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### Supplementary Material

#### **Betulonic acid regulates oviduct epithelial cell inflammation through the TLR4, MAPK, and JAK/STAT signalling pathways**

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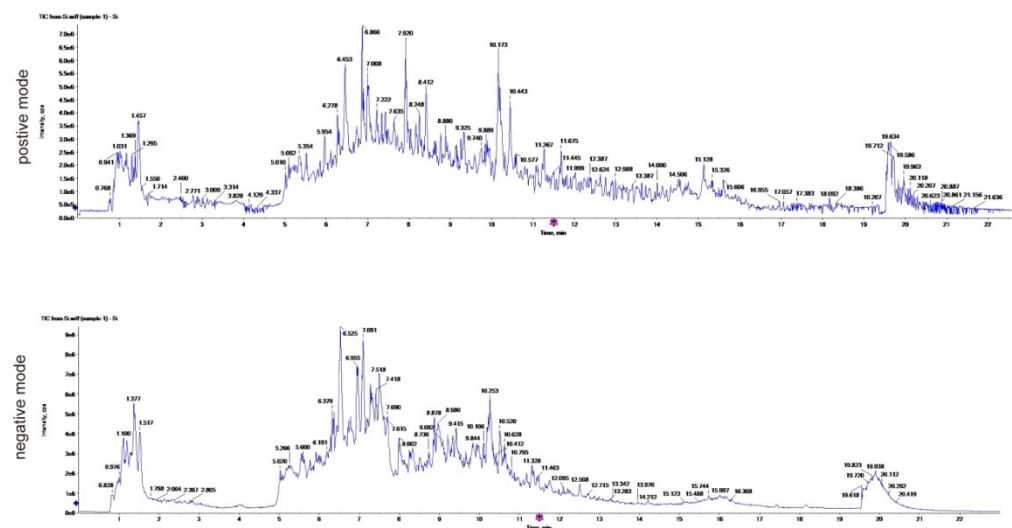
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Supplementary Fig. S1. Basal peak ion flow chromatogram image of the Oviduct Futong decoction under the positive and negative mode.



Supplementary Table S1. Ingredients of the Oviduct Futong decoction under the positive and negative mode.

Component Name	Library Hit	Retention Time	Area	Adduct / Charge	Formula	Precursor Mass	Found At Mass
827.2712 / 4.90 [M-H]-	Maltopentaose [Smart Confirmation]	4.89	5.37E+02	[M-H]-	{828.27907}	827.272	827.2698

96.9606 / 3.34 [M-H]-	FURFURYL ALCOHOL [Smart Confirmation]	3.35	1.39E+03	[M-H]-	{97.96843}	96.962	96.9601
665.2170 / 3.32 [M-H]-	Fungitetraose [Smart Confirmation]	3.37	2.11E+03	[M-H]-	{666.22484}	665.218	665.2145
665.1408 / 6.12 [2M+K-2H]-	STACHYOSE [Smart Confirmation]	6.15	3.09E+03	[2M+K-2H]-	{314.09666}	665.142	665.1489
197.0466 / 5.64	Mimosine [Smart Confirmation]	5.63	3.30E+03	[M-H]-	{198.05446}	197.048	197.0476
433.0454 / 6.72	Geniposide + HCOOH [Smart Confirmation]	6.67	3.79E+03	[M-H]-	{434.05320}	433.046	433.0459
269.0475 / 12.22	Emodin [Smart Confirmation]	12.23	3.99E+03	[M-H]-	{270.05537}	269.049	269.0446
493.1160 / 8.56 [M-H]-	Salvianolic acid A [Smart Confirmation]	8.57	4.22E+03	[M-H]-	{494.12386}	493.117	493.1152
195.0306 / 7.80	(3,4-Dimethoxyphenyl) Acetic Acid [Smart Confirmation]	7.79	4.36E+03	[M-H]-	{196.03841}	195.032	195.0295
405.1205 / 7.43 [M-H]-	Dipsacoside B [Smart Confirmation]	7.45	4.63E+03	[M-H]-	{406.12836}	405.122	405.1261
191.0572 / 5.34	Citric acid [Smart Confirmation]	5.36	6.57E+03	[M-H]-	{192.06499}	191.058	191.056
711.2228 / 3.31 [M+FA-H]-	Fungitetraose [Smart Confirmation]	3.38	8.22E+03	[M+FA-H]-	{666.22513}	711.224	711.2192
455.3542 / 15.40	Oleanolic acid [Smart Confirmation]	15.41	1.22E+04	[M-H]-	{456.36207}	455.355	455.354
297.2449 / 13.69	Nonadecanoic acid [Smart Confirmation]	13.76	1.66E+04	[M-H]-	{298.25270}	297.246	297.2442
515.1415 / 5.48	3,5-DCQA Isochlorogenic acid A [Smart Confirmation]	5.48	1.71E+04	[M-H]-	{516.14936}	515.143	515.1409
299.0580 / 9.77	Hydroxygenkwanin [Smart Confirmation]	9.74	1.80E+04	[M-H]-	{300.06578}	299.059	299.0569
96.9602 / 6.63	FURFURYL ALCOHOL [Smart Confirmation]	6.69	1.84E+04	[M-H]-	{97.96799}	96.961	96.9604
89.0246 / 5.40	GLYCERALDEHYDE [Smart Confirmation]	5.41	1.88E+04	[M-H]-	{90.03247}	89.026	89.0241
227.1046 / 6.09	3,5-Dinitrosalicylate [Smart Confirmation]	6.09	1.95E+04	[M-H]-	{228.11243}	227.106	227.1045
431.0998 / 7.81	Genistin [Smart Confirmation]	7.82	1.99E+04	[M-H]-	{432.10765}	431.101	431.0989
471.3476 / 13.45	Hederagenin [Smart Confirmation]	13.45	2.25E+04	[M-H]-	{472.35539}	471.349	471.3477
681.2973 / 15.61	ATenuifoliside A [Smart Confirmation]	15.61	2.48E+04	[M-H]-	{682.30511}	681.298	681.2977
115.9208 / 19.55 [M-H]-	INDOLE [Smart Confirmation]	19.55	2.54E+04	[M-H]-	{116.92863}	115.922	115.9209
335.0928 / 12.82	Leukotriene B4 [Smart Confirmation]	12.83	2.56E+04	[M-H]-	{336.10059}	335.094	335.0929
469.3331 / 14.78	Glycyrrhetic acid [Smart Confirmation]	14.79	2.64E+04	[M-H]-	{470.34088}	469.334	469.3336

517.3166 / 11.66	A5Sibiricose A5 [Smart Confirmation]	11.66	2.65E+04	[M-H]-	{518.32442}	517.318	517.3182
345.1554 / 7.86	Salidroside +HCOOH [Smart Confirmation]	7.85	2.68E+04	[M-H]-	{346.16326}	345.157	345.1557
191.0572 / 6.42	Quinic acid [Smart Confirmation]	6.43	2.69E+04	[M-H]-	{192.06502}	191.058	191.057
337.1081 / 11.10 [M-H <sub>2</sub> O-H]-	AICAR [Smart Confirmation]	11.11	2.76E+04	[M-H <sub>2</sub> O-H]-	{356.12648}	337.109	337.1087
331.2508 / 9.70	CP 47,497 C8-homolog Negative Mode [Smart Confirmation]	9.72	2.87E+04	[M-H]-	{332.25859}	331.252	331.2496
159.0668 / 6.70	6-CARBOXYHEXANOATE [Smart Confirmation]	6.7	3.00E+04	[M-H]-	{160.07464}	159.068	159.067
644.2673 / 8.61 [M]-	Ustiloxin B [Smart Confirmation]	8.62	3.25E+04	[M]-	{644.26734}	644.268	644.2663
485.3270 / 12.48	Andrastin A [Smart Confirmation]	12.49	3.44E+04	[M-H]-	{486.33479}	485.328	485.3271
267.1617 / 9.69	Paspalic acid [Smart Confirmation]	9.71	3.50E+04	[M-H]-	{268.16949}	267.163	267.1611
251.1653 / 11.17 [M-H]-	Hexazinone [Smart Confirmation]	11.16	3.56E+04	[M-H]-	{252.17311}	251.166	251.1659
242.1779 / 9.73	4-Bromophenylalanine [Smart Confirmation]	9.75	3.65E+04	[M-H]-	{243.18572}	242.179	242.177
627.1579 / 6.09	PFHxA in-source dimer (perfluoro-n-hexanoic acid) (neg) [Smart Confirmation]	6.09	3.67E+04	[M-H]-	{628.16573}	627.159	627.1585
115.0033 / 2.95	MALEATE [Smart Confirmation]	2.95	3.74E+04	[M-H]-	{116.01112}	115.004	115.0038
153.0199 / 6.66	Protocatechuic acid [Smart Confirmation]	6.66	3.76E+04	[M-H]-	{154.02770}	153.021	153.0198
777.4085 / 11.84	Heterophyllin B [Smart Confirmation]	11.84	3.80E+04	[M-H]-	{778.41630}	777.41	777.408
873.2767 / 2.16 [M+FA-H]-	Maltopentaose [Smart Confirmation]	2.14	3.81E+04	[M+FA-H]-	{828.27902}	873.278	873.2751
285.0421 / 8.93	Luteolin [Smart Confirmation]	8.94	3.82E+04	[M-H]-	{286.04995}	285.043	285.0415
499.3064 / 11.95	Qingyangshengenin [Smart Confirmation]	11.96	3.89E+04	[M-H]-	{500.31424}	499.308	499.3075
637.2121 / 7.97	Ciso-Cistanoside C [Smart Confirmation]	7.99	3.95E+04	[M-H]-	{638.21992}	637.213	637.2133
236.0937 / 5.42	Biopterin [Smart Confirmation]	5.44	4.00E+04	[M-H]-	{237.10150}	236.095	236.0936
707.1846 / 6.42 [2M-H]-	4-O-Caffeoyl quinic acid [Smart Confirmation]	6.44	4.31E+04	[2M-H]-	{354.09648}	707.186	707.1851
287.0887 / 5.43 [M+FA-H]-	Thymidine-1 [Smart Confirmation]	5.42	4.37E+04	[M+FA-H]-	{242.09104}	287.09	287.089
387.1670 / 6.67	Geniposide [Smart Confirmation]	6.66	4.45E+04	[M-H]-	{388.17479}	387.168	387.1667

264.9343 / 0.95 [2M+K-2H]-	1-Methylhydantoin [Smart Confirmation]	0.94	4.45E+04	[2M+K-2H]-	{113.99338}	264.936	264.9348
665.2150 / 1.81 [M-H <sub>2</sub> O-H]-	STACHYOSE [Smart Confirmation]	1.83	4.46E+04	[M-H <sub>2</sub> O-H]-	{684.23334}	665.216	665.2159
191.0206 / 5.19	Citric acid [Smart Confirmation]	5.22	4.47E+04	[M-H]-	{192.02847}	191.022	191.0205
407.1565 / 5.85 [M-H]-	Catalpol [Smart Confirmation]	5.85	4.76E+04	[M-H]-	{408.16437}	407.158	407.1563
213.0042 / 5.49	Agistatin B [Smart Confirmation]	5.49	4.95E+04	[M-H]-	{214.01206}	213.005	213.0051
89.0241 / 1.81	GLYCERALDEHYDE [Smart Confirmation]	1.8	4.98E+04	[M-H]-	{90.03192}	89.025	89.0244
515.1413 / 6.30	3,5-DCQA Isochlorogenic acid A [Smart Confirmation]	6.18	5.04E+04	[M-H]-	{516.14917}	515.142	515.1418
112.9852 / 0.95 [M-H]-	Gamma-Caprolactone [Smart Confirmation]	0.94	5.11E+04	[M-H]-	{113.99305}	112.986	112.9856
129.0191 / 4.18	ITACONATE [Smart Confirmation]	4.17	5.18E+04	[M-H]-	{130.02689}	129.02	129.0195
354.0926 / 6.42 [M]-	Chlorogenic Acid [Smart Confirmation]	6.44	5.31E+04	[M]-	{354.09260}	354.094	354.0914
161.0611 / 8.40 [M-H <sub>2</sub> O-H]-	4-Hydroxycoumarin [Smart Confirmation]	8.41	5.46E+04	[M-H <sub>2</sub> O-H]-	{180.07953}	161.062	161.0614
116.9284 / 10.15	MESOXALATE [Smart Confirmation]	10.11	5.54E+04	[M-H]-	{117.93623}	116.93	116.9289
293.2130 / 13.62	Methylinoleate [Smart Confirmation]	13.61	5.61E+04	[M-H]-	{294.22079}	293.214	293.213
527.1412 / 6.07	Pachymic acid [Smart Confirmation]	6.07	5.65E+04	[M-H]-	{528.14898}	527.142	527.1415
165.0562 / 7.65	L-3-Phenyllactic acid [Smart Confirmation]	7.64	5.66E+04	[M-H]-	{166.06400}	165.057	165.0562
277.2184 / 15.09	Sulfamethazine [Smart Confirmation]	15.1	5.68E+04	[M-H]-	{278.22624}	277.22	277.2184
337.1083 / 11.93	AICAR [Smart Confirmation]	11.92	5.77E+04	[M-H]-	{338.11612}	337.109	337.1086
233.1551 / 11.03 [M-H <sub>2</sub> O-H]-	Dichlorprop [Smart Confirmation]	11.03	5.82E+04	[M-H <sub>2</sub> O-H]-	{252.17346}	233.156	233.1553
531.1923 / 5.17 [2M-H]-	Sambucinol [Smart Confirmation]	5.17	6.15E+04	[2M-H]-	{266.10032}	531.194	531.1929
463.0882 / 5.43	Hyperin [Smart Confirmation]	5.43	6.22E+04	[M-H]-	{464.09606}	463.089	463.0889
281.2499 / 16.46	Vaccenic acid [Smart Confirmation]	16.47	6.36E+04	[M-H]-	{282.25772}	281.251	281.2495
147.0301 / 2.27	CITRAMALATE [Smart Confirmation]	2.22	6.38E+04	[M-H]-	{148.03791}	147.031	147.03
461.1660 / 5.87	Scutellarin [Smart Confirmation]	5.87	6.53E+04	[M-H]-	{462.17383}	461.167	461.1667
283.0628 / 9.01	Acacetin [Smart Confirmation]	9.01	6.56E+04	[M-H]-	{284.07064}	283.064	283.0628
159.0299 / 2.95	Diethyl malonate [Smart Confirmation]	2.93	6.65E+04	[M-H]-	{160.03772}	159.031	159.0307

487.3424 / 11.46	Polygalic acid [Smart Confirmation]	11.47	6.71E+04	[M-H]-	{488.35021}	487.343	487.3428
827.2702 / 2.16 [M-H]-	Maltopentaose [Smart Confirmation]	2.15	6.93E+04	[M-H]-	{828.27800}	827.271	827.2695
313.0370 / 9.38	PFHxA (perfluoro-n-hexanoic acid) (neg) [Smart Confirmation]	9.37	6.93E+04	[M-H]-	{314.04484}	313.038	313.0364
315.2543 / 12.69	Isorhamnetin [Smart Confirmation]	12.69	6.98E+04	[M-H]-	{316.26214}	315.255	315.2544
467.1206 / 5.53	Prim-O-glucosylcimifugin [Smart Confirmation]	5.52	7.07E+04	[M-H]-	{468.12839}	467.122	467.1209
128.9602 / 0.95 [M-H]-	Heptanoic acid [Smart Confirmation]	0.95	7.09E+04	[M-H]-	{129.96802}	128.961	128.9596
285.0618 / 6.15 [M+AcO-H]-	Porphobilinogen [Smart Confirmation]	6.15	7.17E+04	[M+AcO-H]-	{226.04850}	285.063	285.0621
531.2241 / 8.46 [M-H]-	Phytolaccagenin [Smart Confirmation]	8.46	7.41E+04	[M-H]-	{532.23188}	531.225	531.2243
515.1209 / 6.83	1,4-Dicaffeoylquinic Acid (Cynarin) [Smart Confirmation]	6.82	7.50E+04	[M-H]-	{516.12871}	515.122	515.1205
595.1462 / 6.16	Tracheloside +HCOOH [Smart Confirmation]	6.18	7.69E+04	[M-H]-	{596.15401}	595.147	595.1469
221.0826 / 9.17	Ethyl ferulate [Smart Confirmation]	9.17	7.73E+04	[M-H]-	{222.09045}	221.084	221.0824
307.0741 / 9.15	Fulvic acid [Smart Confirmation]	9.16	7.95E+04	[M-H]-	{308.08188}	307.075	307.0737
375.1302 / 5.84 [M-H <sub>2</sub> O-H]-	8-epiloganic acid [Smart Confirmation]	5.83	7.97E+04	[M-H <sub>2</sub> O-H]-	{394.14855}	375.131	375.1301
453.3372 / 16.17	Betulonic acid [Smart Confirmation]	16.18	8.22E+04	[M-H]-	{454.34506}	453.338	453.338
186.0409 / 2.90	Indoleacrylic acid [Smart Confirmation]	2.87	8.30E+04	[M-H]-	{187.04871}	186.042	186.0413
431.1565 / 6.28 [M-H]-	Emodin-8-glucoside [Smart Confirmation]	6.3	8.36E+04	[M-H]-	{432.16428}	431.158	431.1563
243.1244 / 8.51 [M-H]-	1,11-Undecanedicarboxylic acid [Smart Confirmation]	8.51	8.46E+04	[M-H]-	{244.13224}	243.126	243.1247
651.2296 / 8.50	DCistanoside D [Smart Confirmation]	8.5	8.56E+04	[M-H]-	{652.23747}	651.231	651.2301
335.0925 / 12.25	Leukotriene B4 [Smart Confirmation]	12.25	8.72E+04	[M-H]-	{336.10028}	335.094	335.093
289.0678 / 1.61 [M+FA-H]-	Uridine [Smart Confirmation]	1.62	8.77E+04	[M+FA-H]-	{244.07018}	289.069	289.0688
131.0457 / 1.01	ASPARAGINE [Smart Confirmation]	1.01	8.85E+04	[M-H]-	{132.05356}	131.047	131.046
229.1457 / 10.16	Dodecanedioic acid [Smart Confirmation]	10.17	8.85E+04	[M-H]-	{230.15353}	229.147	229.1454
353.1031 / 11.17	Prostaglandin F2A [Smart Confirmation]	11.17	9.05E+04	[M-H]-	{354.11096}	353.104	353.1035

132.0299 / 1.02	Aspartic acid [Smart Confirmation]	1.02	9.11E+04	[M-H]-	{133.03775}	132.031	132.0302
239.0932 / 8.50 [M+AcO-H]-	ANSERINE [Smart Confirmation]	8.5	9.29E+04	[M+AcO-H]-	{180.07989}	239.094	239.093
183.1030 / 9.32	3,4 DIHYDROXYMANDELATE [Smart Confirmation]	9.32	9.56E+04	[M-H]-	{184.11079}	183.104	183.1033
173.1045 / 1.00	L(+)-Arginine [Smart Confirmation]	0.99	9.72E+04	[M-H]-	{174.11235}	173.106	173.1047
469.3319 / 14.20	Glycyrrhetic acid [Smart Confirmation]	14.2	9.91E+04	[M-H]-	{470.33977}	469.333	469.3322
121.0295 / 7.27 [M-H]-	4-HYDROXYBENZALDEHYDE [Smart Confirmation]	7.27	1.01E+05	[M-H]-	{122.03737}	121.031	121.0296
147.0299 / 3.43	CITRAMALATE [Smart Confirmation]	3.42	1.02E+05	[M-H]-	{148.03769}	147.031	147.0302
225.0412 / 5.87 [M-H]-	Porphobilinogen [Smart Confirmation]	5.87	1.03E+05	[M-H]-	{226.04905}	225.042	225.0414
188.0573 / 3.31	N-ACETYLGLUTAMATE [Smart Confirmation]	3.3	1.04E+05	[M-H]-	{189.06515}	188.058	188.057
279.2345 / 15.72	Linoleic acid [Smart Confirmation]	15.73	1.07E+05	[M-H]-	{280.24237}	279.236	279.234
309.1190 / 6.66	Threonate [Smart Confirmation]	6.66	1.08E+05	[M-H]-	{310.12678}	309.12	309.1195
321.1132 / 11.44 [M-H]-	5-Thymidylic acid [Smart Confirmation]	11.44	1.11E+05	[M-H]-	{322.12105}	321.114	321.1135
487.1821 / 8.32 [M+FA-H]-	Asiatic acid [Smart Confirmation]	8.32	1.11E+05	[M+FA-H]-	{442.18449}	487.183	487.183
164.0718 / 5.41	Phenprobamate [Smart Confirmation]	5.39	1.11E+05	[M-H]-	{165.07966}	164.073	164.0722
117.0192 / 3.23	METHYLMALONATE [Smart Confirmation]	3.21	1.12E+05	[M-H]-	{118.02702}	117.02	117.0196
269.0473 / 9.56	PFHxA in-source fragment (perfluoro-n-hexanoic acid) (neg) [Smart Confirmation]	9.6	1.15E+05	[M-H]-	{270.05511}	269.048	269.0464
445.0784 / 8.32	Baicalin [Smart Confirmation]	8.32	1.17E+05	[M-H]-	{446.08623}	445.08	445.0795
443.1925 / 6.18	6:2 PAP (6:2 fluorotelomer phosphate ester) (neg) [Smart Confirmation]	6.19	1.20E+05	[M-H]-	{444.20035}	443.194	443.1931
295.2281 / 13.29	17a-Ethynylestradiol [Smart Confirmation]	13.29	1.25E+05	[M-H]-	{296.23590}	295.229	295.2286
485.1671 / 8.11 [M-H]-	Andrastin A [Smart Confirmation]	8.11	1.25E+05	[M-H]-	{486.17497}	485.168	485.1683
255.2343 / 16.30	PALMITATE [Smart Confirmation]	16.31	1.26E+05	[M-H]-	{256.24210}	255.235	255.2338
243.0623 / 4.06	Uridine [Smart Confirmation]	4.07	1.26E+05	[M-H]-	{244.07017}	243.063	243.0627

137.0246 / 8.62	4-HYDROXYBENZOATE [Smart Confirmation]	8.62	1.27E+05	[M-H]-	{138.03245}	137.026	137.0249
117.0197 / 2.22	SUCCINATE [Smart Confirmation]	2.15	1.29E+05	[M-H]-	{118.02749}	117.021	117.0197
779.4584 / 10.51	Saikosaponin B2 [Smart Confirmation]	10.53	1.32E+05	[M-H]-	{780.46623}	779.46	779.4587
206.0823 / 7.40	N-Acetyl-L-phenylalanine [Smart Confirmation]	7.41	1.34E+05	[M-H]-	{207.09014}	206.083	206.0828
271.0619 / 9.56	Naringenin [Smart Confirmation]	9.56	1.35E+05	[M-H]-	{272.06977}	271.063	271.062
215.1295 / 9.54	Undecanedioic acid [Smart Confirmation]	9.54	1.36E+05	[M-H]-	{216.13728}	215.131	215.1297
178.9786 / 19.69	3-(4-HYDROXYPHENYL)PYRUVATE [Smart Confirmation]	19.84	1.40E+05	[M-H]-	{179.98640}	178.98	178.9786
193.0873 / 9.67	Butylparaben [Smart Confirmation]	9.67	1.47E+05	[M-H]-	{194.09512}	193.088	193.0876
351.0870 / 11.44	Lipoxin A4 [Smart Confirmation]	11.43	1.51E+05	[M-H]-	{352.09483}	351.088	351.0874
179.0718 / 8.33 [M-H]-	CAFFEATE [Smart Confirmation]	8.34	1.57E+05	[M-H]-	{180.07962}	179.073	179.0719
170.0185 / 5.05	2-Methyl-5-nitroimidazole-1- [Smart Confirmation]	5.1	1.60E+05	[M-H]-	{171.02635}	170.02	170.018
609.1476 / 7.21	Rutin [Smart Confirmation]	7.21	1.60E+05	[M-H]-	{610.15540}	609.149	609.1465
337.1449 / 11.78 [M-H2O-H]-	AICAR [Smart Confirmation]	11.78	1.65E+05	[M-H2O-H]-	{356.16328}	337.146	337.1452
593.1509 / 3.08	Aempferol-3-O-rutinoside [Smart Confirmation]	3.06	1.69E+05	[M-H]-	{594.15876}	593.152	593.1517
821.3977 / 9.02	Glycyrrhizic acid ammonium salt [Smart Confirmation]	9.03	1.76E+05	[M-H]-	{822.40555}	821.399	821.3984
323.1291 / 12.21 [M-H]-	Glabridin [Smart Confirmation]	12.2	1.89E+05	[M-H]-	{324.13692}	323.13	323.1292
283.2648 / 17.43	Ethyl hexadecanoate1 [Smart Confirmation]	17.43	1.94E+05	[M-H]-	{284.27264}	283.266	283.2651
515.1215 / 7.59 [M-H]-	3,4-DCQA Isochlorogenic acid B [Smart Confirmation]	7.59	1.99E+05	[M-H]-	{516.12936}	515.123	515.1206
475.1250 / 8.34	Ononin +HCOOH [Smart Confirmation]	8.35	2.13E+05	[M-H]-	{476.13285}	475.126	475.1254
128.0348 / 1.54 [M-H]-	OXOPROLINE [Smart Confirmation]	1.54	2.14E+05	[M-H]-	{129.04265}	128.036	128.0354
243.0625 / 1.61 [M-H]-	Uridine [Smart Confirmation]	1.62	2.14E+05	[M-H]-	{244.07035}	243.064	243.0628
503.1616 / 1.34	Maltotriose [Smart Confirmation]	1.32	2.14E+05	[M-H]-	{504.16942}	503.163	503.162



499.1671 / 1.51	PFOS (perfluorooctane sulfonate) (neg) [Smart Confirmation]	1.51	2.20E+05	[M-H]-	{500.17489}	499.168	499.1672
611.1618 / 5.55 [M+Na-2H]-	hydroxysafflor yellow A [Smart Confirmation]	5.54	2.20E+05	[M+Na-2H]-	{590.18767}	611.163	611.1625
188.0568 / 1.70 [M+AcO-H]-	N-ACETYLGLUTAMATE [Smart Confirmation]	1.68	2.27E+05	[M+AcO-H]-	{129.04352}	188.058	188.0571
221.0826 / 9.68	Ethyl ferulate [Smart Confirmation]	9.68	2.30E+05	[M-H]-	{222.09039}	221.084	221.0826
203.0832 / 6.04 [M-H]-	L-Tryptophan [Smart Confirmation]	6.04	2.35E+05	[M-H]-	{204.09100}	203.084	203.0834
805.4034 / 11.28 [M-H <sub>2</sub> O-H]-	Oligomycin B [Smart Confirmation]	11.29	2.36E+05	[M-H <sub>2</sub> O-H]-	{824.42176}	805.404	805.4037
305.0676 / 5.76	Gallocatechin [Smart Confirmation]	5.75	2.40E+05	[M-H]-	{306.07541}	305.069	305.0679
311.2231 / 11.48	Phe-Phe [Smart Confirmation]	11.48	2.40E+05	[M-H]-	{312.23088}	311.224	311.2231
289.0727 / 6.48	Catechin [Smart Confirmation]	6.48	2.44E+05	[M-H]-	{290.08048}	289.074	289.0723
971.5236 / 9.66	Saikosaponin C +HCOOH [Smart Confirmation]	9.66	2.52E+05	[M-H]-	{972.53139}	971.525	971.524
973.5382 / 9.75	Asperosaponin VI +HCOOH [Smart Confirmation]	9.76	2.53E+05	[M-H]-	{974.54599}	973.539	973.5383
577.1360 / 6.19 [M+FA-H]-	Procyanidin B2 [Smart Confirmation]	6.18	2.59E+05	[M+FA-H]-	{532.13833}	577.137	577.1362
731.2257 / 5.22 [M-H]-	Rehmannioside D +HCOOH [Smart Confirmation]	5.22	2.81E+05	[M-H]-	{732.23353}	731.227	731.2266
165.0403 / 1.11	D-Xylonic Acid Lithium Salt [Smart Confirmation]	1.11	2.85E+05	[M-H]-	{166.04808}	165.041	165.0408
573.2345 / 9.41 [M-H]-	Isotoosendanin [Smart Confirmation]	9.42	2.88E+05	[M-H]-	{574.24231}	573.236	573.235
823.4131 / 11.10 [M-H]-	Vincristine [Smart Confirmation]	11.12	2.96E+05	[M-H]-	{824.42090}	823.414	823.4136
163.0399 / 7.50	4-COUMARATE [Smart Confirmation]	7.5	3.03E+05	[M-H]-	{164.04775}	163.041	163.0404
179.0574 / 1.12 [M-H]-	D-Galactose [Smart Confirmation]	1.12	3.16E+05	[M-H]-	{180.06525}	179.059	179.0564
353.0888 / 5.97 [M-H]-	Neochlorogenic acid [Smart Confirmation]	5.98	3.25E+05	[M-H]-	{354.09665}	353.09	353.0889
175.0613 / 6.48	2-Isopropylmalic acid [Smart Confirmation]	6.48	3.97E+05	[M-H]-	{176.06916}	175.062	175.0616
187.0988 / 8.16	Azelaic acid [Smart Confirmation]	8.16	4.18E+05	[M-H]-	{188.10663}	187.1	187.0982
407.1196 / 5.03	Catalpol [Smart Confirmation]	5.02	4.19E+05	[M-H]-	{408.12741}	407.121	407.1198

243.1607 / 10.78	1,11-Undecanedicarboxylic acid [Smart Confirmation]	10.79	4.38E+05	[M-H]-	{244.16848}	243.162	243.1606
417.1197 / 8.25	Isoliquiritin [Smart Confirmation]	8.25	4.45E+05	[M-H]-	{418.12749}	417.121	417.1197
619.2403 / 9.41 [M+FA-H]-	Isotoosendanin [Smart Confirmation]	9.42	4.62E+05	[M+FA-H]-	{574.24267}	619.241	619.2408
479.1564 / 8.00 [M-H]-	Albiflorin [Smart Confirmation]	8	5.00E+05	[M-H]-	{480.16423}	479.158	479.157
593.1516 / 7.50	Aempferol-3-O-rutinoside [Smart Confirmation]	7.51	5.02E+05	[M-H]-	{594.15946}	593.153	593.1522
133.0150 / 1.46	MALATE [Smart Confirmation]	1.47	5.36E+05	[M-H]-	{134.02279}	133.016	133.0149
128.0355 / 2.84	OXOPROLINE [Smart Confirmation]	2.83	5.36E+05	[M-H]-	{129.04331}	128.037	128.0357
191.0564 / 1.26	Quinic acid [Smart Confirmation]	1.27	5.56E+05	[M-H]-	{192.06418}	191.057	191.0565
301.0361 / 8.98	Quercetin [Smart Confirmation]	8.99	5.70E+05	[M-H]-	{302.04391}	301.037	301.0363
623.1986 / 7.49	Acteoside; Verbascoside; Kusaginins [Smart Confirmation]	7.5	5.70E+05	[M-H]-	{624.20640}	623.2	623.1989
153.0197 / 5.90	3,4-DIHYDROXYBENZOATE [Smart Confirmation]	5.89	5.84E+05	[M-H]-	{154.02752}	153.021	153.0199
205.0875 / 10.42	Ibuprofen [Smart Confirmation]	10.42	6.13E+05	[M-H]-	{206.09535}	205.089	205.0876
477.1610 / 6.28 [M+FA-H]-	Emodin-8-glucoside [Smart Confirmation]	6.29	6.39E+05	[M+FA-H]-	{432.16332}	477.162	477.1618
193.0512 / 7.74	trans-Ferulic acid [Smart Confirmation]	7.74	6.87E+05	[M-H]-	{194.05903}	193.052	193.0516
197.0097 / 5.74	Mimosine [Smart Confirmation]	5.75	7.33E+05	[M-H]-	{198.01756}	197.011	197.0098
165.0198 / 6.79	Phthalic acid [Smart Confirmation]	6.79	7.93E+05	[M-H]-	{166.02764}	165.021	165.02
493.1197 / 5.32	Salvianolic acid A [Smart Confirmation]	5.3	9.21E+05	[M-H]-	{494.12749}	493.121	493.1199
377.0858 / 1.18 [M+Cl]-	Isomaltose [Smart Confirmation]	1.19	9.55E+05	[M+Cl]-	{342.11699}	377.087	377.0861
825.4641 / 10.53 [M-H]-	Saikosaponin A +HCOOH [Smart Confirmation]	10.52	9.92E+05	[M-H]-	{826.47191}	825.465	825.4645
255.0673 / 8.87	Isoliquiritigenin [Smart Confirmation]	8.87	1.07E+06	[M-H]-	{256.07515}	255.068	255.0675
191.0212 / 1.51	Citric acid [Smart Confirmation]	1.51	1.09E+06	[M-H]-	{192.02902}	191.022	191.0204
167.0353 / 6.89 [M+FA-H]-	PHOSPHOENOLPYRUVATE [Smart Confirmation]	6.89	1.10E+06	[M+FA-H]-	{122.03763}	167.036	167.0355

165.0558 / 6.45	3-(4-Hydroxyphenyl)-Propionic Acid [Smart Confirmation]	6.45	1.20E+06	[M-H]-	{166.06362}	165.057	165.056
191.0210 / 2.59	Citric acid [Smart Confirmation]	2.61	1.53E+06	[M-H]-	{192.02881}	191.022	191.0204
341.1091 / 1.38 [M-H]-	TREHALOSE [Smart Confirmation]	1.38	1.60E+06	[M-H]-	{342.11689}	341.11	341.1092
255.0673 / 10.11 [M-H]-	Isoliquiritigenin [Smart Confirmation]	10.11	1.67E+06	[M-H]-	{256.07516}	255.068	255.0675
525.1635 / 7.99 [M+FA-H]-	Albiflorin [Smart Confirmation]	8	1.72E+06	[M+FA-H]-	{480.16586}	525.165	525.1625
417.1191 / 7.44	Liquiritin [Smart Confirmation]	7.43	1.96E+06	[M-H]-	{418.12694}	417.12	417.1193
195.0513 / 1.11 [M-H]-	Gluconic acid [Smart Confirmation]	1.11	2.03E+06	[M-H]-	{196.05914}	195.052	195.0515
215.0342 / 1.12 [M+Cl]-	D-(+)-Mannose [Smart Confirmation]	1.1	2.07E+06	[M+Cl]-	{180.06538}	215.035	215.0332
387.1145 / 1.38 [M+FA-H]-	TREHALOSE [Smart Confirmation]	1.38	2.33E+06	[M+FA-H]-	{342.11682}	387.116	387.1147
611.1630 / 6.35	hydroxysafflor yellow A [Smart Confirmation]	6.36	4.14E+06	[M-H]-	{612.17082}	611.164	611.1636
502.1568 / 6.52 [M+FA-H]-	Amygdalin [Smart Confirmation]	6.53	5.22E+06	[M+FA-H]-	{457.15912}	502.158	502.1572
525.1631 / 7.08	Paeoniflorin +HCOOH [Smart Confirmation]	7.09	5.59E+06	[M-H]-	{526.17091}	525.164	525.162
821.3990 / 10.26 [M-H]-	Glycyrrhizic acid ammonium salt [Smart Confirmation]	10.25	1.01E+07	[M-H]-	{822.40683}	821.4	821.3997

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