

Title of the course: Methods of protein crystallography

Kvvn9778

Credit: 2

Coordinator: Harmat, Veronika

Department: Department of Organic Chemistry

Pre-requisites: -

Topics covered by the course:

Introduction to X-ray diffraction, the methods of structure determination of biological macromolecules. A practical approach.

1. Theoretical background, possible implications and limitations.
2. The electron density function and the structure factor.
 - Diffraction of X-rays on a crystal lattice
 - The crystallographic phase problem
 - Symmetry
3. Crystallization and data collection strategies
4. Solving the phase problem
 - The Patterson function
 - Molecular replacement
 - Isomorphous replacement methods
 - Use of anomalous dispersion
5. From electron density maps to 2D structure of the molecule: model building and refinement.
 - The model bias
6. Validation of the refined model
7. New directions and challenges in protein crystallography
 - Structural genomics
 - Large structures and poor crystals
8. Applications in drug discovery
 - Structure based and fragment based drug design
9. Membrane proteins
10. A molecular movie: time resolved crystallography

Literature

Compulsory_ -

Suggested:

- Blow, David „Outline of Crystallography for Biologists”, Oxford University Press 2002
- Drenth, Jan „Principles of Protein X-Ray Crystallography” Springer 1999