
2,8,10-trihydroxy-3-r 382.369	2.000	5.250	2.982	222.754	97.595
5,7,8,15-tetrahydrox 434.445	3.000	5.250	3.555	168.456	72.156

[(2S,3R,4S,5S,6R)-3,4	666.848	8.000	17.300	0.987	13.314	4.645
16-O-[(2S,3R,4S,5S,6	920.868	14.000	38.000	-5.707	0.010	0.002
(2R)-2-[(1S)-1-[(8R,9	486.604	3.000	7.950	3.559	267.405	118.902
(3R,4S,6R)-6-[(1R)-1-	474.636	3.000	8.200	3.398	202.479	88.030
3-[(2S,3R,4S,5S,6R)-	740.668	10.000	26.600	-3.175	0.739	0.204
[(2R,3S,4S,5R,6R)-6-	584.746	6.000	14.650	2.037	33.555	12.615
2-[(2Z,4E,6E,8E,10E,1	600.880	2.000	6.150	9.623	1272.902	642.127
(2R)-2-[(1S)-1-[(5R,6	523.065	4.000	8.950	3.473	414.208	313.053
(4S,4aR,6aR,6bS,8aR	440.708	0.000	2.700	6.587	1682.504	868.124
3-[2-[(1R,4aS,5R,6R,ξ	348.438	2.000	8.400	1.359	227.154	99.680
(1aR,3aS,7bS)-1,1,3a	204.355	0.000	0.000	5.072	9906.038	5899.293
(3S,5R,8R,9R,10R,13l	472.707	2.000	6.150	5.117	1283.259	647.776
(3S,3aS,5aS,5bS,7aR,	440.751	0.000	1.700	5.942	9906.038	5899.293
(1R,2R,5R,7S,10R,11l	426.724	1.000	1.700	7.021	4367.777	2434.422
(2R,3R,4S,5S,6R)-2-[[400.511	5.000	10.950	1.087	141.476	59.750
[(8R,9S,27R,29S,30R,	992.721	12.000	25.200	-3.073	0.002	0.000
2-[[[(11R,12R)-12-[(1	1104.762	19.000	27.950	-4.217	0.000	0.000
(1S,2S,6S,7R,8R)-1,3-	204.355	0.000	0.000	5.425	9906.038	5899.293
N-[(10S,12R,16S)-5-h	371.389	2.000	7.500	1.526	194.993	178.670
(3S,3aR,4S,5Z,7S,10Z	266.336	2.000	6.400	1.140	506.203	237.007
(2S,4aS,6R,8aS)-8a-r	220.354	1.000	1.700	3.535	3395.908	1854.601
[(2S,4aS,6R,8aS)-8a-r	320.471	0.000	1.750	5.682	2659.230	1423.839
(3R,4aR,6aS,6bS,8aS,	426.724	1.000	1.700	7.014	4726.688	2651.345
1-(7-hydroxy-5-meth	478.500	3.000	4.250	5.358	359.549	163.748
1-(7-hydroxy-4-meth	462.501	3.000	3.750	5.390	367.313	167.574
(1S,3R,6S,8R,11S,12	454.778	1.000	1.700	8.289	4382.493	2443.288
(1S,3R,8R,11S,12S,1	452.762	0.000	2.000	8.309	4183.404	2323.540
bis[(2S,3R,4S,5S,6R)-	976.975	14.000	38.000	-4.678	0.011	0.002
(1R,3R,4S,5R,8R,9S,1	357.449	2.000	9.400	0.607	137.238	63.965
[(Z)-hex-1-enyl] benz	204.268	0.000	2.500	3.156	3381.149	1845.890
16,20,20-trimethyl-1	345.440	1.000	2.750	4.638	1526.720	781.578
(1R,2S,4S,8R,9S,12S,	1079.194	14.000	40.150	-4.086	0.150	0.037
(1S,2S,4S,5R,10R,11	486.604	2.000	9.200	2.989	161.295	68.846

(1S,2S,4S,5R,10R,11S) 472.620	2.000	8.500	3.471	466.051	216.754
2-[(1R)-1-[(5S,9S,10R) 470.605	3.000	7.250	3.775	266.313	118.377
(1R,3R,4S,5R)-3-[(E)- 530.484	6.000	11.450	1.754	0.629	0.218
(1S,3R,4R,5R)-3-[(E)- 530.484	6.000	11.450	1.729	0.623	0.216
(2R,3R)-2-[[[(2S,3R)-2 540.609	5.000	9.600	3.684	83.219	33.670
[(2S,3R,4S,5S,6R)-3,4 444.478	5.000	13.700	0.149	68.802	27.412
(5E)-5-(2,3,4,5-tetra 216.190	4.000	9.300	-1.552	49.185	19.071
(2S,3S,4S,5R,6R)-6-[[662.816	5.000	15.200	2.898	0.528	0.230
2-[4-[(2S,3R,4R,5R,6S) 297.307	5.000	10.050	-1.277	29.982	22.970
2-[4-[(2S,3R,4R,5S,6S) 459.449	8.000	18.550	-3.064	2.921	1.860
(3S,3aS,5S,6Z,10Z,11 412.479	4.000	13.200	0.196	126.959	53.152
(2R,3R,4S,5S,6R)-2-[2 388.457	6.000	13.600	-0.461	44.244	17.009
sodium;[(2R,3S,4R,5I) 786.970	6.000	19.100	2.701	2.982	1.172
sodium;[(2R,3S,4R,5I) 967.128	11.000	29.300	-0.471	0.040	0.011
(10E,12E,14E)-9,16-d 310.433	3.000	5.400	3.631	36.357	17.497
2,4,6-tris[(4-hydroxy) 576.688	4.000	4.500	7.036	159.030	67.802
3-[2-(4-hydroxy-3-m 486.563	4.000	4.500	5.265	121.095	50.503
3-[2-[3-hydroxy-4-[(4 562.661	5.000	4.500	6.224	59.559	23.454
2-(13,16-dimethyl-1E) 349.472	2.000	1.500	5.534	4961.899	2794.236
methyl (2S,4aS,6S,10 538.547	5.000	16.450	0.209	84.864	34.390
(2S,3R,4S,5S,6S)-2-[(1032.184	13.000	35.750	-3.099	0.216	0.060
methyl (1S,15R,16S,13 70.447	1.000	7.900	2.219	434.095	222.076
[(2R,3S,4S,5R,6S)-3,4 764.690	8.000	22.850	-0.297	0.941	0.265
(1S,2R)-1-(4-hydroxy) 556.608	5.000	11.300	3.219	68.679	27.358
(1S,5S,8R,9S,11R,14F) 327.422	2.000	7.400	0.919	146.747	68.769
(1S,3S,5S,8R,9S,11R, 329.438	3.000	7.100	1.111	228.150	110.801
[(1S,3R,6S,8R,11S,12 679.164	0.000	2.000	14.310	4369.915	2435.710
(1R,2R,10R,11S,14R, 452.589	0.000	6.450	4.199	505.023	236.409
(1R,2R,10R,11S,14R, 436.590	0.000	5.750	4.744	1415.526	720.235
(13aR)-3-methoxy-6, 281.354	1.000	3.500	3.030	707.119	376.313
(13aS)-3-methoxy-6, 281.354	1.000	3.500	3.030	707.120	376.313
6,14-dihydroxy-7-me 448.339	5.000	14.800	-1.854	5.159	1.667
(9R,12R,13Z,16S,17S) 336.433	0.000	5.750	2.224	236.879	127.658

methyl (2R,5S,8S,10F	462.585	1.000	6.750	4.066	298.663	133.993
(1aR,3R,3aS,7R,7aR,	236.353	0.000	2.700	3.241	4398.378	2452.862
5-[2-(3-hydroxyphen	442.510	5.000	3.750	4.254	54.765	21.420
(1R,2S,4S,5'R,6R,7S,	1049.168	12.000	37.500	-3.061	0.845	0.236
(4aR,6aS,6aS,6bR,8a	438.649	1.000	4.750	4.901	663.034	317.286
(2S)-2-amino-N-form	116.119	3.000	4.000	-1.332	52.311	22.552
[(1S,2R,3R,4R,5R,6S,	631.719	3.000	16.950	1.988	137.820	64.258
5-[(E)-2-[(2S,3S)-3-(3	514.531	5.000	6.000	3.924	33.635	12.647
(4aR,5S,6aR,6aS,6bR	634.849	5.000	12.900	3.705	10.956	4.785
(2S,3S,4S,5R)-2,3,4-ti	362.246	6.000	11.350	-1.508	0.022	0.007
(2S,3R,4S,5S,6R)-2-[(722.912	6.000	18.500	2.586	51.149	19.896
(1R,2R,5R,8S,9R)-4,4	238.369	2.000	2.450	2.747	1995.490	1043.922
(1S,4R,4aR)-4,7-dime	204.355	0.000	0.000	5.440	9906.038	5899.293
(1R,2S,3R)-2-(3,5-dih	546.573	6.000	7.700	3.099	13.276	4.630
(1R,2S,3R)-2-(3,5-dih	560.599	6.000	7.700	3.680	13.839	4.843
4-(4-hydroxy-3,5-dirr	466.487	4.000	6.950	2.910	147.826	62.654
[(2R,3S)-7-hydroxy-2	462.498	2.000	5.750	4.570	279.905	124.921
2-[[2-(3,4-dihydroxyr	578.528	9.000	10.900	0.710	1.205	0.346
(3R,3aR,5aR,5bR,7aR	444.740	2.000	2.450	6.553	3012.594	1629.402
(1S,4aR,6aR,6aS,6bR	714.846	12.000	16.700	0.497	0.438	0.147
4-[2,13-dihydroxy-13	622.881	3.000	13.200	5.788	306.844	137.965
(2S)-4-[(E)-2-[(2R)-2-	726.601	10.000	24.800	-2.028	0.000	0.000
methyl (2S,3R,4S)-4-	460.477	4.000	15.900	-0.088	46.186	17.818
(2S,3R,4S,5S,6R)-2-[(780.991	9.000	22.100	0.728	5.142	1.661
(2S,3R,4S,5S,6R)-2-[(943.133	12.000	30.600	-1.416	0.922	0.259
(2S,3R,4S,5S,6R)-2-[(957.160	11.000	30.600	-0.815	4.146	1.316
[(1R,3R,4R,5R)-1,4-di	350.324	3.000	8.950	0.654	71.888	28.743
3-methyl-3-(4-methy	345.440	1.000	2.750	5.181	1798.203	932.826
8,16-dimethyl-19-prc	331.457	1.000	0.750	6.060	8227.422	4826.605
[(1R,9R,10S,12R,13S,	410.512	1.000	8.700	1.599	29.784	13.572
(4aR,6aS,6bS,8aS,12:	424.709	0.000	2.000	6.969	4299.013	2393.022
(3S,4aR,6aR,6bS,8aS,	426.724	1.000	1.700	6.896	4372.729	2437.405
3-[2-[2-hydroxy-5-[(4	562.661	5.000	4.500	6.441	77.195	31.043

4-[(4-hydroxyphenyl] 364.440	2.000	3.000	4.890	914.051	448.914
5-[2-(3-hydroxyphen 456.537	4.000	3.750	5.239	142.016	59.996
3-[2-(3-hydroxyphen 456.537	4.000	3.750	5.279	216.369	94.575
2-[(2'S,7S,8R,8aS)-2'- 378.508	1.000	6.450	3.373	257.108	113.960
(5R,6S,7S)-10-methy 246.305	2.000	3.900	2.199	1993.168	1042.609
8-hydroxy-4,7-dimet 262.305	1.000	5.250	1.784	571.872	270.407
(1R,3S)-3,5-dihydrox 278.304	2.000	5.950	1.487	984.720	486.544
4-[(E)-2-[(2S)-2-carbc 548.459	8.000	17.000	-0.908	0.002	0.001
6,7'-dihydroxy-10'-m 398.414	2.000	4.750	3.593	334.303	151.357
(2R,3R,4S,5S,6R)-2-[[622.881	6.000	12.650	3.180	60.813	23.988
(2R,3R,4S,5S,6R)-2-[[622.881	6.000	12.650	3.114	56.920	22.333
[(2R,3R,4S,5S,6R)-2-[702.939	6.000	14.950	2.930	3.665	1.478
[(2R,3R,4S,5S,6R)-2-[702.939	6.000	14.950	2.959	3.351	1.362
(1S,2S,4S,7R,9S,12R, 598.661	5.000	17.950	0.004	36.866	15.510
N-[[2-(aminomethyl) 354.676	2.000	2.500	3.932	773.198	2175.717
[5-(3-aminoprop-1-y 285.345	3.000	7.200	0.563	50.566	21.740
(2R,3S,4R,5R)-2,3,4, 332.263	5.000	10.800	-1.928	2.313	0.701
3-[[[(2R,3S,4S,5R,6R)- 1195.354	14.000	39.450	-2.382	0.006	0.001
(1R,7R,10R)-7,10,11, 248.364	1.000	2.000	3.564	312.617	179.043
[(10R,15R)-3,4,5,21, 782.535	12.000	21.000	-3.556	0.002	0.000
(1R,22R)-7,8,9,12,13 780.519	12.000	21.000	-3.622	0.005	0.001
3-[(2S,3R,4R,5S,6R)- 626.524	10.000	22.250	-3.301	0.302	0.078
(1S,2R,8R,15R)-15-hy 235.282	1.000	6.700	0.035	210.117	101.365
1-O-[(2S,3R,4R,5S,6R 976.975	14.000	38.000	-4.700	0.010	0.002
7-hydroxy-2-methox 254.242	1.000	5.500	1.240	464.368	215.907
[(1S,2S,4S,5S,6R,10S) 512.466	6.000	19.100	-1.663	24.963	9.163
(E,5R,6S,7R,8R)-1-(3, 342.302	5.000	12.000	-1.523	4.920	1.584
(4E,12E)-octadeca-4, 280.450	1.000	2.000	5.919	312.492	178.965
2-hydroxy-2-[(E)-3-(4 310.260	2.000	6.250	1.697	1.221	0.568
5-[2-(4-hydroxyphen 296.365	3.000	2.250	3.693	363.401	165.645
2,3,4-trideuterio-3,7, 136.236	0.000	0.000	3.959	9906.038	5899.293
(1S,3R,8S,11S,12S,15 426.724	1.000	1.700	7.546	4402.196	2455.163
5-hydroxy-3-(4-hydr 500.501	5.000	12.250	1.145	16.564	5.881

4-[(2R,3R,4R,5S,6S)-	357.360	5.000	8.600	0.708	51.483	20.036
5-[(E)-2-(2,4-dihydro	312.365	4.000	3.000	3.151	231.105	101.555
7,8-dihydroxy-1,1-dii	237.255	4.000	4.500	-1.290	12.469	6.088
(E)-2-hydroxy-5-(4-h	222.197	2.000	5.450	0.624	13.516	6.004
(3R,6R)-6-[(8S,9S,10F	410.682	1.000	1.700	7.583	4369.736	2435.602
2-[(2,2-dimethyl-3,4-	366.413	2.000	5.250	3.371	295.352	132.388
4-hydroxy-2-[[4-hydr	366.413	3.000	5.250	2.490	192.472	83.337
3,5,7-trihydroxy-6-m	284.268	2.000	3.750	2.196	259.969	115.332
[(2R,3S,4S,5R)-3,4-di	1397.007	24.000	34.250	-6.206	0.000	0.000
hexacyclo[12.8.1.01,	292.379	0.000	0.000	6.977	9906.038	5899.293
[(1S,3R,8S,11S,12S,1	484.761	1.000	3.700	7.334	1844.919	959.047
8-[(3R,4R,5S)-3,4-dih	564.499	9.000	19.050	-2.506	0.917	0.258
11,17-dimethoxy-22-	385.416	1.000	8.400	2.096	723.715	385.868
(Z)-N-[2-hydroxy-2-]	351.444	2.000	4.950	4.816	1786.878	926.477
5-(3,5-dimethyl-11H-	349.472	2.000	1.500	5.817	3599.602	1975.128
8,13,13,17-tetrametl	331.457	0.000	0.750	6.077	6538.427	3765.131
7,8-dihydroxy-3,5-dic	372.260	4.000	12.500	-1.725	0.087	0.033
4-[4,13-dihydroxy-13	622.924	3.000	11.500	7.252	254.895	112.901
(3S,5S,10S,13R,17R)-	414.713	1.000	1.700	7.594	3395.446	1854.329
(Z)-N-(3-aminopropy	408.540	6.000	8.750	1.018	2.447	1.008
2-[(1E,3Z,5E,9Z,11E,	1538.898	0.000	0.000	14.466	9906.038	5899.293
11,12,13,22-tetrahy	652.475	9.000	20.600	-2.987	0.014	0.004
(1,16,17,18,21,22,23	952.656	14.000	24.950	-4.060	0.001	0.000
2-[4,5-dihydroxy-6-(1065.211	14.000	37.200	-2.708	0.352	0.092
2-[4-hydroxy-6-(hydr	1197.327	16.000	44.000	-4.462	0.060	0.013
6,7,8,11,12,13,25,26	784.550	12.000	22.400	-4.338	0.005	0.001
2-[6-[[6,15-dihydroxy	921.084	12.000	30.400	-1.519	0.505	0.135
3-[(2S,3R,4S,5S,6R)-	580.498	8.000	19.800	-2.131	2.574	0.786
(2R,3R)-2-(3,4-dihyd	452.414	9.000	13.950	-1.564	5.097	1.645
1-[(2Z)-3,7-dimethyl	333.472	2.000	0.750	5.940	4545.967	2541.945
3-[2-hydroxy-4-meth	370.444	2.000	3.750	4.823	1913.721	997.763
13-(cyclopenten-1-yl	294.433	0.000	3.000	5.070	98.573	51.423
5-hydroxy-3-(3-meth	304.345	0.000	2.250	4.770	1819.520	944.784

(1R,3aS,5aS,5bR,7aR) 472.707	3.000	4.450	5.708	232.533	130.027
methyl (1R,9R,10S,11S) 539.627	2.000	11.000	1.939	14.233	14.315
5,7-dihydroxy-3-(3-methylbut-2-en-1-yl) 320.344	1.000	3.000	4.049	552.124	260.329
(2S)-2-[[4-[(2-amino-5-formylphenyl)amino]phenyl]amino]phenol 441.402	6.250	12.750	-0.377	0.035	0.012
2-[[4-[(2-amino-5-formylphenyl)amino]phenyl]amino]phenol 473.444	7.250	14.250	-0.683	0.022	0.007
2-amino-6-[(1R,2S)-1-cyclohexylethyl]pyridine 237.218	5.000	9.400	-1.770	21.506	7.799
3-(3-methylbut-2-en-1-yl)pyridine 203.246	2.000	4.000	1.373	613.734	291.865
(2S,4E)-4-[2-[(1S)-1-cyclohexylethyl]phenyl]pyridine 390.349	6.000	10.000	0.602	0.019	0.008
(2S,4E)-4-[2-[(1S)-1-cyclohexylethyl]phenyl]pyridine 374.349	5.000	9.250	1.423	0.054	0.025
(2S)-4-[(E)-2-[(2S)-2-cyclohexylethyl]phenyl]pyridine 388.333	5.000	8.500	1.163	0.024	0.010
(Z)-3-(3,3-dimethyl-4-oxobut-1-en-1-yl)pyridine 383.489	0.250	7.750	2.643	903.319	684.673
3H-benzo[h]quinazolin-6-ol 196.208	1.000	3.500	1.588	1211.791	608.872
isoquinolin-6-ol 145.160	1.000	2.500	1.077	1299.772	656.791
9-[(2R,3R,4S,5R)-3,4-dihydroquinolin-2-yl]pyridine 294.266	4.000	11.800	-1.565	35.024	13.212
5-pyrrolidin-1-yl-7H-benzodiazepin-2-one 207.191	1.000	6.500	-0.503	156.438	66.609
(2S,4E)-4-[2-[2-(4-hydroxyphenyl)ethyl]phenyl]pyridine 360.366	4.000	8.000	2.055	1.199	0.557
(2S,4E)-4-[2-[2-(3,4-dihydroquinolin-2-yl)ethyl]phenyl]pyridine 346.339	5.000	8.000	1.239	0.424	0.181
11-(4-hydroxyphenyl)pyridine 294.352	1.000	2.750	3.748	1174.551	588.672
(E)-3-[(1S,2S,4aR,8aF)octahydroquinolin-2-yl]pyridine 381.514	1.000	4.000	5.476	4196.079	2331.150
(1'R,2S,3R,4'S,6R,8'R)octahydroquinolin-2-yl 584.748	2.000	8.350	6.378	906.411	444.860
4,7-dimethoxyphenylpyridine 268.268	0.000	5.500	1.521	928.932	456.819
(1R,4R,5S,8R,9S)-11,11-dimethyl-5,8-dihydroquinolin-2-yl 398.455	3.000	6.700	2.396	239.196	105.404
6-[(3S,3aR,5S,6R,6aS)octahydroquinolin-2-yl]pyridine 280.320	2.000	5.700	1.596	256.898	113.860
(1R,4R,5S,6S)-6,9-dihydroquinolin-2-yl 266.336	2.000	6.450	1.149	636.961	303.822
(1R,4R,5S)-1,8-dimethyl-5,8-dihydroquinolin-2-yl 248.321	0.000	6.000	1.355	1430.243	728.332
(1R,4R,5S)-7-amino-1,8-dihydroquinolin-2-yl 263.336	1.500	7.000	1.030	600.450	285.043
(1R,4R,5S)-7-hydroxy-1,8-dihydroquinolin-2-yl 264.321	1.000	6.750	1.168	676.167	324.085
(1S,4aR,8aR)-4,7-dimethyl-5,8-dihydroquinolin-2-yl 204.355	0.000	0.000	5.600	9906.038	5899.293
(1R,4aR,8aS)-4,7-dimethyl-5,8-dihydroquinolin-2-yl 204.355	0.000	0.000	5.573	9906.038	5899.293
(1S,8S,9R,16S)-8,16-dimethyl-5,8-dihydroquinolin-2-yl 470.478	6.000	6.200	2.304	17.745	6.336
anisole 108.140	0.000	0.750	2.110	9906.038	5899.293
decacyclo[26.6.2.0.2,4.50.538] 450.538	0.000	0.000	9.811	9906.038	5899.293
(4S)-3,3,6-trimethylheptane 154.252	1.000	1.700	2.557	4346.860	2421.823

methyl (2R)-2-[(2,2-c	2.000	7.250	3.131	190.203	82.275
(1R,8S,9S,16R)-8,16-	6.000	6.200	2.339	19.938	7.186
2,4-dimethylbenzo[h	0.000	1.000	4.105	8716.386	5137.388
[(1S,8S,11R,12S,13R,	2.000	7.950	2.157	476.336	221.928
(1R,2R,3E,7S,11E,13	2.000	5.400	2.109	726.441	350.207
methyl 4-hydroxy-2-	3.000	7.250	2.765	76.454	30.721
methyl 4-hydroxy-3-	3.000	7.250	1.340	60.040	23.658
methyl 2-[[3-[(3,3-dii	3.000	9.250	2.295	79.972	32.252
(8aS)-7-methyl-4-me	0.000	0.000	5.596	9906.038	5899.293
[(1S,8S,11S,13R,17S,	1.000	6.250	3.045	913.608	448.679
1,7,7-trimethylbicycl	0.000	2.000	1.943	3958.705	2188.942
1,6-diazatetracyclo[7	0.000	4.000	2.079	1978.636	1034.395
octanoyl octanoate	0.000	4.500	4.077	1982.689	1036.686
5,6-dihydroxy-2-(4-h	2.000	6.000	2.206	194.501	84.286
tripotassium;2-hydr	3.000	5.750	0.132	0.281	0.148
1-butyl-2-ethylcyclo	0.000	0.000	6.055	9906.038	5899.293
(2S)-2-[(2S,5R)-5-eth	0.000	2.750	4.006	5745.062	3273.842
5-[(2R,3R)-6-hydroxy	7.000	6.750	4.750	6.203	2.034
4-[3-(3,5-dihydroxyp	6.000	5.250	2.865	10.571	3.619
(3S,6S)-3-methyl-6-[[3.000	5.000	4.610	189.511	327.792
(2S,3R,4S,5S,6R)-2-[[8.000	13.000	1.522	3.410	1.065
1,4,5-trihydroxy-7-m	0.000	4.000	1.871	143.807	60.815
ethanol	1.000	1.700	-0.310	2857.851	1539.128
2-hydroxy-3-(2-hydr	1.000	5.500	4.610	38.748	18.743
(2R)-6-methyl-2-[(1R	1.000	0.750	4.588	5860.418	3344.952
1,4-dichlorobenzene	0.000	0.000	3.011	9906.038	10000.000
(1S,2R,5S,7S)-2,6,6-ti	0.000	0.000	4.855	9906.038	5899.293
(1R,5S,6R,7S,10R)-1C	0.000	0.000	5.531	9906.038	5899.293
(Z)-hex-2-enal	0.000	2.000	1.219	1707.617	882.138
(1S,4R,6S)-1-methyl-	0.000	4.000	1.134	3598.553	1974.506
(1R,4R,6S)-1-methyl-	0.000	2.000	1.750	9906.038	5899.293

QPlogKp	Absorción oral (%)	Regla de cinco
-4.322	79.748	0
-5.554	43.193	2
-3.813	82.720	0
-4.544	73.921	0
-4.226	60.754	0
-5.696	31.938	0
-5.855	30.185	0
-4.618	52.714	0
-4.341	56.691	0
-7.330	6.598	1
-6.366	35.948	0
-2.683	83.822	0
-3.183	83.963	0
-3.717	63.978	0
-6.978	23.959	0
-3.726	66.477	0
-3.117	84.098	0
-3.833	63.067	0
-3.128	80.775	0
-3.789	100.000	0
-4.098	68.380	0
-7.576	0.000	1
-6.425	36.432	0
-7.882	4.463	0
-2.125	93.997	0
-2.657	80.786	0
-1.626	95.538	0
-2.742	80.433	0
-3.314	74.124	0
-5.090	48.751	0
-4.366	59.792	0

-2.550	85.817	0
-6.303	17.855	0
-1.931	94.380	0
-1.809	100.000	0
-2.307	96.428	0
-1.670	100.000	0
-1.632	100.000	0
-3.378	76.488	0
-2.521	87.874	0
-7.210	4.868	1
-1.844	100.000	0
-5.501	41.342	0
-2.941	84.823	0
-7.797	1.205	0
-3.943	67.617	0
-1.720	96.601	0
-3.340	70.402	0
-5.732	32.027	0
-2.848	88.787	0
-6.258	35.574	0
-7.015	50.685	0
-4.228	65.701	0
-4.109	60.914	0
-3.275	78.199	0
-2.129	93.988	0
-3.910	65.431	0
-2.396	57.480	0
-5.753	53.662	0
-5.102	39.196	0
-4.862	48.956	0
-3.859	65.514	0
-2.704	84.606	0
-2.145	86.967	0

-1.042	100.000	0
-8.220	0.000	1
-6.580	2.927	0
-5.329	42.445	0
-6.098	28.348	0
-2.717	82.932	0
-11.504	0.000	3
-5.565	28.890	1
-0.340	100.000	0
-4.007	74.208	0
-3.304	68.972	0
-3.304	68.972	0
-1.775	100.000	0
-5.066	46.649	0
-1.165	100.000	1
-5.844	31.385	0
-5.656	34.031	0
-4.205	57.467	0
-1.594	100.000	1
-2.172	87.187	1
-0.112	100.000	0
-1.647	100.000	0
-2.001	95.599	0
-2.471	83.671	0
-3.792	85.898	0
-5.347	26.430	0
-4.234	49.682	0
-3.416	73.002	0
-7.543	47.136	0
-3.436	73.803	0
-4.443	56.586	0
-1.520	100.000	0
-5.084	41.758	0

-7.523	32.978	0
-7.225	19.829	1
0.095	100.000	1
-5.201	37.179	0
-3.655	69.588	0
-6.898	25.847	0
-3.757	86.989	0
-5.616	41.850	0
-5.188	45.016	0
-5.818	43.584	0
-3.260	82.039	0
-4.572	32.851	0
-6.736	11.144	0
-1.987	100.000	0
-3.174	68.202	0
-1.787	89.816	1
-4.924	67.770	0
-2.236	94.931	0
-0.835	100.000	1
-3.909	74.105	0
-2.280	96.972	0
-2.804	89.428	0
-1.757	100.000	1
-4.571	79.183	0
-3.393	76.538	0
-4.603	51.222	0
-0.750	100.000	0
-1.940	94.658	0
-1.954	100.000	0
-1.130	100.000	1
-2.105	94.488	0
-1.843	100.000	0
-1.796	100.000	0

-1.714	100.000	0
-1.839	100.000	0
-1.819	100.000	0
-0.791	100.000	0
-2.969	59.818	2
-5.232	45.391	0
-4.422	63.764	0
-4.724	68.119	0
-1.616	100.000	0
-1.129	100.000	0
-2.997	94.638	0
-1.943	100.000	0
-4.443	58.526	0
-3.206	91.737	0
-9.027	0.000	3
-5.489	45.304	2
-1.002	100.000	1
-7.947	66.748	0
-5.868	45.315	0
-3.389	94.485	0
-1.978	95.511	0
-2.681	91.405	0
-5.847	42.905	0
-3.768	66.828	0
-4.240	83.806	0
-1.577	100.000	0
-3.986	61.888	0
-2.696	90.519	0
-2.413	92.694	0
-2.081	90.635	1
-2.131	90.032	0
-5.556	56.239	0
-6.291	65.566	0

-3.245	74.178	0
-1.865	95.838	0
-2.511	92.702	0
-1.850	94.366	0
-8.654	20.686	1
-0.835	100.000	0
-1.409	100.000	0
-2.943	100.000	0
-3.651	79.204	0
-5.416	56.643	0
-3.328	72.111	0
-1.565	100.000	0
-3.552	88.207	0
-1.208	100.000	0
-4.132	51.940	0
-2.847	100.000	0
-4.435	66.595	0
-3.551	92.322	0
-5.007	61.664	0
-3.385	95.115	0
-2.709	84.570	0
-5.280	63.626	0
-4.224	67.472	0
-0.724	100.000	0
-5.327	63.863	0
-1.031	100.000	0
-3.495	72.968	0
-5.078	65.136	0
-2.052	65.197	0
-13.941	0.000	3
-5.395	61.888	0
-2.761	100.000	0
-3.842	87.430	2

-3.796	75.492	0
-4.232	72.640	0
-2.363	100.000	0
-4.851	69.507	0
-4.666	71.677	0
-4.713	76.651	0
-3.510	88.222	0
-3.325	80.813	2
-4.512	30.557	1
-5.239	45.659	0
-3.895	83.029	0
-2.868	100.000	0
-3.058	100.000	0
-6.270	33.148	0
-6.918	23.336	0
-2.975	89.717	0
-7.801	1.172	0
-7.504	50.197	2
-5.885	0.000	2
-2.381	100.000	0
-1.747	100.000	1
-5.156	46.652	0
-7.127	20.803	0
-1.586	100.000	0
-5.511	27.048	1
-3.201	96.503	0
-5.899	43.218	0
-6.361	0.000	2
-5.784	43.043	0
-2.650	93.305	0
-2.512	93.606	0
-1.849	91.832	0
-3.209	75.113	0

-1.520	100.000	0
-3.484	72.784	0
-5.057	25.128	1
-5.958	0.000	2
-7.872	4.578	0
-2.186	100.000	0
-5.436	42.068	3
-3.619	75.315	0
-10.069	0.000	1
-3.167	95.376	0
0.020	100.000	0
-3.856	83.982	0
-2.244	100.000	0
-3.181	87.775	0
-5.469	40.147	0
-3.238	74.322	0
-2.000	100.000	0
-2.416	100.000	0
-1.481	100.000	0
-1.421	100.000	0
-2.692	88.574	0
-2.665	91.509	0
-3.452	75.885	0
-3.213	75.930	0
-1.425	100.000	0
-2.288	100.000	0
-1.419	100.000	0
-3.362	81.507	0
-1.531	100.000	0
-3.495	73.727	0
-0.800	100.000	0
-2.958	100.000	0
-2.264	93.986	0

-2.066	92.351	0
-2.288	95.235	0
-1.916	100.000	0
-2.244	85.346	0
-0.758	100.000	0
-2.203	91.466	0
-3.312	94.095	0
-2.271	90.981	0
-1.497	100.000	1
-1.467	100.000	0
-2.061	100.000	0
-1.782	100.000	0
-2.960	85.324	0
-1.237	100.000	0
-1.138	100.000	0
-1.793	100.000	0
-3.547	90.987	0
-0.840	100.000	0
-2.378	91.666	0
-0.065	100.000	0
-2.462	85.404	0
-0.679	100.000	0
-1.429	100.000	0
-1.920	100.000	0
-1.790	100.000	0
-2.437	87.336	0
-1.661	100.000	0
-4.723	69.436	0
-2.643	92.406	0
-2.547	92.259	0
-2.897	75.559	0
-2.335	91.761	0
-4.021	75.363	0

-1.167	100.000	0
-0.922	100.000	0
-0.905	100.000	0
-1.955	100.000	0
-2.454	93.125	0
-2.155	100.000	0
-2.818	84.508	0
-1.569	100.000	0
-1.903	100.000	0
-1.813	94.773	0
-2.394	84.715	0
-1.674	100.000	0
-3.125	81.696	0
-6.388	0.000	2
-4.642	62.195	0
-1.871	100.000	0
-2.050	100.000	0
-2.849	89.905	0
1.241	100.000	1
-1.092	100.000	0
-1.195	100.000	0
-1.206	100.000	0
-0.967	100.000	0
-4.740	45.080	0
-0.536	100.000	0
-3.835	81.513	0
-1.670	100.000	0
-0.852	100.000	0
-1.591	100.000	0
-1.870	100.000	1
-0.635	100.000	0
-1.798	100.000	0
-2.510	94.351	0

-2.414	96.677	0
-1.856	100.000	0
-1.723	100.000	0
-2.356	96.523	0
-3.082	78.947	0
-2.257	100.000	0
-2.199	100.000	0
-1.894	100.000	0
-2.274	100.000	0
-1.883	100.000	0
-0.981	100.000	0
-5.931	71.894	0
-2.262	100.000	0
-2.163	100.000	0
-0.627	100.000	0
-1.327	100.000	0
-2.495	87.048	0
-1.568	100.000	2
0.141	100.000	0
-0.981	100.000	0
-2.119	100.000	0
-5.895	29.711	1
-4.530	81.214	0
-2.217	87.077	0
-2.189	96.588	1
-3.214	77.670	0
-1.162	100.000	0
-0.841	100.000	0
-2.489	95.748	0
-1.107	100.000	1
-1.878	100.000	0
-2.123	100.000	0
-2.653	90.117	0

-1.234	100.000	0
-4.140	77.533	0
9.579	100.000	1
-2.080	100.000	0
-3.021	84.190	0
-2.089	100.000	0
-2.090	89.407	0
-0.786	100.000	1
-1.871	100.000	0
-2.460	95.849	0
-1.996	100.000	0
-1.542	100.000	0
1.464	100.000	1
-3.172	100.000	0
-2.830	85.007	0
-2.200	100.000	0
-0.704	100.000	1
-1.741	100.000	0
-1.705	100.000	0
-2.036	100.000	0
-2.653	88.970	0
-1.212	100.000	1
2.685	100.000	1
-0.496	100.000	1
-1.610	100.000	0
-2.078	100.000	0
-1.982	100.000	0
-1.119	100.000	1
-1.207	100.000	1
-1.418	100.000	0
-1.321	100.000	0
-1.597	100.000	1
0.080	100.000	1

0.017	100.000	1
-0.938	100.000	1
5.963	100.000	1
-1.820	100.000	0
-1.487	100.000	0
-3.269	78.637	0
-1.026	100.000	1
-0.873	100.000	1
-2.388	95.489	0
-2.962	85.199	0
-2.572	83.878	0
-0.934	100.000	0
-2.125	94.409	0
-0.095	100.000	0
-4.464	81.283	0
-2.721	94.134	0
-2.366	88.195	0
-2.615	91.197	0
-3.794	66.795	0
-1.888	100.000	0
-2.714	85.005	0
-3.244	93.096	1
-2.665	88.865	0
-6.186	22.591	0
-4.067	67.214	0
-2.901	80.204	0
-3.334	78.870	0
-5.439	41.266	0
-2.014	100.000	0
-1.895	96.584	0
-0.579	100.000	0
-1.864	100.000	0
-1.792	100.000	0

-1.520	100.000	0
-1.101	100.000	0
-3.118	77.910	0
-5.038	40.765	0
-2.297	100.000	0
-1.680	100.000	0
-4.475	92.556	0
-4.419	52.227	0
-4.262	58.011	0
-0.785	100.000	0
-1.988	100.000	0
-4.761	59.948	0
-5.329	42.445	0
-0.741	100.000	0
-1.520	100.000	0
-1.520	100.000	0
-1.520	100.000	0
1.717	100.000	1
-3.553	85.887	0
-0.481	100.000	0
-8.548	33.005	0
-4.081	66.159	0
-4.123	57.639	0
-2.718	100.000	2
-4.351	63.190	0
-4.107	82.073	0
-2.158	100.000	0
-2.364	100.000	0
-2.567	100.000	0
-3.845	81.809	1
-1.215	100.000	1
-3.518	100.000	0
-1.639	100.000	0

-2.840	100.000	0
-3.519	100.000	0
-2.608	92.520	0
-3.397	79.548	0
-4.505	66.078	0
-3.666	80.596	0
-2.652	87.152	0
-1.645	100.000	0
-5.029	90.563	1
-1.373	100.000	1
-0.897	100.000	1
-1.616	100.000	0
-0.800	100.000	0
-1.364	100.000	0
-0.733	100.000	0
-2.619	92.007	0
-4.254	82.813	0
-3.168	85.185	0
-1.601	96.987	0
0.604	100.000	0
-0.897	100.000	0
-0.875	100.000	0
-2.587	82.398	0
-5.445	49.194	0
-1.815	100.000	0
-2.302	100.000	0
-0.497	100.000	1
-1.142	100.000	1
-4.169	58.183	0
-2.019	91.457	1
-0.685	100.000	1
-0.057	100.000	1
-1.994	64.849	0

-3.931	66.203	0
-1.932	91.142	1
-1.789	96.132	1
-1.020	100.000	1
-0.362	100.000	1
-2.596	88.573	0
-3.036	95.398	1
-1.766	100.000	0
-1.445	100.000	0
-2.040	100.000	0
-1.316	100.000	0
-2.274	100.000	0
-6.467	0.000	3
-3.761	80.994	0
-1.182	100.000	1
-1.835	91.869	0
-0.842	100.000	0
-3.158	78.399	0
-1.139	100.000	0
-5.702	17.189	1
-1.894	100.000	0
-0.904	100.000	0
-6.600	0.000	2
-0.986	100.000	1
-1.517	100.000	0
-3.860	66.594	0
-2.030	92.451	0
-3.240	82.246	0
-3.611	72.076	0
-4.495	93.505	0
-0.966	100.000	0
-1.930	100.000	0
0.215	100.000	1

-1.527	100.000	1
-3.444	68.939	0
-4.261	62.008	0
-1.821	100.000	0
-2.027	100.000	0
-2.365	95.755	0
4.392	100.000	1
10.935	100.000	1
-2.301	100.000	0
-1.223	100.000	0
-4.539	80.707	0
-0.998	100.000	0
0.001	100.000	2
-2.318	100.000	0
-0.044	100.000	2
0.020	100.000	2
-2.316	93.741	0
-3.569	74.299	0
-1.405	100.000	1
-1.666	100.000	0
-1.388	100.000	0
-2.345	100.000	0
-1.873	100.000	0
-1.373	100.000	0
-1.853	100.000	0
-1.604	100.000	0
-2.608	91.600	0
-2.183	100.000	0
-2.216	96.884	0
-0.804	100.000	0
5.158	100.000	1
8.774	100.000	1
-3.774	67.925	0

-2.952	82.009	0
-4.997	25.647	1
-0.293	100.000	0
-5.272	36.819	0
-2.013	100.000	0
-2.585	86.059	0
-2.127	95.998	0
-2.636	86.995	0
-1.797	100.000	0
-2.454	95.639	0
-1.394	100.000	0
-2.390	100.000	0
-1.507	100.000	0
-1.787	100.000	0
-1.916	100.000	0
-2.392	100.000	0
-1.117	100.000	1
-1.629	100.000	0
-1.039	100.000	0
3.102	100.000	1
3.520	100.000	1
-0.111	100.000	1
-0.058	100.000	1
4.742	100.000	1
5.575	100.000	1
6.378	100.000	1
6.786	100.000	1
8.050	100.000	1
8.437	100.000	1
9.275	100.000	1
9.692	100.000	1
10.521	100.000	1
11.354	100.000	1

12.545	100.000	2
12.132	100.000	1
-2.178	100.000	0
-4.022	69.179	0
-2.461	93.483	0
-1.359	100.000	1
7.245	100.000	1
10.141	100.000	1
-1.372	100.000	0
-3.794	66.804	0
-3.416	93.276	0
7.633	100.000	1
-3.254	75.862	0
-5.459	23.998	1
-0.431	100.000	1
-6.870	23.669	0
-2.166	100.000	0
-2.702	89.154	0
-2.520	94.925	0
-2.138	100.000	0
-2.058	92.904	1
0.306	100.000	1
-1.937	100.000	0
-0.615	100.000	1
-2.220	100.000	0
-4.514	64.772	0
-2.550	81.208	0
-1.798	100.000	0
-2.354	100.000	0
-2.402	100.000	0
-0.722	100.000	1
0.150	100.000	1
-2.376	90.311	0

-2.619	89.037	0
-1.066	100.000	0
-2.840	82.609	0
-3.466	96.453	0
-2.269	100.000	0
-1.520	100.000	0
-2.366	92.301	0
-1.036	100.000	0
-1.319	100.000	0
-2.673	86.444	0
2.266	100.000	1
-0.915	100.000	1
-0.304	100.000	1
-1.859	100.000	0
-2.350	93.643	0
-2.201	95.995	0
-2.127	100.000	0
-1.507	100.000	0
-2.857	100.000	0
-1.416	100.000	0
-8.902	0.000	3
-0.835	100.000	1
-0.207	100.000	0
-0.910	100.000	1
-3.965	100.000	0
-2.023	100.000	0
-1.439	100.000	0
-1.245	100.000	0
-3.005	90.935	0
-4.320	83.886	0
-2.220	100.000	0
1.847	100.000	1
-1.973	100.000	0

-1.465	100.000	0
-1.124	100.000	1
-2.570	85.599	0
-2.421	94.485	0
-0.611	100.000	0
-0.650	100.000	0
-0.719	100.000	0
-1.231	100.000	0
-0.692	100.000	0
-2.050	100.000	0
-0.862	100.000	0
-3.014	100.000	0
-2.126	100.000	0
-1.689	100.000	1
-1.261	100.000	1
-0.038	100.000	2
-1.501	100.000	1
-0.399	100.000	1
-1.792	100.000	0
-4.179	61.825	0
2.199	100.000	1
0.010	100.000	0
-0.884	100.000	1
-2.676	89.937	0
-2.256	100.000	0
-1.647	100.000	0
2.185	100.000	1
-1.282	100.000	0
-3.715	76.716	0
0.113	100.000	1
-5.166	76.967	0
-3.579	78.894	0
-2.656	87.200	0

-0.998	100.000	0
-1.298	100.000	0
-1.552	100.000	0
0.250	100.000	1
-5.173	46.410	0
-4.478	77.971	0
-0.634	100.000	1
-3.222	82.799	0
-1.327	100.000	0
-3.450	72.489	0
-0.596	100.000	0
-1.322	100.000	1
-1.471	100.000	0
-2.928	89.787	0
-0.559	100.000	1
-2.740	86.788	0
-3.764	100.000	0
-2.794	89.988	0
7.958	100.000	1
-2.380	92.587	0
-0.081	100.000	1
-1.142	100.000	0
-2.267	95.436	0
-1.820	100.000	0
-1.687	100.000	0
-2.883	100.000	0
-1.414	100.000	0
-1.270	100.000	1
-4.937	56.520	1
-1.952	100.000	0
-2.691	96.356	0
-0.545	100.000	1
-1.872	96.663	0

-1.190	100.000	0
-0.943	100.000	0
-0.819	100.000	1
-1.146	100.000	0
-1.643	100.000	0
-3.402	82.329	0
-0.015	100.000	1
-3.101	75.736	0
0.111	100.000	0
-4.394	84.693	0
2.611	100.000	1
15.888	100.000	2
-1.399	100.000	1
-1.117	100.000	1
0.787	100.000	0
-3.464	81.827	0
1.311	100.000	1
-3.275	83.633	0
-1.373	100.000	1
-2.591	100.000	0
-1.968	100.000	0
-4.815	52.901	0
-3.080	84.574	0
-1.520	100.000	0
-2.137	100.000	0
-1.775	100.000	0
-4.316	79.872	0
0.926	100.000	0
-0.981	100.000	1
-1.885	100.000	0
-2.976	92.435	0
-5.765	4.015	3
-1.925	94.337	0

-5.728	43.725	0
3.406	100.000	1
-0.208	100.000	1
-1.395	100.000	0
-2.123	100.000	0
11.781	100.000	1
-3.259	78.967	0
-3.446	74.585	0
-1.913	100.000	0
-1.520	100.000	0
-1.344	100.000	0
-2.102	100.000	0
-2.627	90.969	0
1.016	100.000	0
-6.494	16.183	0
2.946	100.000	1
2.531	100.000	1
-1.412	100.000	1
-8.676	0.000	3
-1.607	100.000	0
-1.422	100.000	0
-0.873	100.000	1
-2.420	100.000	0
0.154	100.000	1
2.172	100.000	1
-6.821	40.543	0
-1.783	100.000	0
-2.237	92.532	0
-2.019	100.000	0
-1.972	100.000	0
-3.154	88.907	0
-0.144	100.000	1
-3.420	100.000	0

-2.655	90.524	0
-1.635	100.000	0
-1.451	100.000	0
0.229	100.000	1
-2.222	92.103	0
-0.840	100.000	0
-2.609	93.196	0
-2.279	96.969	0
-3.091	80.369	0
-2.074	100.000	0
-1.710	100.000	0
-2.489	95.187	0
-2.489	100.000	0
-1.248	100.000	1
-1.505	100.000	1
-2.088	100.000	0
-1.788	100.000	0
-2.095	100.000	0
-3.738	75.896	0
-4.443	77.908	0
-1.256	100.000	0
-1.464	100.000	0
-0.708	100.000	1
-2.752	96.529	0
-0.595	100.000	1
-7.782	5.558	0
-3.237	100.000	0
-3.129	87.059	0
-1.150	100.000	1
-4.439	82.060	0
-1.300	100.000	0
-1.225	100.000	0
2.532	100.000	1

3.706	100.000	1
-1.023	100.000	0
-3.162	100.000	0
6.064	100.000	1
-2.448	100.000	0
15.147	100.000	2
-0.456	100.000	1
-0.729	100.000	1
-3.796	87.865	0
-4.542	82.448	0
-5.586	67.122	2
-2.748	100.000	0
-3.955	70.510	0
-4.723	64.083	0
-1.908	100.000	0
-2.120	100.000	0
-2.461	100.000	0
-2.114	100.000	0
-2.649	96.845	0
-3.934	77.294	0
-2.342	100.000	0
-1.358	100.000	0
-2.122	100.000	0
-1.653	100.000	0
-1.889	100.000	0
-1.190	100.000	1
-10.685	0.000	1
-2.216	100.000	0
-0.969	100.000	0
-2.116	100.000	0
-2.631	95.645	0
-2.761	84.070	0
-1.948	100.000	0

-2.975	87.880	0
-0.818	100.000	0
-1.065	100.000	0
-1.595	100.000	0
-1.862	100.000	0
-1.327	100.000	1
-0.623	100.000	1
-2.134	100.000	0
-2.109	100.000	0
-5.239	45.659	0
-3.097	100.000	0
-2.514	100.000	0
-3.050	94.865	1
-3.090	93.595	1
-6.332	4.007	2
-2.780	100.000	1
-1.449	75.018	0
-6.721	23.845	1
-7.461	0.498	2
-5.658	35.126	1
-2.892	82.698	0
-5.921	42.276	0
-5.031	58.518	0
-1.618	100.000	1
-3.697	93.613	1
-1.992	100.000	0
-1.950	100.000	0
-2.526	100.000	0
-5.392	45.690	0
-6.732	58.425	0
-2.001	100.000	0
-1.391	100.000	1
-2.372	94.263	0

-5.686	59.892	0
-2.410	96.109	0
-1.527	100.000	0
-4.014	100.000	0
-0.988	100.000	0
-2.719	78.267	0
2.446	100.000	1
3.183	100.000	1
-3.675	69.570	0
-6.598	62.089	0
-1.206	100.000	0
-1.847	96.926	0
-1.707	100.000	0
-0.979	100.000	0
-1.540	100.000	0
-4.262	59.106	0
-0.169	100.000	1
-2.013	100.000	0
-1.732	100.000	0
-1.629	100.000	0
-1.889	94.575	0
-0.679	100.000	0
0.310	100.000	1
-1.516	100.000	0
0.144	100.000	1
-2.072	93.998	0
0.336	100.000	1
-2.307	90.571	0
-1.537	100.000	0
-2.882	81.660	0
-0.426	100.000	1
-1.449	100.000	0
-3.638	73.039	0

-3.055	77.859	0
-0.892	100.000	1
0.114	100.000	1
-2.928	91.202	0
-1.896	100.000	0
-1.583	94.352	0
-1.820	100.000	0
-3.797	66.506	0
-3.052	78.356	0
-3.063	82.100	0
-0.042	100.000	1
-4.018	65.074	0
-3.555	69.870	0
-3.866	70.818	0
-2.958	80.044	0
-2.444	90.490	0
-2.077	100.000	0
-4.020	75.366	0
-1.365	100.000	1
-5.211	37.691	1
-6.099	52.082	0
-4.728	60.584	0
-5.626	35.808	1
-4.080	75.239	0
-13.146	0.000	3
-0.682	100.000	0
-4.096	63.121	1
-2.537	100.000	1
-3.976	94.467	0
-3.977	94.789	0
-6.100	88.011	0
-1.288	100.000	0
-4.590	76.949	0

-1.746	96.394	1
-7.438	30.800	1
-3.495	96.662	0
-2.282	100.000	0
-3.047	76.696	0
-8.449	0.000	3
-0.805	100.000	0
-2.049	100.000	1
-4.762	59.903	0
-2.062	100.000	1
-10.682	0.000	3
-2.599	100.000	0
-2.285	100.000	0
-3.585	82.517	1
-10.506	0.000	3
-2.695	100.000	0
-4.393	83.360	2
-1.790	100.000	0
-8.364	0.000	3
-7.269	82.983	0
-2.319	100.000	1
-9.551	0.000	3
-3.044	88.422	0
-4.758	53.257	0
-5.443	0.000	3
-4.261	82.555	0
-3.715	82.201	1
-3.830	76.403	0
-1.377	100.000	0
0.472	100.000	1
-0.849	100.000	1
-0.642	100.000	1
-1.833	100.000	0

-0.073	100.000	1
-1.276	100.000	0
-3.756	57.826	0
-0.649	100.000	1
-3.832	68.231	0
-2.869	82.114	0
-0.442	100.000	1
-2.331	92.355	0
-1.300	100.000	0
0.084	100.000	1
-4.160	72.080	0
-3.578	83.816	0
-3.706	55.621	0
-2.235	95.193	0
-4.153	67.957	0
-2.444	95.874	0
-1.141	100.000	0
-1.043	100.000	0
-2.993	82.496	0
-2.360	86.510	0
-3.129	81.590	0
-2.062	100.000	0
1.102	100.000	1
-5.051	47.854	0
-1.297	100.000	0
0.745	100.000	0
-1.993	100.000	0
-1.425	100.000	0
-2.649	94.571	0
-1.191	100.000	0
-1.572	100.000	0
-1.664	100.000	0
-1.743	100.000	0

-2.722	90.094	0
-7.291	13.317	0
-1.231	100.000	0
-4.032	86.363	0
-1.590	100.000	0
-1.438	100.000	0
-0.720	100.000	1
-1.027	100.000	0
-1.732	100.000	0
-2.913	75.794	0
-1.617	100.000	0
-7.199	53.439	0
-0.849	100.000	0
-3.548	72.781	0
-6.996	0.000	3
-3.758	66.563	0
-2.042	100.000	0
-2.311	100.000	0
-6.392	0.000	2
-2.393	100.000	0
-1.888	100.000	0
-1.874	100.000	0
-0.957	100.000	1
-0.917	100.000	1
-0.882	100.000	1
-1.092	100.000	1
-1.306	100.000	1
-1.169	100.000	1
-3.171	96.876	0
-6.250	7.464	0
-0.257	100.000	1
-2.058	100.000	0
-2.013	100.000	0

-4.677	52.996	0
-4.780	48.886	0
-2.898	89.302	0
-1.386	100.000	0
-1.915	100.000	0
-2.592	100.000	0
-3.631	89.395	0
-2.196	100.000	0
-1.521	100.000	0
-1.305	100.000	1
-2.084	93.915	0
-1.982	100.000	0
-1.414	100.000	1
-2.326	100.000	1
-10.122	0.000	3
-2.924	100.000	1
-2.326	100.000	0
-1.837	100.000	0
-2.359	95.991	0
-2.279	100.000	1
-1.327	100.000	0
-9.427	0.000	3
-2.325	100.000	1
-2.066	100.000	1
-1.682	100.000	1
-1.651	100.000	1
-1.555	100.000	0
-0.688	100.000	1
-2.041	100.000	1
-2.073	100.000	1
-1.914	100.000	0
2.187	100.000	1
-1.262	100.000	1

0.927	100.000	0
-0.920	100.000	1
-5.255	22.073	2
-4.460	92.499	0
-0.760	100.000	1
-2.283	100.000	0
-2.449	100.000	0
-1.847	100.000	0
-7.961	0.000	3
-2.706	88.474	0
-2.154	100.000	1
-2.701	100.000	0
-4.081	67.041	0
-2.904	93.323	0
-4.615	82.304	0
-2.157	100.000	0
2.186	100.000	1
-2.292	100.000	0
-1.311	100.000	1
-1.537	100.000	0
-3.166	77.532	0
-2.500	90.673	0
-2.077	95.877	0
-1.782	100.000	0
-1.187	100.000	1
-1.532	100.000	1
-4.157	59.212	0
-1.919	100.000	0
-2.154	100.000	1
1.275	100.000	1
-1.324	100.000	1
-2.785	94.068	0
-2.624	94.121	0

-1.174	100.000	0
-1.886	100.000	0
-2.545	100.000	0
-6.197	29.267	0
0.583	100.000	1
-1.088	100.000	1
-0.996	100.000	0
-1.740	100.000	0
-1.619	100.000	0
-3.667	72.669	0
-2.631	94.613	0
-1.774	100.000	0
-1.164	100.000	0
-1.053	100.000	0
-2.611	94.978	0
-2.337	95.577	0
-2.555	90.274	0
-1.197	100.000	0
-2.376	95.056	0
-0.864	100.000	0
-1.068	100.000	0
-1.623	100.000	1
-1.033	100.000	0
-4.894	68.241	0
-0.971	100.000	0
-0.621	100.000	0
-4.202	86.427	0
-3.617	95.055	0
-1.594	100.000	0
-0.797	100.000	0
-6.616	25.900	0
-2.227	100.000	1
-7.119	24.752	0

-2.328	100.000	1
-2.622	100.000	1
-3.673	64.990	0
2.140	100.000	1
-0.692	100.000	2
-0.943	100.000	0
-2.972	91.217	0
-2.623	100.000	0
-4.280	69.168	0
-2.766	89.680	0
-1.702	100.000	0
-3.206	86.729	0
-4.440	68.889	0
-2.255	100.000	0
-2.359	100.000	0
-2.268	100.000	0
-2.186	100.000	1
-2.914	79.591	0
-1.939	100.000	0
-6.255	90.695	0
-1.638	100.000	1
-1.942	100.000	0
-1.525	100.000	1
-0.647	100.000	0
-2.612	100.000	1
-1.792	100.000	0
-3.499	69.764	0
-1.606	100.000	0
-2.070	100.000	0
-1.420	100.000	0
-2.695	100.000	0
-0.467	100.000	1
-3.250	71.215	0

-6.033	30.877	0
-0.847	100.000	1
-4.456	53.600	2
-6.873	57.186	0
-6.314	44.758	0
-2.084	100.000	0
-0.554	100.000	1
-2.061	100.000	0
-4.109	60.914	0
-5.393	41.742	0
-7.717	0.000	3
-1.261	100.000	0
-6.640	24.724	1
-4.546	52.120	0
-1.816	90.055	1
-2.752	87.191	1
-2.263	100.000	0
-3.182	81.820	0
-2.206	94.801	0
-1.952	100.000	0
-5.040	51.419	0
-2.073	100.000	1
-2.632	92.118	0
-4.023	79.684	1
-4.680	60.666	0
-7.465	0.000	3
-6.775	2.313	2
-5.660	64.500	0
-2.685	100.000	0
-4.321	54.237	0
-4.449	15.517	3
-2.009	100.000	1
-1.208	100.000	1

-1.750	100.000	0
-4.212	55.989	0
-1.387	100.000	2
-4.285	81.943	0
-2.888	100.000	0
-2.022	100.000	1
-6.395	8.018	2
-2.158	100.000	0
-4.243	77.333	0
-3.783	41.046	2
-2.272	89.251	0
-3.923	70.814	0
-1.794	100.000	0
-1.869	100.000	0
-2.135	100.000	0
-7.471	0.000	3
-1.927	100.000	0
-0.897	100.000	0
-3.876	82.085	0
-4.115	76.730	1
-6.097	2.933	3
-4.589	62.925	0
-3.926	76.518	0
-1.287	100.000	1
-0.893	100.000	0
-2.286	100.000	0
-5.743	47.524	0
-6.853	10.191	1
-7.106	0.000	3
-2.192	100.000	0
-2.089	100.000	0
-2.327	100.000	1
-4.554	56.696	0

-3.303	75.415	0
-5.563	0.000	3
-1.409	100.000	0
-3.543	77.731	1
-7.130	0.000	2
-3.959	65.353	0
-3.037	83.145	0
-1.413	86.686	2
-6.097	2.933	3
-1.666	100.000	0
-4.641	59.003	0
-2.912	89.746	0
-0.769	89.084	2
-4.471	86.973	0
-5.817	24.724	1
-3.644	74.502	0
-4.554	56.696	0
-2.109	100.000	0
-2.519	100.000	0
-5.246	43.556	0
-2.737	100.000	0
-0.247	100.000	1
-1.708	100.000	0
-0.901	100.000	1
-1.364	100.000	0
-1.510	100.000	0
-1.049	100.000	0
-1.201	100.000	1
-1.265	100.000	0
-1.269	100.000	0
-4.938	65.615	0
-6.914	0.000	3
-7.370	0.000	3

-13.925	0.000	3
-3.581	57.408	2
-1.706	100.000	0
-3.199	82.945	0
-5.226	41.727	0
-3.120	100.000	1
-6.500	0.000	2
-5.901	14.738	1
-4.077	84.659	0
-0.460	100.000	1
-1.808	100.000	0
-5.003	50.433	0
-2.920	87.739	0
-3.367	93.620	0
-5.513	0.000	3
-5.889	4.642	3
1.136	100.000	1
-6.776	17.927	1
-4.872	82.260	0
-5.187	40.675	0
-2.061	100.000	0
-2.166	100.000	0
-2.294	100.000	0
-4.288	54.935	0
-4.703	79.749	2
-3.189	81.719	0
-6.076	3.123	3
-1.540	100.000	0
-5.521	45.213	0
-3.045	88.449	0
-1.656	100.000	1
-5.572	53.952	0
-3.764	78.453	0

-2.006	100.000	0
-1.770	100.000	0
-3.163	100.000	0
-2.555	92.970	0
-5.529	69.169	2
-3.947	90.705	0
-4.761	50.336	0
-2.218	100.000	1
-7.108	24.786	0
-4.161	96.153	0
-4.425	65.528	1
-7.175	60.470	0
-1.273	100.000	0
-2.301	100.000	0
-3.144	100.000	1
-3.717	90.387	0
-7.489	0.000	3
-6.292	51.924	0
-6.909	30.210	0
-2.115	100.000	0
-5.638	27.136	1
-2.428	93.572	0
-4.008	96.102	0
-4.607	53.836	0
-3.580	68.467	0
-4.410	81.586	0
-4.533	55.801	0
-4.281	86.331	0
-2.169	89.276	1
-5.375	40.562	0
-4.991	89.947	1
-2.451	100.000	0
-5.962	89.834	0

-2.415	100.000	0
-4.440	80.825	0
-2.216	95.608	0
-2.179	100.000	0
-2.033	92.322	1
-3.354	81.791	0
-2.036	100.000	0
-0.579	100.000	1
-2.912	95.589	0
-13.433	0.000	3
-3.091	100.000	1
-7.774	0.000	3
-6.261	68.617	0
-1.977	100.000	0
-2.113	100.000	0
-4.992	58.902	0
-5.714	0.000	3
-1.747	100.000	1
0.353	100.000	2
-3.845	85.979	0
-4.427	68.380	0
-5.717	46.236	1
-2.668	73.223	3
-1.075	100.000	0
-1.873	100.000	0
-2.076	100.000	0
-4.591	66.779	0
-5.017	59.995	0
-1.374	100.000	1
-2.153	100.000	1
-3.711	96.723	0
-2.746	100.000	0
-3.743	80.197	0

-2.026	79.225	2
-1.406	100.000	0
-1.417	100.000	0
-4.243	32.892	2
-2.001	100.000	0
-5.001	79.621	2
-3.094	71.849	0
-1.951	100.000	0
-2.527	100.000	0
-1.874	100.000	0
-0.507	100.000	0
-4.717	60.702	0
-2.260	100.000	0
-0.459	100.000	0
-2.050	100.000	0
-3.842	74.606	0
-3.202	72.377	3
-1.559	100.000	1
-2.374	88.321	0
-3.653	92.654	0
-1.981	94.725	0
-4.977	44.857	0
-3.186	80.680	0
-4.583	53.379	0
-3.121	87.052	0
-2.054	100.000	0
-2.908	90.138	0
-5.964	32.197	0
-0.480	100.000	0
-4.566	71.038	0
-4.628	70.444	0
-3.832	83.736	0
-4.268	66.958	0

-9.949	0.000	3
-3.318	100.000	0
-2.577	94.462	1
-5.540	70.687	2
2.578	100.000	1
-4.344	78.483	0
-1.817	100.000	1
-1.178	100.000	0
-3.611	74.454	1
-5.778	49.624	0
-2.041	100.000	1
-7.114	0.000	3
-6.347	48.678	2
-7.404	0.619	2
-4.005	90.739	0
-4.099	100.000	0
-1.651	100.000	1
-1.495	100.000	1
-4.574	74.398	0
-1.552	100.000	0
-2.294	100.000	0
-1.912	100.000	0
-6.621	60.853	0
-1.215	100.000	1
-1.017	100.000	0
-3.437	73.932	0
4.527	100.000	1
-6.491	42.520	3
0.240	100.000	1
-2.322	100.000	1
-2.311	95.878	0
-4.546	48.338	2
-4.008	100.000	0

-1.871	100.000	0
-1.689	100.000	1
-1.350	100.000	0
-9.112	0.000	3
-3.923	100.000	0
-4.047	83.382	1
-4.122	83.614	1
-4.076	95.334	0
-5.026	68.862	2
-1.949	100.000	1
-6.113	80.326	0
-2.318	100.000	0
-3.528	93.588	0
-4.038	86.413	0
-4.188	75.312	0
-4.419	80.467	0
-4.856	60.266	1
-2.693	93.932	0
-1.058	100.000	1
-1.501	100.000	1
-3.335	74.689	0
-0.205	100.000	0
-2.015	90.062	0
-1.735	100.000	0
-3.391	100.000	0
-4.086	80.495	1
-1.665	100.000	0
-5.314	55.925	0
7.959	100.000	1
-4.426	88.749	0
-2.919	100.000	0
-2.657	100.000	1
-4.805	93.031	0

-2.073	100.000	1
-10.374	0.000	3
-3.105	100.000	0
-1.871	100.000	0
-2.668	92.754	0
-0.341	100.000	2
-1.465	100.000	0
-3.541	95.982	0
-3.337	83.709	0
-2.032	100.000	0
-5.868	20.370	1
-1.734	80.291	2
-2.601	86.781	0
0.234	100.000	0
-1.444	100.000	0
-5.563	52.926	0
-5.421	76.904	1
-1.918	100.000	0
-4.947	44.304	2
-4.628	74.331	2
-1.076	100.000	1
-0.724	100.000	1
-1.480	100.000	1
-1.636	100.000	1
-1.885	100.000	0
-2.041	100.000	0
-0.970	100.000	0
-3.367	87.935	0
-3.914	79.751	0
-0.868	100.000	1
-2.384	95.656	0
-3.621	87.163	0
-4.780	53.213	0

-4.480	57.545	0
-6.157	29.756	0
-1.638	100.000	0
-6.989	19.105	0
-7.094	0.000	3
-1.190	100.000	0
-6.397	46.630	0
-6.974	0.000	1
-7.409	0.000	3
-6.044	0.000	3
3.932	100.000	1
-4.727	52.024	0
-5.490	51.126	0
-2.050	100.000	0
-4.470	85.816	0
-4.523	85.710	0
-2.037	100.000	0
-1.696	100.000	0
-2.742	80.428	0
-6.674	29.805	0
-4.675	53.127	0
-3.058	85.027	0
-8.821	0.000	2
-4.480	83.998	0
-6.024	37.679	0
-4.909	62.194	0
-5.305	36.411	1
-1.265	100.000	1
-1.190	100.000	0
-4.260	82.483	0
-4.417	53.714	0
-1.425	100.000	0
-1.416	100.000	0

-5.660	64.500	0
-1.349	100.000	1
-5.117	47.074	0
-5.017	48.174	0
-3.553	100.000	0
-5.560	100.000	0
-4.315	74.321	0
-2.153	86.867	2
-3.821	62.785	0
-1.752	89.231	2
-3.992	100.000	0
-4.020	59.045	2
-4.630	48.819	2
-4.202	77.857	1
-4.157	84.307	0
-1.988	100.000	1
-4.733	57.275	1
-4.638	57.802	1
-3.042	100.000	1
-7.797	0.000	3
-7.855	0.000	3
-2.696	100.000	1
-5.868	6.494	3
-2.227	100.000	1
-5.573	8.019	3
-3.099	91.212	1
-9.465	0.000	3
-5.461	33.833	1
-3.918	95.449	0
-3.728	82.030	0
-1.909	100.000	1
-3.826	80.881	0
-5.385	63.317	0

-3.858	71.902	0
-3.720	78.671	0
-4.368	94.873	0
-5.612	92.752	0
-2.805	91.380	0
-4.909	27.288	2
-4.557	86.573	0
-2.967	100.000	0
-5.808	92.331	0
-1.411	100.000	0
-4.166	68.835	0
-4.312	84.453	0
-4.858	73.958	2
-1.302	100.000	0
-1.654	100.000	0
-1.366	100.000	1
-1.322	100.000	1
-0.688	100.000	1
-0.676	100.000	1
-1.224	100.000	1
-2.271	100.000	0
-1.420	100.000	0
-2.488	100.000	0
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-3.300	77.263	0
-6.500	0.000	3
-6.387	0.000	3
-6.739	0.000	3
-5.744	0.000	3
-1.414	100.000	0
-2.357	100.000	0
-2.107	100.000	0

-5.927	85.765	0
-3.764	86.389	0
-3.873	77.987	0
-8.813	0.000	3
-1.560	100.000	0
-13.263	0.000	3
-9.280	0.000	3
-8.292	0.000	3
-11.977	0.000	3
-3.134	93.973	0
-2.276	100.000	0
-1.113	100.000	0
-3.841	74.254	0
-3.971	72.383	0
-5.408	52.542	0
-1.397	100.000	1
-3.557	66.156	0
-5.136	3.174	3
-4.479	57.785	0
-4.408	80.689	0
-1.525	100.000	0
-3.059	84.972	0
-2.863	83.107	0
-7.963	0.000	3
-4.417	96.219	1
-6.323	79.744	0
-1.421	100.000	0
-1.123	100.000	0
-2.001	100.000	0
-2.003	100.000	0
-5.536	35.099	0
-6.202	9.560	1
-1.240	100.000	1

-1.804	100.000	0
-3.814	72.639	0
-1.201	100.000	0
-3.153	84.783	0
-4.498	74.754	0
-10.156	0.000	3
-9.734	0.000	3
-5.059	39.950	0
-2.547	79.431	0
-1.754	100.000	1
-1.423	95.191	1
-5.375	36.636	0
-2.901	82.321	0
-1.522	100.000	1
-2.070	87.854	1
-1.853	92.576	1
-4.128	51.668	0
-3.683	67.166	0
-4.549	41.981	0
-0.499	100.000	1
-4.041	88.539	0
-6.276	48.946	0
-4.467	54.485	0
1.584	100.000	2
-1.049	100.000	2
-6.230	32.053	0
-6.380	47.713	0
-4.836	75.645	1
-4.053	85.832	1
-4.742	75.667	1
-4.465	79.731	1
-1.251	100.000	0
-1.651	100.000	1

-1.520	100.000	0
-3.390	71.486	0
-1.473	100.000	0
-2.031	91.833	0
-1.522	100.000	0
-5.890	34.825	1
-1.455	100.000	0
-3.867	94.347	0
-2.370	100.000	0
-4.913	50.943	1
-4.165	76.627	0
-2.199	100.000	0
-3.545	73.233	1
-1.836	100.000	1
-4.883	54.153	1
-0.559	100.000	0
-7.692	9.070	0
-2.297	94.227	0
-1.658	100.000	0
-6.418	36.749	0
-3.412	100.000	1
-6.803	2.027	4
-7.178	0.000	3
-1.639	100.000	1
-5.357	62.611	0
-4.989	49.868	0
-3.117	85.908	0
-2.657	80.786	0
-2.193	93.383	0
-2.728	92.939	0
9.648	100.000	1
-1.629	100.000	0
2.905	100.000	1

-2.639	80.737	0
-2.034	100.000	0
-0.798	100.000	1
8.374	100.000	2
-0.413	100.000	2
-1.937	100.000	0
-1.435	100.000	0
-0.667	100.000	1
-1.446	100.000	0
-0.865	100.000	1
-1.153	100.000	1
-1.546	100.000	0
2.188	100.000	1
1.808	100.000	2
-2.669	91.554	0
-1.208	100.000	0
5.883	100.000	1
3.212	100.000	1
-2.800	85.041	0
-1.620	100.000	0
-1.472	100.000	0
-1.310	100.000	1
-1.386	100.000	1
-1.421	100.000	1
1.199	100.000	0
-2.029	100.000	0
-1.419	100.000	0
-1.511	100.000	1
-1.967	100.000	0
7.571	100.000	1
6.478	100.000	1
-0.960	100.000	0
-0.625	100.000	1

-0.147	100.000	1
19.945	100.000	2
-1.228	100.000	0
-1.039	100.000	0
-1.135	100.000	0
-1.840	100.000	0
-0.862	100.000	2
-1.395	100.000	1
-1.672	100.000	1
-0.943	100.000	0
-1.039	100.000	0
-1.520	100.000	0
-1.284	100.000	0
-0.887	100.000	1
-0.582	100.000	0
-1.609	100.000	0
-1.995	100.000	0
-1.606	100.000	0
-0.708	100.000	1
-1.306	100.000	0
-1.734	100.000	0
-0.295	100.000	1
-0.907	100.000	1
-2.096	100.000	0
-2.146	100.000	0
-2.330	100.000	0
-1.924	100.000	0
-2.013	100.000	0
-1.879	100.000	0
-0.303	100.000	2
-0.867	100.000	0
-1.045	100.000	0
-1.289	100.000	0

-2.355	84.002	0
-1.328	100.000	1
-0.876	100.000	1
-1.307	100.000	0
-0.622	100.000	0
-1.245	100.000	0
-1.297	100.000	0
-0.871	100.000	0
-0.758	100.000	0
-2.246	93.973	0
-2.318	100.000	0
-1.174	100.000	1
-0.582	100.000	0
-2.082	100.000	0
-0.950	100.000	0
-2.356	100.000	0
-1.581	100.000	0
-2.304	95.595	0
-2.581	100.000	0
-2.125	100.000	0
-3.122	77.318	0
-1.482	100.000	0
-3.936	66.226	2
-1.913	100.000	0
-2.103	100.000	0
-1.850	100.000	0
-2.068	100.000	0
4.431	100.000	1
-2.477	100.000	1
-1.647	100.000	1
-1.649	100.000	0
0.593	100.000	2
-1.727	100.000	1

-1.891	100.000	0
-3.430	83.824	1
2.316	100.000	1
-1.546	100.000	1
-1.208	100.000	1
-1.133	100.000	1
-1.768	100.000	0
-1.647	100.000	0
-3.353	82.589	1
-3.852	76.892	0
-4.686	74.969	0
-2.921	100.000	0
-3.972	96.061	0
-6.487	49.333	0
1.538	100.000	1
-1.863	95.117	0
-2.211	86.929	1
-1.248	100.000	1
-1.351	100.000	1
0.093	100.000	1
-7.536	23.040	2
-1.200	100.000	1
-0.234	100.000	0
-0.964	100.000	1
-0.817	100.000	1
-2.588	100.000	0
-2.449	100.000	0
-3.165	87.036	0
-2.656	100.000	0
0.785	100.000	1
5.420	100.000	1
-1.383	100.000	1
-1.921	100.000	0

3.569	100.000	2
-1.082	100.000	0
-2.042	100.000	0
-1.479	100.000	0
-4.523	61.710	0
-4.426	60.897	0
-3.781	64.104	0
-1.499	100.000	0
0.112	100.000	1
-1.262	100.000	1
-1.046	100.000	1
-0.382	100.000	1
0.102	100.000	1
-1.716	100.000	0
0.232	100.000	1
-1.963	100.000	0
-4.100	100.000	0
-4.235	95.249	0
-1.367	100.000	1
-3.839	94.551	0
-1.588	100.000	1
-1.020	100.000	0
-0.916	100.000	1
-5.751	100.000	0
-7.981	46.567	0
5.359	100.000	2
-1.197	100.000	1
-1.613	100.000	0
-0.846	100.000	0
-2.404	95.772	0
1.573	100.000	3
-1.788	100.000	0
-1.408	100.000	1

-1.487	100.000	0
-2.718	96.834	0
0.103	100.000	1
0.646	100.000	1
1.588	100.000	1
-1.403	100.000	1
-2.704	95.873	0
0.694	100.000	2
-1.663	100.000	0
-2.062	100.000	0
-2.682	80.672	0
-2.169	100.000	0
-1.233	100.000	0
-1.780	100.000	0
-1.267	100.000	1
-3.792	100.000	0
0.052	100.000	0
0.155	85.727	1
-1.208	100.000	1
-1.024	100.000	1
-1.957	100.000	0
-1.408	100.000	1
-1.443	100.000	0
-2.474	100.000	0
-1.967	100.000	0
-3.345	78.395	0
-2.823	95.059	0
-1.890	100.000	0
-0.423	100.000	1
-1.588	100.000	1
-1.896	100.000	0
-4.081	70.946	0
-3.861	62.951	0

-0.199	100.000	1
-2.689	96.831	0
-2.243	100.000	0
-2.718	80.280	0
-2.435	100.000	0
-2.026	100.000	0
-1.512	100.000	0
-3.004	81.822	0
-1.572	100.000	0
-4.037	58.290	0
-3.816	68.008	0
-1.145	100.000	1
-2.804	92.225	0
-2.239	100.000	0
-1.550	100.000	0
-0.479	100.000	1
-6.859	0.406	1
-0.615	100.000	1
-1.917	100.000	0
-1.296	100.000	0
0.858	100.000	1
-2.013	100.000	0
-1.508	100.000	0
-2.740	100.000	0
-2.544	95.165	0
-1.054	100.000	0
-3.587	100.000	0
-3.969	70.798	0
-3.383	100.000	0
-2.025	93.043	0
-1.520	100.000	0
-1.327	100.000	0
-2.535	83.676	0

0.200	100.000	0
-2.370	100.000	0
-2.542	100.000	0
-2.153	100.000	0
-2.281	100.000	0
-1.408	100.000	1
-2.174	100.000	0
-1.491	100.000	0
-3.344	73.999	0
-2.027	100.000	0
-3.941	76.193	0
-1.033	100.000	1
-2.188	100.000	0
-4.365	69.780	0
-1.338	100.000	0
-2.701	87.851	0
-1.306	100.000	0
-1.705	100.000	0
-0.565	100.000	0
-1.214	100.000	0
-3.143	83.424	0
-2.050	100.000	0
-2.827	89.776	0
-5.710	74.399	0
-1.320	100.000	0
-1.509	100.000	1
-2.050	100.000	0
-1.418	100.000	1
-1.965	100.000	0
-7.039	60.262	0
0.405	100.000	1
-1.894	100.000	0
-1.726	100.000	0

-1.088	100.000	1
-2.398	100.000	1
-2.274	100.000	0
-3.504	78.342	0
-1.438	100.000	0
-1.799	100.000	0
-0.372	100.000	0
-0.640	100.000	0
-2.809	100.000	0
-0.707	100.000	0
-2.270	100.000	0
-1.317	100.000	1
-2.635	100.000	1
-1.032	100.000	0
-2.672	100.000	0
-3.497	85.469	0
-2.401	95.482	0
-0.796	100.000	0
-1.388	100.000	0
-1.887	100.000	0
-2.942	100.000	0
-2.368	90.446	0
-2.944	87.624	0
-1.004	100.000	1
-3.774	86.306	0
-2.215	100.000	0
-4.001	95.004	0
-1.169	100.000	0
-3.896	100.000	0
-1.497	100.000	1
-1.377	100.000	0
-4.832	66.121	0
-2.854	100.000	0

-5.565	42.615	2
-0.885	100.000	0
-2.826	85.262	0
-3.781	89.262	2
-3.450	72.489	0
-2.924	100.000	0
-3.303	95.527	0
-1.994	95.057	0
-1.165	100.000	1
-1.282	100.000	0
-1.661	100.000	0
-1.896	100.000	0
-3.406	69.196	0
-3.607	67.396	0
-0.718	100.000	0
-2.010	100.000	0
-1.485	100.000	0
-3.754	68.255	0
-0.814	100.000	0
-1.876	100.000	0
-2.162	100.000	0
-2.565	100.000	0
-2.119	100.000	0
-1.140	100.000	0
-1.706	100.000	1
0.095	100.000	1
0.273	100.000	0
-2.561	90.723	0
-3.325	77.719	0
-1.898	100.000	1
-2.380	100.000	0
-2.938	100.000	0
-2.091	96.136	0

0.075	100.000	0
-1.885	100.000	0
-4.717	89.416	0
-2.166	92.483	0
-2.451	96.259	0
-6.347	16.727	0
-2.478	100.000	0
-4.906	43.255	0
-1.198	100.000	1
-1.990	100.000	0
-8.524	0.000	3
-5.848	0.000	2
-2.109	100.000	0
-1.998	100.000	0
-3.800	70.161	0
-2.464	100.000	0
-2.525	90.853	0
-2.236	94.931	0
-4.506	54.229	0
-2.874	84.035	0
-1.366	100.000	0
-0.358	100.000	0
-0.660	100.000	0
-1.755	100.000	0
-4.309	56.538	0
-2.127	96.491	0
-2.723	100.000	0
-3.007	82.392	0
-2.169	100.000	0
-2.081	100.000	0
-5.703	78.384	0
-2.277	100.000	0
-1.928	100.000	0

-4.439	76.828	0
-5.788	45.837	0
-1.848	100.000	0
-1.992	100.000	0
-2.199	100.000	0
-1.769	100.000	0
-0.827	100.000	0
-2.486	88.904	0
-1.712	100.000	0
-1.833	100.000	0
-1.466	100.000	0
-2.566	96.445	0
-1.374	100.000	0
-1.219	100.000	0
-0.645	100.000	0
-1.437	100.000	0
-5.783	21.570	1
-6.186	16.882	1
-6.186	16.876	1
-1.449	100.000	0
-1.343	100.000	0
-4.815	52.901	0
-3.803	66.644	0
-3.663	73.556	0
-1.854	100.000	0
-6.324	32.689	0
-1.508	100.000	0
-1.397	100.000	0
-3.823	71.997	0
-3.903	82.077	0
-1.599	100.000	0
-12.936	0.000	3
-1.991	100.000	0

-2.600	84.372	0
-3.765	64.901	0
-1.798	93.623	1
-3.660	79.906	0
-1.067	100.000	1
-2.868	94.601	0
-3.491	100.000	0
-1.393	100.000	1
-2.270	100.000	1
-6.671	0.000	2
-6.966	0.000	1
-4.252	91.561	0
-1.584	100.000	0
-2.867	92.130	0
-3.811	93.321	0
-1.350	100.000	0
-2.886	87.211	0
-6.089	26.176	1
-1.411	100.000	0
-2.540	96.831	0
-2.934	100.000	1
-0.332	100.000	1
-2.320	100.000	1
-1.980	93.661	1
-1.812	91.923	0
-2.829	93.688	0
-1.207	100.000	0
-3.326	72.271	0
-1.900	100.000	0
-1.841	100.000	0
-5.695	26.830	1
-1.814	100.000	0
-2.148	100.000	0

-4.300	62.553	0
-3.943	67.617	0
-7.359	0.000	3
-5.656	34.031	0
-6.126	77.572	0
-7.756	36.305	0
-2.275	100.000	0
-1.963	93.230	0
-6.347	28.395	0
-0.645	100.000	1
-2.206	100.000	0
0.759	100.000	2
-3.796	93.261	0
-10.532	0.000	3
-5.084	41.758	0
-2.490	100.000	0
-5.322	36.004	0
-0.912	100.000	0
-1.620	100.000	0
-1.179	100.000	0
-3.464	73.029	0
-7.556	0.000	3
-3.845	93.536	0
-6.639	75.234	0
-2.644	77.249	0
-4.235	76.847	0
-2.864	92.735	0
-4.710	62.975	1
-3.918	71.094	0
-7.436	0.000	2
-5.137	72.013	2
-4.111	78.612	0
-2.154	100.000	1

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-5.544	51.649	0
-2.635	85.096	0
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-1.883	100.000	0
-5.002	49.243	0
-1.201	100.000	1
-6.138	24.720	1
-3.027	87.478	0
-4.888	61.205	0
-2.918	84.563	0
-2.027	87.538	1
-2.603	100.000	1
-6.056	12.984	2
-3.065	82.085	0
-4.201	56.329	1
0.788	100.000	2
-2.553	89.123	0
-4.600	47.669	0
-3.128	81.559	0
-5.454	52.736	0
-1.047	100.000	1
-6.218	16.641	1
-6.368	6.661	2
-6.209	29.335	1
-4.753	30.641	2
-4.065	74.191	0
-5.565	30.057	1
-6.228	0.000	3
-4.368	57.873	0
0.875	100.000	2
-1.747	100.000	1

-6.758	0.000	2
-7.479	0.000	3
-3.166	72.158	0
-4.641	63.637	0
-4.222	70.234	0
-0.895	100.000	2
-1.685	92.404	1
-2.093	87.353	1
-3.197	72.099	3
-3.874	72.271	0
-3.566	76.401	0
-1.481	100.000	0
-1.483	100.000	1
-2.388	94.879	0
-1.436	100.000	1
-1.814	93.001	1
-1.902	100.000	0
-1.710	100.000	0
-2.111	96.949	0
-2.723	91.227	0
-6.528	24.074	0
-0.897	100.000	2
-2.339	91.050	2
0.715	100.000	2
-3.484	69.855	0
-0.011	100.000	2
-0.055	100.000	2
-0.052	100.000	2
-0.881	100.000	2
-1.030	100.000	2
1.050	100.000	2
-2.539	94.862	0
-3.535	51.700	2

-4.995	40.009	2
-4.502	65.393	1
-4.288	67.712	1
-1.843	100.000	1
-1.724	100.000	1
-1.779	100.000	1
-3.388	77.136	0
-1.406	100.000	1
-5.229	32.330	1
-1.221	100.000	0
-3.891	69.563	0
-5.526	40.454	0
-2.991	81.115	0
-1.406	100.000	1
-0.676	100.000	1
-0.497	100.000	1
-1.436	100.000	0
-1.403	100.000	1
-1.395	100.000	1
-1.902	100.000	0
-1.957	100.000	0
-0.998	100.000	0
-4.129	70.463	0
-3.699	87.683	0
-5.973	27.809	2
-6.236	25.182	2
-2.065	100.000	0
-4.322	69.826	0
-3.625	76.784	0
-3.921	70.812	0
-4.059	74.255	0
-6.363	0.000	3
-4.823	58.881	0

-3.582	77.220	0
-3.023	87.496	0
-4.650	64.850	0
-3.654	78.006	0
-5.585	51.260	0
-6.668	0.838	2
-3.688	82.228	0
-7.056	0.000	2
-2.751	92.023	0
-4.722	64.655	0
-2.781	91.757	0
-3.561	80.147	0
-5.435	52.750	0
-3.384	95.403	0
-6.439	26.816	1
-6.956	1.203	2
-7.027	0.000	2
-5.143	57.196	0
-6.173	29.500	1
-4.582	65.908	0
-5.718	47.056	0
-7.473	0.000	3
-4.133	75.256	0
-2.855	88.684	0
-3.450	77.070	0
-2.846	83.524	0
-10.448	0.000	3
-2.536	100.000	0
-3.757	70.466	0
-4.458	39.858	1
-2.113	100.000	0
-0.980	100.000	0
-0.905	100.000	0

-7.542	0.000	2
-5.301	41.535	0
-2.474	95.846	0
-2.765	87.259	0
-6.763	0.000	3
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-1.561	100.000	0
-3.430	83.501	0
-5.703	38.342	0
-6.233	17.670	1
-1.914	100.000	0
-2.605	90.609	0
-2.025	94.533	0
-3.198	88.807	0
-5.513	29.490	1
-2.733	100.000	0
-5.070	22.162	2
-3.227	81.116	0
-2.781	85.843	0
-4.268	67.911	0
-2.789	72.826	2
-1.638	100.000	1
-6.701	35.438	0
-2.063	90.136	1
-3.858	75.272	0
-5.202	71.644	0
-4.787	65.703	0
-3.260	80.953	0
-4.313	65.927	0
-5.642	14.198	2
-2.122	100.000	0
-6.537	0.000	3
-6.956	0.000	3

-8.044	0.000	3
-7.021	0.000	2
-0.728	100.000	1
-1.054	100.000	2
-1.010	100.000	1
-2.081	90.635	1
-1.810	91.897	1
-2.322	85.587	1
-2.107	88.493	1
-1.998	91.528	1
-1.850	92.786	1
-1.262	100.000	1
-1.811	95.967	1
-2.151	87.873	1
-1.910	94.933	1
-2.566	91.682	0
-1.036	100.000	0
-1.744	100.000	0
-2.627	91.992	0
-2.504	93.881	0
-2.527	91.717	0
-2.454	96.137	0
-2.358	100.000	0
-2.337	100.000	0
-2.344	100.000	0
-2.240	100.000	0
-2.251	100.000	0
-2.147	100.000	0
-2.051	100.000	0
-1.974	100.000	0
-2.166	100.000	0
-1.747	100.000	1
-1.734	100.000	1

-1.825	100.000	1
-1.683	100.000	1
-1.780	100.000	1
-3.807	86.395	0
-0.613	100.000	1
-0.968	100.000	1
-2.027	100.000	0
-1.101	100.000	0
-0.858	100.000	1
-1.225	100.000	0
-3.455	90.504	0
-4.720	75.983	0
-13.589	0.000	3
-2.068	88.142	1
-2.101	88.943	1
-2.023	90.924	1
-1.797	91.734	1
-2.046	89.552	1
-1.844	91.627	1
-1.833	92.354	1
-2.718	89.746	0
-2.718	79.099	0
-4.093	74.794	0
-1.062	100.000	1
-1.562	100.000	0
-1.352	100.000	0
-3.667	78.177	0
-1.143	100.000	1
-3.353	76.351	2
-1.248	100.000	1
-3.025	79.561	2
-2.358	100.000	0
-5.373	35.552	1

-3.672	80.533	0
-3.183	82.104	0
-2.474	100.000	0
-4.158	59.820	0
-0.471	100.000	0
-2.751	90.537	0
-1.565	100.000	0
-5.618	0.000	3
-2.463	94.426	0
-3.426	79.075	0
-1.793	100.000	0
-4.551	66.072	0
-3.568	82.218	0
-0.521	100.000	1
-4.401	61.765	0
-1.315	100.000	0
-1.343	100.000	0
-1.261	100.000	1
-1.195	100.000	0
-2.453	93.928	0
-3.582	79.230	0
-2.916	84.557	0
-1.314	100.000	1
-2.132	100.000	0
-4.933	52.004	1
2.723	100.000	1
-3.837	59.005	2
-3.708	66.361	0
-2.061	100.000	0
-1.327	100.000	0
-3.882	78.435	0
-0.874	100.000	0
-2.878	85.456	0

-4.679	63.637	1
-7.032	0.000	2
-1.940	100.000	0
-5.718	14.332	2
-2.976	83.491	0
-1.725	100.000	0
-6.621	0.000	2
-6.138	0.000	3
-1.920	100.000	0
-2.791	91.190	0
-2.035	100.000	0
-2.164	100.000	0
-7.341	5.298	1
-6.596	4.195	2
-2.919	84.559	0
-5.108	35.285	1
-0.149	100.000	1
-0.975	100.000	1
-1.094	100.000	1
-1.060	100.000	1
-2.684	92.594	0
-1.135	100.000	0
-1.042	100.000	0
-3.506	83.484	1
-2.037	100.000	0
-3.399	93.194	0
-2.774	100.000	0
-4.094	60.998	1
-5.058	32.849	1
-1.888	100.000	0
-0.955	100.000	0
-2.594	91.548	0
-2.479	93.905	0

-6.828	35.023	0
-2.201	100.000	0
-3.307	91.556	0
-3.523	89.443	0
-3.978	79.192	0
-1.345	100.000	0
-1.118	100.000	0
-1.069	100.000	0
-11.476	0.000	3
-8.173	0.000	3
-7.972	0.000	3
-6.468	7.152	2
-3.755	78.897	0
-7.209	0.000	2
-2.148	100.000	0
-2.342	100.000	0
-6.131	9.793	2
-1.492	100.000	0
-4.247	70.780	0
-2.361	100.000	0
-2.783	88.054	0
-3.170	81.838	0
-3.167	88.739	0
-2.624	94.088	0
-3.653	68.519	0
-3.025	68.466	1
-3.744	78.494	0
1.322	100.000	2
-2.984	100.000	0
-2.503	100.000	0
-1.794	100.000	0
-4.131	85.117	0
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-4.185	75.782	1
-2.248	100.000	1
-6.668	4.475	2
-1.910	100.000	0
-1.303	100.000	0
-0.357	100.000	1
-1.931	100.000	0
-0.310	100.000	1
-1.052	100.000	1
-1.841	100.000	0
-0.712	100.000	0
-1.655	100.000	0
-2.339	100.000	0
-1.071	100.000	1
-1.175	100.000	0
-0.980	100.000	0
-2.851	95.025	0
-1.992	100.000	0
-1.055	100.000	0
-0.300	100.000	1
-1.364	100.000	0
-2.241	100.000	0
-2.135	100.000	0
-2.538	90.234	0
-2.047	100.000	0
-1.801	100.000	0
-1.430	100.000	0
-2.340	94.682	0
-2.194	100.000	0
-2.122	100.000	0
-0.779	100.000	1
-1.172	100.000	1
-2.253	100.000	0

-0.851	100.000	0
-1.207	100.000	1
-1.709	100.000	0
-1.873	100.000	0
-0.194	100.000	1
-0.662	100.000	1
-2.126	100.000	0
-1.153	100.000	0
-0.770	100.000	1
-2.757	91.910	0
-2.364	100.000	0
-2.825	95.005	0
-1.864	100.000	0
-1.464	100.000	1
-1.617	100.000	1
-2.327	100.000	0
-2.783	88.643	0
-2.684	96.834	0
-2.744	100.000	0
-1.884	100.000	1
-1.947	100.000	0
-2.007	100.000	0
-2.393	96.566	0
-0.102	100.000	1
-1.161	100.000	1
-0.465	100.000	1
-0.598	100.000	1
-0.728	100.000	1
-0.513	100.000	1
-0.964	100.000	1
-1.392	100.000	1
-1.175	100.000	1
-0.950	100.000	1

-1.026	100.000	1
-0.125	100.000	1
-0.122	100.000	1
-1.819	100.000	0
0.932	100.000	2
-1.627	100.000	1
-1.366	100.000	1
-1.280	100.000	1
-2.194	100.000	0
-1.967	93.563	1
-2.189	94.161	0
-1.844	100.000	0
-1.748	100.000	0
-1.460	100.000	0
-1.501	100.000	0
1.500	100.000	1
-1.762	100.000	1
-0.641	100.000	1
0.354	100.000	1
-1.726	100.000	0
-1.058	100.000	0
-0.010	100.000	1
-1.108	100.000	1
-0.828	100.000	1
-0.998	100.000	1
-0.614	100.000	1
-1.960	100.000	0
-1.207	100.000	1
-1.046	100.000	1
-1.875	100.000	0
-1.401	100.000	0
-1.251	100.000	0
-2.268	100.000	0

-1.954	100.000	0
-0.877	100.000	1
1.124	100.000	2
-0.378	100.000	1
-2.110	100.000	0
-1.681	100.000	0
-2.994	85.912	0
0.784	100.000	2
-0.124	100.000	1
-0.198	100.000	1
0.011	100.000	1
-1.110	100.000	0
-1.437	100.000	0
-0.705	100.000	1
-0.774	100.000	1
-1.201	100.000	1
1.948	100.000	2
-0.355	100.000	1
-1.261	100.000	0
-0.126	100.000	1
-2.391	100.000	0
-0.910	100.000	1
-1.335	100.000	0
-1.135	100.000	1
-1.034	100.000	1
-1.100	100.000	1
0.019	100.000	1
-2.518	100.000	0
-1.853	100.000	0
-1.322	100.000	0
-1.979	100.000	0
-1.807	100.000	0
-1.417	100.000	1

-1.499	100.000	0
-1.031	100.000	0
-1.205	100.000	0
-2.553	100.000	0
-2.062	100.000	0
-1.174	100.000	0
-1.706	100.000	1
-1.410	100.000	0
-1.035	100.000	0
-0.719	100.000	1
-0.929	100.000	0
-2.279	100.000	0
-1.899	100.000	0
-1.905	100.000	2
-1.287	100.000	1
-1.929	96.191	0
-1.826	100.000	1
0.354	100.000	1
-3.737	70.641	2
-4.242	69.127	0
-5.906	26.951	1
-1.865	100.000	0
-1.548	100.000	0
-1.745	100.000	1
-11.044	0.000	3
-4.407	85.617	0
-2.661	84.613	0
-3.481	100.000	0
-2.869	91.229	1
-2.218	100.000	1
-5.285	53.150	0
-2.323	90.893	0
-3.235	60.605	1

-2.878	92.271	0
-3.444	96.697	0
-4.937	56.520	1
-4.106	87.729	0
-4.300	86.925	0
-4.307	56.958	0
-5.317	37.801	0
-1.042	76.099	3
-3.918	87.390	0
-3.794	88.834	0
-1.058	100.000	0
-0.812	100.000	0
-1.401	94.245	1
-2.313	100.000	0
-0.834	100.000	1
-1.410	100.000	0
-5.940	79.815	0
-6.103	10.937	2
-3.176	88.172	0
-6.143	0.000	3
-3.593	84.288	0
-3.863	87.714	0
-3.769	81.164	0
-3.705	88.557	0
-2.558	100.000	0
-4.787	62.210	0
-1.911	100.000	1
-6.479	0.000	3
-4.283	90.011	0
-3.199	87.657	0
-8.388	0.000	2
-6.836	0.000	3
-3.675	79.941	0

-4.637	63.690	0
-4.550	66.978	0
-5.230	53.854	0
-2.717	100.000	1
-5.269	0.000	3
-5.702	28.687	1
-7.364	0.000	2
-2.378	100.000	0
-0.887	100.000	0
-7.525	0.000	3
-7.645	0.000	3
-6.602	0.000	3
-3.075	100.000	0
-4.080	61.298	3
-3.409	88.322	0
-3.277	74.313	2
-1.823	100.000	1
-0.178	100.000	2
-0.857	100.000	1
-5.163	38.013	1
-6.353	71.814	0
-6.380	22.460	0
-1.247	100.000	0
-1.923	100.000	0
-1.602	100.000	1
-5.091	49.917	0
-6.314	72.360	0
-1.636	100.000	0
-3.819	68.304	0
0.759	100.000	2
-1.206	100.000	1
-1.163	80.881	1
-1.063	100.000	1

-5.350	81.271	0
-1.905	100.000	0
-1.835	91.178	1
-1.057	100.000	1
-0.769	100.000	1
-0.787	100.000	0
-4.251	88.986	0
-1.095	100.000	0
-2.479	100.000	0
-2.151	100.000	0
-1.260	100.000	1
-2.301	100.000	0
-2.023	100.000	0
-0.862	100.000	1
-1.569	100.000	1
-1.327	100.000	0
-1.083	100.000	1
-1.077	100.000	0
-1.734	100.000	0
-2.058	100.000	0
2.292	100.000	1
-1.064	100.000	1
-5.349	65.220	1
-2.037	100.000	0
-2.015	100.000	0
-2.234	100.000	0
-1.391	100.000	0
-1.737	100.000	0
-2.237	100.000	0
-2.225	100.000	0
-2.368	100.000	0
-1.159	100.000	0
-0.995	100.000	0

-1.176	100.000	1
-2.411	100.000	0
-2.028	100.000	0
-2.242	100.000	0
-2.479	100.000	0
-1.935	100.000	0
-1.773	100.000	0
-1.935	100.000	0
-1.612	100.000	0
-1.401	100.000	0
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-1.560	100.000	0
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-2.298	100.000	0
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-4.842	73.751	0
-1.152	100.000	1
-2.053	100.000	0
-1.560	100.000	0
-1.946	100.000	0
-1.128	100.000	1
-1.242	100.000	0
-1.403	100.000	1
-1.087	100.000	1
-1.092	100.000	1
-1.082	100.000	0
-1.086	100.000	0
-1.936	100.000	0
-1.805	100.000	0
-0.971	100.000	1
-1.899	100.000	0
-1.601	100.000	0
-2.152	86.738	1

-1.744	100.000	1
-1.113	100.000	1
-1.883	100.000	0
-1.293	100.000	0
-2.034	100.000	1
-2.683	96.161	0
-2.530	100.000	0
-1.678	100.000	0
-1.262	100.000	1
-1.128	100.000	1
-1.261	100.000	1
-2.245	100.000	0
-2.164	100.000	0
-1.395	100.000	1
-1.556	100.000	1
-1.735	100.000	1
0.956	100.000	0
-2.157	64.105	0
-6.050	18.162	1
-3.488	100.000	0
-5.790	83.417	0
-9.138	6.498	0
-1.998	100.000	0
1.085	100.000	2
-0.699	100.000	1
-2.174	100.000	1
-1.680	100.000	1
-4.778	46.727	0
-4.139	82.244	0
-1.853	92.576	1
-1.856	94.027	1
-0.715	100.000	0
-2.043	95.679	2

-7.115	0.000	3
-4.565	41.161	3
-2.257	90.638	2
-2.359	89.262	2
-3.983	40.251	1
-2.666	100.000	0
-5.658	15.047	3
-1.559	100.000	0
-2.352	100.000	0
-1.887	100.000	1
-1.853	92.576	1
-2.759	91.164	0
-1.849	100.000	2
-2.124	93.117	2
-1.913	90.918	2
-1.733	86.928	1
-1.630	100.000	1
-3.565	85.330	0
-2.118	100.000	0
-2.492	93.357	0
-1.826	100.000	0
-3.074	89.781	0
-3.086	85.538	1
-8.319	0.000	3
-2.142	100.000	0
-2.420	100.000	0
-0.294	100.000	0
-1.941	100.000	1
-3.658	94.396	0
-4.241	93.712	0
-4.958	49.128	0
-1.879	100.000	0
-1.845	100.000	1

-5.496	32.609	1
-5.360	32.705	0
-1.853	92.576	1
-4.932	85.516	0
-3.738	75.896	0
-6.968	0.000	3
-6.646	0.000	3
-6.481	0.000	3
-2.248	100.000	1
-2.686	85.913	0
-4.924	58.802	0
-1.762	100.000	0
-0.690	100.000	0
-1.962	100.000	1
-0.111	100.000	1
-1.429	100.000	1
-1.650	100.000	0
-8.432	0.000	3
-2.673	95.212	0
-4.896	49.576	0
-3.259	74.719	2
-1.446	100.000	0
-2.142	100.000	1
-3.367	76.875	2
-2.209	100.000	0
-2.143	100.000	0
-11.058	0.000	3
-0.917	100.000	1
-3.567	100.000	0
-1.739	100.000	0
-6.346	20.315	0
-3.243	81.367	0
-0.937	100.000	1

-1.996	91.461	0
-3.135	82.682	0
-0.586	100.000	0
-4.331	90.569	0
-3.595	96.646	0
-3.523	80.202	0
-3.113	73.795	1
-1.624	100.000	1
2.228	100.000	1
2.516	100.000	1
2.480	100.000	1
-1.258	100.000	1
2.532	100.000	1
7.032	100.000	1
-1.045	100.000	0
-1.195	100.000	0
-5.613	43.120	0
-6.049	18.358	1
-4.337	50.483	2
-4.107	59.993	0
-3.659	77.717	0
-1.028	100.000	1
-4.232	35.251	1
-1.629	100.000	1
-2.225	91.491	2
0.761	100.000	2
-7.057	24.549	0
-2.486	100.000	1
-4.064	71.623	0
-6.022	0.000	3
-1.206	100.000	1
-3.408	82.587	0
-0.833	100.000	1

-1.449	100.000	2
-7.230	0.000	3
-4.330	52.178	2
-9.304	0.000	3
-6.282	10.384	2
-3.175	94.692	1
-3.548	96.881	0
-8.200	0.000	3
-1.573	100.000	2
-2.399	100.000	1
-1.027	100.000	1
-4.294	62.181	0
-5.939	0.000	3
-5.321	41.336	0
-1.465	100.000	0
-2.110	93.345	2
-1.728	88.928	2
-3.739	79.022	0
-0.980	100.000	0
-0.995	100.000	1
-2.785	87.092	0
-2.953	93.470	0
-5.301	80.229	0
-7.050	0.000	3
-1.492	90.855	2
-2.857	93.441	0
-4.297	83.231	0
0.677	100.000	2
-7.682	0.000	2
-4.241	37.705	2
-12.611	0.000	3
-2.484	94.604	0
-6.600	5.252	3

-2.019	100.000	0
-1.078	100.000	0
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-1.936	100.000	1
-6.135	8.705	2
-5.247	25.607	2
-5.366	9.512	3
-5.437	35.921	2
-0.870	100.000	1
-8.037	0.000	3
-5.391	42.215	0
-6.002	16.962	1
-2.794	95.603	0
-5.311	42.989	0
-9.023	0.000	3
-6.128	27.465	0
-8.263	0.000	3
-1.496	100.000	0
-1.881	100.000	0
-1.691	100.000	0
-5.938	12.129	2
0.792	100.000	2
-1.247	100.000	2
-1.462	100.000	0
-3.177	57.439	2
-2.797	91.497	0
-3.732	74.166	0
-4.751	49.409	0
-3.522	53.469	1
-7.112	0.000	3
-3.294	51.877	2
-2.199	93.722	0
-1.935	100.000	0

-2.017	100.000	0
-10.646	0.000	3
-6.962	0.000	3
-7.672	0.000	3
-5.016	46.318	0
-3.666	72.435	0
-7.530	0.000	3
-1.408	100.000	1
-4.901	24.842	2
-4.757	39.508	1
-5.305	0.000	3
-2.117	100.000	0
-0.760	100.000	1
-2.786	92.076	0
-1.500	100.000	0
-3.709	100.000	0
-2.069	64.330	2
-2.641	100.000	0
-3.640	44.480	2
-5.372	18.347	3
-3.019	100.000	0
-4.458	50.588	1
-2.451	78.785	2
-0.053	100.000	0
-5.329	52.890	0
-0.485	100.000	0
-4.048	85.591	0
-4.333	47.448	2
-2.977	86.376	2
-3.790	89.856	1
-8.153	0.000	3
-5.846	17.941	2
-3.824	42.194	2

-3.283	71.368	0
-2.403	100.000	1
-1.455	100.000	0
-4.580	77.703	1
-2.756	100.000	0
-3.897	84.301	0
-5.838	16.250	3
-6.207	0.000	3
-6.135	11.955	3
-7.018	0.000	3
-6.630	1.292	2
-4.649	52.839	1
-6.289	0.000	3
-6.651	0.000	3
-3.437	87.505	0
-4.652	83.078	0
-2.866	92.226	0
-1.215	100.000	1
-0.314	100.000	1
-7.900	0.000	3
-11.300	0.000	3
-1.094	100.000	1
-2.391	100.000	0
-1.736	41.268	4
-4.242	58.359	0
-1.499	100.000	1
-5.101	50.414	0
-2.772	89.861	0
-8.570	0.000	3
-1.424	100.000	0
-10.364	0.000	3
-1.981	100.000	0
-1.034	100.000	1

-2.022	91.146	0
-1.855	100.000	0
-4.451	57.890	0
-2.475	96.500	0
-3.813	96.546	0
-4.493	30.883	2
-2.672	94.614	0
-1.092	100.000	1
-2.401	100.000	0
-3.222	82.799	0
-0.949	100.000	0
-1.100	100.000	1
-5.908	48.704	0
-3.669	93.028	0
-4.733	60.557	0
-3.508	89.690	0
1.011	100.000	2
-6.835	0.000	2
-3.760	71.538	1
-5.682	26.289	1
-2.559	100.000	0
-1.670	100.000	0
-2.003	100.000	0
-1.870	100.000	0
-1.057	100.000	0
-14.149	0.000	3
-1.410	100.000	1
-0.602	100.000	1
-5.200	61.129	0
-1.094	100.000	1
-1.422	100.000	0
-2.166	100.000	1
-2.019	83.900	2

-2.317	100.000	0
-9.333	0.000	3
-2.391	91.542	0
-2.425	100.000	0
-1.536	100.000	0
-2.486	94.352	0
-2.091	100.000	0
-3.194	85.465	0
-2.887	92.616	0
-0.438	100.000	0
-1.101	100.000	0
-0.238	100.000	0
-7.178	0.000	3
-7.630	0.000	3
-4.428	87.735	0
-0.488	100.000	1
-1.819	100.000	0
-3.309	55.654	2
-3.485	94.524	0
-1.144	100.000	1
-3.263	89.882	0
-2.253	96.279	1
-0.475	100.000	0
-3.517	79.874	0
-2.296	100.000	0
-1.924	100.000	0
-2.793	100.000	0
-1.897	90.674	0
-2.818	90.846	1
-0.412	100.000	0
-4.817	62.627	0
-3.142	54.188	2
-4.847	41.260	0

-5.622	19.456	2
-5.131	42.868	1
-4.415	67.169	0
-5.599	52.421	1
-4.556	44.507	0
-5.848	0.000	3
-1.463	100.000	1
-7.035	0.000	3
-6.370	3.505	2
-2.160	96.529	2
-5.544	0.000	3
-5.026	45.387	0
-5.438	12.903	2
-2.890	93.388	0
-5.190	16.096	2
-6.171	0.000	3
-2.684	100.000	0
-5.537	80.317	0
-4.044	83.974	1
-5.710	0.000	3
-3.326	86.764	0
-6.740	0.000	2
-1.621	100.000	0
-2.951	100.000	0
-0.562	100.000	0
-3.103	90.173	0
-2.100	100.000	0
-3.316	52.211	2
-2.786	90.848	0
-6.665	9.746	1
-2.127	100.000	0
-3.963	78.504	1
-1.377	100.000	1

-5.340	67.960	0
-1.942	100.000	0
-5.053	2.708	3
-4.386	8.047	3
-1.933	100.000	1
-4.491	54.387	0
-1.649	100.000	0
-2.022	100.000	0
-2.061	100.000	0
-4.506	70.198	1
-3.798	77.945	0
-5.888	0.000	3
-4.893	4.484	3
-4.823	63.891	0
-3.124	92.931	0
-7.742	0.000	2
-3.451	100.000	0
-2.984	100.000	0
-1.898	100.000	0
0.194	100.000	1
-1.777	100.000	0
-0.275	100.000	0
-3.330	76.517	0
-3.349	100.000	0
-2.052	91.749	1
-2.678	91.188	0
-3.260	82.039	0
-1.948	100.000	0
-1.790	100.000	0
-5.323	80.611	0
-1.360	100.000	2
-1.083	100.000	1
-1.347	100.000	0

-1.499	100.000	1
-1.642	100.000	1
-1.799	100.000	0
-1.042	100.000	1
-5.965	89.443	0
-2.997	100.000	1
-1.650	100.000	1
-6.922	80.477	0
-5.959	96.180	0
-1.322	100.000	1
-1.964	100.000	0
-1.679	100.000	0
-3.042	100.000	1
-2.328	100.000	1
-2.862	95.224	0
-1.188	100.000	0
-2.973	92.609	0
-6.281	7.470	2
-1.439	100.000	0
-1.981	100.000	0
-2.072	100.000	0
-1.906	100.000	1
-1.978	100.000	1
-4.020	96.181	0
-4.025	85.178	0
-1.816	100.000	1
-2.052	100.000	0
-5.710	31.314	1
-4.823	51.816	0
-1.256	100.000	1
-1.258	100.000	1
-1.281	100.000	1
-1.354	100.000	1

-6.122	77.806	0
-2.333	100.000	0
-3.825	76.498	0
-1.282	100.000	1
-1.396	100.000	1
-1.312	100.000	0
-3.043	77.182	2
-6.225	8.383	2
-0.997	100.000	1
-3.099	100.000	0
-1.235	100.000	1
-2.426	100.000	0
-5.989	19.247	1
-2.215	100.000	0
-4.163	73.002	0
-1.412	100.000	0
-1.262	100.000	1
-3.844	95.251	0
-4.528	65.169	0
-4.620	75.704	0
-4.762	42.604	2
-5.125	78.295	0
-1.948	100.000	0
-1.692	100.000	1
-1.881	100.000	1
-1.609	88.684	2
-2.627	100.000	0
-2.500	100.000	0
-4.040	93.746	0
-4.444	61.956	1
-0.968	100.000	0
-1.211	100.000	1
-2.155	100.000	0

-2.037	100.000	0
0.024	100.000	1
-1.050	100.000	1
-1.306	100.000	0
-1.808	100.000	0
-2.056	100.000	0
-1.631	100.000	1
-1.539	100.000	1
-1.753	100.000	1
-0.056	100.000	1
-4.400	51.097	2
-2.160	100.000	0
-1.640	100.000	0
-1.523	100.000	1
-1.118	100.000	0
-2.999	95.421	0
-6.838	33.663	0
-1.094	100.000	1
-3.460	100.000	0
-0.122	100.000	1
0.828	100.000	1
-4.738	73.805	0
-5.558	36.770	2
-1.202	100.000	0
-4.947	49.926	0
-2.429	95.105	0
-1.465	100.000	0
-7.916	0.000	3
-1.680	100.000	0
-7.009	0.162	4
-3.945	40.709	1
-4.266	51.098	1
-1.883	100.000	0

-2.099	100.000	1
-1.608	100.000	1
-1.466	100.000	1
-7.212	0.000	3
-5.663	49.672	0
-6.253	0.000	3
-1.872	100.000	0
-1.705	100.000	1
-3.268	86.504	0
-4.919	48.634	0
-3.476	70.213	0
0.098	100.000	0
-0.881	100.000	1
-2.469	93.882	0
-3.353	80.584	0
-10.125	0.000	3
-2.099	100.000	0
-2.938	92.392	0
-1.976	100.000	0
-1.912	100.000	0
-1.652	100.000	1
-3.917	57.738	0
-6.831	0.000	2
-1.186	100.000	1
-6.959	0.000	3
-2.788	86.551	0
-4.615	50.459	0
-1.262	100.000	1
-3.981	73.728	0
-4.606	57.547	0
-1.441	100.000	1
-5.290	10.749	2
-3.371	100.000	0

-3.104	100.000	0
-9.120	0.000	3
-1.904	100.000	0
-3.368	74.037	0
-4.094	74.207	1
-7.078	0.000	2
-3.592	43.373	1
-2.449	100.000	0
-4.082	61.356	0
-11.859	0.000	3
-2.069	100.000	1
-2.692	96.931	0
-1.145	100.000	1
-3.218	90.109	0
-4.951	42.206	1
-7.122	0.000	2
-1.765	100.000	1
-3.296	77.098	2
-3.461	73.386	2
-3.317	96.122	0
-0.511	100.000	2
-2.662	90.858	1
-2.294	94.668	1
-1.560	100.000	0
2.048	100.000	1
-0.889	100.000	0
-5.675	15.421	3
-3.195	79.457	2
-3.119	91.199	0
-2.038	100.000	1
-3.236	95.210	0
-3.487	68.270	2
-3.243	68.622	2

-1.836	100.000	0
-6.388	21.176	1
-1.282	100.000	1
-3.530	80.267	0
-1.745	100.000	1
-2.967	83.933	0
-1.825	100.000	1
-1.583	100.000	1
-0.922	100.000	0
-2.112	100.000	0
-2.859	89.194	0
-4.093	88.270	0
-2.848	91.887	0
-1.503	100.000	1
-4.366	58.880	0
-2.031	100.000	0
-2.826	0.433	3
-4.743	78.905	0
-2.786	100.000	0
-3.899	87.322	0
-1.896	100.000	0
-3.670	61.492	0
-1.032	100.000	0
-4.310	55.412	0
-1.605	100.000	1
-6.159	0.000	1
-7.254	68.496	0
-2.219	100.000	0
-1.516	100.000	1
-1.305	100.000	1
-2.653	90.087	0
-3.263	40.692	3
-4.915	76.723	0

-0.385	100.000	0
-0.669	100.000	0
-0.148	100.000	0
-3.462	75.425	0
-6.214	6.305	2
-1.987	100.000	0
-4.576	61.544	0
-3.764	91.082	0
-5.539	40.478	0
0.902	100.000	1
-4.367	89.160	0
-3.850	90.531	0
-5.250	55.312	1
-4.277	91.217	0
-0.777	100.000	1
0.419	100.000	1
-3.178	95.392	0
-6.415	22.815	4
-0.187	100.000	0
-14.521	0.000	3
-14.901	0.000	3
-6.484	4.327	4
-14.895	0.000	3
-13.385	0.000	3
-5.568	44.387	0
2.094	100.000	1
-6.678	50.134	1
-5.241	29.593	1
-4.085	74.441	0
-4.479	66.624	0
-1.417	100.000	0
-3.421	67.852	0
-3.133	79.108	0

-1.333	100.000	1
-7.050	0.000	3
-6.366	87.151	0
-1.612	100.000	0
-1.022	100.000	1
-5.310	25.377	1
-1.789	100.000	1
-3.227	94.990	0
-5.174	39.851	2
-2.034	100.000	1
-1.568	100.000	0
-0.808	100.000	0
-4.306	100.000	1
-3.433	69.064	0
-5.812	0.000	3
-3.111	90.834	0
-1.677	100.000	1
-0.313	100.000	0
-5.033	26.409	2
-3.649	81.830	1
-4.072	78.091	1
-2.122	100.000	1
-5.192	16.661	3
-4.674	89.505	0
-4.181	81.331	0
-3.545	51.297	2
-9.086	0.000	3
-3.485	53.323	1
-6.127	14.710	1
-3.452	76.347	0
-3.685	93.846	1
-12.031	0.000	3
-3.960	87.084	0

-2.160	100.000	1
-1.589	100.000	1
-8.122	0.000	3
-6.848	37.685	0
-3.144	100.000	0
-3.088	100.000	0
-3.320	96.468	0
-2.819	100.000	0
-1.580	100.000	0
-1.962	95.157	0
-1.299	100.000	0
-2.621	100.000	0
-0.881	100.000	1
-6.504	70.258	0
-2.074	100.000	1
-2.597	100.000	0
-4.866	38.251	2
-4.246	93.946	0
-7.615	49.029	0
-3.970	88.893	0
-0.353	100.000	0
-1.550	95.938	0
-0.644	100.000	0
0.347	100.000	0
0.370	100.000	0
-3.145	100.000	0
-1.625	100.000	1
-4.075	100.000	0
-1.725	100.000	1
0.215	100.000	0
-1.473	100.000	1
10.026	100.000	1
-2.663	91.278	0

-0.725	100.000	0
-1.616	100.000	1
-2.620	100.000	1
-1.849	100.000	1
-1.457	100.000	0
-0.234	100.000	1
-6.931	0.000	3
-5.255	27.463	1
-3.421	96.777	0
-3.360	100.000	0
-3.339	100.000	0
-3.638	91.244	0
-4.077	87.169	0
-6.472	14.906	2
-2.873	87.680	0
-6.140	48.642	0
-7.311	0.000	2
-5.718	85.415	0
-5.510	30.757	1
-3.236	86.170	0
-4.525	34.003	1
-1.050	100.000	1
-2.329	100.000	0
-4.401	49.578	2
-2.318	100.000	0
-4.389	2.589	3
-4.257	1.457	3
-3.999	72.447	2
-3.472	100.000	0
-3.926	92.734	0
-2.935	100.000	0
-3.022	90.750	0
-2.662	100.000	0

-3.372	87.298	0
-2.964	100.000	0
-2.121	95.362	1
-1.237	100.000	0
-1.787	100.000	0
-3.178	88.071	0
-0.966	100.000	1
-1.462	100.000	1
-1.320	100.000	1
-4.660	53.469	0
-3.802	88.383	0
-3.571	76.098	0
-1.783	100.000	0
-3.420	85.332	0
-5.063	5.488	3
-2.697	100.000	0
-2.130	100.000	0
-2.197	100.000	0
-1.426	100.000	1
-1.282	100.000	1
-2.101	100.000	0
-2.225	96.024	0
-4.407	63.884	0
-5.018	60.053	0
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-3.520	82.402	0
-5.276	100.000	1
-3.646	80.293	0
-1.852	100.000	0
-2.918	96.063	0
-5.482	17.715	2
-5.801	7.747	2
-6.592	1.261	2

-2.405	95.592	0
-2.794	92.373	0
-2.957	100.000	0
-2.566	100.000	0
-9.480	0.000	3
-6.018	0.000	3
-6.070	26.875	1
-7.199	0.000	3
-4.642	68.671	0
-2.180	100.000	1
-1.894	100.000	1
-5.831	8.070	2
-4.843	37.405	1
-6.955	0.000	3
-3.840	79.485	1
-3.328	76.349	2
-7.204	0.000	3
-5.870	0.000	3
-6.947	0.000	2
-8.051	0.000	3
-7.271	0.000	3
-7.131	0.000	2
-8.735	0.000	3
-2.758	94.739	0
-5.161	58.061	0
-1.971	89.006	2
-1.819	86.117	2
-3.602	74.840	0
-0.692	100.000	1
-0.799	100.000	1
-0.512	100.000	1
-4.480	71.960	1
-7.485	0.000	3

-1.550	89.954	2
-1.630	89.297	2
-2.373	100.000	0
-2.895	100.000	0
-9.717	0.000	3
-1.955	83.790	2
-1.700	100.000	1
-2.350	95.803	0
-4.239	72.596	0
-3.162	86.821	0
-4.794	59.574	0
-5.020	56.796	0
-4.379	55.142	0
-0.435	100.000	1
-2.449	74.746	0
-4.667	66.664	0
-1.947	100.000	0
-1.971	89.006	2
-11.881	0.000	3
-1.095	82.717	2
-1.135	83.953	2
-5.446	22.542	2
-5.859	18.905	1
-3.107	94.398	1
-6.620	0.000	3
-3.255	81.013	0
-9.351	0.000	3
-8.925	0.000	3
-6.648	0.000	3
-5.670	31.282	0
-3.403	86.754	0
-2.837	100.000	0
-2.946	100.000	0

-4.558	57.139	0
-6.389	6.533	2
-2.476	100.000	0
-2.008	100.000	1
-3.008	100.000	0
-3.843	66.836	0
-1.537	100.000	0
-1.420	100.000	0
-7.619	0.000	3
-1.246	100.000	1
-4.863	51.252	0
-1.319	100.000	0
-9.970	0.000	3
-1.147	100.000	0
-2.900	44.753	3
-2.604	91.453	0
-1.875	92.789	1
-4.936	59.197	0
-2.413	92.694	0
-5.721	74.379	1
-2.395	94.842	0
-1.882	100.000	0
-1.656	100.000	1
-1.597	100.000	1
-6.567	0.000	2
-1.524	100.000	1
-2.091	90.617	1
-5.652	43.927	0
-5.646	43.925	0
-3.717	63.979	0
-3.372	76.082	0
-1.882	92.184	2
-4.951	41.709	2

-3.088	86.925	0
-2.304	93.219	0
-0.934	100.000	1
-1.527	100.000	0
-1.486	100.000	0
1.114	100.000	1
-4.172	88.055	0
-1.321	100.000	1
-0.826	100.000	0
-2.810	86.008	0
-5.035	52.211	0
-5.718	39.147	1
-5.255	44.004	1
-2.771	95.712	0
-1.848	100.000	2
-3.554	81.364	0
-1.939	100.000	0
-2.793	81.280	0
-0.962	100.000	2
-1.380	100.000	0
-1.128	100.000	0
-0.740	100.000	0
-4.880	68.021	0
-1.682	100.000	1
-1.152	100.000	0
-1.322	100.000	1
-6.179	0.000	3
-3.852	42.452	2
-2.897	78.646	2
-3.271	75.010	2
-1.471	100.000	1
-14.641	0.000	3
-8.816	0.000	2

-6.843	0.000	3
-2.672	100.000	1
-4.876	51.764	0
-2.154	95.896	1
-1.897	92.640	1
1.139	100.000	1
-2.886	93.132	0
-0.144	100.000	1
-1.812	100.000	1
-0.997	100.000	1
-6.168	12.867	1
-1.917	100.000	0
-3.598	88.999	0
-3.649	93.492	0
-3.408	94.854	0
-3.914	65.630	0
-7.640	0.000	3
-2.213	100.000	0
-3.163	100.000	0
-5.194	51.924	0
-5.464	43.036	0
-1.090	100.000	1
-0.878	100.000	2
-1.659	96.055	0
-6.619	0.000	3
-5.363	17.518	3
-2.001	100.000	1
-4.371	37.762	2
-1.267	100.000	0
-2.267	94.428	0
-1.433	100.000	0
-6.545	22.796	1
-6.957	0.000	3

-1.760	100.000	1
-8.113	0.000	2
-1.353	100.000	0
-7.103	0.116	1
-6.975	0.000	3
-1.906	81.293	2
-3.055	80.124	0
-2.097	92.688	0
-4.753	95.953	0
-8.369	0.000	2
-5.912	12.820	3
-0.992	100.000	1
-0.651	100.000	1
-2.616	80.418	0
-2.473	100.000	0
-1.011	100.000	0
0.301	100.000	2
-1.055	100.000	1
-6.819	0.114	2
1.757	100.000	2
-2.933	68.041	2
-2.620	93.122	0
-2.453	95.750	0
-1.723	100.000	0
-2.553	100.000	0
-0.510	100.000	1
-3.211	100.000	0
-2.944	100.000	1
-3.498	100.000	0
-2.724	86.409	0
-6.293	0.000	3
-1.099	100.000	1
-0.957	100.000	1

-0.112	100.000	1
1.301	100.000	2
-4.093	91.022	0
-4.512	85.928	0
-3.932	85.709	1
-1.287	100.000	2
-0.798	100.000	1
-2.166	100.000	0
-1.664	100.000	1
-2.441	100.000	1
-1.314	100.000	0
-1.065	100.000	1
-0.580	100.000	1
-1.585	100.000	0
-1.294	100.000	1
-0.033	100.000	2
-1.716	100.000	1
-2.744	100.000	1
-1.518	100.000	0
0.284	100.000	0
-1.774	100.000	1
-1.286	100.000	0
-2.414	100.000	0
-1.902	100.000	0
-1.282	100.000	1
-1.722	100.000	0
-1.918	100.000	0
-2.092	100.000	0
-1.228	100.000	1
-1.672	100.000	0
-2.118	100.000	0
-1.942	100.000	0
-0.983	100.000	1

-0.997	100.000	0
-4.005	87.124	0
-1.664	100.000	0
-1.423	100.000	0
-8.726	0.000	3
-5.277	22.943	2
-3.338	84.061	0
-4.868	9.873	3
-3.396	83.043	0
-3.638	81.601	1
-5.455	2.998	3
-5.431	17.991	3
-5.875	20.676	1
-5.983	0.000	3
-4.288	59.814	0
-1.914	100.000	0
-2.429	100.000	0
-4.589	84.424	0
-6.235	10.152	3
-2.484	100.000	0
-4.321	65.930	0
-1.665	100.000	0
-4.259	69.061	0
-4.182	60.343	1
-1.605	100.000	1
-0.224	100.000	2
-1.747	100.000	1
-2.096	100.000	1
-3.263	84.468	0
-4.651	62.367	0
-3.588	91.094	0
-2.493	88.934	0
-4.469	74.767	0

1.128	100.000	2
-0.338	100.000	2
-10.864	0.000	3
-11.435	0.000	3
-11.661	0.000	3
-10.953	0.000	3
-6.873	0.000	3
-2.287	100.000	0
-9.575	0.000	3
-5.784	36.364	0
-2.302	100.000	1
-5.272	83.833	1
-1.558	100.000	0
-3.536	91.904	0
-3.900	88.533	0
-1.883	100.000	0
-4.859	85.537	0
-2.323	100.000	0
-2.024	100.000	0
-1.546	100.000	1
-1.680	100.000	1
-1.250	100.000	1
-4.754	0.000	3
-6.108	1.072	3
-7.351	0.000	3
-5.742	6.399	3
-6.762	0.000	3
-2.780	93.928	0
-3.140	78.422	0
-8.560	0.000	3
-1.206	100.000	1
-3.557	86.428	0
-3.743	87.612	0

-5.790	13.971	3
-8.813	0.000	3
-3.520	91.227	0
-4.219	88.120	0
-7.094	0.000	3
-4.738	40.263	2
-1.009	100.000	2
-3.352	81.165	1
-2.759	100.000	1
-4.033	77.074	0
-1.513	100.000	1
-2.873	100.000	1
-1.279	100.000	1
-2.115	100.000	1
-4.143	71.804	0
-12.445	0.000	3
-13.048	0.000	3
-1.322	100.000	1
-3.516	76.867	0
-3.800	82.020	0
-2.033	100.000	0
-1.939	100.000	1
-2.000	100.000	1
-2.087	91.104	1
-2.211	91.455	1
-1.472	100.000	1
-1.602	100.000	1
-8.880	0.000	3
-5.720	68.759	0
-1.181	100.000	0
-2.330	100.000	0
-7.999	0.000	3
-4.146	83.962	0

-3.458	95.029	0
-3.751	92.460	0
-6.124	0.000	3
-6.121	0.000	3
-3.241	69.924	1
-4.621	60.705	0
-4.811	48.137	0
-6.581	0.075	3
-4.754	45.899	0
-6.141	0.000	2
-4.472	65.745	0
-5.015	40.748	1
-6.081	12.379	3
-8.529	0.000	3
-3.337	76.140	0
-1.805	81.627	2
-2.703	82.096	1
-2.707	69.240	2
-1.154	100.000	1
-4.190	36.773	2
-9.159	0.000	3
-4.389	87.147	0
-6.299	0.000	3
-3.324	65.713	1
-5.680	71.106	0
-5.212	75.658	0
-0.200	100.000	2
-3.445	100.000	0
-2.762	100.000	0
-3.645	95.686	0
-3.645	95.686	0
-6.792	15.882	1
-5.958	82.466	0

-4.015	95.052	0
-1.914	100.000	0
-3.204	82.968	0
-7.219	0.000	3
-3.487	100.000	0
-6.644	49.907	0
-4.408	50.957	2
-4.217	64.287	1
-5.181	41.331	2
-8.670	0.000	2
-4.805	33.795	3
-2.680	100.000	0
-1.269	100.000	1
-5.196	39.275	2
-4.969	42.999	2
-3.833	82.819	0
-3.167	100.000	0
-6.813	0.000	3
-2.236	100.000	1
-7.223	0.000	3
-2.227	79.428	2
-11.103	0.000	3
-4.541	43.262	1
-6.239	5.058	3
-7.114	0.000	3
-5.901	0.000	3
-4.444	64.008	0
-1.617	100.000	1
-0.768	100.000	1
-7.547	62.692	0
-2.175	100.000	1
-2.078	100.000	1
-2.382	72.527	2

-1.576	100.000	0
-2.461	83.185	1
-2.165	86.689	1
-4.106	89.834	0
-2.176	100.000	0
-3.513	86.742	0
-3.198	89.229	0
-9.523	0.000	3
-3.039	93.161	0
-4.954	51.578	2
-4.914	50.679	2
-5.974	15.324	3
-5.954	14.793	3
-4.773	29.093	2
-3.213	100.000	0
-5.945	60.740	0
-6.941	9.219	1
-9.247	0.000	3
-3.181	92.472	0
-12.283	0.000	3
-11.918	0.000	3
-7.999	0.000	3
-5.427	68.720	0
-8.980	0.000	3
-3.099	81.935	0
-4.786	3.340	3
-5.892	17.456	1
-1.849	93.298	1
-5.394	38.436	0
-2.556	94.393	0
-1.382	100.000	0
-1.679	100.000	1
-5.015	29.553	2

-4.716	61.724	0
-2.788	87.705	0
-6.276	39.004	0
-4.636	50.841	0
-1.366	100.000	1
-3.267	90.897	0
-3.599	82.411	0
-3.333	83.027	0
-15.023	0.000	3
0.209	100.000	1
-2.317	100.000	1
-7.630	0.000	3
-3.805	90.397	0
-0.730	100.000	0
-0.973	100.000	1
-1.207	100.000	1
-8.264	0.000	1
-1.944	86.560	2
-1.682	100.000	1
-7.085	26.903	1
0.691	100.000	2
-10.177	0.000	3
-13.150	0.000	3
-7.302	0.000	3
-8.433	0.000	3
-12.225	0.000	3
-7.557	0.000	3
-6.297	0.000	3
-6.481	4.529	2
-0.864	100.000	1
-1.781	100.000	0
-2.865	79.358	1
-1.196	100.000	0

-3.057	89.764	1
-7.458	45.985	1
-2.254	100.000	0
-8.111	0.000	2
-8.684	0.000	2
-6.013	40.432	0
-3.130	84.885	0
-7.638	0.000	1
-6.635	12.521	0
-7.838	4.619	0
-2.352	95.327	0
-2.227	91.429	0
-2.365	88.986	0
-5.442	45.423	0
-4.935	63.273	0
-5.296	40.386	0
-6.115	27.525	0
-2.521	100.000	0
-1.314	100.000	1
-1.987	91.304	2
-2.610	88.972	0
-3.990	83.552	0
-4.328	79.420	0
-3.527	83.861	0
-2.969	91.358	0
-3.690	82.704	0
-3.583	84.436	0
-1.258	100.000	1
-1.256	100.000	1
-5.017	49.836	1
-0.685	100.000	0
0.958	100.000	1
-1.702	100.000	0

-3.742	86.074	0
-4.913	50.943	1
-0.640	100.000	0
-3.437	87.505	0
-3.455	90.504	0
-4.235	76.847	0
-4.479	66.624	0
-4.085	74.441	0
-1.262	100.000	1
-2.984	100.000	0
-2.294	100.000	0
-1.655	100.000	0
-1.725	100.000	0
-3.694	80.830	0
-6.303	17.855	0
1.791	100.000	1
-1.343	100.000	0
-5.017	43.023	2
-5.054	49.093	1
-2.751	94.702	0
-5.562	6.517	3
-4.217	76.522	0
-2.473	86.988	0
-3.635	82.367	0
-1.316	100.000	0
-0.920	100.000	0
-1.422	100.000	0
-1.311	100.000	1
-2.620	91.937	0
-2.169	100.000	0
-1.313	100.000	0