Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

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

Zhe Wang,[a] Huiyong Sun,[a] Xiaojun Yao,[c] Dan Li,[a] Lei Xu,[d] Youyong Li,[e] Sheng Tian[e] and Tingjun Hou[a,b,*]

[a]College of Pharmaceutical Sciences, Zhejiang University, Hangzhou, Zhejiang 310058, China.

[b]State Key Lab of CAD&CG, Zhejiang University, Hangzhou, Zhejiang 310058, China.

[c]State Key Laboratory of Quality Research in Chinese Medicine, Macau Institute For Applied Research in Medicine and Health, Macau University of Science and Technology, Avenida Wai Long, Taipa, Macau (SAR), China

[d]Institute of Functional Nano and Soft Materials (FUNSOM), Soochow University, Suzhou, Jiangsu 215123, China.

[e]Institute of Bioinformatics and Medical Engineering, School of Electrical and Information Engineering, Jiangsu University of Technology, Changzhou 213001, China

Corresponding Author

E-mail: tingjunhou@zju.edu.cn or tingjunhou@hotmail.com;

Phone: +86-571-88208412

Keywords: Molecular docking, Benchmark, Pose sampling, Scoring function, Virtual screening

Supporting Information

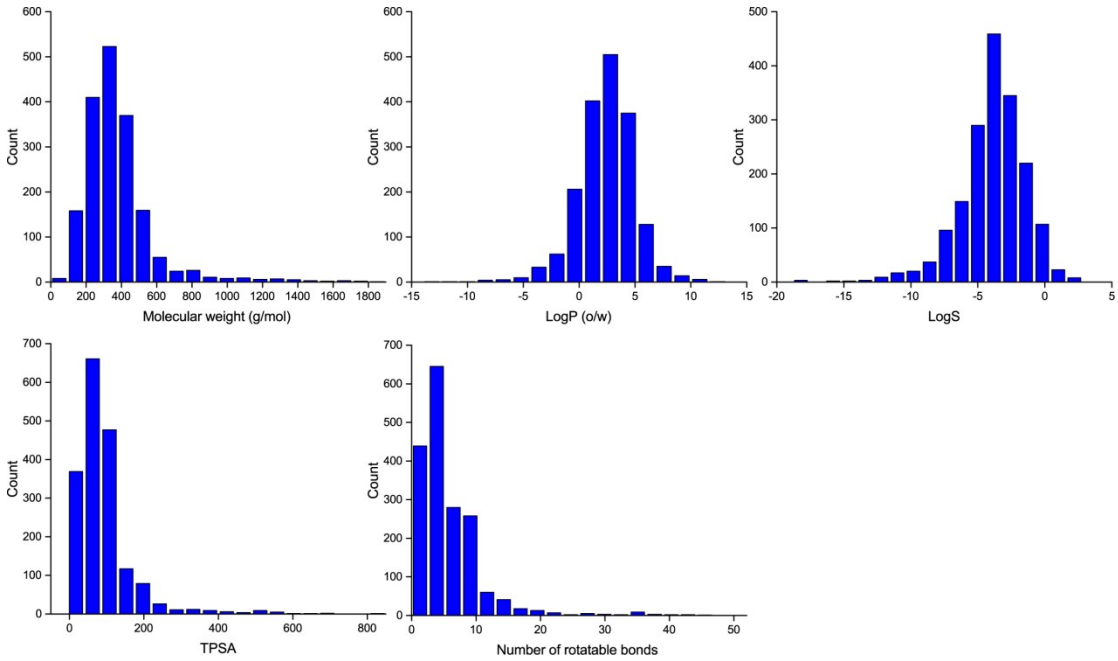

Figure S1. Distributions of five properties of 1790 FDA approved drugs. The structures were downloaded from e-Drug3D.[1]

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

1. Pihan, E.; Colliandre, L.; Guichou, J. F.; Douguet, D., e-Drug3D: 3D structure collections dedicated to drug repurposing and fragment-based drug design. *Bioinformatics* **2012**, 28, 1540-1.