

**Table S1. Virtual Screening Results of 300 Flavonoids (Molecular Weight < 500 Da).**

Compound	NPC ID	Pubchem ID	Docking score (kcal/mol)	Compound	NPC ID	Pubchem ID.	Docking score (kcal/mol)	Compound	NPC ID	Pubchem ID	Docking score. (kcal/mol)
(+)-(2R) Kazinol I	NPC32630	46871916	-5.9	3'-O-Methyl Epicatechin	NPC16435	11420256	-6.9	6-Hydroxy-5,7-Dimethoxy-2-(4-Methoxyphenyl) Chromen-4-One	NPC22519	243760	-6.7
(+)-30-O-Methyltaxifolin	NPC13858	26194552	-7.2	Isobavachin	NPC164980	193679	-6.8	4'-Hydroxy-5,6,7,8-tetramethoxyflavone	NPC226973	3010100	-6.4
(+)-Epicatechin	NPC261619	182232	-6.9	5,7-Dihydroxy-2-(4-Hydroxyphenyl)-6,8-Dimethyl-2,3-Dihydrochromen-4-one	NPC166482	91144	-6.6	3,5,4'-Trihydroxy-,6,7,3'-trimethoxyflavone	NPC227192	6453535	-7.3
(25)-6,3',4'-Trihydroxy-7-Methoxyflavan	NPC107551	71746435	-7.0	2-(3,4-Dimethoxyphenyl)-3,5-Dihydroxy-7-Methoxychromen-4-one	NPC166753	5748558	-7.2	5-Hydroxy-2-(4-Hydroxy-3-Methoxyphenyl)-6,7,8-Trimethoxychromen-4-One	NPC227325	181092	-6.6
1(S)-4-(7-Methoxychroman-2-yl) Phenol	NPC100099	185609	-6.9	Citrusinol	NPC166757	44259051	nan	5-Methoxy-2-phenyl-2,3-Dihydrochromen-4-One	NPC228184	147795	-7.0
Eupafolin	NPC100887	5317284	-7.1	Pongabrone	NPC167479	10957726	-8.1	7-Hydroxy-3,5-Dimethoxy-2-phenylchromen-4-One	NPC230285	44392177	-6.8
Chrysoplenol G	NPC100916	5315858	-6.5	2-(4-Hydroxyphenyl)-3,4-Dihydro-2H-Chromene-3,5,7-Triol	NPC167571	282014	-6.7	Xanthomicrol	NPC231018	73207	-6.7
Trimethylapigenin	NPC101294	79730	-6.9	Farrerol	NPC167624	442396	-6.6	2-(2,5-Dimethoxyphenyl) Furo[2,3-H] Chromen-4-One	NPC233776	11045499	-7.2
Penduletin	NPC101830	5320462	-7.0	4'-Demethylnobiletin	NPC167815	21593928	-6.5	Kazinol B	NPC233980	480869	-6.3
(2S)-6,4'-Dihydroxy-7,3'-Dimethoxyflavan	NPC102904	71746244	-7.2	Artochamin C	NPC170492	10247422	-8.0	4'-O-Me-Ent-Gallocatechin	NPC234333	10087345	-6.4
Morusunnansins F	NPC103420	57333040	-6.1	5,4,40-Trimethoxyflavan	NPC172253	44437744	-6.8	Kazinol U	NPC234952	46871902	-6.6

Continued Table S1.

Compound	NPC ID	Pubchem ID	Docking score (kcal/mol)	Compound	NPC ID	Pubchem ID.	Docking score (kcal/mol)	Compound	NPC ID	Pubchem ID	Docking score. (kcal/mol)
<b>Tupichinol</b>	NPC103799	637885	-6.5	<b>7-Hydroxy-2-(4-Hydroxyphenyl) chromen-4-one</b>	NPC172262	5282073	-6.9	<b>5,7-Dihydroxy-6-Methoxy-2-Phenyl-2,3-Dihydrochromen-4-One</b>	NPC235165	5316733	-7.1
<b>Hydroxy-3,7-Dimethoxyflavone</b>	NPC103904	5748697	-7.6	<b>Hypolaetin</b>	NPC17286	5281648	-7.1	<b>7-Hydroxy-2-(4-Hydroxy-3-Methoxyphenyl)-3,5-Dimethoxychromen-4-One</b>	NPC236223	14162697	-6.6
<b>(2S)-4'-Hydroxy-6,7,3'-Trimethoxyflavan</b>	NPC103976	71746243	-7.2	<b>Licoflavone B</b>	NPC172986	11349817	-8.4	<b>Homoeriodicytol</b>	NPC236637	73635	-7.0
<b>(2S,3S)-2,3-Trans-5,7-Dihydroxy-6,8-Dimethyldihydroflavanol</b>	NPC105136	49831444	-6.8	<b>Sigmoidin</b>	NPC174953	129362	-7.9	<b>Retusin</b>	NPC236769	5352005	-6.3
<b>Calycopterin</b>	NPC105242	10429470	-6.1	<b>(2S)-5-Hydroxy-7-Methoxy-8-[€-3-oxo-1-Butenyl] Flavanone</b>	NPC175504	10980660	-6.2	<b>Abyssinone I</b>	NPC23728	442152	-8.2
<b>(2S)-4,7-Dihydroxy-8-Methylflavan</b>	NPC106914	442361	-7.0	<b>(2S)-3',4'-Dihydroxy-6,7-Dimethoxyflavan</b>	NPC176051	71746434	-6.5	<b>2-(1,3-Benzodioxol-5-yl)-3,5,7,8-Tetramethoxychromen-4-One</b>	NPC238405	386319	-7.1
<b>Sigmoidin B</b>	NPC106976	73205	-7.5	<b>Obovatin</b>	NPC176229	13940733	-7.9	<b>Mosflavone</b>	NPC239128	471722	-7.5
<b>Sophoraflavaone B</b>	NPC107572	509245	-6.6	<b>Artimetin</b>	NPC176300	5320351	-6.6	<b>3',4',5,6-Tetramethoxy Flavone</b>	NPC23955	14055876	-7.4
<b>(2S)-5,7,2'-Trihydroxyflavanone</b>	NPC107586	13889010	-7.1	<b>2-(3,4-Dihydroxyphenyl)-5,7-Dihydroxy-3,8-Dimethoxychromen-4-one</b>	NPC176665	5748553	-6.5	<b>(2S,3S)-3,3',4',5,7-Pentahydroxy Flavanonol</b>	NPC240476	712316	-7.2
<b>2-(3,4-Dihydroxyphenyl)-5-Hydroxy-7-Methoxychromen-4-One</b>	NPC108406	5318214	-7.0	<b>Gardenin B</b>	NPC176775	96539	-8.7	<b>Artocarpetin</b>	NPC241100	390520	-6.5

Continued Table S1.

Compound	NPC ID	Pubchem ID	Docking score (kcal/mol)	Compound	NPC ID	Pubchem ID.	Docking score (kcal/mol)	Compound	NPC ID	Pubchem ID	Docking score. (kcal/mol)
4'-Isobutyrylhomoeiodictyol	NPC108456	44576022	-7.3	7-O-Methyl-Aromadendrin	NPC176869	181132	-7.1	(S)-5-Hydroxy-7-Methoxy-6-Methyl-4-Oxo-2-phenylchroman-8-Carbaldehyde	NPC2416	12132943	-7.4
(S)-5,7-Dihydroxy-6-Prenylflavanone	NPC1089	6546086	-7.3	Lethedocin	NPC177298	5496476	-6.5	3,3',4'-Trihydroxy-4H-Furo[2,3-H] chromen-4-One	NPC241820	44537939	-7.4
(2S)-Abyssinone II	NPC10937	14218027	-7.4	(S)-7-Hydroxy-5-Methoxy-8-Methyl-2-phenylchroman-4-One	NPC177354	52943439	-6.6	Kaempferide	NPC241838	5281666	-7.1
(S)-5-Hydroxy-7-Methoxy-6,8-Dimethyl-2-Phenylchroman-4-one	NPC110038	21142052	-6.9	(2S)-4,5-Dihydroxy-7-Methoxy-8-Methylflavan	NPC17809	44257197	-6.4	Pinocembrin	NPC243083	68071	-7.2
5-Hydroxy-3,6,7-Trimethoxy-2-(4-Methoxyphenyl) Chromen-4-One	NPC110070	5318355	-6.8	8-O-Methylretusin	NPC178854	10200272	-6.2	Guaphallin	NPC245546	9972910	-7.5
Alpinetin	NPC110228	45273057	-6.6	2-(4-Hydroxy-3-Methoxyphenyl)-3,5,7-Trimethoxychromen-4-One	NPC179126	13942543	-6.8	Chrysosplenol E	NPC246204	5315857	-6.6
Abyssinones III	NPC110303	10408069	-7.8	3',5,5',7-Tetrahydroxyflavanone	NPC18244	52945930	-6.8	3,7,3',4'-Tetrahydroxyflavanone	NPC246328	246330	-7.3
(2S)-3',4'-Dihydroxy-5,7-Dimethoxyflavan	NPC11060	73356683	-6.9	5-Hydroxy-7-Methoxy-6-Methyl-2-phenylchromen-4-One	NPC18260	369599	-7.7	2S)-7,4'-Dihydroxy-8-Prenylflavan	NPC246648	57402293	-6.2
5,7,8,3',4'-Pentamethoxyflavaone	NPC110639	632135	-6.7	2-(3,4-Dimethoxyphenyl)-5,7-Dihydroxy-6,8--Dimethoxychromen-4-one	NPC183597	171488	-6.8	5-Demethylnobiletin	NPC2476	358832	-6.7
Bavachinin	NPC110969	44584224	-7.6	5-Hydroxy-2-(2-Hydroxyphenyl)-6,7,8-Trimethoxychromen-4-One	NPC183878	159029	-6.8	Licoflavonol	NPC24821	5481964	-7.0

Continued Table S1.

Compound	NPC ID	Pubchem ID	Docking score (kcal/mol)	Compound	NPC ID	Pubchem ID.	Docking score (kcal/mol)	Compound	NPC ID	Pubchem ID	Docking score. (kcal/mol)
(2S)-4'-Hydroxy-7,3'-Dimethoxyflavan	NPC112246	14017332	-7.0	Chrysoeriol	NPC183950	5280666	-7.0	Demethoxymatteucinol	NPC248372	180550	-6.8
3-O-Acetylpadmatin	NPC112418	10406203	-7.2	3',4',7'-Trihydroxyflavaone	NPC183959	3496769	-7.1	Anastatin A	NPC248593	10134240	-7.8
(2S)-8,5'-Dihydroxy-7,3',4'-Trimethoxyflavan	NPC112939	44567056	-6.9	4'-O-Methylscutellarein	NPC184136	11174076	-6.8	Agrandol	NPC250214	15895373	-6.8
7,3',4'-Trimethoxyflavone	NPC113089	154227	-7.0	Ombuine	NPC20074	5320287	-7.2	2-(4-Hydroxyphenyl)-7-Methoxychromen-4-One	NPC250266	676307	-6.9
(2S)-7-Methoxy-8-(3-Methoxy-3-Methylbut-1-Enyl)Flaavanone	NPC11566	73349082	-6.7	Chrysosplenol C	NPC18607	189065	-7.0	(2R,3S)-4'-O-Methyl-2,3-Dihydromyricetin	NPC25092	11244528	-7.1
5,7-Dihydroxy-3,3',4',6-Tetramethoxyflavone	NPC115798	5379563	-6.8	7-Methoxyhesperetin	NPC18727	14157910	-6.6	Rhamnazin	NPC252933	5320945	-7.1
Sigmoidin C	NPC118256	44424648	-7.9	Isowogonin	NPC187498	20489	-7.6	5,7-Dihydroxy-2-(4-Hydroxy-3-Methoxyphenyl)-3,8-Dimethoxychromen-4-One	NPC253634	5386961	-6.1
6,7,3',4'-Tetrahydroxyflavone	NPC118726	24721539	-7.2	Chrysosplenol D	NPC18772	5280699	-7.1	Casticin	NPC25495	5315263	-6.4
Ophioglonol	NPC119059	11347622	-7.1	(2R)-7,4'-Dihydroxy-5-Methoxy-8-Methylflavan	NPC188022	44479223	-6.6	Dihydrooroxylin	NPC255106	177032	-7.1
Tricin	NPC120464	5281702	-7.0	2(3,4-Dihydroxyphenyl)5,7-Dihydroxy-8-Methoxychromen-4-One	NPC188203	5316843	-6.9	Eupatilin	NPC255350	5273755	-7.0

Continued Table S1.

Compound	NPC ID	Pubchem ID	Docking score (kcal/mol)	Compound	NPC ID	Pubchem ID.	Docking score (kcal/mol)	Compound	NPC ID	Pubchem ID	Docking score. (kcal/mol)
(2S)-8-Hydroxy-7,3',4'-Tetramethoxyflavan	NPC121812	44567048	-6.4	6-4'-Dimethyl-Naringenin	NPC188243	21721822	-6.6	5,7-Dihydroxy-2-(3-Hydroxy-4-Methoxyphenyl)-6-Methoxychromen-4-One	NPC256283	5469524	-7.0
2-(3,4-Dimethoxyphenyl)-5,7-Dihydroxychromen-4-One	NPC12200	5351234	-7.0	(2R)-2-(3,4-Dihydroxyphenyl)-5,7-Dihydroxy-2,3-Dihydroxychromen-4-One	NPC188679	373261	-7.1	Dihydrorobinetin	NPC256346	17751005	-6.9
Abyssinoflavanone Vi	NPC122365	16737096	-7.9	3,7-O-Dimethylquercetin	NPC188871	5280417	-7.1	7-Hydroxy-3',4',6,8-Tetramethoxyflavone	NPC256612	72204299	-6.9
(2R,3R)-Alpinone	NPC122828	46883390	-6.8	3,5,3'-Trihydroxy-6,7,8,4'-Tetramethoxyflavone	NPC189179	10000451	-6.5	(Rac)-Abyssinone II	NPC257097	10064832	-7.8
6,7-Dihydroxy-2-(4-Hydroxyphenyl)Chromen-4-One	NPC12367	10355753	-7.0	3,7,8-Trimethoxy-5-Hydroxyflavone	NPC189960	21632881	-6.5	Rugosaflavonoid B	NPC258331	72701894	-7.1
5,7,3',5'-Tetrahydroxy-3,4'-Dimethoxyflavone	NPC123886	44259718	-6.9	3,7-Dihydroxy-2-(4-Hydroxyphenyl)-3,6,8-Trimethoxychromen-4-One	NPC191459	5386960	-6.2	6-Hydroxy-8,8-Dimethyl-2-Phenylpyrano[2,3-H]Chromen-4-One	NPC259456	38364007	-8.2
2(S)-5,7-Dimethoxy-8-(2S-Hydroxy-3-Methyl-3-Butenyl)-Flavanone	NPC124780	11046839	-6.4	Cyrtominetin	NPC192083	125309	-6.9	Norwogonin	NPC259713	5281674	-7.4
Artocarpetin	NPC124784	12308618	-7.3	2'-Hydroxyflavone	NPC193805	161860	-6.9	(2R,3S)-2-(3,4-Dihydroxyphenyl)-3,5,7-Trihydroxy-2,3-Dihydrochromen-4-One	NPC260491	712318	-6.9
2-(4-Methoxyphenyl)-6-MethylChromen-4-One	NPC125887	688682	-7.3	Diplotrin A	NPC193842	54672084	-6.5	7,3',4'-Trihydroxy-3-Methoxyflavone	NPC260895	9839293	-6.7
Techtochrysin	NPC127447	5281954	-7.5	Garbonzol	NPC1940	442410	-7.0	4'-O-Methyl-Gallocatechin	NPC260898	44257120	-7.2

Continued Table S1.

Compound	NPC ID	Pubchem ID	Docking score (kcal/mol)	Compound	NPC ID	Pubchem ID.	Docking score (kcal/mol)	Compound	NPC ID	Pubchem ID	Docking score. (kcal/mol)
Malvidin	NPC127624	159287	-6.3	7-Hydroxy-5-Methoxy-2-phenylchromen-4-One	NPC194281	5490127	-6.7	Chrysosplenol B	NPC2601004	5281608	-6.8
5,6-Dihydroxy-2-(4-Hydroxy-3-Methoxyphenyl)-7,8-DimethoxyChromen-4-One	NPC128863	442662	-6.6	(S)-5-Hydroxy-7-Methoxy-8-Methyl-2-phenylchroman-4-One	NPC194432	51520434	-6.4	Kanzonol D	NPC261227	15291875	-7.8
3'-Methoxy-[2'',3'':7,8]Furanoflavone	NPC130015	636768	-7.7	7,3',4'-Tri-O-Methyluteolin	NPC195202	5272653	-7.1	2-(3,4-Dimethoxyphenyl)-3-Hydroxy-5,7-Dimethoxychromen-4-One	NPC261548	97142	-6.9
Scutellarein	NPC130230	5281697	-6.4	6-Hydroxykaempferol	NPC195351	52816348	-7.1	Neophellamuretin	NPC262038	44559644	-6.9
2-(3,4-Dihydroxyphenyl)-5,7-Dihydroxy-3,6,8-Trimethoxychromen-4-one	NPC130894	5386962	-7.1	3',5-Dihydroxy-4',6,7,8-Tetramrthoxyflavone	NPC196439	3080750	-6.9	Norartocarpetin	NPC274121	5481970	-8.3
5,3'-Dihydroxy-4'-Methoxy-7-Carbomethoxy flavonol	NPC130955	10043920	-6.6	(2R,3R)-3,5,7-Trihydroxy-2-(3,4,5-Trihydroxyphenyl)-2,3-Dihydrochromen-4-One	NPC19721	161557	-7.1	Alnusin	NPC26227	12305751	-7.3
Meliteratin	NPC131557	386320	-8.0	(2S)-7,4'-Dihydroxy-3'-Prenylflavon	NPC197351	10990534	-7.5	Inustinol	NPC263449	44446838	-6.9
Wogonin	NPC131624	5281703	-7.3	7-O-Methylscutellarein	NPC198826	3084390	-7.3	Kazinol A	NPC265075	442414	-6.1
Laricytrin	NPC133953	5282154	-7.3	Oxyayanin	NPC200383	5281676	-6.4	Diplotrin B	NPC265511	54669843	-6.7
(2R)-4'-Hydroxy-7-Methoxy-8-Methylflavan	NPC134195	44445076	-6.6	Isolicoflavonol	NPC200694	5318585	-7.7	7-Hydroxy-5-Methoxyflavanone	NPC265871	4053302	-6.7
(S)-5,7,8'-Trihydroxy-2',2'-Dimethyl-2,6'-Bichroman-4,4'-Dione	NPC134783	44589231	-8.1	Abyssinin II	NPC200761	442457	-7.0	Pratol	NPC266597	5320693	-7.1

Continued Table S1.

Compound	NPC ID	Pubchem ID	Docking score (kcal/mol)	Compound	NPC ID	Pubchem ID.	Docking score (kcal/mol)	Compound	NPC ID	Pubchem ID	Docking score. (kcal/mol)
4',7'-Dihydroxy-3-Methoxyflavone	NPC136840	14804705	-6.7	Sideritiflavone	NPC201136	155493	-6.9	(2S)-2,7-Dihydroxy-5-Methoxy-6,8-Dimethylflavanone	NPC266725	49831445	-6.8
Velutin	NPC137062	5464381	-7.1	5,7-Dihydroxy-6-Methyl-2-phenylchromen-4-one	NPC201395	11536318	-7.5	Gallocatechin	NPC268342	65084	-7.2
(R)-Pinocebrin	NPC13768	667544	-7.3	Prudomestin	NPC201451	10404353	-7.0	Ayanin	NPC270620	5280682	-6.7
3',4'-Didemethylnobiletin	NPC138360	5318041	-6.8	Santin	NPC203891	5281695	-6.6	Licoflavanone A	NPC270883	5319000	-7.6
(+)-30-O-Methyltaxifolin	NPC13858	26194552	-7.2	(2S)-Dihydrobaicalein	NPC204515	14135323	-7.0	Gossypetin	NPC27208	5280647	-7.1
(S)-5-Hydroxy-7-Methoxy-2-(2,4,6-Trimethoxy phenyl) chroman-4-one	NPC140890	15298900	-5.9	5,7,3'-Trihydroxy-3,6,8,4-Tetramethoxyflavone	NPC204854	21599528	-6.5	Kaempferol 3,7,4'-trimethyl ether	NPC262094	5468749	-6.1
Viscidulin III	NPC142540	5271991	-6.4	Buceracidin B	NPC20488	44584124	-8.5	Amorphigenin	NPC128293	92207	-7.3
Rhamnocitrin	NPC143799	5320946	-7.1	Uralenol	NPC205046	5315126	-7.8	Licopyranocoumarin	NPC103116	122851	-7.4
5-Hydroxyauranetin	NPC143828	11079623	-6.3	3',4',6,7,8-Pentamethoxyflavone	NPC205522	44584772	-6.9	Glabridin	NPC119985	124052	-8.1
Abyssinone IV	NPC143896	7330513	-7.7	5,7-Dihydroxy-2-(4-Methoxyphenyl) chromen-4-one	NPC20709	5118250	-6.5	Erythrabyssin I	NPC124085	126540	-8.8
Salvigenin	NPC145379	161271	-6.7	(2S)-2',3,5,6',7-Pentahydroxyflavanone	NPC208176	157633	-7.0	Barbigerone	NPC128961	156793	-5.7
Acerosin	NPC146165	177696	-7.1	3',8-Dihydroxy-4',5',6,7-Tetramethoxyflavone	NPC208197	72204300	-7.1	(+)-Maackiain	NPC11422	161298	-6.8
Kumatakenin	NPC146679	5318869	-6.8	Cirsilineol	NPC20830	14235159	-7.3	(2-Methyl-4-Oxo-3-Phenylchroman-7-yl) acetate	NPC103001	268208	-7.9
(2S)-2,3-Dihydrotephroapollin C	NPC147145	52316190	-6.7	(2S)-7-Methoxy-4',6-Dihydroxyisoflavanone	NPC210084	25181514	-7.2	Toxicarol	NPC120593	442826	-6.7

Continued Table S1.

Compound	NPC ID	Pubchem ID	Docking score (kcal/mol)	Compound	NPC ID	Pubchem ID.	Docking score (kcal/mol)	Compound	NPC ID	Pubchem ID	Docking score. (kcal/mol)
Liquiritigenin	NPC147686	114829	-6.7	3,5,7-Trihydroxy-4'-Methoxyflavanol	NPC211466	21721857	-7.0	Glabrene	NPC134360	480774	-6.6
(2R,3R)-3,7-Dihydroxyflavanone	NPC148011	14730799	-7.1	5,6-Dihydroxy-2-(3-Hydroxy-4-Methoxyphenyl)-7-Methoxychromen-4-One, 1	NPC212678	373260	-7.0	6-Methoxyboeravinone	NPC108202	487169	-7.3
Pinnatin	NPC14871	5320607	-7.5	5,7-Dihydroxy-2-(2-Hydroxyphenyl) Chromen-4-One	NPC213216	5322064	-7.1	6,7-Dimethoxy-3-(4-Methoxyphenyl) Chromen-4-one	NPC120924	688655	-6.9
6-Cinnamylchrysin	NPC14831	636685	-8.1	(S)-5,7-Dihydroxy-8-Methyl-2-Phenylchroman-4-One	NPC213322	6453244	-6.6	7-O-Acetylformononetin	NPC136095	908827	6.7
4'-o-Mrthyl-8-Prenylnaringenin	NPC148757	45272659	-6.7	Amyrisin C	NPC213622	57381728	-7.4	nan	nan	5280551	-7.1
Lespeflorin A2	NPC149026	25243165	-6.8	2-(3,4-Dihydroxyphenyl)-5,6,7-Trihydroxy-3-Methoxychromen-4-one	NPC214138	5320475	-7.0	Castanin	NPC121522	5281704	-6.9
2-(3,4-Dihydroxyphenyl)-7-Hydroxy-3,5-Dimethoxychromen-4-one	NPC149127	5489501	-6.9	Zapotin	NPC214919	629965	-6.3	Puerarin	NPC124478	5281807	-7.4
Tetramethylscutellarein	NPC14958	96118	-6.3	(S)-5-Hydroxy-7-Methoxy-8-Methyl-4-Oxo-2-Phenylchroman-6-Carbaldehyde	Npc215885	52945746	-6.8	Formonetin	NPC10467	5281812	-7.3
4'-Hydroxy-7,8(2'',2'')-Dimethylpyran)Flavan	NPC149796	3012489	-7.2	5,6,7,8-Tetrahydroxy-2-(4-Hydroxyphenyl) Chromen-4-One,	NPCc216318	96506	-7.1	Corylin	NPC104406	5316097	-9.1
Glabrol	NPC150408	11596309	-7.9	Sophoflavescenol	NPC216538	9929189	-6.6	Lupiwighteonone	NPC144118	5317480	-7.5
Izalpinin	NPC152042	5318691	-7.4	7-Hydroxy-5-Methoxy-6,8-Dimethyl-2-Phenylchromen-4-One	NPC217186	14753671	-6.8	Isoerysegalensin E	NPC117836	5318561	-6.5



Continued Table S1.

Compound	NPC ID	Pubchem ID	Docking score (kcal/mol)	Compound	NPC ID	Pubchem ID.	Docking score (kcal/mol)	Compound	NPC ID	Pubchem ID	Docking score. (kcal/mol)
Teratin	NPC152166	5459184	-6.2	Yukovanol	NPC217706	44584009	-7.3	3'-Methoxydaidzein	NPC139364	5319422	-7.1
Ophioglonin	NPC153512	11461162	-7.3	(2R,3R)-3,3',5,5',7-Pentahydroxy Flavanonol	NPC21835	5320468	-7.1	5-O-Methylglycryol	NPC11543	5319666	-7.9
Pongapinone B	NPC155063	127022	-6.8	3,5,7-Trihydroxy-3',4',5'-trimethoxyflavone	NPC219330	5481248	-7.2	1,3,8-Trihydroxy-[1]Benzofuro[2,3-B]Chromen-11-One	NPC13879	5324349	-7.8
Hamilton A	NPC156057	44566483	-6.4	8-Prenylapigenin	NPC220062	10246505	-6.7	Psi-Tectorigenin	NPC131266	5353911	-7.0
Gancaonin P	NPC157784	5481966	-7.6	Epigallocatechin	NPC220825	72277	-6.9	4',7-Dimethoxy-5-Hydroxygenistein	NPC116632	5386259	-6.9
2'',2''-Dimethylchromene-[5'',6'':7,8]-Flavon	NPC157855	11358607	-8.1	Munduleaflavanone B	NPC220998	42608071	-6.3	2'-O-Methylarbonisofalvone	NPC101366	5482494	-6.9
Quercetin-3',4'-Di-O-Methyl Ether	NPC159103	5487855	-6.5	Abyssinin II	NPC221432	7330517	-7.8	Cladrin	NPC12377	5748605	-7.2
Sideroxylin	NPC159275	3083788	-6.7	5,7-dihydroxy-2-(2-hydroxyphenyl)-8-methoxychromen-4-one	NPC222830	5321205	-6.6	Wistin	NPC135345	10095770	-7.3
Butin	NPC1612	92775	-7.1	Cudraflavanone B	NPC223500	509244	-6.5	Derrisin	NPC103307	10274158	-7.9
2-(3,4-Dihydroxyphenyl)-5,6-Dihydroxy-7-Methoxychromen-4-one	NPC162313	31161	-7.2	5-Hydroxy-2-(3-Hydroxy-4-Methoxyphenyl)-7-Methoxychromen-4-One	NPC223579	5320496	-7.0	R-Coluteol	NPC127218	10336847	-6.8
Myricetin 3,3',4'-Trimethylether	NPC162351	44259719	-6.5	Kushenol V	NPC223787	10572194	-7.5	Crotafuran B	NPC109180	10358740	-7.5
Axillarlin	NPC163524	5281603	-6.8	(2S)-5,7-Dimethoxy-8-Formylflavanone	NPC22467	10335676	-7.2	Erystagallin A	NPC117048	10410005	-6.8
5-8-Dihydroxy-3',4',6,7-Tetramethoxyflavone	NPC163780	72714814	-6.6	2-(3,4-Dihydroxyphenyl)-5-Hydroxy-3,6,7,8-Tetramethoxychromen-4-One	NPC22472	54799	-6.6	Isoformonetin	NPC181124	3764	-5.8