

Supplementary Materials

Antioxidant and Anti-Skin Aging Potential of Selected Thai Plants: In Vitro Evaluation and In Silico Target Prediction

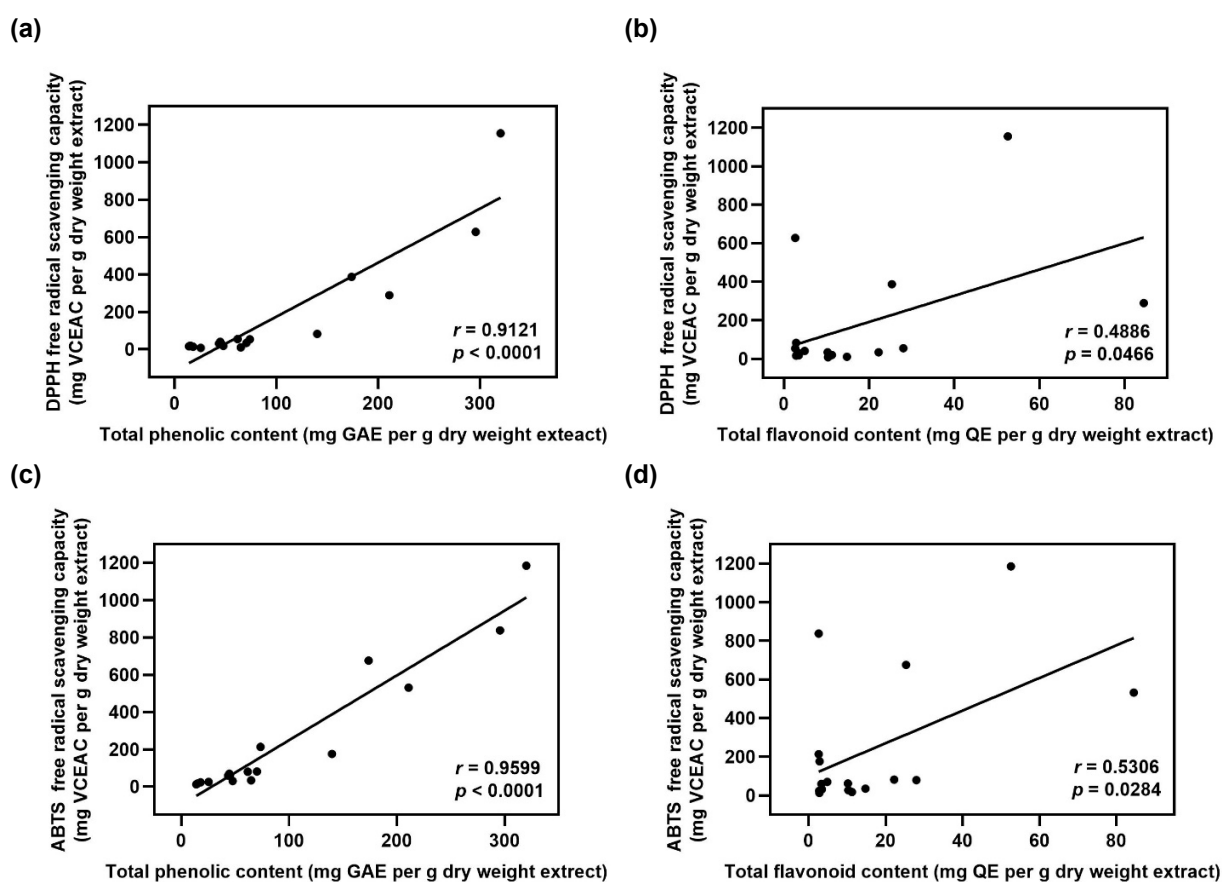


Figure S1. Correlation analysis between phytochemical contents and antioxidant capacities among the studied plants. The correlations are expressed as Pearson's correlation coefficients (r) between **(a)** total phenolic content and DPPH free radical scavenging activity, **(b)** total phenolic content and ABTS free radical scavenging activity, **(c)** total flavonoid content and DPPH free radical scavenging activity, **(d)** total phenolic content and ABTS free radical scavenging activity.

Table S1. The percent inhibition of elastase activity by Thai plants at various concentrations.

<i>Anacardium occidentale</i> L. (Leaf)	
Concentration (µg/ml)	Inhibition (%)
500.00	84.78 ± 2.16
100.00	78.09 ± 3.91
50.00	71.73 ± 6.58
25.00	62.23 ± 7.48
12.50	36.87 ± 10.05
6.25	7.90 ± 4.67
<i>Areca catechu</i> L. (Fruit)	
Concentration (µg/ml)	Inhibition (%)
500.00	88.31 ± 0.41
250.00	78.08 ± 4.51
125.00	52.35 ± 10.44
62.50	28.66 ± 2.80
31.25	13.75 ± 1.30
15.63	8.49 ± 2.19
7.81	8.57 ± 4.85
<i>Glochidion zeylanicum</i> (Gaertn.) A. Juss. (Leaf)	
Concentration (µg/ml)	Inhibition (%)
500.00	87.43 ± 3.80
100.00	66.00 ± 10.67
50.00	54.16 ± 10.29
25.00	34.94 ± 18.68
12.50	25.03 ± 16.41
6.25	20.66 ± 9.82
<i>Senna alata</i> (L.) Roxb. (Leaf)	
Concentration (µg/ml)	Inhibition (%)
500.00	73.95 ± 1.46
250.00	65.61 ± 1.35
125.00	57.85 ± 1.81
62.50	44.81 ± 6.25
31.25	29.04 ± 10.78
15.63	19.75 ± 12.27
7.81	16.19 ± 12.76
<i>Streblus asper</i> Lour. (Leaf)	
Concentration (µg/ml)	Inhibition (%)
400.00	75.25 ± 8.25
200.00	58.30 ± 2.26
100.00	35.74 ± 0.94
50.00	13.01 ± 4.66

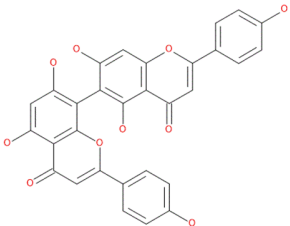
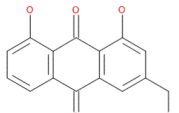
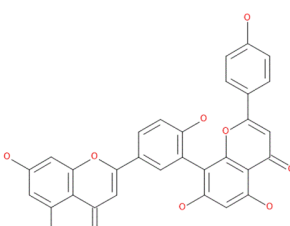
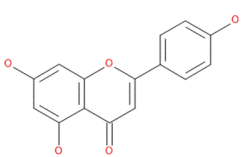
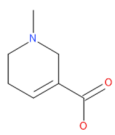
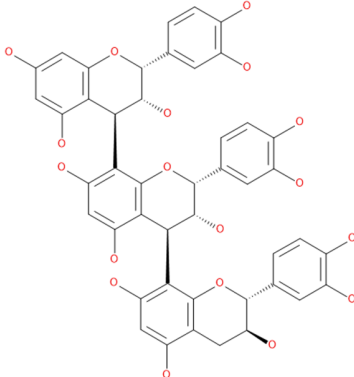
Values show mean ± standard deviation (SD) of at least three independent experiments.

Table S2. The percent inhibition of tyrosinase activity by Thai plants at various concentrations.

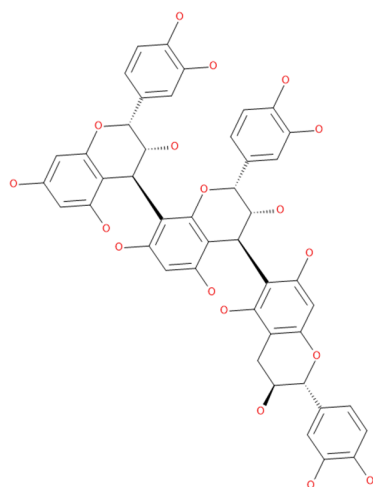
<i>Anacardium occidentale</i> L. (Leaf)	
Concentration (µg/ml)	Inhibition (%)
2000.00	84.41 ± 4.30
1000.00	81.01 ± 2.96
500.00	66.13 ± 8.01
250.00	41.10 ± 11.78
125.00	18.12 ± 10.02
62.50	8.27 ± 2.64
31.25	2.90 ± 0.79
<i>Areca catechu</i> L. (Fruit)	
Concentration (µg/ml)	Inhibition (%)
1000.00	75.38 ± 1.57
500.00	72.94 ± 1.48
250.00	66.88 ± 3.60
125.00	60.94 ± 3.61
62.50	41.82 ± 1.43
31.25	30.14 ± 9.51
15.63	24.86 ± 7.30
<i>Glochidion zeylanicum</i> (Gaertn.) A. Juss. (Leaf)	
Concentration (µg/ml)	Inhibition (%)
500.00	90.43 ± 1.57
250.00	87.70 ± 1.19
125.00	74.47 ± 1.47
62.50	38.05 ± 4.30
31.25	5.45 ± 4.95
<i>Mangifera caloneura</i> Kurz. (Leaf)	
Concentration (µg/ml)	Inhibition (%)
1000.00	76.12 ± 3.98
500.00	52.96 ± 5.12
250.00	34.55 ± 4.40
125.00	21.92 ± 1.46
62.50	12.53 ± 3.71

Values show mean ± standard deviation (SD) of at least three independent experiments.

Table S3. List of compounds derived from three most effective plants on inhibition against elastase and/or tyrosinase.

Compound	Structure	Source	Reference
Agathisflavone		<i>Anacardium occidentale</i>	[26]
Aloe-emodin		<i>Senna alata</i>	[50,57]
Amentoflavone		<i>Anacardium occidentale</i>	[25]
Apigenin		<i>Senna alata</i>	[55]
Arecaidine		<i>Areca catechu</i>	[30,51]
Arecatannin A1		<i>Areca catechu</i>	[31]

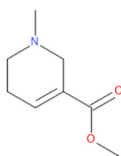
Arecatannin B1



Areca catechu

[31]

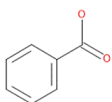
Arecoline



Areca catechu

[30,51]

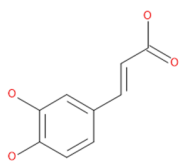
Benzoic acid



Glochidion zeylanicum

[42]

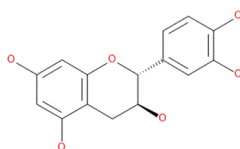
Caffeic acid



Areca catechu

[30]

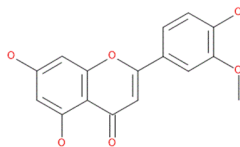
Catechin



Areca catechu,
Anacardium occidentale,
Glochidion zeylanicum

[25,27,30-
32,42,53,
59]

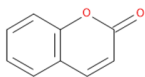
Chrysoeriol



Senna alata,
Areca catechu

[52,61]

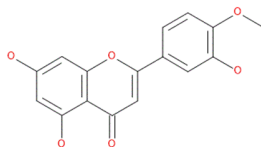
Coumarin



Areca catechu

[30]

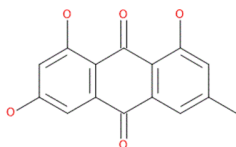
Diosmetin



Senna alata

[57]

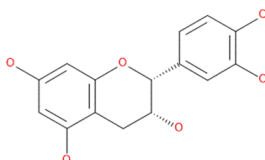
Emodin



Senna alata

[50,54,57]

Epicatechin



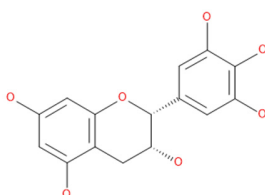
Areca catechu,

[25,30,31,

Anacardium occidentale

53,59,60]

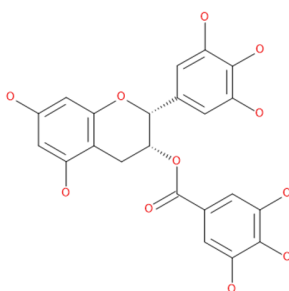
Epigallocatechin



Areca catechu

[30,53]

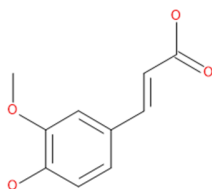
Epigallocatechin gallate



Areca catechu

[53]

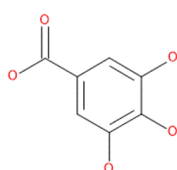
Ferulic acid



Areca catechu

[30]

Gallic acid



Areca catechu,

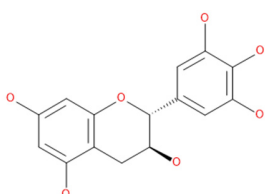
[27,30,32,

Anacardium occidentale,

42,53]

Glochidion zeylanicum

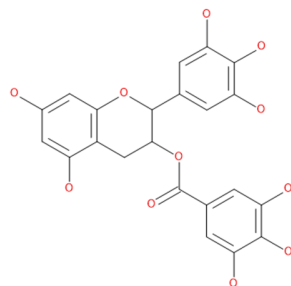
Gallocatechin



Areca catechu

[30]

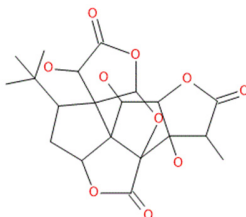
Gallocatechin gallate



Areca catechu

[30]

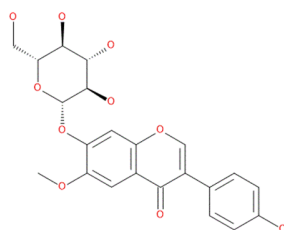
Ginkgolide B



Glochidion zeylanicum

[42]

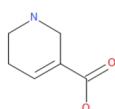
Glycitin



Glochidion zeylanicum

[42]

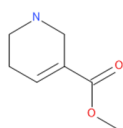
Guvacine



Areca catechu

[30,51]

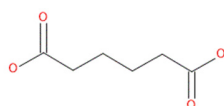
Guvacoline



Areca catechu

[30,51]

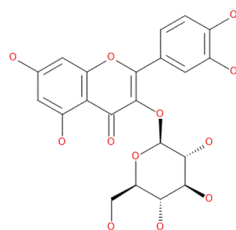
Hexanedioic acid



Glochidion zeylanicum

[42]

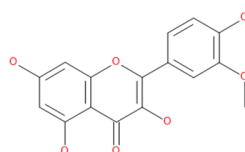
Isoquercetin



Anacardium occidentale

[27]

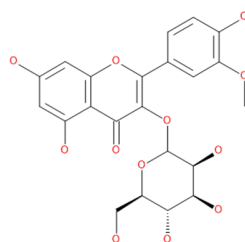
Isorhamnetin



Areca catechu

[61]

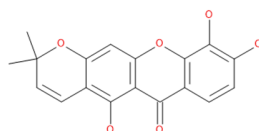
Isorhamnetin-3-O-galactoside



Areca catechu

[30]

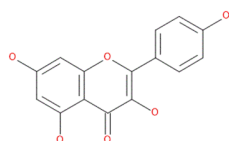
Jacareubin



Areca catechu

[61]

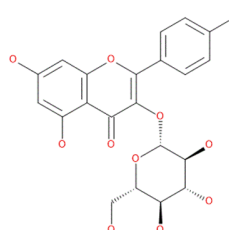
Kaempferol



Areca catechu,
Senna alata

[30,50,52,
57,58]

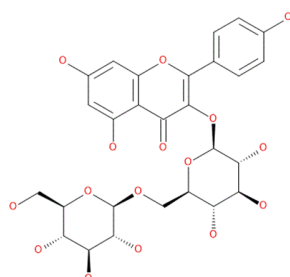
Kaempferol 3-O-beta-L-glucopyranoside



Senna alata

[52]

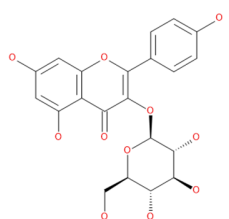
Kaempferol 3-O-gentiobioside



Senna alata

[28]

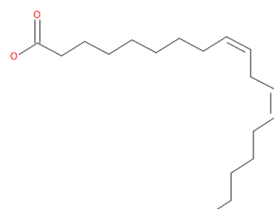
Kaempferol-3-O-glucoside



Areca catechu

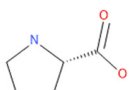
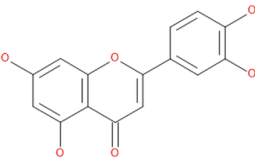
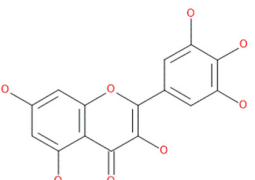
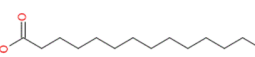
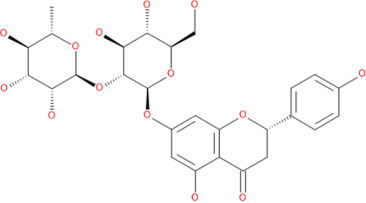
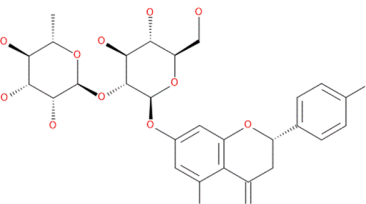
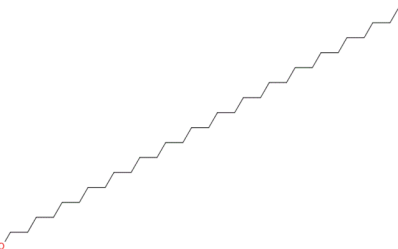
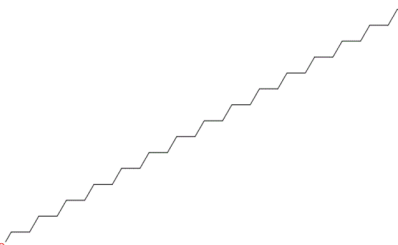
[30]

Linoleic acid

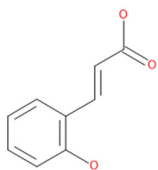


Senna alata

[54]

L-proline		<i>Glochidion zeylanicum</i>	[42]
Luteolin		<i>Areca catechu</i>	[61]
Myricetin		<i>Anacardium occidentale</i>	[25]
Myristic acid		<i>Senna alata</i>	[54]
Naringenin		<i>Areca catechu</i>	[30]
Naringin		<i>Senna alata</i>	[55]
n-dotriacontanol		<i>Senna alata</i>	[52]
n-triacontanol		<i>Senna alata</i>	[52]

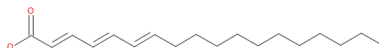
o-Coumaric acid



Areca catechu

[30]

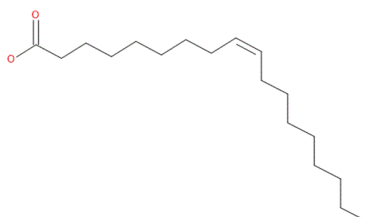
Octadecatrienoic acid



Glochidion zeylanicum

[42]

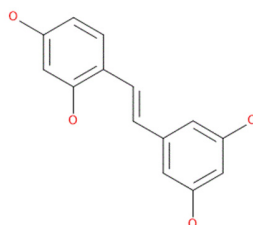
Oleic acid



Senna alata

[54]

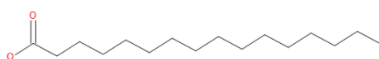
Oxyresveratrol



Glochidion zeylanicum

[42]

Palmitic acid

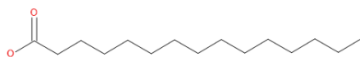


Anacardium occidentale, [32,42,52,

Glochidion zeylanicum, 54]

Senna alata

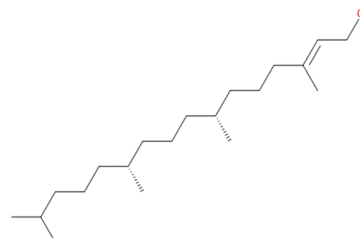
Pentadecanoic acid



Glochidion zeylanicum

[42]

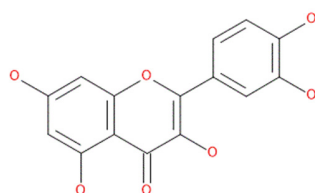
Phytol



Glochidion zeylanicum

[42]

Quercetin



Areca catechu,

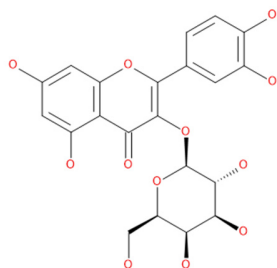
[25,26,30,

Anacardium occidentale, 32,42,52]

Glochidion zeylanicum,

Senna alata

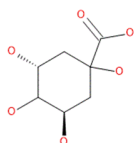
Quercetin-3-O-galactoside



Areca catechu

[30]

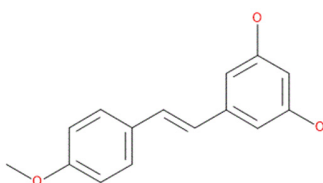
Quinic acid



Glochidion zeylanicum

[42]

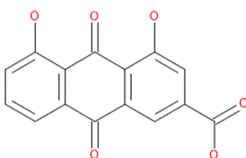
Resveratrol 4'-methyl ether



Glochidion zeylanicum

[42]

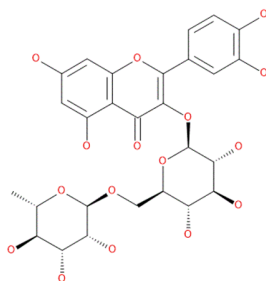
Rhein



Senna alata

[50,54,56,
58]

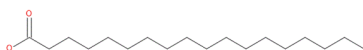
Rutin



Anacardium occidentale

[26,27]

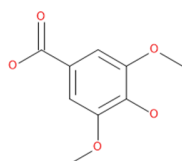
Stearic acid



Senna alata

[52,54]

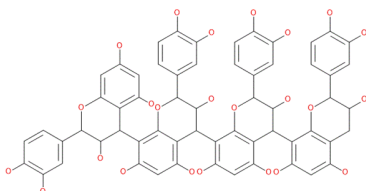
Syringic acid



Areca catechu

[60]

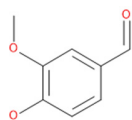
Tetramer of proanthocyanidin



Anacardium occidentale

[25]

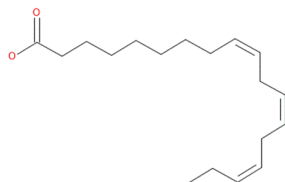
Vanillin



Areca catechu

[30]

α -linolenic acid



Anacardium occidentale,

[32,42]

Glochidion zeylanicum

Table S4. Molecular docking results between phytochemical compounds and the binding site of elastase (3HGP).

No.	Compound	MW	Binding energy (kcal/mol)	Inhibition Constant	Number of hydrogen bond	Amino acid interaction	Bond length (Å)
1	FRW (original inhibitor)	513.51	-7.14	5.80 μ M	9	A:HIS57	2.52350
						A:HIS57	2.75545
						A:THR175	2.24654
						A:GLY193	2.33614
						A:GLY193	2.47173
						A:SER195	2.46901
						A:VAL216	2.18525
						A:VAL216	2.21136
						A:GLN192	2.64759
	Epigallocatechin gallate (positive control)	458.37	-9.69	79.13 nM	16	A:THR41	2.57071
						A:ARG61	2.53699
						A:ARG61	2.34579
						A:CYS191	2.70525
						A:GLY193	2.13234
						A:GLY193	1.99259
						A:ASP194	2.85786
						A:ASP194	2.95908
						A:SER195	2.27809
						A:SER195	2.85192
						A:VAL216	2.32268
						A:SER217	2.68922
						A:CYS191	3.08133
						A:CYS191	2.48834
						A:THR41	3.24692
						A:THR41	3.04781
	Tetramer of proanthocyanidin	1155.02	-11.95	1.75 nM	18	A:HIS57	2.78926
						A:VAL99	2.06369
						A:GLY193	2.67412
						A:SER195	2.67016
						A:VAL216	2.58477
						A:ARG217A	2.14988
						A:ASP97	2.49907
						A:VAL216	3.23714
						A:CYS191	3.28470
						A:SER195	2.59907
						A:SER195	2.58138

						A:THR41	2.90533
						A:CYS42	3.17172
						A:CYS42	2.90763
						A:HIS57	3.36115
						A:CYS58	3.15629
						A:ASP97	2.52302
						A:CYS58	2.85453
2	Amentoflavone	538.46	-11.81	2.21 nM	7	A:VAL99	2.04173
						A:GLY193	1.97784
						A:ASP194	2.81399
						A:SER195	2.08605
						A:VAL216	2.95069
						A:VAL216	3.13572
						A:ARG217A	3.56022
3	Rutin	610.52	-10.12	38.08 nM	12	A:VAL99	2.15421
						A:GLY193	2.01978
						A:ASP194	2.68737
						A:SER195	2.03458
						A:ARG217A	2.89183
						A:ARG217A	2.16727
						A:ARG217A	3.00142
						A:ARG217A	2.77342
						A:ASP97	3.13763
						A:CYS191	2.70211
						A:GLN192	2.85245
						A:ASP97	2.94995
4	Agathisflavone	538.46	-9.92	53.93 nM	0		
5	Kaempferol 3-O-gentiobioside	610.52	-9.73	73.92 nM	8	A:HIS57	3.05099
						A:VAL99	2.83989
						A:ARG217A	1.83288
						A:ARG217A	2.67981
						A:ASP97	2.69662
						A:ASP98	3.35512
						A:ASP98	3.27145
						A:PHE215	4.19666
6	Kaempferol 3-O-beta-L-glucopyranoside	448.38	-9.36	136.73 nM	9	A:VAL99	2.35829
						A:GLY193	2.07372
						A:ASP194	2.84954
						A:SER195	2.16655
						A:VAL216	2.54727
						A:ASP97	3.15783

7	Isoquercetin	464.38	-9.26	162.78 nM	9	A:ASP97	3.22664
						A:PHE215	2.94950
						A:VAL216	3.24286
						A:ARG61	2.97515
						A:ARG61	2.54804
						A:ARG61	2.90630
						A:GLY193	2.03511
						A:ASP194	2.58534
						A:SER195	2.03300
8	Naringin	580.53	-9.16	192.85 nM	16	A:VAL216	2.68435
						A:VAL216	2.75760
						A:PHE215	2.95244
						A:ARG61	2.66162
						A:ARG61	3.06606
						A:GLN192	2.03957
						A:GLY193	1.99418
						A:GLY193	2.19799
						A:ASP194	2.67659
						A:SER195	3.05382
						A:SER195	2.27226
						A:CYS191	2.79285
						A:VAL216	2.79621
						A:SER214	2.75276
						A:ARG61	3.35884
						A:ARG217A	3.35938
9	Glycitin	446.40	-8.67	439.04 nM	10	A:SER217	3.02352
						A:HIS57	2.98501
						A:HIS57	3.97829
						A:HIS57	2.85020
						A:ALA99A	1.87321
						A:CYS191	2.94348
						A:ASP194	2.72853
						A:SER195	2.47003
						A:CYS191	2.54852
						A:ASP98	3.36807
10	Myricetin	318.24	-8.53	561.70 nM	8	A:ASP97	3.09022
						A:VAL216	2.84750
						A:VAL216	3.13688
						A:GLY193	2.07707
						A:ASP194	2.86297
						A:SER195	2.21726

						A:VAL216	2.50270
						A:ARG217A	3.06755
						A:SER217	3.21367
						A:ARG217A	3.73332
						A:VAL216	3.19504
11	Epicatechin	290.27	-8.47	618.86 nM	8	A:HIS57	3.01160
						A:GLY193	2.04469
						A:ASP194	2.83623
						A:SER195	2.17262
						A:VAL216	2.60128
						A:SER214	2.84466
						A:VAL216	3.24085
						A:HIS57	4.04784
12	Quercetin	302.24	-8.39	707.97 nM	6	A:GLY193	2.07626
						A:ASP194	2.85099
						A:SER195	2.20819
						A:VAL216	2.49512
						A:SER217	2.95390
						A:VAL216	3.20176
13	Catechin	290.27	-8.31	812.28 nM	5	A:GLY193	2.04521
						A:ASP194	2.83797
						A:SER195	2.17203
						A:VAL216	2.62754
						A:VAL216	3.09925
14	Ginkgolide B	424.40	-8.28	855.21 nM	7	A:HIS57	2.16026
						A:GLN192	2.28679
						A:GLY193	2.44387
						A:SER195	2.42828
						A:VAL216	2.77862
						A:VAL216	2.26792
						A:GLN192	3.22896
15	Chrysoeriol	300.26	-8.15	1.06 μ M	5	A:GLY193	2.09633
						A:ASP194	2.86127
						A:SER195	2.24263
						A:VAL216	2.43954
						A:VAL216	3.25443
16	Diosmetin	300.26	-8.14	1.08 μ M	6	A:GLY193	2.09905
						A:ASP194	2.87765
						A:SER195	2.25027
						A:VAL216	2.43233
						A:SER217	3.02011

17	Kaempferol	286.24	-8.14	1.09 μ M	5	A:VAL216	3.28497
						A:GLY193	2.08399
						A:ASP194	2.85703
						A:SER195	2.22547
18	Apigenin	270.24	-7.98	1.42 μ M	5	A:VAL216	2.48090
						A:VAL216	3.15619
						A:GLY193	2.08842
						A:ASP194	2.85822
19	Oxyresveratrol	244.24	-7.75	2.08 μ M	5	A:SER195	2.23099
						A:VAL216	2.45696
						A:VAL216	3.28784
						A:GLY193	1.98392
20	Emodin	270.24	-7.67	2.39 μ M	5	A:ASP194	2.50978
						A:SER195	1.99662
						A:VAL216	2.00620
						A:VAL216	2.70284
21	Aloe-emodin	270.24	-7.65	2.47 μ M	7	A:GLY193	2.83596
						A:GLY193	1.98415
						A:ASP194	2.49870
						A:SER195	1.99120
22	Rhein	284.22	-7.35	4.11 μ M	10	A:VAL216	2.06841
						A:GLY193	2.80483
						A:GLY193	2.00453
						A:ASP194	2.49731
23	Resveratrol 4'-methyl ether	242.27	-7.12	6.05 μ M	4	A:SER195	2.01419
						A:VAL216	2.13841
						A:PHE215	2.98478
						A:PHE215	3.14578
						A:ARG61	2.09898
						A:ARG61	2.07925
						A:GLY193	1.86295
						A:GLY193	2.02935
						A:ASP194	2.95764
						A:SER195	3.08050
						A:SER195	2.23777
						A:CYS191	2.88867
						A:THR41	2.61189
						A:CYS42	3.68229
						A:SER195	2.03502
						A:GLY193	2.00145
						A:ASP194	2.56312

24	Gallic acid	170.12	-5.92	45.66 μ M	6	A:ARG217A	2.54819
						A:GLY193	2.08325
						A:ASP194	2.63537
						A:SER195	2.63215
						A:SER195	2.15255
						A:VAL216	2.09269
25	Octadecatrienoic acid	278.43	-5.70	65.93 μ M	2	A:CYS191	2.89322
						A:ARG217A	1.99352
26	Phytol	296.53	-5.53	88.41 μ M	2	A:ARG217A	2.50481
						A:ARG217A	2.18541
27	α -linolenic acid	278.43	-5.21	151.38 μ M	2	A:VAL216	3.16650
						A:ARG217A	2.41950
28	Quinic acid	192.17	-5.14	170.27 μ M	7	A:ARG217A	2.12768
						A:GLY193	2.14684
						A:ASP194	2.27959
						A:SER195	2.09585
						A:VAL216	2.13330
						A:CYS191	2.47275
29	Linoleic acid	280.45	-4.91	9.09 μ M	1	A:CYS191	2.66879
						A:SER195	2.72310
						A:ARG217A	2.45050
						A:ARG217A	2.09175
						A:ARG217A	1.92107
						A:ARG217A	2.14678
30	Oleic acid	282.46	-4.83	287.10 μ M	1	A:ARG217A	2.88731
						A:ARG217A	2.88731
31	Palmitic acid	256.42	-4.58	438.97 μ M	1	A:GLY193	1.94803
						A:ARG217A	2.66437
32	Pentadecanoic acid	242.40	-4.45	543.69 μ M	2	A:ARG217A	3.05706
						A:ARG217A	3.05706
33	Benzoic acid	122.12	-4.24	779.03 μ M	1	A:GLY193	1.94803
34	Stearic acid	284.48	-4.24	782.65 μ M	2	A:ARG217A	2.66437
						A:ARG217A	3.05706
35	Myristic acid	228.37	-4.22	802.18 μ M	0		
36	L-proline	115.13	-3.87	1.46 mM	3	A:ARG61	2.71531
						A:ASP60	3.20048
						A:ASP60	3.49653
37	Hexanedioic acid	146.14	-3.74	1.80 mM	4	A:ARG217A	1.99619
						A:ARG217A	1.83030
						A:ARG217A	1.97210
						A:VAL216	2.99642
38	n-dotriacontanol	466.87	-3.18	4.67 mM	3	A:ARG61	3.19083
						A:HIS57	3.27872
						A:ASP97	3.67089
39	n-triacontanol	438.81	-2.26	21.96 mM	1	A:THR175	2.14124

Table S5. Molecular docking results between phytochemical compounds and the binding site of tyrosinase (2Y9X).

No.	Compound	MW	Binding energy (kcal/mol)	Inhibition Constant	Number of hydrogen bond	Amino acid interaction	Bond length (Å)
	Tropolone (original inhibitor)	122.12	-4.69	364.55 μ M	1	A:HIS61	2.93039
	Kojic acid (positive control)	142.11	-4.59	430.35 μ M	8	A:ASN81	2.08063
						A:HIS85	2.32738
						A:GLU322	2.13654
						A:GLU322	3.04204
						A:CYS83	2.90731
						A:ASN320	3.42295
						A:GLU322	3.50682
						A:HIS85	2.51019
1	o-Coumaric acid	164.16	-10.42	23.09 nM	4	A:HIS263	2.97779
						A:HIS296	3.00656
						A:MET280	2.94362
						A:HIS263	3.80402
2	Tetramer of proanthocyanidin	1155.02	-10.42	22.83 nM	8	A:ASN81	1.94291
						A:ASN81	2.77879
						A:HIS244	2.25277
						A:ARG268	2.89527
						A:GLU322	3.20562
						A:MET280	2.71019
						A:HIS263	3.58654
						A:HIS263	3.11783
3	Caffeic acid	180.16	-10.10	39.74 nM	4	A:HIS61	3.00165
						A:HIS263	3.35274
						A:HIS296	2.79428
						A:GLY281	3.27655
4	Ferulic acid	194.18	-10.00	46.75 nM	5	A:HIS61	3.04213
						A:HIS263	3.29735
						A:HIS296	2.80888
						A:GLY281	3.32939
						A:ASN260	3.13639
5	Arecatannin A1	866.77	-9.94	110.38 nM	10	A:ASN81	2.38646
						A:ARG268	3.05168
						A:GLY281	2.84476
						A:SER282	2.74566
						A:ALA246	2.90249

						A:ALA323	3.06850
						A:CYS83	2.57007
						A:PRO284	3.04284
						A:ASN81	3.22583
						A:HIS244	3.54321
6	Octadecatrienoic acid	278.43	-9.87	58.62 nM	2	A:HIS94	3.16054
						A:HIS296	2.82951
7	Gallic acid	170.12	-9.65	84.78 nM	5	A:SER282	3.06267
						A:HIS263	3.09352
						A:HIS296	2.81572
						A:MET280	3.15132
						A:ASN260	2.88933
8	Quinic acid	192.17	-9.63	88.03 nM	6	A:ASN260	3.18435
						A:MET280	2.74930
						A:HIS61	3.32578
						A:HIS263	3.55667
						A:HIS263	3.32810
						A:HIS85	2.93841
9	Syringic acid	198.17	-9.56	98.46 nM	4	A:HIS263	2.89886
						A:HIS296	3.13860
						A:MET280	3.35634
						A:GLU256	3.11772
10	Arecatannin B1	866.77	-9.52	104.57 nM	11	A:HIS85	2.74069
						A:HIS85	1.66258
						A:VAL248	2.01703
						A:ARG268	1.95436
						A:ALA246	2.65678
						A:ALA246	3.25979
						A:GLU322	3.39371
						A:MET257	3.34050
						A:CYS83	3.17367
						A:CYS83	2.92554
						A:HIS244	3.48197
11	Amentoflavone	538.46	-9.37	136.28 nM	6	A:ASN81	2.32368
						A:ASN81	2.09600
						A:GLU322	3.01671
						A:CYS83	2.80356
						A:HIS85	2.79983
						A:HIS263	3.30620
12	α -linolenic acid	278.43	-9.32	146.97 nM	2	A:HIS94	3.22968
						A:HIS94	3.83676

13	Benzoic acid	122.12	-9.26	163.00 nM	1	A:HIS94	3.36341
14	Pentadecanoic acid	242.40	-8.90	300.01 nM	2	A:HIS263	3.03186
						A:HIS296	2.88041
15	Palmitic acid	256.42	-8.86	318.21 nM	2	A:HIS61	2.79886
						A:HIS296	2.77369
16	Hexanedioic acid	146.14	-8.68	433.58 nM	3	A:HIS94	3.16234
						A:HIS94	3.76420
						A:HIS263	3.40059
17	Arecaidine	141.17	-8.59	502.24 nM	3	A:HIS263	2.92899
						A:HIS296	3.09977
						A:ASN260	3.00512
18	Galocatechin gallate	458.37	-8.41	679.90 nM	9	A:ASN260	2.09290
						A:ARG268	2.17559
						A:VAL283	1.77894
						A:SER282	3.26428
						A:HIS61	3.51813
						A:HIS85	2.99297
						A:HIS259	2.97683
						A:ARG268	3.56983
						A:HIS263	3.39447
19	Agathisflavone	538.46	-8.23	934.62 nM	5	A:ASN81	2.58158
						A:ASN260	2.99061
						A:ASN260	3.75864
						A:HIS85	2.54527
						A:VAL283	2.89718
20	Epigallocatechin gallate	458.37	-8.08	1.19 μ M	6	A:ASN260	2.28274
						A:SER282	3.03305
						A:MET280	3.02781
						A:HIS61	3.22370
						A:HIS259	3.11352
						A:HIS263	3.53154
21	Guvacine	127.14	-7.93	1.53 μ M	0		
22	Isorhamnetin-3-O-galactoside	478.40	-7.78	1.97 μ M	10	A:ARG268	2.61244
						A:ARG268	2.15888
						A:MET280	3.23812
						A:MET280	2.88616
						A:ASN260	2.74567
						A:HIS259	3.24854
						A:HIS263	3.50211
						A:PHE264	3.92479
						A:PHE264	3.89086

23	Isoquercetin	464.38	-7.74	2.11 μ M	7	A:HIS263	3.31541
						A:VAL283	1.95856
						A:HIS259	3.58479
						A:ARG268	2.92003
						A:PRO284	3.18679
						A:GLY281	2.96963
						A:HIS263	3.04766
						A:HIS263	4.03417
						A:VAL283	1.85543
						A:SER282	3.32748
24	Quercetin-3-O-galactoside	464.38	-7.67	2.37 μ M	8	A:HIS61	3.72991
						A:HIS259	3.40187
						A:ARG268	2.91088
						A:PRO284	3.11048
						A:GLY281	2.91699
						A:HIS263	3.14255
						A:HIS244	1.71048
						A:ASN260	2.93145
						A:GLY281	3.22566
						A:HIS61	3.65135
25	Rutin	610.52	-7.65	2.48 μ M	7	A:HIS259	3.37472
						A:PRO284	3.47025
						A:HIS263	3.19461
						A:ARG268	2.01129
						A:ARG268	2.11496
						A:ARG268	2.66378
						A:ARG268	1.79570
						A:VAL283	1.91848
						A:GLY281	2.78962
						A:ARG268	2.88437
26	Kaempferol-3-O-glucoside	448.38	-7.40	3.79 μ M	7	A:HIS244	1.98915
						A:HIS244	2.87322
						A:HIS61	3.14519
						A:HIS85	3.25815
						A:HIS296	3.36954
						A:HIS61	3.08605
						A:HIS244	3.69317
						A:HIS263	3.77767
						A:HIS244	1.84683
						A:HIS263	2.96751
27	Myricetin	318.24	-7.04	6.92 μ M	8	A:SER282	3.07269
28	Gallocatechin	306.27	-6.94	8.21 μ M	5		

						A:MET280	2.71186
						A:HIS244	3.94980
29	Catechin	290.27	-6.85	9.60 μ M	3	A:ASN260	2.82593
						A:HIS61	2.90610
						A:PHE264	3.84711
30	L-proline	115.13	-6.85	9.59 μ M	3	A:HIS263	2.82224
						A:HIS296	3.06908
						A:HIS259	3.74845
31	Quercetin	302.24	-6.78	10.76 μ M	7	A:HIS244	2.13838
						A:HIS244	2.89602
						A:HIS61	3.16356
						A:HIS85	3.24592
						A:HIS296	3.36613
						A:HIS61	3.09307
						A:HIS244	3.80014
32	Epicatechin	290.27	-6.69	12.58 μ M	5	A:ASN260	2.79798
						A:HIS263	2.887000
						A:VAL283	2.87757
						A:MET280	2.73467
						A:HIS85	2.90708
33	Epigallocatechin	306.27	-6.68	12.71 μ M	5	A:HIS263	2.89927
						A:VAL283	2.86357
						A:MET280	2.74093
						A:HIS85	2.86647
						A:HIS263	3.62499
34	Jacareubin	326.30	-6.56	15.53 μ M	3	A:GLY281	2.99526
						A:HIS85	2.95688
						A:HIS259	2.99294
35	Glycitin	446.40	-6.47	18.22 μ M	4	A:VAL283	2.64301
						A:MET280	2.62857
						A:HIS61	2.89798
						A:HIS263	3.31631
36	Isorhamnetin	316.26	-6.47	18.03 μ M	7	A:HIS244	2.54417
						A:HIS263	2.94940
						A:SER282	2.80771
						A:MET280	2.49056
						A:HIS85	2.85990
						A:HIS259	3.71081
						A:HIS263	3.83165
37	Luteolin	286.24	-6.44	18.97 μ M	3	A:ASN260	2.99906
						A:MET280	3.36915

38	Naringenin	272.25	-6.42	19.81 μ M	4	A:HIS263	3.67221
						A:SER282	2.50052
						A:MET280	2.57025
						A:HIS85	2.97900
39	Kaempferol	286.24	-6.39	20.80 μ M	6	A:HIS259	3.20637
						A:HIS244	2.58376
						A:HIS263	2.93476
						A:SER282	2.81249
						A:MET280	2.48505
40	Chrysoeriol	300.26	-6.36	21.87 μ M	3	A:HIS85	2.82651
						A:HIS259	3.58735
						A:ASN260	2.68258
						A:MET280	3.29794
41	Ginkgolide B	424.40	-6.16	30.38 μ M	3	A:HIS263	3.58794
						A:HIS244	1.72866
						A:ARG268	3.09288
42	Oxyresveratrol	244.24	-5.93	44.90 μ M	3	A:ASN260	3.06936
						A:ARG268	2.13044
						A:MET280	2.81813
						A:HIS263	3.77046
43	Coumarin	146.14	-5.70	66.40 μ M	1	A:HIS259	3.30589
44	Resveratrol 4'-methyl ether	242.27	-5.66	71.36 μ M	2	A:SER282	2.73416
						A:MET280	2.77858
45	Vanillin	152.15	-5.00	217.70 μ M	2	A:ASN260	3.28389
						A:PHE264	3.77041
46	Guvacoline	141.17	-4.95	234.06 μ M	6	A:ARG321	2.24586
						A:ARG321	1.70808
						A:HIS244	3.79383
						A:GLY86	3.15994
						A:GLU322	2.82850
						A:GLU322	3.10460
47	Phytol	296.53	-4.64	394.43 μ M	0		
48	Arecoline	155.19	-4.56	450.69 μ M	6	A:CYS83	3.57655
						A:HIS85	1.93297
						A:ALA323	3.23921
						A:THR84	3.69370
						A:ASN320	3.21035
						A:GLU322	3.59248
