BIOINFORMATION

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Supplementary material:

Table 1: Mol inspiration analysis of Banana Flower Flavonoids

SNo	Compound	milogP	TPSA	n atoms	MW	nON	nOHNH	n violations	n rotb	Volume
1	LEUCOCYANIDIN	0.378	130.602	22	306.27	7	6	1	1	252.19
2	CYANIDIN	-0.746	112.31	21	287.25	6	5	0	1	234.81
3	MALVIDIN	-0.422	110.55	24	331.3	7	4	0	3	277.88
3	MALVIDIN	-0.422	110.55	24	331.3	7	4	0	3	277.88
5	PEONIDIN	-0.438	101.316	22	301.27	6	4	0	2	252.33
6	HESPERETIN	1.935	96.223	22	302.28	6	2	0	2	255.80
7	NARINGENIN	2.117	86.989	20	272.26	5	3	0	1	230.26
8	HESPERETIN TRIACETATE	2.193	114.454	32	444.44	9	0	0	10	393.05
9	HESPERETIN DIHYDROCHALCONE	2.475	107.217	22	304.30	6	4	0	5	265.65
10	NARINGENIN FLAVANONE	-1.146	89.818		271.24	5	2	0	1	227.51
11	NARINGENIN PELARGIDANON	2.117	86.989	20	272.26	5	3	0	1	230.26
12	HESPERETIN (ANION)	-1.327	99.052	22	301.27	6	2	0	2	253.06

Table 2: Binding energy values of the docked ligands

S.No	Name Of Flavonoid	AUTODOCK.4.0 (kcal/mol)	AUTODOCK VINA (kcal/mol)
1	HESPERETIN TRIACETATE	-6.08	-8.2
2	NARINGENIN	-6.02	-8.1
3	NARINGENIN PELARGONIDIN	-6.02	-8.1
4	NARINGENIN FLAVANONE	-5.82	-8.0
5	HESPERETIN	-5.78	-8.4
6	MALVIDIN	-5.26	-7.3
7	CYANIDIN	-5.18	-7.9
8	PELARGONIDIN	-4.93	-7.7
9	PEONIDIN	-4.80	-7.7
10	HESPERETIN DIHYDROCHALCONE	-4.78	-7.0