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Functional Plant Biology

Supplementary Material

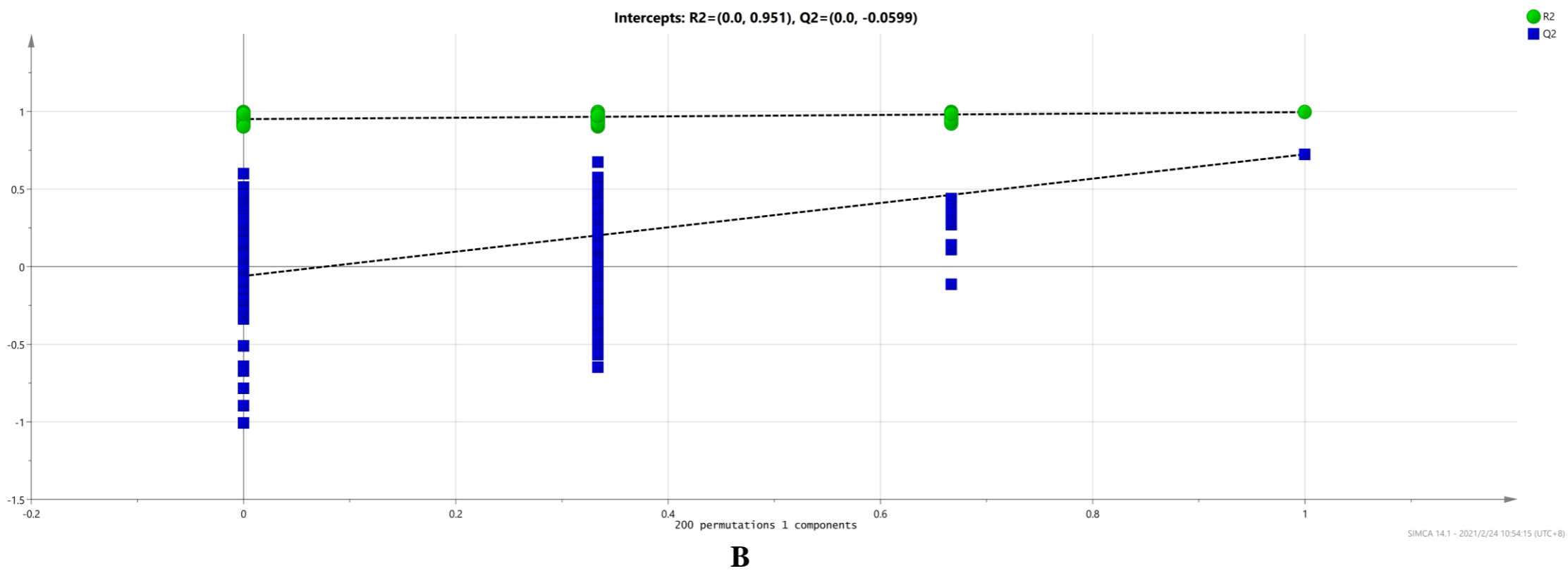
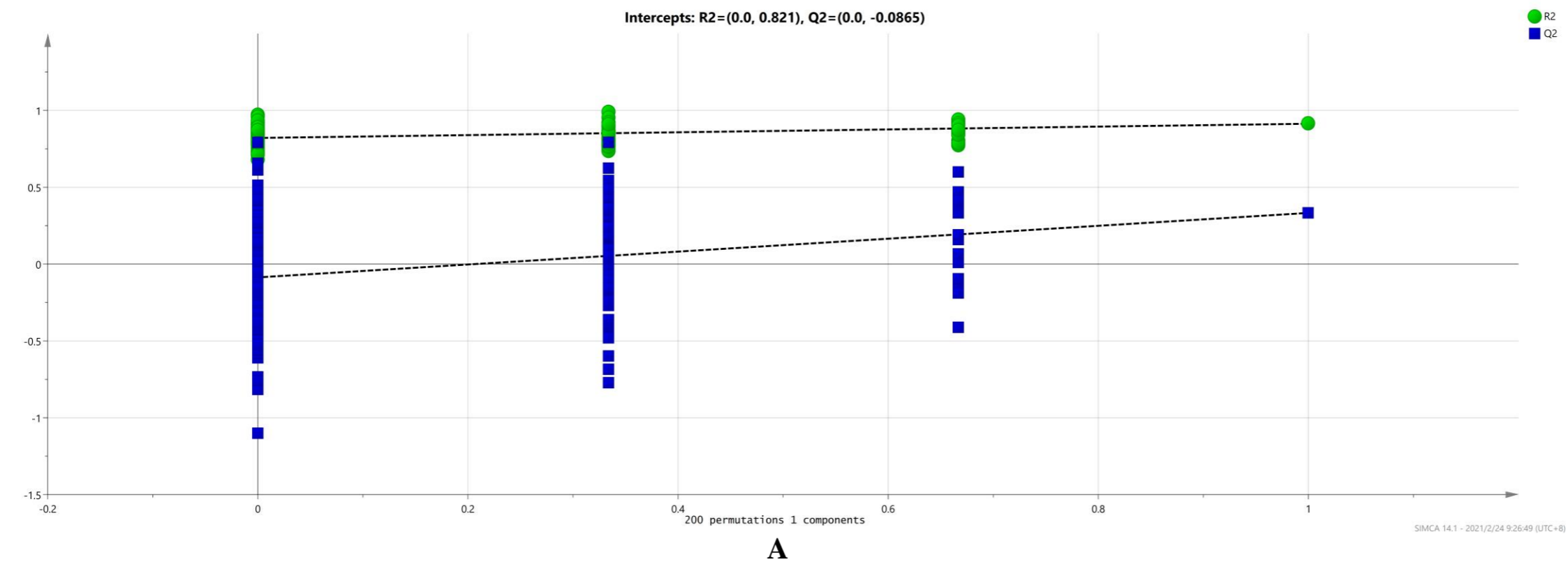
Untargeted metabolomic analysis of the metabolites in roots of *Pugionium cornutum* seedlings under drought stress

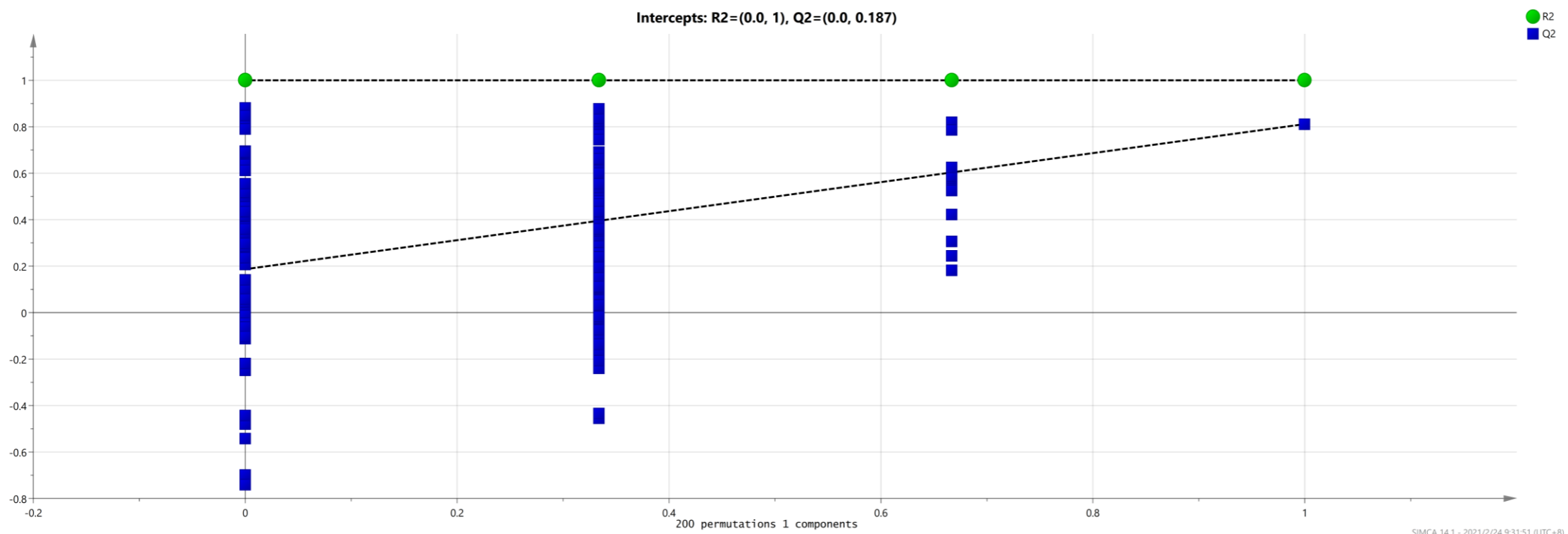
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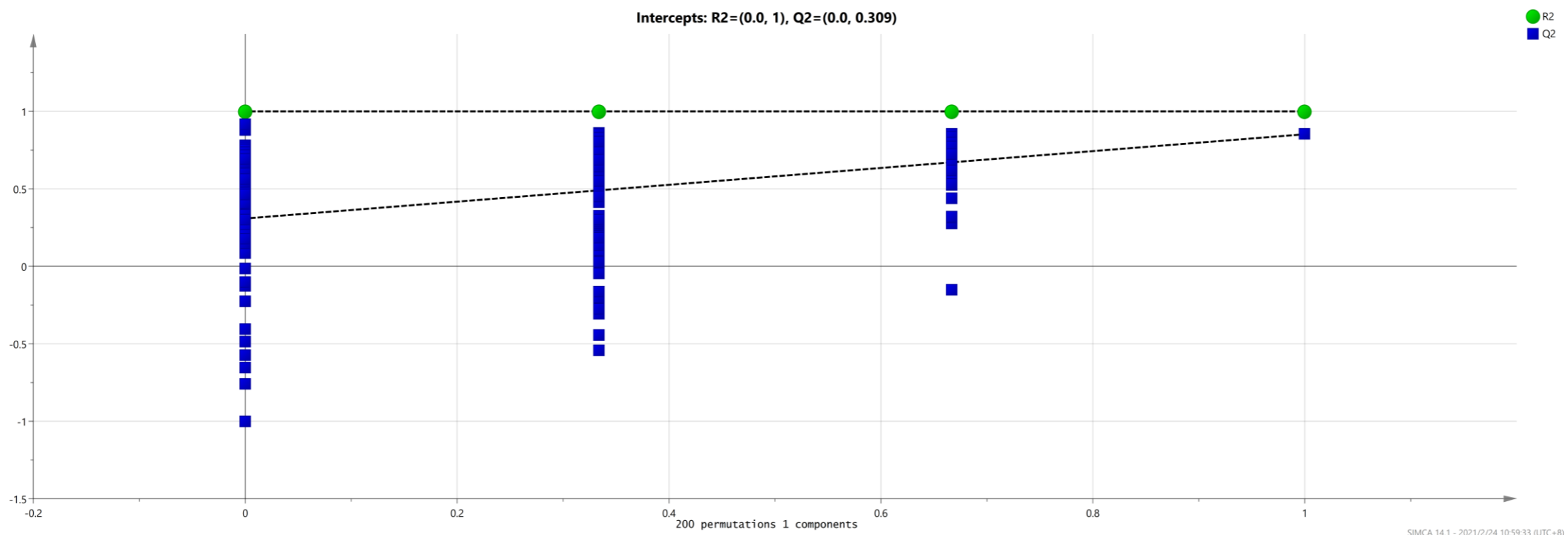
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Fig. S1 Permutation test of OPLS-DA (A: positive ion mode of R1-R2 control, B: negative ion mode of R1-R2, C: positive ion mode of R1-R3 and negative ion mode of R1-R3. The abscissa represents the permutation retention of the permutation test, and the ordinate represents the value of R2 or Q2. The green dots represent the R2 value obtained by the permutation test, the blue squares represent the Q2 value, and the two dashed lines represent the regression lines of R2 and Q2, respectively, n=200)





C



D

Table S1 Table of differential expressed metabolites

id	Peak	VIP	Pvalue	FoldChange	significant
R1-R2 正离子					
35	4-hydroxy-6-[2-(2-methyl-1,2,4a,5,6,7,8,8a-octahydronaphthalen-1-yl)ethyl]oxan-2-one	1.7422	0.0432	0.3629	Down
102	6-Methoxyquinoline	1.3588	0.0252	0.3991	Down
141	N-(1-acetyl-2,3-dihydro-1H-indol-5-yl)-N'-(2-thienylmethyl)thiourea	1.5156	0.0245	0.2878	Down
186	2-[2-(2-acetamido-4-methylpentanamido)propanamido]-3-hydroxypropanoic acid	1.6098	0.0465	0.6777	Down
196	Cytarabine	1.9125	0.0066	0.4954	Down
206	Cytosine	2.1238	0.0027	0.5235	Down
219	Argininosuccinic acid	1.6550	0.0349	1.9251	Up
258	\hat{P}^3 -Linolenic acid ethyl ester	1.5774	0.0281	0.5053	Down
280	Erucamide	1.7823	0.0348	2.9043	Up
321	Penicillic acid	1.4501	0.0276	0.6329	Down
396	4-Aminonicotinic acid	1.7642	0.0323	0.1747	Down
R1-R2 负离子					
14	3,5-di-tert-Butyl-4-hydroxybenzyl alcohol	1.5708	0.0114	1.1517	Up
50	N-(2-hydroxy-1,3-dioxo-2,3-dihydro-1H-inden-2-yl)-4-(1,2,3-thiadiazol-4-yl)benzamide	1.4188	0.0460	0.2036	Down
61	Vanillin	1.5246	0.0357	2.3844	Up
65	3-tert-Butyladipic acid	1.5231	0.0144	1.1401	Up
66	4-Acetyl-3-hydroxy-5-methylphenyl \hat{P}^2 -D-glucopyranoside	1.4837	0.0380	2.4218	Up
72	3-Methylsalicylic acid	1.6784	0.0071	0.4889	Down
94	Pentadecanoic acid	1.4420	0.0450	0.6339	Down
104	4-Nitrophenol	1.6498	0.0047	1.1257	Up
123	3-[(1-Carboxyvinyl)oxy]benzoic acid	1.4735	0.0338	0.4175	Down

125	D(+)-Phenyllactic acid	1.4875	0.0375	2.5329	Up
137	Prostaglandin A3	1.6286	0.0085	1.2035	Up
171	2-Aminooctanedioic acid	1.3858	0.0447	0.4700	Down
182	O,O-Diethyl thiophosphate	1.4147	0.0463	5.2059	Up
206	7-Methylxanthine	1.6727	0.0089	0.7941	Down
220	(1S,4aS,7S,7aS)-7-Hydroxy-1-[[6-O-(4-hydroxybenzoyl)- β -D-glucopyranosyl]oxy]-7-methyl-1,4a,5,6,7,7a-hexahydrocyclopenta[c]pyran-4-carboxylic acid	1.6016	0.0083	1.1413	Up
240	Methylmalonic acid	1.8683	0.0007	0.5763	Down
247	Prostaglandin F 2α 1-11-lactone	2.0431	0.0000	1.3465	Up
273	(2E)-N-(4-acetamidobutyl)-3-(4-hydroxy-3-methoxyphenyl)prop-2-enamide	1.6586	0.0130	3.0445	Up
293	1-[[3-(4-fluorophenyl)-1H-pyrazol-4-yl]methyl]-4-(2-methoxyphenyl)piperidine	1.5175	0.0313	0.4700	Down
299	O1-morpholinocarbonyl-3-(trifluoromethyl)-1-benzenecarbohydroximamide	1.4937	0.0306	0.2464	Down
332	Benzoic acid	1.7326	0.0033	0.4670	Down
357	3-[3-(beta-D-Glucopyranosyloxy)-2-hydroxyphenyl]propanoic acid	1.4772	0.0291	2.1566	Up
372	5-Aminovaleric acid	1.4063	0.0374	2.0608	Up
373	N-(1-adamantyl)-N'-(2,2-diethoxyethyl)thiourea	1.4631	0.0430	0.3705	Down
379	mephedrone-d3	1.6717	0.0081	1.6136	Up
R1-R3 正离子					
8	2-Morpholino-1,3-thiazol-4(5H)-one	1.5343	0.0314	0.4465	Down
35	4-hydroxy-6-[2-(2-methyl-1,2,4a,5,6,7,8,8a-octahydronaphthalen-1-yl)ethyl]oxan-2-one	1.5142	0.0328	0.3031	Down
71	1,2-dihydroxyheptadec-16-yn-4-yl acetate	1.5849	0.0215	0.1781	Down
90	N1-[4-(propylsulfonyl)-3-thienyl]-2-({2-[(4-	1.5369	0.0211	0.2382	Down

	chlorophenyl)sulfonyl]ethyl}thio)acetamide				
96	methyl 3-(1H-indol-3-yl)-2- [(phenylmethylene)amino]propanoate	1.5256	0.0352	0.3312	Down
102	6-Methoxyquinoline	1.6183	0.0193	0.3672	Down
115	Coniferin	1.5076	0.0368	2.5177	Up
141	N-(1-acetyl-2,3-dihydro-1H-indol-5-yl)-N'-(2- thienylmethyl)thiourea	1.6442	0.0215	0.2572	Down
156	Stearoyl Ethanolamide	1.4996	0.0403	2.6125	Up
161	D-(-)-Quinic acid	1.7414	0.0053	0.6002	Down
180	3-hydroxy-3,4-bis[(4-hydroxy-3- methoxyphenyl)methyl]oxolan-2-one	1.4947	0.0337	3.1451	Up
186	2-[2-(2-acetamido-4- methylpentanamido)propanamido]-3- hydroxypropanoic acid	1.4295	0.0463	0.6381	Down
196	Cytarabine	1.6708	0.0096	0.5064	Down
201	D-(+)-Glucose	1.5714	0.0258	0.4648	Down
206	Cytosine	1.6034	0.0149	0.5956	Down
211	4-[(1S,3aR,4S,6aR)-4-(4-hydroxy-3- methoxyphenyl)-hexahydrofuro[3,4-c]furan-1-yl]-2- methoxyphenol	1.4641	0.0478	0.4998	Down
219	Argininosuccinic acid	1.9110	0.0007	2.9570	Up
258	\hat{I}^3 -Linolenic acid ethyl ester	1.5087	0.0261	0.4389	Down
318	7-Hydroxycoumarinyl arachidonate	1.9258	0.0011	0.3223	Down
321	Penicillic acid	1.4578	0.0380	0.6505	Down
351	methyl 2-[(2-acetyl-3-oxo-1-butenyl)amino]acetate	1.4503	0.0477	4.3342	Up
358	2-Amino-3-methoxybenzoic acid	1.6273	0.0147	0.4097	Down
399	N-(p-Coumaroyl) serotonin	1.5847	0.0320	4.0460	Up
R1-R3 负离子					
1	(2E)-3-Phenyl-2-propen-1-yl 6-O-beta-D-	1.3112	0.0402	2.6290	Up

arabinofuranosyl-beta-D-glucopyranoside					
3	Isopropyl 4-hydroxybenzoate	1.3632	0.0212	0.3230	Down
13	8-(4-Sulfophenyl) octanoic acid	1.5193	0.0096	18.3332	Up
19	4-Coumaric acid	1.6271	0.0020	5.5467	Up
30	3-Coumaric acid	1.5046	0.0047	2.8747	Up
31	Suberic acid	1.3074	0.0306	0.6795	Down
38	1-(Carboxymethyl)cyclohexanecarboxylic acid	1.4479	0.0090	0.3339	Down
47	4-oxo-4,5,6,7-tetrahydrobenzo[b]furan-3-carboxylic acid	1.5331	0.0105	0.1689	Down
55	4-[[4,6-Dimethoxypyrimidin-2-yl)amino]methylidene]-2-phenyl-4,5-dihydro-1,3-oxazol-5-one	1.3152	0.0450	3.5036	Up
56	Salsolinol	1.3070	0.0436	0.1372	Down
66	4-Acetyl-3-hydroxy-5-methylphenyl β ² -D-glucopyranoside	1.5387	0.0037	3.5983	Up
67	3-Phenyllactic acid	1.3532	0.0330	5.8447	Up
79	Pimelic acid	1.5643	0.0043	0.4413	Down
90	D-Saccharic acid	1.3145	0.0259	0.5906	Down
101	Methyl 3-{1-[3-hydroxy-4-(hydroxymethyl)tetrahydrofuran-2-yl]-2,4-dioxo-1,2,3,4-tetrahydropyrimidin-5-yl}acrylate	1.5342	0.0083	9.7177	Up
106	(4aS,5R,6S,8aS)-5-[(3E)-5-methoxy-3-methyl-5-oxopent-3-en-1-yl]-5,6,8a-trimethyl-3,4,4a,5,6,7,8,8a-octahydronaphthalene-1-carboxylic acid	1.4042	0.0147	1.3145	Up
123	3-[(1-Carboxyvinyl)oxy]benzoic acid	1.5685	0.0069	0.1309	Down
124	2-Methylbenzoic acid	1.4208	0.0279	6.7371	Up
125	D(+)-Phenyllactic acid	1.5539	0.0034	3.9486	Up
137	Prostaglandin A3	1.3394	0.0188	1.1626	Up

140	13,14-Dihydro-15-keto-tetranor prostaglandin F1 \hat{I} \pm	1.4787	0.0103	0.3056	Down
149	2-Furoic acid	1.4668	0.0085	1.3769	Up
171	2-Aminooctanedioic acid	1.3971	0.0194	0.3309	Down
172	(1,3-Phenylenedioxy)diacetic acid	1.3786	0.0207	0.3815	Down
175	N-(4-Bromo-3-methylphenyl)acetamide	1.4399	0.0167	0.2396	Down
180	Citraconic acid	1.3005	0.0279	1.3173	Up
186	2-(Acetylamino)-4-phenylbutanoic acid	1.3447	0.0340	0.1661	Down
191	Ferulic acid	1.2666	0.0433	2.3532	Up
196	(-)-Corey lactone	1.5254	0.0037	0.3889	Down
202	Azelaic acid	1.3415	0.0364	0.6053	Down
206	7-Methylxanthine	1.6497	0.0008	0.5258	Down
221	Riboflavin	1.4908	0.0065	0.6853	Down
223	Terephthalic acid	1.3705	0.0206	0.4078	Down
240	Methylmalonic acid	1.6903	0.0002	0.4398	Down
247	Prostaglandin F2 \hat{I} \pm 1-11-lactone	1.5155	0.0076	1.4019	Up
256	Uridine	1.5768	0.0020	0.6060	Down
257	Prostaglandin E3	1.3063	0.0347	0.4378	Down
263	L-Tyrosine	1.5883	0.0016	2.4572	Up
276	Erucic acid	1.5044	0.0042	3.0381	Up
279	Caffeic acid	1.3912	0.0335	5.9130	Up
293	1-([3-(4-fluorophenyl)-1H-pyrazol-4-yl]methyl)-4-(2-methoxyphenyl)piperidine	1.3720	0.0290	0.4591	Down
319	2,3-Dihydro-1-benzofuran-2-carboxylic acid	1.2608	0.0341	1.9293	Up
331	Prostaglandin D2	1.4082	0.0182	0.3669	Down
332	Benzoic acid	1.5242	0.0032	0.4411	Down
354	(2R)-2,3-Dihydroxypropanoic acid	1.4859	0.0052	0.4999	Down
360	Porphobilinogen	1.3926	0.0192	2.0205	Up
362	N2-(2,3-dihydrobenzo[b]furan-5-ylmethyl)-2-thiophenesulfonamide	1.2401	0.0438	1.5394	Up

369	N-(1-methyl-1H-indazol-3-yl)-2-[3-(trifluoromethyl)-1H-pyrazol-1-yl]acetamide	1.4639	0.0069	0.3821	Down
372	5-Aminovaleric acid	1.3191	0.0440	2.8089	Up
