COURSE UNIT (MODULE) DESCRIPTION

Course unit (module) title	Code
Structural biology of macromolecules (X-ray crystallography of biological macromolecules)	

Lecturer(s)	Department(s) where the course unit (module) is delivered
Coordinator: Assoc. Prof. dr. Saulius GRAŽULIS **Other(s):**	Faculty of Natural Sciences, Department of Biochemistry and Molecular biology

Study cycle	Type of the course unit (module)
Second level	Elective

Mode of delivery	Period when the course unit (module) is delivered	Language(s) of instruction
Face to face	2nd semester, spring	Lithuanian (English)

Requirements for students	
Prerequisites: Biochemistry, organic chemistry, physical chemistry, physics, calculus, linear algebra	**Additional requirements (if any):** Work experience in Unix or Linux operating systems and basic familiarity with a tree file system and command line interpreter (Unix shell) are desirable.

Course (module) volume in credits	Total student's workload	Contact hours	Self directed learning
4	112	48	64

Purpose of the course unit (module): programme competences to be developed

Upon the successful completion of this course, students will acquire:
Subject-specific competences:

- knowledge of macromolecular structure analysis methods, necessary for independent scientific research;
- skills to select and apply macromolecular structure analysis methods for research and to interpret reasonably the results obtained through those methods;
- skills to integrate the knowledge of different sciences;

General competences:

- analytical and synthetic thinking;
- abilities of self-learning;
- ability to present knowledge in the field of structural biology in talks in written form;
- abilities to participate in scientific discussion;

Learning outcomes of the course unit (module)	Teaching and learning methods	Assessment
Describes the state-of-the-art X-ray crystallography capabilities, and other structure analysis methods. Skills to choose an appropriate structure analysis method for a	Lectures, problem-based learning, practical classes, self-study.	Midterm exams; final exam; topic-related practical classes, practical work report.

given problem.		
Determines, on his/her own, the 3D structure of a macromolecule from collected diffraction data (X-ray diffraction images, HKLFobs data).	Lectures, problem-based learning, practical classes, self-study.	Midterm exams; final exam; topic-related practical classes, practical work report.
Assesses quality of the own constructed macromolecule models and of the macromolecule models published in databases or in scientific press.	Lectures, problem-based learning, practical classes, self-study.	Midterm exams; final exam; topic-related practical classes, practical work report.
Assesses critically the structural information obtained by X-ray crystallography and other methods and extracts biologically relevant knowledge from structural data.	Analysis of structures provided in the PDB, lectures, problem-based learning, practical classes, self-study.	Midterm exams; final exam; topic-related practical classes, practical work report.

Content: breakdown of the topics	**Contact hours**							**Self-study work: time and assignments**	
	Lectures	Tutorials	Seminars	Exercises	Practical work	Work placement	**Contact hours**	**Self-study hours**	**Assignments**
1. Importance of structural information and methods of obtaining it	**4**				**2**		**6**	**8**	Critical assessment of books, scientific papers and Web material on the topic. Self-directed learning.
1a. Structural information about biological macromolecules: types of structural information and its uses	2				1			4	
1b. Experimental methods for macromolecule structure determination (NMR, ESR, EXAFS/XANES, X-ray crystallography)	2				1			4	
2. Theory of X-ray crystallography	**8**				**4**		**12**	**16**	Critical assessment of books, scientific papers and Web material on the topic. Self-directed learning.
2a. Introduction into X-ray diffraction theory	4				2			8	
2b. Phase problem and methods of its solution	4				2			8	
3. Symmetry of crystals	**6**				**3**		**9**	**12**	Critical assessment of books, scientific papers and Web material on the topic. Self-directed learning.
3a. Plane and space symmetry groups	2				1			4	
3b. Elements of crystallographic symmetry	2				1			4	
3c. Use and interpretation of symmetry: International Tables for Crystallography	2				1			4	
4. Analysis of macromolecule crystals	**6**				**3**		**9**	**12**	Critical assessment of books, scientific papers and Web material on the topic.

									Practical work with crystallographic data and models, including ones from the PDB. Self-directed learning.
4a. Methods of crystal preparation	1								
4b. Diffraction experiment and data collection	1				1			4	
4c. Processing of diffraction data and phase determination	2				1			4	
4d. Model building and refinement	2				1			4	
5. Structural models and their interpretation	**8**				**4**		**12**	**16**	Critical assessment of books, scientific papers and Web material on the topic. Practical work with crystallographic data and models, including ones from the PDB. Self-directed learning.
5a. Data and model quality criteria	2				1			4	
5b. Structural databases (PDB, NDB, COD, etc.)	2				1			4	
5c. Model overlay and comparison	2				1			4	
5d. Biochemical interpretation of structural models	2				1			4	
Total	**32**				**16**		**48**	**64**	

Assessment strategy	**Weight,%**	**Deadline**	**Assessment criteria**
Classwork assessment	10	Beginning of each practical seminar	A quiz (virtual learning environment) of 4 questions from topics the topics covered in the previous lectures. The scores from all answers in all quizzes are summed up; maximal sum is 100 points.
Midterm exam	30	Middle of the course	Test (virtual learning environment) of 50 questions from topics 1-3; maximum score from this test is 300 points.
Presentation of the practical work results	30	Last week of the course	Students must upload a report (type-setted according to the presentation standards of the Vilnius University) to the Virtual Learning Environment and prepare a 5 – 10 min. talk on his/her work. The evaluation criteria will include: achievement of the goals set for the practical work – up to 100 points; general understanding of the topic (as judged from the answers to 3 topic related questions) – up to 100 points; written presentation of the work – up to 50 points; oral presentation – up to 50 points; total sum up to 300 points.
Exam	30	Exam session	Test (virtual learning environment) of 50 questions from all topics of the course; maximum score from this test is 300 points.
Total	100		The final mark is obtained by summing up points earned in all quizzes and tests (summing up to 1000 points), dividing by 100 and rounding to the next largest integer (thus a sum, for instance, of 901 point would give the final mark 10).

Author	**Year of public ation**	**Title**	**Issue of a periodical or volume of a publication**	**Publishing place and house or web link**

Compulsory reading				
S. Gražulis	2012	Virtual learning environment: course "X-ray crystallography of biological macromolecules"		http://saulius-grazulis.lt/moodle/.
wwPDB konsorciumas	2013	PDB, The Protein Data Bank		http://www.pdb.org/
	1971 – 2013	*papers describing macromolecule structures as cited in the PDB*		http://www.pdb.org/
Jan Drenth	1994	Principles of Protein X-Ray Crystallography (Springer Advanced Texts in Chemistry)		Springer Verlag, New York, ISBN 0-387-94091-X
Duncan McRee	1999	Practical Protein Crystallography, Second Edition		Academic Press/Elseview, London, ISBN-13 978-0-12-486052-0
Theo Hahn (Editor)	2002	International Tables for Crystallography, Brief Teaching Edition of Volume A		Kluwer Academic Publishers Dortrecht/Boston/London, ISBN 0-7923-6591-7
Optional reading				
IUCr	2013	IUCr Educational resources		http://www.iucr.org/education, http://www.iucr.org/education/pamphlets
Jack D. Dunitz	1995	X-Ray analysis and the Structure of Organic Molecules		Verlag Helvetica Chimica Acta, Basel, ISBN 3-906390-14-4
Carmelo Giacovazzo (Editor), et al.	1995	Fundamentals of Crystallography		Oxford university Press, Oxford, New York, ISBN 0-19-855578-4
Theo Hahn (Editor)	2002	International Tables for Crystallography, Volume A		Kluwer Academic Publishers Dortrecht/Boston/London, ISBN 0-7923-6590-9