COURSE UNIT DESCRIPTION

Course unit title		Course unit code
Bioinformatics III		6BIOB3

Lecturer(s)	Department where the course unit is delivered
Coordinator: Saulius Gražulis **Other lecturers:**	Department of Mathematical Computer Science Faculty of Mathematics and Informatics Vilnius University

Cycle	Type of the course unit
1st (BA)	Compulsory

Mode of delivery	Semester or period when the course unit is delivered	Language of instruction
Face-to-face	6-th semester	Lithuanian, English

Prerequisites
Prerequisites:

Number of credits allocated	Student's workload	Contact hours	Individual work
5	138	66	72

Purpose of the course unit: programme competences to be developed

Purpose of the course unit is to teach students to find the necessary structural information in open access structural databases, process the obtained data using existing programs and their own coded algorithms, critically asses the obtained results and draw biologically relevant conclusions from them.

Generic competences:
- Ability to search, analyse, represent and organise the information *(GK1).*
- Ability to apply the knowledge in practice *(GK2).*

Specific competences:
- Nature and life sciences (*SK7*).
- Software engineering (*SK8*).
- Data coding, representation and mining. (*SK9*).
- Extracting, representation and analysis of bioinformatics data (*SK11*).

Learning outcomes of the course unit: students will be able to	Teaching and learning methods	Assessment methods
Understand information provided in 3D structural models, structure-function relationship; know the state-of-the art methods of three-dimensional structure determination.	Lectures, seminars, problem-based learning, individual assignments, practical classes, self-study.	Midterm exams; final exam; topic-related practical classes, practical work report.
Use structural information about biological macromolecules, evaluate reliability of structural models, use the existing structure analysis methods.		
Create bioinformatics programs with known or novel algorithms and to apply these programs for processing structural data.		
Critically asses the results of computations from the pre-existing software and from the newly created programs.		
Draw biologically relevant conclusions from the results of bioinformatics computations on structural data.		

| Course content: breakdown of the topics | Contact hours | | | | | | | Individual work: time and assignments |
	Lectures	Tutorials	Seminars	Practice	Laboratory work	Contact hours	Individual work	Assignments
1. Structural organization of proteins and nucleic acids, primary, secondary, tertiary and quaternary structure levels	2			2		**4**	**4**	Self-study of scientific publications and other sources; individual assignments as provided in the http://saulius-grazulis.lt/~saulius/pask aitos/VU/bioinformatika -III/užduotys-praktikai/ course teacher's web-site.
2. Representation of spacial structures in computers: coordinate systems, file formats (PDB, CIF, etc.)	6			6		**12**	**11**	
3. Geometry of the protein chain.	2			2		**4**	**4**	
4. Physical interactions determining structure of proteins and nucleic acids; the use of interaction information for validation and prediction of 3D structures	6			6		**12**	**11**	
5. Crystal symmetry and its use for macromolecule structure description	4			4		**8**	**8**	
6. Experimental methods for 3D structure determination and information that they provide	4			4		**8**	**8**	
7. Algorithms for 3D structure analysis (Kabsch algorithm and others)	6			6		**12**	**13**	
8. Prediction and validation of 3D structures	2			2		**4**	**3**	
9. Preparation for exam, exam		2				**2**	**10**	
Total	**32**	**2**		**32**		**66**	**72**	

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	15	Middle of the course	Test (virtual learning environment) of 50 questions from topics 1-3; maximum score from this test is 150 points.
Assessment of individual assignments	50	After each assignment, according to the schedule provided in the Virtual Learning Environment	Students must upload their assignment to the Virtual Learning Environment. The evaluation criteria of each practical assignment will include: achievement of the goals set for the practical work – up to 30% of the score; coding style and readability of the code – up to 30%; general knowledge on the subject – up to 40%.
Presentation of the practical work results	10	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 30 points; general understanding of the topic (as judged from the answers to 3 topic related questions) – up to 30 points; written presentation of the work – up to 20 points; oral presentation – up to 20 points; total

			sum up to 100 points.
Exam	15	Exam session	Test (virtual learning environment) of 50 questions from all topics of the course; maximum score from this test is 150 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	Publishing year	Title	Number or volume	Publisher or URL
Required reading				
Anna Tramontano	2006	Protein Structure Prediction		Wiley-VCH
Janusz Bujnicki (Editor)	2004	Practical Bioinformatics		Springer
Carl Branden, John Tooze	1991	Introduction to Protein Structure		
А. В. Финкельштейн, О. Б. Птицын	2005	Физика Белка		Москва, КДУ
Recommended reading				
Arthur M. Lesk	2002	Introduction to Bioinformatics		Oxford University Press
Dong, Q. & Wu, Z.	2002	A linear-time algorithm for solving the molecular distance geometry problem with exact inter-atomic distances. *Journal of Global Optimization*	vol. 22, pp. 365-375	Springer
Kabsch, W.	1976	A solution for best rotation to relate two sets of vectors. *Acta Crystallographica A*	vol. 32, pp. 922-923	IUCr/Wiley
	1968-2058	*Original papers reporting structure analysis algorithms from Acta Crystallographica, Bioinformatics and other scientific journals*		IUCr, Wiley, OUP, Academic Press, Springer, etc.