Virtual screening for drug discovery

Virtual screening has become an essential element of the drug discovery process. Virtual screening is used to search a large library of small molecules for binding to a target protein and select a small subset of compounds for subsequent experimental validation and optimization. In this block course we will discuss the methodological basis and practical applications of structure-based and ligand-based virtual screening methods such as docking, shape-based, pharmacophore and fingerprint concepts. The course alternates lectures and practical sections in the computer lab.

Tuesday, June 27: Structure-based virtual screening, Theory

- Interactions in protein-ligand complexes
- Free energy, enthalpy and entropy
- Docking algorithms
- Docking applications
- Protein flexibility in docking
- Virtual screening using docking

Wednesday, June 28: Structure-based virtual screening, Practical applications

- Docking
- Virtual screening using docking

Thursday, June 29: Ligand-based virtual screening, Theory

- Similarity principle
- Shape-based methods
- Pharmacophore models
- Fingerprints

Friday, June 30: Ligand-based virtual screening, Practical applications

- Library design
- Shape-based virtual screening
- Pharmacophore models and colored shape-based virtual screening
- Fingerprint-based virtual screening