

Improving Blind Docking in DOCK6 through an Automated Preliminary Fragment Probing Strategy

Supplementary Material

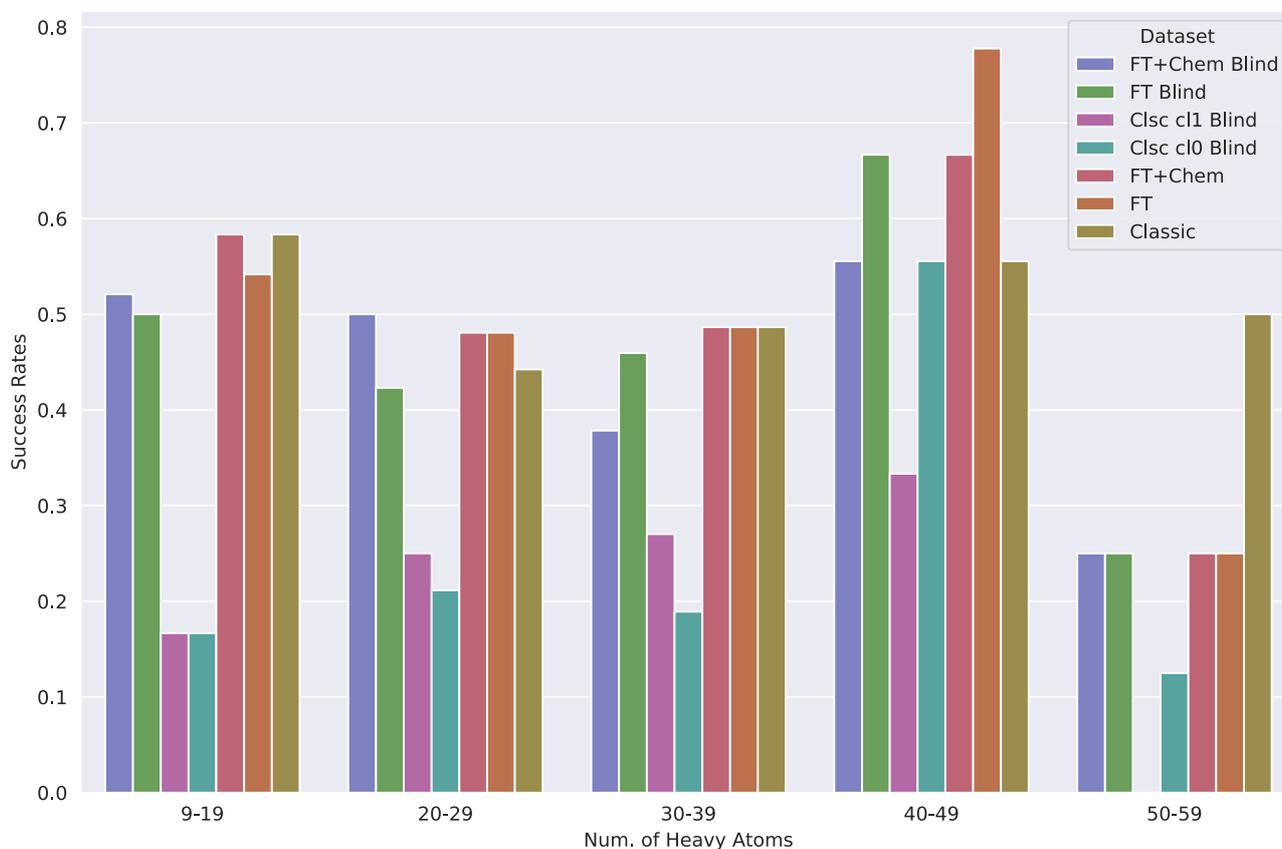


Figure S1: Distribution of success rates (RMSD < 2.0Å) for each PDBbind benchmarking protocol and for six different ligand size categories, distinguished by ligand number of heavy atoms. Minimum number of ligand heavy atoms was 9 and maximum was 70. Although we had 3 ligands in category 60-70, none were docked with RMSD < 2Å. The number of complexes in each category are: 9-19: 48; 20-29: 52; 30-39: 37; 40-49: 9; 50-59: 8; 60-70: 3.