

Molecular Modelling

By Dr. Krisztina Fehér

The course outline is the following:

- Molecular Structure: Conformation, Supramolecular structure
- Basics of Molecular Mechanics
- Quantum Chemistry versus Molecular Mechanics
- Potential Energy Surface
- Force fields
- Potential Energy Function terms
- Parameters, atom types, topology
- Simulations methods
- Energy minimisation for Geometry optimization
- Molecular dynamics and its variants.
- Conformational search methods
- Systematic conformational searches.
- Random conformational searches, Monte Carlo methods.
- Analysis of conformational ensembles and trajectories: geometric and dynamic descriptors, RMSD, RMSD, order parameter, clustering, PCA, machine learning methods