ЦЕНТЪР ЗА ОБУЧЕНИЕ – БАН

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TEMPLATE FOR A SPECIALIZED DOCTORAL COURSE (in English)

Basic Information:
Course Title: Structural Biology
Lecturer: Assoc. Prof. Kiril Kirilov, PhD
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Total Teaching Hours: 30

Annotation (up to 150 words)
ctions, and the energetic basis of protein conformational stability, as well as the mechanical properties and dynamics of macromolecules. Major experimental methods for determining three-dimensional structures—including X-ray crystallography, cryo-electron microscopy, and nuclear magnetic resonance—are presented together with modern computational approaches in structural bioinformatics.

Course content (brief description by topics or modules)
Topic / Module 1 – Structural Organization of Biomolecules
Fundamentals of structural biology. Levels of protein structural organization. Structure of nucleic acids. Relationship between structure and biological function.
Topic / Module 2 – Energetics, Dynamics, and Molecular Interactions
Molecular interactions and energetic factors determining the stability of biomolecular structures. Organization of protein–ligand and protein–protein complexes. Fundamentals of molecular dynamics – force fields, computer simulations, and trajectory analysis.
Topic / Module 3 – Methods and Computational Approaches in Structural Biology
Comparative overview of experimental methods (X-ray crystallography, cryo-electron microscopy, and NMR) and the structural information they provide. Structural bioinformatics and molecular modeling – structural alignment, structure prediction, and analysis of molecular interactions. Calculation of binding free energies using MM/PBSA and MM/GBSA methods.

Teaching and assessment methods
lectures;
computer-based practical exercises;
analysis of structural datasets;
assessment through written test and oral discussion.

Competencies acquired as a result of training (3–5 points)
After completing the course, doctoral students will be able to:

1. interpret three-dimensional biomolecular structures;
2. perform structural analysis using bioinformatics tools;
3. analyze molecular interactions;
4. conduct molecular dynamics simulations;
5. evaluate stability and energetics of biomolecular complexes.

Literature:

Branden C., Tooze J. – Introduction to Protein Structure
Petsko G., Ringe D. – Protein Structure and Function
Leach A. – Molecular Modelling: Principles and Applications

Additional information (optional) (e.g., special requirements, laboratory equipment, prior knowledge)
Recommended background:
biochemistry, molecular biology, or bioinformatics.
Software used in the course:
GROMACS, AMBER, NAMD, VMD, PyMOL.