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Computational method for calculating ligand binding affinities

分子シミュレーションの創薬への応用 : リガンド結合親和性予測の計算科学的手法

Atsushi Suenaga / 末永 敦

Molecular Profiling Research Center for Drug Discovery (MOLPROF)
National Institute of Advanced Industrial Science and Technology (AIST)
産業技術総合研究所　創薬分子プロファイリング研究センター

Virtual compound screening using molecular docking is widely used in the discovery of new lead compounds for drug design. However, the docking scores are not sufficiently precise to represent the protein-ligand binding affinity. The candidates of drugs should strongly and specifically bind to the target proteins, thus the accurate prediction of the binding affinity of a ligand for a protein is a critical element in computer-aided drug discovery. Here, we will review different computational methods currently available to calculate ligand binding affinitis, and introduce an efficient method that we developed.

Keywords: Molecular simulation, Computer-aided drug design, free energy