Course unit (module) title	Code
Thermodynamics of Protein Interactions with Ligands	

Lecturer(s)	Department(s) where the course unit (module) is delivered
Coordinator: Prof. Daumantas Matulis **Other(s):**	Life Sciences Center, Vilnius University, Saulėtekio 7, Vilnius

Study cycle	Type of the course unit (module)
Master	**Elective**

Mode of delivery	Period when the course unit (module) is delivered	Language(s) of instruction
Seminars	**Autumn semester**	**Lithuanian/English upon request**

Requirements for students	
Prerequisites: Biochemistry, general, inorganic, organic and physical chemistries, physics, mathematics	**Additional requirements (if any):** **None**

Course (module) volume in credits	Total student's workload	Contact hours	Self-study hours
5	**125**	**15**	**110**

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

The goal is to learn the main principles, mechanisms and thermodynamics of protein stability and interaction with other proteins, small molecule compounds and drugs. The course is technique-oriented to ITC, SPR, FTSA, NMR, X-Ray crystallography and their application in scientific publications.

Learning outcomes of the program	Learning outcomes of the course unit (module)	Teaching and learning methods	Assessment
Personal skills 1.1.	To be able to learn, improve and update the acquired knowledge and practical skills continuously, and seek the new knowledge and professional development independently.	Seminars, discussion of scientific manuscripts, practical training.	Exam
Social skills 2.1.	Critical and self-critical thinking; analyze and sinthesize; apply knowledge in practice.		
Knowledge and its application 3.2., 3.3.	After completion of the course the student is supposed to apply biothermodynamic and kinetic models for experimental data of protein-ligand interactions and will be able to explain equilibria with natural and drug molecules.		
Special skills 4.1., 4.2.	learn the main principles, mechanisms and thermodynamics of protein stability and interaction with other proteins, small molecule compounds and drugs.		

Content: breakdown of the topics	Contact hours							Self-study work: time and assignments	
	Lectures	Tutorials	Seminars	Exercises	Laboratory work	Internship/work placement	**Contact hours**	**Self-study hours**	**Assignments**
Structural model of water. Water at protein surfaces, Biothermodynamics, Gibbs energy, enthalpy, entropy, heat capacity, energetic of intermolecular interactions, Structural biothermodynamics. Protein structure and ligand recognition			**4**				**4**	**30**	Manuscript to read

Ionic and hydrophobic interactions, hydrophobic effect, Aggregation and pKa shift. Drug aggregation, Isothermal titration calorimetry for protein-ligand enthalpy and Gibbs energy determination, Differential scanning calorimetry for protein stability and unfolding enthalpy, Calculation of protein-ligand intrinsic binding parameters			**4**				**4**	**30**	Manuscript to read
Fluorescence, design of fluorescent probes, relation between absorbance and fluorescence, Simulation of dosing curves by fluorescent thermal shift assay, Models of interactions – polyamino acids, stacking, solubility of Tyr, Derivatives and integration by using thermodynamics of HOH formation			**4**				**4**	**30**	Manuscript to read
Nuclear magnetic resonance. Compound and protein 2D spectra for structure and dynamics, Kinetics of protein-ligand interactions via surface Plasmon resonance. Reaction time and residence time, Protein folding and misfolding, aggregation, amyloidosis, Optical tweezers of single molecules			**3**				**3**	**20**	Manuscript to read
Total			**15**					**110**	

Assessment strategy	**Weight,%**	**Deadline**	**Assessment criteria**
Final exam	100	Exam session	Written exam of 25 questions, evaluated on 10 grade basis Test (virtual learning environment) of 25 questions. <12 answered questions - 2-4 (insufficient) 12 answered questions - 5 (sufficient) 13-15 answered questions -6 (satisfactory) 16-19 answered questions - 7(highly satisfactory) 20-21 answered questions -8 (good) 22-23 answered questions -9 (very good) 24-25 answered questions -10 (excellent)

Author	**Year of publication**	**Title**	**Issue of a periodical or volume of a publication**	**Publishing place and house or web link**
Compulsary reading				
Assigned manuscripts				
Kuriyan, J., Konforti, R., Wemmer, D.	2013	The Molecules of Life		Garland Science
Optional reading				
Bahar, I, Jernigan, R.L, Dill, K.	2017	Protein Actions. Principles and Modeling		Garland Science