

Supplementary Table S1 -Identification, quantification and annotation for metabolites of T0 and T1

index	T0-1	T0-2	T0-3	T0-4	T0-5	T0-6	T1-1	T1-2	T1-3	T1-4	control_n	MS2 name	MS1 name	mz	Cloud	RT [min]	Molecular Formula	CAS	Appm	-	C_ID	Pathway	KEGG_B	KEGG_A	class			
NEG0000	731.0619	320.9292	635.7339	637.0337	132.1392	304.9866	767.8762	595.7486	595.4935	743.2116	654.9647	802.6902	460.3141	693.3308	0.590925	0.049972	0.068885	0.558132	Glycolic acid	96.829	76.01421	C2H4O3	79-14-1	24 Hydroxy	C00160	ko01100/ CarbohydrateMetabolism		
NEG0000	683.917	74510	77537.07	59282.47	70497.59	78686.56	72163.04	70469	84852.42	67766.95	80604.33	92618.07	711.2823	78084.97	0.133487	0.183909	0.22034	2.866921	Pyruvate	96.829	76.01421	C2H4O3	127-17-3	19 Keto acid	C00022	ko01100/ Amino acid Human Diseases;Metabolism		
NEG0000	297.5743	13.02077	2486.069	248.7477	8.550722	293.2841	258.5615	276.5405	234.6932	405.4603	850.1639	691.1899	71.0743	480.3375	0.132891	0.094335	0.128184	0.071723	Lactic acid L-(+)-Lact	99.6	14.365	90.02995	C3H6O3	50-21-5	18 Hydroxy -	-		
NEG0000	11486.14	4391.525	10416.29	8862.845	10409.18	6507.202	6919.776	5059.186	5410.908	7455.936	10942.16	10097.785	860.365	7641.277	-0.19479	0.46241	0.496278	0.581337	Sulfuric acid	1.054	97.9666	H2SO4	7664-93-9	7 -	C00059	ko01100/ Amino acid Environmental Information Processing;Metabolism		
NEG0000	665.8937	453.1285	455.5463	333.3244	686.1867	512.4626	405.8253	613.4826	474.3469	264.6227	293.1457	272.7034	517.757	384.5211	-0.19479	0.1259	0.179791	0.366385	Phosphoric acid	0.937	97.97509	H3PO4	7664-38-2	18 Non-met-	C00009	ko01100/ Energy m Environmental Information Processing;Metabolism		
NEG0000	31.64964	15.20255	26.8057	22.674	14.07441	16.68754	21.03821	13.09207	11.13363	13.75373	28.01928	15.32142	21.8828	17.09922	-0.31226	0.312485	0.0394	0.043138	Succinic anhydride	1.237	100.0143	C4H4O3	108-30-5	17 Oxolanes -	-	-		
NEG0000	311.2677	276.3947	399.9924	279.9043	171.7781	291.0095	424.11	401.5449	350.5039	416.5136	516.6937	420.058	283.3745	421.629	0.057324	0.000413	0.00416	0.509895	2-Ketobutyrate D-Oxobuty	90.4	1.264	102.0299	C4H6O5	600-18-0	17 Keto acid	C00109	ko01100/ Amino acid Metabolism	
NEG0000	128.997	167.8752	149.8552	139.3614	173.8963	175.1639	315.7282	342.946	327.5367	248.8642	391.1843	438.9786	155.825	333.367	0.139823	0.086705	0.07209	0.652528	Malonic acid	0.941	104.0892	C3H4O4	141-82-2	16 Carboxyl	C00083	ko00240/ Metabolism;Metabolism		
NEG0000	399.4893	284.4863	354.7202	269.2611	261.5547	338.3396	305.1984	315.3849	279.9414	207.3707	309.3656	405.2851	138.0603	303.5912	-0.08717	0.048269	0.071474	0.018357	Glycolic acid (2R)-2,3-D	73.9	1.877	102.0248	C3H6O4	473-81-4	17 Organoos	C00258	ko01100/ Amino acid Metabolism	
NEG0000	1117.816	391.9286	397.9824	782.2864	744.082	761.8086	587.9008	538.2317	716.7672	444.9921	912.06	698.9788	0.38383	15.05433	0.183701	0.449094	2-Furonic acid	69.1	127.0213	99.619	102.0143	C5H4O3	88-14-2	15 Furans	C01546	ko0120/ Global	metabolism	
NEG0000	12.82926	12.82037	20.35758	16.29855	57.11546	13.33565	94.67912	31.15946	36.01139	30.70068	59.53301	33.82603	10.38883	47.65121	1.810092	0.009179	0.015969	0.256507	Uracil	89.9	1.237	102.0255	C4H4N2O2	66-22-8	15 Diazines	C00106	ko01100/ Global	metabolism
NEG0000	6.625987	9.977318	11.58793	9.83395	7.20511	14.89009	134.8814	162.2558	141.4874	249.0708	152.8899	217.0853	10.1244	13.9413	0.00645	0.4886705	0.575665	L-Proline	86.4	0.837	151.0615	C5H9NO2	147-85-3	15 Carboxyl	C00148	ko01100/ Amino acid Environmental Information Processing;Genetic Information Processing;Metabolism		
NEG0000	659.8666	981.2837	883.1646	679.7339	823.73	1227.903	1019.518	564.2551	929.0646	518.2965	882.6469	1031.606	87.947	824.2343	-0.08779	0.691185	0.020739	0.051093	Leucic acid	1.182	116.0092	C4H8O4	110-16-7	15 Carboxyl	C001384	ko01120/ Amino acid Metabolism		
NEG0000	39.77975	21.06836	45.7647	39.7966	23.89408	23.75837	95.22046	79.52882	57.10687	79.06313	83.16241	100.6406	32.9445	35.3082	0.549E-05	0.071026	0.031909	Maleic anhydride	86.4	1.297	116.0416	C5H4O3	123-72-6	15 Keto acid -	-	-		
NEG0000	164.8674	71.63453	178.936	123.1272	11.10759	86.99467	22.66817	41.57861	39.53432	42.39365	36.43446	58.37693	106.1291	40.16436	-1.4017	0.029546	0.047939	0.311314	Succinic acid	1.336	118.0249	C4H6O4	110-15-6	14 Carboxyl	C000442	ko01100/ Amino acid Metabolism		
NEG0000	22.89941	47.91498	82.59718	60.92622	16.24691	60.45275	33.94383	38.87781	24.35411	38.76748	20.61791	49.37932	45.0624	29.48041	0.12194	0.136186	0.166799	0.145648	Purine	0.793	120.0416	C5H4N4	120-73-0	5 Imidazop -	-	-		
NEG0000	1.558703	0.491823	1.072434	0.277605	0.466535	0.512161	187.8786	176.5194	155.3993	188.1197	423.949	226.0567	1	222.9858	7.800808	0.00028	0.00084	0.683852	acetophenone	99.5	2.697	120.0558	C8H8O	98-86-2	14 Organoos	C07113	ko01120/ Global	metabolism
NEG0000	10.12627	7.371586	87.04915	9.244133	11.37105	7.91237	76.4148	73.4388	69.90762	63.51915	75.3324	71.4496	22.17909	17.67704	0.1692311	0.003656	0.007719	0.296588	Benzonitrile	96	2.841	122.0351	C7H6N2	65-85-0	13 Benzene	c00180	ko01100/ Amino acid Metabolism	
NEG0000	69.53637	46.34816	78.65214	62.6149	55.20181	53.3589	38.1866	14.722	95.94832	39.3931	28.25732	206.003	60.9155	92.5585	0.602661	0.312515	0.24914	0.163265	Pyrrogallol	96.7	0.917	129.0408	C6H2O3	98-79-3	13 Carboxyl	C001879	ko01100/ Amino acid Metabolism	
NEG0000	2367.548	1762.489	2556.617	1717.015	2127.238	2515.234	2072.239	2105.67	1868.939	1239.309	2093.606	231.787	217.435	1915.591	-0.18054	0.034801	0.28148	0.367078	Iaconic acid	98.8	1.367	130.0248	C5H6O4	97-65-4	13 Fatty	Acy C00490	ko00660/ CarbohydrateMetabolism	
NEG0000	46.8331	27.76115	43.30042	39.58238	22.66526	44.99593	264.0316	151.4671	100.1259	207.2181	180.8553	74.7565	37.85027	179.7424	2.247555	0.727E-05	0.000402	0.546945	Ketoleuic acid	2.347	130.0613	C6H10O3	816-66-0	13 Keto acid	C00233	ko01100/ Amino acid Metabolism		
NEG0000	180.6674	115.8781	219.465	157.4339	127.1328	202.9077	360.0644	410.0726	279.1623	338.9553	344.7658	482.8635	72.6323	64.5614	0.1310233	0.000426	0.046561	DL-β-Leu	99.4	1.316	131.0929	C6H13NO2	5699-54-7	13 Carboxyl -	-	-		
NEG0000	173.9067	219.6884	287.6929	209.8768	91.22637	213.3021	663.367	321.815	441.285	607.481	650.304	770.8684	199.3156	609.1867	1.61183	1.86E-05	0.11804	0.954178	Glutaric acid	0.824	132.0405	C5H8O4	110-94-1	13 Carboxyl	C000489	ko01120/ Amino acid Metabolism		
NEG0000	156.2179	142.3566	122.8219	103.506	133.9929	149.1035	197.166	112.8694	119.2281	91.498	136.5229	270.1127	134.9998	171.2321	0.347727	0.108533	0.221009	0.177273	L-Asparagine	0.785	132.0517	C4H7NO2	70-47-3	13 Carboxyl	C001512	ko01100/ Amino acid Genetic Information Processing;Metabolism		
NEG0000	9.67317	8.947858	8.22214	7.442248	4.065446	9.355493	15.32153	11.67505	13.56403	15.81818	12.8762	18.93002	8.00576	14.69528	0.877087	0.000572	0.01014	0.113999	Ornithine	98.5	0.717	132.0881	C5H12N2	70-84-8	13 Carboxyl -	-	-	
NEG0000	954.3516	1604.821	825.1164	1801.329	398.382	3382.842	2484.006	3572.989	2439.264	4136.299	585.765	3372.956	1346.458	9.66E-05	2.200803	L-Aspartic acid	0.788	133.0357	C4H7NO2	0.788	133.0357	C4H7NO2	14191-95-8	8 Benzene	c -	-	-	
NEG0000	699.456	643.2549	648.5787	622.7689	403.5283	610.1523	1479.264	545.703	995.261	2468.674	1039.257	228.599	576.286	1486.103	1.366677	0.018191	0.03016	1.138715	Deoxybenzoylbenzotriole	0.888	134.0269	C20H18O2	97-67-6	4 Hydroxy	C00149	ko00030/ CarbohydrateMetabolism		
NEG0000	176.0316	122.5982	180.8622	120.8941	168.0232	186.221	155.0562	71.23172	299.4551	94.3531	171.7481	273.9941	153.2498	6.309541	0.434	0.4676102	0.073731	Malic acid	1.302	134.0164	CSH1004	533-67-5	13 Organoos	C01801	ko01100/ Global	metabolism		
NEG0000	246.13	196.37	296.7483	258.8234	125.2606	247.6741	458.088	295.439	226.431	373.3234	368.4626	296.633	356.805	0.023635	0.021303	0.071432	Deoxyrib. DEOXYRIBOSE	85.3	1.267	135.0526	CSH5N5	73-24-5	12 Imidazop	C00147	ko01100/ Global	metabolism		
NEG0000	16.36257	23.6722	18.10817	11.44447	12.0082	17.93077	116.0996	80.47378	81.66612	152.9633	66.78871	46.80028	165.70106	90.74563	2.453162	0.000789	0.001099	0.347475	Adenine	0.811	136.0535	C4H5N5	7306-96-9	12 Organoos	C01620	ko00053/ CarbohydrateMetabolism		
NEG0000	181.1992	1.750676	2.354151	1.599353	1.341794	1.920314	142.9353	68.2388	33.40145	145.2019	199.6082	141.8478	1.79541	121.8723	0.684912	0.000638	0.001665	0.498638	2-Methyl-2-Methyl	96.7	2.377	136.0506	C8H8O2	118-90-1	13 Benzene	c00215	ko01100/ Global	metabolism
NEG0000	641.6076	49.79307	66.4594	46.19948	34.59764	42.68647	3.640784	5.527487	2.462061	4.899598	5.852467	50.58622	4.102743	3.82638	3.56E-06	3.99E-05	0.10393	Salicilic acid	96.6	2.042	138.03	C7H6O3	69-72-7	12 Benzene	c00805	ko01100/ Amino acid Environmental Information Processing;Metabolism		
NEG0000	34.99572	54.52326	48.13887	25.56037	10.84011	21.25792	43.1997	44.35601	39.84501	42.92305	46.92354	46.23355	29.21938	43.94852	0.588889	0.020803	0.032483	0.153716	2-Keto-glut-2-Keto-glutaric acid	0.872	145.0369	CSH7N0	18465-15-9	4 Keto acid	C00940	ko00250/ Amino acid Metabolism		
NEG0000	525.407	1218.421	784.5302	553.0498	820.207	1636.987	130.7883	502.6255	121.4918	292.9843	169.4135	128.6748	224.3327	-0.20486	0.000713	0.007218	0.136705	Trans-3-4-Indoleac	99.6	2.374	145.051	C9H7NO	487-89-8	12 Purine	u -	-	-	
NEG0000	32803.44	24518.77	38315	6962.057	19228.08	27708.04	207.424	24985.32	19436.93	16503.18	21793.53	96.146	24922.57	18845.98	-0.4032	0.250804	0.287821	2.188032	Oxoglutarate	87.6	1.237	146.019	CSH6O5	328-50-7	11 Keto acid	C00026	ko01100/ Amino acid Metabolism	
NEG0000	0.287657	0.636741	0.615998	0.212604	0.541937	0.721561	6.904055	4.216028	3.899126	5.463184	3.285317	3.845713	1	4.587397	2.19767	2.54E-05	0.000672	Adipic acid	66.5	1.701	146.0573	C6H10O4	124-04-9	4 Fatty	Acy C06104	ko01100/ Global	metabolism	
NEG0000																												

NEG0008	1.536795	1.205454	1.723155	1.576435	2.422307	1.31636	33.00901	24.97553	9.541541	29.48	62.64735	24.2992	1.630084	33.95442	4.380581	0.002609	0.005523	0.256677	N-Acetyl-D-10-Hydroxy-	96.4	3.76	188.1398	C10H20O12422-37	7 Hydroxy -	-	-	
NEG0008	13.44781	16.38043	19.35621	13.09167	19.93662	17.58399	29.68917	20.06697	17.32869	17.32869	34.66378	26.96678	17.32869	27.6231	0.916026	0.00515	0.01421	0.164207	N-Acetyl-N-Acetylglytamic ac	0.894	189.0621	CTH11N1188-37	8 CarbohydrC00624	ko111001/ Amino ac Metabolism	-	-	
NEG0008	4.843299	5.553598	2.642294	0.973872	4.447979	4.178105	7.099705	3.547818	1.363643	5.929335	4.011429	7.733062	3.773191	5.296644	4.88209	0.21059	0.246876	0.04364	3-Dehydroquinoic acid	1.397	140.0462	CTH10CE10534-44.8	8 Alcohols_C00944	ko111001/ Amino ac Metabolism	-	-	
NEG0008	0.245353	0.10598	0.622462	0.27246	0.107852	0.129488	0.21952	0.042612	0.068925	0.279488	0.288674	0.391162	1	1	0.042221	0.05956	0.012746	5-Hydroxy-5-Hydroxy-	81.9	3.08	191.0568	C10H9NC154-16	7 Indoles ac C05635	ko111001/ Amino ac Metabolism	-	-	
NEG0008	49663.53	48349.55	56653.45	42625.27	30852.36	44023.72	42426.85	52527.43	4051.17	30603.27	44662.72	50063.54	44744.65	45287.5	0.017398	0.899132	0.91567	0.51842	Citric acid:Citric acid	98.8	0.871	192.0255	C6H8O7 77-92.9	7 CarboxylC00158	ko111001/ Amino ac Metabolism	-	-
NEG0009	598.5276	552.8889	485.9422	715.9331	540.6347	682.3872	317.0284	167.7812	140.2656	173.2502	253.5768	311.9301	665.0495	227.3504	-1.52917	0.002042	0.001564	0.889719	Quinic acid:(+)-quinic acid	0.835	192.0617	CTH120E677-95.2	8 Quinolins C0296	ko040040/ Amino ac Metabolism	-	-	
NEG0009	130.8486	1295.427	1909.91	1228.577	659.1651	1717.718	814.6579	973.1895	660.9028	687.8361	1028.668	1058.689	1352.637	805.5573	0.47722	0.01619	0.02138	0.920818	D-Glucuronic acid	0.824	194.0417	C6H10O7 170908.8	4 Furofur-	-	-	-	
NEG0009	1.176222	1.009466	1.137225	3.257183	0.959191	1.23975	161.22	118.1052	77.63165	42.5135	126.682	61.7637	145.6162	262.217	7.483301	0.014721	0.026369	0.36171	ferrulic ac Ferrulic ac	95.4	2.972	194.0562	C10H18O11335-24.6	8 Cinnaam-C01494	ko111001/ BiosyntheMetabolism	-	-
NEG0009	401.631	42337.47	43721.45	42784.71	30852.8	53467.77	14099.65	21215.52	14953.21	15845.86	20739.06	17482.55	43984.63	17389.31	-1.338	0.3166	0.00516	7.47996	Gluconic Gluconic i	60.8	0.809	196.0566	CH20H20252-95.5	8 OrganoC00257	ko111001/ CarbohydMetabolism	-	-
NEG0009	4.470339	5.175476	6.485337	4.972138	4.835527	3.972306	12.29968	29.93528	24.57635	29.0474	32.16936	5.845232	22.75717	1.993984	0.002023	0.000719	0.18916	Syringic acid	1.858	198.0548	CHH10CS530-57.4	10 Benzene c10833	ko111020/ Global ac Metabolism	-	-		
NEG0009	14.45979	17.49291	17.49291	17.49291	17.49291	17.49291	17.49291	17.49291	17.49291	17.49291	17.49291	17.49291	17.49291	17.49291	17.49291	17.49291	17.49291	17.49291	kowallandian	3.472	198.0548	CHH10CS530-57.4	12 Carboxyl-	-	-	-	
NEG0009	73.01166	65.37715	81.33368	64.29631	64.33451	71.21298	64.34289	67.63799	65.85291	65.41	79.48172	70.74847	67.10637	0.07625	0.367914	0.402802	0.040495	Camelidoximalen	1.952	200.0418	C11H18N213533-86	4 Indoles ac	-	-	-		
NEG0009	29.16884	23.39769	33.3941	18.14933	29.1293	19.1461	15.5686	9.12409	13.4093	17.34775	20.4939	30.08425	9.14465	18.62374	-0.06501	0.06095	0.011727	(s)-Camphoric acid	3.242	200.1034	C10H16O1594-33.2	7 Carboxyl-	-	-	-		
NEG0009	9.957632	8.273014	9.6352	8.819683	7.81375	9.881542	14.86913	13.90025	11.20423	10.44355	15.38399	14.79942	9.06384	13.50941	0.575771	0.003959	0.02313	0.089955	Lauric acLauric ac	98.6	8.654	200.1176	C12H24O143-07.7	8 Fatty AcylC02679	ko111001/ Global ac Metabolism	-	-
NEG0009	153.5511	138.1372	195.525	55.46838	143.8785	184.5687	41.44823	39.49867	31.13449	43.91022	39.99867	15.2222	38.0069	-1.9315	0.000663	0.001054	0.40522	Allyl-Le-Ala-Ala-Ala	1.765	202.1303	C9H18N23303-34.2	7 Carboxyl-	-	-	-		
NEG0010	453.7122	267.3629	425.9433	270.1805	263.0399	323.8879	885.5571	768.9756	676.2199	764.0497	759.6775	847.5521	334.7865	1.230336	1.986-06	3.01E-05	1.002725	L-Tryptoph-D-trypt	84	1.244	204.0884	C11H12N723-23	7 Indoles ac C00078	ko111001/ Amino ac Genetic Information Processing;Metabolism	-	-	
NEG0010	1.777514	1.725688	2.366883	2.347495	1.367054	1.372685	0.349662	0.349662	0.349662	0.349662	0.349662	0.349662	0.349662	0.349662	0.349662	0.349662	0.349662	0.349662	0.349662	97.3	2.865	200.1079	C10H8O120-18-3	7 -	-	-	
NEG0010	73.46336	76.41258	109.2693	95.74262	109.8526	103.1551	217.7889	167.6506	107.3006	156.2531	159.5321	53.74856	94.01595	143.7123	0.612206	0.065587	0.08768	0.243701	Garcinia acid	0.953	205.2025	C6H8O8 27750-10.3	7 Carboxyl-	-	-	-	
NEG0010	0.17577	0.127069	0.206622	0.138989	0.130221	0.157977	0.356693	1.064791	1.947607	4.893644	1.484239	2.275674	0.054175	0.054175	0.054175	0.054175	0.054175	0.054175	0.054175	2.396	208.0358	C10H8O5574-84.5	6 -	-	-	-	
NEG0010	125.0738	102.4466	140.5039	135.8991	209.4422	130.0497	545.2549	397.144	223.8758	408.6441	468.2103	522.2491	140.6002	427.563	1.604538	0.000176	0.000588	0.798042	Lipic acid, reduced	0.841	208.0568	CHH16C2462-20.4	11 Fatty Acyl-	-	-	-	
NEG0010	15.7954	10.20166	13.5288	14.28968	16.02293	10.12886	10.91246	6.984143	11.28886	10.34195	-0.35233	13.11295	10.34195	13.11295	0.13092	0.16247	0.050565	Chalcone	0.826	208.0915	C15H12O194-41.7	12 Linear 1,3-	-	-	-		
NEG0010	46666.3	49920.49	58852.24	41.0543	30960.69	49930.32	47561.81	57079.3	47855.92	40343.3	51975.49	55054.79	46028.58	49978.43	0.117084	0.40189	0.43742	1.832749	GalactaricMUCIC Acid	0.826	210.035	CHH10C526-99.8	7 OrganoC00879	ko00053/ CarbohydMetabolism	-	-	
NEG0010	29.15337	26.36273	32.16419	25.05265	38.04816	26.68512	30.04816	32.04816	36.96176	39.57504	14.57834	34.57834	60.07969	119.0171	0.16175	0.029929	0.23998	5-Galactaric-D-4-diacetylphlorogl	2.392	210.0165	C10H18O110642-42	6 Cinnaam-C05619	ko00710/ Energy m Metabolism	-	-		
NEG0010	821.5811	1258.534	19522083	1203.573	643.289	1263.841	70.51326	883.1625	705.3202	781.0881	856.7895	996.9679	116.8108	859.1442	-0.44408	0.133173	0.164736	0.539802	Sedobutepulose	0.858	210.0174	CTH10C73019-74.7	7 OrganoC02076	ko00710/ Energy m Metabolism	-	-	
NEG0010	2.628544	3.195252	3.27494	3.685337	3.27494	3.685337	3.195252	3.27494	3.685337	3.195252	3.27494	3.685337	3.195252	3.27494	3.685337	3.195252	3.27494	3.685337	3.195252	2.103	212.012	CTH10C73019-74.7	6 Benzene c-	-	-	-	
NEG0010	5.915165	4.728788	5.28985	4.728788	5.28985	4.728788	5.28985	4.728788	5.28985	4.728788	5.28985	4.728788	5.28985	4.728788	5.28985	4.728788	5.28985	4.728788	5.28985	4.942	212.012	CTH10C73019-74.7	6 Benzene c-	-	-	-	
NEG0011	17.3318	13.3301	13.2581	85.02611	74.10092	144.2221	39.10611	88.98978	26.82648	50.63533	49.01405	64.83895	14.4785	48.22326	-1.24728	0.00045	0.00216	0.353992	Dihydroxymannic acid	5.25	212.0129	C12H22O198674-52.3	6 Linolic a-	-	-	-	
NEG0011	837.8523	61.1744	8807.887	585.4374	586.4734	586.4734	586.4734	586.4734	586.4734	586.4734	586.4734	586.4734	586.4734	586.4734	586.4734	586.4734	586.4734	586.4734	586.4734	0.854	214.0231	CSH110719007-18	5 OrganoC011437	ko111001/ Global ac Metabolism	-	-	
NEG0011	1.744178	1.342576	2.527886	1.960914	2.60806	1.740418	2.15757	2.183338	1.762514	1.715533	1.930895	2.174922	1.982572	1.987463	0.033555	0.982763	0.982763	0.019958	Succinylproline	1.879	215.078	CHH13N63250-32.2	6 -	-	-	-	
NEG0011	16.80957	27.86391	25.84519	32.14142	30.88398	15.43875	44.97371	32.99558	35.66263	27.96321	46.73991	0.742519	0.303575	0.343211	0.007039	0.303575	0.343211	0.007039	N-Nonanoylglycine	3.276	215.1508	C11H21NNA	6 Carboxyl-	-	-	-	
NEG0011	2.444704	0.145574	0.885798	0.207413	1.315732	0.959789	0.203167	0.189796	0.718611	0.162657	0.191826	0.237823	1.145057	0.536607	0.732283	0.760218	0.005826	L-2,3,4-Tetrahydro-beta-car	4.405	216.0884	C12H12N242430-90.4	6 Indoles ac	-	-	-		
NEG0011	2.012302	1.386173	1.78997	1.432845	1.617547	1.401114	84.55327	144.10934	15.24278	50.81791	123.5685	45.42477	1.606809	0.614943	5.23751	0.006832	0.34457	12-Hydroxy-D-Hydroxy-	89.8	2.162	217.1212	C14H20O505-95.3	6 Hydroxy -	-	-		
NEG0011	192.9153	130.328	237.9794	187.1676	145.2879	206.5455	154.9371	125.7119	100.9115	125.9198	142.2667	128.9273	183.354	129.7891	-0.49846	0.013228	0.022104	0.28306	Pantothnic acid	1.768	219.0147	CHH17N137-08.6	5 Alcohols_C00864	ko111001/ Global ac Metabolism	-	-	
NEG0011	116.087	170.0893	105.9872	103.1462	102.8023	107.4852	32.61951	45.74294	54.7294	19.42666	19.42666	39.79607	-1.11634	0.004048	0.0775	0.308941	Isofraxidin	4.56	222.0549	C11H18O486-21.6	9 -	-	-	-			
NEG0011	17.77018	12.59623	19.80467	14.9689	9.250489	14.29866	11.06094	10.00176	11.79603	13.00035	14.77885	19.32368	14.77885	19.32368	-0.21444	0.340478	0.378884	0.034881	Flavone	0.835	222.0725	C15H10O525-82.6	19 Flavonoid-	-	-	-	
NEG0012	789.7399	662.4962	761.6149	523.4191	623.4191	623.4191	623.4191	623.4191	623.4191	623.4191	623.4191	623.4191	623.4191	623.4191	623.4191	623.4191	623.4191	623.4191	623.4191	0.855	224.0517	C14H8O3129-43.1	19 -	-	-	-	
NEG0012	7.91964	6.400213	6.358442	4.229824	6.664488	5.122194	5.122194	5.122194	5.122194	5.122194	5.122194	5.122194	5.122194	5.122194	5.122194	5.122194	5.122194	5.122194	5.122194	86.3	2.717	224.067	C11H20O530-59.6	6 -	-	-	-
NEG0012	0.366106	0.56106	0.375142	0.286405	1.339035	0.338674	5.371004	0.586985	2.193722	14.41616	10.29016	17.10973	1.955473	2.574216	0.00067	0.001736	0.017149	Chenisiid-5-(1-Carboxyvinyl)-	1.5								

NEG0017	7.166736	7.570067	9.158924	7.504921	6.334216	8.19152	75.90867	48.18593	43.69478	76.08661	61.40489	82.24203	7.654397	64.58715	3.076886	5.76E-06	5.35E-05	0.352948	α -LinolenOleic acid	97.5	7.983	278.2232	C18H33O2	463-40-1	4 Fatty Acy C06427	ko011001/	Global an Metabolism	
NEG0017	70.24949	44.34879	74.06522	45.06057	53.19739	73.08882	54.18128	46.7853	53.34926	37.2473	47.21703	52.88899	60.00171	48.61138	-0.03071	0.101244	0.129442	0.109156	Asparagiasin-phe		1.87	279.1208	C13H17N1NA		3 Carboxyli-	-	-	
NEG0017	96.70146	68.82228	95.7855	69.28034	78.13914	100.2918	50.88267	57.89241	74.02191	48.48018	42.63095	72.15631	84.83829	57.6774	-0.055671	0.000398	0.011553	0.021804	L-beta-asn-Aspa-	94.2	1.974	280.1049	C13H16N1NA		3 -	-	-	
NEG0017	656.8136	878.402	732.4917	502.5731	724.9071	731.5367	45.31634	3197.62	2629.475	2662.641	3901.907	3095.937	704.4542	3333.955	2.242657	6.35E-06	5.55E-05	2.473759	Linoleic a(Z),11(E)	99.6	10.363	280.2389	C18H32O2	60-33-3	4 Fatty Acy C01595	ko011001/	Global an Metabolism	
NEG0017	14.75651	12.21739	15.03738	17.67013	18.4322	19.0542	11.95606	14.18431	12.19137	17.47313	17.00294	16.24495	15.51619	12.32188	-0.19753	0.32449	0.360439	0.02841	4-Hydrox-N-hydroxyphenyl		2.595	281.0888	C13H15N1S	1029120-37	4 -	C05595	ko003501/	Amino ac Metabolism
NEG0017	1.623689	1.269781	2.076127	1.286184	1.536013	1.379248	8.900482	4.203678	1.59492	6.105951	8.1765	7.941102	1.528522	6.154467	2.009497	0.002473	0.000524	0.098365	Xylobiose		1.313	282.0938	C10H18O2	6860-47-5	5 Organoos	C01630	ko020101/	MembranEnvironmental Information Processing
NEG0017	63.28544	36.02274	72.31965	61.26745	88.30336	58.31136	13.03095	17.1801	11.52009	5.691522	9.365151	74.87396	63.51272	10.71778	2.55385	2.69E-05	0.001419	0.328089	ArtemisinNP-00519	88.5	2.378	282.1458	C15H22O2	63968-64-9	3 -	-	-	
NEG0017	0.192895	1.627666	2.649781	3.580158	0.193955	258.7044	61.56605	59.90596	156.207	127.8643	175.8818	5.083147	138.5151	4.768177	0.001838	0.001419	0.518997	(6E,8R,10J,(6E,8R,10J)-8-Hydrox		5.526	282.1819	C16H22O2	2190485-67	4 -	-	-		
NEG0017	15572.759	1195.826	1508.623	1141.571	1508.865	1190.035	2317.194	2578.341	1762.896	156.2164	2256.505	1843.868	1352.947	1996.737	0.561539	0.000428	0.000809	1.153291	Acic OleicOleic acid	99.6	11.085	282.2546	C18H34O2	112-80-1	4 Fatty Acy C00712	ko010401/	Lipid metMetabolism	
NEG0018	0.180806	0.174853	0.12713	0.137745	0.134243	0.203789	0.369016	0.233126	0.419844	0.52112	4.742001	1.198328	1.531126	1.4249638	1.24806	0.010738	0.014264	0.0457032	Rhein		4.322	284.0311	C15H18O2	478-43-3	3 Anthrac-	-	-	
NEG0018	1268.851	1055.515	1535.572	885.3814	995.0433	1156.478	1272.701	1353.018	1642.739	1184.889	1632.908	1885.62	1149.531	1570.311	0.458004	0.013535	0.022285	0.893911	Stearic acidStearic acid	99.7	12.227	284.2702	C18H36O2	211-28	4 Fatty Acy C01530	ko010401/	Lipid metMetabolism	
NEG0018	152.731	131.5347	185.2524	127.2355	86.4521	201.6712	122.1266	67.59115	91.96106	98.34079	74.75127	129.3235	149.332	97.48447	-0.6155	0.024596	-0.001734	0.278529	Morphine C1280000		1.585	285.1314	C17H19N5	57-27-2	2 Morphine	C01516	ko011001/	BiosyntheMetabolism
NEG0018	36.94168	6.149897	3.312389	7.598541	5.330326	5.872137	684.2088	364.2357	93.46006	236.4786	681.1965	205.3818	10.86829	377.4936	1.183255	0.005148	0.009476	0.858893	Luteolin Luteolin	98	4.32	286.0466	C15H10O2	491-70-3	3 Flavonoi	C01514	ko011001/	BiosyntheMetabolism
NEG0018	0.76553	0.543553	0.321167	0.198719	0.530192	0.232576	5.690909	9.496163	5.887031	1.00665	1.923043	1.375361	1	1.4231224	0.281075	0.020038	0.031679	0.075189	Kaempfer(4E)-5-(4-Methoxy		2.389	286.0519	C15H10O2	520-18-3	7 Flavonoi	C05903	ko011001/	BiosyntheMetabolism
NEG0018	3.69022	2.097313	4.219035	2.91102	2.054461	4.59061	28.16302	20.53866	14.34352	32.50275	30.58625	35.23824	33.44626	26.89524	0.050493	2.78E-05	0.000151	0.22512	2,4,6-trihydro-2,4,6-Trihy	90.9	3.267	288.0622	C15H12O2NA		4 -	-	-	
NEG0018	10.78834	6.26086	13.35248	10.33732	4.882287	10.28927	13.8204	22.98888	36.82331	28.3927	27.78167	25.33307	21.6181	28.7632	2.97E-05	0.000157	0.192105	Phlorin 1,5-Anhydro-1-(2,4,6		2.51	288.0835	C12H16O2	28217-60-9	3 Carbohyd-	-	-	-	
NEG0018	53.42715	21.40374	29.93347	28.93986	16.83986	32.1811	7.131033	13.33038	11.16127	8.739515	6.607391	17.24162	30.4542	10.70194	-1.5087	0.000453	0.000549	0.184501	Atropine		1.691	289.1626	C17H23N	55-48-1	17 Tropae	eC01479	ko011001/	BiosyntheMetabolism
NEG0018	50.27501	47.63635	55.100212	26.76002	45.9162	55.7348	56.14508	30.22381	27.87081	7.848779	44.44564	12.96611	46.22075	29.91534	-0.62766	0.085296	0.116765	0.116261	Sedohexulose 7-phosphate		0.851	290.0139	C7H15O2	2646-35-7	4 Organic	cC0582	ko011001/	CarbohydMetabolism
NEG0018	270.9691	367.8493	352.4793	246.5144	122.8294	196.0657	29.2257	21.13495	28.54351	28.31574	14.74425	35.95829	22.7161	26.32041	-0.31082	0.000138	0.000511	0.635594	Catechin		1.824	290.0755	C15H14O2	154-23-4	12 Flavonoi	-	-	-
NEG0019	6.366384	3.878641	10.04417	7.4748	3.473006	4.158796	4.11216	2.458108	2.014476	3.048828	3.174105	2.707811	1.811	5.8993	2.968986	-0.99057	0.023662	0.036648	0.06439	N-gammagamma-Glutamyl-S-		0.56	290.0926	C11H18NNA		3 Carboxyli-	-	-
NEG0019	6.429564	7.192065	7.607952	4.772012	5.045358	8.809763	71.7919	36.22241	26.82836	60.47048	63.4774	53.58636	6.642801	52.0627	2.970387	7.44E-05	0.000332	0.313102	Argininos Argininosuccinic acid		0.787	290.1213	C10H18N	2387-71-5	4 Carboxyli	C03406	ko011001/	Amino ac Metabolism
NEG0019	41.95884	31.79243	46.35224	35.98348	37.12665	45.11826	20.76882	22.40065	23.37055	19.41853	19.04911	30.59263	39.77219	22.60005	-0.81361	0.000153	0.000535	0.18469	Glutamin phe-gln		1.877	293.1366	C14H19N	92327-75-8	3 Carboxyli-	-	-	-
NEG0019	94.08712	71.08546	104.6938	72.94247	75.28319	89.78859	52.098	51.38731	53.72438	40.10378	40.46613	56.46952	84.64678	49.19619	-0.078291	0.000195	0.000635	0.263202	Tyrosyl-L-4-Hydroxyprolylthn		1.953	294.1205	C14H18N	936346-34	3 Carboxyli-	-	-	-
NEG0019	28.69405	17.86211	29.38618	18.12975	8.834593	29.31031	15.77669	15.51224	6.224062	12.26418	14.64128	10.39236	12.20367	12.46219	-0.82232	0.029407	0.043973	0.116772	Leucyl-L-Leucyltyrosine		1.982	294.157	C15H22NNA		3 Carboxyli-	-	-	-
NEG0019	186.5005	292.1907	303.4504	223.8746	46.90186	295.602	295.3478	229.7635	145.3064	45.97767	276.6022	43.03225	224.7533	237.7033	0.008082	0.851952	0.874916	0.120669	6-Gingerol (+)-6J-Gingerol		5.899	294.1821	C17H26O2	58253-27-3	3 Phenols	C10462	ko011001/	BiosyntheMetabolism
NEG0019	6.078651	3.722301	4.447232	2.834608	3.229115	3.043336	7977.722	4407.325	2176.975	8218.303	13636.56	8771.049	93.25124	7531.388	0.190696	0.000809	0.000248	0.394806	Phenyl-phalic acid		2.381	296.0519	C13H12O2	53735-05-4	4 Fatty Acy-	-	-	-
NEG0019	30.79828	25.84035	5.977138	13.26635	21.50528	29.08455	49.26335	51.20862	30.29015	26.66511	46.75801	29.83343	21.07154	39.06204	0.888827	0.014136	0.022125	0.1792	Avaneticin-13-HOde		8.739	296.2338	C18H32O2	177931-23	5 Fatty Acy C14762	ko005911/	Lipid metMetabolism	
NEG0019	2.219429	1.552006	3.932662	4.118761	0.905746	1.565554	0.033606	4.907624	3.275996	3.652256	8.824862	0.983873	2.382391	49.90396	0.009628	0.0032114	0.0467	0.065667	12,13-Ept (+)-12J13	90.4	9.273	296.2338	C18H32O2NA		4 Fatty Acy C14826	ko011001/	Global an Metabolism	
NEG0019	10.08438	376.0714	1209.859	960.6756	121.3075	483.3071	62.98753	33.74907	46.26303	48.82149	63.17639	66.12558	271.1338	53.85385	-3.74315	0.000285	0.000857	1.091569	OestruthrinOestruthrin	91.1	9.881	298.1589	C19H22O2	148-82-4	6 -	-	-	
NEG0020	37.67546	16.2728	42.2036	25.11405	3.172795	13.12541	11.59075	11.42297	5.618085	6.208192	5.703693	7.453899	22.92769	7.833801	0.035172	0.051424	0.141771	OestruthrinNP-01154	80.1	8.258	288.2495	C18H34O2	114-22-0	4 Fatty Acy-	-	-	-	
NEG0020	31.06430	467.395	387.3068	288.776	211.8812	475.7522	45.67304	59.15884	21.54202	26.40514	27.36341	355.3619	348.3815	32.0868	2.46E-05	0.000144	0.080512	4-(beta-D-GlC-4-beta-D-Glucosylo		2.049	300.0834	C13H16N1NA		3 Carboxyli-	-	-	-	
NEG0020	0.163269	0.126823	0.189611	0.141742	0.123573	0.193977	11.27633	3.989551	1.081982	6.933381	16.90656	4.986587	1	7.529066	2.912471	0.010049	0.017324	0.177508	QuercetinQuercetin	92.7	3.699	302.0415	C15H10O2	117-39-5	3 Flavonoi	C00389	ko011001/	BiosyntheMetabolism
NEG0020	87.31686	61.65524	85.97424	55.76128	37.24431	56.46426	227.9785	93.56784	24.66466	15.82328	173.4265	184.3129	64.96338	173.2957	1.346287	0.001665	0.003776	0.465436	Tributytritybutyrin		3.992	302.1718	C15H26O2	21920	3 Glyceroli-	-	-	-
NEG0020	28.41881	22.40184	29.78538	26.55018	18.05219	26.75561	50.7437	5.080713	44.97931	44.16544	41.43487	53.85895	25.32244	48.31158	0.931598	1.25E-05	0.93E-05	0.220889	Nicotianinicotianin		0.779	303.1416	C12H21N	34441-14-0	7 Flavonoi	-	-	-
NEG0020	24.48019	15.64198	13.67814	33.50034	21.50867	7.725844	18.13061	9.810184	6.95966	12.96238	13.9201	29.15248	11.58334	13.9137	0.003766	0.000468	0.174458	Gallocate(2S,3S)-2-(3,4,5-trihy		2.381	306.0764	C15H14O2	970-73-0	7 Flavonoi	C01217	ko011001/	BiosyntheMetabolism	
NEG0020	0.3101959	33.86139	31.5509	27.1092	32.76354	31.25094	231.2881	272.8309	216.5596	151.8654	300.779	24.234	31.25926	235.9438	2.916088	1.92E-06	0.01E-05	0.685757	Dihomo-82,11Z,14	99.3	10.624	306.2545	C20H34O2	1783-84-2	4 Fatty Acy C03242	ko011001/	Global an Metabolism	

NEG0025	5.931669	2.433829	6.959275	4.583903	1.703831	4.667658	255.476	384.7796	110.1962	359.0683	412.4579	212.636	4.380027	289.1023	6.044497	0.000138	0.000511	0.750228	Centiopic	Centiopicrin	2.285	356.1094	C16h42O2N	NA	3	-	C09782	ko01110/	Global	ac	Metabolism		
NEG0025	29.0428	24.26137	39.86655	35.1997	26.2366	93.26877	4.80839	9.009579	3.120766	4.923177	5.448779	9.042274	41.31192	6.058822	2.766495	0.008010	0.014356	0.253344	Tarenoside		1.57	338.1285	C16h22O16	61081-59-2	15	-	-	-	-	-			
NEG0025	21.18525	16.61467	23.44167	15.24762	20.4284	26.10698	39.11951	50.32583	51.12677	37.48829	39.38771	56.06465	55.05401	1.512632	1.526321	0.000545	0.000201	0.226791	Irigenin		1.373	360.0789	C18H16O	NA	5	-	-	-	-	-			
NEG0026	1299.111	1384.553	1652.903	1575.551	735.1407	1546.294	453.0986	715.7467	503.264	455.446	702.7824	408.6478	1365.592	539.8309	1.338995	0.000228	0.000212	1.292355	Rosmarinate		0.825	360.0886	C18H16O	537-15-5	11	Cinnamic	C01850	ko00350/	Amino	ac	Metabolism		
NEG0026	3.089618	10.37305	3.269216	2.369427	39.7343	17.96362	27.50014	17.96362	27.50014	17.96362	27.50014	23.05061	12.82973	36.04261	1.490213	0.009847	0.012619	0.179952	guaniosino	Guanosine-5'-monophosphate	1.239	363.0566	C10H14N8-32-5		3	Purine	nuC00144	ko01100/	Global	ac	Metabolism		
NEG0026	0.132513	0.119157	0.204337	0.126432	0.109624	0.270259	96.68077	66.81469	42.45671	94.29344	127.4487	129.5208	1	92.86199	6.537128	5.496705	0.000208	0.000215	0.144251	XMP		2.378	364.0393	C10H13N	523-98-8	7	Purine	nuC00655	ko01100/	Global	ac	Metabolism	
NEG0026	108.8743	21.83894	27.91023	17.40251	17.67975	37.63642	24.88975	58.76192	49.17704	50.26192	134.387	73.01366	38.5703	68.41681	0.000735	0.180634	0.012710	0.177735	Neuronic	Neuronic	99.5	12.901	366.3481	C24H46O	506-37-6	4	Fatty	Ac	C08323	ko01040/	Lipid	met	Metabolism
NEG0026	0.378822	3.317767	12.38232	10.68813	2.02382	4.333612	17.55356	39.8201	116.3582	156.1615	272.2344	157.2349	6.780081	196.5608	4.857529	0.000096	0.000207	0.59856	3-Fenulol	(1R,3R,4S,5R)-1,3,4-trihydroxy-5-phenylpentan-3-ol	2.183	368.192	C17H20O	62929-69-5	4	Alcohols	-	-	-	-	-		
NEG0026	0.12599	0.607884	0.212587	0.146426	1.367911	0.171373	1.009917	3.820818	2.025029	0.767229	0.993237	1.719527	1	1.722626	0.78461	0.029533	0.040679	0.042608	Gomphidic acid		2.403	372.075	C18H20O	25328-77-2	9	Benzene	e-	-	-	-	-		
NEG0026	20.64478	11.1589	20.79795	14.4494	2.98836	1.721387	1.444745	1.161004	1.89714	2.058985	2.157912	13.18890	17.25327	2.93429	0.002135	0.004701	0.14232	Dihydroxy	(2S,3S,4S,5R,6R)-6-(3-hydroxy-2-methylbut-3-en-1-yl)-2,3-dihydroxy-4-methyl-5-oxohexanoic acid	2.459	372.194	C16H20O	NA	4	-	-	-	-	-				
NEG0026	55.59338	59.0121	66.18397	49.81753	49.43376	44.60164	36.03376	23.46146	28.13826	23.94302	24.73971	43.12598	58.82026	29.91497	0.88997	7.25E-05	0.000318	0.220204	Syringin	beta-Syringin	2.888	372.1406	C17H24O	118-34-3	3	-	C01533	ko00940/	Biosynthe	Metabolism			
NEG0026	20.66363	13.40251	22.1293	10.22725	10.6269	16.91519	68.84561	51.87954	38.6491	40.11489	70.8404	91.42215	17.29656	60.26196	1.800762	0.000052	0.000149	0.348133	Tetrahydrocurcumin		2.785	372.1587	C22H24O	36862-04-1	3	Diaryl	hydro-	-	-	-	-		
NEG0026	0.604136	0.823927	1.118285	0.977146	0.59034	0.505784	0.820731	1.290083	0.458464	0.728813	1.027331	1.348463	1	1	0	0.330211	0.364668	0.013653	Suacrenin		6.551	372.1956	C22H28O	8377-13-3	5	-	-	-	-	-			
NEG0027	0.4084873	2.696258	4.610286	3.307222	3.952548	3.728154	28.52625	21.37512	23.05995	16.16943	24.73302	17.46256	3.72989	21.88777	2.55292	2.40E-06	0.114E-05	0.02541	Iscodiospyrin		2.561	374.0837	C22H14O	20175-84-2	12	Dihydro-	-	-	-	-	-		
NEG0027	33.28452	50.80991	26.81392	24.05264	41.95676	36.39719	1152.764	45.25273	509.3309	675.4099	963.8496	722.1253	35.55247	774.7895	44.5782	1.86E-05	0.000118	1.296967	Triplidoide		9.739	376.1538	C20H24O	38647-10-8	4	-	-	-	-	-			
NEG0027	12.0712	10.71721	7.917184	4.922821	5.671906	5.756415	165.6577	277.2899	231.0105	109.5851	136.8958	174.0097	6.973465	195.9111	4.81218	0.000001	0.000014	0.601566	Tomenin		2.394	384.1042	C17H18O	28446-08-4	3	Coumarin	-	-	-	-	-		
NEG0027	6.800101	3.803796	6.620292	4.561408	4.234595	3.589973	36.17126	24.08617	17.83676	25.60903	22.71975	27.4517	5.229944	25.64579	2.293854	1.14E-05	8.86E-05	0.213105	Kanzonol	-	1.942	384.1518	C22H24O	156250-71-1	14	Isoflavono-	-	-	-	-	-		
NEG0027	278.0948	292.9824	292.9824	277.7221	277.7221	277.7221	277.7221	277.7221	277.7221	277.7221	277.7221	277.7221	277.7221	277.7221	277.7221	277.7221	277.7221	277.7221	277.7221	277.7221	2.574	386.1199	C17H22O	NA	3	-	-	-	-	-			
NEG0027	1032.072	1204.332	1823.338	1523.176	1041.079	1305.884	819.7032	533.3536	704.8892	964.1684	758.5771	875.6693	1321.642	776.0601	-0.76809	0.002854	0.005907	1.003662	Corchoiol-3-Hydrox-		2.284	386.192	C19H30O	NA	5	Fatty	Ac	-	-	-			
NEG0027	13.25254	26.46071	2.000554	3.338322	4.736492	24.13653	4.664665	4.757208	7.561734	0.251672	5.008123	0.164313	12.65131	3.734619	-1.76025	0.073237	0.096887	0.101857	Globocarissapin		2.139	387.0612	C12H21N	19041-10-2	11	Organo-	-	-	-	-	-		
NEG0027	1228.74	1224.216	1798.488	1134.784	599.8192	617.766	574.2528	804.7621	527.8795	544.7756	815.8899	477.5005	1267.636	624.1767	-1.02211	0.000509	0.005959	1.060388	Betanidin		0.826	388.0837	C20H16N	2181-76-7	17	Indoles	ac	C0859	ko01110/	Global	ac	Metabolism	
NEG0027	41.55143	1221.782	686.8764	53.66293	1547.357	3759.763	177.9529	124.3216	176.0642	181.8552	199.6789	138.429	176.0718	3.305545	0.006658	0.008668	1.25881	Artemetin	D-(+)-Mal	70.3	1.007	388.12	C20H20O	469-78-2	10	Flavonoid	C00208	ko01100/	Carbohydr	Environmental Information Processing	Metabolism		
NEG0027	1.92324	0.951845	1.915449	1.551947	5.262561	1.508755	30.90782	27.14657	6.374113	28.17544	26.37905	30.47121	2.185633	24.99093	3.510566	0.000145	0.000053	0.220343	Geniposic	geniposide	1.978	388.1357	C17H24O	24512-63-8	3	-	-	-	-	-			
NEG0028	0.15936	0.397625	1.606581	0.146307	0.366194	0.285982	262.2007	197.839	94.08761	164.7928	211.4271	135.1106	1	177.5763	7.472295	2.60E-05	0.000148	0.625562	trans-Picoid		2.657	390.13	C20H22O	27208-80-4	4	Stilbenes	-	-	-	-	-		
NEG0028	157.652	118.8171	169.8982	127.0968	94.27253	156.5845	274.8926	296.3011	238.4118	261.9076	223.964	363.8734	137.4627	276.5538	1.00852	0.000147	0.004034	0.533515	Shanzhiside		7.692	392.1275	C16H24O	NA	11	-	-	-	-	-			
NEG0028	2.806423	3.137369	2.590638	1.793854	3.899271	2.170119	13.70127	8.866291	10.31488	4.644016	13.09492	5.099473	7.327296	9.290142	1.765244	0.002173	0.004708	0.159947	Acidissimolol		4.414	393.2346	C25H31N	126006-00-8	10	Prenol	lip-	-	-	-	-		
NEG0028	17.15159	12.07882	20.1522	13.67948	12.36096	18.99923	14.61912	14.51091	11.3485	10.70577	12.2192	13.53167	15.7312	12.82145	-0.29507	0.094643	0.121821	0.056379	Rotenone	Rotenone	8.299	394.1432	C23H22O	83-79-4	3	Isoflavono	C07593	ko01110/	Global	ac	Metabolism		
NEG0028	6.038234	4.998485	4.998485	4.998485	4.998485	4.998485	4.998485	4.998485	4.998485	4.998485	4.998485	4.998485	4.998485	4.998485	4.998485	4.998485	4.998485	4.998485	4.998485	4.998485	7.875	396.1586	C23H24O	31271-07-5	3	Benzopyr-	-	-	-	-	-		
NEG0028	0.632196	0.495994	0.685215	0.501311	0.454239	0.307687	2.224699	0.224848	0.205554	4.64577	0.812427	1.359443	1	1.581015	0.668051	0.164131	0.199153	0.028678	5-Hydroxy-4-hydroxy-9-(4-hydroxy-3-methylbut-3-en-1-yl)-2,3-dihydroxy-4-methyl-5-oxohexanoic acid		3.293	440.1144	C21H20O	17802-04-5	3	Flavonoid	-	-	-	-	-		
NEG0028	0.824833	1.378075	0.495289	0.254361	3.618164	1.25961	160.8573	254.3372	151.1022	279.4266	54.86386	52.23015	13.76181	4.476489	0.00896	0.01256	0.45457	Shoyuflavone		2.389	442.0883	C19H14O	190712-88-8	3	Isoflavono-	-	-	-	-	-			
NEG0028	163.1455	25.84973	226.3382	190.9584	83.7352	246.7174	71.22622	1.112583	69.4487	43.7556	102.5832	35.95614	1.31633	75.7788	1.05808	0.051225	0.071956	0.348333	Apigenin	7-cycloside	0.824	402.0983	C20H18O	NA	10	-	-	-	-	-			
NEG0028	101.2314	53.94247	121.6293	86.60557	67.36516	72.64094	168.7529	162.8555	86.70727	231.5771	40.16621	289.2178	83.89614	183.3544	12.7888	0.007844	0.013965	0.410186	Opin	N-(1S)-4-Carbamin	2.868	404.1667	C25H24O	482-53-1	10	-	-	-	-	-			
NEG0028	8.783878	591.491	3.144998	0.132373	0.510643	4.378429	49.23806	56.28549	50.98084	33.57189	40.44614	67.20140	15.83032	49.00197	3.250817	4.53E-06	4.80E-05	0.317085	Lancerin		2.114	406.0858	C19H18O	81991-99-3	3	Neoflavo-	-	-	-	-	-		
NEG0029	96.67532	54.86787	116.1387	76.14994	77.0209	60.83932	37.70682	31.58602	30.91035	43.46962	35.21717	46.74794	80.2027	37.60632	-1.0941	0.003137	0.003078	0.278964	Malmeisins		2.851	406.1741	C25H26O	18483-64-2	9	Purine	nuC00206	ko01100/	Global	ac	Metabolism		
NEG0029	6.303532	6.68714	4.763146	3.510693	4.489947	46.25766	24.53702	19.77458	17.36331	25.34606	18.51272	15.20247	25.29861	25.29861	-1.0941	0.003137	0.003078	0.278964	malDAP		8.74	411.0331	C10H15N	326322	3	Purine	nuC00206	ko011					

[illegible]

POSO0048	294.8154	168.5048	222.0014	179.2235	135.7389	171.0871	243.4095	227.2924	224.5782	222.0945	182.2788	214.2191	195.23	218.9788	0.165616	0.352615	0.423916	0.095015	Allylsine	Allylsine	0.86	145.0734	C6H11NC	1740725	3	CarboxyliC04076	ko01100/	Amino ac	Metabolism	
POSO0045	143.4645	18.57507	106.6628	105.8122	109.7756	22.8569	35.98181	12.28934	15.40382	12.18599	82.06134	64.6256	84.4493	37.09132	-1.18695	0.080191	0.118119	0.252461	SpermidiolSpermidine		0.598	145.1573	C7H19N3	124-20-9	4	OrganoC00315	ko01100/	Amino ac	Environmental Information Processing;Metabolism	
POSO0056	649.7729	403.9493	522.9647	459.9042	308.1138	408.1001	257.3972	350.3191	285.0865	228.2966	435.8852	297.3911	458.6879	309.06	-0.56963	0.024797	0.043817	0.506969	Oxoglutaralapha-Cetoglutaric a		1.224	146.0212	C5H6O5	328-50-2	2	Keto acidC00026	ko01100/	Amino ac	Metabolism	
POSO0051	20.46335	16.90934	10.53499	6.328527	10.26212	10.63683	47.50958	537.4904	38.64602	33.5432	43.00451	52.57379	12.52244	125.391	3.322915	0.201169	0.262651	0.346714	CoumarinCumarin		2.303	146.0362	C9H6O2	91-64-5	3	CoumarinC00581	ko01110/	Biosynthe	Metabolism	
POSO0052	5903.149	10549.08	11760.65	9336.125	7414.702	8351.599	7647.166	6591.884	2808.127	18105.23	8639.281	3375.166	8885.884	786.143	-0.17678	0.680718	0.762505	0.351553	L-Glutam D-L-Glutamine		0.888	146.0685	C5H9NO2	56-85-0	4	CarboxyliC00064	ko01100/	Amino ac	Environmental Information Processing;Genetic Information Processing;Metabolism	
POSO0053	756.8134	487.2343	493.7944	444.0086	355.6794	425.3543	991.5709	890.9201	856.2896	712.1297	1193.137	851.2532	493.8141	914.2633	0.888674	0.000683	0.022351	0.997788	L-Lysine DL-Lysine		0.687	146.1049	C6H14N2	56-87-0	4	CarboxyliC00047	ko01100/	Amino ac	Environmental Information Processing;Genetic Information Processing;Metabolism	
POSO0054	5152.525	3732.65	4379.335	3579.009	2523.523	3508.914	3774.609	2894.102	2746.89	4497.504	4258.266	3609.608	3812.699	304.163	-0.07076	0.701528	0.704284	0.226118	L-Glutam L-Glutamic acid		0.8	147.0525	C5H9NO2	56-86-0	4	CarboxyliC00025	ko01100/	Amino ac	Environmental Information Processing;Genetic Information Processing;Metabolism	
POSO0055	12213.06	7338.08	7389.719	4361.251	17548.3	6139.571	3883.924	4049.851	1299.386	1876.257	2746.237	2866.986	9164.96	2787.107	-0.17337	0.010594	0.20062	0.374226	Gamma(4R)-5-Hydroxy-L-lysine		0.862	147.0891	C6H13NC	53185-12-9	3	Piperidin-	-	-	-	
POSO0056	29.99153	12.89943	18.88657	18.32584	8.26685	12.84089	9.762713	7.391213	8.04138	7.985235	26.899	8.154067	10.65738	11.3669	-0.57016	0.237406	0.306603	0.066603	CuminalolEL960000		2.272	148.0882	C10H12O	122-03-2	4	Prend lipC06577	ko01120/	Global	an	Metabolism
POSO0057	866.705	838.9514	899.3899	514.7655	461.2676	708.2691	917.4646	1018.074	1134.785	660.6202	378.952	1022.697	174.7814	1022.969	0.51796	0.032027	0.054843	0.72199	L-Methiol(-)-Methionine		0.858	149.0505	C5H11NC	63-68-3	3	CarboxyliC00073	ko01100/	Amino ac	Genetic Information Processing;Metabolism	
POSO0058	30.35647	10.36248	17.69534	16.50222	41.5443	9.49604	95.38782	106.0854	95.8277	33.81083	99.17031	95.55056	21.0032	72.59974	1.787458	0.003442	0.008693	0.345138	Asparaginsparaginic acid		1.257	149.9802	C6H14O2S	118374	3	Dithiolan-	-	-	-	
POSO0059	35.02563	9.69125	26.60794	18.4273	44.79783	15.253134	24.551	18.7252	13.87845	17.95637	64.46193	173.1964	1.87947	0.091945	0.091197	0.258149	Guanine	Guanine		1.147	151.0489	C5H5N5	73-40-5	3	ImidazopC00242	ko01100/	Global	an	Metabolism	
POSO0066	17.85928	10.65672	13.13325	10.18685	8.657664	11.93122	21.46694	19.37288	20.53106	14.12289	20.70457	18.31877	12.07083	19.05663	0.658786	0.002144	0.005787	0.118632	p-Hydroxyphenyllactic acid		1.223	152.0459	C8H8O3	156-38-7	9	Phenols C00642	ko01120/	Amino ac	Metabolism	
POSO0061	14.43192	31.11802	32.70562	3.645472	23.2275	24.40588	31.22217	33.68766	27.63109	25.29317	32.95627	28.26176	19.92261	29.92355	0.586961	0.094158	0.135638	0.125251	3-Phenylpropyl-3-(4,4-dihydroxyph-2-methyl		2	152.1195	C10H16O	2102-58-1	1	Order lipC00964	ko01110/	Global	an	Metabolism
POSO0062	96.96422	53.34929	50.63626	50.37829	47.10427	51.90268	18.82423	179.5414	108.732	182.0823	181.1386	144.93	58.35425	164.1113	1.491764	3.29E-05	0.002099	0.523762	L-HistidinL-Histidine		0.694	155.0689	C6H9N3	71-00-1	3	CarboxyliC00135	ko01100/	Amino ac	Environmental Information Processing;Genetic Information Processing;Metabolism	
POSO0063	1997.048	1692.52	1678.954	1468.319	1746.752	1842.228	1744.204	1717.933	1987.731	1899.553	1788.962	2414.991	1443.335	1660.554	1780.417	0.171459	0.21149	0.275527	0.507309	Phosphorylphosphocolate		14.512	155.9829	C2HSO6	13147-57-5	3	Organic pC00988	ko01100/	Carboxhyd	Metabolism
POSO0064	17.37523	49.01314	18.47432	13.26744	7.149943	62.10533	30.01062	38.61451	21.62967	21.3831	39.33381	23.40771	27.8957	29.06357	0.059073	0.09639	0.934983	0.025575	6-Methox-6-Methoxyquinoline		2.791	159.0677	C10H9N	5263-87-6	3	-	-	-	-	
POSO0065	105.3211	41.20419	93.36255	75.20389	33.40641	43.75532	75.78998	73.26876	49.20441	61.54724	63.91121	59.1546	65.87551	62.6618	-0.07344	0.805313	0.843843	0.033183	CalsyestiGuaucoline		0.859	159.0887	C7H13NC	131580-36-	5	Tropane cI00850	ko00960/	Biosynthe	Metabolism	
POSO0066	59.04901	38.04528	58.4528	48.23513	26.85423	33.87607	35.9949	48.03328	34.12725	31.59242	61.22931	26.6147	43.18548	39.59864	-0.1251	0.630625	0.682829	0.027897	L-2-Amin.alpha.-Aminoadipic		1.221	161.0681	C6H11NC	1118-90-7	4	CarboxyliC00956	ko01100/	Amino ac	Metabolism	
POSO0067	3585.952	2850.66	3459.787	2784.751	1960.917	3034.275	5565.155	4824.727	2946.058	4499.126	50.0099	0.0026	0.006721	1.924889	LevoLugLugucosan		0.829	162.0521	C6H10O5	498-07-7	4	Oxepanes-	-	-	-					
POSO0068	2127.344	1501.15	827.5239	1744.649	527.4563	67.9955	2744.998	2418.412	1621.397	2818.359	2645.629	2585.582	1234.353	2472.396	1.002155	0.003011	0.007682	1.642431	D-1,5-Anil,5-Anhydro-L-Arab		1.099	162.0521	C6H10O5	75414-43-6	3	Carboxyli-	-	-	-	
POSO0069	14.8482	5.679948	7.549314	7.147268	8.454976	5.352548	11.41592	45.98167	3.64558	8.752113	5.97207	17.43864	8.171876	5.92637	0.287166	0.358409	0.078571	Methyl cil-3-Methyl-3-sulfinylar		1.892	162.0707	C10H10O	103-26-4	16	Cinnamic-	-	-	-		
POSO0072	62.62342	9.981695	17.09948	14.68207	21.76893	16.91929	36.64637	20.60914	24.34672	11.73526	42.60076	32.61404	23.84581	28.80925	0.236426	0.653028	0.702435	0.034071	L-Nicotin(+)-nicotine		14.473	162.1151	C10H14N	20033	3	PyridinesC16150	ko01120/	Global	an	Metabolism
POSO0071	125.1136	85.41032	71.7896	61.89757	39.76342	77.13481	38.46201	17.48554	35.21839	47.29449	41.23373	31.6605	76.8431	35.22578	-0.12528	0.007	0.014763	0.380108	Homothomomethomethionine		0.472	163.066	C6H13NC	25148-30-5	3	CarboxyliC17213	ko01110/	Biosynthe	Metabolism	
POSO0072	181.676	119.394	139.2408	113.0002	101.0363	113.409	338.7923	374.7769	243.193	268.7285	378.0491	253.2748	126.6201	309.4688	1.289287	6.58E-05	0.000444	0.689449	EthionineL-Ethionine		1.226	163.066	C6H13NC	13073-35-3	4	-	-	-	-	
POSO0073	1773.141	944.6804	997.398	789.7015	661.4187	988.0963	2226.72	2063.873	1848.162	1939.032	2334.767	1782.727	1022.359	2032.547	0.993547	0.000241	0.002161	0.159444	Phenylpropyl-3-(4,4-dihydroxyph-		1.248	164.0467	C9H8O3	156-06-9	3	Benzene cC00166	ko01100/	Amino ac	Metabolism	
POSO0074	132.2058	77.07222	20.21085	2.516539	53.47943	20.22601	49.8325	641.8776	536.6687	338.1331	429.893	521.7685	50.94331	494.0274	3.27798	2.39E-06	4.95E-05	1.042744	2-Hydroxycinnamic		2.101	164.0467	C9H8O3	583-17-5	3	CinnamicC001772	ko01100/	Amino ac	Metabolism	
POSO0075	49.93052	37.57626	71.16578	19.38171	21.41636	24.34058	1155.385	860.6103	93.1313	129.9233	2488.274	1410.427	25.63517	14.10427	5.734767	0.000227	0.001201	0.896633	4-Coumaric acid		2.649	164.0468	C9H8O3	501-98-4	3	CinnamicC00811	ko01100/	Amino ac	Metabolism	
POSO0077	717.7824	411.2252	530.5431	443.588	333.0428	496.5307	318.6196	347.666	299.9778	346.5536	384.3738	401.8783	488.2702	349.845	-0.4825	0.02369	0.04843	0.505901	S-2-Amin-5-Aminoethyl-L-cys		0.643	164.0612	C5H12N2	2936-69-8	5	Carboxyli-	-	-	-	
POSO0077	71.45608	33.13679	40.41494	29.94848	27.01275	43.98841	98.20258	42.2323	51.98814	98.20258	43.98841	37.76963	53.79642	42.22791	0.373945	0.0379714	0.064393	0.185427	cis-JasmonicFenipic acid		4.526	164.1195	C11H16O4	62-61-4	3	Organoo-	-	-	-	
POSO0078	229.1197	138.9732	171.2754	224.2318	148.0732	46.94196	46.94196	46.94196	46.94196	42.39657	38.96556	42.84303	100.7603	130.6407	2.14193	4.40E-05	0.000346	0.612061	DL-Methyl-Methionine sulfox		0.8	165.0454	C5H11NC	3226-65-1	3	Carboxyli-	-	-	-	
POSO0078	84.23182	54.18582	59.68844	56.1679	34.22984	50.74627	132.1966	112.3814	81.50977	96.73924	115.0098	93.92879	56.4935	105.2948	0.900199	0.002219	0.000444	0.340178	1-Methyl;Epiguanine		1.226	165.0684	C6H7NS	938-85-2	3	Imidazop-	-	-	-	
POSO0086	9205.581	5044.205	5490.648	4670.363	491.405	5209.045	1602.37	9866.129	11923.72	13800.02	9747.007	9866.129	541.563	11668.97	1.050051	0.000124	0.00079	3.854208	L-Phenyl-L-Phenylalanine		1.678	165.0684	C9H9NO	63-91-2	4	CarboxyliC00079	ko01100/	Amino ac	Environmental Information Processing;Genetic Information Processing;Metabolism	
POSO0081	964.0938	527.2129	581.5244	516.1481	422.3859	521.7967	1370.847	1141.725	985.6212	1224.656	1420.172	981.9644	588.8513	1187.498	0.101949	0.000264	0.001218	1.205026	1-Deoxy-13-D-4-Methyl-3-pente		1.679	166.0814	C6H14O	18545-96-5	16	Organoo-	-	-	-	
POSO0082	28.48651	14.50052	10.58743	14.44357	21.24081	15.12104	50.99533	55.51899	46.17415	37.46868	67.78853	31.85043	18.27797	48.29879	1.401895	0.000385	0.00161	0.272347	Pentol(2E,4E,7E)-2,4,7-Dec		3.276	166.0988	C11H14O	NA	3	-	-	-		

PO00132	62.64109	20.11309	14.31743	15.25398	13.86378	16.06934	12.91525	14.29535	17.60827	15.15214	19.83504	14.0165	16.70999	15.30386	-0.1268	0.05158	0.08729	0.032095	Tetradecyl-L-Tetradecyloleamine	5.11	213.2447	C14H31N	2016-42-4	4	-																																																																																																																																																																																																																																																																																																																																																																																																						
PO00133	26.40092	363.0745	40.4784	39.5747	371.6442	34.8587	495.1461	477.3641	477.9633	475.9349	572.4488	572.4488	572.4488	516.3401	0.322165	0.05313	0.048629	0.339214	Valylprolyl Valylproline	1.558	214.131	C10H18N	2048-27-1	3	Carboxylic																																																																																																																																																																																																																																																																																																																																																																																																						
PO00134	5.11376	2.735264	5.01581	2.739222	0.874141	4.391302	3.393818	5.816944	3.704606	4.029717	6.389572	4.088894	3.643145	4.7505	0.276168	0.28954	0.358635	0.031961	SuccinylplSuccinyl proline	1.866	215.0785	C9H13N	63250-32-8	4	-																																																																																																																																																																																																																																																																																																																																																																																																						
PO00137	39.01332	39.66362	40.37689	44.5638	81.84333	45.59474	44.33843	43.5245	84.78154	24.19731	71.66229	51.31671	46.84598	47.4606	0.900798	0.254885	0.324309	0.19087	N-Nonan-N-Nonaronylglycine	3.267	215.5114	C11H21NN	-	3	Carboxylic																																																																																																																																																																																																																																																																																																																																																																																																						
PO00138	40.01672	2.265941	1.6795318	2.903485	14.019159	9.927346	4.232635	2.601069	80.87268	1.86453	3.896222	1.84022	12.66707	15.58846	0.326543	0.825387	0.859768	0.018912	L-1,2,3,4;1,2,3,4-tetrahydro-β	4.598	216.0889	C12H21N	2438-90-4	4	Indoles ar-																																																																																																																																																																																																																																																																																																																																																																																																						
PO00139	155.6214	95.47525	12.2879	103.465	64.61989	87.46197	103.826	81.0673	87.06213	86.55669	110.9773	92.74013	105.0954	58.4594	0.16021	0.440653	0.507373	0.036919	Prolyl-Thr-pro-thr	0.855	216.111	C9H16N2NA	-	4	Carboxylic																																																																																																																																																																																																																																																																																																																																																																																																						
PO00144	65.83112	41.05175	45.29359	38.58622	28.39858	42.9265	47.81947	47.44874	43.93146	43.53579	50.49217	28.98262	43.6796	45.36837	0.0756401	0.795315	0.013296	β-Alanyl-β-Ala-Lys	0.664	217.1419	C9H19N2NA	-	3	-																																																																																																																																																																																																																																																																																																																																																																																																							
PO00141	0.740992	0.57671	0.60099	0.58692	0.384036	0.400169	17.57977	27.8761	12.32082	31.94664	12.54195	-	19.7384	3.402933	0.009019	0.001035	0.224414	EupatorioicEUPATORIOICHOCH	2.511	218.0935	C13H24O	19013-03-7	4	Carboxylic																																																																																																																																																																																																																																																																																																																																																																																																							
PO00142	820.2423	656.0199	598.2827	564.5856	480.1959	637.8576	490.0061	448.5787	448.5787	480.6145	448.5787	490.3224	534.8857	33.9307	0.428204	0.125621	0.175754	0.308163	PanthoicPanthoic acid	1.753	219.1101	C9H17N	137-08-4	2	Alcohols																																																																																																																																																																																																																																																																																																																																																																																																						
PO00143	824.3943	486.9511	728.9602	728.9602	480.1959	506.427	572.9621	728.5897	438.258	61.3653	799.5778	931.7475	567.9844	67.3611	0.2466	0.376429	0.447824	0.309465	(-)-Sedam-sedamide	2.695	219.1614	C14H21N	497-88-1	4	C10171																																																																																																																																																																																																																																																																																																																																																																																																						
PO00144	185.0015	148.9696	110.0328	113.5575	86.24731	132.8837	18.80928	19.5742	20.2661	15.67904	33.55857	22.74959	12.74743	21.78288	-2.5711	2.04E-05	0.000223	0.528555	Chrysoir(-) 3-tris-isodihomo	0.879	220.0575	C12H21O	91362-90-2	7	Oxanes																																																																																																																																																																																																																																																																																																																																																																																																						
PO00145	11.37565	9.84399	14.84394	13.56406	7.314616	4.926783	5.784468	4056.962	32.6628	37.43123	6532.736	3632.725	17.94673	4302.824	9.227739	6.66E-05	0.000444	0.3449271	Snapiac-acSnapiac acid	2.699	224.0675	C11H22O	530-59-6	4	-																																																																																																																																																																																																																																																																																																																																																																																																						
PO00146	96.82756	42.91452	70.37066	84.16622	32.10807	36.86912	23.75371	14.24032	13.06776	24.72272	25.9832	12.98632	60.54269	19.12567	-1.6644	0.004415	0.010025	0.295417	Methyl-methyl Jasmonate	2.551	224.1404	C13H20O	39924-52-2	3	Fatty Acy C11512																																																																																																																																																																																																																																																																																																																																																																																																						
PO00147	103.4454	51.07975	70.37066	84.16622	32.10807	36.86912	23.75371	14.24032	13.06776	24.72272	25.9832	12.98632	60.54269	19.12567	-1.6644	0.004415	0.010025	0.295417	Methyl-methyl Jasmonate	3.976	226.1196	C12H18O	125263-70-4	4	Pyrans																																																																																																																																																																																																																																																																																																																																																																																																						
PO00148	214.9368	102.9396	130.116	110.6054	55.5008	107.1219	353.712	257.8705	374.2939	269.3919	349.0329	297.6865	120.2034	317.0138	1.399068	5.14E-05	0.000382	0.677273	TraumaticNP-008952	4.526	228.1352	C12H20O	6402-36-4	4	Fatty Acy C16308																																																																																																																																																																																																																																																																																																																																																																																																						
PO00149	1585.361	928.6555	998.6138	998.6138	998.6138	998.6138	998.6138	998.6138	998.6138	998.6138	998.6138	998.6138	998.6138	998.6138	998.6138	998.6138	998.6138	998.6138	998.6138	1.834	228.1465	C11H20N	6403-35-6	3	Carboxylic																																																																																																																																																																																																																																																																																																																																																																																																						
PO00150	15.76972	21.4749	23.6239	52.6108	61.09521	64.0168	1.2168	2.26675	0.362551	0.365182	2.213627	0.396999	30.5924	11.38655	4.75004	0.009679	0.019067	0.225783	Cyclobars 160492	6.878	234.0275	C11H18N	105748-58-	4	Indoles ar-																																																																																																																																																																																																																																																																																																																																																																																																						
PO00151	286.6831	187.8187	216.7829	230.3188	105.6211	163.7651	226.5757	190.1969	213.1714	276.7829	211.7331	194.4468	193.1966	213.1714	276.7829	0.375927	0.447824	0.115489	Glutaryl-glu-ser	0.79	234.0841	C10H18N	25075-38-7	4	Carboxylic																																																																																																																																																																																																																																																																																																																																																																																																						
PO00152	57.60503	36.66211	33.81952	30.91798	58.67996	30.22035	165.302	166.9171	46.41969	205.3437	83.68055	41.65107	138.1926	1.720255	0.000514	0.474343	Valericen(-) 9β-Pentadecanoic	4.091	234.161	C14H27O	698970	4	Fenol lip-																																																																																																																																																																																																																																																																																																																																																																																																								
PO00153	14.81818	1.87242	1.880228	0.837642	1.038032	0.899279	1.038032	0.837642	1.038032	0.899279	1.038032	0.837642	1.038032	0.899279	1.038032	0.837642	1.038032	0.899279	1.038032	0.837642	1.038032	0.899279	1.038032	0.837642	1.038032	0.899279	1.038032	0.837642	1.038032	0.899279	1.038032	0.837642	1.038032	0.899279	1.038032	0.837642	1.038032	0.899279	1.038032	0.837642	1.038032	0.899279	1.038032	0.837642	1.038032	0.899279	1.038032	0.837642	1.038032	0.899279	1.038032	0.837642	1.038032	0.899279	1.038032	0.837642	1.038032	0.899279	1.038032	0.837642	1.038032	0.899279	1.038032	0.837642	1.038032	0.899279	1.038032	0.837642	1.038032	0.899279	1.038032	0.837642	1.038032	0.899279	1.038032	0.837642	1.038032	0.899279	1.038032	0.837642	1.038032	0.899279	1.038032	0.837642	1.038032	0.899279	1.038032	0.837642	1.038032	0.899279	1.038032	0.837642	1.038032	0.899279	1.038032	0.837642	1.038032	0.899279	1.038032	0.837642	1.038032	0.899279	1.038032	0.837642	1.038032	0.899279	1.038032	0.837642	1.038032	0.899279	1.038032	0.837642	1.038032	0.899279	1.038032	0.837642	1.038032	0.899279	1.038032	0.837642	1.038032	0.899279	1.038032	0.837642	1.038032	0.899279	1.038032	0.837642	1.038032	0.899279	1.038032	0.837642	1.038032	0.899279	1.038032	0.837642	1.038032	0.899279	1.038032	0.837642	1.038032	0.899279	1.038032	0.837642	1.038032	0.899279	1.038032	0.837642	1.038032	0.899279	1.038032	0.837642	1.038032	0.899279	1.038032	0.837642	1.038032	0.899279	1.038032	0.837642	1.038032	0.899279	1.038032	0.837642	1.038032	0.899279	1.038032	0.837642	1.038032	0.899279	1.038032	0.837642	1.038032	0.899279	1.038032	0.837642	1.038032	0.899279	1.038032	0.837642	1.038032	0.899279	1.038032	0.837642	1.038032	0.899279	1.038032	0.837642	1.038032	0.899279	1.038032	0.837642	1.038032	0.899279	1.038032	0.837642	1.038032	0.899279	1.038032	0.837642	1.038032	0.899279	1.038032	0.837642	1.038032	0.899279	1.038032	0.837642	1.038032	0.899279	1.038032	0.837642	1.038032	0.899279	1.038032	0.837642	1.038032	0.899279	1.038032	0.837642	1.038032	0.899279	1.038032	0.837642	1.038032	0.899279	1.038032	0.837642	1.038032	0.899279	1.038032	0.837642	1.038032	0.899279	1.038032	0.837642	1.038032	0.899279	1.038032	0.837642	1.038032	0.899279	1.038032	0.837642	1.038032	0.899279	1.038032	0.837642	1.038032	0.899279	1.038032	0.837642	1.038032	0.899279	1.038032	0.837642	1.038032	0.899279	1.038032	0.837642	1.038032	0.899279	1.038032	0.837642	1.038032	0.899279	1.038032	0.837642	1.038032	0.899279	1.038032	0.837642	1.038032	0.899279	1.038032	0.837642	1.038032	0.899279	1.038032	0.837642	1.038032	0.899279	1.038032	0.837642	1.038032	0.899279	1.038032	0.837642	1.038032	0.899279	1.038032	0.837642	1.038032	0.899279	1.038032	0.837642	1.038032	0.899279	1.038032	0.837642	1.038032	0.899279	1.038032	0.837642	1.038032	0.899279	1.038032	0.837642	1.038032	0.899279	1.038032	0.837642	1.038032	0.899279	1.038032	0.837642	1.038032	0.899279	1.038032	0.837642	1.038032	0.899279	1.038032	0.837642	1.038032	0.899279	1.038032	0.837642	1.038032	0.899279	1.038032	0.837642	1.038032	0.899279	1.038032	0.837642	1.038032	0.899279	1.038032	0.837642	1.038032	0.899279	1.038032	0.837642	1.038032	0.899279	1.038032	0.837642	1.038032	0.899279	1.038032	0.837642	1.038032	0.899279	1.038032	0.837642	1.038032	0.899279	1.038032	0.837642	1.038032	0.899279	1.038032	0.837642	1.038032	0.899279	1.038032	0.837642	1.038032	0.899279	1.038032	0.837642	1.038032	0.899279	1.038032	0.837642	1.038032	0.899279	1.038032	0.837642	1.038032	0.899279	1.038032	0.837642	1.038032	0.899279	1.038032	0.837642	1.038032	0.899279	1.038032	0.837642	1.038032	0.899279	1.038032	0.837642	1.038032	0.899279	1.038032	0.837642	1.038032	0.899279	1.038032	0.837642	1.038032	0.899279	1.038032	0.837642	1.038032	0.899279	1.038032	0.837642	1.038032	0.899279	1.038032</

[illegible]

POS00306	0.412677	0.312348	0.33188	0.269741	0.338158	0.323557	0.498678	1.051551	1.178368	0.708708	1.012502	0.29473	1	1	0	0.009416	0.018661	0.029042	Mycalami(2R)-3-(((2-Aminoethyl	7.559	503.2986	C24H41N	115185-92-	4 -	-	-	-	-
POS00307	17.04865	10.02859	6.251783	7.336502	21.69774	5.099452	106.0482	86.3763	74.60076	21.8856	122.332	29.06492	11.24379	73.38464	2.70635	0.004123	0.009562	0.37725	Protobass(1 α ,2 α ,3 β ,5 ξ ,9 ξ ,18 ξ)	4.088	504.3427	C30H48O	37905-13-8	4 Prenol lip-	-	-	-	-
POS00308	10.50964	9.214663	6.714518	6.106799	17.34728	7.059409	18.15422	11.73702	12.27164	11.84211	15.97261	10.11499	9.492052	13.34877	0.491915	0.098403	0.141131	0.075372	LysoPC(1 1-Stearoyl-sn-glycer	8.907	523.3613	C26H54N	19420-57-6	4 GlyceroplC04230	ko00564//	Lipid metMetabolism		
POS00309	1.09343	0.743178	0.731822	0.707306	0.581868	0.670773	0.773083	0.680459	0.669265	0.568437	0.842007	0.621223	1	1	0	0.467844	0.531198	0.006739	Diosbulbinoside F	9.489	538.1993	C26H34O	66756-58-9	10 Prenol lip-	-	-	-	-
POS00310	31.4964	27.426	24.06964	22.39117	19.33992	17.7775	277.0355	197.1968	124.8378	96.4246	295.3213	131.5312	23.7501	187.0579	2.977479	0.000761	0.00254	0.649083	Isochama(1S,4 α S,7 α S)-7-(((2E	0.797	542.1224	C30H22O	NA	2 -	-	-	-	-
POS00311	408.4234	386.4677	337.5129	399.8241	316.7454	385.8055	371.7943	532.0009	589.059	476.3401	560.1984	591.6601	372.4631	520.1755	0.481901	0.002798	0.007093	0.545007	Echineno(13cis,15cis)-2',3',4',5'	12.657	550.4149	C40H54O	NA	4 -	C08592	ko01110//	Global anMetabolism	
POS00312	524.1001	210.7017	184.6452	151.73	422.8029	268.0478	2020.897	1446.67	1124.52	1064.449	1893.853	838.3419	293.6713	1398.122	2.251216	0.000292	0.001291	1.671325	PhosphorPhosphoribide A	11.126	592.2649	C35H36N	15664-29-6	6 -	C18021	ko01110//	Global anMetabolism	
POS00313	413.6247	238.8792	238.773	281.8683	139.9181	214.0325	483.3767	291.7267	318.8828	307.3091	366.7865	388.1348	254.516	359.3694	0.497712	0.05011	0.079159	0.392499	Auroxant 2-Acetamido-4-(5-an	11.576	600.4148	C40H56O	27785-15-5	5 Prenol lip-	-	-	-	-
POS00314	216.5543	105.5662	100.2072	85.01778	188.4361	144.4975	561.6225	375.7394	349.9969	295.7079	630.1414	290.7698	140.0465	417.263	1.575051	0.001266	0.000663	0.82521	Phosphoribide b	9.766	606.244	C39H34N	20239-99-0	6 Tetrapyr-	-	-	-	-
POS00315	233.1564	188.569	86.60123	143.857	212.4283	227.8823	767.0187	993.3702	689.3184	557.9559	1110.047	550.3944	182.0824	778.0174	2.095211	0.000107	0.000637	1.25011	Cepharan(1S,2S,3 α R,4S,5S,9R,	12.419	606.2804	C37H38N	481-49-2	12 -	-	-	-	-
POS00316	245.2418	116.7165	224.3851	219.039	101.1834	103.2517	207.2962	491.3179	232.0233	220.4965	534.6513	249.3581	168.3029	322.5239	0.938346	0.043533	0.070472	0.5451	Rutin NP-008131	2.014	610.1496	C27H30O	153-18-4	6 FlavonoidC05625	ko01100//	BiosyntheMetabolism		
POS00317	18.87419	7.981249	9.305362	8.152813	12.6743	33.55774	335.807	306.1121	271.7911	470.1813	288.9618	182.049	15.09094	309.1504	4.356554	1.87E-05	0.000211	0.861074	Cyanidin 3-glucogalactoside	2.364	611.153	C27H31O	142562-01-	13 Flavonoid-	-	-	-	-
POS00318	34.13643	38.45629	9.240112	17.05809	25.42369	31.64784	252.8423	229.3923	347.7896	217.1361	295.9582	203.8342	25.99378	257.8255	3.310157	1.35E-06	3.40E-05	0.75639	Glutathio Epigallocatechin	0.86	612.1489	C20H32N	27025-41-8	5 FlavonoidC12136	ko01110//	BiosyntheMetabolism		
POS00319	61.23578	32.38861	36.60869	34.72423	81.90498	49.04297	30.81126	24.23178	46.83434	14.00441	23.90342	16.7204	49.31754	26.08427	-0.91892	0.030641	0.052734	0.213916	Kanokoside D	10.391	624.2551	C27H44O	64703-88-4	12 Prenol lip-	-	-	-	-
POS00320	0.589498	0.28641	0.272166	0.268376	0.260881	0.27817	46.3816	58.87296	34.54469	100.8124	69.34733	92.44574	1	67.06746	0.606754	8.63E-05	0.000543	0.411229	QuercetinNCGC00385380-021	1.913	626.1447	C27H30O	42900-82-3	5 Flavonoid-	-	-	-	-
POS00321	6.817182	3.636357	2.598566	2.321796	5.860211	0.962366	43.62523	28.09715	24.55887	9.152912	40.66983	9.783724	3.699413	25.98129	2.812105	0.004297	0.009825	0.224748	Ginsenoside Rh1	4.088	638.4356	C36H62O	63223-86-9	5 Prenol lip-	-	-	-	-
POS00322	1.375682	0.489998	1.22433	0.873806	0.258824	1.010555	39.24405	11.0455	35.12296	19.79816	13.36233	11.41545	1	21.66474	4.437277	0.002235	0.005941	0.200355	Rhamneti-3-(((2S,3R,4S,5S,6R)-	2.276	640.1598	C28H32O	259234-17-	6 Flavonoid-	-	-	-	-
POS00323	167.0083	107.1296	123.2664	117.4913	139.714	143.0205	136.004	137.6904	118.3112	131.9106	176.5777	149.4598	132.9383	141.659	0.091665	0.48181	0.543283	0.087643	Pittoside.-2-[5-[2-[4-[5-[2-[2-[5-	12.519	768.4732	C41H68O	75303-44-5	9 -	-	-	-	-
POS00324	0.51147	0.359769	0.358201	0.298078	0.255776	0.31296	121.1887	60.31629	34.50587	69.97777	141.0501	76.61033	1	83.94151	6.391312	0.000431	0.001717	0.474646	Cyanidin 3-glucoside 5-caffeoyl	2.429	772.18	C36H36O-		6 -	C16372	ko00942//	BiosyntheMetabolism	
POS00325	200.1007	146.9042	149.8563	153.4018	119.1432	246.243	525.7871	824.1286	566.2722	309.9272	879.688	316.274	169.2749	570.3462	1.75247	0.00261	0.006721	0.970632	Quercetin[Similar to: NP-0081	1.789	772.2009	C33H40O	50867-29-3	6 Flavonoid-	-	-	-	-
POS00326	0.536098	0.383079	0.407005	0.333914	0.272916	0.34352	62.87643	40.30318	38.78703	32.99397	63.44936	46.19924	1	47.43487	5.567876	4.38E-06	7.42E-05	0.399156	Kaempferol 3-sophoroside 7-g	2.576	786.1947	C33H38O	140163-56-	11 -	-	-	-	-
POS00327	0.509155	0.307551	0.344268	0.277543	0.241348	0.295539	71.24865	88.87151	75.71025	94.07227	120.9546	85.2026	1	89.34331	6.481288	2.19E-07	1.02E-05	0.497647	MoracetinNCGC00179992-021	1.738	788.1961	C33H40O	61474-16-6	6 Flavonoid-	-	-	-	-

