

Table S1. Redocking setting and RMSD result

Protein	Native Ligand	RMSD (Å)	Grid box set up				
			x	y	z	Box size (Å ³)	Spacing (Å)
MDM-2	Nutlin-3a	0.385	-23.945	8.091	-13.667	15x15x15	1.000
Bcl-2	THIQ-PP	0.583	1.861	0.439	19.153		