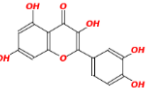
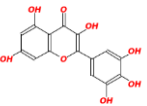
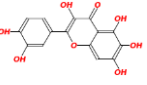
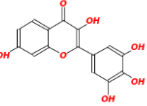
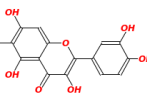
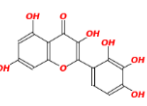
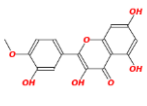
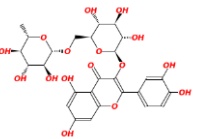
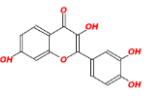
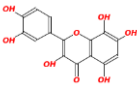
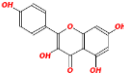
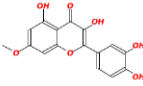
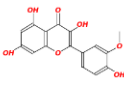
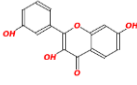
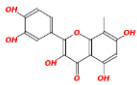
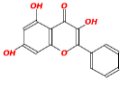
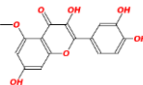
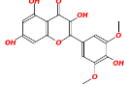
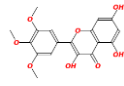
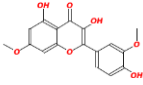
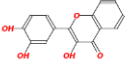
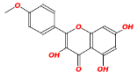
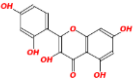
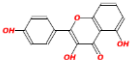
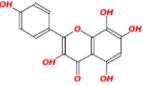
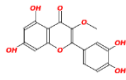
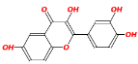
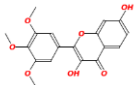
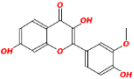
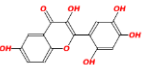
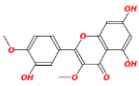


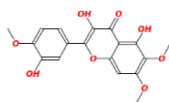
- 1 **Supplementary**
2 **Table T1. Quercetin derivatives used in this study**
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S.NO	Compounds	Structure	ZINC
1.	Quercetin		ZINC03869685
2.	Myricetin		ZINC03874317
3.	Quercetagetin		ZINC05784821
4.	Robinetin		ZINC04098600
5.	Pinoquercetin		ZINC06520226
6.	Myricetin		ZINC14436449
7.	Tamarixetin		ZINC06484604
8.	Quercetin-3-O-Rutinoside		ZINC53683228
9.	Fisetin		ZINC00039111

10.	Gossypetin		ZINC06525297
11.	Kaempferol		ZINC03869768
12.	Rhamnetin		ZINC03875620
13.	Isorhamnetin		ZINC00517261
14.	3,7,3'-Trihydroxyflavone		ZINC00057845
15.	2-(3,4-Dihydroxyphenyl)- 3,5,7-Trihydroxy-8- Methyl-Chromen-4-One		ZINC04731234
16.	Galangin		ZINC00120273
17.	Azaleatin		ZINC05998785
18.	Syringetin		ZINC06483609
19.	3,5,7-Trihydroxy-3',4',5'- Trimethoxyflavone		ZINC06483700
20.	Rhamnazin		ZINC06403375

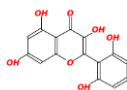
21.	3,3',4'-Trihydroxyflavone		ZINC00039321
22.	Kaempferide		ZINC06411540
23.	Morin		ZINC03881558
24.	3,6,4'-Trihydroxyflavone		ZINC00057752
25.	3,4',5,7,8-Pentahydroxyflavone		ZINC06536276
26.	3-O-Methyl Quercetin		ZINC05998596
27.	3,6,3',4'-Tetrahydroxyflavone		ZINC00008662
28.	3,7-Dihydroxy-3',4',5'-Trimethoxyflavone; (Robinetin Trimethylether)		ZINC02146994
29.	3'-Methoxy-3,7,4'-Trihydroxyflavone		ZINC05732763
30.	3,6,2',4',5'-Pentahydroxyflavone		ZINC48057104
31.	Quercetin 3,4'-Dimethyl Ether		ZINC05640267

32. **3,3',5-Trihydroxy-4',6,7-Trimethoxyflavone**



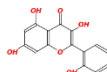
ZINC05733650

33. **2-(2,6-Dihydroxyphenyl)-3,5,7-Trihydroxy-Chromen-4-One**



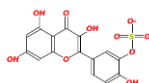
ZINC14644239

34. **Datisacetin**



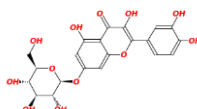
ZINC06095498

35. **Quercetin 3-O-Sulfate**



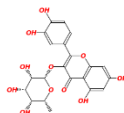
ZINC14644472

36. **Quercetin-7-O-Glucoside**



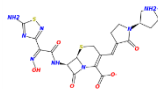
ZINC04654813

37. **Quercitrin**



ZINC04416338

38. **Ceftobiprole**



ZINC04424091

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1 **Table T2. Docking result of Quercetin 3-O-rutinoside and Ceftobiprole in allosteric site of PBP2a.**

Ligands	Glide Score	Number of H-Bond	H-bond forming Residues	H-bond length (Å)
Quercetin 3-O-rutinoside	-7.790318	6	ASN104	1.82
			ASN146	2.22
			VAL277	2.04
			ASP295	2.07
			HIS293	2.11
			GLN292	1.84
Ceftobiprole	-5.194946	3	Tyr105	3.09
			Lys273	2.68
			Lys316	2.71

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