Supporting Information

Quinolizidine-Type Alkaloids: Chemodiversity, Occurrence and Bioactivity

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Table S1. Names and SMILES of compiled 397 quinolizidine alkaloids (QAs)

QAs	Name	SMILES
1	(-)-sophcence A	[H][C@]12CCCC(N1[C@@H]([C@]3(CCC[N+]4(CCC[C@]2([C@]34[H])[H])[O-])[H])O)=O
2	(+)-oxymatrine	[H][C@]12CCCC(N1C[C@@]3(CCC[N+]4(CCC[C@]2([C@]34[H])[H])[O-])[H])=O
3	(+)-oxysophocarpine	[H][C@]1([C@@](CCC2)3[H])CCCN([C@]14[H])CCC[C@@]4(O)C([H])N3C2=O
4	(+)-sophoranol	[H][C@]1([C@@](CCC2)3[H])CCCN([C@]14[H])CCC[C@@]4([H])[C@@H](O)N3C2=O
5	17β-hydroxysophoridine	[H][C@]1([C@@](CCC2)3[H])CCCN([C@]14[H])CCC[C@]4([H])CN3C2=O
6	sophoridine	[H][C@]1([C@@](CCC2)3[H])CCCN([C@]14[H])CCC[C@]4([H])CN3C2=O
7	(+)-matrine	[H][C@]1([C@@](CC=C2)3[H])CCCN([C@]14[H])CCC[C@]4([H])CN3C2=O
8	(+)-9α-hydroxymatrine	O=C1N2C[C@@]([H])([C@@]34[H])CCCN4C[C@@H](O)C[C@]3([H])[C@@]2([H])CCC1
9	(-)-sophocarpine	[H][C@]12CC=CC(N1C[C@]3([H])CCCN4CCC[C@]2([C@]34[H])[H])=O
10	(-)-Δ^{7}-dehydrosophoramine	O=C1C=CC=C2C([C@]34[H])=CCCN4CCC[C@@]3([H])CN12
11	15-deoxymatrine	[H][C@]12CCCCN1C[C@@]3(CCCN4CCC[C@@]2([H])[C@]34[H])[H]
12	darvasamine	[H][C@@]([C@](CCC1)2[H])([C@]34[H])CCCN4CCC[C@]3([H])CN2C1=O
13	allomatrine	[H][C@@]([C@@](CCC1)2[H])([C@@]34[H])CCCN4CCC[C@@]3([H])CN2C1=O
14	sophoramine	O=C1C=CC=C2[C@@]([C@]34[H])([H])CCCN4CCC[C@@]3([H])CN12
15	lehmannine	[H][C@]12CCCN3CCC[C@]([C@]4(C=CCC(N4C1)=O)[H])([C@]23[H])[H]
16	leontalbinine	[H][C@]12CCCN3CCCC([C@]23[H])=C4CCCC(N4C1)=O
17	(+)-5α-hydroxyoxymatrine	O=C1CCC[C@]2([H])[C@@]([C@]34[H])([H])CCC[N+]4([O-])CCC[C@@]3(O)CN12
18	14β-hydroxyoxymatrine	[H][C@@]([C@@](CC[C@@H]1O)2[H])([C@]34[H])CCC[N+]4([O-])CCC[C@@]3([H])CN2C1=O
19	5a,14β-dihydroxymatrine	[H][C@]12CC[C@@H](C(N1C[C@@]3(CCCN4CCC[C@]2([C@]34[H])[H])O)=O)O

20	7b-sophoramine	[H][C@]12CCCN3CCC[C@@](C4=CC=CC(N4C1)=O)([C@]23[H])[H]
21	14 β -hydroxymatrine	[H][C@]12CCCN3CCC[C@]([C@]4(CC[C@@H](C(N4C1)=O)O)[H])([C@]23[H])[H]
22	sophaline F	[H][C@@]12CCCN3C(C(CC(C4=CNC5=C4C=CC=C5)=O)=C[C@@]([C@]6(CCCC(N6C1)=O)[H])([C@]23[H])[H])=O
23	13b-butoxymatrine	[H][C@@]([C@@](C[C@H](OCCCC)C1)2[H])([C@]34[H])CCCN4CCC[C@@]3([H])CN2C1=O
24	(+)-(14β)-14-ethylmatridin-15-one	CC[C@H]1CC[C@]2(N(C1=O)C[C@]3([H])CCCN4CCC[C@]2([C@]34[H])[H])[H]
25	9,10-dehydrosophocarpine	[H][C@]12CCCN3C=CC[C@]([C@]4(CC=CC(N4C1)=O)[H])([C@]23[H])[H]
26	2,3-dehydrosophocarpine	[H][C@]12CC=CN3CCC[C@]([C@]4(CC=CC(N4C1)=O)[H])([C@]23[H])[H]
27	isomatrine	[H][C@@]12CCCN3CCC[C@@]([C@]4(CCCC(N4C1)=O)[H])([C@@]23[H])[H]
28	7,11-dehydromatrine	O=C1CCCC2=C([C@]34[H])CCCN4CCC[C@]3([H])CN12
29	9α-hydroxy-7,11-dehydromatrine	O[C@@H](CC([C@]12[H])=C3CCC4)CN2CCC[C@@]1([H])CN3C4=O
30	9α-hydroxy-13,14-dehydromatrine	[H][C@]12CCCN3C[C@H](C[C@]([C@]4(CC=CC(N4C1)=O)[H])([C@]23[H])[H])O
31	9α-hydroxysophoramine	O=C1C=CC=C2N1C[C@@]3(CCCN4C[C@H](C[C@]2([C@]34[H])[H])O)[H]
32	sophtonseedline B	O[C@]12CCCN3C[C@H](C[C@]([C@]4(CC=CC(N4C1)=O)[H])([C@]23[H])[H])O
33	sophtonseedline C	O[C@]12CCCN3C[C@H](C[C@]([C@]4(CC=CC(N4C1)=O)[H])([C@]23[H])[H])OC(C)=O
34	sophtonseedline D	O[C@]12CCCN3C[C@H](C[C@]([C@]4(CC=CC(N4C1)=O)[H])([C@]23[H])[H])OCSC
35	sophtonseedline E	O[C@]12CCCN3C[C@H](C[C@]([C@]4(CCCC(N4C1)=O)[H])([C@]23[H])[H])OC(C)=O
36	sophtonseedline F	O[C@]12CCCN3C[C@H](C[C@]([C@]4(CCCC(N4C1)=O)[H])([C@]23[H])[H])OCSC
37	sophtonseedline G	[H][C@]12CCC[N+]3([O-])C[C@H](C[C@]([C@]4(CCCC(N4C1)=O)[H])([C@]23[H])[H])O
38	sophtonseedline H	O[C@]12CCCN3C[C@H](C[C@]([C@]4(CCCC(N4C1)=O)[H])([C@]23[H])[H])OC
39	sophtonseedline I	O[C@@]12CCCN3C[C@H](CC([C@]4(CCCC(N4C2)=O)[H])=C13)OC(C)=O
40	sophtonseedline J	O[C@]12CCCN3CCC[C@@]4([C@]23O4)[C@]5(CC=CC(N5C1)=O)[H]

41	sophtonseedline K	[H][C@@]1(CC=C2)[C@@]([C@]34O5)(O)CCCN4CCC[C@@]35CN1C2=O
42	(−)-5α-hydroxysophocarpine	O[C@]12CCCN3CCC[C@]([C@]4(CC=CC(N4C1)=O)[H])([C@]23[H])[H]
43	(+)-5α,9α-dihydroxymatrine	O[C@]12CCCN3C[C@@H](O)C[C@]([C@]4(CCCC(N4C1)=O)[H])([C@]23[H])[H]
44	6,7-dehydromatrine	[H][C@@]12CCCN3CCCC([C@]4(CCCC(N4C2)=O)[H])=C13
45	5-hydroxy-6,7-dehydromatrine	O[C@@]12CCCN3CCCC([C@]4(CCCC(N4C2)=O)[H])=C13
46	5,6-dehydro-matrine	[H][C@@]1(CCCC(N1C2)=O)[C@@]3([H])CCCN4CCCC2=C34
47	(+)-12α-Hydroxysophocarpine	[H][C@@]([C@@]([C@@H](O)C=C1)2[H])([C@]34[H])CCCN4CCC[C@@]3([H])CN2C1=O
48	(−)-13,14-dehydrosophoridine	[H][C@@]([C@@](CC=C1)2[H])([C@]34[H])CCCN4CCC[C@]3([H])CN2C1=O
49	7a-hydroxysophoramine	[H][C@@](C1=CC=C2)([C@]34O)CCCN4CCC[C@@]3([H])CN1C2=O
50	12β-hydroxysophocarpine	[H][C@@]([C@@]([C@H](O)C=C1)2[H])([C@]34[H])CCCN4CCC[C@@]3([H])CN2C1=O
51	(-)-14α-Acetoxymatrine	[H][C@]12CCCN3CCC[C@]([C@]4(CC[C@H](C(N4C1)=O)OC(C)=O)[H])([C@]23[H])[H]
52	(-)-14β-Acetoxymatrine	[H][C@@]([C@@](CC[C@@H]1OC(C)=O)2[H])([C@]34[H])CCCN4CCC[C@@]3([H])CN2C1=O
53	14α-hydroxymatrine	[H][C@]12CCCN3CCC[C@]([C@]4(CC[C@H](C(N4C1)=O)O)[H])([C@]23[H])[H]
54	(-)-14β-Hydroxysophoridine	[H][C@]1([C@@](CC[C@@H]2O)3[H])CCCN([C@]14[H])CCC[C@]4([H])CN3C2=O
55	5,6-dehydro-lupanine	[H][C@@]12CCCCN1C[C@H]3C[C@@H]2CN4C(CCC=C34)=O
56	(-)-lupanine	[H][C@@]12CCCCN1C[C@H]3C[C@@H]2CN4C(CCC[C@]34[H])=O
57	5α-hydoxylupanine	[H][C@@]12CCCCN1C[C@H]3C[C@@H]2CN4C(CC[C@@H]([C@]34[H])O)=O
58	7β-hydoxylupanine	[H][C@@]12CCCCN1C[C@]3(O)C[C@H]2CN4C(CCC[C@]34[H])=O
59	oxylupanine	[H][C@@]12CCCCN1C[C@H]3C[C@@H]2C[N+]4([O-])C(CCC[C@]34[H])=O
60	17α-hydroxylupanine	[H][C@@]12CCCCN1[C@@H]([C@@H]3C[C@H]2CN4C(CCC[C@]34[H])=O)O
61	(+)-lupanine	[H][C@@]12CCCCN1C[C@@H]3C[C@H]2CN4C(CCC[C@]34[H])=O

62	α-isolupanine	[H][C@]12CCCCN1C[C@H]3C[C@@H]2CN4C(CCC[C@]34[H])=O
63	13α-hydroxylupanine	[H][C@]12CCCC(N1C[C@H]3C[C@@H]2CN4CC[C@@H](C[C@@]34[H])O)=O
64	13α-tigloyloxylupanine	[H][C@@]12C[C@@H](OC(/C(C)=C/C)=O)CCN1C[C@H]3C[C@@H]2CN4C(CCC[C@]34[H])=O
65	6,7-dihydroxylupanine	O=C1N2C[C@]([H])(C3)[C@]4([H])CCCCN4C[C@@]3(O)[C@@]2(O)CCC1
66	lanatine A	[H][C@]12CCCC(N1C[C@@H]3C[C@H]2CN4CC[C@H](OC(C5=CC=CC=C5N)=O)C[C@@]34[H])=O
67	13α-*E*-cinnamoyloxylupanine	[H][C@]12CCCC(N1C[C@@H]3C[C@H]2CN4CC[C@H](OC(/C=C/C5=CC=CC=C5)=O)C[C@@]34[H])=O
68	13α-angeloyloxylupanine	[H][C@]12CCCC(N1C[C@@H]3C[C@H]2CN4CC[C@@H](C[C@@]34[H])OC(/C(C)=C/C)=O)=O
69	17-oxolupanine	[H][C@@]12CCCCN1C([C@@H]3C[C@H]2CN4C(CCC[C@]34[H])=O)=O
70	13α-*cis*-cinnamoyloxylupanine	[H][C@]12CCCC(N1C[C@@H]3C[C@H]2CN4CC[C@H](OC(/C=C/C5=CC=CC=C5)=O)C[C@@]34[H])=O
71	13β-methoxylupanine	[H][C@]12CCCC(N1C[C@@H]3C[C@H]2CN4CC[C@@H](OC)C[C@@]34[H])=O
72	4α-hydroxy-13β-methoxylupanine	[H][C@]12C[C@@H](O)CC(N1C[C@@H]3C[C@H]2CN4CC[C@@H](OC)C[C@@]34[H])=O
73	3β,4α-dihydroxy-13β-methoxylupanine	[H][C@]12C[C@H]([C@H](O)C(N1C[C@@H]3C[C@H]2CN4CC[C@H](C[C@@]34[H])OC)=O)O
74	3β,13β-dihydroxylupanine	[H][C@]12CC[C@H](O)C(N1C[C@@H]3C[C@H]2CN4CC[C@H](O)C[C@@]34[H])=O
75	(-)-3β-Hydroxy-l3α-tigloyloxylupanine	[H][C@]12CC[C@H](O)C(N1C[C@@H]3C[C@H]2CN4CC[C@H](O/C=C(C)/CC=O)C[C@@]34[H])=O
76	(+)-15β-hydroxy-17-oxolupanine	[H][C@]12CCCC(N1C[C@@H]3C[C@H]2C(N4[C@@H](O)CCC[C@@]34[H])=O)=O
77	5α-hydroxy-7,17-dehydroisolupanine	[H][C@]12[C@@H](O)CCC(N1C[C@@H]3CC2=CN4CCCC[C@@]34[H])=O
78	(+)-3α-hydroxylupanine	[H][C@]12CC[C@@H](O)C(N1C[C@@H]3C[C@H]2CN4CCCC[C@@]34[H])=O
79	3β-hydroxylupanine	[H][C@]12CC[C@H](O)C(N1C[C@@H]3C[C@H]2CN4CCCC[C@@]34[H])=O
80	3β,13α-dihydroxylupanine	[H][C@]12CC[C@H](O)C(N1C[C@@H]3C[C@H]2CN4CC[C@H](O)C[C@@]34[H])=O
81	8α,13α-dihydroxylupanine	[H][C@]12CCCC(N1C[C@@H]3C(O)[C@H]2CN4CC[C@H](O)C[C@@]34[H])=O
82	3β,8α,13α-trihydroxylupanine	[H][C@]12CC[C@H](O)C(N1C[C@@H]3C(O)[C@H]2CN4CC[C@H](O)C[C@@]34[H])=O

83	(+)-13α-(4’-hydroxytigloyloxy) lupanine	[H][C@]12CCCC(N1C[C@@H]3C[C@H]2CN4CC[C@H](OC(/C(C)=C/CO)=O)C[C@@]34[H])=O
84	13α-methoxylupanine	[H][C@]12CCCC(N1C[C@@H]3C[C@H]2CN4CC[C@H](OC)C[C@@]34[H])=O
85	(+)-12α-Hydroxylupanine	[H][C@@]12CCCC(N1C[C@H]3C[C@@H]2CN4CCC[C@H](O)[C@]34[H])=O
86	lebeckianine	[H][C@]12C[C@@H](O)[C@H](O)C(N1C[C@@H]3C[C@H]2CN4CCCC[C@@]34[H])=O
87	pearsonine	[H][C@]12CC([C@@H](C(N1C[C@@H]3C(O)[C@H]2CN4CC[C@H](OC(/C(C)=C/C)=O)C[C@@]34[H])=O)O)[H]
88	3β-hydroxylupanine-4α-*O*-angelate	[H][C@]12C[C@H]([C@H](O)C(N1C[C@@H]3C[C@H]2CN4CCCC[C@@]34[H])=O)OC(/C(C)=C\C)=O
89	3β,13α-dihydroxylupanine	[H][C@]12CC[C@H](O)C(N1C[C@@H]3C[C@H]2CN4CC[C@H](O)C[C@@]34[H])=O
90	13-(2´-pirroylcarboxyl)calpurmenine	[H][C@]12CCCC(N1C[C@@H]3C[C@H]2CN4CC[C@@H]([C@@H](O)[C@@]34[H])OC(C5=CC=CN5)=O)=O
91	8α-hydroxylupanine-13α-*O*-angelate	[H][C@]12CCCC(N1C[C@@H]3C(O)[C@H]2CN4CC[C@H](OC(/C(C)=C\C)=O)C[C@@]34[H])=O
92	Nuttalline	[H][C@]12C[C@H](O)CC(N1C[C@@H]3C[C@H]2CN4CCCC[C@@]34[H])=O
93	3β-hydroxylupanine-13α-*O*-angelate	[H][C@]12CC[C@H](O)C(N1C[C@@H]3C[C@H]2CN4CC[C@H](OC(/C(C)=C\C)=O)C[C@@]34[H])=O
94	anagyrine	[H][C@]12CCCCN1C[C@H]3C[C@@H]2CN(C3=CC=C4)C4=O
95	thermopsine	[H][C@@]12CCCCN1C[C@H]3C[C@@H]2CN(C3=CC=C4)C4=O
96	sophaline E	O=C1C=CC=C2N1C[C@H]3C[C@@H]2CN4[C@]3([H])C[C@H](O)C[C@@]4([H])C(C5=CNC6=C5C=CC=C6)=O
97	(-)-13α-hydroxy-15α-(1-hydroxyethyl)-anagyrine	O=C1C=CC=C2N1C[C@H]3C[C@@H]2CN4[C@]3([H])C[C@@H](O)C[C@H]4[C@@H](C)O
98	(-)-baptifoline	O=C1C=CC=C2N1C[C@H]3C[C@@H]2CN4[C@]3([H])C[C@@H](O)CC4
99	(-)-epibaptifoline	O=C1C=CC=C2N1C[C@H]3C[C@@H]2CN4[C@]3([H])C[C@H](O)CC4
100	(+)-sophazrine	O=C1C=CC=C2N1C[C@H]3C[C@@H]2CN4[C@@]3([H])CN(C(CCC=C)=O)CC4
101	*O*-acetylbaptifoline	O=C1C=CC=C2N1C[C@H]3C[C@@H]2CN4[C@]3([H])C[C@H](OC(C)=O)CC4
102	thermseedline H	O=C1C=CC=C2N1C[C@H]3C[C@@H]2[C@H](CC(OC)=O)N4[C@@]3([H])CCCC4
103	thermseedline I	O=C1C=CC=C2N1C[C@H]3C[C@@H]2CN4[C@]3([H])C[C@@H](O)C[C@@]4([H])C(OC)=O

104	thermseedline J	O=C1C=CC=C2N1C[C@H]3C[C@@H]2CN4[C@]3([H])[C@H](O)C=CC4
105	thermseedline K	O=C1C=CC=C2N1C[C@H]3C[C@@H]2CN4[C@@]3([H])[C@@H](O5)[C@@H]5CC4
106	thermseedline L	O=C1C=CC=C2N1C[C@H]([C@@]3([H])N4CCCC3)C[C@@H]2C4=O
107	thermseedline M	O=C1C=CC=C2N1C[C@H]3C[C@@H]2CN4[C@@]3([H])CC[C@H](O)C4
108	thermseedline N	O=C1C=CC=C2N1C[C@H]3C[C@@H]2C[N+]4([O-])[C@@]3([H])CCCC4
109	thermseedline 0	O=C1C=CC=C2N1C[C@H]3C[C@@H]2CN4[C@]3([H])CC(CC4)=O
110	(+)-sparteine	[H][C@]12N(C[C@H]3C[C@@H]2CN4[C@]3([H])CCCC4)CCCC1
111	(-)-sparteine	[H][C@@]12N(C[C@H]3C[C@@H]2CN4[C@@]3([H])CCCC4)CCCC1
112	(-)-β-isosparteine	[H][C@]12N(C[C@@H]3C[C@H]2CN4[C@@]3([H])CCCC4)CCCC1
113	(-)-α-sparteine	[H][C@]12N(C[C@H]3C[C@@H]2CN4[C@@]3([H])CCCC4)CCCC1
114	11,12-dehydrosparteine	[H][C@]12N(C[C@H]3C[C@@H]2CN4C3=CCCC4)CCCC1
115	2-phenyl-2,3-didehydrosparteine	[H][C@]12N(C[C@H]3C[C@@H]2CN4[C@]3([H])CCCC4)C(C5=CC=CC=C5)=CCC1
116	15-phenyl-14,15-didehydrosparteine	[H][C@]12N(C[C@H]3C[C@@H]2CN4[C@]3([H])CCC=C4C5=CC=CC=C5)CCCC1
117	2-cyano-2-methylsparteine	[H][C@]12N(C[C@H]3C[C@@H]2CN4[C@]3([H])CCCC4)C(C)(C#N)CCC1
118	2,17-dimethylsparteine	[H][C@]12N(C[C@H]3C[C@@H]2C(C)N4[C@]3([H])CCCC4)C(C)CCC1
119	2-methyl-17-oxosparteine	[H][C@]12N(C[C@H]([C@]3([H])N4CCCC3)C[C@@H]2C4=O)C(C)CCC1
120	acosminine	[H][C@]12N([C@H](C3=CN(C(C)=O)CCC3)[C@H]4C[C@@H]2CN5[C@]4([H])C[C@@H](O)CC5)CCCC1
121	(-)-aphyllidine	[H][C@]12[C@@H]3C(N4CCCC=C4[C@H](CN1CCCC2)C3)=O
122	aphyline	[H][C@]12[C@@H]3C(N4CCCC[C@]4([H])[C@H](CN1CCCC2)C3)=O
123	monspessulanine	[H][C@@]12[C@@H]3C(N4CCCC=C4[C@H](CN1CCCC2)C3)=O
124	(+)-2,3-dehydro-10-oxo-a-isosparteine	[H][C@@]12[C@@H]3C(N4C=CCC[C@]4([H])[C@H](CN1CCCC2)C3)=O

125	7-hydroxy-β-isosparteine	[H][C@@]12C3([H])C(N4CCCC[C@]4([H])C(CN1CCCC2)(O)C3)=O
126	(+)-retamine	[H][C@@]12[C@]3(C(N4CCC[C@H](O)[C@@]4([C@H](C3)CN1CCCC2)[H])=O)[H]
127	10α-Hydroxymethylsparteine	[H][C@@]12N([C@@]([H])(CO)[C@H]3C[C@@H]2CN4[C@@]3([H])CCCC4)CCCC1
128	14α-hydroxysparteine	[H][C@]12N(C[C@H]3C[C@@H]2CN4[C@]3([H])CC[C@@H](O)C4)CCCC1
129	(+)-2β-hydroxyaphylline	[H][C@]12N(C([C@H]3C[C@@H]2CN4[C@]3([H])CCCC4)=O)[C@@H](O)CCC1
130	(+)-13β-hydroxyaphyllidine	[H][C@@]12[C@H]3C(N4CCCC=C4[C@@H](CN1CC[C@H](O)C2)C3)=O
131	oxy-*N*-methylcytisine	O=C1C=CC=C2N1C[C@H]3C[C@@H]2C[N+](C)([O-])C3
132	(-)-cytisine	O=C1C=CC=C2N1C[C@H]3C[C@@H]2CNC3
133	*N*-methylcytisine	O=C1C=CC=C2N1C[C@H]3C[C@@H]2CN(C)C3
134	*N*-butylcytisine	O=C1C=CC=C2N1C[C@H]3C[C@@H]2CN(CCCC)C3
135	(-)-rhombifoline	O=C1C=CC=C2N1C[C@H]3C[C@@H]2CN(CCC=C)C3
136	cytisine-12-carboxyethylester	O=C1C=CC=C2N1C[C@H]3C[C@@H]2CN(C(OCC)=O)C3
137	11-allylcytisine	O=C1C=CC=C2N1C[C@H]3C[C@@H]2CN[C@@H]3CC=C
138	*N*-methylenehydroxycytisine	O=C1C=CC=C2N1C([H])([H])[C@@]3([H])C[C@]2([H])CN(CO)C3
139	*N*-formylcytisine	O=C1C=CC=C2N1C[C@@H]3C[C@H]2CN(C=O)C3
140	9-hydroxy-*N*-methylcytisine	O=C1C=CC=C2N1C[C@@]3(O)C[C@]2([H])CN(C)C3
141	*N*-acetylcytisine	O=C1C=CC=C2N1C[C@H]3C[C@@H]2CN(OC(C)=O)C3
142	*N*-carboxymetylencytisine	O=C1C=CC=C2N1C[C@H]3C[C@@H]2CN(CC(O)=O)C3
143	(-)-12-cytisineacetamide	O=C1C=CC=C2N1C[C@H]3C[C@@H]2CN(CC(N)=O)C3
144	*N*-hydroxycytisine	O=C1C=CC=C2N1C[C@H]3C[C@@H]2CN(O)C3
145	sophorasine A	O=C1C=CC=C2N1CC3([H])CC2([H])CN(CC([C@](O)([H])C)=O)C3

146	sophorasine B	O=C1C=CC=C2N1CC3([H])CC2([H])CN(CC([C@]([H])(O)C)=O)C3
147	cytisine-12-carboxy-methylester	O=C1C=CC=C2N1C[C@H]3C[C@@H]2CN(C(OC)=O)C3
148	thermseedline A	O=C1[C@H]2CN3C(C=CC=C3[C@@H](CN1CCC)C2)=O
149	thermseedline B	O=C1[C@H]2CN3C(C=CC=C3[C@@H](CN1CCCO)C2)=O
150	thermseedline C	O=C1[C@H]2CN3C(C=CC=C3[C@@H](CN1CCCC(N(CC)CC)=O)C2)=O
151	thermseedline D	O=C1C=CC=C2N1C[C@H]3C[C@@H]2CN(C4=CCOC4=O)C3
152	thermseedline E	O=C1C=CC=C2N1C[C@H]3C[C@@H]2CN(C4=CC=C(CO)N=C4)C3
153	thermseedline P	O=C1C=CC=C2N1C[C@H]3C[C@@H]2CN(CC(C4=CNC5=C4C=CC=C5)=O)C3
154	thermseedline Q	O=C1C=CC=C2N1C[C@H]3C[C@@H]2CN(O[C@H]([C@@H]4O)O[C@H](CO)[C@@H](O)[C@@H]4O)C3
155	thermlanseedline G	O=C1[C@H]2CN3C(C=CC=C3[C@@H](CN1CCCC(C)=O)C2)=O
156	3-hydroxy-11-norcytisine	O=C1C(O)=CC=C2N1C[C@H]3C[C@@H]2NC3
157	kushenine	O=C1CCC[C@@]2([H])N1C[C@@H]3C[C@H]2CN(C)C3
158	tetrahydrocytisine	O=C1CCC[C@@]2([H])N1C[C@H]3C[C@@H]2CNC3
159	lupanacosmine	O=C1CCC[C@@]2([H])N1[C@H](C3=CN(C(C)=O)CCC3)[C@@H]4C[C@H]2CN(C)[C@@]4([H])CC=C
160	tetrahydrorhombifoline	O=C1CCC[C@@]2([H])N1C[C@@H]3C[C@H]2CN(CCC=C)C3
161	angustifoline	O=C1CCC[C@@]2([H])N1C[C@@H]3C[C@H]2CN[C@@]3([H])CC=C
162	*N*- methyltetrahydrocytisine epimer	[H][C@]12N(C[C@H]3C[C@@H]2CN(C)C3)CCCC1
163	*N*- formyltetrahydrocytisine	O=C1CCC[C@@]2([H])N1C[C@H]3C[C@@H]2CN(C=O)C3
164	*N*- methyltetrahydrocytisine	O=C1CCC[C@@]2([H])N1C[C@H]3C[C@@H]2CN(C)C3
165	termisine	[H][C@]12N(C[C@@H]3C[C@H]2CN(CO)[C@]3([H])CCCC(O)=O)CCCC1
166	desoxyangustifoline	[H][C@@]12N(C[C@@H]3C[C@H]2CN[C@@]3([H])CC=C)CCCC1

167	(-)-Δ^5-dehydroalbine	O=C1C=CN(C[C@@H]2C[C@H]3[C@](CC=C)([H])NC2)C3=C1
168	(-)-albine	O=C1C=CN(C[C@@H]2C[C@H]3[C@](CC=C)([H])NC2)[C@]3([H])C1
169	11,12-seco-12,13-didehydromultiflorine	O=C1C=CN(C[C@@H]2C[C@H]3CN(CCC=C)C2)[C@]3([H])C1
170	virgilidone	[H][C@@]12N(C([C@]3([H])C[C@@]2([H])CNC3)=O)CCCC1
171	virgiboidine	[H][C@@]12N(C([C@@H]3C[C@H]2CN(CCC=C)C3)=O)CCCC1
172	*N*-methylalbine	O=C1C=CN(C[C@@H]2C[C@H]3[C@](CC=C)([H])N(C)C2)[C@]3([H])C1
173	*N*-methylangustifoline	O=C1CCC[C@@]2([H])N1C[C@@H]3C[C@H]2CN(C)[C@@]3([H])CC=C
174	(-)-lupinine	OC[C@H]1[C@]2([H])N(CCC1)CCCC2
175	(+)-epilupinine	OC[C@@H]1[C@]2([H])N(CCC1)CCCC2
176	(-)-lusitanine	CC(N/C=C1CCCN2CCCC[C@@]2/1[H])=O
177	2-hydroxylupinine	[H][C@@]12N(CC[C@H](O)[C@@H]2CO)CCCC1
178	lycocernuskine C	[H][C@@]12N(CCCC2)[C@@H](C)C[C@](C)(O)C1
179	cermizine C	[H][C@@]12N(CCCC2)[C@@H](C)C[C@@H](C)C1
180	cermizine D	[H][C@@]12N(CCCC2)[C@](C[C@]3([H])NCCCC3)([H])C[C@@H](C)C1
181	cermizine D N-oxide	[H][C@@]12[N+](CCCC2)([O-])[C@](C[C@]3([H])NCCCC3)([H])C[C@@H](C)C1
182	(−)-senepodine G	[H][C@@]12[N+](CCCC2)=C(C)C[C@@H](C)C1
183	(−)-senepodine H	[H][C@@]12[N+]([C@H](C[C@H](C)O)CCC2)=C(C)C[C@@H](C)C1
184	(+)-myrtine	[H][C@@]12N([C@H](C)CC(C2)=O)CCCC1
185	(−)-epimyrtine	[H][C@@]12N([C@H](C)CC(C2)=O)CCCC1
186	(+)-epiquinamide	[H][C@@]12N(CCC[C@@H]2NC(C)=O)CCCC1
187	(+)-clavepictine A	[H][C@]12N([C@@H](C)[C@H](OC(C)=O)CC2)[C@H](/C=C\C=C\CCCCCC)CCC1

188	(+)-clavepictine B	[H][C@]12N([C@@H](C)[C@H](O)CC2)[C@H](/C=C\C=C\CCCCCC)CCC1
189	(-)-Pictamine	[H][C@@]12N([C@H](/C=C\C=C\CCCC)CCC2)[C@@H](C)[C@H](OC(C)=O)CC1
190	quinolizidine 275I-2	C=CCCC[C@H]1CCCC2N1[C@H](CCCC=C)CCC2
191	quinolizidine 249F	[H][C@@]12N(CCCC2)C/C(C[C@@H]1O)=C/C=C\CCC
192	quinolizidine 217A	[H][C@@]12N(CCCC2)[C@H](C/C=C\C#C)CC[C@H]1C
193	quinolizidine 195C	[H][C@@]12N([C@H](CCC)CCC2)[C@@H](C)CCC1
194	quinolizidine-207I	[H][C@@]12N(CCCC2)[C@H](CC=C)CC[C@@H]1CC
195	quinolizidine-231A	[H][C@@]12N(CCCC2)[C@H](C/C=C\C#C)CC[C@@H]1CC
196	quinolizidine-233A	[H][C@@]12N(CCCC2)[C@H](C/C=C\C#C)CC[C@H]1CC
197	quinolizidine-235E	[H][C@@]12N(CCCC2)[C@H](CCCCC=C)CC[C@@H]1C
198	hupermine A	CN(C)CCCCCC[C@H]1C[C@@H](C)C[C@@]2([H])N1CCCC2
199	mamanine	OC[C@H]1C[C@](C2=CC=CC(N2)=O)([H])CN3CCCC[C@@]31[H]
200	pohakuline	OC[C@H]1C[C@]([C@]2([H])CCCC(N2)=O)([H])CN3CCCC[C@@]31[H]
201	Jussiaeiine B	[H][C@@]12N(C[C@H](C3=CC=CC(OC)=N3)C[C@@H]2CO)CC([H])C([H])C1
202	Jussiaeiine C	[H][C@@]12N(C[C@H](C3=CC=CC(OC)=N3)C[C@@H]2CO)CC([H])[C@@H](O)C1
203	Jussiaeiine D	[H][C@@]12N(C[C@H](C3=CC=CC(OC)=N3)C[C@@H]2CO)C[C@@H](O)C([H])C1
204	(+)-13β-hydroxymamanine	[H][C@@]12N(C[C@H](C3=CC=CC(N3)=O)C[C@@H]2CO)CC[C@@H](O)C1
205	4-(3-hydroxy-4-methoxyphenyl)-quinolizidin-2-acetate	[H][C@@]12N([C@H](C3=CC=C(OC)C(O)=C3)C[C@@H](OC(C)=O)C2)CCCC1
206	julandine	[H][C@]12N(CC(C3=CC=C(OC)C=C3)=C(C4=CC(OC)=C(OC)C=C4)C2)CCCC1
207	cylicomorphins A	[H][C@@]12N([C@@H](CC(O)=O)CCC2)[C@@H](C)[C@H](OC(C3=CC=CC=C3)=O)CC1
208	cylicomorphins B	[H][C@@]12N([C@@H](CC(O)=O)CCC2)[C@@H](C)[C@H](OC(C3=CC(OC)=C(OC)C=C3)=O)CC1

209	cylicomorphins C	[H][C@@]12N([C@@H](CC(O)=O)CCC2)[C@@H](C)[C@H](OC(C3=CC=C(OC)C=C3OC)=O)CC1
210	cylicomorphins D	[H][C@@]12N([C@@H](CC(O)=O)CCC2)[C@@H](C)[C@H](OC(/C=C\C3=CC=CC=C3)=O)CC1
211	cylicomorphins E	[H][C@@]12N([C@@H](CC(O)=O)CCC2)[C@@H](C)[C@H](OC(/C=C\C3=CC=C(OC)C=C3)=O)CC1
212	(-)-*(E)*-(3-methoxy-4-α-rhamnosyloxycinnamoyl)epilupinine	[H][C@@]12N(CCC[C@@H]2COC(/C=C/C3=CC=C(OC4O[C@H](C)[C@H](O)[C@H](O)[C@@H]4O)C(OC)=C3)=O)CCCC1
213	lamprolobine	[H][C@]12N(CCC[C@]2([H])CN3C(CCCC3=O)=O)CCCC1
214	17-desoxy-*cis*-lamprolobine	[H][C@]12N(CCC[C@@]2(CN3C(CCCC3)=O)[H])CCCC1
215	epilupinine benzoate	[H][C@]12N(CC(C3=CC=C(OC)C=C3)=C(C4=CC(OC)=C(OC)C=C4)C2)CCCC1
216	nupharidine	[H][C@@]12[N+](C[C@@H](C)CC2)([O-])[C@H](C3=COC=C3)CC[C@H]1C
217	deoxynupharidine	[H][C@@]12N(C[C@@H](C)CC2)[C@H](C3=COC=C3)CC[C@H]1C
218	7-epideoxynupharidine	[H][C@@]12N(C[C@H](C)CC2)C(C3=COC=C3)CC[C@H]1C
219	nupharolutine	[H][C@@]12N(C[C@](C)(O)CC2)[C@H](C3=COC=C3)CC[C@H]1C
220	nupharic acid	[H][C@@]12N(C[C@@H](C)CC2)[C@H]([C@H](C=O)/C=C/C(O)=O)CC[C@H]1C
221	thermlanseedline A	CC(N1CCCC[C@]1([H])[C@@](C2)([H])CN3C(C=CC=C3C2=O)=O)=O
222	(+)-senepodine A	[H][C@@]12N([C@H](CC3=C4[C@](N(C)CCC4)([H])C[C@@H](C)C3)CCC2)[C@@H](C)C[C@@H](C)C1
223	(-)-senepodine A	[H][C@]12N([C@@H](CC3=C4[C@@](N(C)CCC4)([H])C[C@H](C)C3)CCC2)[C@H](C)C[C@H](C)C1
224	senepodine B	[H][C@@]12[N+]([C@H](CC3=C4[C@](N(C)CCC4)([H])C[C@@H](C)C3)CCC2)=C(C)C[C@@H](C)C1
225	senepodine C	[H][C@@]12N([C@H](CC3=C4[C@](NCCC4)([H])C[C@@H](C)C3)CCC2)[C@@H](C)C[C@@H](C)C1
226	senepodine D	[H][C@@]12N([C@H](CC3=C4[C@](N(C=O)CCC4)([H])C[C@@H](C)C3)CCC2)[C@@H](C)C[C@@H](C)C1
227	senepodine E	[H][C@@]12N([C@H](CC3=C4[C@](N(C(C)=O)CCC4)([H])C[C@@H](C)C3)CCC2)[C@@H](C)C[C@@H](C)C1
228	(−)-senepodine F	[H][C@@]12N([C@H](C[C@]3([H])C[C@H](C)C[C@@]4([H])[C@@]3([H])CCCN4C)CCC2)[C@@H](C)C[C@@H](C)C1
229	acetylsenepodine F	[H][C@@]12N([C@H](C[C@]3([H])C[C@H](C)C[C@@]4([H])[C@@]3([H])CCCN4C(C)=O)CCC2)[C@@H](C)C[C@@H](C)C1

230	lycochinine A	[H][C@@]12N([C@H](CC3=C4[C@](N(C)CCC4)([H])C[C@@H](C)C3)CCC2)[C@@H](C[C@]5([H])CCCCN5)C[C@@H](C)C1
231	lycochinine B	[H][C@@]12N([C@H](CC3=C4[C@](NCCC4)([H])C[C@@H](C)C3)CCC2)[C@@H](C[C@]5([H])CCCCN5)C[C@@H](C)C1
232	lycochinine C	[H][C@@]12N([C@H](C[C@]3([H])C[C@H](C)C[C@@]4([H])[C@@]3([H])CCCN4C=O)CCC2)[C@@H](C[C@]5([H])CCCCN5)C[C@@H](C)C1
233	Himeradine A	O=C(C)N1C[C@@H]2[C@@]34CC[C@@H](C[C@@H]5CCC[C@@H]6N5CCCC6)N=C3C[C@@H]7CCC[C@@]41[C@@H]7C2
234	aloperine	[H][C@]12CCCCN1C[C@@H]3[C@]4([H])NCCCC4=C[C@H]2C3
235	ochrocephalamine B	[H][C@]12CCCCN1C[C@@H]3[C@]4([H])N(C=O)CCCC4=C[C@H]2C3
236	ochrocephalamine C	[H][C@]12CCCCN1C[C@@H]3C4=[N+]([O-])CCCC4=C[C@H]2C3
237	ochrocephalamine F	[H][C@@]1(CCCCN21)[C@H](C[C@@H]3C2=O)CC4=C3N=CC=C4
238	ochrocephalamine D	[H][C@@]12N([C@@](C3=O)([H])[C@H]4[C@@](N3CCC5)([H])C5=C[C@H]2C4)CCCC1
239	(-)-multiflorine	[H][C@@]12[C@H](C[C@@H]3CN1CCCC2)CN([C@]3([H])C4)C=CC4=O
240	5,6-didehydromultiflorine	[H][C@@]12[C@H](C[C@@H]3CN1CCCC2)CN(C3=C4)C=CC4=O
241	13α-hydroxy-5,6-didehydromultiflorine	[H][C@@]12[C@H](C[C@@H]3CN1CC[C@H](O)C2)CN(C3=C4)C=CC4=O
242	13α-hydroxymultiflorine	[H][C@@]12[C@H](C[C@@H]3CN1CC[C@H](O)C2)CN([C@]3([H])C4)C=CC4=O
243	multiflorine *N*-oxide	[H][C@@]12[C@@H](C[C@H]3C[N+]1([O-])CCCC2)CN([C@]3([H])C4)C=CC4=O
244	13α-tigloyloxymultiflorine	[H][C@]12[C@H](CN(C=C3)[C@@]4(CC3=O)[H])C[C@H]4CN1CC[C@@H](C2)OC(/C(C)=C/C)=O
245	leontidine	O=C1C=CC=C2N1C[C@@H]3C[C@H]2CN4[C@]3([H])CCC4
246	camoensine	O=C1C=CC=C2N1C[C@H]3C[C@@H]2CN4[C@]3([H])CCC4
247	camoensidine	O=C1CCC[C@]2([H])N1C[C@H]3C[C@@H]2CN4[C@]3([H])CCC4
248	α-guianodendrine	[H][C@@]12[C@H]3C(N4C=CCC[C@]4([H])[C@@H](CN1CCC2)C3)=O
249	β-guianodendrine	[H][C@@]12[C@@H]3C(N4C=CCC[C@]4([H])[C@H](CN1CCC2)C3)=O
250	(-)-camoensidine *N*-oxide	O=C1CCC[C@]2([H])N1C[C@H]3C[C@@H]2C[N+]4([O-])[C@]3([H])CCC4

251	velutinine	O=C1C=CC=C2N1C([H])([H])[C@]3([H])C(O)C2=CN4C3=CC5=C4OCO5
252	lycocernuine *N*-oxide	O=C1CCC[C@]2([H])N1[C@](CC[C@H]3O)([H])[N+]([C@]3([H])C[C@H](C)C4)([O-])[C@@]4([H])C2
253	cernuine *N*-oxide	O=C1CCC[C@]2([H])N1[C@](CCC3[H])([H])[N+]([C@]3([H])C[C@H](C)C4)([O-])[C@@]4([H])C2
254	cernuine	O=C1CCC[C@]2([H])N1[C@](CCC3[H])([H])N([C@]3([H])C[C@H](C)C4)[C@@]4([H])C2
255	2α-hydroxycernuine	O=C1[C@H](O)CC[C@]2([H])N1[C@](CCC3)([H])N([C@]3([H])C[C@H](C)C4)[C@@]4([H])C2
256	lycocernuine	O=C1CCC[C@]2([H])N1[C@](CC[C@H]3O)([H])N([C@]3([H])C[C@H](C)C4)[C@@]4([H])C2
257	*O*-acetyllycocernuine	O=C1CCC[C@]2([H])N1[C@](CC[C@H]3OC(C)=O)([H])N([C@]3([H])C[C@H](C)C4)[C@@]4([H])C2
258	14,15-didehydro-lycocernuine	O=C1C=CC[C@]2([H])N1[C@](CC[C@H]3O)([H])N([C@]3([H])C=C(C)C4)[C@@]4([H])C2
259	*O*-Acetylcarolinianine	O=C1C=CC[C@]2([H])N1[C@](CC[C@H]3OC(C)=O)([H])N([C@]3([H])C=C(C)C4)[C@@]4([H])C2
260	(+)-ormosanine	[H][C@@]12NCCC[C@@]1([H])C[C@H]([C@]3([H])N(CCCC3)C4)C[C@@]24[C@]5([H])NCCCC5
261	(-)-piptanthine	[H][C@]12NCCC[C@]1([H])C[C@@H]([C@]3([H])N(CCCC3)C4)C[C@]24[C@@]5([H])NCCCC5
262	(-)-podopetaline	[H][C@]12NCCCC1=C[C@@H]([C@@]3([H])N(CCCC3)C4)C[C@]24[C@@]5([H])NCCCC5
263	18-epiormosanine	[H][C@@]12NCCC[C@@]1([H])C[C@H]([C@]3([H])N(CCCC3)C4)C[C@@]24[C@@]5([H])NCCCC5
264	(-)-ormosanine	[H][C@]12C[C@H]3C[C@](N1CCCC2)([C@@]4([H])NCCCC4)C[C@@]5([H])NCCC[C@@]53[H]
265	(+)-pipthanthine	[H][C@]12C[C@@H]3C[C@@](N1CCCC2)([C@]4([H])NCCCC4)C[C@]5([H])NCCC[C@]53[H]
266	(-)-templetine	[H][C@@]12C[C@H]3C[C@](N1CCCC2)([C@@]4([H])NCCCC4)C[C@]5([H])NCCC[C@@]53[H]
267	homoormosanine	[H][C@@]12N3CCC[C@@]1([H])C[C@H]([C@]4([H])N(CCCC4)C5)C[C@@]25[C@]6([H])N(CCCC6)C3
268	homo-18-epiormosanine	[H][C@@]12N3CCC[C@@]1([H])C[C@H]([C@]4([H])N(CCCC4)C5)C[C@@]25[C@@]6([H])N(CCCC6)C3
269	homopiptanthine	[H][C@]12N3CCC[C@]1([H])C[C@@H]([C@]4([H])N(CCCC4)C5)C[C@]25[C@@]6([H])N(CCCC6)C3
270	(+)-jamine	[H][C@]12N3CCC[C@]1([H])C[C@@H]([C@@]4([H])N(CCCC4)C5)C[C@]25[C@@]6([H])N(CCCC6)C3
271	panamine	[H][C@@]12C3N(C(N4)CCCC4[C@@]3(C5)C[C@H]([C@@]6([H])N5CCCC6)C2)CCC1

272	15β-hydroxycryptopleurine *N*-oxide	COC(C=C1)=CC2=C1C(C[N+](CCCC3)([O-])[C@@]3([H])[C@]4([H])O)=C4C5=C2C=C(OC)C(OC)=C5
273	pileamartine C	COC(C=C1)=CC2=C1C(CN(CCCC3)[C@]3([H])C4)=C4C5=C2C(OC)=C(OC)C=C5
274	pileamartine D	COC(C=C1)=CC2=C1C(CN(CCCC3)[C@]3([H])C4)=C4C5=C2C=C(O)C(OC)=C5
275	(+)-cryptopleurine	COC(C=C1)=CC2=C1C(CN(CCCC3)[C@]3([H])C4)=C4C5=C2C=C(OC)C(OC)=C5
276	6-O-desmethylcryptopleurine	OC(C=C1)=CC2=C1C(CN(CCCC3)[C@@]3([H])C4)=C4C5=C2C=C(OC)C(OC)=C5
277	(-)-cryptopleurine	COC(C=C1)=CC2=C1C(CN(CCCC3)[C@@]3([H])C4)=C4C5=C2C=C(OC)C(OC)=C5
278	boeshmeriasin A	COC(C(OC)=C1)=CC2=C1C(CN(CCCC3)[C@@]3([H])C4)=C4C5=C2C=C(OC)C=C5
279	boeshmeriasin B	OC(C(OC)=C1)=CC2=C1C(CN(CCCC3)[C@@]3([H])C4)=C4C5=C2C=C(OC)C=C5
280	acosmine	C=CC[C@@H]1[N@@]2[C@@H]3[C@@H]4C[C@H]1C[N@@]([C@H]4CCCCO)[C@H]2CC/C3=C\NC(C)=O
281	acosmine acetate	C=CC[C@@H]1[N@@]2[C@@H]3[C@@H]4C[C@H]1C[N@@]([C@H]4CCCCOC(C)=O)[C@H]2CC/C3=C\NC(C)=O
282	bovdichine	C=CC[C@@H]1[N@@]2[C@@H]3[C@@H]4C[C@H]1C[N@@]([C@H]4CCCCOC(C5=CC(OC)=C(OC)C(OC)=C5)=O)[C@H]2CC/C3=C\NC(C)=O
283	dasycarpumine	C=CC[C@@H]1[N@@]2[C@@H]3[C@@H]4C[C@H]1C[N@@]([C@H]4CC=C)[C@H]2CC/C3=C\NC(C)=O
284	panacosmine	C=CC[C@@H]1[C@@H]2C[C@H]3[C@H]4[N@]([C@H](CCC4)[N@@]1C3)[C@H]2C5=CN(C(C)=O)CCC5
285	neosecurinane	[H][C@@]12N([C@H](C3)CC[C@]24C3=CCO4)CCCC1
286	(+)-2-episecurinol A	O=C(O1)C=C2[C@]31[C@]4([H])N([C@H](C2)[C@@H](O)C3)CCCC4
287	(-)-2-episecurinol A	[H][C@]12N([C@@H](C3)[C@H](O)C[C@@]24C3=CC(O4)=O)CCCC1
288	secua'mamine E	O=C(O1)C=C2[C@]31[C@@]4([H])N([C@H](C2)[C@H](O)C3)CCCC4
289	virosine A	O=C(O1)C=C2[C@@]31[C@]4([H])N([C@@H](C2)[C@@H](O)C3)CCCC4
290	(-)-securinol A	O=C(O1)C=C2[C@]31[C@@]4([H])N([C@H](C2)[C@@H](O)C3)CCCC4
291	(+)-securinol A	O=C(O1)C=C2[C@@]31[C@]4([H])N([C@@H](C2)[C@H](O)C3)CCCC4
292	(+)-virosine B	O=C(O1)C=C2[C@]31[C@]4([H])N([C@H](C2)[C@H](O)C3)CCCC4

293	(-)-virosine B	O=C(O1)C=C2[C@@]31[C@@]4([H])N([C@@H](C2)[C@@H](O)C3)CCCC4
294	(±)-β-myrifabral A (13β-OH anomer)	O[C@H]1O[C@H]2[C@@H]3[C@@]4([H])CCCCN4C[C@]2(CCC3)CC1
295	(±)-α-myrifabral A (13α-OH anomer)	O[C@@H]1O[C@H]2[C@@H]3[C@@]4([H])CCCCN4C[C@]2(CCC3)CC1
296	(±)-β-myrifabral B (13β-OH anomer)	O[C@H]1O[C@H]2[C@@H]3[C@@]4([H])CCCCN4C[C@]2(CCC3)C[C@]1([H])CN(CC)CC
297	(±)-α-myrifabral B (13α-OH anomer)	O[C@@H]1O[C@H]2[C@@H]3[C@@]4([H])CCCCN4C[C@]2(CCC3)C[C@@]1(CN(CC)CC)[H]
298	flavesine G	OC(CCCC1=NC=C2C3=C1CCCN3CCC2)=O
299	flavesine H	OC(CCC[C@@](N=C1)([H])[C@]2([H])CCCN3CCCC1=C32)=O
300	flavesine I	OC(CCCC1=NC[C@]2([H])C3=C1CCCN3CCC2)=O
301	flavesine J	O=C(N1CCCCC1)CCCC2=NC=C3C4=C2CCCN4CCC3
302	alopecurine A	O=C1CCC[C@](N1C2)([H])[C@]3(O)CCCN(C3=O)CCCC2=O
303	alopecurine B	O=C1CCC[C@]2([H])C(CCCN(C3=O)CCC[C@]3(O)CN21)=O
304	ochrocephalamine E	O=C1CC[C@]2([H])[C@]3([H])[C@]4([H])[C@](CCCN4CCC3)([H])CN21
305	14α-hydroxydecodine	O=C(C[C@@H]1O)O[C@@H]2C[C@@H](C3=CC([H])=C(OC)C(O)=C3C4=C(O)C=CC1=C4)N5CCCC([H])[C@@]5([H])C2
306	14β-hydroxydecodine	O=C(C[C@H]1O)O[C@@H]2C[C@@H](C3=CC([H])=C(OC)C(O)=C3C4=C(O)C=CC1=C4)N5CCCC([H])[C@@]5([H])C2
307	4"-*O*-demethylheimidine	O=C(C[C@@H]1O)O[C@@H]2C[C@@H](C3=CC(O)=C(OC)C=C3C4=C(O)C=CC1=C4)N5CCCC[C@]5([H])C2
308	4"-*O*-demethyl-9β-hydroxyvertine	O=C(/C=C\1)O[C@@H]2C[C@@H](C3=CC(O)=C(OC)C=C3C4=C(O)C=CC1=C4)N5CCC[C@@H](O)[C@]5([H])C2
309	4"-*O*-demethylvertine *N*-oxide	O=C(/C=C\1)O[C@@H]2C[C@@H](C3=CC(O)=C(OC)C=C3C4=C(O)C=CC1=C4)[N+]5([O-])CCCC([H])[C@]5([H])C2
310	4"-*O*-demethyl-9β-hydroxyvertine *N*-oxide	O=C(/C=C\1)O[C@@H]2C[C@@H](C3=CC(OC)=C(OC)C=C3C4=C(O)C=CC1=C4)[N+]5([O-])CCCC([H])[C@]5([H])C2
311	4"-*O*-demethyllythridine	O=C(C[C@@H]1O)O[C@@H]2C[C@@H](C3=CC(O)=C(OC)C=C3C4=C(O)C=CC1=C4)N5CCCC[C@@]5([H])C2
312	4"-*O*-demethyllythridine *N*-oxide	O=C(C[C@@H]1O)O[C@@H]2C[C@@H](C3=CC(O)=C(OC)C=C3C4=C(O)C=CC1=C4)N5CCCC[C@@]5([H])C2
313	14-*epi*-4"-*O*-demethyllythridine	O=C(C[C@H]1O)O[C@@H]2C[C@@H](C3=CC(O)=C(OC)C=C3C4=C(O)C=CC1=C4)N5CCCC[C@@]5([H])C2

314	14-*epi*-4"-*O*-demethyl- 14-O-methyllythridine	O=C(C[C@H]1OC)O[C@@H]2C[C@@H](C3=CC(O)=C(OC)C=C3C4=C(O)C=CC1=C4)N5CCCC[C@@]5([H])C2
315	5-epi-dihydrolyfoline N-oxide	O=C(CC1)O[C@H]2C[C@@](C3=CC(O)=C(OC)C([H])=C3C4=C(O)C=CC1=C4)([H])[N+]5([O-])CCCC[C@@]5([H])C2
316	decamine *N*-oxide	O=C(CC1)O[C@H]2C[C@@](C3=CC(OC)=C(OC)C([H])=C3C4=C(O)C=CC1=C4)([H])[N+]5([O-])CCCC[C@@]5([H])C2
317	lagerstroemine N-oxide	O=C(CC1)O[C@H]2C[C@@](C3=CC([H])=C(OC)C(OC)=C3C4=C(O)C=CC1=C4)([H])[N+]5([O-])CCCC[C@@]5([H])C2
318	9β-hydroxyvertine	O=C(/C=C\1)O[C@@H]2C[C@@H](C3=CC(OC)=C(OC)C([H])=C3C4=C(O)C=CC1=C4)N5CCC[C@@H](O)[C@]5([H])C2
319	lythrine	O=C(/C=C\1)O[C@@H]2C[C@@H](C3=CC(OC)=C(OC)C([H])=C3C4=C(O)C=CC1=C4)N5CCCC([H])[C@@]5([H])C2
320	α-dehydrodecodine	O=C(/C=C\1)O[C@@H]2C[C@@H](C3=CC=C(OC)C(O)=C3C4=C(O)C=CC1=C4)N5CCCC[C@@]5([H])C2
321	lythridine	O=C(C[C@@H]1O)O[C@@H]2C[C@@H](C3=CC(OC)=C(OC)C=C3C4=C(O)C=CC1=C4)N5CCCC[C@@]5([H])C2
322	vertine	O=C(/C=C\1)O[C@@H]2C[C@@H](C3=CC(OC)=C(OC)C=C3C4=C(O)C=CC1=C4)N5CCCC[C@]5([H])C2
323	heimidine	O=C(C[C@@H]1O)O[C@@H]2C[C@@H](C3=CC(OC)=C(OC)C=C3C4=C(O)C=CC1=C4)N5CCCC[C@]5([H])C2
324	lyfoline	O=C(/C=C\1)O[C@@H]2C[C@@H](C3=CC(O)=C(OC)C=C3C4=C(O)C=CC1=C4)N5CCCC[C@@]5([H])C2
325	*epi*-lyfoline	O=C(/C=C\1)O[C@@H]2C[C@@H](C3=CC(O)=C(OC)C=C3C4=C(O)C=CC1=C4)N5CCCC[C@]5([H])C2
326	4"-*O*-demethyl-14-hydroxyvertaline.	O=C(C[C@@H]1O)O[C@@H]2C[C@@H](C3=CC(O)=C(OC)C=C3OC4=CC1=CC=C4)N5CCCC[C@]5([H])C2
327	14-hydroxylagerine	O=C(C[C@@H]1O)O[C@@H]2C[C@@H](C3=CC=C(OC)C(O)=C3OC4=CC1=CC=C4)N5CCCC[C@]5([H])C2
328	4"-*O*-demethyl-14-hydroxydecaline.	O=C(C[C@@H]1O)O[C@@H]2C[C@@H](C3=CC(O)=C(OC)C=C3OC4=CC1=CC=C4)N5CCCC[C@@]5([H])C2
329	lagerine *N*-oxide	O=C(CC1)O[C@H]2C[C@@](C3=CC=C(OC)C(O)=C3OC4=CC=C1C=C4)([H])[N+]5([O-])CCCC[C@@]5([H])C2
330	vertaline	O=C(CC1)O[C@@H]2C[C@@H](C3=CC(OC)=C(OC)C=C3OC4=CC1=CC=C4)N5CCCC[C@]5([H])C2
331	lagerine	O=C(CC1)O[C@@H]2C[C@@H](C3=CC=C(OC)C(O)=C3OC4=CC1=CC=C4)N5CCCC[C@]5([H])C2
332	decaline	O=C(CC1)O[C@@H]2C[C@@H](C3=CC(OC)=C(OC)C=C3OC4=CC1=CC=C4)N5CCCC[C@@]5([H])C2
333	araguspongine A	[H][C@]12N(CCC[C@@H]2CCCCCC3)CC[C@@H](CCCCCC[C@@]4(O)CCCN5[C@@]4([H])O[C@H]3CC5)O1

334	araguspongine B	[H][C@@]12N(CCC[C@H]2CCCCCC3)CC[C@H](CCCCCC[C@@H]4CCCN5[C@]4([H])O[C@@H]3CC5)O1
335	araguspongine C	[H][C@]12N(CCC[C@]2(O)CCCCCC3)CC[C@@H](CCCCCC[C@@]4(O)CCCN5[C@@]4([H])O[C@H]3CC5)O1
336	araguspongine D	[H][C@@]12N(CCC[C@@H]2CCCCCC3)CC[C@H](CCCCCC[C@H]4CCCN5[C@]4([H])O[C@@H]3CC5)O1
337	(+)-araguspongine E	[H][C@]12N(CCC[C@@H]2CCCCCC3)CC[C@@H](CCCCCC[C@H]4CCCN5[C@@]4([H])O[C@H]3CC5)O1
338	(-)-araguspongine E	[H][C@@]12N(CCC[C@@H]2CCCCCC3)CC[C@H](CCCCCC[C@@H]4CCCN5[C@]4([H])O[C@@H]3CC5)O1
339	araguspongine F	[H][C@]12N(CCC[C@H]2CCCCCC3)CC[C@@H](CCCCCC[C@@H]4CCCN5[C@@]4([H])O[C@H]3[C@@H](C)C5)O1
340	araguspongine G	[H][C@]12N(CCC[C@H]2CCCCCC3)CC[C@@H](CCCCCC[C@@H]4CCCN5[C@@]4([H])O[C@H]3[C@H](C)C5)O1
341	araguspongine H	[H][C@]12N(CCC[C@H]2CCCCCC3)C[C@H](C)[C@@H](CCCCCC[C@@H]4CCCN5[C@@]4([H])O[C@H]3[C@H](C)C5)O1
342	araguspongine J	[H][C@]12N(CCC[C@H]2CCCCCC3)C[C@@H](C)[C@@H](CCCCCC[C@@H]4CCCN5[C@@]4([H])O[C@H]3[C@H](C)C5)O1
343	araguspongine K	[H][C@]12N(CCC[C@H]2CCCCCC3)CC[C@@H](CCCCCC[C@@]4(O)CCC[N@+]5([O-])[C@@]4([H])O[C@H]3CC5)O1
344	araguspongine L	[H][C@]12N(CCC[C@]2(O)CCCCCC3)CC[C@@H](CCCCCC[C@@]4(O)CCC[N+]5([O-])[C@@]4([H])O[C@H]3CC5)O1
345	araguspongine M	[H][C@]12N(CCC[C@H]2CCCCCC3)CC[C@H](CCCCCC[C@@H]4CCCN5[C@@]4([H])O[C@@H]3CC5)O1
346	araguspongine N	[H][C@]12N(CCC[C@]2(O)CCCCCC3)C[C@H](C)[C@@H](CCCCCC[C@@]4(O)CCCN5[C@@]4([H])O[C@H]3[C@@H](C)C5)O1
347	araguspongine O	[H][C@]12N(CCC[C@@H]2CCCCCC3)C[C@H](C)[C@@H](CCCCCC[C@@]4(O)CCCN5[C@@]4([H])O[C@H]3[C@@H](C)C5)O1
348	araguspongine P	[H][C@]12N(CCC[C@]2(O)CCCCCC3)C[C@H](C)[C@@H](CCCCCC[C@@]4(O)CCCN5[C@@]4([H])O[C@H]3CC5)O1
349	meso-araguspongine C	[H][C@@]12N(CCC[C@@]2(O)CCCCCC3)CC[C@H](CCCCCC[C@@]4(O)CCCN5[C@@]4([H])O[C@H]3CC5)O1
350	3α-methylaraguspongine C	[H][C@]12N(CCC[C@]2(O)CCCCCC3)CC[C@@H](CCCCCC[C@@]4(O)CCCN5[C@@]4([H])O[C@H]3[C@@H](C)C5)O1
351	xestospongine A	[H][C@@]12N(CCC[C@@H]2CCCCCC3)CC[C@H](CCCCCC[C@H]4CCCN5[C@]4([H])O[C@@H]3CC5)O1
352	xestospongine B	[H][C@@]12N(CCC[C@H]2CCCCCC3)C[C@@H](C)[C@H](CCCCCC[C@]4(O)CCCN5[C@]4([H])O[C@@H]3CC5)O1
353	xestospongine C	[H][C@@]12N(CCC[C@@H]2CCCCCC3)CC[C@H](CCCCCC[C@@H]4CCCN5[C@]4([H])O[C@@H]3CC5)O1

354	xestospongine D	[H][C@@]12N(CCC[C@@H]2CCCCCC3)CC[C@H](CCCCCC[C@]4(O)CCCN5[C@]4([H])O[C@@H]3CC5)O1
355	xestospongine E	[H][C@@]12N(CCC[C@]2(O)CCCCCC3)CC[C@@H](CCCCCC[C@@]4(O)CCCN5[C@]4([H])O[C@H]3CC5)O1
356	xestospongine F	[H][C@@]12[N@+](CCC[C@]2(O)CCCCCC3)([O-])CC[C@@H](CCCCCC[C@@]4(O)CCCN5[C@]4([H])O[C@H]3CC5)O1
357	xestospongine G	[H][C@@]12[N@+](CCC[C@]2(O)CCCCCC3)([O-])CC[C@@H](CCCCCC[C@@]4(O)CCC[N@@+]5([O-])[C@]4([H])O[C@H]3CC5)O1
358	xestospongine H	[H][C@@]12N(CCC[C@@H]2CCCCCC3)CC[C@@H](CCCCCC[C@H]4CCCN5[C@]4([H])O[C@H]3[C@@H](C)C5)O1
359	xestospongine I	[H][C@@]12N(CCC[C@]2(O)CCCCCC3)CC[C@@H](CCCCCC[C@H]4CCCN5[C@]4([H])O[C@H]3[C@@H](C)C5)O1
360	(+)-7S-hydroxyxestospongine A	[H][C@]12N(CCC[C@H]2CCCCCC3)CC[C@@H](CCCCCC[C@@H]4C[C@H](O)CN5[C@@]4([H])O[C@H]3CC5)O1
361	demethylxetospongine B	[H][C@@]12N(CCC[C@H]2CCCCCC3)CC[C@H](CCCCCC[C@]4(O)CCCN5[C@]4([H])O[C@@H]3CC5)O1
362	3β,3'β-dimethylxestospongine C	[H][C@]12N(CCC[C@@H]2CCCCCC3)C[C@@H](C)[C@H](CCCCCC[C@@H]4CCCN5[C@@]4([H])O[C@@H]3[C@H](C)C5)O1
363	9'epi-3β,3'β-dimethylxestospongine C	[H][C@]12N(CCC[C@H]2CCCCCC3)C[C@@H](C)[C@H](CCCCCC[C@@H]4CCCN5[C@@]4([H])O[C@@H]3[C@H](C)C5)O1
364	petrosin	[H][C@]1([C@@H]2CCCCC[C@@H]3CCCN4C[C@H](C)C5=O)[C@H](CCCCC[C@H]5[C@]43[H])CCCN1C[C@H](C)C2=O
365	petrosin A	[H][C@@]1([C@H]2CCCCC[C@@H]3CCCN4C[C@H](C)C5=O)[C@@H](CCCCC[C@H]5[C@]43[H])CCCN1C[C@@H](C)C2=O
366	petrosin B	[H][C@@]1([C@H]2CCCCC[C@H]3CCCN4C[C@H](C)C5=O)[C@@H](CCCCC[C@@H]5[C@]43[H])CCCN1C[C@@H](C)C2=O
367	xestosin A	[H][C@]1([C@]2([H])CCCCC[C@@]3([H])CCCN4C[C@](C)([H])C5=O)[C@@](CCCCC[C@@]5([H])[C@@]43[H])([H])CCCN1C[C@@H](C)C2=O
368	neopetrosiasin A	[H][C@]1([C@]2([H])CCCCC[C@@]3([H])CCCN4C[C@@H](C)C5=O)[C@@](CCCCC[C@@]5([H])[C@@]43[H])([H])CCCN1C[C@H](C)C2=O
369	neopetrosiasin B	[H][C@]1([C@]2([H])CCCCC[C@@]3([H])CCCN4C[C@H](C)C5=O)[C@@](CCCCC[C@@]5([H])[C@@]43[H])([H])CCCN1C[C@H](C)C2=O
370	thermlanseedline B	O=C1C=CC=C2N1C[C@H]3C[C@]24[C@@]([C@@](CC([C@]5([H])N6C[C@@H]7C[C@@H]5CN8C7=CC=CC8=O)=O)([H])[C@@]6([H])O4)([H])N9[C@@]3([H])CCCC9
371	thermlanseedline C	O=C1C=CC=C2N1C[C@H]3C[C@@H]2CN4[C@@]3([H])[C@@](/C=C/CN(C[C@H]5C[C@@H]6CN7C5=CC=CC7=O)C6=O)(O)CCC4
372	thermlanseedline D	O=C1C=CC=C2N1C[C@H]3C[C@@H]2CN4[C@@]3([H])[C@@](/C=C/CCN(C[C@H]5C[C@@H]6CN7C5=CC=CC7=O)C6=O)(O)CCC4
373	thermlanseedline E	O=C1[C@H]2CN3C(C=CC=C3[C@@H](CN1CCCC(CCCN4C[C@@H]5C6=CC=CC(N6C[C@H](C4=O)C5)=O)=O)C2)=O

374	thermlanseedline F	O=C1[C@H]2CN3C(C=CC=C3[C@@H](CN1CCCC(/C=C/CCN(C[C@H]4C[C@@H]5CN6C4=CC=CC6=O)C5=O)=O)C2)=O
375	thermseedline F	O=C1[C@H]2CN3C(C=CC=C3[C@@H](CN1CCCC(CCN(C[C@H]4C[C@@H]5CN6C4=CC=CC6=O)C5=O)=O)C2)=O
376	thermseedline G	O=C1[C@H]2CN3C(C=CC=C3[C@@H](CN1CCCC(OCCCN(C[C@H]4C[C@@H]5CN6C4=CC=CC6=O)C5=O)=O)C2)=O
377	alopecuroide B	O=C1CCC[C@](N1C2)([H])[C@@]3([H])[C@H]4[C@]([C@@]5([H])CC[C@]6([H])[C@]7([H])N5CCC[C@]7([H])[C@](CCCC8=O)([H])N8C6)(O4)[C@H](C#N)N9CCC[C@]2([H])[C@]93[H]
378	alopecuroide A	[H][C@]1([C@@]23[C@H](O3)[C@]4([H])[C@]5([H])N(CCC[C@]5([H])[C@](CCCC6=O)([H])N6C4)[C@@H]2C#N)N7CCC[C@]8([H])[C@@]7([H])[C@]([C@](CCCC9=O)([H])N9C8)([H])CC1
379	alopecuroide C	O=C1CCC[C@](N1C2)([H])[C@@]3([H])CC([C@@]4([H])CC[C@]5([H])[C@]6([H])N4CCC[C@]6([H])[C@](CCCC7=O)([H])N7C5)=CN8CCC[C@]2([H])[C@]83[H]
380	alopecuroide D	[H][C@]1(C2=CN(CCC[C@]3([H])[C@](CCCC4=O)([H])N4C5)[C@@]3([H])[C@@]5([H])C2)N6CCC[C@]7([H])[C@@]6([H])[C@]([C@](CCCC8=O)([H])N8C7)([H])CC1
381	alopecuroide E	O=C1CCC[C@](N1C2)([H])[C@@]3([H])CCCN4C[C@@]([H])(CCC[C@]5([H])CN6[C@@](CCCC6=O)([H])[C@]7([H])[C@@]5([H])NCCC7)C[C@]2([H])[C@]43[H]
382	ochrocephalamine A	[H][C@]12[C@]3([H])N(CCC[C@]3([H])C(N4C2)=CC=C([C@]5([H])CC(N(C[C@@]6([H])[C@@]7([H])[C@]8([H])CCCN7CCC6)[C@]8([H])C5)=O)C4=O)CCC1
383	sophaline I	[H][C@]12[C@]3([H])N(CCC[C@]3([H])[C@](CC=C([C@@]4([H])N5CCC[C@@]6([H])[C@@]5([H])[C@]([C@](CC=CC7=O)([H])N7C6)([H])CC4)C8=O)([H])N8C2)CCC1
384	sophoraline A	O=C1C=CC([C@H]2[C@@H]3C(N(C[C@@]4([H])[C@@]5([H])[C@]6([H])CCCN5CCC4)[C@]6([H])C2)=O)[C@]3(N1C7)[C@@]8([H])CCCN9CCC[C@@]7([H])[C@]98[H]
385	sophoraline B	O=C1CCC([C@H]2[C@@H]3C(N(C[C@@]4([H])[C@@]5([H])[C@]6([H])CCC[N+]5([O-])CCC4)[C@]6([H])C2)=O)[C@]3(N1C7)[C@@]8([H])CCCN9CCC[C@@]7([H])[C@]98[H]
386	sophoraline C	O=C1CCC([C@H]2[C@@H]3C(N(C[C@@]4([H])[C@@]5([H])[C@]6([H])CCCN5CCC4)[C@]6([H])C2)=O)[C@]3(N1C7)[C@@]8([H])CCCN9CCC[C@@]7([H])[C@]98[H]
387	sophaline G	O=C1CCC[C@]2([H])[C@](CC3=CC(CCC4)=C(N4CCC5)C5=C3)([H])[C@@]6([H])NCCC[C@@]6([H])CN21
388	sophaline H	O=C1CCC[C@]2([H])[C@](CC3=CC(CCC4)=C(N4CCC5)C5=C3)([H])[C@@]6([H])NCCC[C@]6([H])CN21
389	thiobinupharidine	C[C@H](CC[C@H]1C2=COC=C2)[C@](N1C3)([H])CC[C@@]43C[C@]5(CS4)CN6[C@H](C7=COC=C7)CC[C@@H](C)[C@]6([H])CC5
390	*syn*-thiobinupharadine sulfoxide	C[C@H](CC[C@H]1C2=COC=C2)[C@](N1C3)([H])CC[C@@]43C[C@]5(C[S@]4=O)CN6[C@H](C7=COC=C7)CC[C@@H](C)[C@]6([H])CC5
391	6-hydroxythiobinupharadine	C[C@H](CC[C@H]1C2=COC=C2)[C@](N1[C@@H]3O)([H])CC[C@@]43C[C@]5(CS4)CN6[C@H](C7=COC=C7)CC[C@@H](C)[C@]6([H])CC5
392	6,6'-dihydroxythiobinupharadine	C[C@H](CC[C@H]1C2=COC=C2)[C@](N1[C@@H]3O)([H])CC[C@@]43C[C@]5(CS4)[C@@H](O)N6[C@H](C7=COC=C7)CC[C@@H](C)[C@]6([H])CC5
393	neothiobinupharidine	[H][C@]12[C@@H](CC[C@H](N1C[C@]3(C[C@@](CS3)(CN4[C@@H](CC5)C6=COC=C6)CC[C@]4([C@@H]5C)[H])CC2)C7=COC=C7)C

394	neothiobinupharidine β-sulfoxide	[H][C@]12[C@@H](CC[C@H](N1C[C@]3(C[C@@](C[S@]3=O)(CN4[C@@H](CC5)C6=COC=C6)CC[C@]4([C@@H]5C)[H])CC2)C7=COC=C7)C
395	thionuphlutine B	C[C@H]1[C@@]2([H])N(C[C@](C[C@]34CN5[C@@H](CC[C@H]([C@@]5(CC4)[H])C)C6=COC=C6)(CS3)CC2)[C@H](C7=COC=C7)CC1
396	thionuphlutine B β-sulfoxide	C[C@H]1[C@@]2([H])N(C[C@](C[C@]34CN5[C@@H](CC[C@H]([C@@]5(CC4)[H])C)C6=COC=C6)(C[S@]3=O)CC2)[C@H](C7=COC=C7)CC1
397	6-hydroxythionuphlutine B	C[C@H]1[C@@]2([H])N(C[C@](C[C@]34[C@@H](O)N5[C@@H](CC[C@H]([C@@]5(CC4)[H])C)C6=COC=C6)(CS3)CC2)[C@H](C7=COC=C7)CC1

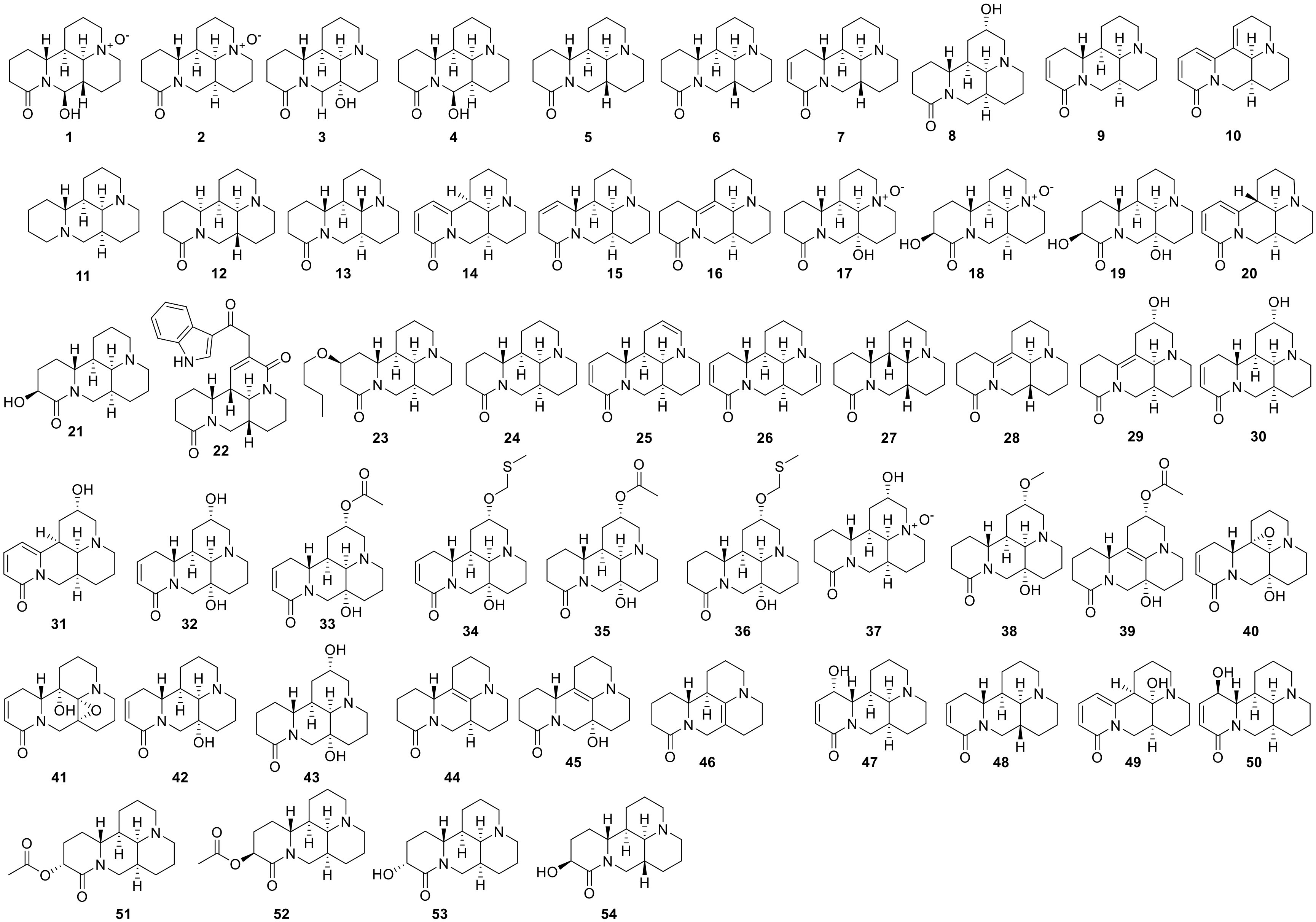


Figure S1. Matrine-type quinolizidine alkaloids **1-54**

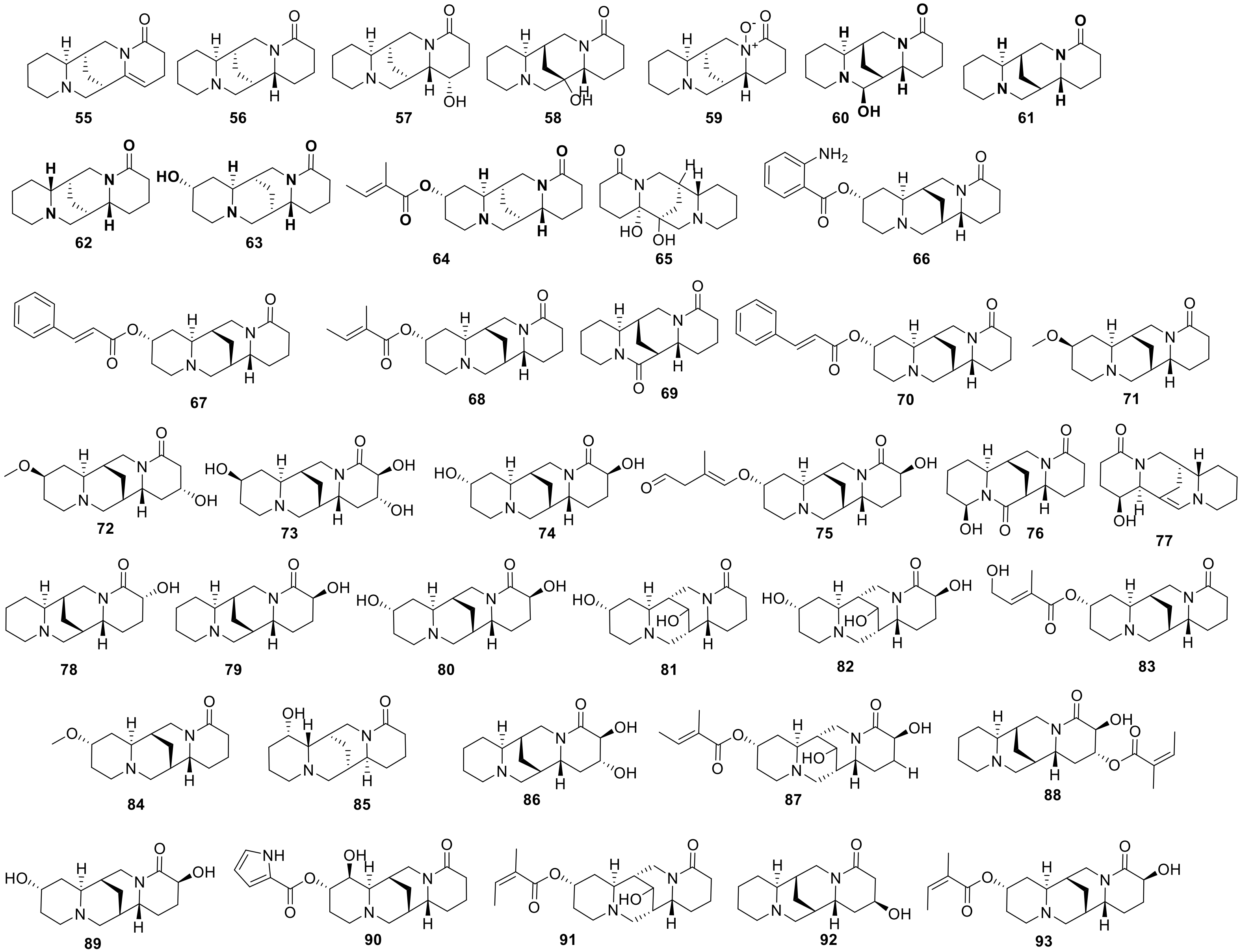
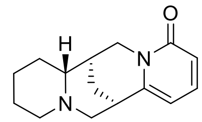


Figure S2. Lupanine-type quinolizidine alkaloids **55-93**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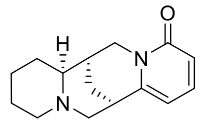
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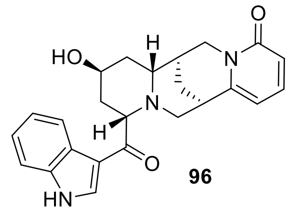
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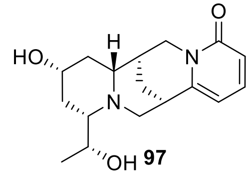
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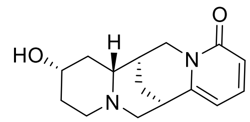
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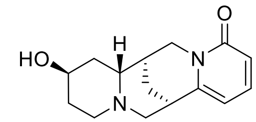
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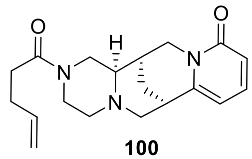
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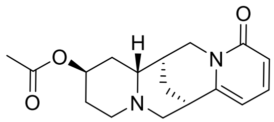
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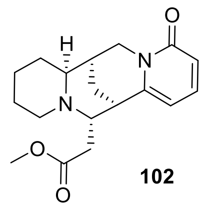
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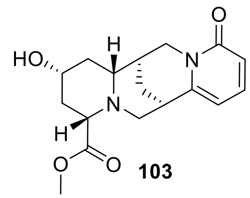
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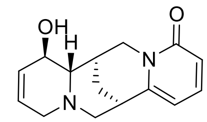
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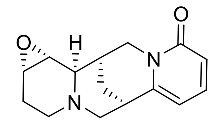
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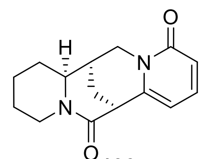
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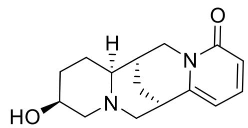
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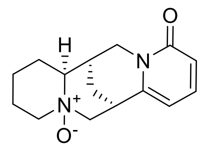
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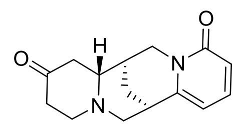
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Figure S3. Anagyrine-type quinolizidine alkaloids **94-109**

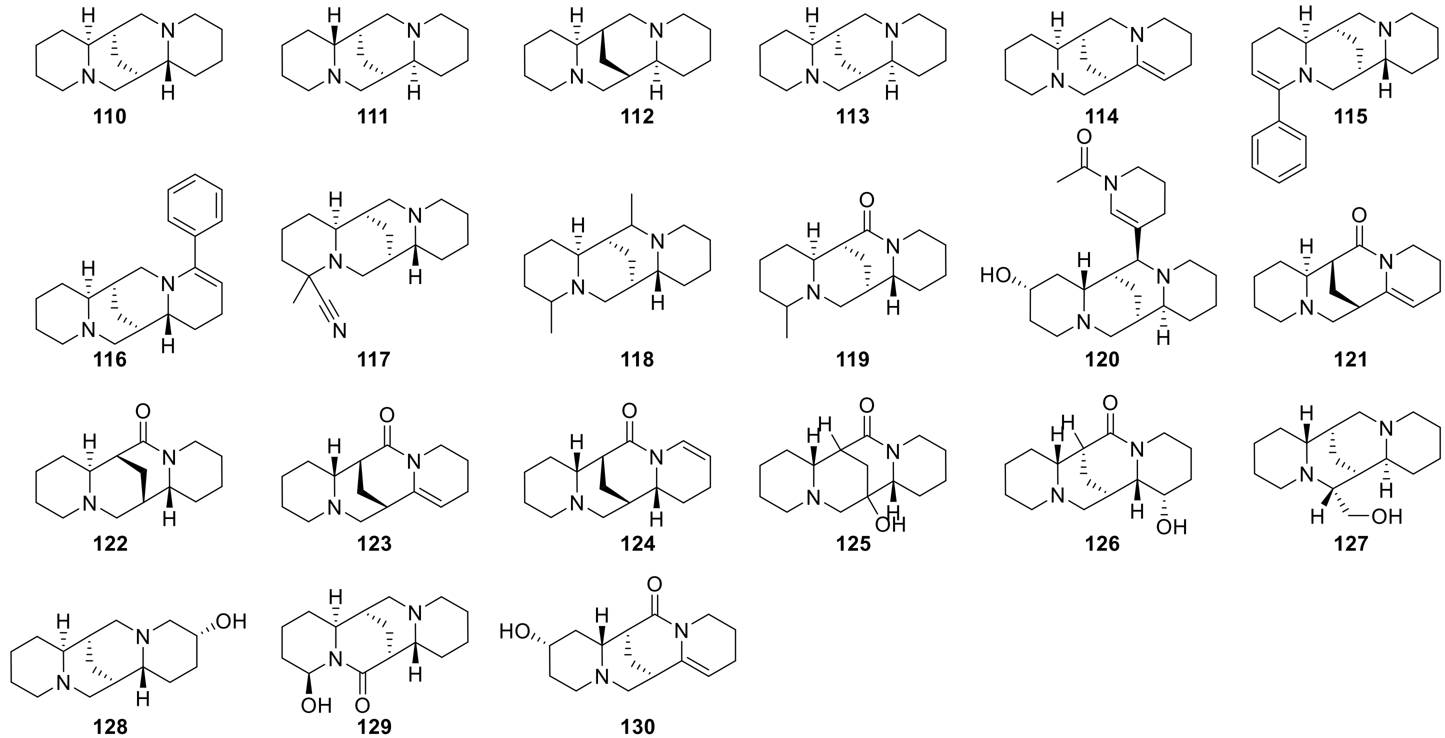

Figure S4. Sparteine-type quinolizidine alkaloids **110-130**

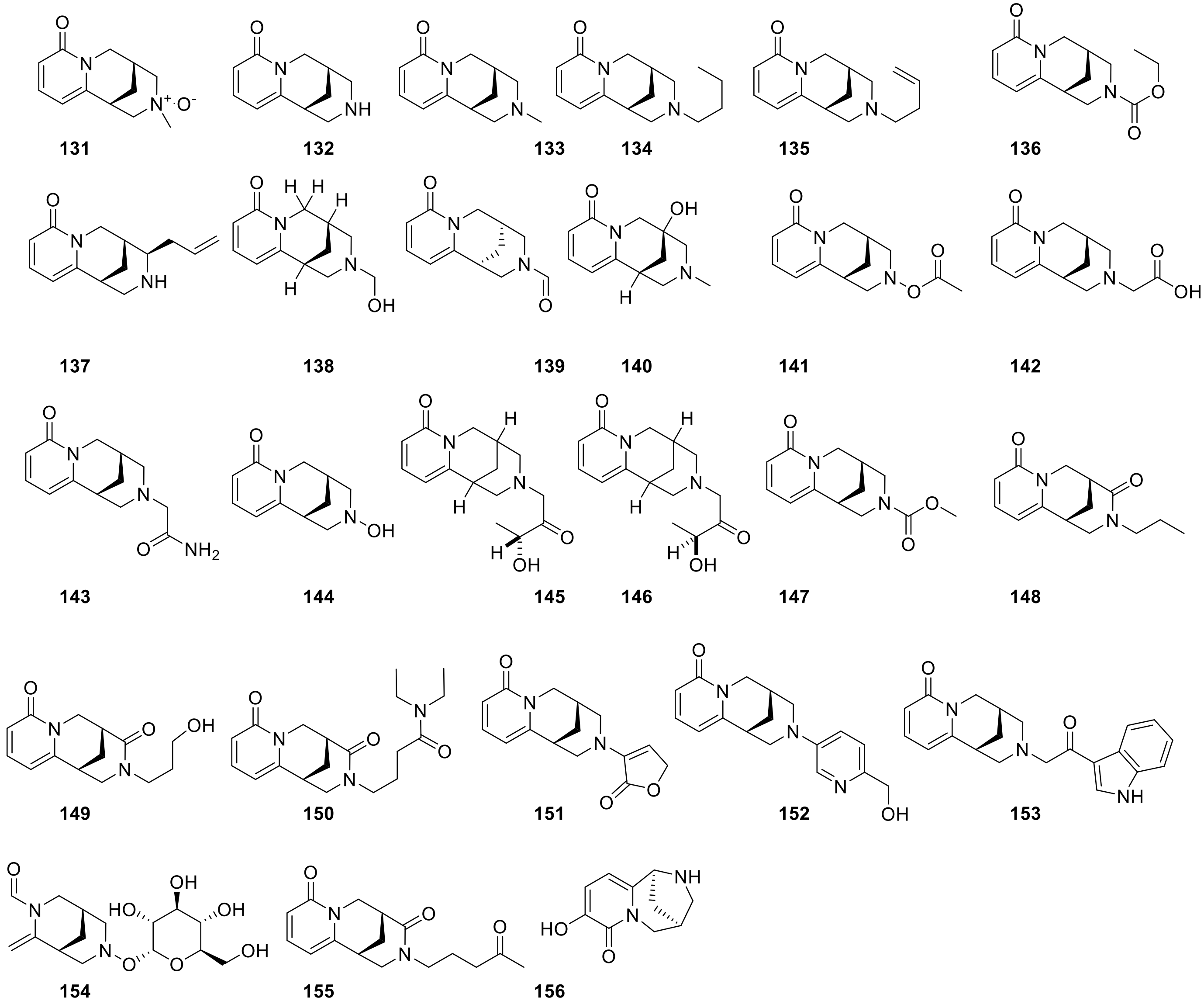

Figure S5. Cytisine-type quinolizidine alkaloids **131-156**

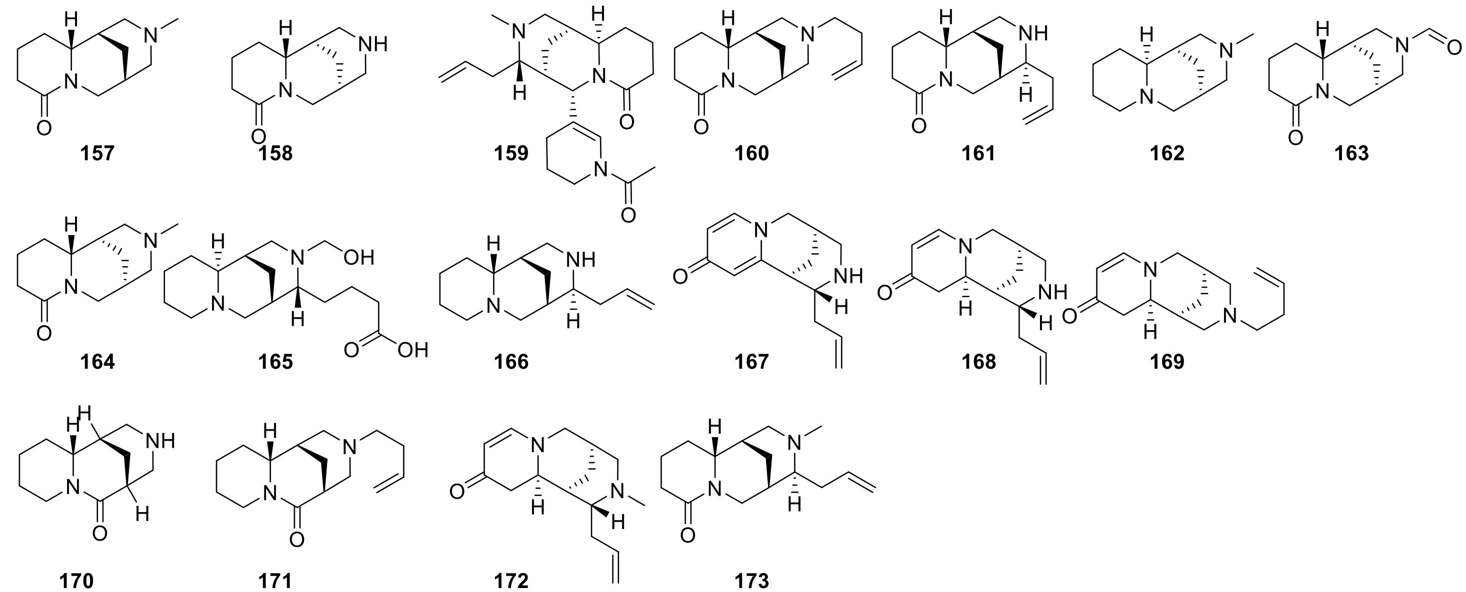

Figure S6. Tetrahydrocytisine-type quinolizidine alkaloids **157-173**

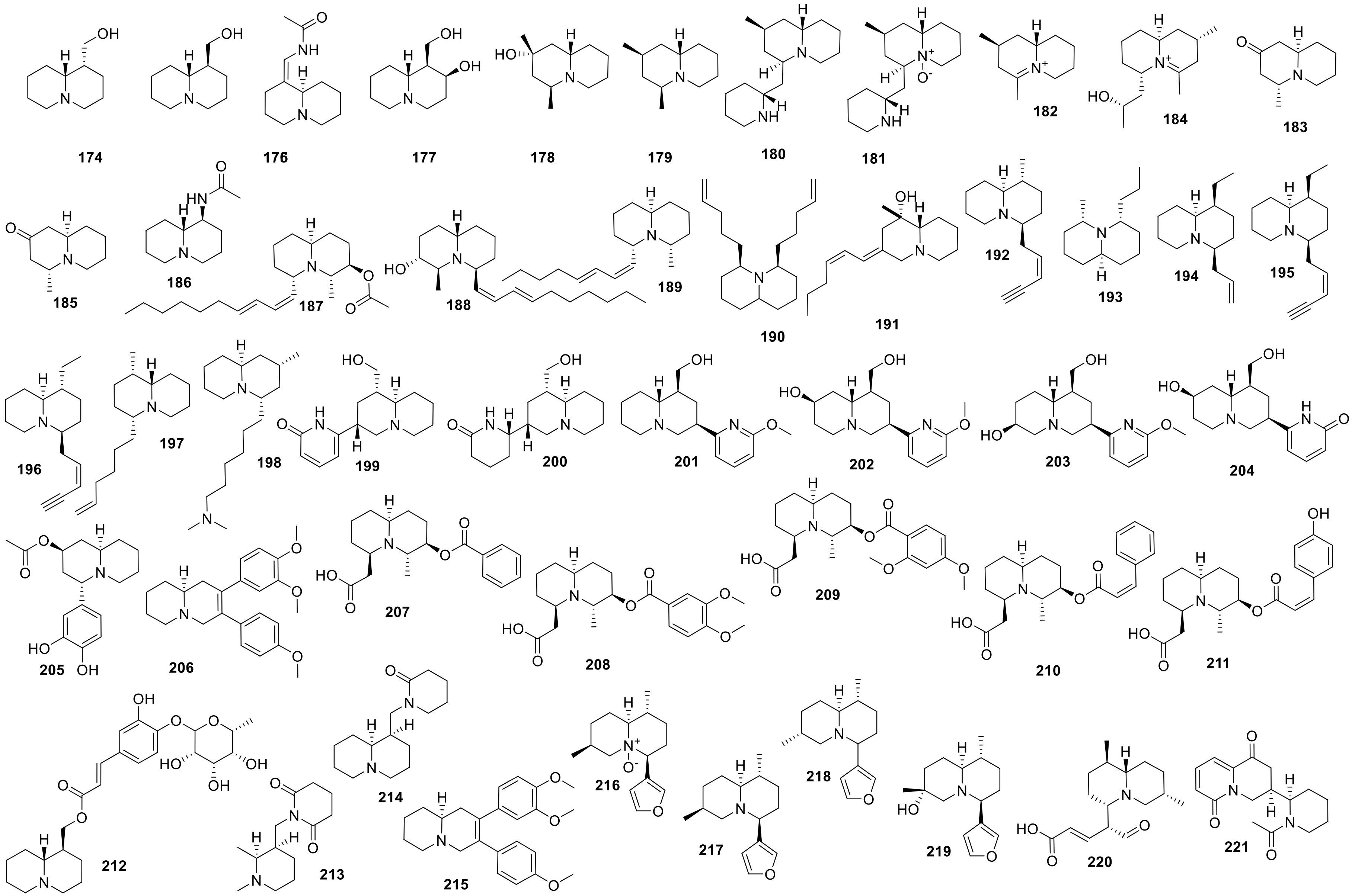

Figure S7. Lupinine-type quinolizidine alkaloids **174-221**

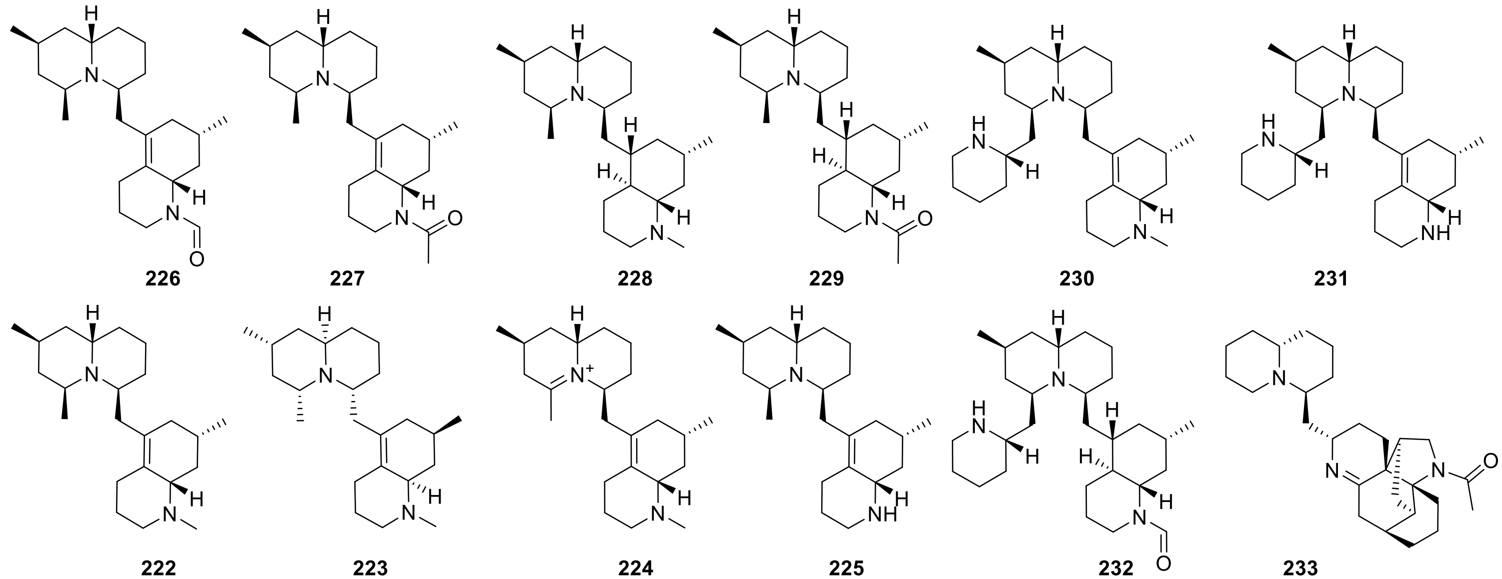

Figure S8. Senepodine-type quinolizidine alkaloids **222-233**

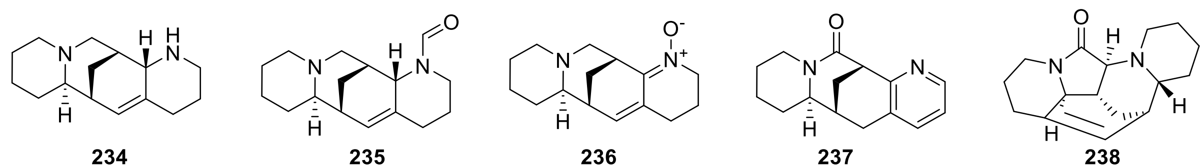

Figure S9. Aloperine-type quinolizidine alkaloids **234-238**

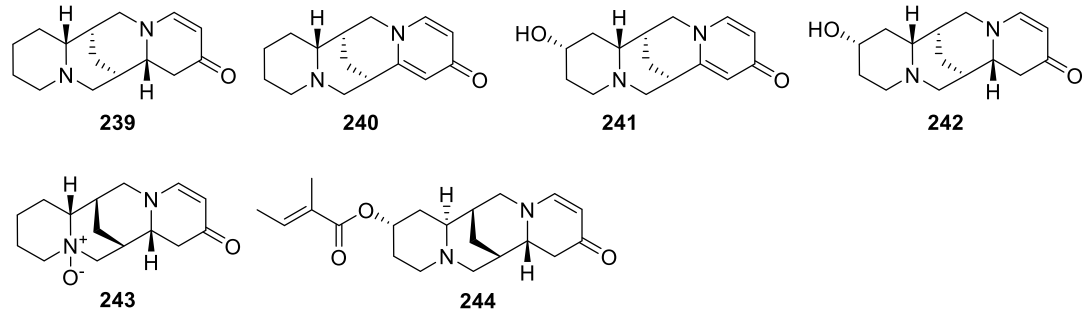

Figure S10. Multiflorine-type quinolizidine alkaloids **239-244**

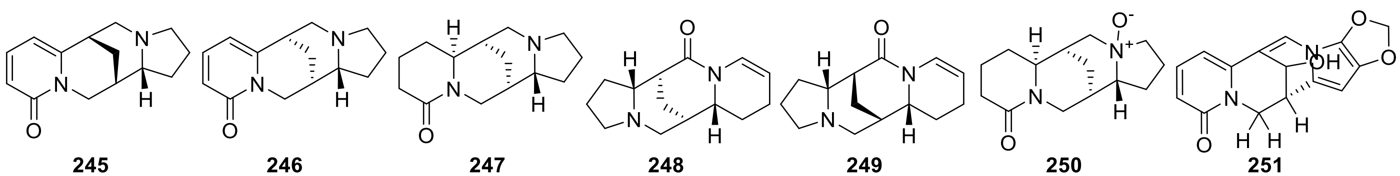

Figure S11. Leontidine-type quinolizidine alkaloids **245-250**

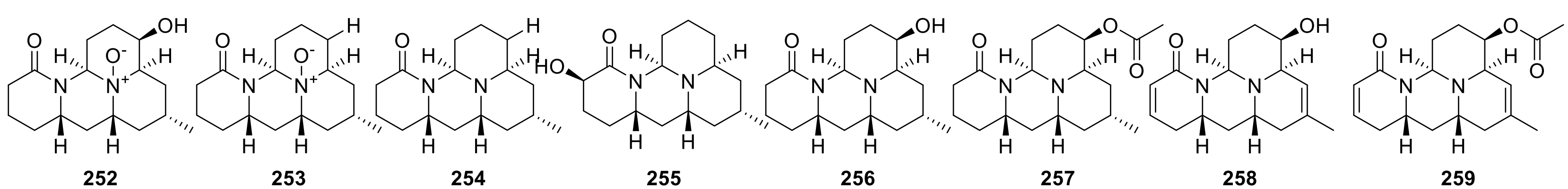

Figure S12. Cernuine-type quinolizidine alkaloids **252-259**

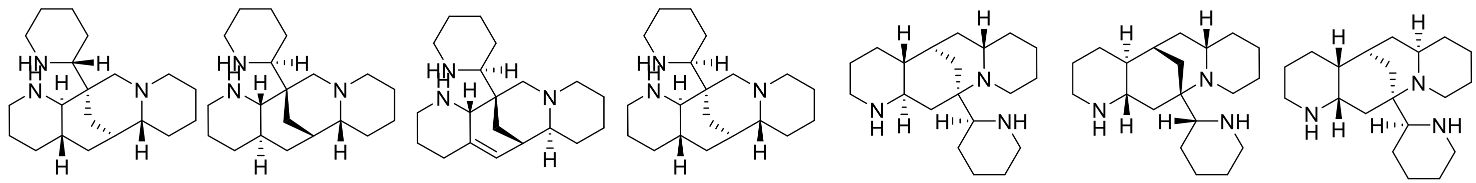

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Figure S13. Ormosanine-type quinolizidine alkaloids **260-266**

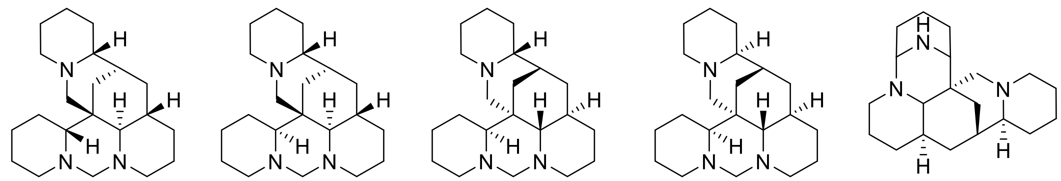

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Figure S14. Homoormosanine-type quinolizidine alkaloids **267-271**

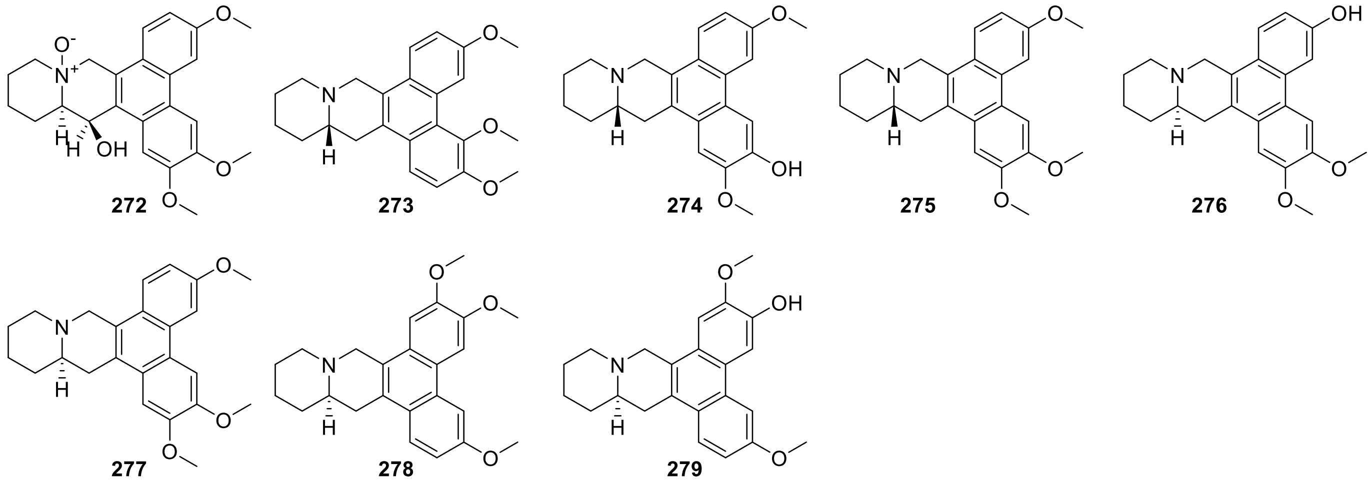

Figure S15. Phenanthroquinolizidine-type quinolizidine alkaloids **272-279**

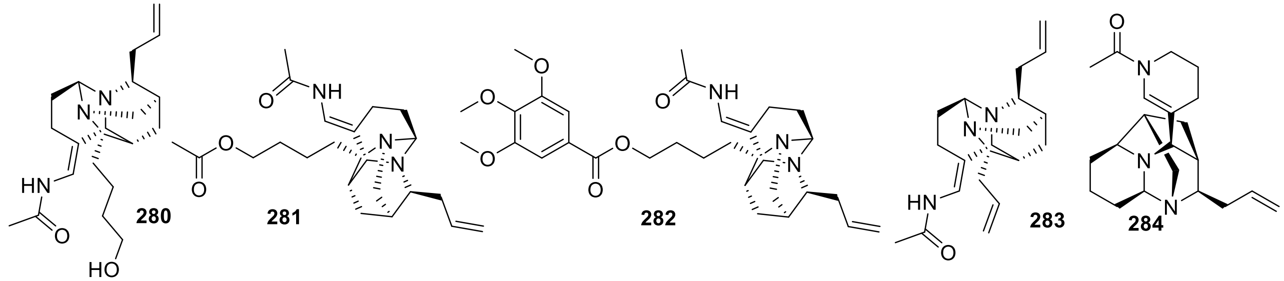

Figure S16. Acosmine-type quinolizidine alkaloids **280-284**

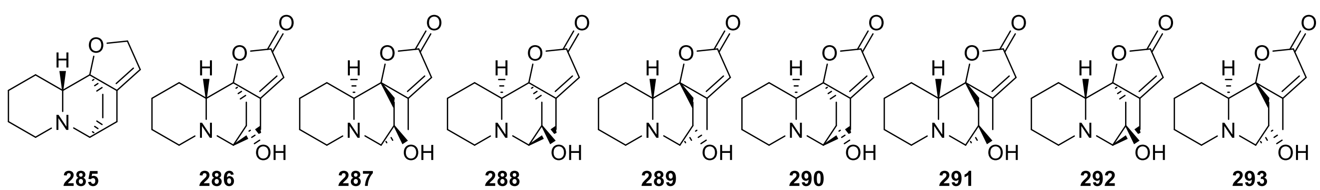

Figure S17. Neosecurinan-type quinolizidine alkaloids **285-293**

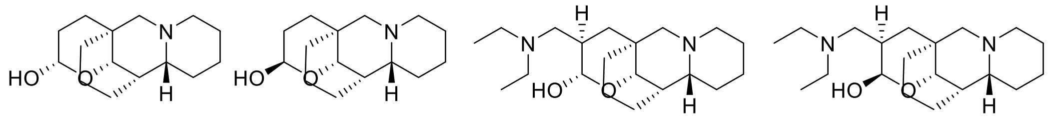

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Figure S18. Myrifabral-type quinolizidine alkaloids **294-297**

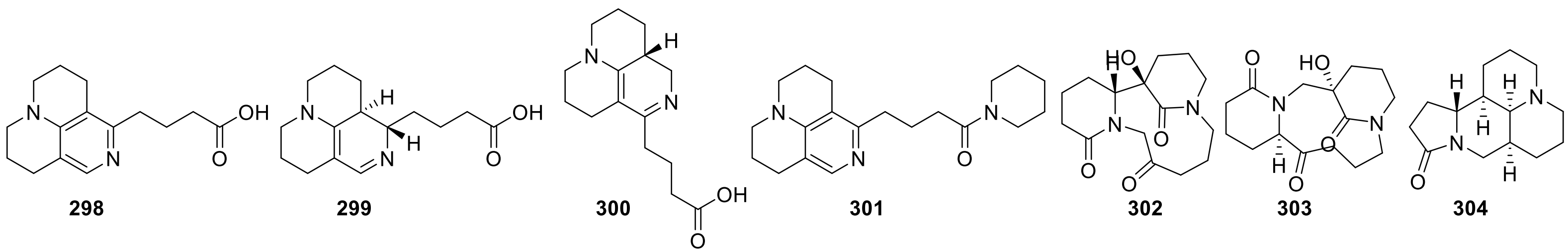

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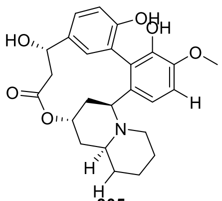
Figure S19. Flavesine- and alopecurine-type quinolizidine alkaloids **298-304**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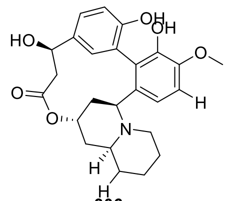
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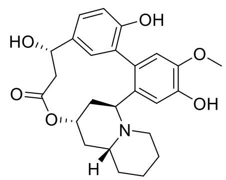
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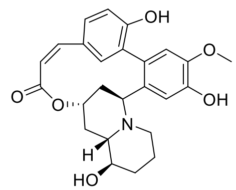
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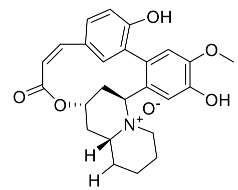
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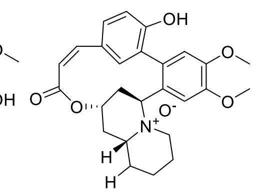
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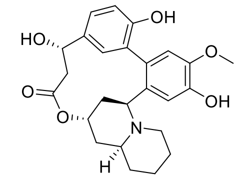
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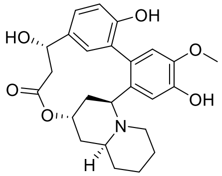
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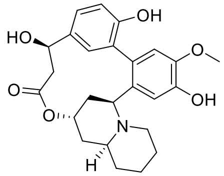
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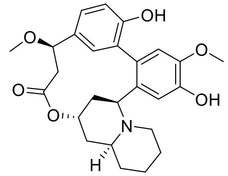
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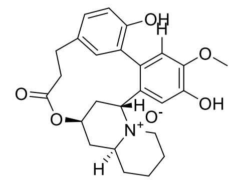
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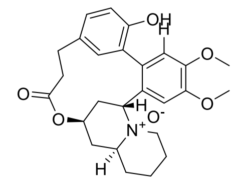
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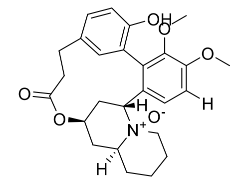
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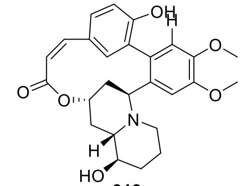
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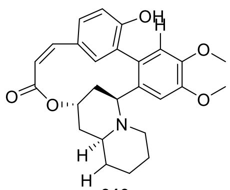
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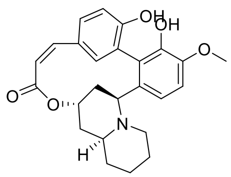
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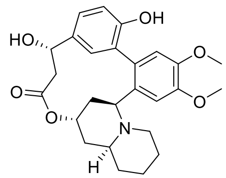
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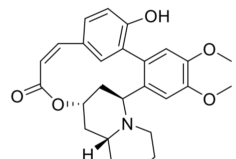
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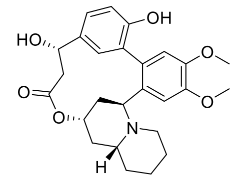
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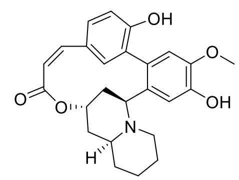
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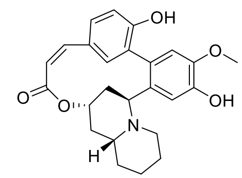
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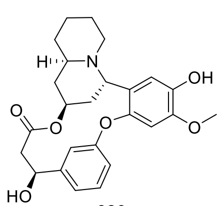
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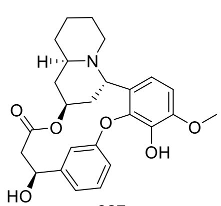
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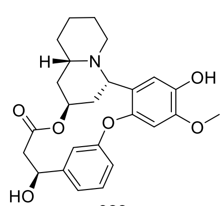
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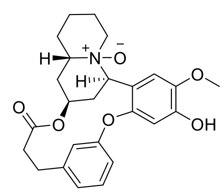
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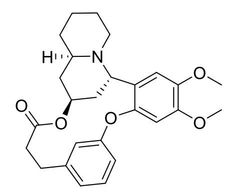
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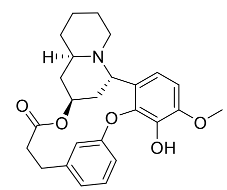
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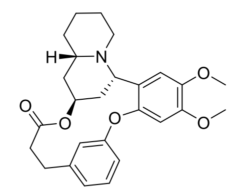
332

Figure S20. Biphenyl and phenyl ether quinolizidine lactones **305-332**

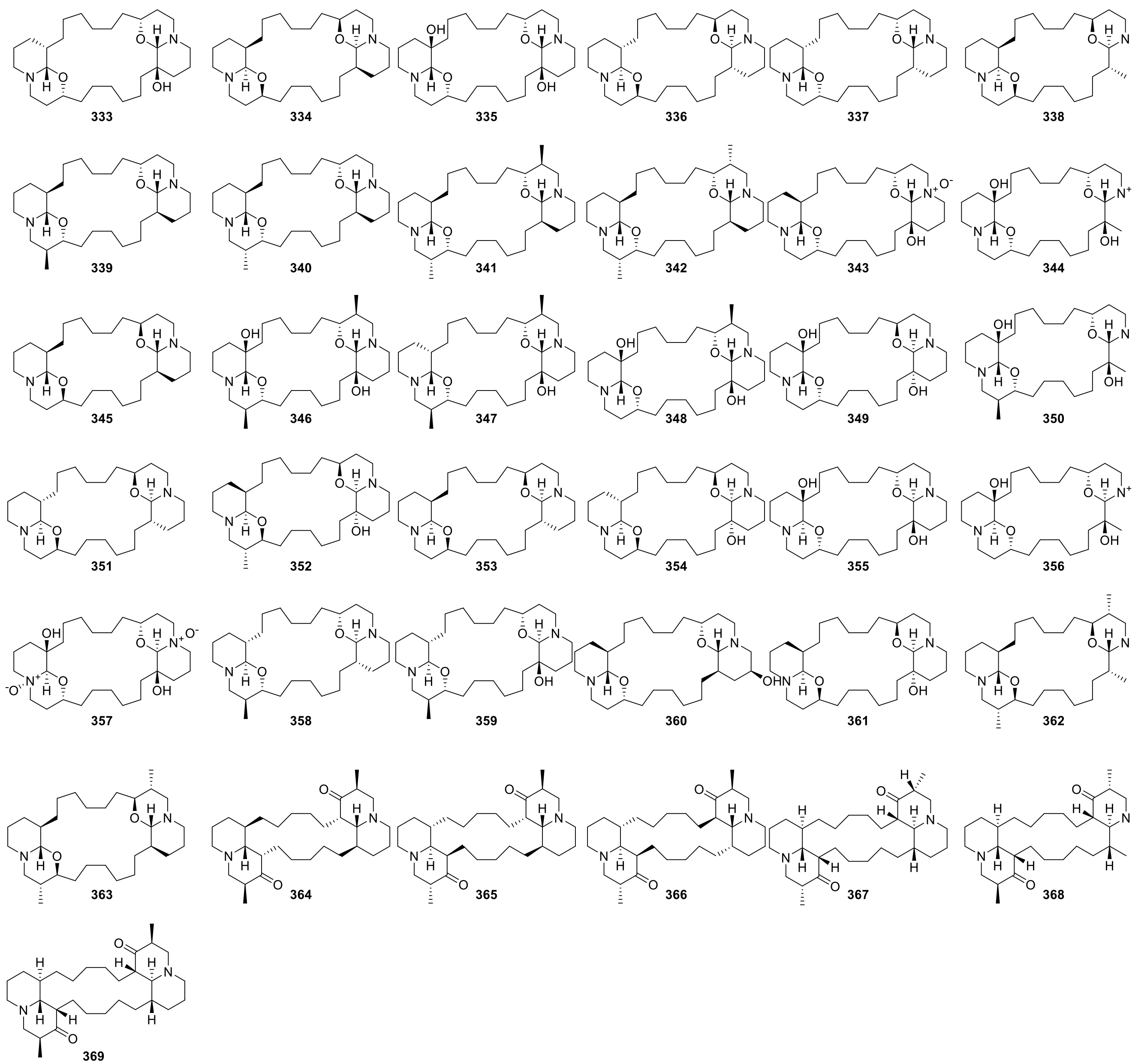

Figure S21. Macrocyclic *bis*-quinolizidines **333-369**

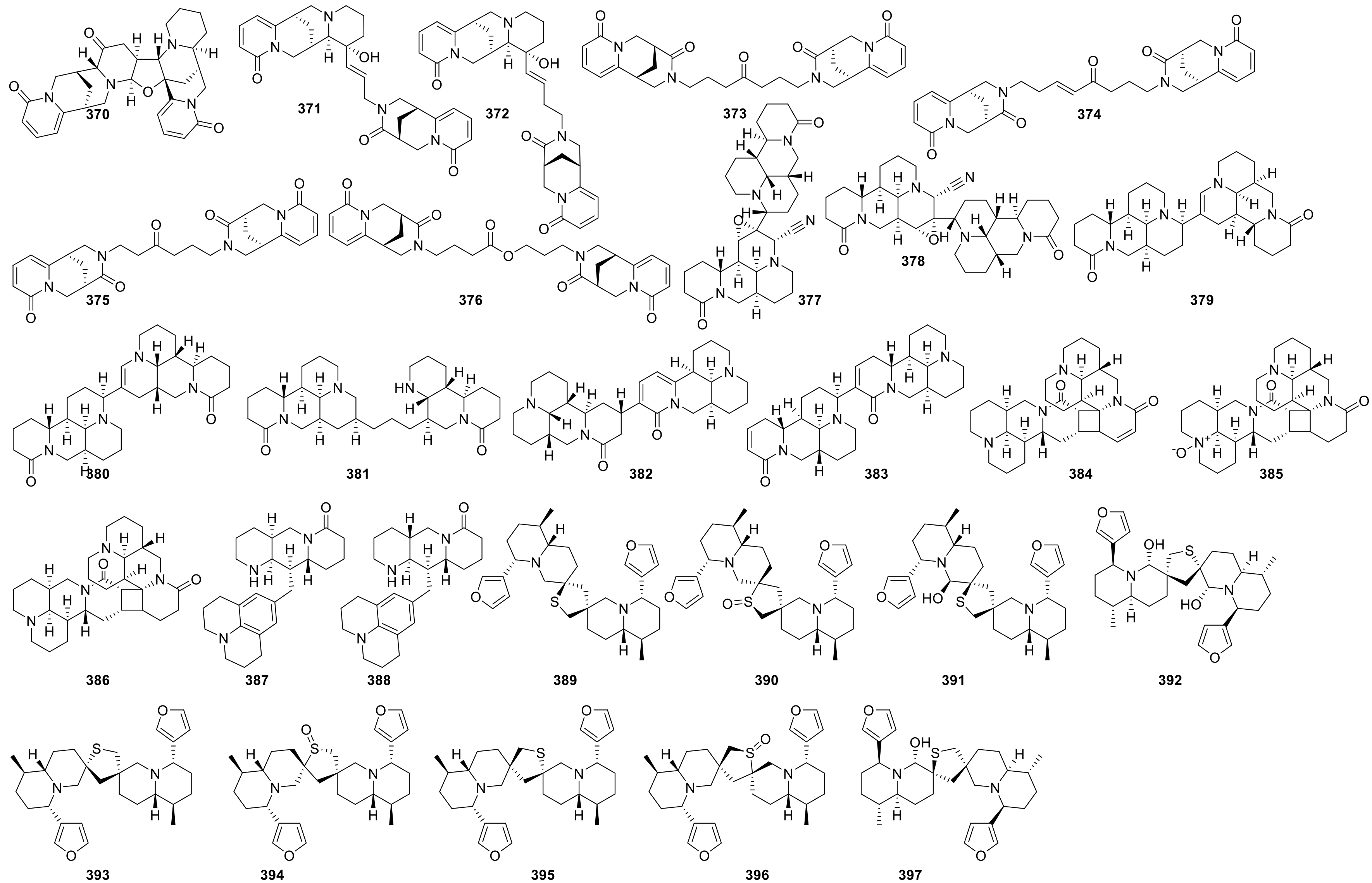

Figure S22. Dimeric quinolizidines alkaloids **370-397**

Table S2. Compendium of reported biological activity of the 397 quinolizidine alkaloids.

QA	Activity tested	Outcome	Ref
1	Anti-inflammatory effects	**TNF-α** IC_{50} = 35.6 ± 0.5 µmol/L and **IL-6** IC_{50} = 41.7 ± 0.8 µmol/L,	1
2	Hepatitis B infection inhibition	Treatment (**2**) for 3 months (0.6 g/d, i.v., for the first month; 0.2 g, oral, bid for another 2 months) reduced Hsc70 mRNA in liver biopsy samples by 50%	2
3	Anticonvulsant and Neuroprotective Effects Antiviral Activities against Influenza Virus A/Hanfang/359/95 (H3N2)	Percentage SE (%) = 35% and Percentage survival (%)=83.3% IC_{50} 402.82 µM	3 4
4	Potent anti-HBV activity Antiviral activity against the Coxsackie virus B3 (CVB3)	Inhibitory potency against HBsAg secretion of 31.1% and against HBeAg secretion of 26.3% IC_{50} 252.18 µM	5 4
5	Cytotoxicity against human tumor HL-60, SMMC-7721, A-549, MCF-7, and SW-480 cell lines	**5** showed no cytotoxic activity for five human cancer cell lines.	6
6	Anticancer activity (human pancreatic cancer)	**6** exhibited remarkable inhibition effects to the growth of human pancreatic, gastric, liver, colon, gallbladder, and prostate carcinoma cells with IC_{50} values of about 20 µmol/L to 200 µmol/L.	7
7	Antiarrhythmic effects Activity anticancer against human lung cancer and hepatoma cells Antiviral Activities against the Hepatitis B Virus Anti-inflammatory activity in LPS-Stimulated RAW 264.7 Cells Biopesticide against four pest species of agricultural importance	LD_{50} in mice was 72.1 mg/kg IC_{50} for the growth of SMMC-7721 and A549 cells were more than 1.0 mg/mL and less than 0.5 mg/mL, respectively, after the cells were treated with matrine for 72 h. HBsAg secretion = 34.9% (concentration of 0.035 mM) HBeAg secretion = 21.8% (concentration of 0.035 mM) TNF-α (%) = 72.48 ± 3.83 IL-6 (%) = 65.49 ± 3.64 Exposure times (h): 120/ LC_{50} and LC_{90} (ppm) *Diaphorina citri:* LC_{50}=1247 and LC_{90} 5712 *Panonychus citri:* LC_{50}= 42 and LC_{90} 73.7 *Sitophilus zeamais:* LC_{50}= 463.9 and LC_{90} 1121	8 9 10 11 12

	Inhibition effect on cancer cell proliferation Antiviral Effect against Human Enterovirus 71	*Spodoptera frugiperda*: LC_{50}= 384.3 and LC_{90} 1034 HepG2: the inhibitory rates were 28±0.42, 14.81±0.81, and 18.25±0.99 %, respectively, for 24, 48, and 72 h at concentration of 1.0 mg/ mL The viral RNA copy number detected by quantitative RT-PCR (qRT-PCR) in the infected RD cells were suppressed in a set of concentrations between 4 and 128 µg/mL	13 14
8	Antiviral activity against the Coxsackie virus B3 (CVB3)	IC_{50} 197.22 µM	4
9	Antiviral Activity: Inhibition of HHV-6 Replication	IC_{50} 3.9 mM	15
10	No reported activity	Structural elucidation only	-
11	No reported activity	Structural elucidation only	-
12	No reported activity	Structural elucidation only	-
13	Antiviral activity against hepatitis B virus (in HepG 2.2.15 cells)	HBsAg (inhibition %) = 26.3	16
14	Antiviral Activities against Influenza Virus A/Hanfang/359/95 (H3N2)	IC_{50} 63.07 µM	4
15	antiviral activity against hepatitis B virus (HBV)	HBsAg (inhibition %)= 52.6 HBeAg (inhibition %)= 25.4	17
16	No reported activity		-
17	Anti-inflammatory effects on RAW264.7 cells	Cytokine: TNF-α (%) = 73.53 ± 9.35	18
18	Anti-HBV activity	HBsAg secretion of 22.6% HBeAg secretion of 30.4%	5
19	No activity	Structural elucidation only	-
20	No activity	Structural elucidation only	-
21	Anti-HBV activity Antiviral activity against the Coxsackie virus B3 (CVB3)	Inhibitory potency against HBsAg secretion of 22.6% and against HBeAg secretion of 30.4% IC_{50} 184.14 µM	5 4
22	Antiviral. Activities against the Hepatitis B Virus	HBsAg secretion = 53.8% (concentration of 0.035 mM) HBeAg secretion = 39.8% (concentration of 0.035 mM)	10
23	cytotoxicity assays against the acute myelogenous leukemia (HL-60) or human lung cancer (A-549) cell line	(IC_{50} > 20 µM) (not exhibit significant Activity)	19
24	Antiproliferative Activity Assay	(IC_{50} > 20 µM) (not exhibit significant Activity)	20

25	No reported activity	Structural elucidation only	-
26	No reported activity	Structural elucidation only	-
27	cytotoxicity activity against HL-60, SMMC-7721, A-549, MCF-7, and SW480 cancer cell lines	**27** was not active against the above five human cancer cell lines	6
28	Antiviral activity against hepatitis B virus (in HepG 2.2.15 cells)	HBsAg (inhibition %) = 25.4 HBeAg (inhibition%) = 22.6	16
29	No reported activity	Structural elucidation only	-
30	No reported activity	Structural elucidation only	-
31	No reported activity	Structural elucidation only	-
32	Significant anti-TMV biological activity (in *N. glutinosa*)	Average inhibition rate (%): Protective effect: 64.2%; Curative effect: 68.4%	21
33	Significant anti-TMV biological activity (in *N. glutinosa*)	Average inhibition rate (%): Protective effect: 62.7%; Curative effect: 59.4%	21
34	Significant anti-TMV biological activity (in *N. glutinosa*)	Average inhibition rate (%): Protective effect: 81.2%; Curative effect: 78.3%	21
35	Significant anti-TMV biological activity (in *N. glutinosa*)	Average inhibition rate (%): Protective effect: 64.3%; Curative effect: 65.2%	21
36	Significant anti-TMV biological activity (in *N. glutinosa*)	Average inhibition rate (%): Protective effect: 78.8%; Curative effect: 33.9%	21
37	Significant anti-TMV biological activity (in *N. glutinosa*) Insecticidal Activity against *A. fabae*	Average inhibition rate (%): Protective effect: 52.6%; Curative effect: 55% LC_{50} = 38.29 µM	21 21
38	Significant anti-TMV biological activity (in *N. glutinosa*)	Average inhibition rate (%): Protective effect: 64.3%; Curative effect: 44.1%	21
39	Significant anti-TMV biological activity (in *N. glutinosa*)	Average inhibition rate (%): Protective effect: 61.9%; Curative effect: 58.2%	21
40	Significant anti-TMV biological activity (in *N. glutinosa*)	Average inhibition rate (%): Protective effect: 66.0%; Curative effect: 52.4%	21
41	Significant anti-TMV biological activity (in *N. glutinosa*)	Average inhibition rate (%): Protective effect: 69.2%; Curative effect: 60.5%	21
42	Antiviral Activities against Influenza Virus A/Hanfang/359/95 (H3N2)	IC_{50} 440.14 µM	4
43	Antiviral Activity: Inhibition Effect of 43 on TMV in *N. glutinosa*	Average inhibition rate (%): Protective effect: 64.1%; Curative effect: 35.0 %	21
44	Antiviral Activity: Inhibition Effect of 43 on TMV in *N. glutinosa*	Average inhibition rate (%): Protective effect: 53.4%; Curative effect: 32.4 %	21

45	Antiviral Activity: Inhibition Effect of 43 on TMV in *N. glutinosa*	Average inhibition rate (%): Protective effect: 51.7%; Curative effect: 21.2 %	21
46	Antiviral Activity: Inhibition Effect of 43 on TMV in *N. glutinosa*	Average inhibition rate (%): Protective effect: 61.3%; Curative effect: 42.2 %	21
47	Antiviral Activities against Influenza Virus A/Hanfang/359/95 (H3N2)	IC_{50} 84.70 μM	4
48	Activity against hepatitis B virus (HBV). Secretion in HepG2 2.2.15 cell line	HBsAg (inhibition %) = 79.3 (0.8 (μmol/mL) HBeAg (inhibition%) = 27.6 (0.8 (μmol/mL)	17
49	No reported activity	Structural elucidation only	-
50	Antiviral Activities against Influenza Virus A/Hanfang/359/95 (H3N2)	IC_{50} 242.46 μM	4
51	No reported activity	Structural elucidation only	-
52	No reported activity	Structural elucidation only	-
53	No reported activity	Structural elucidation only	-
54	No reported activity	Structural elucidation only	-
55	cytotoxicity effects against five human tumor cell lines	IC_{50} >100 μM	22
56	cytotoxic activities against three human glioma stem cells (GSC-3#, GSC-12# and GSC-18#) Antifungal activity against Fusarium oxysporum	Compound 56 was found to inhibit the growth of human glioma stem cells GSC-3# at 20 μg/mL IC_{50} >100 μM	23 24
57	Antibacterial activity	*S. aureus* MIC ± SD = 32 ± 2.4 μg/mL *E. coli* MIC ± SD = 32 ± 1.9 μg/mL	25
58	Antibacterial activity	*S. aureus* MIC ± SD = 16 ± 0.9 μg/mL *E. coli* MIC ± SD = 32 ± 1.5 μg/mL	25
59	Antibacterial activity	*S. aureus* MIC ± SD = 64 ± 3.8 μg/mL *E. coli* MIC ± SD = > 128 μg/mL	25
60	No reported activity	Structural elucidation only	-
61	No reported activity	Structural elucidation only	-
62	No reported activity	Structural elucidation only	-
63	Antifungal activity against Fusarium oxysporum	IC_{50} 78.45 μM	24
64	No reported activity	Structural elucidation only	-
65	Antibacterial activity against E. faecalis	MIC ± SD = 208.33 μg/mL	26
66	Antimicrobial activity (*S.aureus*, *S. epidermides*, *S. saprophyticum* and *S. pyogenes*); three Gram-negative bacteria: *E. coli*, *K. pneumonia* and *S. sonei*	MIC = 25.0-50.0 μg/mL against all bacteria tested.	27

67	Antimicrobial activity (*S.aureus*, *S. epidermides*, *S. saprophyticum* and *S. pyogenes*); three Gram-negative bacteria: *E. coli*, *K. pneumonia* and *S. sonei*	MIC = >100 µg /mL against all bacteria tested.	27
68	No reported activity	Structural elucidation only	-
69	No reported activity	Structural elucidation only	-
70	No reported activity	Structural elucidation only	-
71	No reported activity	Structural elucidation only	-
72	No reported activity	Structural elucidation only	-
73	No reported activity	Structural elucidation only	-
74	No reported activity	Structural elucidation only	-
75	No reported activity	Structural elucidation only	-
76	No reported activity	Structural elucidation only	-
77	No reported activity	Structural elucidation only	-
78	No reported activity	Structural elucidation only	-
79	No reported activity	Structural elucidation only	-
80	No reported activity	Structural elucidation only	-
81	No reported activity	Structural elucidation only	-
82	No reported activity	Structural elucidation only	-
83	No reported activity	Structural elucidation only	-
84	No reported activity	Structural elucidation only	-
85	No reported activity	Structural elucidation only	-
86	No reported activity	Structural elucidation only	-
87	No reported activity	Structural elucidation only	-
88	No reported activity	Structural elucidation only	-
89	No reported activity	Structural elucidation only	-
90	No reported activity	Structural elucidation only	-
91	No reported activity	Structural elucidation only	-
92	Antifungal activity against Fusarium oxysporum	IC_{50} 36.63 µM	24
93	No reported activity	Structural elucidation only	-
94	Anti-inflammatory effects on RAW264.7 cells Antifungal activity against *Fusarium oxysporum* Insecticide activity against *C. pipiens* Cytotoxicity activity	Cytokine: TNF-α (%) = 46.96 ± 0.04; Cytokine: IL-6(%):41.76 ± 1.74 IC_{50} 27.68 µM LC_{50} (ppm)= 3.42; LC_{90} (ppm)= 43.83 IC_{50} MCF-7= 27.3 ± 0.7; HEPG-2= 30.2 ± 1.9	18 24 28 28

95	Antibacterial activity against *E. faecalis*	MIC ± SD = 125.0 µg/mL	26
96	Antiviral Activities against the Hepatitis B Virus	HBsAg secretion = 39.5% (concentration of 0.035 mM) HBeAg secretion = 13.8% (concentration of 0.035 mM)	10
97	No reported activity	Structural elucidation only	-
98	No reported activity	Structural elucidation only	-
99	No reported activity	Structural elucidation only	-
100	No reported activity	Structural elucidation only	-
101	No reported activity	Structural elucidation only	-
102	Insecticidal Activity against *A. fabae*, *N. lugens* (Stal), and *T. urticae*	Average inhibition rate (%): *A. fabae*: 53.2 ± 2.6; *N. lugens* (Stal): 64.7 ± 11.8; *T. urticae*: 59.3 ± 2.5	29
103	Insecticidal Activity against T. urticae	LC_{50} (mg/L)= 65.09	29
104	Insecticidal Activity against T. urticae	LC_{50} (mg/L)= 49.41	29
105	Insecticidal Activity against *A. fabae*, *N. lugens* (Stal), and *T. urticae*	Average inhibition rate (%): *A. fabae*: 35.7 ± 1.8; *N. lugens* (Stal): 56.8 ± 4.1; *T. urticae*: 45.9 ± 3.0	29
106	Insecticidal Activity against *A. fabae*, *N. lugens* (Stal), and *T. urticae*	Average inhibition rate (%): *A. fabae*: 46.9 ± 1.4; *N. lugens* (Stal): 56.7 ± 1.2; *T. urticae*: 28.7 ± 2.4	29
107	Insecticidal Activity against *A. fabae*, *N. lugens* (Stal), and *T. urticae*	Average inhibition rate (%): *A. fabae*: 27.5 ± 1.6; *N. lugens* (Stal): 46.9 ± 1.4; *T. urticae*: 38.0 ± 5.3	29
108	Insecticidal Activity against *A. fabae*, *N. lugens* (Stal), and *T. urticae*	Average inhibition rate (%): *A. fabae*: 33.9 ± 1.1; *N. lugens* (Stal): 52.1 ± 4.0; *T. urticae*: 41.3 ± 2.3	29
109	Insecticidal Activity against *A. fabae*, *N. lugens* (Stal), and *T. urticae*	Average inhibition rate (%): *A. fabae*: 60.3 ± 3.1; *N. lugens* (Stal): 46.2 ± 2.3; *T. urticae*: 45.0 ± 4.2	29
110	Antifungal activity against *Fusarium oxysporum* *In vitro* Anticholinesterase Activity	IC_{50} 16.53 µM Inhibition (%) at 1 mg/mL: AChE: 41.6 ±1.62; BChE: 73.9±1.03	24 30
111	Hyperexcitability, acetylcholine, and GABA release	**111** has a higher affinity for muscarinic than nicotinic acetylcholine receptors (IC_{50}s 21 vs. 331 µM, respectively)	31
112	No reported activity	Structural elucidation only	-
113	No reported activity	Structural elucidation only	-
114	No reported activity	Structural elucidation only	-
115	No reported activity	Structural elucidation only	-
116	No reported activity	Structural elucidation only	-
117	No reported activity	Structural elucidation only	-

118	No reported activity	Structural elucidation only	-
119	No reported activity	Structural elucidation only	-
120	No reported activity	Structural elucidation only	-
121	No reported activity	Structural elucidation only	-
122	Antifungal activity against Fusarium oxysporum	IC_{50} 7.24 µM	[24]
123	No reported activity	Structural elucidation only	-
124	No reported activity	Structural elucidation only	-
125	No reported activity	Structural elucidation only	-
126	*In vitro* Anticholinesterase Activity	Inhibition (%) at 1 mg/mL; AChE: 15.0 ±1.08; BChE: 66.3±0.88	[30]
127	No reported activity	Structural elucidation only	-
128	No reported activity	Structural elucidation only	-
129	No reported activity	Structural elucidation only	-
130	No reported activity	Structural elucidation only	-
131	No reported activity	Structural elucidation only	-
132	Anti-HBV activity	Inhibitory potency against HBsAg secretion of 33.2% and against HBeAg secretion of 27.38%	[5]
133	Antibacterial activity against *E. faecalis* Insecticide activity against *C. pipiens* Cytotoxicity activity Anti-inflammatory and anti-tumor properties	MIC ± SD = 20.83 µg/mL LC_{50} (ppm)= 8.26; LC_{90} (ppm)= 154.18 IC_{50} (µg/mL): MCF-7= 117 ± 3.8; HEPG-2= 115 ± 3.5 IC_{50} = 33.30 µM (inhibitory effect on LPS-induced NO production in macrophages)	[26] [28] [28] [32]
134	Antibacterial activity	MIC ± SD [µg/mL]: *S. aureus*: 16 ± 1.7; *E. coli*: 8 ± 0.5	[25]
135	Cytotoxicity activity	No activity against MCF-7 and HEPG-2	[33]
136	No reported activity	Structural elucidation only	-
137	No reported activity	Structural elucidation only	-
138	Antibacterial activity against *E. faecalis*	MIC ± SD = 250.0 µg/mL	[26]
139	Antifungal activity against *Fusarium oxysporum* Cytotoxic activity against A549 (human lung epithelia cancer cell line).	IC_{50} 13.61 µM IC_{50} A549 = 22.05 µM	[24] [33]
140	No reported activity	Structural elucidation only	-
141	Cytotoxic activity	Inactive (>50 µM) against all four cell lines (T24, HepG2, SPC-A2, and A549)	[33]
142	No reported activity	Structural elucidation only	-
143	No reported activity	Structural elucidation only	-

144	No reported activity	Structural elucidation only	-
145	No reported activity	Structural elucidation only	-
146	No reported activity	Structural elucidation only	-
147	No reported activity	Structural elucidation only	-
148	Insecticidal activity against *A. fabae* Antiviral activity: Inhibition effect on TSWV in *Nicotiana tabacum* cv.K326.	Corrected mortality rate (%) = 73.4 ± 2.9 Protective effect: 16.2% ± 1.4; Curative effect: 58.6% ± 1.8	34
149	Insecticidal activity against *A. fabae*. Antiviral activity: Inhibition effect on TSWV in *Nicotiana tabacum* cv.K326.	Corrected mortality rate (%) =36.5 ± 2.5 Protective effect: 21.7% ± 9.7; Curative effect: 19.0% ± 1.5	34
150	Insecticidal activity against *A. fabae*. Antiviral activity: Inhibition effect on TSWV in *Nicotiana tabacum* cv.K326.	Corrected mortality rate (%) =48.1 ± 4.3 Protective effect: 23.8% ± 4.3; Curative effect: 47.2% ± 4.9	34
151	Insecticidal activity against *A. fabae*. Antiviral activity: Inhibition effect on TSWV in *Nicotiana tabacum* cv.K326.	Corrected mortality rate (%) =43.2 ± 2.2 Protective effect: 23.2% ± 6.9; Curative effect: 18.5% ± 10.5	34
152	Insecticidal activity against *A. fabae*. Antiviral activity: Inhibition effect on TSWV in *Nicotiana tabacum* cv.K326.	Corrected mortality rate (%) =48.5 ± 4.8 Protective effect: 57.2% ± 6.9; Curative effect: 33.6% ± 6.1	34
153	Insecticidal activity against *A. fabae*. Antiviral activity: Inhibition effect on TSWV in *Nicotiana tabacum* cv.K326.	Corrected mortality rate (%) =64.1 ± 5.8 Protective effect: 18.8% ± 5.7; Curative effect: 26.3% ± 4.1	34
154	Insecticidal activity against *A. fabae*. Antiviral activity: Inhibition effect on TSWV in *Nicotiana tabacum* cv.K326.	Corrected mortality rate (%) =42.6 ± 5.0 Protective effect: 12.5% ± 1.62; Curative effect: 19.6% ± 1.3	34
155	Insecticidal activity against *A. fabae*. Antiviral activity: Inhibition effect on TSWV in *Nicotiana tabacum* cv.K326.	Corrected mortality rate (%) =58.5 ± 5.9 Protective effect: 40.2% ± 4.3; Curative effect: 50.9% ± 1.6	34
156	No reported activity	Structural elucidation only	-
157	Antibacterial activity	MIC ± SD [μg/mL] = *S. aureus*: 32 ± 1.3; *E. coli*: 32 ± 2.5	25

158	No reported activity	Structural elucidation only	-
159	No reported activity	Structural elucidation only	-
160	Antifungal activity against *Fusarium oxysporum*	IC_{50} 21.52 µM	[24]
161	Antifungal activity against Fusarium oxysporum	IC_{50} 43.31 µM	[24]
162	No reported activity	Structural elucidation only	-
163	No reported activity	Structural elucidation only	-
164	No reported activity	Structural elucidation only	-
165	No reported activity	Structural elucidation only	-
166	No reported activity	Structural elucidation only	-
167	No reported activity	Structural elucidation only	-
168	No reported activity	Structural elucidation only	-
169	No reported activity	Structural elucidation only	-
170	No reported activity	Structural elucidation only	-
171	No reported activity	Structural elucidation only	-
172	No reported activity	Structural elucidation only	-
173	No reported activity	Structural elucidation only	-
174	Antifungal activity against *Fusarium oxysporum* Antivirulence activity for Preventing *Cryptococcus neoformans* from Crossing the Blood-Brain Barrier Feeding activity in rainbow trout	IC_{50} 27.40 µM IC_{50} < 10 µM Recommended dietary dose: 500 mg/kg	[24] [35] [36]
175	No reported activity	Structural elucidation only	-
175	No reported activity	Structural elucidation only	-
176	No reported activity	Structural elucidation only	-
177	No reported activity	Structural elucidation only	-
178	No reported activity	Structural elucidation only	-
179	Cytotoxicity activity against murine lymphoma L1210 cells	IC_{50} 4.9 µg/mL	[37]
180	Cytotoxicity activity against murine lymphoma L1210 cells	IC_{50} 7.5 µg/mL	[37]
181	Cytotoxicity activity against murine lymphoma L1210 cells	IC_{50} 6.5 µg/mL	[37]
182	Cytotoxicity activity against murine lymphoma L1210 cells	IC_{50} 7.8 µg/mL	[37]

183	Cytotoxicity activity against murine lymphoma L1210 cells	IC_{50} 8.2 µg/mL	37
184	No reported activity	Structural elucidation only	-
185	No reported activity	Structural elucidation only	-
186	Cytotoxic activity	(IC_{50} µM) TE-671= 8±6 (IC_{50} µM) SH-SY5Y= 51±25 (IC_{50} µM) IMR-32= 15±8 (IC_{50} µM) K-177 = 58±44	38
187	Cytotoxic activity	IC_{50} = 1.8-8.5 µg/mL at 9 µg/mL LC_{50} =10.1-24.7 µg/mL at 25 µg/mL	39
188	Cytotoxic activity (inhibit growth of murine leukemia and human solid tumor cell lines (P-388, A-549, U-251, and SNl2KI)	IC_{50} = 1.8-8.5 µg/mL at 9 µg/mL LC_{50} =10.1-24.7 µg/mL at 25 µg/mL	39
189	Potent blockers of α4β2 and α 7 (Neuronal Nicotinic Acetylcholine Receptors)	IC_{50} = α4β2 (1 µM ACh) = 1.5 µM; α7 (100 µ*M* ACh) = 1.3 µM	40
190	No reported activity	Structural elucidation only	-
191	No reported activity	Structural elucidation only	-
192	No reported activity	Structural elucidation only	-
193	No reported activity	Structural elucidation only	-
194	No reported activity	Structural elucidation only	-
195	No reported activity	Structural elucidation only	-
196	No reported activity	Structural elucidation only	-
197	No reported activity	Structural elucidation only	-
198	Cytotoxic activity against HL-60 cells (Human leukemia)	HL-60 cells (IC_{50} 39 µM)	41
199	Cytotoxicity activity against HL-60, SMMC-7721, A-549, MCF-7, and SW480 cancer cell lines	Inactive against the above five human cancer cell lines (IC_{50} >100 µM).	6
200	No reported activity	Structural elucidation only	-
201	No reported activity	Structural elucidation only	-
202	Antiviral activity against CVB3 (Coxsackievirus B3) Antimicrobial Activity	IC_{50} 4.66 µM *S. aureus* (ATCC 29213) MIC= 6.0 g/L *S. aureus* (ATCC 33591) MIC= 8.0 g/L *E. coli* (ATCC 25922) = 0.8 g/L	42
203	No reported activity	Structural elucidation only	-
204	No reported activity	Structural elucidation only	-
205	No reported activity	Structural elucidation only	-

206	Cytotoxic Activity	KB: IC_{50} 0.554 µM; HepG-2: IC_{50} 0.501 µM; LU-1: IC_{50} 0.607 µM; MCF-7: IC_{50} 0.686 µM	43
207	Cytotoxic Activity against HCT-116 cell line	% Inhibition = -6.2 (No appreciable effect)	44
208	Cytotoxic Activity against HCT-116 cell line	% Inhibition = -13.1 (No appreciable effect)	44
209	Cytotoxic Activity against HCT-116 cell line	% Inhibition = -3.2 (No appreciable effect)	44
210	Cytotoxic Activity against HCT-116 cell line	% Inhibition = 0.7 (No appreciable effect)	44
211	Cytotoxic Activity against HCT-116 cell line	% Inhibition = 80.2	44
212	No reported activity	Structural elucidation only	-
213	No reported activity	Structural elucidation only	-
214	Antibacterial activity	MIC= 100 µg/mL (*Proteus mirabilis*) MIC= 100 µg/mL (*Klebsiella pneumoniae*) MIC= 150 µg/mL (*Escherichia coli*) MIC= 150 µg/mL (*P. vulgaris*) MIC= 150 µg/mL (*Shigellu dysenteriue*)	45
215	No reported activity	Structural elucidation only	-
216	Cytotoxic activity against B16 melanoma cells	Inhibition (%) = 47.2±3.8	46
217	Cytotoxic activity against B16 melanoma cells	Inhibition (%) = 19.21±2.6	46
218	Cytotoxic activity against B16 melanoma cells	Inhibition (%) = 23.0±4.1	46
219	Cytotoxic activity against B16 melanoma cells	Inhibition (%) = -0.6±10.3	46
220	No reported activity	Structural elucidation only	-
221	Antiviral activity (Inhibition effect on TSWV in *Nicotiana tabacum* cv.K326) Insecticidal activity	Average inhibition rate (%): Protective effect: 16.2% ± 1.4; Curative effect: 58.6% ± 1.8 LC_{50} *A. fabae* = 25.2 mg/L,	34
222	Cytotoxicity against murine lymphoma L1210	IC_{50} 0.1 µg/mL	47
223	Cytotoxicity against murine lymphoma L1210	IC_{50} 7.5 µg/mL	37
224	Cytotoxicity against murine lymphoma L1210	IC_{50} 0.1 µg/mL	48
225	Cytotoxicity against murine lymphoma L1210	IC_{50} 1.2 µg/mL	48
226	Cytotoxicity against murine lymphoma L1210	IC_{50} 0.8 µg/mL	48
227	Cytotoxicity against murine lymphoma L1210	IC_{50} 0.6 µg/mL	48
228	No reported activity	Structural elucidation only	-

229	No reported activity	Structural elucidation only	-
230	Cytotoxicity Activity against human blood premyelocytic leukemia (HL-60)	No inhibition at 100 µM	49
231	Cytotoxicity Activity against human blood premyelocytic leukemia (HL-60)	No inhibition at 100 µM	49
232	Cytotoxicity Activity against human blood premyelocytic leukemia (HL-60)	46% inhibition at 100 µM	49
233	Cytotoxicity against murine lymphoma L1210	IC_{50}, 10 µg/mL	50
234	Cytotoxicity against MM cell lines and patient cells Cytotoxicity Activity against MG-63 and U2OS OS cells Cytotoxicity Activity against papillary thyroid carcinoma (IHH-4) and anaplastic thyroid carcinoma (8505c and KMH-2)	IC_{50} = 80–260 µM for all cell lines and primary MM cells The rate of late apoptotic cells at different concentrations (0.1, 0.2, and 0.4 mM) was: **MG-63**: 6.69 ± 0.89, 8.88 ± 1.19 and 14.8 ± 2.87% **U2OS**: 5.94 ± 1.34, 13.99 ± 1.92 and 24.18 ± 1.52% (IHH-4) IC_{50} 423.2, 161.7, and 148.8 µM (8505c) IC_{50}708.8, 222.0, and 214.4 µM (KMH-2) IC_{50} 240.8, 221.2, and 208.0 µM	51 52 53
235	Anti-HBV activities Cytotoxicity Activity against HepG2 2.2.15 cells	% inhibition (10 µmol/mL): HBsAg secretion: 13.94 ± 5.06 HBeAg secretion: 16.33 ± 2.96 HepG2 2.2.15 cells: 2.76 ± 3.91	54
236	Anti-HBV activities Cytotoxicity Activity against HepG2 2.2.15 cells	% inhibition (10 µmol/mL); HBsAg secretion: 7.88 ± 1.21 HBeAg secretion: 24.73 ± 8.85 HepG2 2.2.15 cells: 2.86 ± 4.05	54
237	Anti-HBV activities	% inhibition ($1x10^{-5}$ mol/mL) HBsAg secretion: 22.34 ± 4.38% HBeAg secretion: 18.00 ± 5.01%	55
238	Anti-HBV activities	% inhibition (10 µmol/mL) HBsAg secretion: 2.70 ± 3.36 HBeAg secretion: 26.26 ± 3.67	54
239	Antifungal activity against *Fusarium oxysporum*	IC_{50}, 95.53 µM MIC *ca.* 100 µg/mL	24 27

	Antimicrobial activity against *S. aureus* (ATCC 6538), *S. epidermides* (ATCC 12228), *S. saprophyticum* (ATCC 15305), and *S. pyogenes* (ATCC 19615)		
240	No reported activity	Structural elucidation only	-
241	No reported activity	Structural elucidation only	-
242	No reported activity	Structural elucidation only	-
243	No reported activity	Structural elucidation only	-
244	Cytotoxicity activity against the cancer lines U87 (glioblastoma), 518A2 (melanoma), and HCT116 (colon cancer)	IC_{50} (72 h) < 50 µM	56
245	Cytotoxicity activity against the cancer lines U87 (glioblastoma), 518A2 (melanoma), and HCT116 (colon cancer)	IC_{50} (72 h) < 50 µM	56
246	No reported activity	Structural elucidation only	-
247	No reported activity	Structural elucidation only	-
248	No reported activity	Structural elucidation only	-
249	No reported activity	Structural elucidation only	-
250	No reported activity	Structural elucidation only	-
251	Antibacterial activity against *E. faecalis*	MIC = 208.33 µg/mL	26
252	Cytotoxicity against murine lymphoma L1210	IC_{50} 8.9 µg/mL	37
253	anti-acetylcholinesterase (AChE) activity (from electric eel)	IC_{50} 330 µM	37
254	anti-acetylcholinesterase (AChE) activity (from electric eel)	IC_{50} 220 µM	37
255	anti-acetylcholinesterase (AChE) activity and neuroprotective effects	Inactive	57
256	anti-acetylcholinesterase (AChE) activity and neuroprotective effects	Inactive	57
257	anti-acetylcholinesterase (AChE) activity and neuroprotective effects	Inactive	57
258	anti-acetylcholinesterase (AChE) activity and neuroprotective effects	Inactive	57
259	anti-acetylcholinesterase (AChE) activity and neuroprotective effects	Inactive	57
260	Antimalarial activity against *P. falciparum*	IC_{50} = 5 µg/mL	58
261	No reported activity	Structural elucidation only	-

262	No reported activity	Structural elucidation only	-
263	No reported activity	Structural elucidation only	-
264	No reported activity	Structural elucidation only	-
265	No reported activity	Structural elucidation only	-
266	No reported activity	Structural elucidation only	-
267	Antimalarial activity against *P. falciparum*	IC_{50} >20 µg/mL	58
268	No reported activity	Structural elucidation only	-
269	No reported activity	Structural elucidation only	-
270	No reported activity	Structural elucidation only	-
271	No reported activity	Structural elucidation only	-
272	Antimalarial activity and cytotoxicity	IC_{50} = 2.5 ng/mL (6.11 nM) and 2.1 ng/mL (5.13 nM) against K1 and FCR3 IC_{50} = 10 ng/mL (24.45 nM) against MRC5	59
273	Cytotoxicity against KB (mouth epidermal carcinoma cells, CCL-17), HepG-2 (human liver hepatocellular carcinoma cells, HB-8065), LU-1 (human lung adenocarcinoma cells, HTB-57™), and MCF-7 (human breast cancer cells, HTB-22).	KB: IC_{50}, =0.663 µM HepG-2: IC_{50}, =0.796 µM LU-1: IC_{50}, =0.663 µM MCF-7: IC_{50}, =0.637 µM	43
274	Cytotoxicity against KB (mouth epidermal carcinoma cells, CCL-17), HepG-2 (human liver hepatocellular carcinoma cells, HB-8065), LU-1 (human lung adenocarcinoma cells, HTB-57™), and MCF-7 (human breast cancer cells, HTB-22).	KB: IC_{50}, =0.025 µM HepG-2: IC_{50}, =0.027 µM LU-1: IC_{50}, =0.110 µM MCF-7: IC_{50}, =0.744 µM	43
275	Cytotoxicity against KB (mouth epidermal carcinoma cells, CCL-17), HepG-2 (human liver hepatocellular carcinoma cells, HB-8065), LU-1 (human lung adenocarcinoma cells, HTB-57™), and MCF-7 (human breast cancer cells, HTB-22).	KB: IC_{50}, =0.398 µM HepG-2: IC_{50}, =0.186 µM LU-1: IC_{50}, =0.504 µM MCF-7: IC_{50}, =0.398 µM	43
276	Cytotoxicity	IC_{50} (nM): A549= 0.7 ± 0.1 IC_{50} (nM): MRC-5= 2.6 ± 0.4 IC_{50} (nM): MRC-9= 2.2 ± 0.7 IC_{50} (nM): BEL-7402= 1.7 ± 0.7 IC_{50} (nM): LO2= 2.7 ± 1	60
277	Anticancer Activity against the 9-KB carcinoma	ED_{50} = 0.00078 µg/mL	61

	Anticancer Activity against Human gastric cancer AGS (Hypoxia-Inducible Factor-1)	HIF-1: IC_{50}= 8.7 nM	62
278	Cytotoxicity against 12 cell lines from 6 panels of cancer including lung cancer, colon cancer, breast cancer, prostate cancer, kidney cancer and leukemia	K562: GL_{50} (ng/mL) = 100 HL60: GL_{50} (ng/mL) = 5 DU145: GL_{50} (ng/mL) = 2 PC-3: GL_{50} (ng/mL) = 5 A545: GL_{50} (ng/mL) = 0.3 NCl-H460: GL_{50} (ng/mL) = 0.3 MCF-7: GL_{50} (ng/mL) = 5 MDA-MD-231: GL_{50} (ng/mL) = 3 ACHN: GL_{50} (ng/mL) = 0.3 UO-31: GL_{50} (ng/mL) = 0.4 HT-29: GL_{50} (ng/mL) = 0.2 COLO-205: GL_{50} (ng/mL) = 0.3	63
	Cytotoxicity against three cancer cell lines (CEM, HeLa and L1210) and two endothelial cell lines (HMEC-1, BAEC)	HeLa IC_{50} (nM) = 66 ± 56 CEM IC_{50} (nM) = 185 ± 156 L-1210 IC_{50} (nM) = 19 ± 10 HMEC-1 IC_{50} (nM) = 7.4 ± 1.1 BAEC IC_{50} (nM) = 23 ± 13	64
279	Cytotoxicity against 12 cell lines from 6 panels of cancer including lung cancer, colon cancer, breast cancer, prostate cancer, kidney cancer and leukemia	GL_{50} (ng/mL) >100 (showed lower activity)	63
280	No reported activity	Structural elucidation only	-
281	No reported activity	Structural elucidation only	-
282	No reported activity	Structural elucidation only	-
283	No reported activity	Structural elucidation only	-
284	No reported activity	Structural elucidation only	-
285	Cytotoxicity activity against P388 cells	Inactive against P388 cells (>10 µg/mL).	65
286	Inhibitory activity against hPTP1B (human protein tyrosine phosphatase 1B)	Inactive	66
287	Inhibitory activity against hPTP1B (human protein tyrosine phosphatase 1B	Inactive	66
288	Cytotoxicity activity against P388 cells	Inactive against P388 cells (>10 µg/mL).	65
289	No reported activity	Structural elucidation only	-
290	No reported activity	Structural elucidation only	-
291	No reported activity	Structural elucidation only	-

292	No reported activity	Structural elucidation only	-
293	No reported activity	Structural elucidation only	-
294	Activity against Hepatitis C Virus	CC_{50} (μM) = 119.1; EC_{50} (μM) =4.7	67
295	Activity against Hepatitis C Virus	CC_{50} (μM) = 119.1; EC_{50} (μM) =4.7	67
296	Activity against Hepatitis C Virus	CC_{50} (μM) = 169.3; EC_{50} (μM) =2.2	67
297	Activity against Hepatitis C Virus	CC_{50} (μM) = 169.3; EC_{50} (μM) =2.2	67
298	Antiviral activity against hepatitis B virus (in HepG 2.2.15 cells)	HBsAg (inhibition %) = 37.2; HBeAg (inhibition%) = 33.2	16
299	Antiviral activity against hepatitis B virus (in HepG 2.2.15 cells)	HBsAg (inhibition %) = 30.8; HBeAg (inhibition%) = 16.8	16
300	Antiviral activity against hepatitis B virus (in HepG 2.2.15 cells)	HBsAg (inhibition %) = 29.8; HBeAg (inhibition%) = 15.1	16
301	Antiviral activity against hepatitis B virus (in HepG 2.2.15 cells)	HBsAg (inhibition %) = 44.3; HBeAg (inhibition%) = 38.0	16
302	Antiviral activity against hepatitis B virus (in HepG 2.2.15 cells)	HBsAg (inhibition %) = 14.1	16
303	Antiviral activity against hepatitis B virus (in HepG 2.2.15 cells)	HBsAg (inhibition %) = 46.0; HBeAg (inhibition%) = 40.4	16
304	Antiviral activity against hepatitis B virus (in HepG 2.2.15 cells)	Inactive against the secretion of both HBsAg and HBeAg.	55
305	No reported activity	Structural elucidation only	-
306	No reported activity	Structural elucidation only	-
307	No reported activity	Structural elucidation only	-
308	No reported activity	Structural elucidation only	-
309	No reported activity	Structural elucidation only	-
310	No reported activity	Structural elucidation only	-
311	No reported activity	Structural elucidation only	-
312	No reported activity	Structural elucidation only	-
313	No reported activity	Structural elucidation only	-
314	No reported activity	Structural elucidation only	-
315	RLAR activity (rat lens aldose reductase)	% Inhibition= 25-32% (concentration: 50 μM)	68
316	RLAR activity (rat lens aldose reductase)	% Inhibition= 25-32% (concentration: 50 μM)	68
317	RLAR activity (rat lens aldose reductase)	% Inhibition= 25-32% (concentration: 50 μM)	68
318	Antimalarial activity against *P. falciparum*	Inactive	69
319	Antimalarial activity against *P. falciparum*	Inactive	69
320	Antimalarial activity against *P. falciparum*	Inactive	69
321	Antimalarial activity against *P. falciparum*	Inactive	69

322	Antimalarial activity against *P. falciparum*	IC_{50} 4.76 µg/mL for both D6 and W2 clones	69
323	Antimalarial activity against *P. falciparum*	Inactive	69
324	Antimalarial activity against *P. falciparum*	Inactive	69
325	Antimalarial activity against *P. falciparum*	IC_{50} = 2.8 µg/mL for both D6 and W2 clones	69
326	No reported activity	Structural elucidation only	-
327	No reported activity	Structural elucidation only	-
328	No activity	Structural elucidation only	
329	RLAR activity (rat lens aldose reductase)	% Inhibition= 25-32% (concentration: 50 µM)	68
330	No reported activity	Structural elucidation only	-
331	No reported activity	Structural elucidation only	-
332	No reported activity	Structural elucidation only	-
333	Cytotoxic activity against HepG-2, HL-60, LU-1, MCF-7, and SK-Mel-2 human cancer cells	HepG-2: IC_{50} (µM) = 6.85 ± 0.76 HL-60: IC_{50} (µM) = 9.19 ± 0.72 LU-1: IC_{50} (µM) = 9.88 ± 0.98 MCF-7: IC_{50} (µM) = 7.82 ± 0.53 SK-Mel-2: IC_{50} (µM) = 7.51 ± 0.69	70
334	Cytotoxic effects against SNU-398, HT-29, and Capan-1 cell lines Cytotoxic activity against HL-60	SNU-398 IC_{50} >50 µM HT-29 IC_{50} = 22.6±6.6 µM Capan-1 IC_{50} >50 µM IC_{50} (µM) = 5.5	71 72
335	Cytotoxic activity against HepG-2, HL-60, LU-1, MCF-7, and SK-Mel-2 human cancer cells Antimalarial activity against *P. falciparum* African (D6) clone Antituberculosis activity against H37Rv	HepG-2: IC_{50} (µM) = 0.75 ± 0.11 HL-60: IC_{50} (µM) = 0.88 ± 0.07 LU-1: IC_{50} (µM) = 0.96 ± 0.09 MCF-7: IC_{50} (µM) = 0.79 ± 0.05 SK-Mel-2: IC_{50} (µM) = 1.02 ± 0.11 D6 clone IC_{50} = 670 ng/mL W2 clone IC_{50}= 280 ng/mL MIC= 3.94 µM	70 73 73
336	Cytotoxic effects against SNU-398, HT-29, and Capan-1 cell lines Cytotoxic activity against HL-60	SNU-398 IC_{50} =45.7±3.2 µM HT-29 IC_{50} = 12.0±4.3 µM Capan-1 IC_{50} =32.5±3.3 µM IC_{50} (µM) = 5.5	71 72
337	Cytotoxic activity against HepG-2, HL-60, LU-1, MCF-7, and SK-Mel-2 human cancer cells	HepG-2: IC_{50} (µM) = 30.35 ± 3.04 HL-60: IC_{50} (µM) = 22.95 ± 0.95	70

		LU-1: IC_{50} (µM) = 32.59 ± 2.56 MCF-7: IC_{50} (µM) = 24.85 ± 1.21 SK-Mel-2: IC_{50} (µM) = 35.92 ± 4.87	
338	Cytotoxic effects against SNU-398, HT-29, and Capan-1 cell lines	SNU-398 IC_{50} >50 µM HT-29 IC_{50} = 23.2±2.7 µM Capan-1 IC_{50} >50 µM	71
339	Vasodilative activity	Inactive IC_{50} > 100 µM	74
340	Vasodilative activity	Inactive IC_{50} > 100 µM	74
341	Vasodilative activity	Inactive IC_{50} > 100 µM	74
342	Vasodilative activity	Inactive IC_{50} > 100 µM	74
343	Antimalarial activity against *P. falciparum* African (D6) clone	Inactive	73
344	Cytotoxic activity against HepG-2, HL-60, LU-1, MCF-7, and SK-Mel-2 human cancer cells	HepG-2: IC_{50} (µM) = 19.52 ± 1.45 HL-60: IC_{50} (µM) = 16.79 ± 0.74 LU-1: IC_{50} (µM) = 22.25 ± 1.26 MCF-7: IC_{50} (µM) = 24.85 ± 0.91 SK-Mel-2: IC_{50} (µM) = 23.04 ± 2.47	70
345	Cytotoxic activity against HL-60	IC_{50} (µM) = 5.5	72
346	Cytotoxic activity against HepG-2, HL-60, LU-1, MCF-7, and SK-Mel-2 human cancer cells	HepG-2: IC_{50} (µM) = 6.58 ± 0.94 HL-60: IC_{50} (µM) = 7.84 ± 0.85 LU-1: IC_{50} (µM) = 9.20 ± 1.21 MCF-7: IC_{50} (µM) = 7.36 ± 1.16 SK-Mel-2: IC_{50} (µM) =11.23 ± 0.33	70
347	Cytotoxic activity against HepG-2, HL-60, LU-1, MCF-7, and SK-Mel-2 human cancer cells	HepG-2: IC_{50} (µM) = 5.06 ± 0.39 HL-60: IC_{50} (µM) = 5.65 ± 0.42 LU-1: IC_{50} (µM) = 5.63 ± 0.19 MCF-7: IC_{50} (µM) = 5.32 ± 0.67 SK-Mel-2: IC_{50} (µM) =5.45 ± 0.91	70
348	Cytotoxic activity against HepG-2, HL-60, LU-1, MCF-7, and SK-Mel-2 human cancer cells	HepG-2: IC_{50} (µM) = 5.55 ± 0.98 HL-60: IC_{50} (µM) = 6.58 ± 0.94 LU-1: IC_{50} (µM) = 5.84 ± 0.45 MCF-7: IC_{50} (µM) = 5.68 ± 0.89 SK-Mel-2: IC_{50} (µM) = 6.24 ± 0.96	70
349	Cytotoxic activity against HepG-2, HL-60, LU-1, MCF-7, and SK-Mel-2 human cancer cells	HepG-2: IC_{50} (µM) = 0.43 ± 0.03 HL-60: IC_{50} (µM) = 0.62 ± 0.08 LU-1: IC_{50} (µM) = 0.76 ± 0.09 MCF-7: IC_{50} (µM) = 0.44 ± 0.05 SK-Mel-2: IC_{50} (µM) = 0.77 ± 0.13	70

350	No reported activity	Structural elucidation only	-
351	Activity antimicrobial against a fluconazole-resistant strain of *Candida albicans* ATCC 14503.	(MIC, μg/mL) *C. albicans* ATCC 14503 = 100 *C. albicans* UCD-FR1 = 100 *C. glabrata* = 100 *C. krusei* =100	75
352	Cytotoxic activity against KB and L1210 cells Somatostatin and Vasoactive Intestinal Peptide Inhibitors.	(KB) ED_{50} (μg/mL) = 2.5 (L1210) ED_{50} (μg/mL) = 2.0 IC_{50}= 12 μM	76 77
353	Potent inhibitor of the inositol 1,4,5-trisphosphate receptor and the endoplasmic-reticulum Ca^{2+} pumps Activity antimicrobial against a fluconazole-resistant strain of *Candida albicans* ATCC 14503	78% inhibition (MIC, μg/mL) *C. albicans* ATCC 14503 = 100 *C. albicans* UCD-FR1 = 100 *C. glabrata* = 30 *C. krusei* = 30	78 75
354	Cytotoxic activity against KB and L1210 cells Activity antimicrobial against a fluconazole-resistant strain of *Candida albicans* ATCC 1450	(KB) ED_{50} (μg/mL) = 2.0 (L1210) ED_{50} (μg/mL) = 0.2 (MIC, μg/mL) *C. albicans* ATCC 14503 = 100 *C. albicans* UCD-FR1 = 100 *C. glabrata* = 100 *C. krusei* = 100	76 75
355	Cytotoxic activity against breast-cancer cell lines MCF-7, T-47D, ZR-75-1 and MDA-MB-231	ED_{50} values (μg/mL) MCF-7 >>50 T-47D >50 ZR-75-1= ND MDA-MB-231 = ND	79
356	No reported activity	Structural elucidation only	-
357	No reported activity	Structural elucidation only	-
358	No reported activity	Structural elucidation only	-
359	No reported activity	Structural elucidation only	-

360	Activity antimicrobial against a fluconazole-resistant strain of *Candida albicans* ATCC 14503.	Inactive	75
361	No reported activity	Structural elucidation only	-
362	No reported activity	Structural elucidation only	-
363	No reported activity	Structural elucidation only	-
364	Cytotoxic activity against HepG-2, HL-60, LU-1, MCF-7, and SK-Mel-2 human cancer cells Anti-HIV activity Cytotoxic activity against MT2 cell line	Inactive IC_{50} > 50 μM. EC_{50}= 41.3 μM CC_0 (μM) = 13.4 CC_{50} (μM) = 178.1	70 80 80
365	Cytotoxic activity against HepG-2, HL-60, LU-1, MCF-7, and SK-Mel-2 human cancer cells Anti-HIV activity Cytotoxic activity against MT2 cell line	Inactive IC_{50} > 50 μM. EC_{50}= 52.9 μM CC_0 (μM) = 12.1 CC_{50} (μM) = 371.3	70 80 80
366	No reported activity	Structural elucidation only	-
367	No reported activity	Structural elucidation only	-
368	Cytotoxicity against SNU-398, HT-29, and Capan-1	IC_{50} > 50 μM	71
369	Cytotoxicity against SNU-398, HT-29, and Capan-1	IC_{50} > 50 μM	71
370	Antiviral activity Insecticidal activity against *A. fabae*	Inhibition effect on TSWV in *Nicotiana tabacum* cv.K326 Inhibition rate: Protective effect= 21.7% ± 9.7; Curative effect: 19.0% ± 1.5 Corrected mortality rate (%):36.5 ± 2.5	34
371	Antiviral activity Insecticidal activity against *A. fabae*	Inhibition effect on TSWV in *Nicotiana tabacum* cv.K326 Inhibition rate: Protective effect= 23.8% ± 4.3; Curative effect: 47.2% ± 4.9 Corrected mortality rate (%): 48.1 ± 4.3	34
372	Antiviral activity Insecticidal activity against *A. fabae*	Inhibition effect on TSWV in *Nicotiana tabacum* cv.K326 Inhibition rate: Protective effect= 23.2% ± 6.9; Curative effect: 18.5% ± 10.5 Corrected mortality rate (%):43.2 ± 2.2	34

373	Antiviral activity Insecticidal activity against *A. fabae*	Inhibition effect on TSWV in *Nicotiana tabacum* cv.K326 Inhibition rate: Protective effect= 57.2% ± 6.9; Curative effect: 33.6% ± 6.1 Corrected mortality rate (%):48.5 ± 4.8	34
374	Antiviral activity Insecticidal activity against *A. fabae*	Inhibition effect on TSWV in *Nicotiana tabacum* cv.K326 Inhibition rate: Protective effect= 77.2% ± 4.0; Curative effect: 42.9% ± 2.2 Corrected mortality rate (%):41.2 ± 3.9	34
375	Antiviral activity Insecticidal activity	Inhibition effect on TSWV in *Nicotiana tabacum* cv.K326 Inhibition rate: Protective effect= 62.7 ± 3.7; Curative effect: 75.0 ± 2.9 Corrected mortality rate (%): *A. fabae*: 60.9 ± 1.9 *N. lugens* (Stal): 67.0 ± 8.2 *T. urticae*: 37.6 ± 4.9	29
376	Antiviral activity Insecticidal activity against *A. fabae*	Inhibition effect on TSWV in *Nicotiana tabacum* cv.K326 Inhibition rate: Protective effect= 25.7 ± 2.4; Curative effect: 19.1 ± 5.3 Corrected mortality rate (%): *A. fabae*: 48.5 ± 4.8 *N. lugens* (Stal): 68.7 ± 4.7 *T. urticae*: 56.0 ± 7.1	29
377	Anti-inflammatory activity in LPS-Stimulated RAW 264.7 Cells	TNF-α (%) = 96.64 ± 1.27 IL-6 (%) = 67.85 ± 0.44	11
378	Anti-inflammatory activity in LPS-Stimulated RAW 264.7 Cells	TNF-α (%) = 50.05 ± 6.56 IL-6 (%) = 52.87 ± 3.22	11
379	Anti-inflammatory activity in LPS-Stimulated RAW 264.7 Cells	TNF-α (%) = 49.59 ± 0.51 IL-6 (%) = 73.90 ± 0.34	11
380	Anti-inflammatory activity in LPS-Stimulated RAW 264.7 Cells	TNF-α (%) = 70.86 ± 0.31 IL-6 (%) = 60.08 ± 1.66	11
381	Anti-inflammatory activity in LPS-Stimulated RAW 264.7 Cells	TNF-α (%) = 69.14 ± 2.18 IL-6 (%) = no activity	11
382	Cytotoxic activity against A549, KB, KB-VIN, and MDAMB- 231 cell lines Contact toxicity against *S. litura*	(ED_{50} >20 µM) After five days, 50% of larvae were killed (3 mg/mL in EtOH)	81
383	anti-HBV activity in HepG2.2.15 cells	HBsAg (inhibition %)=15.6 ± 0.7; HBeAg (inhibition %)=11.3 ± 0.2	10

384	Hepatoprotective activity against APAP-induced hepatotoxicity in HepG2 cell	Exhibited excellent hepatoprotective activities in acetaminophen-induced liver injury in vitro and *in vivo*.	82
385	Hepatoprotective activity	Inactive	82
386	Hepatoprotective activity	Inactive	82
387	Antiviral activity against the Hepatitis B Virus	HBsAg secretion = 39.8% (concentration of 0.035 mM) HBeAg secretion = 21.5 % (concentration of 0.035 mM)	10
388	Antiviral activity against the Hepatitis B Virus	HBsAg secretion = 32.4% (concentration of 0.035 mM) HBeAg secretion = 20.8% (concentration of 0.035 mM)	10
389	Potent Anti-metastatic Activity	Inhibition (%) = 22.7 ±8.8 at 100 (µM)	46
390	Potent Anti-metastatic Activity	Inhibition (%) = 32.5 ± 5.3 at 100 (µM)	46
391	Potent Anti-metastatic Activity Inhibitory effects on lung metastasis of B16 melanoma cells in mice	Inhibition (%) = 86.8 ± 2.4 at 100 (µM) Inhibition (%) = 94; Dose(mg/kg, po)= 5; Numbers of colonies: 1.2± 0.7	46 46
392	Anti-metastatic Activity	Inhibition (%) = 86.6 ± 1.54 at 100 (µM)	46
393	Anti-metastatic Activity	Inhibition (%) = 28.3 ± 2.10 at 100 (µM)	46
394	Anti-metastatic Activity	Inhibition (%) = 15.7 ± 4.60 at 100 (µM)	46
395	No reported activity	Structural elucidation only	-
396	Anti-metastatic Activity	Inhibition (%) = 9.2 ± 10.5 at 10 (µM)	46
397	Anti-metastatic Activity	Inhibition (%) = 47.1 ± 4.6 at 100 (µM)	46

Table S3. Calculated properties of compiled QAs **1-397**

QA	MW	*d*	cLogP	cLogS	*H*-A	*H*-D
1	280.4	-4.36	0.384	0.253	5	1
2	264.4	-3.09	0.734	0.067	4	0
3	264.4	0.99	0.884	-1.652	4	1
4	264.4	-0.03	1.357	-1.916	4	1
5	248.4	0.25	1.707	-2.102	3	0
6	248.4	0.25	1.707	-2.102	3	0
7	246.4	1.13	1.432	-1.874	3	0
8	264.4	1.08	0.855	-1.703	4	1
9	246.4	1.13	1.432	-1.874	3	0
10	242.3	2.86	1.404	-1.712	3	0
11	234.4	1.45	2.274	-2.12	2	0
12	248.4	0.25	1.707	-2.102	3	0
13	248.4	0.25	1.707	-2.102	3	0
14	244.3	2.87	1.509	-1.976	3	0
15	246.4	2.34	1.432	-1.874	3	0
16	246.4	0.57	1.955	-2.168	3	0
17	280.4	-2.32	-0.089	0.517	5	1
18	280.4	1.52	-0.118	0.466	5	1
19	280.4	5.19	0.032	-1.253	5	2
20	244.3	2.87	1.509	-1.976	3	0
21	264.4	4.73	0.855	-1.703	4	1
22	417.5	1.30	2.353	-4.091	6	1
23	320.5	-1.43	2.598	-2.671	4	0
24	276.4	5.31	2.431	-2.532	3	0
25	244.3	0.84	1.165	-2.098	3	0
26	244.3	0.84	1.165	-2.098	3	0
27	248.4	0.25	1.707	-2.102	3	0
28	246.4	0.57	1.955	-2.168	3	0
29	262.4	1.39	1.103	-1.769	4	1

QA	MW	*d*	cLogP	cLogS	*H*-A	*H*-D
200	266.4	-2.09	1.007	-2.111	4	2
201	276.4	-2.03	2.291	-2.455	4	1
202	292.4	0.85	1.439	-2.056	5	2
203	292.4	0.05	1.439	-2.056	5	2
204	278.4	1.41	-0.044	-1.586	5	3
205	319.4	0.57	2.602	-2.624	5	1
206	379.5	1.11	3.894	-3.537	4	0
207	331.4	-0.53	1.846	-3.479	5	1
208	391.5	-0.41	1.706	-3.515	7	1
209	391.5	-0.41	1.706	-3.515	7	1
210	357.4	-2.45	2.176	-3.849	5	1
211	387.5	-2.33	2.106	-3.867	6	1
212	491.6	0.16	1.991	-3.515	9	3
213	264.4	-0.59	1.433	-2	4	0
214	250.4	0.55	1.999	-2.018	3	0
215	379.5	1.11	3.894	-3.537	4	0
216	249.4	-3.82	2.085	-0.7	3	0
217	233.4	2.21	3.059	-2.869	2	0
218	233.4	2.21	3.059	-2.869	2	0
219	249.4	3.89	2.235	-2.419	3	1
220	279.4	1.21	0.720	-2.42	4	1
221	288.3	1.86	1.067	-1.904	5	0
222	344.6	3.76	4.852	-3.946	2	0
223	344.6	3.76	4.852	-3.946	2	0
224	343.6	2.08	4.310	-3.823	2	0
225	330.6	1.24	4.599	-4.308	2	1
226	358.6	2.31	4.538	-4.397	3	0
227	372.6	2.26	4.909	-4.228	3	0
228	346.6	3.67	4.786	-4.246	2	0

30	262.4	1.96	0.580	-1.475	4	1
31	260.3	3.68	0.657	-1.577	4	1
32	278.4	2.42	-0.244	-1.025	5	2
33	320.4	2.32	0.241	-1.435	6	1
34	338.5	2.22	0.574	-2.396	5	1
35	322.4	1.39	0.517	-1.663	6	1
36	340.5	1.30	0.849	-2.624	5	1
37	280.4	-2.71	-0.118	0.466	5	1
38	294.4	1.39	0.460	-1.381	5	1
39	320.4	1.66	0.764	-1.729	6	1
40	276.3	2.06	-0.071	-1.138	5	1
41	276.3	1.94	-0.071	-1.138	5	1
42	262.4	1.88	0.609	-1.424	4	1
43	280.4	1.54	0.032	-1.253	5	2
44	246.4	0.57	1.955	-2.168	3	0
45	262.4	1.25	1.132	-1.718	4	1
46	246.4	0.57	1.955	-2.168	3	0
47	262.4	2.54	0.580	-1.475	4	1
48	246.4	1.13	1.432	-1.874	3	0
49	260.3	3.49	1.098	-1.659	4	1
50	262.4	2.54	0.580	-1.475	4	1
51	306.4	4.68	1.340	-2.113	5	0
52	306.4	4.68	1.340	-2.113	5	0
53	264.4	4.73	0.855	-1.703	4	1
54	264.4	4.73	0.855	-1.703	4	1
55	246.4	1.39	1.784	-2.204	3	0
56	248.4	0.55	1.707	-2.102	3	0
57	264.4	2.45	0.855	-1.703	4	1
58	264.4	1.22	0.884	-1.652	4	1
59	264.4	-2.92	0.734	0.067	4	0
60	264.4	0.58	1.357	-1.916	4	1

229	374.6	2.13	4.843	-4.528	3	0
230	427.7	3.31	5.399	-4.735	3	1
231	413.7	0.48	5.146	-5.097	3	2
232	443.7	1.71	5.018	-5.486	4	1
233	423.6	1.95	4.002	-4.81	4	0
234	232.4	1.84	2.029	-2.348	2	1
235	260.4	2.22	1.968	-2.437	3	0
236	246.4	-1.01	2.290	-0.244	3	0
237	242.3	2.10	2.118	-2.45	3	0
238	258.4	2.97	1.562	-2.192	3	0
239	246.4	1.84	1.298	-1.996	3	0
240	244.3	2.61	1.375	-2.098	3	0
241	260.3	5.47	0.523	-1.699	4	1
242	262.4	4.72	0.446	-1.597	4	1
243	262.4	-1.81	0.324	0.173	4	0
244	344.5	2.00	2.193	-2.443	5	0
245	230.3	3.93	1.167	-1.706	3	0
246	230.3	3.93	1.167	-1.706	3	0
247	234.3	1.22	1.365	-1.832	3	0
248	232.3	4.01	1.098	-2.056	3	0
249	232.3	4.01	1.098	-2.056	3	0
250	250.3	-3.09	0.392	0.337	4	0
251	284.3	3.20	1.514	-2.437	6	1
252	294.4	-3.92	0.764	-0.343	5	1
253	278.4	-4.88	1.616	-0.742	4	0
254	262.4	-2.22	2.589	-2.911	3	0
255	278.4	0.71	1.737	-2.512	4	1
256	278.4	-1.23	1.737	-2.512	4	1
257	320.4	-1.26	2.222	-2.922	5	0
258	274.4	-0.33	1.357	-2.02	4	1
259	316.4	-0.27	1.842	-2.43	5	0

61	248.4	0.55	1.707	-2.102	3	0
62	248.4	0.55	1.707	-2.102	3	0
63	264.4	0.50	0.855	-1.703	4	1
64	346.5	-2.18	2.603	-2.549	5	0
65	280.4	1.36	0.473	-1.335	5	2
66	383.5	-0.01	2.106	-3.359	6	1
67	394.5	-2.06	3.113	-3.653	5	0
68	346.5	-2.18	2.603	-2.549	5	0
69	262.4	0.90	1.141	-2.084	4	0
70	394.5	-2.06	3.113	-3.653	5	0
71	278.4	0.19	1.283	-1.831	4	0
72	294.4	5.47	0.431	-1.432	5	1
73	310.4	5.65	-0.421	-1.033	6	2
74	280.4	4.67	0.003	-1.304	5	2
75	362.5	2.61	0.967	-2.328	6	1
76	278.4	0.51	0.791	-1.898	5	1
77	262.4	2.31	0.759	-1.891	4	1
78	264.4	3.12	0.855	-1.703	4	1
79	264.4	3.12	0.855	-1.703	4	1
80	280.4	4.67	0.003	-1.304	5	2
81	280.4	0.55	0.003	-1.304	5	2
82	296.4	4.72	-0.849	-0.905	6	3
83	362.5	0.53	1.676	-2.042	6	1
84	278.4	0.19	1.283	-1.831	4	0
85	264.4	0.74	0.855	-1.703	4	1
86	280.4	2.88	0.003	-1.304	5	2
87	378.5	2.48	0.899	-1.751	7	2
88	362.5	0.62	1.751	-2.15	6	1
89	280.4	4.67	0.003	-1.304	5	2
90	373.5	1.35	0.708	-1.932	7	2
91	362.5	-1.94	1.751	-2.15	6	1

260	317.5	2.11	2.557	-3.308	3	2
261	317.5	2.11	2.557	-3.308	3	2
262	315.5	2.32	2.453	-3.044	3	2
263	317.5	2.11	2.557	-3.308	3	2
264	317.5	1.35	2.579	-3.458	3	2
265	317.5	1.35	2.579	-3.458	3	2
266	317.5	1.35	2.579	-3.458	3	2
267	329.5	1.84	3.215	-3.259	3	0
268	329.5	1.84	3.215	-3.259	3	0
269	329.5	1.84	3.215	-3.259	3	0
270	329.5	1.84	3.215	-3.259	3	0
271	315.5	1.62	2.816	-3.113	3	1
272	409.5	-5.85	2.729	-3.062	6	1
273	377.5	0.52	4.429	-5.779	4	0
274	363.5	0.50	4.153	-5.465	4	1
275	377.5	0.52	4.429	-5.779	4	0
276	363.5	0.50	4.153	-5.465	4	1
277	377.5	0.52	4.429	-5.779	4	0
278	377.5	0.52	4.429	-5.779	4	0
279	363.5	0.50	4.153	-5.465	4	1
280	359.5	-8.69	2.482	-2.906	5	2
281	401.5	-5.45	2.967	-3.316	6	1
282	553.7	-5.23	4.201	-4.54	9	1
283	327.5	0.44	2.769	-3.082	4	1
284	341.5	-0.91	3.030	-2.897	4	0
285	205.3	0.61	1.573	-2.111	2	0
286	235.3	-0.93	0.155	-1.694	4	1
287	235.3	-0.93	0.155	-1.694	4	1
288	235.3	-0.93	0.155	-1.694	4	1
289	235.3	-0.93	0.155	-1.694	4	1
290	235.3	-0.93	0.155	-1.694	4	1

92	264.4	2.83	0.855	-1.703	4	1
93	362.5	2.41	1.751	-2.15	6	1
94	244.3	1.42	1.509	-1.976	3	0
95	244.3	1.42	1.509	-1.976	3	0
96	403.5	4.82	1.575	-3.796	6	2
97	304.4	3.19	0.414	-1.826	5	2
98	260.3	4.34	0.657	-1.577	4	1
99	260.3	4.34	0.657	-1.577	4	1
100	327.4	-1.54	1.689	-1.62	5	0
101	302.4	4.29	1.141	-1.987	5	0
102	316.4	-4.33	1.440	-2.227	5	0
103	318.4	2.23	0.133	-1.558	6	1
104	258.3	3.73	0.381	-1.349	4	1
105	258.3	3.95	0.359	-1.659	4	0
106	258.3	1.75	0.943	-1.958	4	0
107	260.3	3.50	0.657	-1.577	4	1
108	260.3	-2.25	0.536	0.193	4	0
109	258.3	3.96	0.801	-1.628	4	0
110	234.4	1.45	2.274	-2.12	2	0
111	234.4	1.45	2.274	-2.12	2	0
112	234.4	1.45	2.274	-2.12	2	0
113	234.4	1.45	2.274	-2.12	2	0
114	232.4	0.72	2.351	-2.222	2	0
115	308.5	0.72	3.970	-3.43	2	0
116	308.5	0.72	3.970	-3.43	2	0
117	273.4	-4.01	2.142	-2.755	3	0
118	262.4	2.33	2.923	-2.876	2	0
119	262.4	3.59	2.032	-2.48	3	0
120	373.5	2.69	1.996	-2.508	5	1
121	246.4	2.14	1.784	-2.204	3	0
122	248.4	2.80	1.707	-2.102	3	0

291	235.3	-0.93	0.155	-1.694	4	1
292	235.3	-0.93	0.155	-1.694	4	1
293	235.3	-0.93	0.155	-1.694	4	1
294	251.4	1.51	1.989	-2.579	3	1
295	251.4	1.51	1.989	-2.579	3	1
296	336.5	3.47	2.364	-2.462	4	1
297	336.5	3.47	2.364	-2.462	4	1
298	260.3	-2.68	1.898	-2.637	4	1
299	262.4	-0.68	1.865	-2.456	4	1
300	262.4	-0.46	1.800	-2.292	4	1
301	327.5	0.22	3.422	-3.223	4	0
302	294.4	1.63	-0.199	-1.202	6	1
303	294.4	2.10	-0.199	-1.202	6	1
304	234.3	3.56	1.365	-1.832	3	0
305	439.5	-0.20	3.082	-4.185	7	3
306	439.5	-0.20	3.082	-4.185	7	3
307	439.5	-0.20	3.082	-4.185	7	3
308	437.5	0.68	3.177	-4.469	7	3
309	437.5	-7.66	3.056	-2.699	7	2
310	451.5	-7.66	3.331	-3.013	7	1
311	439.5	-0.20	3.082	-4.185	7	3
312	439.5	-0.20	3.082	-4.185	7	3
313	439.5	-0.20	3.082	-4.185	7	3
314	453.5	-1.00	3.510	-4.313	7	2
315	439.5	-8.23	3.179	-2.564	7	2
316	453.5	-8.23	3.455	-2.878	7	1
317	453.5	-8.23	3.455	-2.878	7	1
318	451.5	0.68	3.453	-4.783	7	2
319	435.5	-1.81	4.305	-5.182	6	1
320	421.5	-1.81	4.029	-4.868	6	2
321	453.5	-0.20	3.358	-4.499	7	2

123	246.4	2.14	1.784	-2.204	3	0
124	246.4	1.49	1.440	-2.326	3	0
125	264.4	3.39	0.884	-1.652	4	1
126	264.4	3.19	0.855	-1.703	4	1
127	264.4	1.33	1.672	-1.991	3	1
128	250.4	2.15	1.422	-1.721	3	1
129	264.4	2.87	1.357	-1.916	4	1
130	262.4	4.14	0.932	-1.805	4	1
131	220.3	0.43	-0.336	1.227	4	0
132	190.2	3.16	0.384	-1.304	3	1
133	204.3	5.06	0.637	-0.942	3	0
134	246.4	1.89	1.952	-1.782	3	0
135	244.3	0.86	1.767	-1.721	3	0
136	262.3	-3.10	1.303	-1.839	5	0
137	230.3	0.92	1.432	-2.161	3	1
138	220.3	3.29	0.136	-1.264	4	1
139	218.3	2.64	0.323	-1.393	4	0
140	220.3	5.57	-0.186	-0.492	4	1
141	248.3	-0.29	-0.016	-1.368	5	0
142	248.3	-2.45	-1.159	-0.717	5	1
143	247.3	4.39	-0.631	-0.793	5	1
144	206.2	3.07	-0.276	-1.082	4	1
145	276.3	2.55	-0.123	-1.035	5	1
146	276.3	2.55	-0.123	-1.035	5	1
147	248.3	-0.04	0.897	-1.539	5	0
148	246.3	4.32	0.932	-1.494	4	0
149	262.3	2.28	0.005	-0.987	5	1
150	345.4	4.93	1.143	-1.469	6	0
151	272.3	3.40	0.198	-1.441	5	0
152	297.4	3.21	0.588	-1.9	5	1
153	347.4	3.99	1.637	-3.083	5	1

322	435.5	-1.81	4.305	-5.182	6	1
323	453.5	-0.20	3.358	-4.499	7	2
324	421.5	-1.81	4.029	-4.868	6	2
325	421.5	-1.81	4.029	-4.868	6	2
326	439.5	-0.20	3.164	-4.692	7	2
327	439.5	-0.20	3.164	-4.692	7	2
328	439.5	-0.20	3.164	-4.692	7	2
329	439.5	-8.23	3.261	-3.071	7	1
330	437.5	-2.23	4.510	-5.554	6	0
331	423.5	-2.20	4.234	-5.24	6	1
332	437.5	-2.23	4.510	-5.554	6	0
333	462.7	-1.70	6.276	-4.67	5	1
334	446.7	-2.23	7.100	-5.12	4	0
335	478.7	-1.70	5.453	-4.22	6	2
336	446.7	-2.23	7.100	-5.12	4	0
337	446.7	-2.23	7.100	-5.12	4	0
338	446.7	-2.23	7.100	-5.12	4	0
339	460.7	-1.15	7.369	-5.28	4	0
340	460.7	-1.15	7.369	-5.28	4	0
341	474.8	-1.15	7.638	-5.44	4	0
342	474.8	-1.15	7.638	-5.44	4	0
343	478.7	-4.31	5.303	-2.501	6	1
344	494.7	-4.23	4.480	-2.051	7	2
345	446.7	-2.23	7.100	-5.12	4	0
346	506.8	-0.64	5.992	-4.54	6	2
347	490.8	-0.64	6.815	-4.99	5	1
348	492.7	-0.64	5.722	-4.38	6	2
349	478.7	-1.70	5.453	-4.22	6	2
350	492.7	-0.64	5.722	-4.38	6	2
351	446.7	-2.23	7.100	-5.12	4	0
352	476.7	-0.64	6.546	-4.83	5	1

154	368.4	-0.86	-2.338	-0.658	9	4
155	288.3	1.73	0.788	-1.686	5	0
156	192.2	4.79	-0.402	-1.183	4	2
157	208.3	1.69	0.836	-1.068	3	0
158	194.3	-0.35	0.583	-1.43	3	1
159	371.5	-0.62	2.458	-2.712	5	0
160	248.4	-2.60	1.965	-1.847	3	0
161	234.3	-2.95	1.631	-2.287	3	1
162	194.3	3.35	1.402	-1.086	2	0
163	222.3	-0.81	0.522	-1.519	4	0
164	208.3	1.69	0.836	-1.068	3	0
165	296.4	-0.78	-0.541	-2.071	5	2
166	220.4	-1.06	2.197	-2.305	2	1
167	230.3	2.07	1.298	-2.283	3	1
168	232.3	1.26	1.221	-2.181	3	1
169	246.4	1.62	1.556	-1.741	3	0
170	194.3	2.62	0.583	-1.43	3	1
171	248.4	0.11	1.965	-1.847	3	0
172	246.4	2.88	1.474	-1.819	3	0
173	248.4	-1.35	1.884	-1.925	3	0
174	169.3	-2.45	1.212	-1.45	2	1
175	169.3	-2.45	1.212	-1.45	2	1
176	208.3	1.78	1.135	-1.912	3	1
177	185.3	0.83	0.360	-1.051	3	2
178	183.3	2.70	1.640	-1.885	2	1
179	167.3	1.63	2.463	-2.335	1	0
180	250.4	1.11	3.010	-3.124	2	1
181	266.4	-3.24	2.036	-0.955	3	1
182	166.3	-4.14	1.920	-2.212	1	0
183	224.4	-7.09	2.132	-2.731	2	1
184	167.3	1.45	1.485	-1.827	2	0

353	446.7	-2.23	7.100	-5.12	4	0
354	462.7	-1.70	6.276	-4.67	5	1
355	478.7	-1.70	5.453	-4.22	6	2
356	494.7	-4.23	4.480	-2.051	7	2
357	510.7	-7.65	3.506	0.118	8	2
358	460.7	-1.15	7.369	-5.28	4	0
359	476.7	-0.64	6.546	-4.83	5	1
360	462.7	-0.85	6.248	-4.721	5	1
361	462.7	-1.70	6.276	-4.67	5	1
362	474.8	-1.15	7.638	-5.44	4	0
363	474.8	-1.15	7.638	-5.44	4	0
364	470.7	-0.68	6.527	-5.12	4	0
365	470.7	-0.68	6.527	-5.12	4	0
366	470.7	-0.68	6.527	-5.12	4	0
367	470.7	-0.68	6.527	-5.12	4	0
368	470.7	-0.68	6.527	-5.12	4	0
369	470.7	-0.68	6.527	-5.12	4	0
370	514.6	1.93	1.307	-3.003	8	0
371	502.6	4.07	1.112	-2.238	8	1
372	516.6	2.72	1.566	-2.508	8	1
373	518.6	3.25	1.196	-2.466	9	0
374	530.6	2.22	1.399	-2.508	9	0
375	504.6	3.25	0.742	-2.196	9	0
376	534.6	0.65	0.899	-2.177	10	0
377	533.7	-4.19	1.481	-3.916	8	0
378	533.7	-4.19	1.481	-3.916	8	0
379	492.7	0.08	2.935	-3.946	6	0
380	492.7	0.08	2.935	-3.946	6	0
381	496.7	0.47	3.612	-4.166	6	1
382	490.7	4.78	2.949	-3.378	6	0
383	490.7	2.06	2.652	-3.266	6	0

185	167.3	1.45	1.485	-1.827	2	0	**384**	490.7	3.05	2.291	-3.127	6	0
186	196.3	0.39	1.027	-1.672	3	1	**385**	508.7	1.54	1.593	-1.186	7	0
187	347.5	-16.13	5.736	-4.538	3	0	**386**	492.7	4.12	2.566	-3.355	6	0
188	305.5	-15.64	5.252	-4.128	2	1	**387**	393.6	0.47	3.655	-4.487	4	1
189	319.5	-8.45	4.827	-3.998	3	0	**388**	393.6	0.47	3.655	-4.487	4	1
191	235.4	-2.78	3.213	-2.416	2	1	**389**	494.7	3.32	5.724	-5.302	4	0
192	217.4	-0.54	3.195	-3.241	1	0	**390**	510.7	1.32	4.384	-4.219	5	0
193	195.3	-2.09	3.427	-3.093	1	0	**391**	510.7	3.72	5.373	-5.116	5	1
194	207.4	-2.13	3.641	-3.084	1	0	**392**	526.7	2.46	5.023	-4.93	6	2
195	231.4	-0.75	3.649	-3.511	1	0	**393**	494.7	3.32	5.724	-5.302	4	0
196	231.4	-0.75	3.649	-3.511	1	0	**394**	510.7	1.32	4.384	-4.219	5	0
197	235.4	-8.60	4.550	-3.624	1	0	**395**	494.7	3.32	5.724	-5.302	4	0
198	280.5	-1.86	4.029	-2.808	2	0	**396**	510.7	1.32	4.384	-4.219	5	0
199	262.4	-1.54	0.808	-1.985	4	2	**397**	510.7	3.72	5.373	-5.116	5	1

MW = molecular weight; d = druglikeness score; cLogP = logarithmic partition coefficient between *n*-octanol and water, i.e., $Log(C_{n\text{-}octanol}/C_{water})$; cLogS = logarithmic water solubility (M); *H*-A = hydrogen acceptors; *H*-D = hydrogen donnors.

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