COURSE UNIT DESCRIPTION - BIOPHYSICAL CHEMISTRY OF PROTEINS

Course unit title	
BIOPHYSICAL CHEMISTRY OF PROTEINS	

Lecturer(s)	**Department**
Prof. Daumantas Matulis	Institute of Biotechnology of Vilnius University, V.A. Graičiūno 8, Vilnius LT-02241

Cycle		**Type of the course unit**
First		Elective

Mode of delivery	**Period of delivery**	**Language of instruction**
Face to face	5th semester	Lithuanian

Prerequisites and co-requisites
Biochemistry, general and physical chemistry, physics, and mathematics.

Number of credits	**Student's total workload**	**Contact hours**	**Self-study hours**
4	**120**	**48**	**72**

Programme competences to be developed.

The course unit aims to develop:

Specific competences:

- ability to apply concepts of chemistry, physics, mathematics for analysis and description of biological molecules and biological processes;
- skills to assess the properties of biological molecules and biological processes using methods of molecular protein science;

General competences:

- ability to communicate in written and verbal forms using correct Lithuanian in professional field;
- ability to use information sources in English in professional field;
- skills for self-development, learning skills in order to study general science resources;

Learning outcomes of the course unit	**Teaching and learning methods**	**Assessment methods**
After successful completion of this course student should be able to: • Explain the current structural and energetic models of water and aqueous solutions; • Be able to interpret the enthalpic, entropic, Gibbs free energy data in protein folding, ligand binding, stabilities; • Analyze thermal shift assay, ITC, DSC data of binding and unfolding; • Calculate and interpret the pKa of protein ionic functional groups; • Calculate intrinsic binding parameters from observed data; • Be able to understand and interpret fluorescence spectra of organic compounds; • Be able to interpret the NMR spectra of small molecules and protein.		

Topics	**Contact work hours**	**Time and tasks of self-study**

	Lectures	Consultations	Seminars	Tutorials	Laboratory work	Total contact hours	Self-study	**Tasks**
Structure and energetics of water	3					3	5	Study the properties of water according to website by Chaplin
Essentials of biothermodynamics	3					3	5	enthalpies, entropies, heat capacities, Gibbs free energies
Energetics of interaction between small molecules	3					3	5	heats of interaction, dilution, aggregation
Energetics of protein – ligand interactions	3					3	4	Read Ladbury et al 2010
Aggregation and calculation of pKa shifts				3		3	5	Read assigned manuscript on aggregation, Alzheimers
Calculation of the intrinsic parameters of protein-ligand interactions				3		3	4	Read assigned manuscript on carbonic anhydrases,
Essentials of fluorescence, structures of fluorophores	3					3	5	Read Matulis 2008 chapter 2, Matulis ANS fluorescence
Fluorescent thermal shift assay, determination of protein – ligand binding parameters				3		3	5	Complete the assigned task on the ligand-protein pair
Essentials of NMR in organic chemistry and protein structure and dynamics	3					3	4	Read assigned manuscript on NMR
Deconvolution of NMR spectra				3		3	5	NMR problem solving
Isothermal titration calorimetry, differential scanning calorimetry, protein stability and folding	3					3	5	Read assigned manuscript on ITC and DSC
Analysis of isothermal titration calorimetry data				4		4	5	ITC data problem solving
Structural biothermodynamics	3					3	5	Read assigned manuscript on biothermodynamics
Nanotechnology and single-molecule techniques, optical tweezers	4					4	5	Read assigned manuscript on optical tweezers
The path of target-oriented drug design	4					4	5	Read assigned manuscript on drug design
Total	**32**			**16**		**48**	**72**	

Assesment strategy	**Weight %**	**Assessment period**	**Assessment criteria**
Lectures	25%	weekly	Presentation of studied manuscript or textbook chapter
Tutorials	25%	5 times	Completion of the calculation/solving tasks
Midterm exam	25%	November	Open notebook (closed book and other printed material) problem solving and short answers to theoretical problems
Final exam	25%	January	Open notebook (closed book and other printed material) problem solving and short answers to theoretical problems 2-4 (insufficient) 5 (sufficient) 6 (satisfactory) 7(highly satisfactory) 8 (good)

			9 (very good) 10 (excellent)

Reading list

Author	Year of publ.	Title	Publisher	Number of volumes in the library of faculty
Main reading list				
Matulis, D.	2008	e-textbook on biothermodynamics	Kaunas	50
Scientific manuscripts assigned at each lecture				
Additional reading list				
Dill, K et al	2010	Molecular driving forces	Garland Science	1
Klotz, et al	2000	Chemical Thermodynamics	Wiley	1