Comprehensive evaluation of ten docking programs on a diverse set of protein-ligand complexes: prediction accuracy of sampling power and scoring power

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Figure S1. Distributions of five properties of 1790 FDA approved drugs. The structures were downloaded from e-Drug3D.¹
Table S1. The unsuccessful docking instances of individual tested docking program in benchmark. Optimized ligands were used as the input and 2.0 Å was used as RMSD cutoff.

See in TableS1.xlsx

Table S2. The formal charge and number of rotatable bonds of ligands for the 72 failure cases that could not be unsuccessfully predicted by any docking program.

See in TableS2.xlsx

References