

**Table S1.** Redocking of structures of Furin with their ligands co-crystallized.

Structure Furin (PDB ID)	Resolution (Å)	Ligands	Free Energy of Binding (Kcal/mol) VINA	RMSD	Free Energy of Binding (Kcal/mol) Autodock 4.2	RMSD
7QXZ	1.8	3-(3,5-Dichlorophenyl) pyridine-derived	-10.4	1.444	-14.16	1.05
5MIM	1.9	2,5-dideoxystreptamine derived	-7.8	2.104	-7.31	2.61
7LCU	1.34	BOS-318	-10.3	0.00	-13.98	1.13
7IOY	1.7	Guanyldihydroquinazolinone-based inhibitor 2	-6.1	3.37	-6.6	2.31