SEMMELWEIS UNIVERSITY FACULTY OF PHARMACY **INSTITUTE OF ORGANIC CHEMISTRY** 7 Hőgyes E. u., Budapest, H-1092, HUNGARY tel./fax.: (36-1)-2170851 http://semmelweis.hu/orgchem/en/

Head of the Institute: Dr. István Mándity, Ph.D. Associate professor

# **GUIDELINES FOR STUDENTS**

# Academic Year 2024/2025

Welcome to Students of Organic Chemistry

The following pages provide information on the subject-matter of the main **Organic Chemistry** course, of the optional *Name Reactions in Organic Chemistry* course, the literature recommended for the studies, themes proposed for the diploma work, and the evaluation of the student's progress. The introduction includes a short overview of the history and scientific activities of the Institute.

Budapest, August 2024

István Mándity Director/Head of the Institute

# **TEACHING STAFF**

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#### **Directors of Institute:**

Dr. Ottó Clauder	1957-1977	
Dr. László Szabó	1977-1996	
Dr. Ákos Kocsis	1996-1997	(acting director)
Dr. Péter Mátyus	1997-2016	
Dr. Gábor Krajsovszky	2016-2017	(acting director)
Dr. István Mándity	2017-	

#### History

The Institute of Organic Chemistry was founded in 1957 and its first head was Prof. Ottó Clauder. The infrastructure of the Institute (the students' and tutors' laboratories, the equipment for preparative work and the library) was gradually built up and finally a spectroscopic unit was established. In 1977, Prof. László Szabó took over as head of the Institute and after it, in 1997 Dr. Ákos Kocsis was appointed as acting director. After that from 1997 Prof. Péter Mátyus was the head of the Institute. Since 2016 to June 2017 Dr. Gábor Krajsovszky was the acting director. The present head of the Institute is Dr. István Mándity.

Aim and structure of the teaching and research activities are summarized in the following paragraphs.

The aim of the education in organic chemistry is to create an organic chemical basis for subsequent subjects in the curriculum of students at the Faculty of Pharmacy. To attain this goal, besides the main lectures (112 hours in the 3<sup>rd</sup> and 4<sup>th</sup> semesters) and parallel laboratory practicals (110 hours) in organic chemistry, the Institute offers a choice of a special course to its students (Drug Syntheses), and meanwhile, continuous enlargement of number of special courses is planned. The available methods based on Computational Chemistry and Molecular Modelling have been involved in the official education material since 1998. The teaching activities at the Institute also include the introduction of selected students into research in organic and medicinal chemistry, the direction of diploma work and participation in the postgraduate (Ph.D.) education. The Institute takes part in several international research and educational cooperation programs (such as ERASMUS).

The Institute additionally plays an important role in the postgraduate education of pharmacists, as organizer of the Medicinal Chemistry Programme, and offers a two-year postgraduate program in Drug Research and Development.

The main research fields at the Institute were the synthesis and chemical properties of heterocycles, including some natural products. In the last few years, important results have been achieved in the fields of synthesis strategies, including palladium-catalysed cross-coupling reactions of pyridazines and uracils, and mechanistic studies and the synthetic development of certain thermal rearrangement reactions. Another research field was at the Institute involves medicinal chemistry with the design and synthesis of antiarrhythmic compounds, ligands of  $\alpha$ -adrenoceptors and inhibitors of semicarbazide-sensitive amine-oxidase.

The Institute cooperates in both research and education with several academic (e.g. the Semmelweis University Institute of Pharmacodynamics, Institute of Pharmacology and Pharmacotherapy, Institute of Ophthalmology, and II. Institute of Internal Medicine; Peter Pazmany Catholic University Faculty of Information Technology, the University of Debrecen, Pécs, and Szeged; the Hungarian Academy of Sciences Chemical Research Centre; the University of Vienna, Palermo, Cagliari, Universidad de CEU San Pablo (Madrid), National University Singapore); and industrial (Richter Gedeon, EGIS, Pannonpharma) organizations.

The main research profiles in the Institute are involving primarily – preserving the Institutional traditions at least partially – heterocyclic syntheses, preparation of compounds with chloride ion transporter effect, peptide chemistry, chemistry of bifunctional compounds, introduction of processes of "green chemistry" (such as use of solvents carbon dioxide neutral, elaboration of organic chemical reactions taking place in water, application of continuous-flow chemical technologies). The research work is facilitated by separation, spectroscopic and computational methods.

Website: http://semmelweis.hu/orgchem/en/

### The Subject of Organic Chemistry

### https://semmelweis.hu/registrar/pharmaceutical-sciences/pharmaceutical-sciences-curriculum/

#### Aims of the Course

The course includes and discusses the state-of the art knowledge of synthetic and structural organic chemistry subjects to develop problem-solving skills for organic chemistry and biomolecular sciences. To satisfy the requirements of the Faculty of Pharmacy, the course in organic chemistry has two main purposes:

a) The presentation of modern concepts and subject-matter concerning the structures, syntheses, physical and chemical properties, structure – property relationships, and practical applications of organic compounds, with special emphasis on bioactive molecules. The presentation and practical applications of the most important methods and tools of organic chemistry.

b) To provide a solid molecular, organic chemical basis for subsequent subjects in the curriculum of students at the Faculty of Pharmacy.

#### **Timetable of the Subject of Organic Chemistry**

The subject of organic chemistry is included in both semesters of the second year of the curriculum of students at the Faculty of Pharmaceutical Sciences.

Number of lectures in the main course: 112 hours (4 hours per week). Length of the practical course: 72 hours (6 hours every second week). Number of seminars: 40 hours (3 hours every second week).

# Schedule for the Academic Year 2024/2025 Faculty of Pharmacy https://semmelweis.hu/registrar/information/year-books/

### First Semester

Registration Period: 26 August 2024 – 30 August 2024 First day of the Semester (1<sup>st</sup>-4<sup>th</sup> Years): 2 September 2024 Last day of the Semester (1<sup>st</sup>-4<sup>th</sup> Years): 6 December 2024 Examination period: 1<sup>st</sup>-5<sup>th</sup> Years 9 December 2024 – 20 December 6 January 2025 – 7 February

### Second Semester

**Registration Period:** 3 February 2025 – 7 February 2025 First day of the Semester (1<sup>st</sup>-4<sup>th</sup> Years): 10 February 2025 Last day of the Semester (1<sup>st</sup>-4<sup>th</sup> Years): 16 May 2025 Examination period: 1<sup>st</sup>-4<sup>th</sup> Years 19 May 2025 – 4 July 2025

### **Holidays**

Winter holiday: 23 December 2024 – 5 January 2025 Spring holiday: 18 April 2025 – 21 April 2025

National/public holidays:

23 October 2024 1 November 2024 1 May 2025

#### **Topics of the Main Lectures**

#### **First Semester**

History and subject of organic chemistry. Atomic and molecular orbitals. Chemical bonds: localized and delocalized bonds,  $\sigma$  and  $\pi$  bonds. Qualitative molecular orbital theory of organic compounds. MO-LCAO method. Hybridization. The Lewis-Langmuir theory. Resonance. The valence bond method. Bond distance and bond energy. Conjugation: orbital structure of the allyl system and butadiene. Energy profile of reactions.

Classification of organic compounds. Principles of the IUPAC nomenclature. Nomenclature systems. Stereochemistry of organic compounds. Isomerism: constitutional isomerism and stereoi-somerism. Configurational isomers. Compounds containing one centre of chirality. Conformational isomerism. Importance of stereochemistry in biological activity. Geometrical isomerism. The Cahn-Ingold-Prelog convention. Newman and Fischer projections. Tautomerism.

Saturated acyclic and cyclic hydrocarbons: constitution, conformation, preparation and reactions, physical and chemical properties. Mono- and disubstituted cycloalkanes. Organic halogen compounds: synthesis and physical, chemical and biological properties. Classification of chemical reactions. Electronegativity, ionic character. Structure-reactivity. Steric and electronic effects in organic compounds and reactions. Acidity and basicity of organic compounds. Alkylations. Reaction mechanisms. Survey of the principles of reaction kinetics: reactions of first and second order, parallel reactions, principle of the stationary state. Nucleophilic substitution in aliphatic ( $S_N1$ ,  $S_N2$ ,  $S_N$ and  $S_{Ni}$ ) and aromatic compounds, eliminations (E1, E2 and E1cb). Effects of substrate, reagent, and reaction conditions (solvent and temperature), and stereochemical consequences (MO interpretation).

Alkenes, alkynes, and their cyclic analogues: synthesis and physical, chemical, and biological properties. Geometric isomerism. Types of addition reactions. Addition to carbon-carbon double bonds. Interpretation of Markovnikov and anti-Markovnikov orientations. Radical reactions and their mechanisms. Addition vs. substitution. Polymerization. Diolefins. Diels-Alder reaction I. Woodward-Hoffmann rules I. Acetylenes: synthesis and physical, chemical, and biological properties. Nucleophilic additions.

Linear and cyclic  $\pi$ -delocalized systems. Aromaticity and anti-aromaticity. Interpretation of concerted reactions. Aromatic hydrocarbons, nomenclature.

Mechanism and direction rules of electrophilic aromatic substitution. Aromatic halogen compounds. Aromatic nucleophilic substitution. Linear free energy relationship.

Organic compounds containing C-O or C-S single bonds (alcohols, phenols, ethers, thioanalogues, and their derivatives): syntheses and physical, chemical, and biological properties. Protecting groups. Amines, nitro and diazonium compounds: syntheses and physical, chemical, and biological properties. Organophosphorus compounds.

Aldehydes and ketones: syntheses and physical, chemical, and biological properties. Addition to the carbonyl group. C-H acids. Umpolung, synthon principle. (Enolates I.)

Carboxylic acids and their derivatives: nucleophilic reactions at the acyl carbon atom, physical, chemical, and biological properties. (Enolates II.) Carbonic acid and derivatives.

#### Second Semester

Carbon-carbon bond forming reaction with palladium catalysis, organometallic compounds of zinc and magnesium. Inter- and intramolecular reactions.

Heterocyclic and heteroaromatic compounds.  $\pi$ -Electron-excessive and  $\pi$ -electron-deficient heteroaromatic compounds. Three-, four-, five- and six-membered rings containing one or more heteroatoms. Some benzo- and heterofused ring systems. Azepines, diazepines and azocines; Heterocyclic polyenes. Synthetic principles, reactivity, (electrophilic and nucleophilic reactions) and biological importance. Natural compounds:

Structures of nucleosides, nucleotides, and nucleic acids.

Alkaloids, and some representative compounds of these classes.

Isoprenoid compounds (terpenoids, carotenoids, steroids).

Stereochemistry of the citric acid cycle. Vitamins. Sulfonamides. Woodward-Hoffmann rules II. Diels-Alder reaction II.

Polyfunctional organic compounds. Polymers: general properties, synthesis, structure. Carbohydrates. Stereochemistry of organic compounds containing more than one centre of chirality. Amino acids, peptides, proteins: syntheses (including solid-phase synthesis) and physical, chemical, and biological properties. Determination of the amino acid sequence in peptides.

### **Optional courses:**

# Name Reactions in Organic Chemistry (14×2 hours)

In Spring semesters, for 2-4<sup>th</sup> year students Lecturer: Dr. Andrea Czompa, Ph.D.

# Brief course summary:

Description of the most important name reactions used in organic chemistry and discussion of their mechanism. The use of name reactions found in literature and modifications in order to prepare different compounds, like drugs or candidates. Detailed analysis of chemo-, regio- and enantiose-lective synthesis, flow chemistry, microwave reactions, one-pot, tandem and domino synthetic pathways.

### List of teaching materials:

László Kürthy and Barbara Czakó: Strategic Applications of Named Reactions in Organic Synthesis, Elsevier Academic Press, 2005.

Bradford P. Mundy, Michael G. Ellerd, Frank G. Favaloro Jr.: Name Reactions and Reagents in Organic Synthesis, Second Edition, John Wiley & Sons, 2005.

Smith M. B., March J. Advanced Organic Chemistry: Reactions, Mechanisms and Structure, 6th Edition, New York, Wiley-Interscience, 2007.

Jie Jack Li: Name Reactions, Fifth Edition, Springer International Publishing, 2014.

http://www.name-reaction.com/ https://www.organic-chemistry.org/namedreactions/ https://en.wikipedia.org/wiki/List\_of\_organic\_reactions

# Schedule Practicals

# First Semester

16 Sep – 20 Sep	Recrystallization of 4-bromoacetanilide, TLC and melting point
30 Sep – 4 Oct	Acetylsalicylic acid and acetanilide
14 Oct – 18 Oct	4-Bromoacetanilide (from own acetanilide) and column chromatography
28 Oct – 31 Oct	4-Bromo-2-nitroacetanilide (from own 4-bromoacetanilide) and $\beta$ -naph-tholorange
11 Nov – 15 Nov	Purification of crude ethyl acetate by extraction and simple distillation
25 Nov – 29 Dec	Introduction to cheminformatics
2 Dec – 6 Dec	Extra practice

# Second Semester

24 Feb – 28 Feb	Chemical bibliography and databases
10 Mar – 14 Mar	4-Nitrobenzoic acid and phthalimide
24 Mar – 28 Mar	Ethyl-4-nitrobenzoate (from own 4-nitrobenzoic acid) and cyclohexanone oxime
7 Apr – 11 Apr	Ethyl-4-aminobenzoate ( <i>from own ethyl-4-nitrobenzoate</i> ) and <i>N</i> , <i>N</i> '- ethylenebis(salicylimine)
22 Apr – 25 Apr	(E,E)-1,5-Diphenylpenta-1,4-dien-3-one and students' presentations
5 May – 9 May	Diethyl 3,5-dimethylpyrrole-2,4-dicarboxylate
12 May – 16 May	Extra practice

# Schedule Seminars

### First Semester

- 9 Sep 13 Sep Mesomeric structures, hybridisation states. Type of  $\pi$ -electron systems. Classification of reagents: electrophilic, nucleophilic, radical. Reaction types: S<sub>N</sub>1 and S<sub>N</sub>2 mechanisms.
- 23 Sep 27 Sep 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.
- 7 Oct 11 Oct Aromatic, antiaromatic and non-aromatic systems. Synthesis of aromatic hydrocarbons, reactions of aromatic compounds.
- 4 Nov 8 Nov Preparations, applications, and reactions of quinones and ethers. Organic sulfur compounds, preparations of sulfonamides, reactions. Chemical properties of amines, basicity, preparations, reactions, diazotation.
- 18 Nov 22 Nov Aldehydes and ketones: nucleophilic addition reactions. Reactions of  $\alpha$ -hydrogen of aldehydes and ketones.
- 2 Dec 6 Dec Reactivity of carboxylic acids and their derivatives (acylation), reactions involving  $\alpha$ -hydrogen. Carbonic acid derivatives.

# Second Semester

17 Feb – 21 Feb	Nomenclature examples from semester I-II, nomenclature of heterocyclic compounds. https://mek.oszk.hu/17200/17281/17281.pdf
3 Mar – 7 Mar	Heterocyclic compounds – advanced synthetic routes and reaction pathways. 3-, 4- and 5-membered heterocycles and possible benzologues.
17 Mar – 21 Mar	Heterocyclic compounds – advanced synthetic routes and reaction path- ways. 6-, 7- and 8-membered heterocycles and possible benzologues.
31 Mar – 4 Apr	Amino acids, peptides, proteins.
14 Apr – 17 Apr	Carbohydrates. General properties and applications of polymers.
28 Apr – 2 May	Solving of stereochemical organic chemistry problems. Alkaloids – chemistry, structure, and syntheses. Some examples for drug synthesis.
12 May – 16 May	Solving of organic chemistry problems. Isoprenoids and steroids – chem- istry, structure, and syntheses. <u>https://mek.oszk.hu/17200/17281/17281.pdf</u>

### **Requirements for Evaluation of Progress in Studies**

### Written semi-final examination at the end of the first semester

Students have to answer in a written form questions on the subject-matter of the main lectures, the introductory lectures to the practicals and the practicals themselves.

### Written final examination at the end of the second semester

Students have to answer in a written form questions on the theoretical and practical subject-matter from both semesters. The subject-matter involves all topics involved in the main lectures and the introductory lectures to the practicals, and related topics not necessarily directly indicated in the list of questions.

### Attendance on the classes

Students must attend at least 75% of the practices and the seminars.

### **Evaluation of the midterm test**

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 pass mark, 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 both the mid-term tests (excluding the retake tests) during the semester will have a 5-point advantage in the written exam.

# Evaluation of the students' work on seminars

Course material for the seminars (problem sets) are provided in advance to the students. Students are expected to consult these materials before the respective seminars. Attendance is mandatory at the seminars. Missed seminars could be attended at the same week (with another group) upon prior permission from the leading instructor. If anyone has 2 or more absences from the seminars, they must pass a report from the topics of missing seminars, and this report must be accepted. Attendance on at least 75% of the practical course necessary for the signature by the end of the semester.

#### Practical course grade

Based on the attendance and the results described in the protocol, the performance of the practical tasks is validated by the signature of the leading instructor. If necessary, students may make up for missed or unsuccessful experiments at a proper time after preliminary agreement with the leading instructor at the end of the semester. Without permission, the repetition of unsuccessful experiments is not allowed. The presence of the student at the main lecture is a necessary requirement for a consultation.

Evaluation of the compounds is based on their yield and purity. The appropriate parts of the laboratory note-book should be prepared in advance and after the completion of each practical, the notebook should be submitted to the leading instructor, together with the product of the experiment.

At the beginning of each laboratory practical, students must write a short test on the theoretical and practical subject-matter of the experiment, in order to prove gaining proficiency of the subject-matter, consisting of simple questions. These short tests will be immediately corrected by the leading instructor. Success in this test is required before the practical work can be started. If the test is not successful, the preparation in question can be performed only at the end of the semester, if the short test written then is accepted.

Conditions for approval of the preparations: you must reach at least 50% of the usual chemical yield, provided in the prescription:

0-49.9%:	1
50-62.4%:	2
62.5-74.9%:	3
75-87.4%:	4
87.5%-:	5

Further conditions:

- melting range of the crystalline product cannot be more than 10°C less, compared to the literature melting range
- acceptance of the notebook.

The leading instructor can change the actual mark on a range of +1/-1, according to the quality of the notebook. The **mark of preparations** will be the simple average of marks of the preparations. At least 75% preparations must be completed by at least pass mark.

Evaluation of non-preparative practices will be carried out by providing marks in a range of 1 to 5.

The *practical mark* of the Semester will be calculated, as a weighted average of the following 2 values, rounded to a number without decimals:

30% average mark of preparations70% mark of midterm test

#### Requirements for successful completion of the semester

- 1. The midterm test must reach pass mark.
- 2. Attendance on at least 75% of the seminars necessary for the signature by the end of the semester.
- 3. The grade for the practical course must be at least 2.

#### System of examinations

Students are allowed to sit in intermediate examinations only if they have obtained at least a passmark for the **practical course**. Examination dates will be set one month before the starting of the examination period, and students must register themselves for an appropriate date before the beginning of the examination period. Postponement of the examination is allowed only if the student has obtained permission previously - within two days before the examination - from the educational secretary of the Institute, or if a written medical certificate is provided. Otherwise, any absence from the exam decreases the number of the chances they can have in organic chemistry. A request for postponement is possible by discussion with the educational secretary, either personally or by phone or by email.

Failed examinations may be repeated not sooner than on the 3<sup>rd</sup> day following the unsuccessful examination only (unless exceptional permission is granted by the Head of the Institute). Re-sits of intermediate examinations will be on set dates.

The same examination rules are valid for students on CV course. If a student attends on a CV course for Organic chemistry I, then they must complete this course with combined examination at the beginning of the following examination period, then they are allowed to sit in the final combined examination. If a student attends on a CV course for Organic chemistry II, then they must complete this course with combined examination.

At the end of the semester, students must clean the contents of their cupboards. The schedule of the practicals, introductory lectures and seminars is listed in the written material provided.

#### Administrative issues:

https://semmelweis.hu/registrar/contacts/contacts-academic-inquiries/

### The Study and Examination Policy – Faculty of Medicine, Dentistry and Pharmacy

https://semmelweis.hu/registrar/files/2024/02/Study\_and\_examination\_regulations\_2023\_11.pdf

#### Code of Conduct of Semmelweis University:

http://semmelweis.hu/jogigfoig/files/2018/11/Etikai\_Kodex\_hataly\_2017XII09\_tol\_ENG.pdf

### Syllabus for the Semi-Final Examination

1/ Chemical bond. Basic terms. Atomic and molecular orbitals. Hybridization. Bond formation and dissociation energy, with some typical examples. Isoconjugation.

2/ Basic terms of description of chemical bond – conjugation: butadiene, allyl systems; hyperconjugation. Homolysis and heterolysis. Resonance theory.

3/ Types of tautomers, with examples. Classification of protecting groups. Protecting groups of amino and hydroxy compounds.

4/ Nomenclature systems with examples. Rules for selection of the principal chain.

5/ Kinetics and thermodynamic principles; kinetic and thermodynamic control. Classification of organic reactions. Molecularity and order of reactions.

6/ Nomenclature and structures of alkanes, constitutional isomerism; conformational isomerism of ethane and butane.

7/ Preparation of alkanes by synthetic methods, characteristics of homologous series and physical and chemical properties of alkanes. Reactivity and selectivity, Hammond's Principle for radical halogenation of alkanes.

8/ Synthesis and stereochemistry of alicyclic compounds. Strains in alicyclic compounds. Some important cycloalkanes and their derivatives.

9/ Nomenclature of alkenes. (*E*) and (*Z*) isomers: geometric isomers. Structures and preparation of alkenes by synthetic methods. Physical and chemical properties of alkenes. Addition and oxidation reactions.

10/ Elimination reactions. E1, E2 and E1cb reaction mechanisms. The main characteristics of  $S_N1$  and  $S_N2$  reactions and of  $S_N$ ' and  $S_Ni$  reactions. Factors influencing elimination and substitution reactions of aliphatic compounds.

11/ Diolefins. Cumulated, conjugated and isolated dienes. Preparation and chemical reactions. Woodward-Hoffmann Rules.

12/ Structures, preparation, physical and chemical properties of alkynes. Petroleum and natural gas. 13/ Aliphatic and aromatic halogen compounds. Nomenclature, preparation, physical and chemical properties of aliphatic and aromatic halogen compounds. Phase-transfer catalysis: principle and examples.

14/ Alcohols: nomenclature, preparation, acidity, physical and chemical properties. Optical isomerism. More important alcohol derivatives with one or more OH groups.

15/ Phenols: nomenclature, preparation, acidity, physical and chemical properties. More important phenol derivatives with one or more OH groups. Ethers, crown ethers and quinones.

16/ Symmetry elements in organic compounds. Representation and notation of configuration – Cahn-Ingold-Prelog system. Enantiomers, diastereomers, racemic and meso compounds. Prochiral molecules, enantiotopic and diastereotopic surfaces.

17/ Organic amino compounds. Structures, nomenclature, and preparation.

18/ Basicity and acidity of aliphatic and aromatic amines. Influence of the medium. Structures of amine oxides and ylides. Some more important aliphatic, aromatic and arylalkanolamines.

19/ Comparative discussion of the chemical properties of amines.

20/ Organic nitro compounds.

21/ Organic compounds containing C-S bond(s). Sulfonic acids and sulfonamides.

22/ Organic compounds containing C-P bond(s).

23/ Definition of aromaticity (thermodynamic and structural aspects). Hückel's and Möbius's terms of aromaticity. Aromatic and antiaromatic compounds. Extension of aromaticity to systems different from benzene.

24/ Mechanism and direction rules of electrophilic aromatic substitution. Linear functions of free enthalpy.

25/ Chemical reactions of benzene with examples. Preparations of benzene homologues. Isomerism and nomenclature of benzene derivatives. Coal tar.

26/ Fused and isolated polycyclic hydrocarbons: structure and preparation.

27/ Factors affecting the acidity and basicity of organic compounds. Electronic effects in organic compounds.

28/ Aromatic diazonium compounds, preparation, and chemical reactions. Aromatic azo compounds, diazomethane.

29/ Structure, reactivity, and methods for preparation of aliphatic and aromatic aldehydes.

30/ Structures, reactivity, and methods for preparation of aliphatic and aromatic ketones.

31/ Carbonyl compounds: mechanisms of nucleophilic addition reactions, addition to  $\alpha$ , $\beta$ -unsaturated carbonyl compounds.

32/ Aldehydes and ketones: stereochemical aspects of nucleophilic addition reactions. Aldehydes and ketones: oxidation and reduction.

33/ Tautomerism of aldehydes and ketones. Electrophilic substitution on  $\alpha$ -carbon of carbonyl compounds. Aldol type reactions. Preparation of hydroxyoxo and dioxo compounds.

34/ Carboxylic acids and their derivatives: classification, physical properties, preparation, and chemical properties of carboxylic acids. Important carboxylic acids.

35/ Carboxylic acids and their derivatives: mechanism of acylation reactions. Preparation and chemical reactions of acyl halides, anhydrides, esters, and ketene.

36/ Mechanisms of preparation and hydrolysis of esters. Amides and nitriles, acid azides, acid hydrazides and hydroxamic acids. Preparation and chemical reactions of ortho esters.

37/ Electronic effects and interconversion of carboxylic acids and their derivatives: acylation reactions, reactivity order in acylation reactions and its interpretation, with examples.

38/ Carboxylic acids and their derivatives: reactions on the  $\alpha$ -carbon. Halogenation, intermolecular and intramolecular Claisen condensation.

39/ Preparation, chemical properties and synthetic values of ethyl acetoacetate and diethyl malonate. 40/ Carbonic acid derivatives.

41/ Halogenated carboxylic acids and dicarboxylic acids: preparation and chemical properties of them.

42/ Hydroxycarboxylic acids and oxocarboxylic acids: preparation and chemical properties of them.

### **Syllabus for the Final Examination**

1/ Chemical bond. Basic terms. Atomic and molecular orbitals. Hybridization. Bond formation and dissociation energy, with some typical examples. Isoconjugation.

2/ Basic terms of description of chemical bond – conjugation: butadiene, allyl systems; hyperconjugation. Homolysis and heterolysis. Resonance theory.

3/ Nomenclature systems with examples. Main types of heterocycles.

4/ Kinetics and thermodynamic principles; kinetic and thermodynamic control. Classification of organic reactions. Molecularity and order of reactions.

5/ Nomenclature and structures of alkanes, constitutional isomerism; conformational isomerism of ethane and butane.

6/ Preparation of alkanes by synthetic methods, characteristics of homologous series and physical and chemical properties of alkanes. Reactivity and selectivity, Hammond's Principle for radical halogenation of alkanes.

7/ Synthesis and stereochemistry of alicyclic compounds. Strains in alicyclic compounds. Some important cycloalkanes and their derivatives.

8/ Comparative discussion of inter- and intramolecular reactions (enthalpy and entropy). Steric acceleration and steric hindrance.

9/ Nomenclature of alkenes. (*E*) and (*Z*) isomers: geometric isomers. Structures and preparation of alkenes by synthetic methods. Physical and chemical properties of alkenes. Addition and oxidation reactions.

10/ Elimination reactions. E1, E2 and E1cb reaction mechanisms. The main characteristics of  $S_N1$  and  $S_N2$  reactions and of  $S_N$ ' and  $S_Ni$  reactions. Factors influencing elimination and substitution reactions of aliphatic compounds.

11/ Diolefins. Cumulated, conjugated, and isolated dienes. Preparation and chemical reactions. Woodward-Hoffmann Rules.

12/ Structures, preparation, physical and chemical properties of alkynes. Petroleum and natural gas. 13/ Aliphatic and aromatic halogen compounds. Nomenclature, preparation, physical and chemical properties of aliphatic and aromatic halogen compounds. Phase-transfer catalysis: principle and examples.

14/ Alcohols: nomenclature, preparation, acidity, physical and chemical properties. Optical isomerism. More important alcohol derivatives with one or more OH groups.

15/ Phenols: nomenclature, preparation, acidity, physical and chemical properties. More important phenol derivatives with one or more OH groups. Ethers, crown ethers and quinones.

16/ Symmetry elements in organic compounds. Representation and notation of configuration – Cahn-Ingold-Prelog system. Enantiomers, diastereomers, racemic and meso compounds. Prochiral molecules, enantiotopic and diastereotopic surfaces.

17/ Organic amino compounds. Structures, nomenclature, and preparation.

18/ Basicity and acidity of aliphatic and aromatic amines. Influence of the medium. Organic nitro compounds.

19/ Comparative discussion of the chemical properties of amines. Structure of amine-oxides and ylides. Some more important amines and aminoalcohols.

20/ Organic compounds containing C-S bond(s). Sulfonic acids and sulfonamides.

21/ Organic compounds containing C-P bond(s). Use of organic compounds containing zinc, magnesium for organic syntheses. Suzuki cross coupling reaction.

22/ Definition of aromaticity (thermodynamic, structural, and spectroscopic aspects). Hückel's and Möbius's terms of aromaticity. Aromatic and antiaromatic compounds. Extension of aromaticity to systems different from benzene.

23/ Mechanism and direction rules of electrophilic aromatic substitution. Linear functions of free enthalpy.

24/ Chemical reactions of benzene with examples. Preparations of benzene homologues. Nucleophilic substitution reactions of heteroaromatic halogen compounds. Isomerism and nomenclature of benzene derivatives. Coal tar.

25/ Factors affecting the acidity and basicity of organic compounds. Electronic effects in organic

compounds. Classification of protecting groups. Protecting groups of amino and hydroxy compounds.

26/ Aromatic diazonium compounds, preparation, and chemical reactions. Aromatic azo compounds, diazomethane.

27/ Fused and isolated polycyclic hydrocarbons: structure and preparation.

28/ Structure, reactivity, and methods for preparation of aliphatic and aromatic aldehydes.

29/ Structures, reactivity, and methods for preparation of aliphatic and aromatic ketones.

30/ Carbonyl compounds: mechanisms of nucleophilic addition reactions, addition to  $\alpha$ , $\beta$ -unsaturated carbonyl compounds.

31/ Aldehydes and ketones: stereochemical aspects of nucleophilic addition reactions. Aldehydes and ketones: oxidation and reduction.

32/Tautomerism of aldehydes and ketones. Electrophilic substitution on  $\alpha$ -carbon of carbonyl compounds. Aldol type reactions. Preparation of hydroxyoxo and dioxo compounds.

33/ Carboxylic acids and their derivatives: classification, physical properties, preparation, and chemical properties of carboxylic acids. Important carboxylic acids.

34/ Carboxylic acids and their derivatives: mechanism of acylation reactions. Preparation and chemical reactions of acyl halides, anhydrides, esters, and ketene.

35/ Mechanisms of preparation and hydrolysis of esters. Amides and nitriles, acid azides, acid hydrazides and hydroxamic acids. Preparation and chemical reactions of ortho esters.

36/ Electronic effects and interconversion of carboxylic acids and their derivatives: acylation reactions, reactivity order in acylation reactions and its interpretation, with examples.

37/ Carboxylic acids and their derivatives: reactions on the  $\alpha$ -carbon. Halogenation, intermolecular and intramolecular Claisen condensation.

38/ Preparation, chemical properties and synthetic values of ethyl acetoacetate and diethyl malonate.39/ Carbonic acid derivatives.

40/ Carbohydrates: structure (configuration and conformation) and its representation. Reactions of the carbonyl group.

41/ Carbohydrates: chemical reactions of the hydroxy groups. Anomeric effect. Glycosides.

42/ Preparation and chemical properties of amino acids. Protecting groups. Principles of peptide synthesis and synthetic methods.

43/ Sequence determination of peptides. Structure of proteins.

44/ Halogenated carboxylic acids and dicarboxylic acids: preparation and chemical properties of them.

45/ Hydroxycarboxylic acids and oxocarboxylic acids: preparation and chemical properties of them. 46/ Nomenclature system of heterocyclic compounds (with examples). Preparations and chemical reactions of alkylated derivatives of heteroaromatic compounds with examples.

47/ Preparations of  $\pi$ -excessive aromatic heterocyclic compounds with one heteroatom.

48/ Preparations of  $\pi$ -excessive aromatic heterocyclic compounds with 2 heteroatoms, having at least one nitrogen as heteroatom.

49/ Reactivity in electrophilic and nucleophilic substitution reactions as well as acid-base properties of  $\pi$ -excessive aromatic heterocyclic compounds with 1 or 2 heteroatoms, having at least one nitrogen atom.

50/ Preparations of  $\pi$ -deficient aromatic heterocyclic compounds with one heteroatom.

51/Preparations of  $\pi$ -deficient aromatic heterocyclic compounds with 2 heteroatoms, having at least one nitrogen as heteroatom.

52/Reactivity in electrophilic and nucleophilic substitution reactions as well as acid-base properties of  $\pi$ -deficient aromatic heterocyclic compounds with 1 or 2 heteroatoms, having at least one nitrogen atom.

53/ Types of tautomerism in heterocyclic compounds. Double reactivity of azinone, diazinone and similar systems.

54/ Benzo-fused analogues of five- and six-membered aromatic heterocycles.

55/ Three-, four-, seven- and eight-membered nitrogen-containing heterocycles: structures, chemical reactivity, and pharmaceutical importance. 56/ Alkaloids generally. Terms of proto-, pseudo- and real alkaloids. I. Alkaloids derived from aliphatic amino acids (a/ protoalkaloids with N in chain: ephedrine, pseudoephedrine; b/ alkaloids with pyridine-, piperidine- and pyrrolidine skeletone; c/ alkaloids with tropane skeletone). II. Alkaloids derived from aromatic amino acids (a/ alkaloids with phenylethylamine skeletone: hordenine, mescaline; b/ alkaloids with isoquinoline skeletone; c/ alkaloids with morphinane skeletone).

57/ Isolation of alkaloids. Some more important biogenic amines. III. Alkaloids derived from heterocyclic amino acids (tryptophane) (a/ alkaloids with indole skeletone; b/ alkaloids with rubane skeletone; c/ alkaloids with ergoline skeletone; d/ other alkaloids: tabersonine, camptothecine).

58/ Isoprenoid structures with some examples. Nomenclature of steroids. Bioactive steroids (with examples).

59/ Nucleosides and nucleotides. DNA and RNA bases.

#### **Practical work**

Students should bear in mind that the subject-matter of the examination comprises the total subject-matter of the lectures, with special attention to examples from medicinal chemistry discussed in the practicals and seminars, even if they are not directly indicated in the syllabus. At the final examinations, students should also know the subject-matter involved in the practicals.

For the examinations, students should also revise the following basic concepts of other chemical courses: acids and bases, reaction kinetics, order and molecularity of reactions, Arrhenius equation, basic concepts of thermodynamics, entropy, enthalpy, activation parameters, and related concepts and topics.

#### **Recommended textbooks**

F.A. Carey, R.M. Giuliano: Organic Chemistry, 10th Ed. McGraw Hill: New York, 2016 ISBN 0073511218

T.W.Gr. Solomons, C.B. Fryhle, S.A. Snyder: Organic Chemistry, 12th Ed. John Wiley & Sons, Inc., 2016 ISBN 1118875761

Experimental Organic Chemistry for students at the 2nd year of the Faculty of PharmacyCompiled by teaching staff of Institute of Organic Chemistry under the supervision of Péter Mátyus. Institute of Organic Chemistry, 2012

Gábor Krajsovszky: Heterocyclic compounds Semmelweis University, Pharmaceutical Faculty, Institute of Organic Chemistry, 2018 Editor: Gábor Krajsovszky ISBN: 978-615-5722-01-1 http://mek.oszk.hu/19100/19197

Gábor Krajsovszky: Collection of Organic chemical problems Semmelweis University, Pharmaceutical Faculty, Institute of Organic Chemistry, 2017 Editor: Gábor Krajsovszky ISBN 978-963-06-5345-9 http://mek.oszk.hu/17200/17281/

László Szabó, Gábor Krajsovszky: Isomerism in Organic Compounds Semmelweis University, Pharmaceutical Faculty, Institute of Organic Chemistry, 2017 Editor: Gábor Krajsovszky ISBN 978-963-12-9206-0 http://mek.oszk.hu/17200/17283/

J. Clayden, N. Greeves, S. Warren: Organic chemistry (paperback) Oxford University Press, 2012 ISBN 978-0-19-927029-3

A. Corbella, E. Marcantoni, G. Renzi: Seminars in Organic Synthesis. Royal Society of Chemistry, 2011 ISBN 978-88-86208-64-2

J.W. Zubrich: The Organic Chem Lab Survival Manual. A Student's Guide to Techniques. John Wiley & Sons, Inc., 2012
ISBN 978-1-118-08339-0
K.L. Williamson, K.M. Masters: Techniques Labs for Macroscale and Microscale Organic Experiments.
Brooks Cole 2016, 7th Ed
ISBN 1305577191

E. Pretsch, P. Bühlmann, M. Badertscher: Structure Determination of Organic Compounds. Springer-Verlag, Berlin • Heidelberg, 2009 ISBN 3540938095

#### **Diploma Work**

#### Aims of diploma work

In case of experimental work: obtaining expertise in organic chemical preparative work and in methods of electronic searches of the literature.

In case of computer chemical and modelling work: mastering and application of the most important methods.

#### **Requirements of diploma work**

The diploma work should include the literature references (minimum 30) relevant to the subject.

The diploma work must contain a minimum of 40 pages. The cover page should indicate the words "Diploma Work", the relevant year and the name of the student. The first inner page should give the title of the work, the name of the student and the place and year of elaboration.

#### **Preparation of diploma work**

The student may select freely from among the themes offered by the Institute. With preliminary approval of the Head of the Institute, the student may choose a subject different from those proposed officially. The diploma work should preferably be written in English or otherwise in German.

After the student has chosen a topic, this must be reported to the Head of the Institute not later than 15 October in the fourth academic year. After approval of the selection, the Head of the Institute registers it and appoints a supervisor to help with the work. The supervisor may be an external expert. The student is required to consult with the supervisor at least three times. At the first consultation (not later than 15 December in the fourth academic year), the supervisor informs the student about the requirements of the diploma work and its main characteristics. At the second consultation (by 15 May in the fourth academic year), the student reports on the work accomplished and third consultation at the (not later than 15 November in the fifth academic year), the supervisor evaluates the work and gives instructions as to the final form.

After coordination with and final approval by the supervisor and the Head of the Institute, two bound copies of the complete diploma are presented to the Institute by 15 December in the fifth academic year. The reviewer appointed by the Head of the Institute evaluates the work in written form, using a five-scale grading system.

The diploma work is defended in the presence of an examining board, the members of which are the Head of the Institute or a deputy, the supervisor, and the reviewer. Participation in the defence is open to the teaching staff and students at the University.

If the diploma work is not accepted (grade: 1), the Institute informs the student, who is not allowed to take the general board examinations. A new or revised diploma work may be submitted, but not within 2 months.

Students may receive exemption from writing a diploma work if they have won a Rector's prize for an essay competition or published an article (written by one or two students) in a scientific journal (generally with an impact factor). Exemption must be requested in writing from the Dean of the Faculty. The Dean asks for the opinion and grading of the Institute.

# List of themes for diploma / research students work for Year of 2024/2025

- 1. Synthesis and chemical transformations of quinazoline derivatives (Gábor Krajsovszky, Krisztina Süttő-Kaczeus, István Mándity)
- 2. Azocoupling under sustainable conditions (Andrea Czompa, István Mándity)
- 3. Simplified Sandmeyer reactions (Andrea Czompa, István Mándity)
- 4. Cross-coupling reactions under "green" conditions (Andrea Czompa, István Mándity)
- 5. Examinations of interactions of cell penetrating peptide with lipid membrane, by using theoretical chemical calculations (Balázs Balogh, István Mándity)
- 6. Investigation cell-penetrating peptides trough computational modelling (István Mándity, Balázs Balogh)
- 7. Synthesis and structural analysis of modified peptides (Mándity István)
- 8. Chemical flow synthesis of oxindole analogues (István Mándity)
- 9. Solid phase synthesis, purification and quality checking of biologically active peptide (István Mándity)
- 10. Development of artificial peptides (István Mándity)
- 11. Synthesis and applications of photolabile protecting groups (Petra Dunkel)
- 12. Synthesis of nitrogen heterocycles (Petra Dunkel)
- 13. Structure determination with NMR spectroscopy (Dóra Bogdán, Eszter Kalydi, István Mándity)

### Work of research students

If students have a keen interest in the organic chemical and drug chemical preparative or computational work at the Institute, pass their final examination in organic chemistry with a mark not lower than 3, and have sufficient free time for additional work, they may request admission into the Union of Research Students of the Institute. Further information can be obtained from the Secretary of the Union of Research Students or the Head of the Institute.

http://semmelweis.hu/tdk/en/

### Postgraduate work towards a Ph.D. degree

Students who have completed their undergraduate studies, received a diploma in pharmacy and have special interest in research work in the field of organic chemistry may continue their studies towards obtaining the scientific degree of Ph.D. (Doctor of Philosophy) at the University. Additional information may be obtained from the Head of the Institute.

Title of the programme: Modern research trends in pharmaceutical sciences.

1. Synthesis and applications of photoremovable protecting groups (Supervisor: Dr. Petra Dunkel Ph.D.)

2. Chloride-ion transporter synthesis using micro-flow reaction system, peptide conformation analysis using NMR, MS, CD, UV measurements (Supervisor: Dr. István Mándity Ph.D.)

3. Synthesis of azo compound under sustainable conditions (Supervisor: Dr. Andrea Czompa Ph.D., Dr. István Mándity Ph.D.)

4. Cross-coupling reactions under "green" conditions (Supervisor: Dr. Andrea Czompa Ph.D., Dr. István Mándity Ph.D.)

http://semmelweis.hu/phd/en/

### **Selected Publications**

### From 2010

- Dunkel P., Túrós Gy., Bényei A., Ludányi K., Mátyus P.: Synthesis of novel fused azecine ring systems through application of the *tert*-amino effect. *Tetrahedron*, **66**, 2331-2339 (2010). IF 3.011
- Haider N., Hochholdinger I., Mátyus P., Wobus A.: Synthesis of *ortho*-functionalized 4-aminomethylpyridazines as substrate-like semicarbazidesensitive amine oxidase inhibitors. *Chem. Pharm. Bull.*, 58, 964-970 (2010). IF 1.507
- Földi Á.A., Ludányi K., Bényei A.Cs., Mátyus P.: tert-Amino effect in peri-substituted naphthalenes: Syntheses of naphthazepine and naphthazonine ring systems. Synlett, 14, 2109-2113 (2010). IF 2.447
- 4. Énzsöly A., Dunkel P., Récsán Zs., Győrffy H., Tóth J., Marics G., Bori Z., Tóth M., Zelkó R., Di Paolo M.L., Mátyus P., Németh J.: Preliminary studies of the effects of vascular adhesion protein-1 inhibitors on experimental corneal neovascularization. *J. Neural. Transm.*, **118**, 1065-1069 (2011). IF 2.732
- Pop L.A., Czompa A., Paizs Cs., Tosa M.I., Vass E., Mátyus P., Irimie F.D.: Lipase catalyzed synthesis of both enantiomers of 3-chloro-1-phenylpropan-1-ols. *Synthesis*, 18, 2921-2928 (2011). IF 2.466
- Dunkel P., Balogh B., Meleddu R., Maccioni E., Gyires K., Mátyus P.: Semicarbazide sensitive amine oxidase/vascular adhesion protein-1: A patent survey. *Expert Opin. Ther. Patents*, 21, 1453-1471 (2011). IF 3.571
- Maccioni E., Alcaro S., Cirilli R., Vigo S., Cardia C. M., Sanna M.L., Meleddu R., Yanez M., Costa G., Casu L., Mátyus P., Distinto S.: 3-Acetyl-2,5-diaryl-2,3-dihydro-1,3,4-oxadiazoles: A new scaffold for the selective inhibition of monoamine oxidase B. *J. Med. Chem.*, 54, 6394-6398 (2011). IF 5.248
- Dunkel P., Chai C.L.L., Sperlágh B., Huleatt P.B., Mátyus P.: Clinical utility of neuroprotective agents in neurodegenerative diseases: Current status of drug development for Alzheimer's, Parkinson's and Huntington's diseases, and amyotrophic lateral sclerosis. *Expert Opin. Investig. Drugs*, 21, 1267-1308 (2012). IF 4.744

- Bottino P., Dunkel P., Schlich M., Galavotti L., Deme R., Regdon G. Jr., Bényei A., Pintye-Hódi K., Ronsisvalle G., Mátyus P.: Study on the scope of *tert*-amino effect: New extensions of type 2 reactions to bridged biaryls. *J. Phys. Org. Chem.*, 25, 1033-1041 (2012). IF 1.578
- Ilić M., Ilaš J., Dunkel P., Mátyus P., Bohác A., Liekens S., Kikelj D.: Novel 1,4-benzoxazine and 1,4-benzodioxine inhibitors of angiogenesis. *Eur. J. Med. Chem.*, 58, 160-170 (2012). IF 3.499
- Arany Á., Bolgár B., Balogh B., Antal P., Mátyus P.: Multi-aspect candidates for repositioning: Data fusion methods using heterogeneous information sources. *Curr. Med. Chem.*, 20, 95-107 (2013). IF 3.715
- Tábi T., Szökő É., Mérey A., Tóth V., Mátyus P., Gyires K.: Study on SSAO enzyme activity and anti-inflammatory effect of SSAO inhibitors in animal model of inflammation. *J. Neural Transm.*, **120**, 963-967 (2013). IF 2.871
- Ilić M., Dunkel P., Ilaš J., Chabielska E., Zakrzeska A., Mátyus P., Kikelj D.: Towards dual antithrombotic compounds – Balancing thrombin inhibitory and fibrinogen GPIIb/IIIa binding inhibitory activities of 2,3-dihydro-1,4-benzodioxine derivatives through regio- and stereoisomerism. *Eur. J. Med. Chem.*, **62**, 329-340 (2013). IF 3.432
- Bolgár B., Arany Á., Temesi G., Balogh B., Antal P., Mátyus P.: Drug repositioning for treatment of movement disorders: From serendipity to rational discovery strategies. *Curr. Top. Med. Chem.*, 13, 2337-2367 (2013). IF 3.453
- Temesi G., Bolgár B., Arany Á., Szalai Cs., Antal P., Mátyus P.: Early repositioning through compound set enrichment analysis: A knowledge recycling strategy. *Future Med. Chem.*, 6, 563-575 (2014). IF 3.744
- 16. Krajsovszky G., Tóth E., Ludányi K.: Tandem mass spectrometric study of annelation isomers of the novel thieno[3',2':4,5]pyrido[2,3-d]pyridazine ring system. *Arkivoc*, 158-169 (2014). IF 1.165

- Meleddu R., Distinto S., Corona A., Bianco G., Cannas V., Esposito F., Artese A., Alcaro S., Mátyus P., Bogdán D., Tramontano E., Maccioni E.:
  (Z)-3-(2-(4-arylthiazol-2-yl)hydrazono)indolin-2-one derivatives as dual inhibitors of HIV-1 RT. *Eur. J. Med. Chem.*, 9, 452-460 (2015).
  IF 3.447 (2014)
- Antus Cs., Radnai B., Dombóvári P., Fónai F., Avar P., Mátyus P., Rácz B., Sümegi B., Veres B.: Anti-inflammatory effects of a triple-bond resveratrol analog: Structure and function relationship. *Eur. J. Pharmacol.*, **748**, 61-67 (2015). IF 2.532 (2014)
- Huleatt P.B., Khoo M.L., Chua Y.Y., Tan T.W., Liew R.S., Balogh B., Deme R., Gölöncsér F., Magyar K., Sheela D.P., Ho H.K., Sperlágh B., Mátyus P., Chai C.L.L.: Novel arylalkenylpropargylamines as neuroprotective, potent, and selective monoamine oxidase B inhibitors for the treatment of Parkinson's disease. J. Med. Chem., 58, 1400-1419 (2015). IF 5.447 (2014)
- 20. Balogh B., Pázmány T., Mátyus P.: Analysis of Edg-Like LPA receptor-ligand interactions. *Curr. Pharm. Des.* 21, 3533-3547 (2015). IF 3.452 (2014)
- Hársing L.G. Jr., Timár J., Szabó G., Udvari Sz., Nagy K.M., Markó B., Zsilla G., Czompa A., Tapolcsányi P., Kocsis Á., Mátyus P.: Sarcosine-based glycine transporter type-1 (GlyT-1) inhibitors containing pyridazine moiety: a further search for drugs with potential to influence schizophrenia negative symptoms. *Curr. Pharm. Des.*, **21**, 2291-2303 (2015). IF 3.452 (2014)
- Baranyi M., Porceddu P.F., Gölöncsér F., Kulcsár Sz., Otrokocsi L., Kittel Á., Pinna A., Frau L., Huleatt P.B., Khoo M-L., Chai C.L.L., Dunkel P., Mátyus P., Morelli M. and Sperlágh B.: Novel (Hetero)arylalkenyl propargylamine compounds are protective in toxin-induced models of Parkinson's disease. *Mol. Neurodegener.*, **11**, (6) 1-21 (2016). IF: 6.563 (2014)
- 23. Payrits M., Sághy É., Mátyus P., Czompa A., Ludmerczki R., Deme R., Sándor Z., Helyes Zs., Szőke É.:
  A novel 3-(4,5-Diphenyl-1,3-oxazol-2-yl)propanal oxime compound is a potent Transient Receptor Potential Ankyrin 1 and Vanilloid 1 (TRPA1 and V1) receptor antagonist. *Neurosci.*, **324**,151-162 (2016). IF 3.357 (2014)

- 24. Balogh B., Carbone A., Spanò V., Montalbano A., Barraja P., Cascioferro S., Diana P., Parrino **B**.: Investigation of Isoindolo[2,1-a]quinoxaline-6-imines as Topoisomerase I Inhibitors with Molecular Modeling Methods. Curr. Comput.-Aided Drug Des., 13, 208-221 (2017). IF 1.155 (2015)
- Horváth Á., Awt Menghis, Botz B., Borbély É., Csepregi J., Mócsai A., Czompa A., Tóth-Sarudy 25. É., Juhász T., Zákány R., Mátyus P., Keeble J., Pintér E., Helyes Zs.: Analgesic and anti-inflammatory effects of the novel semicarbazide-sensitive amine-oxidase inhibitor SZV-1287 in chronic arthritis models of the mouse. Scientific Reports 7, 39863. Doi: 10.1038/srep39863 (2017). IF 5.228 (2015)
- Meleddu R., Distinto S., Cirilli R., Alcaro S., Yanez M., Sanna ML., Corona A., Melis C., Bianco 26. G., Matyus P., Cottiglia F., Maccioni E.: Through scaffold modification to 3,5-diaryl-4,5-dihydroisoxazoles: new potent and selective inhibitors of monoamine oxidase B. J Enzyme Inhib Med Chem., 32, 264-270 (2017). IF 3.428 (2015)
- 27. Bogdán D., Haessner R., Vágvölgyi M., Passarella D., Hunyadi A., Gáti T., Tóth G.: Stereochemistry, and complete 1H and 13C NMR signal assignment of C-20-oxime derivatives of posterone 2,3-acetonide in solution state. Magnetic Resonance in Chemistry (2018).
- Szabó Z-I., Deme R., Mucsi Z., Rusu A., Mare A.D., Fiser B., Toma F., Sipos E., Tóth G.: 28. Equilibrium, structural and antibacterial characterization of moxifloxacin-β-cyclodextrin complex. Journal of Molecular Structure, 1166, 228-236 (2018).
- 29. Nekkaa I., Palko M., Mandity I.M., Fulop F.: Continuous-flow retro-Diels-Alder reaction: an efficient method for the preparation of pyrimidinone derivatives. Beilstein Journal of Organic Chemistry, 14, 318-324 (2018).
- 30. Nekkaa I., Bogdan D., Gati T., Beni Sz., Juhasz T., Palko M., Paragi G., Toth G.K., Fulop F., Mandity I.M.: Flow-chemistry enabled efficient synthesis of beta-peptides: backbone topology vs. helix formation. Chem. Comm., 55, 3061-3064 (2019).

- Czompa, Andrea; Pásztor, Balázs László; Sahar, Jennifer Alizadeh; Mucsi, Zoltán; Bogdán, Dóra; Ludányi, Krisztina; Varga, Zoltán; Mándity, István M.: Scope and limitation of propylene carbonate as a sustainable solvent in the Suzuki–Miyaura reaction. *RSC Advances*, 9, 37818-37824 (2019).
- Jakab, Géza; Bogdán, Dóra; Mazák, Károly; Deme, Ruth; Mucsi, Zoltán; Mándity, István M.; Noszál, Béla; Kállai-Szabó, Nikolett; Antal, István:
  Physicochemical Profiling of Baicalin Along with the Development and Characterization of Cyclodextrin Inclusion Complexes
  AAPS Pharm.Sci.Tech., 20, Paper: 314, 12 p. (2019).
- 33. Nizami, Bilal; Bereczki-Szakál, Dorottya; Varró, Nikolett; el Battioui, Kamal; Nagaraj, Vignesh U; Szigyártó, Imola Cs; Mándity, István; Beke-Somfai, Tamás: FoldamerDB: a database of peptidic foldamers. *Nucleic Acids Research*, 48, D1122-D1128 (2020).
- Ludmerczki, Robert; Malfatti, Luca; Stagi, Luigi; Meloni, Manuela; Carbonaro, Carlo Maria; Casula, Maria Francesca; Bogdán, Dóra; Mura, Stefania; Mándity, István M.; Innocenzi, Plinio: Polymerization-Driven Photoluminescence in Alkanolamine-Based C-Dots. *Chemistry-A European Journal*, 27, 2543-2550. (2021).
- Balogh, Balázs; Ivánczi, Márton; Nizami, Bilal; Beke-Somfai, Tamás; Mándity, István M: ConjuPepDB: a database of peptide–drug conjugates. *Nucleic Acids Research* 49, D1 D1102-D1112 (2021).
- 36. Batta, Gyula; Kárpáti, Levente; Henrique, Gabriela Fulaneto; Tóth, Gabriella; Tarapcsák, Szabolcs; Kovács, Tamás; Zákány, Florina; Mándity, István M.; Nagy, Peter: Statin-boosted cellular uptake and endosomal escape of penetratin due to reduced membrane dipole potential. British Journal of Pharmacology In press Paper: bph.15509 (2021).

# From 2022

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