COURSE UNIT DESCRIPTION - X-RAY CRYSTALLOGRAPHY OF BIOLOGICAL MACROMOLECULES

Course unit title	Code
X-RAY CRYSTALLOGRAPHY OF BIOLOGICAL MACROMOLECULES	

Lecturer(s)	Department(s)
Coordinator: Assoc. Prof. dr. Saulius GRAŽULIS **Other(s):**	Institute of Biotechnology of Vilnius University, V.A.Graičiūno 8, Vilnius LT-02241

Cycle	Level of the course unit	Type of the course unit
Full-time studies (2nd stage)	1 out of 1	Elective

Mode of delivery	Period of delivered	Language(s) of instruction
Face to face	2nd semester, spring	Lithuanian (English)

Prerequisites and corequisities	
Prerequisites: Biochemistry, organic chemistry, physical chemistry, physics, calculus, linear algebra	**Corequisities (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.

Number of credits allocated to the course unit	Student's total workload	Contact hours	Self-study and research hours
4	107	48	59

Purpose of the course unit: 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	Teaching and learning methods	Assessment methods
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 given problem.	Lectures, problem-based learning, practical classes, self-study.	Midterm exams; final exam; topic-related practical classes, practical work report.
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,	Midterm exams; final exam; topic-related practical classes, practical work report.

	self-study.	

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		**3**	4	
1b. Experimental methods for macromolecule structure determination (NMR, ESR, EXAFS/XANES, X-ray crystallography)	2				1		**3**	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		**6**	8	
2b. Phase problem and methods of its solution	4				2		**6**	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		3	4	
3b. Elements of crystallographic symmetry	2				1		3	4	
3c. Use and interpretation of symmetry: International Tables for Crystallography	2				1		3	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						1		
4b. Diffraction experiment and data collection	1				1		2	4	
4c. Processing of diffraction data and phase determination	2				1		3	4	
4d. Model building and refinement	2				1		3	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		3	4	
5b. Structural databases (PDB, NDB, COD, etc.)	2				1		3	4	
5c. Model overlay and comparison	2				1		3	4	
5d. Biochemical interpretation of structural models	2				1		3	4	
Total	**32**				**16**		**48**	**64**	

Assessment strategy	**Weight,%**	**Assessment period**	**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 publica-tion	Title	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