Electronic Supplementary Material (ESI) for Molecular Omics.

Supplementary data

A Q-marker screening strategy based on ADME studies and systems biology for Chinese herbal medicine, taking Qianghuo Shengshi decoction in treating rheumatoid arthritis as an example

Jiao Wang [a], Cimin Tao [a], Guangzheng Xu [a], Jiawei Ling [a], Jie Tong [b], Bey Hing Goh [a, c], Yipeng Xu [d], Linghui Qian [a], Yong Chen [a], Xuesong Liu [a], Yongjiang Wu [a], Tengfei Xu [a], *

[a] *College of Pharmaceutical Sciences, Zhejiang University, Hangzhou 310058, China*

[b] *PET Center, Department of Radiology and Biomedical Imaging, Yale School of Medicine, New Haven, CT 06520, USA*

[c] *Biofunctional Molecule Exploratory Research Group, School of Pharmacy, Monash University Malaysia, Bandar Sunway 47500, Malaysia*

[d] *Department of urology, Zhejiang Cancer Hospital, Hangzhou, Zhejiang 310022, China*

[*] **Corresponding author**

E-mail addresses: tfxu@zju.edu.cn.

Contents

Text S1. Information of the standards for compound identification comparison.

The standards including adenine, adenosine, uridine, guanosine, phenylalanine, chlorogenic acid, protocatechuic acid, neochlorogenic acid, chlorogenic acid, cryptochlorogenic acid, caffeic acid, isoorientin, orientin, prim-o-glucosylcimifugin, ferulic acid, neoliquiritin, liquiritin, liquiritin apioside, cimifugin, nodakenin, 3,4-dicaffeoylquinic acid, 3,5-dicaffeoylquinic acid, 5-O-methylvisammioside, 4,5-dicaffeoylquinic acid, isoliquiritin apioside, isoliquiritin, ononin, liquiritigenin, sec-O-glucosylhamaudol, isoliquiritigenin, glycyrrhizic acid, casticin, notopterol, osthole, isoimperatorin, columbianadin, ligustilide, levistolide A (with purity > 98.0%) were purchased from Systech Standard Technical Services Co., Ltd. (Shanghai, China).

Table S1 Identification of 159 compounds in QHSSD by UPLC-Triple-TOF MS.

No	Identification	Formula	mol wt.	Ion form	Measured *m/z*	Predicted *m/z*	Error ppm	RT min	MS^n	Classification	Absorbable component	Refs.
1	Sucrose	$C_{12}H_{22}O_{11}$	342.1162	$[M-H]^-$	341.1089	341.1088	-0.5	1.53	59.0182, 71.0163, 89.0254, 101.0245	Saccharide	No	1
2	Adenine*	$C_5H_5N_5$	135.0545	$[M+H]^+$	136.0618	136.0626	5.9	1.55	65.0174, 54.0037, 67.0329, 119.0376	Nucleoside	No	2
3	Citric acid	$C_6H_8O_7$	192.0270	$[M-H]^-$	191.0197	191.0208	5.4	1.98	57.0432, 67.0214, 85.0326, 87.0095, 111.0113	Organic acid	No	2
4	DL-Pyroglutamic acid	$C_5H_7O_3N$	129.0426	$[M+H]^+$	130.0499	130.0508	6.8	2.14	56.0546, 84.0466	Amino acid	No	2
5	Uridine*	$C_9H_{12}O_6N_2$	244.0695	$[M-H]^-$	243.0623	243.0628	2.1	2.94	82.0321, 81.0306, 110.0277	Nucleoside	No	2
				$[M+H]^+$	245.0768	245.0807	9.6	2.94	133.0150, 150.0408, 108.0202			
6	3',5'-Cyclic GMP	$C_{10}H_{12}N_5O_7P$	345.0474	$[M-H]^-$	344.0402	344.0405	0.8	6.42	113.0345, 113.0467, 96.0087, 70.0301	Nucleoside	Yes	2
				$[M+H]^+$	346.0547	346.0550	0.9	6.43	152.0569, 135.0309, 110.0367, 153.0411			
7	Guanosine*	$C_{10}H_{13}O_5N_5$	283.0917	$[M-H]^-$	282.0844	282.0848	1.3	6.48	133.0153, 150.0415, 108.0201, 66.0123	Nucleoside	No	2
				$[M+H]^+$	284.0990	284.0989	-0.1	6.48	135.0310, 152.0568, 153.04133, 110.0360			
8	Adenosine*	$C_{10}H_{13}O_4N_5$	267.0968	$[M+H]^+$	268.1040	268.1040	-0.2	6.99	136.0621, 119.0358	Nucleoside	No	2
9	Phenylalanine*	$C_9H_{11}O_2N$	165.0790	$[M+H]^+$	166.0863	166.0864	1.1	7.94	103.0556, 77.0415, 120.0820	Amino acid	No	2
10	Protocatechuic acid*	$C_7H_6O_4$	154.0266	$[M-H]^-$	153.0193	153.0204	6.8	8.83	108.0221, 109.0308, 65.0131	Organic acid	No	2
11	L-histidyl-L-proline	$C_{11}H_{16}O_3N_4$	252.1222	$[M+H]^+$	253.1295	253.1298	1.1	9.37	68.0518, 70.0687, 80.0518, 120.0814, 122.0963	Amino acid	No	2
12	Tryptophan	$C_{11}H_{12}O_2N_2$	204.0899	$[M-H]^-$	203.0826	203.0834	3.8	10.42	116.0506, 142.0656, 72.0139	Amino acid	No	2
				$[M+H]^+$	205.0972	205.0974	1.0	10.47	91.0567, 115.0560, 130.0661, 143.0736, 141.0579			
13	Neochlorogenic acid*	$C_{16}H_{18}O_9$	354.0951	$[M-H]^-$	353.0878	353.0877	-0.3	10.43	191.0549, 85.0303, 179.0347, 153.0452	Phenylpropanoid	No	3
14	4-Hydroxybenzoic acid	$C_7H_6O_3$	138.0317	$[M-H]^-$	137.0244	137.0261	8.5	11.49	93.0348, 75.0244, 65.0406	Organic acid	No	4
15	5-Hydroxyferulic acid	$C_{10}H_{10}O_5$	210.0528	$[M-H]^-$	209.0456	209.0463	3.6	11.59	119.0494, 93.0354	Phenylpropanoid	No	2
16	Hydroxy-	$C_7H_{12}O_5$	176.0685	$[M-H]^-$	175.0612	175.0622	5.5	12.02	115.0394	Organic acid	No	2

	heptanedioic acid											
17	Chlorogenic acid glucoside	$C_{22}H_{28}O_{14}$	516.1479	$[M-H]^-$	515.1406	515.1388	0.8	12.11	191.0558, 161.0238, 133.0291, 323.0779	Phenylpropanoid	No	5
				$[M+H]^+$	517.1552	517.1573	0.8	12.11	163.0393, 145.0293, 135.0454			
18	Ferulic acid glucoside	$C_{16}H_{20}O_9$	356.1107	$[M-H]^-$	355.1035	355.1028	0.3	12.54	134.0367, 149.0593, 178.0259	Phenylpropanoid	No	6
				$[M+HCOO]^-$	401.1084	401.1078	1.5	12.54	134.0366, 149.0599, 178.0264			
19	Caffeic acid O-Glucoside	$C_{15}H_{18}O_9$	342.0951	$[M-H]^-$	341.0878	341.0878	-0.1	12.66	179.0338, 135.0446, 134.0364	Phenylpropanoid	No	2
				$[M-H]^-$	341.0878	341.0873	-0.1	12.66	135.0446, 134.0364, 179.0338			
20	Dihydrophaseic acid-O-glucoside	$C_{21}H_{32}O_{10}$	444.1996	$[M-H]^-$	443.1923	443.1908	0.5	12.69	59.0168, 71.0152, 113.0245, 189.1273, 237.1480	Sesquiterpene	No	5
21	Lycoperodine-1	$C_{12}H_{12}O_2N_2$	216.0899	$[M+H]^+$	217.0972	217.0972	0.2	12.94	144.0807, 143.0736, 130.0642, 117.0673	Amino acid	No	5
22	Heliotropic acid	$C_8H_6O_4$	166.0266	$[M-H]^-$	165.0193	165.0201	4.4	13.02	77.0379, 147.8875	Organic acid	No	7
23	Adicardin	$C_{20}H_{24}O_{12}$	456.1268	$[M+H]^+$	457.1341	457.1343	0.5	13.07	163.0391, 136.0782	Coumarin	No	
24	Chlorogenic acid*	$C_{16}H_{18}O_9$	354.0951	$[M-H]^-$	353.0878	353.0882	1.0	13.19	191.0553, 127.0397, 85.0313	Phenylpropanoid	No	3
				$[M+H]^+$	355.1024	355.1027	0.9	13.19	163.0397, 145.0295, 135.0453, 89.0417, 193.0499			
25	Vanillic acid	$C_8H_8O_4$	168.0423	$[M-H]^-$	167.0350	167.0358	5.1	13.65	77.0468	Organic acid	No	8
26	Cryptochlorogenic acid*	$C_{16}H_{18}O_9$	354.0951	$[M-H]^-$	353.0878	353.0881	0.8	13.72	191.0550, 179.0337, 135.0442, 85.0302	Phenylpropanoid	No	4
				$[M+H]^+$	355.1024	355.1032	2.4	13.72	163.0391, 145.0290, 133.0288, 89.0419, 193.0498			
27	Caffeic acid*	$C_9H_8O_4$	180.0423	$[M-H]^-$	179.0350	179.0361	6.2	13.97	134.0375, 135.0448, 89.0413	Phenylpropanoid	Yes	7
28	Liquiritigenin-7, 4'-diglucoside	$C_{27}H_{32}O_{14}$	580.1792	$[M-H]^-$	579.1719	579.1724	0.9	15.01	255.0656, 135.0081, 119.0498, 91.0185, 417.1198	Dihydroflavonoid	No	8
29	3-p-Coumaroylquinic acid	$C_{16}H_{18}O_8$	338.1002	$[M-H]^-$	337.0929	337.0932	0.8	15.89	191.0553, 119.0496	Phenylpropanoid	No	4
30	Vicenin-2	$C_{27}H_{30}O_{15}$	594.1585	$[M-H]^-$	593.1512	593.1512	0.2	16.76	353.0671, 383.0783, 203.0362, 503.1213	Flavonoid	No	1
				$[M+H]^+$	595.1658	595.1659	0.3	16.76	409.0959, 457.1163, 307.0592, 295.0621			
31	Angelitriol	$C_{15}H_{18}O_6$	294.1103	$[M+H]^+$	295.1176	295.1179	0.8	17.22	191.0344, 175.0393, 131.0501, 91.0566,	Coumarin	Yes	9

									205.0499			
32	Trans-P-Hydroxycinnamic acid	$C_9H_8O_3$	164.0473	$[M-H]^-$	163.0401	163.0415	8.7	17.70	119.0507, 117.0351, 116.0266, 93.0356	Phenylpropanoid	No	10
33	Methyl chlorogenate	$C_{17}H_{20}O_9$	368.1107	$[M-H]^-$	367.1035	367.1037	0.7	17.78	191.0554, 193.0497, 134.0373, 93.0359	Phenylpropanoid	Yes	11
				$[M+H]^+$	369.1180	369.1183	0.9	17.88	145.0296, 177.0553, 117.0350, 89.0413			
34	Schaftoside	$C_{26}H_{28}O_{14}$	564.1479	$[M-H]^-$	563.1406	563.1408	0.3	19.79	353.0674, 383.0785, 443.0998, 473.1107, 297.0771	Flavonoid	No	1
35	Isoorientin*	$C_{21}H_{20}O_{11}$	448.1006	$[M-H]^-$	447.0933	447.0934	0.3	19.84	327.0511, 357.0639, 297.0414, 298.0493, 285.0408, 133.0289	Flavonoid	No	4
				$[M+H]^+$	449.1078	449.1084	0.6	19.84	299.0546, 329.0648, 325.0720, 311.0546, 283.0603, 165.0184			
36	Orientin	$C_{21}H_{20}O_{11}$	448.1006	$[M-H]^-$	447.0933	447.0935	0.3	20.23	327.0508, 357.0662, 297.0398, 285.0412, 133.0285	Flavonoid	No	4
				$[M+H]^+$	449.1078	449.1081	1.3	20.23	311.0547, 165.0179, 299.0542			
37	Scopoletin/iso	$C_{10}H_8O_4$	192.0423	$[M+H]^+$	193.0495	193.0497	0.8	20.54	133.0285, 122.0365, 178.0235, 81.0380, 53.0430	Coumarin	No	3
38	Prim-O-Glucosylcimifugin*	$C_{22}H_{28}O_{11}$	468.1632	$[M+H]^+$	469.1704	469.1706	0.4	20.63	307.1174, 290.1149, 259.0599, 233.0447, 213.0552, 189.0550, 159.0445	Chromone	Yes	12
39	Ferulic acid*	$C_{10}H_{10}O_4$	194.0579	$[M-H]^-$	193.0506	193.0516	5.0	20.68	133.0291, 132.0211, 134.0376, 104.0265	Phenylpropanoid	Yes	10
				$[M+H]^+$	195.0652	195.0653	0.6	20.82	89.0420, 78.0502, 134.0371			
40	Agnuside	$C_{22}H_{26}O_{11}$	466.1475	$[M-H]^-$	465.1402	465.1403	0.2	20.85	285.0770, 137.0241, 92.0274, 165.0548	Iridoid	No	4
41	Bisabolangelone	$C_{15}H_{20}O_3$	248.1412	$[M+H]^+$	249.1485	249.1487	0.7	20.90	123.0808, 128.0632, 131.0504, 91.0557, 159.0812	Sesquiterpene	No	9
42	Heratomol-6-O-β-D-glucopyranoside	$C_{17}H_{16}O_9$	364.0794	$[M+H]^+$	365.0867	365.0873	1.6	21.37	203.0333, 147.0440, 131.0494, 91.0559	Coumarin	No	3
43	Neoliquiritin*	$C_{21}H_{22}O_9$	418.1264	$[M-H]^-$	417.1191	417.1191	0.0	21.84	119.0505, 135.0082, 91.0198, 255.0658	Dihydroflavonoid	No	2
				$[M+H]^+$	419.1337	419.1347	2.5	21.84	137.0243, 147.0452, 119.0511, 257.0816			
44	Decuroside V	$C_{20}H_{24}O_{10}$	424.1370	$[M+H]^+$	425.1442	425.1446	0.9	21.86	187.0395, 191.0330, 184.0532, 131.0495, 143.0498, 91.0608	Coumarin	No	13

45	Psoralen/iso	$C_{11}H_6O_3$	186.0317	$[M+H]^+$	187.0390	187.0394	2.3	21.88	131.0494, 115.0545, 53.0435, 89.0428	Coumarin	Yes	13
46	Liquiritin*	$C_{21}H_{22}O_9$	418.1264	$[M-H]^-$	417.1191	417.1190	-0.2	22.54	119.0500, 135.0081, 91.0200, 148.0157, 255.0650	Dihydroflavonoid	Yes	2
				$[M+H]^+$	419.1337	419.1345	2.0	22.54	137.0248, 147.0451, 165.0721, 257.0816			
47	Liquiritin apioside*	$C_{26}H_{30}O_{13}$	550.1686	$[M-H]^-$	549.1614	549.1619	0.9	23.08	255.0656, 135.0083, 119.0503, 91.0201	Dihydroflavonoid	Yes	2
				$[M+H]^+$	551.1759	551.1759	0.0	23.08	137.0250, 147.0444, 257.0826			
48	Columbianin	$C_{26}H_{34}O_{14}$	570.1949	$[M+H]^+$	571.2021	571.2027	0.9	23.08	137.0242, 165.0706, 81.0369	Coumarin	No	9
49	Ammijin	$C_{20}H_{24}O_9$	408.1420	$[M+HCOO]^-$	453.1397	453.1401	0.9	24.12	227.0700, 211.0386	Coumarin	No	3
				$[M+H-glu]^+$	247.0970	247.0970	0.0	24.12	91.0571, 147.0442, 175.0386, 213.0527, 229.0862			
50	Senkyunolide G/K	$C_{12}H_{16}O_3$	208.1099	$[M+H]^+$	209.1172	209.1174	1.0	24.13	53.0456, 65.0428, 79.0574, 77.0419, 91.0574, 107.0503, 115.0545, 128.0628, 153.0544	Phthalide	No	7
51	Cimifugin*	$C_{16}H_{18}O_6$	306.1103	$[M+H]^+$	307.1176	307.1180	1.1	24.22	259.0604, 221.0452, 177.0554, 187.0402, 161.0609, 91.0580	Chromone	Yes	12
52	(+)-Peucedanol	$C_{14}H_{16}O_5$	264.0998	$[M-H]^-$	263.0925	263.0926	0.5	24.24	175.0386, 211.0392, 227.0701, 147.0445, 119.0501, 91.0570	Coumarin	Yes	2
53	Nodakenin*	$C_{20}H_{24}O_9$	408.1420	$[M+HCOO]^-$	453.1397	453.1399	0.4	24.36	227.0694, 211.0382	Coumarin	No	10
				$[M+H]^+$	409.1493	409.1502	2.2	24.36	187.0395, 175.0393, 131.0503, 143.0501, 229.0859, 247.0967			
54	Columbianetin-β-D-glucopyranoside	$C_{20}H_{24}O_9$	408.1420	$[M+H]^+$	409.1493	409.1508	0.6	24.36	187.0395, 175.0393, 131.0503, 143.0501, 229.0859, 247.0967	Coumarin	No	6
55	3,4-Dicaffeoylquinic acid*	$C_{25}H_{24}O_{12}$	516.1268	$[M-H]^-$	515.1195	515.1190	-1.0	24.37	191.0551, 173.0444, 135.0450, 161.0234	Phenylpropanoid	No	11
56	3,5-Dicaffeoylquinic acid*	$C_{25}H_{24}O_{12}$	516.1268	$[M-H]^-$	515.1195	515.1194	-0.2	24.55	191.0558	Phenylpropanoid	No	7
				$[M+H]^+$	517.1341	517.1345	0.9	24.55	163.0396, 145.0295			
57	Columbianetin	$C_{14}H_{14}O_4$	246.0892	$[M+H]^+$	247.0965	247.0967	0.9	24.80	147.0452, 175.0396, 91.0575	Coumarin	Yes	6

58	5-O-Methylvisammiosi de*	$C_{22}H_{28}O_{10}$	452.1683	$[M+H]^+$	453.1755	453.1751	-0.9	24.84	243.0645, 241.0865, 216.0413, 217.0492, 205.0496, 291.1226	Chromone	Yes	14
59	6'-Acetyl glycyrrhizin	$C_{24}H_{24}O_{12}$	504.1268	$[M-H]^-$	503.1195	503.1195	-0.1	24.88	135.0075, 119.0491, 91.0189, 255.0649	Dihydroflavo noid	No	15
					505.1341	505.1346	1.0	24.91	137.0233, 147.0443, 217.0458, 244.0683, 292.1263			
60	6''-O-Acetylliquiritin	$C_{23}H_{24}O_{10}$	460.1370	$[M-H]^-$	459.1297	459.1301	0.9	24.89	135.0083, 119.0497, 91.0193, 148.0150	Dihydroflavo noid	No	2
				$[M+H]^+$	461.1442	461.1439	-0.7	24.89	137.0242, 147.0453, 257.0808, 279.0882			
61	Azelaic acid	$C_9H_{16}O_4$	188.1049	$[M-H]^-$	187.0976	187.0987	6.1	24.96	95.0571, 123.0791	Organic acid	No	2
62	Diosmin	$C_{28}H_{32}O_{15}$	608.1741	$[M+H]^+$	609.1814	609.1820	1.0	24.96	301.0705, 286.0478, 258.0527	Flavonoid	No	3
63	4,5-Dicaffeoylquinic acid*	$C_{25}H_{24}O_{12}$	516.1268	$[M-H]^-$	515.1195	515.1187	-1.5	25.00	191.0557, 173.0454, 179.0350, 135.0455	Phenylpropa noid	No	11
64	Klysimplexin I	$C_{40}H_{70}O_8$	678.5071	$[M+H]^+$	679.5144	679.5143	-0.1	25.07	301.0703, 308.1233, 286.0471, 258.0524, 209.1635, 661.5085	Diterpene ester	No	11
65	10-O-Vanilloylaucubin	$C_{23}H_{28}O_{12}$	496.1581	$[M-H]^-$	495.1508	495.1508	0.0	25.20	227.0708, 211.0395, 59.0175, 152.0096, 255.0687	Iridoid	Yes	4
66	Isoliquiritin apioside*	$C_{26}H_{30}O_{13}$	550.1686	$[M-H]^-$	549.1614	549.1616	0.4	25.36	135.0086, 119.0502, 255.0663, 91.0197, 148.0160	Chalcone	Yes	2
				$[M+H]^+$	551.1759	551.1756	-0.6	25.36	137.0240, 147.0449, 239.0700, 257.0808			
67	Glycyroside	$C_{27}H_{30}O_{13}$	562.1686	$[M-H]^-$	561.1614	561.1615	0.2	25.49	267.0661, 252.0427, 195.0439	Isoflavonoid	No	2
				$[M+H]^+$	563.1759	563.1759	0.0	25.49	269.0808, 254.0571, 213.0911			
68	Senkyunolide F/iso	$C_{12}H_{14}O_3$	206.0943	$[M+H]^+$	207.1016	207.1019	1.5	25.54	91.0574, 79.0579, 115.0556, 131.0503	Phthalide	Yes	16
69	Isoliquiritin*	$C_{21}H_{22}O_9$	418.1264	$[M-H]^-$	417.1191	417.1198	1.7	25.61	148.0166, 135.0089, 119.506, 255.0664	Chalcone	Yes	2
				$[M+H]^+$	419.1337	419.1340	0.9	25.62	137.0248, 147.0454, 211.0758, 257.0813, 119.0514			
70	4-Methoxycinnamic acid	$C_{10}H_{10}O_3$	178.0630	$[M+H]^+$	179.0703	179.0709	3.5	25.61	65.0424, 91.0586, 147.0447	Phenylpropa noid	No	4
71	Ononin*	$C_{22}H_{22}O_9$	430.1264	$[M+H]^+$	431.1337	431.1340	0.8	25.76	269.0811, 253.0503, 213.0917, 181.0653	Isoflavonoid	No	17

72	Ulopterol	$C_{15}H_{18}O_5$	278.1154	$[M+H]^+$	279.1227	279.1232	1.9	26.02	161.0604, 177.0548, 203.0704, 131.0503, 105.0713	Coumarin	No	9
73	Liquiritigenin*	$C_{15}H_{12}O_4$	256.0736	$[M-H]^-$	255.0663	255.0671	3.0	26.23	119.0509, 91.0202	Dihydroflavonoid	Yes	2
				$[M+H]^+$	257.0808	257.0812	1.4	26.23	137.0242, 147.0453, 91.0567, 81.0368			
74	24-Hydroxy-licoricesaponin A3	$C_{48}H_{72}O_{22}$	1000.4515	$[M-H]^-$	999.4443	999.4444	0.4	26.38	8377.4054, 351.0582, 193.0354	Triterpene saponin	No	2
				$[M+H]^+$	1001.4588	1001.4597	0.9	26.39	469.3300, 487.3404, 451.3184, 217.0492, 205.0492, 631.3810, 649.3952, 825.4259			
75	Khellinquinone	$C_{12}H_6O_5$	230.0215	$[M+H]^+$	231.0288	231.0288	-1.3	26.39	188.0117, 160.0178, 132.0213	Anthraquinon	Yes	18
76	Bergaptol	$C_{11}H_6O_4$	202.0266	$[M-H]^-$	201.0193	201.0206	6.1	26.40	117.0354, 145.0300, 173.0239, 65.0058	Coumarin	Yes	13
77	5-O-Methylvisamminol	$C_{16}H_{18}O_5$	290.1154	$[M+H]^+$	291.1227	291.1232	1.6	26.50	243.0656, 205.0498, 203.0347, 161.0603	Chromone	Yes	12
78	Formononetin	$C_{16}H_{12}O_4$	268.0736	$[M-H]^-$	267.0663	267.0671	3.0	26.51	195.0447, 223.0401, 167.0496, 251.0359, 252.0438	Isoflavonoid	No	2
79	Sec-O-Glucosylhamaudol*	$C_{21}H_{26}O_{10}$	438.1526	$[M+H]^+$	439.1599	439.1599	0.1	26.55	205.0499, 259.0970, 277.1077, 217.0498, 189.0551, 177.0550	Chromone	Yes	14
80	6'-O-Trans-feruloylnodakenin	$C_{30}H_{32}O_{12}$	584.1894	$[M-H]^-$	583.1821	583.1837	2.7	26.72	175.0394, 160.0155, 193.0498, 211.0389, 227.0703, 235.0605	Coumarin	No	3
81	Oxypeucedanin hydrate	$C_{16}H_{16}O_6$	304.0947	$[M+H]^+$	305.1020	305.1022	0.7	26.73	147.0449, 203.0340, 131.0502	Coumarin	Yes	13
82	Uralsaponin F	$C_{44}H_{64}O_{19}$	896.4042	$[M-H]^-$	895.3969	895.3988	2.1	26.76	351.0580, 193.0352, 113.0242	Triterpene saponin	No	12
				$[M+H]^+$	897.4115	897.4117	0.3	26.76	527.3357, 545.3468, 509.3246, 467.3154			
83	Licoricesaponin A3	$C_{48}H_{72}O_{21}$	984.4566	$[M-H]^-$	983.4493	983.4523	3.0	26.84	821.4083, 803.3977, 645.3701, 351.0578, 193.0349	Triterpene saponin	No	12
				$[M+H]^+$	985.4639	985.4631	-0.8	26.85	453.3356, 471.3465, 615.3886			
84	22-Hydroxy-licoricesaponin G2	$C_{42}H_{62}O_{18}$	854.3936	$[M+H]^+$	855.4009	855.4065	0.4	26.87	485.3260, 503.3353, 467.3152	Triterpene saponin	No	15
85	5-Hydroxyaurapten	$C_{19}H_{22}O_4$	314.1518	$[M+H]^+$	315.1591	315.1597	1.0	27.01	163.0397, 107.0503, 175.0383, 79.0638	Coumarin	No	3

	e											
86	Uralsaponin X	$C_{50}H_{74}O_{22}$	1026.4672	$[M-H]^-$	1025.4599	1025.4636	3.6	27.02	497.1175, 321.0821	Triterpene saponin	No	2
87	Rubranoside A	$C_{25}H_{34}O_{10}$	494.2152	$[M+H]^+$	495.2225	495.2224	-0.1	27.02	163.0394, 153.1275, 175.0393, 135.1177, 107.0872	Polyphenol glycoside	No	11
88	Persicogenin	$C_{17}H_{16}O_6$	316.0947	$[M+H]^+$	317.1020	317.1019	-0.4	27.03	163.0397, 175.0383, 107.0503, 79.0638, 200.0499, 297.1481	Dihydroflavonoid	No	13
89	22β-Acetoxyl-glycyrrhizin	$C_{44}H_{64}O_{18}$	880.4093	$[M-H]^-$	879.4020	879.4046	3.0	27.46	351.0585, 193.0350, 175.0242, 113.0248	Triterpene saponin	No	2
90	Psoralen/iso	$C_{11}H_6O_3$	186.0317	$[M+H]^+$	187.0390	187.0395	2.8	27.78	131.0502, 115.0558, 77.0427, 53.0449	Coumarin	Yes	18
91	3-Butylidenephthalide	$C_{12}H_{12}O_2$	188.0837	$[M+H]^+$	189.0910	189.0913	1.5	27.85	128.0630, 115.0556, 91.0571, 141.0717	Phthalide	No	16
92	24-Hydroxyl-licoricesaponin E2	$C_{42}H_{60}O_{17}$	836.3831	$[M-H]^-$	835.3758	835.3764	2.8	27.85	351.0571, 269.0814, 193.0347, 113.0232	Triterpene saponin	No	2
93	Bergapten or iso	$C_{12}H_8O_4$	216.0423	$[M+H]^+$	217.0495	217.0498	1.0	28.50	89.0417, 90.0487, 174.0315, 161.0600	Coumarin	No	12
94	Licoricesaponine E2/iso	$C_{42}H_{60}O_{16}$	820.3881	$[M-H]^-$	819.3809	819.3844	4.3	29.00	351.0571, 193.0338, 175.0235	Triterpene saponin	No	2
95	Licoricesaponin G2	$C_{42}H_{62}O_{17}$	838.3987	$[M-H]^-$	837.3914	837.3946	3.8	29.06	351.0578, 661.3670, 289.0562, 193.0346, 175.0241, 113.0248	Triterpene saponin	No	2
				$[M+H]^+$	839.4060	839.4058	-0.2	29.07	469.3302, 487.3417, 451.3208, 439.3202, 141.0190			
96	Isoliquiritigenin*	$C_{15}H_{12}O_4$	256.0736	$[M-H]^-$	255.0663	255.0668	2.0	29.20	119.0504, 91.0194	Chalcone	Yes	2
				$[M+H]^+$	257.0808	257.0810	0.6	29.20	137.0244, 165.0403, 81.0368,91.0569			
97	Angelol A/ D/ K / G	$C_{20}H_{24}O_7$	376.1522	$[M-H]^-$	375.1449	375.1452	0.8	29.25	99.0453, 161.0239, 189.0174, 227.0692, 255.0624	Coumarin	No	13
				$[M+H]^+$	377.1595	377.1593	-0.6	29.27	191.0337, 160.0526, 131.0507, 205.0497			
98	Cnidilin	$C_{17}H_{16}O_5$	300.0998	$[M+H]^+$	301.1071	301.1073	0.8	29.27	131.0499, 55.0605, 83.0515, 187.0400, 219.0671	Coumarin	No	13
99	Scoparone	$C_{11}H_{10}O_4$	206.0579	$[M+H]^+$	207.0652	207.0651	-0.5	29.40	149.0240, 91.0569, 164.0466, 163.0400, 191.0345	Coumarin	No	9
100	3-Butyl-4-hydroxyphthalein/ 3-Butyl-5-hydroxyphthalein	$C_{12}H_{14}O_3$	206.0943	$[M-H]^-$	205.0870	205.0879	4.3	29.45	92.0266, 130.0432, 161.0986	Phthalide	No	8

101	Angelol L/C/iso	$C_{20}H_{26}O_7$	378.1679	$[M-H]^-$	377.1606	377.1607	0.2	29.63	101.0606, 157.0289, 257.0821	Coumarin	Yes	13
102	Phellopterin	$C_{17}H_{16}O_5$	300.0998	$[M+H]^+$	301.1071	301.1074	0.8	29.78	131.0497, 55.0605, 83.0533, 187.0393, 219.0640, 217.0479	Coumarin	No	11
103	3′-O-Angeloylhamaudol	$C_{20}H_{22}O_6$	358.1416	$[M+H]^+$	359.1489	359.1490	0.1	29.78	187.0394, 131.0504, 55.0609, 83.0527, 219.0651, 273.1107	Chromone	No	9
104	6,7-Epoxyligustilide	$C_{12}H_{14}O_3$	206.0943	$[M-H]^-$	205.0870	205.0881	5.3	29.89	130.0426, 161.0989, 81.0356	Phthalide	No	7
105	Bergapten or iso	$C_{12}H_8O_4$	216.0423	$[M+H]^+$	217.0495	217.0497	1.0	29.95	89.0420, 174.0321, 90.0497, 118.0429	Coumarin	No	14
106	Pimpinellin	$C_{13}H_{10}O_5$	246.0528	$[M+H]^+$	247.0601	247.0603	0.7	30.16	217.0127, 189.0179, 133.0288, 95.0150	Coumarin	No	12
107	Senkyunolide G/K	$C_{12}H_{16}O_3$	208.1099	$[M-H]^-$	207.1027	207.1038	5.6	30.21	83.0505, 107.0576, 161.0987	Phthalide	No	7
108	Angelol L/C/iso	$C_{20}H_{26}O_7$	378.1679	$[M+H]^+$	379.1751	379.1748	-0.9	30.40	191.0340, 205.0492, 259.0956, 175.0391, 131.0503, 91.0572	Coumarin	Yes	13
109	Columbianetin propionate	$C_{17}H_{18}O_5$	302.1154	$[M+H]^+$	303.1227	303.1227	0.1	30.41	131.0503, 187.0390, 219.0658, 135.0812, 57.0763	Coumarin	No	9
110	Glycyrrhizic acid*	$C_{42}H_{62}O_{16}$	822.4038	$[M-H]^-$	821.3965	821.3982	2.1	30.47	351.0575, 645.3729, 289.0569, 193.0351, 113.0255	Triterpene saponin	Yes	2
				$[M+H]^+$	823.4111	823.4089	-2.6	30.50	453.3349, 435.3246, 471.3454			
111	Melliferone	$C_{30}H_{44}O_3$	452.3291	$[M+H]^+$	453.3363	453.3356	-1.5	30.51	107.0879, 189.1644, 217.1589, 241.1954, 389.3209	Triterpene	No	17
112	Senkyunolide F	$C_{12}H_{14}O_3$	206.0943	$[M-H]^-$	205.0870	205.0879	4.5	30.78	131.0508, 130.0424, 161.0992, 106.0422, 65.0087	Phthalide	No	16
113	7-O-Isoprene-umbellifolactone	$C_{14}H_{14}O_3$	230.0943	$[M-H]^-$	229.0870	229.0871	3.2	31.15	145.0293, 173.0234, 174.0318, 117.0352	Coumarin	No	3
114	4-Hydroxy-3-butylidenephthalide/5-Hydroxy-3-butylidenephthalide	$C_{12}H_{12}O_3$	204.0786	$[M-H]^-$	203.0714	203.0723	4.6	31.33	145.0286, 173.0241	Phthalide	No	16
115	4-Hydroxy-3-butylidenephthalide/5-Hydroxy-3-butylidenephthalide	$C_{12}H_{12}O_3$	204.0786	$[M-H]^-$	203.0714	203.0730	8.0	32.35	145.0299, 173.0243, 117.0371, 92.0292	Phthalide	No	16

116	Uralsaponin C/Licoricesaponin J2	$C_{42}H_{64}O_{16}$	824.4194	$[M-H]^-$	823.4122	823.4148	3.2	31.69	351.0567, 193.0342, 113.0234	Triterpene saponin	No	2
117	Uralsaponin C/Licoricesaponin J2	$C_{42}H_{64}O_{16}$	824.4194	$[M-H]^-$	823.4122	823.4041	-9.8	32.30	351.0583, 193.0354, 175.0253	Triterpene saponin	No	2
118	Uralsaponin C/Licoricesaponin J2	$C_{42}H_{64}O_{16}$	824.4194	$[M-H]^-$	823.4122	823.4147	3.1	33.83	351.0574, 193.0351, 113.0253	Triterpene saponin	No	2
119	Licoricesaponin B2/iso	$C_{42}H_{64}O_{15}$	808.4245	$[M-H]^-$	807.4173	807.4195	2.8	31.96	351.0579, 193.0345, 113.0242	Triterpene saponin	No	2
120	Licoricesaponin K2/H2	$C_{42}H_{62}O_{16}$	822.4038	$[M-H]^-$	821.3965	821.4011	5.6	32.30	351.0580, 645.3728, 193.0353, 113.0255	Triterpene saponin	No	2
				$[M+H]^+$	823.4111	823.4082	-3.5	32.30	453.3373, 435.3242, 471.3459			
121	4-Phenyl-2-butanone	$C_{10}H_{12}O$	148.0888	$[M+H]^+$	149.0961	149.0970	5.9	32.51	91.0570, 79.0578, 115.0562, 105.0716	Aromatic ketone	No	2
122	Thymylisobutyrate	$C_{14}H_{20}O_2$	220.1463	$[M+H]^+$	221.1536	221.1536	0.2	32.51	53.0553, 128.0647	Monoterpene	No	4
123	Licoricesaponin K2/H2	$C_{42}H_{62}O_{16}$	822.4038	$[M-H]^-$	821.3965	821.3990	3.0	33.09	351.0578, 193.0346, 113.0245	Triterpene saponin	No	2
				$[M+H]^+$	823.4111	823.4084	-3.2	33.09	453.3367, 435.3263, 141.0197			
124	Casticin*	$C_{19}H_{18}O_8$	374.1002	$[M+H]^+$	375.1074	375.1075	0.2	33.29	299.0551, 317.0659, 359.0759, 256.0366, 228.0422	Flavonol	No	4
125	Columbianetin acetate	$C_{16}H_{16}O_5$	288.0998	$[M+H]^+$	289.1071	289.1068	-0.7	33.30	131.0503, 187.0391, 91.0570	Coumarin	No	9
126	Isoangenomalin	$C_{14}H_{12}O_3$	228.0786	$[M+H]^+$	229.0859	229.0862	1.4	33.30	131.0497, 129.0708, 128.0637, 187.0383, 53.0495, 213.0519	Coumarin	No	9
127	Psoralen/iso	$C_{11}H_6O_3$	186.0317	$[M+H]^+$	187.0390	187.0395	2.8	33.31	131.0504, 115.0553, 51.0285, 53.0515	Coumarin	Yes	18
128	7-Hydroxy-3-butylidenephthalide	$C_{12}H_{12}O_3$	204.0786	$[M-H]^-$	203.0714	203.0718	5.3	33.86	143.0482, 174.0928, 117.0420	Phthalide	No	16
129	Phenylacetaldehyde	C_8H_8O	120.0575	$[M+H]^+$	121.0648	121.0662	8.9	34.73	51.0296, 51.0441, 50.0345	Aromatic aldehyde	No	2
130	7-O-Prenylscopoletin	$C_{15}H_{16}O_4$	260.1049	$[M-H]^-$	259.0976	259.0982	2.2	34.75	201.0181, 189.0167, 228.0402, 145.0293, 117.0348, 129.0359	Coumarin	No	13
131	Licoricesaponin C2	$C_{42}H_{62}O_{15}$	806.4089	$[M+H]^+$	805.4016	805.4035	2.4	35.10	351.0575, 193.0348, 113.0241	Triterpene saponin	No	2

132	24-Phenylchol-5-ene-3, 24-diol	$C_{30}H_{44}O_2$	436.3341	$[M+H]^+$	437.3414	437.3411	-0.7	35.12	147.1165, 135.0448, 133.1018, 153.0553, 159.1174, 259.1750, 285.1841	Triterpene	No	17
133	Senkyunolide A	$C_{12}H_{16}O_2$	192.1150	$[M+H]^+$	193.1223	193.1226	1.7	35.54	91.0581, 77.0431, 79.0585, 115.0560	Phthalide	No	17
134	Imperatorin	$C_{16}H_{14}O_4$	270.0892	$[M-H]^-$	269.0819	269.0825	2.0	35.63	225.0556, 253.0509, 254.0583, 209.0605, 197.0606, 183.0448	Coumarin	Yes	14
				$[M+H]^+$	271.0965	271.0967	0.6	35.70	131.0503, 91.0565,145.0657			
135	Isolicoflavonol	$C_{20}H_{18}O_6$	354.1103	$[M-H]^-$	353.1031	353.1033	0.6	37.60	125.0239, 57.0383, 199.0392, 216.0414, 201.0910, 228.0777, 284.0317	Flavonol	No	1
136	3′-O-Acetylhamaudol	$C_{17}H_{18}O_6$	318.1103	$[M+H]^+$	319.1176	319.1177	0.2	39.07	205.0492, 217.0496, 189.0549, 149.0230, 128.0639, 243.0659	Chromone	No	14
137	Notoptol	$C_{21}H_{22}O_5$	354.1467	$[M+Na]^+$	377.1359	377.1358	-0.4	39.65	147.0450, 203.0341, 239.0343, 91.0573	Coumarin	No	3
				$[M+H-H_2O]^+$	337.1434	337.1439	1.4	39.65	147.0446, 203.0335, 211.0395			
138	Notopterol*	$C_{21}H_{22}O_5$	354.1467	$[M+H-H_2O]^+$	337.1434	337.1432	-0.7	39.97	147.0453, 203.0349, 91.0576	Coumarin	Yes	11
139	Cnidilide	$C_{12}H_{18}O_2$	194.1307	$[M+H]^+$	195.1380	195.1382	1.0	39.83	79.0577, 77.0425, 93.0713	Phthalide	No	19
140	Bergaptol	$C_{11}H_6O_4$	202.0266	$[M+H]^+$	203.0339	203.0342	1.6	39.95	91.0577, 65.0440, 119.0511, 131.0509, 147.0452	Coumarin	Yes	3
141	Phenethyl-ferulate	$C_{18}H_{18}O_4$	298.1205	$[M-H]^-$	297.1132	297.1137	1.5	39.97	133.0293, 132.0212, 160.0154, 77.0410, 105.0353, 282.0889	Phenylpropanoid	No	11
142	Butylphthalide	$C_{12}H_{14}O_2$	190.0994	$[M+H]^+$	191.1067	191.1068	1.2	40.04	115.0562, 91.0571, 128.0636, 129.0713, 117.0712	Phthalide	No	8
143	Umbelliferone-7-O-β-D-glucopyranoside	$C_{15}H_{16}O_8$	324.0845	$[M+H]^+$	325.0918	325.0930	1.4	40.04	123.0450, 128.0627, 147.0424, 69.0055	Coumarin	No	5
144	Octadecanedioic acid	$C_{18}H_{34}O_4$	314.2457	$[M-H]^-$	313.2384	313.2387	0.8	40.10	127.1103, 137.0967, 171.1026, 201.1130, 199.0977, 277.2147	Organic acid	No	4
145	Osthole*	$C_{15}H_{16}O_3$	244.1099	$[M+H]^+$	245.1172	245.1171	-0.3	40.51	77.0430, 131.0501, 115.0561	Coumarin	No	13
146	Gancaonin M	$C_{20}H_{16}O_6$	352.0947	$[M-H]^-$	351.0874	351.0877	0.8	40.88	199.0758, 267.0648, 283.0963, 183.0442, 107.0510	Isoflavonoid	No	5
147	Isoimperatorin*	$C_{16}H_{14}O_4$	270.0892	$[M+H]^+$	271.0965	271.0964	0.6	41.03	147.0448, 203.0341, 91.0573	Coumarin	No	3
148	Xanthotoxol	$C_{11}H_6O_4$	202.0266	$[M+H]^+$	203.0339	203.0341	0.9	41.03	91.0573, 65.0434, 119.0500, 131.0506, 147.0448	Coumarin	No	3

149	Hydroxylinolenic acid/iso	$C_{18}H_{30}O_3$	294.2195	$[M-H]^-$	293.2122	293.2124	0.6	41.28	96.9604, 148.0513, 205.1194	Organic acid	No	5
150	Hydroxylinolenic acid/iso	$C_{18}H_{30}O_3$	294.2195	$[M-H]^-$	293.2122	293.2125	0.6	42.41	96.9604, 205.1194	Organic acid	No	5
151	(Alpha)-Hydroxylinoleic acid	$C_{18}H_{32}O_3$	296.2352	$[M-H]^-$	295.2279	295.2285	2.1	42.00	277.2166, 195.1385, 182.5665, 171.1001, 113.0949, 98.9551, 57.0418	Organic acid	No	4
152	Columbianadin*	$C_{19}H_{20}O_5$	328.1311	$[M+H]^+$	329.1384	329.1382	-0.5	41.40	131.0503, 187.0387, 147.0442, 128.0627	Coumarin	No	13
153	Glyasperin A	$C_{25}H_{26}O_6$	422.1729	$[M+H]^+$	423.1802	423.1797	-1.3	42.09	299.0543, 311.0550, 367.1171, 255.0656, 147.0457, 137.0236	Flavonol	No	2
154	Ostruthin	$C_{19}H_{22}O_3$	298.1569	$[M-H]^-$	297.1496	297.1498	0.6	42.34	211.0396, 213.0544, 174.0314, 227.0699, 225.0554	Coumarin	No	3
				$[M+H]^+$	299.1642	299.1639	-1.1	42.34	147.0447, 175.0393, 176.0468, 91.0564, 131.0496			
155	Senkyunolide P	$C_{24}H_{30}O_4$	382.2144	$[M+H]^+$	383.2217	383.2220	0.8	42.67	149.0600, 163.1120, 135.0451, 191.1079, 91.0561, 79.0566	Phthalide	No	8
156	Ligustilide*	$C_{12}H_{14}O_2$	190.0994	$[M+H]^+$	191.1067	191.1069	1.3	42.81	91.0578, 115.0561, 127.0567, 77.0418	Phthalide	No	16
157	Levistolide A*	$C_{24}H_{28}O_4$	380.1988	$[M+H]^+$	381.2060	381.2064	0.9	42.85	191.1069, 173.0962, 149.0604, 135.0451, 91.0567, 79.0689	Diterpene ester	No	17
158	Glycyrrhetinic acid	$C_{30}H_{46}O_4$	470.3396	$[M+H]^+$	471.3469	471.3454	-3.2	42.95	149.0984, 119.0870, 229.8111, 235.1708, 317.2121	Triterpene	Yes	2
159	Ricinolic acid	$C_{18}H_{34}O_3$	298.2508	$[M-H]^-$	297.2435	297.2438	1.0	43.19	183.0122, 79.9570	Organic acid	No	4

* The peak information was compared with the standard compounds

Reference:

1 Y. He, Z. Tu, A. Zhou, H. Liu, L. Gao, Y. Li and C. Li, *Drugs & Clin.*, 2021, **36**, 2246–2254.

2 PubChem, PubChem, https://pubchem.ncbi.nlm.nih.gov/, (accessed January 9, 2023).

3 H. Guo, Beijing University of Chinese Medicine, 2019.

4 Z. Zhang, Y. Huang, Y. Guo, H. Liu, S. Fang and H. Zhang, *J. Chin. Med. Mater.*, 2021, **44**, 1142–1148.

5 X.-F. Cai, Y. Xu, H.-P. Liu, Q. Shang, J.-Q. Qiu and W. Xu, *Zhongguo Zhong Yao Za Zhi Zhongguo Zhongyao Zazhi China J. Chin. Mater. Medica*, 2022, **47**, 343–357.

6 G.-Q. Liu, J. Dong, H. Wang, Y. Hashi and S.-Z. Chen, *Eur. J. Mass Spectrom. Chichester Engl.*, 2012, **18**, 59–69.

7 J. Liu, Y. Zhang, R. Bu, H. Zhao, Y. Zhao, H. Zhang, J. Xu, T. Zhang, L. Wang and C. Liu, *Chin. Tradit. Herb. Drugs*, 2021, **52**, 5496–5513.

8 J. Liu, J. Wei, J. Wu, C. Du and Y. Yan, *Chin. J. Exp. Tradit. Med. Formulae*, 2021, **27**, 1–12.

9 M. Wan, Y. Zhang, Y. Yang, X. Liu, L. Jia and X. Yang, *J. Chin. Pharm. Sci.*, 2019, **28**, 145–159.

10 X. Liu, S. Jiang, K. Xu, H. Sun, Y. Zhou, X. Xu, J. Yi, Y. Gu and L. S. Ding, *J. Ethnopharmacol.*, 2009, **126**, 474–479.

11 X. Ma, Y. Wu, Y. Li, Y. Huang, Y. Liu, P. Luo and Z. Zhang, *Phytochem. Anal. PCA*, 2020, **31**, 355–365.

12 Z. Batsukh, K. Toume, B. Javzan, K. Kazuma, S.-Q. Cai, S. Hayashi, N. Kawahara, T. Maruyama and K. Komatsu, *J. Nat. Med.*, 2020, **74**, 170–188.

13 L. Ai, Central South University, 2007.

14 M. Jia, Shanghai Jiao Tong University, 2016.

15 W. Duan, Y. Li, Y. Zheng, C. Li, T. Lu, L. Chen and G. Peng, *Chin. Tradit. Pat. Med.*, 2020, **42**, 1237–1243.

16 X. Zhang, Peking Union Medical College, 2020.

17 G. Sun, J. Huo, S. Zhang and S. Wang, *Chin. Tradit. Pat. Med.*, 2019, **41**, 3052–3060.

18 S. Wang, J. Huo and G. Sun, *Chin. J. Tradit. Med. Sci. Technol.*, 2019, **26**, 362-367+483.

19 Y. Rong, S. Feng, D. Liu, C. Wu, S. Liang and S. Wang, *Chin. Tradit. Pat. Med.*, 2016, **38**, 1544–1550.

Table S2 The *in vivo* metabolites of the absorbable prototypes detected in plasma, urinary, and fecal samples.

NO.	Biotransformation	Formula	*m/z*	Error/ppm	RT/min	% Score	Source	Parent Compound
1	Loss of C_5H_8+Demethylation and Glucuronide Conjugation	$C_{16}H_{12}O_{10}$	363.0352	-1.7	7.71	84.8	F	Imperatorin
2	Glutathione Conjugation and Oxidation	$C_{25}H_{35}N_3O_{13}S$	618.1973	1.5	8.07	88.4	F	Angelitriol
3	Loss of O and O+Loss of Water	$C_{17}H_{18}O_6$	317.1030	-0.2	9.47	82.0	F	Methyl chlorogenate
4	Loss of $C_{30}H_{44}O_3$+Oxidation and Internal Hydrolysis	$C_{12}H_{20}O_{15}$	403.0724	-1.3	11.80	81.7	F	Glycyrrhizic acid
5	Loss of O+Ethyl to Alcohol	$C_{15}H_{16}O_9$	339.0721	-0.2	12.75	82.8	U	Methyl chlorogenate
6	Sulfate Conjugation	$C_{14}H_{14}O_7S$	327.0526	-2.1	12.84	91.6	F	Columbianetin
7	Loss of $C_{30}H_{44}O_3$+Oxidation and Internal Hydrolysis	$C_{12}H_{20}O_{15}$	403.0723	-1.7	13.26	80.4	F	Glycyrrhizic acid
8	Loss of $C_{30}H_{44}O_3$+Loss of CO	$C_{11}H_{18}O_{12}$	341.0719	-2.0	13.47	84.7	F	Glycyrrhizic acid
9	Loss of CH_2+Glycine Conjugation	$C_{16}H_{19}NO_7$	338.1236	0.5	13.71	88.8	U	Angelitriol
	Loss of C_5H_8O and CH_2+Glycine Conjugation	$C_{16}H_{19}NO_7$	338.1236	0.5	13.71	84.3	U	Angelol L/ Angelol C
10	Oxidation and Glucuronide Conjugation	$C_{21}H_{20}O_{11}$	447.0930	-0.6	13.77	83.9	U	Liquiritigenin
11	Tri-Oxidation	$C_{16}H_{18}O_9$	355.1016	-2.1	13.79	91.6	F	Cimifugin
12	Di-Oxidation and Glucuronide Conjugation	$C_{21}H_{20}O_{12}$	463.0878	-0.8	14.67	82.6	U	Liquiritigenin
13	Demethylation and Di-Oxidation	$C_{20}H_{20}O_{11}$	435.0926	-1.5	14.82	80.0	U	Liquiritin
14	Di-Oxidation	$C_{21}H_{22}O_{11}$	449.1085	-0.9	14.82	83.8	U	Liquiritin

15	Loss of $C_5H_8O_2$+Ethyl to Alcohol	$C_{13}H_{14}O_6$	267.0854	-3.5	15.14	82.6	F	Angelol L/ Angelol C
16	Oxidation and Glucuronide Conjugation	$C_{21}H_{20}O_{11}$	447.0931	-0.4	15.41	85.3	U	Isoliquiritigenin
17	Di-Oxidation and Glucuronide Conjugation	$C_{21}H_{20}O_{12}$	463.0876	-1.2	15.48	83.1	U	Isoliquiritigenin
18	Demethylation to Carboxylic Acid	$C_{16}H_{16}O_8$	337.0912	-1.7	15.50	87.1	F	Cimifugin
19	Di-Oxidation	$C_{21}H_{22}O_{11}$	449.1088	-0.4	15.50	84.3	U	Isoliquiritin
20	Loss of CH_2+Oxidation and Internal Hydrolysis	$C_{15}H_{18}O_7$	311.1114	-3.6	15.65	83.5	F	5-O-Methylvisamminol
	Loss of CH_2+Internal Hydrolysis	$C_{15}H_{18}O_7$	311.1114	-3.6	15.65	83.7	F	Cimifugin
21	Loss of CH_2+Loss of Water	$C_{21}H_{24}O_{10}$	437.1443	0.1	15.71	81.8	F, U	Prim-O-glucosylcimifugin
22	Glucuronide Conjugation	$C_{21}H_{26}O_{12}$	471.1488	-1.9	16.49	83.6	F	Angelitriol
23	Loss of CH_2+Oxidation and Internal Hydrolysis	$C_{15}H_{18}O_7$	311.1130	1.4	16.81	88.5	P	5-O-Methylvisamminol
	Loss of CH_2+Internal Hydrolysis	$C_{15}H_{18}O_7$	311.1130	1.4	16.81	88.5	P	Cimifugin
24	Loss of CH_2+Demethylation and Hydrogenation	$C_{14}H_{16}O_6$	281.1011	-3.2	16.82	87.3	F	Cimifugin
	Loss of CH_2 and $C_6H_{10}O_5$+Demethylation and Hydrogenation	$C_{14}H_{16}O_6$	281.1011	-3.2	16.82	84.2	F	Prim-O-glucosylcimifugin
25	Parent	$C_{15}H_{18}O_6$	295.1167	-3.2	16.82	87.8	F, P	Angelitriol
26	Loss of CH_2+Internal Hydrolysis	$C_{15}H_{18}O_6$	295.1177	0.3	17.16	95.3	P	5-O-Methylvisamminol
27	Parent	$C_{15}H_{18}O_6$	295.1180	1.5	17.17	84.7	U	Angelitriol
28	Loss of O+Methylation	$C_{21}H_{28}O_6$	377.1961	0.6	17.24	84.9	U	Angelol L/ Angelol C
29	Loss of CH_2O and O+Glycine Conjugation	$C_{16}H_{19}NO_5$	306.1330	-2.0	17.65	81.8	F	Angelitriol
	Loss of $C_5H_8O_2$ and CH_2O+Glycine Conjugation	$C_{16}H_{19}NO_5$	306.1330	-2.0	17.65	89.1	F	Angelol L/ Angelol C
30	Parent	$C_{17}H_{20}O_9$	367.1033	-0.4	17.69	81.9	U	Methyl chlorogenate
31	Loss of $C_{30}H_{44}O_3$+Oxidation and Internal Hydrolysis	$C_{12}H_{20}O_{15}$	403.0718	-2.8	18.23	84.0	F	Glycyrrhizic acid
32	Tri-Oxidation and Glucuronide Conjugation	$C_{27}H_{30}O_{14}$	579.1698	-1.8	18.30	90.8	U	Notopterol
33	Loss of CH_2O+Di-Hydrogenation	$C_{16}H_{22}O_8$	341.1249	2.1	18.32	80.0	F	Methyl chlorogenate
34	Loss of CH_2+Di-Oxidation	$C_{21}H_{26}O_{12}$	471.1488	-1.9	18.33	95.1	P	5-O-methylvisammioside
35	Loss of $C_{15}H_{10}O_3$+Demethylation and Glucuronide Conjugation	$C_{16}H_{26}O_{16}$	473.1134	-2.9	18.44	80.0	F	Liquiritin apioside
36	Demethylation to Carboxylic Acid	$C_{16}H_{16}O_7$	321.0960	-2.8	18.53	91.3	F, P	5-O-Methylvisamminol
	Ketone Formation	$C_{16}H_{16}O_7$	321.0960	-2.8	18.53	92.0	F, P	Cimifugin
37	Oxidation and Glucuronide Conjugation	$C_{22}H_{22}O_{11}$	461.1083	-1.3	18.80	81.0	U	Imperatorin
38	Loss of CH_2+Loss of Water	$C_{14}H_{14}O_5$	263.0914	0.0	19.79	94.8	P	Angelitriol
39	Loss of CH_2+Demethylation	$C_{14}H_{14}O_5$	263.0914	0.0	19.79	94.6	P	5-O-Methylvisamminol
	Loss of CH_2O+Demethylation	$C_{14}H_{14}O_5$	263.0914	0.0	19.79	95.1	P	Cimifugin
40	Di-Oxidation	$C_{21}H_{22}O_{11}$	449.1080	-2.2	20.03	84.8	U	Liquiritin
41	Oxidation	$C_{22}H_{28}O_{11}$	469.1702	-0.5	20.05	83.1	F	5-O-methylvisammioside

42	Di-Oxidation	$C_{16}H_{18}O_7$	323.1120	-1.5	20.19	95.4	F, P	5-O-Methylvisamminol
	Oxidation	$C_{16}H_{18}O_7$	323.1120	-1.5	20.19	96.7	F, P	Cimifugin
43	Sulfate Conjugation	$C_{21}H_{22}O_{12}S$	497.0751	-1.7	20.22	86.1	U	Liquiritin
44	Loss of CH_2+Di-Oxidation	$C_{15}H_{16}O_7$	309.0959	-3.1	20.26	80.8	F	5-O-Methylvisamminol
	Loss of CH_2+Oxidation	$C_{15}H_{16}O_7$	309.0959	-3.1	20.26	81.0	F	Cimifugin
45	Demethylation	$C_{13}H_{14}O_5$	251.0912	-0.9	20.30	81.5	F	(+)-Peusedanol
46	Loss of $C_5H_8O_2$ and O+S-Cysteine Conjugation	$C_{18}H_{23}NO_6S$	382.1315	-0.9	20.43	88.6	F	Angelol L/ Angelol C
47	Parent	$C_{22}H_{28}O_{11}$	469.1704	0.0	20.48	81.3	P	Prim-O-glucosylcimifugin
48	Loss of Water	$C_{16}H_{14}O_5$	287.0916	0.7	20.69	80.3	U	Oxypeucedanin hydrate
49	Oxidation and Glucuronide Conjugation	$C_{22}H_{26}O_{12}$	483.1496	-0.3	20.71	81.3	P	5-O-Methylvisamminol
	Glucuronide Conjugation	$C_{22}H_{26}O_{12}$	483.1496	-0.3	20.71	90.9	P	Cimifugin
50	Internal Hydrolysis and Di-Oxidation	$C_{14}H_{16}O_7$	297.0965	-1.3	20.89	81.8	F	Columbianetin
51	Oxidation and Sulfate Conjugation	$C_{16}H_{18}O_9S$	387.0742	-0.7	21.05	92.6	F	5-O-Methylvisamminol
	Sulfate Conjugation	$C_{16}H_{18}O_9S$	387.0742	-0.7	21.05	95.1	F	Cimifugin
52	Loss of $C_{15}H_{10}O_3$+Demethylation and Glucuronide Conjugation	$C_{16}H_{26}O_{16}$	473.1139	-2.0	21.25	88.1	F	Liquiritin apioside
53	Oxidation and Glucuronide Conjugation	$C_{22}H_{22}O_{11}$	461.1083	-1.4	21.36	86.3	U	Imperatorin
54	Loss of O and O+Methylation	$C_{21}H_{28}O_5$	361.2007	-0.6	21.40	85.3	U	Angelol L/ Angelol C
55	Bis-Ketone Formation	$C_{16}H_{14}O_7$	319.0808	-1.3	21.41	82.5	F	5-O-Methylvisamminol
56	Loss of $C_5H_{10}O_2$+Glucuronide Conjugation	$C_{17}H_{14}O_{10}$	379.0661	0.4	21.52	83.1	P	Oxypeucedanin hydrate
57	Loss of $C_5H_{10}O_3$	$C_{11}H_6O_3$	187.0390	0.4	21.75	84.3	P	Oxypeucedanin hydrate
58	Loss of CH_2+Loss of Water	$C_{14}H_{14}O_5$	263.0905	-3.3	21.77	81.8	F	Angelitriol
59	Oxidation	$C_{14}H_{14}O_5$	263.0905	-3.3	21.77	82.0	F	Columbianetin
60	Loss of O+Ethyl to Alcohol	$C_{14}H_{14}O_5$	263.0905	-3.3	21.77	82.0	F	5-O-Methylvisamminol
	Loss of $C_6H_{10}O_6$+Ethyl to Alcohol	$C_{14}H_{14}O_5$	263.0905	-3.3	21.77	81.6	F	5-O-methylvisammioside
	Loss of O and O+Ethyl to Alcohol	$C_{14}H_{14}O_5$	263.0905	-3.3	21.77	82.0	F	Cimifugin
61	Parent	$C_{21}H_{22}O_9$	417.1202	2.6	21.89	85.9	F	Liquiritin
62	Loss of CH_2O+Di-Hydrogenation	$C_{15}H_{20}O_4$	265.1437	1.1	22.04	81.9	U	5-O-Methylvisamminol
63	Internal Hydrolysis and Di-Oxidation	$C_{11}H_8O_7$	253.0336	-2.6	22.46	83.7	F	Bergaptol
64	Decarboxylation	$C_{19}H_{26}O_5$	335.1855	0.7	22.55	86.6	U	Angelol L/ Angelol C
65	Loss of $C_{30}H_{44}O_4$+Demethylation	$C_{11}H_{16}O_{12}$	339.0564	-1.3	22.65	81.4	F	Glycyrrhizic acid
66	Loss of $C_6H_{10}O_5$+Sulfate and Glucuronide Conjugation	$C_{21}H_{20}O_{13}S$	511.0542	-1.9	22.66	80.2	U	Liquiritin
67	Loss of $C_{15}H_{10}O_3$+Demethylation and Glucuronide Conjugation	$C_{16}H_{26}O_{16}$	473.1141	-1.4	22.93	81.1	F	Liquiritin apioside
68	Sulfate Conjugation	$C_{21}H_{22}O_{12}S$	497.0753	-1.3	22.96	81.6	U	Liquiritin
69	Loss of C_5H_8O and CH_2+Demethylation	$C_{13}H_{14}O_6$	267.0866	1.0	23.15	80.8	U	Angelol L/ Angelol C
70	Sulfate Conjugation	$C_{20}H_{26}O_{10}S$	459.1319	-0.2	23.40	87.9	F	Angelol L/ Angelol C

71	Loss of $C_5H_8O_2$ and CH_2O+Glucose Conjugation	$C_{20}H_{26}O_9$	411.1647	-0.6	23.40	98.5	F	Angelol L/ Angelol C
72	Loss of CH_2+Internal Hydrolysis	$C_{15}H_{18}O_6$	295.1171	-1.6	23.48	97.0	F, P	5-O-Methylvisamminol
	Loss of CH_2O+Internal Hydrolysis	$C_{15}H_{18}O_6$	295.1171	-1.6	23.48	97.0	F, P	Cimifugin
73	Loss of $C_9H_6O_4$ and O+Bis-Glucuronide Conjugation	$C_{20}H_{30}O_{16}$	525.1460	-0.2	23.54	81.7	F	Methyl chlorogenate
74	Demethylation and Hydrogenation	$C_{11}H_{14}O_3$	195.1017	0.8	23.70	82.0	U	Senkyunolide F
75	Loss of O	$C_{14}H_{16}O_4$	249.1123	0.8	23.77	91.6	U	(+)-Peusedanol
	Loss of CH_2O and O	$C_{14}H_{16}O_4$	249.1123	0.8	23.77	92.4	U	Angelitriol
76	Oxidation and Methylation	$C_{17}H_{20}O_6$	321.1326	-2.1	23.84	85.6	F	5-O-Methylvisamminol
77	Loss of $C_6H_{10}O_5$+Oxidation and Methylation	$C_{17}H_{20}O_6$	321.1326	-2.1	23.84	84.3	F	5-O-methylvisammioside
	Methylation	$C_{17}H_{20}O_6$	321.1326	-2.1	23.84	85.7	F	Cimifugin
78	Demethylation to Carboxylic Acid	$C_{14}H_{12}O_6$	277.0701	-1.9	23.85	90.0	F, P	Columbianetin
79	Di-Oxidation and Glucuronide Conjugation	$C_{22}H_{22}O_{12}$	477.1027	-2.4	23.98	92.2	U	Imperatorin
80	Oxidation	$C_{16}H_{18}O_6$	307.1168	-2.7	24.06	91.5	F, P	5-O-Methylvisamminol
	Parent	$C_{16}H_{18}O_6$	307.1168	-2.7	24.06	92.0	F, P, U	Cimifugin
81	Ethyl to Carboxylic Acid	$C_{15}H_{14}O_7$	307.0808	-1.3	24.20	92.9	F, P	5-O-Methylvisamminol
	Demethylation and Methylene to Ketone	$C_{15}H_{14}O_7$	307.0808	-1.3	24.20	96.2	F, P	Cimifugin
82	Loss of $C_{30}H_{44}O_4$+Methylation	$C_{13}H_{20}O_{12}$	367.0872	-2.7	24.22	82.9	F	Glycyrrhizic acid
83	Oxidation and Sulfate Conjugation	$C_{15}H_{12}O_8S$	351.0178	-0.5	24.22	92.3	U	Liquiritigenin
84	Parent	$C_{14}H_{16}O_5$	265.1078	2.7	24.28	80.3	P	(+)-Peusedanol
	Loss of CH_2O	$C_{14}H_{16}O_5$	265.1078	2.7	24.28	84.4	P	Angelitriol
85	Glucuronide Conjugation	$C_{20}H_{22}O_{10}$	423.1280	-1.3	24.46	82.3	P	Columbianetin
86	Demethylation	$C_{13}H_{12}O_4$	233.0806	-0.8	24.55	80.3	P	Columbianetin
87	Ketone Formation	$C_{16}H_{12}O_5$	283.0620	2.7	24.59	91.0	U	Imperatorin
88	Oxidation and Glucuronide Conjugation	$C_{21}H_{20}O_{11}$	447.0926	-1.5	24.65	91.7	U	Isoliquiritigenin
	Demethylation to Carboxylic Acid	$C_{21}H_{20}O_{11}$	447.0926	-1.5	24.65	92.1	U	Isoliquiritin
89	Glucuronide Conjugation	$C_{27}H_{30}O_{15}$	593.1502	-1.6	24.72	85.6	U	Isoliquiritin
90	Oxidation	$C_{14}H_{14}O_5$	263.0914	-0.1	24.74	92.3	P	Columbianetin
91	Loss of O+Ethyl to Alcohol	$C_{14}H_{14}O_5$	263.0914	-0.1	24.74	94.8	P	5-O-Methylvisamminol
	Loss of O and O+Ethyl to Alcohol	$C_{14}H_{14}O_5$	263.0914	-0.1	24.74	94.6	P	Cimifugin
92	Loss of O+Loss of Water	$C_{15}H_{16}O_4$	261.1121	-0.3	24.74	89.8	U	Angelitriol
	Loss of $C_5H_8O_2$+Loss of Water	$C_{15}H_{16}O_4$	261.1121	-0.3	24.74	91.4	U	Angelol L/ Angelol C
93	Parent	$C_{22}H_{28}O_{10}$	453.1753	-0.6	24.77	86.4	F	5-O-methylvisammioside
94	Parent	$C_{21}H_{22}O_9$	417.1185	-1.5	24.79	98.1	U	Liquiritin iso
95	Loss of $C_9H_6O_3$+Glucuronide Conjugation	$C_{14}H_{22}O_{12}$	381.1032	-1.6	24.84	86.3	F	Methyl chlorogenate
96	Glucose Conjugation	$C_{22}H_{28}O_{10}$	453.1744	-2.4	24.84	90.6	P	5-O-Methylvisamminol
97	Oxidation and Methylation	$C_{17}H_{18}O_7$	335.1118	-2.2	24.86	84.1	F, P	Oxypeucedanin hydrate
98	Loss of O and O+Sulfoxide to Thioether	$C_{14}H_{16}O_2$	217.1227	1.9	25.02	84.8	U	(+)-Peusedanol

99	Oxidation and Sulfate Conjugation	$C_{16}H_{14}O_8S$	365.0336	-0.2	25.03	87.3	U	Imperatorin
100	Loss of O and O+Methylation	$C_{16}H_{20}O_4$	277.1439	1.7	25.05	93.1	U	Angelitriol
101	Oxidation and Sulfate Conjugation	$C_{15}H_{12}O_8S$	351.0184	1.2	25.17	89.2	U	Liquiritigenin
102	Loss of CH_2O+Di-Acetylation of Amines	$C_{18}H_{20}O_7$	349.1275	-2.0	25.27	84.5	F	Angelitriol
103	Tetra-Oxidation	$C_{21}H_{22}O_9$	419.1332	-1.0	25.30	89.9	F	Notopterol
104	Demethylation and Hydrogenation	$C_{15}H_{14}O_4$	257.0830	4.1	25.34	80.6	U	Imperatorin
105	Loss of $C_6H_{10}O_6$+Internal Hydrolysis	$C_{15}H_{14}O_4$	257.0830	4.1	25.34	83.0	U	Isoliquiritin
106	Loss of O and O+Methylation	$C_{16}H_{20}O_4$	277.1438	1.5	25.35	87.8	U	Angelitriol
	Loss of $C_5H_8O_2$ and O+Methylation	$C_{16}H_{20}O_4$	277.1438	1.5	25.35	90.9	U	Angelol L/ Angelol C
107	Loss of CH_2+Decarboxylation	$C_{20}H_{26}O_8$	395.1694	-1.7	25.49	88.6	F	5-O-methylvisammioside
108	Loss of O and CH_2O+Demethylation to Carboxylic Acid	$C_{15}H_{14}O_5$	275.0916	0.9	25.53	80.1	U	5-O-Methylvisamminol
109	Loss of O and O+Ethyl to Alcohol	$C_{18}H_{22}O_6$	335.1480	-2.6	25.53	89.6	F	Angelol L/ Angelol C
110	Bis-Ketone Formation	$C_{21}H_{18}O_7$	383.1126	0.1	25.57	93.9	U	Notopterol
111	Parent	$C_{21}H_{22}O_9$	417.1186	-1.2	25.57	95.6	U	Isoliquiritin
112	Loss of $C_6H_{10}O_6$+Demethylation to Carboxylic Acid	$C_{15}H_{10}O_5$	269.0462	2.4	25.59	86.2	U	Isoliquiritin
113	Ketone Formation	$C_{20}H_{24}O_8$	393.1541	-0.8	25.60	97.9	F	Angelol L/ Angelol C
114	Oxidation	$C_{21}H_{22}O_{10}$	433.1129	-2.6	25.65	84.8	P	Isoliquiritin
115	Loss of CH_2+Oxidation	$C_{19}H_{24}O_8$	381.1544	-0.1	25.77	85.1	U	Angelol L/ Angelol C
116	Loss of CH_2O+Glycine Conjugation	$C_{21}H_{27}NO_7$	406.1860	-0.1	25.77	85.9	U	Angelol L/ Angelol C
117	Loss of CH_2+Oxidation	$C_{15}H_{16}O_6$	293.1009	-3.5	25.82	85.9	F, P	5-O-Methylvisamminol
	Loss of CH_2	$C_{15}H_{16}O_6$	293.1009	-3.5	25.82	85.9	F, P	Cimifugin
118	Loss of O and O+Loss of Water	$C_{14}H_{14}O_2$	215.1067	0.0	25.93	88.3	U	(+)-Peusedanol
119	Loss of CH_2O+Internal Hydrolysis	$C_{15}H_{18}O_5$	279.1217	-3.5	25.95	88.0	F	5-O-Methylvisamminol
	Loss of CO	$C_{15}H_{18}O_5$	279.1217	-3.5	25.95	87.9	F	Cimifugin
120	Di-Oxidation	$C_{16}H_{14}O_6$	301.0723	1.7	25.97	87.9	U	Imperatorin
121	Desaturation	$C_{16}H_{16}O_5$	289.1071	0.3	26.00	84.9	U	5-O-Methylvisamminol
122	Decarboxylation	$C_{20}H_{22}O_7$	373.1286	-1.8	26.00	85.9	P	Isoliquiritin
123	Oxidation	$C_{21}H_{22}O_{10}$	433.1133	-1.7	26.00	89.0	U	Isoliquiritin
124	Loss of O+Bis-Ketone Formation	$C_{21}H_{18}O_6$	367.1170	-1.6	26.05	87.3	F	Notopterol
125	Loss of $C_5H_{10}O_3$+Hydrogenation	$C_{11}H_8O_3$	189.0549	1.5	26.07	80.1	P	Oxypeucedanin hydrate
126	Loss of CH_2O+Loss of Water	$C_{15}H_{14}O_3$	243.1014	-0.6	26.07	86.9	P	5-O-Methylvisamminol
127	Loss of CH_2O	$C_{15}H_{16}O_4$	261.1122	0.1	26.07	94.4	P	5-O-Methylvisamminol
128	Loss of CH_2O and O	$C_{15}H_{16}O_4$	261.1122	0.1	26.07	94.4	P	Cimifugin
129	Parent	$C_{15}H_{12}O_4$	255.0665	0.8	26.22	89.0	P	Liquiritigenin
130	Loss of CH_2O and O+Di-Acetylation of Amines	$C_{20}H_{22}O_9$	405.1202	2.6	26.23	85.5	F	Methyl chlorogenate
131	Bis-Ketone Formation	$C_{20}H_{22}O_9$	407.1335	-0.5	26.26	88.1	F	Angelol L/ Angelol C

132	Glucuronide Conjugation	$C_{26}H_{34}O_{13}$	555.2065	-1.2	26.33	85.8	F	Angelol L/ Angelol C
133	Loss of CH_2O+Di-Hydrogenation	$C_{16}H_{22}O_8$	341.1244	0.6	26.35	82.3	U	Methyl chlorogenate
134	Loss of CH_2O+Demethylation	$C_{14}H_{14}O_4$	247.0966	0.4	26.37	94.6	F, P	5-O-Methylvisamminol
	Loss of CH_2O and O+Demethylation	$C_{14}H_{14}O_4$	247.0966	0.4	26.37	96.6	F, P	Cimifugin
135	Hydrogenation	$C_{12}H_{16}O_3$	209.1173	0.2	26.40	80.6	U	Senkyunolide F
136	Parent	$C_{16}H_{18}O_5$	291.1217	-3.6	26.43	87.6	F	5-O-Methylvisamminol
	Loss of O	$C_{16}H_{18}O_5$	291.1230	1.0	26.50	96.3	P, F	Cimifugin
137	Ketone Formation	$C_{12}H_{12}O_4$	221.0810	0.7	26.53	80.6	U	Senkyunolide F
138	Loss of O+Sulfate Conjugation	$C_{14}H_{14}O_6S$	311.0585	0.3	26.64	87.2	P	Columbianetin
139	Oxidation and Methylation	$C_{18}H_{22}O_{10}$	397.1138	-0.5	26.66	89.8	U	Methyl chlorogenate
140	Decarboxylation	$C_{15}H_{18}O_3$	247.1331	0.8	26.67	88.5	U	5-O-Methylvisamminol
141	Parent	$C_{16}H_{16}O_6$	305.1012	-2.5	26.67	91.3	F, P	Oxypeucedanin hydrate
142	Loss of O and CH_2O+Methylation	$C_{16}H_{18}O_3$	259.1329	0.1	26.67	83.4	U	5-O-Methylvisamminol
143	Ketone Formation	$C_{16}H_{16}O_6$	305.1017	-0.8	26.72	86.1	P	5-O-Methylvisamminol
	Desaturation	$C_{16}H_{16}O_6$	305.1017	-0.8	26.72	86.6	P	Cimifugin
144	Loss of CH_2O+Di-Acetylation of Amines	$C_{18}H_{20}O_7$	349.1282	-0.1	26.76	84.1	P	Angelitriol
145	Loss of CH_2+Loss of CO	$C_{13}H_{16}O_5$	253.1069	-0.5	26.84	90.4	U	Angelitriol
	Loss of C_5H_8O and CH_2+Loss of CO	$C_{13}H_{16}O_5$	253.1069	-0.5	26.84	89.2	U	Angelol L/ Angelol C
146	Glucuronide Conjugation	$C_{21}H_{20}O_{10}$	431.0975	-2.1	26.94	93.2	U	Liquiritigenin
	Loss of $C_6H_{10}O_5$+Glucuronide Conjugation	$C_{21}H_{20}O_{10}$	431.0975	-2.1	26.94	80.5	U	Liquiritin
147	Loss of CH_2O and O+Demethylation	$C_{13}H_{14}O_4$	235.0962	-1.0	26.98	83.2	P	Angelitriol
148	Demethylation and Hydrogenation	$C_{13}H_{14}O_4$	235.0962	-1.0	26.98	83.3	P	Columbianetin
149	Loss of CH_2O+Di-Hydrogenation	$C_{14}H_{20}O_5$	269.1381	-1.0	26.99	87.3	U	Angelitriol
150	Oxidation and Internal Hydrolysis	$C_{21}H_{24}O_7$	389.1590	-1.3	27.06	95.1	F	Notopterol
151	Ketone Formation	$C_{16}H_{14}O_7$	319.0817	1.4	27.08	81.0	P	Oxypeucedanin hydrate
152	Loss of O and O+Sulfoxide to Thioether	$C_{20}H_{26}O_4$	331.1914	3.0	27.15	84.0	U	Angelol L/ Angelol C
153	Desaturation	$C_{14}H_{12}O_4$	245.0812	1.6	27.17	90.4	P	Columbianetin
154	Demethylation and Oxidation	$C_{15}H_{12}O_5$	271.0618	2.1	27.19	95.2	U	Imperatorin
155	Ethyl to Carboxylic Acid	$C_{20}H_{18}O_7$	371.1121	-1.1	27.30	91.9	F	Notopterol
156	Loss of CH_2O and O+Di-Hydrogenation	$C_{14}H_{20}O_4$	253.1432	-0.8	27.40	93.3	U	Angelitriol
	Loss of $C_5H_8O_2$ and CH_2O+Di-Hydrogenation	$C_{14}H_{20}O_4$	253.1432	-0.8	27.40	92.0	U	Angelol L/ Angelol C
157	Loss of O and O+Demethylation	$C_{15}H_{14}O_4$	259.0966	0.4	27.47	87.1	P	Oxypeucedanin hydrate
158	Loss of CH_2+Loss of Water	$C_{15}H_{14}O_4$	259.0966	0.4	27.47	93.1	P	5-O-Methylvisamminol
	Loss of CH_2O+Loss of Water	$C_{15}H_{14}O_4$	259.0966	0.4	27.47	93.8	P	Cimifugin
159	Loss of CO	$C_{19}H_{26}O_6$	351.1804	0.6	27.51	82.1	U	Angelol L/ Angelol C
160	Loss of CH_2+Decarboxylation	$C_{13}H_{16}O_4$	237.1120	-0.6	27.57	93.2	U	Angelitriol
	Loss of C_5H_8O and CH_2+Decarboxylation	$C_{13}H_{16}O_4$	237.1120	-0.6	27.57	92.9	U	Angelol L/ Angelol C
161	Loss of O+Loss of Water	$C_{16}H_{14}O_4$	271.0962	-1.0	27.57	87.8	U	Oxypeucedanin hydrate
162	Glucuronide Conjugation	$C_{22}H_{22}O_{10}$	445.1134	-1.3	27.58	86.4	U	Imperatorin

163	Oxidation and Methylation	$C_{22}H_{24}O_{10}$	447.1288	-1.9	27.66	87.6	P	Isoliquiritin
164	Loss of $C_6H_{10}O_6$+Demethylation to Carboxylic Acid	$C_{15}H_{10}O_5$	269.0464	3.0	27.70	87.0	U	Isoliquiritin
165	Loss of CH_2O	$C_{21}H_{26}O_9$	423.1649	-0.2	27.71	83.4	F	5-O-methylvisammioside
166	Loss of $C_5H_8O_2$+Glycine Conjugation	$C_{17}H_{21}NO_6$	336.1438	-1.2	27.78	83.9	U	Angelol L/ Angelol C
167	Loss of CH_2O+Loss of Water	$C_{15}H_{14}O_3$	243.1015	-0.4	27.81	94.4	U	5-O-Methylvisamminol
	Loss of CH_2O and O+Loss of Water	$C_{15}H_{14}O_3$	243.1015	-0.4	27.81	81.9	U	Cimifugin
168	Loss of O	$C_{17}H_{20}O_8$	351.1091	1.7	27.86	85.7	F	Methyl chlorogenate
169	Methylation	$C_{22}H_{24}O_5$	369.1695	-0.4	27.91	89.9	F	Notopterol
170	Loss of O	$C_{14}H_{14}O_3$	231.1015	-0.2	28.10	87.6	P	Columbianetin
171	Loss of O and CH_2O+Methylation	$C_{16}H_{18}O_3$	259.1328	-0.2	28.24	86.1	P	5-O-Methylvisamminol
	Loss of O and O+Sulfoxide to Thioether	$C_{16}H_{18}O_3$	259.1328	-0.2	28.24	88.1	P	Cimifugin
172	Loss of O+Hydrogenation	$C_{16}H_{20}O_4$	277.1434	-0.1	28.24	86.4	P	5-O-Methylvisamminol
173	Decarboxylation	$C_{14}H_{18}O_4$	251.1282	1.8	28.27	89.1	U	Angelitriol
	Loss of C_5H_8O+Decarboxylation	$C_{14}H_{18}O_4$	251.1282	1.8	28.27	90.2	U	Angelol L/ Angelol C
174	Oxidation	$C_{21}H_{22}O_6$	371.1483	-1.5	28.31	94.0	F	Notopterol
175	Loss of Water	$C_{14}H_{12}O_3$	229.0860	0.4	28.32	82.2	P	Columbianetin
176	Ketone Formation	$C_{15}H_{10}O_5$	269.0462	2.3	28.38	80.2	U	Isoliquiritigenin
177	Loss of Hydroxymethylene	$C_{15}H_{14}O_5$	275.0915	0.4	28.71	81.9	P	Oxypeucedanin hydrate
178	Loss of O and CH_2O+Demethylation to Carboxylic Acid	$C_{15}H_{14}O_5$	275.0915	0.4	28.71	95.8	P	5-O-Methylvisamminol
179	Loss of CH_2+Loss of Water	$C_{15}H_{14}O_5$	275.0915	0.4	28.71	96.1	P	Cimifugin
180	Oxidation and Methylation	$C_{15}H_{16}O_5$	277.1060	-3.6	28.90	80.7	F	Columbianetin
181	Loss of O	$C_{16}H_{18}O_4$	275.1280	0.9	29.19	84.6	U	5-O-Methylvisamminol
182	Loss of O+Methylation	$C_{16}H_{20}O_5$	293.1376	-2.4	29.19	88.0	U	Angelitriol
183	Internal Hydrolysis	$C_{16}H_{16}O_5$	287.0933	2.8	29.31	81.5	U	Imperatorin
184	Parent	$C_{20}H_{26}O_7$	379.1745	-1.7	29.42	93.3	F	Angelol L/ Angelol C
185	Loss of CH_2+Internal Hydrolysis and Di-Oxidation	$C_{14}H_{18}O_9$	331.1028	1.3	29.43	84.3	U	Angelitriol
	Loss of C_5H_8O and CH_2+Internal Hydrolysis and Di-Oxidation	$C_{14}H_{18}O_9$	331.1028	1.3	29.43	84.2	U	Angelol L/ Angelol C
186	Loss of O and O+Internal Hydrolysis	$C_{16}H_{18}O_5$	291.1227	0.1	29.59	85.7	U	Oxypeucedanin hydrate
187	Desaturation	$C_{20}H_{24}O_7$	377.1586	-2.4	29.66	94.6	F	Angelol L/ Angelol C
188	Loss of O+Demethylation	$C_{20}H_{20}O_4$	325.1426	-2.6	29.79	87.4	F	Notopterol
189	Loss of O and O+Sulfoxide to Thioether	$C_{16}H_{16}O_3$	257.1173	0.4	29.81	84.6	U	Oxypeucedanin hydrate
190	Loss of $C_6H_{10}O_6$ and O	$C_{16}H_{18}O_4$	275.1278	0.0	29.81	84.1	U	Prim-O-glucosylcimifugin
191	Loss of O+Methylation	$C_{16}H_{20}O_5$	293.1383	0.0	29.81	87.1	U	Angelitriol
	Loss of $C_5H_8O_2$+Methylation	$C_{16}H_{20}O_5$	293.1383	0.0	29.81	89.9	U	Angelol L/ Angelol C
192	Loss of CH_2	$C_{15}H_{16}O_5$	277.1059	-4.3	30.23	81.5	F	5-O-Methylvisamminol

	Loss of CH_2O	$C_{15}H_{16}O_5$	277.1059	-4.3	30.23	81.4	F	Cimifugin
193	Parent	$C_{20}H_{26}O_7$	379.1744	-1.9	30.29	95.2	F	Angelol L/ Angelol C
194	Loss of O+Ketone Formation	$C_{21}H_{20}O_5$	353.1376	-2.1	31.36	89.7	F	Notopterol
195	Loss of O and O	$C_{14}H_{16}O_3$	233.1175	1.3	31.77	85.1	U	(+)-Peusedanol
	Loss of O and O+Loss of Hydroxymethylene	$C_{14}H_{16}O_3$	233.1175	1.3	31.77	90.4	U	Angelitriol
	Loss of $C_5H_8O_2$ and O+Loss of Hydroxymethylene	$C_{14}H_{16}O_3$	233.1175	1.3	31.77	91.3	U	Angelol L/ Angelol C
196	Loss of O+Methylation	$C_{13}H_{16}O_2$	205.1224	0.3	31.79	86.9	U	Senkyunolide F
197	Desaturation	$C_{16}H_{14}O_6$	303.0857	-1.9	34.47	85.3	F	Oxypeucedanin hydrate
198	Tri-Oxidation and Demethylation	$C_{20}H_{20}O_8$	389.1222	-2.3	34.66	85.5	F	Notopterol
199	Demethylation and Oxidation	$C_{20}H_{20}O_6$	357.1325	-2.1	34.73	93.6	F	Notopterol
200	Loss of O+Demethylation to Carboxylic Acid	$C_{21}H_{20}O_6$	369.1323	-2.5	34.78	89.1	F	Notopterol
201	Loss of O+Internal Hydrolysis	$C_{21}H_{24}O_5$	357.1690	-1.7	35.25	94.1	F	Notopterol
202	Loss of $C_{16}H_{16}O_6$ and O+Phosphorylation	$C_6H_{13}O_7P$	229.0476	1.7	35.47	81.8	F	Prim-O-glucosylcimifugin
203	Demethylation and Oxidation	$C_{29}H_{44}O_5$	471.3107	-1.9	38.70	95.9	P	Glycyrrhetinic acid
204	Loss of CO	$C_{20}H_{22}O_4$	327.1581	-3.1	39.47	80.5	F	Notopterol
205	Loss of $C_6H_8O_6$	$C_{36}H_{54}O_{10}$	645.3668	3.7	39.80	82.8	F	Glycyrrhizic acid
206	Loss of Water	$C_{21}H_{20}O_4$	337.1422	-3.7	39.84	84.6	F	Notopterol
207	Glucuronide Conjugation	$C_{36}H_{54}O_{10}$	645.3670	3.9	39.92	80.4	F, P	Glycyrrhetinic acid
208	Methylation	$C_{23}H_{30}O_{11}$	483.1864	0.6	40.96	88.4	F	Prim-O-glucosylcimifugin
209	Parent	$C_{30}H_{46}O_4$	469.3341	3.7	42.92	85.1	F, P	Glycyrrhetinic acid
	Loss of $C_{12}H_{16}O_{12}$	$C_{30}H_{46}O_4$	469.3341	3.7	42.92	82.6	F	Glycyrrhizic acid
210	Loss of O+Demethylation and Methylene to Ketone	$C_{29}H_{42}O_4$	453.3024	3.0	42.99	82.1	F	Glycyrrhetinic acid

Table S3 The core genes screening through degree evaluation by CytoHubba.

node_name	MCC	DMNC	MNC	Degree	EPC	BottleNeck	EcCentricity	Closeness	Radiality	Betweenness	Stress	ClusteringCoefficient
STAT3	3257418	0.50959	53	53	28.234	4	0.25	97.58333	6.23333	1336.9	10290	0.31567
SRC	2094684	0.46176	50	52	28.069	9	0.25	96.5	6.21333	2369.616	14570	0.26923
HSP90AA1	1186380	0.43803	52	52	27.763	10	0.2	95.78333	6.17333	1301.028	10018	0.273
AKT1	2991577	0.44523	51	52	27.653	22	0.25	97.41667	6.24	2429.687	15750	0.26848
EGFR	3720089	0.50065	49	50	27.789	54	0.25	96.91667	6.25333	1807.361	12388	0.30531
MAPK3	3781662	0.51003	49	49	28.064	4	0.25	95.91667	6.22	1262.103	10732	0.32398
MAPK1	1987507	0.51293	41	42	25.883	10	0.25	90.83333	6.11333	892.824	7142	0.32869
VEGFA	1862886	0.55684	38	38	25.255	1	0.25	89.25	6.1	719.4835	6402	0.38407
JUN	2619170	0.56071	36	36	24.519	2	0.2	88.23333	6.07333	495.8252	4990	0.39365
PIK3CA	276204	0.56809	34	34	23.147	1	0.25	84.91667	5.98	398.5622	3764	0.40642
TNF	1174004	0.40603	32	32	20.557	4	0.2	84.95	6	1377.296	9346	0.29637
ESR1	1075463	0.52184	31	32	22.894	4	0.25	84.91667	6.00667	941.5557	7332	0.36089
CASP3	1666134	0.52184	31	31	22.033	3	0.2	83.85	5.95333	363.1861	3388	0.38495
GAPDH	461300	0.49911	28	30	21.301	6	0.2	85.61667	6.06	1225.967	7854	0.33103
MAPK14	1578786	0.60082	29	29	23.26	3	0.2	82.9	5.95333	242.6259	2458	0.4532
PTPN11	479506	0.6858	27	29	22.505	3	0.25	82.08333	5.93333	613.8244	4020	0.45813
CXCL12	195729	0.63457	25	28	21.149	7	0.25	83.16667	5.99333	1510.094	8370	0.40212
PTK2	906122	0.68948	27	27	22.225	1	0.25	80.75	5.9	135.4384	1506	0.53276
JAK2	409225	0.60095	25	26	20.609	4	0.25	79	5.84	325.1381	2630	0.44
LCK	724088	0.66819	25	25	21.254	1	0.25	80.08333	5.90667	226.5129	1956	0.53
FGF2	65872	0.54053	24	24	20.224	4	0.2	80.03333	5.90667	232.3133	2238	0.43478
MMP9	791317	0.50845	23	24	18.372	4	0.25	80.83333	5.94667	958.7931	6966	0.38043
CREBBP	75474	0.52298	23	23	18.861	3	0.2	80.48333	5.93333	430.0254	3796	0.42688
AR	7469	0.53428	20	23	18.319	7	0.2	79.4	5.89333	704.2778	5458	0.34783
MTOR	421224	0.56172	23	23	20.049	1	0.2	77.35	5.8	90.15744	1038	0.4585
APP	7721	0.44088	21	22	17.477	8	0.2	78.2	5.86667	813.1936	5984	0.33766

NFKB1	25454	0.52748	22	22	18.757	1	0.2	78.98333	5.88667	140.1805	1686	0.43723
CDC42	393726	0.75205	22	22	20.612	1	0.25	77.33333	5.83333	36.85099	628	0.62338
KDR	102657	0.59915	21	22	18.264	1	0.25	77.33333	5.82667	217.0398	1696	0.45887
PRKCA	46984	0.40132	21	21	17.797	1	0.2	75.9	5.76667	180.7261	1592	0.3381
NR3C1	63716	0.58966	19	21	18.129	4	0.2	78.18333	5.85333	718.3628	5862	0.42381
RAC1	514953	0.7308	20	21	19.488	1	0.25	77.16667	5.84	196.2621	1894	0.56667
PIK3CD	19476	0.50871	21	21	16.714	1	0.2	74.48333	5.71333	103.677	1080	0.42857
MAP2K1	45760	0.52567	21	21	17.826	1	0.25	76.91667	5.80667	178.2607	1444	0.44286
FOS	873610	0.59569	20	20	17.741	3	0.2	77.4	5.85333	192.7572	1664	0.51053
IGF1R	211878	0.58955	20	20	18.334	2	0.2	76.48333	5.81333	231.0205	2334	0.50526
HSPA8	3375	0.52948	16	19	15.757	4	0.2	77.48333	5.87333	881.4366	5480	0.34503
IL2	967200	0.75718	19	19	18.999	1	0.2	76.18333	5.80667	35.38596	548	0.66082
GSK3B	3286	0.43554	19	19	14.914	1	0.2	75.4	5.78667	232.3675	2042	0.38012
MAPT	11384	0.5142	18	18	16.703	1	0.2	76.28333	5.84667	187.2887	2000	0.45752
MET	187446	0.74927	18	18	17.966	1	0.2	74.56667	5.76	21.48974	372	0.66667
PTGS2	363728	0.46953	17	17	14.267	5	0.2	75.6	5.81333	959.9037	5656	0.42647
SIRT1	3841	0.60089	15	16	15.425	2	0.2	73.1	5.72	107.9447	948	0.5
KIT	19932	0.5564	16	16	17.134	1	0.25	73.83333	5.76667	85.8658	968	0.51667
NTRK1	1171	0.49073	15	16	16.216	1	0.2	73.35	5.72667	101.763	1072	0.40833
SNCA	3799	0.52077	15	16	13.601	4	0.2	74.45	5.8	1087.34	5922	0.43333
CDK2	3470	0.53079	15	15	15.164	2	0.2	71.93333	5.68667	51.97384	582	0.50476
JAK3	142200	0.74324	14	14	15.23	1	0.2	71.93333	5.7	11.45095	214	0.72527
CDK1	228	0.37162	14	14	12.352	1	0.2	71.06667	5.66	125.989	1108	0.36264
PLG	276	0.32197	12	14	8.062	4	0.2	69.45	5.62	737.8993	4678	0.24176
HSPA5	3134	0.5237	13	13	12.053	1	0.2	73.61667	5.80667	206.1849	1750	0.52564
HSPA1A	1518	0.58756	13	13	13.685	1	0.2	72.9	5.76667	44.6676	540	0.58974
CDK4	848	0.49815	13	13	12.352	1	0.2	70.65	5.66	44.70128	532	0.5
FLT1	43488	0.67697	13	13	14.205	1	0.25	69.66667	5.63333	16.19088	218	0.67949

MMP2	13080	0.68784	12	12	14.481	1	0.25	73	5.79333	48.05803	782	0.71212
PIK3CG	2904	0.6293	12	12	13.671	1	0.25	69.83333	5.65333	11.32936	184	0.65152
FGF1	298	0.38051	12	12	11.87	1	0.2	68.01667	5.56667	18.14216	266	0.39394
MAP2K7	758	0.55613	12	12	14.255	1	0.2	70.1	5.64667	14.20552	214	0.57576
F2	155	0.46652	8	11	10.412	4	0.25	68.91667	5.62667	421.6281	2846	0.30909
TERT	942	0.59388	11	11	12.251	1	0.2	69.26667	5.62667	10.35815	142	0.63636
NOS2	508	0.45814	11	11	12.929	2	0.2	72.23333	5.76	137.8482	1152	0.49091
ESR2	403202	0.7466	11	11	13.356	1	0.2	71.65	5.74	56.11026	756	0.8
IKBKB	774	0.57691	11	11	12.914	1	0.2	71.31667	5.72667	13.16544	212	0.61818
PLA2G4A	756	0.4242	11	11	7.987	3	0.2	67.1	5.53333	226.6756	1750	0.45455
CDK6	816	0.59388	11	11	12.061	1	0.2	69.23333	5.62667	21.14066	274	0.63636
MMP1	1806	0.54298	11	11	9.941	2	0.2	67.35	5.54667	201.0688	1842	0.58182
AHR	58	0.33919	10	10	9.351	5	0.2	68.48333	5.60667	183.6636	1344	0.37778
PARP1	194	0.49882	10	10	11.654	1	0.2	68.1	5.6	18.14209	224	0.55556
PTPN2	3002	0.61853	10	10	12.018	1	0.2	68.56667	5.62667	13.30254	176	0.68889
FLT3	386	0.52506	9	9	11.661	1	0.2	67.93333	5.6	6.80234	142	0.61111
CCNB1	68	0.40573	9	9	8.685	1	0.2	65.35	5.49333	33.32721	358	0.47222
ALOX15	723	0.71324	6	9	3.956	2	0.16667	60.6	5.25333	204.1599	824	0.44444
MMP3	1562	0.59666	9	9	9.406	1	0.2	68.61667	5.64667	24.46578	286	0.69444
FLT4	1488	0.62053	9	9	10.461	1	0.2	65.81667	5.52	3.70406	68	0.72222
CYP3A4	15	0.25611	7	8	2.412	1	0.16667	53.33333	4.84667	110.939	392	0.25
NFE2L2	132	0.43736	8	8	10.04	1	0.2	65.58333	5.50667	11.45219	144	0.53571
CYP1A1	18	0.26242	8	8	3.826	1	0.16667	57.83333	5.13333	175.6554	1416	0.32143
SLC2A1	38	0.34989	8	8	7.402	1	0.2	65.85	5.52667	498.3941	3714	0.42857
PLA2G2A	727	0.62199	7	8	4.481	3	0.2	62.66667	5.38	113.8601	916	0.60714
PTGS1	723	0.5854	7	8	3.257	1	0.16667	55.46667	5.01333	40.36232	134	0.57143
INSR	74	0.47564	7	7	7.683	2	0.2	63.25	5.41333	15.16172	148	0.61905
CASP7	22	0.32929	7	7	7.39	1	0.2	64.26667	5.47333	9.48525	108	0.42857

CALM1	33	0.42794	6	7	8.368	1	0.2	66.06667	5.55333	37.94229	350	0.42857
CDK5R1	18	0.2927	7	7	7.64	1	0.2	63.18333	5.43333	6.47166	86	0.38095
ADAM17	24	0.42794	6	6	7.857	1	0.2	66.9	5.60667	8.23855	130	0.6
CYP1A2	11	0.32413	5	6	4.153	1	0.2	60.26667	5.32667	126.197	740	0.33333
ALOX12	720	0.71324	6	6	3.065	1	0.16667	54.13333	4.98	0	0	1
ALOX5	720	0.71324	6	6	3.083	1	0.16667	54.13333	4.98	0	0	1
CYP19A1	8	0.2842	4	6	4.783	1	0.2	58.5	5.2	94.33565	720	0.26667
NLRP3	9	0.25931	5	6	6.677	2	0.2	64.6	5.50667	52.6534	418	0.26667
AURKA	10	0.32413	5	5	4.906	1	0.2	62.01667	5.40667	11.21601	124	0.5
HK2	10	0.32413	5	5	3.252	4	0.2	60	5.3	407.157	2308	0.5
EIF4E	18	0.45378	5	5	6.565	1	0.2	62.16667	5.4	1.80052	22	0.7
CFTR	10	0.32413	5	5	7.012	1	0.25	65.33333	5.56	24.28077	234	0.5
HSD11B1	8	0.46346	3	5	3.18	1	0.16667	53.98333	4.96667	95.09433	778	0.4
LGALS3	6	0.30898	3	5	4.077	6	0.2	62.45	5.44667	375.7154	2012	0.2
ELANE	7	0.2842	4	5	2.951	3	0.2	53.86667	5	43.60137	434	0.3
CYP2D6	8	0.37893	4	4	1.694	1	0.14286	45.30952	4.38	3.58333	10	0.66667
DPP4	4	0	1	4	2.694	4	0.2	57.26667	5.2	803.4385	4088	0
IDO1	7	0.46346	3	4	3.817	1	0.2	56.58333	5.14667	34.48272	236	0.5
PSEN1	24	0.56839	4	4	4.506	1	0.16667	55.81667	5.11333	0	0	1
PLK1	8	0.37893	4	4	4.504	1	0.16667	58.68333	5.22667	3.00299	52	0.66667
CD38	5	0.30898	3	4	4.963	1	0.2	57.68333	5.2	1.61379	16	0.33333
PTPN22	7	0.46346	3	4	5.804	1	0.2	62.9	5.46667	7.96497	74	0.5
MPO	5	0.30898	3	4	3.602	1	0.2	57.33333	5.17333	39.80463	230	0.33333
F3	4	0.30779	2	4	3.496	1	0.2	57.6	5.20667	67.52682	338	0.33333
HK1	8	0.37893	4	4	1.633	1	0.16667	46.8	4.56	13.22314	102	0.66667
INSRR	24	0.56839	4	4	3.833	1	0.2	55.41667	5.07333	0	0	1
ABCB1	3	0.30779	2	3	2.156	2	0.16667	52.35	4.94667	75.55687	488	0.33333
ADA	3	0	1	3	1.216	3	0.16667	42.88333	4.27333	515.0914	2560	0

TTR	6	0.46346	3	3	4.211	1	0.2	53.48333	5.03333	0	0	1
PKN1	3	0.30779	2	3	3.946	1	0.2	55.83333	5.11333	1.08219	10	0.33333
SHBG	4	0.30898	3	3	3.919	1	0.2	55.58333	5.11333	0.69815	16	0.66667
TRPV1	3	0	1	3	3.854	1	0.2	58.56667	5.26	3.33683	34	0
SLC6A2	3	0	1	3	2.085	3	0.2	50.65	4.87333	662.2115	3002	0
MMP7	4	0.30898	3	3	2.384	1	0.16667	49.5	4.76667	2.88083	20	0.66667
RPS6KA3	6	0.46346	3	3	4.768	1	0.2	59.93333	5.34667	0	0	1
F10	3	0.30779	2	3	2.372	1	0.2	50.55	4.84	11.6905	52	0.33333
PIM1	6	0.46346	3	3	4.111	1	0.2	58.83333	5.27333	0	0	1
RORC	6	0.46346	3	3	4.204	1	0.2	58.83333	5.27333	0	0	1
PFKFB3	6	0.46346	3	3	1.606	1	0.16667	46.3	4.55333	0	0	1
PRKCH	6	0.46346	3	3	5.629	1	0.2	62.06667	5.43333	0	0	1
ABCG2	2	0	1	2	2.549	2	0.2	59.26667	5.33333	76.36231	490	0
ADORA2A	2	0	1	2	1.133	1	0.14286	34.99286	3.44	21.8468	50	0
DRD2	2	0	1	2	1.269	1	0.16667	38.85	3.93333	95.32684	440	0
AGTR1	2	0	1	2	2.712	1	0.2	52.65	4.96	1.08182	8	0
NOX4	2	0	1	2	3.192	1	0.2	59.5	5.32667	0.57771	12	0
BCHE	2	0.30779	2	2	2.686	1	0.2	52.05	4.95333	0	0	1
ARG1	2	0.30779	2	2	3.093	1	0.2	54.33333	5.08	0	0	1
CTSL	2	0	1	2	3.888	1	0.2	58.85	5.31333	0.65255	14	0
CXCR1	2	0.30779	2	2	2.604	1	0.2	52.71667	5.00667	0	0	1
GRK6	2	0.30779	2	2	2.39	1	0.2	52.71667	5.00667	0	0	1
MMP8	2	0	1	2	1.508	1	0.16667	47.41667	4.65333	2.88083	20	0
TREH	2	0.30779	2	2	1.369	1	0.16667	42.88333	4.31333	0	0	1
HSD11B2	2	0.30779	2	2	2.108	1	0.16667	51.23333	4.88667	0	0	1
MMP12	2	0.30779	2	2	2.972	1	0.2	53.21667	5.03333	0	0	1
MMP13	2	0.30779	2	2	3.072	1	0.16667	54.35	5.07333	0	0	1
TLR9	2	0.30779	2	2	2.773	1	0.16667	53.66667	5.03333	0	0	1

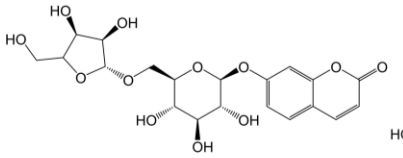
P2RX1	2	0	1	2	1.19	2	0.16667	42.18333	4.26667	298	1260	0
P2RY1	2	0	1	2	2.516	3	0.2	57.81667	5.24667	592	2516	0
PTGES	2	0.30779	2	2	1.896	1	0.16667	49.96667	4.83333	0	0	1
ADORA3	1	0	1	1	1.063	1	0.14286	33.13571	3.28	0	0	0
CHRNA7	1	0	1	1	2.037	1	0.16667	50.21667	4.87333	0	0	0
BRD4	1	0	1	1	1.968	1	0.16667	50.71667	4.9	0	0	0
CD14	1	0	1	1	2.451	1	0.2	51.58333	4.94	0	0	0
MPG	1	0	1	1	2.121	1	0.2	52.75	5.01333	0	0	0
HPRT1	1	0	1	1	2.492	1	0.16667	53.26667	5.06667	0	0	0
RNASE1	1	0	1	1	2.197	1	0.16667	50.1	4.88	0	0	0
HTR2A	1	0	1	1	1.096	1	0.16667	37.66667	3.88	0	0	0
LGALS9	1	0	1	1	1.25	1	0.16667	43.71667	4.45333	0	0	0
P2RY11	1	0	1	1	1.054	1	0.14286	32.90238	3.27333	0	0	0

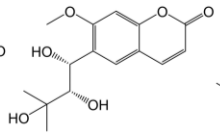
Table S4 The degree of each compound in the QHSSD-absorbable compound-target-RA network.

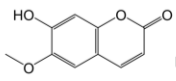
Name	Degree	Type	Selected (TOP 8)
Isoliquiritin	61	mol	√
Glycyrrhizic Acid	60	mol	√
Cimifugin	38	mol	√
Ferulic Acid	37	mol	√
Imperatorin	26	mol	√
Angelitriol	22	mol	√
Notopterol	18	mol	√
Senkyunolide F	18	mol	√
Isoliquiritigenin	17	mol	-
Caffeic Acid	16	mol	-
Liquiritin	16	mol	-
3',5'-Cyclic GMP	14	mol	-
Khellinquinone	13	mol	-
Methyl Chlorogenate	12	mol	-
5-O-Methylvisammioside	12	mol	-
Glycyrrhetinic Acid	9	mol	-
Prim-O-Glucosylcimifugin	9	mol	-
liquiritin apioside	8	mol	-
Psoralen	8	mol	-
(+)-Peucedanol	7	mol	-
Liquiritigenin	6	mol	-
Oxypeucedanin Hydrate	5	mol	-
5-O-Methylvisamminol	5	mol	-
Angelol L	5	mol	-
Columbianetin	3	mol	
Angelol C	2	mol	

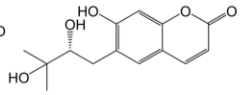
Coumarins

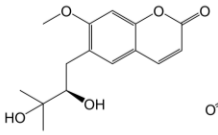
Simple coumarins

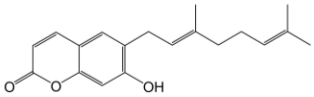

Adicardin

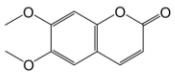

Angelitriol

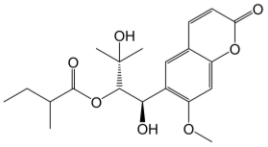

Scopoletin

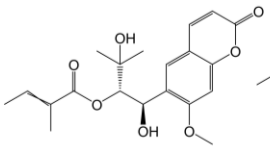

(+)-Peucedanol

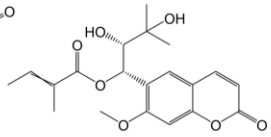

Ulopterol

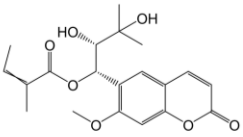

Ostruthin

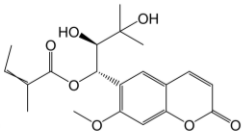

Scoparone

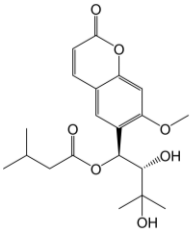

Angelol C

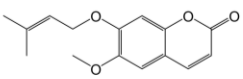

Angelol A

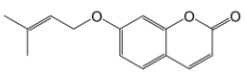

Angelol D

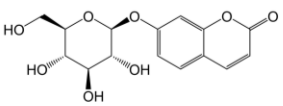

Angelol K

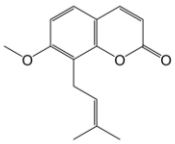

Angelol G

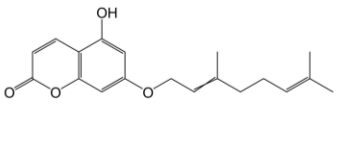

Angelol L


7-O-Prenylscopoletin

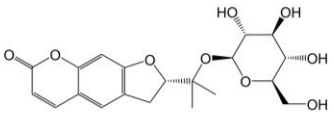

Umbelliferone-7-O-isoprene


Umbelliferone-7-O-β-D-glucopyranoside

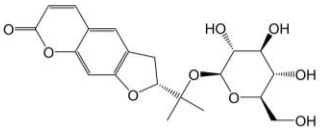

Osthole


5-Hydroxyauraptene

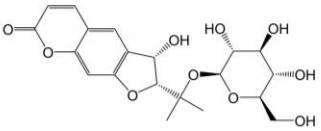
Linear furanocoumarins



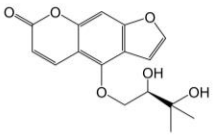
Ammijin



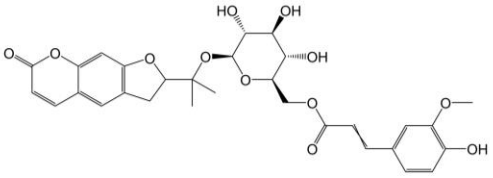
Nodakenin



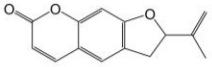
Decuroside V



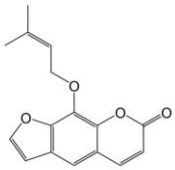
Oxypeucedanin hydrate



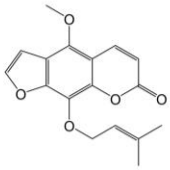
6'-O-Trans-Feruloylnodakenin



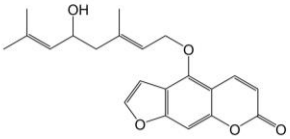
Isoangenomalin



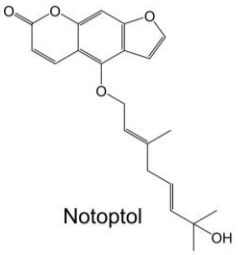
Imperatorin



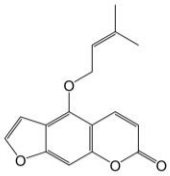
Phellopterin



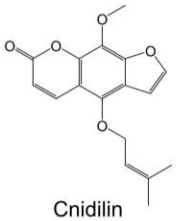
Notopterol



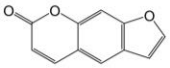
Notoptol



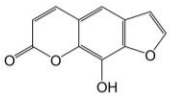
Isoimperatorin



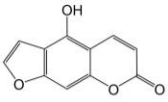
Cnidilin



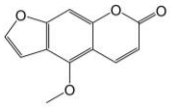
Psoralen



Xanthotoxol

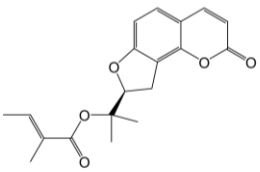


Bergaptol

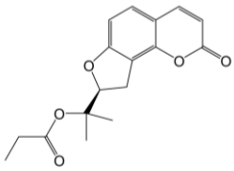


Bergapten

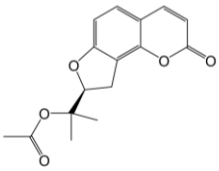
Angular furanocoumarins



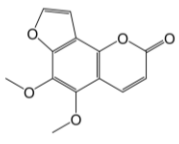
Columbianadin



Columbianetin propionate



Columbianetin acetate



Pimpinellin

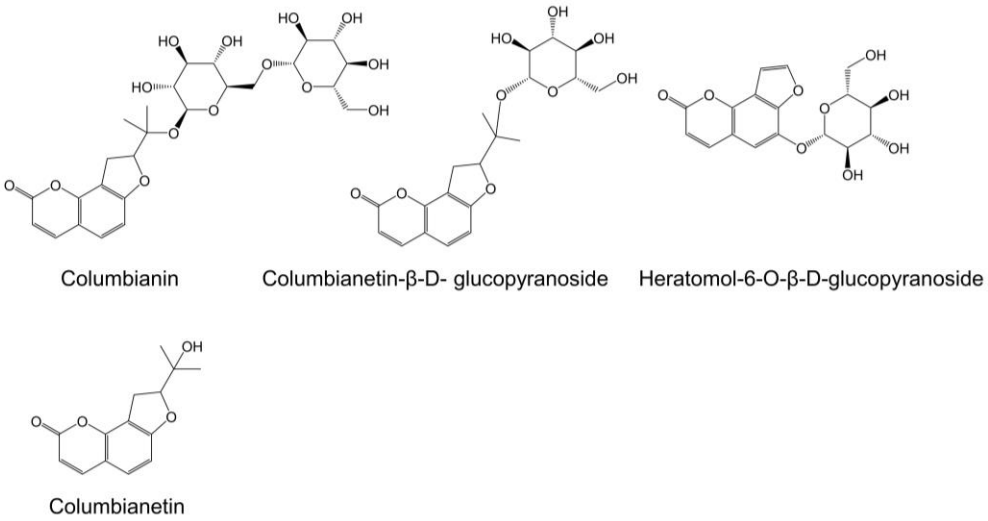
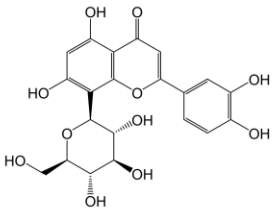


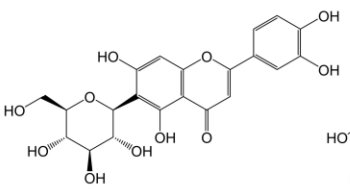
Fig. S1. Chemical structures of the coumarins in QHSSD.

Flavones

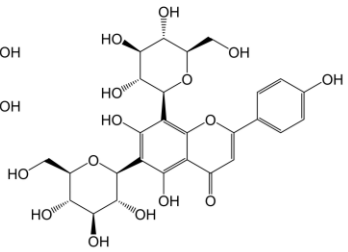
Flavonoids



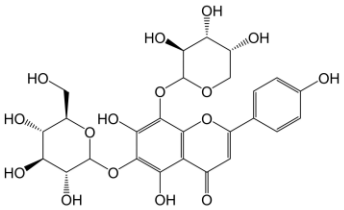
Orientin



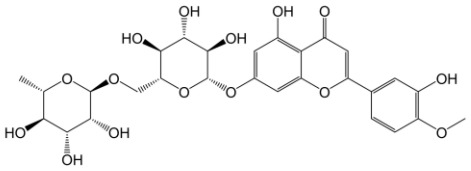
Isoorientin



Vicenin-2

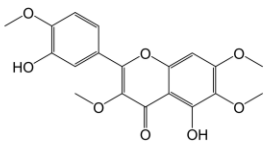


Schaftoside

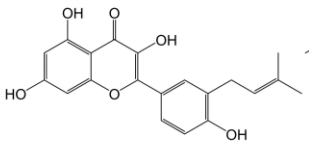


Diosmin

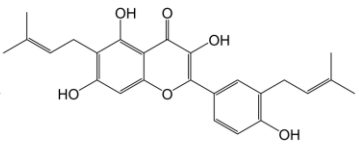
Flavonols



Casticin

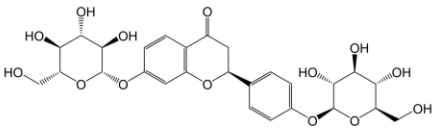


Isolicoflavonol

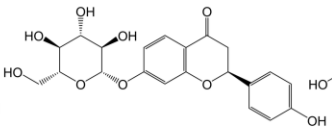


Glyasperin A

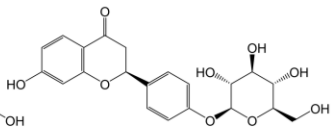
Dihydroflavonoids



Liquiritigenin 4',7-diglucoside



Neoliquiritin



Liquiritin

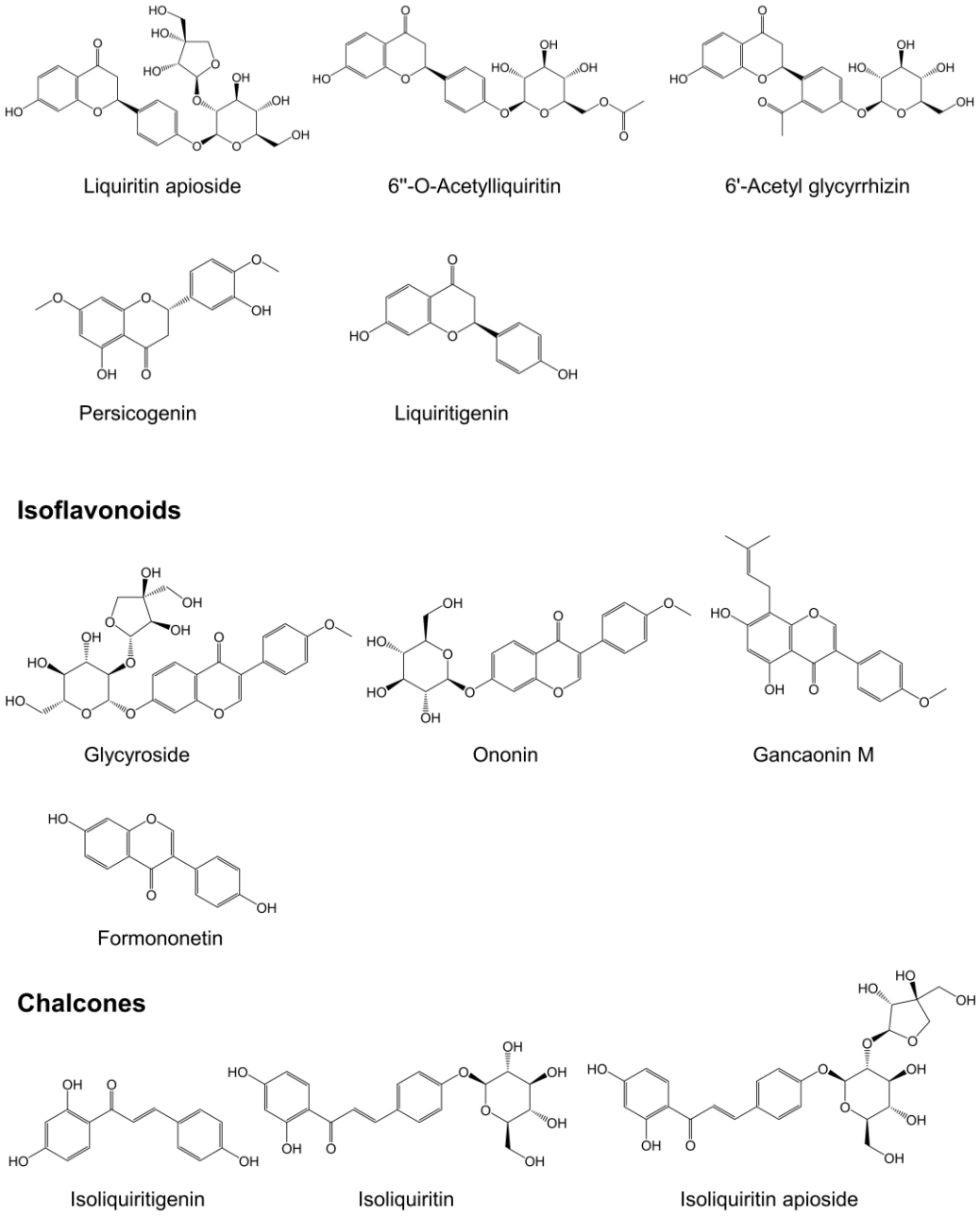


Fig. S2. Chemical structures of the flavones in QHSSD.

Chromones

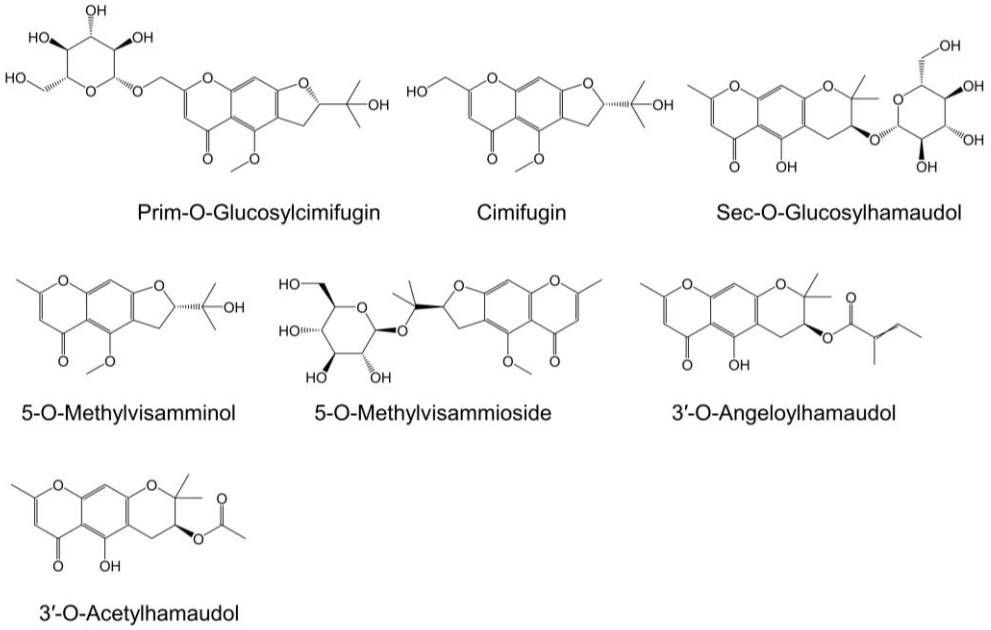
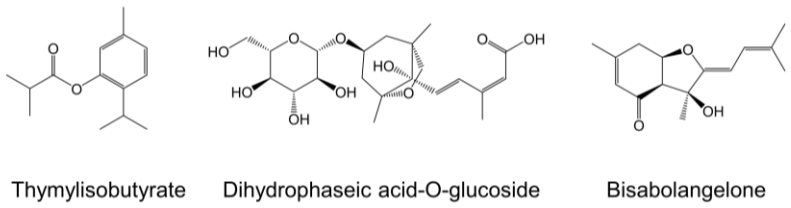


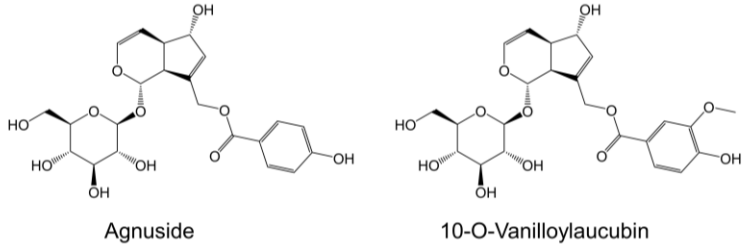
Fig. S3. Chemical structures of the chromones in QHSSD.

Terpenoids

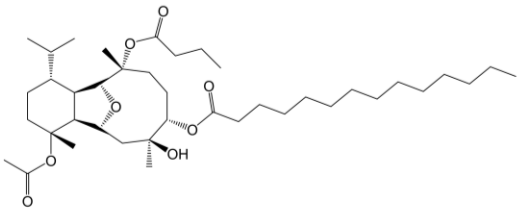
Monoterpene **Sesquiterpenes**



Iridoids

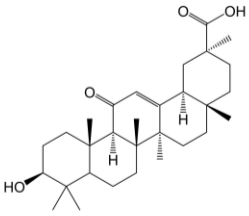


Diterpene esters

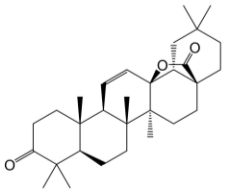


Klysimplexin

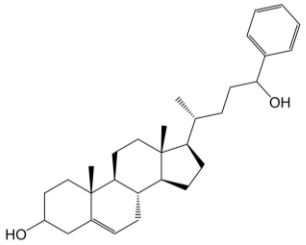
Triterpenes



Glycyrrhetinic acid

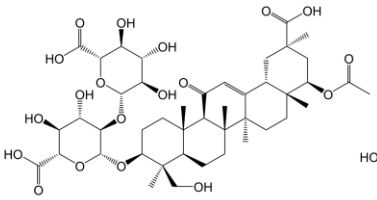


Melliferone

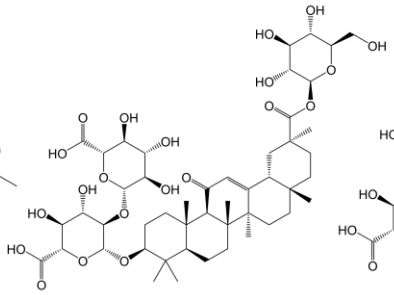


24-Phenylchol-5-ene-3, 24-diol

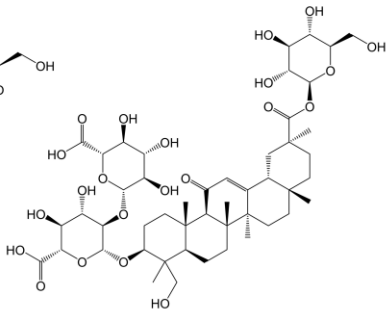
Triterpene saponins



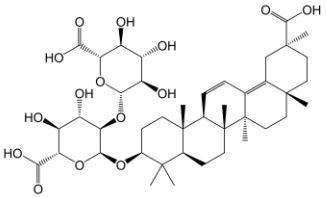
Uralsaponin F



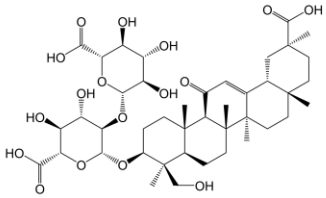
Licoricesaponin A3



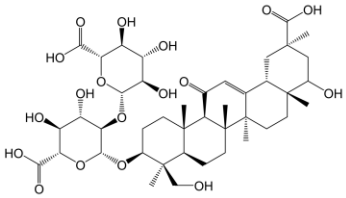
24-Hydroxy-licoricesaponin A3



Licoricesaponin C2



Licoricesaponin G2



22-Hydroxy-licoricesaponin G2

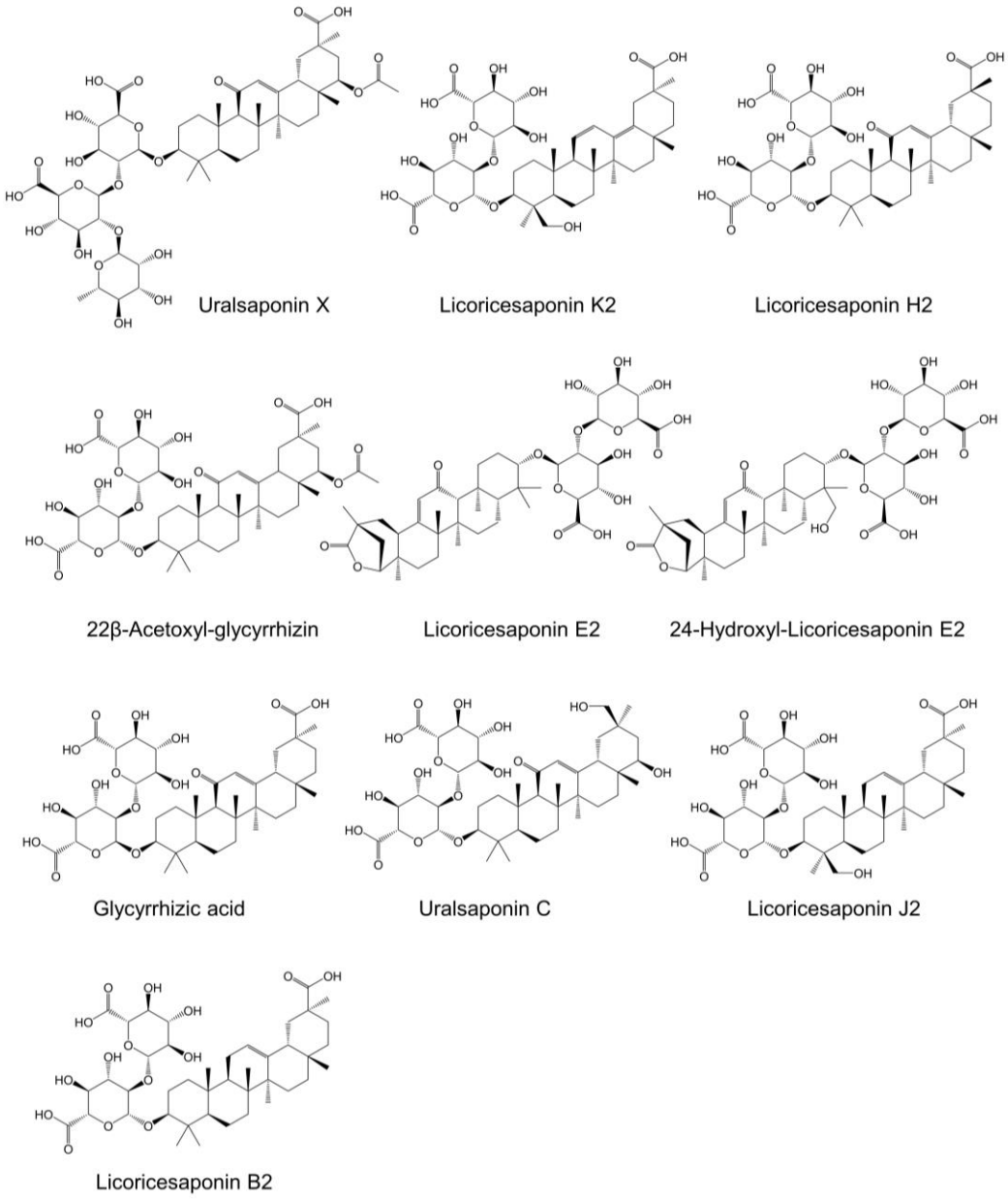


Fig. S4. Chemical structures of the terpenoids in QHSSD.

Phenylpropionic acids

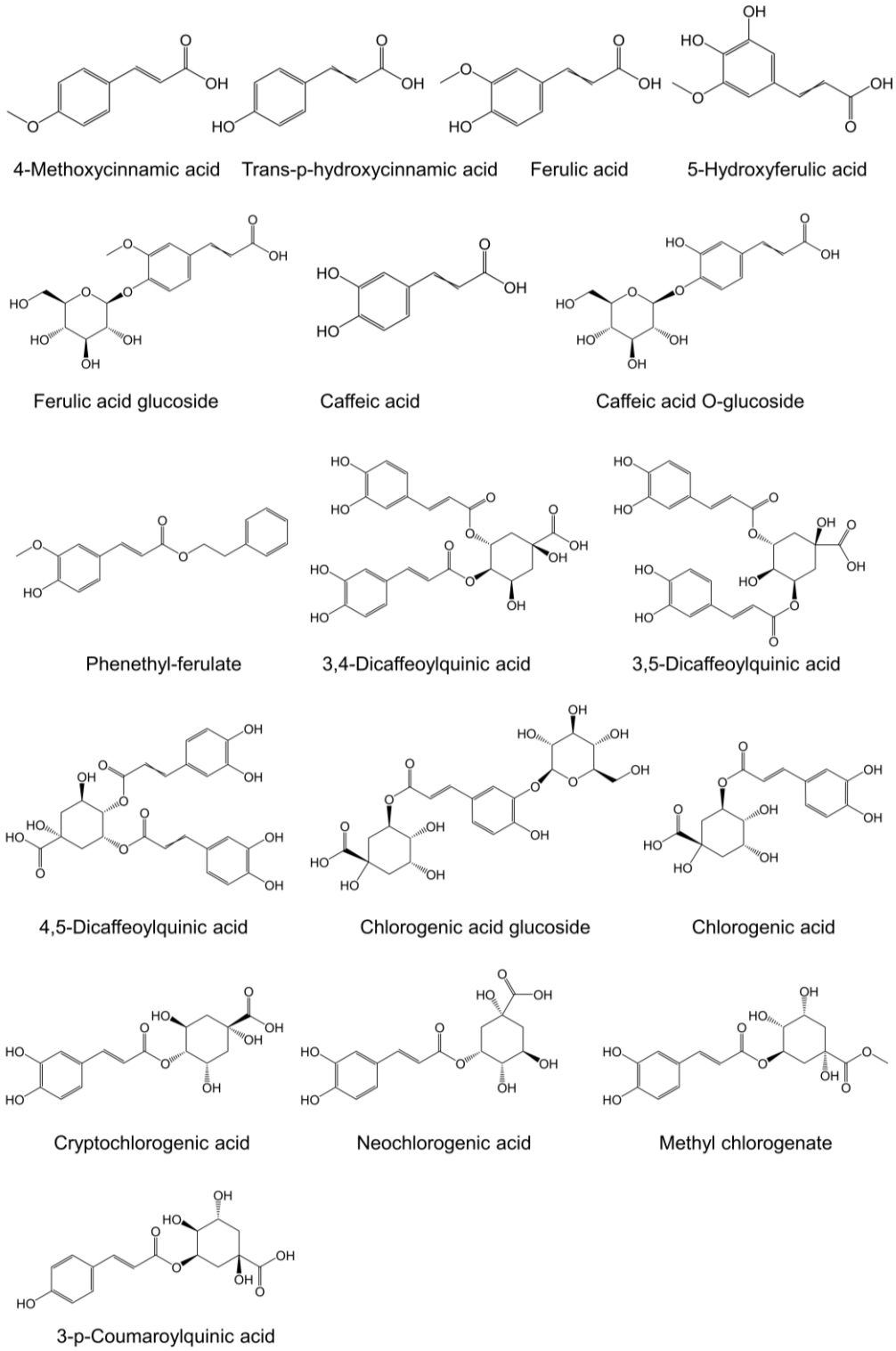


Fig. S5. Chemical structures of the phenylpropionic acids in QHSSD.

Phthalides

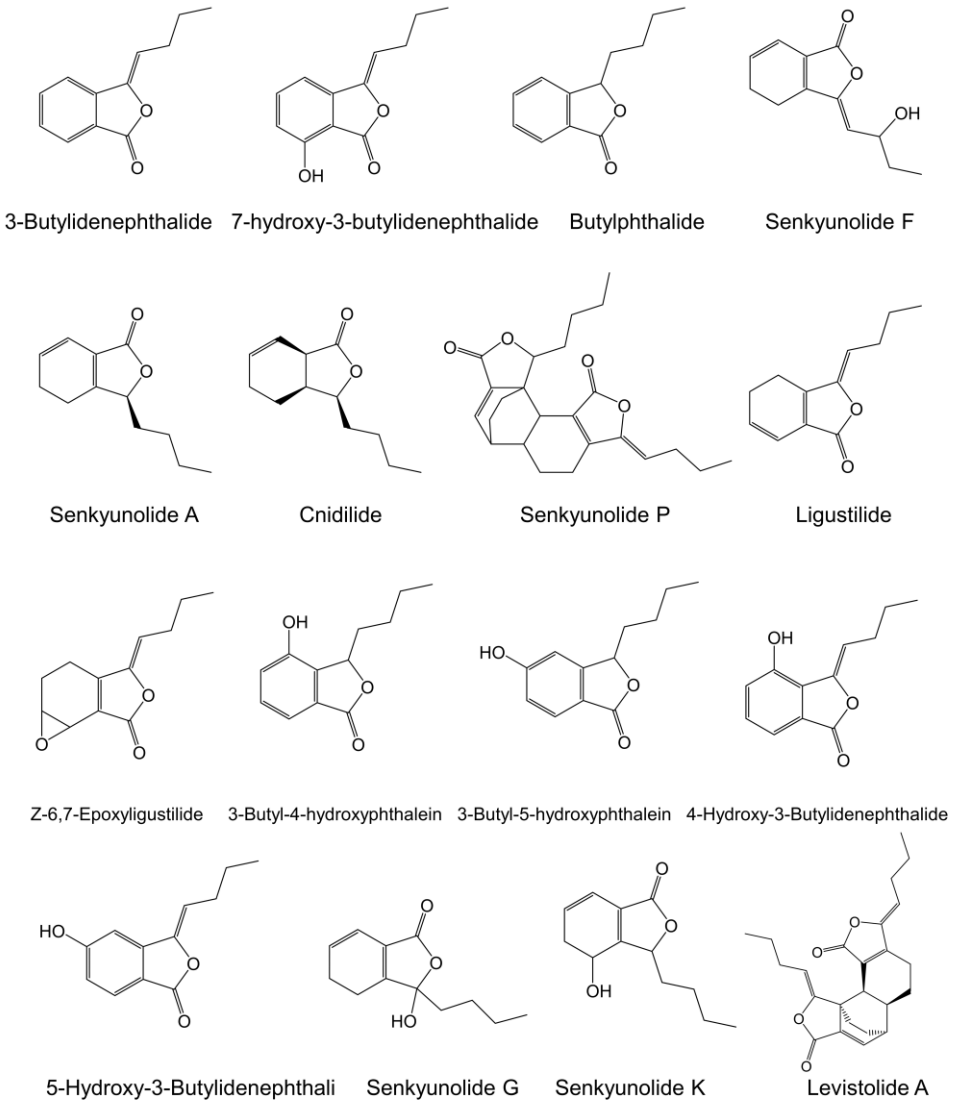


Fig. S6. Chemical structures of the phthalides in QHSSD.

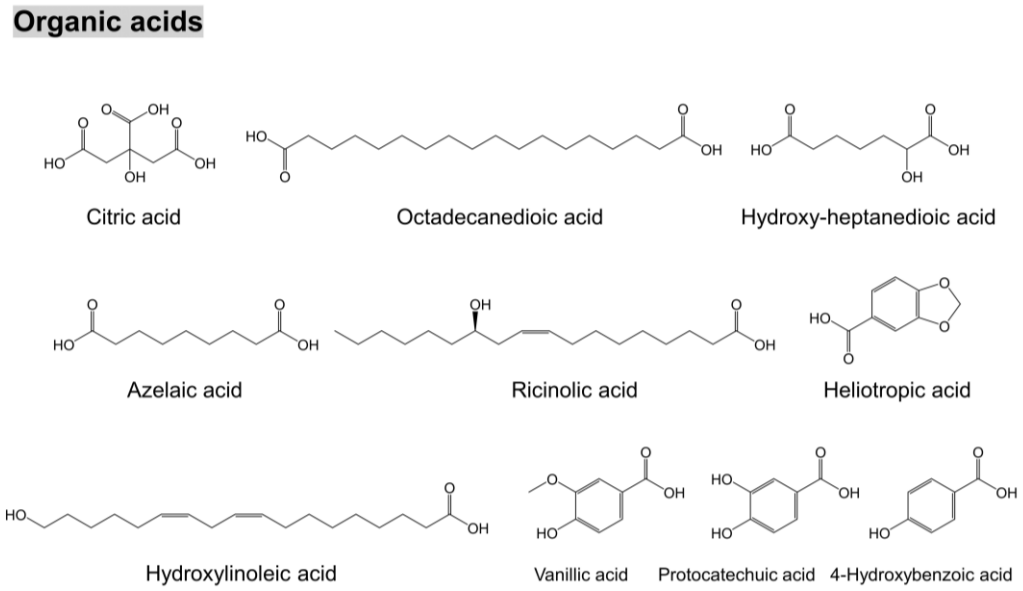


Fig. S7. Chemical structures of the organic acids in QHSSD.

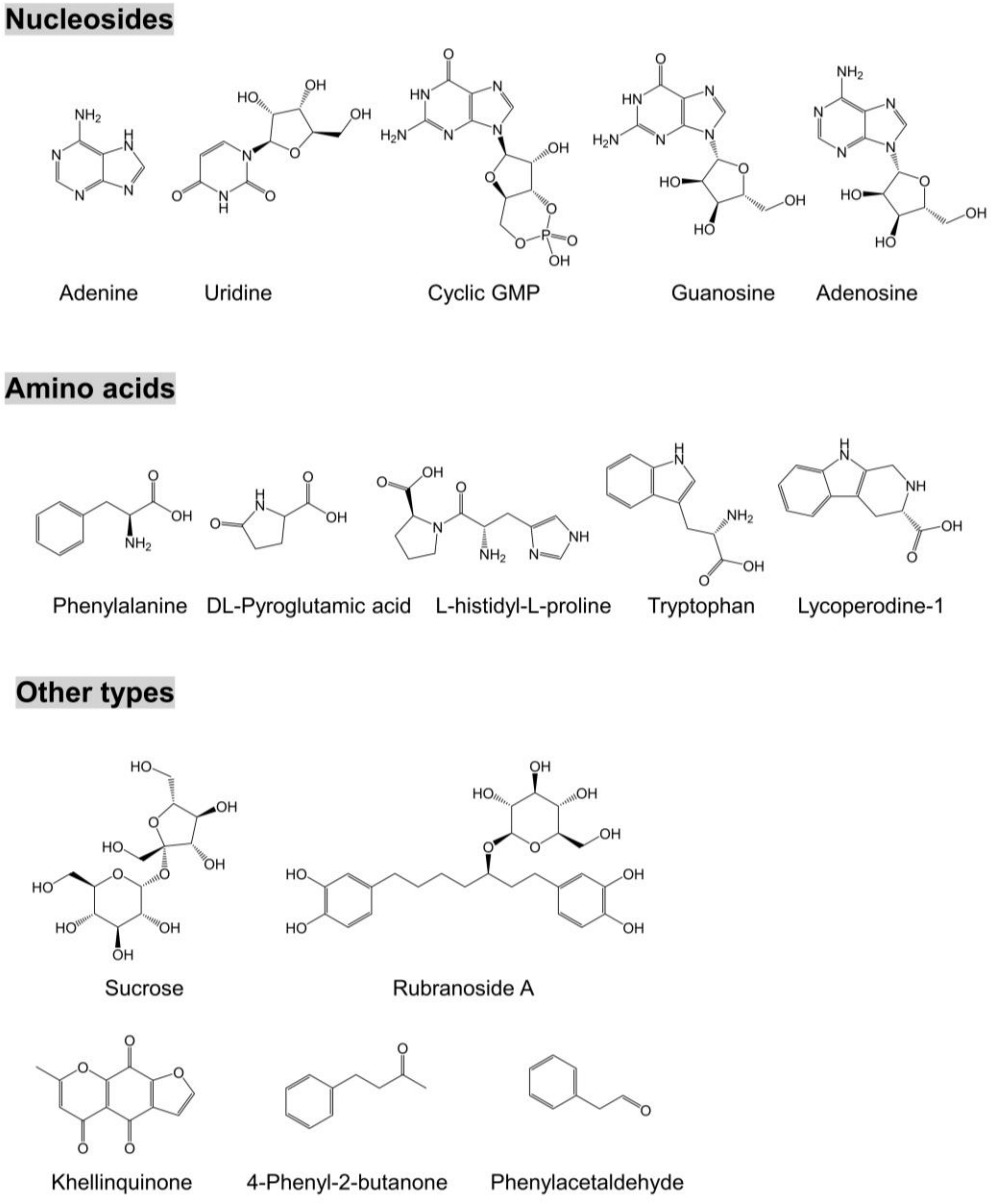


Fig. S8. Chemical structures of the nucleosides, amino acids and other types of compounds in QHSSD.

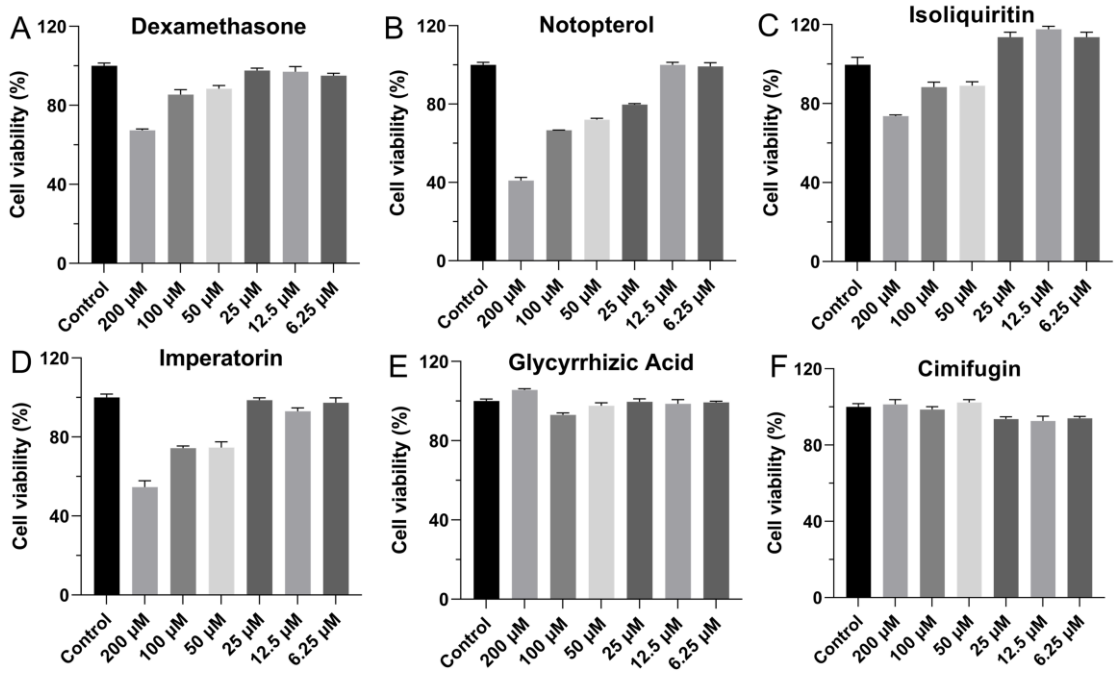


Fig. S9. Effects of (A) dexamethasone, (B) notopterol, (C) isoliquiritin, (D) imperatorin, (E) glycyrrhizic acid, (F) cimifugin on viability of RAW 264.7 cells. Safe dosing concentrations were chosen with cell viability > 90% after administration.

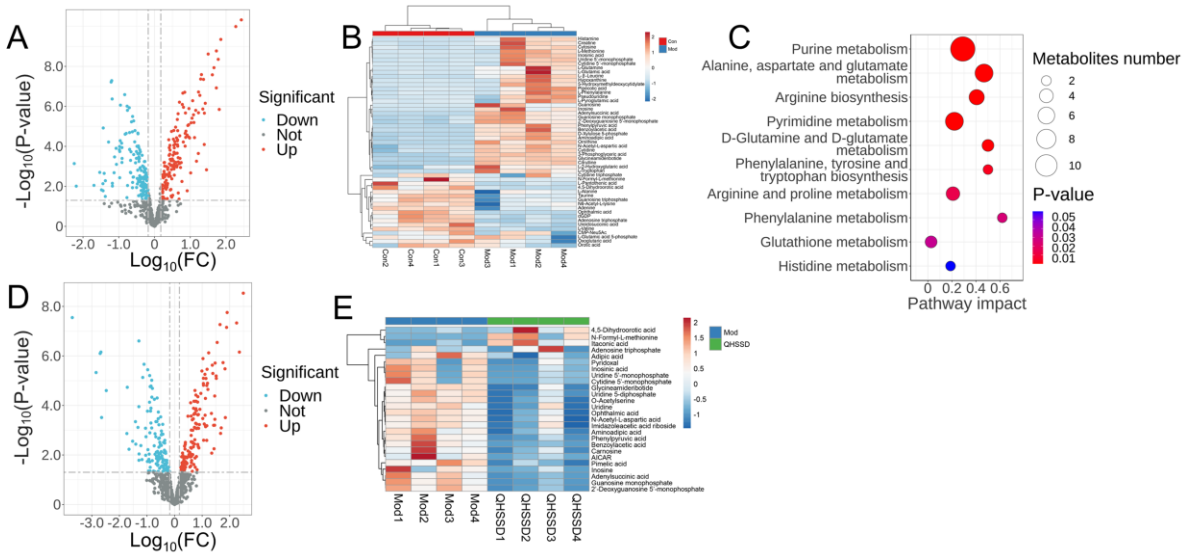


Fig. S10. Phenotypic metabolism changes in LPS-induced RAW264.7 cellular metabolomics study. Volcano plots of the samples from model group and control group in the (A) negative mode or (D) positive mode. Heatmap of the differential metabolites in (B) model and control groups or in (E) QHSSD and model groups. (C) The metabolic pathway enrichment analysis of LPS on RAW264.7 cells.

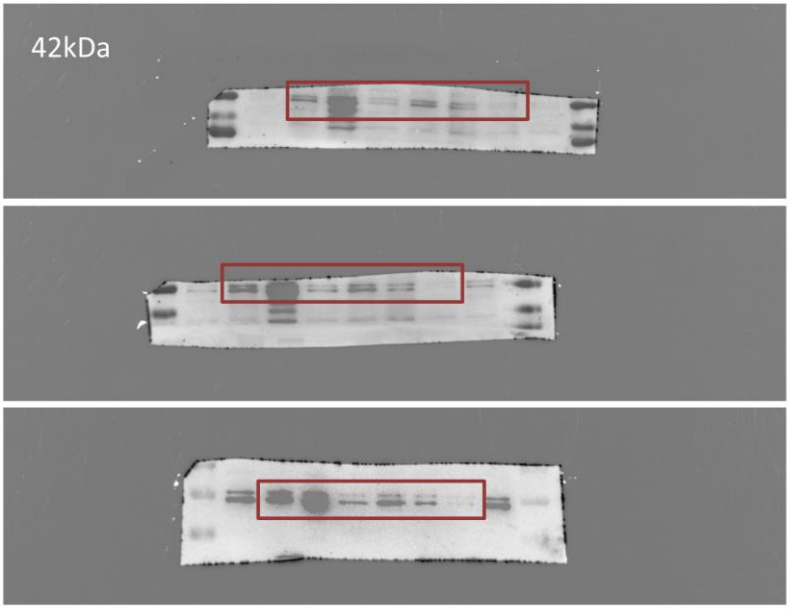


Fig. S11. Original image of the western blot experiments (strips of P-ERK, n=3).

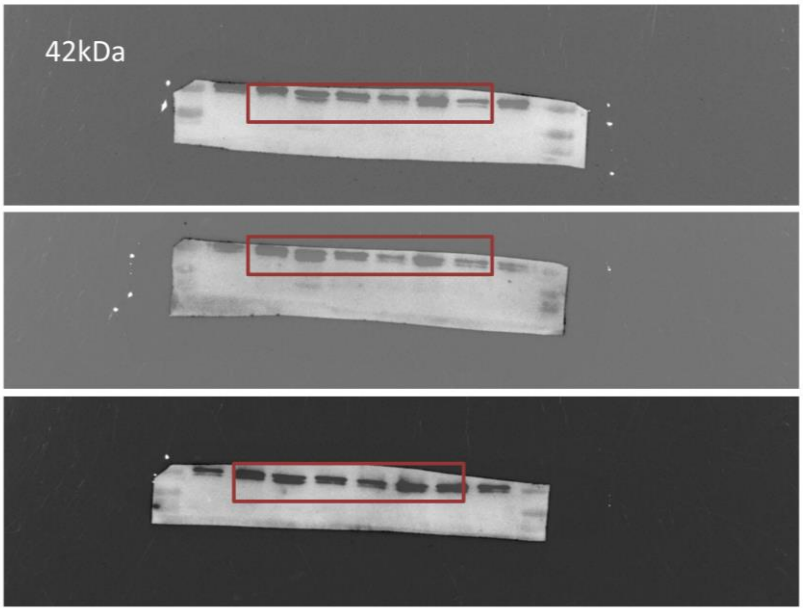


Fig. S12. Original image of the western blot experiments (strips of ERK, n=3).

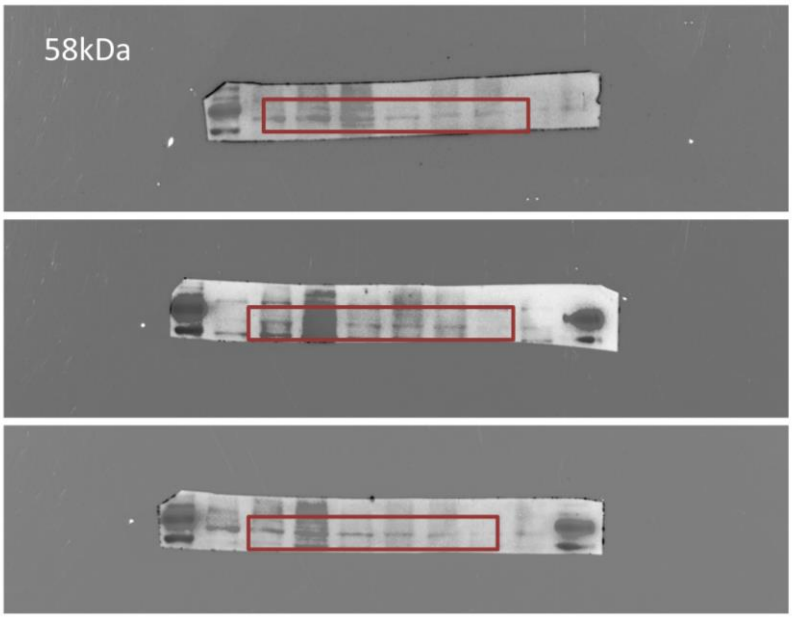


Fig. S13. Original image of the western blot experiments (strips of P-AKT, n=3).

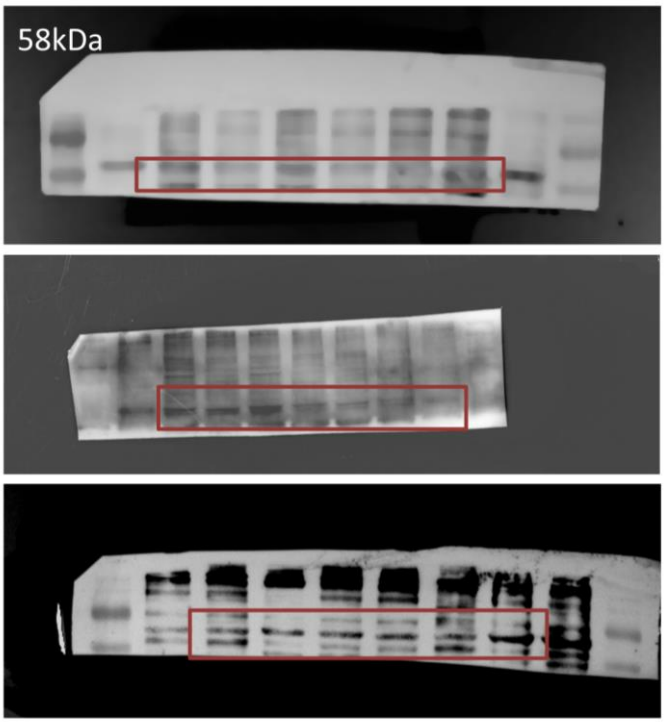


Fig. S14. Original image of the western blot experiments (strips of AKT, n=3).

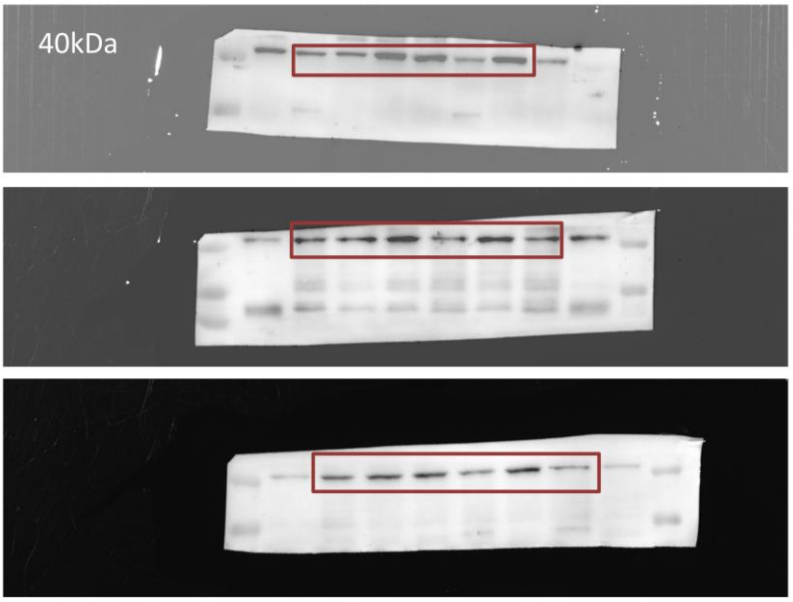


Fig. S15. Original image of the western blot experiments (strips of β-actin, n=3).