
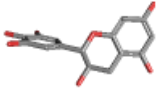
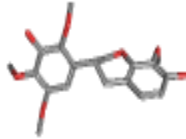
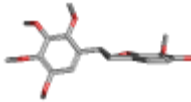
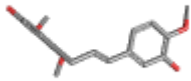
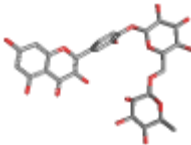
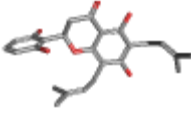
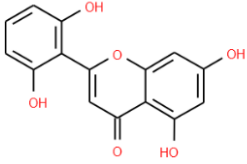
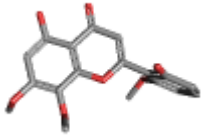
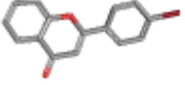
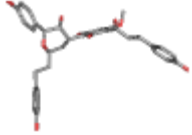
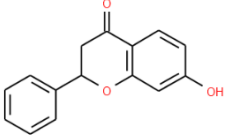
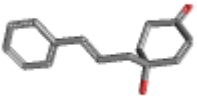
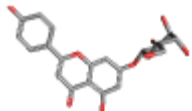
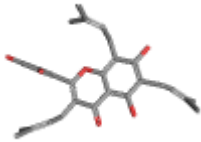
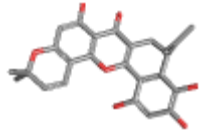
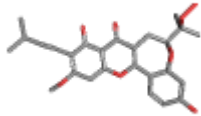
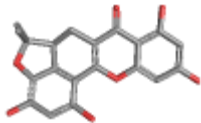
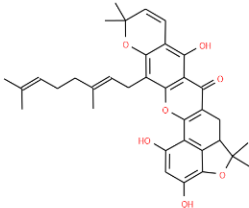
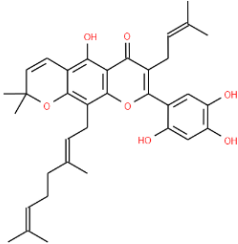
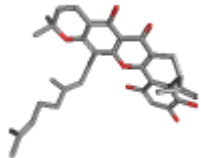
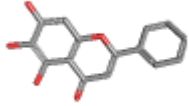
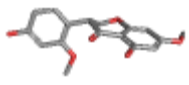
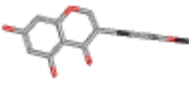
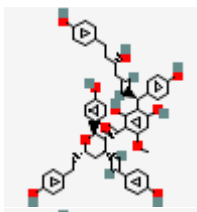
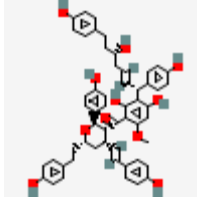
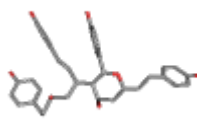
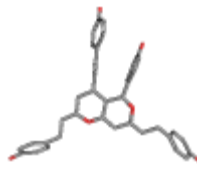
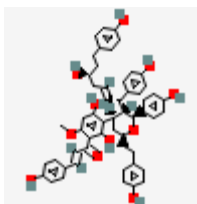


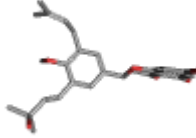
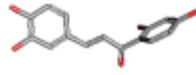
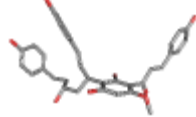
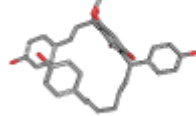
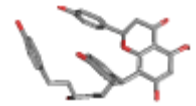
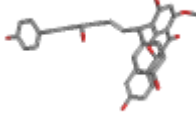
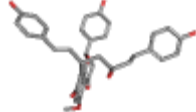
Table S1. List of forty-six phytochemicals from flavonoids and their respective PubChem id and including 3D and 2D.

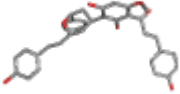
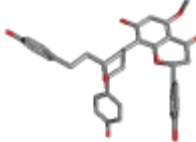
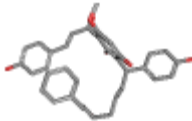
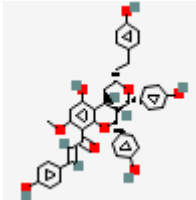
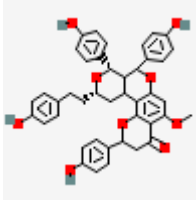
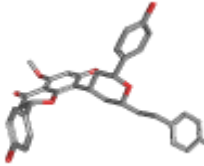
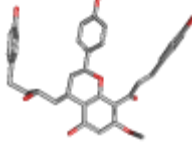
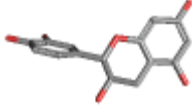
S.NO	PHYTOCOMPOUND	PUBCHEM ID	STRUCTURE (3D and 2D STRUCTURE)
1.	(-)-Epicatechin	72276	
2.	(+)-Gallocatechin	65084	
3.	(3S)-3',7-dihydroxy-2',4',5',8-tetramethoxyisoflavan	471695	
4.	(3S)-7-hydroxy-2',3',4',5',8-pentamethoxyisoflavan	471694	
5.	condenatenin A	44254875	
6.	2',3',5,7-Tetrahydroxy flavone	5321864	
7.	2',5,6',7-Tetrahydroxy Flavanone	42607849	

8.	2',5,6'7-Tetrahydroxy flavone	53212865	
9..	2',5-Dihydroxy-6,7,8-trimethoxyflavone	159029	
10.	4'-bromoflavone	1686	
11,	6-hydroxycalyxin F	10393772	
12.	7-OH-flavanone	1890	
13	candenatenin B	44254876	
14.	apigenin-7-O-beta-D-glucopyranoside	12304093	

15	Artelasticin	5471311	
16	Artobiloxanthone	46887866	
17.	Artoindonesianin B	10096171	
18	Artoindonesianin P	10316935	
19	Artoindonesianins A	10603133	
20	Artoindonesianins U	10030972	
21	Artoindonesianins V	10053761	

22	Baicalein	5281605	
23	Cajanol	442670	
24	Biochanin A	5280373	
25	Blepharocalyxins A7	10819468	
26	Blepharocalyxins B	10677118	
27	Blepharocalyxins C	11801874	
28	Blepharocalyxins D	9985898	
29	Blepharocalyxins E	9988230	

30	Burttinone	42607959	
31	Butein	5281222	
32	Calyxins A	10817087	
33	Calyxins B	9829786	
34	Calyxins C	10460896	
35	Calyxins D	10008443	
36	Calyxins E	44559999	

37	Calyxins F	44559998	
38	Calyxins G	42608059	
39	Calyxins H	10793085	
40	Calyxins I	10327269	
41	Calyxins J	42608060	
42	Calyxins K	42608061	
43	Calyxins L	10722001	
44	Catechin	9064	

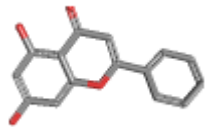
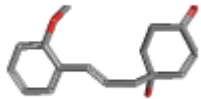
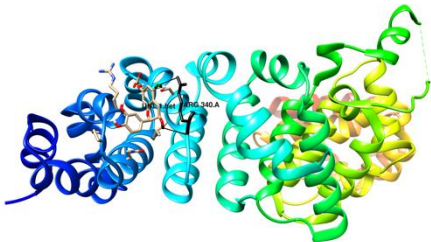
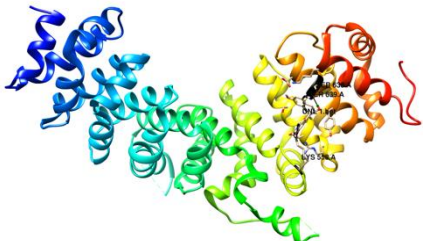
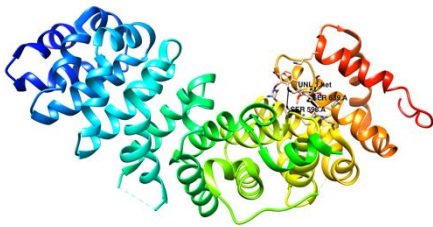
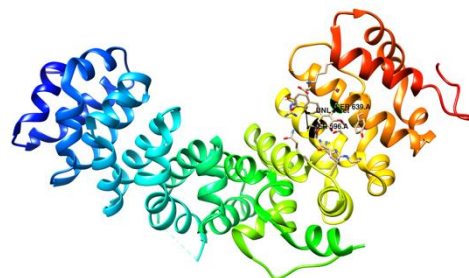
45	Chrysin	5281607	
46	condenatenin C	44254877	

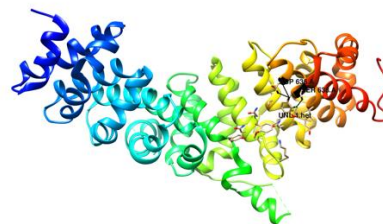
Table S2. Analysis of Patch Dock [Receptor molecule is PKP1 (IXM9), and ligands are flavonoids.]

S.NO.	Ligand	Score	Area	Ace	Complex
1.	(-)-Epicatechin	3200	364.50	-146.28	
2.	(+)-Gallocatechin	3068	344.90	6.66	
3.	(3S)-3',7-dihydroxy-2',4',5',8-tetramethoxyisoflavan	4198	496.30	31.66	

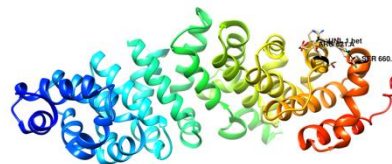
4. (3S)-7-hydroxy-2',3',4',5',8-pentamethoxyisoflavan 4198 496.30 31.66



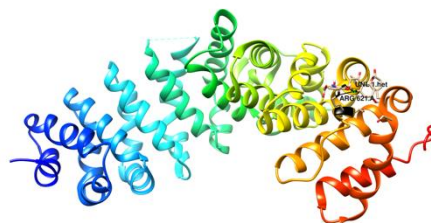
5. candenatenin A 4080 439.40 -48.98



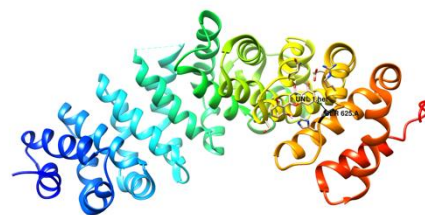
6. 2',3',5,7-Tetrahydroxy flavone 3442 401.50 -69.76

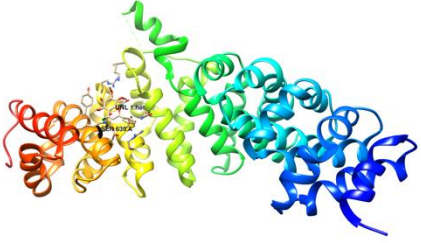
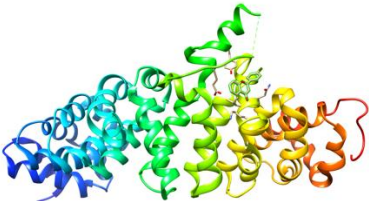
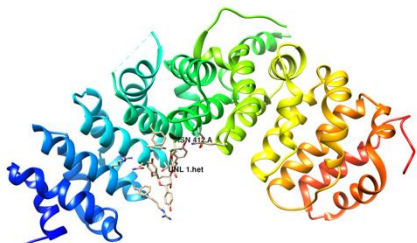
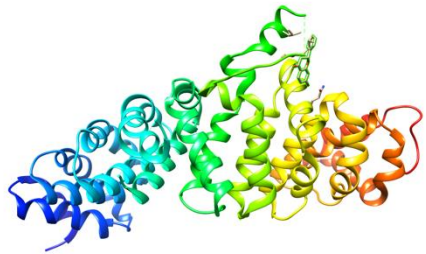
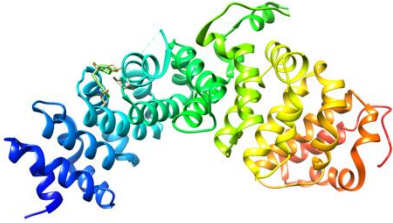


7. 2',5,6',7-Tetrahydroxy Flavanone 3356 380.30 -68.78

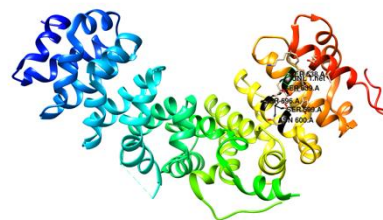


8. 2',5,6'7-Tetrahydroxy flavone 3296 362.90 -147.99

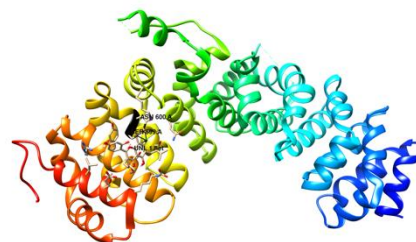


9.	2',5-Dihydroxy-6,7,8-trimethoxyflavone	3922	444.80	52.35	
10.	4'-bromoflavone	3254	389.50	-81.40	
11.	6-hydroxycalyxin F	5150	585.90	-54.87	
12.	7-OH-flavanone	3648	447.90	-181.30	
13.	candenatenin B	3080	333.90	-115.42	

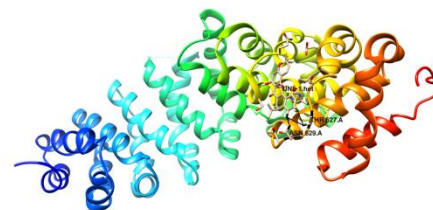
14. apigenin-7-O-beta-D-glucopyranoside 4346 485.00 -78.98



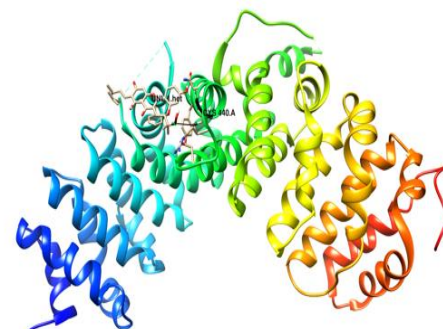
15. Artelasticin 4878 555.20 -80.40



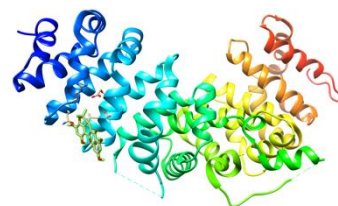
16. Artobiloxanthone 4256 455.60 -172.79

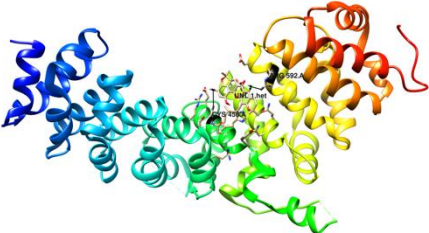
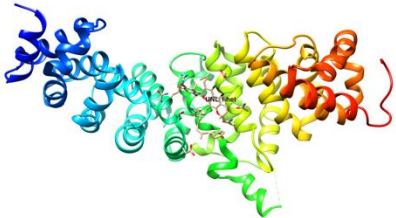
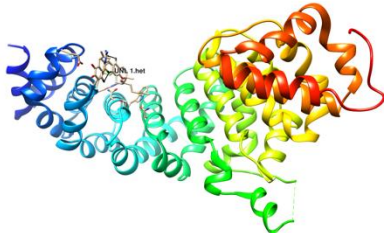
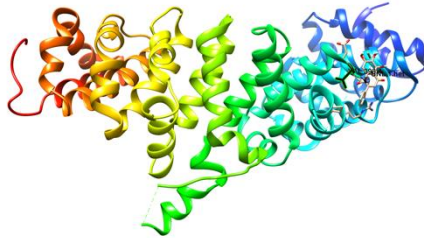
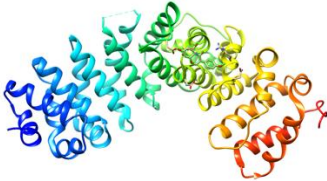
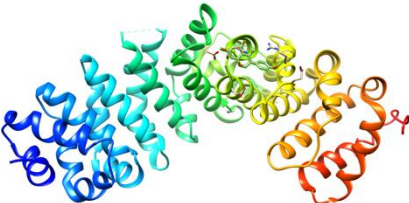


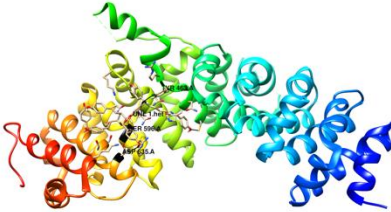
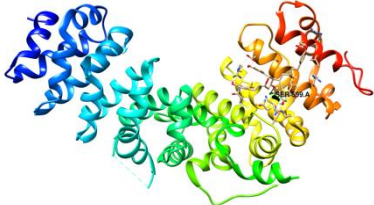
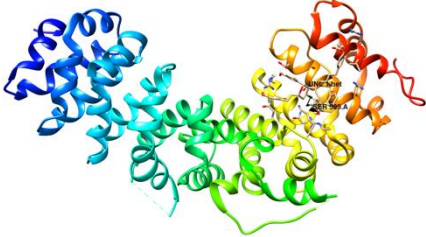
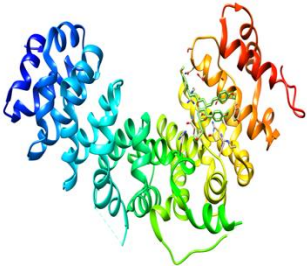
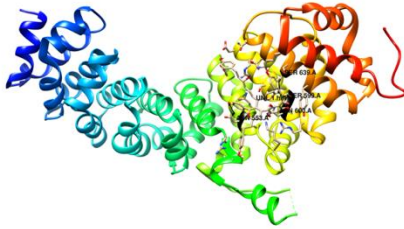
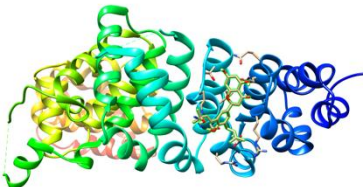
17. Artoindonesianin B 5002 595.50 -269.97

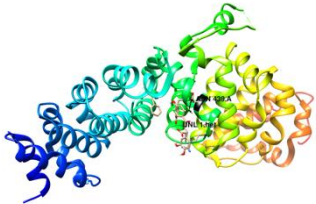
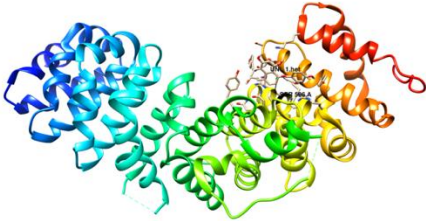
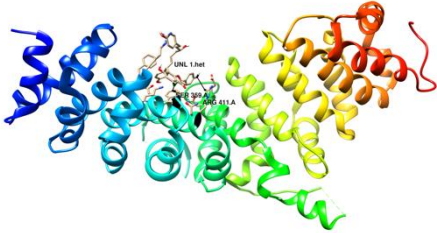
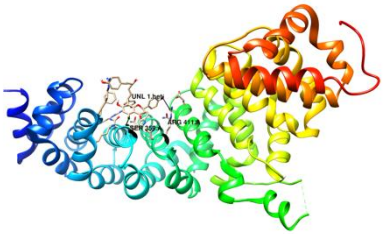
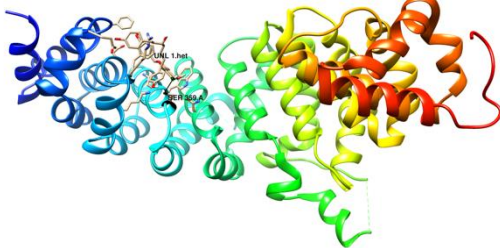
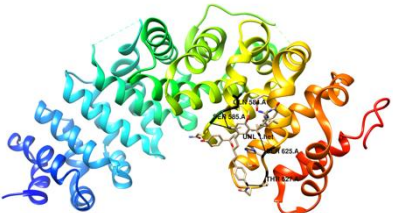


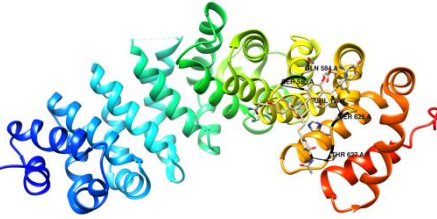
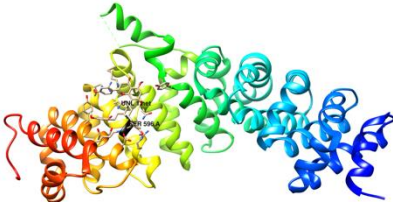
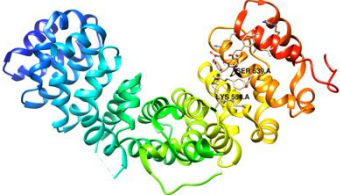
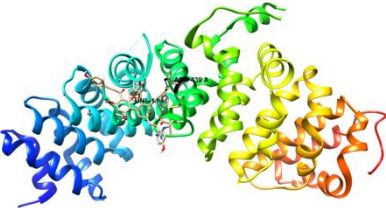
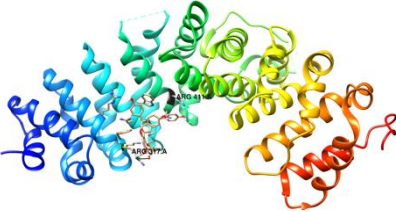
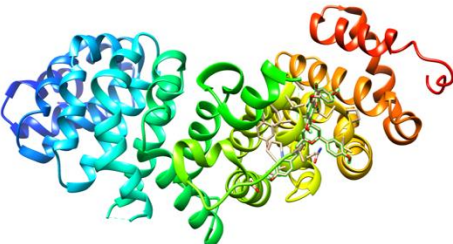
18. Artoindonesianin P 4046 477.00 -138.98



19.	Artoindonesianins A	5484	639.90	-21.91	
20.	Artoindonesianins U	5548	639.40	-39.93	
21.	Artoindonesianins V	5424	719.90	-151.34	
22.	Baicalein	3290	369.10	-146.83	
23.	Cajanol	3686	449.20	-59.91	
24.	Biochanin A	3686	449.20	-59.91	

25.	Blepharocalyxins A	6676	854.00	-132.68	
26.	Blepharocalyxins B	5878	739.80	-19.83	
27.	Blepharocalyxins C	5878	739.40	-19.83	
28.	Blepharocalyxins D	5758	675.60	-49.26	
29.	Blepharocalyxins E	7150	882.30	50.20	
30.	Burtinone	5004	663.60	-143.67	

31.	Butein	3556	402.30	-72.24	
32.	Calyxins A	5480	586.60	78.97	
33.	Calyxins B	5094	602.60	-48.58	
34.	Calyxins C	5094	602.60	-48.58	
35.	Calyxins D	5236	715.20	-146.00	
36.	Calyxins E	5766	770.00	-229.15	

37.	Calyxins F	5766	770.00	-229.15	
38.	Calyxins G	5440	681.70	-7.05	
39.	Calyxins H	5282	628.20	-21.25	
40.	Calyxins I	5908	708.20	-250.73	
41.	Calyxins J	5642	686.40	-142.53	
42.	Calyxins K	5106	681.20	-292.88	

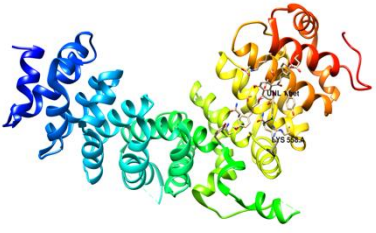
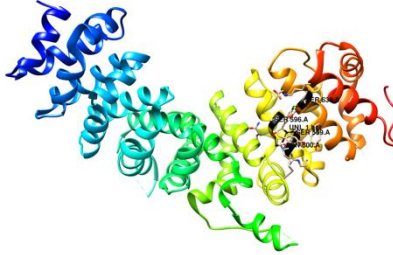
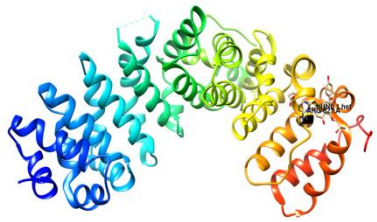
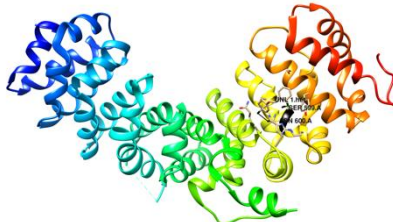
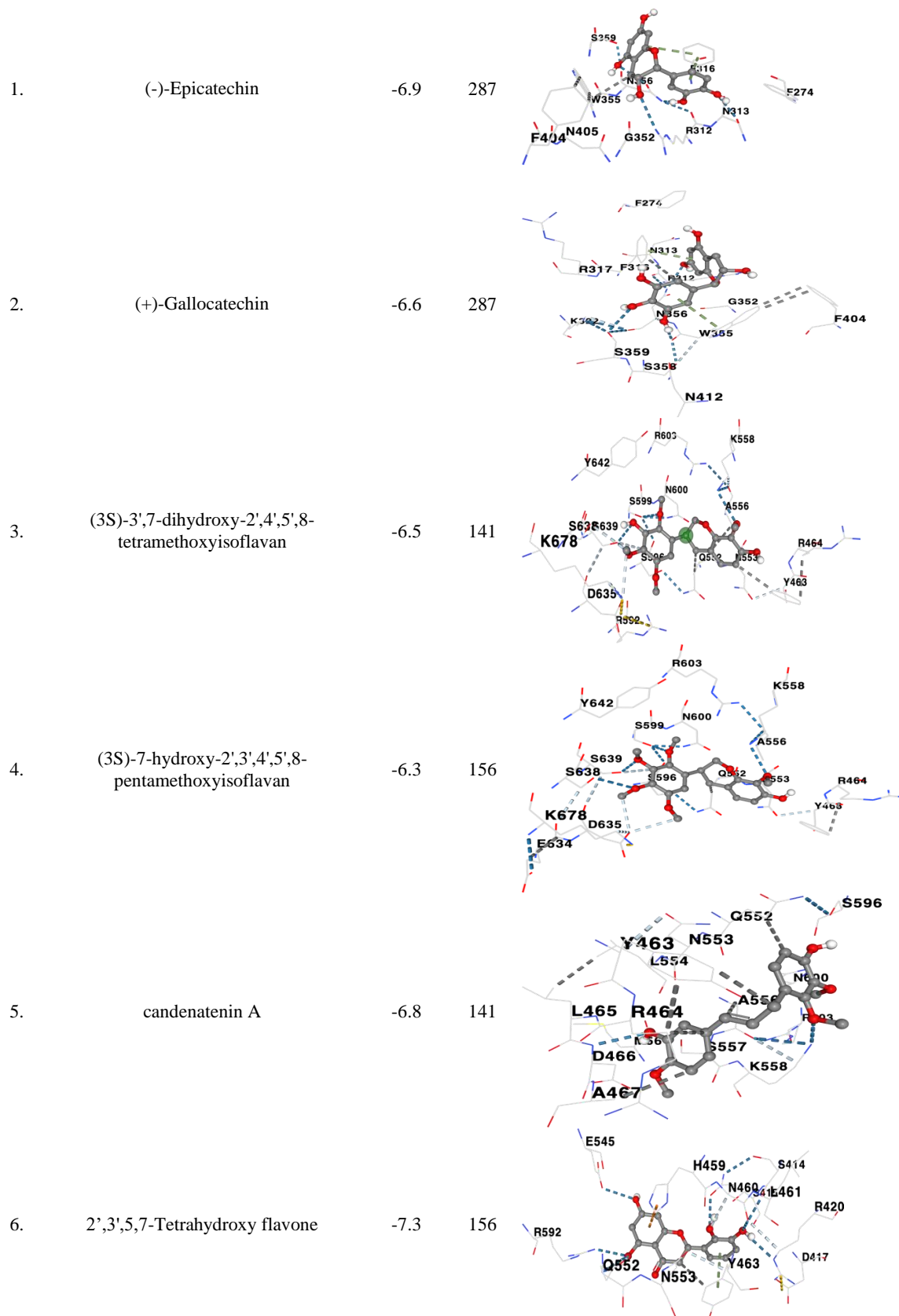
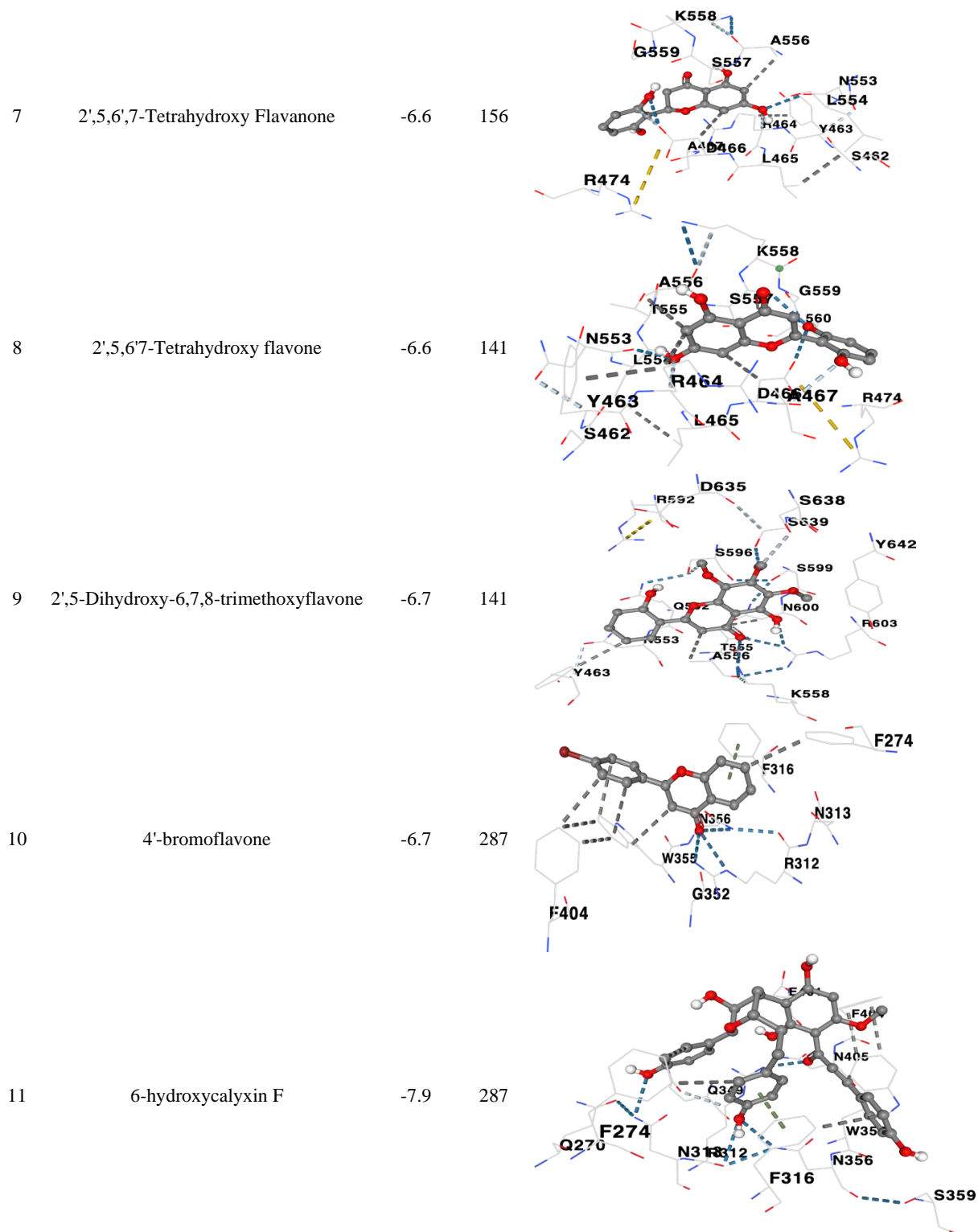
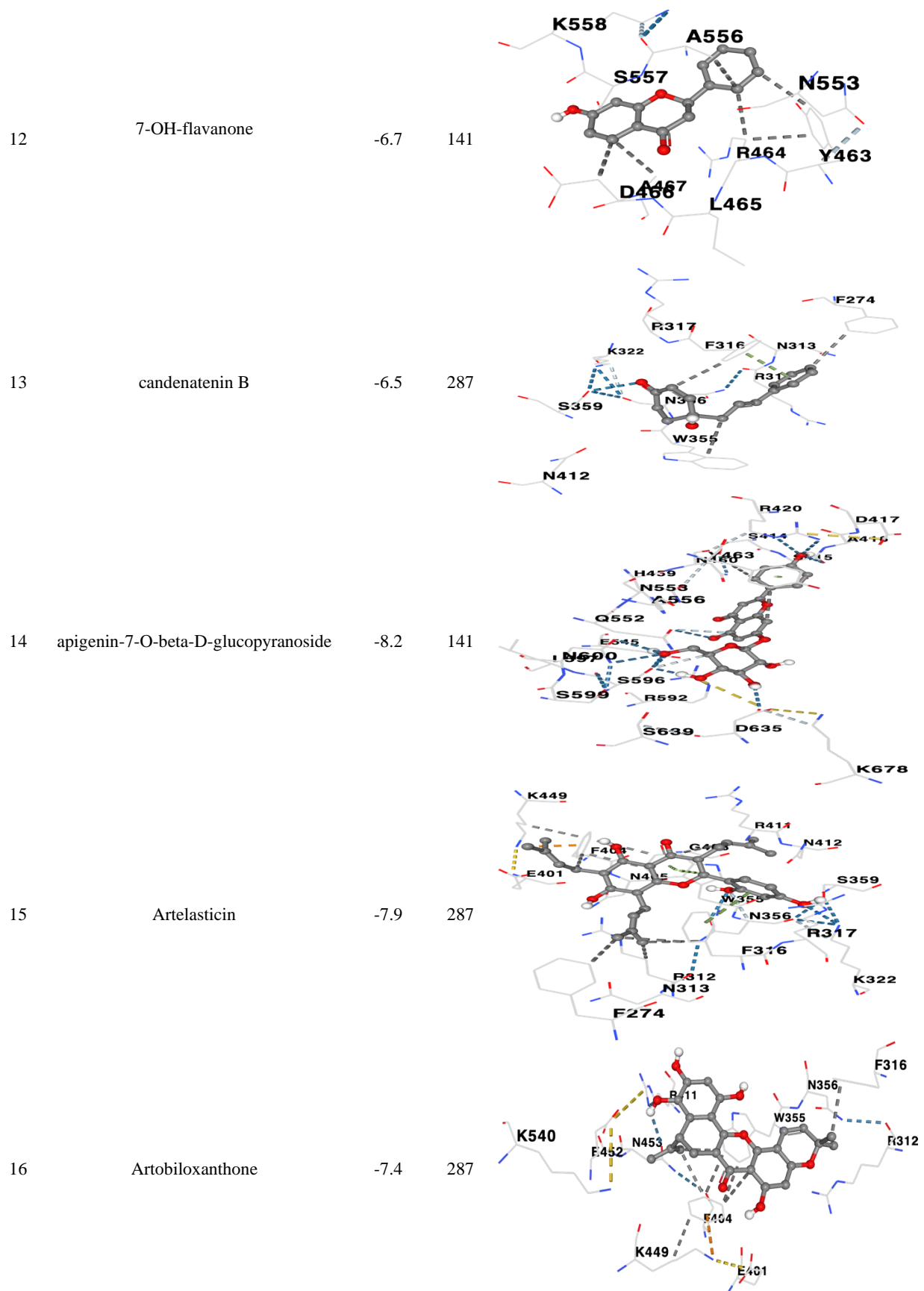
43.	Calyxins L	5940	710.10	-117.89	
44.	Catechin	3176	347.60	17.05	
45.	Chrysin	3382	391.90	-65.96	
46.	condenatenin C	3270	338.60	-45.00	

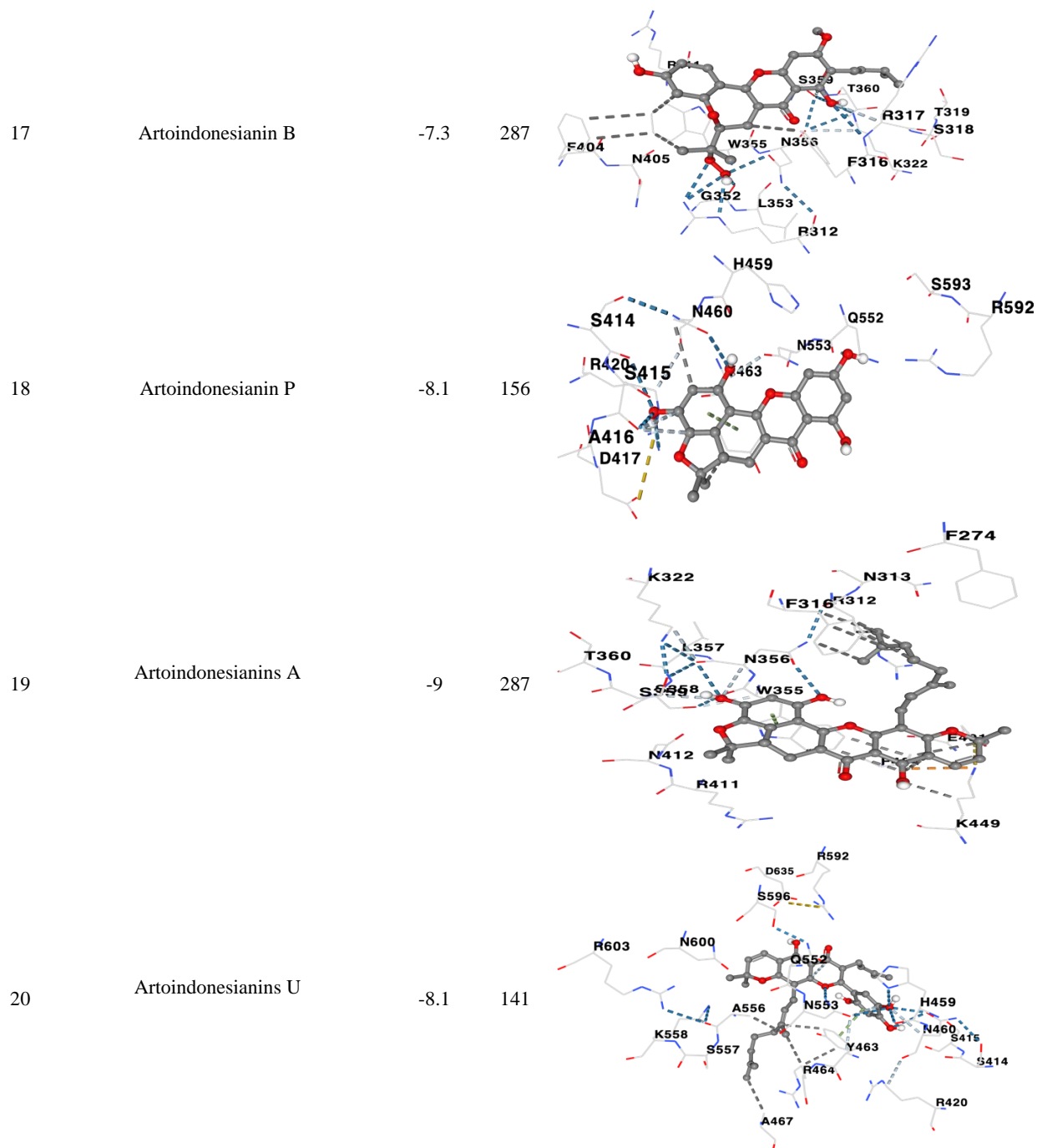
Table S3. (Analysis of CB dock results) [Receptor molecule is PKP1 (IXM9), and ligands are flavonoids]

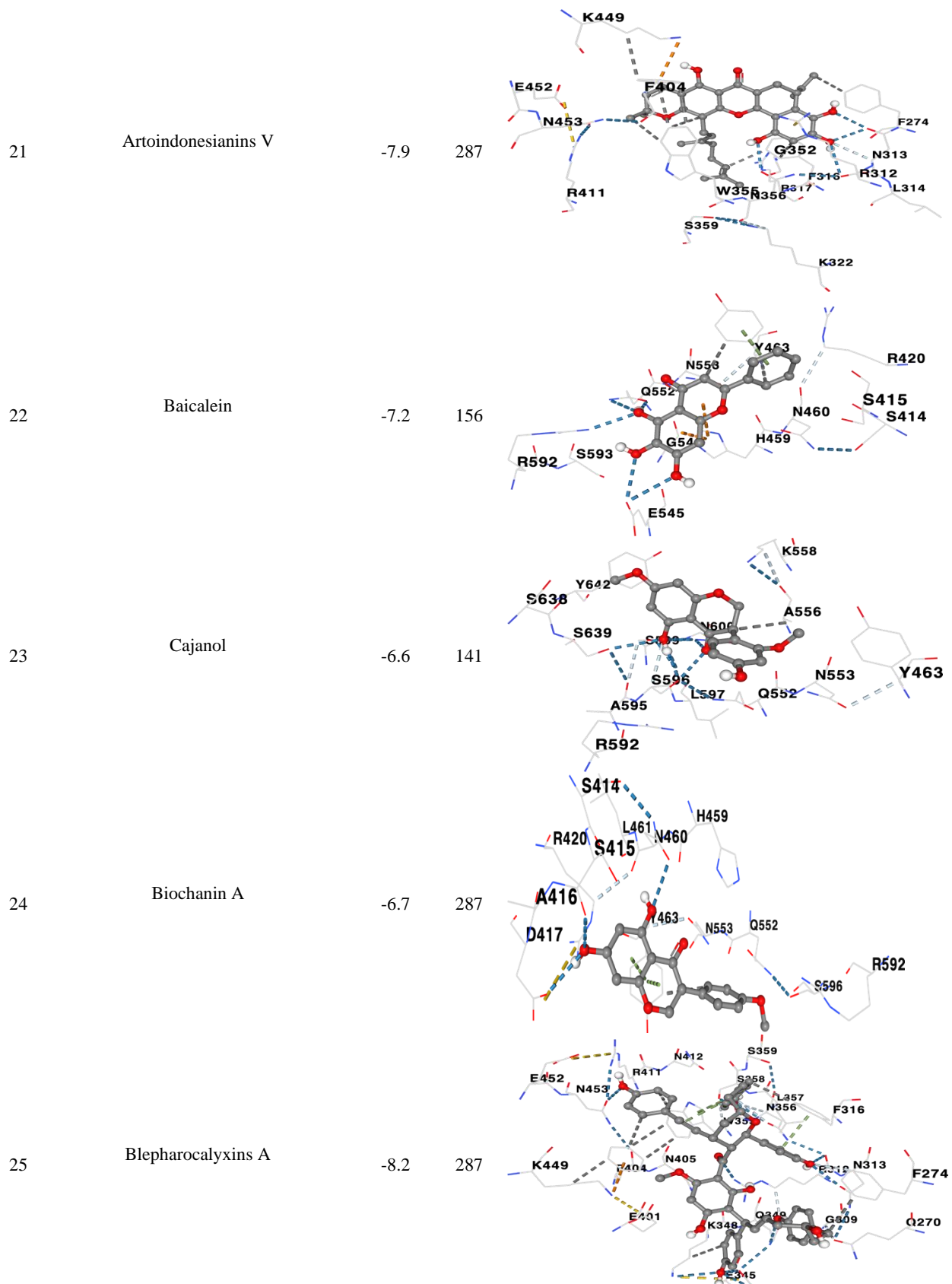
S no.	Phytocompound name	Vina score	Cavity size	Structure of complex
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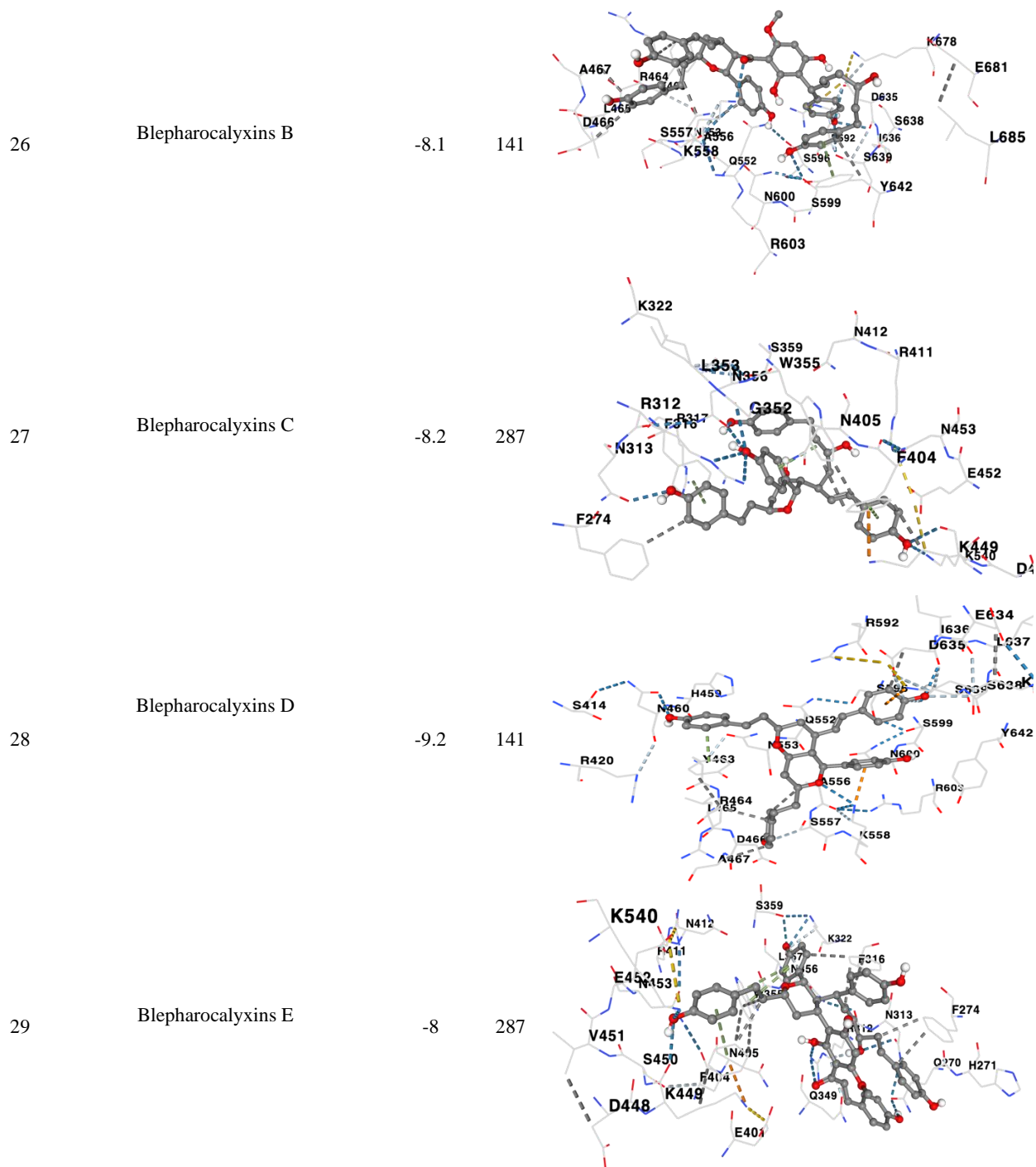


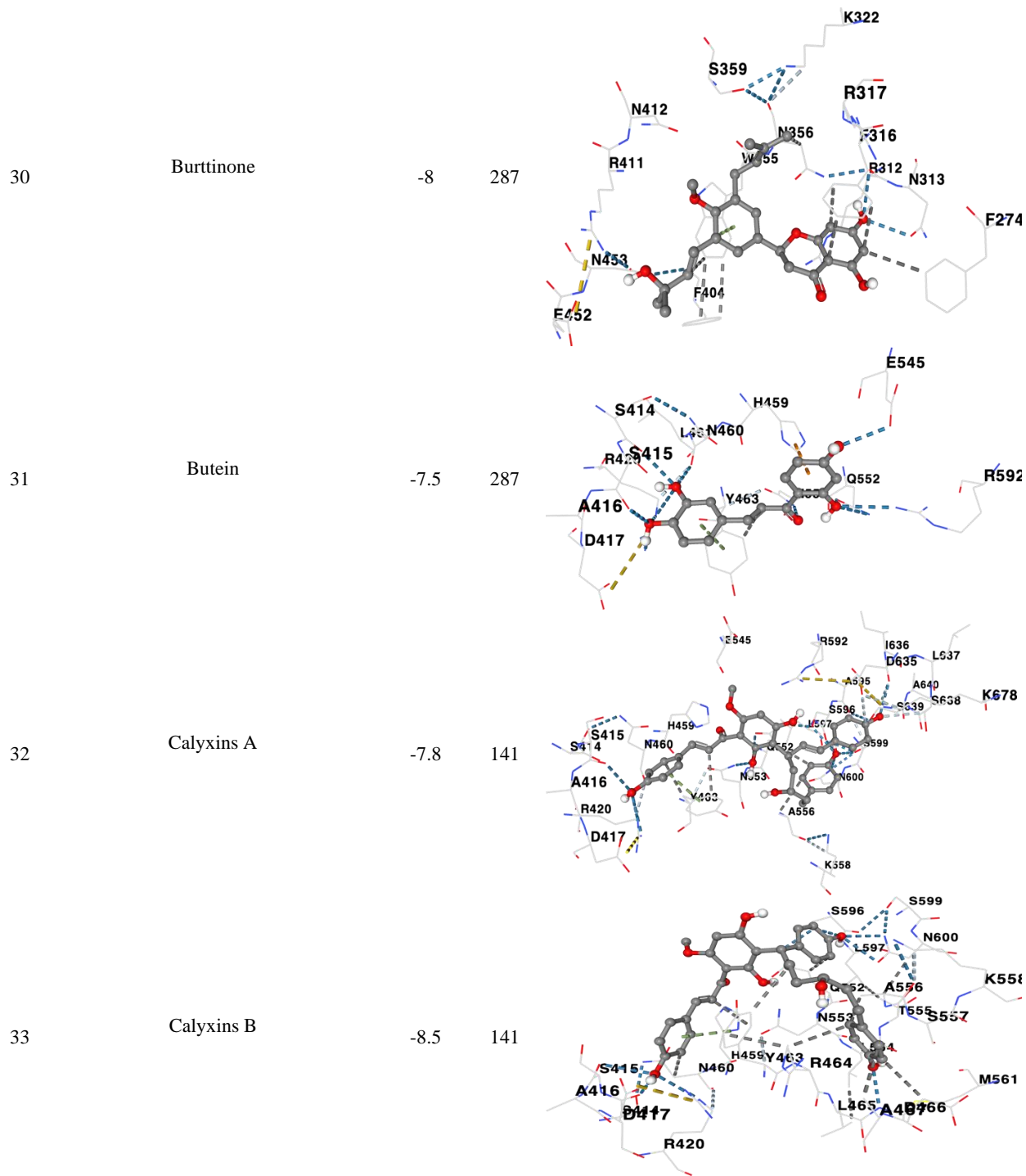


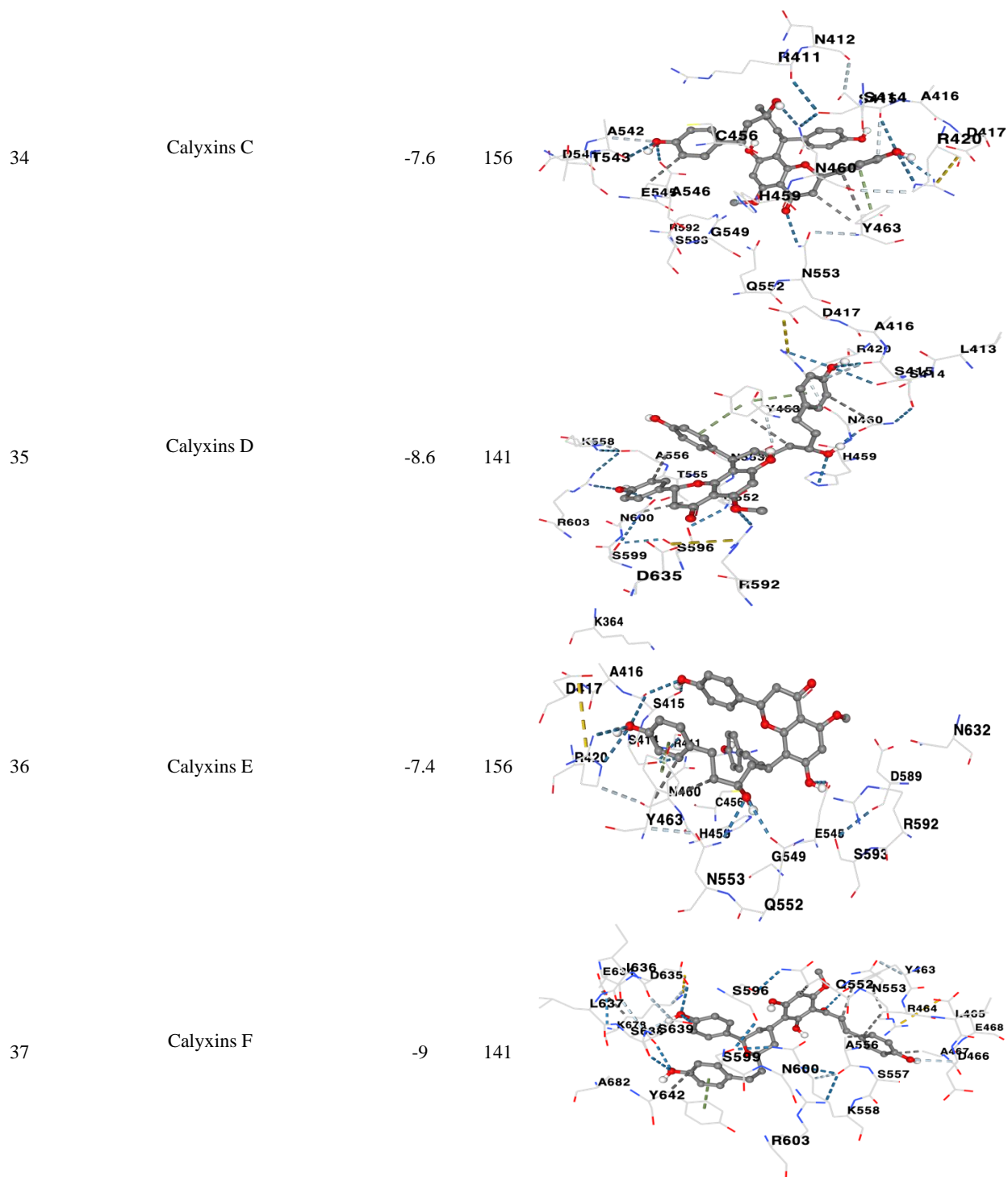


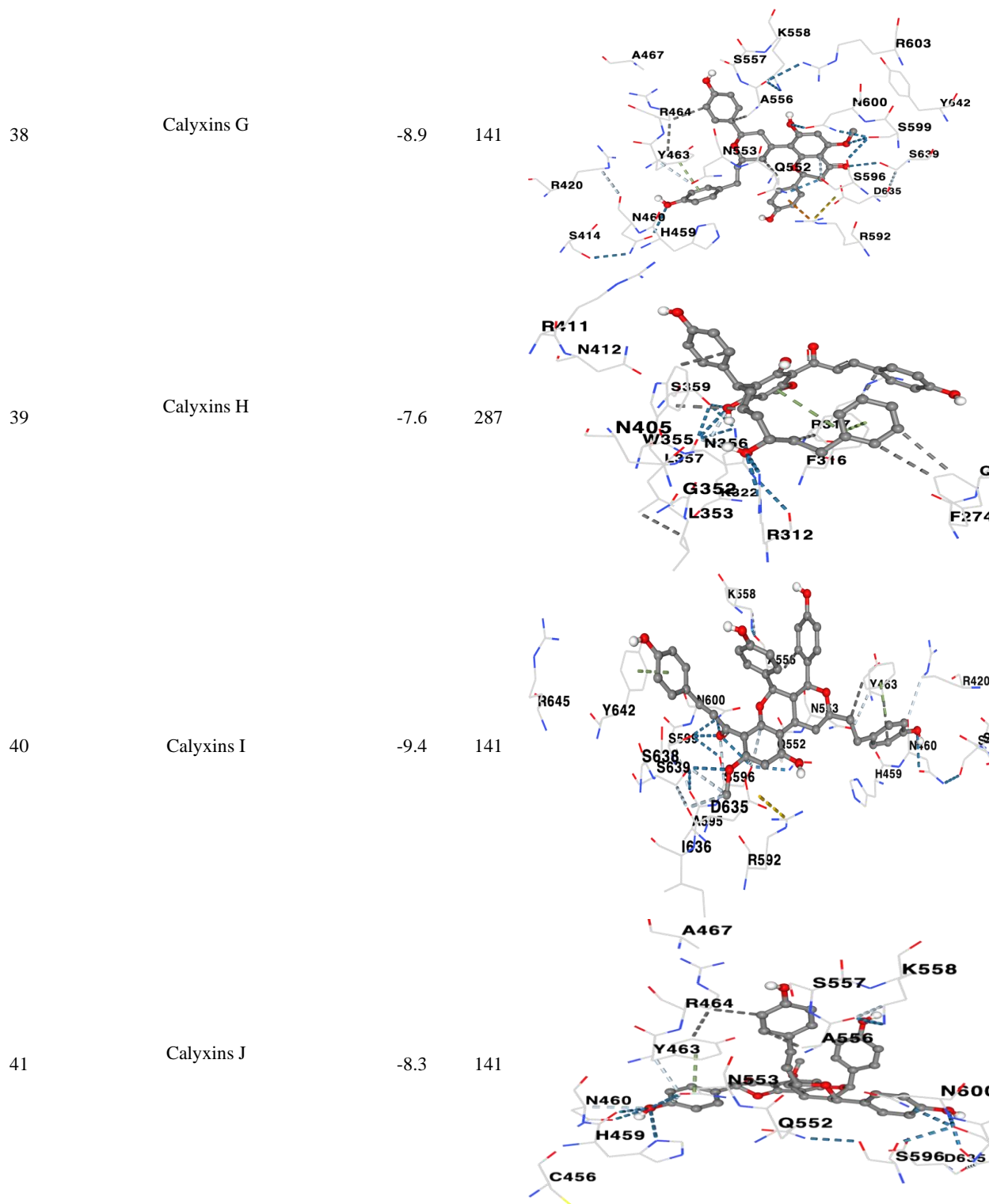


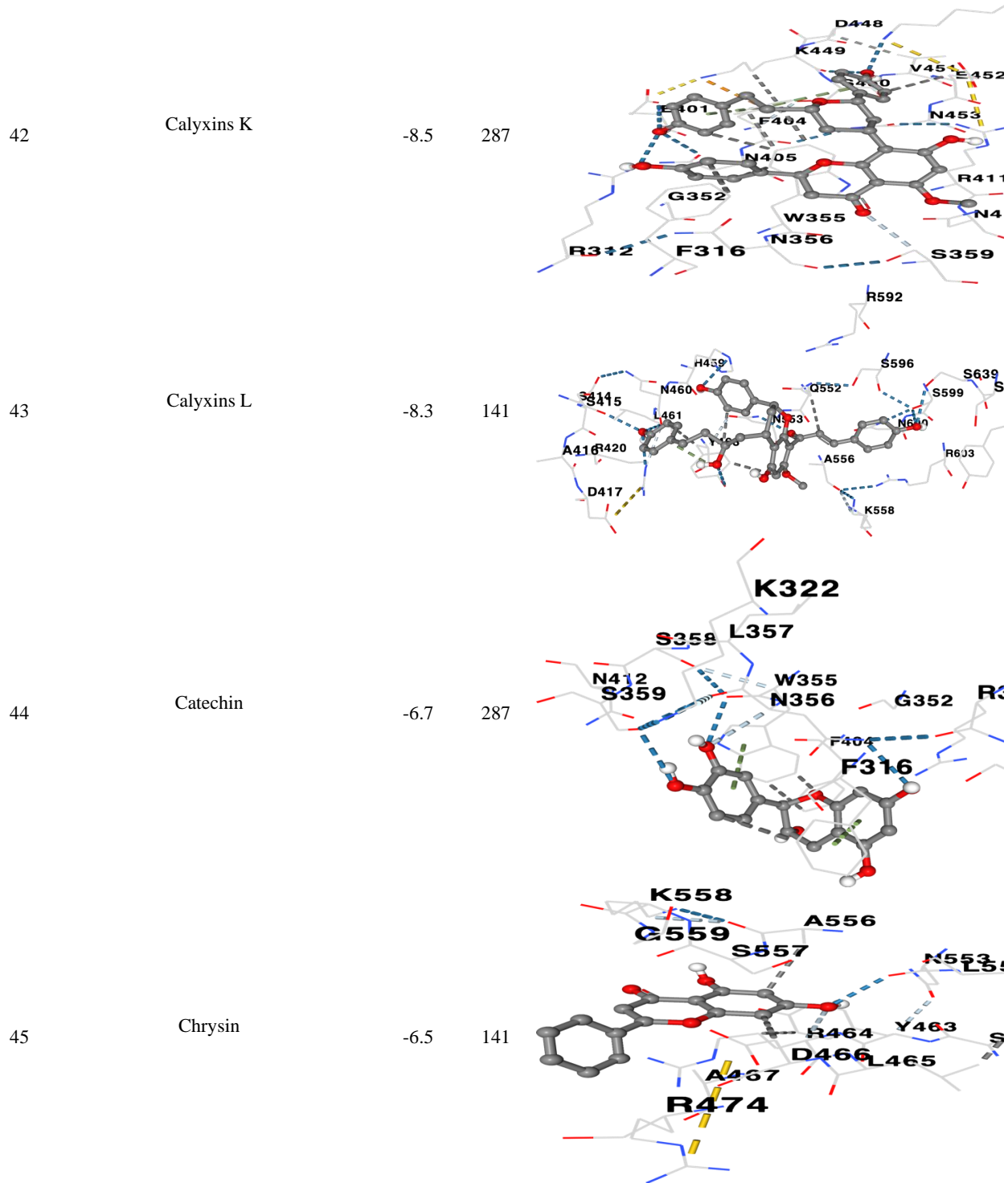












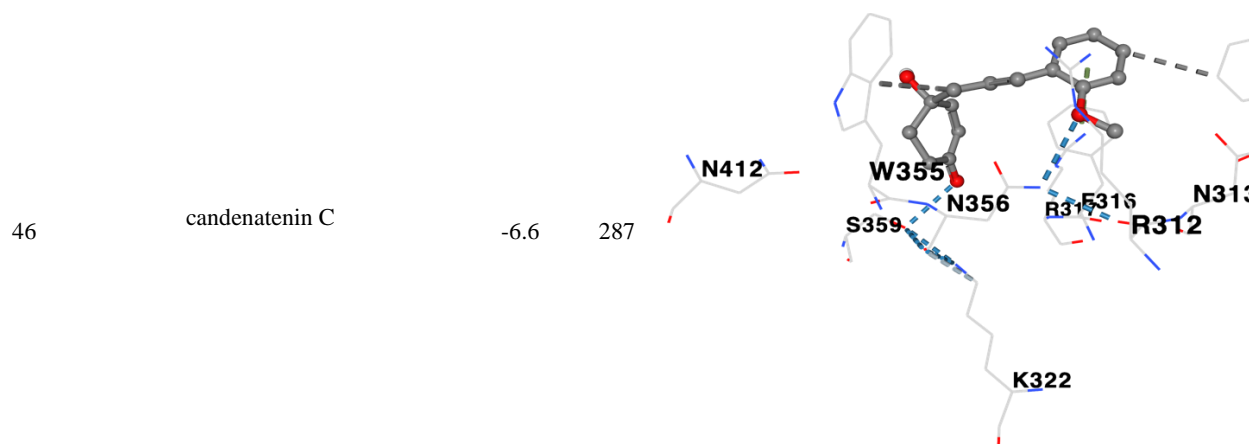


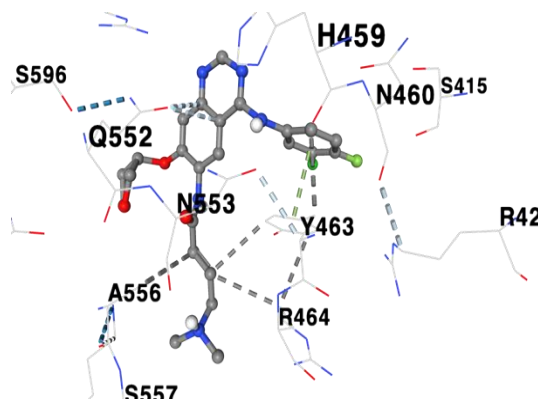
Table S4. Comparison of phytochemicals versus referenced standard drug afatinib.

S no.	Compound name	Binding score by Patchdock	Binding score by CBdock	Complex structure
1.	calyxinsJ	8322	-8.3	
2.	calyxinsI	5908	-9.4	

3. Afatinib

5610

-7.8



4. Blepharocalyxins
E

7150

-8

