Program of Studies:	**Master Program Bioinformatics**
Name of the module:	**Special Lecture Bioinformatics: Structural Bioinformatics**
Abbreviation:	**BI-BM-1**
Subtitle:	-
Modules:	Lecture: 2 h (weekly) Tutorial: 1 h (weekly)
Semester:	1st – 3rd semester; winter semester
Responsible lecturer:	Prof. Dr. Olga Kalinina
Lecturer:	Prof. Dr. Olga Kalinina
Language:	English
Level of the unit/ Mandatory or not :	Graduate course / mandatory elective
Total workload:	150 h = 48 h of classes and 102 h private study and assignments
Credits:	5
Entrance requirements:	Bioinformatics I and II, Molecular Biology/Organic Chemistry, Programming skills in Python
Aims/Competences to be developed:	Expected gained theoretical competencies: - Understanding physical and chemical basics of three-dimensional structure of biomolecules - Understanding relationship between similarity and evolution - Knowledge of basic principles of algorithms for sequence similarity search - Knowledge of basic steps of algorithms for modelling of protein 3D structures - Understanding the concepts of comparison and alignment of protein 3D structures; knowledge of measures for comparison of protein 3D structures - Understanding basic principles of molecular dynamics simulation methods Expected gained practical competencies: - Given a protein sequence, identify its potential functional family, make guesses about cellular localization - Search for experimentally resolved protein 3D structures, related information in publicly available resources - Understanding the common formats of storing structural data - Be able to programmatically analyze and manipulate corresponding files - Visualize protein 3D structures, describe it, analyze it with respect to potential protein function - Build 3D models of protein structures based on homology-modelling approach using online resources and programmatically

Content:	Structural bioinformatics studies protein structures resolved in 3D by experimental methods. Recent years have witnessed an exponential growth of experimental data on protein structure and interactions due to projects such as Structural Genomics Initiative. This opens new venues for bioinformatics studies related to protein structure prediction, comparison and analysis. The course will take you from the very basic concepts of how structural data are obtained and organized in databases to sophisticated topics of relationships between protein structure and function and the evolution of the two; and insights from comparison of protein structures. In the exercises, we will learn basic techniques for structure search, comparison, analysis, and protein structure modelling.
Assessment/Exams:	written exam
Grade:	exam grade
Literature:	The course is largely based on "Structural Bioinformatics", 2nd edition, eds. Jenny Gu, Philip E. Bourne. Where appropriate, the material from the book will be supplemented with data from recent literature. These will be made available in the password protected area.