Electronic Supplementary Material (ESI) for Molecular BioSystems.

Name	Compound ID	logD	logP	Num_RotatableBonds	H-acceptor	H-donor	Molecular Weight	LibDockScore	MM/PBSA Binding Free Energy(kJ mol-1)
C1	F321-0926	4.21	4.14	4	5	1	353.802	163.958	-89.27±2.89
C2	G295-0796	3.68	2.29	6	5	1	354.403	172.488	-56.65±1.85
C3(FL1607)	G415-4990	3.42	2.48	6	5	2	356.417	161.211	-47.32±1.49
C4	G777-0185	2.82	2.8	5	5	1	357.423	161.97	-40.06±2.03
C5	G331-0699	4.83	3.13	7	3	2	367.417	166.656	-17.49±3.10
C6	G862-0627	3.32	1.99	9	4	2	384.449	161.144	-53.30±1.99
C7	F235-0059	-0.47	2.03	5	7	2	384.795	164.764	-110.74±2.2
C8	G765-0264	5.49	2.94	6	3	2	394.51	173.171	-93.73±1.88
C9	G542-0518	4.12	2.43	8	4	1	398.499	165.842	-69.97±2.05
C10	F462-0367	-0.58	1.23	6	7	1	409.371	178.356	-27.50±1.85