

PHD STUDIES COURSE UNIT DESCRIPTION

Name of subject	Field of science, code	Faculty / Center	Department
Organic chemistry: Mechanisms	Chemistry N 003	CHGF	Organic chemistry
Student's workload	Credits	Student's workload	Credits
Lectures	-	Consultations	4
Independent study	5	Seminars	-

Course annotation

Mechanisms of chemical processes in organic reactions are mandatory in understanding entire reaction protocol and purposely modifying this protocol to desired outcome of the reaction. PhD students in pursuit of deeper knowledge in organic reaction mechanisms are given the task of preparing report on certain relevant topic and presents it to doctoral exam committee and other members of the VU community and answers questions after presentation.

Basic coverage of topics is as follows:

The concept of reaction mechanism, means to determine type of the reaction mechanism, kinetics. Nucleophilic substitution reactions (S_N1 , S_N2 , S_Ni). Nucleophilicity. Nucleophilicity in enzymatic reactions.

Elimination reactions ($E2$, $E1$, $E1cb$), stereochemistry of elimination reactions. Nucleophilic substitution versus elimination reactions, impact of reaction conditions to course of the reaction.

Addition to carbon-carbon double bond (electrophilic - A_e and nucleophilic - and additions).

Carbenium, carbonium ions. Non-classical carbocations, electrophilic rearrangements.

Electrophilic substitution in aromatics (S_EAr). Effect of substituent groups. Nucleophilic substitution in aromatics (S_NAr), addition-elimination and elimination-addition mechanisms. Aromaticity.

Free-radical reactions. Generation of free-radicals, diagnostics of radical species. Free-radical substitution, addition and cyclization reactions.

Acids and bases in organic reactions. Acidity of carbonyl compounds, enolates.

Addition and substitution reactions of carbon-heteroatom double bond. Condensation reactions of carbonyl compounds.

Pericyclic reactions, classification, frontier molecular orbital theory (HOMO and LUMO interaction).

Cycloaddition and cycloelimination reactions.

Electrocyclic reactions. Sigmatropic rearrangements.

Photochemical reactions. Transition metal complexes with organic compounds.

A PhD student without basic understanding of the reaction mechanisms in organic chemistry may choose to attend the lectures of this course given to master students.

Reading list

F.A. Carey, R.J.Sandberg. 2007; Advanced Organic Chemistry; Springer.

M. B. Smith, J.March. 2007; March's Advanced Organic Chemistry: Reactions, Mechanisms, and Structure; Wiley-Interscience.

E. Butkus, V. Masevičius, S. Stončius, 2012; Organinių reakcijų mechanizmų uždaviniai (Problems in organic reaction mechanisms); UAB TEV.

F. A. Carroll, 2010; Perspectives on Structure and Mechanism in Organic Chemistry; Wiley.

J. Clayden, N. Greeves, S. Warren, P. Wothers, 2000; Organic chemistry; Oxford University Press.

The names of consulting teachers	Science degree	Main scientific works published in a scientific field in last 5 year period
Viktoras Masevičius	Dr.	1. Rakauskaitė, R., Urbanavičiūtė, G., Simanavičius, M., Lasickienė, R., Vaitiekaitė, A., Petraitytė, G., Masevičius, V., Žvirblienė, A., Klimašauskas, S., Photocage-Selective Capture and Light-Controlled Release of Target Proteins, ISCIENCE (2020), doi: https://doi.org/10.1016/j.isci.2020.101833 .

		<p>2. Gražina Petraitytė, Vytenis Vaitkevičius, Besra Özer, Viktoras Masevičius. Synthesis of 5-substituted and 5,6-disubstituted furo[2,3-d]pyrimidines from 2-methylthio-4,6-pyrimidindione and bifunctional electrophiles. <i>Tetrahedron Lett.</i> 2019, 1019-1021.</p> <p>3. Milda Mickutė, Milda Nainytė, Lina Vasiliauskaitė, Alexandra Plotnikova, Viktoras Masevičius, Saulius Klimašauskas, Giedrius Vilkaitis. Animal Hen1 2'-O-methyltransferases as tools for 3'-terminal functionalization and labelling of single-stranded RNAs. <i>NAR</i> 2018, 46, e104.</p> <p>4. Aleksandr Osipenko, Alexandra Plotnikova, Milda Nainytė, Viktoras Masevičius, Saulius Klimašauskas, and Giedrius Vilkaitis. Oligonucleotide-Addressed Covalent 3'-Terminal Derivatization of Small RNA Strands for Enrichment and Visualization. <i>Angew. Chem. Int. Ed.</i> 2017, 56, 6507–6510.</p>
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Certified during Doctoral Committee session on September 28th, 2021. Protocol No. 610000-KT-142.

Committee Chairman prof. habil. dr. Aivaras Kareiva