RTU Course "Physical Organic Chemistry"

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General data

Code	ĶOS730
Course title	Physical Organic Chemistry
Course status in the programme	Compulsory/Courses of Limited Choice
Responsible instructor	Māris Turks
Volume of the course: parts and credits points	1 part, 6.0 credits
Language of instruction	LV, EN
Annotation	The study course demonstrates how to apply the fundamental theoretical principles of thermodynamics and kinetics to determine and understand the reaction mechanisms of organic compounds, the reaction outcome and selectivity. The study course deals with the basics of quantum chemical calculations, which are used to determine the equilibrium and reaction transition states of substances. It also provides an insight into the determination of non-covalent binding that underlies ligand-protein docking for medicinal chemistry.
Goals and objectives of the course in terms of competences and skills	The aim of the study course is to create an understanding of the fundamental principles of physical chemistry and the relationship between the stereoelectronic effects of organic compounds and organic synthesis. The tasks of the study course are 1) to teach to evaluate the thermochemical feasibility of a given organic reaction; 2) to demonstrate a link between kinetic and thermodynamic parameters and their effect on the reaction outcome; 3) to teach basics of quantum chemical calculations for determining the mechanism of reaction; 4) to teach basics of ligand-protein docking.
Structure and tasks of independent studies	Literature studies. Preparation for practical work, tests and exam.
Recommended literature	Anslyn, Eric V.. Modern physical organic chemistry / Eric V. Anslyn, Dennis A. Dougherty. Sausalito (Cal.) : University Science Books, c2006., xxviii, 1099 lpp. : il. Pierre Vogel, Kendall N. Houk. Organic Chemistry: Theory, Reactivity and Mechanisms in Modern Synthesis Weinheim: Wiley-VCH, 2019., xxx, 1352 lpp Ian Fleming. Molecular Orbitals and Organic Chemical Reactions Reference Edition 2010 John Wiley & Sons, Ltd Singh, Maya Shankar. Reactive intermediates in organic chemistry : structure, mechanism, and reactions /Maya Shankar Singh. Weinheim : Wiley-VCH, ©2014., x, 283 lpp. : il. ; 25 cm. Carey, Francis A.,. Advanced organic chemistry / Frank A. Carey and Richard J. Sundberg. New York : Springer, c2007., 2 sēj. : il. ; 26 cm. Carroll, Felix A.. Perspectives on structure and mechanism in organic chemistry / Felix A. Carroll. Pacific Grove [etc.] : Brooks/Cole, c1998., xxiv, 919 lpp. : il. Eusebio Juaristi, Gabriel Cuevas. The Anomeric Effect CRC Press, 1994 Jaemoon Yang. SixMembered Transition States in Organic Synthesis John Wiley & Sons, Inc., 2008
Course prerequisites	Organic chemistry and physical chemistry.

Course contents

Content	Full- and part-time intramural studies		Part time extramural studies	
	Contact Hours	Indep. work	Contact Hours	Indep. work
1. Introduction. Chemical equilibrium and thermochemistry. Bond dissociation energy. The standard group equiv. and their entropy increments. Additivity rules for thermodyn. parameters and deviations.	2	4	0	0
2. Thermodynamics in organic chemistry I. Enthalpy, entropy and Gibbs free energy influence on chemical equilibrium. Calculation of reaction equilibrium constants.	2	5	0	0
3. Thermodynamics in organic chemistry II. Entropy as a synthetic tool. Calculation of physical parameters for the equilibrium reaction and their experimental determination by NMR.	4	6	0	0
4. Kinetics in organic chemistry I. Evaluation of the energy required for the implementation of chemical transformations. Kinetics of multi-step chemical transformations.	4	6	0	0
5. Kinetics in organic chemistry II. Experimental determination of reaction kinetics by spectroscopic methods. Finding the rate determining step.	4	6	0	0
6. Reaction kinetics and investigation of the mechanism I. Kinetic isotope effects, cross-reactions, radical clocks.	4	6	0	0
Test I	2	0	0	0
7. Reaction kinetics and investigation of the mechanism II. Types of catalysis in organic chemistry. Research methods for unstable intermediates. Investigation of catalysis mechanism.	4	6	0	0
8. Linking Kinetics to Thermodynamics I. Hammond postulate, Curtin-Hammett principle, Bell–Evans–Polanyi principle.	3	6	0	0
9. Linking Kinetics to Thermodynamics II. Linear-free enthalpy correlations: Hammett equation. Mayr classification of nucleophiles and electrophiles.	4	6	0	0

10. Stereoelectronic effects: conformational equilibrium, anomeric effect, Baldwin's rules. Corelation between conformation and reactivity.	4	6	0	0
11. Medium effects. Solvation. Acid-bases equilibria in non-aqueous media. Solvent influence on chemical equilibria and reaction rates.	3	6	0	0
Test II	2	0	0	0
12. Ab initio quantum chem. principles of calculations I. Basic principles of Gaussian, Schroedinger and Gamess, compilation of tasks and processing of results. Local / global minima of conformations.	8	12	0	0
13. Ab initio II. Transition states of reactions. Infrared frequency calculations. Charge distribution in the molecule. Calculation and visualization of HOMO and LUMO energies.	8	12	0	0
14. Types of non-covalent interactions. Basics of ligand and protein docking calculations. Basic operational mode of Autodock.	6	9	0	0
Total:	64	96	0	0

Learning outcomes and assessment

Learning outcomes	Assessment methods
Knows the concepts of thermodynamics and kinetics required for organic chemistry, stereoelectronic and environmental effects, their total effect on the regio- and stereoselectivity of the reaction.	Examination: passing problem solving in seminars (practical work), tests, exam.
is able to compile available experimental data and / or recommend experiments to determine the parameters of equilibrium processes, the rate-limiting step of a multi-step process. Students are able to determine the thermodynamic and kinetic products of a given transformation.	Examination: passing problem solving in seminars (practical work), tests, exam.
Is able to generate the input files for ab initio quantum chemical calculations and ligand-protein binding calculations. Students are able to follow and discuss experimental work and theoretical calculations for the elucidation of reaction mechanisms described in modern scientific lit.	Examination: passing problem solving in seminars (practical work), tests, exam.
Can solve the problems arising from preparative organic synthesis: theoretical and practical determination of the reaction mechanism, suggesting solutions to improve the yield and selectivity; are able to recommend modifications to a ligand to make it better binding to the target protein.	Examination: passing problem solving in seminars (practical work), tests, exam.

Evaluation criteria of study results

Criterion	%
Test I	20
Test II	20
Passing seminars (practical work)	20
Exam	40
Total:	100

Study subject structure

Part	CP	Hours			Tests		
		Lectures	Practical	Lab.	Test	Exam	Work
1.	6.0	2.0	2.0	0.0		*	