2024/2025. ACADEMIC YEAR

PROGRAM OF STUDY (FOR STUDENTS OF 2ND YEAR)

Full (Hun) name of the subject: Szerves kémia I.

Program: Undivided program (pharmaceutical)

Schedule: full-time

Short name of the subject: Org Chem

English name of the subject: Organic Chemistry I.

German name of the subject: Organische Chemie I

Type of registration: obligatory/obligatory elective/elective/criteria requirement

Neptun code of the subject: GYKSZK337E1A

Responsible Department: Semmelweis University, Institute of Organic Chemistry

Responsible tutor	**Title, academic degree:**
Dr. Petra Dunkel **Contact information:** - **phone:** +36-1-476-3600/53006 - **email:** dunkel.petra@semmelweis.hu	assistant professor, PhD

Name of the persons responsible for the teaching of the subject:	**Title, academic degree:**
Dr. Balázs Balogh	assistant professor, PhD
Dr. Dóra Bogdán	assistant lecturer, PhD
Dr. Andrea Czompa	assistant professor, PhD
Dr. Ruth Deme	assistant lecturer, PhD
Dr. Petra Dunkel	assistant professor, PhD
Dr. Zoltán Kaleta	assistant professor, PhD
Dr. Róbert Ludmerczki	assistant lecturer, PhD
Dr. Krisztina Süttőné Kaczeus	research associate
Bence Kontra	PhD student
Dr. László Piros	PhD student
Patrik Pollák	PhD student
Gergő Riszter	PhD student

Class per week:	**Credit point(s):**
4 lecture(s) **4** practice(s)	**8** credits

Professional content, intent of acquirement and it's function in order to implement the goals of the program:

The course discusses state-of the art synthetic and structural organic chemistry subjects to develop problem-solving skills for organic chemistry and biomolecular sciences. Students will acquire the basics of organic chemistry, develop an organic chemistry perspective and acquire the theoretical, practical and material knowledge base for their future studies.

Short description of the subject:

The course in Organic Chemistry at the Faculty of Pharmaceutical Sciences has two main objectives:

a) to provide a modern organic chemistry curriculum and to develop an organic chemistry approach, by presenting typical synthesis methods for the preparation of the different types of compounds and, with particular emphasis, by illustrating and interpreting their chemical reactivity. Introduction to and practical application of the main methods and tools of preparative organic chemistry.

b) To provide a solid molecular, organic chemistry base for subsequent subjects in the curriculum of students at the Faculty of Pharmaceutical Sciences and, in particular, to strengthen the molecular approach necessary for biomedical disciplines.

Course data

Recommended term	Contact hours (lecture)	Contact hours (practice)	Contact hours (seminar)	Individual lectures	Total number of contact hours/semester	Normal course offer	Consultations
3. semester	4	6 (biweekly)	3 (biweekly)	-	56+36+20	Autumn semester Spring semester Both semesters *(* Please underline)*	upon demand

Program of semester**

Topics of theoretical classes (pro week):

1. week: Introduction to Organic Chemistry. MO theory 1. Atomic orbitals, LCAO-MO method, σ and π orbitals, molecular orbitals, delocalisation. MO theory 2. Hybridisation, Lewis-Langmuir theory of bonds, valence bond method, resonance. Conjugation: allyl system, pentadienyl system, electron system of butadiene and hexatriene. Classification of organic compounds. Isomers: constitutional and conformational isomers, stereoisomers. Enantiomers and diastereomers.

2. week: Chirality, absolute configuration according to Cahn-Ingold-Prelog. Stereochemistry of organic compounds containing more than one center of chirality. Axial chirality, determination of absolute configuration. Tautomerism. Newman and Fischer-projection. Energy profile of reactions. Reaction mechanisms. Factors affecting reactivity. Electronegativity, reactivity of reagents: inductive, mesomeric and steric effects.

3. week: Classification of reactions. Kinetic and thermodynamic control. Nomenclature of organic compounds I.

4. week: Alkanes and cycloalkanes: physical and chemical properties, preparations, reactions. Mono- and disubstituted cyclohexanes. Alkenes: preparations, physical, chemical and biological properties. Cis-trans isomerization. Addition reactions. Markovnikov and anti-Markovnikov addition. Radical reactions and their mechanism. Addition vs substitution.

5. week: Polymerisation. Diolefins. Diels-Alder reaction. Pericyclic reactions. Woodward-Hoffmann rules. Alkynes: preparations, physical, chemical and biological properties. Nucleophilic addition reactions.

6. week: Benzene and aromaticity. Extension of the aromatic system. Antiaromatic and non-aromatic structures. S_EAr reactions of aromatic compounds. Activating and deactivating groups, direction rules. S_NAr reactions of aromatic compounds. Linear free energy relationships. Structure of halogenated hydrocarbons, physical, biological properties, preparations.

7. week: Nucleophilic substitution reactions: S_N1, S_N2, S_Ni, elimination reactions: E1, E2, E1cB - factors influencing ratio of S_N vs. E reactions: substrate, solvent, temperature effects, role of the base, of the leaving group, stereochemical consequences. Alcohols, phenols, ethers: preparations, physical, chemical and biological properties. Protecting groups. Acid-base theories. Acidity and basicity of organic compounds. Acid-base reactions.

8. week: Organic sulfur compounds: structure, classification, reactivity, chirality, sulfonic acids, sulfonamides.

9. week: Amines: preparations, physical, chemical and biological properties. Aromatic diazonium and nitro compounds, organophosphorus compounds: preparations, physical, chemical and biological properties.

10. week: Nomenclature of organic compounds II. Oxo compounds: aldehydes and ketones - preparations, physical, chemical and biological properties. Addition to the carbonyl group. (Enolate chemistry I.)

11. week: Carboxylic acids and their derivatives: preparation, reactivity, nucleophilic reactions at the acyl carbon atom, physical, chemical and biological properties. (Enolate chemistry II.)

12. week: Substituted carboxylic acids, dicarboxylic acids and their derivatives. Synthetic applications of ethyl acetoacetate and diethyl malonate.

13. week: Carbonic acid derivatives: classification, nomenclature, synthetic applications. Carbamates, polymers, protecting groups, transformations.

14. week: Summary of organic chemical reactions, reaction mechanisms, synthesis planning.

Topics of practical classes (pro week):

1. week: ---

2. week: *Mesomeric structures, hybridisation states. Type of π-electron systems. Classification of reagents: electrophilic, nucleophilic, radical. Reaction types: S_N1 and S_N2 mechanisms.*

3. week: Recrystallization of 4-bromoacetanilide, thin-layer chromatography.

4. week: *Identification of cis-trans stereoisomers, E/Z notation. Recognition of chirality (stereogenic) centres in molecules. Identify and draw the enantiomers. Identify the configuration of chirality centres (R/S notation). Identify the stereochemical relationship between two compounds. Recognition of diastereomeric and meso compounds. Determining configuration from Fischer projection, drawing Fischer projection. Conformation analysis using Newman projection. Cyclohexane conformers.*

5. week: Preparation of acetanilide and acetylsalicylic acid.

6. week: *Aromatic, antiaromatic and non-aromatic systems. Synthesis of aromatic hydrocarbons, reactions of aromatic compounds.*

7. week: Preparation of 4-bromoacetanilide, column chromatography.

8. week: *Stereochemistry of S_N2 and S_E2 reactions and interpretation of the transition state. Aliphatic and aromatic hydroxy- and halogen compounds: basic properties of substitution and elimination reactions and their mechanism. Kinetic and thermodynamic control.*

9. week: Preparation of 4-bromo-2-nitroacetanilide and β-naphtholorange.

10. week: *Preparations, applications, and reactions of quinones and ethers. Organic sulfur compounds, preparations of sulfonamides, reactions. Chemical properties of amines, basicity, preparations, reactions, diazotation.*

11. week: Purification of ethyl acetate with extraction and distillation.

12. week: *Aldehydes and ketones: nucleophilic addition reactions. Reactions of α-hydrogen of aldehydes and ketones.*

13. week: Introduction into cheminformatics.

14. week: Supplement. Inventory. *Reactivity of carboxylic acids and their derivatives (acylation), reactions involving α-hydrogen. Carbonic acid derivatives.*

Schedule of consultations: consultation upon request, at least 1 week before the date of consultation

Course requirements

Prerequisites:

GYKASK266E2A	General and inorganic chemistry II.

Conditions of attending the classes, amount of acceptable absents, way of presentation of leave, opportunity for makeup:
If necessary, students may make up for a limited number of missed or failed preparative experiments after preliminary agreement with the leading instructor at the end of the semester. Without permission, the repetition of unsuccessful experiments is not allowed. Course material for the seminars (problem sets) are provided in advance to the students *via* Moodle. Students are expected to consult these materials before the respective seminars. These problem sets will form the basis of the discussion. Attendance is mandatory at the seminars. No more than one seminar absence per semester will be accepted without special consequences. A student who misses more seminar classes in their group may attend a seminar of another group (in the same week) if possible (only a limited number of students may be allowed to do so), always by notifying the seminar leaders in advance. If this is not possible, the student (who has more than 2 absences) will be briefly debriefed by the seminar leader on the relevant topics by the end of the semester (however, regular absences are not permitted). The Study and Examination Regulations also require attendance at 75% of the practical sessions and attendance at the seminars (which count as practical sessions) according to the above criteria in order to be signed off at the end of the semester.

The grading method; the conditions for getting the signature; the number, topic(s) and date(s) of the mid-term assessments (reports, term tests), and the process in which they contribute to the final grade; and the possibility of their retake or their upgrading retake (as provided in §§ 25-28 of the STUDY AND EXAMINATION REGULATIONS):

Number, topics and dates of tests during the semester, opportunities of makeup and improvement of results: Theory: At the mid-term tests (one/semester) students have to answer in a written form questions on the subject-matter of the main lectures, the practicals and the seminars, the dates of which are fixed at the beginning of the semesters. The value of the midterm test can be either ranging 2-5 or failed. If the test is failed or the student did not attend it, the student must attend the following makeup test. If the makeup test is failed, a second makeup test should be written. If any of the makeup tests reach the passmark, then the midterm test is accepted. If also the second makeup test is failed, the student does not get signature for the semester, they are not allowed to sit in the semi-final examination. Grades for the main and makeup mid-term tests of the same topic are not averaged. Students who have a result of at least 90% in the mid-term test (excluding the retake tests) during the semester will have a 5-point advantage in the written exam.
Practical: at the beginning of each laboratory practical, students must write a short test on the theoretical and practical subject-matter of the experiment. These tests are immediately corrected by the leading instructor, and the practical work can be started only if the short test is accepted. If the test is failed, the experiment in question can be performed only at the end of the semester.
Completing successfully the non-preparative practicals during the two semesters is also a condition of the signature and 75% of the maximum number of laboratory notebooks that can be submitted must be also approved.

Requirements of signature(as provided for in STUDY AND EXAMINATION REGULATIONS § 29): mid-term test, obtaining a signature, attending practicals and seminars as specified above

Number and type of projects students have to perform independently during the semester and their deadlines: completion of the mid-term assessment, completion of practical work, attendance of a sufficient number of seminars (final deadline: last day of the semester)

Type of the semester-end examination: signature*/practical grade*/<u>semi-final</u>*/final* *(* Please underline)*

Examination requirements: as published by the institute on the MOODLE course site by the start of the academic term

Form of the semester-end examination*:* <u>written</u>*/oral*/combinated examination/**practical examination/the assessment of completing project work (according to STUDY AND EXAMINATION REGULATIONS 30.§)*** *(* Please underline)*

The possibility and conditions for offering grades: -

A list of the basic notes, textbooks, resources and literature that can be used to acquire the knowledge necessary to master the curriculum and to complete the assessments, with exact description about which of them is required to acquire which part of the syllabus (e.g. description based on topics)), as well as the main technical and other aids and study aids that can be used:

Materials of the lectures and practices can be downloaded from Moodle
P.C. Vollhardt; N.E. Schore: Organic Chemistry: Structure and Function, 8th Edition (W. H. Freeman)
D.R. Klein: Organic Chemistry, 3rd Edition (Wiley)
K.L. Williamson, K.M. Masters: Techniques Labs for Macroscale and Microscale Organic Experiments, 7th Edition (Cengage Learning)

In the case of a subject lasting more than one semester, the position of the teaching/research department on the possibility of parallel enrolment and the conditions for admission**:**

yes*/no*/<u>on an individual assesment basis</u>* *(* Please underline)*

The course description was prepared by:
Dr. Petra Dunkel (assistant professor, PhD)

***** A tantárgy tematikáját oly módon kell meghatározni, hogy az lehetővé tegye más intézményben a kreditelismerési döntéshozatalt, tartalmazza a megszerzendő ismeretek, elsajátítandó alkalmazási (rész)készségek, (rész)kompetenciák és attitűdök leírását, reflektálva a szak képzési és kimeneti követelményeire.***