

Supplementary material

Table S1 Precursor ions list of 164 alkaloids

No.	Components name	Formula	Calculated mass (m/z)	Fragment ions (m/z)
1	N-demethyl dihydrosinomenine	C ₁₈ H ₂₃ NO ₄	318.16998	128.8697, 181.0698, 209.0607, 318.1702
2	Sinomenine glucoside	C ₂₅ H ₃₄ NO ₉	493.23063	211.0985, 255.1016, 273.1115, 287.1272, 415.1202
3	Higenamine glucoside	C ₂₂ H ₂₇ NO ₈	434.17367	118.0866, 158.9624, 194.1177, 272.1307, 346.1639
4	Laudanosoline-1-O-xylopyranose	C ₂₂ H ₂₇ NO ₈	434.17367	107.0499, 161.0524, 194.1176, 255.1012, 272.1378, 316.1541, 346.1639, 394.1788,
5	cephatonine-2-O-β-D-glucopyranoside	C ₂₆ H ₃₅ NO ₁₀	522.23337	243.1069, 271.0964, 285.1122, 303.1240, 317.1403, 360.1779, 465.1739
6	Salsolidine	C ₁₂ H ₁₇ NO ₂	208.13321	149.0592, 160.0889, 176.0832, 191.1059

7	N-methylsinomenine	C ₂₀ H ₂₅ NO ₄	344.18563	153.0708, 181.0645, 207.0448, 239.0695, 255.0959, 306.4597
8	Dihydrosinomenine	C ₁₉ H ₂₅ NO ₄	332.18563	137.0599, 153.0694, 165.0698, 181.0657, 193.0647, 213.1069, 241.1040
9	N-demethylsinomenine	C ₁₈ H ₂₁ NO ₄	316.15433	137.0602, 151.0765, 167.0822, 181.0651, 195.0799, 239.0704, 256.1344
10	Feruloyltyramine glucoside	C ₂₅ H ₃₃ NO ₈	476.22789	137.0577, 185.8287, 227.8863, 258.8621, 316.1089
11	Higenamine	C ₁₆ H ₁₇ NO ₃	272.12812	107.0492, 123.0438, 145.0643, 167.0594, 255.1018
12	7'8'-dihydro-1, 1'-disinomenine	C ₃₈ H ₄₆ N ₂ O ₈	659.3269	118.0904, 181.0586, 207.0360, 239.0739, 255.7602, 321.5459, 330.1706
13	Coclaurine glucoside	C ₂₃ H ₂₉ NO ₈	448.19659	107.0496, 175.0742, 192.0953, 237.0917, 269.1183, 286.1445
14	Unknown	C ₁₈ H ₂₂ ClNO ₅	368.12593	148.0801, 213.0532, 241.0965, 257.0815, 289.1069, 332.1470, 351.1006

15	N-methylcocclaurine glucoside	C ₂₄ H ₃₁ NO ₈	462.21224	192.1022, 237.0903, 257.1175, 269.1174, 300.1597
16	3'-hydroxy-N-methyl cocclaurine-O-glucoside	C ₂₄ H ₃₁ NO ₉	477.20716	123.0441, 192.1027, 316.1551, 358.1605
17	3'-hydroxy-N-methylcocclaurine	C ₁₈ H ₂₁ NO ₄	316.15433	123.0438, 143.0488, 175.0752, 192.1016, 269.1176, 285.1124
18	N-norsinoacutine	C ₁₈ H ₁₉ NO ₄	314.13868	151.0754, 238.0850, 283.0845, 298.1075
19	Magnocurarine 4'-O-glucopyranoside	C ₂₅ H ₃₄ NO ₈	477.23575	107.0494, 121.0647, 143.0483, 192.1015; 237.0914, 269.1180, 314.1751
20	Amberline	C ₁₈ H ₂₁ NO ₅	332.14925	153.0696, 165.0700, 181.0650, 193.0629, 213.1077
21	N-methylcocclaurine	C ₁₈ H ₂₁ NO ₃	300.15942	107.0490, 137.0640, 175.0747, 237.0997, 269.1167
22	Isocorydine N-oxide	C ₂₀ H ₂₃ NO ₅	358.16490	253.0810, 263.0696, 285.1095, 295.0957, 313.1069, 340.1551

23	Tembetarine	C ₂₀ H ₂₆ NO ₄	345.19346	227.1056, 238.0990, 255.0998, 269.1167, 282.1233, 313.1442
24	Michelalbine	C ₁₇ H ₁₅ NO ₃	282.11247	136.9338, 165.0689, 180.0873, 239.0700, 249.0526, 267.0637
25	Isosinomenine	C ₁₉ H ₂₃ NO ₄	330.16998	137.0605, 153.069, 181.0653, 209.0612, 223.0748, 245.1168
26	Isosinoacutine or its isomer	C ₁₉ H ₂₁ NO ₄	328.15433	137.0577, 153.0694, 181.0648, 207.0440, 298.1095
27	Magnocurarine	C ₁₉ H ₂₄ NO ₃	315.18290	107.0493, 143.0498, 192.1011, 269.0669,
28	8-demethoxycephatonine	C ₁₉ H ₂₃ NO ₄	330.16998	137.0596, 175.0748, 192.1019, 273.1162, 299.1269 159.6765, 229.0941,
29	1-O-acetyl-daurocumine	C ₂₁ H ₂₆ ClNO ₇	440.14706	277.1082, 287.0900, 305.1000, 323.0673, 383.0913

30	Oxypalmatine	C ₂₁ H ₂₁ NO ₅	368.14925	306.0738, 321.0975, 336.1225, 352.1251
31	(-) -8-oxotetrahydrothalifendine	C ₁₉ H ₁₇ NO ₅	340.11795	151.0764, 163.0622, 178.0864, 206.1174, 297.1157
32	N-methylcorydine	C ₂₁ H ₂₆ NO ₄	357.19346	237.0911, 265.0854, 281.0846, 296.1025, 311.1280, 343.4614
33	Corydine methyl ether	C ₂₁ H ₂₅ NO ₄	356.18563	151.0649, 181.9300, 244.0304, 280.1073, 296.1009, 311.1279
34	Pseudoberberine	C ₂₀ H ₁₈ NO ₄	337.13086	262.0861, 279.0895, 292.0970, 307.0839, 320.0918, 323.1146
35	Dehydrocorydalmine	C ₂₀ H ₂₀ NO ₄	339.14654	262.0846, 279.0879, 294.1104, 307.0850, 323.1154
36	Columbamine	C ₂₀ H ₂₀ NO ₄	339.14654	279.0899, 294.1131, 207.0859, 322.1067
37	Unknown	C ₁₆ H ₃₃ NO ₁₀	400.21772	167.0718, 209.9304, 255.9227, 288.7135, 312.9564, 334.2930, 367.9322

38	N-methylcorydine glucoside	C ₂₆ H ₃₆ NO ₉	507.24628	266.0768, 280.0952, 295.0984, 308.0899, 500.1718
39	Unknown	C ₂₈ H ₃₉ NO ₁₃	598.24942	145.0660, 167.0695, 173.0587, 205.0856, 217.0865, 271.0970
40	Tetrohydrogroenlandicine glucoside	C ₂₀ H ₄₁ NO ₁₂	488.27015	133.0875, 161.0804, 177.1114, 205.1039, 221.1461, 415.2538, 443.2477
41	N-cis-feruloyltyramine	C ₁₈ H ₁₉ NO ₄	314.13868	103.0649, 117.0332, 121.0656, 145.0278
42	Unknown	C ₁₇ H ₂₉ NO	264.23219	105.0683, 119.0849, 133.1011, 203.1451, 219.1740
43	N-trans-feruloyltyramine	C ₁₈ H ₁₉ NO ₄	314.13868	121.0652, 145.0278, 177.0553, 314.1371
44	N-trans-feruloylmethoxytyramine	C ₁₉ H ₂₁ NO ₅	344.14925	117.0341, 145.0286, 177.0551, 201.8803, 314.1393
45	Unknown	C ₂₁ H ₃₅ NO	318.27914	119.0858, 161.1310, 187.1131, 203.1433, 219.1734

46	Analogue of Menisporphine	C ₁₆ H ₃₅ NO ₂	274.27406	115.9768, 128.8718, 149.9088, 174.9391, 204.0750, 245.8988
47	Analogue of Menisporphine	C ₁₈ H ₃₉ NO ₃	318.30027	128.8716, 214.8333, 237.8787, 256.2609, 279.0872, 307.0901
48	Analogue of Michelalbine	C ₁₃ H ₂₅ NO ₃	344.19072	101.9395, 117.9328, 141.9576, 157.9631, 180.1773
49	Unknown	C ₁₃ H ₂₅ NO ₂	228.19581	109.1008, 119.0855, 133.1018, 137.0947, 147.1177, 175.1477
50	Sinotumines H or I	C ₂₀ H ₂₀ NO ₅	355.14142	164.0476, 176.0716, 279.1015, 310.1089, 324.0893, 339.1090
51	Sallisonien D	C ₁₇ H ₃₇ NO	252.13829	128.9992, 140.8669, 172.9394, 195.1585, 224.8458
52	6-O-demethylmenisporphine	C ₁₈ H ₁₃ NO ₄	307.09173	116.9176, 144.9167, 194.0600, 219.0682, 236.0710, 264.0656, 293.0784
53	Unknown	C ₂₂ H ₂₅ N ₆ O ₄	438.20100	133.1006, 185.8839, 241.9761, 293.1837, 376.2663, 437.1864

54	Sinomenine	C ₁₉ H ₂₃ NO ₄	330.16998	137.0594, 153.0756, 181.0657, 207.0460, 213.0913, 239.0726, 255.1027
55	N-1, 7-dimethoxy-phenan-threnyl-acemide	C ₁₈ H ₁₇ NO ₃	296.12812	
56	3-methoxymorphinane	C ₁₇ H ₂₃ NO	258.18524	
57	3-methoxy-17-methyl-morphinane	C ₁₈ H ₂₅ NO	272.20089	
58	3-methoxy-6-hydroxy-17-methylmorphinane	C ₁₈ H ₂₅ NO ₂	288.19581	
59	3-methoxy-17-methylmorphinane-6-one	C ₁₈ H ₂₃ NO ₂	286.18016	
60	3-methoxy-14-hydroxy-17-methylmorphinane-6-one	C ₁₈ H ₂₃ NO ₃	302.17507	
61	3-methoxy-7, 8-didehydro-17-methylmorphinane-6-one	C ₁₈ H ₂ NO ₂	264	

62	Sinoacutine	$C_{19}H_{21}NO_4$	328.15433	137.0577, 153.0694, 165.0693, 181.0648, 207.0430, 298.1095
63	13, 13a-didehydro-9, 10-dimethoxy-2, 3- (methylenedioxy) -berbine	$C_{20}H_{19}NO_4$	338.13868	
64	Sinomendine	$C_{20}H_{19}NO_4$	338.13868	
65	7-methoxylsinomendine	$C_{21}H_{21}NO_4$	352.15433	
66	8-Demethoxyrunanine	$C_{20}H_{25}NO_4$	344.18563	
67	3-methoxy-6-hydroxy-17-methylmorphinan	$C_{19}H_{27}NO_2$	302.21146	
68	2, 2'-disinomenine	$C_{38}H_{44}N_2O_8$	658.32487	239.0739, 255.7602, 330.1706, 568.2294, 584.2102, 594.2525, 600.2525

69	1'-disinomenine	$C_{38}H_{46}N_2O_8$	659.33269
70	7', 8'-dihydro-1, 1'-disinomenine	$C_{38}H_{46}N_2O_8$	659.33269
71	Sinomendine-A	$C_{20}H_{19}NO_4$	338.13868
72	Sallisonine A	$C_{38}H_{24}N_2O_7$	621.16563
73	Sallisonine B	$C_{38}H_{40}N_2O_7$	637.29083
74	Sallisonine C	$C_{37}H_{40}N_2O_7$	625.29083
75	Sallisonine D	$C_{16}H_{17}NO_3$	272.12812
76	Sallisonine E	$C_{19}H_{15}NO_4$	322.10738

77	Acutumine	$C_{19}H_{24}NO_6Cl$	398.13649	213.0571, 241.0500, 255.0648, 273.0767, 305.1025, 341.0792, 362.1583
78	Duaricumine	$C_{19}H_{24}NO_6Cl$	398.13649	
79	Cephamonine	$C_{20}H_{25}NO_5$	360.18055	211.0728, 243.0684, 271.0966, 285.1137, 303.1218
80	(+)-tannagine	$C_{21}H_{27}NO_5$	374.19620	
81	14-episinomenine	$C_{19}H_{23}NO_4$	330.16998	
82	O-methylflainantine	$C_{20}H_{23}NO_4$	342.16998	
83	Protostephanone	$C_{21}H_{25}NO_5$	372.18055	

84	2, 3-dimethoxy-6-hydroxymorphinandienone	C ₂₁ H ₂₃ NO ₅	358.16490	243.0996, 254.0913, 271.0956, 285.1136, 303.1227, 313.1068
85	Liriodenine	C ₁₇ H ₉ NO ₃	276.06552	
86	Telitoxine	C ₁₇ H ₁₃ NO ₃	280.09682	
87	5, 6-dimethoxy-7H-Dibenzo[de, h]quinolin-7-one	C ₁₈ H ₁₃ NO ₃	292.09682	
88	Bianfugecine	C ₁₈ H ₁₃ NO ₃	292.09682	100.1124, 225.1958, 234.9152, 249.0827, 264.0947
89	Menisporphine	C ₁₉ H ₁₅ NO ₄	322.10738	128.8737, 191.0693, 219.0675, 250.0866, 262.0851, 278.0809, 292.0963
90	Dauriporphine	C ₂₀ H ₁₇ NO ₅	352.11795	

91	Tetrahydro-palmatine	C ₂₁ H ₂₅ NO ₄	356.18563	
92	Discretamine	C ₁₉ H ₂₁ NO ₄	328.15433	137.0439, 151.0654, 195.0800, 211.0751, 241.0810, 267.0998, 298.1134
93	Tetrahydrocolumbamine	C ₂₀ H ₂₃ NO ₄	342.16998	
94	Cheilanthifoline	C ₁₉ H ₁₉ NO ₄	326.13868	119.0494, 151.0749, 178.0874, 269.8322, 326.1406
95	Tetrahydrogroenlandicine	C ₁₉ H ₁₉ NO ₄	326.13868	
96	(-) -sinactine	C ₂₀ H ₂₁ NO ₄	340.15433	165.0914, 192.1009, 266.0872, 284.0999, 297.1145
97	8-oxo-epiberberine	C ₂₀ H ₁₇ NO ₅	352.11795	

98	Coclaurine	C ₁₇ H ₁₉ NO ₃	286.14377	107.0497, 175.0758, 209.0968, 237.0913, 269.1175
99	N-methyl-coclaurine	C ₁₈ H ₂₁ NO ₃	300.15942	
100	FK1000	C ₂₀ H ₂₇ NO ₅	362.19620	
101	3-methoxy-6-hydroxy-17-methylmorphine	C ₁₉ H ₂₇ NO ₂	302.21146	
102	3-methoxymorphine	C ₁₈ H ₂₅ NO	272.20089	
103	3-methoxy-17-morphine	C ₁₉ H ₂₇ NO ₂	302.21146	
104	8-dmethoxyranine	C ₂₁ H ₂₉ NO ₅	376.21185	
105	1,1'-disinomenine	C ₄₁ H ₄₆ N ₂ O ₅	647.4795	

106	2,2'-disinomenine	C ₄₁ H ₄₆ N ₂ O ₅	647.4795	
107	Tuduranine	C ₁₈ H ₁₉ NO ₃	298.14377	
108	Magnoflorine	C ₂₀ H ₂₄ NO ₄	343.17781	237.0910, 265.0864, 282.0892, 297.1127, 311.1301
109	8, 14-dihydrosalutaridine	C ₂₀ H ₂₅ NO ₄	344.18563	
110	Bianfugenine	C ₂₁ H ₁₇ NO ₅	352.11795	223.0684, 251.0587, 265.0704, 294.0769, 308.0938, 322.0719
111	Dauriporphinoline	C ₁₈ H ₁₅ NO ₅	338.10230	251.0587, 294.0768, 309.1000, 323.0767
112	Tetrahydroepiberberine	C ₂₁ H ₂₃ NO ₆	386.15981	
113	Tetrahydropalmatine	C ₂₁ H ₂₅ NO ₄	356.18563	165.0909, 192.1006, 342.1707

114	8-oxocanadine	C ₂₁ H ₂₅ NO ₄	356.18563	
115	8-oxotetrahydropalmatine	C ₂₁ H ₂₅ NO ₄	356.18563	
116	Oxoisocorypalmine	C ₂₀ H ₂₃ NO ₄	342.16998	
117	Acutumidine	C ₁₈ H ₂₂ ClNO ₆	384.12084	169.0278, 185.0583, 199.0741, 213.0489, 227.0694, 241.0798, 323.0758
118	Dauricumine	C ₂₀ H ₂₆ ClNO ₆	412.15214	
119	(1, 7-dimethoxyl-phenanthren-yl) - acetamide	C ₁₇ H ₁₇ NO ₃	284.12812	
120	N-trans-feruloylmrthyramine	C ₂₀ H ₂₁ NO ₅	356.14925	
121	Gasanol	C ₁₈ H ₁₈ NO ₃	297.13594	

122	N-trans-feruloyl tyramine	C ₁₈ H ₁₉ NO ₄	314.13868	
123	Sinoracutine	C ₁₇ H ₁₇ NO ₂	268.13321	
124	2,7dimethoxy-4-dehydroxy-sinoraculine	C ₂₁ H ₂₃ NO ₆	386.15981	
125	10-chlorine-miharumine	C ₁₉ H ₂₂ NCIO ₆	396.12084	
126	(+) zippelianine	C ₂₀ H ₂₅ NO ₅	360.18055	
127	O-demethylprotostephanone	C ₂₀ H ₂₃ NO ₅	358.16490	
128	Salutaridine	C ₂₀ H ₂₃ NO ₄	342.16998	115.0529, 137.0577, 153.0694, 181.0648, 207.0440, 298.1095
129	(+) -14-hydroxy-isostephodeline	C ₂₁ H ₂₇ NO ₆	390.19111	

130	Sinomenine N-oxide	C ₁₉ H ₂₁ NO ₅	323/324	146.0593, 207.0913, 239.0716, 255.0977, 314.1366
131	1-hydroxy-10-oxo-sinomenine	C ₁₉ H ₂₁ NO ₆	361.15199	187.0762, 211.0730, 225.0877, 254.0911, 285.1120, 303.1210, 317.1386
132	Xylopinine	C ₁₈ H ₁₇ NO ₃	296.12812	136.0517, 164.0507, 178.0849, 340.1119
133	9-methoxy-Omethylnoschatoine	C ₂₀ H ₁₇ NO ₅	352.11795	
134	N-formyldehydroanonaine	C ₁₈ H ₁₃ NO ₃	292.09682	
135	N-demethyl-N-formyldehydronuciferine	C ₁₉ H ₁₇ NO ₃	308.12812	
136	Govadine	C ₁₉ H ₂₁ NO ₄	328.15433	
137	Aurotensine	C ₁₉ H ₂₁ NO ₄	328.15433	

138	Argemexirine	$C_{17}H_{19}NO_3$	286.14377	
139	6, 7-isoquinolinediol, 1, 2, 3, 4-Tetrahydro-[(4-methoxyphenyl) methyl]-methyl	$C_{18}H_{21}NO_3$	300.15942	
140	Dauricumine	$C_{19}H_{24}ClNO_6$	398.13469	
141	N-trans-p-coumaroyl-O-methyldopamine	$C_{18}H_{19}NO_4$	314.13868	
142	N-cinnamoyltyramine	$C_{17}H_{17}NO_2$	268.13321	
143	Dehydrodiscretine	$C_{20}H_{20}NO_4^+$	339.14654	265.0732, 279.0894, 294.1160, 307.0850, 322.1074, 323.1154,
144	Thalifaurine	$C_{19}H_{16}NO_4^+$	323.11521	221.0815, 237.0732, 250.0864, 279.0881, 307.0842

145	Pseudocolumbamine	$C_{20}H_{20}NO_4^+$	339.14654	250.0866, 265.0727, 279.0901, 294.1127, 307.0851, 322.1067
146	Stepholidine	$C_{19}H_{21}NO_4$	328.15433	137.0577, 151.0694, 163.0633, 178.0853, 265.0674, 298.1095
147	Menisperine	$C_{21}H_{26}NO_4$	357.19346	248.0837, 264.0787, 279.1027, 296.1048, 311.1289, 325.1506
148	Stepharanine	$C_{19}H_{18}NO_4^+$	325.13086	238.0855, 266.0812, 294.0764, 309.0997
149	Palmatine	$C_{21}H_{22}NO_4$	353.16216	188.9044, 201.9610, 224.8873, 267.0940, 292.0977, 308.1261, 337.1238
150	Epiberberine	$C_{17}H_{18}N^+$	237.15120	277, 292, 306, 321, 336
151	8-demethoxyrunanine	$C_{21}H_{27}NO_4$	358.20128	
152	Tetrahydricheilanthifolinium	$C_{18}H_{16}NO_4^+$	311.11521	

153	sinopyrines A	C ₁₃ H ₁₅ NO ₃	234.11247	
154	Sinopyrines B	C ₁₃ H ₁₀ NO ₃	229.07334	
155	Sinopyrines C	C ₁₃ H ₁₇ NO ₂	220.13321	
156	CCRIS 3818	C ₁₉ H ₁₅ NO ₄	322.10738	
157	Acutuminine	C ₂₀ H ₂₆ ClNO ₅	384.15723	229.0849, 257.0794, 289.1084, 325.0832
158	(-) -8-oxotetrahydrothalifendine	C ₁₇ H ₁₂ NO ₅ ⁺	310.07882	
159	Stepharine	C ₁₈ H ₁₉ NO ₃	198.14377	161.0836, 192.1019, 238.0996, 254.0956, 269.1174
160	Tsuduranine	C ₁₈ H ₁₉ NO ₃	298.14733	146.0598, 161.0834, 192.1020, 238.0989, 254.0963, 269.1173

161	Menisperine	C ₂₂ H ₂₆ NO ₄	369.19346	
162	Reticuline	C ₁₉ H ₂₃ NO ₄	330.16998	106.0869, 140.9169, 172.8902, 213.0894, 287.3114, 330.32931
163	Laurifoline	C ₂₀ H ₂₄ NO ₄	343.17781	194.0724, 205.0645, 233.0597, 265.0861, 282.0887, 311.1301
164	Stephamiersine	C ₂₁ H ₂₇ NO ₆	390.15473	149.0253, 254.0560, 269.0807, 285.0740, 330.0736, 345.0988

Figure S1 Chemical structure of Aporphine alkaloids

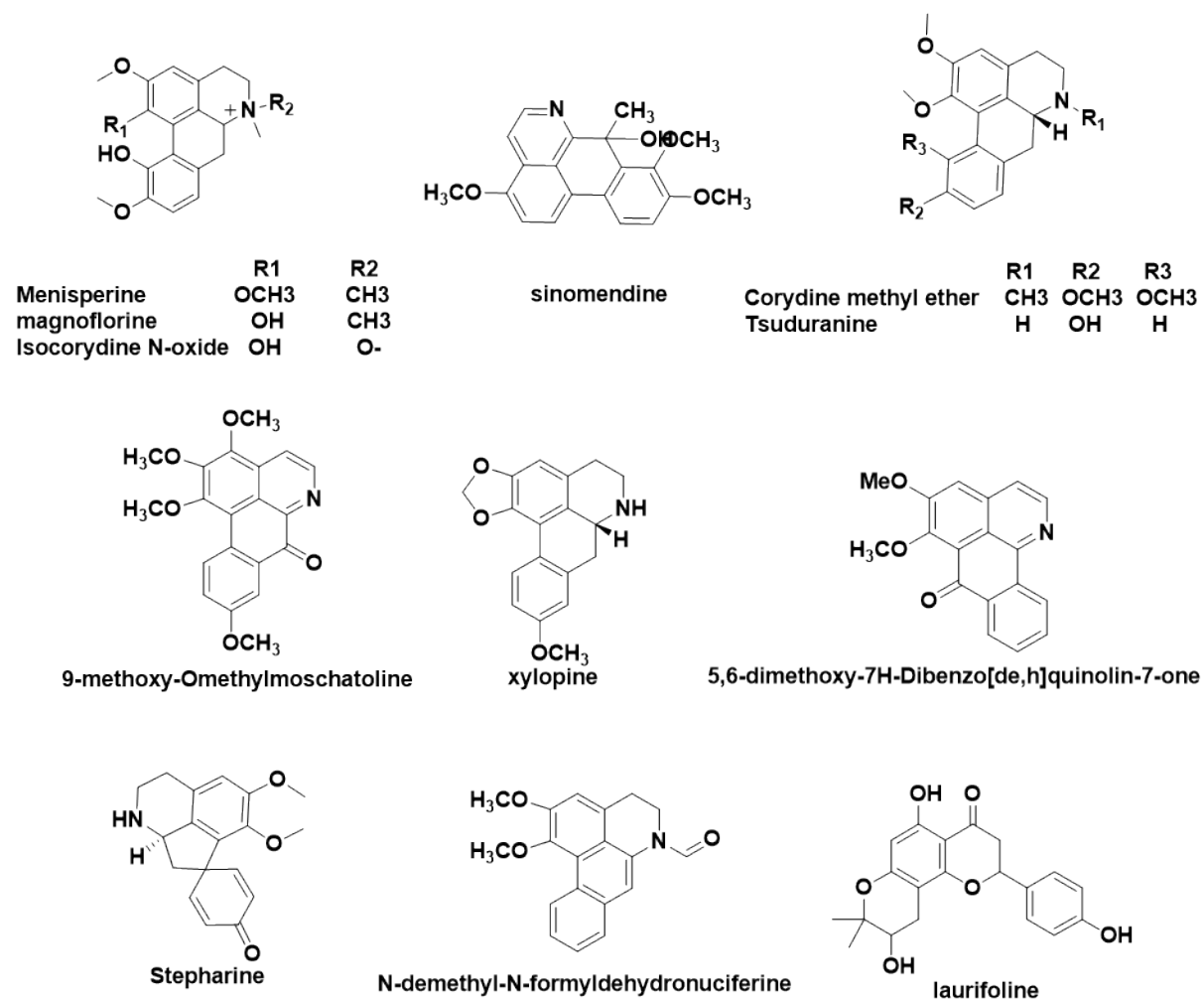
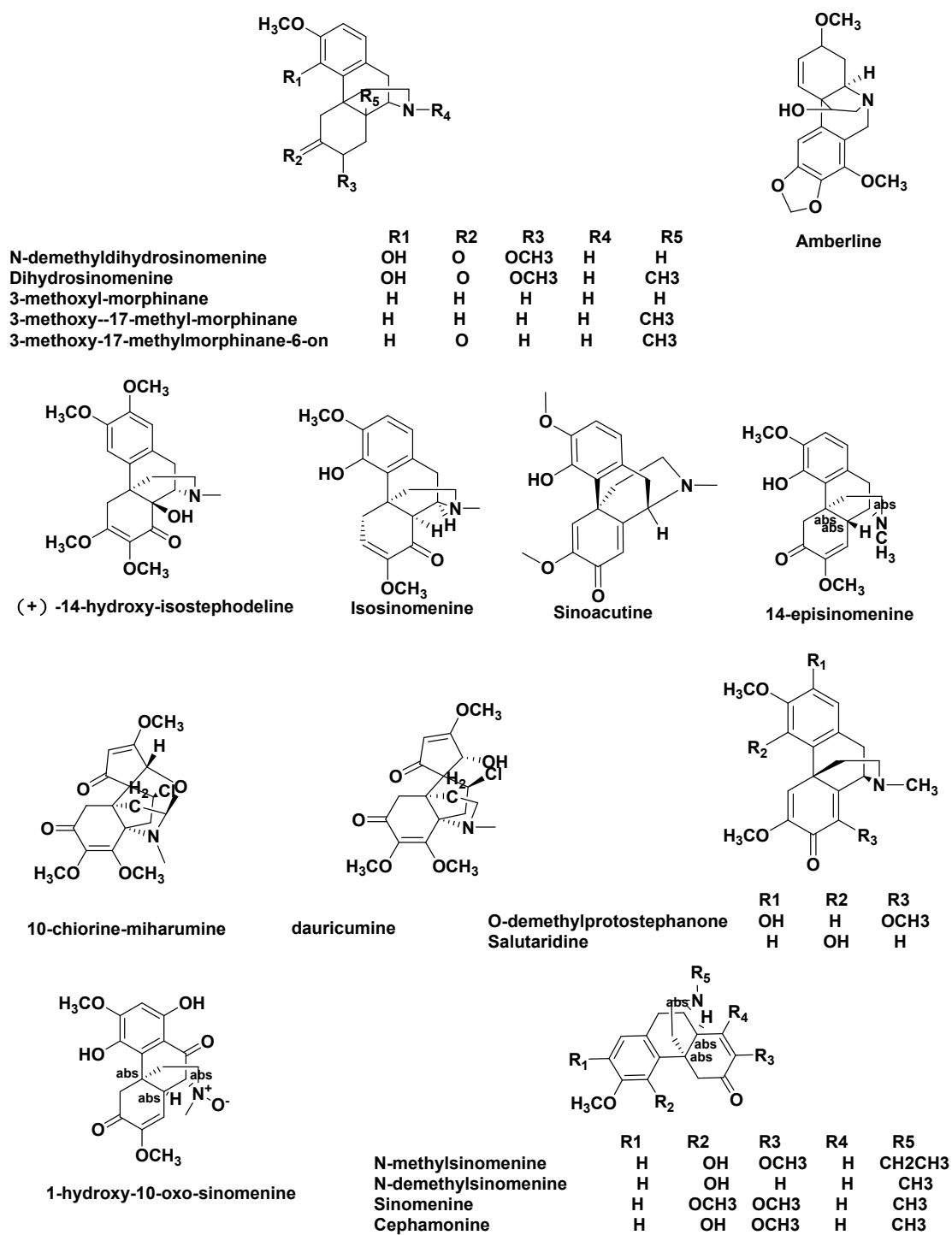
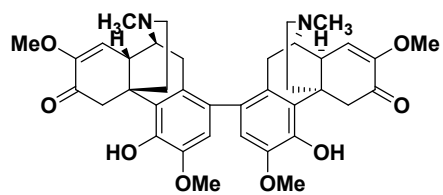
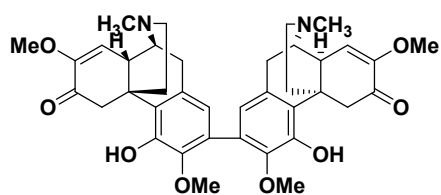


Figure S2 Chemical structure of morphine alkaloids

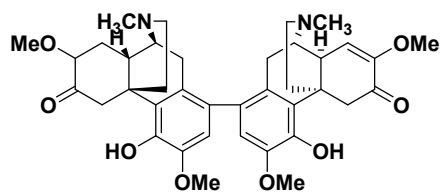




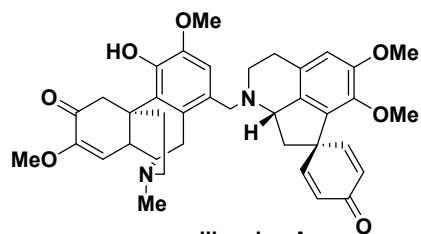
1,1'-disinomenine



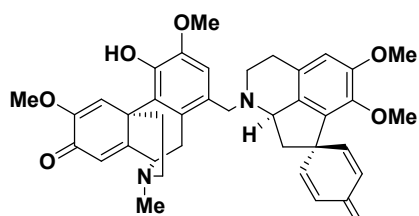
2,2'-disinomenine



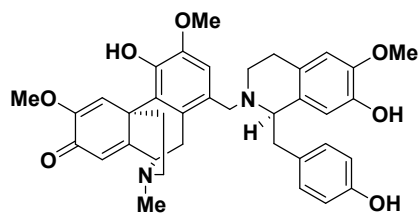
7',8'-dihydro-1,1'-disinomenine



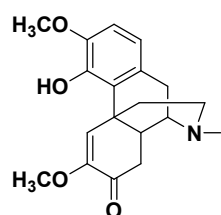
sallisonine A



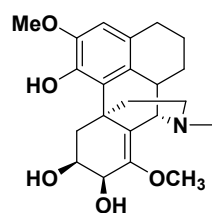
sallisonine B



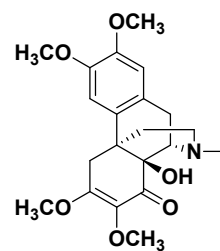
sallisonine C



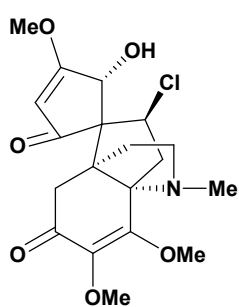
8,14-dihydrosalutaridine



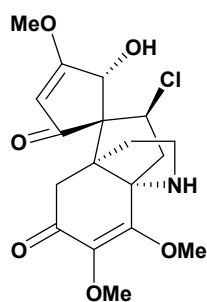
FK1000



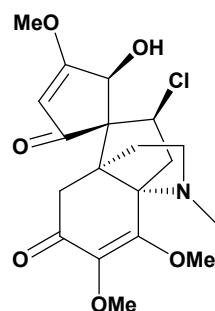
(+)-14-hydroxy-isostephodeline



duaricumine



acutumidine



dauricumine

Figure S3 Chemical structure of protoberberine alkaloids

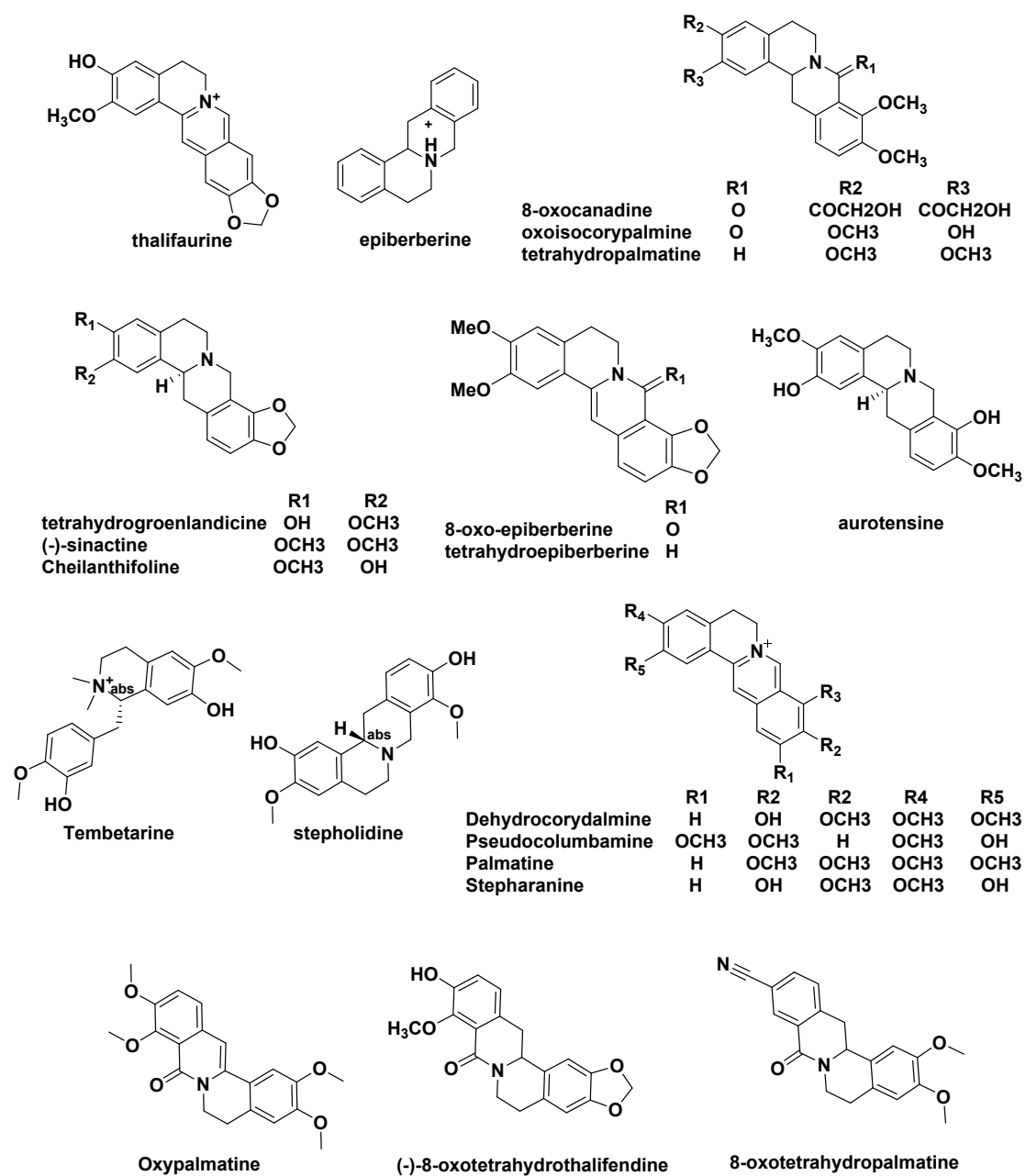
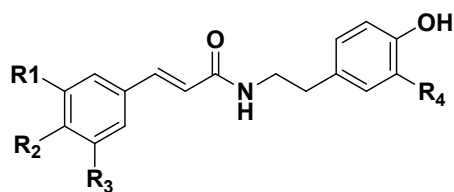


Figure S4 Chemical structure of other types alkaloids



	R1	R2	R3	R4
N-cis-feruloyltyramine	H	OH	OCH3	OCH3
N-trans-feruloyltyramine	OCH3	OH	H	H
N-trans-feruloylmethoxytyramine	OCH3	OH	H	OCH3
N-trans-p-coumaroyl-3-O-methyldopamin	H	OH	H	OCH3
N-cinnamoyltyramine	H	H	H	H

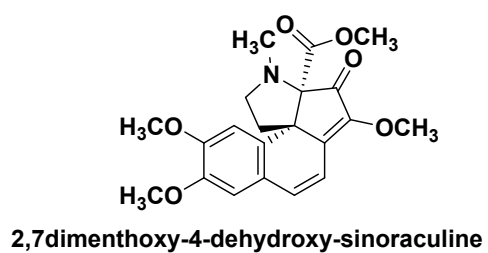
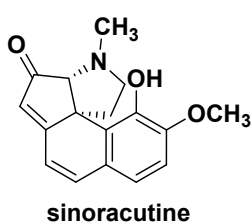


Figure S5 79 core targets were screened from the PPI network based on $2 \times DC$, $2 \times BC$, and $2 \times CC$

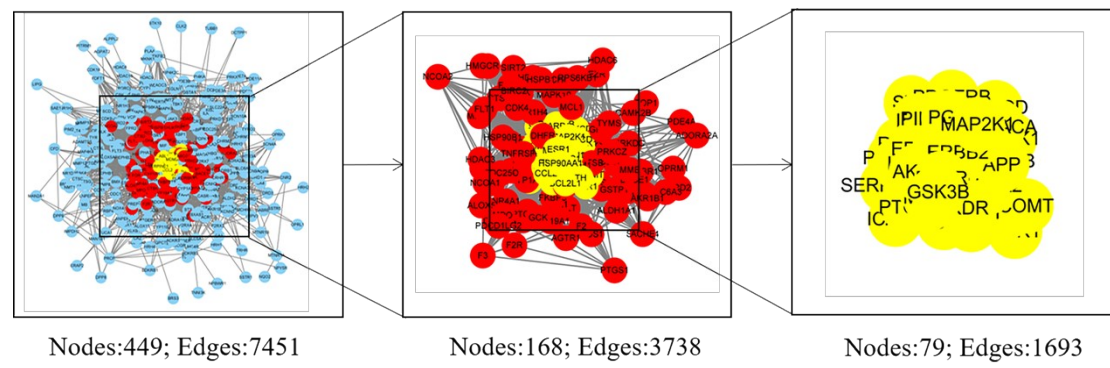


Figure S6 The C-P-T network of SC for the treatment of RA

