

**Table S4** MMPBSA based on total binding free energies along with its constituent energies for top three bioactive molecules.

Protein	Complex	Total Binding	Van der Waals	Electrostatic	Polar Solvation	SASA Energy
		Free Energy	Energy	Energy	Energy	(Kcal/mol)
		(Kcal/mol)	(Kcal/mol)	(Kcal/mol)	(Kcal/mol)	
6M17	Luteolin	-20.7415	-24.6780	-15.8804	23.1922	-3.3753
6M17	CBGVA	-22.9144	-26.5570	-18.3969	25.5149	-3.4755
6M17	CBNA	-10.9932	-15.0076	-7.6496	13.7080	-2.0440
3R4D	Luteolin	-12.7945	-18.2797	-22.3411	30.6544	-2.8280
3R4D	Stigmasterol	-28.0828	-35.6418	-6.9927	18.7811	-4.2294
3R4D	CBNA	-17.0425	-18.6689	-22.9830	27.2120	-2.6027