

Supplementary materials

Identification of Dietary Bioflavonoids as Potential Inhibitors against KRAS G12D Mutant—Novel Insights from Computer-Aided Drug Discovery

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Supplementary Table S1: Binding energies of all 514 bioflavonoids with the KRAS G12D mutant protein. The binding energy (Kcal/mol) of all the compounds were tabulated according to their higher negative values and the BI-2852 was shown in bold.

Ligand model number	Flavonoid/ Compound name	Canonical SMILES	Binding Affinity
model_684	5-Dehydroxyparatocarpin K	<chem>Oc1ccc(cc1)C1CC(=O)c2c(O1)cc1c(c2)C=CC(O1)(C)C</chem>	-8.8
model_298	Carpachromene	<chem>Oc1ccc(cc1)c1cc(=O)c2c(O1)cc1c(c2O)C=CC(O1)(C)C</chem>	-8.6
model_765	Sanggenone H	<chem>Oc1cc2OC(CC(=O)c2c(c1O)c1ccc(c2c1OC(C)(C)C=C2)O</chem>	-8.6
model_654	Kuwanol C	<chem>CC(=CCCC1(C)C=Cc2c(O1)cc1c(c2O)C(=O)CC(O1)c1ccc(c1O)O)C</chem>	-8.5
Reference	BI-2852	<chem>CN1C=C(N=C1)CN2C=CC3=C2C=C(C=C3)CNCC4=C(C5=CC=CC=C5N4)C6C7=C(C=CC(=C7)O)C(=O)N6</chem>	-8.5
model_379	Kazinol B	<chem>CC(=CCc1c(cc2c(c1O)OC(C=C2)(C)C)C1CCc2c(O1)cc(cc2)O)C</chem>	-8.4
model_395	Cyclomorusin	<chem>CC(=CC1Oc2cc(O)ccc2c2c1c(=O)c1c(O2)c2C=CC(Oc2cc1O)(C)C)C</chem>	-8.4
model_874	Furano(2'',3'',7,6)-4'-hydroxyflavanone	<chem>Oc1ccc(cc1)C1CC(=O)c2c(O1)cc1c(c2)cco1</chem>	-8.4
model_138	Barbacarpan	<chem>CC(=C)C1Oc2c(C1)c1OC3C(c1cc2)COc1c3ccc(c1)O</chem>	-8.3
model_816	Licoisoflavone B	<chem>Oc1cc(O)c2c(c1)occ(c2=O)c1ccc2c(c1O)C=CC(O2)(C)C</chem>	-8.3
model_100	Maackiain	<chem>Oc1ccc2c(c1)OCC1C2Oc2c1cc1c(c2)OCO1</chem>	-8.2
model_799	Ophiopogonanone A	<chem>O=C1C(COc2c1c(O)c(c(c2O)C)Cc1ccc2c(c1)OCO2</chem>	-8.2
model_92	Glabridin	<chem>Oc1ccc(c(c1O)C1COc2c(C1)ccc1c2C=CC(O1)(C)C</chem>	-8.2
model_970	Cudraflavone B	<chem>CC(=CCc1c(oc2c(c1=O)c(O)c1c(c2)OC(C=C1)(C)C)c1ccc(c1O)O)C</chem>	-8.2
model_814	Glabrene	<chem>Oc1ccc2c(c1)OCC(=C2)c1ccc(c2c1OC(C)(C)C=C2)O</chem>	-8.1
model_257	Methylophiopogonanone A	<chem>O=C1C(COc2c1c(O)c(C)c(c2C)O)Cc1ccc2c(c1)OCO2</chem>	-8
model_400	Butin	<chem>Oc1ccc2c(c1)OC(CC2=O)c1ccc(c(c1)O)O</chem>	-8
model_689	Methylophiopogonone A	<chem>Cc1c(O)c(C)c2c(c1O)c(=O)c(co2)Cc1ccc2c(c1)OCO2</chem>	-8
model_758	Semilicoisoflavone B	<chem>Oc1cc(O)c2c(c1)occ(c2=O)c1cc(O)c2c(c1)C=CC(O2)(C)C</chem>	-8
model_785	7,8-Benzoflavone	<chem>O=c1cc(oc2c1ccc1c2cccc1)c1cccc1</chem>	-8
model_1002	Methylophiopogonone B	<chem>COc1ccc(cc1)Cc1coc2c(c1=O)c(O)c(c(c2C)O)C</chem>	-7.9
model_1056	Ophiopogonanone B	<chem>COc1ccc(cc1)CC1COc2c(C1=O)c(O)c(c(c2O)C</chem>	-7.9
model_128	Bavachin	<chem>CC(=CCc1cc2C(=O)CC(Oc2cc1O)c1ccc(cc1)O)C</chem>	-7.9
model_134	Fustin	<chem>Oc1ccc2c(c1)OC(C(C2=O)O)c1ccc(c(c1)O)O</chem>	-7.9

model_258	Methylophiopogonanone B	<chem>COc1ccc(cc1)CC1COc2c(C1=O)c(O)c(c(c2C)O)C</chem>	-7.9
model_286	Corylin	<chem>Oc1ccc2c(c1)occ(c2=O)c1ccc2c(c1)C=CC(O2)(C)C</chem>	-7.9
model_49	Liquiritigenin	<chem>Oc1ccc(cc1)C1CC(=O)c2c(O1)cc(cc2)O</chem>	-7.9
model_581	7-Hydroxy-3-(4-hydroxybenzyl)chromic	<chem>Oc1ccc(cc1)CC1COc2c(C1)ccc(c2)O</chem>	-7.9
model_604	Isoderrone	<chem>Oc1cc(O)c2c(c1)occ(c2=O)c1ccc2c(c1)C=CC(O2)(C)C</chem>	-7.9
model_624	Cedeodarin	<chem>Oc1ccc(cc1O)C1Oc2cc(O)c(c(c2C(=O)C1O)O)C</chem>	-7.9
model_839	Poriol	<chem>Oc1ccc(cc1)C1CC(=O)c2c(O1)cc(c(c2O)C)O</chem>	-7.9
model_1038	Pomiferin	<chem>CC(=CCc1c2OC(C)(C)C=Cc2c2c(c1O)c(=O)c(co2)c1ccc(c(c1)O)O)C</chem>	-7.8
model_1060	Licoflavone A	<chem>CC(=CCc1cc2c(=O)cc(oc2cc1O)c1ccc(cc1)O)C</chem>	-7.8
model_1066	Glyasperin F	<chem>Oc1cc(O)c2c(c1)OCC(C2=O)c1ccc(c2c1OC(C)(C)C=C2)O</chem>	-7.8
model_118	Dihydromorin	<chem>Oc1ccc(c(c1)O)C1Oc2cc(O)cc(c2C(=O)C1O)O</chem>	-7.8
model_169	Fisetin	<chem>Oc1ccc2c(c1)oc(c(c2=O)O)c1ccc(c(c1)O)O</chem>	-7.8
model_17	3-Deoxysappanone B	<chem>Oc1ccc2c(c1)OCC(C2=O)Cc1ccc(c(c1)O)O</chem>	-7.8
model_218	Anhydrotuberosin	<chem>Oc1ccc2c(c1)OCc1c2oc2c1cc1c(c2)OC(C=C1)(C)C</chem>	-7.8
model_266	7-O-Methyleriodictyol	<chem>COc1cc2OC(CC(=O)c2c(c1)O)c1ccc(c(c1)O)O</chem>	-7.8
model_280	Scillascillin	<chem>Oc1cc(O)c2c(c1)OCC1(C2=O)Cc2c1cc1c(c2)OCO1</chem>	-7.8
model_304	Isobonducellin	<chem>COc1ccc(cc1)C=C1COc2c(C1=O)ccc(c2)O</chem>	-7.8
model_726	Demethylvestitol	<chem>Oc1ccc2c(c1)OCC(C2)c1ccc(cc1O)O</chem>	-7.8
model_768	Coccineone B	<chem>Oc1cc(O)c2c(c1)oc1c(c2=O)c2ccccc2OC1O</chem>	-7.8
model_788	4'-Hydroxyflavanone	<chem>Oc1ccc(cc1)C1CC(=O)c2c(O1)cccc2</chem>	-7.8
model_833	Plathymenin	<chem>O=C1CC(Oc2c1cc(O)c(c2)O)c1ccc(c(c1)O)O</chem>	-7.8
model_834	Garbanzol	<chem>Oc1ccc(cc1)C1Oc2cc(O)ccc2C(=O)C1O</chem>	-7.8
model_87	Eriodictyol	<chem>Oc1cc2OC(CC(=O)c2c(c1)O)c1ccc(c(c1)O)O</chem>	-7.8
model_1036	Glabrone	<chem>Oc1ccc2c(c1)occ(c2=O)c1ccc2c(c1O)C=CC(O2)(C)C</chem>	-7.7
model_1062	Licoflavone B	<chem>CC(=CCc1cc2c(=O)cc(oc2cc1O)c1ccc(c(c1)CC=C(C)C)O)C</chem>	-7.7
model_121	Morin	<chem>Oc1ccc(c(c1)O)c1oc2cc(O)cc(c2c(=O)c1O)O</chem>	-7.7
model_167	Sakuranetin	<chem>COc1cc2OC(CC(=O)c2c(c1)O)c1ccc(cc1)O</chem>	-7.7
model_188	Alpinumisoflavone	<chem>Oc1ccc(cc1)c1coc2c(c1=O)c(O)c1c(c2)OC(C=C1)(C)C</chem>	-7.7
model_206	7,4'-Dihydroxy-3'-prenylflavan	<chem>CC(=CCc1cc(ccc1O)C1CCc2c(O1)cc(cc2)O)C</chem>	-7.7
model_231	Taxifolin	<chem>Oc1cc2OC(c3ccc(c(c3)O)O)C(C(=O)c2c(c1)O)O</chem>	-7.7
model_239	Naringenin	<chem>Oc1ccc(cc1)C1CC(=O)c2c(O1)cc(cc2O)O</chem>	-7.7
model_253	Luteolin	<chem>Oc1cc(O)c2c(c1)oc(cc2=O)c1ccc(c(c1)O)O</chem>	-7.7

model_292	Steppogenin	<chem>Oc1ccc(c(c1)O)C1CC(=O)c2c(O1)cc(cc2O)O</chem>	-7.7
model_388	Derrone	<chem>Oc1ccc(cc1)c1coc2c(c1=O)c(O)cc1c2C=CC(O1)(C)C</chem>	-7.7
model_411	7,3',4'-Trihydroxyflavone	<chem>Oc1ccc(cc1)c1oc2cc(O)ccc2c(=O)c1O</chem>	-7.7
model_578	Euchrenone A10	<chem>CC(=CCc1c(O)cc(c2c1OC(CC2=O)c1ccc2c(c1)C=CC(O2)(C)C)O)C</chem>	-7.7
model_626	Osajin	<chem>CC(=CCc1c2OC(C)(C)C=Cc2c2c(c1O)c(=O)c(co2)c1ccc(cc1)O)C</chem>	-7.7
model_644	Atalantoflavone	<chem>Oc1ccc(cc1)c1cc(=O)c2c(o1)c1C=CC(Oc1cc2O)(C)C</chem>	-7.7
model_697	6-Aldehydoisooophiopogonanone A	<chem>O=Cc1c(O)c2C(=O)C(COc2c(c1O)C)Cc1ccc2c(c1)OCO2</chem>	-7.7
model_773	Isookanin	<chem>O=C1CC(Oc2c1ccc(c2O)O)c1ccc(c(c1)O)O</chem>	-7.7
model_796	Ophiopogonanone C	<chem>O=Cc1c2OCC(C(=O)c2c(c(c1O)C)O)Cc1ccc2c(c1)OCO2</chem>	-7.7
model_971	Shuterin	<chem>CC(=CCc1c(O)cc2c(c1O)C(=O)C(C(O2)c1ccc(cc1)O)O)C</chem>	-7.7
model_975	Hyperxanthone E	<chem>Oc1cc(O)c2c(c1)oc1c(c2=O)c2CCC(Oc2c(c1)O)(C)C</chem>	-7.7
model_13	7,3',4'-Trihydroxy-3-benzyl-2H-chromene	<chem>Oc1ccc2c(c1)OCC(=C2)Cc1ccc(c(c1)O)O</chem>	-7.6
model_130	Hydroxygenkwanin	<chem>COc1cc(O)c2c(c1)oc(cc2=O)c1ccc(c(c1)O)O</chem>	-7.6
model_222	Genkwanin	<chem>COc1cc(O)c2c(c1)oc(cc2=O)c1ccc(cc1)O</chem>	-7.6
model_23	Quercetin	<chem>Oc1cc(O)c2c(c1)oc(c(c2=O)O)c1ccc(c(c1)O)O</chem>	-7.6
model_233	Aromadendrin	<chem>Oc1ccc(cc1)C1Oc2cc(O)cc(c2C(=O)C1O)O</chem>	-7.6
model_242	Hydrangenol	<chem>Oc1ccc(cc1)C1OC(=O)c2c(C1)cccc2O</chem>	-7.6
model_267	Kaempferol	<chem>Oc1ccc(cc1)c1oc2cc(O)cc(c2c(=O)c1O)O</chem>	-7.6
model_272	Apigenin	<chem>Oc1ccc(cc1)c1cc(=O)c2c(o1)cc(cc2O)O</chem>	-7.6
model_306	5-O-Methylnaringenin	<chem>COc1cc(O)cc2c1C(=O)CC(O2)c1ccc(cc1)O</chem>	-7.6
model_327	Isowighteone	<chem>CC(=CCc1cc(ccc1O)c1coc2c(c1=O)c(O)cc(c2)O)C</chem>	-7.6
model_340	Padmatin	<chem>COc1cc2OC(c3ccc(c(c3)O)O)C(C(=O)c2c(c1)O)O</chem>	-7.6
model_382	Hydroxytuberosone	<chem>O=C1C=CC2(C(=C1)OCC1(C2Oc2c1cc1c(c2)OC(C=C1)(C)C)O)O</chem>	-7.6
model_444	6-Prenylnaringenin	<chem>CC(=CCc1c(O)cc2c(c1O)C(=O)CC(O2)c1ccc(cc1)O)C</chem>	-7.6
model_525	Albanin A	<chem>CC(=CCc1c(oc2c(c1=O)c(O)cc(c2)O)c1ccc(cc1O)O)C</chem>	-7.6
model_526	beta-Rhamnocitrin	<chem>COc1cc(O)c2c(c1)oc(c(c2=O)O)c1ccc(c(c1)O)O</chem>	-7.6
model_591	Sanggenol A	<chem>CC(=CCc1c(O)ccc(c1O)C1CC(=O)c2c(O1)cc(cc2O)O)CCC=C(C)C</chem>	-7.6
model_605	Yukovanol	<chem>Oc1ccc(cc1)C1Oc2c(C(=O)C1O)c(O)cc1c2C=CC(O1)(C)C</chem>	-7.6
model_610	Dihydrobonducellin	<chem>COc1ccc(cc1)CC1COc2c(C1=O)ccc(c2)O</chem>	-7.6
model_637	2-Hydroxynaringenin	<chem>Oc1ccc(cc1)C1(O)CC(=O)c2c(O1)cc(cc2O)O</chem>	-7.6

model_668	Dihydroobovatin	<chem>O=C1CC(Oc2c1c(O)cc1c2CCC(O1)(C)C)c1cccc1</chem>	-7.6
model_798	6-Aldehydo-isoophiopogonone A	<chem>O=Cc1c(O)c(C)c2c(c1O)c(=O)c(o2)Cc1ccc2c(c1)OCO2</chem>	-7.6
model_856	3,9-Dihydroeucomin	<chem>COc1ccc(cc1)CC1COc2c(C1=O)c(O)cc(c2)O</chem>	-7.6
model_890	4-O-Methylbutein	<chem>COc1ccc(cc1O)C=CC(=O)c1ccc(cc1O)O</chem>	-7.6
model_923	Eucomol	<chem>COc1ccc(cc1)CC1(O)COc2c(C1=O)c(O)cc(c2)O</chem>	-7.6
model_973	Gericudranin E	<chem>Oc1ccc(cc1)Cc1c(O)cc2c(c1O)C(=O)C(C(O2)c1ccc(cc1)O)O</chem>	-7.6
model_974	Artocarpesin	<chem>CC(=CCc1c(O)cc2c(c1O)c(=O)cc(o2)c1ccc(cc1O)O)C</chem>	-7.6
model_988	5,7-Dimethoxyluteolin	<chem>COc1cc(OC)c2c(c1)oc(cc2=O)c1ccc(c(c1)O)O</chem>	-7.6
model_1011	Azaleatin	<chem>COc1cc(O)cc2c1c(=O)c(c(o2)c1ccc(c(c1)O)O)O</chem>	-7.5
model_1083	Tuberosin	<chem>Oc1ccc2c(c1)OCC1(C2Oe2c1cc1c(c2)OC(C=C1)(C)C)O</chem>	-7.5
model_127	Bavachinin	<chem>COc1cc2OC(CC(=O)c2cc1CC=C(C)C)c1ccc(cc1)O</chem>	-7.5
model_139	Agrimonolide	<chem>COc1ccc(cc1)CCC1OC(=O)c2c(C1)cc(cc2O)O</chem>	-7.5
model_153	(-)-Epiafzelechin	<chem>Oc1ccc(cc1)C1Oc2cc(O)cc(c2CC1O)O</chem>	-7.5
model_210	Scutellarein	<chem>Oc1ccc(cc1)c1cc(=O)c2c(o1)cc(c(c2O)O)O</chem>	-7.5
model_250	Epicatechin	<chem>Oc1cc2OC(c3ccc(c(c3)O)O)C(Cc2c(c1)O)O</chem>	-7.5
model_311	Morusin	<chem>CC(=CCc1c(o2c(c1=O)c(O)cc1c2C=CC(O1)(C)C)c1ccc(cc1O)O)C</chem>	-7.5
model_316	Dihydroalpinumisoflavone	<chem>Oc1ccc(cc1)c1coc2c(c1=O)c(O)c1c(c2)OC(CC1)(C)C</chem>	-7.5
model_320	4',5-Dihydroxyflavone	<chem>Oc1ccc(cc1)c1cc(=O)c2c(o1)cccc2O</chem>	-7.5
model_326	4',5,7-Trihydroxy-6-prenylflavone/ 6-Prenylapigenin	<chem>CC(=CCc1c(O)cc2c(c1O)c(=O)cc(o2)c1ccc(cc1)O)C</chem>	-7.5
model_363	6-Methoxynaringenin	<chem>COc1c(O)cc2c(c1O)C(=O)CC(O2)c1ccc(cc1)O</chem>	-7.5
model_381	8-Isomulberrin hydrate	<chem>Oc1ccc(c(c1)O)c1oc2c3CCC(Oc3cc(c2c(=O)c1CCC(O)(C)C)O)(C)C</chem>	-7.5
model_399	Rhamnocitrin	<chem>COc1cc(O)c2c(c1)oc(c(c2=O)O)c1ccc(cc1)O</chem>	-7.5
model_487	8-Demethylsideroxylin	<chem>COc1cc2oc(cc(=O)c2c(c1C)O)c1ccc(cc1)O</chem>	-7.5
model_506	Isonobavaisoflavone	<chem>Oc1ccc2c(c1)occ(c2=O)c1ccc2c(c1)CCC(O2)(C)C</chem>	-7.5
model_509	Erythrinin A	<chem>Oc1ccc(cc1)c1coc2c(c1=O)cc1c(c2)OC(C=C1)(C)C</chem>	-7.5
model_538	6-Hydroxykaempferol	<chem>Oc1ccc(cc1)c1oc2cc(O)c(c(c2c(=O)c1O)O)O</chem>	-7.5
model_553	Cyclomulberrin	<chem>CC(=CCc1c(O)cc(c2c1oc1c3ccc(cc3OC(c1c2=O)C=C(C)C)O)O)C</chem>	-7.5
model_556	5,7-Di-O-methylquercetin	<chem>COc1cc(O)c2c(c1)oc(c(c2=O)OC)c1ccc(c(c1)O)O</chem>	-7.5
model_560	Kaempferol 5-methyl ether	<chem>COc1cc(O)cc2c1c(=O)c(c(o2)c1ccc(cc1)O)O</chem>	-7.5
model_563	Cudraflavanone B	<chem>CC(=CCc1c(O)cc2c(c1O)C(=O)CC(O2)c1ccc(cc1O)O)C</chem>	-7.5
model_568	Eriosematin A	<chem>CC(=CCc1c(O)cc(c2c1occc2=O)O)C</chem>	-7.5

model_593	6-Methoxyluteolin	<chem>COc1c(O)cc2c(c1O)c(=O)cc(o2)c1ccc(c(c1)O)O</chem>	-7.5
model_603	Sanggenol L	<chem>CC(=CCCC1(C)C=Cc2c(O1)cc(c1c2OC(CC1=O)c1ccc(cc1O)O)O)C</chem>	-7.5
model_628	Neorauflavane	<chem>COc1c2CC(COc2cc2c1C=CC(O2)(C)C)c1ccc(cc1O)O</chem>	-7.5
model_643	Neorauflavene	<chem>COc1c2C=C(COc2cc2c1C=CC(O2)(C)C)c1ccc(cc1O)O</chem>	-7.5
model_656	7-O-Methylporiol	<chem>COc1cc2OC(CC(=O)c2c(c1C)O)c1ccc(cc1)O</chem>	-7.5
model_676	Isokaempferide	<chem>COc1c(oc2c(c1=O)c(O)cc(c2)O)c1ccc(cc1)O</chem>	-7.5
model_696	4',7-Isoflavandiol	<chem>Oc1ccc(cc1)C1COc2c(C1)ccc(c2)O</chem>	-7.5
model_704	Thevetiaflavone	<chem>COc1cc(O)cc2c1c(=O)cc(o2)c1ccc(cc1)O</chem>	-7.5
model_73	Thunberginol C	<chem>Oc1ccc(cc1)C1OC(=O)c2c(C1)cc(cc2O)O</chem>	-7.5
model_76	3-O-Methylquercetin	<chem>COc1c(oc2c(c1=O)c(O)cc(c2)O)c1ccc(c(c1)O)O</chem>	-7.5
model_763	Kuwanon A	<chem>CC(=CCc1c(oc2c(c1=O)c(O)cc(c2)O)c1ccc(c2c1OC(C)(C)C=C2)O)C</chem>	-7.5
model_850	Sophoraisoflavone A	<chem>Oc1cc(O)c2c(c1)occ(c2=O)c1ccc(c2c1OC(C)(C)C=C2)O</chem>	-7.5
model_857	Topazolin	<chem>COc1c(oc2c(c1=O)c(O)c(c2)O)CC=C(C)C)c1ccc(cc1)O</chem>	-7.5
model_9	3'-Hydroxy-3,9-dihydroeucomin	<chem>COc1ccc(cc1O)CC1COc2c(C1=O)c(O)cc(c2)O</chem>	-7.5
model_932	Licoflavonol	<chem>CC(=CCc1c(O)cc2c(c1O)c(=O)c(c(o2)c1ccc(cc1)O)O)C</chem>	-7.5
model_96	Cyanidin Chloride	<chem>Oc1cc(O)c2c(c1)[o+](c(c2)O)c1ccc(c(c1)O)O.[Cl-]</chem>	-7.5
model_969	Mesopsin	<chem>Oc1ccc(cc1)CC1(O)Oc2c(C1=O)c(O)cc(c2)O</chem>	-7.5
model_10	4-Demethyl-3,9-dihydroeucomin	<chem>Oc1ccc(cc1)CC1COc2c(C1=O)c(O)cc(c2)O</chem>	-7.4
model_1055	Cochliophilin A	<chem>O=c1cc(oc2c1c(O)c1c(c2)OCO1)c1cccc1</chem>	-7.4
model_211	3,4,4',7-Tetrahydroxyflavan	<chem>Oc1ccc(cc1)C1Oc2cc(O)ccc2C(C1O)O</chem>	-7.4
model_219	Luteone	<chem>CC(=CCc1c(O)cc2c(c1O)c(=O)c(co2)c1ccc(cc1O)O)C</chem>	-7.4
model_263	Wighteone	<chem>CC(=CCc1c(O)cc2c(c1O)c(=O)c(co2)c1ccc(cc1)O)C</chem>	-7.4
model_397	Demethoxycapillarisin	<chem>Oc1ccc(cc1)Oc1cc(=O)c2c(o1)cc(cc2O)O</chem>	-7.4
model_426	Kazinol U	<chem>CC(=CCc1c(ccc(c1O)O)C1CCc2c(O1)cc(cc2)O)C</chem>	-7.4
model_446	6-Geranylaringenin	<chem>CC(=CCc1c(O)cc2c(c1O)C(=O)CC(O2)c1ccc(cc1)O)CCC=C(C)C</chem>	-7.4
model_480	Pelargonidin chloride	<chem>Oc1ccc(cc1)c1[o+](c2cc(O)cc(c2cc1O)O.[Cl-]</chem>	-7.4
model_505	Neobavaisoflavone	<chem>CC(=CCc1cc(ccc1O)c1coc2c(c1=O)ccc(c2)O)C</chem>	-7.4
model_584	7,4'-Dihydroxyhomoisoflavanone	<chem>Oc1ccc(cc1)CC1COc2c(C1=O)ccc(c2)O</chem>	-7.4
model_62	Hispidulin	<chem>COc1c(O)cc2c(c1O)c(=O)cc(o2)c1ccc(cc1)O</chem>	-7.4
model_625	Warangalone	<chem>CC(=CCc1c2OC(C)(C)C=Cc2c(c2c1occ(c2=O)c1ccc(cc1)O)O)C</chem>	-7.4

model_641	Glepidotin B	<chem>CC(=CCc1c(O)cc(c2c1OC(c1ccccc1)C(C2=O)O)O)C</chem>	-7.4
model_645	Bidwillol A	<chem>COc1c(ccc(c1CC=C(C)C)O)C1=Cc2c(OC1)cc(cc2)O</chem>	-7.4
model_665	Auricularin	<chem>CC(=CCc1c2OC(C)(C)C=Cc2c(c2c1occ(c2=O)c1ccc(c(c1)O)O)O)C</chem>	-7.4
model_683	6-Methyl-7-O-methylaromadendrin	<chem>COc1cc2OC(c3ccc(cc3)O)C(C(=O)c2c(c1C)O)O</chem>	-7.4
model_715	9-O-Methyl-4-hydroxyboeravinone B	<chem>COc1cc2oc3C(O)Oc4c(c3c(=O)c2c(c1C)O)cccc4O</chem>	-7.4
model_757	Glycyrrhisoflavone	<chem>CC(=CCc1cc(cc(c1O)O)c1coc2c(c1=O)c(O)cc(c2)O)C</chem>	-7.4
model_770	Boeravinone B	<chem>OC1Oc2ccccc2c2c1oc1cc(O)c(c(c1c2=O)O)C</chem>	-7.4
model_797	Ophiopogonanone E	<chem>COc1ccc(c(c1)O)CC1COc2c(C1=O)c(O)c(c(c2OC)O)C</chem>	-7.4
model_815	Boeravinone O	<chem>COc1cc(O)c2c(c1)oc1c(c2=O)c2cccc(c2OC1O)O</chem>	-7.4
model_981	Citrusinol	<chem>Oc1ccc(cc1)c1oc2c3C=CC(Oc3cc(c2c(=O)c1O)O)(C)C</chem>	-7.4
model_1003	Lupinalbin A	<chem>Oc1ccc2c(c1)oc1c2c(=O)c2c(o1)cc(cc2O)O</chem>	-7.3
model_1041	Karanjin	<chem>COc1c(oc2c(c1=O)ccc1c2ccol)c1ccccc1</chem>	-7.3
model_12	7-Hydroxy-3-(4-hydroxybenzylidene)chroman-4-one	<chem>Oc1ccc(cc1)C=C1COc2c(C1=O)ccc(c2)O</chem>	-7.3
model_183	Kumatakenin	<chem>COc1c(oc2c(c1=O)c(O)cc(c2)OC)c1ccc(cc1)O</chem>	-7.3
model_223	Dihydorobinetin	<chem>Oc1ccc2c(c1)OC(C(C2=O)O)c1cc(O)c(c(c1)O)O</chem>	-7.3
model_224	Robtin	<chem>Oc1ccc2c(c1)OC(CC2=O)c1cc(O)c(c(c1)O)O</chem>	-7.3
model_313	Morusinol	<chem>Oc1ccc(c(c1)O)c1oc2c3C=CC(Oc3cc(c2c(=O)c1CCC(O)(C)C)O)(C)C</chem>	-7.3
model_356	Viscidulin I	<chem>Oc1cc(O)c2c(c1)oc(c(c2=O)O)c1c(O)cccc1O</chem>	-7.3
model_414	Eurycarpin A	<chem>CC(=CCc1c(O)ccc(c1O)c1coc2c(c1=O)ccc(c2)O)C</chem>	-7.3
model_442	Sappanone A	<chem>Oc1ccc2c(c1)OCC(=Cc1ccc(c(c1)O)O)C2=O</chem>	-7.3
model_554	Cyclocommunol	<chem>CC(=CC1Oc2cc(O)ccc2c2c1c(=O)c1c(o2)cc(cc1O)O)C</chem>	-7.3
model_577	3',5'-Diprenylgenistein	<chem>CC(=CCc1cc(cc(c1O)CC=C(C)C)c1coc2c(c1=O)c(O)cc(c2)O)C</chem>	-7.3
model_582	2H-1-Benzopyran-7-yloxy	<chem>Oc1ccc2c(c1)OC(CC2=O)c1ccccc1</chem>	-7.3
model_640	3,6-Dimethoxyapigenin	<chem>COc1c(O)cc2c(c1O)c(=O)c(c(o2)c1ccc(cc1)O)OC</chem>	-7.3
model_642	Sanggenon N	<chem>CC(=CCCC1(C)C=Cc2c(O1)ccc(c2O)C1CC(=O)c2c(O1)cc(c(c2O)O)C</chem>	-7.3
model_728	Boeravinone E	<chem>Oc1ccc2c(c1)OC(c1c2c(=O)c2c(o1)cc(c(c2O)C)O)O</chem>	-7.3
model_837	(+/-)-Vestitol	<chem>COc1ccc(c(c1)O)C1COc2c(C1)ccc(c2)O</chem>	-7.3
model_848	Abyssinone V	<chem>CC(=CCc1cc(cc(c1O)CC=C(C)C)C1CC(=O)c2c(O1)cc(cc2O)O)C</chem>	-7.3
model_886	Licorisoflavan A	<chem>CC(=CCc1c(O)ccc(c1O)c1coc2c(c1=O)c(O)cc(c2)O)C</chem>	-7.3

model_941	Gancaonin G	<chem>COc1cc2occc(=O)c2c(c1CC=C(C)C)O)c1ccc(cc1)O</chem>	-7.3
model_989	Axillarin	<chem>COc1c(O)cc2c(c1O)c(=O)c(c(o2)c1ccc(c(c1)O)O)OC</chem>	-7.3
model_1037	Glabrol	<chem>CC(=CCc1cc(ccc1O)C1CC(=O)c2c(O1)c(CC=C(C)C)c(cc2)O)C</chem>	-7.2
model_1047	Eriosematin	<chem>CC(=CCc1c2OC(C)(C)C=Cc2c(c2c1occc2=O)O)C</chem>	-7.2
model_1079	Irilone	<chem>Oc1ccc(cc1)c1coc2c(c1=O)c(O)c1c(c2)OCO1</chem>	-7.2
model_11	Pinocembrin 7-acetate	<chem>CC(=O)Oc1cc2OC(CC(=O)c2c(c1)O)c1ccccc1</chem>	-7.2
model_112	Herbacetin	<chem>Oc1ccc(cc1)c1oc2c(O)c(O)cc(c2c(=O)c1O)O</chem>	-7.2
model_141	Erysubin B	<chem>OCC1(C)C=Cc2c(O1)cc1c(c2O)c(=O)c(co1)c1ccc(cc1)O</chem>	-7.2
model_156	5-Hydroxy-7-methoxy-3-(4-hydroxybenzylidene)chroman-4-one	<chem>COc1cc(O)c2c(c1)OCC(=Cc1ccc(cc1)O)C2=O</chem>	-7.2
model_220	Glabranin	<chem>CC(=CCc1c(O)cc(c2c1OC(CC2=O)c1ccccc1)O)C</chem>	-7.2
model_305	3,9-Dihydroxypterocarpan	<chem>Oc1ccc2c(c1)OCC1C2Oc2c1ccc(c2)O</chem>	-7.2
model_315	Erythrinin C	<chem>Oc1ccc(cc1)c1coc2c(c1=O)c(O)c1c(c2)OC(C1)C(O)(C)C</chem>	-7.2
model_333	Isomedicarpin	<chem>COc1ccc2c(c1)OC[C@@H]1[C@H]2Oc2c1cccc2</chem>	-7.2
model_336	Lupalbigenin	<chem>CC(=CCc1cc(ccc1O)c1coc2c(c1=O)c(O)c(c(c2)O)CC=C(C)C)C</chem>	-7.2
model_387	2'-Hydroxydaidzein	<chem>Oc1ccc(c(c1)O)c1coc2c(c1=O)ccc(c2)O</chem>	-7.2
model_427	Sulfuretin	<chem>Oc1ccc2c(c1)OC(=Cc1ccc(c(c1)O)O)C2=O</chem>	-7.2
model_428	Honyucitrin	<chem>CC(=CCc1cc(cc(c1O)CC=C(C)C)c1cc(=O)c2c(o1)cc(cc2O)O)C</chem>	-7.2
model_431	Barpisoflavone A	<chem>COc1cc(O)cc2c1c(=O)c(co2)c1ccc(cc1O)O</chem>	-7.2
model_575	Cathayanon H	<chem>CC(=CCc1cc(cc(c1O)CC=C(C)C)C1Oc2cc(O)cc(c2C(=O)C1O)O)C</chem>	-7.2
model_590	Neocyclomorusin	<chem>Oc1ccc2c(c1)OC(Cc1c2oc2c3C=CC(Oc3cc(c2c1=O)O))(C)C)C(O)(C)C</chem>	-7.2
model_6	3,7-O-Diacetylpinobanksin	<chem>CC(=O)Oc1cc(O)c2c(c1)OC(C(C2=O)OC(=O)C)c1ccccc1</chem>	-7.2
model_633	6,8-Diprenylgenistein	<chem>CC(=CCc1c(O)c(CC=C(C)C)c2c(c1O)c(=O)c(co2)c1ccc(cc1)O)C</chem>	-7.2
model_664	Syzalterin	<chem>Oc1ccc(cc1)c1cc(=O)c2c(o1)c(C)c(c(c2O)C)O</chem>	-7.2
model_838	Sativan	<chem>COc1cc(OC)ccc1C1COc2c(C1)ccc(c2)O</chem>	-7.2
model_1018	Odoriflavene	<chem>COc1c(OC)ccc(c1O)C1=Cc2c(OC1)cc(cc2)O</chem>	-7.1
model_1029	Glyasperin C	<chem>COc1c2CC(COc2cc(c1CC=C(C)C)O)c1ccc(cc1O)O</chem>	-7.1
model_104	3-Hydroxy-5,7-dimethoxy-3',4'-methylenedioxyflavan	<chem>COc1cc2OC(C(Cc2c(c1)OC)O)c1ccc2c(c1)OCO2</chem>	-7.1
model_1042	Dihydrolicoisoflavone	<chem>CC(=CCc1c(O)ccc(c1O)C1COc2c(C1=O)c(O)cc(c2)O)C</chem>	-7.1

model_1092	Glycinol	<chem>Oc1ccc2c(c1)OCC1(C2Oc2c1ccc(c2)O)O</chem>	-7.1
model_140	Erysubin A	<chem>Oc1ccc(cc1)c1coc2c(c1=O)c(O)c1c(c2)oc(c1)C(O)(C)C</chem>	-7.1
model_174	Sideroxylin	<chem>COc1c(C)c2oc(cc(=O)c2c(c1C)O)c1ccc(cc1)O</chem>	-7.1
model_21	2'-Hydroxygenistein	<chem>Oc1ccc(c(c1)O)c1coc2c(c1=O)c(O)cc(c2)O</chem>	-7.1
model_236	Pinostrobin	<chem>COc1cc2OC(CC(=O)c2c(c1)O)c1cccc1</chem>	-7.1
model_238	Chrysin	<chem>Oc1cc(O)c2c(c1)oc(cc2=O)c1cccc1</chem>	-7.1
model_249	Robinetin	<chem>Oc1ccc2c(c1)oc(c(c2=O)O)c1cc(O)c(c(c1)O)O</chem>	-7.1
model_269	Tectochrysin	<chem>COc1cc(O)c2c(c1)oc(cc2=O)c1cccc1</chem>	-7.1
model_290	Galangin	<chem>Oc1cc(O)c2c(c1)oc(c(c2=O)O)c1cccc1</chem>	-7.1
model_317	alpha-Isowighteone	<chem>Oc1ccc(cc1)c1coc2c(c1=O)c1OC(C)(C)CCc1c(c2)O</chem>	-7.1
model_318	Cirsimaritin	<chem>COc1cc2oc(cc(=O)c2c(c1OC)O)c1ccc(cc1)O</chem>	-7.1
model_322	5-Hydroxy-7-acetoxyflavone	<chem>CC(=O)Oc1cc(O)c2c(c1)oc(cc2=O)c1cccc1</chem>	-7.1
model_331	2,3-Dehydrokievitone	<chem>CC(=CCc1c(O)cc(c2c1occ(c2=O)c1ccc(cc1O)O)O)C</chem>	-7.1
model_357	8-O-Demethyl-7-O-methyl-3,9-dihdropunctatin	<chem>COc1cc(O)c2c(c1O)OCC(C2=O)Cc1ccc(cc1)O</chem>	-7.1
model_370	5,7-Dihydroxy-2-isopropylchromone	<chem>Oc1cc(O)c2c(c1)oc(cc2=O)C(C)C</chem>	-7.1
model_377	Isothymusin	<chem>COc1c(O)c2oc(cc(=O)c2c(c1OC)O)c1ccc(cc1)O</chem>	-7.1
model_504	Norwogonin	<chem>Oc1cc(O)c2c(c1O)oc(cc2=O)c1cccc1</chem>	-7.1
model_592	Eupatoletin	<chem>COc1cc2oc(c3ccc(c(c3)O)O)c(c(=O)c2c(c1OC)O)O</chem>	-7.1
model_595	7-Hydroxyflavone	<chem>Oc1ccc2c(c1)oc(cc2=O)c1cccc1</chem>	-7.1
model_658	Pedalitin	<chem>COc1cc2oc(cc(=O)c2c(c1O)O)c1ccc(c(c1)O)O</chem>	-7.1
model_666	Isoerysenegalensein E	<chem>CC(=CCc1c(O)c(CC(C(=C)C)O)c(c2c1occ(c2=O)c1ccc(cc1)O)O)C</chem>	-7.1
model_716	1"-Hydroxyerythrinin C	<chem>Oc1ccc(cc1)c1coc2c(c1=O)c(O)c1c(c2)OC(C1O)C(O)(C)C</chem>	-7.1
model_734	Dihydrobaicalein	<chem>O=C1CC(Oc2c1c(O)c(c(c2)O)O)c1cccc1</chem>	-7.1
model_775	8,3'-Diprenylapigenin	<chem>CC(=CCc1cc(ccc1O)c1cc(=O)c2c(c1)c(CC=C(C)C)c(cc2O)O)C</chem>	-7.1
model_827	Homoeriodictyol	<chem>COc1cc(ccc1O)C1CC(=O)c2c(O1)cc(cc2O)O</chem>	-7.1
model_849	7,8-Dihydroxyflavone	<chem>Oc1ccc2c(c1O)oc(cc2=O)c1cccc1</chem>	-7.1
model_859	Isolupalbigenin	<chem>CC(=CCc1cc(ccc1O)c1coc2c(c1=O)c(O)cc(c2CC=C(C)C)O)C</chem>	-7.1
model_877	6-Methylgenistein	<chem>Oc1ccc(cc1)c1coc2c(c1=O)c(O)c(c(c2)O)C</chem>	-7.1
model_933	Dehydroglyasperin D	<chem>COc1c2C=C(COc2cc(c1CC=C(C)C)OC)c1ccc(cc1O)O</chem>	-7.1
model_942	Euchrestaflavanone B	<chem>CC(=CCc1cc(c(cc1O)O)C1CC(=O)c2c(O1)c(CC=C(C)C)c(cc2O)O)C</chem>	-7.1

model_990	Eriodictyol 7,3'-dimethyl ether	<chem>COc1cc2OC(CC(=O)c2c(c1)O)c1ccc(c(c1)OC)O</chem>	-7.1
model_1020	Pendulone	<chem>COC1=C(OC)C(=O)C=C(C1=O)C1COc2c(C1)ccc(c2)O</chem>	-7
model_1028	Glicoricone	<chem>COc1c(CC=C(C)C)c(O)cc(c1c1coc2c(c1=O)ccc(c2)O)O</chem>	-7
model_1067	Kushenol S	<chem>CC(=CCc1c(O)cc(c2c1OC(CC2=O)c1ccccc1O)O)C</chem>	-7
model_14	Pinocembrin diacetate	<chem>CC(=O)Oc1cc2OC(CC(=O)c2c(c1)OC(=O)C)c1ccccc1</chem>	-7
model_148	Amaranol B	<chem>COc1c(O)cc(cc1O)CC1(O)Oc2c(C1=O)c(O)cc(c2)O</chem>	-7
model_176	Isobavachin	<chem>CC(=CCc1c(O)ccc2c1OC(CC2=O)c1ccc(cc1)O)C</chem>	-7
model_192	4'-Demethyleucomin	<chem>Oc1ccc(cc1)C=C1COc2c(C1=O)c(O)cc(c2)O</chem>	-7
model_201	Oroxylin A	<chem>COc1c(O)cc2c(c1O)c(=O)cc(o2)c1ccccc1</chem>	-7
model_227	Brazilin/Brasilin	<chem>Oc1ccc2c(c1)OCC1(C2c2cc(O)c(cc2C1)O)O</chem>	-7
model_237	Pinocembrin	<chem>Oc1cc2OC(CC(=O)c2c(c1)O)c1ccccc1</chem>	-7
model_252	Baicalein	<chem>Oc1cc2oc(cc(=O)c2c(c1O)O)c1ccccc1</chem>	-7
model_254	Chrysoeriol	<chem>COc1cc(ccc1O)c1cc(=O)c2c(o1)cc(cc2O)O</chem>	-7
model_289	Pinobanksin	<chem>Oc1cc2OC(c3ccccc3)C(C(=O)c2c(c1)O)O</chem>	-7
model_335	5-Deoxycajanin	<chem>COc1ccc2c(c1)occ(c2=O)c1ccc(cc1O)O</chem>	-7
model_376	Leachianone A	<chem>COc1cc(O)ccc1C1CC(=O)c2c(O1)c(CC(C(=C)C)CC=C(C)C)c(cc2O)O</chem>	-7
model_418	8-Prenylaidzein	<chem>CC(=CCc1c(O)ccc2c1occ(c2=O)c1ccc(cc1)O)C</chem>	-7
model_443	8-Prenylnaringenin	<chem>CC(=CCc1c(O)cc(c2c1OC(CC2=O)c1ccc(cc1)O)O)C</chem>	-7
model_508	Corylifol C	<chem>CC(=CCc1c(O)ccc2c1oc(cc2=O)c1ccc(c(c1)O)O)C</chem>	-7
model_574	5,7-Dimethoxyflavanone	<chem>COc1cc2OC(CC(=O)c2c(c1)OC)c1ccccc1</chem>	-7
model_602	Izalpinine	<chem>COc1cc(O)c2c(c1)oc(c(c2=O)O)c1ccccc1</chem>	-7
model_613	Eriosemation	<chem>CC(=CCc1c(O)c(CC=C(C)C)c2c(c1O)c(=O)cco2)C</chem>	-7
model_614	4',7-Dihydroxyflavone	<chem>Oc1ccc2c(c1)oc(cc2=O)c1cc(c(c(c1)C(C)(C)C)O)C(C)(C)C</chem>	-7
model_627	Furowanin A	<chem>CC(=CCc1c2OC(Cc2c(c2c1occ(c2=O)c1ccc(c(c1)O)O)O)C(O)(C)C)C</chem>	-7
model_630	Dalbergioidin	<chem>Oc1ccc(c(c1)O)C1COc2c(C1=O)c(O)cc(c2)O</chem>	-7
model_638	4'-O-Methyllicoflavanone	<chem>COc1ccc(cc1CC=C(C)C)C1CC(=O)c2c(O1)cc(cc2O)O</chem>	-7
model_646	5,7,4-Trihydroxy-3,6-dimethoxy-3-prenylflavone	<chem>COc1c(O)cc2c(c1O)c(=O)c(c(o2)c1ccc(c(c1)CC=C(C)C)O)OC</chem>	-7
model_77	Chrysosplenol D	<chem>COc1c(oc2c(c1=O)c(O)c(c(c2)OC)OC)c1ccc(c(c1)O)O</chem>	-7
model_801	5,7-Dihydroxy-3-(4-hydroxy-3,5-dimethoxybenzyl)-6,8-dimethylchroman-4-one	<chem>COc1cc(CC2COc3c(C2=O)c(O)c(c(c3C)O)C)cc(c1O)OC</chem>	-7
model_825	Chrysindimethylether	<chem>COc1cc(OC)c2c(c1)oc(cc2=O)c1ccccc1</chem>	-7

model_828	Hematoxylin	<chem>Oc1cc2CC3(C(c2cc1O)c1ccc(c(c1OC3)O)O)O</chem>	-7
model_845	Cirsiliol	<chem>COc1cc2oc(cc(=O)c2c(c1OC)O)c1ccc(c(c1)O)O</chem>	-7
model_865	7,4'-Dihydroxy-8-methylflavan	<chem>Oc1ccc(cc1)C1CCc2c(O1)c(C)c(cc2)O</chem>	-7
model_983	Negletein	<chem>COc1cc2oc(cc(=O)c2c(c1O)O)c1ccccc1</chem>	-7
model_99	3',5,5',7-Tetrahydroxyflavanone	<chem>Oc1cc(O)cc(c1)C1CC(=O)c2c(O1)cc(cc2O)O</chem>	-7
model_151	5,7-Diacetoxy-8-methoxyflavone	<chem>COc1c(OC(=O)C)cc(c2c1oc(cc2=O)c1ccccc1)OC(=O)C</chem>	-6.9
model_179	Medicarpin	<chem>COc1ccc2c(c1)OC1C2COc2c1ccc(c2)O</chem>	-6.9
model_200	Alpinetin	<chem>COc1cc(O)cc2c1C(=O)CC(O2)c1ccccc1</chem>	-6.9
model_202	3'-O-Methylorobol	<chem>COc1cc(ccc1O)c1coc2c(c1=O)c(O)cc(c2)O</chem>	-6.9
model_226	Genistein	<chem>Oc1ccc(cc1)c1coc2c(c1=O)c(O)cc(c2)O</chem>	-6.9
model_234	Orobol	<chem>Oc1cc(O)c2c(c1)occ(c2=O)c1ccc(c(c1)O)O</chem>	-6.9
model_248	Daidzein	<chem>Oc1ccc(cc1)c1coc2c(c1=O)ccc(c2)O</chem>	-6.9
model_25	Blumeatin	<chem>COc1cc2OC(CC(=O)c2c(c1)O)c1cc(O)cc(c1)O</chem>	-6.9
model_271	Hesperetin	<chem>COc1ccc(cc1O)C1CC(=O)c2c(O1)cc(cc2O)O</chem>	-6.9
model_294	Penduletin	<chem>COc1c(oc2c(c1=O)c(O)c(c(c2)OC)OC)c1ccc(cc1)O</chem>	-6.9
model_321	5,7-Diacetoxyflavone	<chem>CC(=O)Oc1cc(OC(=O)C)c2c(c1)oc(cc2=O)c1ccccc1</chem>	-6.9
model_334	Artocarpin	<chem>COc1cc2oc(c3ccc(cc3O)O)c(c(=O)c2c(c1C=CC(C)C)O)CC=C(C)C</chem>	-6.9
model_34	5-Acetoxy-7-hydroxyflavone	<chem>CC(=O)Oc1cc(O)cc2c1c(=O)cc(o2)c1ccccc1</chem>	-6.9
model_372	Diosmetin	<chem>COc1ccc(cc1O)c1cc(=O)c2c(o1)cc(cc2O)O</chem>	-6.9
model_375	3,4'-Dihydroxy-3,5',7-trimethoxyflavan	<chem>COc1cc2OC(C(Cc2c(c1)OC)O)c1ccc(c(c1)OC)O</chem>	-6.9
model_406	Farrerol	<chem>Oc1ccc(cc1)C1CC(=O)c2c(O1)c(C)c(c(c2O)C)O</chem>	-6.9
model_434	Dracorhodin perchlorate	<chem>[O-][Cl](=O)(=O)=O.COc1c(C)c(O)cc2c1ccc([O+])c1ccccc1</chem>	-6.9
model_531	8-Prenylkaempferol	<chem>CC(=CCc1c(O)cc(c2c1oc(c1ccc(cc1)O)c(c2=O)O)O)C</chem>	-6.9
model_555	Onysilin	<chem>COc1cc2OC(CC(=O)c2c(c1OC)O)c1ccccc1</chem>	-6.9
model_557	Kazinol A	<chem>CC(=CCc1c(cc(c(c1O)O)CC=C(C)C)C1CCc2c(O1)cc(cc2O)O)C</chem>	-6.9
model_571	Dihydrooroxylin A	<chem>COc1c(O)cc2c(c1O)C(=O)CC(O2)c1ccccc1</chem>	-6.9
model_580	Euchrestaflavanone A	<chem>CC(=CCc1cc(ccc1O)C1CC(=O)c2c(O1)c(CC=C(C)C)c(cc2O)O)C</chem>	-6.9
model_599	Cathayanon I	<chem>CC(=CCc1cc(c(c(c1O)CC=C(C)C)O)C1Oc2cc(O)cc(c2C(=O)C1O)O)C</chem>	-6.9
model_617	Homoferreirin	<chem>COc1ccc(c(c1)OC)C1COc2c(C1=O)c(O)cc(c2)O</chem>	-6.9
model_631	12-Deoxo-12alpha-acetoxyelliptone	<chem>COc1cc2c(cc1OC)OCC1C2C(OC(=O)C)c2c(O1)c1ccoc1cc2</chem>	-6.9

model_662	Angophorol	<chem>COc1c(C)c2OC(CC(=O)c2c(c1C)O)c1ccc(cc1)O</chem>	-6.9
model_667	Erysenegalensein E	<chem>CC(=CCc1c(O)c(CC(C(=C)C)O)c2c(c1O)c(=O)c(co2)c1ccc(c1)O)C</chem>	-6.9
model_691	5,7,4'-Trihydroxy-8-methylflavanone	<chem>Oc1ccc(cc1)C1CC(=O)c2c(O1)c(C)c(cc2O)O</chem>	-6.9
model_710	Lupiwighteone	<chem>CC(=CCc1c(O)cc(c2c1occ(c2=O)c1ccc(cc1)O)O)C</chem>	-6.9
model_717	Mirabijalone D	<chem>COc1cc2oc3C(O)Oc4c(c3c(=O)c2c(c1C)O)ccc(c4)O</chem>	-6.9
model_824	Mosloflavone	<chem>COc1cc2oc(cc(=O)c2c(c1OC)O)c1ccccc1</chem>	-6.9
model_858	Maackiaflavanone	<chem>COc1cc(O)c2c(c1CC=C(C)C)OC(CC2=O)c1cc(CC=C(C)C)c(cc1O)O</chem>	-6.9
model_943	Dodovisone A	<chem>COc1c(O)cc2c(c1O)c(=O)c(c(o2)c1cc(CC=C(C)C)c2c(c1)CC(C(O2)(C)C)O)OC</chem>	-6.9
model_1010	Isoformononetin	<chem>COc1ccc2c(c1)occ(c2=O)c1ccc(cc1)O</chem>	-6.8
model_182	Cajanin	<chem>COc1cc(O)c2c(c1)occ(c2=O)c1ccc(cc1O)O</chem>	-6.8
model_240	Isosakuranetin	<chem>COc1ccc(cc1)C1CC(=O)c2c(O1)cc(cc2O)O</chem>	-6.8
model_295	4'-Hydroxywogonin	<chem>COc1c(O)cc(c2c1oc(cc2=O)c1ccc(cc1)O)O</chem>	-6.8
model_314	Wogonin	<chem>COc1c(O)cc(c2c1oc(cc2=O)c1ccccc1)O</chem>	-6.8
model_365	Prunetin	<chem>COc1cc(O)c2c(c1)occ(c2=O)c1ccc(cc1)O</chem>	-6.8
model_4	Noreugenin	<chem>Oc1cc(O)c2c(c1)oc(cc2=O)C</chem>	-6.8
model_452	Peonidin chloride	<chem>COc1cc(ccc1O)c1[o+]c2cc(O)cc(c2cc1O)O.[Cl-]</chem>	-6.8
model_454	Petunidin chloride	<chem>COc1cc(cc(c1O)O)c1[o+]c2cc(O)cc(c2cc1O)O.[Cl-]</chem>	-6.8
model_519	Licoflavone C	<chem>CC(=CCc1c(O)cc(c2c1oc(cc2=O)c1ccc(cc1)O)O)C</chem>	-6.8
model_547	7,3'-Dihydroxy-5'-methoxyisoflavone	<chem>COc1cc(O)cc(c1)c1coc2c(c1=O)ccc(c2)O</chem>	-6.8
model_601	Galangin 3-methyl ether	<chem>COc1c(oc2c(c1=O)c(O)cc(c2)O)c1ccccc1</chem>	-6.8
model_611	Sappanol	<chem>Oc1ccc2c(c1)OCC(C2O)(O)Cc1ccc(c(c1)O)O</chem>	-6.8
model_634	Lupinol C	<chem>CC(=CCc1c(O)cc2c(c1O)C(=O)C1(C(O2)Oc2c1ccc(c2)O)O)C</chem>	-6.8
model_655	Dodoviscin J	<chem>COc1cc(cc(c1O)CC=C(C)C)c1oc2cc(O)cc(c2c(=O)c1OC)O</chem>	-6.8
model_661	Phaseollidin hydrate	<chem>Oc1ccc2c(c1)OCC1C2Oc2c1ccc(c2CCC(O)(C)C)O</chem>	-6.8
model_723	Sophoflavescenol	<chem>COc1cc(O)c(c2c1c(=O)c(O)c(o2)c1ccc(cc1)O)CC=C(C)C</chem>	-6.8
model_724	Isoxanthohumol	<chem>COc1cc(O)c(c2c1C(=O)CC(O2)c1ccc(cc1)O)CC=C(C)C</chem>	-6.8
model_727	3'-Methoxydaidzein	<chem>COc1cc(ccc1O)c1coc2c(c1=O)ccc(c2)O</chem>	-6.8
model_733	6,7,4'-Trihydroxyisoflavone	<chem>Oc1ccc(cc1)c1coc2c(c1=O)cc(c(c2)O)O</chem>	-6.8
model_752	Isoanhydroicaritin	<chem>COc1cc(O)c2c(c1CC=C(C)C)oc(c(c2=O)O)c1ccc(cc1)O</chem>	-6.8
model_823	Dehydroglyasperin C	<chem>COc1c2C=C(COc2cc(c1CC=C(C)C)O)c1ccc(cc1O)O</chem>	-6.8

model_841	Licoricone	<chem>COc1c(CC=C(C)C)c(OC)cc(c1c1coc2c(c1=O)ccc(c2)O)O</chem>	-6.8
model_860	Glyasperin D	<chem>COc1c2CC(CO2cc(c1CC=C(C)C)OC)c1ccc(cc1O)O</chem>	-6.8
model_93	Biochanin A	<chem>COc1ccc(cc1)c1coc2c(c1=O)c(O)cc(c2)O</chem>	-6.8
model_1093	Norwogonin 5,7,8-trimethyl ether	<chem>COc1cc(OC)c2c(c1OC)oc(cc2=O)c1cccc1</chem>	-6.7
model_119	Tectorigenin	<chem>COc1c(O)cc2c(c1O)c(=O)c(co2)c1ccc(cc1)O</chem>	-6.7
model_155	Velutin	<chem>COc1cc(O)c2c(c1)oc(cc2=O)c1ccc(c(c1)OC)O</chem>	-6.7
model_198	Moslosooflavone	<chem>COc1c(OC)cc(c2c1oc(cc2=O)c1cccc1)O</chem>	-6.7
model_205	Naringenin triacetate	<chem>CC(=O)Oc1ccc(cc1)C1CC(=O)c2c(O1)cc(cc2OC(=O)C)OC(=O)C</chem>	-6.7
model_217	Skullcapflavone I	<chem>COc1cc(O)c2c(c1OC)oc(cc2=O)c1cccc1O</chem>	-6.7
model_232	Isorhamnetin	<chem>COc1cc(ccc1O)c1oc2cc(O)cc(c2c(=O)c1O)O</chem>	-6.7
model_241	Acacetin	<chem>COc1ccc(cc1)c1cc(=O)c2c(o1)cc(cc2O)O</chem>	-6.7
model_301	Isosativan	<chem>COc1ccc2c(c1)OCC(C2)c1ccc(cc1O)OC</chem>	-6.7
model_303	Tamarixetin	<chem>COc1ccc(cc1O)c1oc2cc(O)cc(c2c(=O)c1O)O</chem>	-6.7
model_329	Dihydrotamarixetin	<chem>COc1ccc(cc1O)C1Oc2cc(O)cc(c2C(=O)C1O)O</chem>	-6.7
model_33	Glycitein	<chem>COc1cc2c(cc1O)occ(c2=O)c1ccc(cc1)O</chem>	-6.7
model_330	Sepinol	<chem>COc1c(O)cc(cc1O)C1Oc2cc(O)ccc2C(=O)C1O</chem>	-6.7
model_341	2',5,6',7-Tetrahydroxyflavanone	<chem>Oc1cc2OC(CC(=O)c2c(c1)O)c1c(O)cccc1O</chem>	-6.7
model_415	7,3'-Dihydroxy-4'-methoxyflavan	<chem>COc1ccc(cc1O)C1CCc2c(O1)cc(cc2)O</chem>	-6.7
model_503	Rivularin	<chem>COc1cccc(c1c1cc(=O)c2c(o1)c(OC)c(cc2O)OC)O</chem>	-6.7
model_522	Kuwanon E	<chem>CC(=CCc1cc(c(cc1O)O)C1CC(=O)c2c(O1)cc(cc2O)O)CCC=C(C)C</chem>	-6.7
model_529	Kushenol L	<chem>CC(=CCc1c2OC(c3ccc(cc3O)O)C(C(=O)c2c(c(c1O)CC=C(C)C)O)O)C</chem>	-6.7
model_551	(+/-)-Sigmoidin A	<chem>CC(=CCc1c(cc(c(c1O)O)CC=C(C)C)C1CC(=O)c2c(O1)cc(cc2O)O)C</chem>	-6.7
model_564	Kurarinol	<chem>COc1cc(O)c(c2c1C(=O)CC(O2)c1ccc(cc1O)O)CC(C(=C)C)C CC(O)(C)C</chem>	-6.7
model_620	Isochandalone	<chem>CC(=CCc1c(O)cc2c(c1O)c(=O)c(co2)c1ccc2c(c1)C=CC(O2)(C)C)C</chem>	-6.7
model_650	Dodoviscin	<chem>OCC(CCc1cc(ccc1O)c1oc2cc(O)cc(c2c(=O)c1OC)O)C</chem>	-6.7
model_686	Dihydrodaidzein	<chem>Oc1ccc(cc1)C1COc2c(C1=O)ccc(c2)O</chem>	-6.7
model_754	Pratensein	<chem>COc1ccc(cc1O)c1coc2c(c1=O)c(O)cc(c2)O</chem>	-6.7
model_790	6-Hydroxywogonin	<chem>COc1c(O)c(O)c(c2c1oc(cc2=O)c1cccc1)O</chem>	-6.7
model_802	3-(2,4-Dihydroxybenzyl)-5-hydroxy-7,8-dimethoxy-6-methylchroman-4-one	<chem>COc1c2OCC(C(=O)c2c(c(c1OC)C)O)Cc1ccc(cc1O)O</chem>	-6.7

model_822	Trilepisflavan	<chem>COc1cc(ccc1OC)C1CCc2c(O1)cc(cc2)O</chem>	-6.7
model_972	Montixanthone	<chem>COc1cc(O)cc2c1c(=O)c1c(o2)cc(c(c1)O)O</chem>	-6.7
model_1034	5-Methyl-7-methoxyisoflavone	<chem>COc1cc(C)c2c(c1)occ(c2=O)c1ccccc1</chem>	-6.6
model_1064	Parvisoflavanone	<chem>COc1c(ccc(c1OC)O)C1COc2c(C1=O)c(O)cc(c2)O</chem>	-6.6
model_1070	5,7,2',4'-Tetrahydroxy-8,3'-di(gamma,gamma-dimethylallyl)-isoflavanone	<chem>CC(=CCc1c(O)ccc(c1O)C1COc2c(C1=O)c(O)cc(c2CC=C(C)C)O)C</chem>	-6.6
model_135	Formononetin	<chem>COc1ccc(cc1)c1coc2c(c1=O)ccc(c2)O</chem>	-6.6
model_177	6-Methoxywogonin	<chem>COc1c(O)c(OC)c2c(c1O)c(=O)cc(o2)c1ccccc1</chem>	-6.6
model_185	Pachypodol	<chem>COc1cc(O)c2c(c1)oc(c(c2=O)OC)c1ccc(c(c1)OC)O</chem>	-6.6
model_20	5-Hydroxy-7,8-dimethoxyflavanone	<chem>COc1c(OC)cc(c2c1OC(CC2=O)c1ccccc1)O</chem>	-6.6
model_207	Phaseollidin	<chem>CC(=CCc1c(O)ccc2c1OC1C2COc2c1ccc(c2)O)C</chem>	-6.6
model_270	Tricin	<chem>COc1cc(cc(c1O)OC)c1cc(=O)c2c(o1)cc(cc2O)O</chem>	-6.6
model_274	3-O-Acetylpinobanksin	<chem>CC(=O)OC1C(Oc2c(C1=O)c(O)cc(c2)O)c1ccccc1</chem>	-6.6
model_325	Trifolirhizin	<chem>OCC1OC(Oc2ccc3c(c2)OCC2C3Oc3c2cc2c(c3)OCO2)C(C(C1O)O)O</chem>	-6.6
model_339	2',3,5,6',7-Pentahydroxyflavanone	<chem>Oc1cc2OC(c3c(O)cccc3O)C(C(=O)c2c(c1)O)O</chem>	-6.6
model_416	Jaceosidin	<chem>COc1cc(ccc1O)c1cc(=O)c2c(o1)cc(c(c2O)OC)O</chem>	-6.6
model_500	Viscidulin II	<chem>COc1cc(O)c2c(c1OC)oc(cc2=O)c1c(O)cccc1O</chem>	-6.6
model_528	Leachianone G	<chem>CC(=CCc1c(O)cc(c2c1OC(CC2=O)c1ccc(cc1O)O)O)C</chem>	-6.6
model_546	Kushenol E	<chem>CC(=CCc1c2OC(CC(=O)c2c(c(c1O)CC=C(C)C)O)c1ccc(cc1O)O)C</chem>	-6.6
model_597	3'-Deoxy-4-O-methylsappanol	<chem>COC1c2ccc(cc2OCC1(O)Cc1ccc(cc1)O)O</chem>	-6.6
model_659	Derrisisoflavone B	<chem>CC(=CCc1c(O)cc2c(c1O)c(=O)c(c2)c1ccc(c(c1)CC(C(=C)C)O)O)C</chem>	-6.6
model_8	4-O-Methylsappanol	<chem>COC1c2ccc(cc2OCC1(O)Cc1ccc(c(c1)O)O)O</chem>	-6.6
model_831	5,7-Dihydroxy-3',4',5'-trimethoxyflavone	<chem>COc1c(OC)cc(cc1OC)c1cc(=O)c2c(o1)cc(cc2O)O</chem>	-6.6
model_136	Ermanin	<chem>COc1ccc(cc1)c1oc2cc(O)cc(c2c(=O)c1OC)O</chem>	-6.5
model_195	Anhydroicaritin	<chem>COc1ccc(cc1)c1oc2c3CCC(Oc3cc(c2c(=O)c1O)O)(C)C</chem>	-6.5
model_197	Noricaritin	<chem>Oc1ccc(cc1)c1oc2c(CCC(O)(C)C)c(O)cc(c2c(=O)c1O)O</chem>	-6.5
model_209	Naringenintrimethyl ether	<chem>COc1ccc(cc1)C1CC(=O)c2c(O1)cc(cc2OC)OC</chem>	-6.5
model_251	Kaempferide	<chem>COc1ccc(cc1)c1oc2cc(O)cc(c2c(=O)c1O)O</chem>	-6.5
model_368	5-Hydroxy-7-acetoxy-8-methoxyflavone	<chem>COc1c(OC(=O)C)cc(c2c1oc(cc2=O)c1ccccc1)O</chem>	-6.5
model_401	Isopedicin	<chem>COc1c2OC(CC(=O)c2c(c(c1OC)O)OC)c1ccccc1</chem>	-6.5

model_438	Kurarinone	<chem>COc1cc(O)c(c2c1C(=O)CC(O2)c1ccc(cc1O)O)CC(C(=C)C)C=C(C)C</chem>	-6.5
model_440	Sophoraflavanone G	<chem>CC(=CCC(C(=C)C)Cc1c(O)cc(c2c1OC(CC2=O)c1ccc(cc1O)O)O)C</chem>	-6.5
model_445	6,8-Diprenylnaringenin	<chem>CC(=CCc1c2OC(CC(=O)c2c(c(c1O)CC=C(C)C)O)c1ccc(cc1)O)C</chem>	-6.5
model_45	Calycosin	<chem>COc1ccc(cc1O)c1coc2c(c1=O)ccc(c2)O</chem>	-6.5
model_453	Malvidin chloride	<chem>COc1cc(cc(c1O)OC)c1[o+]c2cc(O)cc(c2cc1O)O.[Cl-]</chem>	-6.5
model_502	Skullcapflavone II	<chem>COc1cccc(c1c1cc(=O)c2c(o1)c(OC)c(c(c2O)OC)OC)O</chem>	-6.5
model_558	Isothymonin	<chem>COc1cc(ccc1O)c1cc(=O)c2c(o1)c(O)c(c(c2O)OC)OC</chem>	-6.5
model_649	Aliarin	<chem>COc1ccc(cc1CCC(O)C)c1oc2cc(O)c(c(c2c(=O)c1OC)O)OC</chem>	-6.5
model_813	Sideritoflavone	<chem>COc1c(OC)c(OC)c(c2c1oc(cc2=O)c1ccc(c(c1)O)O)O</chem>	-6.5
model_820	Hesperetin-7-methyl ether	<chem>COc1cc2OC(CC(=O)c2c(c1)O)c1ccc(c(c1)O)OC</chem>	-6.5
model_868	2',4'-Dihydroxy-7-methoxy-8-prenylflavan	<chem>COc1ccc2c(c1CC=C(C)C)OC(CC2)c1ccc(cc1O)O</chem>	-6.5
model_920	Piloin	<chem>COc1cc(O)c2c(c1)oc(cc2=O)c1ccc(c(c1)O)OC</chem>	-6.5
model_979	Trimethylapigenin	<chem>COc1ccc(cc1)c1cc(=O)c2c(o1)cc(cc2OC)OC</chem>	-6.5
model_1	Pectolinarigenin	<chem>COc1ccc(cc1)c1cc(=O)c2c(o1)cc(c(c2O)OC)O</chem>	-6.4
model_1030	Gancaonin N	<chem>COc1ccc(c(c1)O)c1coc2c(c1=O)c(O)c(c(c2O)CC=C(C)C</chem>	-6.4
model_16	2',5,7-Trihydroxy-8-methoxyflavanone	<chem>COc1c(O)cc(c2c1OC(CC2=O)c1cccc1O)O</chem>	-6.4
model_175	Eucalyptin	<chem>COc1ccc(cc1)c1cc(=O)c2c(o1)c(C)c(c(c2O)C)OC</chem>	-6.4
model_184	Quercetin 3,4'-dimethyl ether	<chem>COc1ccc(cc1O)c1oc2cc(O)cc(c2c(=O)c1OC)O</chem>	-6.4
model_2	7-Hydroxy-2',5,8-trimethoxyflavanone	<chem>COc1cccc1C1CC(=O)c2c(O1)c(OC)c(cc2OC)O</chem>	-6.4
model_22	3',4',7-Trimethoxyflavan	<chem>COc1cc(cc(c1OC)O)C1CCc2c(O1)c(O)c(cc2)OC</chem>	-6.4
model_281	Ombuin	<chem>COc1cc(O)c2c(c1)oc(c(c2=O)O)c1ccc(c(c1)O)OC</chem>	-6.4
model_288	7-Hydroxy-5,8-dimethoxyflavanone	<chem>COc1c(O)cc(c2c1OC(CC2=O)c1cccc1)OC</chem>	-6.4
model_344	Visnagin	<chem>COc1c2c(=O)cc(oc2cc2c1cco2)C</chem>	-6.4
model_424	5,7,3'-Trihydroxy-4'-methoxy-8-prenylflavanone	<chem>COc1ccc(cc1O)C1CC(=O)c2c(O1)c(CC=C(C)C)c(cc2O)O</chem>	-6.4
model_435	Kushenol A	<chem>CC(=CCC(C(=C)C)Cc1c(O)cc(c2c1OC(CC2=O)c1cccc1O)O)C</chem>	-6.4
model_436	Kushenol I	<chem>COc1cc(O)c(c2c1C(=O)C(O)C(O2)c1ccc(cc1O)O)CC(C(=C)C)CC=C(C)C</chem>	-6.4
model_5	Jaceidin	<chem>COc1cc(ccc1O)c1oc2cc(O)c(c(c2c(=O)c1OC)O)OC</chem>	-6.4
model_570	4'-Hydroxy-7-methoxyflavan	<chem>COc1ccc2c(c1)OC(CC2)c1ccc(cc1)O</chem>	-6.4
model_616	Gancaonin M	<chem>COc1ccc(cc1)c1coc2c(c1=O)c(O)cc(c2CC=C(C)C)O</chem>	-6.4

model_708	2',7-Dihydroxy-5,8-dimethoxyflavanone	<chem>COc1c(O)cc(c2c1OC(CC=O)c1cccc1O)OC</chem>	-6.4
model_713	Ayanin	<chem>COc1cc(O)c2c(c1)oc(c(=O)OC)c1ccc(c(c1)O)OC</chem>	-6.4
model_743	6-Demethoxytangeretin	<chem>COc1ccc(cc1)c1cc(=O)c2c(o1)c(OC)c(cc2OC)OC</chem>	-6.4
model_772	Toxicarolisoflavone	<chem>COc1cc(OC)c(cc1c1coc2c(c1=O)c(O)cc1c2C=CC(O1)(C)C)OC</chem>	-6.4
model_809	Ladanein	<chem>COc1ccc(cc1)c1cc(=O)c2c(o1)cc(c(c2O)O)OC</chem>	-6.4
model_811	Licoricidin	<chem>COc1c2CC(COc2cc(c1CC=C(C)C)O)c1ccc(c(c1O)CC=C(C)C)O</chem>	-6.4
model_89	3,5-Dihydroxy-4',7-dimethoxyflavone	<chem>COc1ccc(cc1)c1oc2cc(OC)cc(c2c(=O)c1O)O</chem>	-6.4
model_934	7-O-Methyleucomol	<chem>COc1ccc(cc1)CC1(O)COc2c(C1=O)c(O)cc(c2)OC</chem>	-6.4
model_1053	Daidzein diacetate	<chem>CC(=O)Oc1ccc(cc1)c1coc2c(c1=O)ccc(c2)OC(=O)C</chem>	-6.3
model_149	Desmethoxycentaureidin	<chem>COc1ccc(cc1O)c1cc(=O)c2c(o1)cc(c(c2O)OC)O</chem>	-6.3
model_166	4',7-Di-O-methylnaringenin	<chem>COc1ccc(cc1)C1CC(=O)c2c(O1)cc(cc2O)OC</chem>	-6.3
model_173	5,7,3'-Trihydroxy-6,4',5'-trimethoxyflavanone	<chem>COc1c(O)cc(cc1OC)C1CC(=O)c2c(O1)cc(c(c2O)OC)O</chem>	-6.3
model_208	Cimifugin	<chem>COc1c2CC(Oc2cc2c1c(=O)cc(o2)CO)C(O)(C)C</chem>	-6.3
model_265	7,4'-Di-O-methylapigenin / Apigenin 7,4'-dimethyl ether	<chem>COc1ccc(cc1)c1cc(=O)c2c(o1)cc(cc2O)OC</chem>	-6.3
model_273	2-Hydroxy-7-O-methylscillascillin	<chem>COc1cc(O)c2c(c1)OC(C1(C2=O)Cc2c1cc1c(c2)OCO1)O</chem>	-6.3
model_302	Chrysosplenetin	<chem>COc1cc2oc(c3ccc(c(c3)OC)O)c(c(=O)c2c(c1OC)O)OC</chem>	-6.3
model_354	8-Methoxybonducellin	<chem>COc1ccc(cc1)C=C1COc2c(C1=O)ccc(c2OC)O</chem>	-6.3
model_355	Viscidulin III/ Ganhuangenin	<chem>COc1c(O)ccc(c1c1cc(=O)c2c(o1)c(OC)c(cc2O)O)O</chem>	-6.3
model_405	5,7-Dihydroxychromone	<chem>Oc1cc(O)c2c(c1)occc2=O</chem>	-6.3
model_420	4-Hydroxycoumarin	<chem>O=c1cc(O)c2c(o1)cccc2</chem>	-6.3
model_421	Centaureidin	<chem>COc1ccc(cc1O)c1oc2cc(O)c(c(c2c(=O)c1OC)O)OC</chem>	-6.3
model_501	5,2',5'-Trihydroxy-6,7,8-trimethoxyflavone	<chem>COc1c(OC)c(OC)c(c2c1oc(cc2=O)c1cc(O)ccc1O)O</chem>	-6.3
model_521	Tephrosin	<chem>COc1cc2c(cc1OC)OCC1C2(O)C(=O)c2c(O1)c1C=CC(Oc1cc2)(C)C</chem>	-6.3
model_527	Kushenol W	<chem>COc1cc(C2CC(=O)c3c(O2)c(CC=C(C)C)c(cc3O)O)c(cc1O)O</chem>	-6.3
model_541	8-Methoxykaempferol / Sexangularetin	<chem>COc1c(O)cc(c2c1oc(c1ccc(cc1)O)c(c2=O)O)O</chem>	-6.3
model_705	Tsugafolin	<chem>COc1ccc(cc1)C1CC(=O)c2c(O1)cc(cc2OC)O</chem>	-6.3
model_729	Kaempferol 3,7,4'-trimethylether	<chem>COc1ccc(cc1)c1oc2cc(OC)cc(c2c(=O)c1OC)O</chem>	-6.3
model_745	5,7,3'-Trihydroxy-6,4',5'-trimethoxyflavone	<chem>COc1c(O)cc(cc1OC)c1cc(=O)c2c(o1)cc(c(c2O)OC)O</chem>	-6.3
model_771	Alpha-Toxicarol	<chem>COc1cc2OCC3C(c2cc1OC)C(=O)c1c(O3)c2C=CC(Oc2cc1O)(C)C</chem>	-6.3

model_117	Naringenin-4',7-diacetate	<chem>CC(=O)Oc1ccc(cc1)C1CC(=O)c2c(O1)cc(cc2O)OC(=O)C</chem>	-6.2
model_165	5-Hydroxy-3',4',7-trimethoxyflavone	<chem>COc1cc(O)c2c(c1)oc(cc2=O)c1ccc(c(c1)OC)OC</chem>	-6.2
model_225	Norkhellol	<chem>OCc1cc(=O)c2c(o1)cc1c(c2O)cco1</chem>	-6.2
model_255	Angelicaicain	<chem>OCc1cc(=O)c2c(o1)cc1c(c2O)CC(O1)C(O)(C)C</chem>	-6.2
model_28	3',5,5',7-Tetrahydroxy-4',6-dimethoxyflavone	<chem>COc1c(O)cc(cc1O)c1cc(=O)c2c(o1)cc(c(c2O)OC)O</chem>	-6.2
model_293	8-Demethyleucalyptin	<chem>COc1ccc(cc1)c1cc(=O)c2c(o1)cc(c(c2O)C)OC</chem>	-6.2
model_337	3-Hydroxy-4',5,7-trimethoxyflavanone	<chem>COc1ccc(cc1)C1Oe2cc(OC)cc(c2C(=O)C1O)OC</chem>	-6.2
model_338	Blumeatin B	<chem>COc1cc2OC(c3ccc(c(c3)O)OC)C(C(=O)c2c(c1)O)O</chem>	-6.2
model_366	Eupatilin	<chem>COc1cc(ccc1OC)c1cc(=O)c2c(o1)cc(c(c2O)OC)O</chem>	-6.2
model_404	Capillarisin	<chem>COc1c(O)cc2c(c1O)c(=O)cc(o2)Oc1ccc(cc1)O</chem>	-6.2
model_439	2'-Methoxykurarinone	<chem>COc1cc(O)c(c2c1C(=O)CC(O2)c1ccc(cc1OC)O)CC(C(=C)C)CC=C(C)C</chem>	-6.2
model_755	Isosinensetin	<chem>COc1cc(ccc1OC)c1cc(=O)c2c(o1)c(OC)c(cc2OC)OC</chem>	-6.2
model_980	Tetramethylkaempferol	<chem>COc1ccc(cc1)c1oc2cc(OC)cc(c2c(=O)c1OC)OC</chem>	-6.2
model_1031	4"-methyloxy-Daidzin	<chem>OCC1OC(Oc2ccc3c(c2)occ(c3=O)c2ccc(cc2)O)C(C(C1OC)O)O</chem>	-6.1
model_398	Homopterocarpin	<chem>COc1ccc2c(c1)OCC1C2Oc2c1ccc(c2)OC</chem>	-6.1
model_419	Cirsilineol	<chem>COc1cc2oc(cc(=O)c2c(c1OC)O)c1ccc(c(c1)OC)O</chem>	-6.1
model_532	Aformosine	<chem>COc1ccc(cc1)c1coc2c(c1=O)cc(c(c2)O)OC</chem>	-6.1
model_573	Sophoraflavanone C	<chem>CC(=CCc1c(O)cc(c2c1OC(CC2=O)c1ccc(cc1O)O)O)CCC=C(C)C</chem>	-6.1
model_632	Deguelin	<chem>COc1cc2c(cc1OC)OCC1C2C(=O)c2c(O1)c1C=CC(Oc1cc2)(C)C</chem>	-6.1
model_657	5,7,4'-Tri-O-methylcatechin	<chem>COc1cc2OC(c3ccc(c(c3)O)OC)C(Cc2c(c1)OC)O</chem>	-6.1
model_880	Pierreione B	<chem>COc1cc(ccc1OCC(C(O)(C)C)O)c1coc2c(c1=O)cc1c(c2)OC(C=C1)(C)C</chem>	-6.1
model_935	7,3'-Di-O-methylorobol	<chem>COc1cc(O)c2c(c1)occ(c2=O)c1ccc(c(c1)OC)O</chem>	-6.1
model_1017	Colutehydroquinone	<chem>COc1ccc2c(c1)OCC(C2)c1cc(O)c(c(c1O)OC)OC</chem>	-6
model_1024	4',5,6,7-Tetramethoxyflavone	<chem>COc1ccc(cc1)c1cc(=O)c2c(o1)cc(c(c2OC)OC)OC</chem>	-6
model_1045	Irisolidone	<chem>COc1ccc(cc1)c1coc2c(c1=O)c(O)c(c(c2)O)OC</chem>	-6
model_1085	Hamaudol	<chem>Cc1cc(=O)c2c(o1)cc1c(c2O)CC(C(O1)(C)C)O</chem>	-6
model_15	3',5-Dihydroxy-4',5',6,7-tetramethoxyflavone	<chem>COc1c(O)cc(cc1OC)c1cc(=O)c2c(o1)cc(c(c2O)OC)OC</chem>	-6
model_190	Prudomestin	<chem>COc1ccc(cc1)c1oc2c(OC)c(O)cc(c2c(=O)c1O)O</chem>	-6
model_196	Icaritin	<chem>COc1ccc(cc1)c1oc2c(CC=C(C)C)c(O)cc(c2c(=O)c1O)O</chem>	-6

model_342	2',5,6',7-Tetraacetoxyflavanone	<chem>CC(=O)Oc1cc(OC(=O)C)c2c(c1)OC(CC2=O)c1c(ccc1OC(=O)C)OC(=O)C</chem>	-6
model_345	4',5-Dihydroxy-3',5',6,7-tetramethoxyflavone	<chem>COc1cc2oc(cc(=O)c2c(c1OC)O)c1cc(OC)c(c(c1)OC)O</chem>	-6
model_348	Eupatorin	<chem>COc1cc2oc(cc(=O)c2c(c1OC)O)c1ccc(c(c1)O)OC</chem>	-6
model_383	Isolicoflavonol	<chem>CC(=CCc1cc(ccc1O)c1oc2cc(O)cc(c2c(=O)c1O)O)C</chem>	-6
model_50	Eucalyptin acetate	<chem>COc1c(C)c2oc(cc(=O)c2c(c1C)OC(=O)C)c1ccc(cc1)OC</chem>	-6
model_507	Corylifol A	<chem>CC(=CCc1cc(ccc1O)c1coc2c(c1=O)ccc(c2)O)CCC=C(C)C</chem>	-6
model_544	Limocitrin	<chem>COc1cc(ccc1O)c1oc2c(OC)c(O)cc(c2c(=O)c1O)O</chem>	-6
model_622	Dehydrodeguelin	<chem>COc1cc2c(cc1OC)OCc1c2c(=O)c2c(o1)c1C=CC(Oc1cc2)(C)C</chem>	-6
model_1013	7-O-Methylbiochanin A	<chem>COc1ccc(cc1)c1coc2c(c1=O)c(O)cc(c2)OC</chem>	-5.9
model_123	Epimedin A	<chem>COc1ccc(cc1)c1cc(=O)c2c(o1)cc(c(c2O)OC)OC</chem>	-5.9
model_328	6-Acetyl-2,2-dimethylchroman-4-one	<chem>O=C1CC(C)(C)Oc2c1cc(cc2)C(=O)C</chem>	-5.9
model_736	Irigenin	<chem>COc1cc(cc(c1OC)O)c1coc2c(c1=O)c(O)c(c(c2O)OC)OC</chem>	-5.9
model_79	Sinensetin	<chem>COc1ccc(cc1OC)c1cc(=O)c2c(o1)cc(c(c2OC)OC)OC</chem>	-5.9
model_1051	3'-Demethylnobiletin	<chem>COc1ccc(cc1O)c1cc(=O)c2c(o1)c(OC)c(c(c2OC)OC)OC</chem>	-5.8
model_137	2',4',5'-Trimethoxy-2'',2''-dimethylpyrano[5'',6'':6,7]isoflavone	<chem>COc1cc(OC)c(cc1c1coc2c(c1=O)cc1c(c2)OC(C=C1)(C)C)O</chem>	-5.8
model_647	11-Hydroxytephrosin	<chem>COc1cc2OCC3C(c2cc1OC)(O)C(=O)c1c(O3)c2C=CC(Oc2cc1O)(C)C</chem>	-5.8
model_740	Gardenin B	<chem>COc1ccc(cc1)c1cc(=O)c2c(o1)c(OC)c(c(c2O)OC)OC</chem>	-5.8
model_836	Alpinumisoflavone acetate	<chem>CC(=O)Oc1ccc(cc1)c1coc2c(c1=O)c(O)c1c(c2)OC(C=C1)(C)C</chem>	-5.8
model_899	Daidzein dimethyl ether	<chem>COc1ccc(cc1)c1coc2c(c1=O)ccc(c2)OC</chem>	-5.8
model_915	Corymbosin	<chem>COc1cc(O)c2c(c1)oc(cc2=O)c1cc(OC)c(c(c1)OC)OC</chem>	-5.8
model_94	5,7-Dihydroxy-3,4',8-trimethoxyflavone	<chem>COc1ccc(cc1)c1oc2c(OC)c(O)cc(c2c(=O)c1OC)O</chem>	-5.8
model_114	Irisfloreutin	<chem>COc1cc(cc(c1OC)OC)c1coc2c(c1=O)c(OC)c1c(c2)OCO1</chem>	-5.7
model_264	5,7-Diacetoxy-3,4',8-trimethoxyflavone	<chem>COc1ccc(cc1)c1oc2c(OC)c(OC(=O)C)cc(c2c(=O)c1OC)OC(=O)C</chem>	-5.7
model_389	Tangeretin	<chem>COc1ccc(cc1)c1cc(=O)c2c(o1)c(OC)c(c(c2OC)OC)OC</chem>	-5.7
model_41	Ononin	<chem>OCC1OC(Oc2ccc3c(c2)occ(c3=O)c2ccc(cc2)OC)C(C(C1O)O)O</chem>	-5.7
model_55	Kaempferol 3,4,7-triacetate	<chem>CC(=O)Oc1ccc(cc1)c1oc2cc(OC(=O)C)cc(c2c(=O)c1OC(=O)C)O</chem>	-5.7
model_583	2H-1-Benzopyran-5-ol	<chem>CCCCCc1ccc2c(c1O)C=CC(O2)(C)C</chem>	-5.7

model_669	Dehydrotoxicarol	<chem>COc1cc2OCc3c(c2cc1OC)c(=O)c1c(o3)c2C=CC(Oc2cc1O)(C)C</chem>	-5.7
model_800	Ophiopogonanone F	<chem>COc1ccc(c(c1)O)CC1COc2c(C1=O)c(OC)c(c(c2OC)O)C</chem>	-5.7
model_847	Arteanoflavone	<chem>COc1c(OC)cc(cc1OC)c1cc(=O)c2c(o1)cc(c(c2O)OC)O</chem>	-5.7
model_910	Nevadensin	<chem>COc1ccc(cc1)c1cc(=O)c2c(o1)c(OC)c(c(c2O)OC)O</chem>	-5.7
model_1050	Hexamethylquercetagenin	<chem>COc1ccc(cc1OC)c1oc2cc(OC)c(c(c2c(=O)c1OC)OC)OC</chem>	-5.6
model_164	Vitexicarpin/Casticin	<chem>COc1cc2oc(c3ccc(c(c3)O)OC)c(c(=O)c2c(c1OC)O)OC</chem>	-5.6
model_229	Artemetin	<chem>COc1ccc(cc1OC)c1oc2cc(OC)c(c(c2c(=O)c1OC)O)OC</chem>	-5.6
model_751	5-O-Demethylnobiletin	<chem>COc1cc(ccc1OC)c1cc(=O)c2c(o1)c(OC)c(c(c2O)OC)OC</chem>	-5.6
model_189	Isoapetalic acid	<chem>CCCC(c1c2OC(C)C(C(=O)c2c(c2c1OC(C)(C)C=C2)O)C)CC(=O)O</chem>	-5.5
model_364	Artemetin acetate	<chem>COc1ccc(cc1OC)c1oc2cc(OC)c(c(c2c(=O)c1OC)OC(=O)C)O</chem>	-5.5
model_131	8-Hydroxy-3,5,7,3',4',5'-hexamethoxyflavone	<chem>COc1cc(cc(c1OC)OC)c1oc2c(O)c(OC)cc(c2c(=O)c1OC)OC</chem>	-5.4
model_343	Khellin	<chem>COc1c2c(=O)cc(oc2c(c2c1cco2)OC)C</chem>	-5.4
model_968	5'-Methoxynobiletin	<chem>COc1c(OC)cc(cc1OC)c1cc(=O)c2c(o1)c(OC)c(c(c2OC)OC)OC</chem>	-5.4
model_256	Araneosol	<chem>COc1ccc(cc1)c1oc2c(OC)c(O)c(c(c2c(=O)c1OC)O)OC</chem>	-5.3
model_1009	3,3',4',5,6,7,8-heptamethoxyflavone	<chem>COc1cc(ccc1OC)c1oc2c(OC)c(OC)c(c(c2c(=O)c1OC)OC)O</chem>	-5.2
model_636	Maltol	<chem>O=c1ccoc(c1O)C</chem>	-5.2
model_109	3',4',5',3,5,6,7-Heptamethoxyflavone	<chem>COc1c(OC)cc(cc1OC)c1oc2cc(OC)c(c(c2c(=O)c1OC)OC)O</chem>	-5
model_36	Exoticin	<chem>COc1c(OC)cc(cc1OC)c1oc2c(OC)c(OC)c(c(c2c(=O)c1OC)O)C)OC</chem>	-5

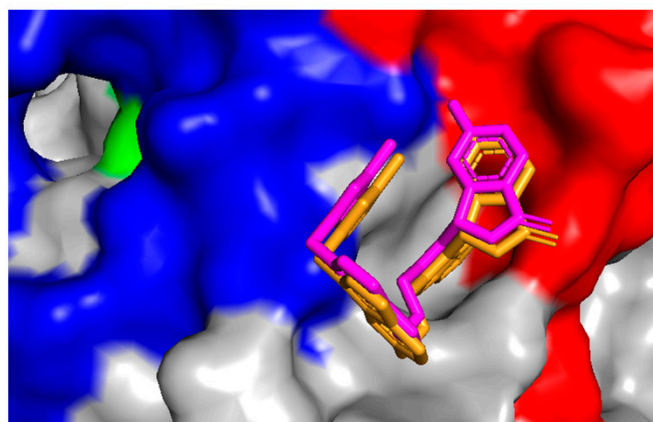
Supplementary Table S2: Kinase targets of top 4 lead flavonoids (The top 4 lead flavonoids, 5-Dehydroxyparatocarpin K, Carpachromene, Sanggenone H, and Kuwanol C were represented as L1, L2, L3, and L4 respectively).

Target	Common name	Uniprot ID	ChEMBL ID	L1	L2	L3	L4
3-phosphoinositide dependent protein kinase-1	PDPK1	O15530	CHEMBL2534			Yes	
CaM kinase II	CAMK2D	Q13557	CHEMBL2801				Yes
Casein kinase I gamma 1	CSNK1G1	Q9HCP0	CHEMBL2426			Yes	
Casein kinase II alpha	CSNK2A1	P68400	CHEMBL3629		Yes		
CDC7/DBF4 (Cell division cycle 7-related protein kinase/Activator of S phase kinase)	CDC7	O00311	CHEMBL5443	Yes			
CDK2/Cyclin A	CCNA2 CDK2	P20248 P24941	CHEMBL30384 69				Yes
c-Jun N-terminal kinase 3	MAPK10	P53779	CHEMBL2637				Yes
Cyclin-dependent kinase 1	CDK1	P06493	CHEMBL308	Yes			
Cyclin-dependent kinase 2	CDK2	P24941	CHEMBL301			Yes	
Cyclin-dependent kinase 2/cyclin E1	CCNE1 CDK2	P24864 P24941	CHEMBL19076 05				Yes
Cyclin-dependent kinase 4	CDK4	P11802	CHEMBL331			Yes	
Cyclin-dependent kinase 5/CDK5 activator 1	CDK5R1 CDK5	Q15078 Q00535	CHEMBL19076 00		Yes		Yes
Cyclin-dependent kinase 6	CDK6	Q00534	CHEMBL2508		Yes		
Dual specificity protein kinase TTK	TTK	P33981	CHEMBL3983				Yes
Ephrin receptor	EPHB4	P54760	CHEMBL5147			Yes	
Epidermal growth factor receptor erbB1	EGFR	P00533	CHEMBL203			Yes	Yes
Focal adhesion kinase 1	PTK2	Q05397	CHEMBL2695			Yes	
G protein-coupled receptor kinase 6	GRK6	P43250	CHEMBL6144		Yes		
Glycogen synthase kinase-3 alpha	GSK3A	P49840	CHEMBL2850			Yes	
Glycogen synthase kinase-3 beta	GSK3B	P49841	CHEMBL262			Yes	
Inhibitor of nuclear factor kappa B kinase epsilon subunit	IKBKE	Q14164	CHEMBL3529	Yes			
Kinesin-1 heavy chain/ Tyrosine-protein kinase receptor RET	RET	P07949	CHEMBL2041				Yes
LIM domain kinase 1	LIMK1	P53667	CHEMBL3836				Yes
LIM domain kinase 2	LIMK2	P53671	CHEMBL5932				Yes
MAP kinase ERK2	MAPK1	P28482	CHEMBL4040	Yes		Yes	

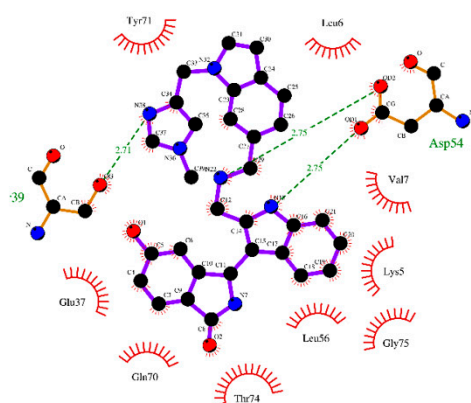
MAP kinase p38 beta	MAPK11	Q15759	CHEMBL3961				Yes
MAP kinase signal-integrating kinase 2	MKNK2	Q9HBH9	CHEMBL4204			Yes	
Maternal embryonic leucine zipper kinase	MELK	Q14680	CHEMBL4578				Yes
Mitogen-activated protein kinase kinase kinase 4	MAP4K4	O95819	CHEMBL6166			Yes	
Platelet-derived growth factor receptor beta	PDGFRB	P09619	CHEMBL1913				Yes
Protein kinase C alpha	PRKCA	P17252	CHEMBL299		Yes		
Protein kinase C beta	PRKCB	P05771	CHEMBL3045		Yes		
Protein kinase C delta	PRKCD	Q05655	CHEMBL2996		Yes		
Protein kinase C epsilon	PRKCE	Q02156	CHEMBL3582		Yes		
Protein kinase C eta	PRKCH	P24723	CHEMBL3616		Yes		
Protein kinase C gamma	PRKCG	P05129	CHEMBL2938		Yes		
Proto-oncogene tyrosine-protein kinase MER	MERTK	Q12866	CHEMBL5331	Yes			
Pyruvate dehydrogenase kinase isoform 1	PDK1	Q15118	CHEMBL4766			Yes	Yes
Receptor protein-tyrosine kinase erbB-2	ERBB2	P04626	CHEMBL1824		Yes		Yes
Rho-associated protein kinase 1	ROCK1	Q13464	CHEMBL3231	Yes		Yes	Yes
Rho-associated protein kinase 2	ROCK2	O75116	CHEMBL2973	Yes	Yes		Yes
Ribosomal protein S6 kinase 1	RPS6KB1	P23443	CHEMBL4501			Yes	
Ribosomal protein S6 kinase alpha 1	RPS6KA1	Q15418	CHEMBL2553			Yes	
Serine/threonine-protein kinase 17B	STK17B	O94768	CHEMBL3980	Yes			Yes
Serine/threonine-protein kinase Aurora-A	AURKA	O14965	CHEMBL4722	Yes		Yes	Yes
Serine/threonine-protein kinase Aurora-B	AURKB	Q96GD4	CHEMBL2185	Yes		Yes	Yes
Serine/threonine-protein kinase B-raf	BRAF	P15056	CHEMBL5145	Yes		Yes	Yes
Serine/threonine-protein kinase Chk1	CHEK1	O14757	CHEMBL4630	Yes		Yes	Yes
Serine/threonine-protein kinase Chk2	CHEK2	O96017	CHEMBL2527	Yes	Yes		
Serine/threonine-protein kinase mTOR	MTOR	P42345	CHEMBL2842			Yes	
Serine/threonine-protein kinase PLK1	PLK1	P53350	CHEMBL3024	Yes			
Serine/threonine-protein kinase RAF	RAF1	P04049	CHEMBL1906			Yes	Yes
Serine/threonine-protein kinase Sgk1	SGK1	O00141	CHEMBL2343			Yes	
Serine/threonine-protein kinase TAO1	TAOK1	Q7L7X3	CHEMBL5261	Yes			
Serine/threonine-protein kinase TAO3	TAOK3	Q9H2K8	CHEMBL5701	Yes			
Serine/threonine-protein kinase TBK1	TBK1	Q9UHD2	CHEMBL5408	Yes			
Serine/threonine-protein kinase WEE1	WEE1	P30291	CHEMBL5491			Yes	
Serine/threonine-protein kinase/endoribonuclease IRE1	ERN1	O75460	CHEMBL1163101	Yes		Yes	Yes

Sphingosine kinase 1	SPHK1	Q9NYA1	CHEMBL4394			Yes	
Sphingosine kinase 2	SPHK2	Q9NRA0	CHEMBL3023			Yes	
Tyrosine-protein kinase ABL	ABL1	P00519	CHEMBL1862		Yes		Yes
Tyrosine-protein kinase ITK/TSK	ITK	Q08881	CHEMBL2959				Yes
Tyrosine-protein kinase LCK	LCK	P06239	CHEMBL258				Yes
Tyrosine-protein kinase receptor FLT3	FLT3	P36888	CHEMBL1974	Yes			Yes
Tyrosine-protein kinase SYK	SYK	P43405	CHEMBL2599	Yes	Yes		Yes
Tyrosine-protein kinase SYK	SYK	P43405	CHEMBL2599			Yes	
Vascular endothelial growth factor receptor 1	FLT1	P17948	CHEMBL1868				Yes

A

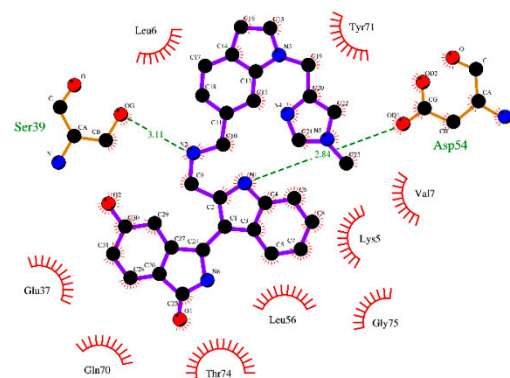


B



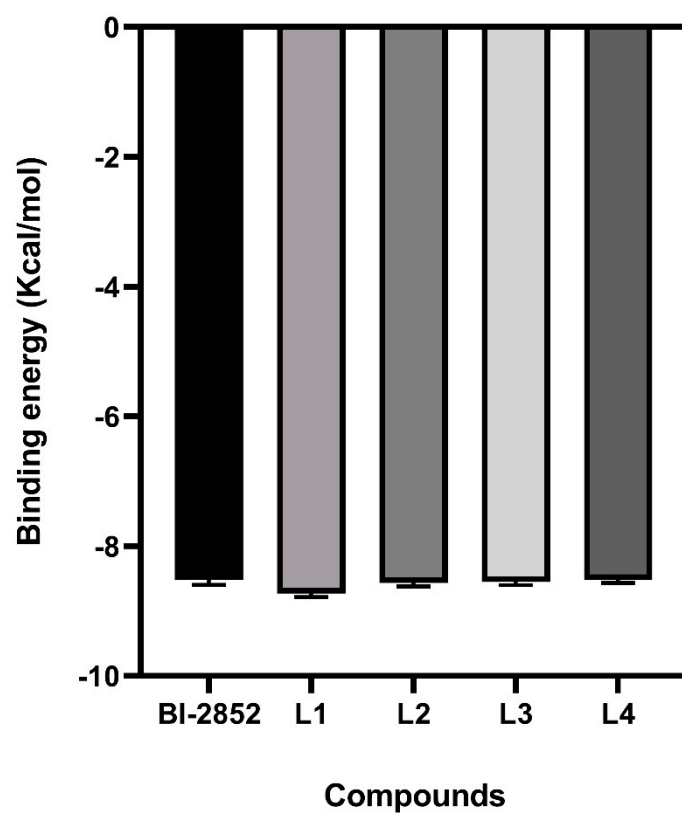
KRAS G12D-BI-2852 crystalline

C



KRAS G12D_BI-2852 docked

Supplementary Figure S1: Binding poses and molecular interactions of BI-2852 in crystallized and docked forms. [A] The P-loop (residues 10-17), Switch I (residues 25-40), and Switch II (residues 57-76) were shown in green, blue, and red color respectively, and the crystallized and docked forms of BI-2852 were shown in magenta and bright yellow color respectively. [B] Molecular interactions of BI-2852 in crystallized form. [C] Molecular interactions of BI-2852 in docked form. In both crystallized and docked forms, the Indole group near to the Isatin group of BI-2852 have closer interaction in the SI/II region, and also showed similar type of interactions with the residues of KRAS G12D mutant protein.



Supplementary Figure S2: Binding energies of BI-2852 and top 4 lead flavonoids against KRAS G12D mutant protein.