



Figure S2. Docking validation of AutoDock Vina 1.2.0. (A) The original ligand position (pink) for PDB code 8SKL and the ligand position after AutoDock docking (green). RMSD = 0.84 Å. (B) The original ligand position (pink) for PDB code 2F71 and the ligand position after AutoDock docking (green). RMSD = 0.87 Å.