

Supplementary materials

Table S1 Chemical constituents isolated from *Rhizoma Coptidis*

Types	Chemical name	Formula	Molecular weight	Reference
Alkaloids				
1	berberine	C ₂₀ H ₁₈ NO ₄	336.1236	1
2	berberrubine	C ₁₉ H ₁₆ NO ₄	322.1079	1
3	coptisine	C ₁₉ H ₁₄ NO ₄	320.0923	1
4	palmatine	C ₂₁ H ₂₂ NO ₄	352.1549	1
5	epiberberine	C ₂₀ H ₁₈ NO ₄	336.1236	1
6	columbamine	C ₂₀ H ₂₀ NO ₄	338.1392	1
7	tetradehydroscoulerine	C ₁₉ H ₁₆ NO ₄	322.1079	1
8	jatrorrhizine	C ₂₀ H ₂₀ NO ₄	338.1392	1
9	groenlandicine	C ₁₉ H ₁₆ NO ₄	322.1079	1
10	berberastine	C ₂₀ H ₁₈ NO ₅	352.1185	1
11	worenine	C ₂₀ H ₁₆ NO ₄	334.1079	1
12	8-oxyberberine	C ₂₀ H ₁₇ NO ₅	351.1107	1
13	8-oxycoptisine	C ₁₉ H ₁₃ NO ₅	335.0794	1
14	3-hydroxy-2-methoxy-9,10-methylenedioxy-8-oxyptoberberine	C ₁₉ H ₁₅ NO ₅	337.0950	1
15	8-oxypiberberine	C ₂₀ H ₁₇ NO ₅	351.1107	1
16	8-oxyberberrubine	C ₁₉ H ₁₅ NO ₅	337.0950	1
17	(-)-5-hydroxyl-8-oxyberberine	C ₂₀ H ₁₇ NO ₆	367.1056	1
18	(+)-5-hydroxyl-8-oxyberberine	C ₂₀ H ₁₇ NO ₆	367.1056	1
19	tetrahydroberberine	C ₂₀ H ₂₁ NO ₄	339.1471	1
20	8,13-dioxocoptisine hydroxide	C ₁₉ H ₁₂ NO ₆ HO	367.0692	1
21	1,3-dioxolo[4,5-g] isoquinolin-5(6H)-one	C ₁₀ H ₇ NO ₃	189.0426	1
22	noroxyhydrastinine	C ₁₀ H ₉ NO ₃	191.0582	1

Supplementary materials

23	corydaldine	$C_{11}H_{13}NO_3$	207.0895	1
24	thalifoline	$C_{11}H_{13}NO_3$	207.0895	1
25	6-([1,3]dioxolo[4,5-g]isoquinoline-5-carbonyl)-2,3-dimethoxy benzoic acid methyl ester	$C_{21}H_{17}NO_7$	395.1005	1
26	berbithine	$C_{19}H_{17}NO_5$	339.1107	1
27	coptisonine	$C_{19}H_{14}NO_5HO$	353.0899	1
28	tetrandrine	$C_{38}H_{42}N_2O_6$	622.3043	1
29	obamegine	$C_{36}H_{38}N_2O_6$	594.2730	1
30	magnoflorine	$C_{20}H_{24}NO_4$	342.1705	1
31	sanguinarine	$C_{20}H_{14}NO_4$	332.0923	1
32	norsanguinarine	$C_{19}H_{11}NO_4$	317.0688	1
33	oxysanguinarine	$C_{20}H_{13}NO_5$	347.0794	1
34	6-acetyl-5,6-dihydrosanguinarine	$C_{23}H_{19}NO_5$	389.1263	1
35	chilenine	$C_{20}H_{17}NO_7$	383.1005	1
36	(<i>Z</i>)- <i>N</i> -Feruloyltyramine	$C_{18}H_{19}NO_4$	313.1314	1
37	(<i>E</i>)- <i>N</i> -Feruloyltyramine	$C_{18}H_{19}NO_4$	313.1314	1
38	3-hydroxy-1-(4-hydroxyphenethyl) pyrrolidine-2,5-dione pyrrolidine-2,5-dione	$C_{12}H_{13}NO_4$	235.0845	1
39	4'-[formyl-5-(hydroxymethyl)-1H-pyrrol-1-yl] butanoate butanoate	$C_{11}H_{15}NO_4$	225.1001	1
40	8,9-dihydroxy-1,5,6,10- β -tetrahydro-2H-pyrrolo[2,1-a]-isoquinolin-5-one	$C_{12}H_{13}NO_3$	219.0895	1
41	ethyl-2-pyrrolidinone-5(S)-carboxylate	$C_7H_{11}NO_3$	157.0739	1
42	methyl-5-hydroxy-2-pyridinecarboxylate	$C_7H_7NO_3$	153.0426	1
43	1H-indole-3-carboxaldehyde	C_9H_7NO	145.0528	1
44	choline	$C_5H_{14}NO$	104.1075	1
Lignans				1
45	woorenogenin	$C_{22}H_{26}O_7$	402.1679	1
46	woorenoside I	$C_{28}H_{36}O_{12}$	564.2207	1
47	longifolroside A	$C_{27}H_{34}O_{11}$	534.2101	1

Supplementary materials

48	woorenoside II	$C_{30}H_{38}O_{13}$	606.2312	1
49	woorenoside V	$C_{31}H_{38}O_{13}$	618.2312	1
50	woorenoside III	$C_{33}H_{42}O_{14}$	662.2575	1
51	woorenoside IV	$C_{35}H_{44}O_{15}$	704.2680	1
52	(+)-pinoresinol	$C_{20}H_{22}O_6$	358.1416	1
53	(+)-medioresinol	$C_{21}H_{24}O_7$	388.1522	1
54	(+)-pinoresinol-4'- <i>O</i> - β -glucopyranoside	$C_{26}H_{32}O_{11}$	520.1945	1
55	(+)-pinoresinol-4,4'- <i>O</i> - β -D-diglucopyranoside	$C_{32}H_{42}O_{16}$	682.2473	1
56	(+)-Syringaresinol-4'- <i>O</i> - β -glucopyranoside	$C_{28}H_{36}O_{13}$	580.2156	1
57	(+)-lariciresinol	$C_{20}H_{24}O_6$	360.1573	1
58	(\pm)-5,5'-dimethoxylariciresinol	$C_{22}H_{28}O_8$	420.1784	1
59	(+)-5'-methoxylariciresinol	$C_{21}H_{26}O_7$	390.1679	1
60	(+)-lariciresinol glucoside	$C_{26}H_{34}O_{11}$	522.2101	1
61	7S,8R,8'R-(+)-lariciresinol-4,4'- <i>O</i> - β -D-diglucopyranoside	$C_{32}H_{44}O_{16}$	684.2629	1
62	lanicepside A	$C_{26}H_{34}O_{12}$	538.2050	1
63	9-acetyl lanicepside B	$C_{28}H_{36}O_{13}$	580.2156	1
64	(+)-Isolariciresinol	$C_{20}H_{24}O_6$	360.1573	1
65	isolarisiresinol-9- <i>O</i> - β -D-glucopyranoside	$C_{26}H_{34}O_{11}$	522.2101	1
66	woorenoside XI	$C_{26}H_{34}O_{11}$	522.2101	1
67	cleomiscosin A	$C_{20}H_{18}O_8$	386.1002	1
68	aquillochin	$C_{21}H_{20}O_9$	416.1107	1
69	2,3-bis[(4-hydroxy-3,5-dimethoxyphenyl)-methyl]-1,4-butanediol	$C_{22}H_{30}O_8$	422.1941	1
70	secoisolariciresinol	$C_{20}H_{26}O_6$	362.1729	1
71	erythro-guaiacylglycerol-8- <i>O</i> -4'-(coniferylalcohol) ether	$C_{20}H_{24}O_7$	376.1522	1
72	threo-guaiacylglycerol-8- <i>O</i> -4'-(coniferylalcohol) ether	$C_{20}H_{24}O_7$	376.1522	1
73	woorenoside X	$C_{29}H_{40}O_{14}$	612.2418	1

Supplementary materials

74	dihydrodehydrodiconiferyl alcohol	C ₂₀ H ₂₄ O ₆	360.1573	1
75	woorenol	C ₃₂ H ₄₀ O ₁₃	632.2469	1
Simple phenylpropanoids				
76	<i>Z</i> -octadecyl cafeate	C ₂₇ H ₄₄ O ₇	480.3087	1
77	<i>E</i> -3-methoxycinnamic acid	C ₁₀ H ₁₀ O ₃	178.0630	1
78	ferulic acid	C ₁₀ H ₁₀ O ₄	194.0579	1
79	ethyl ferulate	C ₁₂ H ₁₄ O ₄	222.0892	1
80	<i>n</i> -butyl ferulate	C ₁₄ H ₁₈ O ₄	250.1205	1
81	<i>p</i> -hydroxyphenethyl <i>E</i> -ferulate	C ₁₈ H ₁₈ O ₅	314.1154	1
82	<i>E</i> -3,4-dimethoxycinnamic acid	C ₁₁ H ₁₂ O ₄	208.0736	1
83	4- <i>O</i> -feruloylquinic acid	C ₁₇ H ₂₀ O ₉	368.1107	1
84	methyl 4- <i>O</i> -feruloylquicinate	C ₁₈ H ₂₂ O ₉	382.1264	1
85	ethyl 4- <i>O</i> -feruloylquicinate	C ₁₉ H ₂₄ O ₉	396.1420	1
86	4- <i>O</i> -feruloylquinic acid butyl ester	C ₂₁ H ₂₈ O ₉	424.1733	1
87	5- <i>O</i> -feruloylquinic acid	C ₁₇ H ₂₀ O ₉	368.1107	1
88	methyl 5- <i>O</i> -feruloylquicinate	C ₁₈ H ₂₂ O ₉	382.1264	1
89	ethyl 5- <i>O</i> -feruloylquicinate	C ₁₉ H ₂₄ O ₉	396.1420	1
90	5- <i>O</i> -feruloylquinic acid butyl ester	C ₂₁ H ₂₈ O ₉	424.1733	1
91	chlorogenic acid	C ₁₆ H ₁₈ O ₉	354.0951	1
92	methyl 3- <i>O</i> -feruloylquicinate	C ₁₈ H ₂₂ O ₉	382.1264	1
93	<i>N</i> -butyl 3- <i>O</i> -feruloylquicinate	C ₂₁ H ₂₈ O ₉	424.1733	1
94	3-(4'-hydroxyphenyl)-(2 <i>R</i>)-lactic acid	C ₉ H ₁₀ O ₄	182.0579	1
95	3-(3',4'-hydroxyphenyl)-(2 <i>R</i>)-lactic acid	C ₉ H ₁₀ O ₅	198.0528	1
96	3-(3',4'-dihydroxyphenyl)-(2 <i>R</i>)-lactic acid-4'- <i>O</i> -β- <i>D</i> -glucopyranoside	C ₁₅ H ₂₀ O ₁₀	360.1056	1
97	methyl-3-(4'- <i>O</i> -β- <i>D</i> -glucopyranosyl-3',4'-dihydroxyphenyl)-lactate	C ₁₆ H ₂₂ O ₁₀	374.1213	1
98	methyl-3,4-dihydroxyphenyl lactate	C ₁₀ H ₁₂ O ₅	212.0685	1

Supplementary materials

99	ethyl-3,4-dihydroxyphenyl lactate	C ₁₁ H ₁₄ O ₅	226.0841	1
100	<i>n</i> -butyl-3,4-dihydroxyphenyl lactate	C ₁₃ H ₁₈ O ₅	254.1154	1
101	3-(2,3,4-trihydroxyphenyl) propanoic acid	C ₉ H ₁₀ O ₅	198.0528	1
Flavonoids				
102	6,8-dimethyl-3,5,7-trihydroxyfavone	C ₁₇ H ₁₄ O ₅	298.0841	1
103	rhamnetin	C ₁₆ H ₁₂ O ₇	316.0583	1
104	wogonin	C ₁₆ H ₁₂ O ₅	284.0685	1
105	7,4'-dihydroxy-5-methoxyfavanone	C ₁₆ H ₁₄ O ₅	286.0841	1
106	2',4,4'-trihydroxy-6'-methoxydihydrochalcone	C ₁₆ H ₁₆ O ₅	288.0998	1
107	coptiside I	C ₄₆ H ₅₈ O ₂₇	1042.3165	1
108	coptiside II	C ₂₁ H ₂₀ O ₁₂	464.0955	1
109	woorenoside XII	C ₄₂ H ₅₄ O ₂₅	958.2954	1
Others				
110	limonin	C ₂₆ H ₃₀ O ₈	470.1941	1
111	3,4-dihydroxyphenylethyl alcohol	C ₈ H ₁₀ O ₃	154.0630	1
112	3',4'-dihydroxyphenethyl alcohol-1-O-β-D-glucopyranoside	C ₁₄ H ₂₀ O ₈	316.1158	1
113	3,5-dihydroxyphenethyl alcohol-3-O-β-D-glucopyranoside	C ₁₄ H ₂₀ O ₈	316.1158	1
114	protocatechuic aldehyde	C ₇ H ₆ O ₃	138.0317	1
115	gentisic acid-5-O-β-D-glucopyranoside	C ₁₃ H ₁₆ O ₉	316.0794	1
116	apocynol	C ₉ H ₁₂ O ₃	168.0786	1
117	1,2-dihydroxy-benzene	C ₆ H ₆ O ₂	110.0368	1
118	protocatechuic acid	C ₇ H ₆ O ₄	154.0266	1
119	vanillic acid	C ₈ H ₈ O ₄	168.0423	1
120	vanillic acid-4-O-β-D-glucopyranoside	C ₁₄ H ₁₈ O ₉	330.0951	1
121	protocatechuic acid methyl ester	C ₈ H ₈ O ₄	168.0423	1
122	protocatechuic acid ethyl ester	C ₉ H ₁₀ O ₄	182.0579	1

Supplementary materials

123	woorenoside VI	$C_{11}H_{20}O_7$	264.1209	1
124	woorenoside VII	$C_{16}H_{26}O_9$	362.1577	1
125	woorenoside VIII	$C_{11}H_{20}O_7$	264.1209	1
126	woorenoside IX	$C_{16}H_{26}O_9$	362.1577	1
127	cyclo-(Phe-Val)	$C_{14}H_{18}N_2O_2$	246.1368	1
128	cyclo-(Phe-Leu)	$C_{15}H_{20}N_2O_2$	260.1525	1
129	β -sitosterol	$C_{29}H_{50}O$	414.3862	1

Reference:

1. J. Wang, L. Wang, G.-H. Lou, H.-R. Zeng, J. Hu, Q.-W. Huang, W. Peng and X.-B. Yang, *Pharmaceutical Biology*, 2019, **57**, 193-225.

Table S2 The chemical constituents in Rhizoma Coptidis used for targets prediction

No	Characterization	SMILE format of structures
2	quinic acid	<chem>O[C@@H]1[C@H](O)C[C@@](O)(C(O)=O)C[C@H]1O</chem>
4	3-(3',4'-dihydroxyphenyl)-(2R)-lactic acid-4'-O-β-D-glucopyranoside	<chem>OC(C(O)=O)CC1=CC(O)=C(O[C@H]2[C@H](O)[C@@H](O)[C@H](O)[C@@H](CO)O2)C=C1</chem>
5	vanillic acid-4-O-β-D-glucopyranoside	<chem>O=C(O)C1=CC(OC)=C(O[C@H]2[C@H](O)[C@@H](O)[C@H](O)[C@@H](CO)O2)C=C1</chem>
6	gentisic acid-5-O-β-D-glucopyranoside	<chem>OC1=CC=C(O[C@H]2[C@H](O)C(O)[C@H](O)[C@@H](CO)O2)C=C1C(O)=O</chem>
7	5-feruloylquinic acid-4'-O-β-D-glucopyranoside	<chem>O[C@@H]1[C@H](OC/C=C/C2=CC(OC)=C(O[C@H]3[C@H](O)[C@@H](O)[C@H](O)[C@@H](CO)O3)C=C2)O)C[C@@](O)(C(O)=O)C[C@H]1O</chem>
8	vanillic acid	<chem>O=C(O)C1=CC(OC)=C(O)C=C1</chem>
9	3-(2,3,4-trihydroxyphenyl) propanoic acid	<chem>OC1=C(O)C(O)=CC(CCC(O)=O)=C1</chem>
10	3',4'-dihydroxyphenethyl alcohol-1-O-β-D-glucopyranoside	<chem>OC1=C(O)C=C(CCO[C@H]2[C@H](O)[C@@H](O)[C@H](O)[C@@H](CO)O2)C=C1</chem>
12	3,5-dihydroxyphenethyl alcohol-3-O-β-D-glucopyranoside	<chem>OCCC1=CC(O[C@H]2[C@H](O)[C@@H](O)[C@H](O)[C@@H](CO)O2)=CC(O)=C1</chem>
13	3-feruloylquinic acid-4'-O-β-D-glucopyranoside	<chem>O[C@@H]1[C@H](O)C[C@@](O)(C(O)=O)C[C@H]1OC/C=C/C2=CC(OC)=C(O[C@@H]3[C@@H](O)[C@H](O)[C@@H](O)[C@H](CO)O3)C=C2)O</chem>
14	3-(3',4'-hydroxyphenyl)-(2R)-lactic acid	<chem>OC(C(O)=O)CC1=CC(O)=C(O)C=C1</chem>
15	rebouoside B	<chem>OC1=C(O)C=CC(CCO[C@H]2[C@H](O)[C@@H](O)[C@H](O)[C@@H](CO[C@H]3[C@H](O)[C@@H](O)[C@H](O)CO3)O2)=C1</chem>
16	5-O-caffeoylquinic acid	<chem>O[C@@H]1[C@H](OC/C=C/C2=CC(O)=C(O)C=C2)O)C[C@@](O)(C(O)=O)C[C@H]1O</chem>
17	4-feruloylquinic acid-4'-O-β-D-glucopyranoside	<chem>O[C@]1(C(O)=O)C[C@@H](O)[C@H](OC/C=C/C2=CC(OC)=C(O[C@@H]3[C@@H](O)[C@H](O)[C@@H](CO)O3)C=C2)O)[C@H](O)C1</chem>
18	3-(4'-hydroxyphenyl)-(2R)-lactic acid	<chem>OC(C(O)=O)CC1=CC=C(O)C=C1</chem>
19	methyl-3-(4'-O-β-D-glucopyranosyl-3',4'-dihydroxyphenyl)-lactate	<chem>OC(C(O)=O)CC1=CC(OC)=C(O[C@H]2[C@H](O)[C@@H](O)[C@H](O)[C@@H](CO)O2)C=C1</chem>

20	darendoside A	<chem>OC1=CC=C(CCO[C@H]2[C@H](O)[C@@H](O)[C@H](O)[C@@H](CO[C@H]3[C@H](O)[C@@H](O)[C@H](O)CO3)O2)C=C1</chem>
21	chlorogenic acid	<chem>O[C@@H]1[C@H](O)C[C@@](O)(C(O)=O)C[C@H]1OC(/C=C/C2=CC(O)=C(O)C=C2)=O</chem>
22	4-O-caffeoylquinic acid	<chem>O[C@]1(C(O)=O)C[C@@H](O)[C@H](OC(/C=C/C2=CC(O)=C(O)C=C2)=O)[C@H](O)C1</chem>
23	7S, 8R, 8'R-(+)-lariciresinol-4,4'-O-β-D-diglucofuranoside	<chem>OC[C@H]([C@@H](C1=CC(OC)=C(O)[C@H]2[C@H](O)C(O)[C@H](O)[C@@H](CO)O2)C=C1)OC3[C@H]3CC4=CC=C(O[C@H]5[C@H](O)C(O)[C@H](O)[C@@H](CO)O5)C(OC)=C4</chem>
24	5-O-feruloylquinic acid	<chem>O[C@@H]1[C@H](OC(/C=C/C2=CC(OC)=C(O)C=C2)=O)C[C@@](O)(C(O)=O)C[C@H]1O</chem>
26	(+)-pinoresinol-4,4'-O-β-D-diglucofuranoside	<chem>O[C@@H]1[C@@H](O)[C@H](O)[C@@H](CO)O[C@H]1OC2=CC=C([C@H]3OCC4C3CO[C@@H]4C5=CC(OC)=C(O)[C@H]6[C@H](O)[C@@H](O)[C@H](O)[C@@H](CO)O6)C=C5)C=C2O</chem>
27	magnoflorine	<chem>OC1=C(OC)C=C2C3=C1C(C(O)=C(OC)C=C4)=C4CC3[N+](C)(C)CC2</chem>
28	4-O-feruloylquinic acid	<chem>O[C@]1(C(O)=O)C[C@@H](O)[C@H](OC(/C=C/C2=CC(OC)=C(O)C=C2)=O)[C@H](O)C1</chem>
29	2,3-bis-[(4-hydroxy-3,5-dimethoxyphenyl)-methyl]-1,4-butanediol glycoside	<chem>OC(C(OC)=C1)=CC=C1CC(CO)C(CO)CC2=CC(OC)=C(O[C@H]3[C@H](O)[C@@H](O)[C@H](O)[C@@H](CO)O3)C=C2</chem>
30	(+)-lariciresinol glucoside	<chem>OC[C@H]([C@@H](C1=CC(OC)=C(O)C=C1)OC2)[C@H]2CC3=CC=C(O[C@H]4[C@H](O)C(O)[C@H](O)[C@@H](CO)O4)C(OC)=C3</chem>
31	methyl 5-O-feruloylquinic acid	<chem>O[C@@H]1[C@H](OC(/C=C/C2=CC(OC)=C(O)C=C2)=O)C[C@@](O)(C(OC)=O)C[C@H]1O</chem>
33	isolarisiresinol-9-O-β-D-glucopyranoside	<chem>OC[C@H]1[C@H](CO[C@H]2[C@H](O)[C@@H](O)[C@H](O)[C@@H](CO)O2)[C@@H](C3=CC=C(O)C(OC)=C3)C4=CC(O)=C(OC)C=C4C1</chem>
34	methyl 3-O-feruloylquinic acid	<chem>O[C@@H]1[C@H](O)C[C@@](O)(C(OC)=O)C[C@H]1OC(/C=C/C2=CC(OC)=C(O)C=C2)=O</chem>
35	menisperine	<chem>OC1=C(OC)C=CC(C2)=C1C3=C(C2[N+](C)(C)CC4)C4=CC(OC)=C3OC</chem>
36	woorenoside XI	<chem>OC[C@H]1[C@H](CO)[C@@H](C2=CC=C(O)C(OC)=C2)C3=CC(O[C@H]4[C@H](O)[C@@H](O)[C@H](O)[C@@H](CO)O4)=C(OC)C=C3C1</chem>
37	(+)-pinoresinol glucoside	<chem>OC1=CC=C([C@H]2OCC3C2CO[C@@H]3C4=CC(OC)=C(O[C@H]5[C@H](O)[C@@H](O)[C@H](O)[C@@H](CO)O5)C=C4)C=C1OC</chem>
38	berberrubine	<chem>OC1=C(OC)C=CC2=C1C=[N+]3C(C4=CC5=C(OCO5)C=C4CC3)=C2</chem>

Supplementary materials

39	methyl 4-O-feruloylquicinate	<chem>O[C@]1(C(OC)=O)C[C@@H](O)[C@H](OC(/C=C/C2=CC(OC)=C(O)C=C2)=O)[C@H](O)C1</chem>
40	8-oxyberberine	<chem>O=C1C2=C(C=CC(OC)=C2OC)C=C3C4=CC5=C(OCO5)C=C4CCN31</chem>
42	columbamine	<chem>OC1=C(OC)C=C2C(C3=CC(C=CC(OC)=C4OC)=C4C=[N+]3CC2)=C1</chem>
43	epiberberine	<chem>COC1=C(OC)C=C(C2=CC(C=CC3=C4OCO3)=C4C=[N+]2CC5)C5=C1</chem>
44	jatrorrhizine	<chem>OC1=C(OC)C=C(C2=CC(C=CC(OC)=C3OC)=C3C=[N+]2CC4)C4=C1</chem>
45	coptisine	<chem>C1(OCO2)=C2C=C(C3=CC(C=CC4=C5OCO4)=C5C=[N+]3CC6)C6=C1</chem>
46	groenlandicine	<chem>OC1=C(OC)C=C(C2=CC(C=CC3=C4OCO3)=C4C=[N+]2CC5)C5=C1</chem>
47/52	13-methyl berberine	<chem>CC1=C2C3=CC4=C(OCO4)C=C3CC[N+]2=CC5=C1C=CC(OC)=C5OC</chem>
48/49	worenine or its isomers	<chem>CC1=C2C3=CC4=C(OCO4)C=C3CC[N+]2=CC5=C1C=CC6=C5OCO6</chem>
50	palmatine	<chem>COC1=C(OC)C=C(C2=CC(C=CC(OC)=C3OC)=C3C=[N+]2CC4)C4=C1</chem>
51	berberine	<chem>COC1=C(OC)C=CC2=C1C=[N+]3C(C4=CC5=C(OCO5)C=C4CC3)=C2</chem>
53	7,4'-dihydroxy-5-methoxyfavanone	<chem>OC1=CC(OC)=C(C(CC(C2=CC=C(O)C=C2)O3)=O)C3=C1</chem>
55	wogonin	<chem>OC1=CC(O)=C(C(C=C(C2=CC=CC=C2)O3)=O)C3=C1OC</chem>