

Table S2. List of colorectal abnormal associated metabolites

Metabolite feature	Metabolite annotation	approach	F meanN	F meanC	F meanA	anova nc adj	anova na adj	anova ca adj	F cvNp raw log2	F cvCp raw log2	F fc nc raw	F fc na raw	F fc ac raw
X10.3_339.237mz_pos	(-)-Folicanthine	exact mass match	7748.846605	5053.536056	5527.387681	0.00000527	7.36E-08	0.016360165	1.066851507	3.045501184	0.732979425	0.686815097	1.062715076
X12.4_340.269mz_pos	(-)-Ormosanine	exact mass match	45226.06503	31316.75757	27721.72218	0.0000798	0.0000327	0.374105369	0.82512597	0.830862497	0.687636808	0.562694393	1.222043114
X10.9_313.166mz_neg	(-)-trans-Carveol glucosid	exact mass match	364.3974089	8542.0151	9965.786895	0.002652316	0.000960176	0.295523934	7.802344415	1.555479803	8.146636736	8.049968526	1.01200852
X15_265.108mz_neg	(+)-2,5-epi Goniothalesdiol	exact mass match	32595.35307	22986.25282	25975.3202	0.001250629	0.001302286	0.43224324	1.276557314	2.675216985	0.752619218	0.720752853	1.04421261
X20.8_388.119mz_neg	(+/-)-6-Acetylthiodiols	exact mass match	6812.396901	10133.51548	3573.206732	0.004217867	0.0002535	0.116465099	6.234319405	7.015515802	1.484891164	0.526968596	2.817798206
X12.5_321.241mz_pos	(±)15-HETE	exact mass match	11931.10675	8063.355578	8309.938888	3.99E-10	3.99E-10	0.00389225	1.0537419	2.554831014	0.707014986	0.657446626	1.075395262
X14.9_265.108mz_pos	(±)-Goniothalesdiol	exact mass match	24851.58866	16540.4257	15696.90897	0.002211296	0.000178788	0.127514798	0.650486116	0.819995262	0.718165912	0.582429257	1.233052604
X15.1_333.226mz_pos	(±)-Pandamarine	exact mass match	78154.92166	37693.09503	61456.22917	0.00000158	0.000472756	0.950049258	1.398514317	1.360676174	0.471657455	0.682169628	0.691407878
X24_357.235mz_neg	(1S)-1-hydroxy-23-oxo-2	exact mass match	2067.046116	6783.212071	10613.37145	0.00000682	0.00010632	0.584324567	2.877609538	13.07421455	2.452112148	3.00547459	0.815881843
X20.7_645.438mz_pos	(20R)-Ginsenoside Rh2	exact mass match	19519.16483	12756.37371	12327.32875	4.39E-10	4.01E-10	0.003733196	1.465309488	2.612138841	0.666444891	0.589918254	1.12972147
X11_428.321mz_pos	(22E)-1α-hydroxy-24-oxo	exact mass match	97120.90614	72845.20464	62220.94605	3.99E-10	3.99E-10	0.0064595	0.841975269	0.930335036	0.716145838	0.559366987	1.280279057
X12.4_546.383mz_pos	(22S)-Acetoxy-3α,15α	exact mass match	9231.270141	6429.061705	6092.236396	0.0000161	0.0000601	0.397096351	1.227501645	3.258940702	0.743957672	0.630497745	1.179952946
X18.7_445.296mz_neg	(23S,25R)-1α,25-dihydrox	exact mass match	19301.02292	32357.61626	37626.34194	0.0000078	0.001813676	0.985522683	0.507675713	0.769683063	1.729323187	1.728930055	1.000227384
X4.8_524.344mz_pos	(25R)-3α,7α,15α-dihy	exact mass match	42278.66705	14322.95252	13266.55609	0.000000306	0.000571753	0.999569714	1.459558199	4.480875598	0.342545041	0.286060852	1.197455154
X9_530.336mz_pos	(25S)-11α,20,26-trihy	exact mass match	38023.71975	26906.34985	25382.98412	3.99E-10	4E-10	0.022765966	0.916553919	2.051186976	0.708744036	0.614803877	1.152796954
X12.2_502.357mz_pos	(25S)-3-oxo-12β-acetyl	exact mass match	31958.1137	23103.82901	21531.79709	4.03E-10	3.99E-10	0.003719973	0.682227397	1.154315774	0.722037656	0.619163391	1.166150433
X11.6_286.201mz_pos	(2E)-octenoylcarnitine	MS/MS spectrum match	13453.00627	33364.91448	33905.72166	0.000017	0.002253687	0.971075742	4.188632551	2.955775791	2.306003701	2.18233241	1.056669318
X20.3_715.487mz_pos	(2'S)-Deoxyoxylol 2'-α-L-	exact mass match	7748.409131	5609.9888	3555.197895	0.0000691	0.00000981	0.104453542	4.288444982	7.967021716	0.788635377	0.463329937	1.702103218
X18.1_587.394mz_pos	(3b,16a,21b,22a)-12-Olea	exact mass match	10628.13143	7185.808936	5500.136528	0.00000153	1.32E-08	0.009300059	4.374952618	5.498801314	0.718968946	0.50677689	1.418709022
X12.2_364.232mz_pos	(3S,4S)-3-hydroxytetradec	exact mass match	15772.88487	35269.11483	37464.98325	0.00000016	0.000855232	0.964062627	7.835010397	3.687203575	2.089298558	2.068529643	1.010040424
X10.7_400.29mz_pos	(3S,5R,6R)-3,5-dihydroxy-	exact mass match	21795.06161	12037.97684	12218.58863	0.000342243	0.00000602	0.037985192	1.595370636	2.189918456	0.5725328	0.5305283	1.079174853
X13_421.295mz_pos	(4R,4aS,6aS,8R,9R,11aR,11	exact mass match	11934.10061	8360.047954	6466.344251	4.19E-10	1.65E-09	0.183096218	1.699455832	2.957412625	0.730073449	0.522233108	1.397983848
X14.7_442.337mz_pos	(5E)-(24R)-24,25-dihydrox	exact mass match	49108.46688	36348.05832	29371.42209	4.11E-10	5.26E-08	0.684818542	1.027109275	1.550868479	0.727598766	0.547509065	1.328925515
X22.2_445.311mz_pos	(6R)-6-methylvitamin D3	exact mass match	4926.046547	2706.184577	3686.166487	6.53E-08	0.0000379	0.872966193	2.26998756	12.96484117	0.689016018	0.705749569	0.976289676
X25.6_449.311mz_pos	(6R)-vitamin D3 6,19-sulf	exact mass match	12298.18161	7151.685256	9222.914069	4.2E-10	0.0000248	0.801573237	8.812450938	14.90745789	0.618853611	0.718597583	0.861196343
X27.8_353.212mz_neg	(E)-2-(4,8-dimethylnona-9	MS/MS spectrum match	148979.4135	661207.0536	1133916.741	3.99E-10	3.99E-10	0.134267366	1.84115847	2.063421286	4.322471299	6.715949982	0.643612798
X15.8_555.713mz_pos	Galβ1-4[Fucα1-3]GlcNAc	exact mass match	6637.175039	4303.392169	2880.885392	0.000108407	4.14E-10	0.000002363	7.311820369	14.74482086	0.471581349	0.443439817	1.672338207
X15.8_511.018mz_pos	(N-Sulfolindol-3-yl)methyl	exact mass match	29186.40004	22499.90694	18837.38392	3.6E-09	1.38E-09	0.02828573	0.807437688	1.75709615	0.768422291	0.59427491	1.293041786
X19.1_542.03mz_pos	(R)-AM1241	exact mass match	13839.90492	10689.70452	11501.07819	0.000187398	0.0000275	0.124521706	1.540117563	1.51315139	0.791771246	0.776948566	1.01907807
X10.3_505.194mz_pos	(S)-Multifidol-2-[apiosyl-(exact mass match	10268.06979	14535.29099	8224.276358	0.00000304	0.0000435	0.292377203	3.615316308	4.012332721	1.382979398	0.743269311	1.860670657
X17.5_470.368mz_pos	(Z)-2-pentacos-16-enam	exact mass match	1541720.215	1112842.585	1113302.922	4.17E-10	6.75E-08	0.685039559	0.869028884	1.211919695	0.665229088	0.654200409	1.016858258
X15.7_456.352mz_pos	(Z)-2-tetracos-15-enamid	exact mass match	914827.0994	669049.7222	578207.027	3.99E-10	3.99E-10	0.032418565	0.418785076	0.873093345	0.66058611	0.539320574	1.224848712
X14.3_329.233mz_neg	(Z)-5,8,11-trihydroxyoctad	MS/MS spectrum match	23391.65438	4700.138831	6893.331033	3.99E-10	4.06E-10	0.998593315	0.734687355	2.734289476	0.264405313	0.298388796	0.886110057
X26.3_514.705mz_pos	(des-Gly-NH2)-Argβ-Va	exact mass match	58954.23862	47623.94754	31991.28776	1.72E-09	3.99E-10	0.00000488	0.887991852	2.109944	0.786544048	0.494575448	1.590341881
X7.4_461.196mz_pos	(6-Acetoxy-7-(chloromethyl	exact mass match	12066.52463	17821.67127	7037.00706	0.00000921	5.19E-09	0.001743429	12.56187005	8.351417788	1.436937087	0.553086768	2.598031938
X22.1_471.004mz_pos	(1-(2,4-Dichlorophenyl)-2-	exact mass match	56381.39632	44502.78039	30959.61396	4.14E-10	3.99E-10	0.000657242	0.969642274	1.655607854	0.769882315	0.50166789	1.534645392
X26.2_848.629mz_pos	1-(2E,6E-phytyadienyl)-2-(exact mass match	391197.9318	272991.3841	220232.0235	3.99E-10	3.99E-10	0.001260118	0.321296523	1.59319371	0.651961453	0.484717969	1.345032564
X7.2_744.501mz_pos	1-(6-[5]-ladderane-hexan	exact mass match	58212.88359	20344.06023	16941.07618	5.8E-10	0.000000293	0.688047446	1.116039125	2.349430668	0.35885376	0.269034778	1.333856397
X16.7_778.551mz_pos	1-(8-[5]-ladderane-octan	exact mass match	284763.3151	198505.2832	176867.2336	3.99E-10	3.99E-10	0.006982728	0.295853122	1.130526924	0.645267598	0.539044479	1.197058171
X16.5_822.578mz_pos	1-(8-[5]-ladderane-octan	exact mass match	33376.57516	22110.9712	19406.84485	3.99E-10	3.99E-10	0.013617049	0.303285778	1.504875559	0.668207154	0.539273705	1.239087217
X22.9_715.519mz_pos	1-(O-alpha-D-glucopyran	exact mass match	50245.21063	38147.52833	36806.61214	1.61E-09	1.64E-09	0.047439362	1.486759725	1.955617727	0.737649139	0.654686491	1.126721185
X17.9_775.54mz_pos	1,2-di-(9Z,12Z,15Z)-octade	exact mass match	89183.85876	60018.2244	69117.56912	3.99E-10	3.99E-10	0.001776808	1.414861814	1.385130578	0.639182096	0.670567659	0.95319553
X15.9_447.806mz_pos	1,2,3,4,6,7,8-Heptachloroc	exact mass match	7098.001182	4970.489235	5209.674882	0.00000106	1.97E-09	0.008199487	0.761805982	4.028440188	0.782156344	0.704316829	1.110517756
X6.8_326.253mz_pos	1,2,3-Tris(1-ethoxyethoxy)	exact mass match	143458.3827	141128.6631	91529.16404	3.99E-10	4E-10	0.011970207	1.93022627	1.488043386	0.663452782	0.550567111	1.20503526
X8.6_208.073mz_pos	1,2,4-Triazolol[4,3-a]pyrid	exact mass match	15083.93153	8850.525113	11917.94535	0.000259009	0.001530194	0.662066759	2.190461061	2.322421687	0.629665027	0.704246466	0.894097531
X20.1_723.486mz_pos	1,26-Dicaffeoylhexacosan	exact mass match	176311.9344	121292.8809	156319.0252	3.99E-10	3.99E-10	0.077374897	1.727010774	2.550051883	0.643953558	0.769519291	0.836828089
X28.5_150.002mz_neg	1,2-Benzisothiazol-(3,2H)-	exact mass match	14441.17101	90295.82037	106319.3668	3.99E-10	4.97E-10	0.333541554	1.113873426	1.142490098	5.994711572	6.283797138	0.953995083
X15.7_287.186mz_neg	1,2-Dihexanoyl-sn-glycer	exact mass match	6336.906579	3559.391053	4594.014677	0.000176849	0.000596874	0.52531918	1.127243807	4.324910384	0.695608489	0.669882884	1.038403139
X14.7_359.058mz_pos	1,2-Glycerol dinitrate gluc	exact mass match	12251.93067	7760.521706	5557.277127	0.0000507	0.004965976	0.98505884	2.906042748	3.387978596	0.665648981	0.439437677	1.514774483
X15_476.299mz_pos	10-Deoxymethylmycin	exact mass match	5885.348673	13219.61069	8762.396788	0.000100097	0.000940998	0.68140257	3.198066655	1.214359722	2.109204605	1.293012464	1.631233003
X18.2_311.223mz_neg	10-hydroperoxy-8E,12Z-d	exact mass match	5063.170423	8679.332009	18142.25467	0.002400476	0.000228448	0.141814414	4.997379095	6.689255249	1.666344498	2.686069856	0.620365287
X20.2_499.307mz_neg	11-Deoxocurbitacin I	exact mass match	4065.241461	8295.740168	9158.779055	0.000000476	0.000702485	0.999836788	3.16683007	2.286369472	1.854277751	1.699326074	1.091184193
X9.1_548.363mz_pos	11-KETOROCOGENIN A	exact mass match	5291.983662	3340.963914	2202.407209	0.000053	3.99E-10	2.68E-08	0.817116117	7.311112797	0.751158781	0.420239499	1.787454015
X14.5_530.389mz_pos	11-OXOIRSOLIC ACID A	exact mass match	592116.5201	436257.8408	400555.272	3.99E-10	3.99E-10	0.039757223	0.565335518	0.826351643	0.66783221	0.582449258	1.146592945

X18.3_311.223mz_neg	12-hydroperoxy-9Z,13E-d	exact mass match	4305.860679	7697.849797	14688.90263	0.000929524	0.000202302	0.195819394	3.402651825	6.785334145	1.70438976	2.469295422	0.690233232
X5.7_661.428mz_pos	12-O-Palmitoyl-16-hydro	exact mass match	6430.163581	1957.709238	2030.682587	0.000001133	0.000488252	0.9611712024	1.24090691	14.19047637	0.34752259	0.305734036	1.136682704
X8.9_650.736mz_pos	13,17-Dimethyltritetracon	exact mass match	10625.3727	7049.394923	5165.3284	0.00000336	0.000487486	0.68295772	5.53532297	10.00510291	0.706585856	0.482968114	1.46300726
X28.1_483.368mz_pos	13-beta-D-Glucosyloxyd	exact mass match	209495.4434	139732.1143	160916.8388	4.08E-10	0.002925594	0.080463355	1.049839199	1.846689527	0.619672806	0.669303783	0.92584686
X8.7_525.329mz_pos	15(S)-HETE-biotin	exact mass match	24101.02013	15623.46535	14384.02687	4E-10	3.99E-10	0.004963082	1.557361846	3.00887842	0.655729321	0.556301978	1.178729084
X30.6_355.228mz_neg	16-Dehydropregnenolone	exact mass match	6129.909826	25665.19637	32837.39163	3.99E-10	8.24E-10	0.361662155	1.308984371	1.013063562	3.744820086	4.092463242	0.915052834
X33.6_429.159mz_neg	17β-hydroxy Wortmannin	exact mass match	99903.68964	129257.7167	153044.2159	0.002471367	0.003949029	0.56235936	1.116970096	1.040841562	1.295712248	1.355857518	0.95564042
X25.5_475.341mz_pos	18-acetoxy-1α,25-dihydro	exact mass match	25147.65987	17405.6408	14119.92571	4.33E-10	1.01E-09	0.013573069	2.886307912	4.153587353	0.69385052	0.522063735	1.329053282
X21.3_601.413mz_pos	19-Methoxypomolic acid	exact mass match	9667.130465	5358.849275	6909.142575	2.04E-09	4.01E-10	0.000602164	3.190131158	4.216566742	0.621651025	0.674054019	0.922256982
X15.2_442.318mz_pos	1b,3a,7a,12a-Tetrahydrox	exact mass match	22781.28885	17816.70311	14052.21346	3.28E-09	8.73E-08	0.274385874	1.405586451	2.41431713	0.77927117	0.571668355	1.363152541
X20.2_510.359mz_pos	1-heptadecanoyl-2-hydr	MS/MS spectrum match	122310.4042	100429.4874	70564.20246	3.02E-08	4.54E-10	0.00141886	0.83353428	1.477246266	0.781130047	0.502785721	1.553604278
X18.3_510.359mz_pos	1-heptadecanoyl-sn-glyc	exact mass match	41328.57911	31204.87845	23139.80057	1.16E-09	4.01E-10	0.000878654	1.032052308	1.217389792	0.751031431	0.518638005	1.448084066
X35.1_577.369mz_pos	1-Hydroxyvitamin D3-3-D	exact mass match	40107.24749	18526.2236	19574.2956	0.000017	0.001832291	0.952910166	8.684007565	4.192429966	0.464930247	0.443697843	1.047853295
X16.4_399.052mz_pos	1-Methyl-2-galloyl-galact	exact mass match	55993.78295	42064.13039	26777.66844	0.000129331	0.00000229	0.032900117	2.405389678	2.040964884	0.735567516	0.431603997	1.704264837
X8.9_650.4mz_pos	1-Palmitoyl-2-(5-hydroxy	exact mass match	41354.74236	28734.10069	24891.89888	3.99E-10	3.99E-10	0.000780168	0.849447688	3.672958156	0.690530062	0.555447209	1.243196563
X11.4_722.489mz_pos	1-tetradecanyl-2-(8-[3]-H	exact mass match	381267.3351	304022.5008	276495.5061	4.02E-10	4.13E-10	0.035751107	0.588539921	1.045616131	0.740005511	0.627381531	1.179514338
X12.4_486.363mz_pos	1α,25-dihydroxy-11-(3-h	exact mass match	52635.07907	39186.97759	33764.8404	4.17E-10	5.34E-10	0.065026498	0.735188712	1.339905676	0.728303711	0.581873146	1.251653761
X15.2_550.373mz_pos	1α,25-dihydroxy-22-oxav	exact mass match	16614.06022	10740.54052	10261.83568	1.04E-08	0.000000296	0.322455189	2.054227676	3.984484186	0.662318939	0.580567507	1.140812965
X25.4_541.37mz_pos	1α,25-dihydroxy-25,25-di	exact mass match	185553.3603	149195.1098	159781.752	5.65E-10	4.36E-10	0.013127749	0.602346095	1.272943955	0.750751952	0.756995945	0.991751616
X30.4_530.368mz_pos	2-(8-[3]-ladderane-octan	exact mass match	261229.8523	192001.5591	180656.4139	4.83E-08	0.000110078	0.987255433	4.093381401	1.792217526	0.680041863	0.604473774	1.125014668
X16.7_629.446mz_pos	2-(9R-(15Z)-docosenoylo	exact mass match	58279.26633	40177.22982	44464.08735	3.99E-10	3.99E-10	0.0000182	1.583689022	1.483819398	0.668470687	0.669568449	0.998360493
X24.8_504.691mz_pos	2,2',4,5'-Tetrabromodiphe	exact mass match	54781.18719	42277.37796	33182.49598	6.27E-10	3.99E-10	0.00000324	0.440825386	1.761897217	0.754112033	0.550436415	1.370025697
X13.4_343.211mz_pos	2,3-dinor, 6-keto-PGF1α	exact mass match	3126.002783	26999.97613	28448.68655	0.0000103	0.003108296	0.999330453	5.73381753	1.358644524	6.22604859	6.119212419	1.017459137
X16.8_327.216mz_pos	2,3-Dinor-11b-PGF2a	exact mass match	13693.4327	25196.27472	26969.33791	0.000108144	0.00000094	0.019966876	2.245939944	1.357980504	1.745650566	1.735055033	1.006119268
X18.9_341.233mz_neg	2,3-Dinor-TXB1	exact mass match	15862.78327	5503.47846	10310.79453	3.99E-10	0.000605969	0.058673164	2.798822661	3.949520047	0.421169175	0.502535993	0.710773359
X21.9_489.338mz_pos	2,3-epoxyphyloquinone	exact mass match	42514.18532	33381.0583	36641.41646	0.000000129	7.99E-10	0.002849027	1.153036885	1.69035611	0.774328427	0.777888075	0.995423958
X18.2_514.017mz_pos	2,5-Diamino-6-(5'-triphos	exact mass match	16483.10223	12592.80659	11669.41389	0.000001178	0.00000118	0.131403788	1.999435081	3.333977291	0.771347025	0.65885004	1.170747481
X7.2_153.092mz_neg	2,6-nonadienoic acid	exact mass match	21444.75996	14284.63665	11948.86327	0.00076858	0.001277486	0.48919605	2.167769949	1.677091998	0.719887263	0.51140468	1.074666554
X23_509.019mz_pos	2,7-Dichlorodihydrofluor	exact mass match	31536.86429	23824.466	25000.94231	0.000000728	0.000000697	0.136508001	0.615172924	2.252284305	0.756098658	0.728556269	1.037804066
X6.7_588.375mz_pos	2-[2-[(19-Acetamido-16,1	exact mass match	36104.14791	11531.65658	12029.29501	6.62E-09	0.000000402	0.041556909	1.382213894	2.05380845	0.345298346	0.307861048	1.121604532
X10.6_708.473mz_pos	2-[6-[5-Hydroxy-3-(2-hy)	exact mass match	253778.24	212051.0251	181794.6211	2.24E-09	3.31E-08	0.207270878	0.873351055	1.971957382	0.775281236	0.62314048	1.244151618
X18.9_597.407mz_pos	24Z-ethylidene-cholest-5	exact mass match	13354.5312	10417.16367	7665.306768	0.0000222	6.77E-09	0.0012885	1.914997642	4.242982077	0.798953296	0.550564599	1.451152685
X26.3_514.37mz_pos	25-Hydroxy-24-epi-brass	exact mass match	179966.0944	137152.047	98311.68968	3.99E-10	3.99E-10	0.000243156	0.774623156	1.429822839	0.713963776	0.47360542	1.507507612
X17.3_514.395mz_pos	26,27-diethyl-1α,25-dihy	exact mass match	2152165.581	1583385.893	1486733.164	4E-10	1.06E-09	0.328714854	0.571230554	1.063205734	0.678139864	0.629963828	1.07647429
X17.5_446.289mz_pos	2-Angeloyl-9-(3-methyl-)	exact mass match	4540.275933	11160.56407	12161.21188	0.0000495	0.000170163	0.447626635	3.390391704	1.468451401	2.158997307	2.142226859	1.007828512
X14.6_662.468mz_pos	2-carboxy-2-amino-3-O-	exact mass match	175651.7247	126087.5843	119100.6983	3.99E-10	3.99E-10	0.024270611	0.384041601	1.09811425	0.668044968	0.586550815	1.138937925
X21.5_515.03mz_pos	2'-Deoxy-5-hydroxymeth	exact mass match	270998.6743	228606.7424	188769.234	0.00000025	0.000000224	0.110954318	0.531178382	0.93243685	0.785290907	0.608486838	1.290563506
X16.1_412.326mz_pos	2-docosanamidoethanesul	exact mass match	145475.0576	106591.7285	91473.41753	4.01E-10	3.99E-10	0.002748238	1.418143122	0.748057437	0.690501405	0.54030554	1.277983204
X26.6_427.268mz_pos	2-glyceryl-PGD2	exact mass match	21330.50775	14409.31864	15821.07909	0.0000172	0.0000226	0.25901201	1.518015993	3.431419344	0.677428414	0.678467296	0.998468781
X49.2_381.337mz_neg	2-hydroxy-15Z-tetracosel	exact mass match	13771.8846	25238.38324	49556.7157	0.000382488	0.003896058	0.799625822	3.928781138	3.854854595	1.779504656	3.047814898	0.583862444
X38.9_315.288mz_pos	2-hydroxy-nonadecanoic	exact mass match	33385.93058	54513.17969	117786.0858	0.000431305	0.001262144	0.559685693	2.259889012	2.612178912	1.543649559	2.999942735	0.514559675
X18.1_539.71mz_pos	2-Hydroxyphytanoyl-CoA	exact mass match	81953.51182	64129.14522	53234.66914	1.27E-09	1.97E-09	0.060750028	0.795797097	0.98864077	0.750247743	0.568842872	1.318901545
X34.4_165.979mz_neg	2-Mercaptobenzothiazole	exact mass match	213.8743864	1308.799008	2158.413238	7.19E-08	0.001526405	0.836387307	11.44752797	6.929486453	4.443474084	4.660488779	0.953435207
X16.4_369.049mz_pos	2-O-Caffeoylhydroxycitric	exact mass match	32718.23548	20893.24297	11970.60228	0.000230906	0.001341105	0.64995002	2.835763932	2.821486933	0.689522275	0.348816413	1.976748366
X24.5_524.708mz_pos	2S-Pristanoyl-CoA	exact mass match	249505.0657	209087.2478	148131.0953	1.26E-09	4.01E-10	0.000748233	0.747489423	1.400208468	0.780241399	0.521930156	1.494915346
X20.3_440.358mz_pos	2-tetracosanamidoethanes	exact mass match	59826.97622	42485.38807	29435.78727	4.72E-10	3.99E-10	0.000505687	0.729675687	1.370476992	0.696904421	0.448311632	1.554508899
X17.8_426.342mz_pos	2-tricosanamidoethanesul	exact mass match	350504.315	257006.2958	195734.0945	4.25E-10	4.05E-10	0.009386705	0.721735602	0.814417254	0.688567872	0.4892718457	1.407485475
X14.9_313.202mz_neg	2-Undecyl-4(1H)-quinolin	exact mass match	6478.425965	17832.98385	20601.86977	0.00000352	0.000714007	0.946273839	0.843657168	0.739998542	2.597680028	2.551528599	1.018087757
X21.3_533.364mz_pos	2α-(benzyloxy)-1α,25-dih	exact mass match	64435.69901	52729.16283	54431.56652	0.00000967	0.0000026	0.107964758	0.624225322	1.510303281	0.789865901	0.742705955	1.063497467
X14.3_442.337mz_pos	2α-Fluoro-19-nor-22-oxi	exact mass match	572977.4451	432362.4619	405889.29	3.99E-10	3.99E-10	0.03217799	0.41997006	0.947013425	0.688005724	0.608150448	1.131308422
X17.8_657.112mz_pos	3'-(2'',3''-Digalloyl)glucosy	exact mass match	13656.6401	10062.59038	7309.712105	0.00000575	0.003445402	0.994261157	3.37740977	5.929380019	0.758566505	0.516536353	1.468563639
X16.1_593.356mz_pos	3,14,25-Trihydroxy-2,10,1	exact mass match	1517.341789	5072.032705	6240.440407	0.0000182	0.0019457						

X29.3 319.264mz_neg	3,7,11,15-Tetramethylhexyl	exact mass match	21465.21929	10591.33726	12358.25876	2.66E-08	0.000224763	0.987906466	2.837269658	2.902809047	0.538142393	0.527853885	1.019491205
X18 592.735mz_pos	3a,7a-Dihydroxy-5b-chole	exact mass match	15647.28892	11113.88126	6964.01185	0.00000158	0.000618865	0.972820364	4.184349758	3.401437751	0.725363506	0.430435528	1.685185025
X13.7 544.404mz_pos	3alpha-Acetomethoxy-11	exact mass match	26966.71172	19689.93683	15755.60298	0.000389437	0.00003353	0.105942629	0.854208283	2.880907672	0.730992643	0.540145731	1.353324855
X22.4 439.302mz_pos	3beta-(3-methyl-butanoyl	exact mass match	7164.48903	4426.137375	4836.080945	2.91E-08	4.04E-10	0.000225229	1.816408318	5.233060042	0.713214506	0.658351644	1.083333676
X14.6 557.389mz_pos	3beta.15alpha-Diacetoxyl	exact mass match	113519.3635	81387.46113	98812.59102	3.99E-10	4E-10	0.024232515	1.103453533	1.478498983	0.673583653	0.751388542	0.896451856
X27.5 549.061mz_pos	3-carboxy-1-hydroxyprop	exact mass match	80347.92818	59062.60285	38206.13762	7.05E-10	4E-10	0.000655543	1.411419301	2.131461659	0.706932045	0.426044566	1.659291305
X24.7 729.535mz_pos	3-dodecanoyl-NBD Chole	exact mass match	557479.3334	426205.875	446935.2165	4.02E-10	4E-10	0.00917566	0.641897861	1.273800489	0.700997579	0.684654888	1.023869699
X19.9 605.403mz_pos	3-Epipapyriferic acid	exact mass match	24657.24796	17740.47522	16648.84064	0.00000121	0.000000139	0.046955753	0.841924115	1.185663053	0.72467897	0.630669019	1.149063848
X13 645.441mz_pos	3-hexanoyl-NBD Choleste	exact mass match	77203.56868	48695.56068	39580.96086	4E-10	3.99E-10	0.002497843	1.480830901	3.150584499	0.607013705	0.455699639	1.332047808
X24.8 585.397mz_pos	3-Hexaprenyl-4,5-Dihydr	exact mass match	729495.4561	618664.333	547935.0519	2.82E-08	1.24E-09	0.010056215	0.347499478	1.171669527	0.77682921	0.651389783	1.19257199
X15.8 525.693mz_pos	3-Hydroxyoctadecanoyl-Q	exact mass match	31115.93434	23682.07544	17088.37567	7.83E-10	3.99E-10	0.000131933	1.100989243	2.212832871	0.759486757	0.51102898	1.486191169
X8.9 307.05mz_pos	3-Hydroxyphenytoin	exact mass match	21907.91261	6525.076782	2594.049516	0.003375581	0.001149482	0.29650248	4.445329485	6.210508172	0.330807465	0.124252335	2.662384298
X14.5 441.248mz_pos	3'-HydroxyPravastatin	exact mass match	7562.560915	18897.63986	17396.73643	0.00000635	0.000411191	0.827797932	2.840421376	2.866105656	2.340515748	0.702567093	1.156628686
X18.1 523.017mz_pos	3'-Keto-3'-deoxy-ATP	exact mass match	15548.05622	11955.17155	13335.11707	1.25E-08	6.62E-10	0.006840705	1.208841348	1.754471868	0.777958473	0.787909493	0.987370352
X9.8 166.087mz_neg	3-Methoxytyramine	exact mass match	5316.376778	2648.089551	4550.902525	0.00000259	0.0000312	0.478556385	1.975710599	5.529397995	0.662718942	0.755262934	0.877467489
X1.5 165.042mz_neg	3-Methylxanthine	exact mass match	49839.01904	12039.75114	11204.19926	0.00000359	0.000319092	0.596409682	0.339380462	0.754838432	0.285017684	0.264632238	1.077033115
X12.7 618.442mz_pos	3'-N-Acetyl-4'-O-(14-me	exact mass match	575918.0696	423504.5863	402295.4816	3.99E-10	3.99E-10	0.068359068	0.536867177	0.711723619	0.668474248	0.602545063	1.109417849
X25.9 616.427mz_pos	3'-N-Acetyl-4'-O-(9-octa	exact mass match	9546.061276	7080.658117	5990.22164	0.00497497	0.003512046	0.441743313	2.167525352	2.839098235	0.786311772	0.610683012	1.287593983
X11.6 212.02mz_pos	3-NITROPHTHALIC ACID	MS/MS spectrum match	283498.5887	31963.65412	45100.69707	3.99E-10	3.23E-08	0.824986033	1.925677835	1.048051204	0.116926168	0.161871024	0.722341564
X7.4 761.174mz_pos	3-O-beta-D-Galactopyra	exact mass match	4568.32125	10035.26362	11435.36862	0.001600917	0.000127199	0.120666338	5.460991682	4.720649784	1.964606006	2.021682212	0.971767963
X16.5 601.394mz_pos	3-O-cis-Coumaroylmaslin	exact mass match	8014.925057	5168.995395	5289.213756	0.0000004	4.98E-10	0.000530342	3.489731523	3.946016029	0.71951033	0.633622852	1.135549844
X6.5 522.365mz_pos	3-O-L-rhamnosyl-3-hydr	exact mass match	41199.28048	12786.06415	12767.79194	4.81E-08	0.000680391	0.92244231	1.469962987	2.88297861	0.316377288	0.283214594	1.117093876
X16.4 412.046mz_neg	3'-O-Methyl-(-)-epicatec	exact mass match	165717.0348	109100.7622	44628.49953	0.0000712	0.0000851	0.305767538	3.730674616	3.592213108	0.691924251	0.249911872	2.768673
X27.5 412.16mz_neg	3-O-Methylrimiterol gluc	exact mass match	966.2147378	3226.02994	3196.730366	0.0000702	0.002573526	0.895496328	4.801533596	1.425376085	2.43717887	1.862721446	1.308396849
X16.4 319.2mz_pos	3-Oxa-9-azonitricyclo[3	exact mass match	7254.705197	14672.8257	14036.15549	0.00000303	0.0000814	0.10000814	1.60419488	1.636528697	1.921440133	1.697092126	1.130452265
X8.5 529.664mz_pos	3-Oxo-OPC8-CoA	exact mass match	6822.899004	4272.299389	3250.257831	5.95E-09	3.99E-10	0.00000145	2.200365048	7.9444735	0.730737138	0.486661856	1.50152951
X15.1 474.644mz_pos	3Z-dodecenoyl-CoA	exact mass match	5662.39706	3828.696391	4667.311843	0.003339893	0.000205861	0.114711495	1.745539672	4.429981222	0.786842686	0.775140505	1.015096851
X18.6 423.271mz_pos	3a,7b,12a-Trihydroxy-6-g	exact mass match	4034.521352	16332.22216	8659.412905	0.0000043	0.000672938	0.927610371	9.429722977	7.952648288	3.38293076	1.74203227	1.941980717
X10 549.22mz_pos	3β-ACETOXY-23-BROMOC	exact mass match	88462.84121	123234.28117	64960.54489	0.000567186	0.0000518	0.12528986	3.316119794	2.937158933	1.30294622	0.643957939	2.023340567
X18 569.06mz_pos	4,6-Dideoxy-4-oxo-dTDP	exact mass match	68912.26569	53704.24182	45628.59807	2.35E-09	0.000000918	0.635399505	0.942667806	1.378931224	0.751690729	0.579420831	1.297246875
X16.7 247.17mz_neg	4,7,10,13-hexadecatetrae	exact mass match	3035.020864	6779.194838	12945.08337	0.00000889	0.0000076	0.496978393	2.60276654	2.067485888	1.904048029	2.922294052	0.651559355
X37.7 462.148mz_neg	4-(5-amino-1-methyl-1H	exact mass match	52707.99729	84404.70166	74407.53535	0.0000631	0.0000495	0.247992137	2.814843303	3.270793903	1.618184842	1.250075881	1.094462923
X27.4 531.26mz_pos	4a,7b-Dihydroxy-3-(hydr	exact mass match	32602.94925	25632.08277	20117.77482	4.32E-10	9.1E-09	0.342785985	0.723200347	1.83071554	0.778724148	0.770395322	1.218811106
X25 489.347mz_pos	4'-Apo-3,4-didehydrolycc	exact mass match	53901.17746	42653.7406	33980.50883	5.36E-10	3.99E-10	0.0000143	0.45139856	1.528867892	0.771694681	0.569381628	1.355320655
X26.4 503.019mz_pos	4-Hydroxyglucobrassicin	exact mass match	33217.73651	25347.28828	24948.47493	6.74E-10	3.99E-10	0.000107527	0.714101749	1.277430274	0.760268259	0.689097705	1.103280788
X16.4 381.086mz_pos	4-Methoxybenzyl-O-(2-su	exact mass match	45039.45344	30945.79721	20600.63003	0.000116627	0.0000975	0.279819345	3.903139138	2.622816958	0.680630272	0.421236599	1.615790921
X16.4 364.084mz_pos	4-Methylthiobutyl-desulf	exact mass match	15465.23697	9365.447383	7507.802103	0.0000741	0.000116347	0.346016429	8.946776796	2.635446011	0.635673768	0.467716705	1.359099988
X18.1 578.06mz_pos	4'-O-Demethylrebeccamy	exact mass match	16823.32051	12116.90269	9010.059972	0.00000017	0.000000333	0.153278657	2.850183369	2.550223632	0.7334453	0.511665737	1.433446189
X7.4 524.112mz_neg	4'-O-Methyldephinidin 3	exact mass match	65201.03952	98155.17966	10493.77089	0.001599157	0.000491401	0.853309089	9.276919172	9.435097411	1.543267691	0.157075538	10.21520566
X32.1 452.103mz_pos	4-Phenylbutyl glucosinol	exact mass match	30418.50064	57543.73353	62568.38352	0.0000268	0.000570002	0.737186692	3.293912579	4.486213476	1.824398297	1.771112673	1.03008596
X12.1 268.167mz_pos	4-Piperidinmethanol, a,a	exact mass match	26531.22244	10984.9061	7026.845769	0.0000677	0.00000244	0.046444879	7.678964606	7.107482464	0.443227432	0.248845522	1.781134853
X17.7 504.339mz_pos	4S,5R-antillatoxin A	exact mass match	6124.725207	4134.949834	4718.32068	0.000150625	1.54E-09	0.0000878	2.553427905	8.069360209	0.777444912	0.735966631	1.056358914
X27.2 563.068mz_pos	5,7,2',3',4'-Pentahydroxy-9	exact mass match	127826.6749	105740.2173	67409.38129	7.73E-09	4E-10	0.000175105	1.225306052	2.103839128	0.78356593	0.459476954	1.705343267
X15.8 329.233mz_neg	5,8,12-trihydroxy-9-octad	exact mass match	16009.28642	2546.475325	3963.17829	3.99E-10	4.03E-10	0.990533214	0.659973464	4.396005362	0.238674511	0.267936195	0.890788611
X1 197.068mz_neg	5-Acetylamino-6-amino-1	exact mass match	19266.12133	7937.270052	8973.06363	0.000989544	0.001282599	0.458379874	0.523986114	1.978630877	0.487736351	0.489330868	0.996741434
X26.7 502.015mz_pos	5-Azacytidine 5'-triphosp	exact mass match	10276.8588	7468.872471	7563.104929	3.98E-09	3.99E-10	4.91E-08	1.824348998	4.144736822	0.764503704	0.699114283	1.093531805
X9.7 641.069mz_pos	5-Carboxypyranocyanidin	exact mass match	84079.948834	61838.89966	37840.85134	3.99E-10	3.99E-10	0.01652262	4.426014468	3.717289765	0.707330818	0.402587539	1.756961529
X16.3 354.263mz_pos	5-Hydroperoxy-6-trans-8	exact mass match	1868.263081	7149.075314	5221.64663	0.0000229	0.001331929	0.892784728	5.898606348	5.418202431	2.732631559	1.848601445	1.478215635
X37.7 426.171mz_neg	5-hydroxyfluvastatin	exact mass match	73728.27568	119966.6132	131128.8101	0.0000924	0.0000714	0.260759186	2.979286487	2.644021767	1.629083845	1.565075508	1.040897923
X19.1 568.39mz_pos	5-O-β-D-Mycaminosyltyl	exact mass match	12993.98442	9924.759578	7167.849047	0.00000468	0.0000132	0.2984289	2.139049875	3.061359802	0.784535155	0.528973862	1.483126504
X19.4 524.03mz_pos	6-(3'-Triphosphoryl-1'-m	exact mass match	9418.226149	5590.568972	4390.084528	0.000000854	3.05E-08	0.021475631	2.812283217	4.034526183	0.656322907	0.469517926	1.397865493
X23 520.037mz_pos	6-(Methylsulfonyl)hexyl gl	exact mass match	258558.0128	222171.5666	173327.0016	4.68E-09	4.73E-10	0.004710575	0.753337931	1.72034273	0.795676954	0.588283253	1.352540549
X23.1 660.119mz_pos	6-(N-Acetyl-alpha-D-glu	exact mass match	10620.54554	7882.774542	5203.312879	0.001448758	0.003913201	0.633719325	5.106900578	8.051958323	0.782336239	0.485510232	1.611369212
X8.4 488.307mz_pos	6-bromo-5,9-hexacosadi	exact mass match	15685.95529	10548.18919	9319.66859	3.99E-10	3.99E-10	0.003282733	0.511671627	2.712639041	0.69061643	0.562821296	1.227061652
X28.5 391.157mz_pos	6-Butyryl-5-hydroxy-4-p	exact mass match	5654.463974	361177.9533	25970.21846	3.99E-10	4.82E-10	0.739929071	6.987475306	1.765569133	5.543506894	3.724369151	1.488441846
X22.8 553.047mz_pos	6-desmethylgriseofulvin g	exact mass match	16579.62608	11403.67745	9084.362781	0.0000323	0.0000211	0.205659692</					

X39.2_407.19mz_neg	6-Hydroxydexamethasone	exact mass match	7779.166893	14877.48579	19268.49947	0.003316107	0.001106944	0.292826099	5.032706569	5.618884025	1.802626935	1.982935671	0.904069801
X14.6_388.268mz_pos	6-Keto-PGF1 α	exact mass match	10546.25369	16943.58454	19324.09114	6.25E-10	0.0000075	0.833013873	4.541991127	4.079752516	1.558885534	1.626141585	0.958640716
X23.2_494.01mz_pos	6-Methoxyluteolin 3',4'-di	exact mass match	63442.92079	48827.33342	49944.38062	8E-10	4.08E-10	0.003420955	0.816782194	0.894060531	0.741273705	0.69184848	1.071439379
X33.8_359.305mz_pos	6Z,9Z-Tricosadiene	exact mass match	7612.650144	14552.03903	35871.60542	0.000959517	0.002688238	6.1017603	4.993043009	3.208199202	1.846129775	3.884515701	1.475253524
X28.2_595.382mz_pos	7,8-Didehydroastaxanthin	exact mass match	48811.99115	75921.96818	44090.13626	0.000143639	0.000954531	0.640925474	7.756528385	5.593383861	1.469353452	0.879100008	1.842426349
X21.6_489.003mz_pos	7',8'-Dihydro-8'-hydroxy	exact mass match	36775.32413	28978.07599	29675.08581	0.000000128	4E-10	0.0000248	1.072280139	1.430084545	0.779759153	0.732789936	1.064096427
X25_497.009mz_pos	7-methylguanosine 5'-diph	exact mass match	42262.25682	31498.82535	31138.24407	4.14E-10	3.99E-10	0.000128715	5.424174527	3.926547181	0.735894772	0.67109105	1.096564724
X17.2_660.945mz_pos	8-Hydroxyapigenin 8-(2''	exact mass match	13696.21545	9459.031892	10120.35715	0.000000104	0.000941673	0.931631415	0.002392946	1.732733446	0.712494362	0.689676913	1.033084259
X19.3_545.049mz_pos	8-Hydroxyluteolin 8-gluc	exact mass match	16280.298	10085.53849	7774.305734	0.000000191	0.000000153	0.290290413	2.867797104	3.392919638	0.640395199	0.458479177	1.396781429
X18.1_548.709mz_pos	8Z,11Z,14Z-eicosatrienoyl	exact mass match	31748.27318	23153.83461	16854.86985	4.16E-09	6.85E-09	0.076387864	1.914194343	2.208981067	0.728724752	0.494064468	1.474958835
X9.1_618.891mz_pos	9,10,12,13-tetrabromo-st	exact mass match	9901.133834	4739.572268	4389.255532	3.99E-10	4E-10	0.124000205	2.384117024	5.411841681	0.557035088	0.445283685	1.250966759
X14.8_329.233mz_neg	9,10,13-trihydroxy-11-oc	exact mass match	9448.58364	4327.394413	7208.156678	4.27E-08	0.001455056	0.798872314	0.773507381	2.274484522	0.57395857	0.702331888	0.817214596
X7.3_342.248mz_pos	9a-Fluoro-B-hydroxyandri	exact mass match	502370.1503	370732.1204	368860.9394	3.99E-10	3.99E-10	0.075069286	1.222154988	1.036195239	0.671758654	0.632673156	1.061778342
X28.7_311.223mz_neg	9-hydroperoxy-10E,12-oc	exact mass match	42195.1966	15807.86316	17847.30057	0.0000252	0.001460197	0.898033489	1.053921518	1.116878585	0.41558844	0.686791295	1.074451378
X10.8_300.216mz_pos	AcAr 9:1	MS/MS spectrum match	146420.2288	113359.8661	118695.4936	0.003570834	0.004785157	0.055171104	1.035734306	1.6017336	0.726139971	0.702888879	1.033078321
X17.2_579.732mz_pos	ACETRIAZOIC ACID	exact mass match	10087.12938	7489.358887	6045.758887	0.00057715	0.00000122	0.009111493	2.127196982	2.884215944	0.777430702	0.579360986	1.341876171
X14.7_513.362mz_pos	Acetyl-11-keto-B-Boswel	exact mass match	30069.69688	19471.43507	18272.69274	1.22E-08	1.12E-08	0.066802028	2.134832052	1.420375847	0.649559085	0.560926806	1.158010417
X27.1_548.392mz_pos	Acinosisperigenin A	exact mass match	54911.28567	45005.18931	29124.22505	0.000119572	0.000000184	0.02962475	2.945859065	2.254516393	0.799641033	0.484933514	1.648970446
X20.8_657.12mz_pos	Actinorhodin	exact mass match	12751.90206	8925.178099	4469.968123	0.00000829	0.004734218	0.988354104	4.76784643	6.662540495	0.732595548	0.354737133	2.065178637
X22_465.997mz_pos	Acyclovir triphosphate	exact mass match	12632.0355	8140.682119	6257.637462	1.05E-09	4.31E-10	0.006470216	3.202754599	6.581896871	0.674574477	0.483688321	1.394647025
X18.2_525.034mz_pos	Adenosine triphosphate (A	exact mass match	80413.6574	61477.66887	50370.16984	4.1E-10	4.02E-10	0.008398298	1.829014997	2.151561013	0.734218007	0.549215895	1.336847702
X15.7_500.379mz_pos	Adlupone	exact mass match	1546437.221	1138536.614	1083377.949	3.99E-10	4.01E-10	0.259107982	0.42563522	0.805723533	0.671448663	0.632580988	1.061443003
X15.2_521.021mz_pos	Aerophobin 2	exact mass match	16523.21851	12138.16942	10058.63439	6.59E-09	0.000005533	0.796234709	1.546747863	2.31777556	0.747436532	0.572193689	1.3062649
X7.4_481.154mz_pos	a-L-Fucopyranosyl-(1->2	exact mass match	63694.24496	96290.93072	43951.58945	0.000112097	0.000303453	0.456169951	3.678724057	3.768153925	1.422493462	0.608798006	2.336560646
X8.7_383.034mz_pos	Alginic acid	exact mass match	9998.008752	5596.711712	4696.846222	0.002018704	0.0000087	0.086191559	3.570621429	2.739951424	0.617375362	0.43021731	1.435030795
X27.7_743.457mz_pos	Alliosterol 1-rhamnoside	exact mass match	5083.044698	7654.340022	8751.103948	0.000230481	0.00050661	0.463889788	2.151785882	7.846156111	1.4363446398	1.451493719	0.989564322
X21.7_483.328mz_pos	all-trans-Carophyll yellow	exact mass match	62368.83604	49585.25105	56250.05178	3.12E-09	2.68E-08	0.168512021	2.265017766	1.167455353	0.7654766	0.760217144	1.006918361
X29.7_585.071mz_pos	alpha-D-Galactopyranuro	exact mass match	10637.87201	6992.11196	6484.131865	0.000434541	0.00000664	0.035906085	4.210866048	2.302570947	0.702115287	0.619164814	1.133971554
X19.9_422.186mz_pos	AM1235	exact mass match	3602.881908	8616.221108	8092.308983	0.000100931	0.002188004	0.866266893	4.698529189	2.39317366	2.051116356	1.736412968	1.18123764
X13.6_306.19mz_pos	AMIPRILOSE	exact mass match	4438.48227	8547.029892	8191.009018	0.000000231	0.001530126	0.923444695	2.779788274	3.207511042	1.752999278	1.536513752	1.140893973
X16.3_258.177mz_pos	amitraz	exact mass match	27210.28616	46712.96854	47836.19856	0.00000523	0.00479234	0.971112032	0.822446404	0.881393743	1.622462696	1.524194835	1.064471981
X13.2_241.144mz_neg	AMPROLIUM	exact mass match	4413.475436	5362.035072	8504.586566	0.003086444	0.002451276	0.000000101	4.904019105	7.069253988	1.223922676	1.470376225	0.832387423
X42.1_572.415mz_pos	Anhydroeschscholtzanthi	exact mass match	14211.1121	28021.77491	32312.80263	0.000000624	0.002584266	0.921491223	4.216816556	1.256986011	1.883216279	1.962750956	0.959477958
X42.3_572.415mz_pos	Anhydroeschscholtzanthi	exact mass match	21042.37451	37440.42732	44581.98915	0.0000275	0.0000422	0.297009806	3.564680542	0.743843871	1.69333163	1.838194938	0.92119263
X11.4_705.463mz_pos	Antanapeptin C	exact mass match	136439.9858	105986.024	118922.5482	4.09E-10	4.78E-10	0.060471002	0.967089277	1.25852693	0.726223411	0.753680639	0.963569148
X9.7_641.404mz_pos	Apicidin	exact mass match	44853.55175	33136.58002	23823.44644	3.99E-10	3.99E-10	0.016174014	3.242508445	3.856263547	0.730655205	0.49551459	1.474538227
X12.7_323.242mz_pos	Aprindine	exact mass match	10390.13551	7423.167584	7027.067658	4.13E-10	3.99E-10	0.000000423	1.656927671	1.294391783	0.751895717	0.644973914	1.165776942
X14.3_354.284mz_pos	Arachidic acid(d3)	exact mass match	55549.66455	41822.08364	39289.42982	1.11E-09	6.18E-10	0.021277432	0.914338789	1.014420709	0.732887718	0.628168637	1.166705364
X15.6_615.431mz_pos	Arachidonic Acid-biotin	exact mass match	164938.5101	116241.4512	132514.1231	3.99E-10	3.99E-10	0.031632262	0.983611273	1.137482059	0.659503085	0.697937031	0.944932074
X18.2_383.287mz_pos	Arachidonoyl 2'-Chloroet	exact mass match	31705.13081	21052.42341	19710.14673	3.99E-10	3.99E-10	0.0000234	1.32057606	2.569797492	0.669467739	0.572616512	1.169138027
X18.1_748.541mz_pos	Arachidonoyl thio-PC	exact mass match	2434524.299	1701520.037	1619289.947	3.99E-10	4E-10	0.140779539	0.488637674	0.968883812	0.649031865	0.60446602	1.073727626
X30.6_357.241mz_pos	Arachidonyl Trifluorometh	exact mass match	3295.296569	12746.22806	15481.59591	3.99E-10	5.14E-10	0.243088635	4.806390762	1.198158377	3.167083717	3.446115504	0.919030054
X14.9_348.237mz_pos	Arginyl-Arginine	exact mass match	15723.10368	26550.50031	28427.71649	0.00000337	0.0000869	0.625846131	3.745027687	1.155216756	1.605841936	1.585245032	1.012992883
X13.6_289.164mz_pos	Arginyl-Asparagine	exact mass match	15129.67169	28169.71303	23813.48664	0.00000158	0.000325218	0.909222043	2.949955121	2.49841728	1.760343695	2.394491157	1.258744959
X8.5_322.185mz_pos	Arginyl-Phenylalanine	exact mass match	9814.429714	18772.48653	22447.87013	1.25E-08	0.000477801	0.874043412	5.516247103	4.7583324	1.832355443	2.004239758	0.914239644
X10_464.217mz_pos	Aspergamide A; 6b-hydro	exact mass match	9098.069659	15165.91704	15353.38547	0.001151791	0.002547822	0.574302654	2.351073947	1.053956769	1.622759631	1.528229118	1.061856244
X17.1_583.056mz_pos	ATB-343	exact mass match	4761.612901	3202.144606	2808.546005	0.001188246	0.0000004	0.014571114	5.773320306	11.70399662	0.791480322	0.567600425	1.394432221
X19.9_620.363mz_pos	Avermectin A2b aglycone	exact mass match	21507.59472	33373.06652	32023.69218	0.00085124	0.0000402	0.080771119	7.661509525	4.977529995	1.478653482	1.310675201	1.128161638
X22.3_732.546mz_pos	bacteriohopane-32,33,34	exact mass match	1961321.012	1389724.511	1263959.366	3.99E-10	3.99E-10	0.092395945	0.248466609	1.031683535	0.652658984	0.587903209	1.110147
X22.4_688.52mz_pos	bacteriohopane-31,32,33	exact mass match	47067.39258	32822.44117	25851.27706	4.03E-10	4.03E-10	0.016235155	0.888171127	1.68934874	0.693485392	0.506782621	1.368407998
X19.7_614.447mz_pos	Bacteriorubixanthinal	exact mass match	10182.31827	7369.127986	5974.472257	0.000000017	1.75E-09	0.017281643	1.246416327	2.605531565	0.767256612	0.570111785	1.345800301
X15.7_412.325mz_pos	benzethonium	exact mass match	803926.4394	620943.556	684157.4716	3.99E-10	5.59E-09	0.792313821	0.530090521	1.432557166	0.701107211	0.744634375	0.941545589
X22.1_465.328mz_pos	benzethonium chloride	exact mass match	73919.72358	53620.14315	50136.26226	3.99E-10	4E-10	0.027190353	0.633308528	1.13338886	0.697385201	0.591936556	1.178141802
X22_453.977mz_pos	BENZTHIAZIDE	exact mass match	15655.77882	12273.3874	13633.72914	1.83E-08	4.01E-10	0.000131795	1.496470511	1.690392583	0.792017918	0.798616388	0.991737623
X32.1_401.148mz_neg	Benzyl beta-primeverosid	exact mass match	11328.29302	22325.97467	22202.27801	0.0000173	0.0000202	0.24527604	3.328117422	3.24390999	1.934716709	1.630964841	1.186240598
X10.8_367.269mz_pos	BEPRIDIL	exact mass match	27443.73908	20700.11173	12711.83315	0.00000125	3.99E-10	0.000002604	1.407632045	3.183618249	0.754133298	0.432818062	1.742379454
X12.1_394.084mz_pos	Berberine chloride	exact mass match											

X37.7_704.433mz_neg	beta1-Chaconine	exact mass match	47303.72374	79937.28659	139060.0576	0.002301321	0.00112474	0.335170954	1.79768479	2.054960634	1.688113138	2.566133569	0.657843052
X19.1_982.687mz_pos	beta-D-Mannosylphosph	exact mass match	133053.0355	84613.86118	67809.9807	3.99E-10	3.99E-10	0.005743365	0.558173756	1.860135268	0.602007857	0.441423458	1.363787643
X22.4_724.831mz_pos	Bisdiphosphoinositol tetra	exact mass match	9171.164529	6616.354579	3716.434322	0.000593502	0.000275548	0.26929265	5.211217404	5.385284108	0.776761215	0.41412268	1.875679002
X37.7_382.204mz_pos	Bisphenol A dimethylacrylat	exact mass match	354668.6942	511480.6217	898403.9558	0.00184973	0.000505649	0.243607939	1.516098243	1.956703549	1.305357549	2.219441588	1.588146837
X14.3_431.12mz_pos	Bispyribac	exact mass match	7947.848155	10174.13371	6271.020917	0.002200925	0.000279706	0.165231618	5.638037089	4.153262452	1.273533502	0.74238127	1.714547141
X26.2_543.102mz_neg	Bis-γ-glutamylcystine	exact mass match	340.314991	8605.702205	2695.606503	3.99E-10	5.02E-10	0.015027268	0	8.146293047	21.46331269	6.781354965	3.165047812
X26.2_423.209mz_pos	Blasticidin S	exact mass match	50374.72952	518812.5319	444499.3151	3.99E-10	1.26E-08	0.992475604	5.645345917	0.568658054	9.683809901	7.6795731	1.26098284
X10.2_472.311mz_pos	Borrelidin	exact mass match	13157.2306	9333.351572	8735.932554	9.86E-10	0.000000634	0.693909772	0.951914788	2.146129576	0.735388515	0.626410394	1.173972401
X25.6_448.98mz_pos	butoconazole	exact mass match	5000.984662	2489.772287	3093.570521	0.00000569	2.66E-09	0.001299639	4.742666582	9.612414805	0.644750092	0.590441238	1.091980117
X18.7_621.417mz_pos	Butyl 4'-O-hexadecanoyl	exact mass match	84140.54849	60767.80635	75908.67933	4E-10	3.99E-10	0.001013908	2.09222165	2.522206956	0.685531778	0.777975948	0.881173485
X19.3_513.013mz_pos	C.I. Pigment Yellow 100	exact mass match	8184.343276	5704.550205	6083.372626	0.0000059	7.2E-09	0.000737374	1.358045342	2.567823807	0.762748644	0.708398659	1.076722316
X12.8_411.295mz_pos	C19 Sphingosine-1-phosph	exact mass match	9128.559467	6669.156405	7357.700505	0.00000124	2.64E-08	0.016500059	2.355042449	2.096913147	0.778597348	0.760076584	1.024366972
X18_836.593mz_pos	C20 Sulfate	exact mass match	1286095.317	903235.2766	829359.2682	3.99E-10	3.99E-10	0.126247899	0.522482276	0.950499118	0.650831537	0.589008169	1.104961817
X17.8_880.62mz_pos	C22-OH Sulfate	exact mass match	505033.0433	332563.3415	331915.3867	3.99E-10	3.99E-10	0.016169133	0.82578879	0.771142282	0.604447364	0.558426399	1.082411872
X25.6_892.656mz_pos	C24 Sulfate	exact mass match	946149.1274	648849.0734	620841.2296	3.99E-10	3.99E-10	0.007550541	0.544975192	1.182908616	0.616929897	0.563189763	1.095421005
X22.9_453.825mz_pos	C24:1-OH Sulfate	exact mass match	351054.843	224855.2202	269866.0293	3.99E-10	3.99E-10	0.008454452	1.228990963	1.149028264	0.643173068	0.655394469	0.984356462
X10.2_272.185mz_pos	C75	exact mass match	29631.01167	50454.75066	54467.27786	0.00012866	0.003653492	0.896345178	3.365282034	2.410540541	1.618733809	1.602515614	1.01012046
X16.4_253.133mz_pos	Camoensine	exact mass match	39252.24237	25507.63867	26557.40172	0.0000088	0.000634461	0.620700876	1.260146487	0.815424858	0.647134919	0.609452728	1.061829556
X16.2_343.263mz_pos	Cannabidiol dimethyl ethe	exact mass match	67010.89503	114259.9813	170781.7554	0.002680022	0.0005477	0.220385748	1.89609399	1.21287771	1.615489816	2.151708632	0.750793947
X11.2_678.463mz_pos	Carbaprostacyclin-biotin	exact mass match	613373.1974	474228.8786	416957.0004	3.99E-10	4E-10	0.073201899	0.450166384	1.18385167	0.699500144	0.582228679	1.201418222
X17.2_544.037mz_pos	Carmoisine	exact mass match	28131.50894	22185.9172	19208.84479	0.000000051	2.26E-09	0.012903545	1.276458762	1.846810545	0.786203805	0.62926319	1.249476987
X4.1_479.1mz_pos	CCG-100602	exact mass match	12883.00927	17610.65638	7157.276909	0.004860157	0.000540741	0.10704172	10.69683213	7.768594547	1.332607794	0.526494392	2.531095892
X9.5_604.047mz_pos	CDP-glucose	exact mass match	83059.89357	60936.47058	47676.23278	3.99E-10	3.99E-10	0.000204026	1.339915954	2.173432863	0.703740745	0.501515427	1.40322851
X26.5_516.022mz_pos	CDP-glycerol	exact mass match	48126.17183	33699.42999	32831.48093	1.93E-09	4.8E-10	0.008119975	1.598717843	2.230461669	0.689325931	0.618186364	1.115077864
X26.6_502.337mz_pos	Ceanothine D	exact mass match	1726535.078	1112015.411	1058706.589	1.76E-09	0.00000101	0.685783644	2.322257474	2.227332954	0.584123271	0.552318673	1.057583782
X22.7_535.046mz_pos	Cefamandole nafate	exact mass match	156484.9147	131621.2615	106263.0908	0.00000168	5.07E-08	0.021898016	0.656743561	1.37589232	0.789300255	0.591064922	1.335386733
X17.8_643.105mz_pos	CEFDITORIN PIVOXIL	exact mass match	8930.326842	6056.484016	3260.266602	0.0000123	0.000324184	0.719638825	3.289565606	6.559087195	0.734545026	0.37969691	1.934556238
X23.4_492.003mz_pos	Cefixime	exact mass match	41294.71676	29553.72593	31498.97973	5.79E-10	4.12E-10	0.006354567	1.627793369	3.001069968	0.70803944	0.692042441	1.023115633
X18.3_534.034mz_pos	Cefmenoxime	exact mass match	44065.00841	31715.03726	25640.86167	8.91E-10	4.08E-10	0.002965821	1.717916357	1.927101751	0.71403899	0.535761401	1.332755568
X9.2_567.024mz_pos	Cefodizime	exact mass match	70506.43578	49727.32116	46101.27462	3.99E-10	3.99E-10	0.006015513	0.510293765	1.649963383	0.678879285	0.57099244	1.188946188
X24_543.042mz_pos	Cefonicid	exact mass match	43330.02556	34550.51532	36777.93103	0.00000695	0.00000012	0.019789357	0.933901155	1.964161327	0.78614963	0.768040388	1.023578503
X22_632.106mz_pos	Cefoperazone sodium	exact mass match	52526.47285	41643.52563	30774.62231	0.00000174	0.000000236	0.055125276	1.794995828	2.120268188	0.772758851	0.535378522	1.443387845
X27.2_558.062mz_pos	ceforanide	exact mass match	22768.08702	16780.66016	10542.14099	0.00000276	4.88E-10	0.00151071	3.747384909	3.297711464	0.74129663	0.439348783	1.68726228
X27.1_494.019mz_pos	Cefotaxime	exact mass match	19129.2944	13065.18505	8292.912445	0.000000306	2.27E-09	0.005496107	5.093535095	3.895217283	0.694687406	0.417569372	1.663645499
X10.3_382.03mz_neg	Ceftizoxime	exact mass match	31356.26489	40533.51278	5408.727405	0.000272808	0.00432058	2.48E-08	7.264876308	7.594777911	1.337398116	0.177452026	7.536674261
X18.1_555.053mz_pos	Ceftriaxone	exact mass match	23044.22947	15939.14807	14064.81121	1.97E-08	0.000000396	0.306436803	1.592909195	1.626591096	0.696681378	0.56883254	1.224756549
X23.3_485.01mz_pos	Cefuroxime sodium	exact mass match	53009.59518	41724.46655	34676.34814	4.94E-10	3.99E-10	0.000159992	0.691077321	1.081772876	0.770810489	0.593746969	1.298213766
X8.3_451.283mz_pos	Celastrol	exact mass match	23159.02844	11775.61542	10388.59307	3.99E-10	3.99E-10	0.027435543	1.908756066	5.495372043	0.525308257	0.421866219	1.245201045
X21.9_483.997mz_pos	Cephapirin sodium	exact mass match	16079.27987	11558.6179	13346.32766	0.00000304	0.000000151	0.033331239	1.946335802	2.726010807	0.733350688	0.76966653	0.952816134
X21.8_776.572mz_pos	Cerebroside C	exact mass match	2488546.779	1766236.564	1449631.057	3.99E-10	3.99E-10	0.044689393	0.352932811	1.273817471	0.661306589	0.525324254	1.258854096
X18.6_656.442mz_pos	CerP(d18:1/16:0)	exact mass match	9035.643646	5938.744627	6941.566021	0.00000936	0.00000133	0.075356963	8.494263872	8.733785003	0.714003301	0.723203437	0.987278634
X14.4_381.284mz_pos	Cetyltrimethylammonium	exact mass match	41201.59686	30449.31553	34413.51445	3.99E-10	3.99E-10	0.013505785	1.02784508	1.511681208	0.752856505	0.967543885	
X37.7_379.179mz_neg	Chaparrin	exact mass match	23556.08696	41428.58112	45272.3575	0.00038049	0.00002293	0.095979071	3.902545771	4.501546595	1.731186106	1.654756187	1.046188024
X16.4_360.088mz_neg	Chelirubine	exact mass match	4216.585718	8590.239275	2585.259	0.001028037	0.000258196	0.214238482	8.572447785	7.376671331	1.918183307	0.612704781	3.130681148
X19.1_571.714mz_pos	Chenodeoxycholoyl-CoA	exact mass match	9103.687473	6085.001091	6859.390497	0.000774521	0.0000101	0.035034163	2.279314427	2.990616107	0.726453511	0.716799427	1.013468321
X20.7_460.99mz_pos	Chloramphenicol succinat	exact mass match	22228.80696	15887.39965	13171.40782	1.72E-08	4.03E-10	0.000247998	1.025970002	1.509244605	0.722632509	0.55560241	1.300628822
X23_508.685mz_pos	Chlordecone	exact mass match	80279.67948	65696.03724	67970.57161	0.000000259	6.33E-09	0.0013015406	0.577712996	1.244323588	0.781463623	0.740873802	1.454786418
X18.3_510.693mz_pos	Chlordecone alcohol	exact mass match	28161.54789	21344.12441	14077.49467	2.41E-09	2.1E-09	0.046629572	2.014994897	2.849144668	0.753197293	0.468237865	1.608578353
X13.3_373.273mz_pos	cholocalcic acid / 25,26,	exact mass match	7507.522817	15997.64981	16950.26787	0.00000418	0.000536347	0.901618829	2.627241977	1.452515948	2.024328528	1.983838857	1.020409758
X7.3_587.376mz_pos	cholesteryl beta-D-glucos	exact mass match	9659.465034	3400.712124	3145.563133	5.07E-08	1.04E-08	0.036594061	1.481350101	10.11553173	0.430282057	0.320968233	1.340575211
X17.4_491.011mz_pos	Cl Acid Orange 3	exact mass match	42608.69674	32226.07504	26187.80423	6.89E-10	5.61E-10	0.025574287	0.785119059	1.100298633	0.750501726	0.565191844	1.327870763
X6_147.045mz_neg	Cinnamic acid	exact mass match	13165.32169	7434.146186	9601.432202	0.00000029	0.000218895	0.800879279	0.737534468	1.43812915	0.645979544	0.663600673	0.973446185
X15.5_383.205mz_pos	Cinnacissol C3	exact mass match	7915.480307	12899.8187	12193.95904	0.00000162	0.001898197	0.958378085	0.944422912	2.288151965	1.572317072	1.36795313	1.149393964
X14_427.232mz_pos													

X10.9_615.244mz_pos	Clomiphene citrate	exact mass match	10472.21252	15551.7806	14708.13592	0.00066049	0.000307143	0.273732304	9.792903929	6.446578784	1.461539716	1.265045783	1.15532555
X19.3_538.705mz_pos	CoA(20:0(3Ke))	exact mass match	9418.678733	6723.773392	4755.15053	0.00000268	6.31E-10	0.00037586	1.981850374	4.06363546	0.763210746	0.502203692	1.519723488
X27.2_566.727mz_pos	CoA(24:0(3Ke))	exact mass match	14962.09779	11206.29042	11441.80733	0.000178718	0.000145511	0.294290012	6.509054909	4.785819863	0.761867791	0.712314316	1.069566866
X28.7_567.74mz_pos	CoA(24:0(3OH))	exact mass match	66120.52425	52431.38168	30936.33099	9.14E-10	3.99E-10	0.000289807	1.511633552	2.528964204	0.765774975	0.424790665	1.8021714
X22.8_715.518mz_pos	COCONUT;(CNP0084305)	Sirius match	181061.7858	112394.6573	140528.2161	4.06E-10	3.98E-09	0.352796506	1.759274969	2.70084258	0.586149267	0.674943597	0.868441852
X27.8_355.226mz_pos	COCONUT;(CNP0118734)	Sirius match	59892.13113	283317.1587	362636.5033	3.99E-10	6.56E-10	0.952924823	3.535997821	0.82947159	4.449510629	5.522390251	0.805721875
X15.6_265.108mz_neg	COCONUT;(CNP0238385)	Sirius match	25529.35911	13917.64524	18657.71794	0.000000509	0.000427651	0.988616178	0.669352647	1.11258567	0.589482762	0.670147967	0.879630755
X15.9_329.233mz_neg	COCONUT;(CNP0275063)	Sirius match	20803.62898	3870.435653	5424.408682	3.99E-10	3.99E-10	0.859946279	0.752873952	1.437090409	0.256417051	0.27445059	0.93429222
X18.1_455.317mz_pos	Coenzyme Q4	exact mass match	23246.52757	18674.33602	3583.89468	0.0000332	3.99E-10	1.55E-09	4.920428726	7.68688881	0.799135265	0.158775787	5.03310538
X20.1_613.419mz_pos	Coenzyme Q6	exact mass match	28573.3779	18337.21181	15693.59601	4.34E-10	4.02E-10	0.005310773	1.763596102	2.224728784	0.648232363	0.514623274	1.259625041
X14.5_387.2mz_pos	Corchoinol C 9- glucoside	exact mass match	5643.380311	8357.602105	9127.216708	0.00026758	0.002118389	0.722857501	2.199450923	3.193520677	1.429221918	1.402070871	1.01936496
X15.4_269.174mz_pos	Corey PG-Lactone Diol	exact mass match	6416.635847	8573.371738	9131.720888	0.000746262	0.000316767	0.266539228	1.422733675	2.119196566	1.315718405	1.266342463	1.038990986
X12.1_305.195mz_pos	CPX	exact mass match	662219.0338	411672.5756	520203.4841	0.00000152	0.000608609	0.980822723	0.933243892	1.418559901	0.572448844	0.674879228	0.848224128
X28.9_497.291mz_neg	Cucurbitacin S	exact mass match	16570.20033	5325.225324	4939.764703	0.0000015	0.002171067	0.982263743	3.183055061	10.24081286	0.353241795	0.293447576	1.203764571
X16.4_360.237mz_pos	Curaclin D	exact mass match	8816.056607	13839.77236	15988.31719	0.0000718	0.001597137	0.81676705	3.708793133	3.388299647	1.518651384	1.605794066	0.945733042
X22.647.117mz_pos	Cyanidin 3-(2''-glucuronol	exact mass match	19274.67153	14258.43581	9251.571334	0.0000661	0.000714568	0.677243821	4.810317782	6.139949832	0.462899199	0.562869553	1.621403191
X20.593.079mz_pos	Cyanidin 3-(6''-dioxalylglu	exact mass match	55333.28941	42795.30214	36079.54293	5.75E-09	0.00000056	0.462207623	0.910412403	1.495757394	0.753316219	0.589551747	1.277777944
X12.1_448.104mz_neg	Cyanidin 3-galactoside	exact mass match	14035.60323	7741.824582	2102.486267	0.0000964	0.000024	0.149510133	6.130598915	11.51384024	0.627574439	0.172737523	3.6331101
X5.7_462.118mz_pos	Cyanidin 3-O-(6''-acetyl-	exact mass match	8058.87515	12658.58198	5472.026961	0.001029728	0.0000786	0.110662434	5.138741142	7.499122533	1.518627027	0.649416898	2.338447046
X25.8_544.056mz_pos	Cyanidin 3-O-(6''-malony	exact mass match	141879.434	118683.0588	81169.67849	4.61E-09	3.99E-10	0.0000855	0.978667999	1.418934081	0.789434829	0.497085168	1.588127911
X3.7_202.053mz_pos	Cyclamate	exact mass match	3636.398928	12369.01307	12358.48037	0.000653195	0.000656489	0.38899022	5.499291341	6.534835554	2.808324391	2.558490394	1.097648988
X27.5_537.376mz_pos	Cyclotricuspidogenin C	exact mass match	46378.63528	34081.91851	32533.51774	6.24E-10	4.05E-10	0.003351758	1.026672177	1.106485898	0.726974916	1.106485898	1.134552902
X21.8_861.48mz_pos	Cyclotricuspidoside C	exact mass match	16125.56909	40756.88352	40191.43181	0.00277228	0.000207222	0.125567314	3.819659525	2.884133124	2.334040806	2.130226082	1.095677509
X13.432.099mz_pos	Cyhalothrin	exact mass match	6230.46337	7583.640929	3499.822158	0.000713321	0.00000591	0.025594974	6.235964615	5.689876111	1.214560582	0.564079231	2.15317373
X16.5_501.014mz_pos	Cytarabine triphosphate	exact mass match	36191.23811	27149.68758	22075.34177	7.66E-10	3.99E-10	0.000144843	0.780235209	1.374113396	0.748817952	0.560466231	1.327676735
X26.4_509.029mz_pos	dATP	exact mass match	48067.77051	37785.44644	29631.88473	8.07E-10	3.99E-10	0.0000221	0.398929929	1.317088465	0.773742691	0.56782467	1.362643668
X12.1_358.107mz_pos	Deacetoxycephalosporin C	exact mass match	27061.04227	15805.42905	17908.90352	0.00000924	0.000675052	0.870215861	4.411640005	2.511904565	0.591986558	0.600511507	0.985803853
X28.516.691mz_pos	Decachlorobiphenyl	exact mass match	16118.68749	12102.52163	12689.73336	2.18E-09	3.99E-10	0.000000234	1.634604748	1.823128687	0.759421311	0.736516598	1.031098706
X19.583.345mz_pos	Deferoxamine	exact mass match	34831.47929	44999.23018	12988.05083	0.003912646	0.000545073	0.188331802	13.144819	8.684483621	1.247541166	0.348209943	3.582727007
X13.8_417.164mz_pos	Dehydronimidopine	exact mass match	53202.55345	30293.66202	44143.13322	0.002199255	0.00033967	0.184141646	1.733256532	2.999136299	0.710750922	0.794793041	
X10.5_752.137mz_pos	Delphinidin 3-(6''-malony	exact mass match	36037.16324	25695.19306	11373.9621	4.01E-10	4.04E-10	0.025787856	9.952239142	8.66960851	0.714277343	0.301684975	2.367626506
X21.9_676.133mz_pos	Delphinidin 3-O-(2''-O-g	exact mass match	11289.95133	8186.57567	5343.730212	0.0000452	0.000548403	0.671232369	6.772713949	5.874766493	0.76142155	0.476949854	1.596439424
X19.9_637.105mz_pos	Delphinidin 3-O-3'',6''-O-	exact mass match	24242.09686	17918.50407	13942.88375	0.000000364	4.32E-08	0.048516016	1.343618619	2.709067097	0.7424881708	0.539702702	1.375723533
X22.661.123mz_pos	delphinidin-3-O-(6-p-co	exact mass match	21148.07649	16116.58033	10831.75163	0.00000407	0.00000247	0.143139823	3.218281587	4.468176527	0.766296292	0.486394524	1.575462415
X21.7_486.014mz_pos	Deoxyuridine triphosphate	exact mass match	31724.65198	24074.38672	18754.06852	5.59E-08	1.08E-09	0.006320408	1.554052916	1.570485968	0.761709894	0.551958154	1.380013845
X13.1_472.347mz_pos	DEQUALINIUM	exact mass match	233003.6307	172305.5129	161727.178	3.99E-10	4.03E-10	0.137205236	0.309284836	1.311070526	0.68601885	0.603740461	1.136281058
X37.7_442.09mz_neg	Desmethylhalofantrine	exact mass match	1470615.332	2391225.158	3618180.499	0.000516919	0.000290053	0.288985934	1.424108606	1.190382105	1.543510444	2.30349838	0.670072294
X10.2_530.39mz_pos	DG(14:0/0:0/14:0) (d5)	exact mass match	8681.450944	6240.323043	6558.024987	0.00000145	0.000699563	0.984069822	1.372516499	3.815475775	0.772649026	0.713705675	1.082587757
X17.1_558.421mz_pos	DG(15:0/0:0/15:0) (d5)	exact mass match	2444817.07	1763915.581	1637255.888	3.99E-10	4.28E-10	0.150464587	0.620339095	1.065445507	0.678522335	0.613081295	1.106741211
X21.3_586.452mz_pos	DG(16:0/0:0/16:0) (d5)	exact mass match	1344766.867	985790.5964	887564.5191	4E-10	4.58E-10	0.113352459	0.484583768	0.919883991	0.675956913	0.596278434	1.133626297
X12.9_706.494mz_pos	DG(20:2(11Z,14Z)/0:0/20:2	exact mass match	632773.882	452214.0058	395501.6806	3.99E-10	3.99E-10	0.017388325	0.281882466	0.863019125	0.643843683	0.533197882	1.207513578
X16.9_673.473mz_pos	DG(20:5(5Z,8Z,11Z,14Z,17	exact mass match	385865.1499	262020.056	313494.9909	3.99E-10	3.99E-10	0.084632743	1.10713988	1.340049356	0.629391298	0.692432377	0.90895706
X10.3_356.264mz_pos	DHA (d5)	exact mass match	24844.40923	15660.12419	14127.83047	0.00000115	4.46E-08	0.02397828	0.789698541	1.444539636	0.63831185	0.530197711	1.203912874
X16.4_367.048mz_neg	DIACERIN	exact mass match	72801.26686	45903.31776	32422.61088	0.0000664	0.001456486	0.808625584	2.061138584	1.686413869	0.663648006	0.406608341	1.634325895
X16.4_391.989mz_neg	Dialifor	exact mass match	164158.3531	93818.8842	65171.90641	0.0000309	0.000707237	0.760746187	1.518640678	1.080410903	0.597788537	0.37241672	1.605160308
X4.9_505.302mz_pos	Digitoxigenin monodigitox	exact mass match	37490.63979	11380.33625	11661.62038	7.07E-08	0.000257607	0.999499533	1.551817494	2.426708466	0.31026318	0.28403209	1.09235256
X25.3_601.288mz_pos	Dihydro Isorescinnamine	exact mass match	16923.68771	27410.82381	13918.51146	0.0000174	0.000144912	0.356557178	6.227702133	3.594152872	1.547188411	0.748392782	2.067522166
X10.515.269mz_pos	DIHYDROFISSINOLIDE	exact mass match	43446.45487	73644.19386	295673.93	0.000282023	0.002170923	0.721386646	7.499597788	7.83460714	1.542418429	5.606557574	0.27510971
X10.2_287.184mz_pos	Dihydrolysergic acid amid	exact mass match	7128.436872	9431.902325	9818.558038	0.000107378	0.000853963	0.654268249	1.238197154	2.716316555	1.302332716	1.234550357	1.054904491
X20.1_528.357mz_pos	Dihydroproprymycin	exact mass match	74653.99668	58435.72468	60147.55709	1.66E-09	3.99E-10	0.00000534	1.321222594	2.100752456	0.753129215	0.704678884	1.06875519
X16.4_259.19mz_pos	Diisobutyl adipate	MS/MS spectrum match	9673.641073	17385.1384	22018.27208	0.0000543	0.000447923	0.611662037	4.521621163	2.827616856	1.714274458	1.972981163	0.868875228
X25.1_634.256mz_pos	Dimoracin	exact mass match	7370.688133	13198.22631	3852.143421	0.00000184	0.002247561	0.986471516	6.815403066	7.543526617	1.709299465	0.511473813	3.341910026
X23.4_479mz_pos	Dioxation	exact mass match	25750.74197	19116.86371	18218.08735	0.0000135	0.0000412	0.358141975	1.880674544	0.745004837	0.654699781	1.137933536	
X9.4_241.108mz_neg	Diphenylcarbazine	exact mass match	9536.639959	5380.908198	6740.465201	2.18E-08	0.00000018	0.215693333	0.98510778	1.897307066	0.663629315	0.646166306	1.027025564
X12.1_350.253mz_pos	Dipipanone	exact mass match	710797.1638	453087.0356	622659.7714	0.00000126	0.000374979	0.939996985	3.273491482	1.882074995	0.587836763	0.752904943	0.780758273
X25.483.672mz_pos	Diallosyl galactosyl glob	exact mass match	52698.38892	46292.88198	44292.88198	4.27E-10	4.01E-10	0.004231704	0.888217725	1.24437679	0.752069125	0.715188941	1.05156705
X16.1_432.259mz_pos	Distigmine	exact mass match	14658.13										

X28.1_519.042mz_pos	Dithiazanine iodide	exact mass match	73750.65234	55892.08519	36385.65594	3.99E-10	3.99E-10	0.0000115	1.046012953	1.974946861	0.729780023	0.442353824	1.649765378
X17.9_497.368mz_pos	DL-PPMP	exact mass match	10041.1745	7280.57713	8535.196222	2.36E-09	0.000000103	0.321792465	1.52308441	2.035203065	0.765280668	0.792476186	0.965682883
X14.2_398.311mz_pos	Docosatraenoyl Ethanol	exact mass match	590700.0086	460782.9277	437523.6337	3.99E-10	3.99E-10	0.052639509	0.398278	0.93710133	0.710663391	0.63567609	1.117964641
X19.3_544.715mz_pos	Docosenoyl-CoA	exact mass match	45303.12543	34359.06154	23695.965	2.41E-08	4.57E-10	0.001679921	1.22229657	2.159271012	0.749354806	0.484088448	1.54797085
X26.1_421.226mz_neg	docusate	exact mass match	165494.3586	334439.8348	517680.8609	0.000000142	0.0003528199	0.744176206	3.587542998	3.045054821	2.030638286	2.957300911	0.686652575
X23.7_479.335mz_pos	Dolicholide	exact mass match	48887.12414	37698.88491	40922.61316	8.35E-09	0.00000581	0.786556807	1.140732212	1.44141527	0.755605169	0.747009896	1.011506237
X5.5_463.291mz_pos	dolichyl phosphate	exact mass match	45274.02015	13788.22321	14736.33535	0.00000191	0.000124721	0.748802329	1.552005936	2.499213316	0.312682052	0.297224212	1.052007338
X19.1_568.056mz_pos	dTDP-3-amino-2,3,6-trideo	exact mass match	14703.67856	10252.18141	7693.958533	0.000000111	0.000000005	0.067067467	2.849476805	2.304979871	0.715675186	0.503875879	1.420340239
X17.2_553.037mz_pos	dTDP-4-oxo-2,3,6-trideo	exact mass match	28346.87718	19396.43368	22932.61964	0.000000686	0.0000583	0.724897407	1.835150052	3.600954997	0.691756223	0.739827025	0.935024268
X19.1_583.065mz_pos	dTDP-4-oxo-5-C-methyl	exact mass match	9044.669028	6715.4167	4565.071925	0.001842564	0.000083	0.087525108	2.789905572	3.344572135	0.794584038	0.500879143	1.58637877
X17.2_579.064mz_pos	dTDP-D-galacturonate	exact mass match	60620.22317	46892.50038	42276.32155	7.65E-10	2.77E-09	0.101432362	0.729490247	1.142497932	0.748723672	0.618550399	1.210448936
X23.7_587.072mz_pos	dTDP-D-glucose	exact mass match	33167.23177	24519.94393	17502.35907	0.0000548	0.001541494	0.687581013	4.669778283	4.068186007	0.739765799	0.494993187	1.494496932
X35.8_307.262mz_pos	Eicosatrienoic acid	exact mass match	6627.464272	9681.434063	20163.28616	0.001834808	0.000100947	0.089794822	4.843425421	1.417335389	2.534339306	0.55925242	
X14.3_377.206mz_pos	Enalapril	exact mass match	6297.459115	8931.446362	8946.021533	0.000268137	0.0001542667	0.659407526	1.498875233	2.828278785	1.389671328	1.260945641	1.102086627
X12.7_329.195mz_pos	endo-1-methyl-N-(9-me	exact mass match	3695.244914	6295.020421	6354.536844	0.00000271	0.0003126265	0.978164125	2.062148697	3.019892772	1.534585622	1.391210747	1.103057624
X8.3_622.401mz_pos	Enniatin B	exact mass match	25818.82936	20195.35102	19268.22512	5.67E-08	0.00000106	0.342572054	0.625883427	1.246889666	0.779987231	1.140553332	
X22_646.782mz_pos	Epoxomicin	exact mass match	51915.9717	40970.10063	31352.27006	0.00000253	0.00000428	0.217773604	2.441781163	2.621392965	0.769885971	0.550023557	1.399732724
X8.9_405.245mz_pos	Estradiol-17-phenylprop	exact mass match	8162.816409	5882.41904	15315.71133	0.0000242	1.29E-08	0.002052336	7.491130394	13.3332295	0.779039756	1.622768992	0.48006818
X14.7_328.06mz_pos	Etaconazole	exact mass match	21404.76943	14459.24631	11847.26726	0.000106721	0.001468023	0.758917757	5.336093562	3.786893698	0.68371651	0.510402134	1.339564364
X37.7_497.166mz_neg	Eucaglobulin	exact mass match	10888.18381	17143.82131	16611.04997	0.000253522	0.000738842	0.522014977	1.821324802	2.036237059	1.571250195	1.289777786	1.218233258
X28.9_477.129mz_pos	Eupachlorin acetate	exact mass match	33859.78144	198711.5037	205306.8761	3.99E-10	1.84E-08	0.999921347	5.820751675	2.256086151	5.568978352	5.408303405	1.029708937
X27.4_717.441mz_pos	Evasterioside E	exact mass match	4261.227837	7236.863583	8188.319582	0.004625893	0.003812908	0.468034621	1.993315523	6.726016346	1.570749648	1.568106897	1.001685313
X30.2_357.289mz_pos	Evocarpine	exact mass match	8748.829345	14660.65375	20997.44899	0.004434213	0.00000286	0.004828851	4.014037027	6.739973521	1.627753964	2.058850139	0.790613136
X13_329.233mz_neg	FA 18:1+3O	MS/MS spectrum match	81953.07437	139126.4007	257642.4639	0.00000971	0.0000697	0.472965188	2.17843853	1.818537746	1.75297647	0.87708637	0.609288789
X16.4_223.134mz_pos	FA13:3+1O	MS/MS spectrum match	36502.19486	222701.9558	242938.4952	0.0000457	0.001167377	0.4680385619	0.432870583	0.812357024	0.622763651	2.627030544	0.985337904
X6.1_326.217mz_pos	Farnesylcysteine	exact mass match	15502.28202	11596.98057	10617.67501	0.000000636	0.00000701	0.387433713	1.144713425	1.982966931	0.761710901	0.637915773	1.19406187
X37.7_708.427mz_pos	Fasciculin acid C	exact mass match	110749.299	237909.0035	257213.3603	0.000162107	0.000197657	0.347185483	3.73710247	4.288370611	2.07756987	0.514720503	1.014725537
X25_495.023mz_pos	Fd& red no. 1--prohibite	exact mass match	109547.8092	85586.26791	65142.24929	4.21E-10	3.99E-10	0.000181817	0.841852139	0.909605778	0.74540631	0.204783607	1.434070449
X10.3_788.823mz_pos	Fistularin 1	exact mass match	54029.23911	35714.06865	14772.72003	4.21E-10	4.59E-09	0.290826546	12.61241599	8.023282523	0.652270454	0.26073833	2.501628565
X16.3_348.077mz_pos	Flumipropyn	exact mass match	23359.04544	18152.27672	10574.27004	0.001179434	0.000101175	0.129828248	4.375294372	3.450118459	0.779027691	0.42810887	1.819695282
X37.7_424.124mz_neg	Fluotrimazole	exact mass match	19329.19291	35921.53202	38272.42027	0.000235569	0.0000582	0.170637662	2.608139653	3.180426418	1.850887045	1.690736363	1.094722445
X22.6_966.692mz_pos	FMC-5(d18:1/20:0)	exact mass match	133396.3406	65257.64609	55886.97328	3.99E-10	3.99E-10	0.038907781	0.819381244	2.582757693	0.466614184	0.361742882	1.28990564
X26.7_994.724mz_pos	FMC-5(d18:1/22:0)	exact mass match	34484.51987	20610.30781	12033.83563	3.99E-10	3.99E-10	1.32E-08	1.725347863	2.804486637	0.603862783	0.330483238	1.827211531
X22.4_1010.718mz_pos	FMC-6(d18:1/22:0(2-OH))	exact mass match	314587.0889	208862.051	166323.03	3.99E-10	3.99E-10	0.009686308	0.411751929	1.491260597	0.616447023	0.460333108	1.339132492
X26.3_1038.75mz_pos	FMC-6(d18:1/24:0(2-OH))	exact mass match	65682.69031	39441.65821	24262.3873	3.99E-10	3.99E-10	0.0000128	1.849623073	4.133564875	0.588392962	0.338415395	1.738669991
X5.1_301.177mz_neg	Formestane	exact mass match	7758.131783	11622.87162	12794.36572	0.000118272	0.000305994	0.451580719	5.399510279	5.467228242	1.49541355	1.364447373	1.095984777
X28.7_659.436mz_pos	Fucoxanthin	exact mass match	9543.289563	16280.20566	16689.40925	0.000015	0.000437603	0.752648127	2.441878591	3.082997362	1.646082239	1.551709396	1.060818633
X37.7_690.366mz_neg	Fumonisin C2	exact mass match	52268.77618	105078.9278	130431.2501	0.000085	0.0000401	0.203071979	2.488063787	3.243785736	2.005377331	2.182562108	0.918817991
X22.7_534.377mz_pos	Fusidic acid	exact mass match	296481.844	245396.7476	167236.8822	0.00000041	4.56E-10	0.000338024	0.79426108	1.55422079	0.769200733	0.496562767	1.58505036
X18.1_549.043mz_pos	gadopentetic acid	exact mass match	24033.45626	19051.34747	13496.28444	0.00000336	0.00000555	0.224603973	1.917402915	2.447844724	0.79464588	0.525226723	1.512957824
X21.4_598.085mz_pos	Gadoteridol	exact mass match	40032.94554	29668.32397	20647.13709	2.84E-08	0.00000038	0.273962527	3.300564705	3.232986668	0.741428061	0.483173948	1.534495111
X37.7_944.677mz_neg	Galabiosylceramide (d18:1	exact mass match	16529.3983	43025.16452	62638.61563	0.000567068	0.002495308	0.662735569	8.242902299	6.665083442	2.513783942	3.217424639	0.78130313
X20.7_996.703mz_pos	Galabiosylceramide (d18:1	exact mass match	329846.7047	217840.3983	179489.2875	3.99E-10	3.99E-10	0.01469791	0.400550054	1.547155939	0.617051229	0.475281421	1.298286027
X18.9_1026.713mz_pos	Galabiosylceramide (d18:1	exact mass match	33012.70427	19705.39867	14889.95237	3.99E-10	3.99E-10	0.000186722	2.180647751	2.932614694	0.605805402	0.422995739	1.432178498
X20.3_1040.729mz_pos	Galabiosylceramide (d18:1	exact mass match	96309.80479	61902.76648	46167.92643	3.99E-10	3.99E-10	0.0000132	0.868215391	2.027872533	0.615031723	0.416948182	1.47507952
X11.5_560.4mz_pos	gamma-Chaconine	exact mass match	810602.8658	602037.5345	557634.8173	3.99E-10	3.99E-10	0.04738518	0.596879137	1.000468233	0.665270989	0.588164948	1.131095947
X19.3_477.004mz_pos	GAMGLEOIDIN ACETATE	exact mass match	19191.31666	14100.3127	8179.42015	4.15E-08	7.22E-10	0.004364755	1.901035967	4.242610431	0.743727074	0.411375604	1.808012109
X26.8_572.402mz_pos	Ganoderic acid Me	exact mass match	28902.65106	21457.36839	15011.72123	1.16E-09	3.99E-10	0.000101797	0.884613356	2.795882177	0.74452681	0.486784397	1.529479611
X32.1_603.394mz_pos	Ganoderic acid Mg	exact mass match	83211.45831	174363.6335	223720.0719	0.0000785	0.0000616	0.256241747	2.017050905	3.798243375	1.968831725	2.28470938	0.861742742
X23.3_527.338mz_neg	Ganoderic acid V	exact mass match	33135.34541	16420.59656	23443.87681	0.000000122	0.002037857	0.83262302	0.907912181	0.91463988	0.533292666	0.649511048	0.821067891
X12.7_430.295mz_pos	GANT 61	exact mass match	11089.37725	26874.08289	22158.73929	0.003027858	0.004965002	0.583027443	8.215852896	0.715400853	2.276774709	1.745545251	1.304334395
X27.1_552.051mz_pos	GDP-4-Dehydro-6-deoxy	exact mass match	32661.25558	25098.54769	24052.99698	0.00000953	0.00000269	0.110444539	1.021572728	1.497879559	0.764328606	0.675982687	1.130692576
X20.7_454.98mz_pos	Geodin hydrate; 3,5-Dichl	exact mass match	9118.508077	6798.131437	7320.317743	9.73E-08	7.23E-10	0.00283408	1.117788191	3.321427359	0.794037531	0.75769614	1.047999704
X33.6_377.164mz_neg	Gibberellin A17	exact mass match	26399.01677	39689.85225	38411.38707	0.003633801	0.000259072	0.126584614	2.815199246	3.565577439	1.500553742	1.264030102	1.187118677
X37.7_380.208mz_pos	Gibberellin A36	exact mass match	692638.6943	1001072.405	1756536.091	0.00187689	0.000459151	0.230447945	1.791187946	1.706337012	1.295675122	2.24932168	0.576029268
X39.2_365.198mz_pos	Gibberellin A44 diacid	exact mass match	20169.3699	33844.64452	59803.71007	0.003371977	0.00062119	0.120201124	3.877550248	3.708096494	1.602304089	2.550684464	0.628185929
X13.5_409.149mz_pos	Ginkgolide A	exact mass match	74743.34619	52765.30883	51492.17481	0							

X22.4_543.376mz_pos	Ginsenoyno A linoleate	exact mass match	145190.9338	117915.8133	100396.9482	4.66E-08	1.01E-09	0.006370227	0.42995583	1.237421118	0.764567672	0.601681787	1.270717658
X16.7_692.505mz_pos	GlcCer(d14:1/18:1)	exact mass match	14289.00821	7332.592178	5796.820189	3.99E-10	5.9E-10	0.937441163	1.94608456	5.884402533	0.550766784	0.397083667	1.387029559
X12.9_664.474mz_pos	GlcCer(d14:2(4E,6E)/16:0)	exact mass match	6766.066546	3373.792523	2203.047931	0.000000981	0.00000856	0.376371991	3.526171985	4.874427204	0.614770562	0.346383536	1.774826161
X21.3_632.484mz_pos	GlcCer(d14:2(4E,6E)/18:1(9Z))	exact mass match	9163.576604	3872.425457	2985.858237	4E-10	5.16E-10	0.158967233	1.011222892	12.70556499	0.514220461	0.341328225	1.506527806
X33.8_490.179mz_neg	Glipizide	exact mass match	16214.45154	27654.03761	25507.69542	0.000440937	0.001719814	0.628091014	3.064439525	3.156407552	1.719500945	1.331381926	1.291515914
X24.9_490.016mz_pos	Glucosylsyringic acid	exact mass match	36608.5667	25822.16179	18602.64057	6.65E-10	3.99E-10	0.000397109	0.907978355	1.84081776	0.710583311	0.476027049	1.492737257
X16.3_406.083mz_pos	Glucocleomin	exact mass match	21987.59739	32725.79809	17090.47894	0.000274305	0.004145994	0.846466316	3.764456377	3.399846966	1.421167779	0.710360829	2.00062802
X37.7_448.08mz_neg	Glucosylquercetin	exact mass match	32809.69945	58665.1787	87766.53876	0.000135417	0.000519736	0.531324406	2.024095888	1.485307329	1.785921976	2.344320723	0.761807869
X23.7_476.01mz_pos	Glucoraphanin	exact mass match	28616.78598	20611.66971	11646.29959	5.14E-10	3.99E-10	0.00016281	2.501776375	3.806953155	0.724499118	0.386029768	1.876795984
X16.4_408.052mz_neg	Glucotropaeolin	exact mass match	20394.82945	11983.98515	4735.919822	0.0000301	0.001454475	0.882846233	5.142316973	7.021202291	0.65534029	0.238608438	2.747321239
X11_259.119mz_neg	Glycerol tripropanoate	exact mass match	13463.24989	23500.52423	27609.02673	0.0000142	0.000661859	0.828308745	0.537781147	0.908687543	1.756425183	1.759027394	0.998520654
X33.1_339.289mz_pos	Glycidyl oleate	exact mass match	64364.26688	104850.9985	216998.3225	0.003671682	0.000414882	0.165878688	3.237444352	2.662771437	1.545305213	2.897150844	0.533387903
X26.2_581.329mz_pos	Goshonolide F6	exact mass match	20555.04309	40419.92637	33341.92442	0.0000735	0.003894855	0.945875851	8.499412027	6.156794118	1.850508837	1.427039362	1.296697572
X17.3_524.02mz_pos	Gossypetin 7,8-dimethyl ether	exact mass match	24358.28332	18830.23143	20984.05249	5.14E-08	0.000000193	0.172697299	1.114418514	1.973151198	0.769374164	0.710696131	1.010782459
X6_649.428mz_pos	Goyaglycoside A	exact mass match	14364.54952	4394.862891	3965.969532	0.00000423	0.00000774	0.580789949	1.615166401	8.235704407	0.324099287	0.256963974	1.248265365
X25.5_702.536mz_pos	GPNEtn(16:0/18:1(9Z))	exact mass match	154742.9578	113050.4254	83076.10491	4.1E-10	3.05E-08	0.609041406	1.194068176	2.058816478	0.692951597	0.464271888	1.492555582
X10.3_715.115mz_pos	Guanosine diphosphate adenylylated	exact mass match	33510.99118	23029.56907	19764.79537	3.99E-10	4.01E-10	0.082352947	4.740496342	3.802815968	0.690393391	0.55107848	1.252804122
X18.7_612.082mz_pos	Guanosine diphosphofuranosylated	exact mass match	5935.781356	4210.5675	2739.037581	0.00257807	0.000372186	0.181387897	4.356630471	12.12554134	0.798049811	0.469869101	1.698451357
X24.2_541.035mz_pos	Guanosine triphosphate (GTP)	exact mass match	82797.62592	66599.37058	72131.05981	0.00000234	6.42E-08	0.021891157	2.836718972	3.99076929	0.763966087	0.757673277	1.00830544
X37.7_440.095mz_neg	GW 848687X	exact mass match	73770.30794	124216.6025	185527.7855	0.00012543	0.000444677	0.511515845	1.688745307	1.26332152	1.672039261	2.232587327	0.748924461
X5.8_508.349mz_pos	Gymnodimine	exact mass match	14905.04418	4465.673907	4467.433339	1.59E-08	0.000521089	0.880341006	1.575800839	6.224215479	0.308140993	0.279658502	1.101847398
X11.4_382.024mz_neg	H 151/73	exact mass match	6125.856701	8619.79686	5280.200559	0.004639974	0.00000377	3.532789119	3.223736037	1.400999209	0.766294695	1.828277318	0.7337318
X25_484.006mz_pos	H-89	exact mass match	50693.62058	38232.80758	38864.29308	5.03E-10	4E-10	0.011331222	0.586834824	1.26151782	0.74030229	0.691223845	1.071002246
X34.6_531.178mz_neg	Haplodimerine	exact mass match	370430.6479	1628913.24	1889527.769	3.99E-10	8.13E-10	0.971593655	0.838406267	0.884072411	4.122907748	4.525458506	0.911047449
X23.3_490.351mz_pos	HECODOGEMIN ACETATE	exact mass match	154378.9613	116350.2221	72734.75659	4.06E-10	3.99E-10	0.00000564	0.150202823	1.746178139	0.710100987	0.409291839	1.734950272
X18.7_647.108mz_pos	Hectochlorin	exact mass match	19157.58294	15138.16572	9477.579191	0.000023	0.00000269	0.078353037	1.981368936	2.37698918	0.794215053	0.471871152	1.683118473
X20_605.403mz_pos	Hederagenin 3-O-arabinoside	exact mass match	26600.52912	18446.0329	18614.07701	6.01E-08	9.18E-09	0.031626793	0.971979435	1.485942196	0.698311256	0.647306893	1.078794716
X53.4_627.458mz_pos	Heptanoyl thio-PC	exact mass match	7787.95767	18861.1187	23930.19127	0.002334882	0.001369888	0.365884016	13.02529402	5.966919171	2.183992901	2.520201906	0.866594417
X15.7_588.431mz_pos	Hericenone C	exact mass match	1119190.78	812458.6742	767044.741	3.99E-10	3.99E-10	0.190926049	0.353211487	0.865215502	0.668356001	0.615035273	1.086695397
X18.7_616.462mz_pos	Hericenone D	exact mass match	3878637.814	2777465.823	2599722.966	3.99E-10	4.14E-10	0.095942182	0.612689993	0.896653241	0.686756357	0.616241368	1.114427548
X21.3_612.425mz_pos	Hericenone E	exact mass match	15594.00562	11612.82835	6675.950886	0.0000037	0.000442552	0.88551165	5.635978094	6.252749221	0.761771153	0.419341126	1.816590615
X15.1_331.213mz_neg	Hexadecanedioic acid	exact mass match	34800.0408	15739.4038	25681.51568	0.000000901	0.000283333	0.930523412	1.246385334	1.336437711	0.486773425	0.660116486	0.737405345
X20.7_460.656mz_pos	Hexaflumuron	exact mass match	21056.55521	16597.41338	13966.00695	2.96E-08	4.02E-10	0.000140138	0.79185828	2.083705543	0.788295311	0.615863428	1.279893961
X7.9_295.211mz_pos	HMDB:(4669);SuperNatural	Sirius match	77859.4292	53337.6941	44642.35416	3.99E-10	3.99E-10	0.00000192	1.430252329	0.49908278	0.658358326	0.500876007	1.314413781
X18.9_562.379mz_pos	Hovenidulcigenin A	exact mass match	11991.95041	7876.927768	9001.233245	3.07E-08	4.07E-10	0.000328481	2.867490493	2.60799815	0.690480273	0.702937047	0.982278961
X15.7_476.284mz_pos	Hydrocortamate	exact mass match	9665.33242	13255.2073	14417.05727	0.003261803	0.0000249	0.029281277	4.191738635	1.840285477	1.344100856	1.334551362	1.007155584
X6.3_574.36mz_pos	Hydroxydestruxin B	exact mass match	41720.02512	12846.66407	13362.84635	0.000000762	0.00000788	0.387666967	1.026856232	1.776940941	0.326596573	0.293932979	1.111125993
X32.1_440.151mz_neg	Hydroxydomperidone(M2)	exact mass match	13675.55424	22813.88202	26357.45433	0.000123325	0.003589828	0.89730755	2.967457942	2.479680645	1.673726039	1.632912811	1.024994125
X21.7_480.343mz_pos	Hydroxysintaxanthin 5,6-epoxide	exact mass match	32800.9658	180186.6954	193925.6481	0.000310443	0.00453981	0.849748816	1.012267499	0.9822246	0.499774	0.510522385	0.978946301
X27.4_543.052mz_pos	Hypericin	exact mass match	36614.06081	29183.96999	23912.56184	1.38E-09	3.99E-10	0.0000284	0.627919024	1.446616552	0.792860004	0.604783502	1.310981536
X16.5_530.7mz_pos	Icosenoyl-CoA	exact mass match	49611.85041	39060.777	33106.52922	1.44E-08	8.08E-10	0.008583931	0.83389839	1.182773073	0.769155381	0.601169584	1.279431631
X14.7_341.232mz_pos	Idebenone Metabolite (1,4-dihydroxy-2,3,5-trimethoxybenzene)	exact mass match	4574.02852	18641.98539	16262.69537	0.00000723	0.001436629	0.972719927	5.495641087	2.052773544	3.421809642	2.838178016	1.205636018
X15.1_355.209mz_pos	Idebenone Metabolite (Benzoic acid derivative)	exact mass match	17275.07728	10071.92013	11198.22227	0.0000206	0.003277172	0.989079781	5.24117424	6.695842097	0.606814949	0.596410543	1.017445041
X13.5_604.426mz_pos	Ilexonide A	exact mass match	52002.82252	37566.25225	36731.81734	3.99E-10	4E-10	0.03974063	0.617171016	1.419309997	0.704249286	0.631126933	1.115859978
X6.8_281.195mz_pos	Imipramine	exact mass match	224052.6172	163241.1145	152517.4466	3.99E-10	3.99E-10	0.002532567	1.073583546	0.542458191	0.679005985	0.591607068	1.14773136
X21.4_566.049mz_pos	Indoxacarb	exact mass match	10882.12716	7480.196853	8832.024393	0.0000301	0.0000192	0.201115623	1.815918037	1.573631847	0.724934971	0.760903066	0.952729727
X16.4_366.084mz_pos	Inosine 5'-monophosphate	exact mass match	12194.70398	8002.496249	5135.989263	0.000649645	0.0000356	0.085053421	2.398736929	2.880546997	0.698446915	0.411517588	1.692746813
X15.8_509.001mz_pos	Inosine triphosphate	exact mass match	13182.69098	9394.9611	10337.00279	0.000000175	0.00000604	0.488796702	1.336555278	1.646414647	0.734524017	0.731239419	1.004491823
X8.7_312.192mz_pos	Isoleucyl-Tyrosine	exact mass match	13793.36926	9272.640781	10876.326	0.000717797	0.003880918	0.723826261	5.20763084	8.245098336	0.712254529	0.725412902	0.981808051
X27.8_534.052mz_pos	Isopentenyladenosine-5'-phosphate	exact mass match	115954.7355	91165.29385	56218.02903	4.17E-10	3.99E-10	0.0000223	1.187351906	1.996378076	0.750377617	0.423388766	1.772313481
X9.9_598.043mz_pos	Isopentenyladenosine-5'-triphosphate	exact mass match	7856.209974	3906.972153	2713.910171	3.99E-10	3.99E-10	0.0000446	2.13304043	10.97679445	0.602562763	0.363837212	1.656132863
X15.8_555.045mz_pos	Isorhamnetin 3-glucuronide	exact mass match	33754.67132	26004.66361	19672.17156	0.00000152	0.000000613	0.098582935	1.536027623	1.137809453	0.767730936	0.538434182	1.425858464
X17.2_565.057mz_pos	Isoctellarein 4'-methyl ether	exact mass match	25533.10457	19470.31253	13303.7518	4.75E-08	9.09E-08	0.123557876	1.922247738	2.502980962	0.764896025	0.490877353	1.558222274
X7.8_386.274mz_pos	Istamycin C	exact mass match	642653.5882	519304.8567	491477.1435	3.99E-10	4.2E-10	0.09522969	0.845910891	0.786664458	0.730078237	0.652377812	1.119103415
X6.8_432.28mz_pos	Istamycin C1	exact mass match	8461.928545	5293.385042	3715.592555	0.00000447	2.57E-08	0.008656098	1.805438355	5.902290724	0.698393216	0.4452977	1.568373731
X37.7_400.148mz_neg	JWH 369	exact mass match	1102277.192	1824398.222	2307529.938	0.000335681	0.00000299	0.02415493	2.827366119	2.506794523	1.578507471	1.932343115	0.816887777
X17.3_521.031mz_pos	Kaempferol 3-sulfate-7-oxide	exact mass match	22632.95221	16223.89367									

X16.4_507.278mz_neg	Kazinol E	exact mass match	70967.09851	34967.94968	58339.26873	1.29E-08	0.002880855	0.544541825	2.50997612	2.185605312	0.504476536	0.745672877	0.675638669
X8.1_502.979mz_pos	KB2115	exact mass match	7389.873531	3717.2915	3095.096728	6.79E-10	0.000000015	0.24670384	2.612021155	10.51030953	0.611342514	0.429736332	1.422599087
X23.7_611.914mz_pos	KDNaIpha2-3Galbeta1-4G	exact mass match	39297.39974	26410.4724	30346.93503	3.99E-10	3.99E-10	0.010997243	8.299227905	10.22604311	0.66799161	0.701496542	0.952237923
X20.7_671.796mz_pos	Kelevan	exact mass match	10264.38752	7189.984673	2645.983822	0.0000759	3.67E-09	0.00034461	7.248556097	8.868155016	0.744240856	0.273899305	0.712720682
X28.8_562.065mz_pos	KRP_203-phosphate	exact mass match	37067.52271	27406.09416	18161.52824	2.49E-08	3.99E-10	0.000000672	0.897620428	2.057146281	0.740931003	0.459603979	1.612107458
X25.8_629.395mz_neg	Kurilensoside F	exact mass match	1965.939867	7095.915903	11349.97551	0.00000157	0.001058757	0.998216059	2.08759117	5.127804341	2.734760572	3.633409887	0.752670537
X21.7_500.689mz_pos	Lacto-N-difucopentaose	exact mass match	115667.8241	93242.57992	78601.75827	2.48E-09	4.02E-10	0.000580572	0.708500766	0.789902443	0.764503041	0.591820313	1.29178236
X11.1_336.237mz_pos	L-Citronellol glucoside	exact mass match	8255.671859	4676.478172	6738.337204	0.0000668	0.000861518	0.711628083	4.062672864	8.006984794	0.654518527	0.745623498	0.877813707
X16.8_464.834mz_pos	Leptophos	exact mass match	46363.18622	33242.21678	26089.84733	3.99E-10	3.99E-10	0.006042514	0.757830554	1.853058587	0.711883248	0.5187988	1.372175973
X14.3_280.263mz_pos	Linoleamide	exact mass match	19791.902	6443.667643	4286.158577	0.002205765	0.002533146	0.486454931	1.774804615	9.56348862	0.352608594	0.220500392	1.599129107
X33.6_279.233mz_neg	Linoleic acid	exact mass match	87634.02438	123303.2813	224898.3076	0.004658983	0.00082873	0.220715361	2.099623731	2.10159988	1.391129893	2.250852264	0.618045847
X19.1_574.066mz_pos	Lipoyl-AMP	exact mass match	48308.4849	35761.56497	28792.19961	7.51E-10	4.21E-10	0.006726778	0.717429373	2.108192174	0.728787189	0.547417568	1.3313186
X28.4_577.074mz_pos	Lithospermic acid	exact mass match	25152.50953	18862.507	11097.65817	0.00000655	4.46E-10	0.000217077	1.497652737	2.699602196	0.754231926	0.420315162	1.794443775
X20.9_515.286mz_neg	L-Olivosyl-oleandolide	exact mass match	1928.412741	5219.156217	6481.779133	0.004843737	0.002001514	0.342995449	5.514982328	3.422340184	2.07179856	2.026005678	1.022602544
X24.5_519.033mz_pos	Lorazepam glucuronide	exact mass match	164615.7179	136891.8115	111809.2847	1.93E-09	4.06E-10	0.001394577	0.452120953	1.078929687	0.776733616	0.58991914	1.316678107
X19.5_536.299mz_neg	LPC 16:2	MS/MS spectrum match	67855.68239	42083.93371	53014.53472	0.0000526	0.003150175	0.942908695	1.182024908	1.181751324	0.636908614	0.706937929	0.901652442
X21.4_512.336mz_neg	LPC O-15:0	MS/MS spectrum match	126018.7642	81489.15177	97841.78973	0.000703949	0.000968223	0.44826505	1.798624605	1.471844081	0.665211627	0.693490314	0.959222664
X32.1_444.145mz_neg	Lucinamide	exact mass match	18180.03792	33519.02655	33972.70951	0.0000518	0.000532151	0.649785499	2.857614529	2.75480607	1.84228698	1.607563459	1.146011978
X10.8_612.373mz_pos	L-Urobilin	exact mass match	6526.427872	12771.38917	14965.43509	0.000592899	0.002890248	0.687303914	9.630848904	6.511973511	1.82946983	1.945902873	0.940165028
X25.2_463.99mz_pos	Luteolin 7,3'-disulfate	exact mass match	5962.150971	3136.643118	3589.343138	0.0000117	0.0000104	0.204058447	2.649907635	1.10128512	0.649333458	0.583077348	1.113631769
X16.1_460.289mz_pos	Lyngbyatoxin	exact mass match	36104.67266	48920.10987	65326.73102	0.000693406	0.000000928	0.006947016	10.53120774	6.653191151	1.299605981	1.593254942	0.815692421
X16.2_269.128mz_pos	Lysergic acid	exact mass match	7257.410197	9882.900619	10584.79666	0.000476762	0.001312817	0.554795189	4.131556619	4.044623631	1.350348055	1.286246034	1.049836516
X5.6_616.37mz_pos	LysoPC(22:1(13Z))	exact mass match	36978.06596	11110.21181	10797.23318	0.000000303	0.0000118	0.540812363	1.179626885	2.484368751	0.321615977	0.269352659	1.194033048
X16.9_637.157mz_neg	Malvidin 3-(6''-p-coumar	exact mass match	17768.4909	8955.899702	7216.065606	4.58E-10	4E-10	0.002325777	1.072790457	2.643059142	0.573135346	0.389892433	1.46998325
X8.7_613.378mz_pos	Mancinellin	exact mass match	15718.12067	9695.834379	7572.472895	4.34E-10	3.99E-10	0.003093531	1.631544602	4.82658982	0.639027418	0.464829504	1.374756577
X28.1_597.091mz_pos	Mangiferin 6'-gallate	exact mass match	135410.266	114573.1111	82360.72377	0.00000196	0.000000001	0.000871309	0.693503856	1.41528344	0.797148691	0.530746023	1.501940019
X18.8_731.514mz_pos	Mannosyl-1beta-phospho	exact mass match	22300.09288	15739.55978	17608.33915	3.99E-10	4.13E-10	0.125267486	1.438178809	1.690481911	0.710690128	0.723378882	0.982459049
X5.9_312.238mz_pos	Margaric acid(d3)	exact mass match	34464.39588	27651.86716	26569.38769	0.00000604	0.000118993	0.849356567	2.162602843	3.059561393	0.792623794	0.766118653	1.122507939
X19.1_520.361mz_pos	Medicaginic acid	exact mass match	92286.5421	74264.91462	50553.86509	0.00000172	2.12E-09	0.002081334	0.88829774	1.232659744	0.773507599	0.485009926	1.594828388
X16.4_325.082mz_neg	Methyl nigakinone	exact mass match	43987.34926	27497.59434	13103.97724	0.00000778	0.0000351	0.096191325	2.798898713	3.629594413	0.666816527	0.283153129	2.65486789
X17_448.315mz_pos	METHYLBENZETHONIUM	exact mass match	63820.6562	49963.7685	48804.65738	0.00000054	0.001182763	0.986354106	0.774798872	1.430865395	0.750179845	0.63220769	1.131116336
X24.2_539.384mz_pos	Methylcarbonyl PAF C-16	exact mass match	306375.5459	263864.8979	188707.0573	1.02E-08	4.11E-10	0.000807596	0.819912364	1.48030187	0.794663295	0.534753114	1.486037714
X11.9_357.111mz_pos	Met-Val-OH	exact mass match	10433.96473	13565.00912	8560.68912	0.00000347	0.000285165	0.826195784	3.575979915	3.114997173	1.288648599	0.76198341	1.691176712
X7.4_556.122mz_neg	Mezlocillin penicilloate	exact mass match	15802.65468	20717.98158	3535.550171	0.000960255	0.00000138	0.00764872	10.65427841	11.05468794	1.352806877	0.245247766	5.516082371
X27.8_329.268mz_pos	MG(0:0/16:1(9Z)/0:0)	exact mass match	9164.009285	13455.19357	19241.25848	0.002144853	0.000835443	0.297358999	1.022863707	2.64270019	1.448534993	1.825996227	0.793284768
X28.5_329.268mz_pos	MG(16:1(9Z)/0:0/0:0)	exact mass match	16547.0588	29034.38272	47802.34886	0.00066351	0.001412321	0.527225616	2.131206597	2.179699529	1.710488162	2.468385519	0.692958271
X15.8_747.509mz_pos	MGDG(18:3(9Z,12Z,15Z)/1	exact mass match	6048.334599	3162.415282	4013.343053	2.35E-08	0.000000083	0.148553941	2.038956051	5.667693407	0.651988196	0.641180442	1.016856026
X18.1_775.54mz_pos	MGDG(18:3(9Z,12Z,15Z)/1	exact mass match	304662.8481	210562.0224	239597.4304	3.99E-10	3.99E-10	0.010725478	1.134872505	1.189847168	0.637408447	0.672645377	0.947614403
X16.4_405.111mz_pos	Mollicellin D	exact mass match	7425.631806	4027.164318	2931.560776	0.00014884	0.000173277	0.33616848	10.96874795	4.641623532	0.634399493	0.38770365	1.636172225
X30.4_564.922mz_pos	Molybdoenzyme molybde	exact mass match	56037.0182	34573.07184	16893.34819	4.05E-10	3.99E-10	0.000571176	2.105886583	3.923179213	0.61032816	0.278785841	2.189236573
X9.7_714.443mz_pos	Momordicoside E	exact mass match	47968.51918	33754.05815	10375.52892	3.99E-10	3.99E-10	0.00000784	13.55095271	12.42252515	0.69581497	0.209649406	3.318945577
X6.4_649.428mz_pos	Momordicoside K	exact mass match	8096.870595	2483.648789	2268.209784	4.07E-08	0.002122388	0.723372595	1.799240169	13.15684164	0.330737698	0.280057917	1.180961787
X14.9_315.216mz_pos	Mono-N-desisopropylidist	exact mass match	9388.584667	21695.84279	18716.92647	2.22E-08	0.00000378	0.621871349	3.343729471	3.36865347	2.18680053	1.761704634	1.241298052
X6.8_699.443mz_pos	Mycinamicin III	exact mass match	12055.78148	3919.801063	4382.592352	5.64E-09	0.0000112	0.905986046	1.945625229	8.516387055	0.390671582	0.33230531	1.105996078
X6.7_685.428mz_pos	Mycinamicin VI	exact mass match	19459.77549	6560.757763	6424.002082	1.05E-08	0.000000928	0.476990002	1.49662479	2.945116807	0.378020157	0.309179553	1.222655748
X15.8_570.054mz_pos	Myricatin	exact mass match	16579.91201	11693.14192	9406.220401	5.22E-08	1.34E-09	0.00158636	1.207877523	1.986789973	0.72113292	0.53763882	1.341296226
X20.7_671.127mz_pos	Myricetin 3,7-diglucuronic	exact mass match	15627.17639	12120.11689	7379.6883	0.00000554	0.00000743	0.20436842	3.952732041	6.013308186	0.790218214	0.457630223	1.726761421
X32.1_354.173mz_pos	N-(9-FLUORENYLMETHC	exact mass match	29735.52561	50635.0602	64885.4405	0.0000431	0.00037129	0.603440596	1.854324977	2.498054138	1.640577995	1.87818684	0.873490305
X16.5_515.69mz_pos	N-(1-Deoxy-1-fructosyl)h	exact mass match	68771.32415	51810.4458	42223.55696	4.1E-10	3.99E-10	0.002189006	0.683424904	1.169465579	0.725219326	0.544746259	1.331297488
X12.6_298.201mz_pos	N-(3-oxododecanoyl) hor	exact mass match	51917.15091	79365.65783	76129.28321	0.00000109	0.001069198	0.999957483	7.360306662	2.374177827	1.459207445	1.29004906	1.13112557
X6.9_488.135mz_neg	N-(4-acetamidophenyl)-li	exact mass match	5764.030791	11286.28747	2246.954956	0.001017157	0.00000113	0.00633193	13.0944772	12.21790532	1.86283923	0.419890403	4.436489184
X16.4_211.122mz_pos	N,N-Dimethyltryptamine	exact mass match	5778.072276	3704.805983	3715.963484	0.002483574	0.0000204	0.02983481	1.708650656	4.449221922	0.745565624	0.594945942	1.253165324
X8.4_492.307mz_pos	N2'-Acetylgentamicin C1a	exact mass match	14144.3342	8507.439236	6080.877863	3.99E-10	4E-10	0.04182978	6.845872751	0.632780425	0.421267459	1.502087122	
X28.5_382.18mz_pos	N-Acetylmuramoyl-Ala	exact mass match	10411.5224	19997.33515	23894.8848	0.0001666	0.002963857	0.838574479	4.290895078	2.616512192	1.861385859	1.948075208	0.95499999
X7.8_295.211mz_pos	N-Acetylprocainamide	exact mass match	20349.03249	14082.32612	12697.49383	3.61E-09	6.87E-09	0.00861103	1.385018875	0.806277192	0.698933292	0.577792094	1.209662263
X23.1_666.13mz_pos	NADH	exact mass match	32216.56247	25166.79115	12908.46715	0.0000133	1.56E-08	0.00365627	2.750814818	3.815383593	0.779790097	0.383240954	2.034725382
X19.1_548.039mz_pos	Naphthal AS-BI α -D-gluc	exact mass match	10632.36731	7975.043331	7937.9505								

X8.5_474.327mz_pos	Narbomycin	exact mass match	599796.8834	497247.885	490989.4807	4.02E-10	2.02E-09	0.337295918	0.484756201	0.837858777	0.749745729	0.694870938	1.078971199
X17.3_416.173mz_pos	N-Desmethylnepomam glu	exact mass match	8698.650913	11107.9777	6258.693609	0.001595637	0.0000017	0.006457694	7.758913285	5.726343856	1.267086112	0.683806848	1.852988334
X15.1_378.284mz_pos	N-docosahexaenoyl GABA	exact mass match	54971.88232	26608.87925	39355.99644	0.00000097	0.000362895	0.951349313	2.468212039	1.836257402	0.478196466	0.627874003	0.761612144
X16.7_483.333mz_pos	N-docosahexaenoyl histid	exact mass match	4909.08754	2695.043818	3971.581884	0.0000689	0.0000331	0.198643102	2.084506026	9.221037876	0.681239088	0.738782729	0.922110197
X30.3_587.087mz_pos	Neobetanin	exact mass match	9008.468096	6080.723419	2239.722215	0.001433445	0.001706916	0.465686759	4.953273749	7.520110147	0.735015975	0.266942389	2.975462938
X8.5_529.329mz_pos	Neolinderachalcone	exact mass match	16235.6096	9375.565311	6313.716035	3.99E-10	3.99E-10	0.00074692	4.030522118	4.497011299	0.603436151	0.381004952	1.583801333
X30.4_535.324mz_pos	neriifolin	exact mass match	59718.46891	39629.164	20490.77902	0.00000149	0.0000237	0.490931209	10.03605074	6.84193954	0.643014807	0.318457867	2.0191519
X16.3_317.195mz_pos	Neryl glucoside	exact mass match	1245849.894	2110150.618	1996653.1	0.000253887	0.001131604	0.604490476	1.137823996	1.440575562	1.519300873	1.450314497	1.047566494
X28.9_475.116mz_neg	N-Ethylmaleimide-S-gluta	exact mass match	9795.832766	58651.99116	66745.35987	3.99E-10	5.19E-09	0.999822743	0.492458513	0.870386715	5.594084892	5.681107286	0.984682142
X26.4_497.678mz_pos	Neu5Aca2-8Neu5Aca2-3	exact mass match	11776.54291	9006.85189	9345.308624	0.0000007	3.99E-10	1.26E-08	2.104580203	2.588813289	0.790075238	0.745868159	1.059269293
X19.6_646.104mz_pos	Nicotinamide adenine din	exact mass match	11709.95106	8604.856793	5968.21687	0.000112213	0.001805599	0.79167574	4.080019507	4.539512799	0.766881024	0.497550821	1.541311946
X11.8_242.175mz_pos	N-nonanoyl-L-Homoserin	exact mass match	3734.946843	10688.09582	10390.58776	0.0000316	0.001052743	0.827760243	3.400976963	2.633702256	2.425153475	2.178847256	1.11304428
X10.5_414.305mz_pos	N-oleoyl methionine	exact mass match	10180.74044	7553.778182	7491.733262	2.29E-09	5.36E-10	0.010420913	1.005989024	2.202274041	0.781319804	0.695816265	1.122882351
X17.1_623.089mz_pos	NORSTICTIC ACID PENTA	exact mass match	20856.56963	16054.46595	11138.57194	3.25E-08	1.63E-08	0.056855005	1.691331267	2.754101169	0.504321877	1.534933397	
X20.7_572.379mz_pos	Notoginsenoside R10	exact mass match	11238.34515	6461.242161	8242.384438	3.99E-10	4.08E-10	0.280430661	1.944647991	6.6486534	0.623460661	0.68848045	0.905560442
X25.4_475.006mz_pos	Novaluron	exact mass match	43774.18469	31610.24434	26018.09775	4E-10	3.99E-10	0.00180818	0.658951044	1.750590505	0.718234004	0.549482693	1.30710942
X16.4_590.18mz_pos	Novclobiocin 104	exact mass match	148512.9404	80325.16556	63488.61705	0.0000195	0.000512385	0.752454114	2.97854872	1.912169773	0.511358585	0.381606677	1.340014776
X11.4_370.279mz_pos	N-palmitoyl methionine	exact mass match	64455.15048	48789.43663	42384.95359	4.02E-10	3.99E-10	0.002724838	0.747722205	1.051104972	0.730010544	0.57984197	1.258981898
X6.3_328.233mz_pos	N-palmitoyl taurine	exact mass match	345921.9902	294178.8277	290553.0843	4.63E-09	8.45E-09	0.082329936	1.198237437	0.769540125	0.785166268	0.719009903	1.092010367
X15.9_368.3mz_pos	N-propyl arachidonoyl an	exact mass match	115008.7783	93747.13916	77619.0725	0.0000179	1.85E-08	0.003234975	1.292199924	0.326028433	0.773834826	0.584964978	1.322873769
X15.7_439.326mz_pos	NSC 23766	exact mass match	358462.1138	265260.4262	300321.9968	3.99E-10	4E-10	0.021702974	1.112202285	1.169175576	0.689239131	0.719983285	0.957298795
X16.4_322.094mz_pos	NSC 663284	exact mass match	5586.108114	3445.915051	2370.407265	0.002566982	0.0000201	0.02901078	2.380224433	5.779489067	0.728202913	0.414718543	1.755896681
X8.4_356.264mz_pos	N-stearoyl taurine	exact mass match	45879.9181	336217.6577	317125.0781	3.99E-10	3.99E-10	0.030278249	1.01843436	0.661124418	0.673837003	0.592295013	1.137671242
X17.9_317.231mz_pos	NYLIDROL	exact mass match	4246.893534	6039.422325	6893.107281	0.0000054	0.000327653	0.806522438	1.222882584	3.287104842	1.347739009	1.346033044	1.001267402
X37.7_472.176mz_neg	OA-6129 B1	exact mass match	176039.3362	270169.3232	371743.2932	0.0000789	0.000200363	0.424549934	2.078135907	1.999939047	1.539725961	1.922334374	0.800966773
X26.7_499.695mz_pos	O-b-D-glucopyranosyl-(D	exact mass match	24164.90001	16766.95477	14573.49739	4.99E-10	5.02E-10	0.030052711	2.1620473	2.48548516	0.700062749	0.55994846	1.250227117
X7_398.751mz_pos	Octachlorostyrene	exact mass match	37127.12594	12428.20102	12373.18573	4.01E-10	8.37E-09	0.566985527	1.141031858	2.165654369	0.360141847	0.316001428	1.13752439
X17.7_583.405mz_pos	OH-Diaponeurosporene g	exact mass match	7725.258215	4754.888437	3736.07168	1.55E-09	6.18E-10	0.017417834	2.559885073	5.855601903	0.700994459	0.491001064	1.427684196
X21.7_542.426mz_pos	OLEANANOIC ACID ACET	exact mass match	56109.62338	39521.52176	25798.33767	5.62E-10	3.99E-10	0.000136251	0.675365751	2.131563269	0.694957834	0.424970896	1.635306889
X37.7_281.248mz_neg	Oleic Acid	exact mass match	60664.91368	104051.1427	220940.5338	0.000152491	0.0000524	0.189407652	3.81848135	2.932861274	1.670063593	3.169321358	0.275646233
X13.1_794.546mz_pos	Oligomycin D	exact mass match	496826.2722	360797.3562	323929.7924	3.99E-10	3.99E-10	0.114282776	0.349509113	1.022191639	0.658898321	0.59162712	1.178365989
X18.6_659.954mz_pos	Omphalotin A	exact mass match	37781.80119	25161.3868	19456.7179	4.02E-10	4.02E-10	0.013777916	2.663630503	2.214457657	0.664731048	0.480079526	1.384626947
X26.1_529.046mz_pos	Orange B	exact mass match	209219.6728	169025.3132	130146.7609	1.37E-09	4.01E-10	0.000775004	0.525327281	1.244794208	0.754290546	0.544580115	1.385086464
X28.6_551.048mz_pos	Orientin 7-O-sulfate	exact mass match	31287.43691	21646.79243	22662.09782	0.000000099	3.65E-09	0.013679625	2.579998313	2.043939106	0.689393565	0.665397892	1.03606214
X18.1_554.385mz_pos	PA(12:0/12:0)[U]	exact mass match	69012.87734	56078.696	47194.93552	2.21E-08	9.47E-10	0.008050201	0.737800517	1.438310046	0.783390784	0.60310888	1.298920992
X28.8_568.409mz_pos	PA(12:0/13:0)	exact mass match	19477.54074	13705.84137	3760.86061	0.0000156	4.55E-10	0.0000321	3.653001666	9.570777319	0.71606822	0.203478992	3.519126052
X37.7_618.429mz_pos	PA(12:0/15:1(9Z))	exact mass match	723782.8503	1074289.558	1882746.576	0.004964269	0.001150491	0.25659335	3.383379459	2.74596899	1.319811481	2.343526887	0.563173176
X19.1_587.403mz_pos	PA(12:0/17:1(9Z))	exact mass match	19920.45017	13644.15962	12212.023	3.99E-10	3.99E-10	0.0000196	0.613542368	1.7348411	0.691486252	0.569700977	1.213770521
X19.6_603.396mz_pos	PA(12:0/17:2(9Z,12Z))	exact mass match	12294.09725	6969.655044	8327.708562	3.99E-10	4.26E-10	0.123687579	1.696343697	3.110147133	0.608938182	0.637593189	0.955057539
X18.3_617.413mz_pos	PA(12:0/18:2(9Z,12Z))	exact mass match	13284.81748	8839.839827	8176.290067	3.99E-10	3.99E-10	0.000456543	1.189251941	2.462126326	0.691194611	0.585610685	1.180297132
X15.6_659.457mz_pos	PA(13:0/20:2(11Z,14Z))	exact mass match	45981.33237	32666.14957	35083.69127	3.99E-10	3.99E-10	0.004420634	1.144720387	0.543882002	0.700579576	0.689970085	1.01537674
X17.8_657.447mz_pos	PA(13:0/20:3(8Z,11Z,14Z))	exact mass match	15652.53375	11245.80142	6390.197434	0.000000248	0.00000719	0.481505908	2.88464446	6.284303862	0.736073917	0.401235275	1.834519451
X5.6_679.439mz_pos	PA(13:0/22:6(4Z,7Z,10Z,13Z))	exact mass match	35807.72186	10775.13726	8879.535739	0.00000559	0.0000632	0.515589069	1.668564496	3.652045365	0.316705916	0.230343355	1.374929681
X28.5_582.416mz_pos	PA(14:0/12:0)	exact mass match	68060.34864	54395.45179	38399.62879	6.29E-09	1.05E-09	0.005800485	0.996992536	1.9224387	0.770920037	0.504768252	1.527275208
X25.5_685.509mz_pos	PA(16:0e/18:0)	exact mass match	131715.0377	93369.5763	102607.1521	4E-10	3.99E-10	0.005718917	1.150997041	1.231738498	0.66807447	0.671799109	0.994455724
X13.8_749.509mz_pos	PA(18:0/22:6(4Z,7Z,10Z,13Z))	exact mass match	35951.49471	27325.47776	21565.01657	0.003485393	0.001038166	0.278347592	1.293083604	3.046231396	0.75314036	0.548399788	1.373341815
X27.5_715.428mz_neg	PA(18:3(6Z,9Z,12Z)/20:5(5Z))	exact mass match	25858.09167	42707.67447	56861.52988	0.000574285	0.003893963	0.752036432	0.847050846	1.364329675	1.678068873	1.900880055	0.882785249
X19.7_791.562mz_pos	PA(21:0/22:6(4Z,7Z,10Z,13Z))	exact mass match	19801.59604	11642.65866	13446.36263	3.99E-10	3.99E-10	0.051970796	1.621032248	1.921819624	0.603846243	0.626755846	0.963447325
X13_601.415mz_pos	PA(O-16:0/12:0)	exact mass match	23421.41004	14577.89579	18743.07218	3.99E-10	4.12E-10	0.116618102	1.570508976	2.359717641	0.631908542	0.7358986	0.856896962
X14.8_615.431mz_pos	PA(O-16:0/13:0)	exact mass match	8946.749417	4612.949126	6628.702684	0.000000815	0.000159372	0.865928114	3.219744827	4.692424891	0.598166629	0.69583418	0.859639618
X20.4_659.483mz_pos	PA(O-16:0/O-16:0)[U]	exact mass match	21383.38437	12679.71089	14044.66941	4E-10	4.3E-10	0.077901268	2.109554449	1.915361262	0.607369198	0.604484016	1.004772965
X22.9_671.493mz_pos	PA(O-18:0/15:0)	exact mass match	372763.3511	278161.9363	288158.3225	4.01E-10	4.54E-10	0.08232873	1.291044708	1.756868273	0.687736684	0.655943259	1.048469779
X21.4_705.485mz_pos	PA(P-11:0/22:6(4Z,7Z,10Z,13Z))	exact mass match	14868.03375	11457.86342	5089.694717	0.00027864	0.00000234	0.022553301	4.633408925	8.734348831	0.789701057	0.343726156	2.29747153
X8.7_566.352mz_pos	PAF C-16-d4	exact mass match	13134.1388	8679.274604	5252.275739	4.77E-08	0.000000289	0.211631658	4.309505173	13.0491054	0.691086735	0.401216167	1.722479781
X6.7_298.222mz_pos	Palmitic acid(d3)	exact mass match	8932.171544	6105.979959	5123.316281	0.000194346	0.0000172	0.093881568	4.068641547	4.820362221	0.740043986	0.563562882	1.313152461
X16.2_503.679mz_pos	Palmitoyl CoA	exact mass match	60750.70388	50349.49207	51274.12789	0.00000192	9.04E-08	0.029717452	0.636894233	1.086980505	0.799218268	0.74952048	

X19.7_605.403mz_pos	Papyriferic acid	exact mass match	12244.4117	8627.743861	9969.774985	0.000283365	0.0000184	0.083209501	1.881170455	2.518189886	0.731620018	0.757841792	0.96539941
X8.9_492.979mz_pos	Patuletin 3,3'-di-O-sulfate	exact mass match	5121.028158	3388.446211	3446.392177	0.000012	0.000000012	0.002921032	1.106984692	7.95557718	0.78803534	0.651105881	1.210302905
X9.3_666.428mz_pos	PAz-PC	exact mass match	5980.601082	3901.425777	2325.664016	0.000228583	0.00000615	0.046893024	4.82127767	7.973809184	0.75888487	0.398467899	1.904506917
X21.4_566.384mz_pos	PC(10:0/10:0)	exact mass match	13874.88213	9715.645538	10701.5324	0.00000297	0.00000146	0.122041023	2.623969178	2.583472126	0.720652974	0.716511658	1.00577983
X23.5_572.403mz_pos	PC(10:0/13:0)[U]	exact mass match	14562.41545	8087.234017	6085.306162	9.38E-09	4.34E-10	0.001912595	3.637199627	6.163942377	0.582993951	0.410640513	1.419718546
X18.1_607.41mz_pos	PC(11:1(10E)/11:1(10E))[U]	exact mass match	6652.611621	4019.872114	3198.27529	0.0000302	0.000202628	0.533264398	4.110976594	7.652385456	0.707148846	0.486514109	1.45350121
X18.3_704.515mz_pos	PC(12:0/18:1(9Z))	exact mass match	3603955.745	2540327.715	2348198.3	3.99E-10	3.99E-10	0.077716305	0.560598557	0.973159129	0.66545263	0.596809228	1.115017327
X19.6_724.488mz_pos	PC(14:1(9Z)/18:4(6Z,9Z,12Z))	exact mass match	14651.0498	8685.451824	10180.17301	3.09E-08	2.3E-09	0.016409983	1.941161363	3.100156668	0.616932908	0.652036874	0.946162606
X20.4_464.315mz_pos	PC(15:0/0:0)	exact mass match	7320.36562	5218.739034	5991.909218	0.000765144	0.000000051	0.004158197	3.006593774	4.157354865	0.7897994	0.774763873	1.019406592
X14.2_513.363mz_pos	PC(16:0/0:0)[U] / PC(16:0/0:0)	exact mass match	13046.07965	9121.096362	10974.57697	0.000000902	0.000000051	0.107077143	1.979451952	2.539937833	0.720956906	0.774421917	0.930961392
X24_555.376mz_pos	PC(16:0/2:0)	exact mass match	92665.81625	74949.21594	81830.39837	0.00000216	0.000000864	0.104155177	3.277919791	3.144652157	0.766760781	0.768625239	0.997574294
X21.8_822.604mz_pos	PC(16:0/23:5(8E,11E,14E,17E))	exact mass match	42465.66732	24809.90206	20602.1868	3.99E-10	3.99E-10	0.069577578	1.636242364	2.890642945	0.590864925	0.450304901	1.312144114
X16.8_690.499mz_pos	PC(18:0/11:1(10E))	exact mass match	1480932.675	1049584.641	907788.757	3.99E-10	3.99E-10	0.047656468	0.355037976	0.871826298	0.656911205	0.560790658	1.171025963
X21.4_592.41mz_pos	PC(18:1(9Z)/4:0)	exact mass match	20334.49717	14296.00335	16085.75474	0.000000113	0.000000699	0.555791328	2.828394799	3.140850605	0.711390645	0.724647218	0.98170617
X21.4_847.598mz_pos	PC(18:2(9Z,12Z)/22:6(4Z,7Z))	exact mass match	403316.3445	260927.3668	296682.0294	3.99E-10	3.99E-10	0.02634781	1.151216376	1.372847883	0.601384291	0.630143501	0.954360856
X11.5_766.515mz_pos	PC(18:3(6Z,9Z,12Z)/20:5(5Z,8Z))	exact mass match	265275.1298	205493.4159	202323.7249	4.01E-10	9.76E-10	0.257279474	0.397318265	1.005832036	0.715748852	0.654358854	1.093817021
X51.8_845.574mz_pos	PC(18:3(6Z,9Z,12Z)/22:6(4Z,7Z))	exact mass match	36346.241	65336.46638	56077.55097	0.0000133	0.000736591	0.851706627	8.727370397	6.605681745	1.697412444	1.350473552	1.256901656
X54.6_875.62mz_pos	PC(20:2(11Z,14Z)/22:6(4Z,7Z))	exact mass match	32221.75079	107284.1925	207330.0093	0.0000661	0.004316824	0.962595293	13.94799978	7.343236281	3.1080313	5.572722508	0.557722244
X53_873.605mz_pos	PC(20:3(5Z,8Z,11Z)/22:6(4Z,7Z))	exact mass match	212850.1499	398116.1436	507593.1489	0.00072513	0.001751812	0.558639595	6.208193255	4.295721624	1.685579858	2.058640926	0.818782837
X8.8_518.353mz_pos	PC(O-1:0/O-16:0)[U]	exact mass match	462340.0827	391494.1408	380324.3266	6.65E-10	2.05E-08	0.283789984	0.588991448	0.81754405	0.775083611	0.714758879	1.084398717
X11.3_546.385mz_pos	PC(O-1:0/O-18:0)	exact mass match	27276.56695	20869.95584	17761.50512	4.09E-10	3.99E-10	0.0000933	0.801133707	2.520458945	0.766049827	0.599857388	1.277053251
X12.3_560.401mz_pos	PC(O-10:0/O-10:0)[U]	exact mass match	29252.90649	20547.76145	18794.01773	4.04E-10	6.55E-10	0.135517571	0.769077676	1.977658284	0.708066593	0.591648718	1.196768576
X19.5_454.328mz_pos	PC(O-12:0/O-2:0)	exact mass match	175654.0425	97289.11194	92784.40188	0.0000246	0.002282701	0.953787035	9.62633235	1.31684578	0.526610472	0.460688093	1.143095468
X16.7_736.531mz_pos	PC(O-14:0/18:3(9Z,12Z,15Z))	exact mass match	14454.85805	7477.824334	5545.73149	3.99E-10	0.00000435	0.674944514	2.650048544	2.780599408	0.556184884	0.379337289	1.466201453
X21.4_468.343mz_pos	PC(O-14:0/O-1:0)	exact mass match	182059.3965	128439.8064	129895.4755	0.000302092	0.002728627	0.758186865	5.196458945	1.301697683	0.666237265	0.619850572	1.074835284
X13.5_574.416mz_pos	PC(O-16:0/O-5:0)[U]	exact mass match	29327.55206	19368.53666	13594.97683	3.99E-10	3.99E-10	0.000000541	1.266107067	1.464321279	0.666534177	0.430835816	1.547072347
X21.6_480.004mz_pos	PC(O-16:1(9E)/0:0)[U]	exact mass match	25102.91517	19496.86666	14863.39561	0.00000163	0.00000108	0.128902655	1.140300063	2.350351654	0.778640533	0.555258524	1.402302711
X22_525.399mz_pos	PC(O-18:1(9E)/0:0)[S]	exact mass match	132494.6475	99247.68307	112365.6596	4.04E-10	4.05E-10	0.019018788	1.370708198	1.238171787	0.705342868	0.73137826	0.964402289
X17.3_544.37mz_pos	PC(O-18:1(9E)/O-1:0)[U]	exact mass match	32279.81944	24398.04419	16977.93218	2.83E-09	1.59E-09	0.035461699	1.561946493	2.359033673	0.754677009	0.490658365	1.538090579
X16.4_548.365mz_pos	PC(O-18:2(9Z,12Z)/2:0)	exact mass match	11211.65686	8521.103956	9009.834908	0.0000476	0.000000684	0.024422754	1.812076351	2.009348676	0.789159005	0.3717160001	1.056211527
X27.1_494.354mz_pos	PC(P-17:0/0:0)	exact mass match	16561.20121	10788.64457	6255.490288	5.12E-10	3.99E-10	0.00014022	6.156451895	5.445809623	0.666770908	0.731049998	1.796983999
X26.4_483.003mz_pos	PD 0325901	exact mass match	6936.490652	4723.418336	4747.673539	0.000115201	5.18E-10	0.00001447	2.262032698	3.546640072	0.769330763	0.659007634	1.167407968
X24.7_755.531mz_pos	PE(14:0/22:5(4Z,7Z,10Z,13Z))	exact mass match	542939.594	440750.9466	333777.2596	4.07E-10	3.99E-10	0.001467775	0.641960964	1.412037734	0.746489828	0.530266688	1.407922317
X21.3_674.504mz_pos	PE(14:0/P-18:1(11Z))	exact mass match	46062.24211	31189.05542	28560.61486	3.99E-10	3.99E-10	0.002726029	0.718663323	1.699095895	0.674742469	0.567534595	1.188901037
X21.3_632.431mz_pos	PE(14:1(9Z)/14:1(9Z))	exact mass match	27963.53071	21526.55143	17995.35628	0.00000165	5.49E-09	0.004698693	0.920167877	1.624489895	0.772827402	0.596596144	1.295394565
X37.7_646.427mz_neg	PE(14:1(9Z)/15:0)	exact mass match	515708.9129	1006541.54	966365.639	0.000446326	0.00000125	0.011218986	5.080845803	4.968008947	1.826441419	1.66410665	1.0975507
X20.1_718.53mz_pos	PE(16:0/18:1(9Z))	exact mass match	4658194.075	3290001.53	2997956.293	3.99E-10	4.43E-10	0.198867749	0.427472003	0.918514328	0.676607379	0.616430068	1.097622284
X15.9_688.484mz_pos	PE(16:1(9Z)/16:1(9Z))[U]	exact mass match	25180.01468	19146.27596	15700.62754	4.3E-10	3.99E-10	0.0000597	0.893282313	2.358271567	0.759287324	0.572268966	1.326801503
X13.8_676.483mz_pos	PE(17:0/14:1(9Z))	exact mass match	424397.9424	321941.9345	303729.1869	4E-10	4.07E-10	0.047641876	0.346438777	1.056221702	0.695755895	0.611093144	1.13854312
X6.5_760.496mz_pos	PE(18:3(6Z,9Z,12Z)/20:5(5Z,8Z))	exact mass match	28350.76361	9002.270271	7109.527615	0.0000331	0.00000117	0.040775267	2.265966672	6.730419611	0.344534173	0.234076334	1.471888109
X11.6_736.468mz_pos	PE(18:3(6Z,9Z,12Z)/P-16:0)	exact mass match	42710.27568	33078.52137	30006.51113	0.0000199	0.000283912	0.642036669	1.195970054	1.800136215	0.767201208	0.639099814	1.200440354
X7.3_810.511mz_pos	PE(20:5(5Z,8Z,11Z,14Z,17Z))	exact mass match	12001.5087	4098.490772	3854.147855	1.01E-09	1.21E-08	0.182109236	2.575345978	12.04330013	0.413921612	0.313908021	1.318607949
X28_906.671mz_pos	PE(22:1(13Z)/24:1(15Z))	exact mass match	32503.76866	19763.62695	12965.36897	3.99E-10	3.99E-10	0.001889257	1.722496979	2.803190867	0.615528133	0.373066835	1.649913837
X23.3_878.64mz_pos	PE(22:4(7Z,10Z,13Z,16Z)/2:0)	exact mass match	2225326.967	1577182.918	1360293.111	3.99E-10	4.11E-10	0.385810649	0.51728168	1.15784591	0.656373444	0.563461847	1.164894211
X7.6_810.512mz_pos	PE(22:6(4Z,7Z,10Z,13Z,16Z))	exact mass match	9913.441251	3616.374291	2979.772923	9.59E-09	5E-10	0.004047594	2.071541755	12.51337281	0.451492844	0.304544019	1.482520805
X13.2_455.321mz_pos	PE(P-16:0/0:0)	exact mass match	32292.4088	23784.7336	25278.1343	2.82E-08	1.26E-09	0.010234953	1.712184235	1.236410267	0.726744784	0.713963556	1.017901366
X20.8_642.445mz_pos	PE(P-16:0/12:0)	exact mass match	12138.92972	8724.158505	3957.857611	0.0000118	0.00037039	0.444488576	4.713364221	0.749927556	0.633605511	2.231561234	1.164894211
X18.5_660.489mz_pos	PE(P-16:0/15:1(9Z))	exact mass match	4158706.048	2949169.349	2780379.141	3.99E-10	4.03E-10	0.110095743	0.514230312	0.797461066	0.673870904	0.615159053	1.095441742
X12.8_708.5mz_pos	PE(P-16:0/17:2(9Z,12Z))	exact mass match	8103.400684	4603.203266	3784.662145	6.37E-10	4.85E-10	0.018935477	1.457902211	6.226391346	0.657370488	0.474808003	1.38449749
X21.1_631.481mz_pos	PE-Cer(d14:1(4E)/18:1(9Z))	exact mass match	33306.44808	15736.76271	8789.030028	0.004590793	0.000188036	0.092914015	2.573585025	3.707656333	0.490464588	0.248112458	1.976783402
X18_598.411mz_pos	Pectenolone	exact mass match	27680.23323	21229.6062	16326.36426	0.00000154	0.000079						

X17.4_479.66mz_pos	Pentaglutamyl folate	exact mass match	16467.32078	11623.56416	10382.52174	9.75E-10	1.08E-09	0.044744301	1.537704513	3.086530928	0.717134151	0.589416528	1.216684835
X37.7_464.145mz_neg	Perphenazine sulfoxide	exact mass match	36050.32046	57297.71079	272361.2144	0.0000839	0.004514127	0.9539384	9.152196118	8.155035526	1.517242296	6.448381508	0.235290405
X2.2_211.083mz_neg	PERSEITOL	exact mass match	14697.40892	3934.237839	3839.365102	0.0000933	0.001687635	0.799258983	0.489504416	3.593400783	0.300022054	0.266125446	1.127370788
X13.7_553.303mz_neg	PG(10:0/10:0)[U]	exact mass match	5527.044572	11213.90651	13785.33357	0.000603172	0.000702696	0.409673816	1.59717863	0.858368525	1.884438929	1.94284794	0.969936396
X20.8_635.433mz_pos	PG(12:0/15:0)	exact mass match	71706.99931	50957.78664	58719.73784	4E-10	3.99E-10	0.000592751	2.439371634	3.432673037	0.676628457	0.709324637	0.95388099
X20.4_679.459mz_pos	PG(12:0/17:1(9Z))	exact mass match	74673.3541	50887.48061	61326.08165	3.99E-10	3.99E-10	0.012611272	2.578922048	3.686718571	0.648490661	0.70891203	0.914768877
X9.1_687.424mz_pos	PG(12:0/18:4(6Z,9Z,12Z,15Z))	exact mass match	58654.13041	37273.44452	25277.67278	3.99E-10	3.99E-10	0.016045492	2.980179878	3.35384467	0.622537264	0.396771606	1.569006589
X10.3_715.449mz_pos	PG(12:0/20:4(5Z,8Z,11Z,14Z))	exact mass match	51025.46681	36978.56463	24501.03577	3.99E-10	4.01E-10	0.037797534	6.209945173	5.199326173	0.711599818	0.4444404986	1.601241753
X20.7_679.459mz_pos	PG(13:0/16:1(9Z))	exact mass match	108382.0797	71571.85253	94684.9382	3.99E-10	4.55E-10	0.225767455	3.827982397	4.25130254	0.624399172	0.748737766	0.833935726
X14.9_761.526mz_pos	PG(13:0/22:2(13Z,16Z))	exact mass match	16534.9014	10131.00552	10867.96128	0.000000174	0.00000418	0.803775499	0.94635487	2.535855934	0.632722247	0.612628499	1.032799238
X20.7_656.451mz_pos	PG(14:0/12:0)	exact mass match	32410.4632	24824.47705	14149.95243	0.000000569	0.000000147	0.065527019	2.700135385	3.694923544	0.763935494	0.414613336	1.84252514
X13.3_497.275mz_neg	PG(17:0/0:0)	exact mass match	305964.5815	170175.0641	175135.0305	0.003093026	0.00429612	0.548945783	1.040654251	1.768674366	0.549958011	0.523168059	1.051207162
X25.9_831.603mz_pos	PG(18:0/22:2(13Z,16Z))	exact mass match	13141.62852	9013.554983	9887.743368	4.07E-10	3.99E-10	0.000016	1.59430306	1.904621317	0.710717675	0.501869653	1.012606361
X8.2_539.334mz_pos	PG(20:1(11Z)/0:0)	exact mass match	16934.91515	10731.92137	9625.402882	5.01E-10	4.04E-10	0.004593172	2.338206799	3.702392171	0.651042833	0.537774561	1.21062408
X21.1_909.654mz_pos	PG(22:0/22:2(13Z,16Z))	exact mass match	252156.1887	150055.6617	122705.5384	3.99E-10	3.99E-10	0.026598816	0.603581921	1.894000798	0.556078487	0.420846119	1.32133448
X9.2_567.359mz_pos	PG(22:1(11Z)/0:0)	exact mass match	47519.18735	34543.08581	31098.26393	3.99E-10	3.99E-10	0.047905864	0.624049088	2.035911812	0.716852213	0.598529087	1.197689852
X20.7_675.452mz_pos	PG(O-16:0/12:0)	exact mass match	30384.44944	20381.77746	21563.78928	4E-10	4E-10	0.011675042	1.217040593	1.180369943	0.674353951	0.654749376	1.029942105
X12.8_689.468mz_pos	PG(O-16:0/13:0)	exact mass match	106948.3663	82369.39933	88927.55703	4.84E-10	1.38E-09	0.106058369	0.520534084	1.083477633	0.725094439	0.722028974	1.004254625
X15.7_703.483mz_pos	PG(O-16:0/14:0)	exact mass match	20460.44744	12206.99032	14115.91478	3.99E-10	1.55E-09	0.455056463	0.98748052	1.173964491	0.610561066	0.636013568	0.959981196
X14.9_717.499mz_pos	PG(O-16:0/15:0)	exact mass match	19811.23622	13665.29574	14223.59977	0.00000612	0.001849848	0.992898767	0.833428352	2.40490181	0.694799975	0.659334284	1.053790151
X21.7_759.547mz_pos	PG(O-18:0/18:3(6Z,9Z,12Z))	exact mass match	106671.281	72131.23518	74704.5431	3.99E-10	3.99E-10	0.0000893	1.157014683	2.013918388	0.640923693	0.606304063	1.057099451
X14.2_353.234mz_neg	PGE1	exact mass match	5105.808929	7836.559724	9610.961712	0.002134704	0.000689093	0.270616803	1.49342353	2.030135133	1.532070886	1.49925404	1.021888783
X17.8_410.319mz_pos	PGF2α diethyl amide	exact mass match	28906.22163	20568.11011	22376.52889	5.35E-10	4.07E-10	0.005406726	1.57489638	1.293236496	0.711925671	0.70709543	1.006831102
X27.1_395.28mz_neg	PGF2α isopropyl ester	exact mass match	7314.947775	4378.608741	6106.667678	0.00000139	0.003039437	0.950315456	1.083308902	1.766073175	0.70368881	0.74686219	0.942193647
X25.9_527.029mz_pos	Ph4Cl-Ph4Cl-OH	exact mass match	22532.23984	17178.54778	19311.15895	0.0000797	1.87E-08	0.001324331	2.318890174	1.807948864	0.792605764	0.792233366	1.000470061
X12.1_618.405mz_pos	Phorbol 12-tiglate 13-deca	exact mass match	89060.17046	73970.8111	64101.45694	5.11E-08	0.000000129	0.143119874	0.729356843	1.039977844	0.79223624	0.626679457	1.264180964
X8.4_455.955mz_pos	Phosphiphen	exact mass match	7137.747425	4296.751421	2915.403819	9.72E-10	8.62E-10	0.036133904	3.16765271	7.406858102	0.702763692	0.424290949	1.656324966
X16.4_395.999mz_pos	Phosphonoformyl-CMP	exact mass match	15271.75326	10336.12323	2710.721088	0.00405052	0.000237673	0.275074287	5.660940416	6.850436803	0.704388103	0.187319636	3.760353784
X7.4_497.151mz_neg	Phylloflavan	exact mass match	7162.720413	12867.43916	3052.6199	0.002468977	5.17E-10	0.000001114	14.62989304	11.55834356	1.781033047	0.450082539	3.957125401
X10.3_493.19mz_pos	Physalin C	exact mass match	10745.46614	14637.42638	6485.862219	0.000099	0.000311901	0.475014184	7.685345298	6.437525249	1.335562065	0.577551516	2.312440885
X21.6_825.554mz_pos	PI(12:0/21:0)	exact mass match	42197.82703	26430.34954	37362.41572	3.99E-10	3.99E-10	0.02866009	6.612414786	10.78605087	0.620310991	0.789342214	0.785858123
X12.4_868.583mz_pos	PI(13:0/22:1(11Z))	exact mass match	21201.10297	14060.24094	13649.33106	2.67E-08	0.0000184	0.848233546	1.066489962	2.863866227	0.66973386	0.595164457	1.125292098
X6.1_727.439mz_pos	PI(14:0/12:0)	exact mass match	16326.66839	5023.827503	4464.900497	0.00000584	0.000494952	0.863665864	1.923619694	6.847002258	0.351979363	0.263781539	1.334359347
X33.8_853.527mz_pos	PI(15:1(9Z)/22:4(7Z,10Z,13Z))	exact mass match	161531.8963	280914.2027	251441.0935	0.000135315	0.001478248	0.733161188	2.790739069	1.766985873	1.58246846	1.315750028	1.202712085
X14.9_910.63mz_pos	PI(16:0/22:1(11Z))	exact mass match	23235.35263	13588.81519	9753.170345	1.01E-09	7.59E-08	0.376878162	2.248722124	2.598201221	0.594168729	0.399313196	1.487976694
X17.6_924.645mz_pos	PI(17:0/22:1(11Z))	exact mass match	41946.13018	26785.81908	21699.86727	3.99E-10	3.99E-10	0.000349239	0.559274178	2.489283022	0.643116314	0.481253471	1.33633595
X19.3_921.634mz_pos	PI(18:0/22:1(11Z))	exact mass match	18492.44323	11589.02169	13840.50208	4E-10	1.41E-08	0.727303969	1.151151767	1.583040132	0.63977255	0.68382265	0.935582566
X21.3_952.677mz_pos	PI(19:0/22:1(11Z))	exact mass match	100944.9572	63400.03709	50820.3153	3.99E-10	3.99E-10	0.001684459	0.591311963	2.106284865	0.601409974	0.435165152	1.382026965
X24.8_963.681mz_pos	PI(21:0/22:1(11Z))	exact mass match	15297.44775	8892.006869	10683.09415	3.99E-10	3.99E-10	0.000372809	2.219940016	3.357008613	0.603931544	0.645134957	0.936132103
X19.9_767.512mz_pos	PI(O-16:0/14:1(9Z))	exact mass match	50306.90669	31291.24483	43475.57687	3.99E-10	3.99E-10	0.002668322	4.41321884	5.256163351	0.609447618	0.757973512	0.804048701
X15_866.604mz_pos	PI(O-16:0/20:2(11Z,14Z))	exact mass match	24526.82589	16527.99837	13032.03397	5.2E-09	0.000000483	0.450465521	1.117339218	2.585861925	0.680280853	0.497157448	1.368340866
X18.9_894.635mz_pos	PI(O-16:0/22:2(13Z,16Z))	exact mass match	35901.90776	20925.92763	14724.13467	3.99E-10	3.99E-10	0.0000277	0.905795123	3.399382476	0.591266786	0.377048192	1.527630921
X7_871.564mz_pos	PI(O-18:0/20:5(5Z,8Z,11Z,14Z))	exact mass match	11198.67843	3786.905646	2538.086576	0.000193694	0.000014	0.083526533	6.309570192	10.27161026	0.403496853	0.231195627	1.74526045
X23_905.64mz_pos	PI(O-18:0/22:2(13Z,16Z))	exact mass match	199207.5195	136505.7775	147261.5278	3.99E-10	3.99E-10	0.107618732	1.74828831	1.626352611	0.637352611	0.644068528	0.989572668
X27.4_950.698mz_pos	PI(O-20:0/22:2(13Z,16Z))	exact mass match	97186.0431	60932.56769	40703.26733	3.99E-10	3.99E-10	0.0000301	1.082787737	2.200418129	0.60215813	0.366381236	1.643528847
X8_966.639mz_pos	PI(O-20:0/22:6(4Z,7Z,10Z,13Z))	exact mass match	25549.75436	9868.15589	4309.091668	4.01E-10	4.03E-10	0.021091276	3.456723739	10.67123837	0.412055429	0.169047775	2.437508737
X20_767.512mz_pos	PI(P-16:0/14:0)	exact mass match	57440.68392	35642.73873	50951.90765	3.99E-10	3.99E-10	0.0262674	4.362918393	4.881054265	0.600327654	0.767057162	0.78263744
X21.3_891.624mz_pos	PI(P-20:0/19:1(9Z))	exact mass match	67635.39587	42307.18905	53861.32151	3.99E-10	3.99E-10	0.074711436	1.370681268	1.828423801	0.601083631	0.689146387	0.872214731
X18.2_543.367mz_pos	Pikromycin	exact mass match	77869.55441	52794.67746	43934.27833	3.99E-10	3.99E-10	0.008347616	0.535300596	1.432428429	0.654296164	0.494869914	1.322157896
X41_744.488mz_pos	Piloceraine	exact mass match	263501.1351	499057.5119	478354.5425	5.11E-08	0.000493525	0.958969221	2.287983854	0.629016249	1.731425887	1.559735242	1.110076787
X11.4_287.138mz_pos	Pilosine	exact mass match	5811.908219	10487.09754	9976.392901	0.0000325	0.000720522	0.758948414	6.92189784	3.995147641	1.712766896	1.457989481	1.174745715
X16.4_626.157mz_pos	Pinotin A	exact mass match	78025.19922	42246.74888	20312.09909	0.0000424	0.0000873	0.358217939	2.600070059	3.414757383	0.525107718	0.235268005	2.231955499
X37.7_398.153mz_neg	Pipazethate	exact mass match	32452.28035	56260.77226	70122.07237	0.000151191	0.0000181	0.107360837	4.331538632	3.523220868	1.746813506	1.881394514	0.928467418
X8.6_324.193mz_pos	PIPERIDOLATE	exact mass match	17341.404	10501.54395	14023.96083	0.000350295	0.002206053	0.698172252	3.059475128	5.646124552	0.640421995	0.725757977	0.882418127
X12.6_340.269mz_pos	Piptanthine	exact mass match	60006.35986	42358.81805	37209.41101	3.99E-10	3.99E-10	0.000569536	1.164488571	0.3959913	0.684943209	0.554875059	1.234409797
X20.4_481.007mz_pos	Ponceau SX	exact mass match	45001.21697	35440.8335									

X14.7_300.065mz_pos	PPM-18	exact mass match	12993.79855	8846.77241	8919.772717	0.00010622	0.001846689	0.801627424	5.530041292	3.725693046	0.703392172	0.637618309	1.103155543
X16.4_858.311mz_pos	Pradimicin A	exact mass match	40180.29946	19640.92448	8864.256666	0.000307814	0.000587589	0.456587743	3.707099525	7.582701314	0.478193479	0.203923149	2.34496908
X18.1_425.25mz_pos	Pravastatin	exact mass match	88684.48342	136381.3763	63155.83577	0.000605209	0.004195088	0.760630905	7.87548108	6.092011635	1.429444688	0.62090988	2.302177392
X27.9_387.254mz_neg	Pregn-4-en-20-one, 3b,1	exact mass match	9511.655483	6194.569047	7148.663468	0.0000116	0.002273748	0.986086126	1.401319019	2.313232087	0.727331795	0.679730339	1.070209912
X16.4_209.117mz_pos	Primin	MS/MS spectrum match	911990.0857	628369.5706	602887.4005	0.0000188	0.000427552	0.723725878	0.952049735	0.544817987	0.617802703	0.604914224	1.021306291
X8.6_393.063mz_pos	Prochloraz	exact mass match	27025.60782	15661.63346	16309.77433	0.00010409	0.001046601	0.697317535	4.385425589	2.799378439	0.60115338	0.537474935	1.11847705
X16.4_604.076mz_pos	Prochlorperazine mesylate	exact mass match	13341.27629	10089.29199	10663.14677	0.00000474	0.000115492	0.639010318	1.768536053	4.266454945	0.776157837	1.740555235	1.048075552
X37.7_450.123mz_neg	Prochlorperazine sulfone	exact mass match	5549.023838	9665.222034	10503.17577	0.001004323	0.00000534	0.019712016	3.17903558	3.337486614	1.674667396	0.493646465	1.121193961
X11.1_502.358mz_pos	Propapyriogenin A2	exact mass match	34328.25409	26149.07407	24325.23005	4.02E-10	4.04E-10	0.020331305	0.713827944	1.409868182	0.760981393	0.651135307	1.168699324
X10.3_386.067mz_neg	Propiconazole	exact mass match	6185.99314	8452.435924	3891.040466	0.003052593	0.00168914	5.89E-08	6.046805182	5.503316061	1.369102531	0.595846621	2.297743216
X20.3_686.137mz_pos	Propidium Iodide Solution	exact mass match	16438.58847	12681.79715	9506.38263	0.000168869	0.00000715	0.05929307	2.293818815	2.632739877	0.784126667	0.548822305	1.428744168
X23.1_514.026mz_pos	Protogonyautoxin 3	exact mass match	169841.798	142525.022	117832.9987	1.97E-08	8.38E-10	0.007754531	0.485669602	1.25984978	0.784482273	0.605869565	1.294803896
X32.1_662.292mz_pos	Protorifamycin I	exact mass match	23289.21466	49266.65657	53954.84568	0.000154123	0.000625172	0.550591004	1.827573616	5.870358149	2.033073608	1.979736697	1.026941416
X37.7_698.398mz_neg	PS(12:0/18:4(6Z,9Z,12Z,15Z))	exact mass match	23842.95677	51960.8862	36772.97402	0.00038403	0.000000153	0.002564704	7.135454942	8.890499595	2.153419559	1.325123616	1.625070697
X40.7_744.487mz_pos	PS(13:0/20:3(8Z,11Z,14Z))	exact mass match	87312.63095	203785.0336	170408.0689	2.02E-08	0.0000645	0.985796821	2.26378569	1.456572894	2.14639512	1.657241082	1.295161666
X11_752.472mz_pos	PS(14:1(9Z)/20:5(5Z,8Z,11Z))	exact mass match	21351.91088	15389.24651	16771.71907	0.000000256	0.00000157	0.605611279	3.196180548	3.458954788	0.727195296	0.59552353	1.221102541
X12.1_736.505mz_pos	PS(16:0/16:0)	exact mass match	647186.1748	487901.3949	451480.3016	3.99E-10	3.99E-10	0.073364854	0.329022539	1.080754693	0.679235228	0.599027237	1.13389707
X39.7_788.544mz_pos	PS(18:1(9Z)/18:1(9Z))U	exact mass match	45237.08269	125987.9942	228575.8801	0.001725132	0.0000088	0.093959319	6.77611179	7.205339347	2.591415538	4.523904869	0.572827151
X25.9_848.63mz_pos	PS(19:0/21:0)	exact mass match	115731.2175	79418.94008	55176.31227	3.99E-10	3.99E-10	0.000000868	0.892870268	1.289078869	0.655117334	0.413220416	1.585394402
X23.2_546.282mz_neg	PS(20:3(8Z,11Z,14Z)/0:0)	exact mass match	5397.449904	6934.206641	9124.237288	0.001834914	0.004739772	0.642719229	5.018853434	4.135492111	1.300418784	1.353201423	0.960994248
X20.9_910.656mz_pos	PS(21:0/22:1(11Z))	exact mass match	30027.89377	16150.2085	11715.16518	3.99E-10	3.99E-10	0.003532607	0.445246339	3.722865258	0.551761356	0.369010248	1.495246704
X23.9_764.536mz_pos	PS(22:0/12:0)	exact mass match	396706.0005	300411.879	273057.0584	3.99E-10	4.01E-10	0.025969329	0.473449357	1.093132524	0.700207532	0.592435372	1.181913784
X14.1_940.64mz_pos	PS(22:0/22:1(11Z))	exact mass match	24161.46971	14184.75588	9740.96974	4.04E-10	4.09E-10	0.025168063	1.632221489	3.79710667	0.598370551	0.381959965	1.566579239
X13.9_720.51mz_pos	PS(O-16:0/16:1(9Z))	exact mass match	528128.6444	400840.7455	374185.6345	3.99E-10	4.03E-10	0.043428024	0.373071979	0.977989843	0.68567048	0.608228669	1.127323514
X16.8_734.525mz_pos	PS(O-16:0/17:1(9Z))	exact mass match	1111891.254	786818.6995	679934.0866	3.99E-10	3.99E-10	0.01905885	0.326729243	1.024788836	0.648074229	0.536826763	1.207231595
X6.1_790.507mz_pos	PS(O-16:0/20:5(5Z,8Z,11Z))	exact mass match	16037.18395	50625.277881	3292.363796	0.00000841	0.000142553	0.613521061	3.0533387	8.330564776	0.35975927	0.202593406	1.775769891
X26.7_804.603mz_pos	PS(O-16:0/22:1(11Z))	exact mass match	86224.18875	62743.94372	43741.60086	3.99E-10	3.99E-10	0.00000455	0.74046015	1.831529728	0.702423522	0.445484929	1.579953516
X23.3_690.473mz_pos	PS(P-16:0/14:1(9Z))	exact mass match	14771.45379	10954.67403	7910.027238	0.000462701	0.000211987	0.257793123	2.371939535	3.250178486	0.759540247	0.513056723	1.480421586
X19.1_718.494mz_pos	PS(P-16:0/16:1(9Z))	exact mass match	11115.70981	6684.358487	4660.080871	0.000000236	0.000000109	0.07266213	5.866226831	5.450889678	0.646934334	0.417059077	1.551181523
X18_838.599mz_pos	PS(P-20:0/19:1(9Z))	exact mass match	28944.77079	16481.26683	12563.13091	3.99E-10	3.99E-10	0.026133174	0.933674561	5.067099419	0.578567288	0.405353364	1.427315868
X18.4_703.981mz_pos	Psamaplin A	exact mass match	42631.67149	27775.21053	22951.12072	4.01E-10	4.11E-10	0.040510114	3.150852737	3.773587617	0.646738835	0.495670945	1.30477455
X16.6_866.604mz_pos	PubChem:(100928965)	Sirius match	28103.71617	17554.53317	14872.85307	3.99E-10	3.99E-10	0.007614685	0.66031068	2.422494512	0.633336471	0.492677569	1.285498986
X29.9_447.312mz_neg	PubChem:(101300969)	Sirius match	23806.79818	11431.04914	14278.74982	5.54E-08	0.004453381	0.600329735	2.112764209	2.324184508	0.522965881	0.559073132	0.93541587
X19.3_877.608mz_pos	PubChem:(101402222)	Sirius match	212381.7041	141487.9057	157695.3455	3.99E-10	3.99E-10	0.056262694	0.894698351	1.131702876	0.62217202	0.645832938	0.963363718
X34.6_578.25mz_pos	PubChem:(101486042)	Sirius match	114136.1713	640073.9993	1058219.548	3.99E-10	1.37E-08	0.876282629	7.009585731	6.533157712	5.290487436	8.664811174	0.610571579
X9.8_414.306mz_pos	PubChem:(102045845)	Sirius match	517854.2381	389070.457	365600.3863	3.99E-10	3.99E-10	0.047954764	0.406815172	1.688506332	0.683827952	0.606830613	1.126884401
X10_576.395mz_pos	PubChem:(102068876)	Sirius match	609960.0834	496033.0139	467922.9581	3.99E-10	4.89E-10	0.205777782	0.479108416	0.809494295	0.735034939	0.656328442	1.119919375
X20.8_630.478mz_pos	PubChem:(102077830)	Sirius match	2374941.357	1703600.371	1605165.941	4.01E-10	7.1E-10	0.200163944	0.54711412	1.045462043	0.667225556	0.620300419	1.07645511
X16.8_778.551mz_pos	PubChem:(102449434)	Sirius match	410345.7064	286815.7084	258320.0349	3.99E-10	3.99E-10	0.019229426	0.569257446	1.075783834	0.648199209	0.540852646	1.198476543
X32.1_367.18mz_pos	PubChem:(104076871040)	Sirius match	244873.7019	382957.456	509156.9384	0.000272042	0.00331383	0.807037141	3.567977145	2.676904999	1.425302662	1.76531726	0.807391789
X16.4_289.106mz_neg	PubChem:(108167690)	Sirius match	166071.1185	100266.1803	98533.44019	0.0000763	0.001068104	0.737005213	1.336617251	1.28207984	0.630328953	0.559714975	1.126160603
X34.6_382.182mz_pos	PubChem:(110119094125)	Sirius match	10875.26084	66785.00194	103562.7866	6.15E-10	0.000762245	0.420779245	10.50849101	2.82675696	5.708018646	8.140014439	0.701229548
X14.1_354.284mz_pos	PubChem:(111279841)	Sirius match	112958.1224	83615.24046	75701.35616	9.84E-10	4.04E-10	0.001973357	0.992748819	0.741212991	0.700297145	0.578049291	1.211484344
X9.7_532.369mz_pos	PubChem:(11307370)	Sirius match	773013.1418	613645.2148	589648.8192	3.99E-10	4.03E-10	0.152673356	0.667993553	0.970827751	0.712861662	0.655774401	1.087053201
X17_602.447mz_pos	PubChem:(117883478)	Sirius match	2456447.423	1738403.97	1626412.775	3.99E-10	4.01E-10	0.165028306	0.54749429	1.165939277	0.661768998	0.609848585	1.085136563
X12_692.479mz_pos	PubChem:(117904446)	Sirius match	837418.3393	626496.0337	562095.203	3.99E-10	3.99E-10	0.059478037	0.389841441	0.991098004	0.669542767	0.572323923	1.169866818
X1.6_213.098mz_pos	PubChem:(118244276)	Sirius match	19423.91613	5342.420308	6920.377731	0.00067642	0.004954424	0.780465712	2.120717393	6.595156555	0.29036262	0.347672478	0.835611359
X19_572.436mz_pos	PubChem:(118569846)	Sirius match	3123213.006	2285057.427	2129331.002	4.02E-10	5.47E-10	0.118079411	0.434967956	1.018091321	0.684311186	0.613937906	1.114626054
X18_819.567mz_pos	PubChem:(11857590)	Sirius match	108872.5187	73332.9637	83185.95144	3.99E-10	3.99E-10	0.014433681	1.169113008	0.956423856	0.635746523	0.658604064	0.965293957
X20.9_476.358mz_pos	PubChem:(121391961139)	Sirius match	130711.6207	187774.2738	264705.5207	0.001867438	0.0000272	0.042560687	6.280755586	3.009771301	1.3524515	1.739999585	0.777271162
X20.8_891.624mz_pos	PubChem:(122201608)	Sirius match	67068.77946	44421.32485	48573.48492	3.99E-10	3.99E-10	0.0000278	1.209295827	1.656640282	0.636202886	0.630505058	1.009036927
X22.8_905.639mz_pos	PubChem:(122201636)	Sirius match	62164.78132	36243.22965	50659.12719	0.00000144	0.00000136	0.15135996	4.996871858	7.131636585	0.565353212	0.707665331	0.798899123
X37.7_452.119mz_neg	PubChem:(122306767)	Sirius match	236347.4965	385899.2946	431918.581	0.000100105	0.0000417	0.195777653	1.277730779	1.760548479	1.630703206	1.664158349	0.979896659
X18_792.567mz_pos	PubChem:(122389449)	Sirius match	1957225.551	1387032.623	1235231.732	3.99E-10	3.99E-10	0.09859312	0.339000931	1.020048153	0.65510167	0.578524008	1.132367302
X11.4_353.252mz_pos	PubChem:(123299389)	Sirius match	14705.41615	11318.67298	12126.40779	0.00000235	1.46E-08	0.008062564	1.207364008	1.6913524	0.782324929	0.760350566	1.028900305
X13_750.519mz_pos	PubChem:(123308928)	Sirius match	632411.0694										

X24_355.228mz_neg	PubChem:(123461402)	Sirius match	105347.4783	278392.0215	435907.9955	0.0000019	0.00000638	0.281861267	1.262012625	5.650732013	2.645833562	3.613597746	0.732188182
X11_634.437mz_pos	PubChem:(123609703)	Sirius match	825175.2199	627155.6258	613944.1251	3.99E-10	4.05E-10	0.289290411	0.645587487	1.034866444	0.685226396	0.644207824	1.063672888
X9.4_488.343mz_pos	PubChem:(123793792)	Sirius match	849914.377	673322.5806	658157.9666	3.99E-10	6.25E-10	0.421586124	0.69587773	0.952075991	0.714047317	0.675419474	1.057190893
X23.3_861.614mz_pos	PubChem:(127025305);Pu	Sirius match	280362.7181	191098.9522	218774.426	3.99E-10	3.99E-10	0.150764175	0.95880048	1.450068831	0.629754489	0.667238534	0.943822122
X7.8_384.259mz_pos	PubChem:(128935389)	Sirius match	23240.89323	18082.39324	16554.93468	0.00000227	0.00000415	0.1551462	0.700301439	1.610443291	0.778407845	0.654105382	1.190034308
X14.4_486.363mz_pos	PubChem:(129236486)	Sirius match	797850.1099	599701.841	598327.3918	3.99E-10	3.99E-10	0.134811055	0.445632842	0.974660797	0.67443342	0.64468113	1.046150397
X37.7_431.174mz_neg	PubChem:(129292423)	Sirius match	88496.82894	135876.5261	174120.938	0.0000611	0.000101042	0.344068402	1.954552074	1.959607213	1.526890257	1.742023669	0.876503737
X10.3_502.358mz_pos	PubChem:(130291918)	Sirius match	948276.6324	724759.0097	691947.936	3.99E-10	4.04E-10	0.313890739	0.564112662	0.942781245	0.681491373	0.636035492	1.071467522
X9.1_444.316mz_pos	PubChem:(132555253)	Sirius match	858039.8009	665964.1946	644635.7647	3.99E-10	4.02E-10	0.18572879	0.756546498	0.860162954	0.69791021	0.654658772	1.066067147
X9.5_370.279mz_pos	PubChem:(132594475)	Sirius match	162886.6297	121948.0627	112622.2167	3.99E-10	3.99E-10	0.007363546	0.855049019	0.743982559	0.699829352	0.599122955	1.168089698
X21.9_803.571mz_pos	PubChem:(132837452)	Sirius match	230513.5051	157576.0511	180332.4616	3.99E-10	3.99E-10	0.028736874	1.263553411	1.322590182	0.633985677	0.677738211	0.935443312
X8.6_298.177mz_pos	PubChem:(134993681_134	Sirius match	2309466.848	1373935.859	1656148.454	0.0000149	0.0032865	0.996255306	0.713183524	0.916145172	0.577785539	0.64417223	0.896942637
X28.6_340.284mz_pos	PubChem:(135240006_135	Sirius match	46584.80982	20353.84644	21020.44182	3.99E-09	0.0000572	0.996740346	2.463041263	4.211162735	0.449606593	0.423375139	1.061957944
X19.5_850.609mz_pos	PubChem:(135563652);CH	Sirius match	2909637.267	2042332.584	1800610.724	3.99E-10	3.99E-10	0.101558223	0.35234552	0.99328743	0.651944183	0.561649934	1.160766064
X20.6_462.142mz_neg	PubChem:(135965356)	Sirius match	22532.2032	73217.94447	80293.51679	2.01E-08	0.001394891	0.735644622	4.043220882	0.931499222	3.211214835	3.174717362	1.011496291
X14.9_778.55mz_pos	PubChem:(136390100)	Sirius match	169763.1559	118458.0041	97776.1045	3.99E-10	3.99E-10	0.01984759	0.505800513	1.125406076	0.648786938	0.498508915	1.301455038
X24_600.468mz_pos	PubChem:(137308119)	Sirius match	242622.0117	178744.6027	157364.6929	4.02E-10	4E-10	0.00901202	0.375104026	1.090764418	0.686429578	0.562553484	1.220203231
X10_267.12mz_pos	PubChem:(139327660)	Sirius match	4907.711304	8866.309242	8775.933682	0.00000521	0.0000325	0.654165854	14.65471485	13.62413157	1.680390573	1.52020277	1.105375616
X10.3_380.033mz_neg	PubChem:(14128419)	Sirius match	107283.878	137533.5706	23764.35862	0.000253003	0.004562729	2.52E-08	5.959660522	5.657805345	1.316669714	0.203912316	6.457038697
X10.1_458.332mz_pos	PubChem:(18296198)	Sirius match	835886.0436	636746.8246	613118.006	3.99E-10	3.99E-10	0.072385512	1.08201853	2.477691834	0.68505436	0.632213202	1.083581232
X5.7_312.238mz_pos	PubChem:(19141677)	Sirius match	202748.6769	165695.6322	155956.575	1.08E-09	0.000000074	0.364673377	1.186831453	1.978399774	0.76049472	0.670621228	1.134015281
X8.6_527.214mz_pos	PubChem:(19529255)	Sirius match	40497.96079	25859.81557	57918.46074	0.0000944	0.002834918	0.88476406	5.754228183	9.109002892	0.635783276	1.217705125	0.522115957
X16.8_646.473mz_pos	PubChem:(19893390_5432	Sirius match	2349454.304	1652754.26	1569277.126	3.99E-10	4E-10	0.168280981	0.478679185	1.16915685	0.656808155	0.612670915	1.072040698
X23.8_817.587mz_pos	PubChem:(21059301)	Sirius match	118224.1056	86919.09782	96378.50363	3.99E-10	3.99E-10	0.000174558	1.483777261	1.226096213	0.692083466	0.698441683	0.990896566
X34.6_533.192mz_pos	PubChem:(21588517)	Sirius match	1081864.73	4999869.007	6709951.779	3.99E-10	1.14E-09	0.95746507	3.483479576	1.438125088	5.290857032	6.75962634	
X22_542.426mz_pos	PubChem:(21808473_2180	Sirius match	304031.1077	223695.2076	175572.8689	4E-10	4E-10	0.009745675	0.705860826	1.096623209	0.684135919	0.501196147	1.365006342
X26.6_483.297mz_neg	PubChem:(21845541)	Sirius match	44757.70494	21910.19053	25033.32522	3.16E-09	6.22E-08	0.242078837	1.063653632	2.353118017	0.510801923	0.501555994	1.018434491
X37.7_444.087mz_pos	PubChem:(22536862)	Sirius match	1759790.126	2871514.087	4338772.811	0.000634356	0.000359794	0.292901182	1.36477462	1.098813928	1.540888793	2.310389069	0.666939095
X14.9_243.159mz_pos	PubChem:(23052242)	Sirius match	10214.65057	16354.71521	17732.44711	0.0000114	0.004797536	0.995194817	1.769539525	2.677201362	1.548587549	1.540061022	1.005536492
X32.4_372.116mz_neg	PubChem:(2373052_23730	Sirius match	10802.85545	16011.81526	16770.09244	0.002578227	0.000280553	0.154689262	2.612344403	2.671422397	1.497498293	1.312162244	1.141244766
X18.8_687.488mz_pos	PubChem:(25155707)	Sirius match	114213.1396	80232.53605	89202.13674	3.99E-10	3.99E-10	0.049256441	1.011548692	1.083706073	0.626239172	0.671906597	0.986207273
X28.5_370.183mz_pos	PubChem:(25744986)	Sirius match	123640.9829	845388.6331	918903.2965	3.99E-10	5.99E-10	0.980542907	4.661612361	0.689590766	6.350727166	6.845692279	0.92796985
X27.2_483.367mz_pos	PubChem:(4412448)	Sirius match	218625.9811	169766.4878	146713.2907	0.00000178	0.00113011	0.99818126	1.894138785	2.218131106	0.722581277	0.581581082	1.242442884
X32.1_352.177mz_pos	PubChem:(53933216)	Sirius match	83123.07478	131705.0325	170757.8045	0.0000764	0.000803686	0.682904217	1.385764375	2.224735689	1.499354797	1.750229485	0.856661832
X10.2_428.285mz_pos	PubChem:(54054725)	Sirius match	20390.9679	15945.25709	15122.31099	0.000000553	0.0000137	0.503033382	0.962731876	1.36545453	0.787009295	0.678919024	1.159209372
X10.6_546.385mz_pos	PubChem:(57073523)	Sirius match	1018227.933	771066.8542	740749.5357	3.99E-10	4.39E-10	0.444959934	0.395577489	1.056750671	0.683114303	0.640934128	1.065810469
X14_329.233mz_neg	PubChem:(57112208)	Sirius match	25705.63432	6684.929061	9755.626562	3.99E-10	8.43E-10	0.949176203	0.915172517	2.011020692	0.313771452	0.366465905	0.856209124
X5.6_366.238mz_pos	PubChem:(57413668)	Sirius match	53055.8093	16582.99882	17773.42171	1.53E-08	0.00000342	0.643950986	1.784469595	2.631528655	0.322117711	0.301657888	1.067824591
X12.8_645.442mz_pos	PubChem:(57805134_6853	Sirius match	170941.0329	128590.3956	102735.8712	4.01E-10	3.99E-10	0.000290415	1.733755498	1.733755498	0.701547829	0.522205571	1.343432296
X23.3_644.494mz_pos	PubChem:(57840046)	Sirius match	878329.6785	635631.8556	551021.0717	3.99E-10	4E-10	0.021003944	0.422824579	0.999950297	0.657564134	0.536135364	1.226489012
X10.2_620.421mz_pos	PubChem:(58301686_1231	Sirius match	444288.0443	366602.3678	342615.7641	4.01E-10	4.64E-10	0.087999292	0.627986898	0.810189514	0.75488242	0.661199027	1.14168713
X19.9_762.557mz_pos	PubChem:(58302059_1237	Sirius match	4537241.301	3191260.414	2906723.413	3.99E-10	4.07E-10	0.124545442	0.319143067	1.006824553	0.677703264	0.605210322	1.119781404
X34.6_567.155mz_neg	PubChem:(59648218)	Sirius match	24579.50109	128142.6604	77061.65642	3.99E-10	4.01E-10	0.448035744	4.399815946	2.257624822	5.122976548	2.728242219	1.877757229
X30.2_676.499mz_pos	PubChem:(59844531)	Sirius match	257573.3758	431166.957	584259.6459	0.003244338	0.0000291	0.032759451	4.29272017	4.422537108	1.565916543	1.949717168	0.803128124
X20.5_674.504mz_pos	PubChem:(60194116)	Sirius match	3991514.188	2866604.975	2659430.85	4E-10	4.19E-10	0.065125163	0.495035034	0.964214605	0.689013251	0.613792708	1.122550402
X14.4_574.416mz_pos	PubChem:(67222548)	Sirius match	379911.4366	279655.6948	257354.9943	3.99E-10	3.99E-10	0.005187629	0.669256733	0.847092633	0.683879655	0.586249844	1.16653274
X12.8_662.468mz_pos	PubChem:(6722172)	Sirius match	588688.1039	420628.7753	369100.8252	3.99E-10	3.99E-10	0.084249945	0.455171825	0.865661079	0.649261348	0.541109906	1.199871436
X19.4_413.291mz_neg	PubChem:(69516894)	Sirius match	89328.43998	39979.38992	35992.91116	0.0000214	0.000721922	0.802746032	0.506521448	0.992813821	0.458370637	0.368460568	1.244015443
X16.4_267.124mz_neg	PubChem:(69745087)	Sirius match	6322413.316	3945043.097	4354788.963	0.00000181	0.001139875	0.998161048	0.407690009	0.742530881	0.574057405	0.675462017	0.849873702
X11.9_648.453mz_pos	PubChem:(70883444)	Sirius match	952884.7595	716571.159	655045.1535	3.99E-10	3.99E-10	0.157504177	0.466475752	0.926663358	0.672694811	0.595245031	1.130114114
X15_690.498mz_pos	PubChem:(70986616)	Sirius match	26321.68452	19005.87882	14584.95291	2.76E-08	0.000000162	0.192564109	1.248244449	2.564889288	0.725145402	0.516827795	1.403069665
X6_574.36mz_pos	PubChem:(71202655)	Sirius match	35719.40111	10986.63336	11447.89319	0.00000157	0.0000038	0.237923333	1.280366636	2.098996662	0.327068798	0.294253103	1.111522004
X18.9_938.661mz_pos	PubChem:(71451942);Pub	Sirius match	85846.70065	55714.32703	46372.85173	3.99E-10	3.99E-10	0.0000769	0.521300619	1.253234785	0.624463416	0.470924117	1.326038302
X37.7_381.174mz_neg	PubChem:(85711770)	Sirius match	701658.9484	1157712.423	1254155.265	0.000328685	0.00000486	0.033701486	2.629282814	2.808916043	1.565173047	1.621829958	0.96506606
X12.8_367.268mz_pos	PubChem:(87315495)	Sirius match	31747.12273	19660.64861	24321.19842	4.26E-10	7.48E-08	0.662774946	1.254691378	1.738169384	0.621114728	0.698120012	0.889696209
X15.7_544.405mz_pos	PubChem:(8755409)	Sirius match	1335104.865	974670.9688	916298.9265	3.99E-10	3.99E-10	0.19992785	0				

X11.7_604.426mz_pos	PubChem:(89468623)	Sirius match	930599.003	694757.6179	633236.8007	3.99E-10	3.99E-10	0.10390075	0.318499888	1.205512126	0.668619183	0.586578504	1.139863085
X21.2_864.624mz_pos	PubChem:(89625184_1233	Sirius match	2612420.49	1742953.916	1550340.753	3.99E-10	3.99E-10	0.117369178	0.376615055	1.187064829	0.614291101	0.532826293	1.15289187
X8.8_400.29mz_pos	PubChem:(89759680)	Sirius match	872392.7923	653450.0145	626637.0688	3.99E-10	3.99E-10	0.11944484	0.452678756	0.943645234	0.670672202	0.61799864	1.085232488
X37.7_665.43mz_neg	PubChem:(90060284)	Sirius match	57095.79115	103017.5781	124522.5289	0.000082	0.000132797	0.355604228	3.628383661	3.597108277	1.791565213	1.903392103	0.941248632
X10.8_590.411mz_pos	PubChem:(90302461)	Sirius match	965271.1687	734260.7256	701489.9494	3.99E-10	4.02E-10	0.25812342	0.481359212	0.970067665	0.681114357	0.636444796	1.070186072
X28.5_368.169mz_neg	PubChem:(90345383)	Sirius match	7361.44466	56151.50762	64281.06564	3.99E-10	5.55E-10	0.861661866	0.855743463	1.074897225	6.845877738	6.879007495	0.995183934
X24.3_790.588mz_pos	PubChem:(90392164)	Sirius match	1692474.605	1225302.284	1095064.064	3.99E-10	3.99E-10	0.067364257	0.325570492	0.879501881	0.662323587	0.584485876	1.133172954
X26.2_398.18mz_neg	PubChem:(91500978)	Sirius match	25638.91992	260634.6615	244555.1588	3.99E-10	2.7E-09	0.738584379	0.85318627	0.844022055	9.432190143	8.13996588	1.158750575
X37.7_429.179mz_neg	PubChem:(9311457_93114	Sirius match	228620.6195	338406.0678	436375.2171	0.000106236	0.000052	0.213911196	1.788641549	1.718457227	1.477077511	1.746457071	0.845756552
X23.4_474.306mz_pos	PubChem:(9826925_98702	Sirius match	153838.9604	127177.0644	85717.57395	0.002605525	0.000246266	0.142854558	3.072384289	2.324699043	0.767629283	0.483129561	1.588868381
X19.3_476.335mz_pos	Pubesanolide	exact mass match	84362.76768	67602.39877	50743.90887	1.21E-09	4.28E-10	0.005429776	0.976309396	1.507423935	0.773159527	0.529479165	1.460226536
X18.3_511.027mz_pos	Pyriprrole	exact mass match	13737.81028	8943.134499	6259.120546	1.47E-09	0.000000557	0.616039363	6.403470228	9.238287482	0.67501756	0.44429161	1.519311967
X10.1_708.438mz_pos	Quadrigemine A	exact mass match	9552.791787	6893.056769	4897.405983	0.00000376	0.000572717	0.917590445	6.895276278	6.435875394	0.770626026	0.508437594	1.515674756
X16.3_632.228mz_pos	QYNAD	exact mass match	22558.49921	14229.36088	7956.79478	0.000105887	0.000158055	0.356284376	4.411985299	3.110923241	0.64624849	0.342534351	1.886667683
X10.3_193.09mz_neg	R-3-(Methylthio)-1-hexar	exact mass match	89184.79524	385707.7225	556469.6337	9.71E-09	0.00000826	0.823335122	1.169531516	1.329505089	4.583923842	5.940629957	0.771622517
X19.5_509.335mz_pos	Reduced Vitamin K	exact mass match	263098.4817	451882.0414	542985.5251	0.00027026	0.001960685	0.70631389	1.920238817	0.94829873	1.584901349	1.829204382	0.86644301
X7.1_381.076mz_neg	Resorcinolnaphthalein	exact mass match	2760.324506	6999.746682	8619.120107	0.004487095	0.00393128	0.4784411	9.083422492	2.294949691	2.25779069	2.190947676	1.030508722
X18.3_739.493mz_pos	Rhodopin β-D-glucoside/	exact mass match	17209.80867	11396.55376	13192.33526	5.54E-09	0.000000306	0.380975812	2.699682336	2.816294816	0.673814486	0.710090302	0.948913799
X17.9_563.383mz_pos	Rhodoxanthin	exact mass match	51497.7915	37327.08449	35757.84114	3.99E-10	4.01E-10	0.045509294	0.390956451	0.957144574	0.625147976	1.134966383	
X16.4_407.11mz_pos	Rotenonone	exact mass match	49397.35059	32128.46587	20444.35307	0.0000772	0.000280261	0.484424088	2.281497131	1.703773213	0.64339408	0.379277494	1.696367674
X32.1_436.201mz_pos	S32826	exact mass match	17286.5441	27956.53122	32015.87394	0.0000364	0.003950706	0.981829339	2.115741833	1.962931489	1.568133927	1.608779502	0.974735149
X32.1_353.142mz_neg	S-Adenosylmethioninamid	exact mass match	73891.8733	112513.9318	99407.71338	0.0000547	0.003191848	0.941965392	1.842803946	2.042825264	1.553303467	1.20062034	1.293750751
X32.1_395.175mz_pos	Salermide	exact mass match	124520.7442	192208.6049	247240.4793	0.0000561	0.004521711	0.974558688	4.290222012	3.109137208	1.449213063	1.678011189	0.863649225
X23.2_733.494mz_pos	Salinomycin	exact mass match	56507.96646	38744.94919	38364.87667	4.07E-10	4.22E-10	0.03461752	1.09438418	1.457906894	0.669465786	0.611756845	1.094333135
X24.7_493.006mz_pos	Sanguisorbic acid dilacton	exact mass match	100197.2688	78300.36284	87243.58303	5.92E-10	4E-10	0.01310211	1.438904008	1.112641431	0.739055433	0.754963207	0.978929073
X14.7_357.228mz_neg	SB 939	exact mass match	7560.429174	21665.389	27096.5458	6.04E-08	0.000367112	0.985976629	1.585611668	0.902434336	2.742484993	2.906829116	0.94346275
X9.1_636.061mz_pos	Sceptrin	exact mass match	47130.92552	32369.42422	25015.33415	3.99E-10	3.99E-10	0.0000931	2.27640536	2.204972862	0.680857122	0.490515527	1.388043976
X9.4_710.106mz_pos	Selenodiglutathione	exact mass match	44916.92375	31919.79165	11669.76813	4.96E-10	3.99E-10	0.00000145	11.04352942	7.83414256	0.70704474	2.429819004	2.830227996
X10.9_181.974mz_neg	Se-Methylselenocysteine	exact mass match	6415.024645	28177.72681	19014.5448	0.000000128	0.00195372	0.843952862	9.497806457	2.760506543	3.994383141	2.291580044	1.670185846
X34.7_366.193mz_pos	Senkirkine	exact mass match	4866.911426	8490.734225	14690.33393	0.000798549	0.000583175	0.34732956	2.102621585	4.391953451	1.637637474	2.40936531	6.620828785
X18.9_577.056mz_pos	Sennidin A	exact mass match	9980.047114	7529.737909	7453.820587	0.000641186	0.00000728	0.031185692	2.703316801	3.021303333	0.793283587	0.708254021	1.120055183
X16.4_409.081mz_pos	Ser-Phe4Cl-OH	exact mass match	135464.6073	94462.35193	63440.11537	0.0000427	0.000036	0.241941034	3.869984673	2.369824516	0.661914345	0.413393013	1.601174484
X23.3_458.983mz_pos	Sertaconazole	exact mass match	7736.898079	4051.381104	4772.775048	5.83E-08	0.000000135	0.04296562	11.53462505	0.616320714	0.597767226	1.031037981	
X19.9_484.384mz_pos	SM(d18:0/0:0)	exact mass match	458374.0329	345677.7568	271103.2555	4.02E-10	3.99E-10	0.003226203	0.597470523	0.942051136	0.699076037	0.503804992	1.387592518
X21.9_487.33mz_pos	SM(d18:1/0:0)	exact mass match	43515.23415	31024.03266	35695.8681	1.66E-09	4.16E-10	0.003036141	3.796982852	2.978247594	0.704175008	0.74387034	0.946636759
X15.8_482.001mz_pos	Sodium picosulfate	exact mass match	20226.96054	14686.88304	9668.233166	8.68E-10	4E-10	0.000498523	1.375390443	2.510239274	0.731986682	0.452074027	1.619174381
X22.1_471.337mz_pos	Solacapine	exact mass match	17342.89997	13170.46154	8504.491516	0.000000233	0.00000034	0.140018238	8.334070062	2.583754647	0.768956587	0.470474448	1.634447652
X5.6_635.412mz_pos	Soyasapogenol B 3-O-D-	exact mass match	27471.98114	9290.756629	7791.322303	0.00000679	0.000622832	0.884188506	1.576047678	3.216118372	0.351611459	0.261385055	1.34518578
X23.9_607.426mz_pos	Spheroidene	exact mass match	27494.59275	18827.76376	11376.71309	2.95E-08	0.000000109	0.15760614	3.053438015	4.75885561	0.691462407	0.395374656	1.748878934
X6.9_730.485mz_pos	Spinetoram	exact mass match	15339.77618	5014.971799	4639.109405	0.000360748	0.0000119	0.057017969	10.78028178	5.050721924	0.357651695	0.284805604	1.255774779
X24.5_512.018mz_pos	Sporidesmin	exact mass match	39258.69197	31415.23807	31866.9266	3.28E-08	3.94E-09	0.023557182	0.728264808	1.572294885	0.789965216	0.738718482	1.069372482
X15.6_639.431mz_pos	Sporidesmolide I	exact mass match	13382.84704	9911.290077	7397.610028	0.00000078	4E-10	0.00000925	1.270929189	1.798701715	0.529050048	1.434561669	
X17.4_500.011mz_pos	SR 1001	exact mass match	26027.75111	19423.66546	15506.84899	1.1E-09	4.28E-10	0.005843241	1.429930702	2.073639024	0.747189417	0.551935182	1.353762979
X16.4_384.051mz_neg	S-Sulfanylgutathione	exact mass match	54977.74823	37001.22184	14278.55337	0.000146975	0.000123704	0.2903673	4.04833189	4.718707479	0.713610753	0.224822376	2.914810177
X7_841.554mz_pos	Staphyloxanthin	exact mass match	41736.71981	13771.35166	9793.893436	4.02E-10	3.48E-08	0.762789627	1.534558369	3.300683462	0.351976572	0.225188023	1.56303416
X25.9_517.695mz_pos	Stearoyl-CoA	exact mass match	19799.35427	14826.03427	14352.22565	0.000000139	6.56E-09	0.017075683	0.830608288	1.140070487	0.753805579	0.67165758	1.122306368
X12_458.332mz_pos	Suillin	exact mass match	53270.58942	39324.89876	35399.17952	3.99E-10	4.05E-10	0.059184149	0.763716884	0.74552358	0.719307027	0.5992016932	1.20041172
X10.9_789.159mz_pos	Sultamicillin tosilate	exact mass match	58457.21846	40105.29252	15781.27941	3.99E-10	3.99E-10	0.00000162	13.20668958	8.978655891	0.670999084	0.255800736	2.623131952
X25.4_504.022mz_pos	T0901317	exact mass match	70259.57045	57090.89452	47613.89963	1.29E-09	3.99E-10	0.00000831	0.309518342	1.52194311	0.779976515	0.594902804	1.311099074
X17.1_638.099mz_pos	Tannin	exact mass match	23049.98616	17296.25919	12703.29015	0.000000053	3.26E-09	0.016730222	3.058643472	3.51896552	0.754581732	0.494671929	1.525418538
X15.8_466.991mz_pos	TEMEFOS	exact mass match	12467.15807	8680.897133	7675.373888	1.03E-08	0.00000598	0.771109753	1.030770344	1.116848891	0.725264	0.587462435	1.234570853
X7.9_340.269mz_pos	Templetine	exact mass match	52127.49582	35004.88161	28247.80694	3.99E-10	3.99E-10	0.001470864	0.721431129	1.654409717	0.661066486	0.49714579	1.329723593
X34.7_367.158mz_pos	Testosterone sulfate	exact mass match	2637.576261	4615.463923	5954.178406	0.002207843	0.000111722	0.096294002	3.60429187	5.772699904	1.624321785	1.567353995	1.036346473
X28.8_562.733mz_pos	Tetrabromobisphenol A	exact mass match	11043.02437	6789.939148	3278.259208	0.00000222	0.0000019	0.15418324	3.622989582	8.533021763	0.663926345	0.311938382	2.128389399
X16.5_489.663mz_pos	Tetradecanoyl-CoA	exact mass match	11561.438	8304.402468	9589.602232	5.89E-09	6E-10	0.008232401	1.588981934	1.840702098	0.747978751	0.771578815	0.969413282
X17.2_615.337mz_pos	TETRAHYDROAMBOGIC	exact mass match	7737.808921	11365.07809	12022.26045	0.001708827	0.001424036	0.410135519	0.930154491	2.821322659	1.427132989	1.358589661	1.050451825
X17.7_462.826mz_pos	Thelepin	exact mass match	449427.2003	328901.4837	312842.9442	3.99E-10	3.99E-10	0.003886396	0.812911522	0.818374048	0.674357945	0.598127661	1.127448

X18.3_505.016mz_pos	Thiamin triphosphate	exact mass match	19577.83305	14986.75223	10442.47431	6.16E-09	0.000000593	0.463748967	2.428097432	3.676806702	0.770395444	0.503235277	1.530885212
X16.5_543.871mz_pos	Thiifuzamide	exact mass match	17758.25144	13096.86374	12549.98326	5.69E-10	8.53E-10	0.05630675	0.612996838	1.437615962	0.745383497	0.653255952	1.141028252
X16.4_357.093mz_neg	Thr-Ala-OH	exact mass match	13287.64488	8511.731576	6750.008233	0.001071282	0.0000147	0.037919365	2.254454515	2.476714927	0.720101941	0.485500087	1.483216913
X16.4_405.087mz_pos	Thr-Phe4Cl-OH	exact mass match	9786.344556	6527.231598	5399.736756	0.000762983	0.00000255	0.013699784	3.982061135	2.188639801	0.72677182	0.532720527	1.364264719
X23.1_500.019mz_pos	Thymidine 5'-triphosphate	exact mass match	46006.51556	35430.5105	27797.82176	5.77E-09	4.04E-10	0.000587365	0.630963173	1.488410389	0.760923691	0.556289066	1.367856637
X7.4_459.182mz_neg	Tovophyllin B	exact mass match	3539.468929	6882.12645	1951.542004	0.001102515	0.000438255	0.273099638	11.05618329	11.05195536	1.818526222	0.564935866	3.218995877
X17.2_550.047mz_pos	trans-Zeatin riboside diphosphate	exact mass match	65689.67859	52908.06958	46839.48019	0.000000182	6.54E-10	0.00170475	0.621024215	1.437514077	0.776062987	0.626815663	1.238104011
X15_515.178mz_pos	Triamcinolone acetonide sodium salt	exact mass match	4566.903007	6587.692234	3827.031959	0.000105096	0.000000909	0.019819705	9.706514864	9.986612351	1.373503383	0.775660988	1.770752176
X14.9_303.18mz_pos	Tributyrin	exact mass match	48789.92481	90392.83316	78489.58964	0.00000287	0.0000631	0.587077612	2.117933821	1.647874084	1.737335249	1.407857784	1.23402752
X21.9_480.004mz_pos	Tricetin 7,3'-disulfate	exact mass match	94049.97948	75379.35423	63622.86133	6.55E-10	4.01E-10	0.001433101	0.388707571	1.080873705	0.767083398	0.591401502	1.29706028
X19.3_539.039mz_pos	Trisjuglone	exact mass match	7835.578654	5578.132449	4700.493817	0.0000938	2.89E-08	0.001704799	1.625720987	4.631124142	0.778823526	0.591945184	1.315702107
X13.8_522.131mz_pos	Troglitazone sulfate	exact mass match	37953.90696	49005.20836	21586.31772	0.000285288	0.00331017	0.801610139	4.660366857	3.745237808	1.239462464	0.522288659	2.373136851
X15.7_634.463mz_pos	Tsugarioside B	exact mass match	9181.786004	4539.844642	3512.967423	3.99E-10	3.99E-10	0.052662847	1.018691936	7.613841132	0.576838829	0.39290263	1.468147028
X17.4_518.346mz_pos	Tuftsins	exact mass match	96695.78983	74037.07824	81597.95368	4.13E-10	4.01E-10	0.005199108	0.925592141	3.04321616	0.724576022	0.731474939	0.990568485
X12.9_384.295mz_pos	UCM707	exact mass match	101724.5225	70662.72943	64551.96549	3.99E-10	3.99E-10	0.024628102	0.590054719	0.606922022	0.6649264	0.554034002	1.200154499
X18.6_645.091mz_pos	UDP-2,3-diacetamido-2,3-diphosphate	exact mass match	5893.800709	4128.877845	4972.302104	0.000226516	0.000019	0.093158276	3.912040244	5.624036322	0.798009563	0.79209746	1.007463858
X34.6_631.104mz_neg	UDP-2,4-bis(acetamido)-2,4-diphosphate	exact mass match	7550.658811	48719.31811	29512.62121	7.07E-10	7.53E-10	0.039315529	11.4865541	3.460443031	5.984518349	3.196193925	1.872389001
X18_613.086mz_pos	UDP-2-acetamido-4-aminopyrimidin-5(2H)-one	exact mass match	18958.84556	14608.03664	9079.181458	0.00000303	0.0000147	0.350431279	2.333404374	4.714779559	0.77740783	0.459005349	1.693679238
X20.7_549.052mz_pos	UDP-4-dehydro-6-deoxyuridine	exact mass match	7570.34339	5259.286014	3408.66604	0.00000218	4.27E-10	0.0000662	4.897163925	11.04803731	0.770805798	0.459594583	1.677142913
X27.8_528.042mz_pos	UDP-L-Ara4FN	exact mass match	73272.33443	55793.62718	41747.83562	4.36E-10	3.99E-10	0.000515946	0.723929638	1.568182847	0.73213004	0.505368778	1.448704532
X18.1_558.043mz_pos	UDP-L-Ara4N	exact mass match	16547.76361	12036.34252	10991.10076	0.000000948	0.0000822	0.749756788	2.02726663	1.721258501	0.737812978	0.623246807	1.183821513
X17.3_535.037mz_pos	UDP-L-Ara4O	exact mass match	79896.13972	62469.9675	55382.63279	6.06E-10	5.33E-09	0.170170715	0.793722664	1.045990995	0.749884192	0.606004967	1.237422517
X9.9_678.091mz_pos	UDP-N-acetyl-3-(1-carboxyethyl)-5-phosphate	exact mass match	67048.35342	42725.82134	18218.69267	4.56E-10	4E-10	0.001360989	8.487262409	7.339622028	0.628240915	0.257673264	2.438130001
X9_888.082mz_pos	UDP-N-acetyl-6-(D-galactosyl)-5-phosphate	exact mass match	20177.8202	10988.41429	1656.054656	1.03E-08	1.84E-08	0.092849021	12.33119574	13.01423077	0.566202371	0.094945685	5.963434459
X13.2_516.374mz_pos	UNC0321	exact mass match	200292.9458	147786.3797	140343.0499	3.99E-10	4E-10	0.088039577	0.781406145	0.982601703	0.684824418	0.610442469	1.121849237
X22.8_671.492mz_pos	Uvaricin	exact mass match	281906.4428	184568.9007	229241.4642	4.04E-09	6.6E-09	0.07567074	2.843286323	3.466167205	0.619629953	0.702173029	0.882446245
X17.1_582.388mz_pos	Valnemulin	exact mass match	9613.572866	7188.79071	7243.693649	0.0000268	0.000016	0.191348769	2.132630309	4.378916301	0.788773781	0.714057199	1.10463669
X11.6_590.41mz_pos	Vitamin D2 glucosiduronic acid	exact mass match	10312.80548	7853.227597	6383.621301	0.00000618	0.0000128	0.27194542	1.468195322	2.540858922	0.79349504	0.595786122	1.331845457
X15.9_614.08mz_pos	XCT 790	exact mass match	5673.370621	3756.460274	2649.669852	0.000805555	0.000116426	0.153652748	4.286073295	12.00670279	0.765542031	0.470488783	1.627120687
X29.1_553.065mz_pos	Xipamide O-glucuronide	exact mass match	37023.20353	28049.15397	15202.91056	9.93E-09	4E-10	0.0000783	1.73218069	2.833712935	0.755544939	0.38793258	1.947619196
X23.3_507.012mz_pos	Yellow prussiate of soda	exact mass match	41352.90536	31489.55507	33365.96584	1.59E-08	4.29E-10	0.001285266	3.751984924	6.240874171	0.752036476	0.732634877	1.026481949
X12.2_301.164mz_pos	Zinndiol: 1-[4,5-Bis(hydroxymethyl)-2-thiazolyl]ethane-2-thione	exact mass match	10962.51287	24032.3679	23862.77232	0.000000207	0.001015384	0.961064658	1.536081427	1.787099151	2.064818921	1.91052472	1.080760118
X16.4_251.127mz_pos	δ-CEHC	exact mass match	3097794.175	2110034.384	2080346.226	0.0000208	0.001228308	0.88933765	0.739980866	0.860171842	0.61814365	0.646771506	0.955737295