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: Methods of computer program construction, linear algebra, calculus, chemistry, molecular biology

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:*** • Natural 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 course teacher's web-site[1].
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	Day of the lecture or practical	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 test	15	Middle of the course	Test (virtual learning environment) including questions from the topics learned so far; 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, coding style and readability of the code, general knowledge on the subject. Evaluation will be conducted using subtractive method: an assignment that was carried out ideally will be worth 100% of the score; each deficiency will attract negative scores depending on its importance (the importance and the nature of the deficiency will be explained). Additional (bonus) assignments may be issued to help students to correct the previous deficiencies.

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[1] https://saulius-grazulis.lt/~saulius/paskaitos/VU/bioinformatika-III/užduotys-praktikai/

Assessment strategy	**Weight %**	**Deadline**	**Assessment criteria**
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, understanding of the topic (as judged from the answers to several topic related questions), written presentation of the work, oral presentation. The evaluation will be carried out either using the Moodle Rubric method or the subtractive method, as for the assignments.
Exam	15	Exam session	Approx. 30-question quiz covering several recent lectures (Bloom's 1 to 9 level questions) using an electronic teaching environment (Moodle, Open edX or similar). To be eligible for the exam, students must fulfil all following criteria: 1. carry out at least one practical work and get a positive grade for the practicals; 2. have enough accumulated points to be able to pass the exam in principle if they score maximum points at the exam quiz; Participation in the final exam quiz is obligatory to pass the course, regardless of the accumulated points. Students who do not show up in the final exam will be indicated as such in the exam grading report. To pass the exam, on must score at least 50% of possible points.
Total	100		The final mark is obtained by summing up points earned in all quizzes, tests, practicals and other course activities (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).
External students			Taking the exam as an external student is permitted by the decision of the lecturer coordinating the subject. As a rule, taking exam as an external student is permitted for very good students (with the academic average of at least 8) who are able to master the subject on their own and only need a knowledge assessment by a qualified VU representative. The requirements that apply to an external student are the same as those to a regular course attendee. A student applying for external student status may not have academic debts; only non-academic debts are permitted.

Author	**Publ. 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

Author	**Publ. year**	**Title**	**Number or volume**	**Publisher or URL**
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.