第 9 回 2012 年 12 月 21 日（金）14:50 ~ 15:40

Molecular Simulations for drug design

創薬支援のための分子シミュレーション技術

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Molecular simulations, including protein structure prediction, docking simulation and molecular dynamics are an integral part of structure-based drug discovery and design. For example, molecular simulations contribute to the following issues in chemical biology projects: 1) prediction of structural model using protein-protein docking for the protein-protein interaction (PPIs) identified by a protein interaction network analysis system utilizing mass spectrometry, 2) Discovery of seed compounds that regulate biological system using high-throughput docking from commercially available chemical libraries, and 3) Design and optimization of seed compounds or natural products using structure based approach through cooperation with combinatorial library synthesis and molecular dynamics simulations. In this talk, I will present multi strategies for the in silico structure-based drug discovery for PPIs, GPCRs and kinases based on the molecular simulations.

Keywords : structure-based drug design, docking simulation, molecular modeling, molecular dynamics