

Table S1. The docking scores of 158 compounds with tyrosinase and adenylate cyclase.

NO.	Compound	Formula	Binding Energy (kcal/mol)	
			Tyrosinase	Adenylate cyclase
1	dactylorhin A	C ₄₀ H ₅₆ O ₂₂	4.6	-6.3
2	gymnoside I	C ₂₁ H ₃₀ O ₁₁	-5.3	-8.9
3	gymnoside II	C ₂₁ H ₃₀ O ₁₁	-7.8	-8.1
4	gymnoside V	C ₄₉ H ₆₂ O ₂₃	-8.5	-8.8
5	gymnoside IX	C ₅₁ H ₆₄ O ₂₄	23.7	-4.8
6	gymnoside X	C ₅₁ H ₆₄ O ₂₄	-	-
7	militarine	C ₃₄ H ₄₆ O ₁₇	-	-
8	bletilnoside A	C ₃₈ H ₆₂ O ₁₂	-4.2	-8.5
9	bletilnoside B	C ₃₈ H ₆₀ O ₁₂	3.8	-3.8
10	3-O-β-D-glucopyranosyl-3-epiruscogenin	C ₄₁ H ₆₀ O ₁₂	3.5	-4.3
11	3-O-β-D-glucopyranosyl-3-epineoruscogenin	C ₄₁ H ₅₈ O ₁₂	26.4	-7
12	dancosterol	C ₃₅ H ₆₀ O ₆	24.4	-5.1
13	2,7-dihydroxy-4-methoxyphenanthrene-2-O-glucoside	C ₂₁ H ₂₂ O ₈	-5.2	-7.1
14	2,7-dihydroxy-4-methoxyphenanthrene-2,7-O-diglucoside	C ₂₇ H ₃₂ O ₁₃	-9.0	-10.0
15	3,7-dihydroxy-2,4-dimethoxyphenanthrene-3-O-glucoside	C ₂₂ H ₂₄ O ₉	-0.7	-8.5
16	gastrodin	C ₁₃ H ₁₈ O ₇	-9.4	-8.7
17	2,7-dihydroxy-1-(4'-hydroxybenzyl)-9,10-dihydrophenanthrene-4'-O-glucoside	C ₂₈ H ₃₀ O ₉	-7.1	-6.7
18	3'-hydroxy-5-methoxybibenzyl-3-O-β-D-glucopyranoside	C ₂₁ H ₂₆ O ₈	-7.0	-11.3
19	blestritin A	C ₃₇ H ₃₆ O ₆	-8.8	-9.6
20	blestritin B	C ₃₀ H ₃₀ O ₆	-3.6	-10.1
21	blestritin C	C ₃₆ H ₃₄ O ₆	-4.9	-10.0
22	bulbocodin	C ₃₆ H ₃₄ O ₆	-4.6	-10.5
23	bulbocodin C	C ₂₉ H ₂₈ O ₅	-9.1	-11.1
24	bulbocodin D	C ₂₉ H ₂₈ O ₅	-9.3	-9.7
25	bulbocol	C ₂₃ H ₂₄ O ₄	-9.2	-10.1
26	gymconopin D	C ₂₃ H ₂₄ O ₄	-9	-9.7
27	shancigusin B	C ₂₈ H ₂₆ O ₅	-8.9	-9.6
28	shanciguol	C ₂₈ H ₂₆ O ₅	-6.2	-10.1
29	arundinan	C ₂₂ H ₂₂ O ₃	-8.2	-10
30	arundin	C ₂₉ H ₂₈ O ₄	-8.7	-9.5
31	batatasin III	C ₁₅ H ₁₆ O ₃	-7.2	-10.2

32	gigantol	C ₁₆ H ₁₈ O ₄	-8.2	-8.6
33	3,4'-dihydroxy-5,3',5'-trimethoxybibenzyl	C ₁₇ H ₂₀ O ₅	-8.4	-8.2
34	3,3'-dihydroxy-5,4'-dimethoxybibenzyl	C ₁₆ H ₁₈ O ₄	-8.3	-8.3
35	3'-O-methylbatatasin III	C ₁₅ H ₁₈ O ₃	-8.5	-8.2
36	3,3'-dihydroxy-4-(p-hydroxybenzyl)-5-methoxybibenzyl	C ₂₂ H ₂₂ O ₄	-8.2	-8.6
37	3,3'-dihydroxy-2-(p-hydroxybenzyl)-5-methoxybibenzyl	C ₂₂ H ₂₂ O ₄	-8.5	-9.7
38	3',5-dihydroxy-2-(p-hydroxybenzyl)-3-methoxybibenzyl	C ₂₂ H ₂₂ O ₄	-8.9	-9.5
39	2',6'-bis(p-hydroxybenzyl)-5-methoxybibenzyl-3,3'-diol	C ₃₃ H ₃₆ O ₅	-9.0	-9.8
40	2,6-bis(p-hydroxybenzyl)-5,3'-dimethoxybibenzyl-3-ol	C ₃₀ H ₃₀ O ₅	-7.5	-10.4
41	3,3'-dihydroxy-5-methoxy-2,5',6-tris(p-hydroxybenzyl) bibenzyl	C ₄₆ H ₄₄ O ₁₁	-6.9	-10.2
42	3,3',5-trimethoxybibenzyl	C ₁₇ H ₂₀ O ₃	-4.3	-11.6
43	3,5-dimethoxybibenzyl	C ₁₆ H ₁₈ O ₂	-8.0	-8.5
44	5-hydroxy-4-(p-hydroxybenzyl)-3',3-dimethoxybibenzyl	C ₂₃ H ₂₄ O ₄	-7.6	-8.4
45	3,3'-dihydroxy-5-methoxybibenzyl	C ₁₅ H ₁₆ O ₃	-8.5	-9.7
46	5-hydroxy-2-(p-hydroxybenzyl)-3-methoxybibenzyl	C ₂₂ H ₂₂ O ₃	-8.2	-8.6
47	4-methoxyphenanthrene-2,7-diol	C ₁₅ H ₁₂ O ₃	-8.8	-9.6
48	3,4-dimethoxyphenanthrene-2,7-diol	C ₁₆ H ₁₄ O ₄	-8.6	-9.0
49	2,4-dimethoxyphenanthrene-3,7-diol	C ₁₆ H ₁₄ O ₄	-8.4	-8.3
50	3,5-dimethoxyphenanthrene-2,7-diol	C ₁₆ H ₁₄ O ₄	-8.1	-9.2
51	1,5-dimethoxyphenanthrene-2,7-diol	C ₁₆ H ₁₄ O ₄	-7.5	-8.3
52	2,4-dimethoxyphenanthrene-7-ol	C ₁₅ H ₁₄ O ₃	-8.7	-8.5
53	2,4,7-trimethoxyphenanthrene	C ₁₇ H ₁₆ O ₃	-8.1	-9.0
54	2,3,4,7-tetramethoxyphenanthrene	C ₁₈ H ₁₈ O ₄	-7.5	-8.9
55	2,3,4,7-tetramethoxyphenanthrene	C ₁₈ H ₁₈ O ₄	-7.2	-8.1
56	1,8-bis(p-hydroxybenzyl)-4-methoxyphenanthrene-2,7-diol	C ₂₉ H ₂₄ O ₅	-10.2	-10.7
57	1-(p-hydroxybenzyl)-4,8-dimethoxyphenanthrene-2,7-diol	C ₂₃ H ₂₀ O ₅	-9.2	-9.1
58	1-(p-hydroxybenzyl)-4-methoxyphenanthrene	C ₂₂ H ₁₈ O ₄	-9.5	-10.5

	ne-2,7-diol			
59	2-hydroxy-4,7-dimethoxyphenanthrene	C ₁₆ H ₁₄ O ₃	-7.5	-8.7
60	3,7-dihydroxy-2,4,8-trimethoxyphenanthrene	C ₁₇ H ₁₆ O ₅	-8.4	-7.8
61	2,7-dihydroxy-3,4-dimethoxyphenanthrene	C ₁₆ H ₁₄ O ₄	-8.4	-8.3
62	1-(p-hydroxybenzyl)-4,7-dimethoxyphenanthrene-2-ol	C ₂₃ H ₂₀ O ₄	-9.0	-10.5
63	1-(p-hydroxybenzyl)-4,7-dimethoxyphenanthrene-2,8-diol	C ₂₃ H ₂₀ O ₅	-8.4	-9.4
64	1-(p-hydroxybenzyl)-4,7-dimethoxyphenanthrene-2,6-diol	C ₂₃ H ₂₀ O ₅	-9.1	-10.2
65	bleformin B	C ₂₃ H ₂₀ O ₅	-9.3	-8.7
66	blespirol	C ₂₅ H ₁₈ O ₅	-6.1	-10.3
67	1,8-dihydroxy-3-methoxy-6-methylanthracene-9,10-dione	C ₁₆ H ₁₂ O ₅	-9.3	-9.0
68	2-methylanthraquinone	C ₁₅ H ₁₀ O ₂	-9.0	-10.4
69	4,7-dimethoxyphenanthrene-1,2-dione	C ₁₆ H ₁₃ O ₄	-7.7	-9.0
70	7-hydroxy-2-methoxyphenanthrene-3,4-dione	C ₁₅ H ₁₃ O ₄	-9.1	-9.9
71	3',7',7'-trihydroxy-2,2',4'-trimethoxy-[1,8'-biphenanthrene]-3,4-dione	C ₃₁ H ₂₃ O ₈	2.2	-8.5
72	blestrin A	C ₃₀ H ₂₆ O ₆	-6.9	-11.1
73	blestrin B	C ₃₀ H ₂₆ O ₆	-9.6	-11.9
74	blestrin C	C ₃₀ H ₂₄ O ₆	-6.9	-11.2
75	blestrin D	C ₃₀ H ₂₄ O ₆	-10	-12.1
76	blestriarene A	C ₃₀ H ₂₆ O ₆	-5.0	-7.1
77	blestriarene B	C ₃₀ H ₂₄ O ₆	-3.9	-7.9
78	blestriarene C	C ₃₀ H ₂₂ O ₆	-5.3	-9.5
79	blestrianol A	C ₃₀ H ₂₆ O ₆	-5.4	-10.2
80	blestrianol B	C ₃₇ H ₃₂ O ₇	0.2	-10.6
81	blestrianol C	C ₃₇ H ₃₀ O ₇	4.6	-8.0
82	4,7,3'5'-tetramethoxy-9',10'-dihydro-[1,2'-biphenanthrene]-2,7'- diol	C ₃₂ H ₂₇ O ₆	6.5	-9.8
83	4,7,7'-trimethoxy-9',10'-dihydro-[1,3'-biphenanthrene]-2,2',5'- triol	C ₃₁ H ₂₅ O ₆	0.8	-8.6
84	4,7,4'-trimethoxy-9',10'-dihydro-[1,1'-biphenanthrene]-2,2',7'- triol	C ₃₁ H ₂₅ O ₆	-3.4	-8.2

85	4,7,3',5'-tetramethoxy-9',10'-dihydro-[1,1'-biphenanthrene]-2,2',7'-triol	C ₃₂ H ₂₇ O ₇	-2.7	-8.5
86	4,8,4',8'-tetramethoxy-[1,1'-biphenanthrene]-2,7,2',7'-tetrol	C ₃₂ H ₂₆ O ₈	1.1	-7.4
87	bleformin D	C ₃₇ H ₃₂ O ₇	3.7	-8.5
88	4,4'-dimethoxy-9,10-dihydro-[6,1'-biphenanthrene]-2,7,2',7'-tetraol	C ₃₀ H ₂₄ O ₆	-5.5	-10.9
89	gymconopin C	C ₃₀ H ₂₆ O ₆	-5.3	-10.9
90	4,7-dihydroxy-2-methoxy-9,10-dihydrophenanthrene	C ₁₅ H ₁₄ O ₃	-8.8	-9.2
91	2,7-dihydroxy-3-(p-hydroxybenzyl)-4-methoxy-9,10dihydrophenanthrene	C ₂₂ H ₂₀ O ₄	-9.3	-10.2
92	4,7-dihydroxy-1-(p-hydroxybenzyl)-2-methoxy-9,10dihydrophenanthrene	C ₂₂ H ₂₀ O ₄	-9.7	-9.6
93	2,7-dihydroxy-1,6-bis(p-hydroxybenzyl)-4-methoxy-9,10dihydrophenanthrene	C ₂₉ H ₂₆ O ₅	-9.7	-9.6
94	2,7-dihydroxy-1,3-bis(p-hydroxybenzyl)-4-methoxy-9,10dihydrophenanthrene	C ₂₉ H ₂₆ O ₅	-6.8	-10.2
95	2,7-dihydroxy-1-(p-hydroxybenzyl)-4-methoxy-9,10dihydrophenanthrene	C ₂₂ H ₂₀ O ₄	-8.8	-10.8
96	2,4,7-trimethoxy-9,10-dihydrophenanthrene	C ₁₇ H ₁₈ O ₃	-7.3	-8.9
97	2,7-dihydroxy-4-methoxy-9,10-dihydrophenanthrene	C ₁₅ H ₁₄ O ₃	-8.6	-8.8
98	4,5-dihydroxy-2-methoxy-9,10-dihydrophenanthrene	C ₁₅ H ₁₄ O ₃	-8.2	-9.1
99	2,8-dihydroxy-4,7-dimethoxy-9,10-dihydrophenanthrene	C ₁₅ H ₁₄ O ₃	-8.7	-8.3
100	2,8-dihydroxy-1-(p-hydroxybenzyl)-4,7-dimethoxy-9,10dihydrophenanthrene	C ₂₃ H ₂₂ O ₅	-8.3	-9.5

101	pleionesin C	C ₂₇ H ₂₆ O ₇	-7.6	-9.3
102	(2,3-trans)-2-(4-hydroxy-3-methoxyphenyl)-3-hydroxymethyl-10-methoxy-2,3,4,5-tetrahydro-phenanthro[2,1-b]furan-7-ol	C ₂₅ H ₂₄ O ₆	-8.5	-9.7
103	bleochranol A	C ₄₀ H ₃₈ O ₈	4.5	-8.6
104	bleochranol B	C ₂₅ H ₂₄ O ₆	-9.3	-9.9
105	bleochranol C	C ₃₃ H ₃₂ O ₈	-2.3	-9.6
106	bleochranol D	C ₃₄ H ₃₂ O ₈	-3.9	-9.6
107	(2,3-trans)-3-[2-hydroxy-6-(3-hydroxyphenethyl)-4-methoxybenzyl]-2-(4-hydroxy-3-methoxyphenyl)-10-methoxy-2,3,4,5-tetrahydrophenanthro[2,1-b]furan-7-ol	C ₁₇ H ₁₈ O ₄	19.4	-9.0
108	shanciol	C ₂₅ H ₂₄ O ₆	-5.8	-10.6
109	bletlos A	C ₂₈ H ₂₈ O ₈	-3.1	-7.6
110	bletlos B	C ₂₇ H ₂₆ O ₇	-3.9	-9.3
111	bletlos C	C ₂₇ H ₂₆ O	-6.1	-9.5
112	blestriaren A	C ₃₀ H ₂₆ O ₆	-4.7	-7.7
113	Bletilla anthocyanin 1	C ₇₅ H ₈₁ O ₄₀	106.3	16.6
114	Bletilla anthocyanin 2	C ₇₂ H ₇₉ O ₃₇	99.9	29.7
115	Bletilla anthocyanin 3	C ₇₅ H ₈₁ O ₄₃	112.7	46.7
116	Bletilla anthocyanin 4	C ₇₂ H ₇₉ O ₄₀	106.3	36.6
117	3-O-(β-glucopyranoside)-7-O-[6-O-(4-O-(6-O-(4-O-(β-glucopyranosyl)-trans-caffeoyl)-β-glucopyranosyl)-trans-caffeoyl)β-glucopyranoside]	C ₅₇ H ₆₃ O ₃₂	77.0	6.5
118	β-sitosterol	C ₂₉ H ₅₀ O	-5.4	-9.6
119	β-sitosterol palmitate	C ₄₅ H ₈₀ O ₂	0.8	-6.8
120	stigmasterol	C ₂₉ H ₄₈ O	-4.6	-10.5
121	stigmasterol palmitat	C ₄₅ H ₇₈ O ₂	4.4	-6.5
122	3-epiruscogenin	C ₂₇ H ₄₂ O ₄	-0.4	-9.2
123	3-epineoruscogenin	C ₂₇ H ₄₀ O ₄	-0.8	-7.3
124	(20S,22R)-1β,2β,3β,4β,5β,7α-hexahydroxypirost-25(27)-en-6-one	C ₂₇ H ₃₅ O ₉	4.3	-6.2
125	(1α,3α)-1-O-[(β-D-xylopyranosyl-(1→2)-α-L-rhamnopyranosyl)]-3-O-D-glucopyranosyl-5α-spirostan	C ₄₄ H ₇₁ O ₁₇	43.2	-5.9
126	(1α,3α)-1-O-[(β-D-xylopyranosyl-(1→2)-α-L-rhamnopyranosyl)oxy]-3-O-D-glucopyranosyl-25(27)-ene-5α-spirostan	C ₄₄ H ₆₉ O ₁₇	44.5	-2.4

127	(1 α ,3 α)-1-O-[(β -D-xylopyranosyl-(1 $\rightarrow$ 2)- α -L-rhamnopyranosyl)oxy]-epiruscogenin	C ₃₈ H ₅₉ O ₁₂	48.6	-2.1
128	(1 α ,3 α)-1-O-[(β -D-xylopyranosyl-(1 $\rightarrow$ 2)- α -L-rhamnopyranosyl)oxy]-epineoruscogenin	C ₃₈ H ₅₇ O ₁₂	35.5	-3.4
129	cyclomargenol	C ₃₂ H ₅₄ O	-0.7	-8.0
130	cyclomargenone	C ₃₂ H ₅₃ O	-0.6	-8.2
131	cycloneolitsol	C ₃₂ H ₅₄ O	-0.7	-9.0
132	cyclobalanone	C ₃₂ H ₅₃ O	0.8	-8.1
133	24-methylenecycloartanol palmitate	C ₄₇ H ₈₁ O ₂	7.7	-6.7
134	cyclolaudenol	C ₃₁ H ₅₁ O	-1.4	-8.5
135	cyclolaudenone	C ₃₁ H ₅₀ O	0.5	-9.4
	3 β -hydroxyoleane-12-en-28-oic acid			
136	3-O- α -L-rhamnopyranosyl-(1 $\rightarrow$ 2)- β -D-glucopyranoside	C ₄₁ H ₅₅ O ₁₂	13.7	-1.7
137	p-hydroxybenzoic acid	C ₇ H ₆ O ₃	-5.9	-6.0
138	protocatechuic acid	C ₇ H ₆ O ₄	-6.3	-6.1
139	cinnamic acid	C ₉ H ₈ O ₂	-6.5	-7.0
140	caffeic acid	C ₉ H ₈ O ₄	-6.8	-7.0
141	2-hydroxysuccinic acid	C ₄ H ₅ O ₅	-5.2	-4.4
142	palmitic acid	C ₁₆ H ₃₂ O ₂	-5.7	-6.7
143	syringaresinol	C ₂₂ H ₂₆ O ₈	-9.0	-8.5
144	pinoresinol	C ₂₀ H ₂₂ O ₆	-9.2	-9.4
145	3''-methoxynyasol	C ₁₈ H ₁₇ O ₃	-8.5	-8.9
146	p-hydroxybenzaldehyde	C ₇ H ₆ O ₂	-5.6	-5.4
147	ferulic acid	C ₁₀ H ₁₀ O ₄	-6.7	-7.0
148	3-hydroxycinnamic acid	C ₉ H ₈ O ₃	-6.7	-6.9
149	4-hydroxybenzylamine	C ₇ H ₉ NO	-5.5	-5.4
150	4,4'-dihydroxydiphenylmethane	C ₁₃ H ₁₂ O ₂	-7.3	-7.7
151	4,4'-dihydroxybenzyl sulfide	C ₁₄ H ₁₄ SO ₂	-7.2	-8
152	5-(hydroxymethyl)-2-furaldehyde	C ₆ H ₆ O ₃	-5.8	-5.2
153	striatolide	C ₁₈ H ₃₀ O ₃	-7.2	-8.4
154	schizandrin	C ₂₄ H ₃₂ O ₇	-1.3	-7.0
155	brugnanin	C ₅₆ H ₉₀ O ₈	13.0	-5.5
156	bletillanol A	C ₁₈ H ₂₁ O ₅	-8.4	-8.3
157	bletillanol B	C ₁₈ H ₂₀ O ₅	-8.2	-7.6
158	tupichinol A	C ₁₇ H ₁₈ O ₄	-8.2	-8.0
	mimosine		-6.4	
	LER1			-8.5