第 5 回 2013 年 11 月 8 日（金）14:50 ~ 15:40

Computational method for calculating ligand binding affinities

化合物スクリーニングと創薬インフォマティクス

Chie Motono / 本野 千恵

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
Computational Biology Research Center (CBRC)
National Institute of Advanced Industrial Science and Technology (AIST)
産業技術総合研究所　生命情報工学研究センター

There are two major types of rational drug design: ligand-based drug design and structure-based drug design. In this lecture I will explain computer-aided drug design, especially structure-based methods, which relies on knowledge of the three dimensional structure of the target proteins. In structure-based drug design molecular docking screens of chemical databases are widely used for ligand discovery. Typical docking approaches and scoring methods will be reviewed. I will also introduce our alternative docking screen which uses MD simulations and concavity shape comparing.

Keywords: protein structure, molecular dynamics simulation, pharmacoinformatics