

Supplementary material:

Table 1: Table showing the amino acids involved in hydrogen bond interaction with the investigating ligands

No	Ligand	Rule of 5 No.Of Violations	Torsions	ΔG (Kcal/Mol)	K_d (μM)	Amino Acids Involved In Hydrogen Bond Interaction	H -Bond Length (\AA)
01.	Cyanidin	0	6	-6.73	12.0	Cyanidin::FRA1:H	1.91
02.	Chrysin	0	3	-6.56	273.8	KSR:A:LYS365:HZ2 Chrysin:FRA1:H	2.098 2.109
03.	Apigenin	0	4	-6.08	35.04	Apigenin::FRA1:H1	2.03
04.	Delphinidin	0	6	-5.74	15.66	Delphinidin::FRA1:H1 Delphinidin::FRA1:H1	1.83 2.07
05.	Acacetin	0	4	-5.69	67.92	Acacetin::FRA1:H	2.04
06.	Taxifolin	0	6	-4.86	61.58	Taxifolin::FRA1:H1 KSR:A:ASN368:HD21 1	2.09 1.95