Supplementary Information (SI)

A theoretical screening of phytochemical constituents from Millettia Brandisiana as inhibitors against acetylcholinesterase

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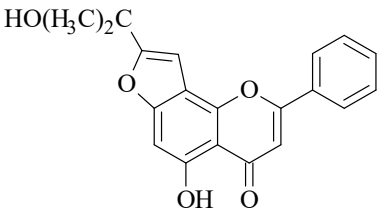
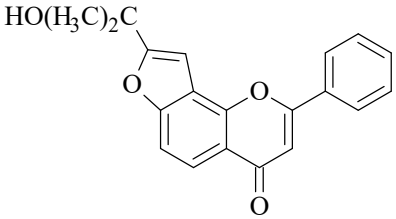
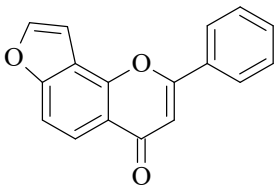
[5] *Faculty of Applied Technology, School of Technology, Van Lang University, Ho Chi Minh City, Vietnam*



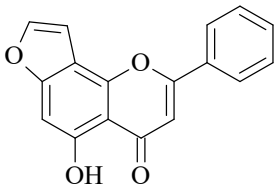
brandisianones A
(1)



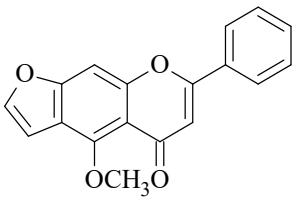
brandisianones B
(2)



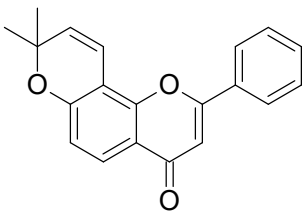
lanceolatin B
(3)



pongaglabol
(4)

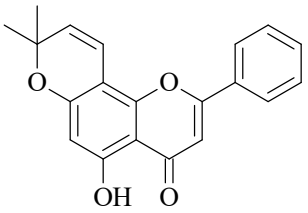


pinnatin
(5)



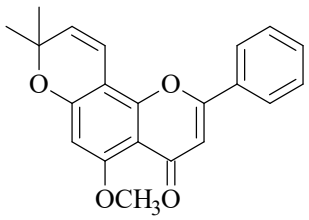
6″,6″−dimethylchromeno−[2″,3″:7,8]−flavone
(6)

Supplementary Information (SI)



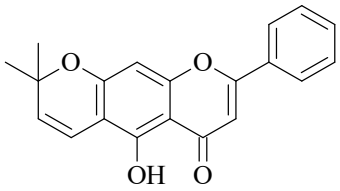
candidine

(**7**)



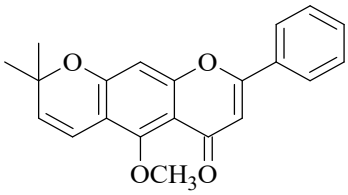
5−methoxy−6″,6″−dimethylchromeno−[2″,3″:7,8]−flavone

(**8**)



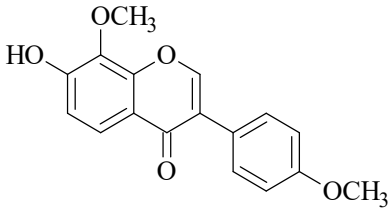
5−hydroxy−6″,6″−dimethylchromeno[2″,3″:7,6]−flavone

(**9**)



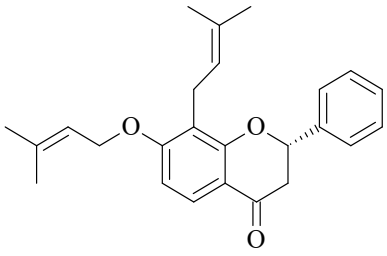
5−methoxy−6″,6″−dimethylchromeno−[2″,3″:7,6]−flavone

(**10**)



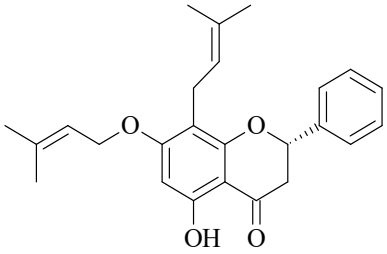
7−hydroxy−8,4′−dimethoxyisoflavone

(**11**)



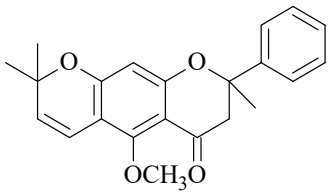
brandisianones C

(12)



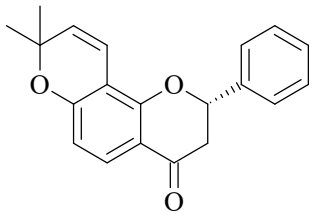
7−o−8−bis−(3,3−dimethylallyl)−5−hydroxyflavanone

(**13**)



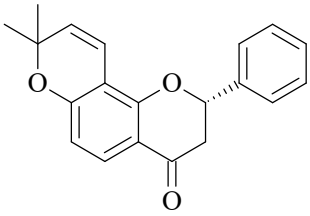
brandisianones D

(14)



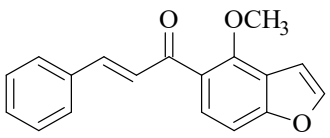
(−)−isolonchocarpin

(**15**)



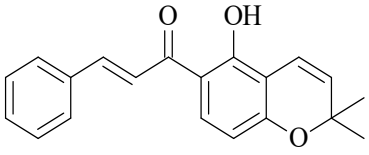
obovatin

(**16**)



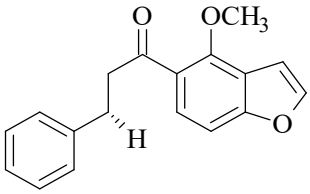
ovalitenin A

(**17**)



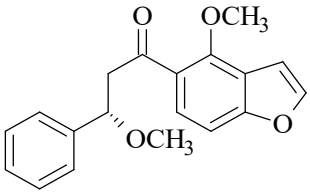
lonchocarpine

(**18**)



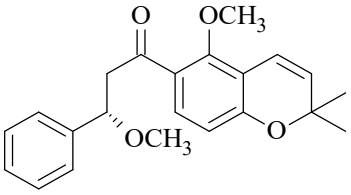
2′−methoxyfurano−[2″,3″:4′,3′] –dihydrochalcone

(**19**)



ovalitenin B

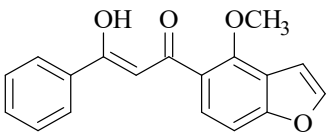
(**20**)



brandisianones E

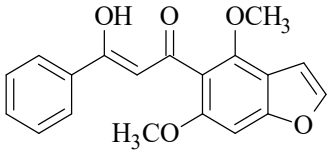
(21)

Supplementary Information (SI)



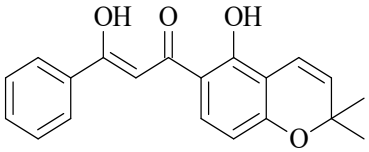
pongamol

(**22**)



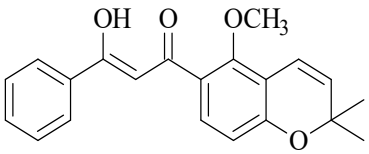
2′,6′−dimethoxyfurano−[2″,3″:4′,3′]−*β*−hydroxydihydrochalcone

(**23**)



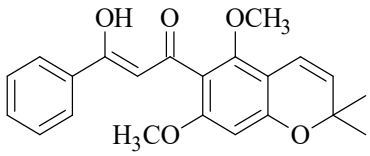
2′−hydroxy−6″,6″−dimethylchromeno−[2″,3″:4′,3′]−*β*−hydroxychalcone

(**24**)



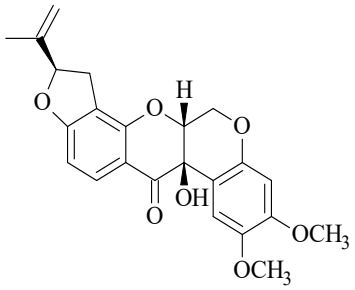
2′−methoxy−6″,6″−dimethylchromeno−[2″,3″:4′,3′]−*β*−hydroxychalcone

(**25**)



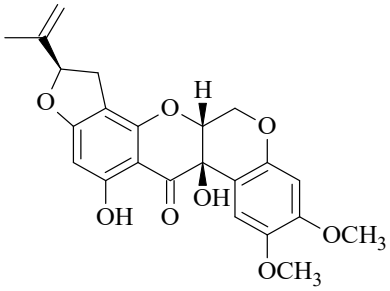
praecansone B

(**26**)



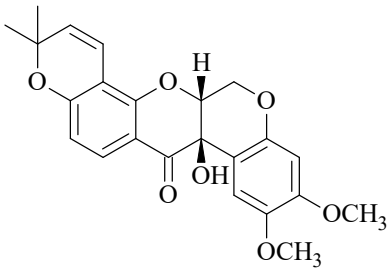
(−)−12*α*−hydroxyrotenone

(**27**)



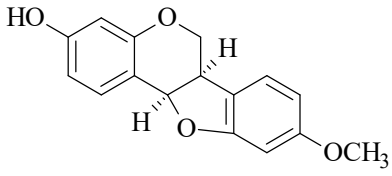
(−)−villosinol

(**28**)



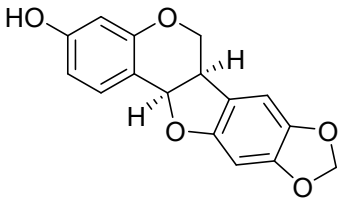
(−)−tephrosin

(**29**)



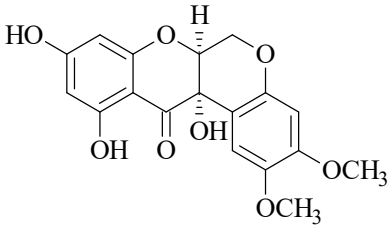
(−)−medicarpin

(**30**)



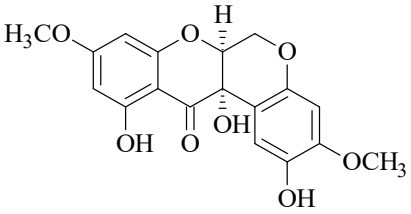
(−)−maackiain

(**31**)



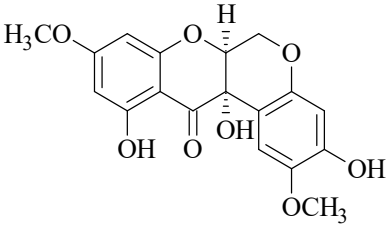
(−)−(6as,12as)−millettiabrandisin A

(**32**)



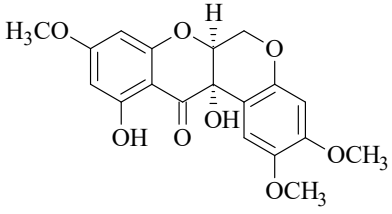
(–)−(6as,12as)−millettiabrandisins B

(33)



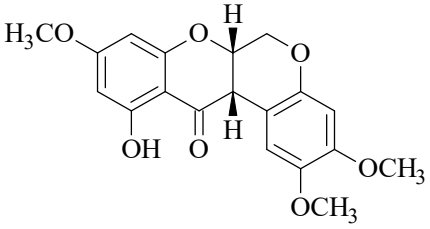
(–)−(6as,12as)− millettiabrandisins C

(**34**)



(–)−(6as,12as)−6−deoxyclitoriacetal

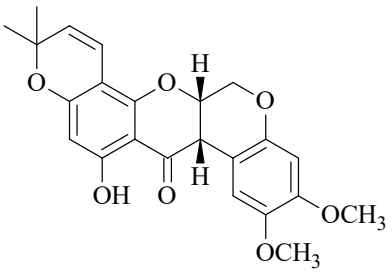
(**35**)



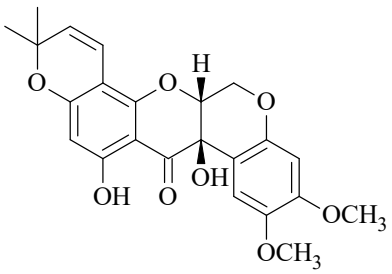
sermundone

(**36**)

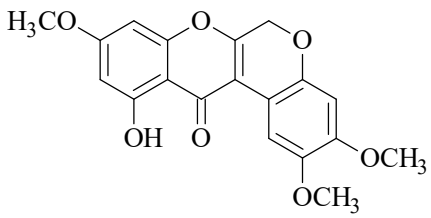
Supplementary Information (SI)



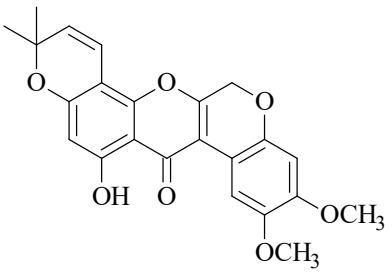
α−toxicarol)
(**37**)



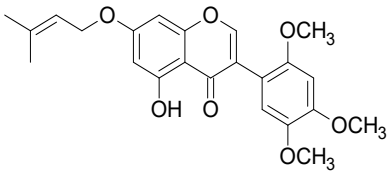
(–)−(6ar,12ar)−12a−hydroxy−α−toxicarol
(**38**)



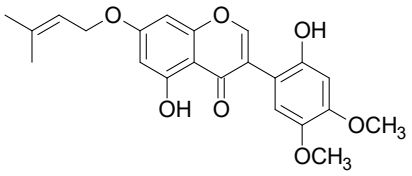
6a,12a−dehydrosurmundone
(**39**)



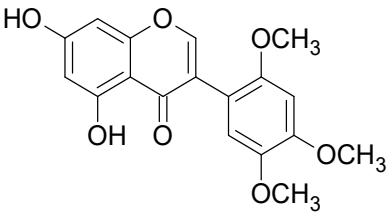
6a,12a−dehydro−α−toxicarol
(**40**)



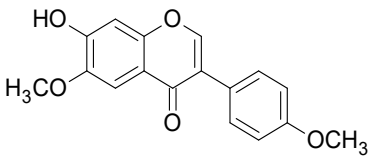
millettiabrandisins D
(**41**)



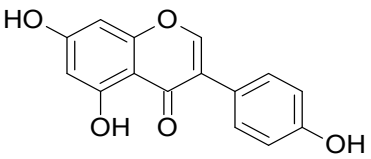
millettiabrandisins E
(**42**)



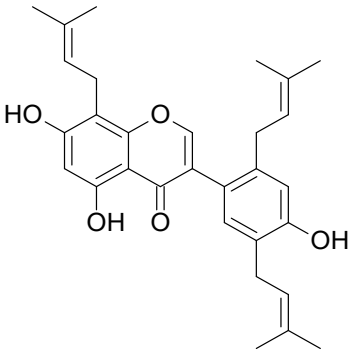
7−demethylrobustigenin
(**43**)



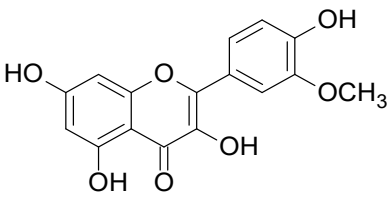
afrormosin
(**44**)



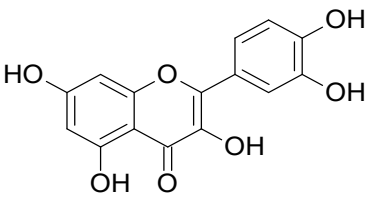
genistein
(**45**)



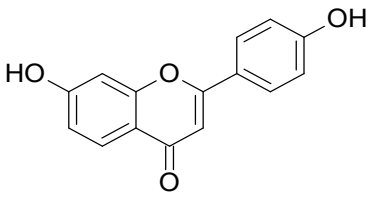
flemiphyllin
(**46**)



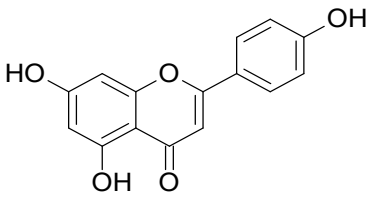
isothamnetin
(**47**)



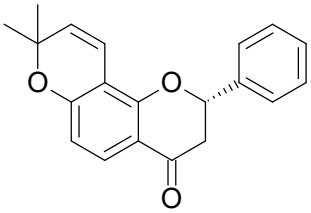
quercetin
(**48**)



4′,7−dihydroxyflavone
(**49**)

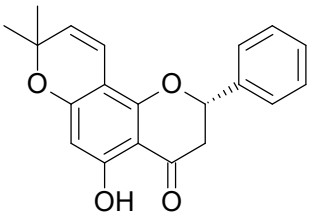


apigenin
(**50**)



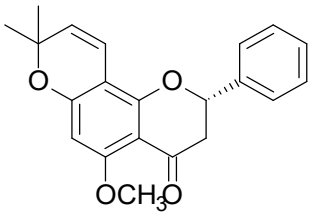
isolonchocarpin
(**51**)

Supplementary Information (SI)



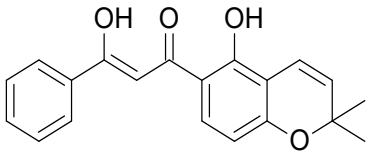
obovatin

(**52**)



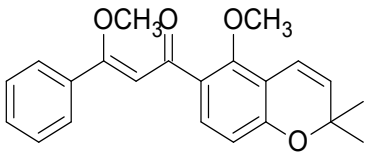
pongachin

(**53**)



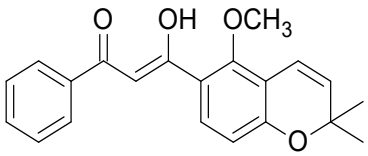
(2z)−3−hydroxy−1−(5−hydroxy−2,2−dimethyl−2h−1−benzopyran−6−yl)−3−phenylprop−2−en−1−one

(**54**)



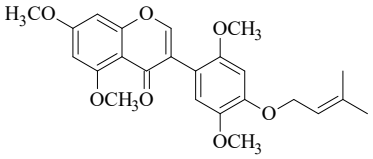
(e)−2′−methoxy−6″,6″−dimethylchromeno−[2″,3″:4′,3’]− 7−methoxychalcone

(**55**)



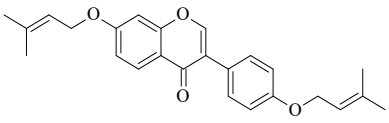
purpurenone

(**56**)



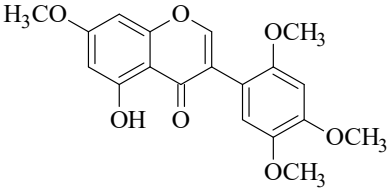
4−γ, γ−dimethylallyloxy−5,7,2,5−tetramethoxyisoflavone

(**57**)



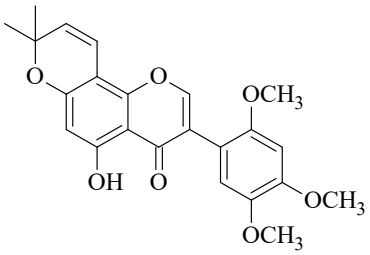
7,4−di−o−prenylgenistein

(**58**)



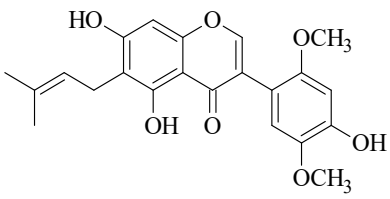
robustigenin

(**59**)



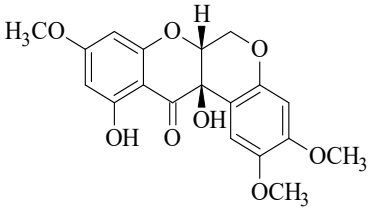
toxicarol isoflavone

(**60**)



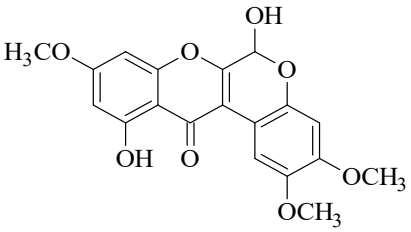
viridiflorin

(**61**)



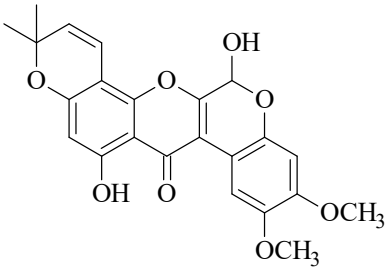
6−deoxyclitoriacetal

(**62**)



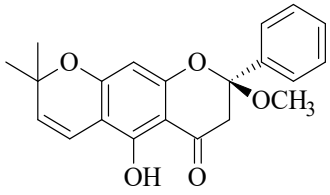
stemonal

(**63**)



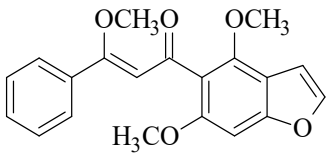
6−hydroxy−6a,12a− dehydro−a−toxicarol

(**64**)



brandisianone F

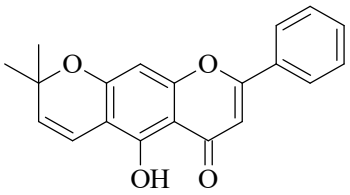
(**65**)



brandisianone G

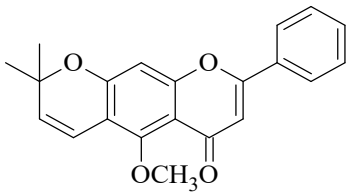
(**66**)

Supplementary Information (SI)



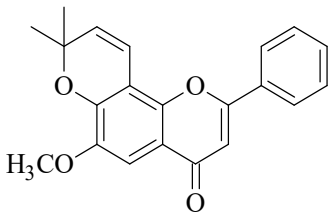
5−hydroxy−6",6"−dimethyl chromeno−[2",3":7,6]−flavone

(**67**)



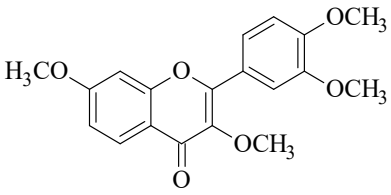
5−methoxy−6",6"−dimethylchromeno−[2",3":7,6]−flavone

(**68**)



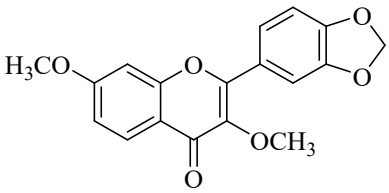
6−methoxy−6",6"−dimethylpyrano−[2",3":7,8]flavone

(**69**)



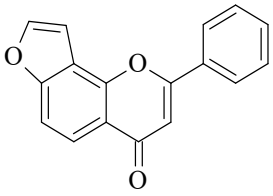
3,3',4',7−tetra−o−methylfisetin

(**70**)



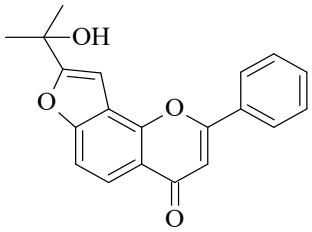
desmethoxykanugin

(**71**)



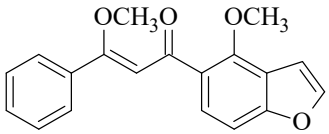
lancelatin B

(**72**)



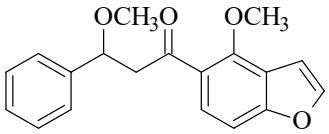
brandisianone B

(**73**)



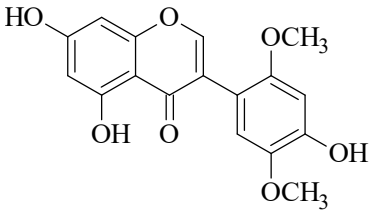
o−methylpongamol

(**74**)



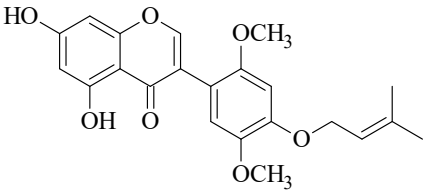
ovalitenin B

(**75**)



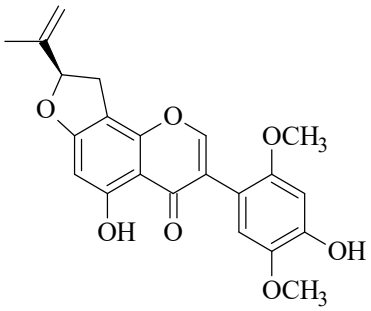
brandisianin A

(**76**)



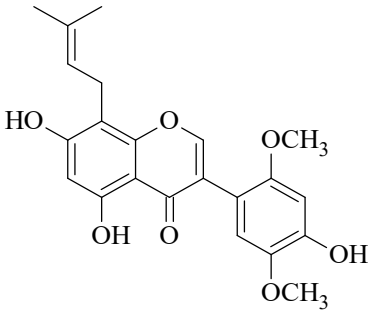
olibergin A

(**77**)



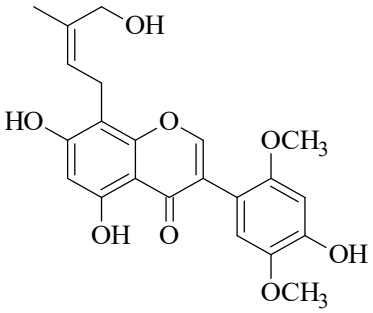
brandisianin B

(**78**)



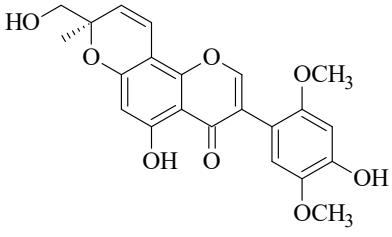
brandisianin C

(**79**)



brandisianin E

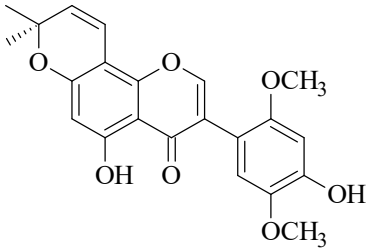
(**80**)



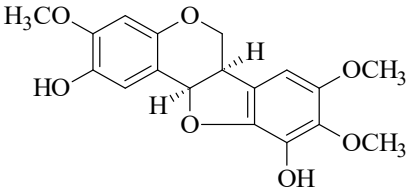
brandisianin D

(**81**)

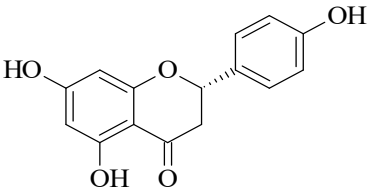
Supplementary Information (SI)



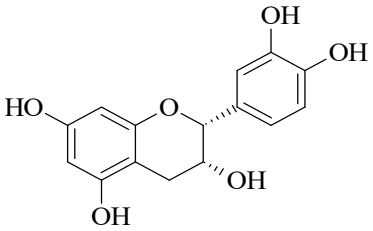
4′−demethyltoxicarol isoflavone
(**82**)



brandisianin F
(**83**)



naringenin
(84)



epicatechin
(**85**)

Figure S1. Structure of 85 compounds extracted from Millettia brandisiana.

Supplementary Information (SI)

Table S1. SMILES strings and predicted free binding energy (GraphConv model) of 85 compounds extracted from Millettia brandisiana

ID	SMILES strings	Predicted ΔG (kcal.mol^{-1})
1	C12=C(C=C(O1)C(C)(C)O)C1=C(C(=C2)O)C(=O)C=C(O1)C1=CC=CC=C1	-7.255
2	C12=C(C=C(O1)C(C)(C)O)C1=C(C=C2)C(=O)C=C(O1)C1=CC=CC=C1	-8.586
3	C12=C(C=CO1)C1=C(C=C2)C(=O)C=C(O1)C1=CC=CC=C1	-6.943
4	C12=C(C=CO1)C1=C(C(=C2)O)C(=O)C=C(O1)C1=CC=CC=C1	-6.157
5	C12=CC3=C(C(=C1C=CO2)OC)C(=O)C=C(O3)C1=CC=CC=C1	-7.393
6	C12=CC=C3C(=C1C=CC(O2)(C)C)OC(=CC3=O)C1=CC=CC=C1	-7.02
7	C12=CC(=C3C(=C1C=CC(O2)(C)C)OC(=CC3=O)C1=CC=CC=C1)O	-6.45
8	C12=CC(=C3C(=C1C=CC(O2)(C)C)OC(=CC3=O)C1=CC=CC=C1)OC	-7.152
9	C12=CC3=C(C(=C1C=CC(O2)(C)C)O)C(=O)C=C(O3)C1=CC=CC=C1	-6.593
10	C12=CC3=C(C(=C1C=CC(O2)(C)C)OC)C(=O)C=C(O3)C1=CC=CC=C1	-7.819
11	C1(=CC=C2C(=C1OC)OC=C(C2=O)C1=CC=C(C=C1)OC)O	-7.879
12	C12=C(C(=O)C[C@H](O1)C1=CC=CC=C1)C=CC(=C2CC=C(C)C)OCC=C(C)C	-6.549
13	C12=C(C(=O)C[C@H](O1)C1=CC=CC=C1)C(=CC(=C2CC=C(C)C)OCC=C(C)C)O	-5.572
14	C12=C(C(=O)C[C@](O1)(C1=CC=CC=C1)OC)C(=C1C(=C2)OC(C=C1)(C)C)OC	-8.207
15	C12=C(C(=O)C[C@H](O1)C1=CC=CC=C1)C=CC1=C2C=CC(O1)(C)C	-5.588
16	C12=C(C(=O)C[C@H](O1)C1=CC=CC=C1)C(=CC1=C2C=CC(O1)(C)C)O	-4.475
17	C1=CC(=CC=C1)/C=C/C(=O)C1=CC=C2C(=C1OC)C=CO2	-7.717
18	C1=CC(=CC=C1)/C=C/C(=O)C1=CC=C2C(=C1O)C=CC(O2)(C)C	-6.933
19	C(C(=O)C1=CC=C2C(=C1OC)C=CO2)CC1=CC=CC=C1	-7.467
20	C(C(=O)C1=CC=C2C(=C1OC)C=CO2)[C@@H](C1=CC=CC=C1)OC	-6.766
21	C1(=CC=C2C(=C1OC)C=CC(O2)(C)C)C(=O)C[C@@H](C1=CC=CC=C1)OC	-5.724
22	C1=CC(=CC=C1)/C(=C/C(=O)C1=CC=C2C(=C1OC)C=CO2)/O	-8.873
23	C1=CC(=CC=C1)/C(=C/C(=O)C1=C(C=C2C(=C1OC)C=CO2)OC)/O	-8.18
24	C1=CC(=CC=C1)/C(=C/C(=O)C1=CC=C2C(=C1O)C=CC(O2)(C)C)/O	-7.8
25	C1=CC(=CC=C1)/C(=C/C(=O)C1=CC=C2C(=C1OC)C=CC(O2)(C)C)/O	-7.999
26	C1=CC(=CC=C1)/C(=C/C(=O)C1=C(C=C2C(=C1OC)C=CC(O2)(C)C)OC)/O	-6.936
27	C12=CC=C3C(=C1C[C@@H](O2)C(=C)C)O[C@H]1[C@@](C3=O)(C2=CC(=C(C=C2OC1)OC)OC)O	-8.126
28	C12=CC(=C3C(=C1C[C@@H](O2)C(=C)C)O[C@H]1[C@@](C3=O)(C2=CC(=C(C=C2OC1)OC)OC)O)O	-6.615
29	C12=C(C3=C(C=C1)C(=O)[C@@]1([C@H](O3)COC3=C1C=C(C(=C3)OC)OC)O)C=CC(O2)(C)C	-8.37
30	C12=C(C=C(C=C1)OC)O[C@@H]1[C@H]2COC2=C1C=CC(=C2)O	-5.506
31	C12=C(C=C3C(=C1)OCO3)O[C@@H]1[C@H]2COC2=C1C=CC(=C2)O	-6.043
32	C1(=CC2=C(C(=C1)O)C(=O)[C@]1([C@@H](O2)COC2=C1C=C(C(=C2)OC)OC)O)O	-8.022

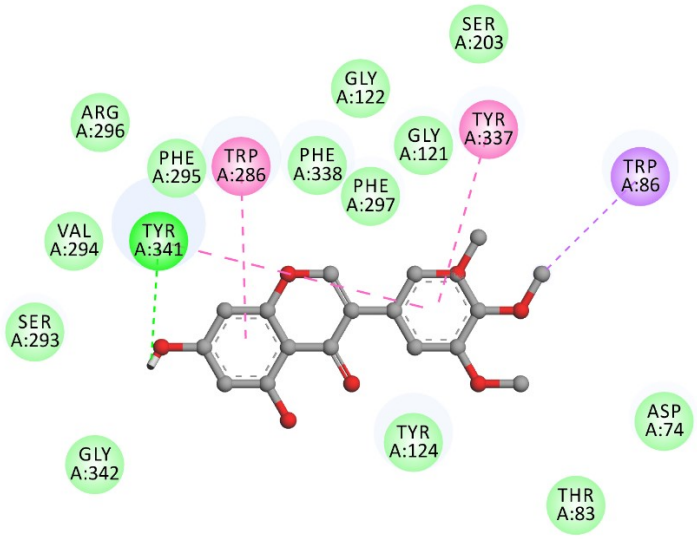
33	C1(=CC2=C(C(=C1)O)C(=O)[C@]1([C@@H](O2)COC2=C1C=C(C(=C2)OC)O)O)OC	-7.956
34	C1(=CC2=C(C(=C1)O)C(=O)[C@]1([C@@H](O2)COC2=C1C=C(C(=C2)O)OC)O)OC	-7.426
35	C1(=CC2=C(C(=C1)O)C(=O)[C@]1([C@@H](O2)COC2=C1C=C(C(=C2)OC)OC)O)OC	-8.237
36	C1(=CC(=C2C(=C1)O[C@H]1[C@@H](C2=O)C2=CC(=C(C=C2OC1)OC)OC)O)OC	-7.944
37	C12=C(C3=C(C(=C1)O)C(=O)[C@@H]1[C@H](O3)COC3=C1C=C(C(=C3)OC)OC)C=CC(O2)(C)C	-7.295
38	C12=C(C3=C(C(=C1)O)C(=O)[C@@]1([C@H](O3)COC3=C1C=C(C(=C3)OC)OC)O)C=CC(O2)(C)C	-8.103
39	C1(=CC2=C(C(=C1)O)C(=O)C1=C(O2)COC2=CC(=C(C=C12)OC)OC)OC	-7.998
40	C12=CC(=C3C(=C1C=CC(O2)(C)C)OC1=C(C3=O)C2=C(OC1)C=C(C(=C2)OC)OC)O	-7.925
41	C1(=CC(=C2C(=C1)OC=C(C2=O)C1=C(C=C(C(=C1)OC)OC)OC)O)OCC=C(C)C	-8.594
42	C1(=CC(=C2C(=C1)OC=C(C2=O)C1=C(C=C(C(=C1)OC)OC)O)O)OCC=C(C)C	-8.687
43	C1(=CC(=C2C(=C1)OC=C(C2=O)C1=C(C=C(C(=C1)OC)OC)OC)O)O	-9.24
44	C1(=C(C=C2C(=C1)OC=C(C2=O)C1=CC=C(C=C1)OC)OC)O	-8.455
45	C1(=CC(=C2C(=C1)OC=C(C2=O)C1=CC=C(C=C1)O)O)O	-6.292
46	C1(=CC(=C2C(=C1CC=C(C)C)OC=C(C2=O)C1=C(C=C(C(=C1)CC=C(C)C)O)CC=C(C)C)O)O	-8.042
47	C1(=CC(=C2C(=C1)OC(=C(C2=O)O)C1=CC=C(C(=C1)OC)O)O)O	-6.595
48	C1(=CC(=C2C(=C1)OC(=C(C2=O)O)C1=CC=C(C(=C1)O)O)O)O	-5.726
49	C1(=CC=C2C(=C1)OC(=CC2=O)C1=CC=C(C=C1)O)O	-5.694
50	C1(=CC(=C2C(=C1)OC(=CC2=O)C1=CC=C(C=C1)O)O)O	-5.678
51	C12=C(C3=C(C=C1)C(=O)C[C@H](O3)C1=CC=CC=C1)C=CC(O2)(C)C	-5.588
52	C12=C(C3=C(C(=C1)O)C(=O)C[C@H](O3)C1=CC=CC=C1)C=CC(O2)(C)C	-4.475
53	C12=C(C3=C(C(=C1)OC)C(=O)C[C@H](O3)C1=CC=CC=C1)C=CC(O2)(C)C	-5.709
54	C1=CC=C(C=C1)/C(=C/C(=O)C1=CC=C2C(=C1O)C=CC(O2)(C)C)/O	-7.8
55	C1=CC=C(C=C1)/C(=C/C(=O)C1=CC=C2C(=C1OC)C=CC(O2)(C)C)/OC	-8.106
56	C1=CC=C(C=C1)C(=O)/C=C(/C1=CC=C2C(=C1OC)C=CC(O2)(C)C)\O	-7.899
57	C1(=CC(=C2C(=C1)OC=C(C2=O)C1=C(C=C(C(=C1)OC)OCC=C(C)C)OC)OC)OC	-9.488
58	C1(=CC=C2C(=C1)OC=C(C2=O)C1=CC=C(C=C1)OCC=C(C)C)OCC=C(C)C	-7.919
59	C1(=CC(=C2C(=C1)OC=C(C2=O)C1=C(C=C(C(=C1)OC)OC)OC)O)OC	-9.012
60	C12=CC(=C3C(=C1C=CC(O2)(C)C)OC=C(C3=O)C1=C(C=C(C(=C1)OC)OC)OC)O	-8.528
61	C1(=C(C(=C2C(=C1)OC=C(C2=O)C1=C(C=C(C(=C1)OC)O)OC)O)CC=C(C)C)O	-7.677
62	C1(=CC(=C2C(=C1)O[C@H]1[C@@](C2=O)(C2=CC(=C(C=C2OC1)OC)OC)O)O)OC	-8.237
63	C1(=CC2=C(C(=C1)O)C(=O)C1=C(O2)[C@@H](OC2=CC(=C(C=C12)OC)OC)O)OC	-8.112
64	C12=CC(=C3C(=C1C=CC(O2)(C)C)OC1=C(C3=O)C2=C(O[C@@H]1O)C=C(C(=C2)OC)OC)O	-8.211
65	C1(C=CC2=C(C3=C(C=C2O1)O[C@@](CC3=O)(C1=CC=CC=C1)OC)O)(C)C	-7.617
66	C1=CC(=CC=C1)/C(=C/C(=O)C1=C(C=C2C(=C1OC)C=CO2)OC)/OC	-7.88
67	C1(C=CC2=C(C3=C(C=C2O1)OC(=CC3=O)C1=CC=CC=C1)O)(C)C	-6.593
68	C1(C=CC2=C(C3=C(C=C2O1)OC(=CC3=O)C1=CC=CC=C1)OC)(C)C	-7.819
69	C12=C(C=C3C(=C1C=CC(O2)(C)C)OC(=CC3=O)C1=CC=CC=C1)OC	-7.767

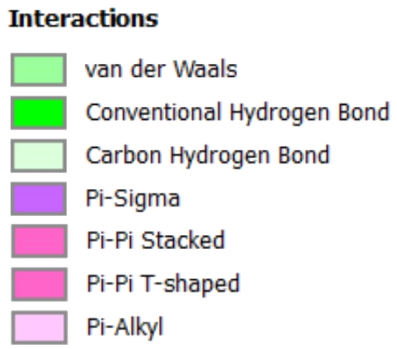
70	C1(=CC=C2C(=C1)OC(=C(C2=O)OC)C1=CC=C(C(=C1)OC)OC)OC	-9.092
71	C1(=CC=C2C(=C1)OC(=C(C2=O)OC)C1=CC2=C(C=C1)OCO2)OC	-9.096
72	C12=C(C3=C(C=C1)C(=O)C=C(O3)C1=CC=CC=C1)C=CO2	-6.943
73	C12=C(C3=C(C=C1)C(=O)C=C(O3)C1=CC=CC=C1)C=C(O2)C(C)(C)O	-8.586
74	C1=CC(=CC=C1)/C(=C/C(=O)C1=CC=C2C(=C1OC)C=CO2)/OC	-8.934
75	C1=CC(=CC=C1)[C@@H](CC(=O)C1=CC=C2C(=C1OC)C=CO2)OC	-6.766
76	C1(=CC(=C2C(=C1)OC=C(C2=O)C1=C(C=C(C(=C1)OC)O)OC)O)O	-8.482
77	C1(=CC(=C2C(=C1)OC=C(C2=O)C1=C(C=C(C(=C1)OC)OCC=C(C)C)OC)O)O	-8.462
78	C12=C(C3=C(C(=C1)O)C(=O)C(=CO3)C1=C(C=C(C(=C1)OC)O)OC)C[C@@H](O2)C(=C)C	-6.844
79	C1(=CC(=C2C(=C1CC=C(C)C)OC=C(C2=O)C1=C(C=C(C(=C1)OC)O)OC)O)O	-7.55
80	C1(=CC(=C2C(=C1C/C=C(/C)\CO)OC=C(C2=O)C1=C(C=C(C(=C1)OC)O)OC)O)O	-7.087
81	C12=CC(=C3C(=C1C=C[C@@](O2)(CO)C)OC=C(C3=O)C1=C(C=C(C(=C1)OC)O)OC)O	-8.007
82	C12=CC(=C3C(=C1C=CC(O2)(C)C)OC=C(C3=O)C1=C(C=C(C(=C1)OC)O)OC)O	-7.038
83	C1(=CC2=C(C=C1O)[C@H]1[C@@H](CO2)C2=C(C(=C(C(=C2)OC)OC)O)O1)OC	-6.926
84	C1(=CC2=C(C(=C1)O)C(=O)C[C@H](O2)C1=CC=C(C=C1)O)O	-4.646
85	C1(=CC2=C(C(=C1)O)C[C@H]([C@H](O2)C1=CC(=C(C=C1)O)O)O)O	-6.261

Supplementary Information (SI)

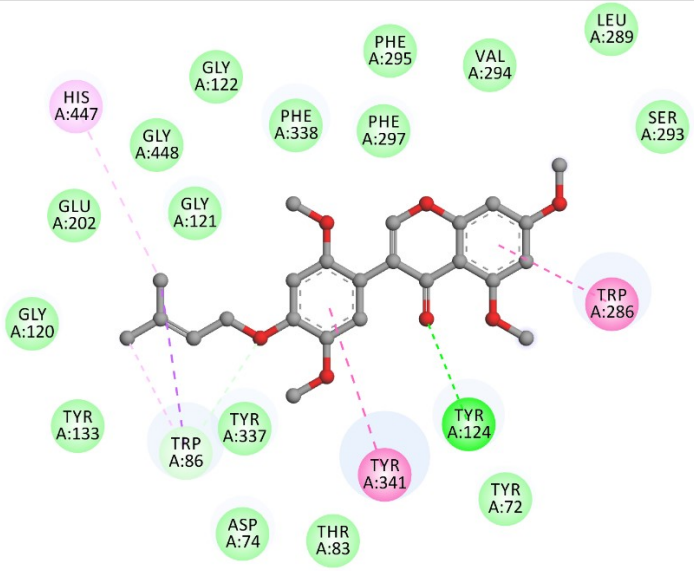
Figure S2. Interactions of compound ID 43, 57, 59, 70, 71 in complex with AChE by molecular docking method.

ID 43

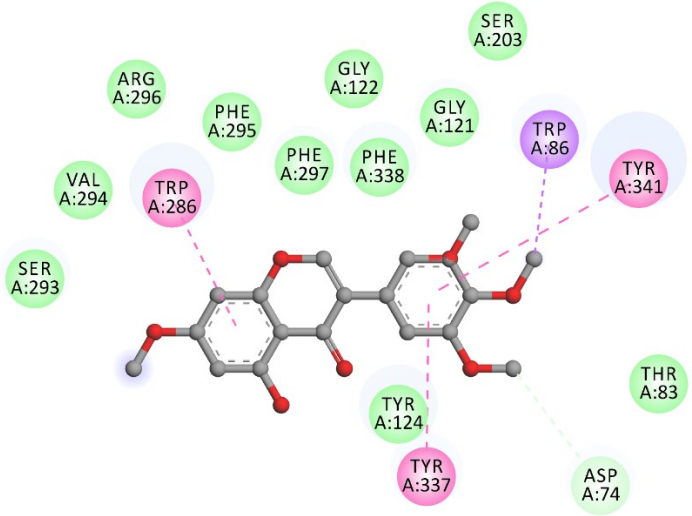




ID 57

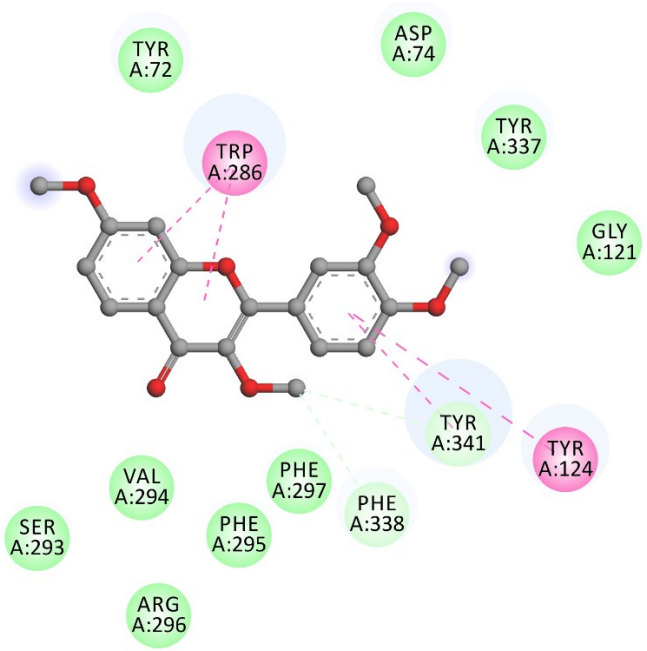


ID 59



Supplementary Information (SI)

ID 70



ID 71