

Supplementary Material

Metabolomics reveals the influences of smoke-water and karrikinolide on the biosynthesis of flavonoids and terpenoids in *Salvia miltiorrhiza*

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Table S1. 178 differential metabolites in positive and negative ion modes were identified between SW and the control

ID	Name_des	Molecular Weight	FC	Log2FC	Pvalue	ROC	VIP
Com_3657_pos	6-chloro-2,4-diphenyl-8-(trifluoromethyl)-3H-1,5-benzodiazepine	398.08198	2.988559556	1.579450293	1.53538E-08	1	1.468071923
Com_377_neg	2,4-Dihydroxybenzoic acid	154.02661	0.19043775	-2.392608603	1.47478E-07	1	2.228315486
Com_4724_pos	Genistein 4'-O-glucuronide	446.08276	18.79477856	4.232260013	3.02298E-07	1	3.912769959
Com_4183_neg	Sanguinarine	332.09196	4.462728721	2.157926111	3.4444E-07	1	1.999198606
Com_2462_pos	N-2-Hydroxycyclopentyladenosine	351.15379	11.84692303	3.566440495	6.36474E-07	1	3.336207471
Com_3709_neg	3-O-p-coumaroyl quinic acid O-hexoside	500.15138	3.692640787	1.884652927	1.40652E-06	1	1.747492247
Com_4383_neg	Glutathione reduced form	307.08381	3.308996777	1.726393886	1.61063E-06	1	1.607264726
Com_1857_pos	LysoPC 20:4	543.33019	0.137508467	-2.862407636	3.68971E-06	1	2.676730095
Com_1776_pos	PC (14:1e/4:0)	521.3461	0.103846491	-3.267475624	3.80805E-06	1	3.001323852
Com_17_neg	DL-Malic acid	134.02143	3.756394126	1.90934844	4.91491E-06	1	1.773804526
Com_1665_pos	4-Acetylbutyric acid	130.0631	3.606886489	1.850754021	5.14467E-06	1	1.709668706
Com_5831_neg	Smyrindioloside	424.13792	3.886699998	1.958545755	7.04949E-06	1	1.818915003
Com_605_neg	N1-[4-(2-thienylthio)phenyl]-4-chlorobenzamide	345.00207	0.212023534	-2.237703683	9.23175E-06	1	2.065871581
Com_6160_neg	Dracorhodin	266.09431	2.693187296	1.429314564	9.50384E-06	1	1.333464479
Com_180_neg	Fumaric Acid	116.01092	3.729902026	1.899137736	1.04821E-05	1	1.754297221
Com_5495_neg	Atractylenolide k	248.14129	2.192947025	1.132870961	1.14796E-05	1	1.048032153
Com_4499_neg	N2-Methylguanosine	297.10811	2.230836396	1.157584714	1.16865E-05	1	1.080204134
Com_4715_neg	Trehalose	342.11641	2.178120547	1.123083802	1.18772E-05	1	1.043555834
Com_565_neg	LPC 18:1	581.36985	0.121407163	-3.042074548	1.2762E-05	1	2.854930661
Com_919_pos	Glycerophospho-N-palmitoyl ethanolamine	453.28524	0.307853865	-1.699682414	1.53532E-05	1	1.587967874
Com_318_neg	4-Oxoproline	83.03711	5.835348943	2.544818929	1.96553E-05	1	2.394329774
Com_1556_neg	Aspartic acid	133.03749	3.514456434	1.813301571	2.06923E-05	1	1.699374869
Com_2551_neg	Cinnamic Acid	148.05242	0.210510906	-2.248033118	2.13567E-05	1	2.065343082
Com_844_pos	(3R)-4,4-Dimethyl-2-oxotetrahydro-3-furanyl beta-D-glucopyranoside	292.11554	3.652025857	1.86869698	2.74501E-05	1	1.755680477
Com_1271_pos	Citral	152.1202	0.24967757	-2.001861872	3.12372E-05	1	1.887256993
Com_2759_neg	LysoPC 15:0	481.31752	0.328863072	-1.604441078	3.33034E-05	1	1.488025105
Com_2049_pos	LPE 18:1	479.30118	0.203012168	-2.300361895	3.41495E-05	1	2.143200433
Com_4999_neg	8-Epiloganic acid	376.13716	2.968120982	1.569549898	4.17695E-05	1	1.445445187
Com_1477_neg	L-Serine	105.04255	4.222110874	2.077964465	4.5342E-05	1	1.904259533
Com_3383_pos	Atractylenolide I	230.13057	3.366212367	1.751126196	4.66917E-05	1	1.612262394

Com_4297_neg	Specnuezhenide	686.24013	3.89358632	1.961099611	4.7165E-05	1	1.838691232
Com_356_neg	L-Valine	117.07894	4.328318358	2.113806617	4.78139E-05	1	1.998922794
Com_122_pos	PC (14:0e/2:0)	495.33236	0.315699487	-1.663376179	5.17565E-05	1	1.53179345
Com_2418_neg	B Eupalinolide	462.18934	5.888887367	2.55799508	5.8701E-05	1	2.413022446
Com_2621_neg	Caffeoyl shikimic acid	336.08601	0.410486242	-1.284594225	6.07695E-05	1	1.188477072
Com_244_pos	Acetyl-N-formyl-5-methoxykynur enamine	264.11456	0.450081937	-1.151740428	7.11863E-05	1	1.072004821
Com_99_pos	trans-3-Indoleacrylic acid	187.06336	0.476494051	-1.069469892	7.25489E-05	1	1.003641972
Com_3027_neg	3-(pyrazin-2-ylamino)-2-(2-thienyl carbonyl)acrylonitrile	256.03718	0.108875352	-3.199250715	7.30112E-05	1	3.067011506
Com_4747_pos	L-Citrulline	175.09575	3.148379854	1.654609614	8.75868E-05	1	1.551075794
Com_2242_pos	N,5-Bis(3-nitrophenyl)oxazol-2-a mine	326.06087	13.27659371	3.730813146	0.000104535	1	3.37566409
Com_208_pos	LPE 18:2	477.28535	0.39610197	-1.33605622	0.000108542	1	1.241309288
Com_2146_pos	LPC 15:1	479.30147	0.219239758	-2.18941865	0.000115498	1	2.03678324
Com_4766_neg	Baohuoside	514.18387	2.536597809	1.342894791	0.000118629	1	1.264879635
Com_754_neg	LPI 16:0	572.29677	0.304893122	-1.713624491	0.000134404	1	1.617518636
Com_299_neg	LPC 16:0	555.35403	0.299013572	-1.741717126	0.000139491	1	1.65370094
Com_1908_pos	O-Phospho-L-Serine	185.009	6.962440426	2.799593078	0.000149995	1	2.674006022
Com_2669_pos	Ellagic acid	302.01201	4.390032179	2.134231515	0.000164559	1	2.034329687
Com_1504_neg	Sweroside	358.12652	2.578351637	1.366449033	0.00017232	1	1.28460062
Com_1847_neg	LPC(1-acyl 16:0)	495.33235	0.337989105	-1.564951352	0.000175793	1	1.483370605
Com_368_neg	Uridine 5'-diphosphogalactose	566.05539	2.466226939	1.302305561	0.000186056	1	1.191462021
Com_3351_pos	Usnic acid	344.08916	0.388241533	-1.364973635	0.000206505	1	1.273245768
Com_1470_neg	D-Xylulose 5-phosphate	230.01907	3.512713806	1.812586039	0.000209528	1	1.705032012
Com_6022_neg	Nicotinamide adenine dinucleotide	663.11078	3.412574276	1.770860447	0.000221979	1	1.612742558
Com_915_pos	Monoolein	356.29197	0.330015223	-1.599395519	0.000224155	1	1.510705343
Com_99_neg	L-Glutamic acid	147.05311	3.617501625	1.854993665	0.000228466	1	1.757765277
Com_210_pos	methyl 4-methyl-2-oxo-2H-pyran-6-carbo xylate	168.04227	0.295500783	-1.758766141	0.000241409	1	1.679828323
Com_1428_pos	8-Hydroxyquinoline	145.05286	0.461090609	-1.116877811	0.000247196	1	1.025106471
Com_2178_pos	β -Nicotyrine	158.08446	0.412814284	-1.276435205	0.000253504	1	1.206478066
Com_426_pos	LPE 18:3	475.26981	0.362920127	-1.462276026	0.000253693	1	1.34416495
Com_419_pos	Kojic acid	142.02672	7.066191621	2.820932873	0.000261674	1	2.548385807
Com_814_neg	Ethyl 3,4-Dihydroxybenzoate (Ethyl protocatechuate)	182.05792	0.389928171	-1.358719706	0.000261934	1	1.276788279
Com_473_pos	Isohomovanillic acid	182.05796	0.430086272	-1.217302013	0.000274924	1	1.114032149
Com_2553_pos	1-Naphthol	144.05758	2.238003306	1.162212168	0.000285037	1	1.076134206
Com_825_neg	L-Aspartic acid	133.03747	3.362343035	1.74946692	0.000292962	1	1.654143992
Com_1040_pos	4-(4-methoxyphenyl)-6-pyridin-4- yl-1,3,5-triazin-2(3H)-one	280.09214	0.316033029	-1.661852749	0.000305831	1	1.576251048

Com_6730_pos	3-Hydroxynaphthalene-2_7-Disulphonic acid	303.97102	3.28048991	1.713911284	0.000311395	1	1.600766151
Com_1401_pos	Carvone	150.10448	0.237616749	-2.073291561	0.000320342	1	1.927869674
Com_545_pos	Vanillin	152.04742	4.048656897	2.017443387	0.00032073	1	1.82836824
Com_2472_pos	Bakuchiol	256.18235	0.374050714	-1.418694209	0.000340157	1	1.336848128
Com_3209_pos	Sebacic acid	202.12056	0.283555333	-1.818297805	0.000341661	1	1.738103861
Com_6194_pos	PC (14:1e/3:0)	507.3315	0.209170531	-2.257248486	0.000386017	1	2.146998034
Com_2014_pos	(2R)-2-[(2R,5S)-5-[(2S)-2-hydroxybutyl]oxolan-2-yl]propanoic acid	216.13609	0.270620706	-1.885655865	0.000386028	1	1.785886245
Com_5523_neg	Gomisin E	514.22029	0.194481239	-2.362297106	0.000418962	1	2.255633337
Com_1873_pos	LPC 15:0	481.3166	0.23217465	-2.106717632	0.000443496	1	1.898773958
Com_1131_pos	2-Arachidonoyl glycerol	378.27404	0.308529536	-1.69651949	0.000458221	1	1.62327483
Com_61_pos	9-Oxo-10(E),12(E)-octadecadienoic acid	294.21913	0.166847961	-2.583394042	0.000461721	1	2.339623877
Com_3624_pos	Disinapoyl sucrose	754.22944	2.763325684	1.466405608	0.000471749	1	1.339376252
Com_2974_neg	LPI 18:1	598.31227	0.225535802	-2.148571626	0.000524493	1	2.044232561
Com_824_neg	LPI 18:2	596.29671	0.39461117	-1.341496299	0.000538333	1	1.24206569
Com_5312_neg	Abscisic acid glucose ester (ABA-GE)	426.18926	5.494269598	2.457927704	0.000562828	1	2.174138865
Com_8289_pos	5-methoxy-8,8-dimethyl-2-phenyl-4H,8H-pyrano[2,3-h]chromen-4-one	334.11591	2.659925463	1.411385819	0.000636582	1	1.332365056
Com_1853_neg	Genipin	226.08422	2.409452199	1.26870518	0.000715971	1	1.205523741
Com_1696_neg	Prunindihydrochalcone	436.13713	2.201784856	1.138673505	0.000747528	1	1.080439259
Com_4603_pos	8-(1,2-dihydroxy-3-methylbut-3-en-1-yl)-7-methoxy-2H-chromen-2-one	314.05516	0.392248047	-1.35016183	0.000852602	1	1.253784322
Com_1063_neg	LPG 18:1	510.29599	0.173376456	-2.528020098	0.000866144	1	2.262219715
Com_312_neg	5-oxoproline	129.04259	3.036060105	1.602200352	0.000872899	1	1.536404147
Com_3899_pos	Norverapamil	440.27465	0.189095479	-2.402813223	0.000917416	0.96	2.234257952
Com_2563_pos	L-Saccharopine	276.13171	0.205865515	-2.280225914	0.001014537	1	2.043383892
Com_268_pos	5'-S-Methyl-5'-thioadenosine	297.08916	2.300506114	1.201951291	0.001043123	1	1.085855966
Com_8298_pos	Ganoderic Acid C2(Sh)	518.32443	0.47394669	-1.077203302	0.001043351	1	1.026526727
Com_5089_pos	2-hydroxy-3,6-diphenylcyclohexyl acetate	332.13805	3.264603194	1.706907646	0.001066173	1	1.655843498
Com_2322_pos	Lactucin	276.09945	2.463517663	1.300719815	0.001122835	1	1.251001206
Com_2446_pos	5,7-dihydroxy-6,8-dimethoxy-2-(4-methoxyphenyl)-4H-chromen-4-one	366.07103	0.35287126	-1.502786161	0.001197449	1	1.451221864
Com_482_pos	β-Alanine	89.0477	3.702441661	1.888477003	0.001273444	1	1.837901529
Com_2812_neg	Farnesyl pyrophosphate	382.12638	3.988114186	1.995706717	0.001280156	1	1.951243179
Com_1037_neg	LPC 18:2	519.33232	0.387388004	-1.368148816	0.001444088	0.96	1.258474888

Com_2263_pos	N', N''-DiFeruloylspermidine	497.25164	0.330726075	-1.596291302	0.001556566	0.96	1.49346257
Com_1916_neg	Plantagoside	466.11161	2.966378786	1.568702832	0.001609275	1	1.401385721
Com_335_neg	LPG 16:0	484.27982	0.412169918	-1.27868888	0.001703078	1	1.170538377
Com_43_pos	PC (16:2e/2:0)	519.33236	0.401853072	-1.315259984	0.001707584	1	1.178364491
Com_1095_pos	(1E,4E)-1,5-bis(4-methoxyphenyl) penta-1,4-dien-3-one	294.12513	0.423889013	-1.238241523	0.001783859	1	1.151784579
Com_2305_pos	LPC(1-acyl 16:1)	493.31645	0.106786536	-3.227198332	0.001820768	1	3.368149935
Com_2374_neg	2,6-Diaminooimelic Acid	190.09538	2.656920444	1.40975503	0.001896214	1	1.372240566
Com_5388_neg	Lobetyolin +HCOOH	442.18466	2.351156977	1.233370865	0.002026415	1	1.189006738
Com_5323_neg	Polygalaxanthone n	494.14289	2.09757046	1.068719273	0.002042027	1	1.03029791
Com_6242_neg	Shanzhiside	392.12889	0.193009457	-2.373256558	0.002087236	1	2.096173934
Com_763_pos	Methyl dihydrojasmonate	226.15674	0.372589438	-1.424341318	0.002151676	0.96	1.39842883
Com_10068_pos	Trifolirhizin	463.14668	3.630311608	1.860093387	0.002153619	1	1.64540684
Com_5828_pos	Juglalin	440.07173	2.142893716	1.099560296	0.002169522	1	1.02803155
Com_5430_pos	PC (16:2e/4:0)	547.36339	0.373348381	-1.421405621	0.002505125	1	1.268138722
Com_992_pos	Asparagine	132.0535	4.474868691	2.161845349	0.002512255	1	2.146891198
Com_2919_pos	Suberic acid	174.08935	2.300718978	1.202084776	0.002695941	1	1.093987499
Com_3167_neg	2-chloro-6-[(2-oxoazepan-3-yl)amino]benzotrile	263.07935	2.853634388	1.512800506	0.002785812	1	1.355217559
Com_875_pos	Dihydrojasmonone	166.13585	0.358003888	-1.48195284	0.002854973	0.96	1.455083017
Com_1089_pos	Thymine	126.04291	5.292446524	2.403934787	0.002877943	1	2.092111495
Com_868_pos	2-methyl-2,3,4,5-tetrahydro-1,5-benzoxazepin-4-one	159.06852	0.399966444	-1.322049127	0.002925087	0.96	1.19416051
Com_5293_pos	C-pentosyl-apigenin O-p-coumaroylhexoside	710.18116	2.39366526	1.259221414	0.003089268	1	1.236122718
Com_4518_pos	1-(7-methoxy-2-oxo-2H-chromen-8-yl)-3-methyl-2-oxobutyl acetate	318.1101	2.782727008	1.476499384	0.003233926	0.96	1.453223454
Com_3280_neg	Pseudolaric acid B +NH3	432.17902	2.759656177	1.464488534	0.003314536	1	1.437414806
Com_502_neg	5,5-Dimethylhydantoin	128.05856	8.090481087	3.016225493	0.003369302	1	3.057680364
Com_6364_pos	Agarotretol	318.11092	0.386702343	-1.370704588	0.00338286	0.96	1.347319107
Com_4263_neg	Oxaloacetate	132.00571	4.39365559	2.135421784	0.003396396	1	1.84105576
Com_462_neg	2-Aminoisobutyric Acid	103.06328	2.332494496	1.221873677	0.003480342	1	1.08750323
Com_389_pos	Kumatakenin	314.07868	0.158192526	-2.660246657	0.003587498	1	2.299633814
Com_2311_pos	Tricin 5-O-hexoside derivative	534.09966	0.46283067	-1.111443625	0.003849466	1	1.040367666
Com_179_pos	Tyramine	137.08411	0.261315387	-1.93613602	0.00389672	1	1.674100506
Com_554_neg	L-Histidine	155.06952	6.150847713	2.620785257	0.003980384	1	2.317432461
Com_1551_pos	Dodecanedioic Acid	230.15151	2.543123978	1.346601796	0.003993947	1	1.219119728
Com_67_neg	9-HpOTrE	310.21441	0.352306985	-1.505095015	0.004020415	0.96	1.458396703
Com_4375_neg	Thymidine	242.08914	0.446796873	-1.162309006	0.004263064	1	1.139121333
Com_2041_pos	Indole	117.05788	0.3954745	-1.33834342	0.0042794	0.96	1.20554135
Com_2067_neg	Sinensetin	372.12092	2.103901583	1.073067219	0.004482164	1	1.031374416
Com_1424_neg	3-Phosphoglyceric acid	185.99297	4.384723362	2.132485824	0.004617086	1	2.133037227

Com_6055_neg	Flavin adenine dinucleotide (FAD)	785.15701	2.771463942	1.470648238	0.004771517	1	1.385334259
Com_3454_pos	Methyl oleate	296.27094	0.410496432	-1.284558412	0.005075816	1	1.126470464
Com_9339_pos	Yamogenin	414.31273	2.439107352	1.286353257	0.005305292	1	1.267858732
Com_182_neg	D-(+)-Malic acid	134.02143	2.151754068	1.105513196	0.005459822	1	1.098094934
Com_1990_pos	gamma-Glutamylglutamine	275.11133	2.38733984	1.25540395	0.006465729	1	1.24738958
Com_191_neg	(+/-)12(13)-DiHOME	296.235	0.297676961	-1.748180529	0.006641898	0.96	1.526282932
Com_2949_pos	Tricin 4'-O-(β-guaiacylglyceryl) ether 5-O-hexoside	688.1993	2.273399801	1.18485142	0.006833486	0.96	1.20187882
Com_4055_pos	2-(2-amino-3-methylbutanamido)-3-phenylpropanoic acid	264.14706	0.242741145	-2.042509424	0.007385788	1	2.219124819
Com_4155_neg	Puerarin	416.11079	2.43760798	1.285466128	0.008184485	0.96	1.189788299
Com_328_pos	(3beta,9xi)-3-(beta-D-Glucopyranosyloxy)-14-hydroxycard-20(22)-enolide	536.29624	2.261239086	1.17711354	0.008230876	1	1.033811376
Com_3707_pos	N-(2-Hydroxyethyl)iminodiacetic acid	177.06371	0.440043945	-1.184280488	0.008662148	0.96	1.040742844
Com_862_neg	α-Phenylacetoacetonitrile	159.0684	0.383825076	-1.381479125	0.009143778	0.96	1.21198882
Com_50_pos	DL-Glutamine	146.06915	3.586177045	1.842446714	0.009339948	1	2.104021358
Com_7788_pos	Oleuropein	540.18403	4.425916266	2.145976157	0.010692735	1	1.765520657
Com_33_pos	D-(-)-Glutamine	146.0692	6.1414792	2.618586176	0.011038604	1	2.82422243
Com_2734_pos	2-[(carboxymethyl)(methylamino)-5-methoxybenzoic acid	239.07927	2.276144745	1.186592305	0.01128069	0.92	1.149878201
Com_1006_pos	2-{1-[2-(1-benzothiophen-5-ylamino)-2-oxoethyl]cyclohexyl}acetic acid	331.1264	3.533784274	1.821213971	0.011813945	1	1.906252616
Com_3650_pos	Isorhamnetin	316.05788	0.395256674	-1.339138272	0.011817068	0.96	1.31186559
Com_35_pos	L-Pyroglutamic acid	129.04253	5.93133779	2.568357536	0.012245492	1	2.785250245
Com_508_pos	Sedanolid	194.13073	0.460889865	-1.117506053	0.012276077	0.92	1.103500565
Com_124_pos	LPC 18:3	517.31689	0.416924533	-1.262141829	0.013210163	0.96	1.098653542
Com_1212_neg	Gallic acid O-Hexoside	332.07449	0.433636665	-1.205441351	0.014026662	1	1.213086588
Com_4601_pos	10-Gingerol	350.24454	0.196632671	-2.346425044	0.01433581	0.92	2.294990232
Com_1902_neg	Demethoxycurcumin	338.11566	2.773282429	1.471594547	0.01647894	0.96	1.398753515
Com_8363_pos	N-Sinapoylputrescine	294.15743	0.336427402	-1.571632878	0.019718097	0.96	1.854100987
Com_534_pos	1-Acetylimidazole	110.04802	4.154688288	2.054740241	0.02034144	1	2.27960053
Com_1790_pos	Vanillactic acid	212.06757	2.665537327	1.414426385	0.021215745	1	1.496026063
Com_141_pos	Maltol	126.03172	0.44378975	-1.172051748	0.021226913	0.88	1.013769163
Com_3173_pos	3-(dimethylamino)-1-[4-(phenylsulfonyl)phenyl]prop-2-en-1-one	315.09271	0.322422632	-1.632975079	0.022436174	0.92	1.585200925
Com_6394_pos	Phenobarbital	232.08464	2.674117128	1.419062658	0.022727567	1	1.165245125
Com_631_pos	Arecoline	155.09465	0.307559674	-1.701061739	0.023781906	1	1.362568798
Com_823_pos	Coumarin	146.03681	0.454745946	-1.136867317	0.024381939	0.92	1.140578223
Com_418_neg	L-Alanine	89.04769	5.114325437	2.354543966	0.024731349	0.84	1.881590175

Com_213_pos	D-Pyrrolidine-2-Carboxylic Acid	115.06335	3.452977258	1.787840832	0.028991203	1	1.969586631
Com_1971_neg	Gingerglycolipid B +HCOOH	678.38392	0.465687124	-1.102567101	0.029370483	0.88	1.19849477
Com_1170_neg	N-Acetylthreonine	161.06873	2.391307382	1.257799588	0.029704413	1	1.387077128
Com_6738_pos	Ethyl Gallate	198.05295	0.364662711	-1.455365411	0.032310224	0.8	2.271613936
Com_4590_pos	8-O-Methylreyusin	298.08354	0.266858304	-1.905854189	0.03283296	1	1.434232708
Com_6914_neg	Quercetin 3-alpha-L-arabinofuranoside (Avicularin)	434.08696	2.092835422	1.065458864	0.033056723	0.96	1.138991664
Com_392_pos	N-Acetyl-Dl-serine	147.05318	2.04233399	1.030218814	0.033344057	0.92	1.021116161
Com_8239_pos	(6E)-7-(2H-1,3-benzodioxol-5-yl)- 1-(piperidin-1-yl)hept-6-en-1-one	337.15801	0.289477563	-1.788476564	0.034548672	0.96	1.461941206
Com_159_pos	Nicotinamide-N-oxide	138.04257	0.021176151	-5.561415822	0.036958105	0.96	3.4016087
Com_2408_neg	6-Deoxycatalpol +HCOOH	392.13211	2.251193967	1.170690367	0.03958428	0.92	1.323693564
Com_971_neg	Ixoside	388.10138	0.395429609	-1.338507194	0.043645953	1	1.50158829
Com_3534_pos	Guanine	151.04943	0.319102105	-1.647909969	0.04734189	0.8	1.390430641

Table S2. 199 differential metabolites in positive and negative ion modes were identified between KAR₁ and the control

ID	Name_des	Molecular Weight	FC	Log2FC	Pvalue	ROC	VIP
Com_3027_neg	3-(pyrazin-2-ylamino)-2-(2-thienyl carbonyl)acrylonitrile	256.03718	0.071305788	-3.809837009	5.02E-09	1	3.375377921
Com_3657_pos	6-chloro-2,4-diphenyl-8-(trifluoro methyl)-3H-1,5-benzodiazepine	398.08198	3.785195512	1.92036782	1.05E-08	1	1.697699855
Com_418_neg	L-Alanine	89.04769	5.237258841	2.388811909	8.66E-08	1	2.117491373
Com_1665_pos	4-Acetylbutyric acid	130.0631	3.841894879	1.941818045	1.24E-07	1	1.715112023
Com_377_neg	2,4-Dihydroxybenzoic acid	154.02661	0.200974031	-2.314919	1.27E-07	1	2.055691793
Com_1477_neg	L-Serine	105.04255	2.920447705	1.546189551	1.69E-07	1	1.366431599
Com_7788_pos	Oleuropein	540.18403	3.173642242	1.666139505	2.23E-07	1	1.477469248
Com_2462_pos	N-2-Hydroxycyclopentyladenosine	351.15379	16.2752395	4.024606868	8.54E-07	1	3.588884688
Com_4724_pos	Genistein 4'-O-glucuronide	446.08276	14.13376266	3.821073682	1.17E-06	1	3.364156168
Com_844_pos	(3R)-4,4-Dimethyl-2-oxotetrahydro-3-furanyl beta-D-glucopyranoside	292.11554	6.492760182	2.698831923	1.24E-06	1	2.398462849
Com_4375_neg	Thymidine	242.08914	0.287183724	-1.799954106	1.27E-06	1	1.588651652
Com_4183_neg	Sanguinarine	332.09196	4.399143733	2.137222739	1.36E-06	1	1.882445828
Com_4499_neg	N2-Methylguanosine	297.10811	2.581139637	1.368008192	3.45E-06	1	1.212706865
Com_605_neg	N1-[4-(2-thienylthio)phenyl]-4-chlorobenzamide	345.00207	0.123230884	-3.020564224	4.06E-06	1	2.644472882
Com_2242_pos	N,5-Bis(3-nitrophenyl)oxazol-2-amine	326.06087	18.09011048	4.177129314	6.47E-06	1	3.761090466
Com_4055_pos	2-(2-amino-3-methylbutanamido)-3-phenylpropanoic acid	264.14706	0.170253496	-2.554243676	7.31E-06	1	2.28572574
Com_2551_neg	Cinnamic Acid	148.05242	0.184869856	-2.435418086	1.00E-05	1	2.141186406
Com_419_pos	Kojic acid	142.02672	9.848742375	3.299939513	1.12E-05	1	2.884637624
Com_1271_pos	Citral	152.1202	0.249801263	-2.001147326	1.19E-05	1	1.788555546
Com_17_neg	DL-Malic acid	134.02143	3.308173548	1.726034921	1.27E-05	1	1.523544794
Com_180_neg	Fumaric Acid	116.01092	3.27374671	1.710942705	1.35E-05	1	1.505164843
Com_1089_pos	Thymine	126.04291	7.60055272	2.926104337	1.53E-05	1	2.558363687
Com_1776_pos	PC (14:1e/4:0)	521.3461	0.157852773	-2.663348493	1.86E-05	1	2.368760182
Com_2014_pos	(2R)-2-[(2R,5S)-5-[(2S)-2-hydroxybutyl]oxolan-2-yl]propanoic acid	216.13609	0.195073697	-2.357908833	2.22E-05	1	2.066830219
Com_318_neg	4-Oxoproline	83.03711	4.047345567	2.016976033	2.42E-05	1	1.7945988
Com_1556_neg	Aspartic acid	133.03749	3.130060415	1.646190504	2.42E-05	1	1.448515949
Com_2669_pos	Ellagic acid	302.01201	5.438160097	2.443118624	2.42E-05	1	2.17923257
Com_814_neg	Ethyl 3,4-Dihydroxybenzoate (Ethyl protocatechuate)	182.05792	0.368993461	-1.438332845	2.77E-05	1	1.261260676
Com_2418_neg	B Eupalinolide	462.18934	5.047029674	2.335434569	2.98E-05	1	2.094722278

Com_1857_pos	LysoPC 20:4	543.33019	0.132522989	-2.915685443	3.00E-05	1	2.631393256
Com_5831_neg	Smyrindioloside	424.13792	3.398557613	1.76492258	3.40E-05	1	1.553482241
Com_3209_pos	Sebacic acid	202.12056	0.24513776	-2.028335367	5.48E-05	1	1.813099443
Com_6364_pos	Agarotetrol	318.11092	0.267323133	-1.903343408	5.88E-05	1	1.664256726
Com_328_pos	(3beta,9xi)-3-(beta-D-Glucopyranosyloxy)-14-hydroxycard-20(22)-enolide	536.29624	2.545427865	1.347908182	7.41E-05	1	1.198300998
Com_1040_pos	4-(4-methoxyphenyl)-6-pyridin-4-yl-1,3,5-triazin-2(3H)-one	280.09214	0.409794135	-1.28702876	8.50E-05	1	1.148357028
Com_1908_pos	O-Phospho-L-Serine	185.009	6.983687547	2.803989014	8.62E-05	1	2.543248381
Com_4383_neg	Glutathione reduced form	307.08381	4.362486	2.125150501	9.18E-05	1	1.844157907
Com_694_neg	Lactobionic acid	358.11118	0.386932138	-1.369847535	9.26E-05	1	1.19710373
Com_6160_neg	Dracorhodin	266.09431	2.797510852	1.484143728	9.87E-05	1	1.299036159
Com_1401_pos	Carvone	150.10448	0.181777358	-2.459755582	0.000101065	1	2.145379719
Com_2974_neg	LPI 18:1	598.31227	0.249026632	-2.005628057	0.000130975	1	1.782673488
Com_268_pos	5'-S-Methyl-5'-thioadenosine	297.08916	2.744598561	1.456595149	0.000135821	1	1.27800531
Com_7_neg	Gluconic acid	196.05814	0.438411958	-1.189640946	0.00014598	1	1.065600257
Com_971_neg	Ixoside	388.10138	0.364569232	-1.455735287	0.00015004	1	1.295435212
Com_473_pos	Isohomovanillic acid	182.05796	0.410006308	-1.286281989	0.00016693	1	1.127383053
Com_545_pos	Vanillin	152.04742	3.808009716	1.92903716	0.000225166	1	1.667578649
Com_99_neg	L-Glutamic acid	147.05311	3.052325977	1.609909045	0.000233314	1	1.453717548
Com_661_pos	(2S)-2-(2-hydroxypropan-2-yl)-2H,3H,7H-furo[3,2-g]chromen-7-one	246.08906	2.522956134	1.335115123	0.000241751	1	1.161420177
Com_5523_neg	Gomisin E	514.22029	0.147731202	-2.758953526	0.000251732	1	2.523450423
Com_1063_neg	LPG 18:1	510.29599	0.160002153	-2.643836779	0.000252743	1	2.292762104
Com_2621_neg	Caffeoyl shikimic acid	336.08601	0.325616062	-1.618756228	0.000258685	1	1.46988444
Com_417_pos	Chlorogenic acid methyl ester	368.11034	2.381681527	1.251980512	0.000260645	1	1.09026081
Com_875_pos	Dihydrojasnone	166.13585	0.333380817	-1.584757003	0.000275066	1	1.397308945
Com_312_neg	5-oxoproline	129.04259	2.964942921	1.568004331	0.000312554	1	1.412351219
Com_3624_pos	Disinapoyl sucrose	754.22944	2.882301862	1.527221436	0.000323752	1	1.332896513
Com_2305_pos	LPC(1-acyl 16:1)	493.31645	0.416937435	-1.262097184	0.00033239	1	1.100204124
Com_1212_neg	Gallic acid O-Hexoside	332.07449	0.446952662	-1.161806054	0.00034036	1	1.027730515
Com_2812_neg	Farnesyl pyrophosphate	382.12638	5.342669037	2.417560649	0.000348408	1	2.213747845
Com_754_neg	LPI 16:0	572.29677	0.283190933	-1.820153018	0.000354029	1	1.6585216
Com_3383_pos	Atractylenolide I	230.13057	3.088151353	1.626743462	0.000356844	1	1.410125055
Com_2471_pos	Fenvalerate	451.15886	0.21267018	-2.233310339	0.000382389	1	1.930896611
Com_6384_pos	Trehalose 6-phosphate	422.08177	2.619853466	1.389486121	0.000392278	1	1.202353222
Com_825_neg	L-Valine	133.03747	2.703031113	1.434578118	0.000394434	1	1.262264
Com_3167_neg	2-chloro-6-[(2-oxoazepan-3-yl)amino]benzotrile	263.07935	2.726896836	1.447260121	0.000399236	1	1.291093222
Com_2919_pos	Suberic acid	174.08935	2.208097446	1.142803841	0.000404821	1	1.04321773
Com_2146_pos	LPC 15:1	479.30147	0.308500544	-1.696655061	0.000406154	1	1.465560113

Com_3510_pos	Biotin	244.0881	2.798072727	1.484433461	0.000451989	1	1.297068979
Com_1696_neg	Prunindihydrochalcone	436.13713	2.365276313	1.24200873	0.000453591	1	1.106073138
Com_3650_pos	Isorhamnetin	316.05788	0.242463431	-2.044160922	0.00046442	1	1.807198443
Com_61_pos	9-Oxo-10(E),12(E)-octadecadienoic acid	294.21913	0.175834964	-2.507706125	0.000482503	1	2.176920384
Com_8457_pos	Bisdemethoxycurcumin	308.10484	2.808935689	1.490023594	0.000513095	1	1.291013083
Com_1594_pos	Pinoresinol-glucoside	520.19415	2.511239808	1.328399804	0.00051876	1	1.176438909
Com_6194_pos	PC (14:1e/3:0)	507.3315	0.247248812	-2.015964503	0.000550521	1	1.808071127
Com_6730_pos	3-Hydroxynaphthalene-2_7-Disulphonic acid	303.97102	2.815083905	1.493177923	0.000565268	1	1.360488228
Com_2759_neg	LysoPC 15:0	481.31752	0.381013711	-1.39208518	0.000594493	1	1.257433317
Com_335_neg	LPG 16:0	484.27982	0.342396293	-1.546261013	0.000596104	0.96	1.367573692
Com_6022_neg	Nicotinamide adenine dinucleotide	663.11078	3.060430026	1.613734383	0.000596172	1	1.389280666
Com_5391_neg	Ciso-Cistanoside C	638.22192	2.498826097	1.321250502	0.000602278	1	1.174065038
Com_210_pos	methyl 4-methyl-2-oxo-2H-pyran-6-carboxylate	168.04227	0.227424357	-2.13654132	0.000622741	1	1.981203578
Com_4155_neg	Puerarin	416.11079	3.419448984	1.773763866	0.000662866	1	1.597541609
Com_67_neg	9-HpOTrE	310.21441	0.261531161	-1.934945242	0.000693353	1	1.741809505
Com_3454_pos	Methyl oleate	296.27094	0.281497018	-1.828808453	0.000704874	1	1.560349308
Com_1853_neg	Genipin	226.08422	2.803740206	1.487352676	0.000717716	1	1.311168413
Com_4747_pos	L-Citrulline	175.09575	2.344078212	1.229020707	0.000773592	1	1.094398679
Com_4766_neg	Baohuoside	514.18387	2.312293145	1.20932431	0.00079758	1	1.060205217
Com_901_pos	8,8-dimethyl-2H,8H-pyrano[3,2-g]chromen-2-one	228.0786	2.381745156	1.252019055	0.000800644	1	1.080929275
Com_2988_pos	(4-methoxyphenyl)(4-nitrophenyl) methanone	257.06642	2.540312899	1.345006209	0.000818293	1	1.184401111
Com_1504_neg	Sweroside	358.12652	2.438223378	1.285830305	0.00083015	1	1.131316734
Com_6242_neg	Shanzhiside	392.12889	0.201970967	-2.307780174	0.000835678	1	1.986861558
Com_2553_pos	1-Naphthol	144.05758	2.22347695	1.152817449	0.000888388	1	1.002705338
Com_4297_neg	Specnuezhenide	686.24013	2.678604303	1.421481474	0.000922834	1	1.292964588
Com_5089_pos	2-hydroxy-3,6-diphenylcyclohexyl acetate	332.13805	3.577367313	1.838898258	0.00100316	1	1.699307384
Com_1847_neg	LPC(1-acyl 16:0)	495.33235	0.265494424	-1.913246534	0.001010366	1	1.776822538
Com_5312_neg	Abscisic acid glucose ester (ABA-GE)	426.18926	5.21290098	2.382086456	0.001041645	1	2.006892895
Com_2049_pos	LPE 18:1	479.30118	0.286290264	-1.804449485	0.001046761	1	1.646692409
Com_2311_pos	Tricin 5-O-hexoside derivative	534.09966	0.401341782	-1.317096738	0.001086721	1	1.166075528
Com_1891_pos	4,5-Dicaffeoylquinic acid	516.12513	2.175251921	1.121182492	0.001187833	1	1.01296613
Com_389_pos	Kumatakenin	314.07868	0.098512438	-3.343550297	0.001269448	1	2.736827421
Com_2374_neg	2,6-Diaminooimelic Acid	190.09538	2.770612656	1.47020503	0.001292777	1	1.354596725
Com_1592_pos	α -Lapachone	264.0784	2.262678096	1.178031351	0.001444766	1	1.034030552

Com_179_pos	Tyramine	137.08411	0.246878779	-2.018125266	0.001463845	1	1.702473275
Com_2242_neg	1,5-Anhydro-2-O-(6-O-benzoyl- α -L-galactopyranosyl)-D-glucitol	430.14774	2.187812134	1.12948886	0.001523428	1	1.035139553
Com_4086_neg	1-(2,4-dihydroxyphenyl)-2-(3,5-dimethoxyphenyl)propan-1-one	302.11729	0.435648523	-1.198763444	0.00160115	1	1.095566814
Com_1407_pos	Neocnidilide	194.13077	0.443833259	-1.171910312	0.001636393	0.96	1.040594014
Com_9513_pos	di-C,C-pentosyl-apigenin	534.13933	3.312386712	1.727871113	0.001753865	1	1.468216508
Com_824_neg	LPI 18:2	596.29671	0.438399711	-1.189681247	0.001784364	0.96	1.064178838
Com_3899_pos	Norverapamil	440.27465	0.21242164	-2.23499735	0.001830684	0.96	2.01678066
Com_7410_pos	Isomucronulatol-7-O-glucoside	464.16612	2.797811361	1.484298694	0.00193635	1	1.260769273
Com_2446_pos	5,7-dihydroxy-6,8-dimethoxy-2-(4-methoxyphenyl)-4H-chromen-4-one	366.07103	0.464380663	-1.106620195	0.002026739	1	1.008625297
Com_4883_pos	Engeletin	434.12003	2.202725468	1.139289699	0.002070535	1	1.031442855
Com_4992_neg	Liguiritigenin-7-O-D-Apiosyl-4'-O-D-Glucoside	550.17057	3.120106308	1.641595185	0.002126692	1	1.421357339
Com_299_neg	LPC 16:0	555.35403	0.372182086	-1.425919477	0.00241045	1	1.327876811
Com_3707_pos	N-(2-Hydroxyethyl)iminodiacetic acid	177.06371	0.351615392	-1.507929871	0.002484015	1	1.280552704
Com_1873_pos	LPC 15:0	481.3166	0.37006538	-1.434147917	0.002518512	0.96	1.270704418
Com_1470_neg	D-Xylulose 5-phosphate	230.01907	2.982801088	1.576667773	0.002535857	1	1.36634091
Com_2041_pos	Indole	117.05788	0.355768293	-1.490990157	0.002600649	1	1.271420135
Com_2563_pos	L-Saccharopine	276.13171	0.245319553	-2.027265866	0.002712041	1	1.674331792
Com_1037_neg	LPC 18:2	519.33232	0.419552907	-1.253075343	0.002751867	0.96	1.105591704
Com_868_pos	2-methyl-2,3,4,5-tetrahydro-1,5-benzoxazepin-4-one	159.06852	0.388799508	-1.362901703	0.00276624	0.96	1.194857126
Com_8363_pos	N-Sinapoylputrescine	294.15743	0.284891217	-1.811516952	0.002825685	1	1.731819922
Com_2263_pos	N', N''-DiFeruloylspermidine	497.25164	0.358261021	-1.48091701	0.0028502	1	1.319461492
Com_1011_neg	D-myo-Inositol 1,4-bisphosphate	339.99605	0.429084436	-1.220666522	0.002871439	1	1.128967035
Com_2949_pos	Tricin 4'-O-(β -guaiacylglyceryl) ether 5-O-hexoside	688.1993	2.626567017	1.393178396	0.003047879	0.96	1.31203268
Com_5293_pos	C-pentosyl-apigenin O-p-coumaroylhexoside	710.18116	2.562111037	1.357333001	0.00328246	0.96	1.225964578
Com_5828_pos	Juglalin	440.07173	2.736602848	1.452386077	0.003430462	0.96	1.248649944
Com_3399_pos	Sulfamethoxazole	253.05189	4.634422743	2.21238965	0.003560802	1	2.158077545
Com_3280_neg	Pseudolaric acid B +NH3	432.17902	3.201256443	1.678638251	0.003679505	1	1.474013687
Com_191_neg	(+/-)12(13)-DiHOME	296.235	0.280549741	-1.833671516	0.003820806	0.96	1.579438053
Com_4601_pos	10-Gingerol	350.24454	0.085491362	-3.548077534	0.003941485	1	2.880351533
Com_5388_neg	Lobetyolin +HCOOH	442.18466	2.126856436	1.088722654	0.003952172	1	1.010934719
Com_9555_pos	Linarin	592.17882	2.502485318	1.323361605	0.004275107	1	1.199070102
Com_122_pos	PC (14:0e/2:0)	495.33236	0.444025966	-1.171284048	0.004281429	1	1.081619825
Com_10068_pos	Trifolirhizin	463.14668	3.697418585	1.88651838	0.004416353	1	1.550549514

Com_565_neg	LPC 18:1	581.36985	0.143539578	-2.800479508	0.004680166	1	2.729717361
Com_2061_pos	Methionine sulfoxide	165.04601	0.418593414	-1.256378482	0.004911625	1	1.058671057
Com_763_pos	Methyl dihydrojasmonate	226.15674	0.415293761	-1.267795895	0.004997352	0.96	1.205804324
Com_2370_pos	6,7-Dimethoxycoumarin	206.05788	2.230192366	1.157168156	0.005245254	0.92	1.07026859
Com_4518_pos	1-(7-methoxy-2-oxo-2H-chromen-8-yl)-3-methyl-2-oxobutyl acetate	318.1101	2.486829552	1.314307628	0.005445555	0.96	1.24637734
Com_1925_neg	FAHFA (18:1/22:3)	614.53122	0.433883676	-1.204619786	0.005500058	0.96	1.054735358
Com_915_pos	Monoolein	356.29197	0.401336408	-1.317116057	0.005758575	0.96	1.266461514
Com_482_pos	β -Alanine	89.0477	2.771978783	1.470916215	0.005839387	1	1.424374283
Com_508_pos	Sedanolid	194.13073	0.440067687	-1.184202651	0.005883345	0.96	1.072319404
Com_4234_neg	di-C,C-pentosyl-luteolin	550.13386	2.362288682	1.240185279	0.006095783	1	1.047573614
Com_4002_pos	Rosuvastatin	481.16935	2.327311641	1.218664409	0.006169894	1	1.124420241
Com_6394_pos	Phenobarbital	232.08464	2.328346907	1.219306025	0.006404386	1	1.019862814
Com_502_neg	5,5-Dimethylhydantoin	128.05856	5.622795218	2.491287505	0.006895249	0.96	2.293786785
Com_3463_pos	N-Feruloylspermidine	321.20488	10.62295793	3.409113631	0.007086113	0.92	3.161782204
Com_4263_neg	Oxaloacetate	132.00571	2.494462531	1.318728999	0.00711126	1	1.079600602
Com_141_pos	Maltol	126.03172	0.338314052	-1.563564992	0.007691533	1	1.29904335
Com_1990_pos	gamma-Glutamylglutamine	275.11133	2.273908622	1.18517428	0.007753733	1	1.120155156
Com_5430_pos	PC (16:2e/4:0)	547.36339	0.43802941	-1.190900357	0.008002649	0.92	1.048308491
Com_1996_neg	Tricin 5-O-hexoside	492.12692	3.806412072	1.928431752	0.008009739	0.96	1.761249235
Com_1391_neg	7-Methylguanosine	299.12155	2.29293498	1.197195445	0.008518449	1	1.002850396
Com_5495_neg	Atractylenolide III	248.14129	2.659466645	1.411136943	0.008821268	1	1.161020937
Com_6696_neg	Hesperetin 7-rutinoside (Hesperidin)	610.19063	2.574720649	1.364415912	0.008952496	0.96	1.270131837
Com_361_neg	2-Ketoadipic acid	160.03714	0.395140214	-1.339563415	0.009020081	0.96	1.124831572
Com_8239_pos	(6E)-7-(2H-1,3-benzodioxol-5-yl)-1-(piperidin-1-yl)hept-6-en-1-one	337.15801	0.193275412	-2.371269982	0.009343169	0.96	2.140819372
Com_2408_neg	6-Deoxycatalpol +HCOOH	392.13211	3.517675959	1.814622591	0.009902801	0.96	1.795930402
Com_1131_pos	2-Arachidonoyl glycerol	378.27404	0.39770196	-1.330240423	0.009955715	0.96	1.320078667
Com_4460_neg	Kaempferol 3-A-L-Arabinopyranoside	418.09032	0.273914786	-1.868200951	0.01054707	0.92	1.5543531
Com_3173_pos	3-(dimethylamino)-1-[4-(phenylsulfonyl)phenyl]prop-2-en-1-one	315.09271	0.280137165	-1.835794703	0.010617219	0.96	1.553331329
Com_478_pos	Prolylleucine	228.14713	2.48719312	1.314518531	0.011313326	1	1.14445599
Com_1416_pos	Sinapinic acid	206.05788	2.777539033	1.473807186	0.01151487	0.92	1.410129342
Com_534_pos	1-Acetylimidazole	110.04802	5.482166299	2.454746092	0.011623983	1	2.440260082
Com_554_neg	L-Histidine	155.06952	4.97104721	2.313549805	0.011646809	0.96	1.947769329
Com_33_pos	D-(-)-Glutamine	146.0692	5.350081531	2.419560877	0.013795447	1	2.503162652
Com_4590_pos	8-O-Methylreyusin	298.08354	0.212003544	-2.23783971	0.014114359	1	1.69150204
Com_264_neg	LPG 18:2	508.2801	0.424630489	-1.235720133	0.014866958	0.92	1.026009334
Com_698_neg	Pipecolic acid	129.07892	3.075536354	1.620838029	0.014897581	0.92	1.45437304
Com_1424_neg	3-Phosphoglyceric acid	185.99297	3.00963959	1.589590732	0.01506265	1	1.576002548

Com_1006_pos	2-{1-[2-(1-benzothiophen-5-ylamino)-2-oxoethyl]cyclohexyl}acetic acid	331.1264	3.175410174	1.66694296	0.015486925	1	1.674399829
Com_6055_neg	Flavin adenine dinucleotide (FAD)	785.15701	2.496307645	1.319795743	0.015946406	0.92	1.159302235
Com_35_pos	L-Pyrogutamic acid	129.04253	5.053902742	2.337397901	0.015973595	1	2.438216218
Com_1729_neg	Chlortetracycline	239.05567	3.748050278	1.906140306	0.015981275	0.92	1.654156075
Com_1848_neg	Selgin 5-O-hexoside	478.11145	4.163161437	2.057679504	0.016236536	0.92	1.850242952
Com_50_pos	DL-Glutamine	146.06915	2.866676699	1.519379208	0.016833902	0.88	1.724011173
Com_4273_pos	Naringin dihydrochalcone	582.19115	2.577501053	1.365973017	0.017157307	1	1.077300572
Com_1315_pos	Thiamine	264.10421	3.383531969	1.75853002	0.017319139	1	1.793202438
Com_3172_pos	2-Isopropylmalate	176.06846	0.310355796	-1.688005004	0.017748073	1	1.283769229
Com_3238_pos	Obscurolid A1	273.09988	0.429837411	-1.218137042	0.020451807	0.92	1.054280533
Com_631_pos	Arecoline	155.09465	0.315422008	-1.66464477	0.021145533	1	1.300986667
Com_1551_pos	Dodecanedioic Acid	230.15151	3.004043459	1.586905684	0.022431137	0.96	1.254585965
Com_6914_neg	Quercetin 3-alpha-L-arabinofuranoside (Avicularin)	434.08696	2.314294452	1.210572433	0.022849537	1	1.196988281
Com_1263_neg	2-[2-(4-benzhydrylpiperazino)-2-oxoethoxy]acetic acid	368.16828	2.751779744	1.460365	0.024399644	1	1.499506811
Com_225_pos	3-Methyl-2-Oxobutanoic Acid	116.04732	0.139300525	-2.843727398	0.024421736	1	1.913957604
Com_3534_pos	Guanine	151.04943	0.229803703	-2.121526049	0.02468766	0.8	1.639456299
Com_1790_pos	Vanillic acid	212.06757	2.501476758	1.322780048	0.025400686	1	1.336966114
Com_5102_neg	Trifolirhizin +HCOOH	446.12147	2.214931197	1.147261885	0.025592431	0.92	1.064566028
Com_992_pos	L-Citrulline	132.0535	3.095321846	1.630089426	0.028109157	0.92	1.39957841
Com_2275_pos	Shikimic acid	174.05296	0.405613433	-1.301822662	0.028412719	0.84	1.036471139
Com_2869_pos	Laricitrin	332.05287	0.352673136	-1.503596407	0.028857995	0.92	1.661288968
Com_813_pos	Glucose 1-phosphate	260.02937	0.047955069	-4.382172857	0.031494744	1	2.562556297
Com_4098_pos	Wedelolactone	314.04238	0.43396312	-1.204355655	0.035197264	0.84	1.336738519
Com_213_pos	D-Pyrrolidine-2-Carboxylic Acid	115.06335	3.107257454	1.635641782	0.036809353	1	1.762080896
Com_1170_neg	N-Acetylthreonine	161.06873	2.222934886	1.15246569	0.037659352	1	1.234331
Com_1902_neg	Demethoxycurcumin	338.11566	2.029304685	1.020985491	0.038595662	0.92	1.011200068
Com_5092_pos	5,7,3'-Trihydroxy-6,4',5'-Trimethoxyflavone	360.08372	3.963118934	1.986636264	0.041719883	0.8	1.465741187
Com_523_pos	Adenosine	267.09651	16.95904252	4.083982815	0.041793025	0.84	2.774853587
Com_1196_pos	Adenine	135.05457	0.405251435	-1.303110799	0.049492168	0.84	1.095706331