

Table 3 The top 10 ligands against Kir5.1

Rank	Ligand	score(kcal/mol)	Hydrogen bond
1	Z2087256678_2	-7.3	ASP113, ASP101, ASP105
2	Z2211139111_1	-7.3	ASP101, GLU141, GLU142
3	Z2211139111_2	-7.3	ASP101, ASP105
4	PV-000592319198_1	-7.3	ASP105
5	Z2211137992_1	-7.2	ASP101, ASP105
6	Z2211137992_2	-7.2	ASP101, ASP105, ASP113, HIS116
7	Z2717222271_1	-7.1	THR109, GLU142, VAL145
8	Z2211137992_4	-7.0	ASP105, ILE108, ASP113, ASN114, GLU141, GLU142
9	Z1411107749_2	-7.0	ASP105, PRO106, ASP113, ASN114
10	PV-000377841410_1	-6.9	ASP101, ASP105, ILE108, ASP113