Master Training in Chemistry at University of Debrecen

1. Title of the training: Master in Chemistry

Program supervisor: Dr. István Fábián professor of chemistry

Faculty: Faculty of Science and Technology

2. The degree received

- MSc in Chemistry

Electable specialization tracks and the corresponding supervisors

Analytical Chemistry: Dr Attila Gáspár, professor of chemistry
Synthetic Chemistry: Dr. Tibor Kurtán, professor of chemistry
Radiochemistry: Dr. Noémi Nagy, professor of chemistry

3. Scientific area of the training: natural sciences

4. Requirements for the admittance to the training program

4.1. The admittance is based on full credits earned in the following BSc trainings:
Chemistry, chemical engineering, various fields of natural sciences and engineering

***4.2. Credit requirements can be satisfied primarily on the basis of the following subjects*:** biology, physics, geography, environmental sciences, mathematics, bioengineering, material sciences, environmental engineering, civil engineering, molecular biology, biotechnology, medical laboratory analysis, medical diagnostic analysis.

4.3. Credits from any field of basic trainig are subject to acceptance by the admittance committee or the program supervisor.

5. The duration of the training: 4 semesters

6. Required credits for earning the MSc degree: 120

- credits earned in core and specialization courses are balanced (40 – 60 %),
- credits earned by the diploma work: 30
- credits from freely elected courses: 6

7. Identification code of the training: 442

8. The objectives of the training and competencies to be gained

The main goal of the program is to train highly qualified chemists to satisfy the demands of the chemical industry. The students will gain high level knowledge in theoretical and practical aspects of chemistry. They will also receive excellent training in related fields such as mathematics, physics and informatics. The graduates of the MSc program will be prepared to use the chemical literature and solve various problems independently in both the chemical industry and chemical laboratories including research and development areas. They will be able to fill high level positions in the chemical and pharmaceutical industry as well as in companies and agencies active in related areas such as environmental protection and management, quality control and assurance, food safety etc. MSc graduates will develop the appropriate skills to continue their studies in doctoral schools of chemistry at the University of Debrecen or at any university throughout the world.

8.1. Gained competencies

a) knowledge

- understanding the main relationships between chemical phenomena and the ability to use theoretical and practical methods for the interpretation of them;
- the knowledge of the latest scientific results related to chemical bonding, structures, reactions; understanding the novel theories, models and appropriate computational methods for the interpretation of the new results.
- understanding the main trends and the limits of the developments in chemistry and the chemical industry;
- understanding the main principles and concepts of natural sciences;
- the ability to use laboratory methods, industrial systems and the corresponding apparatuses as well as understanding the related safety regulations;
- possessing sufficient knowledge to accurately interpret chemical phenomena and to solve practical chemical problems related to natural resources, living systems and natural sciences;
- the knowledge of the inquiring scientific and practical problems of a specific area of chemistry;
- broad knowledge of the relevant literature of a specific area of chemistry.

b) skills

- the ability to use the most important theories, practical tools in chemical research and development and the evaluation of the results obtained;
- the ability to evaluate chemical literature results objectively and recognize overall and specific relationships in chemistry;.
- the ability to make a distinction between real scientific and pseudo scientific statements in chemistry.
- the ability to critically use novel chemical theories and principles in the practice and to design new laboratory and industrial procedures independently;
- the ability to perform new laboratory experiments supported by appropriate measurements, to synthesize new compounds, and to describe and confirm new chemical phenomena by utilizing analytical chemistry
- the ability to evaluate, interpret and analyze experimental data independently, to draw appropriate conclusions on the basis of the results and to identify the main directions of further development.
- the ability to communicate the main chemical problems in a specific area to other chemists and non-specialists in the fields of natural sciences and engineering.
- the ability to support a standpoint in scientific debates with appropriate scientific arguments;
- the ability to utilize her/his acquired chemical knowledge in scientific research and in producing new results;

c) attitude

- to accept the specific professional identity which originates in the natural sciences;
- commitment to give high priority to environmental protection during laboratory and industrial activities and communicate this attitude toward colleagues;
- a commitment to use the most environment friendly approach in solving a chemical problem;
- to follow the ethical norms while handling the intellectual properties produced by her/him or others;

- openness toward introducing and using novel chemical and environmental technologies;
- initiation and participation in professional consultations;
- openness toward inter- and multidisciplinary collaboration;
- appreciation of the skepticism in science;
- active communication of the concepts of natural sciences toward both professional and non-professional audiences;
- openness toward acquiring new knowledge and competences, as well as toward further professional development;
- refraining from taking undue advantage of professional knowledge and strictly following professional and societal ethical norms.

d) autonomy and responsibility

- acting independently in developing general and specific professional concepts;
- responsible collaboration with other professionals;
- independent approach toward personalized tasks and accepting responsibility for individual ideas, decisions and acts;
- understanding the direct and indirect risks of laboratory and industrial procedures and following prudent rules to minimize any potential hazard;
- objective evaluation of the work performed by subordinates;
- understanding the significance of the personal professional statements and taking responsibility for them;
- taking responsibility for operating the laboratory and industrial equipment and supervising the activities of the subordinates.
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9. Features of the training

9.1. Professional features

The disciplines used in the training:

- fundamental courses in natural sciences: 6-18 credits;
- courses in chemistry (inorganic chemistry at least 4 credits, organic chemistry at least 4 credits, physical chemistry at least 4 credits, analytical chemistry at least 4 credits, applied and industrial chemistry at least 4 credits) 30−50 credits;
- special courses: 20−40 credits.

9.2 Contact classes

The number of classes (depends on the specialization) mandatory:1260-1300, freely elected: 350-660.

9.3. Minimum requirements to enter the MSc program:

- general natural sciences (mathematics, physics, informatics, biology etc.): 15 credits;
- chemistry (general and inorganic chemistry: at least 10 credits, organic chemistry: at least 10 credits, analytical chemistry: at least 10 credits, physical chemistry: at least 10 credits,) at least 50 credits.

10. Specialization

The optional specializations are detailed in Chapter 2. In this case, general and specific courses need to be taken as follows:

fundamental courses: 48 credits
specific freely elected courses: 30 credits

11. Final exam

Objectives:
The professional competencies and knowledge of the student is evaluated. The graduate needs to demonstrate proficiency in chemistry and the ability to perform high level chemical tasks independently. The preparedness for professional debates also needs to be shown.

Requirements:
In order to participate in the final exam, the student needs to satisfy all formal and informal requirements. Thus, a minimum of 120 credits need to be earned. Further requirement is the submission of a thesis covering the diploma work of the graduate well before the final exam.

The diploma work

The final exam:
The final exam has two parts. First, the thesis based on the diploma work is presented in front of the examining committee. The graduating student gives a lecture, answers the remarks of the reviewer and the questions of the committee and the audience. In the second part, the student must demonstrate her/his knowledge in chemistry at the masters level. There are the following groups of questions:

A: fundamental topics (inorganic, analytical, physical, organic, applied and biochemistry)
B: specialization in analytical chemistry
C: specialization in synthetic chemistry
D: radiochemistry

The students need to answer one question from group A and another question from the group of her/his specialization. If no specialization was selected, two questions are answered from group A.

STRUCTURE OF THE CURRICULUM IN ECTS CREDITS

Table 1. Science Courses (Total 30 credits BSc + MSc)

Course name *Lecturer*	**Code**	**Hours/week (L+S+P)[a] exam type[b]**	**Prerequisites**	**Credits**
Science (6 credits)				
Crystallography *Gábor Dobosi*	TTGME5101_EN	2e+0+0	none	3
Biochemistry II.[c] *Gyöngyi Gyémánt*	TTKML0304_EN	0+(1+2)p	minimum 3 credits of biochemistry	3
Biochemistry III.[c] *Teréz Barna*	TTKME0304_EN	2e+0+0	minimum 3 credits of biochemistry	3
Measurement Methods in Materials Science (lecture) *Lajos Daróczi*	TTFME0411_BT_EN	2e+0+0	minimum 3 credits of physics	3
Measurement Methods in Materials Science (practice) *Lajos Daróczi*	TTFML0411_BT_EN	0+0+2p	minimum 3 credits of physics	1
Atomic and Molecular Physics *András Csehi*	TTFME0101_EN	2e+1s+0	minimum 12 credits of physics	4
Computational Quantum Chemistry[c] *Mihály Purgel*	TTKMG0902_EN	0+2p+0	minimum 12 credits of mathematics	3

Table 2. Basics of Professional Knowledge

Course name *Lecturer*	**Code**	**Semester Hours/week (L+S+P)[a] exam type[b]**				**Credits**
		I. (fall)	**II. (spring)**	**III. (fall)**	**IV. (spring)**	
Inorganic Chemistry Block (10 cr)						
Inorganic Chemistry V. *Péter Buglyó*	TTKME0203_EN	3e+0+0				4
Inorganic Chemistry VI. *Péter Buglyó*	TTKML0203_EN	0+0+4p				4
Inorganic Chemistry VII. *Katalin Várnagy*	TTKME0204_EN		2e+0+0			3
Physical Chemistry Block (including radio- and colloid chemistry) (10 cr)						
Physical Chemistry VI. *Attila Bényei*	TTKME0401_EN	3e+0+0				4
Physical Chemistry VII. *Ferenc Krisztián Kálmán*	TTKML0405_EN	0+0+3p				3
Physical Chemistry VIII. *Levente Novák*	TTKML0406_EN		0+0+3p			3

Course name *Lecturer*	Code	Semester Hours/week (L+S+P)[a] exam type[b]				Credits
		I. (fall)	**II. (spring)**	**III. (fall)**	**IV. (spring)**	
Organic and Biochemistry Block (11 credits)						
Synthetic Methods in Organic Chemistry I. *Krisztina Kónya*	TTKME0301_EN	2e+0+0				3
Synthetic Methods in Organic Chemistry II. *Éva Bokor*	TTKML0302_EN		0+0+4p			3
Heterocycles *Tibor Kurtán*	TTKME0327_EN		2e+0+0			3
Biochemistry IV. *Teréz Barna*	TTKME0303_EN		2e+0+0			2
Analytical Chemistry and Structure Determination Block (10 credits)						
Instrumental Analysis I. *Attila Gáspár*	TTKME0501_EN		2e+0+0			3
Instrumental Analysis II. *Attila Gáspár*	TTKML0501_EN			0+0+3p		2
Spectroscopic Methods for Structure Investigation I. *Katalin Erdődi Kövér*	TTKME0502_EN		2e+0+0			3
Spectroscopic Methods for Structure Investigation II. *Katalin Erdődi Kövér*	TTKML0502_EN			0+0+3p		2
Engineering Chemistry (6 credits)						
Introduction to Chemical Engineering *Miklós Nagy*	TTKME0601_EN		2e+0+0			3
Advanced Chemical Technology *Katalin Illyés Czifrák*	TTKME0602_EN			2e+0+0		3
Diploma Thesis I. *István Fábián*	TTKML0001_EN			0+0+15p		15
Diploma Thesis II. *István Fábián*	TTKML0002_EN				0+0+15p	15
Industrial placement *Ákos Kuki*	TTKMX0003_EN			4 weeks (summer)	s	0
Total (credits, hours/week, exams)		18 cr, 15h, 3e, 2p	23 cr 19h, 6e, 2p	7+15 cr 8+15h 1e, 3p	15 cr 15h 1p	48+30cr 42+30h 10e+8p

Table 3. Compulsory and Optional courses on Analytical specialization (30 credits)

Course name *Lecturer*	**Code**	**Semester Hours/week (L+S+P)[a] exam type[b]**			**Credits**
		II. (spring)	**III. (fall)**	**IV. (spring)**	
Compulsory Courses					**23**
Chemometrics I. *József Kalmár*	TTKME0511_EN	2e+0+0			3
Separation Tehcniques III. *Attila Kiss*	TTKME0315_EN	2e+0+0			3
Separation Techniques IV. *Attila Kiss*	TTKML0315_EN		0+0+4p		4
Inorganic Methods in Environmental Analysis I. *Edina Baranyai*	TTKME0503_EN		1e+0+0		1
Inorganic Methods in Environmental Analysis II. *Edina Baranyai*	TTKML0503_EN		0+0+4p		4
Quality Assurance in Analytical Chemistry *József Kalmár*	TTKME0513_EN			1e+0+0	1
Mass Spectrometry *Sándor Kéki*	TTKME0317_EN			(2+1)e+0	4
Electrophoretic Techniques *Attila Gáspár*	TTKME0504_EN			2e+0+0	3
Optional Courses					**7**
Sampling, Sample Treatment, Analytical Tests I.[d] *Edina Baranyai*	TTKME0514_EN	1e+0+0 (spring semester)			1
Sampling, Sample Treatment, Analytical Tests II.[d] *Edina Baranyai*	TTKML0514_EN	0+0+4p (spring semester)			4
Chemometrics II. *József Kalmár*	TTKMG0512_EN	0+(1+2)p			3
Nuclear Analysis I. *Noémi Nagy*	TTKME0523_EN		2e+0+0		3
NMR Operator Training II.[e] *Katalin Erdődi Kövér*	TTKML0530_EN		0+0+2p		2
Analysis of Proteins[d] *Attila Gáspár*	TTKME0506_EN			2e+0+0	2
Analytics in Pharma Industry *András Zékány*	TTKME0520_EN		0+4p+0		4

Table 3. Compulsory and Optional courses on Synthetic specialization (30 credits)

Course name *Lecturer*	Code	Semester Hours/week (L+S+P)[a] exam type[b] II. (spring)	III. (fall)	IV. (spring)	Credits
Compulsory Courses					**27**
Reaction Mechanism *László Somsák*	TTKME0311_EN	3e+0+0			4
Asymmetric Syntheses *Attila Mándi*	TTKME0312_EN		2e+0+0		3
Synthetic Methods in Polymer Chemistry *Sándor Kéki*	TTKME0313_EN	2e+0+0			3
Chemical Aspects of Drug Design *László Somsák*	TTKME0314_EN		2e+0+0		3
Separation Techniques III. *Attila Kiss*	TTKME0315_EN	2e+0+0			3
Separation Techniques IV. *Attila Kiss*	TTKML0316_EN		0+0+2p		2
NMR Operator Training II.[e] *Katalin Erdődi Kövér*	TTKML0530_EN		0+0+2p		2
Mass Spectrometry *Sándor Kéki, Lajos Nagy*	TTKME0317_EN			(2+1)e+0	4
High Efficiency Synthetic Methods I. *Krisztina Kónya*	TTKML0319_EN			0+(1+3)p	3
Optional Courses					**3**
2D NMR Methods[e] *Katalin Erdődi Kövér*	TTKMG0318_EN		0+2p+0		2
Glycobiochemitstry *János Kerékgyártó*	TTKME0321_EN			2e+0+0	3
Sterecohemical Structural Elucidation Methods *Tibor Kurtán*	TTKME0322_EN			2e+0+0	3
Carbohydrate Chemistry *László Somsák*	TTKME0323_EN			2e+0+0	3
Organic Chemistry of Drug Syntheses *Éva Juhász Tóth*	TTKME0324_EN		2e+0+0		3

Table 4. Compulsory and Optional courses on Radiochemical specialization (30 credits)

Course name *Lecturer*	Code	Semester Hours/week (L+S+P)[a] exam type[b]			Credits
		II. (spring)	III. (fall)	IV. (spring)	
Compulsory courses					25
Radiochemistry *Noémi Nagy*	TTKME0410_EN	2e+0+0			3
Nuclear Methods for Environmental Protection *Mihály Molnár*	TTKME0426_EN	2e+0+0			3
Medical Applications of Radiopharmaceuticals *László Galuska*	TTKME0429_EN		2e+0+0		3
Nuclear Analysis I. *Noémi Nagy*	TTKME0523_EN		2e+0+0		3
Nuclear Analysis II. *Noémi Nagy*	TTKML0523_EN		Visit a power plan(p)		1
Production of Isotopes *István Kertész*	TTKML0437_EN		1+0+1p		3
Separation Techniques for Radiolabeled Compounds *István Jószai*	TTKME0431_EN		(2+2)e+0		4
Dosimetry, Radiation Health Effects *István Hajdu*	TTKME0432_EN	2e+0+0			3
Radiochemical Exercises *Noémi Nagy*	TTKML0415_EN	0+0+2p			2
Optional Courses					5
Biological Application of Labelled Compounds *István Kertész*	TTKME0434_EN			2e+0+0	3
Syntheses and Quality Control of Radioactive Pharmaceuticals *István Jószai*	TTKML0435_EN			0+0+2p	2
Investigation of Cellular and Tissue Metabolism With Radiochemical Methods *György Trencsényi*	TTKME0436_EN			2e+0+0	3

Table 5. Optional Courses for all specialization (max. 30 credits from this table and other Compulsory/Optional Courses from other specialization)

Course name ***Lecturer***	**CODE**	**Hours/week (L+S+P)[a] exam type[b]**	**Credits**
Complexes of Macrocyclic Ligands *Gyula Tircsó*	TTKME0212_EN	2e+0+0	3
Dangerous and Special Materials [c] *István Lázár*	TTKME0206_EN	2e+0+0	3
Biocolloids[c] *Levente Novák*	TTKME0411_EN	2e+0+0	3
Physical Chemistry of Living Systems *Henrietta Győrvári Horváth*	TTKME0417_EN	2e+0+0	3
Metal Complex Catalyzed Organic Syntheses *Ferenc Joó*	TTKME0420_EN	2e+0+0	3
Environmental Chemistry II. *Mónika Kéri*	TTKME0414_EN	2e+1+1	4
Structure Determination by X-ray Diffraction *Attila Bényei*	TTKME0423_EN	2e+0+0	3
Chemistry of Secondary Metabolites I. *László Juhász*	TTKME0331_EN	2e+0+0	3
Chemistry of Secondary Metabolites II. *László Juhász*	TTKML0332_EN	0+0+4p	3
Enzyme Biotechnology *Teréz Barna*	TTKME0334_EN	2e+0+0	3
NMR Operator Training I.[c] *Gyula Batta*	TTKML0004_EN	0+0+2p	2
Reaction Kinetics/Catalysis *Ferenc Joó*	TTKME0437_EN	2e+0+2p	4
NMR Structure Determination *Krisztina Fehér*	TTKME0507_EN	1e+0+1	3

[a] L: lecture, S: seminar P: laboratory practice;
[b] e: oral or written exam p: practice s: signature
[c] Can be fulfilled on BSc as well, but only once (during BSc and MSc)!
[d] Prerequisite: TTKME0501, Instrumental Analysis I.
[e] Prerequisite: TKBL0004 or TKML0004, NMR Operator Training I.

DESCRIPTION OF SUBJECTS
(in order of their appearance in the tables above)

Title of course: Crystallography **Code**: TTGME5104_EN	**ECTS Credit points: 2**
Type of teaching, contact hours - lecture: 2 hours/week - practice:- - laboratory: -	
Evaluation: mid-term test, end-term test and written final exam	
Workload (estimated), divided into contact hours: - lecture: 28 hours - practice:- - laboratory: - - home assignment: 10 - preparation for the exam:30 Total: 68	
Year, semester: 1st year, 1st semester	
Its prerequisite(s):	
Further courses built on it:-	

Topics of course

Position of crystallography among other fields of science. The definition of space latice, unit cell and crystallographic axes. Bravais lattices. Unit cells and crystallographic axes in crystal systems. Calculation of Miller indices. Symmetry elements, crystal classes, point groups and space groups. Fundamentals of crystal chemistry and the different types of lattices. Rules of coordination and packing. Lattice defects and element substitutions in the lattice. Physical properties of crystals and their explanation through stuctural differences.
The understanding of constitution of unit cells and symmetry elements will be supported by the in-class study of three dimensional crystal models.

Literature

Compulsory:

W. D. Nesse: Introduction to Mineralogy. Oxford University Press. Oxford-New York, 2012 (2nd edition)

Recommended:

Course objective/intended learning outcomes

a) Knowledge

-knows the definition of space lattice, unit cell and crystal cross, the unit cells and crystal systems according to Bravais,

- knows and able to identify the simple and combined symmetry elements and crystal forms,

-knows the possible combination of the symmetry elements, the point groups and crystal classes,

-knows the basics of crystal chemistry and the different types of lattices,

-knows the most important mechanical, electrical, optical properties of crystals and their connections to crystal structures.

b) Ability

-able to identify the different crystal systems, can give directions in crystallography, can calculate Miller indexes for lattice plains,

- able to identify the symmetry elements in macroscopic crystals, in crystal lattices and even in chemical molecules,

-able to apply the general rules of crystallography in structure research,

- able to interprete the connection between the crystal lattices and bond types in compounds,

-able to interprete the connection between the physical properties of crystals and their stuctures.

c) Attitude

-endeavour to completely understand the basic rules in crystallography,

-endeavour to understand the connection between inner structure of crystals and their macroscopic appearance,

- endeavour to understand and identify the symmetry elements,

-endeavour to understand the structure of crystall lattices and their effects on structure and physical/chemical properties of substances,

- endeavour to deeper understand the material structures with the use of gained knowlege in crystallography.

d) Autonomy and responsibility

- accept the scale of values of his/her profession with responsibility,
- cooperates with the experts of other fields of science during his/her work,
- understand the importance of crystallography, especially the symmetry in material structure research,

-able to individually process the scientific literature under the appropriate supervision.

Schedule:

1st week

Subject of crystallography. Properties of crystalline substances, definition of space lattice. Principles of morphology and crystallography.

2nd week

Bravais-type unit cells and crystal systems. Crystal cross in crystallography. Definition of directions, lattice planes and crystal faces. The Miller index.

3rd week

The visible symmetry elements of crystals, simple and combined symmetry elements. The stereographic projection. The translational symmetry.

4th week

Practicing of identification of symmetry elements

5th week

Point groups and the 32 crystal classes. Holohedral, hemihedral and tetrahedral crystal classes.

6th week

Mid-term test. Definition of crystal form. Crytal forms and symmetry elements in triclinic, monoclinic and orthorhombic systems.

7th week

Crystal forms and symmetry elements in trigonal, tetragonal and hexagonal crystal systems

8th week

Crystal forms and symmetry elements in cubic crystal system

9th week

Basics of crystal chemistry. X-ray diffraction and Bragg equation. Types of crystal lattices (atomic, inoic, metallic, molecular lattice).Coordination number, atomic, ionic radii.

10th week

Types of atomic lattices. Metallic lattice and the close packing. Molecular lattices. Properies of ionic lattice substances.

11th week

Isodesmic, anisodesmic and mesodesmic ionic lattices. Stucture of silicates. Ortho, ring, chain, sheet and framework silicates.

12th week

Isomorphism and polymorphism. Real lattice structures, lattice defects. Rules of element substitutions. Crystal growth.

13th week
Crystal physics. Cohesion properties. Cleavage and sliding. Mohs-type hardness scale. Thermoelectric and piezoelectric properties. Structural interpretation of physical properties.

14th week
Crystal optics. Isotropic and anisotropic crystals. Birefrigency and optical activity. Summary

Requirements:
- *for a signature*
Participation at **lecture classes** is not compulsory but highly advised.
During the semester there will be be two tests, the mid-term test in week 6, and theend-term test in week 15. Students have to sit for the tests.
- for a grade
The course ends with a **writing examination** in the exam period, covering the whole material of the semester. The final grade for the course will be determined according to the followings: it is based on the average grade of the mid-term test and end-term test in 10 %, and based on the result of written exam in 90 %.
The minimum requirement for the average grade of end-term test and mid-term test and final exam is 50%, respectively. The examination is given according to the following table:

Score	Grade
0-49	fail (1)
50-59	pass (2)
60-72	satisfactory (3)
73-87	good (4)
88-100	excellent (5)

If the score of the test is below 49, students can take a retake test in conformity with the EDUCATION AND EXAMINATION RULES AND REGULATIONS.

-an offered grade:
it may be offered for students if the average grade of mid-term test and end-term test is at least satisfactory (3).

Person responsible for course: Dr. Gábor Dobosi, professor, DSc

Lecturer: Dr. Dávid Nagy, assistant lecturer, PhD

Title of course: **Biochemistry II** **Code**: TTKML0304_EN	**ECTS Credit points:** 3

Type of teaching, contact hours
- lecture: -
- practice: 1 hours/week
- laboratory: 2 hours/week

Theoretical seminar (2 h), solving independent tasks (use of database, use of simulation program), practical laboratory work (5 h), evaluation and interpretation of results.

Evaluation:
Assessment methods:
An assessment carried out with written examinations at the end of semester.
Written examinations are used during the semester from the theoretical and practical part.
The ratings are not checked by a second examiner.
The examination papers are marked with name.
There is not an examination board.

Workload (estimated), divided into contact hours:
- lecture: -
- practice: 14 hours
- laboratory: 28 hours
- home assignment: 40 hours
- preparation for the exam: -

Total: 82 hours

Year, semester: 3nd year, 2nd semester

Its prerequisite(s): A minimum of 3 credits biochemistry, during earlier studies (BSc).

Further courses built on it: -

Topics of course

Enzymes and mechanisms of enzyme action. Stability of enzymes, the influence of the reaction conditions on enzymatic activity. The Michaelis-Menten model for the kinetic properties of enzymes. Definition, significance and determination of K_M and v_{max}. Specific inhibition of enzymes and determination of the type of inhibition. Regulation of enzymes with allosteric interaction or covalent modification.
Preparation, activity measurement and kinetic investigation of some oxidoreductases and hydrolases.

Literature

Compulsory:
- Kandra Lili: Biokémiai gyakorlatok

Recommended:
- J. M. Berg, J. L. Tymoczko, L. Stryer: Biochemistry V. edition (W. H. Freeman and Co. 2002. ISBN 0-7167-4684-0)
- A. Cornish-Bowden: Fundamentals of enzyme kinetics, 3. reprint (Portland Press, 2002, ISBN 1 85578 072 0)

Course objective/intended learning outcomes

Objective of the course

To provide practical skills in biochemistry especially in enzymology and in characterization of biomolecules.

a) Knowledge

- He/she has the basic biochemical knowledge that will enable to describe basic life processes.
- He/she knows and is able to use the materials, tools and methods used in biochemical laboratories and has the relevant safety engineering knowledge.
- He/she possesses the knowledge whose application is necessary to solve the chemical problems of the living systems.
- He/she understands the essential biochemical, enzyme terminology in the mother tongue.

b) Abilities

- He/she is able to apply the most important terminology, theories, procedures of the given biochemistry field when completing the relevant tasks.
- He/she is able to create fundamental models of engineering systems and processes.

c) Attitude

- He/she seeks out to know the processes in the living organism and to describe their laws.
- He/she is environmentally conscious during his/her laboratory work.
- He/she is open to professional co-operation with professionals working in biochemistry.
- He/she is committed to acquiring new competencies.

d) Autonomy and responsibility

- During his laboratory work, he is able to consider basic professional issues independently, and can produce relevant compilations that can serve as a basis for decisions.
- He/she correctly evaluates the results of his / her own work and compares them with the results of his/her colleagues.
- Assesses the own work and the work of his / her colleagues responsibly during their laboratory activities.

Schedule: practices - 2 hours/week, laboratory - 5 hours/week, two independent tasks

1st week

Labor safety education. Semester schedule. Theory: The concept, structure and grouping of enzymes. Parameters influencing the speed of enzyme reactions. Occurrence, function, structure and activity of lipase enzyme.

2nd week

Laboratory practice: Extraction of lipase enzyme and determination of its activity.

3rd week

Enzyme activity measurement, reaction rate measurement for enzyme reactions. Enzyme structure and function relationship. Coenzymes, prosthetic groups. Enzyme regulation. The occurrence, function and structure of the catalase enzyme. Hem is a prosthetic group. Generation of hydrogen peroxide in living organisms, $FADH_2$ coenzyme, superoxide dismutase. Enzyme databases, molecular modelling.

4th week

Laboratory practice: Extraction of catalase enzyme from plant tissue, measurement of activity.

5th week

The mechanism of enzyme activity. Structural analysis of proteins. How can we develop an enzyme activity measurement method? The function and significance of the amylase enzyme, its mechanism of action and its activity. Definition and calculation of the subsite map.
6th week
Laboratory practice: Study of starch and oligosaccharide hydrolysis catalysed by amylase enzyme
7th week
Overview of the virtual laboratory program. Enzyme assays to **investigate the effects of pH, time, amount of enzyme, incubation temperature and substrate concentration on the activity of different enzymes. Students can also investigate the effects of adding different inhibitors, as well. The students carry out the tasks independently at home.**
8th week
Kinetics of enzymatic reactions, inhibition types. Methods for determining kinetic constants. Computer evaluation of enzyme kinetic measurements. The Grafit enzyme kinetic program. Function of emulsion beta-glucosidase, method of measuring activity.
9th week
Laboratory practice: Determination of kinetic parameters of almond emulsin beta-glucosidase. Enzyme and substrate concentration dependence of reaction rate. Determination of enzyme kinetic parameters K_M and v_{max} and inhibition assay.
10th week
Presentation and discussion of results obtained from a search for a given enzyme in the protein and enzyme databases.
11th week
End term test

Requirements:
- *for a signature*

Participation at **practice and laboratory classes** is compulsory. A student must attend the practice classes and may not miss more than one times during the semester. In case a student does so, the subject will not be signed and the student must repeat the course. A student can't make up any practice with another group. Attendance at practice classes will be recorded by the practice leader. Being late is equivalent with an absence. In case of further absences, a medical certificate needs to be presented. Missed practice classes should be made up for at a later date, to be discussed with the tutor.
During the semester there are tests in every week as a part of practice, which are mandatory.
Students have to submit all the two tasks (database search and virtual laboratory) as a minimum on a sufficient level.
- *for a grade*

The course is evaluated based on the tests, designing tasks and the lab notebooks. The grade is calculated as an average.
The minimum requirement is 60%. The grade for the practice is given according to the following table:

Score	Grade
0-59	fail (1)
60-69	pass (2)
70-79	satisfactory (3)
80-89	good (4)

90-100	excellent (5)

If the score of any test is below 60, students can take a retake test in conformity with the EDUCATION AND EXAMINATION RULES AND REGULATIONS.

Person responsible for course: Dr. Gyöngyi Gyémánt, associate professor, PhD, habil

Lecturer: Dr. Gyöngyi Gyémánt, associate professor, PhD, habil

Title of course: Biochemistry III **Code**: TTKME0304_EN	**ECTS Credit points:** 3
Type of teaching, contact hours - lecture: 2 hours/week - practice: - - laboratory: -	
Evaluation: exam	
Workload (estimated), divided into contact hours: - lecture: 28 hours - practice: - - laboratory: - - home assignment : - preparation for the exam: 60 hours Total: 60 hours	
Year, semester: 2nd year, 2nd semester	
Its prerequisite(s): Biochemistry I	
Further courses built on it: -	

Topics of course

The lectures cover the main features of the protein structures including fibrous proteins and the membrane proteins with their role in transport. There is an insight into the photosynthesis: the light reactions and the carbon-assimilation reactions. The nucleotide metabolism is summarized. The biosynthesis of macromolecules such as DNA, RNA and protein will also be described. Post-translational modification: N-glycosylation is also mentioned.

Literature

Compulsory: The lecture notes
Recommended:
Nelson D.L., Cox M.M.: Lehninger Principles of Biochemistry (W. H. Freeman Sixth edition, 2012) ISBN-13: 978-14234146.
Berg J.M., Tymoczky J.L., Gatto G.J. and Styer L.: Biochemistry (W. H. Freeman; Eighth edition, 2015), ISBN-13: 978-1464126109.

Albert B., Bray D. Essential Cell Biology (Fouth edition, Garland Science, 2014) ISBN: 978-0-8153-4454-4.

Course objective/intended learning outcomes

a) Knowledge

- He/she knows the structural and functional features of the proteins including fibrous and membrane proteins.
- She/he knows the principles that govern the photosynthetic processes.
-She/he is also aware of the characteristics of the nucleic acid and protein biosynthesis.

b) Abilities

- He/she is able to understand the function of the different structural form of the proteins.
- He/she is able to understand the fundamentals of the biosynthetis pathways of the macromolecules.
-He/she is able to understand of the complex events at the different stages of the photosynthesis.

c) Attitude

-He/she is open to the contextual observations of the studied area and is motivated to follow the latest scientific theories in that field.

d) Autonomy and responsibility

- He/she is capable of considering complex questions on the studied scientific field on her/his own as well as in a team.
- He/she shows responsibilities in her/his profession.

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Schedule:

1st week

The different structural level or proteins. Protein folding and chaperons. Protein misfolding. Structural classification of proteins.

2nd week

Fibrous proteins: α-keratin, fibroin and the structure of collagen fibrils. Structural feature of membrane protein.

3rd week

The role of membrane proteins in transport processes of the cell. Facilitated diffusion by transport proteins. Primary and secondary active transport. The ion selective channels.

4th week

The role, the location and the components of photosynthesis. The light driven electron flow in Photosystem I and II. The function and structure of Cythocrome b_6f complex.

5th week

The synthesis of ATP and NADPH in the light reactions of photosynthesis. The cyclic photophosphorylation. The water splitting complex. Comparing the light reactions of the photosynthesis with the oxidative phosphorylation taking place at the mitochondria.

6th week

Photosynthetic assimilation of carbon dioxide. The function, structure and regulation of Rubisco. The three stages of the Calvin cycle. Photorespiratory reactions and the C_4 pathway.

7th week

Nucleotide Metabolism. The biological function of nucleotides. The pyrimidin *de novo* biosynthesis. The interconversion of nucleoside mono- di- and triphosphates.

8th week

The purin *de novo* biosynthesis. The role of tetrahydrofolate in the nucleotide biosynthesis. The Salvage pathway. The function of ribonucleotide reductase in the generation of deoxyribonucleotides. Degradation of purin and pyrimidine nucleotides.

9th week

The biosynthesis of deoxyribonucleic acid. The helical structure of DNA. The Meselson-Stahl experiment. The stages of replication in prokaryotes. The replication forks. DNA synthesis on the leading and lagging strands.

10th week

The function of the protein factors and enzymes involved in the the processes of replication including primase, DNA polymerases I and III, DNA ligase. Termination of chromosome replication in bacterial cell.

11th week

The biosynthesis of ribonucleic acids in prokaryotes. The function and characteristics of the DNA - dependent RNA polymerase. Transcription initiation, elongation and termination.

12th week

The biosynthesis of ribonucleic acids in eukaryotes. The function of the different RNA polymerases. Assembly of the Initiation Complex. RNA processing: 5' capping and 3' Poly(A) Tail. RNA splicing.

13th week

The biosynthesis of proteins. The genetic code. The structure and the function of tRNA. The components of the ribosome. The stages of the protein biosynthesis. Proofreading on the ribosome. Antibiotics inhibit translation.

14th week

Signal sequences and protein targeting. Protein translocation into the ER. Post-translational modification: N-glycosylation and its function.

Requirements:

- *for a signature*

Attendance at **lectures** is recommended, but not compulsory.

- *for a grade*

The course ends in an **examination**.

The grade for the examination is given according to the following table:

Score	Grade
0-59	fail (1)
60-69	pass (2)
70-79	satisfactory (3)
80-89	good (4)
90-100	excellent (5)

If the score of examination is below 60, students can take a retake test in conformity with the EDUCATION AND EXAMINATION RULES AND REGULATIONS.

Person responsible for course: Dr. Teréz Barna, PhD

Lecturer: Dr. Teréz Barna, PhD

Title of course: Measurement Methods in Materials Science (lecture) Code: TTFME0411_BT_EN	ECTS Credit points: 3
Type of teaching, contact hours lecture: 2 hours/week	
Evaluation: exam	
Workload (estimated), divided into contact hours: lecture: 28 hours preparation for the exam: 56 hours Total: 84 hours	
Year, semester: 1^{st}year, 1^{st} semester	
Its prerequisite(s): minimum 3 credits of physics	
Further courses built on it: -	

Topics of course

The series of lectures are based on the topics of modern measurement methods in the materials science. It reviews the fundametals, technical details, practical aspects of the different methods. Topics: mechanical testing: tensile test, hardness tests, Charpy-test. Microscopic methods: optical microscopy, transmission electron microscopy, scanning electron microscopy, field-electron and field-ion microscopy, scanning tunneling microscopy, atomic force microscopy. Magneteic methods: measurement of magnetization curves, magnetometers, Barkhausen-noise measurements. Ionometry: secunder ion mass spectrometry, secondary neutral mass spectrometry, Rutherford backscattering. X-ray spectrometry: electron probe micro analysis, X-ray fluorescence spectrometry, proton induced X-ray emission. Electron spectroscopy: electron energy loss spectroscopy, photoelectron spectroscopy, Auger-electron spectroscopy. Diffraction methods: X-ray diffraction, electron diffraction, neutron diffraction.

Literature

Compulsory:

H. Czichos, T. Saito, L. Smith: Springer Handbook of Materials Measurement Methods, Springer Science+Business Media Inc. 2006

D.J. O'Connor, B.A. Sexton, R. St. C. Smart: Surface Analysis Methods in Materials Science, Springer-Varlag berlin Heidelberg GmbH 1992

Recommended:

C.Giocavazzo: Fundamentals of Crystallography, Oxford University Press 1992

D.B. Williams and C.B.Carter: Transmission Electron Microscopy, Plenum Press 1996

J.A Stroscio, W. J. Kaiser:Methods of Experimental Physics Vol.27 Scanning Tunneling Microscopy, Academic Press (1997)

Course objective/intended learning outcomes

a) Knowledge

- He/she fundamentally knows principles of the most important measurement methods in materials science.

b) Abilities

- He/she is able to choose the most effective measurement method for a particular problem.

He/she is able to interpretate the measurement results.

c) Attitude

- He/she is open to learn and accept professional, technological improvement and innovation in his/her profession and convey it genuinely.
- He/she makes a decision in complex and unexpected decision cases by completely taking into account legal and ethical norms.

d) Autonomy and responsibility

- Even in unexpected decision-making situations he/she is capable of considering complex, fundamental questions from his/her professional field and elaborating them on the basis of the given sources.

. He/she is open to critical remarks which are professionally well-founded.

Schedule:

1st week

Mechanical tests: tensile test, hardness tests, Charpy-test

2nd week

Microscopy I: fundamentals of optical and transmission electron microscopy

3rd week

Microscopy II: Scanning electron microscopy, scanning tunneling microscopy, atomic force microscopy

4th week

Microscopy III.: field-electron and field-ion microscopy, atom-probe

5th week

Magnetic measurements: measurement of magnetization curves, magnetometers, Barkhausen-noise measurements

6th week

Secondary ion and secondary neutral mass spectrometry, Rutherford backscattering

7th week

X-ray spectrometry I.: origin of X-rays, X-ray spectra, emission and absorption

8th week

X-ray spectrometry II: electron-beam microanalysis, wavelength and energy dispersive detectors, qualitative and quantitative analysis.

9th week

X-ray spectrometry III: X-ray fluorescent analysis, proton induced X-ray emission

10th week

Electron spectrometry I.: fundamentals of electron spectroscopy, detectors, applications *11th week* Electron spectrometry II.: electron energy loss spectrometry, photoelectron spectrometry, Auger-electron spectrometry *12th week* Diffraction I.: fundamentals of diffraction, crystal systems, reciprocal lattice, Miller indices, Bragg-equation, Ewald construction *13th week* Diffraction II.: X-ray, electron and neutron diffraction, diffractometers, comparison of methods, applications *14th week* *Summar, discussion*
Requirements: *- for a signature* Attendance at **lectures** is recommended, but not compulsory. *- for a grade* - The course ends in an **exam**. The minimum requirement for the exam is 50%. The grade will be calculated according to the following table: Score Grade 0-50 fail (1) 51-62 pass (2) 63-75 satisfactory (3) 76-87 good (4) 87-100 excellent (5)
Person responsible for course: Lajos Daróczi, associate professor, PhD
Lecturer: Lajos Daróczi, associate professor, PhD

Title of course: Measurement Methods in Materials Science (practice) **Code**: TTFML0411_BT_EN	**ECTS Credit points:** 1
Type of teaching, contact hours laboratory: 2 hours/week	
Evaluation: practice	
Workload (estimated), divided into contact hours: practice: 28 hours home assignment :28 hours Total: 56 hours	

Year, semester: 1^{st} year, 1^{st} semester
Its prerequisite(s): minimum 3 credits of physics
Further courses built on it: -

Topics of course
The series of practices are based on the topics of modern measurement methods in the materials science. It reviews the fundametals, technical details, practical aspects of the different methods. Selection of topics:: Mechanical tests: tensile test, hardness tests,. Microscopic methods: optical microscopy, transmission electron microscopy, scanning electron microscopy, atomic force microscopy. Magneteic methods: measurement of magnetization curves, magnetometers, Barkhausen-noise measurements. Ionometry:, secondary neutral mass spectrometry, Rutherford backscattering. X-ray spectrometry: electron probe micro analysis, proton induced X-ray emission. Electron spectroscopy:, photoelectron spectroscopy, Auger-electron spectroscopy. Diffraction methods: X-ray diffraction, electron diffraction.
Literature
Compulsory: H. Czichos, T. Saito, L. Smith: Springer Handbook of Materials Measurement Methods, Springer Science+Business Media Inc. 2006 D.J. O'Connor, B.A. Sexton, R. St. C. Smart: Surface Analysis Methods in Materials Science, Springer-Varlag berlin Heidelberg GmbH 1992 *Recommended:* C.Giocavazzo: Fundamentals of Crystallography, Oxford University Press 1992 D.B. Williams and C.B.Carter: Transmission Electron Microscopy, Plenum Press 1996 J.A Stroscio, W. J. Kaiser:Methods of Experimental Physics Vol.27 Scanning Tunneling Microscopy, Academic Press (1997)
Course objective/intended learning outcomes
a) Knowledge - He/she fundamentally knows principles of the most important physical measurement methods in materials science. He/she fundamentally knows the most important equipments, the basic rules of operation and data interpretation. **b) Abilities** - He/she is able to apply the most important terminology, theories, procedures of the given field when completing the relevant tasks. - He/she is able to select the most effective measurement method for a given scientific problem. **c) Attitude** - He/she is open to learn and accept professional, technological improvement and innovation in his/her profession and convey it genuinely. - He/she makes a decision in complex and unexpected decision cases by completely taking into account legal and ethical norms. **d) Autonomy and responsibility**

- Even in unexpected decision-making situations he/she is capable of considering complex, fundamental questions from his/her professional field and elaborating them on the basis of the given sources.

. He/she is open to critical remarks which are professionally well-founded.

Schedule:

1st week

Tensile test

2nd week

Hardness test

3rd week

Optical microscopy

4th week

Transmission electron microscopy

5th week

Scanning electron microscopy

6th week

Atomic force microscopy

7th week

Electron probe micro analysis

8th week

X-ray diffraction

9th week

Electron diffraction

10th week

Measurement of magnetization curves

11th week

Barkhausen-noise measurement

12th week

Secondary neutral mass spectrometry

13th week

Rutherfor backsattering, proton induced X-ray emission

14th week

Electron spektroscopy

Requirements:

- for a signature

Participation at **practice classes** is compulsory. A student must attend the practice classes and may not miss more than three times during the semester. In case a student does so, the subject will not be signed and the student must repeat the course. Attendance at practice classes will be recorded by the practice leader. Being late is equivalent with an absence. In case of further absences, a medical certificate needs to be presented. Certificated missed practice classes should be made up for at a later date, to be discussed with the tutor.

In case of assigned practices submission of a written report is obligatory.

During the semester there are two compulsory home works.
Students have to submit both home works within the deadline. The scores have to be better than 50% in both cases.
- *for a grade*
The course ends in a practice mark.
.Based on the scores of the home works and the reports the grade will be calculated according to the following table:

Score	Grade
0-50	fail (1)
51-62	pass (2)
63-75	satisfactory (3)
76-87	good (4)
88-100	excellent (5)

Person responsible for course: Lajos Daróczi, associate professor, PhD

Lecturer: Lajos Daróczi, associate professor, PhD

Title of course: Atomic and molecular physics
Code: TTFME0101_EN

ECTS Credit points: 4

Type of teaching, contact hours
- lecture: 2 hours/week
- practice: 1 hours/week
- laboratory: -

Evaluation: exam

Workload (estimated), divided into contact hours:
- lecture: 28 hours
- practice: 14 hours
- laboratory: -
- home assignment: 20 hours
- preparation for the exam: 28 hours

Total: 90 hours

Year, semester: 1st year, 1st semester

Its prerequisite(s): introductory physics courses (at least 12 credits)

Further courses built on it: -

Topics of course

Electronic structure of one-electron atoms and ions. Energy levels, eigenstates, quantum numbers. Rydberg atoms. Interaction of one-electron atoms with electromagnetic field. Permanent and transition dipole moments of atoms. The dipole approximation. Einstein-coefficients. Selection rules. Intensity and broadening of spectral lines, life times of excited states. Fine- and hyperfine structure of one-electron atoms, Stark-effect, Lamb-shift. Electronic structure of two-electron atoms and ions. Double excitations, autoionization. Electronic structure of many-electron atoms. Central field approximation, LS- and jj-coupling schemes. Interaction of many-electron atoms with electromagnetic field. Selection rules, spectra of alkali metals. Helium atom and alkaline earth metals. Structure of molecules: separation of the electronic and nuclear motions. Rotation and vibration of diatomic molecules. Electronic structure of diatomic molecules. The aspect of polyatomic molecules. Electronic structure of the H2+ molecular ion, atomic and molecular orbitals, formation of the bond. Spectra of diatomic molecules: rotational energy levels, ro-vibrational spectral lines, transitions between electronic states. Atomic scattering processes, potential scattering, cross section, partial waves, the Born-approximation. Electron-atom scattering, elastic scattering, excitation of atoms, ionization, resonances.

Literature

Compulsory:

B.H. Bransden, C.J. Joachain: Physics of atoms and molecules, Longman Scientific & Technical (1995)

D.J. Griffiths: Introduction to Quantum Mechanics, Prentice-Hall, New Jersey (1994)

Recommended:

I.N. Levine: Quantum Chemistry, Prentice Hall, New Jersey (2008)

Course objective/intended learning outcomes

a) Knowledge

- He/she fundamentally knows the interaction of atoms and simple molecules with external electromagnetic fields and understands the resulting spectra. Furthermore he/she knows the basics of scattering processes.

b) Abilities

- He/she is able to apply quantum mechanics in the description of atomic and molecular processes, as well as in the interpretation of simple computations.

c) Attitude

- He/she can accept the fundamental laws of quantum mechanics that constitute the basics of atomic and molecular processes.

d) Autonomy and responsibility

- He/she is open to critical remarks which are professionally well-founded.
- He/she continuously improves his/her abilities.

Schedule:

1st week

Electronic structure of one-electron atoms and ions. Energy levels, eigenstates, quantum numbers. Rydberg atoms.

2nd week
Interaction of one-electron atoms with electromagnetic field I.
Permanent and transition dipole moments of atoms. The dipole approximation. Einstein-coefficients.
3rd week
Interaction of one-electron atoms with electromagnetic field II.
Selection rules. Intensity and broadening of spectral lines, life times of excited states.
4th week
Fine- and hyperfine structure of one-electron atoms. Stark-effect, Lamb-shift.
5th week
Electronic structure of two-electron atoms and ions. Double excitations, autoionization.
6th week
Electronic structure of many-electron atoms. Central field approximation, LS- and jj-coupling schemes.
7th week
Interaction of many-electron atoms with electromagnetic field. Selection rules, spectra of alkali metals. Helium atom and alkaline earth metals.
8th week
Structure of molecules: separation of the electronic and nuclear motions. Rotation and vibration of diatomic molecules. Electronic structure of diatomic molecules. The aspect of polyatomic molecules.
9th week
Electronic structure of the H2+ molecular ion, atomic and molecular orbitals, formation of the bond.
10th week
Spectra of diatomic molecules: rotational energy levels, ro-vibrational spectral lines, transitions between electronic states.
11th week
Atomic scattering processes, potential scattering, cross section, partial waves, the Born-approximation.
12th week
Electron-atom scattering, elastic scattering, excitation of atoms, ionization, resonances.
13th week
Practical test.
14th week
Summary and consultation.

Requirements:
- *for a signature*
Attendance at **lectures** is recommended, but not compulsory.
Participation at **practice classes** is compulsory. A student must attend the practice classes and may not miss more than three times during the semester. In case a student does so, the subject will not be signed and the student must repeat the course.
During the semester there are practical home works which have to be evaluated and submitted by the end of the 14th week of the semester. The requirement for a signature is a successful (> 50%) completion of the home works.
- *for a grade*
The course ends in an **examination**. The requirement for applying for an exam is to have a practical signature.

The grade for the examination is given according to the following table:

Score	Grade
0-49	fail (1)
50-62	pass (2)
63-75	satisfactory (3)
76-88	good (4)
89-100	excellent (5)

Person responsible for course: Dr. András Csehi, senior lecturer, PhD

Lecturer: Dr. András Csehi, senior lecturer, PhD

Title of course: Computational Quantum Chemistry **Code**: TTKMG0902_EN	**ECTS Credit points:** 3

Type of teaching, contact hours
- lecture: -
- practice: 2 hours/week
- laboratory: -

Evaluation: exam

Workload (estimated), divided into contact hours:
- lecture: -
- practice: 28 hours
- laboratory: -
- home assignment: 32 hours
- preparation for the exam: 30 hours

Total: 90 hours

Year, semester: 1st /2nd year, 2nd semester

Its prerequisite(s):
minimum 12 credits of mathematics

Further courses built on it: -

Topics of course

- Hartree-Fock Theory
- Density Functional Theory
- Basis sets
- Solvent effect, Polarizable Continuum Model
- Geometry optimization
- Structural analysis
- Calculating energies of chemical reactions

Literature

Compulsory:
https://maker.pro/linux/tutorial/basic-linux-commands-for-beginners
http://gaussian.com/keywords/

Recommended:
http://barrett-group.mcgill.ca/tutorials/Gaussian%20tutorial.pdf

Course objective/intended learning outcomes

a) Knowledge

He/She knows the basic qualitative and quantitative chemical principles, and the methods based on it.
He/She knows the main models and theories of chemical bonds and molecular structure based on scientific findings.
He/She has a basic chemical knowledge on describing simple chemical processes as well as on recognizing, organizing these in practice.
He/She has the knowledge to test or measure chemical reactions, systems with scientific methods (including computational) under supervision.

b) Abilities

He/She is able to evaluate and discuss the calculations, and create a report about it.
He/She is able to collect and evaluate data on the field of chemistry in order to opining for problems on social, scientific or ethical questions.
He/She is able to argue on scientific problems by his/her knowledge.
He/She is able to communicate on the field of chemistry using foreign language(s).

c) Attitude

He/She is ready to discuss problems on the field of chemistry and other science with professionals.
He/She is able to represent his/her own personal scientific ideology toward professional and unprofessional groups.
He/She is committed learn or get insights into new competence or ideology.
He/She is well aware about his/her propositions and its consequences.

d) Autonomy and responsibility

He/She stands for his/her opinion or ideology in professional discussions.
He/She can make reasonable evaluations about his/her own work comparing to others to the same field.

Schedule:
1st week

Basic theory of the Hartree-Fock method: approximations, LCAO-MO theory. Building structures by the GaussView program.

2nd week

Basic Linux commands, using the WinSCP and Putty programs, connecting by SFTP. Using the Gaussian program package, optimizing simple molecules.

3rd week

Geometry optimizations by different basis sets, comparing and calibrating the methods by structural parameters.

4th week

Frequency analysis, calculating Gibbs free energies of simple reactions. Scanning a reaction pathway, finding the transition state, identifying the stationary points of the Potential Energy Surface.

5th week

Basic theory of the post-Hatree-Fock theories. Recalculating the previously studied systems and comparing them to the HF results.

6th week

Solvent effect, using Polarizable Continuum Models to refine the energies.

7th week

Basic theory of the Density Functional Theory. Recalculating the previously studied systems and comparing them to the (post-)HF results.

8th week

Systems with explicit solvent molecules.

9th week

Calculation on more difficult systems: metal complexes and relativistic effects.

10th week

Mid-term exam about calculations by using Gaussian.

11th week

Conformation analysis, more Linux commands.

12th week

Writing simple scripts in b shell.

13th week

Generating input files by scripts.

14th week

Exam of writing scripts in b shell.

Requirements:

- *for a signature*

Attendance is recommended, maximum 3 absences are accepted.

- *for a grade*

Class performance (33%)

Final examination (67%)

Based on the sum of the final practical exam of performing calculations and the class performance the practical grade is calculated.

The final grade is given according to the following table:

Score (%)	Grade

0-49	fail (1)
50-59	pass (2)
60-74	satisfactory (3)
75-89	good (4)
90-100	excellent (5)

If the score of the final grade is below 50%, students can take a retake test in conformity with the EDUCATION AND EXAMINATION RULES AND REGULATIONS.

Person responsible for course: Dr. Mihály Purgel, assistant professor, PhD

Lecturer: Dr. Mihály Purgel, assistant professor, PhD
Dr. Attila Mándi, assistant professor, PhD

Title of course: Inorganic Chemistry V.
Code: TTKME0203_EN

ECTS Credit points: 4

Type of teaching, contact hours
- lecture: 3 hours/week

Evaluation: examination

Workload (estimated), divided into contact hours:
- lecture: 42 hours
- practice: -
- laboratory: -
- home assignment: -
- preparation for the exam: 84 hours

Total: 168 hours: 4 credit x 42 hours

Year, semester: 1st year, 1st semester

Its prerequisite(s):

Further courses built on it:

Topics of course

Literature

Compulsory:
1) Syllabus provided by the tutor

Recommended:
2) R. H. Crabtree, THE ORGANOMETALLIC CHEMISTRY OF THE TRANSITION METALS (4th Edition), Wiley, 2005, ISBN 0-471-66256-9 (or later edition)

Course objective/intended learning outcomes

a) Knowledge

- He/she knows the definition of organometallic compounds, nature of the metal-carbon bond, the factors influencing the thermal, oxidative and hydrolytic stability of the compounds, their most important chemical reactions, methods to synthesize them and their important use.
- He/she knows the special properties, importance, most important preparation routes and practical use of mesoporous materials, nanoparticles, special ceramics and their composites.

b) Abilities

- He/she is able to apply the most important terminology, theories, and procedures of the given organometallic and modern inorganic chemistry-related field when completing the relevant tasks.
- He/she is able to create fundamental models of organometallic chemical reactions, and processes.

c) Attitude

- He/she is open to learn and accept professional, technological improvement and innovation in his/her profession and convey it genuinely.
- He/she makes a decision in complex and unexpected cases by completely taking into account legal and ethical norms.

d) Autonomy and responsibility

- Even in unexpected decision-making situations he/she is capable of considering complex, fundamental questions from his/her professional field and elaborating them on the basis of the given sources.
- He/she confesses and represents the value system of the qualified chemists and chemical engineers profession with responsibility. He/she is open to critical remarks which are professionally well-founded.

Schedule:

1st week

Brief history of organometallic chemistry. Definition, classification and general characterization of the organometallic compounds.

2nd week

General characterization of the p- and s-group organometallics, structure, physical and chemical properties, use. Methods for the preparation of them.

3rd week

Ionic (polar) organometallic compounds.

4th week

Organometallics containing multicenter bonding(s): organolithium, -magnesium, -boron and -almininum compounds, their importance in the organic synthesis.

5th week

Organic compounds of the silicon, silicone polymers.

6th week

General characterization of the organotransition metal compounds: structure, physical and chemical properties, preparation. Definition of hapticity.

7th week

Transition metal alkyles and aryles: (cross)coupling reactions with Pd-alkyl catalysts (Heck, Negishi, Suzuki reactions). Transition metal carbonyls and their synthetic use (carbonylation reactions: Monsanto process, hydroformylation of alkenes).

8th week
Transition metal alkene and alkyne complexes and some selected applications (Wacker process, Ziegler-Natta polymerization process)
9th week
Important η^3-η^8 organotransition compounds and their practical use. Metallocenes.
10th week
Porous materials, general preparation routes. preparation of mesopores. Special features and practical use of non-silica mesoporous materials, special adsorbents. Procedures and materials based on sol-gel technologies. Aerogels, aerogel composits, hybrides. Silica-based aerogel nanocomposites and their use from catalysis to medical therapy.
11th week
General characterization of nanoparticles and nanowires, their special features. Preparation techniques for nanoparticles, special experimental techniques. Molecular magnets, one dimensional metals.
12th week
Metal-organic frameworks (MOF), properties, preparation and use of self organising metarials. Chemical materials with semiconducting properties. Features of quantum dots, their preparation, experimental techniques for their study and their practical applications.
13th week
Materials for transparent ceramics: ways of preparation, properties, practical use. Solid phase chemical reactions, solid electrolytes, fuel cells. Ceramic metal and metal ceramic composites, metal glasses.
14th week
Colour changing materials, interpretation of the electrochromic, thermochromic, chemochromic and solvatochromic properties. Composition, preparation and use of colour changing materials. Special modifications of carbon. Properties, preparation and use of single and multi-wall carbon nanotubes, graphenes, fullerenes, fullerites and carbon nanowires.

Requirements:
- *for a signature*
Attendance at **lectures** is recommended, but not compulsory.
- *for a grade*
The course ends in an **examination**.
The minimum requirement for the examination is 40 score. Based on the score, the grade for the examination is given according to the following table:

Score	Grade
0-39	fail (1)
40-55	pass (2)
56-70	satisfactory (3)
71-85	good (4)
86-100	excellent (5)

If the score of any test is below 40, students can retake the test in conformity with the EDUCATION AND EXAMINATION RULES AND REGULATIONS.

Person responsible for course: Dr. Péter Buglyó, associate professor, PhD

Lecturers: Dr. Péter Buglyó, associate professor, PhD

Dr. István Lázár, associate professor, PhD

Title of course: Inorganic Chemistry VI. **Code**: TTKML0203_EN	**ECTS Credit points:** 4
Type of teaching, contact hours - lecture: - - practice: - - laboratory: 6 hours/week	
Evaluation: practice grade	
Workload (estimated), divided into contact hours: - lecture: - - practice: - laboratory: 78 hours - home assignment: 102 hours - preparation for the exam: - Total: 180 hours	
Year, semester: 1st year, 1st semester	
Its prerequisite(s):	
Further courses built on it:	

Topics of course
Synthesis and characterization of non-metal and metal compounds and complexes using high/low temperature or pressure, vac-line technique. Qualitative and quantitative analysis of the compounds with classical and instrumental techniques.
Literature
1. Syllabus provided by the tutor. 2. Inorganic Experiments (ed. J. D. Woolins), 2nd Edition, Wiley-VCH, 2003
Course objective/intended learning outcomes
a) Knowledge - He/she fundamentally knows basic principles of preparative inorganic chemistry and characterization of inorganic compounds using various analytical techniques. **b) Abilities** - He/she is able to apply the most important preparative techniques, theories, procedures of the given synthetic work when completing the relevant tasks. - He/she is able to find solutions for the inorganic synthetic/preparative and characterization problems. **c) Attitude**

- He/she is open to learn and accept professional and state-of-the-art synthetic techniques and analytical characterization techniques and innovation in his/her profession and convey it genuinely.
- He/she is capable of making decisions in complex and unexpected cases by completely taking into account legal and ethical norms.

d) Autonomy and responsibility

- Under supervision he/she is responsible in collaboration with other professionals (especially from the field of safety and treatment of hazardous compounds).
- He/she confesses and represents the value system of the inorganic synthetic profession with responsibility. He/she is open to critical remarks which are professionally well-founded.

Schedule: 2 h introduction + 9 x 6 h practice

1st week: Introductory guidance, safety regulations and protection (2h)

2nd week: Preparation of $[Ni(NH_3)_x]Br_2$ and determination of its stoichiometry via classical volumetric analysis.

3rd week: Synthesis and characterization of an copper-oxalate complex, $K_aCu_b(C_2O_4)_c{\cdot}dH_2O$

4th week: Green chemical preparation of copper(I)-iodide and its study

5th week: Synthesis and characterization of metal acetylacetonates

6th week: Synthesis and characterization of transition metal phosphane complexes

7th week: Full sandwich type organometallic compounds of π-donor arene ligands

8th week: Preparation and study of $[MoO_2Br_2(H_2O)_2]{\cdot}$diglyme and $[MoO_2Br_2(DMF)_2]$

9th week: Ni(II) complexes of Schiff-base ligands: template sysnthesis and NMR study

10th week: A model compound for B_{12} vitamin with direct Co-C bond: synthesis and characterization

Requirements:

- *for a signature*

Participation at practices is compulsory. Students must attend every practice during the semester. In case of absence(s), a medical certificate needs to be presented. Missed practice classes should be made up for at a later date, to be discussed with the tutor.

- *for a grade*

Grading is given by considering the following three separate grades:

- the average grade of the short tests written at the beginning of the practices (an average of at least 2.0 is necessary to avoid a ‘fail’ final grade) (30 %)

- the average grade of evaluation of the quality and quantity of the prepared compounds and the laboratory notebook prepared by the student (an average of at least 2.0 is necessary to avoid a 'fail' final grade) (30 %) - the grade of the oral discussion on the topics of the practice and the results of the student with the tutor in the second half of the semester (in case of 'fail' mark the oral discussion can once be repeated and an average grade will be taken into consideration) (40 %)
Person responsible for course: Dr. Péter Buglyó, associate professor, PhD
Tutor: Dr. Péter Buglyó, associate professor, PhD

Title of course: Inorganic Chemistry VII. **Code**: TTKME0204_EN	**ECTS Credit points:** 3
Type of teaching, contact hours - lecture: 2 hours/week - practice: - - laboratory: -	
Evaluation: exam	
Workload (estimated), divided into contact hours: - lecture: 28 hours - practice: - - laboratory: - - home assignment: 32 hours - preparation for the exam: 30 hours Total: 90 hours:	
Year, semester: 1st year, 2nd semester	
Its prerequisite(s): -	
Further courses built on it: TTKME0203_EN, TTKML0203_EN	

Topics of course
To understand the molecular basis of biological role of trace elements and the harmful effects of toxic inorganic compounds; to get to know the possibilities of using these knowledges in medicine, environmental protection and other areas of life.
Literature
Compulsory: 1. Robert Chrichton: Biological Inorganic Chemistry, An introduction, Elsevier, 2008, ISBN: 978-0444-52740-0 2. Rosette Roat-Malone: Bionorgainc chemistry, Wiley-Interscience, 2002, ISBN: 0-471-15976-X. 3. J.A. Cowan, Inorganic Biochemistry, An introduction, Wiley-VCH, 1997, ISBN: 0-471-18895-6

Recommended:
1. Elichiro Ochiai: Bioinorganic chemistry, Elsevier, 2008, ISBN: 978-0-12-088756-9
2. S.J. Lippard, J.M. Berg, Principles of Bioinorganic Chemistry, University Science Books, Mill Valley, CA 1994.
3. E.I. Ochiai, General Principles of Biochemistry of the Elements, Plenum Press, New York, London (1987).
4. W. Kaim, B. Schwederski, Bioinorganic Chemistry, Inorganic Elements in the Chemistry of Life, John Wiley and Sons, Chichester, 1994.

Course objective/intended learning outcomes

a) Knowledge
He/she has the knowledge required for interpreting the processes occurring in biological systems, and for solving fundamental chemistry-related practical problems and questions related to living and non-living systems.
b) Abilities
He/she is able to understand anthropogenic chemical processes that occur in biological systems or are connected to natural processes taking place within these systems. He/she knows how to utilise the scientific literature related to the subject. He/she is able to support his or her standpoint using scientific arguments when debating, both in spoken and in written form.
c) Attitude
He/she accepts the identity that is the basis of the distinctive characteristics and personal/public roles of natural sciences.
He/she uses and treats his or her scientific results, as well as those achieved by others, in accordance with the ethical standards of his or her profession.
He/she is determined to acquire further knowledge and competence, broaden his or her horizons and further polish his or her scientific skills.
He/she does not abuse his or her knowledge, obeys the ethical standards of the society and those of his or her profession.

d) Autonomy and responsibility
He/she acts independently when dealing with general or specific scientific questions, as well as when representing scientific standpoints.
He/she creates his or her standpoint independently, is willing to stand up for his or her views.
He/she is aware of the gravity of his or her statements and takes responsibility of their consequences.

Schedule:
1st week Classification of the elements according to their role in biological systems. Essential, beneficial and toxic elements and their role in biochemical processes. The factors that determined the natural selection of essential elements
2nd week The basis of coordination chemistry; chelate effect. The hard-soft theory. The crystal field theory. The crystal field theory.
3rd week Coordination chemistry of the most common bioligands including amino acids, peptides,

proteins, carbohydrates, nucleotides and porphyrins. Characterization of metalloproteins and metalloenzymes.
4th week Membrane transport process: diffusion, passive and active transport. Cation distribution and membrane transport processes. Involvement of alkaline metal ions biological processes:

5th week The role of magnesium in human body and in the photosynthesis. The main roles of calcium in biological systems (with examples)

6th week Binding, transport and activation of oxygen. The role of iron in the transport and storage of oxygen.

7th week The role of iron in catalysis of redox processes: cytochromes and iron-sulphur proteins. The structure and properties of cytochromes.

8th week The structure and properties of iron-sulphur proteins. The transport and storage of iron.

9th week The structure and properties of copper proteins. The participation copper in biological oxidation reactions. Disorder of copper metabolism. Wilson and Menkes diseases.

10th week Biochemistry of zinc: zinc containing enzymes and zinc finger proteins. The role of zinc in catalysis of acid-base processes (with examples) and in determination of protein structures (Cu,Zn-superoxide dismutase, zinc-finger proteins)

11th week Involvement of other essential elements in biological processes: the enzymes/coenzymes of manganese, cobalt, nickel, molybdenum, vanadium and selenium.

12th week Toxic elements: biochemistry and harmful effects of aluminium, thallium, lead and tin.

13th week 18. The role of metal ions in the brain. The use of inorganic compounds in therapy and diagnosis.

14th week Environmental aspects of inorganic substances.

Requirements:
- *for a signature*

Attendance at **lectures** is recommended, but not compulsory.
- *for a grade*

Preparation a project including a bioinorganic chemistry theme (10 %)
Oral examination: discussion two topics (90 %)
The minimum requirement is 50 %:

Score	Grade
0-50	fail (1)
51-60	pass (2)
61-75	satisfactory (3)

76-89	good (4)
90-100	excellent (5)

In the case of the exam is not successful, the exam is repeatable (two times).

Person responsible for course: Dr. Katalin Várnagy, full professor, PhD

Lecturer: Dr. Katalin Várnagy, full professor, PhD

Title of course: Physical Chemistry VI.
Code: TTKME0401_EN

ECTS Credit points: 4

Type of teaching, contact hours
- lecture: 3 hours/week
- practice: -
- laboratory: -

Evaluation: exam

Workload (estimated), divided into contact hours:
- lecture: 42 hours
- practice: -
- laboratory: -
- home assignment: 40 hours
- preparation for the exam: 40 hours

Total: 122 hours

Year, semester: 1st year, 1st semester

Its prerequisite(s): -

Further courses built on it: -

Topics of course

The series of lectures are based on selected topics of advanced physical chemistry.
Main topics include:
- Thermodynamics in axiomatic approach
- Concepts and applications of irreversible thermodynamics
- Concepts and applications of statistical thermodynamics
- Radiochemistry
- Photochemistry
- Structure of matter and supramolecular chemistry.

Literature

Compulsory:
- P.W. Atkins, J. de Paula (2006): Atkins' Physical Chemistry 8th Edition, W.H. Freeman and Company, New York, ISBN: 0-7167-8759-8.

- J Kónya, N. M. Nagy (2018): Nuclear and Radiochemistry, Elsevier, ISBN: 9780128136430
- P. Érdi, G. Lente (2014): Stochastic Chemical Kinetics, Springer, ISBN: 978-1493903863
- Lecture notes and teaching material available via the e-learning system

Recommended:

-K. K. Rohatgi-Mukherjee: Fundamentals of Photochemistry (revised edition) - e-book; publisher: New Age International, 1978; 371 pages; ISBN: 0852267843, URL: http://www.ebook3000.com/Fundamentals-OfPhotochemistry_126059.html

Course objective/intended learning outcomes

a) Knowledge

- He/She understands the progress and future trends in chemistry and chemical industries.
- He/She has global knowledge on science other than chemistry, and capable to organize this information
- He/She has detailed, updated information on the actual field.

b) Abilities

- He/She is able to communicate, discuss and aim problems to other chemists or engineers of professionals other than chemistry field.
- He/She is able to use his/her knowledge to solve advanced level chemistry problems including proving the solutions.

c) Attitude

- He/She is open to collaborate with professionals on the field of social sciences, economy and environmental safety, treating the new chemical trends critically but carefully.

d) Autonomy and responsibility

- He/She is responsible for his/her own decisions stand in for these decisions and ideologies.

Schedule:

1st week Classical and rational thermodynamics. Axiomatic approach

Concepts: Logical discrepancies in the classical thermodynamics and the different ways of explanation and solution methods. 0th, 1st 2nd and 3rd law of thermodynamics, advanced perspective.

2nd week Irreversible thermodynamics, introduction

Concepts: Basic terminology of irreversible thermodynamics. Entropy production, thermodynamic forces and flows. Onsager relations. Seebeck-, Peltier- and Hall-effect

3rd week Irreversible thermodynamics. Applications.

The fenomenological equations and thermodynamic forces. Chemical affinity. De Donder inequality and direction of chemical processes in irreversible systems. Knudsen gases. Electro-osmosis. Electrokinetic phenomena. Non-equilibrium chemical systems, continuous model.

4th week Statistical thermodynamics, introduction and applications

Concepts: Molecular state, configuration. Internal energy and entropy in discrete systems. Partition functions. Calculation of translational, rotational and vibrational energy contributions. Calculation of heat capacity, zero point entropy and equilibrium constant, main formulas of partition functions. Thermodynamic information content of partition function.

5th week Chemical kinetics

Concepts: Rate equations, simplification methods, collision theory and transition state theory. Types of reactors. Processes in reactors. Continuous stirred tank reactor (CSTR), flow reactors, stochastic models of chemical kinetics

6th week Isotope effects. Interaction of nuclear radiation and matter. Energy transport between alpha particles and electrons.

Concepts: Types of isotope effects and their characterization in physics, chemistry, environmental science, and use in isotope separation. Mechanism of energy transfer between charged particles.

Practical consequences. Physical background of the formulas.

7th week Nuclear reactions

Concepts: Nuclear reactions with neutrons and charged particles.

Thermonuclear reactions. Preparation of radioactive isotopes

8th week Environmental questions of nuclear energy production

Concepts: Nuclear waste, separation, and activity levels. Disposal of nuclear waste and spent fuel elements.

9th week Photochemistry. Interaction of electromagnetic radiation and molecules

Concepts: Franck-Condon principle. Electron transitions, oscillator strength and cross section.

10th week Photophysical processes

Concepts: Fluorescence, phosphorescence and other photophysical processes. Inter- and intramolecular energy transport. Kinetics of photophysical processes.

11th week Photochemistry

Concepts: Photodimerization, photoisomerization, photodissociation and photoaddition, photon induced redox processes. Examples.

12th week Experimental methods of photochemistry.

Concepts: Light sources, their characterization and types. Spectrophotometer, spectrofluorometer, flash photolysis, actinometry. Mathematical description of photochemical reactions.

13th week Critical comparison of structure determination methods.

Concepts: Modern structure determination methods, advantages and disadvantages. Spectroscopic and diffraction methods. Modern methods of surface studies.

14th week Secondary interactions – supramolecular chemistry, biological consequences.

Concepts: Types of secondary interactions and their role in stabilizing solid state structures. Structure and function of biological macromolecules. Basic terminology of supramolecular chemistry.

Requirements:

- *for a signature*

Attendance at **lectures** is recommended, but not compulsory.

During the semester there is a written end-term test in the 15th week. Students have to sit for the test.

- *for a grade*

The course ends in a **written or oral examination**. Based on the result of the examination questions scored according to pre-set maximum points for each sub-questions. The type of the examination (written or oral) is the choice of the student. Questions of the exam with scoring system are provided for the students.

The minimum requirement for the examination is 60%. Based on the score of the tests separately, the grade for the tests and the examination is given according to the following table:

Score	Grade

0-59	fail (1)
60-69	pass (2)
70-79	satisfactory (3)
80-89	good (4)
90-100	excellent (5)

If the score of any test is below 60, students can take a retake test in conformity with the EDUCATION AND EXAMINATION RULES AND REGULATIONS.

-an offered grade:

It may be offered for students on the basis of the result of the end-term test if the grade is at least satisfactory (3).

Person responsible for course: Dr. Attila Bényei, associate professor, PhD

Lecturer: Dr. Noémi Nagy, professor, DSc
Dr. Attila Bényei, associate professor, PhD
Dr. Mihály Purgel, assistant professor, PhD

Title of course: Physical Chemistry VII.
Code: TTKML0405_EN

ECTS Credit points: 3

Type of teaching, contact hours
- lecture: -
- practice: -
- laboratory: 3 hours/week

Evaluation: practice

Workload (estimated), divided into contact hours:
- lecture: -
- practice: -
- laboratory: 42 hours
- home assignment: 48 hours
- preparation for the exam: -

Total: 90 hours

Year, semester: 1st year, 1st semester

Its prerequisite(s): -

Further courses built on it: -

Topics of course

This course is intended to stimulate students for independent work. This means that the students are supposed to have well established basic knowledge of laboratory work and capability to design, perform and elucidate physico-chemical experiments and their results as well as to prepare appropriate laboratory notebook. The tasks detailed here contain mainly thermodynamic, equilibrium and kinetic studies.

Set of measurements:
301. Examining the formation of complex ion by spectrophotometry
302. Kinetic examination of the acetone–iodine reaction
303. Determination of the equilibrium constant in the triiodine ion formation reaction by spectrophotometry
304. Study of mutual solubility of three liquids
305. Determining ion transport number with the Hittorf's and moving boundary method
306. Determination of mean activity coefficient based on solubility measurements
307. Promotor and inhibitor effect in the catalytic decomposition of H_2O_2
308. Effect of temperature and ionic strength on the reaction between iodide and persulfate ions
309. Study of ultraviolet and visible spectra of metal complexes
310. Kinetic analysis of an autocatalytic reaction by spectrophotometric method
311. Study of vapour–liquid equilibrium in two component system
312. Investigation of iodide–persulfate reaction by measuring the change of absorption
313. Effect of ionic strength on the rate of reduction of hexacyanoferrate(III) by ascorbic acid

Literature

- Laboratory notes and additional teaching material available via the e-learning system.
- P.W. Atkins, J. de Paula: Atkins' Physical Chemistry 8th Edition, W.H. Freeman and Company, New York, ISBN: 0-7167-8759-8, 2006
- Á. Kathó, V. Kiss, A. Udvardy, A. Bényei, Physical Chemistry laboratory measurements for MSc students, Egyetemi Kiadó
- K. Ősz, A. Bényei: Physical Chemistry Laboratory Measurements (for students of Pharmacy, Chemistry and Chemical Engineering). Debreceni Egyetemi Kiadó, ISBN: 978-963-318-143-0, 2011

Course objective/intended learning outcomes

a) Knowledge
- He/She has global knowledge on science other than chemistry, and capable to organize this information.
- He/She knows various methods from chemical labs or industries, able to show it to other people and apply them including the equipments and their safe usage.

b) Abilities
- He/She is able to recognize and evaluate the global relationships on the field of chemistry.
- He/She is able to carefully apply the newest chemical theories in practice and design lab experiments or industrial processes based on these results.
- He/She is able to evaluate graphically the experimental data, analyze them and make consequences. Based on these results he/she can present new trends in research or development without supervision.
- He/She is able to use his/her knowledge to solve advanced level chemistry problems including proving the solutions.

c) Attitude
- He/She is committed to protect the environment in both chemical labs and industries. This attitude is shown to other co-workers as well.
- He/She makes effort to apply those technologies that makes lower environmental changes/loads.

d) Autonomy and responsibility
- He/She is responsible in collaboration with other professionals (especially from the field of environmental economy and safety) without supervision.

Schedule: One of the measurements listed above (**Topics of course**) per week except the 1st practice (introduction, general information and safety training).

Requirements:
Participation on the laboratory practice is compulsory. The measurements and knowledge of the associated theory are marked and an overall mark will be given. Safety training (1st week) is mandatory before the first lab practice (2nd week). Everybody should work individually according to the pre-set schedule (which will be provided on the 1st week). Lab practices are 6 hours long every week (from the 2nd until the 7th week). Being late or failed mark on the written test from the appropriate measurement is equivalent with an absence. In accordance with the regulations of University of Debrecen, attendance is compulsory with the exception of health or family problems (the reason of absence should be certified). In this case, the students should agree with the teacher on replacement dates for the missed experiments.

Requirements for the grade:
The measurements (regularly) and written tests (occasionally) according to the knowledge of the associated theory are marked and the overall mark will be given based on these.
- All of the notebooks of the measurements have to be marked as “pass (2)” or better for the successful completion.
- The minimum requirement for the written tests is 60%. Based on the score of the tests separately, the grade for the tests is given according to the following table:

Score	Grade
0-59	fail (1)
60-69	pass (2)
70-79	satisfactory (3)
80-89	good (4)
90-100	excellent (5)

If the average of written tests is below 60% the best grade for the course can be only “pass (2)” in any other cases the final mark is given with weighted average by means of the mark of the written tests and notebooks in 1 to 2 ratio.

Person responsible for course: Dr. Ferenc K. Kálmán, assistant professor, PhD

Lecturer: Dr. Ferenc K. Kálmán, assistant professor, PhD

Title of course: Physical Chemistry VIII.
Code: TTKML0406_EN

ECTS Credit points: 3

Type of teaching, contact hours
- lecture: -

- practice: - - laboratory: 3 hours/week
Evaluation: practice
Workload (estimated), divided into contact hours: - lecture: - hours - practice: - hours - laboratory: 42 hours (7 weeks, 6 hours/week) - home assignment: 50 hours - preparation for the exam: - Total: 92 hours
Year, semester: 1st year, 2nd semester
Its prerequisite(s): -
Further courses built on it: -

Topics of course
The goal of this laboratory practice for the students is to make complex physical chemical measurements based on their theoretical and practical knowledge, beginning from the planning of the measurements, through the effective implementation, until the evaluation of the data and comparison with the literature. They have to be capable to perform these tasks by themselves, helped by a description containing short guidances about the theoretic background of the problem as well as practical advices. On the whole they have to acquire the necessary theoretical and practical proficiency for individual research work. *Set of lab measurements:* - Study of homogeneous isotope exchange in the ethyl iodide-I^- ion system. - Determination of the average size and size distribution of suspended particles with sedimentation. Effect of the electrolyte on the sedimentation. - Determination of the electric surface charge of solid particles by potentiometric titration. The effect of pH and electrolytes on the interfacial electric double layer. Determination of the point of zero charge. - Preparation of a lyosol and study of its coagulation. Effect of electrolytes and polymers on the coagulation (steric and electrostatic inhibition). Validation of the Hardy-Schulze rule. - Preparation of emulsions. Effect of the amount of surfactant on the nature and stability of the emulsion. Rheological properties of emulsions. - Study of radioactive radiation with solid state trace detector. - Investigation of the absorption of a herbicide by radioactive tracer experiment. Familiarization with the measurement technique of low energy β radiation.
Literature
Compulsory:

- Laboratory manual downloadable from the Department's homepage (http://fizkem.unideb.hu)

Recommended:
- J. Kónya and N. M. Nagy: Nuclear and radiochemistry, Elsevier, 1st edition, ISBN: 978-0-12-391430-9, 2012
- W. Bostock,: J. *Scient. Instr.* 29: 209, 1952
- D.J. Shaw: Introduction to Colloid and Surface Chemistry. Butterworth-Heinemann, ISBN 978-0-08-050910-5, 1992
- P. W. Atkins, J. de Paula: Physical Chemistry, W. H. Freeman, ISBN 0-7167-8567-6 & ISBN 0-7167-8569-2, 2006
- Pashley, R. M.: Applied Colloid & Surface Chemistry. Wiley&Sons, ISBN 0-a470-a86883-aX, 2004

Course objective/intended learning outcomes

a) Knowledge
- He/She has global knowledge on science other than chemistry, and capable to organize this information.
- He/She knows various methods from chemical labs or industries, able to show it to other people and apply them including the equipments and their safe usage.

b) Abilities
- He/She is able to recognize and evaluate the global relationships on the field of chemistry.
- He/She is able to carefully apply the newest chemical theories in practice and design lab experiments or industrial processes based on these results.
- He/She is able to evaluate experimental data, analyze them and draw conclusions. Based on these results he/she can present new trend sin research or development without supervision.
- He/She is able to use his/her knowledge to solve advanced level chemistry problems including to prove the solutions.

c) Attitude
- He/She is committed to protect the environment in both chemical labs and industries. This attitude is shown to other coworkers as well. He/she make effort to apply those technologies that makes lower environmental changes/loads.

d) Autonomy and responsibility
- He/She is responsible in collaboration with other professionals (especially from the field of environmental economy and safety) without supervision.
- He/She can operate chemical or industrial instruments or equipments with responsibility, and manage persons working with these.

Schedule:
One of the topics as listed above per week (see under **Topics of course**) except the 1st practice when an introduction, general information and safety training will be given.

Requirements:
The measurements and the knowledge of the associated theory are marked and an overall mark will be given. Safety training (1st week) is mandatory before the first lab practice (2nd week).

Everybody should work in small groups according to the pre-set schedule (which will be provided on the 1st week). Lab practices are 6 hours long every week (from the 2nd until the 7th weeks). Being late is equivalent to an absence. In accordance with the EDUCATION AND EXAMINATION RULES AND REGULATIONS of the University of Debrecen, the attendance is compulsory with the exception of health or family problems (the reason of the absence should be certified). In this case, the students should agree with the teacher on replacement dates for the missed experiments.

- *for a signature*
Attendance at **all laboratory courses** is compulsory (for exceptions see above).
- *for a grade*
The measurements (with appropriate lab notes) and written tests from the associated theory are marked and the overall mark will be given based on the weighted average these marks (a weight of 2 is assigned to the measurement's marks and a weight of 1 to the written test's marks).
- At least 5 notebooks of the measurements (from a total of 6) have to be marked as “pass (2)” or better for the successful completion.
- The minimum requirement for the overall mark is 50%. The grade for the laboratory practice is given according to the following table:

Score	Grade
0-49	fail (1)
50-59	pass (2)
60-74	satisfactory (3)
75-89	good (4)
90-100	excellent (5)

Person responsible for course: Dr. Levente Novák, assistant professor, PhD

Lecturer: Dr. Levente Novák, assistant professor, PhD

Title of course: Synthetic Methods in Organic Chemistry I.
Code: TTKME0301_EN

ECTS Credit points: 3

Type of teaching, contact hours
- lecture: 2 hours/week
- practice:
- laboratory: -

Evaluation: exam

Workload (estimated), divided into contact hours:
- lecture: 28 hours
- practice:
- laboratory: -
- home assignment: 14 hours
- preparation for the exam: 40 hours

Total: 82

Year, semester: 1st 1st semester
Its prerequisite(s): -
Further courses built on it: -

Topics of course

- General characterization of organic syntheses.
- Methods for introducing key functional groups and their interconversion.
- Most important protecting groups and their application.
- Retrosynthetic analysis and its application.

Literature

Compulsory:

1. Lecture slides

Recommended:

2. F. A. Carey, R. J. Sundberg: Advanced Organic Chemistry, Part B, Plenum: New York-London, 1977.
3. M. B. Smith, J. March: Advanced Organic Chemistry, 5th Ed., Wiley: New York, 2001
4. R. C. Larock: Comprehensive Organic Transformations, Wiley: New York, 1999.
5. J. F. W. McOmie: Protective Groups in Organic Chemistry, Plenum: London-New York, 1973.
6. T. W. Greene, P. G. M. Wuts: Protective Groups in Organic Synthesis, Wiley: New York, 1999.
7. P. J. Kocienski: Protecting Groups, Thieme: Stuttgart-New York, 2004.
8. Stuart Warren, Paul Wyatt: Organic Synthesis: The Disconnection Approach, 2nd Edition, 2009.

Course objective/intended learning outcomes

a) Knowledge

- He/she has general knowledge of organic compounds, including the characteristic properties, preparations and transformability of the various functional groups.
- He/she is able to apply his/her knowledge to solve simple tasks on the field of these derivatives. - He/she knows the practical application of different protective groups.
- He/she is able to plan different synthesis routes for producing an organic compound of a particular structure.

b) Abilities

- He/She is able to distinguish between the scientifically proven theories and non-reliable data or information.
- He/She is able to transfer the theoretical knowledge into practical one in research to obtain new results.

c) Attitude

- He/she is open to getting new, scientifically proven knowledge on the subject, but to reject unsubstantiated or possibly misleading claims.
- He/She is responsible and stands in for the professional ethics.

d) Autonomy and responsibility

- He/She is responsible for his/her own decisions, stand in for these decisions and ideologies.
- He/She is well aware about his/her propositions and its consequences.

Schedule:

1st week

Methods for the formation of C=C double bonds.

2nd week

Methods for the formation of C=C double bonds.

3rd week

Methods for the formation of C-Hlg derivatives, metallo-organic compounds and their application for C-C coupling, C-H activation.

4th week

Methods for the formation of C-OH and C-SH bonds.

5th week

Methods for the formation of C-NH_2, C-NHR, C-NRR_1 bonds.

6th week

Methods for the formation of C=O bond.

7th week

Methods for the formation of COOH/COX groups.

8th week

General aspects of the use of protective groups.

9th week

Cleavage classes (Kocienski's classification). Protection of alcoholic / phenolic hydroxyl groups.

10th week

Protection of 1,2- and 1,3-diols.

11th week

Protection of carboxylic acids (carboxyl group).

12th week

Protection of amines (amino group) and carbonyl group.

13th week

Retrosynthesis: basic concepts, retrosynthetic analysis of aromatic compounds.

14th week

C-X disconnections.

Requirements:

- for a signature

Attendance at **lectures** is recommended, but not compulsory. A student may not miss the lecture more than three times during the semester. In case of further absences, a medical certificate needs to be presented. In case a student does not do this, the subject will not be signed and the student must repeat the course.

- for a grade

The course ends in an oral exam in the exam period. The exam grade is the result of the written exam. The minimum requirement for the examination respectively is 50%. The grade for the written exam is given according to the following table:

Score	Grade
0-49	fail (1)
50-62	pass (2)
63-75	satisfactory (3)
76-87	good (4)
88-100	excellent (5)

If the score of any test below 50, students can take a retake test in conformity with the EDUCATION AND EXAMINATION RULES AND REGULATIONS.

Person responsible for course: Krisztina Dr. Kónya, senior lecturer, PhD

Lecturer: Krisztina Dr. Kónya, senior lecturer, PhD.

Title of course: Synthetic Methods in Organic Chemistry II.
Code: TTKML0302_EN

ECTS Credit points: 3

Type of teaching, contact hours
- lecture: -
- practice: -
- laboratory: 4 hours/week

Evaluation: term mark

Workload (estimated), divided into contact hours:
- lecture: -
- practice: -
- laboratory: 56 hours
- home assignment: 34
- preparation for the exam: -

Total: 90 hours

Year, semester: 1st year, 2nd semester

Its prerequisite(s): -

Further courses built on it: -

Topics of course

The aim of the course is to enable students to learn the general synthetic methods of organic chemistry and their practical implementation, to practice the use of literature and the structural analysis of organic small molecules.
The 4-hour laboratory practice is compacted in 7 × 8 hours. Students will get an individual list of tasks including six organic compounds to be synthetized, a literature search and a spectrum analysis task. The execution of the tasks and the order of their implementation are planned by the students.
Preparative work includes:

- synthesis of heterocycles
- preparation of compounds with single and double carbon-carbon bonds
- preparation of organic molecules having C-O and C-N bonds.

Literature

Compulsory:

- J. R. Mohrig, D. G. Alberg, G. E. Hofmeister, P. F. Schatz, C. Noring Hammond: **Laboratory Techniques in Organic Chemistry (**Supporting Inquiry-Driven Experiments)**, 4th edition,** W. H. Freeman and Company. ISBN-13: 978-1-4641-3422-7.

Recommended:

- E.K. Meislich, H. Meislich, J. Sharefkin: 3000 Solved problems in Organic Chemistry, McGraww-Hill INC, 1994.
- R:O:C: Norman, J.M. Coxon: Principles of Organic Synthesis, Blackie Academic & Professional, Glasgow, U.K., 1993.

Course objective/intended learning outcomes

a) Knowledge

- He/She knows the laboratory equipment and techniques of organic chemistry, their theoretical background and their practical scope.
- He has sufficient practical knowledge to synthetize organic compounds and solve problems.
- Based on his/her organic chemistry knowledge, he can interpret the results of experiments.

b) Abilities

- He/She is individually able to design experiments and carry out organic reactions.
- He/She is able to make assessment of his/her own results and draw logical conclusions from them.
- He/She is able to recognize and evaluate chemical relationships on the field of organic chemistry.
- Based on known spectra he/she is able to make suggestion on structures of small molecules.

c) Attitude

- He/She is receptive to the knowledge and practical application of organic synthetic methods.
- He/She is open to expand his organic chemistry knowledge and acquire new laboratory techniques.
- During his/her laboratory practice he/she strives for environmentally conscious work and follows the safety rules.

d) Autonomy and responsibility

- He/She independently organizes his preparative work and takes responsibility for his decisions.
- He/She professionally prepares his experiments and laboratory equipment.
- He/She works carefully, taking into account any potential hazards.

Schedule:

1st week

Introduction:

Timetable and requirements. Receiving of laboratory equipment and list of tasks. Safety education.

Preparative work:

Preparation and purification of a selected organic compound from the individual list. Determination of physical properties (melting point or boiling point) and purity (TLC, R_f). Calculation of yield.

2nd week

Short written test:

Topics: formation of carbon-carbon single and multiple bonds (*Grignard reactions and their applications; β-dicarbonyl compounds as C-nucleophiles; ethinylation reactions; CN , as nucleophile; Wittig reaction; elimination reactions; reductive methods towards partial or complete saturation of multiple carbon-carbon bonds, Aldol condensation and related variants).*

Safety rules, basic concepts of spectroscopy, definitions.

3rd week

Short written test:

Topics: Formation of C-O, C-S, C-O-C, C-S-C bonds *(syntheses of alcohols, phenols, ethers and their thio analogs e.g. acid catalyzed hydration of double/triple bonds, oxymercuration, hydroxy mercuration, hydroboration, halohydrin formation, Kucserov reaction, epoxidation, preparation of vicinal diols: OsO_4; $KMnO_4$; ring-opening of epoxids; formation of acetals and hydrates; S_N reactions with O-nucleophiles; Williamson ether synthesis, preparations of thio analogs).*

Chromatographic purification techniques (*TLC, column chromatography*), recrystallization.

Spectral analysis of known organic compounds.

Preparative work: Preparation and purification of the selected organic compound(s) from the individual list. Determination of physical properties (melting point or boiling point) and purity (TLC, R_f). Calculation of yield(s).

4th week

Short written test:

Topics: formation of C-N, C=N and C≡N bonds *(synthetic routes towards aliphatic and aromatic amines wherein C-N bond is built up: Gabriel synthesis; S_N reactions with N-nucleophiles; Hofmann rearrangement; reductive amination; sytheses of imines, Schiff bases, oxymes, hydrazones; syntheses of nitro és nitroso compounds;; syntheses of azo- and diazo compounds and their transformations)*

Extraction methods. Drying liquids and solids.

Spectral analysis of known organic compounds.

Preparative work: Preparation and purification of the selected organic compound(s) from the individual list. Determination of physical properties (melting point or boiling point) and purity (TLC, R_f). Calculation of yield(s).

5th week

Short written test:

Topics: Oxidative and reductive methods in organic syntheses: their applications, advantages and limitations. *(applications of Jones reagent; PCC; $KMnO_4$; MnO_2; peroxy acids; H_2O_2; DMD (dimethyl dioxirane); O_3 in case of different substrates; Baeyer-Villiger oxidation; Oppenauer oxidation; H_2/Pd (and its variants); Birch reduction; applications of metal hydrides ($NaBH_4$; $LiAlH_4$; $NaCNBH_4$, DIBAL-H etc.); Fe/HCl; $(NH_4)_2S_x$; $SnCl_2$; Meerwein-Ponndorf-Verley reduction; Stephen reduction; reductive amination and their reaction conditions).*

Classification of solvents and their effects on the outcome of the organic reactions.

Spectral analysis of known organic compounds.
Preparative work: Preparation and purification of the selected organic compound(s) from the individual list. Determination of physical properties (melting point or boiling point) and purity (TLC, R_f). Calculation of yield(s).

6th week
Short written test:
Topics: Synthesis and transformation of carbonyl compounds *(syntheses of ketones, aldehydes, carboxylic acids and related derivatives; reactions of oxo derivatives with O, S- and N-nucleophiles reductive, oxidatives, condensation and hydrolytic transformations; interconversions of carboxylic acid derivatives).* Synthesis of heterocycles.
Spectral analysis of known organic compounds.
Deadline for submitting the spectrum analysis and literature task.
Preparative work: Preparation and purification of the selected organic compound(s) from the individual list. Determination of physical properties (melting point or boiling point) and purity (TLC, R_f). Calculation of yield(s).

7th week
Short written test:
Topics: Complex synthesis designing *(Design of multi-step synthesis of a selected compound using the knowledge acquired during the semester. Detailed description and interpretation of the synthesis and isolation steps of the compound.)*
Last occasion to present the synthesized products to the instructor.
Evaluation.

Requirements:

Attendance at laboratory practice is mandatory.

Before starting to prepare a selected compound, students must give an oral report on their theoretical organic chemistry and practical knowledge as well as on the safety rules.
The synthetic work can only be started after a successful discussion.
Minimum requirements for signing the course:
- Syntheses and characterizations of the selected six organic compounds.
- Sufficient level of the discussion (pass, (2)) for each preparation.
- Minimum level of the written test: at least 50 % of the overall score.
- Submission of the spectroscopic task within the given time.
- Presentation of the result of the literature search within the given time.

In case of failure of any subtask, the practice ends with a poor (1) grade.

The final grade will be determined based on the average of the grades of tasks. A weighted average of the grades of subtasks will be calculated in the following manner:
- Activity in laboratory practice, discussion (40 %)
- Short written test (40 %)

- Spectroscopic task (10 %)
- Literature search (10 %)

Final grade: excellent (5): 90 %; good (4): 75 %; satisfactory (3): 60 %; pass (2): 50 %; fail (1): below 50 %.

Person responsible for course: Dr. Éva Bokor, assistant professor, PhD

Lecturer: Dr. Éva Bokor, assistant professor, PhD

Title of course: Heterocycles **Code**: TTKME0327_EN	**ECTS Credit points:** 3

Type of teaching, contact hours
- lecture: 2 hours/week for day-time course, 8 hours/semester for reading course
- practice: -
- laboratory: -

Evaluation: exam

Workload (estimated), divided into contact hours:
- lecture: 28 hours
- practice: -
- laboratory: -
- home assignment: 10 hours
- preparation for the exam: 40 hours

Total: 78 hours

Year, semester: 1st year, 2nd semester

Its prerequisite(s): -

Further courses built on it: -

Topics of course

- Classification and nomenclature of heterocyclic compounds.
- Preparation and reactions of oxiranes, thiiranes and aziridines.
- Characterization, preparatio and reactions of four-membered heterocycles with one heteroatom.
Preparation of azetidine-2-one derivatives and introduction of β-lactam antibiotics.
- Description of five-membered heterocycles with one or more than one
- Characterization of benzene-condensed five-membered heterocycles.
- Characterization, preparation and reactivity of 2H-pyran derivatives.
- Characterization, preparation and reactivity of piridine derivatives.
- Characterization of six-membered heterocycles with more than one heteroatom.
- Six-membered derivatives with one or two heteroatoms.
- Representatives of flavonoids, their preparation and reactions.

Literature
Compulsory: Supporting material with lecture slides available at the homepage of the Department of Organic Chemistry Recommended: Theophil Eicher, Siegfried Hauptmann: The chemistry of heterocycles; structure, reactions, syntheses, and applications, 2nd edition, WILEY-VCH GmbH & Co. KGaA, 2003. John A. Joule, Keith Mills: Heterocyclic chemistry, 5th edition, A John Wiley & Sons, Ltd., 2010.

Course objective/intended learning outcomes
a) Knowledge The student knows the nomenclature, preparations, reactions and occurrence of the major heterocycles containing O, N and S heteroatoms and is able to explain the diffferent characteristics of heterocyclic compounds. He/She has systematic knowledge on the various subject of chemistry, their main principals including the theoretical and practical application built on these principals. He/She has knowledge to solve problems on the field of natural processes, using natural sources, and understanding the chemical background of living and non-living systems. b) Abilities He/She is able to retrieve literature data on the synthesis and reaction of heterocyclic compounds, to process those data and to use the literature data to interpret the results. He/She is able to explain the reactivity of heterocycles. Using the knowledge and experiences acquired during the MSc course, he/she is able to execute laboratory experiments or measurements to demonstrate proper chemical phenomena, or syntheses and characterization of new compounds, and using analytical methods for developing new reactions. c) Attitude He/She is receptive to establish and apply new chemical and environmental technologies. He/She is responsible and stands in for the professional ethics. d) Autonomy and responsibility He/She can make own decisions even in complex professional questions and discussions. He/She recognizes the unsafe conditions both in academic and industrial laboratories and environment and makes decisions according to this.

Schedule:

1st week

Definition and importance of heterocycles. Classification and nomenclature of heterocycles.

The student acquires the conventional and systematic nomenclatures of simple and condensed heterocycles and learn the different subgroups and classification of heterocycles.

2nd week

Preparation, occurrence and reactions of oxiranes. Enantioselective epoxidation.

The student gets acquainted with the three-membered, oxygen-containing heterocycles, their synthesis and reactivity.

3rd week
Characterization of thiiranes and aziridines, their preparation and reactions.
The student gets acquainted with the three-membered, sulfur- or nitrogen-containing heterocycles, their preparation and reactivity.
4th week
Description of four-membered heterocycles with one heteroatom, their preparation and reactions. Preparation of azetidine-2-one derivatives and introduction of β-lactam antibiotics.
The student is able to explain the reactivity of four-membered heterocycles with one heteroatom and knows their preparation. He or She recognizes the importance of azetidine-2-one subunit in β-lactam antibiotics.
5th week
Characterization, preparation and reactions of furan and thiophene derivatives.
The student is able to interpret the preparation and reactivity of furan and thiophene derivatives.
6th week
Synthesis and reactions of pyrrole derivatives.
The student knows the preparation and reactions of pyrrole derivatives and is able to compare them with those benzene and other five-membered heterocycles with one heteroatom.
7th week
Characterization of five-membered heterocycles with more than one heteroatom I.
The student can interpret the reactivity of 1,2- and 1,3-azoles compared to those of other π-excessive heterocycles.
8th week
Characterization of five-membered heterocycles with more than one heteroatom II.
The student learns the main representatives and occurrence of 1,2- and 1,3-azoles.
9th week
Characterization of benzene-condensed five-membered heterocycles.
The student is able to compare the reactivity of benzene-condensed five-membered heterocycles with those of other five-membered heterocycles and explain the differences.
10th week
Characterization, synthesis and reactions of 2*H*-pyrane derivatives.
The student knows the occurrence, synthesis and reactions of 2*H*-pyrane derivatives.
11th week
Representatives, synthesis and reactions of flavonoids.
The student learns the definition, basic skeletons, natural occurrence and reactions of flavonoids.
12th week
Characterization, synthesis and reactions of pyridine derivatives.
The student is able to interpret the reactivity of π-electron deficient heterocycles, knows their occurrence and main transformations.
13th week
Six-memberd heterocycles with more than one heteroatom.
The student can interpret the reactivity of six-membered heterocycles with more than one heteroatom and knows the possible pathways for their preparations.
14th week

Six-membered heterocycles with one or more than one heteroatom. The student knows the structures, preparation and reactivity of seven-membered heterocycles with one or more than one heteroatom.
Requirements: - *for a signature* Attendance at **lectures** is highly recommended, but not compulsory. - *for a grade* The course ends with a written **exam**. The list of short questions used for the written exam is available at the homepage of the Department of Organic Chemistry. The minimum requirement for achieving the course is 50%. Score Grade 0-49 fail (1) 50-59 pass (2) 60-74 satisfactory (3) 75-89 good (4) 90-100 excellent (5)
Person responsible for course: Dr. Tibor Kurtán, D.Sc.
Lecturer: Dr. Tibor Kurtán, D.Sc.

Title of course: Biochemistry IV **Code**: TTKME0303_EN	**ECTS Credit points:** 3
Type of teaching, contact hours - lecture: 2 hours/week - practice: - laboratory: -	
Evaluation: exam	
Workload (estimated), divided into contact hours: - lecture: 28 hours - practice: 0 hours - laboratory: - - home assignment: hours - preparation for the exam: 60 hours Total: 60 hours	
Year, semester: 2nd year, 2nd semester	
Its prerequisite(s):	
Further courses built on it: -	

Topics of course

Bioregulation at the molecular and at the cellular levels. The function of hemoglobin and its regulation. Different strategies in the regulation of enzyme activities: allostery, isoenzymes, reversible covalent modification, limited proteolysis and modulation by small regulatory proteins. Control by limiting the amount of enzyme: regulation of gene expression in prokaryotic and eukaryotic organisms at transcriptional levels. Hormonal regulation: sensing the environment in multicellular eukaryotic organisms. The interplay between metabolic and signaling pathways through heterotrimer G-protein coupled receptors and through insulin receptor. The phosphatidylinositol signaling.

Literature

Compulsory:

- The lecture notes.

Recommended:

Nelson D.L., Cox M.M.: Lehninger Principles of Biochemistry (W. H. Freeman, Sixth edition, 2012) ISBN-13: 978-14234146.

- Albert B., Bray D. Essential Cell Biology (Fourth edition, Garland Science, 2014) ISBN : 978-0-8153-4454-4.

-Gerhard Krauss: Biochemistry of Signal Transduction and Regulation (Wiley￾VCH Verlag GmbH & Co. KGaA, 2014) ISBN:9783527333660.

Course objective/intended learning outcomes

a) Knowledge

-She/he knows the different regulatory mechanisms at the molecular and at the cellular level.

-She/he is aware of the fundamentals of the signaling pathways.

b) Abilities

- She/he is able to understand the basis of the integrated metabolic regulation at the cellular and at the organismal level and the basic principles of gene expression.

He/she is able to understand the molecular mechanism of sensory processes.

b) Attitude

- **-**He/she is open to the contextual observations of the studied area.

-He/she exhibits interest in the latest research discoveries, reads regularly the advised scientific papers.

d) Autonomy and responsibility

- He/she is capable of considering complex, fundamental questions from his/her professional field on her/his own as well as in a team.
- He/she collaborates with other people in solving problematic tasks.

Schedule:

1st week

Bioregulation at the protein level. The storage and the transport of molecular oxygen by heme proteins: myoglobin and hemoglobin. Cooperative binding of molecular oxygen to hemoglobin can be explained by concerted and sequential model. The fetal hemoglobin. Hydrogen ions and carbon dioxide promote the release of oxygen: the Bohr effect. Sickle-cell anemia.

2nd week

Allostery. The characteristics of the allosteric regulation is explained in the case of Aspartate Transcarbamoylase (ATCase). The quaternary structure of ATCase in T and R states. The sigmoidal kinetics of ATCase and its regulatory molecules. Comparison of the Michaelis-Menten kinetics with sigmoidal kinetics.

3rd week

Regulation of glycolysis. The role of the glucose transporters. The irreversible reactions of glycolysis are the regulatory points. The allosteric regulation of phosphofructokinase and pyruvate kinase in liver and in other tissues. The role of phosphofructokinase II and its hormonal regulation. The reciprocally regulated glycolysis and gluconeogenesis.

4th week

Isoenzymes, one of the ways of fine-tuning of metabolism in different cell types or cell compartments. Isoenzymes of hexokinases and lactate dehydrogenases (function, kinetic behaviour, regulation, substrate specificity, location).

5th week

Activation by limited proteolysis – zymogen activation. Pancreatic zymogens: the proteolytic cascade. Structural changes in chymotrypsinogen on its proteolytic cleavage. Substrate specificities and mechanism of serine proteases. Protein protease inhibitors.

6th week

Reversible covalent modification._Post-translational modification by phosphorylation. The driving force of phosphorylation and dephosphorylation. Kinases and phosphatases. The function and regulation of protein kinase A. The phosphorylation of muscle and liver glycogen phosphorylases as well as phosphorylase kinase.

7th week

The overview of signal transduction pathways. Classification of receptors and signal molecules. The receptor-ligand interactions.

8th week

The G protein signal cascade. The structure of the seven transmembrane helix receptors and the heterotrimeric G proteins. The G protein cycle. Turning off the signals. Bacterial toxins target G proteins. Glucagon and ephinephrine.

9th week

The role of G-Protein coupled receptors in sensory perception. Signals which change the resting membrane potential of the nerve cells. Sensory transduction in vision. Light-induced hyperpolarization of rod cells. The termination of the visual signal. Signaling by olphactory receptor neurons.

10th week

Signal cascades based on the membrane lipid phosphatidylinositol. The domain structures of PLC and PKC and their function. Ca^{2+} as a secondary messengers and its sensor protein: Calmodulin.

11th week

Insulin signaling cascade. Processing and secretion of insulin. Insulin receptor and its tyrosine kinase activity. The role of SH2 domain. The activation of protein kinase B and the Glut4

translocation.
12th week
Regulation of blood glucose levels. The coordinated regulation of carbohydrate metabolism. Diabetes Mellitus and hyperglycemia.
13th week
Central dogma of Biology. The structure of DNA and RNA. Regulation of prokaryotic gene expression. Key players and steps of prokaryotic transcription. Promoter recognition. Operon model and its role in gene regulation. Lac operon is under the control of repressor and catabolite activator proteins.
14th week
Regulation of eukaryotic gene expression at different levels. Features of eukaryotic transcription. Cis-regulatory DNA sequence elements and transcription factors. Histone modifications - chromatin remodeling. DNA methylation.

Requirements:
- *for a signature*
Attendance at **lectures** is recommended, but not compulsory.
- *for a grade*
The course ends in an **examination**.
The grade for the examination is given according to the following table:

Score	Grade
0-59	fail (1)
60-69	pass (2)
70-79	satisfactory (3)
80-89	good (4)
90-100	excellent (5)

If the score of the exam is below 60, students can take a retake test in conformity with the EDUCATION AND EXAMINATION RULES AND REGULATIONS.

Person responsible for course: Dr. Teréz Barna , PhD

Lecturer: Dr. Teréz Barna, PhD

Title of course: Instrumental analysis **Code**: TTKME0501_EN	**ECTS Credit points: 2**

Type of teaching, contact hours
- lecture: 2 hours/week
- practice: -
- laboratory:

Evaluation: examination

Workload (estimated), divided into contact hours:

- lecture: 48 hours - practice: - - laboratory: - - home assignment: - - preparation for the exam: 42 Total: 90 hours
Year, semester: 2^{nd} year, 1st semester
Its prerequisite(s):
Further courses built on it:

Topics of course

The course surveys the history, methods, theories, fundamentals and some practical aspects of analysis of several instrumental analytical methods and techniques. Important additional topics are the sampling, electrophoresis, atomic spectrometry, sensors, immunoanalysis, labelling methods, thermal analysis, polarography. The course is connected to some topics of the Instrumental Analysis laboratory practices and complete the knowledge acquired in BSc level.

Literature

Daniel C. Harris: Quantitative Chemical Analysis, 7th Ed., 2007, Freeman and CoH.H.
Willard, L.L. Merritt, J.A. Dean, F.A. Settle: Instrumental methods of Analysis, Wadsworth Publ. Co., Belmont, 1988.
Douglas A. Skoog, Donald M. West, F. James Holler, Stanley R. Crouch: Fundamentals of Analytical Chemistry, 8th. ed., 2004, Brooks/Cole

Course objective/intended learning outcomes

a) Knowledge

- He/she fundamentally knows principles and means of instrumental analysis, sample pretreatment, data evaluation and validation of the measurements.
- He/she expansively knows the operating principles of the instrumental analysis, auxiliary devices.

b) Abilities

- He/she is able to apply the most important terminology, theories, procedures of the given instrumental analysis field when completing the relevant tasks.
- He/she is able to find solutions for the analytical problems.

c) Attitude

- He/she is open to learn and accept professional, analytical improvement and innovation in his/her profession and convey it genuinely.
- He/she makes a decision in complex and unexpected decision cases by completely taking into account legal and ethical norms.

d) Autonomy and responsibility

- Under supervision he/she is responsible in collaboration with other professionals (especially from the field of analytical and environmental economy and safety).

- He/she confesses and represents the value system of the instrumental analytical profession with responsibility. He/she is open to critical remarks which are professionally well-founded.

Schedule:

1st week: Quality ensurance, validation parameters, evaluation methods (2h)

2nd week: Sampling, storing samples (2h)

3rd week: Sample pretreatment methods (2h)

4th week: Atomic emission methods. ICP-AES. Laser ablation sample introduction. ICP-MS. Graphite furnace atomic absorption methods. Background correction methods (2h)

5th week: Labelling analytical methods. Immunoanalysis. ELISA (2h)

6th week: Ion exchange chromatography. Ion chromatography. Supercrtitical fluid chromatography. (2h)

7th week: Gel electrophoresis. Capillary electrophoresis. Electroosmosis. Detection on gels. (2h)

8h week: Microfluidic application in analytical chemistry. Lab-on-a-chip. Bioanalyzer 2100 (2h)

9th week: Characterization and classification of sensors. Electrochemical and semiconductive sensors (2h)

10th week: Attenuated total reflexion spectrometry. Surface plasmon resonance spectroscopy. Molecularly imprinted polymers and their analytical applications. (2h)

11th week: Fundamentals and instrumentation of polarography. Methods of polarography. Cyclic voltammetry. Inverse voltammetry. Bipotentiometry. (2h)

12th week: Continuous analysis. Kinetic analytical methods. (2h)

13th week: Methods of the thermal analysis (TG, DTG, DTA, DSC) (2h)

14th week: Consultations. Survey and classification of the analytical methods. (2h)

Requirements:

Attendance at lectures is recommended, but not compulsory.

The course ends in an examination (written test).

The minimum requirement for the examination is 50%. Based on the score of the test, the grade is given according to the following table:

Score	Grade

0-50	fail (1)
50-69	pass (2)
70-79	satisfactory (3)
80-89	good (4)
90-100	excellent (5)

Person responsible for course: Dr. Attila Gáspár, professor, DSc

Lecturer: Dr. Attila Gáspár, professor, DSc

Title of course: Instrumental analysis II **Code**: TTKML0501_EN	**ECTS Credit points:** 2

Type of teaching, contact hours
- lecture: -
- practice: -
- laboratory: 3 hours/week

Evaluation: practice grade

Workload (estimated), divided into contact hours:
- lecture: -
- practice: 42 hours
- laboratory: -
- home assignment: 28 hours
- preparation for the exam:

Total: 70 hours

Year, semester: 2nd year, 1st semester

Its prerequisite(s):

Further courses built on it: **TTKME0501**

Topics of course

The series of laboratory practices are based on the topics of different intsrumental analysis like electrophoresis, atomic spectrometry, electroanalysis, validation, ion chromatography, circular dichroism. The instrumental laboratories are connected to the topics of the Instrumental Analysis lecture and the those complete the knowledge acquired in BSc level.

Literature

1. Daniel C. Harris: Quantitative Chemical Analysis, 7th Ed., 2007, Freeman and CoH.H.
2. Willard, L.L. Merritt, J.A. Dean, F.A. Settle: Instrumental methods of Analysis, Wadsworth Publ. Co., Belmont, 1988.

3. Douglas A. Skoog, Donald M. West, F. James Holler, Stanley R. Crouch: Fundamentals of Analytical Chemistry, 8th. ed., 2004, Brooks/Cole
4. Syllabuses provided by the tutor.

Course objective/intended learning outcomes

a) Knowledge

- He/she fundamentally knows principles and means of instrumental analysis, sample pretreatment, data evaluation and validation of the measurements.
- He/she expansively knows the operating principles of the analytical instruments, auxiliary devices.

b) Abilities

- He/she is able to apply the most important terminology, theories, procedures of the given instrumental analysis field when completing the relevant tasks.
- He/she is able to find solutions for the analytical problems.

c) Attitude

- He/she is open to learn and accept professional, analytical improvement and innovation in his/her profession and convey it genuinely.
- He/she makes a decision in complex and unexpected decision cases by completely taking into account legal and ethical norms.

d) Autonomy and responsibility

- Under supervision he/she is responsible in collaboration with other professionals (especially from the field of analytical and environmental economy and safety).
- He/she confesses and represents the value system of the instrumental analytical profession with responsibility. He/she is open to critical remarks which are professionally well-founded.

Schedule:

1st week: Introductory guidance, accident protection (2h)

2nd week: Capillary electrophoresis (6h)

3rd week: Graphite furnace atomic absorption spectrometry (6h)

4th week: Cyclic voltammetry (6h)

5th week: Validation of analytical methods (8h)

6th week: Circular dicroism spectroscopy (6h)

7th week: Ion chromatography (6h)

8th week: Final test (2h)

Requirements:

- for a signature

Participation at practices is compulsory. A student must attend every practices during the semester.

Attendance at practices will be recorded by the practice leader. Being late is equivalent with an absence. In case of further absences, a medical certificate needs to be presented. Missed practice classes should be made up for at a later date, to be discussed with the tutor. Active participation is evaluated by the teacher in every class. If a student's behavior or conduct doesn't meet the requirements of active participation, the teacher may evaluate his/her participation as an absence because of the lack of active participation in class.

- *for a grade*

Grading is given by the average of 3 separate grades:

- the average grade of the short tests written at the beginning of the instrumental analysis lab practices (an average of at least 2.0 is necessary to avoid a 'fail' final grade)
- the average grade of evaluation of the analytical data measured by the instrument, the laboratory notebook prepared by the student and final discussion/conclusion made between the student and the supervisor at the end of the lab practice (an average of at least 2.0 is necessary to avoid a 'fail' final grade)
- the grade of the final test

The grade of the final test is calculated according to the following table:

Score	Grade
0-59	fail (1)
60-69	pass (2)
70-79	satisfactory (3)
80-89	good (4)
90-100	excellent (5)

Person responsible for course: Dr. Attila Gáspár, professor, DSc

Lecturer: Dr. Attila Gáspár, professor, DSc

Title of course: **Spectroscopic methods for structure investigation I.**
Code: TTKME0502_EN

ECTS Credit points: 3

Type of teaching, contact hours
- lecture: 2 hours/week
- practice: -
- laboratory: -

Evaluation: exam

Workload (estimated), divided into contact hours:
- lecture: 28 hours
- practice: -
- laboratory: -
- home assignment: 20 hours
- preparation for the exam: 42 hours

Total: 90 hours

Year, semester: 1st year, 2nd semester

Its prerequisite(s): TKBE0503_EN

Further courses built on it: TTKML0502_EN, TTKMG0318_EN, TKML0530_EN,

Topics of course

Basic principles of different spectroscopic and structure elucidation methods. Examples and applications for structural studies of organic compounds.

Literature

1. **P.J. Hore, Nuclear Magnetic Resonance, Oxford Univ. Press (2002)**
2. **N.E. Jacobsen, NMR Spectroscopy Explained: Simplified Theory, Applications and Examples for Organic Chemistry and Structural Biology, Wiley**
3. **T.D.W. Claridge, High-Resolution NMR Techniques in Organic Chemistry, Elsevier**
4. **J.R.Chapman: „Practical Organic Mass Spectrometry", Wiley, 1995**
5. **E.Pretsch, J.T.Clerc: „Interpretation of Organic Compounds", VCH, 1997**

Compulsory:
Recommended:

Course objective/intended learning outcomes

a) Knowledge

- Have basic knowledge on various topics of chemistry, including basics of spectroscopic and analytical methods studied during BSc courses.

b) Abilities

- Using the knowledge and experiences acquired during the course he/she is able to analyse NMR, MS, Fluorescent and UV spectra and accomplish structure verification and/or elucidation of organic compounds using spectral parameters assessed from relevant spectra.

c) Attitude

- He/She is receptive to establish and apply new chemical technologies.
- He/She is open to collaborate with professionals on the field of chemistry, environmental chemistry, treating the new chemical trends critically but carefully.

d) Autonomy and responsibility

- He/She is responsible for his/her own decisions, stand in for these decisions and ideologies.
- He/She recognizes the unsafe chemical environment in laboratory, and makes decisions according to this.
- He/She is well aware about his/her propositions and its consequences.

Schedule:

1st week

The basic concepts of mass spectrometry. Isotopes in mass spectrometry. Resolution and its interpretation. Most important fragmentation processes. The use of nitrogen rule for different type of ions.

2nd week

Soft ionization techniques. Generation of CI spectra, interpretation of the spectra. *3rd week* Soft ionization techniques. Ion formation in liquid chromatography-linked systems. Generation of ESI spectra, interpretation of spectra. Multiple charged ions and their presentation in the spectra. *4th week* Soft ionization techniques. Ion formation in liquid chromatography-linked systems. Generation of APCI spectra, interpretation of spectra. *5th week* pH, pKa, and their significance in MS studies. MS compatible eluent preparation rules. *6th week* Basics of tandem mass spectrometry. Construction and operation of a tandem device. Structure of MSMS experiments, rules for their use. Signal to noise ratio. The most important areas of application of tandem measurements with examples. *7th week* Principles of Fluorescence Spectroscopy and Applications. Fluorophores. Raman spectroscopy: principle and applications. *8th week* NMR - Macroscopic magnetization (M), phenomenological description of time dependence of macroscopic magnetization. Bloch equations in laboratory frame. *9th week* Introduction of rotating frame. Solutions of Bloch equations in the rotating frame in case of specific conditions: shape of resonance signal, concept and occurrence of saturation. *10th week* Relaxation phenomenon. Nuclear spin relaxation: spin-lattice and spin-spin relaxation times. Measurement of T_1 and T_2 relaxation times. *11th week* Relaxation mechanisms - dipolar (DD), chemical shift anisotropy (CSA), quadrupolar (Q), scalar coupling (SC), spin-rotation (SR) and paramagnetic (PR) relaxation. Relaxation and dynamics (molecular motion, rotational diffusion). *12th week* Relaxation and structure. Nuclear Overhauser (NOE) effect. Steady-state and transient NOE experiments. Applications of NOE in solving stereochemical – configurational and conformational - problems. *13th week* Principles of pulsed Fourier NMR spectroscopy. Basic principles of 2D NMR spectroscopy. *14th week* Principles and applications of dynamic NMR. Two- and multisite exchange. NMR time scale (fast, intermediate, slow motional regime) and its implications on spectral properties and parameters.
Requirements: - *for a signature* Attendance at **lectures** is highly recommended, but not compulsory. - *for a grade*

The course ends in a **written exam** during the examination period following the course. The minimum requirement for the end-term test is 60%. Based on the score of the test, the grade for the exam is given according to the following table: Score — Grade 0-59 — fail (1) 60-69 — pass (2) 70-79 — satisfactory (3) 80-89 — good (4) 90-100 — excellent (5) If the score of the written exam is below 60, students can take a retake test in conformity with the EDUCATION AND EXAMINATION RULES AND REGULATIONS.
Person responsible for course: Prof. Katalin E. Kövér, professor, DSc.
Lecturer: Prof. Katalin E. Kövér, professor, DSc. & Dr. Attila Kiss, PhD, associate professor

Title of course: **Spectroscopic methods for structure investigation II.** **Code**: TTKML0502_EN	**ECTS Credit points:** 2
Type of teaching, contact hours - lecture: - - practice: 3 hours/week - laboratory: -	
Evaluation: exam	
Workload (estimated), divided into contact hours: - lecture: - - practice: 42 hours - laboratory: - - home assignment: 18 hours - preparation for the exam: - Total: 60 hours	
Year, semester: 2^{nd} year, 1^{st} semester	
Its prerequisite(s): TTKME0502_EN	
Further courses built on it: -	

Topics of course
The series of practise are based on the topics of ^1H and ^{13}C NMR. It reviews the fundamental relations of the nuclear Zeeman effect, Boltzmann-distribution, nuclear shielding-origin of the chemical shift-

and scalar splitting pattern.
There are two main tasks to elaborate: to obtain structural information from resonance frequencies and splitting patterns and to propose the correct structure based on ^{1}H and ^{13}C NMR data.
Basic principles of different spectroscopic and structure elucidation methods (MS, IR, UV/Vis and NMR). Examples and applications for structural studies of organic compounds.

Literature

1. **R.M.Silverstein, F.X.Webster:"Spectrometric Identification of Organic Compounds", Wiley, 1998.**
2. **J.P.Hore:"Nuclear Magnetic Resonance", Oxford Chemistry Primers, 1995.**
3. **L.D.Field, S.Sternhell, J.R.Kalman: „Organic Structure from Spectra"**

Course objective/intended learning outcomes

a) Knowledge
- Have systematic knowledge on the various subject of chemistry, their main principals including the theoretical and practical application built on these principals.

b) Abilities
- Using the knowledge and experiences acquired during the course he/she is able to solve structural problems by using analytical and spectroscopic methods.

c) Attitude
- He/She is receptive to establish and apply new chemical and environmental technologies.
- He/She is open to collaborate with professionals on the field of social sciences, economy and environmental safety, treating the new chemical trends critically but carefully.

d) Autonomy and responsibility
- He/She is responsible for his/her own decisions, stand in for these decisions and ideologies.
- He/She recognizes the unsafe environment both in laboratory on industry, and makes decisions according to this.
- He/She is well aware about his/her propositions and its consequences.

Schedule:

1st week
Introduction, overview of theoretical basics of IR, UV and MS that are required for complex problem solving.

2nd week
Complex spectral analysis of open chain and branched chain aliphatic compounds, focusing on their IR, UV and MS spectra. Problem Solving.

3rd week
Complex spectral analysis of halogenated organic compounds, focusing on their IR, UV and MS spectra. Problem Solving.

4th week
Complex spectral analysis of aromatic compounds, focusing on their IR, UV and MS spectra. Problem Solving.

5th week
Complex spectral analysis of oxygen containing organic compounds, focusing on their IR, UV and MS spectra. Problem Solving.
6th week
Complex spectral analysis of nitrogen containing organic compounds, focusing on their IR, UV and MS spectra. Problem Solving.
7th week
Spectral analysis of complex organic compounds, focusing on their IR, UV and MS spectra. Problem Solving.
8th week
Zeeman energy levels, Boltzmann-distibution, equilibrium macroscopic magnetization (M_0). The selection rule for NMR.
9th week
Empirical rules for calculation of chemical shifts of different organic compounds (alkanes, alkenes, aromatics).
10th week
Case of strong coupling (second order effects). Examples, rules for chemical shifts calculations.
Process of ^{1}H spectral analysis. Interpretation of simple and more complex ^{1}H NMR spectra.

11th week
Overlapping signals in ^{1}H NMR spectra, extra information. ^{13}C NMR analysis.
12th week
Problem solving: structure elucidation of an organic compound based on combined analysis of ^{1}H and ^{13}C NMR spectra.
13th week
^{1}H and ^{13}C NMR: applications for structure verification of complex organic structures.
14th week
Complex problem solving exercises.

Requirements: - *for a signature*
Participation at **practice classes** is compulsory. A student must attend the practice classes and may not miss more than three times during the semester. In case a student does so, the subject will not be signed and the student must repeat the course.
If a student's behaviour or conduct doesn't meet the requirements of active participation, the teacher may evaluate his/her participation as an absence because of the lack of active participation in class. The course ends in an **end-term test**, the end-term test in the 15th week. Students have to sit for the tests.
- *for a grade*
The minimum requirement for end-term test is 60%. Based on the score of the test, the grade for the test is given according to the following table:

Score	Grade
0-59	fail (1)
60-69	pass (2)
70-79	satisfactory (3)

80-89	good (4)
90-100	excellent (5)

If the score of the test is below 60, students can take a retake test in conformity with the EDUCATION AND EXAMINATION RULES AND REGULATIONS.

Person responsible for course: Prof. Dr. Katalin E. Kövér, professor, DSc.

Lecturer: Prof. Dr. Katalin E. Kövér, professor, DSc.

Title of course: Introduction to Chemical Engineering
Code: TTKME0601_EN

ECTS Credit points: 3

Type of teaching, contact hours
- lecture: 2 hours/week
- practice:
- laboratory: -

Evaluation: exam

Workload (estimated), divided into contact hours:
- lecture: 28 hours
- practice:
- laboratory: -
- home assignment: 30
- preparation for the exam: 32 hours

Total: 90 hours

Year, semester: 1st year, 2nd semester

Its prerequisite(s):

Further courses built on it: -

Topics of course

Similitude. Physical quantities, units, dimensions. Scalars, vectors, tensors. Covariance. Similitude criteria and similitude invariables. Extensive and intensive properties. Balance equations. Currents. Uniqueness criteria. Theory of transport processes, generic transport equation – basic classification of engineering processes. Dimensional analysis: concepts and methods. Dimension matrices. Dimensionless numbers. Classes of dimensionless numbers and connections between them. Dimensional analysis and similitude. Aero- and hydrodynamics: fundamental equations, the Navier-Stokes equations, Bernoulli equation. Equation of momentum transport. Momentum balance. Similarity transformation. Free flow. Effect of changes in uniqueness criteria. Momentum transport in turbulent flow. Simultaneous flow of liquid and solid particles. Balance equations. Similarity transformation. Thermal conductivity and diffusion. Continuity equation fro mass transport. Mass transport in a flowing liquid. Heat exchange in a flowing liquid. Thermal diffusion. Chemical reactions: stoichiometric equations, mass balance, energy balance, momentum balance. Principles of reactor technology. Thermal analysis of chemical reactors. Equilibria: phase equilibrium, equilibrium lines, working lines.

Literature

Compulsory:

McCabe, W.L.; Smith, J.C.; Harriot, P. (1993) Unit Operations Of Chemical Engineering (7th Ed) - McGraw-Hill

Richard G. Griskey:Transport phenomena and unit operations: a combined approach, (2002), Wiley, ISBN 0-47 1-43819-7

Christie J Geankoplis: Transport processes and unit operations (1993), 3rd edition, Prentice-Hall, ISBN 0-13-045253-X

J. M. Coulson, J. F. Richardson: Chemical Engineering. Volume 1-6. Third Edition. Pergamon Press. Oxford

Course objective/intended learning outcomes

a) Knowledge

- Have systematic knowledge on the various subject of chemistry, their main principals including the theoretical and practical application built on these principals.
- He/She understands the progress and future trends in chemistry and chemical industries.
- He/She has knowledge to solve problems on the field of natural processes, using natural sources, and understanding the chemical background of living and non-living systems.

b) Abilities

- He/She is able to communicate discuss and aim problems to other chemists or engineers of professionals other than chemistry field.
- He/She is able to argue his/her opinion in scientific discussions both in oral or written form.
- He/She is able to transfer the theoretical knowledge into practical one in research to obtain new results.

c) Attitude

- He/She accepts those professional identities that defines the uniqueness and importance of science
- He/She is able to represent and distribute his/her own personal scientific ideology toward professional and unprofessional groups, and making the ideal scientific person who is critical to the new results.
- He/She is responsible and stands in for the professional ethics.

d) Autonomy and responsibility

- He/She is responsible for his/her own decisions, stand in for these decisions and ideologies.

Schedule:

1st week
Definition and classification of unit operations. batch and continuous processes. Flowsheets.

2nd week
Physical quantities, units, dimensions. The SI system. Extensive and intensivequantities. Dimensional and tensorial homogenity. Scalar-vector-tensor quantities.

3rd week
The fundamental equation of thermodynamics. Conditions of equilibrium, driving force, rate of processes. Degrees of freedom of a chemical system.

4th week
Flows and fluxes. Scalar and vector fields and their derivatives. The Nabla vector, gardient and divergence. The general transport equation. Differential and integral form of balance equations valid for one and two phase unit operations. The Damköhler equations. The Onsager theory.

5th week
The mathematical model. Initial and boundary conditions. Balance equations for simple systems: Fourier-I and Fick-I laws.

6th week
Similitude and modelling. Dimensional analysis, dimensionless numbers.

7th week
Mass and energy balances for simple and complex unit operations.

8th week
The heat equation. Types and calculation of heat transport. Steady state heat conduction in plane pipe walls. Fourier-I equation and thermal insulation. Heat exchanngers. Stationary heat transmission with constant temperature difference through flat and cylindrical wall. Determination of heat flow and thermal resistances.
Direct and indirect heat exchange. Determination of the power requirement for a stationary recuperative heat exchanger. Temperature-space function of co-current and counter current heat exchangers. Logarithmic mean temperature difference. Types and apparatus of heat exchangers.

9th week
Flow in unpacked pipes and in pipelines: Fluids in rest, Pascal's law. Navier-Stokes equations. Bernoulli equation. Cavitation. Newtonian and non-Newtonian fluids. Newton's law of viscosity.

10th week
Basic types of fluid flow. Reynolds' experiment. Hagen-Poisseuille equation. Modified Bernoulli equation. Fanning equation. Moody diagram. Energy requirement of fluid transport. Types of pumps.

11th week
Mass transfer theories. Two-film and boundary layer theory of component transfer. Absorption-desorption: Concentration-space diagram of a continuous counter current absorption unit operation. Equation of operating line.

12th week
Basics of filtration. Darcy's law of filtration. Batch filtration using constant pressure, continuous filtration using constant flow rate. Filtration units. Filtration using centrifugal force. Types of centrifuges. Basics of membrane filtration. Concentration polarization.

13th week
Introduction to chemical reactors.

14th week
Classification of reactors based on flow, operation mode, component stream and heat. Operation time, residence time. Concentration-time and concentration-space functions of batch and continuous reactors.
Heat balance of a reactor. Stability of reactors.

Requirements:
- *for a signature*

Attendance at **lectures** is recommended, but not compulsory.
Participation at **practice classes** is compulsory. A student must attend the practice classes and may not miss more than three times during the semester. In case a student does so, the subject will not be signed and the student must repeat the course. A student can't make up any practice with another group. Attendance at practice classes will be recorded by the practice leader. Being late is equivalent with an absence. In case of further absences, a medical certificate needs to be presented. Missed practice classes should be made up for at a later date, to be discussed with the tutor.

During the semester there are two tests: the mid-term test in the 8th week and the end-term test in the 15th week. Students have to sit for the tests.
- *for a grade*

The course ends in an **examination**.
The minimum requirement for the mid-term and end-term tests and the examination respectively is 60%. Based on the score of the tests separately, the grade for the tests and the examination is given according to the following table:

Score	Grade
0-59	fail (1)

60-69	pass (2)
70-79	satisfactory (3)
80-89	good (4)
90-100	excellent (5)

If the score of any test is below 60, students can take a retake test in conformity with the EDUCATION AND EXAMINATION RULES AND REGULATIONS.

-an offered grade:

it may be offered for students if the average grade of the mid-term and end-term tests is at least satisfactory (3). The offered grade is the average of them.

Person responsible for course: Dr. Miklós Nagy, associate professor, PhD

Lecturer: Dr. Miklós Nagy, associate professor, PhD

Title of course: Advanced Chemical Technology **Code**: TTKME0602_EN	**ECTS Credit points:** 3

Type of teaching, contact hours
- lecture: 2 hours/week
- practice: - hours/week
- laboratory: -

Evaluation: exam

Workload (estimated), divided into contact hours:
- lecture: 28 hours
- practice: - hours
- laboratory: -
- home assignment: 22 hours
- preparation for the exam: 40 hours

Total: 90 hours

Year, semester: 2^{nd} year, 1^{st} semester

Its prerequisite(s): -

Further courses built on it: -

Topics of course

Introducing the procedures of chemical technology in the organic chemistry industry. Advanced petrochemical processes and the production of organic chemical raw materials.
- Environment and industry relations.
- Occurrence and extraction of petroleum, coal and natural gas.
- More detailed discussion of oil processing.
- Description of Petrochemical Procedures.

- Production and transformation of paraffins, olefins and aromatic industries.
- Production and transformation of polymeric raw materials.
- Other areas of organic chemistry.

Literature

Compulsory:
- P. J. Chenier: Survey of industrial chemistry, VCH, N.Y. 1992.
- Ullmann's Encyclopedia of Industrial Chemistry, Wiley, 2000.
- Ullman's Enciklopedia of Industrial Chemistry 5th ed, Weinheim, Federal republic of Germany, VCH, Volumes A1-A28.1985-1996.

Recommended:
- Ronald Bailey, Herbert Clark, James Ferris, Sonja Krause, Robert Strong: Chemistry of the Environment 2nd Edition, Academic Press.

Course objective/intended learning outcomes

a) Knowledge
- He/She understands the progress and future trends in chemistry and chemical industries.
- He/She knows various methods from chemical labs or industries, able to show it to other people and apply them including the equipments and their safe usage.
- He/She has knowledge to solve problems on the field of natural processes, using natural sources, and understanding the chemical background of living and non-living systems.

b) Abilities
- He/She is able to carefully apply the newest chemical theories in practice and design lab experiments or industrial processes based on these results.
- Using the knowledge and experiences during the MSc coursed he/she is able to execute laboratory experiments or measurements to demonstrate proper chemical phenomena, or syntheses of new compounds and characterize them, and using analytical methods for provement of new reactions.

c) Attitude
- He/She is committed to protect the environment in both chemical labs and industries. These attitudes are shown to other coworkers as well. He/she makes effort to apply those technologies that makes lower environmental changes/loads.
- He/She is receptive to establish and apply new chemical and environmental technologies.
- He/She is being active to start and participate in professional discussions.

d) Autonomy and responsibility
- He/She can make own decisions even in complex professional questions, discussions.
- He/She is responsible for his/her own decisions, stand in for these decisions and ideologies.
- He/She recognizes the unsafe environment both in laboratory on industry, and makes decisions according to this.

Schedule:
1st week: The relationship between industry and the environment. Know the 12 laws of environmentally friendly chemistry. Equipment used in the main organic chemical industry.

The student gains knowledge of the relationship between industry and the environment. Know the equipment used in the organic chemical industry.
2nd week: The occurrence, composition and extraction of crude oil, natural gas and coal.
Basic concepts of combustion engineering.
Students acquire knowledge of major fossil fuels.
3rd week: A more detailed description of the atmospheric and vacuum distillation processing of crude oil. Motor fuels and lubricants.
The student gains knowledge of the steps of oil refining and the composition of the propulsion materials.
4th week: Description of petrochemical processes (viscosity breakdown, delayed chamber coking, flex coking, catalytic cracking, catalytic reforming).
The student gains knowledge of the catalytic petrochemical processes that are aimed at the production of motor carriers.
5th week: Description of Petrochemical Procedures (hydrocracking, aliphatic and aromatic alkylation procedures, isomerization procedures).
The student acquires knowledge of petrochemical processes, which aim to produce propellants by increasing hydrocarbons branching.
6th week: Description of catalysts used in petrochemical processes.
The student becomes acquainted with the construction and operation of catalysts in the industry.
7th week: Olefin production with thermal cracking (TVK olefin plant and technology used therein).
The student gets acquainted with the technology of olefin production in TVK.
8th week: Industrial production and use of synthetic gas.
Students acquire knowledge about synthesis gas production and utilization.
9th week: Methods of transformation of petrochemical products - paraffin hydrocarbons.
The student gets acquainted with the industrial production and conversion processes of paraffin hydrocarbons.
10th week: Transformations of petrochemicals - olefins into organic chemical raw materials.
Students learn about the industrial conversion processes of olefins (ethylene, propylene).
11th week: Production of Petrochemicals Products Olefins Conversion-Polymers (PE, PPP, PVC ..)
Students are familiar with the industrial production and properties of the major polymers.
12th week: Transformations of Petrochemicals - Aromatic (BTX Fraction) into organic chemical raw materials.
The student gets acquainted with the industrial transformations of the BTX fraction.
13th week: Other sectors of organic chemistry - plant protection products, pharmaceutical active ingredients.
The student becomes acquainted with the plant protection products, the most important known pharmaceutical active ingredients.
14th week: Other sectors of organic chemistry - dyes, surfactants and paper production.
The student is familiar with the industrial use of dyes, tensides and the paper manufacturing process.

Requirements:
- *for a signature*
Attendance at **lectures** is recommended, but not compulsory. Presentation from a published topic is

compulsory.
Active participation is evaluated by the teacher in every class. If a student's behaviour or conduct doesn't meet the requirements of active participation, the teacher may evaluate his/her participation as an absence because of the lack of active participation in class.
Students have to **submit all the two designing tasks** as scheduled minimum on a sufficient level.
Students must present the presentation before the written exam.
At the end of the semester there are a test: in the 15th week. Students have to sit for the tests
- *for a grade*
The course ends in written **examination**. The final grade calculated on the average of the grades of oral presentation and the examination. The exam grade calculated from the result of examination.
The minimum requirement for examination respectively is 50%. Based on the score of the tests separately, the grade for the tests and the examination is given according to the following table:

Score	Grade
0-50	fail (1)
51-69	pass (2)
70-79	satisfactory (3)
80-89	good (4)
90-100	excellent (5)

If the score of any test is below 50, students can take a retake test in conformity with the EDUCATION AND EXAMINATION RULES AND REGULATIONS.

Person responsible for course: Katalin Illyés Czifrák, assistant professor

Lecturer: Katalin Illyés Czifrák, assistant professor

Title of course: Diploma Thesis I.
Code: TTKML0001_EN

ECTS Credit points: 15

Type of teaching, contact hours
- lecture: -
- practice: -
- laboratory: 15 hours/week

Evaluation: practical grade

Workload (estimated), divided into contact hours:
- lecture: -
- practice: -
- laboratory: 210 hours
- home assignment: 70 hours
- preparation for the exam: -

Total: 280 hours

Year, semester: 2nd year, 1st semester

Its prerequisite(s): -

Further courses built on it: Diploma Thesis II. TTKML0002_EN

Topics of course

The purpose of the diploma work is to demonstrate that the graduate is prepared to perform independent chemical work. Thus, the diploma work is based on chemical research performed by the graduate under the supervision of a senior staff member. The corresponding thesis should include a literature survey, a detailed description of the experimental methods used, the results of the experiments and a thorough discussion of the data. The length of the thesis is 35 – 45 pages and it is evaluated by an independent reviewer who proposes a mark. The final mark is given by the final exam committee.

Literature

Provided by the supervisor.

Course objective/intended learning outcomes

a) Knowledge

- He/She has knowledge to solve problems in the field of a particular field of chemistry
- He/She can understand and communicate professionally on chemical subjects at his/her native language.

b) Abilities

- He/She is able to use the previously learned paradigms, theories and laws in the field of chemical, natural science; to plan, execute and evaluate laboratory experiments.
- He/She is able to evaluate and discuss the laboratory measurements, and create a report about it.

c) Attitude

- He/She is committed learn or get insights into new competence or ideology.
- He/She is well aware about his/her propositions and its consequences.

d) Autonomy and responsibility

- He/She takes part in scientific project(s) under supervision.

Schedule:
The student works by following the instructions of the supervisor.

Requirements:
- *for a signature*

The student have to take part in the research project coordinated by the supervisor.

- *for a grade*

The work of the student is evaluated by the supervisor considering many aspects, e.g. the quality of the work in the laboratory or industry, the ability to work alone or in a team, the competence for process the literature about the given topic, the problem solving ability and the presentation of the results.

Person responsible for course: Dr. István Fábián, full professor, responsible for the MSc in Chemistry studies

Lecturer: supervisors are staff members of the Institute of Chemistry, UD

Title of course: Diploma Thesis II. **Code**: TTKML0002_EN	**ECTS Credit points:** 15
Type of teaching, contact hours - lecture: - - practice: - - laboratory: 15 hours/week	
Evaluation: practical grade	
Workload (estimated), divided into contact hours: - lecture: - - practice: - - laboratory: 210 hours - home assignment: 70 hours - preparation for the exam: - Total: 280 hours	
Year, semester: 2nd year, 2nd semester	
Its prerequisite(s): Diploma Thesis I. TTKML0001_EN	
Further courses built on it: -	

Topics of course

The purpose of the diploma work is to demonstrate that the graduate is prepared to perform independent chemical work. Thus, the diploma work is based on chemical research performed by the graduate under the supervision of a senior staff member. The corresponding thesis should include a literature survey, a detailed description of the experimental methods used, the results of the experiments and a thorough discussion of the data. The length of the thesis is 35 – 45 pages and it is evaluated by an independent reviewer who proposes a mark. The final mark is given by the final exam committee.

Literature

Provided by the supervisor.

Course objective/intended learning outcomes

a) Knowledge

- He/She has knowledge to solve problems in the field of a particular field of chemistry
- He/She can understand and communicate professionally on chemical subjects at his/her native language.

b) Abilities

- He/She is able to use the previously learned paradigms, theories and laws in the field of chemical, natural science; to plan, execute and evaluate laboratory experiments. - He/She is able to evaluate and discuss the laboratory measurements, and create a report about it. **c) Attitude** - He/She is committed learn or get insights into new competence or ideology. - He/She is well aware about his/her propositions and its consequences. **d) Autonomy and responsibility** - He/She takes part in scientific project(s) under supervision.

Schedule: *The student works by following the instructions of the supervisor.*
Requirements: - *for a signature* The student have to take part in the research project coordinated by the supervisor. - *for a grade* The work of the student is evaluated by the supervisor considering many aspects, e.g. the quality of the work in the laboratory or industry, the ability to work alone or in a team, the competence for process the literature about the given topic, the problem solving ability and the presentation of the results.
Person responsible for course: Dr. István Fábián, full professor, responsible for the MSc in Chemistry studies
Lecturer: supervisors are staff members of the Institute of Chemistry, UD

Title of course: Industrial Placement **Code**: TTKMX0003_EN	**ECTS Credit points:** 0
Type of teaching, contact hours 4 weeks	
Evaluation: signature	
Workload (estimated), divided into contact hours: Total: 160 hours	
Year, semester: 1st year, 2nd semester in the Summer	
Its prerequisite(s): -	
Further courses built on it: -	

Topics of course

Industrial placement is an ideal opportunity to apply existing skills and to develop new ones whilst getting a practical insight into working life in chemical industry, it gives real world experience, and a possible step in a career and provides with the opportunities for the future. All these experiences greatly enhance career prospects for when students graduate.
Industrial placement is an extraordinary opportunity to train and develop personal abilities with competent professionals and gain first hand experience of chemical industry and is an ideal grounding for a future career in chemical industry. It provides integrated industrial and professional training in an area such as operation of a chemical plant and a chance to sharpen skills and acquire work experience.

Literature

-

Course objective/intended learning outcomes

a) Knowledge
- He/She knows the most recent theories, models and related computational methods on the scientific results about chemical bonds, structure of compounds, reactions, and chemical interactions.
- He/She understands the progress and future trends in chemistry and chemical industries.
- He/She has knowledge to solve problems on the field of natural processes, using natural sources, and understanding the chemical background of living and non-living systems.

b) Abilities
- He/She is able to use the new approaches on the field of chemical research and innovation to apply the main theories, practical information, application and technology as well as understanding and analyzing scientific data.
- He/She is able to carefully apply the newest chemical theories in practice and design lab experiments or industrial processes based on these results.
- Using the knowledge and experiences during the MSc coursed he/she is able to execute laboratory experiments or measurements to demonstrate proper chemical phenomena, or syntheses of new compounds and characterize them, and using analytical methods for provement of new reactions.
- He/She is able to evaluate experimental data, analyze them and draw conclusions. Based on these results he/she can present new trend sin research or development without supervision.

c) Attitude
- He/She is committed to protect the environment in both chemical labs and industries. These attitudes are shown to other coworkers as well. He/she makes effort to apply those technologies that makes lower environmental changes/loads.
- He/She is receptive to establish and apply new chemical and environmental technologies.
- He/She is being active to start and participate in professional discussions.
He/She is open to collaborate with professionals on the field of social sciences, economy and environmental safety , treating the new chemical trends critically but carefully

d) Autonomy and responsibility
- He/She can make own decisions even in complex professional questions, discussions.
- He/She is responsible in collaboration with other professionals (especially from the field of environmental economy and safety) without supervision.
- He/She recognizes the unsafe environment both in laboratory on industry, and makes decisions according to this.

Requirements:
The students are expected to write a report of about 15 pages on the work accomplished during the internship.

Person responsible for course: Dr. Ákos Kuki, associate professor, PhD

Title of course: Chemometrics I. **Code**: TTKME0511_EN	**ECTS Credit points:** 3
Type of teaching, contact hours - lecture: 2 h / week - practice: – - laboratory: –	
Evaluation: exam	
Workload (estimated), divided into contact hours: - lecture: 26 h - practice: – - laboratory: – - home assignment: – - preparation for the exam: 55 h Total: 81 h	
Year, semester: 1st year, 1st semester	
Its prerequisite(s): –	
Further courses built on it: –	

Topics of course

The material of the lecture covers the fundamental aspects of applied Chemometrics. The course begins with descriptive statistics covering the normal distribution and the Poisson distribution. This is followed by statistical hypothesis testing (Q-test, t-test, ANOVA). Mathematical modelling is demonstrated through linear and non-linear least-squares fitting (regression analysis). Some fundamental aspects of numerical mathematics are covered. Optimization and design of experiment approaches are overviewed. The use of principal component analysis (PCA) and cluster analysis is demonstrated for pattern recognition. Classification is realized by linear discriminant analysis (LDA). Finally, the fundamental strategies of calibration in chemical analysis are covered, including multivariate calibration by the methods of partial least squares and principal component regression.

Literature

Compulsory:

1) Matthias Otto: Chemometrics

WILEY-VCH Verlag GmbH, Weinheim, Germany, 1999.
2) Richard G. Brereton: Applied Chemometrics for Scientists
John Wiley & Sons Ltd, Chichester, England, 2007.
3) D. L. Massart. B. G. M. Vandeginste, S. N. Deming, Y. Michotte, and L. Kaufman: Chemometrics: A textbook. Elsevier, Amsterdam, The Netherlands, 1988.

Course objective/intended learning outcomes

a) Knowledge

- He/she fundamentally knows principles and means of chemometrics, procedures and operating processes of statistics.
- He/she expansively knows the operating principles of hypothesis tests, regression analysis, principal component analysis, cluster analysis, partial least squares regression.

b) Abilities

- He/she is able to apply the most important terminology, theories, procedures of the given chemometrics field when completing the relevant tasks.
- He/she is able to create fundamental models of chemical systems and processes.

c) Attitude

- He/she is open to learn and accept professional, technological improvement and innovation in his/her profession and convey it genuinely.
- He/she makes a decision in complex and unexpected decision cases by completely taking into account legal and ethical norms.

d) Autonomy and responsibility

- Even in unexpected decision-making situations he/she is capable of considering complex, fundamental questions from his/her professional field and elaborating them on the basis of the given sources.
- He/she confesses and represents the value system of the engineering profession with responsibility. He/she is open to critical remarks which are professionally well-founded.

Schedule:

1st week

Introduction. The scope of Chemometrics. Interaction with related fields.

2nd week

Descriptive statistics.

3rd week

Statistical hypothesis testing I: Fundamentals, Q-test, t-test.

4th week

Statistical hypothesis testing II: ANOVA

5th week

Principal component analysis (PCA) I: Fundamentals, mathematics.

6th week

Principal component analysis (PCA) II: Practical examples.

7th week

Cluster analysis and linear discriminant analysis (LDA).

8th week Mathematical modelling I: Regression analysis, linear least-squares fitting. *9th week* Mathematical modelling II: Non-linear least-squares fitting. Practical examples. *10th week* Design of experiment I: Screening. *11th week* Design of experiment II: Optimization. *12th week* Calibration in analytical chemistry. *13th week* Multivariate calibration (PLS, PCR).
Requirements: - *for a signature* Attendance at **lectures** is recommended, but not compulsory. Participating in an exam earns the signature. - *for a grade* The course ends in an **oral examination**. Based on the score of the oral examination the grade is given according to the following table: Score — Grade 0-50 — fail (1) 51-60 — pass (2) 61-70 — satisfactory (3) 71-80 — good (4) 81-100 — excellent (5) If the score of the oral exam is below 51%, students can take a retake the exam in conformity with the EDUCATION AND EXAMINATION RULES AND REGULATIONS.
Person responsible for course: József Kalmár, Ph.D., assistant professor
Lecturer: József Kalmár, Ph.D., assistant professor

Title of course: Separation techniques III. **Code**: TTKME0315_EN	**ECTS Credit points:** 2
Type of teaching, contact hours - lecture: -2 hours/week - practice: - laboratory: -	
Evaluation: exam	

Workload (estimated), divided into contact hours: - lecture: 28 hours - practice: - laboratory: - - home assignment: 20 hours - preparation for the exam: 42 hours Total: 90 hours
Year, semester: 2nd year, 1th semester
Its prerequisite(s): TTKME0315_EN
Further courses built on it: **-**

Topics of course

Basic principles of different modern analytical methods in the field of HPLC, GC, SFC. Examples and applications for chromatographic studies of organic compounds.

Literature

1. **Effective Organic Compound Purification, Teledyne ISCO, Lincoln, USA (2010)**
2. **D.A. Skoog, J.J. Leary: Principles of Instrumental Analysis, New York (1992)**
3. **L.R. Snyder, J.J. Kirkland: Introduction To Modern Liquid Chromatography, Wiley, 1979**
4. **P. Schreider, A. Bernreuter, M. Huffer: Analysis of Chiral Organic Molecules, Walter de Gruyer, 1995**

Course objective/intended learning outcomes

a) Knowledge

- Have systematic knowledge on the various subject of chemistry, their main principals including basics of analytical methods studied during BSc courses.

b) Abilities

- Using the knowledge and experiences acquired during the course he/she is able to analyse HPLC, GC SFC provided results and accomplish structure, purity verification and/or determination of main analytical parameters from relevant chromatograms.

c) Attitude

- He/She is receptive to establish and apply new chemical technologies.
- He/She is open to collaborate with professionals on the field of chemistry, environmental chemistry, treating the new chemical trends critically but carefully.

d) Autonomy and responsibility

- He/She is responsible for his/her own decisions, stand in for these decisions and ideologies.
- He/She recognizes the unsafe environment both in laboratory on industry, and makes decisions according to this.
- He/She is well aware about his/her propositions and its consequences.

Schedule:

1st week
Introduction, overview of major chromatographic concepts. Categorization of chromatographic techniques by stationary and mobile phase. Chromatographic stationary phases. Retention Volume, Retention Time, Peak Height, peak area, Half Width, Bandwidth, Theoretical Plate Number, Theoretical Plate Height, Resolution, Signal, Noise, Drift, Signal / Noise, LOD, LOQ, tailing factor, peak asymmetry. Definition and use of the Kováts index in analytical chemistry.
2nd week
Size Exclusion Chromatography. Principles and mechanism of separation. Stationary phases in chromatography, physical and chemical structures, the newest developments. Instrumentation and operation of the separation processes.
3rd week
Calibration of GPC-SEC. Eluents and detectors.
4th week
Most common errors (GPC-HPLC comparison) and elimination of them.
5th week
Instruments of modern column chromatography and their use. How can a TLC data be used as a pre-experiment? Transfer of TLC data to column chromatography.
6th week
Chiral chromatographic methods. Introduction. Use of chiral GC, HPLC.
Basics of Stereochemistry from chromatographic point of view. The concept of chirality. Different chiral and achiral chromatographic systems.
7th week
Chiral interactions and their application in separation techniques. Enumeration of chiral stationary phases 1. Adapting methods from achiral systems to chiral stationary phases.
8th week
Chiral interactions and their application in separation techniques. Enumeration of chiral stationary phases 2. Adapting methods from achiral systems to chiral stationary phases.
9th week
Hyphenated Techniques. GCMS, HPLCMS SFCMS, and chiral chromatography. Method of development in chiral chromatography 1.
10th week
Hyphenated Techniques. GCMS, HPLCMS SFCMS, and chiral chromatography. Method of development in chiral chromatography 2.
11th week
Stationary Phases, Mobile Phases in Reverse Phase Liquid Chromatography. The role of pH in the separation of proton-active compounds. Preparation of liquid chromatographic buffer solutions, their properties and their application possibilities.
12th week
The usage of gradient chromatography. The possibilities of eliminating the difficulties and pitfalls of it.
13th week
Instrumentation of liquid chromatography.
14th week
Closing test.

Requirements: - *for a signature* Attendance at **lectures** is highly recommended, but not compulsory. - *for a grade* The course ends in a **written exam** during the examination period following the course. The minimum requirement for the end-term test is 60%. Based on the score of the test, the grade for the exam is given according to the following table: Score — Grade 0-59 — fail (1) 60-69 — pass (2) 70-79 — satisfactory (3) 80-89 — good (4) 90-100 — excellent (5) If the score of the written exam is below 60, students can take a retake test in conformity with the EDUCATION AND EXAMINATION RULES AND REGULATIONS.
Person responsible for course: Dr. Attila Kiss, PhD, associate professor
Lecturer: Dr. Attila Kiss, PhD, associate professor and György Deák, PhD, associate professor

Title of course: **Separation techniques IV.** **Code**: TTKML0315_EN	**ECTS Credit points: 4**
Type of teaching, contact hours - lecture: - - practice: - laboratory: 4 hours/week	
Evaluation: exam	
Workload (estimated), divided into contact hours: - lecture: - practice: - laboratory: 56 hours - home assignment: 20 hours - preparation for the exam: 44 hours Total: 120 hours	
Year, semester: 2nd year, 1th semester	
Its prerequisite(s): TTKME0315_EN	
Further courses built on it: TTKME0315_EN	

Topics of course
Basic principles of different modern analytical methods in the field of HPLC, GC, SFC. Examples and

applications for chromatographic studies of organic compounds.

Literature

6. **Effective Organic Compound Purification, Teledyne ISCO, Lincoln, USA (2010)**
7. **D.A. Skoog, J.J. Leary: Principles of Instrumental Analysis, New York (1992)**
8. **L.R. Snyder, J.J. Kirkland: Introduction To Modern Liquid Chromatography, Wiley, 1979**
9. **P. Schreider, A. Bernreuter, M. Huffer: Analysis of Chiral Organic Molecules, Walter de Gruyer, 1995**

Compulsory:
Recommended:

Course objective/intended learning outcomes

a) Knowledge

- Have systematic knowledge on the various subject of chemistry, their main principals including basics of analytical methods studied during BSc courses.

b) Abilities

- Using the knowledge and experiences acquired during the course he/she is able to analyse HPLC, GC SFC provided results and accomplish structure, purity verification and/or determination of main analytical parameters from relevant chromatograms.

c) Attitude

- He/She is receptive to establish and apply new chemical technologies.
- He/She is open to collaborate with professionals on the field of chemistry, environmental chemistry, treating the new chemical trends critically but carefully.

d) Autonomy and responsibility

- He/She is responsible for his/her own decisions, stand in for these decisions and ideologies.
- He/She recognizes the unsafe environment both in laboratory on industry, and makes decisions according to this.
- He/She is well aware about his/her propositions and its consequences.

Schedule:

1st week

Basics of gas chromatography, most important measurement methods. Main parts of the GC device. Practical applications of different types of columns. Chromatographic indexes (Kováts index).
Using the GC for quantification (in alcohol-water mixture, quantitative measurement of alcohol or determination of methane in air-methane gas mixtures).

2nd week

Using the GC for quantification (in alcohol-water mixture, quantitative measurement of alcohol or determination of methane in air-methane gas mixtures)

3rd week

Determination of caffeine or limonene using GC-FID and GC-MS methods after extraction of a solid sample (lemon or caffee). Using the Spectrum Library of the GC to identify an unknown compound.

4th week

Determination of molecular weight of polymer by GPC-SEC method (calibration and measurement).
5th week
Chiral method development 1. CSP-HPLC-UV coupling.
6th week
Chiral method development 2. CSP-HPLC-UV coupling.
7th week
Chiral method development 3. CSP-HPLC-MS coupling.
8th week
Chiral method development 3. CSP- SFC-UV coupling.
9th week
The basics of liquid chromatography, its most important methods of measurement, the construction of the HPLC apparatus. Waters Alliance Liquid Transmission System and UV + DAD Detectors. Things to do after turning on the power. Checking the fluid delivery system.
10th week
Checking the injector and detectors. Application of Empower software, writing of measuring methods, methods for integration of recorded chromatograms. Column types and their application possibilities.
11th week
Chromatographic behavior of acidic substances. The use of Pallas software and predict the logD function of the acids to be tested. Record chromatograms of the acid mixtures at different pH values.
12th week
Evaluation of the chromatograms recorded in the previous week, interpretation of the results. Produce a report on the results obtained. Understand the security features provided by the software.
13th week
Repeating lab practice. Discussing unclear questions.
14th week
Closing test.

Requirements: - *for a signature*
Participation at **laboratory** is compulsory. A student must attend the practice classes and may not miss none of them during the semester. In case a student does so, the subject will not be signed and the student must repeat the course. Attendance at lab courses will be recorded by the practice leader. Being late is equivalent with an absence. In case of further absences, a medical certificate needs to be presented. Missed lab courses should not to be made up for at a later date! Students are required to bring the drawing tasks and drawing instruments of the course to each lab courses. Active participation is evaluated by the teacher in every class. If a student's behavior or conduct doesn't meet the requirements of active participation, the teacher may evaluate his/her participation as an absence because of the lack of active participation in class.
Students have to **submit all the two designing tasks** as scheduled minimum on a sufficient level.
During the semester there are two tests: the mid-term test in the 8th week and the end-term test in the 15th week. Students have to sit for the tests
- *for a grade*
The course ends in an **examination**. Based on the average of the grades of the designing tasks and the examination, the exam grade is calculated as an average of them:

- the average grade of the two designing tasks

- the result of the examination The course ends in a **written exam** during the examination period following the course. The minimum requirement for the end-term test is 60%. Based on the score of the test, the grade for the exam is given according to the following table: Score Grade 0-59 fail (1) 60-69 pass (2) 70-79 satisfactory (3) 80-89 good (4) 90-100 excellent (5) If the score of the written exam is below 60, students can take a retake test in conformity with the EDUCATION AND EXAMINATION RULES AND REGULATIONS.
Person responsible for course: Dr. Attila Kiss, PhD, associate professor
Lecturer: Dr. Attila Kiss, PhD, associate professor and György Deák, PhD, associate professor

Title of course: Inorganic Methods in Environmental Analysis I. **Code**: TTKME0503_EN	**ECTS Credit points:** 1
Type of teaching, contact hours - lecture: 1 hours/week - practice: - - laboratory: -	
Evaluation: essay and presentation	
Workload (estimated), divided into contact hours: - lecture: 14 hours - practice: - - laboratory: - - home assignment: 5 hours - preparation for the exam: 11 hours Total: 30 hours	
Year, semester: 1st year, 1st semester	
Its prerequisite(s): -	
Further courses built on it: -	

Topics of course
The aim of this course is to give a general introduction to the inorganic methods of environmental analysis for chemistry master students. The most important steps from field sampling, sample storage, treatment and analysis techniques will be overviewed focusing on the analytics of inorganic pollutants

such as toxic metals. Rules and theoretical background will be discussed of performing a complex environmental assessment with the corresponding regulations. The most important classical and instrumental possibilities will be introduced widely used in environmental analysis. Water quality parameters and biological indication will be discussed.

Literature

Compulsory:

- J.R. Dean: Methods for Environmental Trace Analysis, Wiley, 2003.
- R. Reeve: Introduction to environmental analysis, Wiley, 2002.

Recommended:

-Environmental Chemistry by banez, J.G., Hernandez-Esparza, M., Doria-Serrano, C., Fregoso-Infante, A., Singh, M.M., Springer-Verlag New York

Course objective/intended learning outcomes

a) Knowledge

- He/She has global knowledge on science other than chemistry, and capable to organize this information.
- He/She knows various methods from chemical labs or industries, able to show it to other people and apply them including the equipments and their safe usage.
- He/She can understand and communicate professionally on chemical subjects at his/her native language

b) Abilities

- He/She is able to recognize and evaluate the global relationships on the field of chemistry.
- He/She is able to distinguish between the scientifically proven theories and non-reliable data or information
- He/She is able to evaluate experimental data, analyze them and draw conclusions. Based on these results he/she can present new trend sin research or development without supervision.

c) Attitude

- He/She is committed to protect the environment in both chemical labs and industries. These attitudes are shown to other coworkers as well. He/she makes effort to apply those technologies that makes lower environmental changes/loads.
- He/She is receptive to establish and apply new chemical and environmental technologies.

d) Autonomy and responsibility

- He/She is responsible for his/her own decisions, stand in for these decisions and ideologies.
- He/She recognizes the unsafe environment both in laboratory on industry, and makes decisions according to this.
- He/She can operate chemical or industrial instruments or equipment with responsibility, and manage persons working with these.

Schedule: The lecture will be held in the first half of the semester, 2 hours/week

1st week

General introduction to the aims and objectives of environmental analysis. Grouping the available methods and stating their connections to other scientific fields. The steps of a complex analysis and the importance of environmental assessment and monitoring. Prevention possibilities.

2nd week

The basic types of environmental samples and their classification regarding spheres, state and homogeneity. Discussion of the features of inorganic and organic compounds usually focused by environmental analysis, however the inorganic analytes will be highlighted. The general rules of sampling, sample storage and preservation. Sampling strategies.

3rd week

Sample pre-treatment strategies and basic rules of dissolution. Solubility features of the analyte, grouping of applied reagents and methods. High temperature reactions under acidic and basic conditions. Mineralization techniques of organic materials. Eliminating the sample matrix and mobilization of the measured compounds.

4th week

The most widely used sampling pre-treatment techniques: dilution, dry and wet digestion, wet digestion at atmospheric pressure and under high pressure, microwave digestion, extraction methods. Chemicals and reagents used to gain the inorganic analyte from the environmental samples. Advantages and disadvantages of the sample treatment possibilities.

5th week

The most important water quality parameters, the theoretical background of them and their direct connection to environmental assessment. Chemical oxygen demand, biological oxygen demand, ions affecting halobity, saprobity categories, oxygen saturation etc. Classical and instrumental analytical methods to determine these parameters. Limits and regulations connected to water quality control.

6th week

Biological indicators and their role in environmental analysis. Biotic and abiotic indicators, active and passive indication, accumulation, biomagnification, bioaccumulation factor. Indicator species and their application possibilities.

7th week

Elemental analytical techniques in environmental chemistry: destructive and non-destructive possibilities. FAAS. GFAAS, ICP-OES and ICP-MS applications in environmental chemistry. The importance of elemental speciation in environmental assessment (Cr, As and Hg species and their effect on biological systems).

Requirements:

- *for a signature*

Attendance at **lectures** is recommended, but not compulsory. However, a 5-6 minutes of power point presentation must be held from a chosen environmental issue and students will talk and discuss about it during the lecture. Giving the presentation is compulsory, missing it means signature denied in the electronic system and one must take the course in the next semester.

- *for a grade*

Students will put together a 5-6 minutes of power point presentation regarding a freely chosen environmental issue and also write a short, maximum 10 pages of essay discussing the problem. The average of the two grades will form the final one.

- *for an offered grade*

no grade will be offered

Person responsible for course: Dr. Edina Baranyai, assistant professor, PhD

Lecturer: Dr. Edina Baranyai, assistant professor, PhD

Title of course: Inorganic Methods in Environmental Analysis II. **Code**: TTKML0503_EN	**ECTS Credit points:** 4
Type of teaching, contact hours - lecture: - - practice: - - laboratory: 4 hours/week	
Evaluation: short tests, general test and laboratory manuals to form the practical grade	
Workload (estimated), divided into contact hours: - lecture: - - practice: - - laboratory: 56 hours - home assignment: 44 hours - preparation for the exam: 20 hours Total: 120 hours	
Year, semester: 1st year, 1st semester	
Its prerequisite(s): -	
Further courses built on it: -	

Topics of course
The aim of the laboratory practice is to introduce the most important chemical analysis to determine the inorganic components of environmental samples. Chemical oxigen demand, dissolved oxigen, anions and cations affecting the halobity will be determined from surface water, inorganic contaminants, trace minerals and macro elements from soil and plants, ammonia from the atmosphere. Students are working in groups and 2 occasions are available to finish one series of experiments. During the last 4 practices own project tasks will be carried out based on the supervisior's instructions.
Literature
Compulsory: - Practical syllabus available at the Department's home page (inorg.unideb.hu) *Recommended:* -Environmental Chemistry by banez, J.G., Hernandez-Esparza, M., Doria-Serrano, C., Fregoso-Infante, A., Singh, M.M., Springer-Verlag New York - R. Reeve: Introduction to environmental analysis, Wiley, 2002. - J.R. Dean: Methods for Environmental Trace Analysis, Wiley, 2003.
Course objective/intended learning outcomes
a) Knowledge

- He/She has global knowledge on science other than chemistry, and capable to organize this information.
- He/She knows various methods from chemical labs or industries, able to show it to other people and apply them including the equipments and their safe usage.
- He/She can understand and communicate professionally on chemical subjects at his/her native language

b) Abilities

- He/She is able to recognize and evaluate the global relationships on the field of chemistry.
- He/She is able to distinguish between the scientifically proven theories and non-reliable data or information
- He/She is able to evaluate experimental data, analyze them and draw conclusions. Based on these results he/she can present new trend sin research or development without supervision.

c) Attitude

- He/She is committed to protect the environment in both chemical labs and industries. These attitudes are shown to other coworkers as well. He/she makes effort to apply those technologies that makes lower environmental changes/loads.
- He/She is receptive to establish and apply new chemical and environmental technologies.

d) Autonomy and responsibility

- He/She is responsible for his/her own decisions, stand in for these decisions and ideologies.
- He/She recognizes the unsafe environment both in laboratory on industry, and makes decisions according to this.
- He/She can operate chemical or industrial instruments or equipment with responsibility, and manage persons working with these.

Schedule: 2 practical occasions (2*4 hours) are available to finish one series of experiments. During the last 3 practices own project tasks will be carried out based on the supervisior's instructions.

1st week

General introduction to the basic laboratory safety rules and applied pieces of laboratory equipment.

2nd week

Short test writing of the theoretical background of the laboratory material. Water sampling from the Botanical garden. Determination of the dissolved oxygen concentration and chemical oxygen demand of surface water by permanganometric and iodometric titration methods. Calculation of the oxygen saturation. (Part I.)

3rd week

Water sampling from the Botanical garden. Determination of the dissolved oxygen concentration and chemical oxygen demand of surface water by permanganometric and iodometric titration methods. Calculation of the oxygen saturation. (Part II.) Laboratory manual due in.

4th week

Short test writing of the theoretical background of the laboratory material. Water sampling from the Botanical garden. Determination of the inorganic ion composition of standing surface water: chloride ion by argentometric titration, sulphate ion by spectrophotometry, carbonate and hydrogen carbonate ion by acid-base titration, sodium, potassium, calcium and magnesium ions by microwave plasma atomic emission spectrometry. Building up the Maucha type diagram indication the ionic concentration of water affecting halobity. (Part I.)

5th week

Water sampling from the Botanical garden. Determination of the inorganic ion composition of standing surface water: chloride ion by argentometric titration, sulphate ion by spectrophotometry, carbonate and hydrogen carbonate ion by acid-base titration, sodium, potassium, calcium and magnesium ions by microwave plasma atomic emission spectrometry. Building up the Maucha type diagram indication the ionic concentration of water affecting halobity. (Part II.) Laboratory manual due in.

6th week

Short test writing of the theoretical background of the laboratory material. Elemental analysis of plant samples. Comparsion of atmospheric wet digestion carried out with the mixture of concentrated acids and oxidizing agents on an electric hot plate with dry digestion in crucibles placed in electric owen. Determination of concentration of a chosen element by flame atomic absorption spectrometry. (Part I.)

7th week

Elemental analysis of plant samples. Comparsion of atmospheric wet digestion carried out with the mixture of concentrated acids and oxidizing agents on an electric hot plate with dry digestion in crucibles placed in electric owen. Determination of concentration of a chosen element by flame atomic absorption spectrometry. (Part II.) Laboratory manual due in.

8th week

Short test writing of the theoretical background of the laboratory material. Wet digestion of soils in either a microwave or a thermal block system by the mixture of concentrated acids and oxidation agents. The complex macro and micro elemental profile will be quantitatively determined by microwave plasma atomic emission spectrometry. (Part I.)

9th week

Determination the elemental composition of soil samples. Wet digestion of soils in either a microwave or a thermal block system by the mixture of concentrated acids and oxidation agents. The complex macro and micro elemental profile will be quantitatively determined by microwave plasma atomic emission spectrometry. (Part II.) Laboratory manual due in.

10th week

Short test writing of the theoretical background of the laboratory material. Nitrite ion detection from water samples by spectrophotometry. Determination of the Arany type texture coefficient as well as the carbonate content of soil samples (Scheibler type calcimeter). (Part I.)

11th week

Determination of ammonium from the laboratory air by absorption method combined with spectrophotometry. Nitrite ion detection from water samples by spectrophotometry. Determination of the Arany type texture coefficient as well as the carbonate content of soil samples (Scheibler type calcimeter). (Part II.) Laboratory manual due in.

12th week

Laboratory work on an own project in groups previously discussed with the supervisor where the studied techniques and methods can be applied. (Project work Part I)

13th week

Laboratory work on an own project in groups previously discussed with the supervisor where the studied techniques and methods can be applied. (Project work Part II)

14th week

General written test of the theoretical background and application of the gained knowledge. Finishing the project work, discussion of the results. Laboratory manual of the project work due in.

Requirements:
- *for a signature*
Attending the laboratory practices is obligatory. Only one absence is allowed but along with a medical certificate proving illness. Students write a short test before each experimental part (all together 5) and also a general test at the very last occasion. The average of the short tests also the general test result must be above 20% to gain a signature. If either the short tests or the general test is under 20%, the signature will be denied in the electronic system and the student must take the course again in the next semester.
- *for a grade*
Students write a short test before each experimental part (all together 5) and also a general test at the very last occasion which will be evaluated according to the following table:

Score	Grade
0-49	fail (1)
50-65	pass (2)
66-79	satisfactory (3)
80-89	good (4)
90-100	excellent (5)

Students will also handle in 5 laboratory manuals considering the practical work and one extra about the chosen project work. They will receive one grade as the average of the laboratory manuals, one as the average of the short tests and one for the general test. The three individual grades will be averaged to get the final one.
If the final grade is not reaching the passing mark then students will have one more occasion to take a written exam in the examination period. The exam is in conformity with the EDUCATION AND EXAMINATION RULES AND REGULATIONS.
- *for an offered grade*
no grade will be offered

Person responsible for course: Dr. Edina Baranyai, assistant professor, PhD

Lecturer: Dr. Edina Baranyai, assistant professor, PhD

Title of course: Quality Assurance in Analytical Chemistry
Code: TTKME0513_EN

ECTS Credit points: 1

Type of teaching, contact hours
- lecture: 1 h / week
- practice: –
- laboratory: –

Evaluation: exam

Workload (estimated), divided into contact hours:
- lecture: 14 h

- practice: – - laboratory: – - home assignment: – - preparation for the exam: 20 h Total: 34 h
Year, semester: 2^{nd} year, 2^{nd} semester
Its prerequisite(s): –
Further courses built on it: –

Topics of course
The material of the lecture covers the fundamental aspects of Quality Assurance (QA) and Quality Control (QC) in the chemical and pharmaceutical industry, and chemical safety. The course begins with describing the controlling and technical requirements of the supporting analytical laboratories. The next chapter covers the most important aspects of quality assurance and quality control in the pharmaceutical industry. The directives and the fundamental requirements of Good Manufacturing Practice (GMP) and Good Laboratory Practice (LCP) are discussed. The rules concerning the active pharmaceutical ingredients and the final pharmaceutical formulations are reviewed. The last chapter is dealing with chemical safety. The rules of the hazard classification of chemicals and their environmental and toxicological effects are overviewed. Environment and health protection, workplace safety regulations (EHS) together with the directives of REACH are reviewed.
Literature
Compulsory: 1) Matthias Otto: Chemometrics WILEY-VCH Verlag GmbH, Weinheim, Germany, 1999. 2) Richard G. Brereton: Applied Chemometrics for Scientists John Wiley & Sons Ltd, Chichester, England, 2007. 3) D. L. Massart. B. G. M. Vandeginste, S. N. Deming, Y. Michotte, and L. Kaufman: Chemometrics: A textbook. Elsevier, Amsterdam, The Netherlands, 1988.
Course objective/intended learning outcomes
a) Knowledge - He/she fundamentally knows principles and means of Quality Assurance, Quality Control and chemical safety. - He/she expansively knows the operating principles of GLP qualified supporting analytical laboratories and GMP qualified manufacturing facilities. - He/she expansively knows the operating principles of Environment, Health and Safety rules. **b) Abilities** - He/she is able to apply the most important terminology, theories, procedures of QC, QA, GLP, GMP, EHS and REACH when completing the relevant tasks. - He/she is able to create fundamental models for QA and QC processes.

c) Attitude

- He/she is open to learn and accept professional, technological improvement and innovation in his/her profession and convey it genuinely.
- He/she makes a decision in complex and unexpected decision cases by completely taking into account legal and ethical norms.

d) Autonomy and responsibility

- Even in unexpected decision-making situations he/she is capable of considering complex, fundamental questions from his/her professional field and elaborating them on the basis of the given sources.
- He/she confesses and represents the value system of the engineering profession with responsibility. He/she is open to critical remarks which are professionally well-founded.

Schedule:

1st week
Quality Control systems. Requirements

2nd week
Controlling requirements for supporting analytical laboratories.

3rd week
Technical requirements for supporting analytical laboratories.

4th week
Good Manufacturing Practice (GMP) and Good Laboratory Practice (GLP).

5th week
Quality Assurance (QA) and Quality Control (QC) in the pharmaceutical industry.

6th week
Regulations concerning chemicals.

7th week
Chemical safety, REACH.

Requirements:

- *for a signature*

Attendance at **lectures** is recommended, but not compulsory. Participating in an exam earns the signature.

- *for a grade*

The course ends in a **written examination**.
Based on the score of the written examination the grade is given according to the following table:

Score	Grade
0-50	fail (1)
51-60	pass (2)
61-70	satisfactory (3)
71-80	good (4)
81-100	excellent (5)

If the score of the oral exam is below 51%, students can take a retake the exam in conformity with the EDUCATION AND EXAMINATION RULES AND REGULATIONS.

Person responsible for course: József Kalmár, Ph.D., assistant professor
Lecturer: József Kalmár, Ph.D., assistant professor

Title of course: Mass Spectrometry **Code**: TTKME0317_EN	**ECTS Credit points:** 4
Type of teaching, contact hours - lecture: 2 hours/week - practice: 1 hour/week - laboratory: -	
Evaluation: exam	
Workload (estimated), divided into contact hours: - lecture: 28 hours - practice: 14 hours - laboratory: - - home assignment: 30 hours - preparation for the exam: 48 hours Total: 120 hours	
Year, semester: 2nd year, 2nd semester	
Its prerequisite(s): -	
Further courses built on it: -	

Topics of course
Operation of ion sources, such as EI, ESI, APPI, APCI, DART, MALDI, their applicability on different compounds. Analysis of additives in household goods and nicotine adsorbed on clothes using DART technique. Studying combined techniques, such as GC-MS and HPLC-MS. Application of combined techniques for the analysis of natural samples, such as hot peppers, tropical fruits, spirits, caffeine. Discussion of scientific articles on mass spectrometry in the literature.
Literature
Compulsory: - Edmond de Hoffmann, Vincent Stroobant: Mass Spectrometry: Principles and Applications (Wiley, 2013) ISBN: 978-0-470-03310-4 - Jürgen H. Gross: Mass Spectrometry – A Textbook (Springer, 2017) ISBN 978-3-319-54398-7 - Michael L. Gross, Richard M. Caprioli: The Encyclopedia of Mass Spectrometry (Elsevier, 2006) ISBN: 9780080438016 *Recommended:* - Alison E. Ashcroft: Ionization Methods in Organic Mass Spectrometry (RSC Publishing, 1997) ISBN: 978-0-85404-570-9

Course objective/intended learning outcomes

a) Knowledge
- He/She knows various methods from chemical labs or industries, able to show it to other people and apply them including the equipments and their safe usage.
- He/She has knowledge to solve problems on the field of natural processes, using natural sources, and understanding the chemical background of living and non-living systems.

b) Abilities
- He/She is able to recognize and evaluate the global relationships on the field of chemistry.
- Using the knowledge and experiences during the MSc coursed he/she is able to execute laboratory experiments or measurements to demonstrate proper chemical phenomena, or syntheses of new compounds and characterize them, and using analytical methods for provement of new reactions.

c) Attitude
- He/She is receptive to establish and apply new chemical and environmental technologies.
- He/She is open to collaborate with professionals on the field of social sciences, economy and environmental safety , treating the new chemical trends critically but carefully.

d) Autonomy and responsibility
- He/She evaluates his coworkers in a professional way.
- He/She is responsible in collaboration with other professionals (especially from the field of environmental economy and safety) without supervision.

Schedule:

1st week
Principles of Electrospray Ionization (ESI), its applications.

2nd week
Principles of Atmospheric Pressure Photoionization (APPI), its applications..

3rd week
Principles of Atmospheric pressure chemical ionization (APCI), its applications.

4th week
Principles of Direct analysis in real time (DART), its applications.

5th week
Principles of Matrix-Assisted Laser Desorption Ionization (MALDI), its applications.

6th week
Review of combined techniques, their applicability.

7th week
Application of HPLC-ESI combined technique to determine the capsaicine concentration in different hot pepper samples.

8th week
Principles of Electron Ionization (EI), the basics of GC-MS technique.

9th week
Application of GC-MS for the identification of volatile oils in tropical fruits.

10th week
Quality analysis of spirits by GC-MS technique.
11th week
Analysis of additives in household goods by DART technique.
12th week
Studying passive smoking by the analysis of nicotine adsorbed on clothes using DART technique.
13th week
Analysis of caffeine in different coffee samples using HPLC-MS technique.
14th week
Discussion of the scientific articles found in the literature.

Requirements:
- *for a signature*
Attendance at **lectures** is recommended, but not compulsory. Active participation is rewarded by the teacher in every class. Participation at **practice classes** is compulsory. A student must attend the practice classes and may not miss more than three times during the semester. In case a student does so, the subject will not be signed and the student must repeat the course. Attendance at practice classes will be recorded by the practice leader. Being late is equivalent with an absence. In case of further absences, a medical certificate needs to be presented. Missed practice classes should be made up for at a later date, to be discussed with the tutor.
During the semester there is one end-term test in the 15th week for an offered grade (optional). Students have to sit for the tests.
- *for a grade*
The course ends in an **examination**.
The minimum requirement for the end-term test and the examination respectively is 50%. Based on the score of the test, the grade for the test and the examination is given according to the following table:

Score	Grade
0-49	fail (1)
50-61	pass (2)
62-74	satisfactory (3)
75-87	good (4)
88-100	excellent (5)

If the score the test is below 50, students can take a retake test in conformity with the Education and Examination Rules and Regulations.
-an offered grade:
it may be offered for students if the grade of the end-term test is at least satisfactory (3).

Person responsible for course: Prof. Sándor Kéki, full professor, PhD, DSc

Lecturers: Prof. Sándor Kéki, full professor, PhD, DSc; Dr. Tibor Nagy, assistant professor

Title of course: Electrophoretic techniques **Code**: TTKME0504_EN	**ECTS Credit points:** 3

Type of teaching, contact hours
- lecture: 2 hours/week, (for corresponding students 8 hours/semester)
- practice: -
- laboratory:

Evaluation: examination

Workload (estimated), divided into contact hours:
- lecture: 48 hours
- practice: -
- laboratory: -
- home assignment: -
- preparation for the exam: 42

Total: 90 hours

Year, semester: 2^{nd} year, 2nd semester

Its prerequisite(s):

Further courses built on it:

Topics of course

The course surveys the history, methods, theories, fundamentals and some practical aspects of analysis of the electrophoresis. Important additional topics are the capillary electrophoresis, chip electrophoresis (lab-on-a-chips) and hyphenation of capillary electrophoresis with mass spectrometry. The course is connected to some topics of the Instrumental Analysis lecture and complete the knowledge acquired in BSc level.

Literature

1. H.Engelhardt, W.Beck, T.Schmitt: Capillary electrophoresis, Friedr.Vieweg & Sohn Verlagsgesellschaft mbH, Braunschweig/Wiesbaden, 1996 (ISBN 3-528-06668-7)
2. R.Kuhn, S.Hoffstetter-Kuhn: Capillary electrophoresis, Springer-Verlag, New York, 1993 (ISBN 0-387-56434-9)
3. F.Foret, L.Kriváanková, P.Bocek: Capillary Zone Electrophoresis, VCH-Weinheim, 1993, (ISBN 3-527-30019-8)
4. D.N.Heiger: High Performance Capillary Electrophoresis, Hewlett-Packard GmbH, Waldbronn, 1992 (ISBN 12-5091-6199E)

Course objective/intended learning outcomes

a) Knowledge
- He/she fundamentally knows principles and means of slab gel electrophoresis and capillary electrophoresis, sample pretreatment, data evaluation and validation of the measurements.
- He/she expansively knows the operating principles of the electrophoresis, auxiliary devices.

b) Abilities

- He/she is able to apply the most important terminology, theories, procedures of the given instrumental analysis field when completing the relevant tasks.
- He/she is able to find solutions for the analytical problems.

c) Attitude

- He/she is open to learn and accept professional, analytical and electrophoretic improvement and innovation in his/her profession and convey it genuinely.
- He/she makes a decision in complex and unexpected decision cases by completely taking into account legal and ethical norms.

d) Autonomy and responsibility

- Under supervision he/she is responsible in collaboration with other professionals (especially from the field of analytical and environmental economy and safety).
- He/she confesses and represents the value system of the instrumental analytical profession with responsibility. He/she is open to critical remarks which are professionally well-founded.

Schedule:

1st week: History and importance of electrophoresis, expected future trends (2h)

2nd week: Theory of the electrophoretic migration (2h)

3rd week: Paper electrophoresis, isoelectric focusing, isotachophoresis (2h)

4th week: Gel electrophoresis, polyacrilamide gel electrophoresis (2h)

5th week: DNA sequencing with automatic capillary electrophoretic systems. Human Genome Project (2h)

6th week: The construction and operation of capillary electrophoresis instrument (2h)

7th week: Detection methods applicable to capillary electrophoresis (UV-Vis, amperometry, conductometry, LIF, MS) (2h)

8h week: Techniques of capillary electrophoresis (2h)

9th week: Principles of optimization for capillary electrophoresis I. (2h)

10th week: Principles of optimization for capillary electrophoresis II. (2h)

11th week: Main application fields of capillary electrophoresis (2h)

12th week: Lab-on-a-chip technology, microfluidics, miniaturized analytical systems (2h)

13th week: Commercial microfluidic analytical devices (Bioanalyzer 2100, LabChip, HPLC-chip MS) (2h)

14th week: Detection methods applicable to capillary electrophoresis (UV-Vis, amperometry, conductometry, LIF, MS) (2h)
Requirements: Attendance at lectures is recommended, but not compulsory. The course ends in an examination. The minimum requirement for the examination is 50%. Based on the score of the test, the grade is given according to the following table: Score Grade 0-50 fail (1) 50-69 pass (2) 70-79 satisfactory (3) 80-89 good (4) 90-100 excellent (5)
Person responsible for course: Dr. Attila Gáspár, professor, DSc
Lecturer: Dr. Attila Gáspár, professor, DSc

Title of course: Sampling, Sample Treatment, Analytical Tests **Code**: TTKME0514_EN	**ECTS Credit points:** 1
Type of teaching, contact hours - lecture: 1 hours/week - practice: - - laboratory: -	
Evaluation: exam	
Workload (estimated), divided into contact hours: - lecture: 14 hours - practice: - - laboratory: - - home assignment: - - preparation for the exam: 16 hours Total: 30 hours	
Year, semester: 1st and 2nd year, 2nd semester	
Its prerequisite(s): -	
Further courses built on it: -	

Topics of course

The aim of the course is to introduce the sampling methods generally applied in environmental chemistry. The most important techniques for sampling soil, sediment, surface and underground water, gases, biotic and abiotic bioloical indicators, biological tissues and fluids, rocks and metal alloys will be discussed. All the relevant and most important pre-treatment techniques will be overviewed which are necessary to get rid of the matrix components prior to the quantitative and qualitative determination of organic and inorganic analytes (such as extraction and dilution techniques, atmospheric and microwave digestion, acidic and basic reactions under high pressure etc.). Sampling and sample pre-treatment methods will be discussed which are used for speciation analysis, for organometallic compounds and biomolecules.

Literature

Compulsory:

-Fundamentals of environmental sampling and analysis by Chunlong Zhang (ISBN: 978-0-471-71097-4)

Recommended:

- N.T. Crosby, I. Patel: General principles of good sampling practice, RSC,1995
- S. Mitra: Sample Preparation Techniques in Analytical Chemistry, Wiley, 2003.
- Sampling for Environmental Data Generation; P. Grieco and R. Trattner, SciTech Publishers, Matawan, NJ 1990.
- https://web.njit.edu/~kebbekus/analysis/SAMPLING.htm

Course objective/intended learning outcomes

a) Knowledge

- Have systematic knowledge on the various subject of chemistry, their main principals including the theoretical and practical application built on these principals.
- He/She has knowledge to solve problems on the field of natural processes, using natural sources, and understanding the chemical background of living and non-living systems.

b) Abilities

- He/She is able to carefully apply the newest chemical theories in practice and design lab experiments or industrial processes based on these results.
- He/She is able to evaluate experimental data, analyze them and draw conclusions. Based on these results he/she can present new trend sin research or development without supervision.

c) Attitude

- He/She is being active to start and participate in professional discussions
- He/She is committed to get new knowledge and competences, widening his/her ideology, and makes effort to evolve him/her.

d) Autonomy and responsibility

- He/She is responsible for his/her own decisions, stand in for these decisions and ideologies.

Schedule: The lecture will be held in the first half of the semester, 2 hours/week

1st week

The grouping of environmental samples, sample types. The thematic classification of the most commonly measured components from environmental samples. The basic rules of sampling and the

general description of sampling techniques.
2nd week
General statistical aspects of sampling. Liquid sampling: surface and underground water, rivers and streams. Solid sampling of metals, alloys and rocks. General guidelines, homogenization methods.
3rd week
Sampling from gases at atmospheric and high pressure. Direct sampling of solid materials from gaseous substances: aerosols and particulate matter (PM 10, PM 2.5). Adsorption and absorption techniques to selectively gain compounds from gaseous state, gas filtration. Sampling of soil, sediment and biological tissues.
4th week
Introduction to basic sample pre-treatment methods: homogenisation and drying of solid substances, circumstances affecting the solubility of the analyte. Storage, preservation and dissolving methods. Extraction techniques.
5th week
Reactions to eliminate the matrix and mobilize the compounds to be determined: dry and wet digestion methods, ignition, digestion at atmospheric pressure, microwave assisted sample pre-treatment. Digestion under acidic and basic conditions, most commonly applied reagents and pieces of equipment.
6th week
General introduction to the sampling and sample pre-treatment carried out for speciation analysis and organometallic substances, as well as biomolecules. Elemental speciation.
7th week
Sample preparation of biological indicators and biological tissues, fluids. Exact examples of a complex sampling and sample pre-treatment process, discussing the steps of tasks to be carried out. Review and consultation possibility.

Requirements:
- for a signature
Attendance at **lectures** is recommended, but not compulsory. However, students attending 5 out of the 7 occasions will have the opportunity to write a written test after the last lecture: if it is successful **a grade will be offered** in the electronic system which can be accepted or denied by the student.
- for a grade
The course ends in an **examination**. The students will either successfully fulfil the requirements to write the written test for an offered grade or take an oral exam in the examination period.
The minimum requirement for the passing mark in the written test and the examination respectively is 50%. For the written test to gain the offered grade the following table will be applied to calculate the result:

Score	Grade
0-49	fail (1)
50-65	pass (2)
66-79	satisfactory (3)
80-89	good (4)
90-100	excellent (5)

If the score of the written test is below 50, students can take the oral exam in the examination period

which is the same for those students not visiting the lectures regularly. The exam is in conformity with the EDUCATION AND EXAMINATION RULES AND REGULATIONS. - *for an offered grade* Please see above highlighted with bold characters.
Person responsible for course: Dr. Edina Baranyai, assistant professor, PhD
Lecturer: Dr. Edina Baranyai, assistant professor, PhD

Title of course: Sampling, Sample Treatment, Analytical Tests **Code**: TTKML0514_EN	**ECTS Credit points:** 4
Type of teaching, contact hours - lecture: - - practice: - - laboratory: 4 hours/week	
Evaluation: practical grade based on laboratory manual and written test	
Workload (estimated), divided into contact hours: - lecture: - - practice: - - laboratory: 56 hours - home assignment: 64 hours - preparation for the exam: - Total: 120 hours	
Year, semester: 1st and 2nd year, 2nd semester	
Its prerequisite(s): -	
Further courses built on it: -	

Topics of course
During the laboratory practice, the complex environmental assessment of a fishing lake will be carried out. Taken plant, water, soil and sediment samples will be analysed with the studied methods for the most important inorganic contaminants: chemical oxygen demand, cations and anions affecting halobity, dissolved oxygen, oxygen saturation, pH, conductivity, elemental composition. Both on site techniques, as well as classical and instrumental methods will be applied.
Literature
Compulsory: - Fundamentals of environmental sampling and analysis by Chunlong Zhang (ISBN: 978-0-471-71097-4) - University syllabus of environmental analysis (available at the Department's home page of inorg.unideb.hu)

Recommended:
- Sampling for Environmental Data Generation; P. Grieco and R. Trattner, SciTech Publishers, Matawan, NJ 1990.
- https://web.njit.edu/~kebbekus/analysis/SAMPLING.htm

Course objective/intended learning outcomes

a) Knowledge

- Have systematic knowledge on the various subject of chemistry, their main principals including the theoretical and practical application built on these principals.
- He/She has knowledge to solve problems on the field of natural processes, using natural sources, and understanding the chemical background of living and non-living systems.

b) Abilities

- He/She is able to carefully apply the newest chemical theories in practice and design lab experiments or industrial processes based on these results.
- He/She is able to evaluate experimental data, analyze them and draw conclusions. Based on these results he/she can present new trend sin research or development without supervision.

c) Attitude

- He/She is being active to start and participate in professional discussions
- He/She is committed to get new knowledge and competences, widening his/her ideology, and makes effort to evolve him/her.

d) Autonomy and responsibility

- He/She is responsible for his/her own decisions, stand in for these decisions and ideologies.

Schedule: The third occasion will be a whole day (8 hours) of sampling at a fishing lake which therefore equals with two practical occasions (2*4 hours).

1st week

Introduction to the general laboratory safety rules highlighting the safety considerations of on-site field study. Overview of the laboratory and on-site pieces of equipment and instruments.

2nd week

Introduction to the fishing lake to be sampled. The sample types to be taken and the compounds to be measured will be discussed, the analytical methods to be applied for the quantitative analysis will be chosen. Students will build up the sampling plan, make a map, indicate the sampling points and collect all the sampling tools from the laboratory which will be necessary to carry out the sampling and on-site measurements.

3rd week (2 4 hours)*

A full day trip to the fishing lake where the collection of surface water, sediment, soil and plant samples will be carried out. On site measurements of water pH and electric conductivity, temperature, preservation of samples for elemental analysis as well as the titration for dissolved oxygen and chemical oxygen demand will be carried out. Samples will be then taken to the laboratory for further measurements.

4th week

Determination of cation (macro and micro elements) concentration of the surface water samples by microwave plasma atomic emission spectrometry (MP-AES). Dilution of standard solutions and calibration required for the quantitative measurements.

5th week

Determination of the anion concentration affecting halobity from surface water samples by classical analytical and instrumental methods: carbonate and hydrogen carbonate ion by acid-base titration, chloride ion by argentometric titration and sulphate ion by spectrophotometric analysis.

6th week

Grinding and drying of soil samples, homogenization. Determination of the moisture content and organic matter content of soil samples and preparing them for elemental analysis by microwave assisted wet digestion at elevated pressure.

7th week

The elemental analysis of soil samples by microwave plasma atomic emission spectrometry (MP-AES). Dilution of standard solutions and calibration required for the quantitative measurements.

8th week

Grinding and drying of plant samples, homogenization. Determination of the moisture content of plant samples and preparing them for elemental analysis by conventional wet digestion at atmospheric pressure.

9th week

The elemental analysis of plant samples by microwave plasma atomic emission spectrometry (MP-AES). Dilution of standard solutions and calibration required for the quantitative measurements.

10th week

Cutting, grinding and drying of sediment samples, homogenization. Determination of the moisture content and organic matter content of sediment samples and preparing them for elemental analysis by microwave assisted wet digestion at elevated pressure.

11th week

The elemental analysis of sediment samples by microwave plasma atomic emission spectrometry (MP-AES). Dilution of standard solutions and calibration required for the quantitative measurements.

12th week

Evaluation of the gained results – calculating the final concentration results from the primer data of samples.

13th week

Written test regarding the field and laboratory work of sampling, sample pre-treatment and analysis of important environmental factors. Discussion of statistical analysis for the final evaluation and interpretation of the gained data. Finishing the laboratory manuals to be handled in. Washing up all the sample containers and pieces of equipment.

Requirements:

- *for a signature*

Attendance at **both the field study and laboratory practices are obligatory.** Maximum one occasion can be missed but only along with a medical certificate. The written test must be above 20% to get a signature, otherwise the student will receive a signature denied and must take the course again in the next semester.

- *for a grade*

The course ends in a written test. The minimum requirement for the passing mark in the written test is 50%. For calculating the grade of the test the following table will be applied:

Score	Grade
0-49	fail (1)
50-65	pass (2)
66-79	satisfactory (3)
80-89	good (4)
90-100	excellent (5)

If the score of the written test is below 50, students can take one final exam in the examination period, which will be similar to the written test. The exam is in conformity with the EDUCATION AND EXAMINATION RULES AND REGULATIONS.

Students will also handle in an electronic laboratory manual interpreting the overall results of the complex environmental assessment of the fishing lake. Grade will be given to this laboratory manual as well.

Final grade will be formed by taking the average of the results of the written test (or exam) and the laboratory manual.

- *for an offered grade*

no grade will be offered

Person responsible for course: Dr. Edina Baranyai, assistant professor, PhD

Lecturer: Dr. Edina Baranyai, assistant professor, PhD

Title of course: Chemometrics II. **Code**: TTKMG0512_EN	**ECTS Credit points:** 3

Type of teaching, contact hours
- lecture: –
- practice: 1 h / week
- laboratory: 2 h / week

Evaluation: midterm tests

Workload (estimated), divided into contact hours:
- lecture: –
- practice: 13 h
- laboratory: 26 h
- home assignment: 60 h
- preparation for the exam: 35 h

Total: 134 h

Year, semester: 1st year, 2nd semester

Its prerequisite(s): –

Further courses built on it: –

Topics of course

The material of the practice covers the fundamental aspects of applied Chemometrics. The course begins with descriptive statistics covering the normal distribution and the Poisson distribution. This is followed by statistical hypothesis testing (Q-test, t-test, ANOVA). Mathematical modelling is demonstrated through linear and non-linear least-squares fitting (regression analysis). The use of principal component analysis (PCA) and cluster analysis is demonstrated for pattern recognition. Classification is realized by linear discriminant analysis (LDA). Finally, the fundamental strategies of calibration in chemical analysis are covered, including multivariate calibration by the methods of partial least squares and principal component regression.

Literature

Compulsory:

1) Matthias Otto: Chemometrics
WILEY-VCH Verlag GmbH, Weinheim, Germany, 1999.
2) Richard G. Brereton: Applied Chemometrics for Scientists
John Wiley & Sons Ltd, Chichester, England, 2007.
3) D. L. Massart. B. G. M. Vandeginste, S. N. Deming, Y. Michotte, and L. Kaufman: Chemometrics: A textbook. Elsevier, Amsterdam, The Netherlands, 1988.

Course objective/intended learning outcomes

a) Knowledge

- He/she fundamentally knows principles and means of chemometrics, procedures and operating processes of statistics.
- He/she expansively knows the operating principles of regression analysis, principal component analysis, cluster analysis, partial least squares regression.

b) Abilities

- He/she is able to apply the most important terminology, theories, procedures of the given chemometrics field when completing the relevant tasks.
- He/she is able to create fundamental models of chemical systems and processes.

c) Attitude

- He/she is open to learn and accept professional, technological improvement and innovation in his/her profession and convey it genuinely.
- He/she makes a decision in complex and unexpected decision cases by completely taking into account legal and ethical norms.

d) Autonomy and responsibility

- Even in unexpected decision-making situations he/she is capable of considering complex, fundamental questions from his/her professional field and elaborating them on the basis of the given sources.
- He/she confesses and represents the value system of the engineering profession with responsibility. He/she is open to critical remarks which are professionally well-founded.

Schedule:

1st week

Descriptive statistics and statistical hypothesis testing through practical examples.

2nd week
Mathematical modelling through practical examples.
3rd week
Principal component analysis and cluster analysis through practical examples and experiments.
4th week
Principal component analysis and linear discriminant analysis through practical examples and experiments.
5th week
Calibration I: Technical aspects of multivariate techniques (PCR, PLS).
6th week
Calibration II: Multivariate techniques (PCR, PLS) through experiments.

Requirements:

- for a signature
Attendance at **practices and laboratories** is obligatory.
- for a grade
During the course, **4 midterm tests** will be written. Based on the average score of the midterm tests the grade is given according to the following table:

Score	Grade
0-50	fail (1)
51-60	pass (2)
61-70	satisfactory (3)
71-80	good (4)
81-100	excellent (5)

If the score of the oral exam is below 51%, students can take a retake the exam in conformity with the EDUCATION AND EXAMINATION RULES AND REGULATIONS.

Person responsible for course: József Kalmár, Ph.D., assistant professor

Lecturer: József Kalmár, Ph.D., assistant professor

Title of course: Nuclear Analysis I.
Code: TTKME0523_EN

ECTS Credit points: 3

Type of teaching, contact hours
- lecture: 2 hours/week
- practice: -
- laboratory: -

Evaluation: exam

Workload (estimated), divided into contact hours:
- lecture: 28 hours
- practice: -

- laboratory: - - home assignment: 22 hours - preparation for the exam: 40 hours Total: 90 hours
Year, semester: 2nd year, 1st semester
Its prerequisite(s): -
Further courses built on it: TTKML0523_EN

Topics of course
- Formation of nuclear, atomic and particle radiations. their interaction with matter, and analytical aspects. - Application of natural stable and radioactive isotope in natural sciences. - Tracer methods. - Nuclear and radioanalytical methods using the interactions of radiation with matter.
Literature
Compulsory: - Kónya, J., Nagy N.M., 2012, 2018. Nuclear and Radiochemistry, Elsevier, Oxford. - Choppin, G.R., Liljenzin, J-O., Rydberg, J. Ekberg, C., 2013. Radiochemistry and Nuclear Chemistry, 4th Edition, Elsevier, Amsterdam. - Kratz, J.-V., Lieser, K.H., 2013. Nuclear and Radiochemistry: Fundamentals and Applications, 3rd Edition, Wiley-VCH Verlag GmbH & Co. KGaA, Weinheim, Germany,
Course objective/intended learning outcomes
a) Knowledge - He/She has systematic knowledge on the nuclear and radioanalysis, their main principles including the theoretical and practical application built on these principals. - He/She understands the progress and future trends in nuclear and radioanalysis. **b) Abilities** - He/She is able to use the obtained chemical knowledge on the field of nuclear and radioanalysis to solve the actual basic problems and prove the obtained solution. - He/She is able to argue his/her opinion in scientific discussions both in oral or written form. **c) Attitude** - He/She is being active to start and participate in professional discussions. - He/She treats the scientific results or intellectual properties with the adequate professional ethics. **d) Autonomy and responsibility** - He/She is responsible in collaboration with other professionals (especially from the field of nuclear and radioanalysis) without supervision. - He/She is responsible for his/her own decisions stand in for these decisions and ideologies.

Schedule:

1st week
Formation and production of nuclear, atomic and particle radiation.
2nd week
Interaction of nuclear, atomic and particle radiation with matter.
3rd week
Analytical methods using natural radioactivity: determination of geological and historical ages.
4th week
Separation of isotopes. Physical, chemical, geological, and biological information obtained by observing isotope separations.
5th week
Basic rules of tracer studies
6th week
Selection of tracers. Production of tracer isotopes.
7th week
Chemical radioanalytical methods: isotope dilution analysis, radiometric titration, radio gravimetry, radiochemical separation methods.
8th week
Radioanalysis in living organisms: in-vitro and in-vivo methods.
9th week
Industrial radioanalysis.
10th week
Nuclear and radioanalytical methods based on radiation-matter interactions: classification, characterization on the basis of the irradiation and emitted particles/photons.
11th week
Applications of neutrons: activation analytical methods, neutron radiography and tomography, neutrons scattering.
12th week
Application of electromagnetic radiation with high energy (gamma, X-ray): X-ray fluorescence analysis, Mössbauer spectroscopy
13th week
Application of beta and electron radiation: beta backscattering, electron microscopes and microprobes.
14th week
Application of ions: Rutherford backscattering, particles induced X-ray and gamma spectroscopy.

Requirements:
- for a signature
Attendance at **lectures** is recommended, but not compulsory.
- for a grade
The course ends in an **examination**. Based on the examination, the exam grade is given according to the following table:

Score	Grade
0-59	fail (1)
60-69	pass (2)
70-79	satisfactory (3)

80-89	good (4)
90-100	excellent (5)

If the score of the examination is below 60, students can take a retake test in conformity with the EDUCATION AND EXAMINATION RULES AND REGULATIONS.

-an offered grade:

It may be offered for students if they write a test on the 14th week and the score of it is at least 60%. The offered grade is calculated as the exam grade (see above).

Person responsible for course: Dr. Noémi Nagy, professor, DSc

Lecturer: Dr. Noémi Nagy, professor, DSc

Title of course: NMR Operator Training **II.** **Code**: TKML0530_EN	**ECTS Credit points:** 2

Type of teaching, contact hours
- practice: 2 hours/week

Evaluation: practical exam

Workload (estimated), divided into contact hours:
- practice: 28 hours
- preparation for the exam: 32 hours

Total: 60 hours:

Year, semester: 2nd year 1st or 2nd semester

Its prerequisite(s): TKBL0004_ EN or TTKML0004_EN

Further courses built on it: TTKMG0318_EN

Topics of course: practical laboratory course with the aim that students accomplishing the course will be able to record basic 2D homo- and heteronuclear correlated spectra on the 400/500 MHz high field NMR spectrometers without external help.

Literature

Compulsory: P.J. Hore, Nuclear Magnetic Resonance, ISBN 963 19 4426 3
Bruker TopSpin 3.x manuals (free download)
Recommended: James Keeler, Understanding NMR Spectroscopy, ISBN 0-470-01787-2
N.E. Jacobsen, NMR Spectroscopy Explained: Simplified Theory, Applications and Examples for Organic Chemistry and Structural Biology

Course objective/intended learning outcomes

a) Knowledge: firm knowledge of the basic principles of high resolution NMR spectroscopy.
Principles of pulsed Fourier NMR spectroscopy.

b) Abilities: to run Bruker NMR spectrometers using TopSpin software, record and process routine 1D and 2D ^{1}H/ ^{13}C NMR spectra, determine basic NMR parameters.
c) Attitude: critical and responsible concerning the obtained NMR spectra, with respect to general quality, accuracy etc.
d) Autonomy and responsibility: The main aim is the independent and autonomous usage of the sophisticated superconducting NMR spectrometers. Must pay attention to saving the technical conditions of the equipments, including the protection of supercon magnets from accidental failure.

Schedule:
1st week Safety rules in NMR laboratory with supercon magnets. Dangers for magnets and human beings. Principle of pulsed Fourier NMR. Hardware of 400/500 MHz spectrometers. Optimizing lock parameters, adjusting field homogeneity (shimming), tuning/matching of probehead for proton and carbon measurements. Calibration of 90 degree hard (non-selective) proton pulse.
2nd week Principle of 2D NMR spectroscopy. Concept of indirectly detected, 2nd dimension. Recording magnitude 2D COSY spectrum. Explanation of important experimental parameters. Choice of spectral window, number of acquired data points, number of incremented delays, number of transients, etc. Processing 2D raw data – 2D Fourier transformation. Explanation of signals, diagonal- and cross-peaks in resulting spectra.
3rd week Exercising tuning/matching of probehead and pulse calibration. Exercising acquisition and processing of 2D COSY spectrum.
4th week Principle of 2D TOCSY experiment. Explanation of relevant experimental parameters. Calculating and/or calibrating the optimal power level for the TOCSY mixing block. Recording phase sensitive 2D TOCSY spectrum. Processing phase-sensitive 2D data – 2D Fourier transformation, phase correction in both dimensions. Explanation of signals in the resulting TOCSY spectra. Assignment of spin systems.
5th week Exercising tuning/matching of probehead and pulse calibration. Calculation of TOCSY power level. Exercising acquisition and processing of 2D TOCSY spectrum. Practicing phase correction.
6th week Principle of 2D HSQC experiment. Explanation of relevant experimental parameters. Recording gradient- and sensitivity enhanced, phase sensitive 2D HSQC spectrum. Processing phase-sensitive 2D data – 2D Fourier transformation, phase correction and chemical shift referencing in both dimensions. Explanation of signals in the resulting HSQC spectra.
7th week Exercising tuning/matching of probehead for proton and carbon frequencies, pulse calibration. Exercising acquisition and processing of 2D HSQC spectrum. Practicing phase correction and chemical shift calibration.
8th week Principle of 2D NOESY/ROESY experiments. Explanation of relevant experimental parameters. Calculating and/or calibrating the optimal power level for the ROESY mixing pulse. Recording phase sensitive 2D ROESY spectrum. Processing phase-sensitive 2D data – 2D Fourier transformation, phase correction in both dimensions. Explanation of signals (intensities and phases of diagonal and crosspeaks) in the resulting ROESY spectra. Merits and limitations: ROESY vs. NOESY.
9th week Exercising acquisition and processing of 2D ROESY spectrum. Practicing phase correction, calibration, chemical shift referencing.
10th week Principle of 2D HMBC experiment. Explanation of relevant experimental parameters. Recording magnitude 2D HMBC spectrum. Processing 2D raw data, chemical shift referencing in both

dimensions. Explanation of signals in the resulting HMBC spectra. *11th week* Exercising tuning/matching of probehead for proton and carbon frequencies, pulse calibration. Exercising acquisition and processing of 2D HMBC spectrum. *12th week* Exercising acquisition and processing of 2D COSY spectrum, one by one. *13th week* Exercising acquisition and processing of 2D HSQC spectrum, one by one. *14th week* Exercising acquisition and processing of 2D spectra, one by one.
Requirements: - *for a signature* Attendance of laboratory exercises is compulsory. A student must attend the practice classes and may not miss more than two times during the semester. In case a student does so, the subject will not be signed and the student must repeat the course. A student can't make up any practice with another group. Attendance at practice classes will be recorded by the practice leader. Being late is equivalent with an absence. In case of further absences, a medical certificate needs to be presented. Missed practice classes should be made up for at a later date, to be discussed with the tutor. Active participation is evaluated by the teacher in every class. If a student's behaviour doesn't meet the requirements of active participation, the teacher may evaluate his/her participation as an absence because of the lack of active participation in class. - *for a grade* The course ends in a **practica**l **exam**. Based on the average of the grades of two practical tasks, the exam grade is calculated as an average of them: - the average grade of the two tasks - recording and processing 2D COSY and HSQC spectra
Person responsible for course: Prof. Katalin E. Kövér, professor, DSc.
Lecturer:

Title of course: Analysis of proteins **Code**: TTKME0506_EN	**ECTS Credit points: 2**
Type of teaching, contact hours - lecture: 2 hours/week, (for corresponding students 8 hours/semester) - practice: - - laboratory:	
Evaluation: examination	
Workload (estimated), divided into contact hours: - lecture: 48 hours - practice: - - laboratory: - - home assignment: - - preparation for the exam: 42 Total: 90 hours	

Year, semester: 2^{nd} year, 2st semester
Its prerequisite(s): TTKME0501_EN
Further courses built on it:

Topics of course

The course surveys the history, methods, theories, fundamentals and some practical aspects of analysis of proteins. Important additional topics are the chromatography, electrophoresis, labelling methods, mass spectrometry and isothermal titration calorimetry. The course is connected to some topics of the Instrumental Analysis laboratory practices and complete the knowledge acquired in BSc and MSc level.

Literature

Daniel C. Harris: Quantitative Chemical Analysis, 7th Ed., 2007, Freeman and CoH.H.
Willard, L.L. Merritt, J.A. Dean, F.A. Settle: Instrumental methods of Analysis, Wadsworth Publ. Co., Belmont, 1988.
Douglas A. Skoog, Donald M. West, F. James Holler, Stanley R. Crouch: Fundamentals of Analytical Chemistry, 8th. ed., 2004, Brooks/Cole

Course objective/intended learning outcomes

a) Knowledge

- He/she fundamentally knows principles and means of instrumental analysis, sample pretreatment, data evaluation and validation of the measurements, which are applicable for the analysis of proteins.
- He/she expansively knows the operating principles of the instrumental analysis, auxiliary devices applicable for protein analysis.

b) Abilities

- He/she is able to apply the most important terminology, theories, procedures of the given instrumental analysis field applicable for protein analysis when completing the relevant tasks.
- He/she is able to find solutions for the analytical problems of proteins.

c) Attitude

- He/she is open to learn and accept professional, analytical improvement and innovation in his/her profession and convey it genuinely.
- He/she makes a decision in complex and unexpected decision cases by completely taking into account legal and ethical norms.

d) Autonomy and responsibility

- Under supervision he/she is responsible in collaboration with other professionals (especially from the field of analytical and environmental economy and safety).
- He/she confesses and represents the value system of the instrumental analytical profession with responsibility. He/she is open to critical remarks which are professionally well-founded.

Schedule:

1^{st} week: Definition, classification and goals of proteomics (2h)

2nd week: Post-translation modifications and their roles in biological activity of proteins (2h)

3rd week: The practice of proteomics. Bottom up and top down proteomics. (2h)

4th week: Chromatography of proteins. SEC, HIC, IEX, AC. (2h)

5th week: Hyphenated chromatographic systems. 2D chromatography, HPLC-MS. (2h)

6th week: Surface plasmon resonance spectroscopy (SPR) (2h)

7th week: Analysis of proteins with capillary electrophoresis (2h)

8h week: Microfluidic application in analytical chemistry. Lab-on-a-chip. Bioanalyzer 2100 (2h)

9th week: Proteomic analysis using mass spectrometry (2h)

10th week: Study of post-translation modifications using mass spectroscopy (2h)

11th week: Sequencing proteins by means of CE-MS/MS I. (2h)

12th week: Sequencing proteins by means of CE-MS/MS II. (2h)

13th week: Biologicum as the important product of the pharmaceutical industry (2h)

14th week: Analysis and study of monoclonal antibodies (2h)

Requirements:

Attendance at lectures is recommended, but not compulsory.
The course ends in an examination (written test).
The minimum requirement for the examination is 50%. Based on the score of the test, the grade is given according to the following table:

Score	Grade
0-50	fail (1)
50-69	pass (2)
70-79	satisfactory (3)
80-89	good (4)
90-100	excellent (5)

Person responsible for course: Dr. Attila Gáspár, professor, DSc

Lecturer: Dr. Attila Gáspár, professor, DSc

Title of course: Analytics in the Pharma Industry	**ECTS Credit points:** 4

Code: TTKML0520_EN	
Type of teaching, contact hours - lecture: - hours/week - practice: - hours/week - laboratory: 4 hours /week	
Evaluation: practical grade based on laboratory manual and written test	
Workload (estimated), divided into contact hours: - lecture: - - practice: - - laboratory: 84 hours - home assignment: 42 hours - preparation for the exam: - Total: 126 hours	
Year, semester: 1st year, 1st semester	
Its prerequisite(s): -	
Further courses built on it: -	

Topics of course

Laboratory course series provided within pharmaceutical laboratories aim to present the basis of analytical investigations as well as pharma regulations (GMP=Good Manufacturing Practice) to the students. The course is focussed on the analysis of the active pharmaceutical ingredients (API) production applying classic and instrumental technics.

The course reviews the significance of the analytical results and their documentation, the calibration of the balances and other instrumentation, the usage of certified weights and other certified standards. Students will deal with qualification of analytical standards and their use for determination of assay and related compound content of API including photometry, liquid chromatography, classic as well as instrumental titration. Non-related compounds of the API, such as counter ions, water and organic solvents will be determined by ion-chromatography, Karl-Fischer (KF) titration and headspace gas-chromatography (HSGC). Purity or composition of the solvents used in production will be analysed by gas-chromatography and near-infrared spectroscopy as an alternative technique. Volatile impurities are determined as loss on drying, the results will be compared with those obtained by HSGC and KF titration. Normal phase chromatography will be used as chiral chromatography for enantiomer separation.

Literature

Compulsory:

- L. Nádasdi (editor) (2010): Laboratory course for pharmaceutical analysis (TEVA in-house publication course attendees)

Course objective/intended learning outcomes

a) Knowledge

- He/she fundamentally knows the basic principles of analytical techniques applied in pharma industry including instrumental and classic techniques
- He/she knows how to use the laboratory instruments for analytical tests, he is aware in their capabilities and limitations, as well as he clearly knows the safety regulations related to analytical laboratories

b) Abilities

- He/she is able to evaluate the analytical results, he understands their significance. He is able to decide if the results are reliable or additional test has to be performed
- He/she is able to create a plan to qualify an API, he is able to perform instrumental and classic analytical tests for qualification of API
- He/she is able to apply his knowledge for innovation, research and development related to pharma industry

c) Attitude

- He/she is engaged against environmentally conscious behaviour in his laboratory work, he is open for application and development of new, environment-friendly analytical methods. He is engaged to accept and apply innovations in his professional field and convey it to his mates
- He/she is willing to perform professional discussion related to technologies and analytics

d) Autonomy and responsibility

- He/she is able to create his own statement related to his work and he is willing to assume the consequences of his decisions.
- He/she is aware of the safety background of the analytical activities, and he can make a decision in his professional filed with appropriate considerations
- He/she is aware of his responsibility on the utilisation of laboratory instrumentation.

Schedule:

1st week Safety training, handling of basic laboratory instruments and equipment (analytical balance, automatic pipettes, ultrasonic water bath) basic calculations, rules of rounding, evaluation and interpretation of the analytical results.

2nd week Basic gmp rules, documentation system of an R&D laboratory.

3rd week Determination of assay by photometry. Reference materials.UV-VIS spectroscopy

4th week Determination of assay by potentiometry. Komplexometry and redox titrations.

5th week Determination of solvent composition by NIR spectroscopy. IR/NIR spectroscopy.

6th week Water content determination by Karl Fischer (KF) titration and as Loss on drying. Basic principal of the KF titration. Coulometry and direct titration.

7th week The basis of the analytical chromatography. The construction of the HPLC, autosampler, pump, degasser, injector and detector. Analytical columns. Eluent/diluent preparation.

8th week Determination of assay of an active pharmaceutical ingredient by HPLC. The Empower software

9th week Chiral chromatography: determination of optical purity. Normal-Phase chromatography.

10th week Counter-ion determination by ion-chromatography. The Chromeleon software

11th week Impurity content determination by HPLC

12th week Impurity identification and quantification by MS detection with HPLC

13th week Identification and chromatographic purity GC. The construction of a gas-chromatograph, autosampler, injector and detector. Analytical columns. The Openlab software

14th week Residual solvent determination by GC

Requirements:

- *for a grade*

Attendance at **practical laboratory courses is** compulsory.

The student must attend the practical classes. If a course is missed, it has to be make up during the semester discussed with the lecturer. In case a student misses a course but does not make up, the subject will not be signed and the student must repeat the course. Being late is equivalent with being absent.

Before starting the lab course, the student has to prepare a lab notebook connected to the actual laboratory work including summary of theoretical principles and the short description of the practice. Before start of the manual work, short oral and/or written test is taken to ensure the lecturer if the student is aware of necessary knowledge to perform the tasks. After finishing the lab-work, the student completes the lab notebook and hand it in to the lecturer within one week. The lab notebook must include all calculations, results as well as the short summary/discussion of the results.

The course ends with a grade. Based on the grades of the individual courses and the oral/written tests, final grade will be calculated as their average.

Average	Final grade
<2.00	fail (1)
2.00-2.50	pass (2)
2.51-3.50	satisfactory (3)
3.51-4.50	good (4)
4.51-5	excellent (5)

Person responsible for course: András Zékány, TEVA Pharmaceutical Works Ltd

Lecturer: Levente Nádasdi, TEVA Pharmaceutical Works Ltd

Title of course: Reaction mechanisms **Code**: TTKME0311_EN	**ECTS Credit points:** 4
Type of teaching, contact hours - lecture: 4 hours/week - practice: - - laboratory: -	
Evaluation: oral examination	
Workload (estimated), divided into contact hours: - lecture: 56 hours - practice: - - laboratory: - - home assignment: - - preparation for the exam: 64 hours Total: 120 hours	
Year, semester: 1st year, 2nd semester	
Its prerequisite(s): -	
Further courses built on it: -	

Topics of course

The students will get acquainted with the most frequently applied methods and theories used to explain thermodynamic and kinetic aspects as well as specificity and selectivity relationships of organic chemical reactions. The following main topics will be handled: summary of thermodynamic and kinetic characteristics of chemical reactions; types of organic reactions and mechanisms; use of VB and MO methods to describe homo- and heteronuclear bonds; understanding of reactions by frontier orbital interactions; principles of least motion; stereoelectronic effects; characterization of solvents, solvent effects; application of the above principles to a range of selected ionic, pericyclic and radical reactions.

Literature

1. Fleming, I. *Frontier Orbitals and Organic Chemical Reactions*, Wiley, 1976.
2. Rauk, A. *Orbital Interaction Theory of Organic Chemistry*, Wiley, 1994.
3. Giese, B. *Radicals in Organic Synthesis: Formation of Carbon-Carbon Bonds*; Pergamon Press: Oxford, 1986.
4. Parsons, A. F. *An Introduction to Free Radical Chemistry*, Blackwell, 2000.
5. Alabugin, I. V. *Stereoelectronic Effects - A Bridge Between Structure and Reactivity,*

Wiley, 2016.
6. Savin, K. *Writing Reaction Mechanisms in Organic Chemistry,* Academic Press, 2014.
7. Moloney, M. G. *How to Solve Organic Reaction Mechanisms,* Wiley, 2015.

Course objective/intended learning outcomes

a) Knowledge

- He/She has systematic knowledge on various subjects of chemistry, their main principles including theoretical and practical applications built on these principles.
- He/She knows the basic and some most recent theories, models and methods about chemical bonds, structure of compounds, reactions, and chemical interactions.

b) Abilities

- He/She is able to distinguish between the scientifically proven theories and non-reliable data or information.
- He/she is able to gain knowledge on the professional chemical language to present his/her knowledge and communicate.

c) Attitude

- He/She is open to collaborate with professionals in the field of social sciences, economy and environmental safety , treating the new chemical trends critically but carefully.

d) Autonomy and responsibility

- He/She can make own decisions even in complex professional questions, discussions.
- He/She is well aware about his/her propositions and its consequences.

Schedule:

1st week

Repetitive survey of VB and LCAO-MO methods and their use for the description of homo- and heteronuclear bonds as well as electron shift phenomena (inductive and mesomeric effects, conjugation, hyperconjugation). Effects of substituents on the energy levels and electron densities of bonds/compounds/intermediates. Reactive intermediates and their properties. The Hammond-postulate and its applications. Interactions between particles, properties of solvents and solutions, classification of solvents. Solvent effects in organic reactions.

2nd week

Perturbation theory of chemical reactions, Klopman-Salem-equation and its explanation. The concept of stereoelectronic effects, their consequnces, Baldwin's rules. Principle of least motion, and its use for understanding of chemical reactions.

3rd week

Substitution on tetrahedral carbon atoms. Aliphatic nucleophilic substitution. Characterization of nucleophiles and leaving groups. Kinetic and stereochemical characterization of the bimolecular mechanism, its stereoelectronic control. Ring closures by S_N2 reactions.

Kinetic and stereochemical characteristics of the monomolecular mechanism. Stereochemical effects of ion-pairs, neighbouring group effects and their consequences. The Walden-cycle. Effects of the nucleophile, the solvent and the structure of the substrate. Ambident and α-effect nucleophiles.

4th week

Eliminations. Types: α-, β- and 1,n-eliminations. Mechanisms of β-eliminations. Syn- and anti-eliminations. Kinetic and stereochemical characterization of the bimolecular mechanism, its stereoelectronic control. Kinetic and stereochemical characteristics of the monomolecular mechanism. Effects of the substrate, the attacking base, and the leaving group in eliminations; orientation of the double bond. Solvent effects, ratio of substitution and elimination.

5th week

Substitutions on trigonal carbon atoms. Nucleophilic substitution on acyl-acarbon. Reactivity oredr of carboxylic acid derivatives and its explanation. Tetrahedral mechanism and its proofs. Effects of the nucleophile and the structure of the substrate on the reactions. Stereoelectronic controls (Bürgi-Dunitz-trajectory, decomposition of the tetrahedral intermediate), and their consequences. Activation and catalysis in acyl nucleophilic substitutions. Ring-closures on acyl carbons.

6th week

Additions. Electrophilic additions on carbon-carbon multiple bonds. Cis- and trans additions, stereospecificity and stereoselectivity. Onium- and carbeniumion type intermediates, stereochemical and solvent effects.

Nucleophilic additions on carbonyl groups. Summary and categorization of the reactions: additions of heteroatomic, hydride, and metalorganic nucleophiles. Nucleophilic additions on carbon-carbon multiple bonds. Preconditions, 1,2- and 1,4-additions, directing the regioselectivity. Ring-closures by addition reactions.

7th week

Concept and types of pericyclic reactions. The main methods used for their explanation (correlation diagrams, FMO analysis). Electrocyclic reactions. Cycloaddition reactions, normal and inverse electron demand Diels-Alder-reactions. Lewis-acid catalysis, position- and periselectivity.

8th week

1,3-Dipolar cycloadditions. Cheletropic reactions, sigmatropic rearrangements. Solvent effects in pericyclic reactions.

9th week

Pericyclic reactions in biological systems, their applications for bioorthogonal labeling.

10th week

Explanation of pericyclic reaction by the aromatic character of the transition states. Comparison of the methods for understanding the pericyclic reactions.

11th week

Concept of free radicals, methods for their generation. Chemical initiators. Structure and elemental reactions of free radicals. Transformations by chain and non-chain mechanisms. Thermodynamic and kinetic stability of carbon-centered radicals, effects of the substituents on the radical centre.

12th week

Abstraction reactions of free radicals: thermochemical, polar, stereoelectronic and steric effects.

13th week

Addition reactions of free radicals: thermochemical, polar, stereoelectronic and steric effects.

14th week

Fragmentations and rearrangements of free radicals. Generation of radical in place of functional groups. Synthetic applications of radicals, condition of selectivity and reactivity.

Comparison of synthetic applications of radical and ionic reactions. The SET mechanism. Determining the radical nature of a reaction.

Requirements:
Attendance at **lectures** is recommended, but not compulsory.

An oral exam to be absolved during the examination period closes the course. A list of topics is provided at the start of the semester, and at the exam two topics chosen randomly are discussed after an approx. 1 hour preparation time.

Person responsible for course: Dr. László Somsák, full professor

Lecturer: Dr. László Somsák, full professor

Title of course: Asymmetric syntheses **Code**: TTKME0312_EN	**ECTS Credit points:** 3
Type of teaching, contact hours - lecture: 2 hours/week - practice: - - laboratory: -	
Evaluation: exam	
Workload (estimated), divided into contact hours: - lecture: 28 hours - practice: - - laboratory: - - home assignment: 8 hours - preparation for the exam: 42 hours Total: 78 hours	
Year, semester: 1^{st} / 2^{nd} year, 1^{st} semester	
Its prerequisite(s): -	
Further courses built on it: -	

Topics of course
- Chirality, stereo isomerism, determination of the relative and the absolute configuration - Biopolymers, readily available enantiopure natural products - Methods for the preparation of enantiopure compounds - „Chiral pool" synthesis - Models describing stereochemistry of reactions - First (substrate-controlled), second (auxiliary-controlled), third (reagent-controlled) and fourth generation (catalyst-controlled) methods - C-C bond-forming reactions - Asymmetric oxidation methods, asymmetric epoxidation - Asymmetric reduction - Multiple asymmetric induction - Organocatalysis - „Memory of chirality" - Kinetic and dynamic kinetic resolution - Enzymatic reactions - Asymmetric total synthesis
Literature
Compulsory:

1. R. A. Aitken, S. N. Kilényi: Asymmetric Synthesis, Springer Science+Business Media Dordrecht, 1992.
2. R. E. Gawley, J. Aubé: Principles of Asymmetric Synthesis, Second Edition, Elsevier, 2012, Kidlington, Oxford.

Recommended:

1. J. P. Riehl: Mirror-Image Asymmetry - An Introduction to the Origin and Consequences of Chirality, John Wiley & Sons, 2010, Hoboken, New Jersey.
2. E. L. Eliel, S. H. Wilen: Stereochemisty of Organic Compounds, Wiley, New York, 1994.
3. Y. Izumi, A Tai: Stereo-Differentiating Reactions - The Nature of Asymmetric Reactions, Kodansha Scientific Books & Academic Press, 1977, New York.
4. R. S. Ward: Selectivity in Organic Synthesis, Wiley, Chichester, 1999.
5. G. Q. Lin, Y. M. Li, A. S. C. Chan: Principles and Applications of Asymmetric Synthesis, Wiley-Interscience, New York, 2001.
6. D. Enders, K. E. Jaeger: Asymmetric Synthesis with Chemical and Biological Methods, Wiley-VCH, Weinheim, 2007.
7. M. Christmann, S. Bräse: Asymmetric Synthesis - The Essentials, Wiley-VCH, Weinheim, 2008.

Course objective/intended learning outcomes

a) Knowledge

They know the most recent theories, models and related computational methods on the scientific results about chemical bonds, structure of compounds, reactions, and chemical interactions. They are familiar with the basic concepts of stereochemistry and asymmetric synthesis, the possibilities of producing enantiomeric pure materials and their major synthesis methods. They know the most important theories and models needed to interpret stereo-selective reactions based on the scientific results of chemistry. In English, they can communicate professionally and understand the conceptual system and terminology of science / organic chemistry, and understands the essence of source literatures.

b) Abilities

They are able to use the new approaches on the field of chemical research and innovation to apply the main theories, practical information, application and technology as well as understanding and analyzing scientific data. They are able to distinguish between the scientifically proven theories and non-reliable data or information. They are able to gain knowledge on the professional chemical language to present their knowledge and communicate. They are able to understand the concepts of stereochemistry and the asymmetry syntheses, data collection, processing of data, and the use of chemical literature. They own ability to apply the learned theories, paradigms and principles. Based on their knowledge, they have the ability to scientifically argue with others in the relevant field of science. They are able to master the English language vocabulary of asymmetric synthesis that they can utilize for processing and summarizing source literatures independently.

c) Attitude

They are committed to protect the environment in both chemical labs and industries. These attitudes are shown to other co-workers as well. By knowing effective stereoselective reactions, they are environmentally conscious and strive to decrease the environmental loads. They are open for professional knowledge exchange.

d) Autonomy and responsibility

They evaluate their co-workers in a professional way. They are well aware about their propositions and the consequences. By being able to consider the basic professional questions of stereochemistry and asymmetric synthesis independently, they can prepare useful summaries for their supervisors. They compare their results with those of similar professional positions (students).

Schedule:

1st week

Significance of chirality in living organisms. Biopolymers. Stereoisomerism. Determination of relative and absolute configuration. Examples for enantiomers / diastereomers with different biological effects from living organisms and synthetic medicines. Possibilities for the production of enantiomerically pure materials. Enantiomerically pure compounds available in large amounts from natural sources.

2nd week

Advantage, disadvantage and examples of "chiral pool" syntheses. Stereoselectivity, stereospecificity. The basic concepts of asymmetric synthesis. Topicity (groups, faces). Prochirality. Symmetry relationships of faces.

3rd week

Cram's rule, Bürgi-Dunitz trajectory, Felkin-Anh model, Conforth-Evans model, Cram-chelate model, Prelog's rule. First (substrate-controlled), second (auxiliary-controlled), third (reagent-controlled) and fourth generation (catalyst-controlled) methods.

4th week

Examples of first and second generation methods.

5th week

Carbon-carbon bond forming reactions (asymmetric alkylation, asymmetric Michael reaction, asymmetric nucleophilic addition of carbonyl compounds).

6th week

Carbon-carbon bond forming reactions (asymmetric nucleophilic addition of carbonyl compounds, asymmetric [2 + 2] cycloaddition, asymmetric Diels-Alder reaction).

7th week

Asymmetric oxidation reactions, epoxidation reactions.

8th week

Asymmetric reduction reactions.

9th week

Multiple asymmetric induction.

10th week

Organocatalysis. „Memory of chirality"

11th week

Kinetic resolution. Dynamic kinetic resolution. Enzymatic reactions.

12th week

Asymmetric total syntheses.

13th week

Short presentation and discussion of independently processed source literature.

14th week

Short presentation and discussion of independently processed source literature.
Requirements: - *for a signature* Attendance at **lectures** is recommended, but not compulsory. - *for a grade* Presentation of an independently processed source literature (20%) Exam (80%) The course ends in an **examination**. Based on the sum of the exam and the presentation points the final grade is calculated. The final grade is given according to the following table: Score (%) Grade 0-49 fail (1) 50-59 pass (2) 60-74 satisfactory (3) 75-89 good (4) 90-100 excellent (5) If the score of the final grade is below 50%, students can take a retake test in conformity with the EDUCATION AND EXAMINATION RULES AND REGULATIONS. *-an offered grade:* It may be offered for students taking a successful early exam.
Person responsible for course: Dr. Attila Mándi, researcher / assistant professor, PhD
Lecturer: Dr. Attila Mándi, researcher / assistant professor, PhD

Title of course: Synthetic Methods in Polymer Chemistry **Code**: TTKME0313_EN	**ECTS Credit points:** 3
Type of teaching, contact hours - lecture: 2 hours/week - practice: - - laboratory: -	
Evaluation: exam	
Workload (estimated), divided into contact hours: - lecture: 28 hours - practice: - - laboratory: - - home assignment: 32 hours - preparation for the exam: 30 hours Total: 90 hours	
Year, semester: 1st year, 2nd semester	

Its prerequisite(s): -
Further courses built on it: -

Topics of course
Nitroxide-mediated radical polymerization (NMP). Atom transfer radical polymerization (ATRP). Reversible addition-fragmentation chain transfer (RAFT) polymerization. Ring opening polymerization (ROP). Ring opening metathesis polymerization (ROMP). Controlled step polymerization methods.
Literature
Compulsory: - George Odian: Principles of Polymerization (Wiley, 2004) ISBN: 978-0-471-27400-1 - Leslie H. Sperling: Introduction to Physical Polymer Science (Wiley, 2006) ISBN: 978-0-471-70606-9 *Recommended:* - Krzysztof Matyjaszewski, Thomas P. Davis: Handbook of Radical Polymerization (Wiley, 2002) ISBN: 978-0-471-39274-3
Course objective/intended learning outcomes
a) Knowledge - He/She has global knowledge on science other than chemistry, and capable to organize this information. - He/She has knowledge to solve problems on the field of natural processes, using natural sources, and understanding the chemical background of living and non-living systems. **b) Abilities** - He/She is able to communicate discuss and aim problems to other chemists or engineers of professionals other than chemistry field. - He/She is able to use his/her knowledge to solve advanced level chemistry problems including to prove the solutions. **c) Attitude** - He/She is receptive to establish and apply new chemical and environmental technologies. - He/She is open to collaborate with professionals on the field of social sciences, economy and environmental safety , treating the new chemical trends critically but carefully. **d) Autonomy and responsibility** - He/She can make own decisions even in complex professional questions, discussions. - He/She is responsible in collaboration with other professionals (especially from the field of environmental economy and safety) without supervision.

Schedule:
1st week
Review of polymerization methods.
2nd week
Laboratory techniques for the exclusion of air and humidity.
3rd week
Nitroxide-mediated radical polymerization (NMP) I.
4th week
Nitroxide-mediated radical polymerization (NMP) II.
5th week
Atom transfer radical polymerization (ATRP) I.
6th week
Atom transfer radical polymerization (ATRP) II.
7th week
Reversible addition-fragmentation chain transfer (RAFT) polymerization I.
8th week
Reversible addition-fragmentation chain transfer (RAFT) polymerization II.
9th week
Ring opening polymerization (ROP) I.
10th week
Ring opening polymerization (ROP) II.
11th week
Ring opening metathesis polymerization (ROMP) I.
12th week
Ring opening metathesis polymerization (ROMP) II.
13th week
Controlled step polymerization methods I.
14th week
Controlled step polymerization methods II.

Requirements:
- *for a signature*

Attendance at **lectures** is recommended, but not compulsory. Active participation is rewarded by the teacher in every class.
During the semester there is one end-term test in the 15th week for an offered grade (optional). Students have to sit for the tests.
- *for a grade*

The course ends in an **examination**.
The minimum requirement for the end-term test and the examination respectively is 50%. Based on the score of the test, the grade for the test and the examination is given according to the following table:

Score	Grade
0-49	fail (1)
50-61	pass (2)
62-74	satisfactory (3)

75-87	good (4)
88-100	excellent (5)

If the score the test is below 50, students can take a retake test in conformity with the Education and Examination Rules and Regulations.

-an offered grade:

it may be offered for students if the grade of the end-term test is at least satisfactory (3).

Person responsible for course: Prof. Sándor Kéki, full professor, PhD, DSc

Lecturer: Prof. Sándor Kéki, full professor, PhD, DSc

Title of course: Chemical aspects of drug design **Code**: TTKME0314_EN	**ECTS Credit points:** 3

Type of teaching, contact hours
- lecture: 2 hours/week
- practice: -
- laboratory: -

Evaluation: oral examination

Workload (estimated), divided into contact hours:
- lecture: 28 hours
- practice: -
- laboratory: -
- home assignment: -
- preparation for the exam: 62 hours

Total: 90 hours

Year, semester: 1st year, 1st semester

Its prerequisite(s): -

Further courses built on it: -

Topics of course

The students will get acquainted with the complex process of finding and/or discovery, design and development of drugs. The following main topics will be handled: drugs as chemical, legal and commercial entities; Intermolecular interactions responsible for the development of drug action; characterization of interactions between a small molecule and a biological target; drug targets, pharmacodynamics and pharmacokinetics; structure-activity relationships. These topics will be illustrated by several case studies.

Literature

1. G. L. Patrick: An introduction to medicinal chemistry, 4th edition, Oxford University Press, New York, 2009. (978-0-19-923447-9)

2. R. B. Silverman, M. W. Holladay: The organic chemistry of drug design and drug action, 3rd ed., Academic Press, 2012. (978-0-12-382030-3)
3. H. J. Smith, C. Simons (Eds.): Enzymes and their inhibition – Drug development. CRC Press, Boca Raton, 2005.

Course objective/intended learning outcomes

a) Knowledge
- He/She understands the progress and future trends in chemistry and chemical industries.
- He/She has knowledge to solve problems in the field of biomolecular interactions.

b) Abilities
- He/She is able to recognize and evaluate the global relationships on the field of chemistry.

c) Attitude
- He/She is receptive to establish and apply new chemical and environmental technologies.
- He/She is responsible and stands in for the professional ethics.

d) Autonomy and responsibility
- He/She can make own decisions even in complex professional questions, discussions.
- He/She is well aware about his/her propositions and its consequences.
- He/She is responsible for his/her own decisions, stand in for these decisions and ideologies.

Schedule:

1st week

Definition of drugs, their types, and modes of action. Intermolecular interactions, hydrophobic/solvophobic effects. Participation of proteinogenic amino acid side chains in secondary chemical bondings.

2nd week

Characterization of interactions between small molecules-biological macromulcules: binding energy and its components (enthalpy, enthropy), flexibility, solvatation, repulsive forces, shape of the molecules, stereoisomerism (configuration, conformation). Enthalpy-enthropy compensation. Isosterism, bioisosterism.

3rd week

Categories of drug targets. Receptors, characterization of small molecule-receptor complexes: affinity (dissociation constant), effectivity. Definition of agonists and antagonists, models.

4th week

Enzymes as drug targets. Characterization of enzyme catalysis on the molecular level. Cofactors, coenzymes and their ways of action.

5th week

Types of enzyme inhibitors: reversible (competitive, non-competitive, uncompetitive, transition-state analogues), irreversible (affinity labels, mechanism-based inactivators). Enzyme inhibitors in drug development.

6th week Nucleic acids as drug targets. Interactions of small molecules with nucleic acids. Alkylation and chain splitting of DNA. Antisense therapy. Transport and structural proteins, lipids as drug targets. *7th week* Pharmacodynamics and pharmacokinetics. ADMET properties. *8th week* Drugs as merchandises. Chemical biology and drug design. The multi- and interdisciplinary process of drug design and development. Phases, current practice and problems of drug development. *9th week* Finding, discovery and design of drugs. Hits, lead molecules, optimized leads. Elements of the early drug development phase. *10th week* Optimization of pharmacodynamic properties. *11th week* Optimization of pharmacokinetic properties. Concept of prodrugs. *12th week* Structure-activity relationships. *13th week* Case studies. *14th week* Case studies.
Requirements: Attendance at **lectures** is recommended, but not compulsory. An oral exam to be absolved during the examination period closes the course. A list of topics is provided at the start of the semester, and at the exam two topics chosen randomly are discussed after an approx. 1 hour preparation time.
Person responsible for course: Dr. László Somsák, full professor
Lecturer: Dr. László Somsák, full professor

Title of course: Separation techniques III. **Code**: TTKME0315_EN	**ECTS Credit points:** 2

Type of teaching, contact hours
- lecture: 2 hours/week
- practice:
- laboratory: -

Evaluation: exam

Workload (estimated), divided into contact hours:
- lecture: 28 hours
- practice:
- laboratory: -
- home assignment: 20 hours
- preparation for the exam: 42 hours

Total: 90 hours

Year, semester: 2nd year, 1th semester

Its prerequisite(s):

Further courses built on it: -

Topics of course

Basic principles of different modern analytical methods in the field of HPLC, GC, SFC. Examples and applications for chromatographic studies of organic compounds.

Literature

1. **Effective Organic Compound Purification, Teledyne ISCO, Lincoln, USA (2010)**
2. **D.A. Skoog, J.J. Leary: Principles of Instrumental Analysis, New York (1992)**
3. **L.R. Snyder, J.J. Kirkland: Introduction To Modern Liquid Chromatography, Wiley, 1979**
4. **P. Schreider, A. Bernreuter, M. Huffer: Analysis of Chiral Organic Molecules, Walter de Gruyer, 1995**

Course objective/intended learning outcomes

a) Knowledge
- Have systematic knowledge on the various subject of chemistry, their main principals including basics of analytical methods studied during BSc courses.

b) Abilities
- Using the knowledge and experiences acquired during the course he/she is able to analyse HPLC, GC SFC provided results and accomplish structure, purity verification and/or determination of main analytical parameters from relevant chromatograms.

c) Attitude
- He/She is receptive to establish and apply new chemical technologies.
- He/She is open to collaborate with professionals on the field of chemistry, environmental chemistry, treating the new chemical trends critically but carefully.

d) Autonomy and responsibility

- He/She is responsible for his/her own decisions, stand in for these decisions and ideologies.
- He/She recognizes the unsafe environment both in laboratory on industry, and makes decisions according to this.
-He/She is well aware about his/her propositions and its consequences.

Schedule:

1st week

Introduction, overview of major chromatographic concepts. Categorization of chromatographic techniques by stationary and mobile phase. Chromatographic stationary phases. Retention Volume, Retention Time, Peak Height, peak area, Half Width, Bandwidth, Theoretical Plate Number, Theoretical Plate Height, Resolution, Signal, Noise, Drift, Signal / Noise, LOD, LOQ, tailing factor, peak asymmetry. Definition and use of the Kováts index in analytical chemistry.

2nd week

Size Exclusion Chromatography. Principles and mechanism of separation. Stationary phases in chromatography, physical and chemical structures, the newest developments. Instrumentation and operation of the separation processes.

3rd week

Calibration of GPC-SEC. Eluents and detectors.

4th week

Most common errors (GPC-HPLC comparison) and elimination of them.

5th week

Instruments of modern column chromatography and their use. How can a TLC data be used as a pre-experiment? Transfer of TLC data to column chromatography.

6th week

Chiral chromatographic methods. Introduction. Use of chiral GC, HPLC.

Basics of Stereochemistry from chromatographic point of view. The concept of chirality. Different chiral and achiral chromatographic systems.

7th week

Chiral interactions and their application in separation techniques. Enumeration of chiral stationary phases 1. Adapting methods from achiral systems to chiral stationary phases.

8th week

Chiral interactions and their application in separation techniques. Enumeration of chiral stationary phases 2. Adapting methods from achiral systems to chiral stationary phases.

9th week

Hyphenated Techniques. GCMS, HPLCMS SFCMS, and chiral chromatography. Method of development in chiral chromatography 1.

10th week

Hyphenated Techniques. GCMS, HPLCMS SFCMS, and chiral chromatography. Method of development in chiral chromatography 2.

11th week

Stationary Phases, Mobile Phases in Reverse Phase Liquid Chromatography. The role of pH in the separation of proton-active compounds. Preparation of liquid chromatographic buffer solutions, their properties and their application possibilities.

12th week The usage of gradient chromatography. The possibilities of eliminating the difficulties and pitfalls of it. *13th week* Instrumentation of liquid chromatography. *14th week* Closing test.
Requirements: - *for a signature* Attendance at **lectures** is highly recommended, but not compulsory. - *for a grade* The course ends in a **written exam** during the examination period following the course. The minimum requirement for the end-term test is 60%. Based on the score of the test, the grade for the exam is given according to the following table: Score Grade 0-59 fail (1) 60-69 pass (2) 70-79 satisfactory (3) 80-89 good (4) 90-100 excellent (5) If the score of the written exam is below 60, students can take a retake test in conformity with the EDUCATION AND EXAMINATION RULES AND REGULATIONS.
Person responsible for course: Dr. Attila Kiss, PhD, associate professor
Lecturer: Dr. Attila Kiss, PhD, associate professor and György Deák, PhD, associate professor

Title of course: Separation techniques V. **Code**: TTKML0316_EN	**ECTS Credit points:** 2
Type of teaching, contact hours - lecture: - - practice: - laboratory: -2 hours/week	
Evaluation: exam	
Workload (estimated), divided into contact hours: - lecture: - practice: - laboratory: -28 hours - home assignment: 20 hours - preparation for the exam: - 42 hours Total: 90 hours	
Year, semester: 2nd year, 1th semester	

Its prerequisite(s): TTKME0315_EN
Further courses built on it: -

Topics of course

Basic principles of different modern analytical methods in the field of HPLC, GC, SFC. Examples and applications for chromatographic studies of organic compounds.

Literature

10. **Effective Organic Compound Purification, Teledyne ISCO, Lincoln, USA (2010)**
11. **D.A. Skoog, J.J. Leary: Principles of Instrumental Analysis, New York (1992)**
12. **L.R. Snyder, J.J. Kirkland: Introduction To Modern Liquid Chromatography, Wiley, 1979**
13. **P. Schreider, A. Bernreuter, M. Huffer: Analysis of Chiral Organic Molecules, Walter de Gruyer, 1995**

Course objective/intended learning outcomes

a) Knowledge

- Have systematic knowledge on the various subject of chemistry, their main principals including basics of analytical methods studied during BSc courses.

b) Abilities

- Using the knowledge and experiences acquired during the course he/she is able to analyse HPLC, GC SFC provided results and accomplish structure, purity verification and/or determination of main analytical parameters from relevant chromatograms.

c) Attitude

- He/She is receptive to establish and apply new chemical technologies.
- He/She is open to collaborate with professionals on the field of chemistry, environmental chemistry, treating the new chemical trends critically but carefully.

d) Autonomy and responsibility

- He/She is responsible for his/her own decisions, stand in for these decisions and ideologies.
- He/She recognizes the unsafe environment both in laboratory on industry, and makes decisions according to this.
- He/She is well aware about his/her propositions and its consequences.

Schedule:

1st week

Basics of gas chromatography, most important measurement methods. Main parts of the GC device. Practical applications of different types of columns. Chromatographic indexes (Kováts index.

Using the GC for quantification (in alcohol-water mixture, quantitative measurement of alcohol or determination of methane in air-methane gas mixtures).

2nd week

Determination of caffeine or limonene using GC-FID and GC-MS methods after extraction of a solid sample (lemon or caffee). Using the Spectrum Library of the GC to identify an unknown compound.

3rd week

Determination of molecular weight of polymer by GPC-SEC method (calibration and measurement).
4th week
Chiral method development 1. CSP-HPLC-UV coupling.
5th week
Chiral method development 3. CSP-HPLC-MS coupling.
6th week
The basics of liquid chromatography, its most important methods of measurement, the construction of the HPLC apparatus. Waters Alliance Liquid Transmission System and UV + DAD Detectors. Things to do after turning on the power. Checking the fluid delivery system.
7th week
Checking the injector and detectors. Application of Empower software, writing of measuring methods, methods for integration of recorded chromatograms. Column types and their application possibilities.
8th week
Closing test.

Requirements: - *for a signature*
Participation at **laboratory** is compulsory. A student must attend the practice classes and may not miss none of them during the semester. In case a student does so, the subject will not be signed and the student must repeat the course. Attendance at lab courses will be recorded by the practice leader. Being late is equivalent with an absence. In case of further absences, a medical certificate needs to be presented. Missed lab courses should not to be made up for at a later date! Students are required to bring the drawing tasks and drawing instruments of the course to each lab courses. Active participation is evaluated by the teacher in every class. If a student's behavior or conduct doesn't meet the requirements of active participation, the teacher may evaluate his/her participation as an absence because of the lack of active participation in class.
Students have to **submit all the two designing tasks** as scheduled minimum on a sufficient level.
During the semester there are two tests: the mid-term test in the 8th week and the end-term test in the 15th week. Students have to sit for the tests
- *for a grade*
The course ends in an **examination**. Based on the average of the grades of the designing tasks and the examination, the exam grade is calculated as an average of them:
- the average grade of the two designing tasks
- the result of the examination

The course ends in a **written exam** during the examination period following the course.

The minimum requirement for the end-term test is 60%. Based on the score of the test, the grade for the exam is given according to the following table:

Score	Grade
0-59	fail (1)
60-69	pass (2)
70-79	satisfactory (3)
80-89	good (4)
90-100	excellent (5)

If the score of the written exam is below 60, students can take a retake test in conformity with the

EDUCATION AND EXAMINATION RULES AND REGULATIONS.
Person responsible for course: Dr. Attila Kiss, PhD, associate professor
Lecturer: Dr. Attila Kiss, PhD, associate professor and György Deák, PhD, associate professor

Title of course: High efficiency synthetic methods I. **Code**: TTKML0319_EN	**ECTS Credit points: 3**
Type of teaching, contact hours - lecture: - - practice: 1 hour/week - laboratory: 3 hours/week	
Evaluation: term mark	
Workload (estimated), divided into contact hours: - lecture: - practice: 14 hours - laboratory: -42 hours - home assignment: 28 hours - preparation for the exam: - Total: 84 hours	
Year, semester: 2nd year, 2nd semester	
Its prerequisite(s): -	
Further courses built on it: -	

Topics of course

- Understanding the theory of the most important high-performance techniques, practice of methods capable for the synthesis of various organic compounds.
- Use of microwave technology, various flow condition methods and cleaning techniques.

Literature

Compulsory:

1. Slides and experimental descriptions provided by the lecturer.

Recommended:

2. O. Kappe: Microwaves in Organic and Medicinal Chemistry, Vol. 25, 2005.
3. O. Kappe: Microwaves in Organic and Medicinal Chemistry, Vol. 52, 2012.
4. Santiago V Luis: Chemical Reactions and Processes under Flow Conditions, 2009.
5. Stefan Bräse: Combinatorial Chemistry on Solid Supports, 2007.

Course objective/intended learning outcomes

a) Knowledge

- He/She knows the most recent theories, models and related computational methods on the scientific results about chemical bonds, structure of compounds, reactions, and chemical interactions.
- He/She knows various methods from chemical labs or industries, able to show it to other people and apply them including the equipments and their safe usage.

b) Abilities

- He/She is able to use the new approaches on the field of chemical research and innovation to apply the main theories, practical information, application and technology as well as understanding and analyzing scientific data.
- He/She is able to recognize and evaluate the global relationships on the field of chemistry.
- He/She is able to distinguish between the scientifically proven theories and non-reliable data or information
- He/She is able to carefully apply the newest chemical theories in practice and design lab experiments or industrial processes based on these results.
- He/she is able to gain knowledge on the professional chemical language to present his/her knowledge and communicate.

c) Attitude

- He/She is receptive to establish and apply new chemical technologies.
- He/She is being active to start and participate in professional discussions.
- He/She is open to collaborate with professionals on the field of chemistry, environmental chemistry, treating the new chemical trends critically but carefully.

d) Autonomy and responsibility

- He/She is responsible for his/her own decisions, stand in for these decisions and ideologies.
- He/She recognizes the unsafe environment both in laboratory on industry, and makes decisions according to this.
- He/She can operate chemical or industrial instruments or equipment with responsibility, and manage persons working with these.
- He/She is well aware about his/her propositions and its consequences.

Schedule:

1st week
Theoretical background of the applied techniques 1.
2nd week
Theoretical background of the applied techniques 2.
3rd week
Use of a CEM microwave reactor 1.
4th week
Use of a CEM microwave reactor 2.
5th week
Use of a TECAN robot 1.
6th week
Use of a TECAN robot 2.
7th week
Use of a BIOTAGE SP4 fluid chromatograph 1.

8th week Use of a BIOTAGE SP4 fluid chromatograph 2. *9th week* Use of a H-cube reactor 1. *10th week* Use of a H-cube reactor 2. *11th week* Use of ASIA flow reactor 1. *12th week* Use of ASIA flow reactor 2. *13th week* Complex problem solving. *14th week* Exam including the theoretical background and the practice.
Requirements: - *for a signature* Participation at **laboratory** is compulsory. A student must attend the practice classes and may not miss none of them during the semester. In case a student does so, the subject will not be signed and the student must repeat the course. Attendance at lab courses will be recorded by the practice leader. Being late is equivalent with an absence. In case of further absences, a medical certificate needs to be presented. Missed lab courses should not to be made up for at a later date! Students are required to bring the drawing tasks and drawing instruments of the course to each lab courses. Active participation is evaluated by the teacher in every class. If a student's behavior or conduct doesn't meet the requirements of active participation, the teacher may evaluate his/her participation as an absence because of the lack of active participation in class. - *for a grade* The course ends in a term mark which is calculated as an average of: - Theoretical knowledge (70%) - Practical grade (30%) Grade: excellent (5) 90 %, good (4) 75 %, satisfactory (3) 60 %, pass (2) 50 %, fail (1) below 50 %
Person responsible for course: Krisztina Dr. Kónya, PhD, senior lecturer
Lecturer: Krisztina Dr. Kónya, PhD, senior lecturer

Title of course: 2D NMR Methods **Code**: TTKMG0318_EN	**ECTS Credit points:** 2
Type of teaching, contact hours - seminar: 2 hours/week	

Evaluation: written exam

Workload (estimated), divided into contact hours:
- seminar: 28 hours
- preparation for the exam: 32 hours

Total: 60 hours:

Year, semester: 2^{nd} year 1^{st} or 2^{nd} semester

Its prerequisite(s): TTKME0502_EN, TTKML0530_EN

Further courses built on it:

Topics of course: seminar with the aim that students accomplishing the course will be able to analyse, evaluate and assign basic 2D homo- and heteronuclear correlated spectra without external help.

Literature

Compulsary: P.J. Hore, Nuclear Magnetic Resonance, ISBN 963 19 4426 3
Recommended: James Keeler, Understanding NMR Spectroscopy, ISBN 0-470-01787-2
N.E. Jacobsen, NMR Spectroscopy Explained: Simplified Theory, Applications and Examples for Organic Chemistry and Structural Biology

Course objective/intended learning outcomes

a) Knowledge: firm knowledge of the basic principles of high resolution NMR spectroscopy. Principles of pulsed Fourier NMR spectroscopy.

b) Abilities: to analyse and interpret routine 2D ^{1}H/ ^{13}C NMR spectra, determine basic NMR parameters.

c) Attitude
- He/She is receptive to establish and apply new NMR technologies.
- He/She is open to collaborate with professionals on the field of chemistry, treating the new spectroscopic trends critically but carefully.

d) Autonomy and responsibility:
- He/She is responsible for his/her own decisions, stand in for these decisions.

Schedule:

1^{st} week Principle of pulsed Fourier NMR. Basic principle of 2D NMR spectroscopy. General scheme of 2D experiments, main building blocks. Concept of indirectly detected, 2^{nd} frequency dimension. Concept of 2D Fourier transformation.

2^{nd} week Introduction of vector model (VM) and product operator formalism (PO). Simple examples and applications of PO. Explanation of 2D COSY (Correlation Spectroscopy) experiment. Clarification of signals - diagonal- and cross-peaks – appearing in the resulting spectra.

3^{rd} week Product operator description of COSY sequence. Concept of coherence transfer. Quadrature detection in the indirectly detected dimension. Magnitude and phase sensitive detection. Analysis of COSY spectrum, assigning coupling partners. Exercises on spectra of different complexity.

4th week Principle of 2D TOCSY (Total Correlation Spectroscopy) experiment. Concept of isotropic mixing. Different mixing sequences (MLEV, DIPSI). Explanation of signals in the resulting TOCSY spectrum. Concept of spin system. Analysis of TOCSY spectrum, assigning spin systems. Exercises on spectra of different complexity.
5th week Practicing proton assignment of simple bio-oligomers (peptides, carbohydrates) based on combined analysis of COSY and TOCSY spectra.
6th week Origin of Nuclear Overhauser Effect (NOE). Dipolar relaxation, cross-relaxation, sign of NOE. Laboratory- and rotating-frame NOE. Steady-state and transient NOE experiments.
Principle of 2D NOESY/ROESY experiments. Explanation of signals – integrated intensities and phases of diagonal and crosspeaks - in the resulting NOESY/ROESY spectra. Merits and limitations of different experiments: ROESY vs. NOESY.
7th week Practicing analysis of 2D ROESY/NOESY spectra. Estimation of relative proton-proton distances based on volume intensities of crosspeaks using the two-spin approximation.
8th week Homo- and heteronuclear spin-echo building blocks. PO analysis of basic elements. INEPT sequence. Principle of 2D HSQC experiment. Explanation of signals in the resulting HSQC spectra.
9th week PO description of HSQC sequence. Practicing analysis of 2D HSQC spectra.
10th week Principle of 2D HMBC experiment. Explanation of signals in the resulting HMBC spectra.
11th week Practicing assignment of 2D HSQC and HMBC spectra. Exercises on spectra of different complexity.
12th week Problem solving exercises with real life examples. Practicing proton and carbon assignment based on combined analysis of different 2D spectra.
13th week Problem solving exercises with real life examples. Practicing proton and carbon assignment based on combined analysis of different 2D spectra.
14th week Problem solving exercises with real life examples. Practicing proton and carbon assignment based on combined analysis of different 2D spectra.

Requirements:
- *for a signature*
Attendance of seminars is compulsory.
A student must attend the seminar classes and may not miss more than two times during the semester. In case a student does so, the subject will not be signed and the student must repeat the course. A student can't make up any seminar with another group. Attendance at seminar classes will be recorded by the seminar leader. Being late is equivalent with an absence. In case of further absences, a medical certificate needs to be presented. Missed seminar classes should be made up for at a later date, to be discussed with the tutor. Active participation is evaluated by the teacher in every class. If a student's behaviour doesn't meet the requirements of active participation, the teacher may evaluate his/her participation as an absence because of the lack of active participation in class.
- *for a grade*
The course ends in a **written exam**. Based on the average of the grades of two tasks – *one theoretical* (basic concepts and principles of 2D NMR experiments) and *one practical* (i.e. assignment of 2D spectra), the exam grade is calculated as an average of them:

Person responsible for course: Prof. Katalin E. Kövér, professor, DSc.

Lecturer: Prof. Katalin E. Kövér, professor, DSc

Title of course: Glycobiochemistry **Code**: TTKME0321_EN	**ECTS Credit points:** 3
Type of teaching, contact hours - lecture: 2 hours/week - seminar:- - laboratory: -	
Evaluation: exam	
Workload (estimated), divided into contact hours: - lecture: 28 hours - practice: - - laboratory: - - home assignment: 40 hours - preparation for the exam: 22 hours Total: 90 hours	
Year, semester: 2nd year, 2nd semester	
Its prerequisite(s):-	
Further courses built on it:-	

Topics of course

Carbohydrates. Biological role of carbohydrates. Monosaccharides are polyhydroxy aldehydes or ketons. Sucrose, lactose, and maltose are the common disaccharides. Polysaccharides. Glycoconjugates. Structure of glycolipids and glycoproteins occurring in cell membranes. Cell surface glycans mediate uncountable biological events such as viral and bacterial infection, tumorigenesis, immune response and receptor-mediated signaling processes. Specific glycosylation patterns are proven to serve as markers at the early stages of disease or malignancy prior to metastasis. Carbohydrate-lectin interactions and functional glycomics. Modern methods for the synthesis and analysis of oligosaccharides.

Literature

Compulsory:

- Lubert Stryer, Biochemistry, W. H. Freeman and Company, New York, 2002, ISBN 1-7167-4684-0.

Recommended:

- Glycoscience-Chemistry and Chemical Biology, (Eds: B. Fraser-Reid, K. Tatsua, J. Thiem) 2001, Springer-Verlag, Berlin
- Essentials of glycobiology (Eds: A.Varki, R. Cummings, J. Esko, H. Freeze, G. Hart, J. Marth, 1999, Cold Spring Harbor, New York, ISBN 0-87969-559-5)

Course objective/intended learning outcomes

a) Knowledge

-He/she fundamentally knows the basic principles of glycobiochemistry.

-He/she expansively knows the areas of glycobiology.

b) Abilities

-He/she is able to apply the most important terminology, theories of the given glycobiochemical field when completing the relevant tasks.

-He/she is able to understand scientific publications in the field of glycobiochemistry.

c) Attitude

-He/she is open to learn and accept professional, technological improvement and innovation in his/her profession and convey it genuinely.

-He/she makes a decision in complex and unexpected decision cases by completely taking into account legal and ethical norms.

d) Autonomy and responsibility

-Even in unexpected decision-making situations he/she is capable of considering complex, fundamental questions from his/her professional field and elaborating them on the basis of the given sources.

-He/she is open to critical remarks which are professionally well-founded.

Schedule:

1st week: Carbohydrates. Biological role of carbohydrates. Monosaccharides, disaccharides, polysaccharides

2nd week: Glycoconjugates. Structures of glycolipids and glycoproteins occurring in cell membranes. Biological role of carbohydrates.

3rd week: Cell surface glycans mediate uncountable biological events such as viral and bacterial infection, tumorigenesis, immune response and receptor-mediated signaling processes. Specific glycosylation patterns are proven to serve as markers at the early stages of disease or malignancy prior to metastasis.

4th week: Modern methods for the synthesis and analysis of oligosaccharides.

5th week: Project work: Finding scientific journals in the field of glycobiochemistry and work out a choosen topics of the course.

6th week: Project work: Finding scientific journals in the field of glycobiochemistry and work out a choosen topics of the course.

7th week: Project work: Finding scientific journals in the field of glycobiochemistry and work out a choosen topics of the course.

8th week: Project work: Finding scientific journals in the field of glycobiochemistry and work out a choosen topics of the course.

9th week: Project work: Finding scientific journals in the field of glycobiochemistry and work out a choosen topics of the course. *10th week:* Project work: Finding scientific journals in the field of glycobiochemistry and work out a choosen topics of the course. *11th week:* Project work: Finding scientific journals in the field of glycobiochemistry and work out a choosen topics of the course. *12th week:* Project work: Finding scientific journals in the field of glycobiochemistry and work out a choosen topics of the course. *13th week:* Consultation. *14th week:* Evaulation of the papers.
Requirements: - *for a signature* Attendance at **lectures** is recommended, but not compulsory. - *for a grade* Students must summarize their projectwork in a written report of 8-10 pages.
Person responsible for course: Dr. János Kerékgyártó, senior research fellow, CSc, PhD
Lecturer: Dr. János Kerékgyártó, senior research fellow, CSc, PhD

Title of course: Stereochemical structural elucidation method **Code**: TTKME0322_EN	**ECTS Credit points:** 3
Type of teaching, contact hours - lecture: 2 hours/week - practice: - - laboratory: -	
Evaluation: exam	
Workload (estimated), divided into contact hours: - lecture: 28 hours - practice: - - laboratory: - - home assignment: 10 hours	

- preparation for the exam: 40 hours Total: 78 hours
Year, semester: -
Its prerequisite(s): -
Further courses built on it: -

Topics of course
- Importance of asymmetry and chirality and stereochemical definitions. - Types of chirality. Conformational and configurational enantiomers and diastereomers - Assignment of absolute configuration. R/S and D/L descriptors, Chan-Ingold-Prelog system. - Chiral drugs and their preparation by enantioselective synthesis. - Methods for determining absolute and relative configuration. Chemical correlation and kinetic resolvation. - NMR methods for determining absolute configuration. Mosher's method and its modifications. - Interaction of substance and light. Circular dichroism and circular birefringence. Chiroptical methods. - Optical rotation, optical rotatory dispersion and circular dichroism spectroscopy. - Semi-empirical ECD rules and exciton-coupled circualr dichroism. - Vibrational circular dichroism and Raman optical activity.
Literature
Compulsory: Supporting material with lecture slides available at the homepage of the Department of Organic Chemistry Recommended: -J. P. Riehl: Mirror-Image Asymmetry - An Introduction to the Origin and Consequences of Chirality, John Wiley & Sons, 2010, Hoboken, New Jersey. -E. L. Eliel, S. H. Wilen: Stereochemisty of Organic Compounds, Wiley, New York, 1994.
Course objective/intended learning outcomes
b) Knowledge The student knows the types and importance of chirality, the Cahn-Ingold-Prelog system for assigning the absolute configuration, the different structural elucidation methods for determining stereochemistry, and owns the ability to determine the absolute configuration of optically active derivatives. c) Abilities The student is able to search and process literature data related to the stereochemical analysis of optically derivatives and to apply the acquired principles and theory in the field of stereochemical analysis. He/She can apply chiroptical methods efficiently for the determination of absolute configuration. He/She is able to evaluate experimental data, analyze them and draw conclusions. Based on these results he/she can present new trends in research or development without supervision.

c) Attitude

He/She is receptive to establish and apply new chemical and environmental technologies. He/She is committed to get new knowledge and competences, widening his/her ideology, and makes effort to evolve him/her.

d) Autonomy and responsibility

He/She is responsible for his/her own decisions, stand in for these decisions and ideologies.

Schedule:

1st week

Importance of asymmetry and chirality and stereochemical definitions. Types of chirality. Conformational and configurational enantiomers and diastereomers.

2nd week

Assignment of absolute configuration. R/S and D/L descriptors, Chan-Ingold-Prelog system.

3rd week

Axial chirality of biaryls and allenes. Planar chirality.

4th week

Chiral drug molecules. Different pharmacological activities of enantiomers.

5th week

Preparation of chiral non-racemic active ingredients with stereoselective synthesis.

6th week

Methods for determining relative and absolute configuration. Chemical correlation.

7th week

Determination of absolute configuration by methods based on kinetic resolution. Horeau and Prelog method.

8th week

NMR methods for the determination of absolute configuration. Mosher's method and its modifications.

9th week

Interaction of substance and light. Circular dichroism and circular birefringence. Chiroptical methods.

10th week

Optical rotation and optical rotatory dispersion spectroscopy for determining configuration.

11th week

Electronic circular dichroism spectroscopy. Rotatory strength, ellipticity.

12th week

Theory and application of exciton-coupled circular dichroism

13th week

Helicity rules, sector rules and their application for determining absolute configuration.

14th week

Vibrational circular dichroism and Raman optical activity and their applications for stereochemical analysis.

Requirements:

- for a signature

Attendance at **lectures** is highly recommended, but not compulsory.

- *for a grade*

The course ends with a written **exam**. The list of short questions used for the written exam is available at the homepage of the Department of Organic Chemistry. The minimum requirement for achieving the course is 50%.

Score	Grade
0-49	fail (1)
50-59	pass (2)
60-74	satisfactory (3)
75-89	good (4)
90-100	excellent (5)

Person responsible for course: Dr. Tibor Kurtán, D.Sc.

Lecturer: Dr. Tibor Kurtán, D.Sc.

Title of course: Carbohydrate chemistry
Code: TTKME0323_EN

ECTS Credit points: 3

Type of teaching, contact hours
- lecture: 2 hours/week
- practice: -
- laboratory: -

Evaluation: oral examination

Workload (estimated), divided into contact hours:
- lecture: 28 hours
- practice: -
- laboratory: -
- home assignment: -
- preparation for the exam: 62 hours

Total: 90 hours

Year, semester: 2nd year, 2nd semester

Its prerequisite(s): -

Further courses built on it: -

Topics of course

Occurence and biological functions of carbohydrates. Categories and utilization of carbohydrates. Constitution, configuration and conformation of monosaccharides, ways for their depiction. Basics of carbohydrate nomenclature. Structural aspects of oligo- and polysaccharides. Microheterogeneity. Structural elucidation methods in carbohydrate chemistry (X-ray, UV, IR, MS, NMR, chiroptical methods). Conformational analysis of monosaccharides. The anomeric effects (endo-, exo and reverse) and their generalization. Transformations of free sugars in aqueous medium; oxidation, reduction, reactions with N-, S-, and C-nucleophiles. Reactions of free sugars with alcohols: formation and hydrolysis of glycosides. Protecting groups: carbohydrate ethers and esters, acetals and ketals. Formation and reactions of peracylated monosaccharides, glycosyl halides, Construction of unsaturated bonds and further carbonyl gropus on carbohydrate skeletons. Nucleophilic substitutions on non-anomeric carbons. Formation and cleavage of epoxides.

Literature

4. El Khadem, H. S. Carbohydrate Chemistry – Monosaccharides and Their Oligomers; Academic Press, 1988.
5. Stoddart, J. F. Stereochemistry of Carbohydrates; Wiley, 1971.
6. Lichtenthaler, F. W. (Ed.) Carbohydrates as Organic Raw Materials; VCH, 1991.
7. Kirby, A. J. The Anomeric Effect and Related Stereoelectronic Effect at Oxygen; Springer, 1983.
8. Levy, D. E.; Fügedi, P. The Organic Chemistry of Sugars; CRC Press, 2006.
9. Lindhorst, T. K. Essentials of Carbohydrate Chemistry; Wiley-VCH, 2000.
10. Collins, P. M.; Ferrier, R. J. Monosaccharides - Their Chemistry and Their Roles in Natural Products; John Wiley & Sons, 1995.
11. Miljkovic, M. Carbohydrates – Synthesis, Mechanisms, and Stereoelectronic Effects; Springer, 2009.
12. Stick, R. V.; Williams, S. J. Carbohydrates: The Essential Molecules of Life; Elsevier, 2009.
13. Gabius, H.-J. (Ed.) The Sugar Code – Fundamentals of Glycosciences; Wiley-Blackwell, 2009.
14. Transforming Glycoscience: A Roadmap for the Future - 2012 (PDF is available from the National Academies Press at http://www.nap.edu/catalog.php?record_id=13446)

Course objective/intended learning outcomes

a) Knowledge

- He/She knows the most recent theories, models and related methods in the field of carbohydrates, structure of compounds, reactions, and chemical interactions.
- He/She has knowledge to solve problems on the field of carbohydrate chemistry, and understanding the chemical background of their action in living systems.

b) Abilities

- He/She is able to carefully apply the newest chemical theories in practice and design lab experiments or industrial processes based on these results in the field of the carbohydrates.

c) Attitude

- He/She is committed to get new knowledge and competences, widening his/her ideology, and makes effort to evolve him/her.
- He/She is committed to protect the environment in both chemical labs and industries. These attitudes are shown to other coworkers as well. He/she makes effort to apply those technologies that makes lower environmental changes/loads.

d) Autonomy and responsibility

- He/She can make own decisions even in complex professional questions, discussions.
- He/She is well aware about his/her propositions and its consequences.
- He/She is responsible for his/her own decisions, stand in for these decisions and ideologies.

Schedule:

1st week
Occurence and biological functions of carbohydrates.

2nd week
Categorization and utility of carbphydrates.

3rd week
Constitution, configuration and conformation of monosaccharides, ways for their depiction.

4th week
Basics of carbohydrate nomenclature.

5th week
Structural properties of oligo- and polysaccharides.

6th week
Application of physical methods of structural elucidation to carbohydrates (X-ray, UV-VIS, IR, MS, ORD/CD, NMR).

7th week
Conformational analysis of monosaccharides. The anomeric effects (endo-, exo and reverse) and their explanation.

8th week
Transformations of free sugars in aqueous media, their oxidation and reduction.

9th week
Reactions of free sugars with alcohol, formation and hydrolysis of glycosides; reactions with N-, S-, and C-nucleophiles.

10th week
Carbohydrate ethers and esters.

11th week
Carbohydrate acetals and ketals.

12th week
Formation and reactions of peracylated monosaccharides and glycosyl halides.

13th week
Synthesis of glycosides with protected monosaccharide derivatives.

14th week

Formation of unsaturated monosaccharide derivatives, creation of further carbonyl groups, reactions of the non-anomeric carbons, formation and cleavage of epoxides.
Requirements: Attendance at **lectures** is recommended, but not compulsory. An oral exam to be absolved during the examination period closes the course. A list of topics is provided at the start of the semester, and at the exam two topics chosen randomly are discussed after an approx. 1 hour preparation time.
Person responsible for course: Dr. László Somsák, full professor
Lecturer: Dr. László Somsák, full professor

Title of course: Organic Chemistry of Drug Synthesis **Code**: TTKME0324_EN	**ECTS Credit points:** 3
Type of teaching - lecture: 2 hours/week - practice: - - laboratory: -	
Evaluation: exam	
Workload (estimated) - lecture: 28 hours - practice: - - laboratory: - - home assignment: - - preparation for the exam: 40 hours Total: 68 hours	
Year, semester: 2rd year, 1st semester	
Its prerequisite(s): -	
Further courses built on it: -	

Topics of course

- History of the development of pharmaceutical chemistry
- The evolution of the Hungarian pharmaceutical industry
- The current state of drug research
- The most important concepts of pharmacology
- Central nervous system drugs (narcotics, sedative anesthetics, anxiolytics, analgesics)
- Classification, structure and synthesis of antibiotics
- Structure and synthesis of antiviral drugs
- Structure and synthesis of antifungal drugs

- Structure and synthesis of natural and synthetic chemotherapeutic agents
- Types of diabetes, the biological background of its development, therapeutic options. Structure and production of insulin and synthetic hypoglycemic agents.

Literature

Compulsory:

1. Slides of the lecture by Éva Juhászné Tóth
2. Ruben Vardanyan and Victor Hruby: Synthesis of Essential Drugs, ISBN: 978-0-444-52166-8, Elsevier 2006
3. M. J. Neal: Medical Pharmacology at a Glance, 7th Edition, ISBN: 978-1-118-30647-5Wiley-Blackwell 2012
4. Francis A. Carey: Organic Chemistry (4th Edition), ISBN 0-07-290501-8; The McGraw-Hill Companies, Inc. 2000 *(recommended)*

Course objective/intended learning outcomes

a) Knowledge History of the development of pharmaceutical chemistry. The evolution of the Hungarian pharmaceutical industry. The current state of drug research. The most important concepts of pharmacology. Pharmacokinetic and pharmacodynamic principles. Central nervous system drugs (narcotics, sedative anesthetics, anxiolytics, analgesics), antibiotics, antiviral drugs, antifungal drugs, natural and synthetic chemotherapeutic agents, insulin, synthetic hypoglycemic agents, their structure, application and detailed synthesis based on general organic chemistry. Have systematic knowledge on the various subject of chemistry, their main principals including the theoretical and practical application built on these principals. He/She can realize and recognize the detectable properties of chemical reactions, their systems and scientific aspects on his/her own field.

b) Abilities He/She is able to participate in professional communication in the development of pharmaceutical chemistry, the formation and its present situation of the Hungarian pharmaceutical industry. He/She has the ability to plan a synthesis route for the preparation of simpler structured drug molecules based on the studies. It is capable of expanding / further developing its pharmaceutical chemistry knowledge.

c) Attitude He/She has opened up to acquiring new scientific knowledge and competences in this subject and recognizing this unfounded, possibly wrong claims. He/She is receptive to establish and apply new chemical and environmental technologies.

d) Autonomy and responsibility In addition to professional management, he or she can perform the subtasks given on the subjects covered by the course independently, to prepare a synthesis plan for the production of certain drug molecules based on literary analogy. He/She is responsible for his/her own decisions.

Schedule:

1st week

The concept of pharmaceutical chemistry.
History and development of drug chemistry.

2nd week

Hungarian pharmaceutical industry and pharmaceutical research.
Current situation and problems of pharmaceutical research.
Production of medicines.
Risk and cost of drug therapy.

3rd week

The basics of the mechanism of action of drugs.
Pharmacokinetic and pharmacodynamic principles.
Drug-receptor interaction.
Drug absorption, distribution and selection.
Drug metabolism.
Define concepts that are relevant to the distribution and judgment of medicines.
Categorization of drugs according to their effects.

4th week

Medicinal products of the central nervous system; sedatives.
Anatomical-functional division of the human nervous system.
Causes of nervous system disorders and diseases.
A historical overview of the use of narcotics.
Surgical narcotics: structure of inhalation and injection narcotics.
Synthesis of inhaled narcotics.

5th week

Synthesis of barbituric acid derivatives, steroids, benzodiazepines and other injectable narcotics.

6th week

Structure and synthesis of sedative-hypnotics; alkaloids, alcohols, glycols, polyalcohols, aldehydes, urethans and ureides.

7th week

Hypnotics and sedative drugs; Structure of the barbituric acid derivatives, their most important effect-structural relationships and their production. Preparation of Dioxo-piperidines. The Thalidomid "scandal"
Anxiolytics; benzodiazepines and their structure and synthesis.

8th week

Analgesics; major and minor analgesics.

Production of morphine and co-alkaloids from poppy straw (János Kabay's invention). Important discoveries about understanding the effects of opioids. Painkillers; grouping and production of strong analgesics (opioids, morphine and semi-synthetic derivatives, synthetic morphine analogs).

9th week
Definition and grouping of antibiotics. Beta-lactam antibiotics: penicillins, cephalosporins, monobactams, their structure and mechanism of action. Discovery, grouping of penicillins (natural and semi-synthetic derivatives) and their synthesis.

10th week
Penicillin resistance. Structure, mechanism of action and production of aminoglycosides, peptide, macrolide and polycyclic Antibiotics.

11th week
Mechanism of action, structure and production of antifungal drugs (polyenes, imidazoles, triazoles, allylamines and other molecules).

12th week
Viruses, viral infections and treatment options. Structure and production of antiviral drugs (amantadine, vidarabine, ribavirin, etc.).

13th week
Structure and production of natural (plant-derived) and synthetic (purine, pyrimidine derivatives, various alkylating agents, antibiotics) chemotherapeutic preparations.

14th week
Types of diabetes, the biological background of its development, therapeutic options. Structure and production of insulin and synthetic hypoglycemic agents.

Requirements:
- *for a signature*
Attendance at **lectures** is recommended, but not compulsory.
- *for a grade*
The course ends in an **examination**.
The exam grade is the result of the written exam.
The minimum requirement for the examination respectively is 50%. The grade for the written exam is given according to the following table:

Score	Grade
0-49	fail (1)
50-62	pass (2)
63-75	satisfactory (3)

76-87	good (4)
88-100	excellent (5)

If the score of any test below 50, students can take a retake test in conformity with the EDUCATION AND EXAMINATION RULES AND REGULATIONS.

Person responsible for course: Dr. Éva Juhászné Tóth, senior lecturer, PhD

Lecturer: Dr. Éva Juhászné Tóth, senior lecturer, PhD

Title of course: Radiochemistry **Code**: TTKME0410_EN	**ECTS Credit points:** 3

Type of teaching, contact hours
- lecture: 2 hours/week
- practice: -
- laboratory: -

Evaluation: exam

Workload (estimated), divided into contact hours:
- lecture: 28 hours
- practice: -
- laboratory: -
- home assignment: 22 hours
- preparation for the exam: 40 hours

Total: 90 hours

Year, semester: 1st year, 2nd semester

Its prerequisite(s): -

Further courses built on it: TTKML0415_EN

Topics of course

- Properties of atomic nuclei, binding energy, fundamental and composite particles.
- Kinetics of radioactive decay.
- Mechanism and type of radioactive decay.
- Interaction of radiation with matter.
- Nuclear reactions, new trends in nuclear energy production.
- Physico-chemical applications of radioisotopes.
- Statistics of radioactive decay, measurement of radiation.

Literature

Compulsory:

- Kónya, J., Nagy N.M., 2012, 2018. Nuclear and Radiochemistry, Elsevier, Oxford.

- Choppin, G.R., Liljenzin, J-O., Rydberg, J. Ekberg, C., 2013. Radiochemistry and Nuclear Chemistry, 4th Edition, Elsevier, Amsterdam.
- Kratz, J. V., Lieser, K.H., 2013. Nuclear and Radiochemistry: Fundamentals and Applications, 3rd Edition, Wiley-VCH Verlag GmbH & Co. KGaA, Weinheim, Germany,

Course objective/intended learning outcomes

a) Knowledge

- He/She has systematic knowledge on the nuclear and radiochemistry, their main principles including the theoretical and practical application built on these principles.
- He/She understands the progress and future trends in nuclear and radiochemistry.

b) Abilities

- He/She is able to use the obtained chemical knowledge on the field of nuclear and radiochemistry to solve the actual basic problems and prove the obtained solution.
- Using the knowledge and experiences during the MSc coursed he/she is able to execute laboratory experiments or measurements to demonstrate proper chemical phenomena, or syntheses of new compounds and characterize them, and using analytical methods for provement of new reactions.

c) Attitude

- He/She is being active to start and participate in professional discussions.
- He/She is committed to get new knowledge and competences, widening his/her ideology, and makes effort to evolve him/herself.

d) Autonomy and responsibility

- He/She is responsible in collaboration with other professionals (especially from the field of radiochemistry) without supervision.
- He/She is responsible for his/her own decisions stand in for these decisions and ideologies.

Schedule:

1st week

Properties and constituents of atomic nuclei. Binding energy, Yukawa potential, meson field. Scientific model of atomic nucleus.

2nd week

Fundamental and composite particles. Models of atomic nucleus. Kinetics of radioactive decay. Statistical description of simple radioactive decay. Description of decay as a function of time.

3rd week

Branching and successive decay. Kinetics of successive decay. Radioactive equilibria and their measuring consequences. Measurement of radionuclides having branching and successive decay.

4th week

Mechanisms of radioactive decay. Alpha decay: recoil of nucleus, interpretation of alpha decay by the particle-wave duality. Application of particle-wave duality.

5th week Beta decays, electron capture, double beta decay, proton and neutron decays, exotic decay, spontaneous fission. Types of radioactive decay.

6th week

Interaction of radiation with matter: what happens to the radiation and matter. Kinetics of radiation-matter interactions. Interaction of alpha radiation with matter: energy loss and scattering.

Characterization and classification of radiation-matter interactions.

7th week

Interaction of beta radiation with matter: interactions with electron shell, nuclear field and molecules. Measuring consequences. Interaction of gamma and X-ray radiation with matter: scattering, photoelectric effect, pair formation, Mössbauer effect. General aspects of the interaction of beta and electromagnetic radiation with matter

8th week

Production of neutrons, properties, interaction with matter. Chemical effects of radiation. Szilárd-Chalmers reactions. Properties and applications of neutrons. Chemical changes following irradiation.

9th week

Nuclear reactions, Conservation rules, kinetics. Nuclear reactions with neutrons. Nuclear reactions with charged particles Spallation reaction. Isotopes produced in nuclear reactor and cyclotron. Transformations of atomic nuclei.

10th week

Nuclear reactions. Thermonuclear reactions. Nucleogenesis. Production of transuranium elements.
Transformations of atomic nuclei.

11th week

Nuclear reactors (energy production). Fission by thermal neutrons. Operation of nuclear reactors (energy production, breeding). Nuclear accidents. Types and operation of nuclear reactors

12th week

New trends in nuclear energy production. Fusion reactors. Natural nuclear reactors. Nuclear weapons. New trend in nuclear energy production

13th week

Radioisotopes in physical chemistry: isotope exchange reactions. Study of physico-chemical processes by radiotracers.

14th week

Detection and measurement of nuclear radiation. Detectors, electric units. Effect of statistics on the evaluation. Detection and measurement of radiation.

Requirements:

- for a signature

Attendance at **lectures** is recommended, but not compulsory.

- for a grade

The course ends in an **examination**. Based on the examination, the exam grade is given according to the following table:

Score	Grade
0-59	fail (1)
60-69	pass (2)
70-79	satisfactory (3)
80-89	good (4)
90-100	excellent (5)

If the score of the examination is below 60, students can take a retake test in conformity with the EDUCATION AND EXAMINATION RULES AND REGULATIONS.

-an offered grade:

it may be offered for students if they write a test on the 14th week and the score of it is at least 60%. The offered grade is calculated as the exam grade (see above).
Person responsible for course: Dr. Noémi Nagy, professor, DSc
Lecturer: Dr. Noémi Nagy, professor, DSc

Title of course: Nuclear Methods for Environmental Protection **Code**: TTKME0426_EN	**ECTS Credit points:** 3
Type of teaching, contact hours - lecture: 2 hours/week - practice: - - laboratory: -	
Evaluation: exam	
Workload (estimated), divided into contact hours: - lecture: 22 hours - practice: - - laboratory: - - home assignment: 20 hours - preparation for the exam: 20 hours Total: 62 hours	
Year, semester: 1st year, 2nd semester	
Its prerequisite(s): NA	
Further courses built on it: -	

Topics of course
The series of lectures are based on the topics of natural and anthropogenic radioactivity. It reviews the sources and level of the natural and industrial radiation. It presents the environmental problems, which could be investigated using isotope analyses. It gives an overview about the applicable analytical methods and their basic parameters (sample matrix, sample amount and suitable physical froms, detection level). Introduction of the complex application of combined isotope methods targeting environmental problems.
Literature
Compulsory: Allegre, J.C. (2008) Isotope Geology. Cambridge University Press, Cambridge, pp: 534, ISBN-13 978-0-521-86228-8 *Recommended:* - Faure, G. (1998) Principles and Applications of Geochemistry. Prentice-Hall Inc., Upper Saddle

River, New Yersey, pp: 600, ISBN: 0-02-336450-5
Brownlow, H.A. (1996) Geocehmistry. Prentice-Hall Inc., Upper Saddle River, New Yersey, pp: 573, ISBN-13: 978-0133982725

Course objective/intended learning outcomes

a) Knowledge

He/She knows the most recent theories, models and related computational methods on the scientific results about chemical bonds, structure of compounds, reactions, and chemical interactions.

He/She understands the progress and future trends in chemistry and chemical industries.

He/She has global knowledge on science other than chemistry, and capable to organize this information**b)**

b) Abilities

He/She is able to distinguish between the scientifically proven theories and non-reliable data or information

Using the knowledge and experiences during the MSc coursed he/she is able to execute laboratory experiments or measurements to demonstrate proper chemical phenomena, or syntheses of new compounds and characterize them, and using analytical methods for provement of new reactions.

c) Attitude

He/She is receptive to establish and apply new chemical and environmental technologies.

d) Autonomy and responsibility

- He/She can make own decisions even in complex professional questions, discussions..

Schedule:

1st week

Generation-II type NPP Rectors and their environmental impact.

2nd week

Radioactive waste management in NNP systems, techniques and strategies.

3rd week

Radioactive emissions during normal operation of NPPs and their impact.

4th week

New generation of NPP rectors, perspective.

5th week

Nuclear waste repository systems, technology and strategies.

6th week

Application of noble gas isotope analyses for diagnostics of nuclear reactors and connected systems.

7th week

Classification of nuclear waste streams, difficult-to-measure isotopes.

8th week

Gas generation in nuclear waste, implications and methods.

9th week

Normal and accidental isotope releases form NPPs. History, recent practice and future perspective. *10th week* Groundwater monitoring systems around NPPs. Strategies and recent practice. *11th week* Overview of isotope analytical methods for NPPs radiochemical purposes. Example of the HEKAL Laboratory at MTA Atomki. *12th week* Cyclotrons for NPP investigations and medical applications. *13th week* Environmental impact of Cyclotron laboratories. *14th week* *Visit at the Cyclotron Lab of MTA Atomki, Debrecen.*
Requirements: *- for a signature* Attendance at **lectures** is recommended, but not compulsory. *- for a grade* The course ends in an **examination**. The minimum requirement for the examination respectively is 60%. Based on the score of the tests separately, the grade of the examination is given according to the following table: Score Grade 0-59 fail (1) 60-69 pass (2) 70-79 satisfactory (3) 80-89 good (4) 90-100 excellent (5) If the score of any test is below 60, students can take a retake test in conformity with the EDUCATION AND EXAMINATION RULES AND REGULATIONS. *-an offered grade:* Not applicable.
Person responsible for course: Dr. Mihály Molnár, Senior research fellow, PhD
Lecturer: Dr. Mihály Molnár, Senior research fellow, PhD

Title of course: Medical applications of radiopharmaceuticals **Code**: TTKME0429_EN	**ECTS Credit points: 3**
Type of teaching, contact hours - lecture: 2 hours/week - practice: 0 hours/week - laboratory: 0-	
Evaluation: terminal exam	

Workload (estimated), divided into contact hours: - lecture: 28 hours - practice: 0 hours - laboratory: 0 - home assignment: 30 hours - preparation for the exam: 32 hours Total: 90 hours
Year, semester: 2nd year, 2nd semester
Its prerequisite(s): -
Further courses built on it: -

Topics of course
The series of lectures are based on the different topics of preclinical and clinical Nuclear medicine. It reviews the physiological fundamentals of the radiopharmaceutical applications the essentials of instrumentation and diagnostic and therapeutic procedures of Nuclear Medicine,.
Literature
Compulsory: -A Concise Guide to Nuclear Medicine (Elgazzar, A. H., Springer, 2011) *Recommended:1.* A Clinician's Guide to Nuclear Medicine (Taylor A., Alazraki N., and Schuster D.M.; SNM, 2006, 2nd ed.) 2. Fred A., Mettler JR., Milton J.,Guiberteau essentials of Nuclear Medicine Imaging 5th. ed. Elsevier 2006
Course objective/intended learning outcomes
a) Knowledge - He/she fundamentally knows principles of nuclear medicine procedures from developmental and physiological basics of radiopharmaceutical applications to technical essentials of detectors and data acquisition with dedicated and hybrid instruments of Nuclear medicine. **b) Abilities** - He/she is able to apply the most important terminology, theories and procedures of preclinical and clinical Nuclear Medicine. - He/she is able to discover the connections between the clinical indications and radiopharmaceuticals and the used imaging protocols, and is able to use reading principles of imaging and quantitative information's of procedures. - **c) Attitude** - He/she is open to learn the new scientific improvements and develop knowledge of professional, technological and innovation in his/her profession but to refuse the unrealistic statements.

d) Autonomy and responsibility

- First with guidance but later independently he/she is capable to participate in team work of preclinical and clinical studies considering fundamental questions from his/her professional.
- He/she is open to critical remarks which are professionally well-founded.

Schedule:

1st week: The anatomy, the developmental and physiological fundamentals of brain, endocrine system and heart and lung system from the aspects of used radiopharmaceuticals.

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*2nd week***:** The anatomy, the developmental and physiological fundamentals of gastrointestinal tract, kidney's, inflammations. Oncology.

3rd week: Instrumentation of Nuclear medicine, single photon technics.

4th week: Instrumentation of Nuclear medicine, double photon (PET) technics.

5th week: Instrumentation of Nuclear medicine, multimodality (hybrid) imaging.

6th week: Nuclear Medicine investigations of illnesses of central nervous and endocrine systems.

7th week: Nuclear Medicine investigations of respiratory, circulatory systems and gastrointestinal and immunologyc disorders

8th week: Imaging of separated kidney function. Oncology 1. Bone scitigraphy.

9th week: Onkologia **2.** PET, PET-CT hybrid imaging.

10th week: Introduction into the field of preclinical interventions.

11th week: Visit the preclinical lab, try the instruments.

12th week: Visit the department of human clinical diagnostic and therapeutic nuclear medicine interventions. Patient booking and management from the aspects of Single photon radiopharmaceuticals. Imaging instrumentation (1 hour)
Patient booking and management from the aspects of PET isotope-labelled radiopharmaceticals. PET Imaging instrumentation (1 hour)

13th week: Protocols of different isotope therapies. From isotope shielding to patient release.

14th week: Discussion, consultation before exam.,

Requirements:

- *for a signature*

Attendance at **lectures** is recommended, but not compulsory.

Participation at **practice classes** is compulsory. A student must attend the practice classes and may not miss more than three times during the semester. In case a student does so, the subject will not be signed and the student must repeat the course. A student can't make up any practice with another group. Attendance at practice classes will be recorded by the practice leader. Being late is equivalent with an absence. In case of further absences, a medical certificate needs to be presented. Missed practice classes should be made up for at a later date, to be discussed with the tutor. Students are required to bring the drawing tasks and drawing instruments of the course to each practice class. Active participation is evaluated by the teacher in every class. If a student's behavior or conduct doesn't meet the requirements of active participation, the teacher may evaluate his/her participation as an absence because of the lack of active participation in class.

Students have to **submit all the designing tasks** as scheduled minimum on a sufficient level.

At the end of course there is a one written exam. Students have to sit for the tests

- *for a grade*

The course ends in an **examination**. Based on the average of the grades of the designing tasks and the examination, the exam grade is calculated as an average of them:

- the average grade of the two designing tasks
- the result of the examination

The minimum requirement for the mid-term and end-term tests and the examination respectively is 60%. Based on the score of the tests separately, the grade for the tests and the examination is given according to the following table:

Score	Grade
0-59	fail (1)
60-69	pass (2)
70-79	satisfactory (3)
80-89	good (4)
90-100	excellent (5)

If the score of test is below 60, students can take a retake test in conformity with the EDUCATION AND EXAMINATION RULES AND REGULATIONS.

-an offered grade:

it may be offered for students if the average grade of the two designing tasks is at least satisfactory (3) and the average of the mid-term and end-term tests is at least satisfactory (3). The offered grade is the average of them.

Person responsible for course: Dr. László Galuska professor emeritus

Lecturer: Dr. László Galuska professor emeritus

Title of course: Nuclear Analysis I. **Code**: TTKME0523_EN	**ECTS Credit points:** 3
Type of teaching, contact hours	

- lecture: 2 hours/week - practice: - - laboratory: -
Evaluation: exam
Workload (estimated), divided into contact hours: - lecture: 28 hours - practice: - - laboratory: - - home assignment: 22 hours - preparation for the exam: 40 hours Total: 90 hours
Year, semester: 2nd year, 1st semester
Its prerequisite(s): -
Further courses built on it: TTKML0523_EN

Topics of course
- Formation of nuclear, atomic and particle radiations. their interaction with matter, and analytical aspects. - Application of natural stable and radioactive isotope in natural sciences. - Tracer methods. - Nuclear and radioanalytical methods using the interactions of radiation with matter.
Literature
Compulsory: - Kónya, J., Nagy N.M., 2012, 2018. Nuclear and Radiochemistry, Elsevier, Oxford. - Choppin, G.R., Liljenzin, J-O., Rydberg, J. Ekberg, C., 2013. Radiochemistry and Nuclear Chemistry, 4th Edition, Elsevier, Amsterdam. - Kratz, J.-V., Lieser, K.H., 2013. Nuclear and Radiochemistry: Fundamentals and Applications, 3rd Edition, Wiley-VCH Verlag GmbH & Co. KGaA, Weinheim, Germany,
Course objective/intended learning outcomes
a) Knowledge - He/She has systematic knowledge on the nuclear and radioanalysis, their main principles including the theoretical and practical application built on these principals. - He/She understands the progress and future trends in nuclear and radioanalysis. **b) Abilities** - He/She is able to use the obtained chemical knowledge on the field of nuclear and radioanalysis to solve the actual basic problems and prove the obtained solution. - He/She is able to argue his/her opinion in scientific discussions both in oral or written form. **c) Attitude** - He/She is being active to start and participate in professional discussions.

- He/She treats the scientific results or intellectual properties with the adequate professional ethics.

d) Autonomy and responsibility

- He/She is responsible in collaboration with other professionals (especially from the field of nuclear and radioanalysis) without supervision.
- He/She is responsible for his/her own decisions stand in for these decisions and ideologies.

Schedule:

1st week
Formation and production of nuclear, atomic and particle radiation.

2nd week
Interaction of nuclear, atomic and particle radiation with matter.

3rd week
Analytical methods using natural radioactivity: determination of geological and historical ages.

4th week
Separation of isotopes. Physical, chemical, geological, and biological information obtained by observing isotope separations.

5th week
Basic rules of tracer studies

6th week
Selection of tracers. Production of tracer isotopes.

7th week
Chemical radioanalytical methods: isotope dilution analysis, radiometric titration, radio gravimetry, radiochemical separation methods.

8th week
Radioanalysis in living organisms: in-vitro and in-vivo methods.

9th week
Industrial radioanalysis.

10th week
Nuclear and radioanalytical methods based on radiation-matter interactions: classification, characterization on the basis of the irradiation and emitted particles/photons.

11th week
Applications of neutrons: activation analytical methods, neutron radiography and tomography, neutrons scattering.

12th week
Application of electromagnetic radiation with high energy (gamma, X-ray): X-ray fluorescence analysis, Mössbauer spectroscopy

13th week
Application of beta and electron radiation: beta backscattering, electron microscopes and microprobes.

14th week
Application of ions: Rutherford backscattering, particles induced X-ray and gamma spectroscopy.

Requirements:

- *for a signature*

Attendance at **lectures** is recommended, but not compulsory.

- *for a grade*

The course ends in an **examination**. Based on the examination, the exam grade is given according to the following table:

Score	Grade
0-59	fail (1)
60-69	pass (2)
70-79	satisfactory (3)
80-89	good (4)
90-100	excellent (5)

If the score of the examination is below 60, students can take a retake test in conformity with the EDUCATION AND EXAMINATION RULES AND REGULATIONS.

-*an offered grade:*

It may be offered for students if they write a test on the 14th week and the score of it is at least 60%. The offered grade is calculated as the exam grade (see above).

Person responsible for course: Dr. Noémi Nagy, professor, DSc

Lecturer: Dr. Noémi Nagy, professor, DSc

Title of course: Nuclear Analysis II.
Code: TTKML0523_EN

ECTS Credit points: 1

Type of teaching, contact hours
- lecture: -
- practice: -
- laboratory: 2 hours/week

Evaluation: practice

Workload (estimated), divided into contact hours:
- lecture: -
- practice: -
- laboratory: 5 days/semester
- home assignment: 20 hours
- preparation for the exam: -

Total: 30 hours

Year, semester: 2nd year, 1st semester

Its prerequisite(s): TTKME0523_EN (same semester)

Further courses built on it: -

Topics of course

- Visits and laboratory practices in nuclear facilities.

Literature

Compulsory:

- Descriptions of practices on the homepage of the department
- Kónya, J., Nagy N. M., 2012, 2018. Nuclear and Radiochemistry, Elsevier, Oxford.
- Choppin, G.R., Liljenzin, J-O., Rydberg, J. Ekberg, C., 2013. Radiochemistry and Nuclear Chemistry, 4th Edition, Elsevier, Amsterdam.

Course objective/intended learning outcomes

a) Knowledge

- He/She has systematic knowledge on the nuclear and radioanalysis, their main principles including the theoretical and practical application built on these principals.
- He/She understands the progress and future trends in nuclear and radioanalysis.

b) Abilities

- He/She is able to use the obtained chemical knowledge on the field of nuclear and radioanalysis to solve the actual basic problems and prove the obtained solution.
- He/She is able to argue his/her opinion in scientific discussions both in oral or written form.

c) Attitude

- He/She is being active to start and participate in professional discussions.
- He/She treats the scientific results or intellectual properties with the adequate professional ethics.

d) Autonomy and responsibility

- He/She is responsible in collaboration with other professionals (especially from the field of nuclear and radioanalysis) without supervision.
- He/She is responsible for his/her own decisions stand in for these decisions and ideologies.

Schedule:

1st day

Visit of a nuclear power plant (Paks). Chemical task in a nuclear power plant (analysis, radiation protection)

2nd day

Visit of a nuclear waste disposal site (Bátaapáti).

3rd day

Visit of Isotope Institute Ltd. (Budapest). Production of radiopharmaceuticals.

4th day

Visit of Energy Science Research Institute (Budapest). Prompt gamma activation analysis laboratory practice.

5th day

Visit of Energy Science Research Institute (Budapest). ICP-MS analysis of uranium and transuranium elements.

Requirements:

The measurements and knowledge of the associated theory are graded and an overall mark will be given.

Safety training is mandatory before the first lab practice. Everybody should work and do the

measurement individually according to the pre-set schedule (it will be provided prior to the first lab. The laboratory practices are 4-hrs long. In accordance with the regulations of University of Debrecen, attendance is compulsory with the exception of health or family problems. In this case, the students should agree with the teacher on replacement dates for the missed experiments. Pregnant and breastfeeding women are not allowed to work in radioactive laboratory.
Person responsible for course: Dr. Noémi Nagy, professor, DSc
Lecturer: Dr. Noémi Nagy, professor, DSc

Title of course: Production of Isotopes **Code**: TTKML0437_EN	**ECTS Credit points: 3**
Type of teaching, contact hours - lecture: 1 hour/week - practice: 0 hours/week - laboratory: 1 hour/week	
Evaluation: practical grade	
Workload (estimated), divided into contact hours: - lecture: 14 hours - practice: 0 hour - laboratory: 14 hours - home assignment: 62 hours - preparation for the exam: 0 hours Total: 90 hours	
Year, semester: 2nd year, 1st semester	
Its prerequisite(s):	
Further courses built on it: -	

Topics of course
The present course is aimed at providing knowledge for the students on the various aspects of production of radioisotopes by the use of cyclotrons, nuclear reactors or isotope-generators. They will obtain the basic overview about the practical aspects of producing biological relevant isotopes, some details about the technical limitations of the processes. They have also opportunity to get very basic practical knowledge about the handling of different isotopes. They will work under supervision of an experienced worker, but independently.
Literature
Compulsory: *Recommended:* - G. Stöcklin, V. Pike: Radiopharmaceuticals for Positron Emission Tomography, ISBN 978-94-015-8204-9

- Cyclotron produced radionuclides, Physical characteristic and production IAEA TECHNICAL REPORTS SERIES No. 468 ISBN 978–92–0–106908–5
- Handbook of Nuclear Chemistry, Editors: Vértes, A., Nagy, S., Klencsár, Z., Lovas, R.G., Rösch, F. ISBN 978-1-4419-0719-6
- Michael J. Welch,Carol S. Redvanly: Handbook of radiopharmaceuticals: radiochemistry and applications ISBN: 978-0-471-49560-4

Course objective/intended learning outcomes

a) Knowledge

- Have systematic knowledge on the various subject of radiochemistry and production of radioactive isotopes.
- Have first-hand experience handling different isotopes and the rules of radiation-protection
- Insert the topic into the global knowledge on science and on chemistry, and capable to organize this information

b) Abilities

- He/She is able to apply the most important terminology, theories, and procedures of the given field when completing the relevant tasks.
- He/she is able to participate in a professional discussion and be able to express her/his opinion about radiochemistry without any stereotype.

c) Attitude

- He/She is being active to start and participate in professional discussions.
- He/she is open to learn and accept professional, technological improvement and innovation in his/her profession and convey it genuinely.
- He/She is able to evaluate the potential risks of the application of radioactivity, but can refuse the rumours

d) Autonomy and responsibility

- Even in unexpected decision-making situations he/she is capable of considering complex, fundamental questions from his/her professional field and elaborating them on the basis of the given sources.
- He/she is able to work independently on the tasks involved in the practical sessions under supervision.
- He/she is open to critical remarks which are professionally well-founded.

Schedule:

1st week The requirements of nuclear reaction, basic definitions

2nd week Nuclear reactors and other neutron sources

3rd week Production of isotopes with neutron excess

4th week Particle accelerators

5th week Production of isotopes with neutron deficient

6th week Targetry, classical PET isotopes

7th week Radionuclide generators

8th week Basic aspect of radiolabelling

9th week Production of a Gallium-68labelled molecule by means of an isotope-generator

10th week Production of a Gallium-68labelled molecule by means of an isotope-generator

11th week Production and application of Fluorine-18 isotope

12th week Production and application of Fluorine-18 isotope

13th week: Production and application of Carbon-11 isotope

14th week Production and application of Carbon-11 isotope

Requirements:

- for a signature

Attendance at **lectures** is recommended, but not compulsory. The participation on the **practical part** is an obligation as well as the preparation of a laboratory report. Attendance at practice classes will be recorded by the practice leader. Being late is equivalent with an absence. In case of further absences, a medical certificate needs to be presented. Missed practice classes should be made up for at a later date, to be discussed with the tutor. Active participation is evaluated by the teacher in every class. If a student's behaviour or conduct doesn't meet the requirements of active participation, the teacher may evaluate his/her participation as an absence because of the lack of active participation in class. Students have to **submit all the 3 laboratory reports** as scheduled minimum on a sufficient level. In case a student does so, the subject will not be signed and the student must repeat the course.

- for a grade

The course ends in an **examination** of the theoretical part. Based on the average of the grades of the reports and the examination, the practical grade is calculated as an average of them:

- the average grade of the reports
- the result of the oral examination

Score	Grade
< 1.5	fail (1)
1.51-2.5	pass (2)
2.51-3.5	satisfactory (3)
3.51-4.5	good (4)
4.5<	excellent (5)

If the score of a report or the oral examination is below „pass", students can take a chance to repeat it,

in conformity with the EDUCATION AND EXAMINATION RULES AND REGULATIONS. *-an offered grade:* It may be offered for students if the average grade of the reports is “excellent” and they prepare a 10 min. slide show in a high quality for the class, from a topic selected by the tutor. The offered grade is “excellent”.
Person responsible for course: Dr. István Kertész, research fellow, PhD
Lecturer: Dr. István Kertész, research fellow, PhD Dr. Hajdú István, senior lecturer, PhD Norbert Pótári, chemist Noémi Dénes Stéfán, PhD. student

Title of course: Separation techniques for radiolabeled compounds **Code**: TTKME0431_EN	**ECTS Credit points:** 3
Type of teaching, contact hours - lecture: 2 hours/week - practice: - - laboratory: -	
Evaluation: exam	
Workload (estimated), divided into contact hours: - lecture: 28 hours - practice: - - laboratory: - - home assignment: 22 hours - preparation for the exam: 40 hours Total: 90 hours	
Year, semester: 2nd year, 1st semester	
Its prerequisite(s): -	
Further courses built on it: -	

Topics of course
- Characteristics of radiochemistry. - Solvent exchange. Solvent elimination in radiolabelling processes. - Solid phase extraction procedures. - Chromatographic techniques. Liquid chromatography. Analytical and semi-preparative techniques. - Radioactive detectors. - Fast chromatography. Ultrahigh efficiency in chromatographic measurements of radioactive samples. - Quality assurance.

Literature

Compulsory:

- 1. Pharmaceutical Radiochemistry, Munich Molecular Imaging Handbook Series. Hans J. Wester. Scintomics, Print Media and Publishing. 2010.

2. J. M. Miller. J.B. Crowther. Analytical chemistry in a GMP environment. Wiley. 2000.

Recommended:

1. L. Huber. Validation and qualification in Analytical Laboratories. Informa Healthcare. 2007.

Course objective/intended learning outcomes

a) Knowledge

- He/she fundamentally knows principles of radiochemistry, rules of radioactive decay, natural and artificial radionuclides, rules of irradiation protection, analytical methods applicable to radioactive samples.

b) Abilities

- He/she is able to apply the most important terminology, theories, procedures of the given chemical field when completing the relevant tasks.
- He/she is able to create fundamental models of analytical systems and processes.

c) Attitude

- He/she is open to learn and accept professional, technological improvement and innovation in his/her profession and convey it genuinely.
- He/she makes a decision in complex and unexpected decision cases by completely taking into account legal and ethical norms.

d) Autonomy and responsibility

- Even in unexpected decision-making situations he/she is capable of considering complex, fundamental questions from his/her professional field and elaborating them on the basis of the given sources.
- He/she confesses and represents the value system of the engineering profession with responsibility. He/she is open to critical remarks which are professionally well-founded.

Schedule:

1st week

Basic separation problems in the field of radiochemistry.

2nd week

Elimination of solvents, solvent exchange, evaporation, lyophilisation.

3rd week

Elimination of solid parts from liquid reaction mixtures. Filtration, centrifuging. Extraction, SPE, SPME techniques. Supercritical fluid extraction. Ion exchange.

4th week

Basics of chromatography. Retention, selectivity, dynamic partition coefficient. van Deemter equation.

5th week
Sample preparation. Extraction. SPE techniques. Filtration. Internal standards. Reverse phase chromatography. Separation of acids, basics and neutral compounds. Gradient elution. pH control.

6th week
Normal phase chromatography. HILIC. Ion exchange. Size exclusion. Chiral chromatography.

7th week
HPLC method development. Preparative separation.

8th week
Fast chromatography. Ultrahighperformance chromatography (UPLC)

9th week
Detecton in HPLC. UV, RI, ELS, EC detectors.

10th week
Radioactive detectors. Gamma spectrometry. Liquid scintillation. Scintillation detectors. Coincidence detectors.

11th week
Gas chromatography. Type of injection, detection. Method development. GC-MS.

12th week
Performance of analytical devices. Troubleshooting. Maintenance.

13th week
Qualification of analytical devices: DQ/IQ/OQ/PQ.

14th week
Validation of analytical methods.

Requirements:
- for a signature
Attendance at **lectures** is recommended, but not compulsory.
- for a grade
The course ends in an **examination**.

Person responsible for course: Dr. István Jószai, chemist, PhD

Lecturer: Dr. István Jószai, chemist, PhD and Dr. Dezső Szikra, chemist, PhD

Title of course: Dosimetry, Radiation Health Effects Code: TTKME0432-EN	ECTS Credit points: 3
Type of teaching, contact hours - lecture: 2 hours/week - practice: - - laboratory: -	
Evaluation: exam	
Workload (estimated), divided into contact hours: - lecture: 28 hours - practice: - - laboratory: - - home assignment: 30 hours - preparation for the exam: 32 hours Total: 90 hours	
Year, semester: 1st year, 2nd semester	
Its prerequisite(s): -	
Further courses built on it: -	

Topics of course

- The interactions of radiation with matter. Radiation detectors. Dose concepts. Devices for dosimetry.
- Constituents of population dose. The biological effects of radiation. Forms of radiation damage. Principles of nuclear safety. Protection against external radiation sources.
- Preparation for participating in handling nuclear incidents.
- System of dose limits. Requirements for staffing and equipments.
- Documentation, supervision by the authorities. Classification of isotope labs. Handling unsealed radioactive materials.
- Handling radioactive waste; decontamination.

Attending the classes and passing the exam entitles the student to obtain an official certificate on radiation protection, advanced level, valid for 5 years.

Literature

Compulsory: Diagnostic Radiology Physics
http://www-pub.iaea.org/MTCD/Publications/PDF/Pub1564webNew-74666420.pdf
Related chapters:

Chapter 1. Fundamentals of Atomic and Nuclear Physics
Chapter 2. Interactions of Radiation with Matter
Chapter 3. Fundamentals of Dosimetry
Chapter 20. Radiation Biology
Chapter 21. Instrumentation for Dosimetry
Chapter 24. Radiation Protection

Course objective/intended learning outcomes

a) Knowledge

- He/she is familiar with the physical characteristics and biological effects of ionizing radiation, the principles, methods and tools of radiation protection.

b) Abilities

- He/she is able to comprehend the tasks of radiation protection;
- to organize and control the radiation protection system of a research or medical isotope laboratory.
- He/she is able to apply the tools and methods of radiation protection in the practice.

c) Attitude

- He/she strives for safe work.
- Is open to form his/her working habits to meet the requirements of radiation protection.
- Searches for the possibility to aquire and utilize new knowledge, apply new procedures and techniques, in order to decrease the risk of radiation to him/herself and co-workers.
- Effectively communicates with co-workers to form their means of work safer.

d) Autonomy and responsibility

- He/she comprehends the danger and risks of working with ionizing radiation, and is prepared for an independent activity so that he/she does not impose a health risk to him/herself, co-workers and the population more than inevitable.

Schedule:

Week	*Topic*
1	Types and origin of ionizing radiation Interactions of charged particles with matter
2	Interactions of electromagnetic radiation with matter
	Detection of X-ray, gamma and beta radiation by inducing light
3	Gas ionization detectors Dose concepts and dosimeters
4	Consultation: physics of ionizing radiation

	How to use dosimeters (practice)
5	Biological effects of radiation Forms of radiation injury
6	Constituents of population dose Radiation protection rules, dose limits
7	How to work with unsealed radioactive preparations? Protection against external radiation
8	Classification and equipment of workplaces applying ionizing radiation. Handling of radioactive waste.
9	Radiation protection of patients. Consultation: radiation biology and protection
10	Nuclear safety. Operations in case of nuclear/radiological incidents
11	Radiation protection in and around a cyclotron facility. Demonstration of the radiation protection system.
12	Requirements for staffing.
13	Decay schemes and tables. Decontamination (practical)
14	Radiation protection of patients in nuclear medicine. Visit to the "in vivo" NM center

Requirements:
Attendance of at least 75% of the classes. Usable understanding of the basic physical phenomena, the concepts of radiation effects and protection, as well as the regulations and practical solutions is required.
Chance *"A"* is a computer-based exam. Chance *"B"* and *"C"* are oral.

Person responsible for course: István Hajdu, PhD, Assistant Professor

Lecturer: István Hajdu, PhD, Assistant Professor; József Varga, PhD, Associate Professor

Title of course: Dosimetry, Radiation Health Effects **Code**: TTKME0432-EN	**ECTS Credit points: 3**
Type of teaching, contact hours	

- lecture: 2 hours/week - practice: - - laboratory: -
Evaluation: exam
Workload (estimated), divided into contact hours: - lecture: 28 hours - practice: - - laboratory: - - home assignment: 30 hours - preparation for the exam: 32 hours Total: 90 hours
Year, semester: 1st year, 2nd semester
Its prerequisite(s): -
Further courses built on it: -

Topics of course

- The interactions of radiation with matter. Radiation detectors. Dose concepts. Devices for dosimetry.
- Constituents of population dose. The biological effects of radiation. Forms of radiation damage. Principles of nuclear safety. Protection against external radiation sources.
- Preparation for participating in handling nuclear incidents.
- System of dose limits. Requirements for staffing and equipments.
- Documentation, supervision by the authorities. Classification of isotope labs. Handling unsealed radioactive materials.
- Handling radioactive waste; decontamination.

Attending the classes and passing the exam entitles the student to obtain an official certificate on radiation protection, advanced level, valid for 5 years.

Literature

Compulsory: Diagnostic Radiology Physics
http://www-pub.iaea.org/MTCD/Publications/PDF/Pub1564webNew-74666420.pdf
Related chapters:
Chapter 1. Fundamentals of Atomic and Nuclear Physics
Chapter 2. Interactions of Radiation with Matter
Chapter 3. Fundamentals of Dosimetry

Chapter 20. Radiation Biology
Chapter 21. Instrumentation for Dosimetry
Chapter 24. Radiation Protection

Course objective/intended learning outcomes

a) Knowledge

- He/she is familiar with the physical characteristics and biological effects of ionizing radiation, the principles, methods and tools of radiation protection.

b) Abilities

- He/she is able to comprehend the tasks of radiation protection;
- to organize and control the radiation protection system of a research or medical isotope laboratory.
- He/she is able to apply the tools and methods of radiation protection in the practice.

c) Attitude

- He/she strives for safe work.
- Is open to form his/her working habits to meet the requirements of radiation protection.
- Searches for the possibility to aquire and utilize new knowledge, apply new procedures and techniques, in order to decrease the risk of radiation to him/herself and co-workers.
- Effectively communicates with co-workers to form their means of work safer.

d) Autonomy and responsibility

- He/she comprehends the danger and risks of working with ionizing radiation, and is prepared for an independent activity so that he/she does not impose a health risk to him/herself, co-workers and the population more than inevitable.

Schedule:
Week 1
Types and origin of ionizing radiation
Interactions of charged particles with matter

Week 2
Interactions of electromagnetic radiation with matter
Detection of X-ray, gamma and beta radiation by inducing light

Week 3
Gas ionization detectors
Dose concepts and dosimeters

Week 4

Consultation: physics of ionizing radiation
How to use dosimeters (practice)

Week 5
Biological effects of radiation
Forms of radiation injury

Week 6
Constituents of population dose
Radiation protection rules, dose limits

Week 7
How to work with unsealed radioactive preparations?
Protection against external radiation

Week 8
Classification and equipment of workplaces applying ionizing radiation.
Handling of radioactive waste.

Week 9
Radiation protection of patients.
Consultation: radiation biology and protection

Week 10
Nuclear safety.
Operations in case of nuclear/radiological incidents

Week 11
Radiation protection in and around a cyclotron facility.
Demonstration of the radiation protection system.

Week 12
Requirements for staffing.

Week 13
Decay schemes and tables.
Decontamination (practical)

Week 14
Radiation protection of patients in nuclear medicine.

Visit to the "in vivo" NM center
Requirements: Attendance of at least 75% of the classes. Usable understanding of the basic physical phenomena, the concepts of radiation effects and protection, as well as the regulations and practical solutions is required. Chance *"A"* is a computer-based exam. Chance *"B"* and *"C"* are oral.
Person responsible for course: István Hajdu, PhD, Assistant Professor
Lecturer: István Hajdu, PhD, Assistant Professor; József Varga, PhD, Associate Professor

Title of course: Radiochemical exercises **Code**: TTKML0415_EN	**ECTS Credit points:** 2
Type of teaching, contact hours - lecture: - - practice: - - laboratory: 2 hours/week	
Evaluation: practice	
Workload (estimated), divided into contact hours: - lecture: - - practice: - - laboratory: 28 hours - home assignment: 32 hours - preparation for the exam: - Total: 60 hours	
Year, semester: 1st year, 2nd semester	
Its prerequisite(s): TTKME0410_EN (same semester)	
Further courses built on it: -	

Topics of course
- Measuring technique practices: adjust of optimal parameters, study of self-absorption, liquid scintillation spectrometry - Basic properties of radioactive decay (half-life, statistics) - Operations with un-sealed radionuclides : radiometric titration, self-absorption (sample preparation) - Simulation of nuclear energy production, computations
Literature
Compulsory:

- Descriptions of practices on the homepage of the department
- Kónya, J., Nagy N. M., 2012, 2018. Nuclear and Radiochemistry, Elsevier, Oxford.
- Choppin, G.R., Liljenzin, J-O., Rydberg, J. Ekberg, C., 2013. Radiochemistry and Nuclear Chemistry, 4th Edition, Elsevier, Amsterdam.

Course objective/intended learning outcomes

a) Knowledge

- He/She knows various methods from radiochemical labs or industries, able to show it to other people and apply them including the equipments and their safe usage.

b) Abilities

- He/She is able to carefully apply the newest chemical theories in practice and design lab experiments or industrial processes based on these results.

c) Attitude

- He/She is committed to protect the environment in both chemical labs and industries. This attitude is shown to other coworkers as well.
- He/She makes effort to apply those technologies that makes lower environmental changes/loads.

d) Autonomy and responsibility

- He/She can operate chemical or industrial instruments or equipments with responsibility, and manage persons working with these.

Schedule:

1st week

Operation of gas ionization detector, adjust of optimal measuring parameters

Optimal parameters of radioactivity detector

2nd week

Liquid scintillation spectrometry

Special technique of beta activity measurement, factors influencing the affectivity, absolute activity measurement

3rd week

Statistics of radioactive decay

Calculations on statistics of radioactive decay, measuring errors, spread-error rules, improvements of accuracy

4th week

Determination of short and long half-life

Determination of short half-life by direct measurement. Determination of long half-life by comparing activity and number of radionuclides.

5th week

Absorption and self-absorption of radiation.

Possibility of the (self-) absorption correction. Handling of unsealed radionuclide during the sample preparation.

6th week

Radiometric titration

Special observation of endpoint of a titrimetric method. Operation with unsealed radionuclide *7^{th} week* Comparison of different types of energy production. Simulation of nuclear reactor. Comparison of environmental impacts of energy production ways.
Requirements: The measurements and knowledge of the associated theory are graded and an overall mark will be given. Safety training is mandatory before the first lab practice. Everybody should work and do the measurement individually according to the pre-set schedule (it will be provided prior to the first lab. The laboratory practices are 4-hrs long. In accordance with the regulations of University of Debrecen, attendance is compulsory with the exception of health or family problems. In this case, the students should agree with the teacher on replacement dates for the missed experiments. Pregnant and breastfeeding women are not allowed to work in radioactive laboratory.
Person responsible for course: Dr. Noémi Nagy, professor, DSc
Lecturer:

Title of course: Biological application of labelled compounds **Code**: TTKME0434_EN	**ECTS Credit points: 3**
Type of teaching, contact hours - lecture: 2 hour/week - practice: 0 hours/week - laboratory: 0 hour/week	
Evaluation: exam	
Workload (estimated), divided into contact hours: - lecture: 28 hours - practice: 0 hour - laboratory: 0 hours - home assignment: 7 hours - preparation for the exam: 55 hours Total: 90 hours	
Year, semester: 2^{nd} year, 2^{nd} semester	
Its prerequisite(s):	
Further courses built on it: -	

Topics of course
The present course is aimed at providing knowledge for the students on the application of different

isotopes on the field of nuclear medicine and biological research. It will summarize the properties can be important for the biological application and provide a short survey about the chemical reactions common in radiolabelling.

Literature

Compulsory:
Recommended:
- Handbook of Nuclear Chemistry, Editors: Vértes, A., Nagy, S., Klencsár, Z., Lovas, R.G., Rösch, F. ISBN 978-1-4419-0719-6
- Michael J. Welch,Carol S. Redvanly: Handbook of radiopharmaceuticals: radiochemistry and applications ISBN: 978-0-471-49560-4
- HJ. Wester: Pharmaceutical Radiochemistry: 1 ISBN: 978-3-98135230-6

Course objective/intended learning outcomes

a) Knowledge

- Have systematic knowledge on the various subjects of radiochemistry and the chemical tools suitable to incorporate isotopes into biological vectors.
- Give examples the application of PET "classical" isotopes, radiolabelling with radiometals for diagnostic or therapeutic purposes, using different halogen isotopes, C-14 or H-3 labelling examples. Moreover it provides some elements of the knowledge of the detection of radiations and a very basic information about the radiopharmaceutical considerations.
- Insert the topic into the global knowledge on science and on chemistry, and capable to organize this information

b) Abilities

- He/She is able to apply the most important terminology, theories, and procedures of the given field when completing the relevant tasks.
- He/she is able to participate in a professional discussion and be able to express her/his opinion about radiochemistry without any stereotype.

c) Attitude

- He/She is being active to start and participate in professional discussions.
- He/she is open to learn and accept professional, technological improvement and innovation in his/her profession and convey it genuinely.
- He/She is able to evaluate the potential risks of the application of radioactivity, but can refuse the rumours

d) Autonomy and responsibility

- Even in unexpected decision-making situations he/she is capable of considering complex, fundamental questions from his/her professional field and elaborating them on the basis of the given sources.
- He/she is open to critical remarks which are professionally well-founded.

Schedule:

1st week The classification of the chemical reactions useful for radiolabelling.

2nd week Radiolabelling with Fluorine-18. Electrophile fluorination.

3rd week Radiolabelling with Fluorine-18. Nucleophile fluorination.

4th week Instrumental developments for improving the efficacy of radiolabelling.

5th week Peptide (sensitive biomolecules) radiolabelling with Fluorine-18.

6th week Peptide (sensitive biomolecules) radiolabelling with Gallium-68 or Technetium-99m .Comparison, benefits, drawbacks.

7th week Radiolabelling. Radiopharmaceutical aspects.

8th week Chemoselective way of radiolabelling. In vivo labelling.

9th week Radiolabelling with Carbon-11.

10th week Radiolabelling with Nitrogen-13, Oxigen-15. Radiohalogenation.

11th week Radiolabelling with therapeutic radiometals.

12th week "Non-common" radiometals for radiolabelling.

13th week: Radiolabelling with Carbon-14 or Tritium.

14th week Consultation. Measurement of radiation.

Requirements:
- *for a signature*

Attendance at **lectures** is recommended, but not compulsory.
- *for a grade*

The course ends in an **examination**. During the oral examination students will get two topics and after the appropriate preparation time they will present their knowledge. The grade of the course will be calculated:

- 30% from the attitude during the lessons (it is possible due to a small number of participants)
- 70% the result of the oral examination

Score	Grade
	fail (1)
	pass (2)
	satisfactory (3)
	good (4)

excellent (5) If the score of the oral examination is below „pass", students can take a chance to repeat it, in conformity with the EDUCATION AND EXAMINATION RULES AND REGULATIONS. *-an offered grade:*
Person responsible for course: Dr. István Kertész, research fellow, PhD
Lecturer: Dr. István Kertész, research fellow, PhD

Title of course: Production and quality control of radiopharmaceuticals **Code**: TTKML0435_EN	**ECTS Credit points:** 2
Type of teaching, contact hours - lecture: - - practice: - - laboratory: 2 hours/week	
Evaluation: practice	
Workload (estimated), divided into contact hours: - lecture: - - practice: - - laboratory: 28 hours - home assignment: 32 hours - preparation for the exam: - Total: 60 hours	
Year, semester: 2nd year, 2nd semester	
Its prerequisite(s): -	
Further courses built on it: -	

Topics of course
- Decontamination procedure. - Radiolabelling with PET isotopes. - Quality control of radiopharmaceuticals. Method development.
Literature
Compulsory: - 1. Pharmaceutical Radiochemistry, Munich Molecular Imaging Handbook Series. Hans J. Wester. Scintomics, Print Media and Publishing. 2010. 2. J. M. Miller. J.B. Crowther. Analytical chemistry in a GMP environment. Wiley. 2000. *Recommended:*

1. L. Huber. Validation and qualification in Analytical Laboratories. Informa Healthcare. 2007.

Course objective/intended learning outcomes

a) Knowledge

- He/she fundamentally knows principles of radiochemistry, rules of radioactive decay, natural and artificial radionuclides, rules of irradiation protection, analytical methods applicable to radioactive samples.

b) Abilities

- He/she is able to apply the most important terminology, theories, procedures of the given chemical field when completing the relevant tasks.
- He/she is able to create fundamental models of analytical systems and processes.

c) Attitude

- He/she is open to learn and accept professional, technological improvement and innovation in his/her profession and convey it genuinely.
- He/she makes a decision in complex and unexpected decision cases by completely taking into account legal and ethical norms.

d) Autonomy and responsibility

- Even in unexpected decision-making situations he/she is capable of considering complex, fundamental questions from his/her professional field and elaborating them on the basis of the given sources.
- He/she confesses and represents the value system of the engineering profession with responsibility. He/she is open to critical remarks which are professionally well-founded.

Schedule:

1st week
Decontamination procedures.

2nd week
Production of [^{18}F]FDG. Preparation of synthesis modules.

3rd week
Production of [^{18}F]FDG. Performance of radiolabelling procedure. Dispensing of radiopharmaceutical into vials.

4th week
Production of [^{11}C]methionine. Preparation of synthesis modules.

5th week
Production of [^{11}C]methionine. Performance of radiolabelling procedure. Dispensing of radiopharmaceutical into vials.

6th week
Preparation of other F-18 and C-11 labelled tracers.

7th week Production of C-11 isotope in cyclotron. *8th week* Production of F-18 isotope in cyclotron. *9th week* Quality control of [^{18}F]FDG. Determination of radiochemical and chemical purity by HPLC. *10th week* Quality control of [^{18}F]FDG. Determination of radiochemical purity by thin layer chromatography. *11th week* Quality control of [^{11}C]methionine. Determination of radiochemical, enantiomeric and chemical purity by HPLC. *12th week* Validation of HPLC methods. *13th week* Determination of solvent content in radiopharmaceuticals by GC. *14th week* Radionuclidic identification and purity test by gamma spectrometry.
Requirements: - *for a signature* Participation at **laboratory practices** is compulsory. A student can't make up any practice with another group. Attendance at practices will be recorded by the practice leader. Being late is equivalent with an absence. In case of further absences, a medical certificate needs to be presented. Missed practices should be made up for at a later date, to be discussed with the tutor. Students are required to bring laboratory coats, calculators and protective glasses. Active participation is evaluated by the teacher in every class. If a student's behaviour or conduct doesn't meet the requirements of active participation, the teacher may evaluate his/her participation as an absence because of the lack of active participation in class. - *for a grade* Laboratory report must be prepared after completion of practical topic. The laboratory practice grade will be calculated as the average grade of reports.
Person responsible for course: Dr. István Jószai, chemist, PhD
Lecturer: Dr. István Jószai, chemist, PhD, Norbert Pótári, chemist, Enikő Németh chemist

Title of course: Investigation of Cellular and Tissue Metabolism With Radiochemical Methods **Code**: TTKME0436_EN	**ECTS Credit points:** 3
Type of teaching, contact hours - lecture: 2 hours/week - practice: - - laboratory: -	
Evaluation: exam	
Workload (estimated), divided into contact hours: - lecture: 28 hours - practice: - - laboratory: - - home assignment: 30 - preparation for the exam: 32 Total: 90 hours	
Year, semester: 2nd year, 2nd semester	
Its prerequisite(s): -	
Further courses built on it: -	

Topics of course

- General characteristics of radionuclides, radiopharmaceuticals and their properties.
- General characterization of normal and pathological metabolic processes.
- Investigation of metabolic processes using radiopharmaceuticals.
- General characterization of receptor expression and their in vitro and in vivo detection using radiopharmaceuticals.
- Examination of diseases with radiopharmaceuticals in vivo.

Literature

Compulsory:

- Sharp, Peter F., Gemmell, Howard G., Murray, Alison D. (Eds.): Practical Nuclear Medicine, Springer, 3rd ed. 2005, X, 382 p. 222 illus., 17 illus. in color. ISBN 978-1-84628-018-4.
- Harvey A. Ziessman, MD and Janis P. O'Malley, MD: Nuclear Medicine: The Requisites, 4th Edition, 2014, I SBN: 978-0-323-08299-0.

Recommended:

- R. A. Powsner, E. R. Powsner: Essential Nuclear Medicine Physics
Blackwell Publishing, 2006 (2nd ed.) Print ISBN: 9781405104845.

Course objective/intended learning outcomes

a) Knowledge
- Have systematic knowledge on the various subject of chemistry, their main principals including the theoretical and practical application built on these principals.
- He/She understands the progress and future trends in chemistry and chemical industries.
- He/She has global knowledge on science other than chemistry, and capable to organize this information.

b) Abilities
- He/She is able to use the new approaches on the field of chemical research and innovation to apply the main theories, practical information, application and technology as well as understanding and analyzing scientific data.
- He/She is able to recognize and evaluate the global relationships on the field of chemistry.
- He/She is able to distinguish between the scientifically proven theories and non-reliable data or information.

c) Attitude
- He/She accepts those professional identities that define the uniqueness and importance of science.

d) Autonomy and responsibility
- He/She can make own decisions even in complex professional questions, discussions.

Schedule:

1st week Introduction: Radioisotopes in medical biology. The structure and operation of a preclinical radiochemistry and imaging laboratory. Authorizations.

2nd week Basic metabolic processes of cells and tissues. Receptors.

3rd week Development of radiopharmaceuticals, experimental radioligands.

4th week In vitro, ex vivo studies with radiopharmaceuticals.

5th week Characterization and investigation of normal and pathological carbohydrate metabolism with radiopharmaceuticals.

6th week Glucose metabolism measurement with 18FDG radiopharmaceutical.

7th week Characterization and investigation of normal and pathological amino acid metabolism with radiopharmaceuticals.

8th week Characterization and investigation of normal and pathological lipid metabolism with radiopharmaceuticals.

9th week Characterization and investigation of normal and pathological cell proliferation with radiopharmaceuticals.

10th week Preclinical radiopharmaceuticals of oncological and immunological diseases.

11th week Preclinical radiopharmaceuticals of neurological and cardiovascular diseases.

12th week Radiopharmaceuticals in drug research and development.

13th week Radiopharmaceuticals in receptor research, receptor-ligand binding assays.

14th week Summary, review.

Requirements:
- *for a signature*

Attendance at **lectures** is compulsory.
A student may not miss more than two times during the semester. In case a student does so, the subject will not be signed and the student must repeat the course. In case of further absences, a medical certificate needs to be presented.
The course ends in an **examination**.
The minimum requirement for the examination is 60%. Based on the score the grade for the examination is given according to the following table:

Score	Grade
0-59	fail (1)
60-69	pass (2)
70-79	satisfactory (3)
80-89	good (4)
90-100	excellent (5)

If the score of the examination is below 60, students can take a retake examination in conformity with the EDUCATION AND EXAMINATION RULES AND REGULATIONS.

Person responsible for course: György Trencsényi, PhD, Habil., associate professor

Lecturer: György Trencsényi, PhD, Habil., associate professor

Title of course: Investigation of Cellular and Tissue Metabolism With Radiochemical Methods
Code: TTKME0436_EN

ECTS Credit points: 3

Type of teaching, contact hours
- lecture: 2 hours/week
- practice: -
- laboratory: -

Evaluation: exam

Workload (estimated), divided into contact hours:
- lecture: 28 hours
- practice: -

- laboratory: - - home assignment: 30 - preparation for the exam: 32 Total: 90 hours
Year, semester: 2^{nd} year, 2^{nd} semester
Its prerequisite(s): -
Further courses built on it: -

Topics of course
- General characteristics of radionuclides, radiopharmaceuticals and their properties. - General characterization of normal and pathological metabolic processes. - Investigation of metabolic processes using radiopharmaceuticals. - General characterization of receptor expression and their in vitro and in vivo detection using radiopharmaceuticals. - Examination of diseases with radiopharmaceuticals in vivo.
Literature
Compulsory: - Sharp, Peter F., Gemmell, Howard G., Murray, Alison D. (Eds.): Practical Nuclear Medicine, Springer, 3rd ed. 2005, X, 382 p. 222 illus., 17 illus. in color. ISBN 978-1-84628-018-4. - Harvey A. Ziessman, MD and Janis P. O'Malley, MD: Nuclear Medicine: The Requisites, 4th Edition, 2014, I SBN: 978-0-323-08299-0. *Recommended:* - R. A. Powsner, E. R. Powsner: Essential Nuclear Medicine Physics Blackwell Publishing, 2006 (2nd ed.) Print ISBN: 9781405104845.
Course objective/intended learning outcomes
a) Knowledge - Have systematic knowledge on the various subject of chemistry, their main principals including the theoretical and practical application built on these principals. - He/She understands the progress and future trends in chemistry and chemical industries. - He/She has global knowledge on science other than chemistry, and capable to organize this information. **b) Abilities** - He/She is able to use the new approaches on the field of chemical research and innovation to apply the main theories, practical information, application and technology as well as understanding and analyzing scientific data. - He/She is able to recognize and evaluate the global relationships on the field of chemistry. - He/She is able to distinguish between the scientifically proven theories and non-reliable data or information. **c) Attitude**

- He/She accepts those professional identities that define the uniqueness and importance of science.

d) Autonomy and responsibility

- He/She can make own decisions even in complex professional questions, discussions.

Schedule:

1st week Introduction: Radioisotopes in medical biology. The structure and operation of a preclinical radiochemistry and imaging laboratory. Authorizations.

2nd week Basic metabolic processes of cells and tissues. Receptors.

3rd week Development of radiopharmaceuticals, experimental radioligands.

4th week In vitro, ex vivo studies with radiopharmaceuticals.

5th week Characterization and investigation of normal and pathological carbohydrate metabolism with radiopharmaceuticals.

6th week Glucose metabolism measurement with 18FDG radiopharmaceutical.

7th week Characterization and investigation of normal and pathological amino acid metabolism with radiopharmaceuticals.

8th week Characterization and investigation of normal and pathological lipid metabolism with radiopharmaceuticals.

9th week Characterization and investigation of normal and pathological cell proliferation with radiopharmaceuticals.

10th week Preclinical radiopharmaceuticals of oncological and immunological diseases.

11th week Preclinical radiopharmaceuticals of neurological and cardiovascular diseases.

12th week Radiopharmaceuticals in drug research and development.

13th week Radiopharmaceuticals in receptor research, receptor-ligand binding assays.

14th week Summary, review.

Requirements:

- *for a signature*

Attendance at **lectures** is compulsory.

A student may not miss more than two times during the semester. In case a student does so, the subject will not be signed and the student must repeat the course. In case of further absences, a medical certificate needs to be presented.

The course ends in an **examination**.

The minimum requirement for the examination is 60%. Based on the score the grade for the examination is given according to the following table:

Score	Grade
0-59	fail (1)
60-69	pass (2)
70-79	satisfactory (3)
80-89	good (4)
90-100	excellent (5)

If the score of the examination is below 60, students can take a retake examination in conformity with the EDUCATION AND EXAMINATION RULES AND REGULATIONS.

Person responsible for course: György Trencsényi, PhD, Habil., associate professor

Lecturer: György Trencsényi, PhD, Habil., associate professor

Title of course: Special and dangerous materials.
Code: TTKME0206_EN

ECTS Credit points: 3

Type of teaching, contact hours
- lecture: 2 hours/week

Evaluation: examination

Workload (estimated), divided into contact hours:
- lecture: 28 hours
- practice: -
- laboratory: -
- home assignment: -
- preparation for the exam: 56 hours

Total: 84 hours: 3 credit x 28 hours

Year, semester: 2nd–4th year, 1st semesters

Its prerequisite(s):

Further courses built on it:
none

Topics of course

Structure, composition, properties and handling/safe use of special materials, which may represent a personal, social or environmental risk or even a life-threatening danger in case of accidents, war, or illicit use.

Literature

Compulsory:

1) Chemical Warfare Agents Chemistry, Pharmacology, Toxicology, and Therapeutics, Edited by James A. Romano, Jr. Brian J. Lukey, Harry Salem, CRC Press, ISBN-13 978-1-4200-4661-8
2) High Energy Materials. Propellants, Explosives and Pyrotechnics, Jai Prakash Agrawal, 2010, Wiley-VCH Verlag GmbH & Co. KGaA, Weinheim
Recommended:
3) Chemistry of Pyrotechnics, Basic Principles and Theory, 2nd Edition, 2010, CRC Press, ISBN-13: 978-1-4200-1809-7
4) The Pleasure Instinct Why We Crave Adventure, Chocolate, Pheromones, and Music, Gene Wallenstein, 2009, John Wiley & Sons, Inc., ISBN 978-0-471-61915-4

Course objective/intended learning outcomes

a) Knowledge
- He/she fundamentally knows major types of dangerous and/or illicit materials, their properties, legal and illegal uses and the danger they represent.

b) Abilities
- He/she is able to recognize the major types of the dangerous materials and to estimate the risk they represent.
- He/she is able to make or take part in a plan to keep the persons/environment safe from dangerous materials. He/she is able to give advice on possible/expected behaviour of the dangerous materials.

c) Attitude
- He/she is open to learn and accept professional, technological improvement and innovation in his/her profession and convey it genuinely.
- He/she makes a decision in complex and unexpected cases by completely taking into account legal and ethical norms.

d) Autonomy and responsibility
- Even in unexpected decision-making situations he/she is capable of considering complex, fundamental questions from his/her professional field and elaborating them on the basis of the given sources.
- He/she confesses and represents the value system of the qualified chemists' or chemical engineers' profession with responsibility. He/she is open to critical remarks which are professionally well-founded.

Schedule:
1st week
Narcotics, hard and soft drugs 1. General properties, groups, addiction, legal state. Treatment of addiction. Cannabis.
2nd week
Narcotics, hard and soft drugs 2. Opium, morphine, heroine, opioids. Treatment of addiction, withdrawal syndroms.
3rd week
Narcotics, hard and soft drugs 3. LSD, mescaline, and related derivatives.
4th week
Narcotics, hard and soft drugs 4. Natural materials: Catinone, harmine, harmaline, bufotenine,

ibogaine, ephedrine, LSA, safrole, iso-safrole, myristicyne.
5th week
Narcotics, hard and soft drugs 5. Synthetics 1. Amphetamine and derivatives, Extasy, etc..
6th week
Narcotics, hard and soft drugs 6. Synthetics 2. DON, DOB, STP, designer drugs.
7th week
Chemical weapons 1. Major groups, target organs, toxicity. Tear gases, lachrymators.
8th week
Chemical weapons 2. Blood poisons, lung poisons, vesicants..
9th week
Chemical weapons 3. Nerve gases. Floroorganic poisons.
10th week
Chemical weapons 4. Binary chemical weapons. Incendiaries, flame materials, heat source materials.
11th week
Explosives, pyrotechnics 1. Basic concepts, definitions, modes of action. Deflagration: gun powder. Energetic materials, propellants, high energy polymers.
12th week
Explosives, pyrotechnics 2. Initiators, shock and spark sensitive materials. Blasting caps, detonators. High energy explosives, binary explosives, and their civilian and military uses.
13th week
Explosives, pyrotechnics 3. Basic experimental techniques to determine explosive characteristics and stability of explosives and gun powders. Pyrotechnical materials and devices. Civilian pyrotechnics, fireworks.
14th week
Pheromones. Basic properties, mode of action, role in the behavior control and in the physiological signaling processes. Use of pheromones in the agriculture, and in the animal life. Pheromone-like materials, the Dirty 12.

Requirements:
- for a signature
Attendance at **lectures** is recommended, but not compulsory.
- for a grade
The course ends in an **examination**.
The minimum requirement for the examination is 50 score. Based on the score, the grade for the examination is given according to the following table:

Score	Grade
0-49	fail (1)
50-62	pass (2)
63-75	satisfactory (3)
76-88	good (4)
89-100	excellent (5)

If the score of any test is below 60, students can take a retake test in conformity with the EDUCATION AND EXAMINATION RULES AND REGULATIONS.

Person responsible for course: Dr. István Lázár, associate professor, PhD

Lecturer: Dr. István Lázár, associate professor, PhD

Title of course: Biocolloids **Code**: TTKME0411_EN	**ECTS Credit points:** 3
Type of teaching, contact hours - lecture: 2 hours/week - practice: - - laboratory: -	
Evaluation: exam	
Workload (estimated), divided into contact hours: - lecture: 14 hours - practice: - - laboratory: - - home assignment: 40 hours - preparation for the exam: 40 hours Total: 94 hours	
Year, semester: 1^{st}/ 2^{rd} year, 2^{nd} semester	
Its prerequisite(s): -	
Further courses built on it: -	

Topics of course

The goal of this series of lectures is to give knowledge about the relationship between biological sciences and colloid/surface phenomena. A further goal is to deepen colloid chemical knowledge of students about biological phenomena related to colloids. It makes them able to approach biological problems from a colloid chemical perspective and to solve possible problems and tasks in this context.

Literature

Compulsory:
- Lecture slides downloadable from the Department's homepage (http://fizkem.unideb.hu)

Recommended:
- D. Fennell Evans, Hakan Wennerstrom: The Colloidal Domain: Where Physics, Chemistry and Biology Meet, 2nd Ed. ,Wiley, 1999
- Pashley, R. M.: Applied Colloid & Surface Chemistry. Wiley&Sons, ISBN 0-a470-a86883-aX, 2004
- Cosgrove T.: Colloid science. Blackwell Publishing ISBN:978-a14051-a2673-a1, 2005

Course objective/intended learning outcomes

a) Knowledge
- Have systematic knowledge on the various subject of chemistry, their main principles

including the theoretical and practical application built on these principles.

- He/She has global knowledge on science other than chemistry, and capable to organize this information.
- He/She has knowledge to solve problems on the field of natural processes, using natural sources, and understanding the chemical background of living and non living systems.

b) Abilities

- He/She is able to recognize and evaluate the global relationships on the field of chemistry.
- He/She is able to communicate discuss and aim problems to other chemists or engineers of professionals other than chemistry field.
- He/She is able to argue his/her opinion in scientific discussions both in oral or written form.

c) Attitude

- He/She accepts those professional identities that defines the uniqueness and importance of science.
- He/She is able to represent and distribute his/her own personal scientific ideology toward professional and unprofessional groups, and making the ideal scientific person who is critical to the new results.
- He/She is committed to get new knowledge and competences, widening his/her ideology, and makes effort to evolve him/herself.

d) Autonomy and responsibility

- He/She can make own decisions even in complex professional questions, discussions.
- He/She is well aware about his/her propositions and its consequences.

Schedule:

1st week

Importance of colloidal state in biology. Hypotheses about the origin of life in the past and nowadays. Occurrence of organic matter in space. Hyperresistant organisms and survival under the conditions found in space. Shadow biosphere and "artificial life".

2nd week

Formation of interfaces. Films and membranes. Langmuir-Blodgett films and liquid crystals. Membrane models, structure of the cell membrane.

3rd week

Diffusion and transport phenomena through membranes, osmosis and dialysis. Transport phenomena in living organisms. Function of the kidneys, artificial kidney.

4th week

Adsorption phenomena in biological systems, processes in biotechnology and separation sciences.

5th week

Surface tension and its importance in nature. Motion of striders on the surface of water. Reproduction using surface tension: ballistospores of fungi. Wetting, contact angle, influencing the surface tension. Capillarity, water transport in plants and the transpiration-adhesion-tension-cohesion hypothesis. The importance of capillarity under arid climates. Adhesion to smooth surfaces. Atherosclerosis and interfacial influences leading to atherosclerosis.

6th week
Association colloids, micelles and inverse micelles. Critical micelle concentration and its importance. Detergents and their uses. Biological detergents in the digestion: bile acids. Solubilization with polar molecules. Lung surfactants and their role in breathing.

7th week
Modern instrumental methods in the study of biomacromolecules (ultracentrifugation, electrophoresis, size exclusion chromatography, scanning confocal microscopy, electron microscopy, scanning probe microscopy, surface plasmon resonance, X-ray diffraction, NMR).

8th week
Macromolecules, types and importance of macromolecules. Characterization and importance of dispersity, shape, and conformation.

9th week
Important and interesting biomacromolecules, their properties, importance and uses (*polysaccharides*: cellulose, starch, chitin, etc.; *proteins*: collagen, silk, green fluorescent protein, etc.; *others*: lignin, chlorophylls, haemoglobin, etc.).

10th week
Dispersion colloids in nature. Bioaerosols and smokes. Importance of foams, emulsions, sols and their biological relevance. Making and breaking of dispersions in different biological, medical, pharmaceutical, etc. processes.

11th week
Coherent systems and lyogels. The eye as a natural lyogel system. Biocomposites: structure and formation of bones. A complex disperse system: the soil.

12th week
Electrokinetic effects, precipitation from liquids. Epitaxis. Kidney and bile stones, processes of their formation.

13th week
Flow properties. Biorheology. Rheology of blood and its importance in blood coagulation.

14th week
Nanotechnology and its development. Nanostructures from non-living matter. Natural nanostructures: diatoms and the fine structure of butterfly scales. Nanodevices. Natural nanomotors: kinesins, dyneins, the actomyosin complex. DNS machines, active molecular tweezers.

Requirements:
- *for a signature*
Attendance at **lectures** is recommended, but not compulsory.
- *for a grade*
The course ends in an **examination**. The minimum requirement for the examination is 50%. The grade for the examination is given according to the following table:

Score	Grade
0-49	fail (1)
50-59	pass (2)
60-74	satisfactory (3)
75-89	good (4)
90-100	excellent (5)

If the score of any test is below 50%, students can make a retake test in conformity with the EDUCATION AND EXAMINATION RULES AND REGULATIONS.

Person responsible for course: Dr. Levente Novák, assistant professor, PhD

Lecturer: Dr. Levente Novák, assistant professor, PhD

Title of course: Physical chemistry of living systems
Code: TTKME0417_EN

ECTS Credit points: 3

Type of teaching, contact hours
- lecture: 2 hours/week

Evaluation: exam

Workload (estimated), divided into contact hours:
- lecture: 28 hours
- practice: -
- laboratory: -
- home assignment: -
- preparation for the exam: 60 hours

Total: 88 hours

Year, semester: **1st/2nd year, 2nd semester**

Its prerequisite(s): -

Further courses built on it: -

Topics of course

- The subject of biophysics-chemistry, thermodynamic concepts
- Structure of macromolecules, interactions with small molecules
- The concept of chemical potential, its effect on thermodynamic parameters, the properties of

solutions.
- Definition and interpretation of pH in biological systems
- The significance of electron transfer reactions in live systems
- Simple and complex reactions, kinetic description of enzymatic catalysed reactions
- Basic concepts related to biochemical pathways
- NMR spectroscopy in biological systems

Literature

Compulsory:
lecture material on the Department of Physical Chemistry website
Recommended:
- P. W. Atkins: Physical Chemistry (8th ed.) Oxford University Press for, 2006. ISBN: 0-7167-8759-8
- P. W. Atkins. J. de Paula: Physical Chemistry for the Life Sciences (2nd ed.) Oxford University Press, 2011, ISBN:978-0-19-956428-6

Course objective/intended learning outcomes

a) Knowledge
The student acquires physico-chemical knowledge that enables him to apply it for the biological systems. Understand the complexity of biological systems and possible methods for their simplified description.
b) Abilities
Be aware of the meaning and correct use of concepts in presentations. Can apply the knowledge of the previous mathematical, physical, physico-chemical, organic chemistry, biochemical, etc. to the physico-chemical description of biological systems.
c) Attitude
The subject helps that the students can apply the appropriate and comprehensive physico-chemical knowledge for biological systems, as well. The student's solid theoretical basis in the field of physical chemistry help him to perform his professional tasks accurately and efficiently.
d) Autonomy and responsibility
The course helps the student to apply his physico-chemical knowledge to specific biochemical and biological systems, and in a professional and non-professional way he can formulate an opinion on physico-chemical and natural science issues.

Schedule:
1st week
The subject of bio-physical chemistry. Environmental and environmentally-independent constraints of biological systems. The basics of thermodynamics. The system and the surroundings. Thermodynamic first and second law. Concept of internal energy, work, heat, enthalpy, entropy, Gibbs energy. Applications in biological systems: calculation of mechanical, electrical, extension work. (Bio)chemistry reactions, energy, enthalpy, and Gibbs energy changes. Introduction of standard

conditions. Hess law The thermodynamics of ATP.

2nd week

First, secondary, tertiary and quaternary structures of proteins. Secondary interactions that determine the tertiary structure of proteins. Interactions between hydrophobic side chains - the role of water. Elevation and repression of proteins change in entropy during conformational change. First and secondary structure of nucleic acid, interactions that determine the secondary structure. Changing of the Gibbs energy while the the double-single DNA threads (fibers) transform.

3rd week

The concept of chemical potential, used to calculate a change in the free-enthalpy accompanying a chemical reaction or a transport process. Concentration dependence of the free-enthalpy, reaction rate and equilibrium constant. Temperature dependence of equlibrium constant.

4th week

Measuring the thermodynamic quantities of the reactions. Binding of small molecules to macromolecules, independent binding, cooperation. Dissociation macro- and microconstants. Average ligand number, saturation degree, number of binding sites. Hughes-Klotz-representation. Scatchard-representation.

5th week

Autoprotolysis of water. Acid-base theory Arrhenius and Bronsted. The pH scale in chemical and biochemical systems. Conjugated acids and bases. Determination of the strength of acids and bases, the concept of pK. Dissociation degree. pK values of free amino acids, pH change its charge, isoelectric focusing. Change of pK with (bio) chemical environment. pH control in biochemical systems: buffer systems, ion transport

6th week

Electron transition reaction. Electrochemical cell: Danielle cell. Electrodes, halfcell-reaction, electromotive force. Standard electrode potential and their application: electrochemical line. Concentration dependence of electromotive force: Nernst equation, hydrogen electrode, glass electrode, combined glass electrode. Electrochemical discussion of terminal oxidation.

7th week

Specifications of solutions. Chemical potential of the solvent. Colligative properties: boiling-point elevation, freezing point depression, osmosis. Vegetable water transport and water potential. Determination of the molecular weight of protein according to their osmotic properties. Osmolarity and tonicity of the solution. Chemical potential of the solute. pH determination with weak acids and bases penetrating the membrane. Membrane potential. Electrochemical gradient as energy storage in the cell. Theory of chemio-osmosis. Stoichiometry of proton pump and ATP synthesis during oxidative phosphorylation.

8th week

Ideal and real system. Properties of the perfect gas. Ideal solution features. Discussing a real, dilute solution. Activity coefficient and affecting its value in solution containing ions: Debye-Hückel's theory. The role of ion strength in practice.

9th week

Chemical reaction rates – kinetics. Thermodynamic and kinetic stability. Specify the velocity of a chemical reaction. The concentration dependence of the chemical reaction rate. Rate equation. Temperature dependence of chemical reaction rate. Ionic strength dependence of the reaction rate. Isotope substitution method for detecting the mechanism of the reaction. Effect of pH on reaction rate.

Kinetics of sequential, parallel and reversible reactions.
10th week
Kinetics of enzymatic catalyzed reactions. Catalysis concept, catalysts. Classification of enzymes. Energy profile of enzyme catalysis. Use of steady-state approximation in enzyme-catalyzed reactions. The application and limitations of the Michaelis-Menten approach. Determination of K_M and V_{max}. Expression of catalytic activity of enzymes. Temperature dependence of the rate of enzymatic catalysis. pH dependent on the rate of enzymatic catalysis reactions.
11th week
Kinetics of multi-substrate enzymes. Activation parameters of multi-substrated enzymatic catalyzed reactions. The role of antigen-specific antibodies in the formation of "artificial enzymes". Discussion of kinetics of dual substrate enzyme catalyzed reaction, three-molecule complex approach and ping-pong mechanism. Inhibition in the enzyme reactions. Interpretation of different inhibition types, changes in K_M and V_{max} for different types of inhibition. The Dixon representation and the information that can be gained from it.
12th week
Industrial utilization of enzymatic catalysis: applications. Myths and facts about the industrial enzyme application area. Basics of enzyme immobilization. Use of ionic liquids as a reaction medium. Enzyme catalysis in non-aqueous medium (ionic liquids): regioselectivity, enantioselectivity.
13th week
Associated chemical reactions and biochemical pathways. Consecutive (serial) coupling of chemical reactions. Parallel coupling of chemical reactions. Structure of biochemical pathways from coupled reactions. Kinetic and thermodynamic control of biochemical pathways. Systemic analysis of kinetic control of biochemical pathways. Metabolic control analysis: control coefficient, elasticity coefficient.
14th week
Briefly about quantum mechanics: particles, waves, quantization of energy. Limitations of classical mechanical description. Interaction of molecules by electromagnetic radiation. General characterization of spectroscopic methods. Electro-dissemination spectra and their biochemical applications. The basics of NMR spectroscopy and its biochemical, medical applications.

Requirements:
- for a signature
Attendance at **lectures** is recommended, but not compulsory.
- for a grade
The course ends in an oral or written **examination**. The minimum requirement for the examination is 50%. The grade for the examination is given according to the following table:

Score	Grade
0-49	fail (1)
50-59	pass (2)
60-74	satisfactory (3)
75-89	good (4)
90-100	excellent (5)

If the score of any test is below 50%, students can make a retake test in conformity with the EDUCATION AND EXAMINATION RULES AND REGULATIONS.

- *offered grade* It may be offered for students if the student gives a 10-15 minute presentation related to the topic of the subject. The possible topics are discussed with the lecturer. The offered grade can be satisfactory (3) or better, in case of lower evaluation exam should be taken.
Person responsible for course: Dr. Henrietta Győrvári Horváth, senior research fellow, PhD
Lecturer: Dr. Henrietta Győrvári Horváth, senior research fellow, PhD

Title of course: Metal Complex Catalyzed Organic Syntheses **Code**: TTKME0420_EN	**ECTS Credit points:** 3
Type of teaching, contact hours - lecture: 2 hours/week - practice: - - laboratory: -	
Evaluation: exam	
Workload (estimated), divided into contact hours: - lecture: 28 hours - practice: - - laboratory: - - home assignment: 28 hours - preparation for the exam: 34 hours Total: 90 hours	
Year, semester: $1^{st}/2^{nd}$ year, 1^{st} semester	
Its prerequisite(s): -	
Further courses built on it: -	

Topics of course
- General questions of activation of small molecules (H_2, HCN, $HSiR_3$, CO, CO_2, O_2). Oxidative addition, reductive elimination. The 18 electron rule. Role of radical processes in metal complex catalyzed reactions. - Practice of homogeneously catalyzed organic synthesis. Recovery of the catalyst. Heterogenized complex catalysts, biphasic reactions, phase transfer assisted complex catalyzed syntheses. - Regio-, stereo-, and enantioselective catalysis. Hydrogenation, hydrocyanation, hydrosilylation of alkenes. Telomerization reactions. Hydrogenation and hydrosilylation of ketones, nitrocompounds and imines. Reductive amination. Dehydrogenation. Hydrogenolysis of C-X bonds (X: oxygen, halogen). Hydroformylation, carbonylation and decarbonylation. Oxidation. - Selected examples of complex catalyzed reactions for synthesis of biologically active compounds including heterocyclic derivatives (quinolines, beta-lactams, lactones, etc.).
Literature

Compulsory:

- P. W. M. N. van Leeuwen, *Homogeneous Catalysis. Understanding the Art.* Kluwer, Dordrecht, 2004.
- D. J. Adams, P. J. Dyson, S. J. Tavener, *Chemistry in Alternative Reaction Media*. Wiley-Interscience: Cambridge, 2004.

Recommended:

- A. Behr, P. Neubert: Applied Homogeneous Catalysis (Wiley-VCH, Weinheim, Germany, 2012)

a) Knowledge

- He/she fundamentally knows principles and means of activation of small molecules and the basic synthetic processes in which such activation plays a crucial role.
- He/she expansively knows the basic questions of practical application of homogeneous catalysis in laboratory and in industrial processes.

b) Abilities

- He/she is able to apply the most important terminology, theories and procedures of homogeneous catalysis when completing the relevant tasks in organic synthesis.
- He/she is able of system level understanding the problems of complex catalysed preparative reactions and is able to participate in professional discussions of such problems.

c) Attitude

- He/she is open to learn and accept professional, scientific and technological improvements and innovation in his/her profession and to refuse unscientific approaches.
- He/she makes a decision in complex and unexpected decision cases

d) Autonomy and responsibility

- Even in unexpected decision-making situations he/she is capable of considering complex, fundamental questions from his/her professional field and elaborating them on the basis of the given sources.
- He/she considers in a responsible manner the environmental risks of organic syntheses and -in order to minimize such risks- evaluates the possible application of metal complex catalyzed synthetic procedures, too.
- He/she is open to critical remarks which are professionally well-founded.

Schedule:

1st week Definition and characteristics of catalysis. Catalysis as efficient means of green chemistry. General questions of activation of small molecules (H_2, HCN, $HSiR_3$, CO, CO_2, O_2), relation between molecular structure and reactivity.

2nd week Characteristic steps and mechanisms of homogeneous catalysis. Oxidative addition, reductive elimination. The 18 electron rule. Role of radical processes in metal complex catalyzed reactions.

3rd week Practice of homogeneously catalyzed organic synthesis. Recovery of the catalyst. Heterogenized complex catalysts, methods of heterogenization on solid supports.

4th week Reactions in liquid biphasic systems, phase transfer assisted complex catalyzed syntheses. Alternative solvents, their properties and their effect on catalytic processes.

5th week Selectivity of catalytic reactions. Explanation of selectivity. Enantioselective reactions. Kinetic resolvation.

6th week Hydrogenation, hydrocyanation and hydrosilylation of alkenes. Catalytic dehydrogenation. Hydrogen transfer reactions. Catalytic isomerization of alkenes. Applications.

7th week Hydrogenation of aldehydes and ketones. Hydrosilylation of ketones. Reductive amination. Hydrogenation of nitrocompounds and imines. Redox isomerization of allylic alcohols.

8th week Hydrogenolysis of C-X (X: oxygen, halogen) bonds. Applications in destruction of environmentally harmful substances. Hydration of alkynes and alkenes. Telomerization.

9th week Hydroformylation. Cobalt-, rhodium- and platinum-based catalysts. Mechanisms of hydroformylations. Asymmetric hydroformylation. Industrial applications.

10th week Carbonylation and decarbonylation. Catalysts and mechanisms. Applications in manufacturing of fine chemicals.

11th week Homogeneously catalyzed oxidations. Catalysts and mechanisms. Practical applications.

12th week Formation of C-C bonds via homogeneous catalysis (Sonogashira-, Suzuki, Heck-cross couplings and other name reactions for catalytic C-C bond formation).

13th week Alkene metathesis. The various ways and mechanisms of the reaction. Most frequently used catalysts.

14th week Organic syntheses based on catalytic reactions of carbon dioxide: production of methanol, formic acid and its derivatives (formate esters, formamides), lactones and polycarbonates. Methods for fast optimization of reaction conditions.

Requirements:

- *for a signature*

Attendance at **lectures** is recommended, but not compulsory.

- *for a grade*

The course ends in a written **examination**.

The minimum requirement for the examination is 60%. Based on the score of the examination the grade is given according to the following table:

Score Grade

0-59	fail (1)
60-69	pass (2)
70-79	satisfactory (3)
80-89	good (4)
90-100	excellent (5)

If the score of the examination is below 60, students can take a retake exam in conformity with the EDUCATION AND EXAMINATION RULES AND REGULATIONS.

Person responsible for course: Dr. Ferenc Joó, Professor, DSc, Member of the Hungarian Academy of Sciences

Lecturer: Dr. Ferenc Joó, Professor, DSc, Member of the Hungarian Academy of Sciences

Title of course: Environmental chemistry II.
Code: TTKME0414_EN

ECTS Credit points: 4

Type of teaching, contact hours
- lecture: 2 hours/week
- practice: 1 hour/week
- laboratory: 1 hour/week

Evaluation: exam

Workload (estimated), divided into contact hours:
- lecture: 28 hours
- practice: 14 hours
- laboratory: 14 hours
- home assignment: 20 hours
- preparation for the exam: 40 hours

Total: 116 hours

Year, semester: 1st/2nd year, 2nd semester

Its prerequisite(s): -

Further courses built on it: -

Topics of course

The aim of the subject is to recognize the physical chemical principles in the natural processes of the atmo-, hydro- and lithosphere, and to apply the acquired knowledge for the description of these processes. Methods of model calculations, correct usage of thermodynamic tables are studied. The lectures review the physical chemistry of energy and work production and supply (internal- and external-combustion engines, electric engines, etc.) and deal with hydrogen and methanol economy and biofuels as well. “Mental pollution” of the environment, i.e. the interpretation of deceiving information about environmental problems is also discussed.
The practical part includes thermodynamic calculations, calculations in equilibrium and complex

formation processes, speciation, chemical kinetics, transport processes, using the knowledge of the chemical processes in the atmo-, hydro- and lithosphere.
In the laboratory, being connected with the lectures and using the acquired knowledge two environmental problems are studied through experimental work, data evaluation, and discussion of the results.

Literature

Compulsory:
- G. W. van Loon, S. J. Duffy (2010): Environmental Chemistry: A global perspective, Oxford Univ. Press. ISBN 9780199228867
- P. Brimblecombe, J. E. Andrews, T. D. Jickells, P. Liss, B. Reid (2003): An Introduction to Environmental Chemistry, Blackwell Publishing. ISBN 0-632-05905-2
- I. Williams (2005): Environmental Chemistry, Wiley. ISBN 978-0-471-48942-9

Recommended:
- T. G. Spiro, K. L. Purvis-Roberts, W. M. Stigliani (2011): Chemistry of the Environment, Univ. Sci. Books.ISBN 978-1-891389-70-2

Course objective/intended learning outcomes

a) Knowledge
- He/she fundamentally knows principles, definitions main questions and problems of environmental chemistry.
- He/she expansively knows the physico-chemical background of phenomena in our environment.
- He/she knows the theory and practice necessary for modelling chemical problems in the environment end elaborating possible solutions.
- He/she knows the specific properties of environmental chemistry compared to the other fields of chemistry.

b) Abilities
- He/she understands the phenomena of environmental chemistry and their physical chemical background. He/she is able to apply the principles in practice.
- He/she is able to grasp the importance of problems associated with environmental chemistry and to judge them and the possible solutions.
- He/she is able to collect, record, evaluate and discuss environmental chemical data on the basis of the acquired methods. With the help of data he/she is able to model the environmental problems and elaborate possible solutions.

c) Attitude
- He/she is open to learn and accept the theories and principles of environmental chemistry. He/she recognizes the relationships of the environmental problems with the other fields of chemistry and associated sciences.
- He/she is open to solve environmental problems on the basis of the acquired knowledge and methods.
- He/she is open to acquire new scientific knowledge in this topic, but decline unestablished, deceptive statements.

d) Autonomy and responsibility
- He/she is capable of considering with responsibility the risk of chemical processes polluting and

loading the environment.

- He/she use the literature of environmental chemistry on his/her own.

Schedule:

1st week

Definitions, development, significance, researching methods and relations of environmental chemistry to the other fields of science and economy. Principles of green chemistry. Basics of physical chemistry.

2nd week

Usage of thermodynamic tables, model calculations. “Mental pollution” of the environment, i.e. deceiving information about environmental problems.

3rd week

Physical chemistry of energy and work production and supply: internal- and external-combustion engines, electric motors, hydrogen and methanol economy, biofuels.

4th week

Composition and regions of the Earth’s atmosphere. Properties of thermosphere, mesosphere, stratosphere and troposphere. Calculation of atmospheric pressure and energy of the light in the thermosphere.

5th week

Definition of climate. Application of the Planck-equation. Energy spectrum of solar radiation, calculation of the surface temperature. Greenhouse effect.

6th week

Definitions of smog types. Reactions and explanations in photochemical smog. Thermodynamic calculations of NO formation considerations of further reactions.

7th week

The chemistry and role of the stratospheric ozone. Environmental problems of ultraviolet radiation, chemical UV protection. Formation and depletion of ozone, an influencing factors. Stationary kinetics, principles of photochemistry. Kinetic modelling of ozone formation.

8th week

Composition of the hydrosphere, water resources. Sea water and fresh water. Solubility of gases, liquids and solids in water. Speciation in aqueous systems.

9th week

Chemical kinetics in the environment. Transport processes: flux, viscosity, diffusion. Cyan pollution on the Tisza river. Role of colloids in transport processes.

10th week

Characterization and significance of interfaces: surface charge and adsorption. Causes, effects, solution and elimination possibilities of the red sludge disaster.

11th week

Water treatment technologies: Arsenic removal and the treatment of arsenic sludge.

Laboratory practise 1. Treatment and elimination of water treatment arsenic sludge, measurements using mobile analytical methods.

12th week

Properties and composition of soils. Weathering processes, soil colloids. Soil colloids. Chemical properties of soils, acid/base buffer capacity. Calculations associated with soil pollution.

13th week
Structure and interfacial reactions of clay minerals.
Laboratory practise 2. Soil-forming minerals: particle size, metal adsorption, effect of pH.
14th week
Lithosphere, formation of rocks and minerals. Chemical aspects of volcanic activities.

Requirements:
- for a signature
Attendance at **lectures** is compulsory, since the **practical part** is integrated into the classes. A student must attend the classes and may not miss more than three times during the semester. In case a student does so, the subject will not be signed and the student must repeat the course. Attendance at practice classes will be recorded by the lecturer. Being late is equivalent with an absence. In case of further absences, a medical certificate needs to be presented.
Students have to **submit a report task** at the end of the semester, the topic of which is chosen from a list. The grade of the report task reflects the processing of the literature and the creative solution of the relating model calculation.
During the semester there are two **laboratory practises** (11th and 13th weeks), where the attendance is compulsory. The students get grades for the lab reports.
- for a grade
The course ends in an **examination**. Based on the average of the grade of the report task, lab reports and the examination, the exam grade is calculated as a weighted average of them:

- the grade of the report task (25%)
- the average grade of the lab reports (25%)
- the result of the examination (50%).

The minimum requirement for the examination is 50%. Based on the score of exam test (70), the grade is given according to the following table:

Score	Grade
0-35	fail (1)
36-44	pass (2)
45-53	satisfactory (3)
54-62	good (4)
63-70	excellent (5)

If the score is below 35, students can take a retake test in conformity with the EDUCATION AND EXAMINATION RULES AND REGULATIONS.

Person responsible for course: Dr. Mónika Kéri, assistant professor, PhD

Lecturer: Dr. Mónika Kéri, assistant professor, PhD
Dr. István Bányai, professor, DSc

Title of course: Structure determination by X-ray diffraction
Code: TTKME0423_EN

ECTS Credit points: 3

Type of teaching, contact hours

- lecture: 2 hours/week
- practice: -
- laboratory: -

Evaluation: exam

Workload (estimated), divided into contact hours:
- lecture: 28 hours
- practice: -
- laboratory: -
- home assignment: 30 hours
- preparation for the exam: 40 hours

Total: 88 hours

Year, semester: 1st/2nd year, 2nd semester

Its prerequisite(s): -

Further courses built on it: -

Topics of course

The series of lectures are based on the topics of X-ray diffraction. The purpose of the course to give strong theoretical background for the students on the methodology and applications of single crystal structure determination via X-ray diffraction. Part of the course of learning basic usage of software tools. Application of single crystal diffraction in preparative chemistry, interpretation and presentation of the results as well as use of crystallographic databases are also discussed. Fields of protein crystallography, polymorphism research as well as powder diffraction are also reviewed.

Literature

Compulsory:
- J. P. Glusker, K. N. Trueblood (2010): Crystal Structure Analysis: a Primer (IUCR Texts on Crystallography), Oxford University Press, ISBN 13 978-0199576357
- http://www.iucr.org/education/pamphlets
- Lecture notes and teaching material available via the e-learning system

Recommended:
- W. Massa (2000): Crystal Structure Determination, Springer, ISBN 3-540-65970-6

Course objective/intended learning outcomes

a) Knowledge
- He/She has a mathematical and scientific background to understand processes in single crystal structure determination.

b) Abilities
- He/She is able to use documentation (both online or printed) related to the current field, including the scientific literature in English.

c) Attitude

- He/She makes effort to improve and apply the practical methods with new results and experiences.
- He/She can collaborate with other people and discuss their opinions in problem solving processes before making new decisions.

d) Autonomy and responsibility

- He/She can make own decisions even in complex professional questions, discussions..

Schedule:

1st week X-ray radiation

Properties of X-rays, practical applications. Diffraction methods in general. Place of single crystal structure determination among structural studies. Fourier transformation and its properties. Least square methods.

2nd week Symmetry

Structure of solids. Crystals. Unit cell, asymmetric unit, Miller indexes. Symmetry notation of IUCR, systematic absences. Reciprocal space. The most frequent space groups and symmetry operators.

3rd week Crystal growing

Thermodynamics and kinetics of crystallization. Methods to grow single crystals. Applications of crystallization in pharmaceutical industry. Basics of neutron diffraction.

4th week X-ray diffraction methods

Generation of X-rays. Development of X-ray diffraction methods. Main parts of the diffractometer. Types of detectors, advantages and disadvantages. Area detectors.

5th week Structure determination

The main steps of structure determination by single crystal diffraction. Determination of the unit cell. Data collection, data/parameter ratio. Symmetry effects in data collection. Phase problem and methods to solve the phase problem for small molecules. Refinement of the structure.

6th week Publication

The Crystallographic Information Format and its advantages. Publication of single crystal structure determination results. Validation of the results. Interpretation and use of crystallographic results. Steps of publication in case of major journals.

7th week Computer programs in structure determination

Basic usage of WINGX and PLATON packages. The MERCURY program. The construction of shelx .ins files.

8th week Cambridge Structural Database

Basic terms of usage of CSD. Computer practice to search the database and making crystallographic calculations. Computer practice.

9th week Powder diffraction

Powder methods. Data collection, geometry, optics, possibility of structure determination from powder data.

10th week Polymorphism

Polymorphism phenomena. Definition of polymorphic forms. Consequences in pharmaceutical industry. Thermodynamic and structural considerations. Polymorphism in everyday life.

11th week Protein crystallography

Comparison of protein and small molecule crystallography. Solving the phase problem for proteins. Refinement of protein structures. Structural motifs and function of proteins. Intrinsically disordered

proteins.
12th week Practical class
Determination of crystal and molecular structure for a relatively simple organometallic compound. Group work.
13th week Chirality and X-ray diffraction
Concepts and definitions. Types of chirality. Determination of absolute configuration. Anomalous dispersion.
14th week Student works
The student give short presentation on their chosen topic in the field of X-ray structure determination.

Requirements:
- *for a signature*
Attendance at **lectures** is recommended, but not compulsory.
- *for a grade*
The course ends in an **examination**. Based on the average of the grades of the **written test or oral exam** the exam grade is calculated. It is the choice of the student to give written or oral exam.
Based on the scores, the grade for the tests and the examination is given according to the following table:

Score	Grade
0-59	fail (1)
60-69	pass (2)
70-79	satisfactory (3)
80-89	good (4)
90-100	excellent (5)

If the score of any test is below 60, students can take a retake test in conformity with the EDUCATION AND EXAMINATION RULES AND REGULATIONS.
-an offered grade:
it may be offered for students if the student prepare a short written report on literature search in the field of X-ray diffraction. The possible topics are discussed with the lecturer and preliminary versions of the paper are iterated to correct errors. The report should have a minimum of 10 A4 sheet and it should be presented at the last class. The offered grade can be satisfactory (3) or better, in case of lower evaluation exam should be taken.

Person responsible for course: Dr. Attila Bényei associate professor, PhD

Lecturer: Dr. Attila Bényei, associate professor, PhD

Title of course: Chemistry of secondary metabolites I **Code**: TKME0331_EN	**ECTS Credit points:** 3

Type of teaching, contact hours
- lecture: 2 hours/week
- practice:

- laboratory: -
Evaluation: exam
Workload (estimated), divided into contact hours: - lecture: 28 hours - practice: - laboratory: - - home assignment: 20 hours - preparation for the exam: 40 hours Total: 88
Year, semester: 1st or 2nd year, 1st semester
Its prerequisite(s): -
Further courses built on it: -

Topics of course

- Classification of metabolic processes, and review the major building blocks, and basic reactions.
- Isolation and structural determination of natural compounds.
- The function of natural compounds and application them as lead compounds in in drug development.
- Discussion of the retrosynthetic analysis and laboratory synthesis of natural compounds through the processing of selected examples.

Literature

Compulsory:

1. K. C. Nicolaou, E. J. Sorensen: Classics in Total Synthesis I., 4th edition (Reprint), Wiley, 2003.
2. K. C. Nicolaou, S. E. Snyder: Classics in Total synthesis II., 1st edition, Wiley, 2003.
3. K. C. Nicolaou, E. J. Sorensen: Classics in Total synthesis III., 1st edition , Wiley, 2011.
4. Selected article by the lecturer

Course objective/intended learning outcomes

a) Knowledge

- He/she knows the method of the retrosynthetic analysis and the processes which can be used to the synthesis of the complex natural organic compounds, they are aware of the predictable pitfalls of chemical synthesis, the use of protective groups and reagents used.

b) Abilities

- He/she is able to apply basic knowledge of simple natural compounds, to plan the synthesis of this type of compounds.
- He/she is able to participate in professional communication on the field of isolation, synthesis and application of secondary metabolites.
- He/she is able to expand and/or develop his/her knowledge from the natural products.

c) Attitude

- He/she is open to getting new, scientifically proven knowledge on the subject, but to reject unsubstantiated or possibly misleading claims

d) Autonomy and responsibility
- He/she is able to independently perform the tasks of the course with professional guidance, and he/she can interpret and evaluate of the results obtained.

Schedule:
1st week
Classification of the most important metabolic processes and metabolites The definition of primary and secondary metabolites. The building blocks and biosynthetic processes of primary metabolites.
2nd week
The building blocks and biosynthetic processes of secondary metabolites. Isolation and structural elucidation of natural compounds. The function of natural compounds and application them as lead compounds in in drug development.
3rd week
Retrosynthetic analysis of the menthol and periplanone-B, bio- and chemical synthesis.
4th week
Retrosynthetic analysis and synthesis of the strychnine and quinine.
5th week
Retrosynthetic analysis of progesterone and estrone, bio- and chemical synthesis.
6th week
Retrosynthetic analysis of prostaglandins, bio- and chemical synthesis.
7th week
Retrosynthetic analysis of β-lactam antibiotics (Penicillin V, Thienamycin) and bio- and chemical synthesis.
8th week
Retrosynthetic analysis and chemical synthesis of rapamycine, indalizomycine
9th week
Retrosynthetic analysis and chemical synthesis of dynemicine.
10th week
Retrosynthetic analysis and chemical synthesis of Bisorbicillinoids.
11th week
Retrosynthetic analysis and chemical synthesis of Taxol
12th week
Retrosynthetic analysis and chemical synthesis of (-)-FR182877
13th week
Retrosynthetic analysis and chemical synthesis of Azaspiracid – I
14th week
Retrosynthetic analysis and chemical synthesis of Littoralisone, Oseltamivir (Tamiflu®), and Hirsutellone B

Requirements:
- *for a signature*
Attendance at **lectures** is recommended, but not compulsory. A student may not miss the lecture more than three times during the semester. In case of further absences, a medical certificate needs to be presented. In case a student does not do this, the subject will not be signed and the student must repeat

the course. - *for a grade* The course ends in an oral exam in the exam period.
Person responsible for course: László Dr. Juhász, associate professor, PhD, dr. habil
Lecturer: László Dr. Juhász, associate professor, PhD, dr. habil.

Title of course: Chemistry of secondary metabolites II. **Code**: TKML0332_EN	**ECTS Credit points:** 3
Type of teaching, contact hours - lecture: - - practice: 4 hours/week - laboratory: -	
Evaluation: term mark	
Workload (estimated), divided into contact hours: - lecture: - practice: 72 hours - laboratory: - - home assignment: 28 hours - preparation for the exam: Total: 100	
Year, semester: 1st or 2nd year, 1st semester	
Its prerequisite(s): -	
Further courses built on it: -	

Topics of course
Isolation and derivatization of nicotine; Isolation of coffein; Isolation and hydrolysis of piperine; Essenes of the rosary resin; Isolation and derivatization of carvone; Isolation of betulin from birch bark, Isolation and derivatization of cholesterol; isolation of anethol and anisic acid; cinnamic acid and cinnamaldehyde; isolation of rutin and quercetin; Isolation and derivatization of hesperidine. Synthesis of azelaic acid; Triglyceride of nutmeg; Isolation of thymol.
Literature
Compulsory: 1. Satyajit D. Sarker, Zahid Latif, Alexander I. Gray; Natural Products Isolation, 2nd edition, Humana Press, 2006 2. Corrado Tringali, Bioactive Compounds From Natural Sources: Isolation, characterisation and biological properties; Taylor and Francis, 2001. 3. Corrado Tringali, Bioactive Compounds From Natural Sources: Natural Products as Lead

Compounds in Drug Discovery, 2nd edition, CRC Press, 2012
4. Jerry R. Mohrig, David Alberg, Gretchen Hofmeister, Paul F. Schatz, Christina Noring Hammond; Laboratory Techniques in Organic Chemistry; 4th edition; W. H. Freeman and Company

Course objective/intended learning outcomes

a) Knowledge
- He/she knows theoretical backgrounds and devices of the classical isolation methods of the natural compounds and he/she can apply it.

b) Abilities
- He/she is able to select and apply the required isolation technique.
- He/she is able to participate in professional communication on the isolation of natural compounds.
- He/she is able to expand and/or develop his/her knowledge.

c) Attitude
- He/she is open to getting new, scientifically proven knowledge on the subject, but to reject unsubstantiated or possibly misleading claims.

d) Autonomy and responsibility
- He/she is able to independently perform the experiments of the lab course with professional guidance, and he/she can interpret and evaluate of the results obtained.

Schedule:

1st week
Isolation of nicotine from Tobacco leaves and derivatization with picric acid. Characterization of the product and calculation of nicotine contain of tobacco leaves.

2nd week
Isolation of coffein from tea leaves and characterization of the product and calculation of coffein contain of tea leaves.

3rd week
Isolation of piperine from black pepper and hydrolysis into piperic acid. Characterization of the product and calculation of piperine contain of black pepper

4th week
Isolation of essential oil from the rosin resin and characterization of the product.

5th week
Isolation of carvone from caraway and derivatization with 2,4-dinitrophenylhydrazone. Characterization of the product and calculation of carvone contain of caraway.

6th week
Isolation of betulin from birch bark and characterization of the product

7th week
Isolation of cholesterol from gall stone and transformation into dibromo derivatives. Characterization of the products.

8th week
Isolation of anethol from anise and transformation into anisic acid. Characterization of the products.

9th week
Isolation of cinnamic aldehyde from cinnamon and transformation into cinnamic acid. Characterization

of the products.
10th week
Isolation of rutin from Japanese acacia flowers and transformation into quercetin. Characterization of the products.
11th week
Isolation of hesperidin from orange peel and transformation into hesperetin. Characterization of the products.
12th week
Isolation of azelaic acid from castor oil. Characterization of the products.
13th week
Isolation and saponification of the glyceride of nutmeg. Characterization of the products.
14th week
Isolation of thymol from thyme. Characterization of the products.

Requirements:
A student must attend the laboratory classes and may not missed during the semester. In case of absences, a medical certificate needs to be presented, otherwise the subject will not be signed, and the student must repeat the course. Being late is equivalent with an absence. The knowledge of the students is controlled every week with a short written test at the beginning of the lab. The results of the experiments must be summarized in the laboratory notebook, which is checked and graded at the end of each practice.
- for a signature
Attendance at **laboratory** is compulsory. The student must be writing every short test and the laboratory notebook.
- for a grade
The minimum requirement for the short written tests respectively is 50%. Based on the score of the tests separately, the grade for the tests is given according to the following table:

Score	Grade
0-49	fail (1)
50-65	pass (2)
66-80	satisfactory (3)
80-89	good (4)
90-100	excellent (5)

The final mark will be calculated as an average of the grades of tests and laboratory notebooks.

Person responsible for course:. László Dr Juhász, associate professor, PhD, dr. habil

Lecturer: László Dr Lázár, associate professor, PhD, dr. habil.

Title of course: Enzyme biotechnology
Code: TTKME0334_EN

ECTS Credit points: 3

Type of teaching, contact hours

- lecture: 2 hours/week - practice: - - laboratory: -
Evaluation: exam
Workload (estimated), divided into contact hours: - lecture: 28 hours - practice: - - laboratory: - - home assignment: - preparation for the exam: 56 hours Total: 56 hours
Year, semester:
Its prerequisite(s):
Further courses built on it: -

Topics of course
The lectures describe the effective catalytic properties of enzymes that have promoted their introduction into several biotechnological processes. From each enzyme class, there is a representative industrial enzyme, which is characterized in details. Approaches to improve enzyme function are also mentioned.
Literature
Compulsory: The lecture notes *Recommended:* Biocatalysts and Enzyme Technology (K. Buchholz, V. Kasche, U.T. Bornscheuer; Wiley-VCH, second edition, 2012, ISBN:978-3-527-32989-2). Biocatalysis biochemical Fundamentals and Applications (P. Grunwald; Imperial College Press, 2009, ISBN:978-1-86094-744-5). Enzyme Technology (Wu-Kuang Yeh, Hsiu-Chiung Yang and J. R. McCarthy; Wiley 2010, 9780470286241). Industrial enzyme (Ed. J. Polaina, A. MacCabe, Springer, 2007, ISBN: 978-1-4020-5377-1). Enzymatic reaction mechanism (P.A. Frey-A.D. Hegeman; Oxford University Press, 2007).
Course objective/intended learning outcomes
a) Knowledge - He/she knows the main characteristics and application of industrial enzyme. -She/he is also aware of strategies for improvement of enzyme function. **b) Abilities** - He/she is able to understand the main criteria for industrial enzymes. - He/she is able to understand the enzymatic processes applied in the different field of biotechnology.

c) Attitude

-He/she is open to the contextual observations of the studied area and is motivated to follow latest scientific theories in that field.

d) Autonomy and responsibility

- He/she is capable of considering complex questions on the studied scientific field on her/his own as well as in a team.
- He/she shows responsibilities in her/his profession.

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Schedule:

1st week

Definition of biotechnology. The scope of biotechnology in energy usage. Sustainable development. Enzyme technology is green technology. The advantage of the application of biocatalysts *versus* conventional processes.

2nd week

Comparison of biocatalysis with other kinds of catalysis. Requirements for industrial enzymes. Industrial enzymes on the global market. Application of enzymes in molecular biology and enzymes used in immunoassays and as a therapeutic agent.

3rd week

Kinetics of enzyme catalyzed reactions. The integrated Michaelis-Menten equation. Substrate and end-product inhibition. *Reversible* enzymatic *reaction.* Conversion of enzyme processes. Two-subsrate enzyme reactions.

4th week

Effect of environmental factors on enzyme activities. The environemntal stability of enzymes. Enzyme assays.

5th week

Classification of enzymes, enzyme databases. Cofactor dependent enzymes in industrial application, the methods of cofactor regeneration. The advantage of the whole cell technology for enzyme catalysed processes.

6th week

The biotechnological importance of NAD(P) dependent dehydrogenases. Mechanism of oxidases. The hydrogen peroxide producing oxidases as industrial enzymes.

7th week

Industrial application of laccase and its enzymatic mechanism. Peroxidases. The enzymes involved in ROS elimination.

8th week

Industrial hydrolases. Characterisation of glycoside hydrolases. CAZY database. Industrial hydrolysis of starch by starch processing enzymes. The cellulolytic and hemicellulolytic enzyme systems. The cellulosome. Enzyme catalysis in bioethanol production.

9th week

Biotechnological application of isomerases. The importance of xilose izomerases in the production of high-*fructose* corn syrup.

10th week

Industrial application of aldolases. Enzymatic processes used for the production of amino acids.
11th week
Metabolic engineering. Improvement of pentose utilisation in yeast. Metabolic engineering of microbes for oligosaccharide synthesis.
12th week
Improving enzyme function by rational design versus directed evolution. Novel substrate specificity, product selectivity, increased stability, decreased protease sensitivity. Screening and selection.
13th week
Improving enzyme stability by immobilisation.classification of enzyme immobilizazion methods. Effects of enzyme immobilization on activity. Immobilization by entrapment and by carrier-binding.
14th week
Immobilization by crosslinking. Magnetic single-enzyme particles with high stability. Application of immobilized enzymes.

Requirements:
- *for a signature*
Attendance at **lectures** is recommended, but not compulsory.
- *for a grade*
The course ends in an **examination**.
The grade for the examination is given according to the following table:

Score	Grade
0-59	fail (1)
60-69	pass (2)
70-79	satisfactory (3)
80-89	good (4)
90-100	excellent (5)

If the score of examination is below 60, students can take a retake test in conformity with the EDUCATION AND EXAMINATION RULES AND REGULATIONS.

Person responsible for course: Dr. Teréz Barna, PhD

Lecturer: Dr. Teréz Barna, PhD

Title of course: NMR Operator Training Practice I.
Code: TTKML0004_EN, TTKBL0004_EN

ECTS Credit points: 2

Type of teaching, contact hours
- practice: 2 hours/week

Evaluation: practical exam

Workload (estimated), divided into contact hours:
- practice: 28 hours
- preparation for the exam: 32 hours

Total: 60 hours:

Year, semester: 2nd year, 2nd semester or 3rd year, 1st or 2nd semester

Its prerequisite(s):

Further courses built on it: TTKMG0530_EN

Topics of course: practical laboratory course with aim that students would be able to pick up ^{1}H and ^{13}C NMR spectra on the 360MHz high field NMR spectrometer without external help

Literature

Compulsory: P.J. Hore, Nuclear Magnetic Resonance, ISBN 963 19 4426 3
Bruker Topspin 3.x manuals (free download)
Recommended: James Keeler, "Understanding NMR Spectroscopy" , 2009, ISBN 0-470-01787-2

Course objective/intended learning outcomes

a) Knowledge: firm knowledge of the basic principles of high resolution NMR spectroscopy. Pulse -Fourier principle of NMR spectroscopy.

b) Abilities: to run Bruker NMR spectrometers using topspin software, pick up 1D ^{1}H NMR and ^{13}C NMR spectra within 1 hr timeframe.

c) Attitude: critical and responsible concerning the obtained NMR spectra, with respect to general quality, accuracy etc.

d) Autonomy and responsibility: The main aim is the independent and autonomous use of the sophisticated superconducting spectrometers. Must pay attention to save the technical conditions of the equipments, including the protection of supercon magnets from accidental failure.

Schedule:

1st week Safety rules in NMR labs. with supercon magnets. Dangers for magnets and human beings. Pulse Fourier measurement principle. Hardware of 360 MHz spectrometer: magnet, probeheads, RF preamplifier, electronic control unit, control PC, manual controls.

2nd week Sample preparation: use of deuterated solvents, quality and cleaning of NMR sample tubes, sample amount and dissolving rules. Positioning the samples before measurement, pneumatic transfer of samples into the magnet. Use of deuterium lock in automatic or manual mode. Lock power, field, phase, gain, finding the lock signal. Optimizing lock parameters avoiding saturation of the deuterium signal.

3rd week Homogenisation of the main magnetic field up to 10^{-9}-10^{-10} accuracy, using the lock signal amplitude. Sample spinning, use of z-shim coils. Non-spinning shims (x,y) combinations. Changing lock phase. Reading and writing shim files (rsh/wsh). Signs of bad shimming. Indicators of good shims in TMS signal.

4th week Recording proton NMR spectra. Measurement principles: pulse program zg and it's visualisation. Acqusition parameters in eda and ased starting windows. Explanation of important parameters: digital sampling and connection between td, sw, aq parameters. Choice of p1 pulse and d1 relaxation delay for quantitative 1H-NMR. Real-time FID shimming in gs mode.

5th week Processing proton NMR spectra. Math rules of Fourier transformation with FFT. TD and SI, zero filling. Window functions for S/N enhancement (em) or resolution (gm) enhancement. Phase correction to pure absorption phase - automatic or manual. Baseline correction for accurate integrals. Integration routine and calibration, correction of integrals.

6th week Recording carbon NMR spectra. Pulse programs zgdc and jmod. Explaining the double impact of proton decoupling: removing splittings caused by proton-carbon spin-spin couplings and heteronuclear NOE that improves carbon sensitivity. Explaining the proton channel power and dB scale, and heating effect danger. Exponential line broadening is a must (em) before FT. Explaining and running the jmod spin-echo sequence.

7th week Recording more carbon NMR spectra with gated (zggd) and inverse gated (zgig) sequences. The former for measuring heteronuclear couplings with better sensitivity, the latter for quantitative ^{13}C-NMR. Adjusting optimal parameters for carbon NMR. Explaining signal multiplicity of deuterated organic solvents. Peak picking (ppm) of spectra.

8th week Excercising ^{1}H NMR signal acquisition and processing one by one.

9th week Excercising ^{13}C NMR signal acquisition and processing one by one.

10th week Excercising ^{1}H NMR signal acquisition and processing one by one.

11th week Excercising ^{13}C NMR signal acquisition and processing one by one.

12th week Excercising ^{1}H NMR and ^{13}C NMR signal acquisition and processing one by one.

13th week Excercising ^{1}H NMR and ^{13}C NMR signal acquisition and processing one by one.

14th week Excercising ^{1}H NMR and ^{13}C NMR signal acquisition and processing one by one.

Requirements:

- *for a signature*

Attendance of laboratory excercises is compulsory.

A student must attend the practice classes and may not miss more than two times during the semester. In case a student does so, the subject will not be signed and the student must repeat the course. A student can’t make up any practice with another group. Attendance at practice classes will be recorded by the practice leader. Being late is equivalent with an absence. In case of further absences, a medical certificate needs to be presented. Missed practice classes should be made up for at a later date, to be discussed with the tutor. Active participation is evaluated by the teacher in every class. If a student’s

behaviour or conduct doesn't meet the requirements of active participation, the teacher may evaluate his/her participation as an absence because of the lack of active participation in class. - *for a grade* The course ends in an **examination**. The student must produce an 1H NMR spectrum with quantitative integrals and a 13C NMR spectrum with peak list within one hour time limit, without external help. They may ask for tutor help, however this may result in lowering their mark. - the result of the practical examination may be 1 (failed) 2,3,4,5 (passed)
Person responsible for course: Dr. Batta Gyula, professor, PhD
Lecturer: Dr. Batta Gyula, professor, PhD

Title of course: Reaction Kinetics/Catalysis **Code**: TTKME0437_EN	**ECTS Credit points:** 4
Type of teaching, contact hours - lecture: 2 hours/week - practice: - - laboratory: 2 hours/week	
Evaluation: exam	
Workload (estimated), divided into contact hours: - lecture: 28 hours - practice: - - laboratory: 28 hours - home assignment: 28 hours - preparation for the exam: 36 hours Total: 120 hours	
Year, semester: $1^{st}/2^{nd}$ year, 2^{nd} semester	
Its prerequisite(s): -	
Further courses built on it: -	

Topics of course
- Basic principles, analysis of kinetic data. - Lindemann theory of unimolecular reactions; theory of associative reactions. - Specific kinetic effects characteristic to reactions in solution. - Basic principles and equations related to composite reactions. - Kinetics of photochemical reactions; governing principles. - Phenomenon, development and significance of catalysis. - Most important features of homogeneous and heterogeneous catalysis. Discussion of the importance if catalysis through industrial examples.

- Major kinetic features of enzymatic catalysis and demonstration of its significance through examples.
- Green chemistry and application of catalysis in green chemical processes.

Every student has to work out the 4 laboratory practices (4 hours each) listed in the detailed course schedule. In these laboratory assignments they will use various methods and equipments, such as flow reactors, and will make measurements on acid-, metal ion-, metal complex-, and enzyme-catalyzed reactions.

Literature

Compulsory:
- M. J. Pilling, P. W. Seakins: *Reaction Kinetics,* Oxford University Press, Oxford, UK, 1995
- P. W. Atkins: *Physical Chemistry*, 6th ed., Oxford University Press, Oxford, UK

Recommended:
- K. J. Laidler, *Physical Chemistry*, 2nd ed., Houghton Mifflin Co., Boston, 1995
- B. C. Gates: *Catalytic Chemistry*, Wiley, 1991.
- G. Rothenberg: *Catalysis,* Wiley, 2008.

a) Knowledge

- He/she knows the fundamental principles, the most important relationships and experimental methods of reaction kinetics. He/she will have an overview of composite reactions, of kinetic effects of light, and of specific kinetic phenomena in solutions. Will know several examples of industrial catalytic processes and of enzymatic catalysis. Will understand the principal role of catalysis in devising green chemical processes. Learns the interaction of reaction kinetics and catalysis with other fields of chemistry. Will acquire the basic skills and methods of studying reaction kinetics, devising kinetic experiments and analysis of kinetic data.

b) Abilities

- He/she is able to apply the most important terminology, theories, procedures of reaction kinetics, homogeneous and heterogeneous catalysis and is able to analyze experimental kinetic data.
- He/she is able of system level understanding the problems of reaction kinetics and catalysis and is able to participate in professional discussions of such problems.

c) Attitude

- He/she is open to learn and accept professional, scientific and technological improvements and innovation in his/her profession and to refuse unscientific approaches.
- He/she makes a decision in complex and unexpected decision cases.
- He/she is sensitive to environmental problems, and is keen on applying chemical principles and methods in order to achieve sustainable development.

d) Autonomy and responsibility

- Even in unexpected decision-making situations he/she is capable of considering complex, fundamental questions from his/her professional field and elaborating them on the basis of the given sources.
- He/she considers in a responsible manner the environmental risks of chemical processes and -in order to minimize such risks- evaluates the possible application of homogeneous or heterogeneous catalysis.
- He/she is open to critical remarks which are professionally well-founded.

Schedule:
1st week Basic principles and analysis of kinetic results: order of reactions, molecularity. Determination of rate constants and coefficients. Analysis of kinetic results: integral and differential methods, isolation method, method of half lives. Temperature dependence of the reaction rate. Connection between reaction kinetics and thermodynamics.
Iodination of acetone:: determination of the order of reactants (or that of the activation energy of the reaction) using iodometry.

2nd week Kinetics and mechanism: principle of reaction mechanism. Rules for explanation of relation of the rate equation and reaction mechanism. Kinetically equivalent reaction schemes.
Catalytic decomposition of H_2O_2: Study of the effect of copper(II)-ion, of various anions, and that of the pH in decomposition of H_2O_2 catalyzed by iron-ions. Determination of H_2O_2 concentration by iodometry..

3rd week Lindemann theory of unimolecular reactions. Comparison of the theory to experimental results. Extrapolation to infinite pressure. Activation and the rate of dissociation. Theory of associative reactions.

4th week Kinetics of solution reactions. Role of the solvent: the cage effect. Formation of a collision complex. Diffusion controlled reactions. Kinetically controlled reactions. Effects of ionic strength and pressure on the rate coefficient.

5th week Kinetics of composite reactions: application of the Bodenstein-principle and that of the fast preequilibria for kinetic description of reaction systems. Parallel and consecutive reactions. Reactions leading to equilibrium. The most important reactions taking place in the atmosphere.

6th week Theory of chain reactions: general scheme of chain reactions. Definition of chain length. Reactions with open chain: hydrogen-halogen reactions, alkane pyrolysis, radical polymerizations. Thermal explosions. Chain reactions with branching: the $H_2 + O_2$ reaction, oxidation of hydrocarbons.

7th week Oscillating chemical reactions in closed systems. The Belouszov-Zhabothinsky reaction and the Field-Körös-Noyes mechanism. The Oregonator model and its dynamics. Chemical chaos.

8th week Kinetics of photochemical reactions: formation and decay of electronically excited molecules. Kinetic laws of photochemistry: Quantum yield coefficient. Lifetimes of fluorescence and phosphorescence. Stern-Volmer diagram.

9th week Definition and characteristics of catalysis. Historical overview of the most important catalytic processes. Principles of green chemistry and comparison of traditional and green processes. Green chemistry and catalysis. Atom efficiency and environmental factor (E-factor) – with examples

10th week Selectivity of catalytic processes. Explanation of selectivity. Enantioselective reactions. Kinetic resolutions.

11th week Characteristic steps and mechanisms of homogeneous catalytic reactions. Examples of industrial homogeneous catalytic processes.

12th week Heterogeneous catalytic reactions. Langmuir-Hinshelwood and Ealy-Rideal mechanisms. Examples of industrial heterogeneous catalytic processes..

13th week Fast optimization of reaction conditions. Flow reactors: the H-Cube hydrogenation reactor. Multiple work-place reactors.
Application of the H-Cube hydrogenation reactor. Demonstration. Hydrogenation of alkynes, the effects of flow rate, temperature and H_2-pressure on the rate and selectivity of the reaction.

14th week Catalysis by enzymes. Classification and general properties of enzymes. Quantification of enzyme activity and its dependence on the temperature and the pH. Kinetics of enzyme reactions. The Michaelis-Menten approach, methods for determination of K_M and V_{max}. Unique and multiple substrate enzymes and their way of action.
Enzyme kinetics and kinetics of enzyme inhibition: decomposition of lactose in the presence of constant amount (activity) of β-galactosidase enzyme in cases of various substrate and inhibitor concentrations and at various pH. Determination of the kinetic parameters, pH-dependence, the type of inhibition and kinetic parameters of inhibition. Dependence of the reaction rate on the amount of enzyme.

Requirements:
- for a signature
All four **laboratory practices** must be finished with the grade: pass. Attendance at **lectures** is recommended, but not compulsory.
- for a grade
The course ends in a written **examination**.
The minimum requirement for the examination is 60%. Based on the score of the examination the grade is given according to the following table:

Score	Grade
0-59	fail (1)
60-69	pass (2)
70-79	satisfactory (3)
80-89	good (4)

90-100	excellent (5)

If the score of the examination is below 60, students can take a retake exam in conformity with the EDUCATION AND EXAMINATION RULES AND REGULATIONS.

Person responsible for course: Dr. Ferenc Joó, professor, DSc, Member of the Hungarian Academy of Sciences

Lecturer: Dr. Ferenc Joó, professor, DSc, Member of the Hungarian Academy of Sciences

Title of course: NMR structure determination
Code: TTKME0507_EN

ECTS Credit points: 3

Type of teaching, contact hours
- lecture: 1 hours/week
- practice: 1 hours/week
- laboratory: -

Evaluation: exam

Workload (estimated), divided into contact hours:
- lecture: 14 hours
- practice: 14 hours
- laboratory: -
- home assignment:
- preparation for the exam: 62 hours

Total: 150 hours

Year, semester: 1st year, 1st semester

Its prerequisite(s):

Further courses built on it: -

Topics of course

The aim of the course is to acquaint the students with principles, possibilities and limitations of NMR based structure determination. During the course, the students will be introduced into the molecule mechanics, which forms the basis of NMR based structure determination process.

Literature

Compulsory:
Andrew R. Leach: Molecular Modelling: Principles and Applications, 2nd Edition, 2001
Quincy Teng: Structural Biology - Practical NMR Applications
G.C.K. Roberts: NMR of Macromolecules A Practical Approach

Course objective/intended learning outcomes

a) Knowledge

Learn the basic principles of molecular mechanics and the most important terms used here.
Learn general and global issues as well as problems with the definition of structure.
Learn about the principle of algorithms used in NMR based structure determination.
Understand the possibilities and limiting factors associated with the use of an NMR structural ensemble.

b) Abilities

Able to select the appropriate structure determination strategy.
Capable of practical implementation of the theory of NMR-based structure determination.
Understands the relationship between the NMR parameters and the molecular structure.
Able to critically evaluate the literature related to the NMR structure and to adapt the methods described.

c) Attitude

Try to get to know the possibilities, limits and areas of application of the NMR based structure determination as much as possible.
Try to continually improve his/her knowledge in structure determination.
Be aware of the advantages and limitations of molecular mechanics-based modeling.

d) Autonomy and responsibility

Open to cooperation with professionals specialised in structural dtermination and modeling.
Critically examines structural issues and make an opinion on them.
Takes responsibility for the results of structure determination.
Under proper guidance, independently reads literature related to NMR based structure determination.

Schedule:

1st week

Concepts related to structure: conformation, supramolecular structure, conformational ensemble - Boltzman distribution, correlation of structure and dynamics.
Experimental methods of structure determination. Theoretical methods of modeling of structure. Principles of Molecular and Quantum Mechanics and their comparison.

2nd week

Molecular mechanics. Introducing the concept of a force field, describing terms. Bonding and non-bonding terms, Description functional forms of individual terms, Description of force constants.

3rd week

Definition of parameters and atom types. Topology. The advantages and limitations of molecular mechanics. Frequently used force fields and their characteristics.

4th week

The potential energy surface and its features. Simulation methods for mapping the potential energy surfaces. Geometry optimization and energy minimization.

5th week

Molecular dynamics. Thermodynamic ensembles. High temperature molecule dynamics, simulated annealing.

6th week

NMR parameters related to structure. Nuclear-Overhauser Effect or NOE.

7th week

Coupling constants. NMR parameters related to hydrogen bonds. Residual dipolar cou-plings. Paramagnetic relaxation effects. Structural parameters of proteins and peptides.

8th week

Process of the NMR structure determination. Methods for generating a structural ensemble. Distance geometry. Molecular dynamics with restraints. Variable Target Function algorithm.

9th week

Implementing restraints. Practical aspects of NOE restraints. Structure refinement. Selection and accuracy of the final ensemble.

10th week

Software for determining NMR structure. Validation of the structural ensemble and the programs applied to it. Structural statistics.

11th week

Structure and dynamics. Time scale of dynamic processes and their effects on NMR struc-tural parameters. Modeling of dynamic structures.

12th week

Structure determination of Maganin in a secondary structure inducing solvent. Assignment of signals in the ^{1}H NMR spectra of Maganin acquired in TFE solvent using homonuclear 2D methods. Structural calculation and refinement with ARIA / CNS programs, structure validation and structural statistics.

13th week

Modeling the structural ensemble of Maganin peptide in aqueous medium without presence of secondary structure elements. Assignment of 1H NMR spectra of Maganin with homonuclear 2D methods acquired in aqueous solution. Calculation Molecular Dynamics using explicit solvents with AMBER simulation engine and comparison of the trajectories with NMR parameters.

14th week

Consultation

Requirements:

- for a signature

Attendance at **lectures** is recommended, but not compulsory.

Participation at **practice classes** is compulsory. A student must attend the practice classes and may not miss more than three times during the semester. In case a student does so, the subject will not be signed and the student must repeat the course. A student can’t make up any practice with another group. Attendance at practice classes will be recorded by the practice leader. Being late is equivalent with an absence. In case of further absences, a medical certificate needs to be presented. Missed practice classes should be made up for at a later date, to be discussed with the tutor. Active participation is evaluated by the teacher in every class. If a student’s behaviour or conduct doesn’t meet the requirements of active participation, the teacher may evaluate his/her participation as an absence because of the lack of active participation in class.

- for a grade

The course ends in an **examination**. The exam grade depends on the performance of the examination

Person responsible for course: Dr. Fehér Krisztina, Research Fellow, PhD

Lecturer: Dr. Fehér Krisztina, Research Fellow, PhD

STAFF HANDBOOK

Name	*Edina Baranyai PhD*
Position	*Assistant Professor, UD*
Academic career	
	doctoral qualification: PhD, UD, Hungary, 2016 *Undergraduate degree, subject: environmentalist Msc (chemistry) and english-hungarian special translator MSc (chemistry), 2010*
Employment	*Assistant Professor, 2016-, UD* *Junior Assistant Professor, 2013-2016, UD*
Research and development projects over the last 5 years	*Name of project or research focus:* TÁMOP-4.2.2.A-11/1/KONV, EU project: *Basic targeted chemical and biological research for the elimination of environmentally hazardous chemicals Period and any other information: 2013-2015* *Partners, if applicable:* *Amount of financing:* *Name of project or research focus:* GINOP-2.3.2-15-2016-00008, EU project: *Chemistry for better life: strategic R&D center at the University of Debrecen.* *Period and any other information: 2016-2020* *Partners, if applicable:* *Amount of financing:*
Industry collaborations over the last 5 years	Novo-Lab Ltd (Agilent Technologies)
Patents and proprietary rights	
Important publications over the last 5 years	*Selected recent publications from a total of approx. (give total number): 19* 1. Cs. N. Tóth, E. Baranyai, I. Csípő, T. Tarr, M. Zeher, J. Posta, I. Fábián: Elemental analysis of whole and protein separated blood serum of patients with systemic lupus erythematosus and Sjögren's syndrome. Biological Trace

	Element Research 179 pp. 14-22. (2017) 2. S. Harangi, E. Baranyai, M. Fehér, Cs. N. Tóth, P. Herman, L. Stündl, I. Fábián, B. Tóthmérész, E. Simon: Accumulation of metals in juvenile carp (Cyprinus carpio) exposed to sublethal levels of iron and manganese: survival, body weight and tissue Biological Trace Element Research 177 (1) pp. 187-195. (2016) 3. E. Baranyai, E. Simon, M. Braun, B. Tóthmérész, J. Posta, I. Fábián: The effect of a fireworks event on the amount and elemental concentration of deposited dust collected in the city of Debrecen, Hungary. Air Quality, Atmosphere and Health 8 359-365. (2015) 4. E. Simon, S. Harangi, E. Baranyai, M. Braun, I. Fábián, Sz. Mizser, L. Nagy, B. Tóthmérész: Distribution of toxic elements between biotic and abiotic components of terrestrial ecosystem along an urbanization gradient: soil, leaf litter and ground beetles. Ecological Indicators, 60. pp. 258-264. (2016) 5. D. Tőzsér, S. Harangi, E. Baranyai, Gy. Lakatos, Z. Fülöp, B. Tóthmérész, E. Simon: Phytoextraction with Salix viminalisin a moderately to strongly contaminated area. Environmental Science and Pollution Research 25: (4) pp. 3275-3290. (2018)
Activities in specialist bodies over the last 5 years	

Name	*Teréz Barna PhD*
Position	*Senior lecturer*
Academic career	*Lecturer (University of Debrecen, Department of Biochemistry, 2004-2009)* *Senior lecturer (University of Debrecen, Department of Genetics and Applied Microbiology, 2010-)*
	Doctoral qualification: PhD, University of Debrecen, 2006. *Doctorate, subject: Structural/functional studies on xenobiotic degrading flavoenzymes.* *University studies:* *MSc in Biotechnology, Newcastle upon Tyne, England,*

	1993. *MSc in Chemistry, Kossuth Lajos University, Debrecen, 1986.*
Employment	*Research Fellow – Enzymology Institute of the Central Biological Centre, Hungarian Academy of Sciences* (Budapest) (1987-1988) *Research fellow -Central Chemical Research Institute of Hungarian Academy of Sciences, Budapest (1989 – 1997)* Postdoctoral Research Fellow - *Department of Biochemistry, University of Leicester, England (1998–2003)* *Research Fellow, Department of Biological and Nutritional Sciences, University of Newcastle upon Tyne, England 1996-1997 (12 month)-* Royal Society Fellowship *Research Fellow, Department of Bioinorganic Chemistry, University of Newcastle upon Tyne, England 1995 (12 month)* EC CHOST Fellowship
Research and development projects over the last 5 years	*Name of project or research focus:* *GINOP-2.3.2-15-2016-00008 : Chemistry for improving the quality of life.* *Period and any other information: 2016-2020* *Partners, if applicable:* *Amount of financing:*
Industry collaborations over the last 5 years	*Project title:* *Partners:*
Patents and proprietary rights	*Title (Year)*
Important publications over the last 5 years	*Selected recent publications from a total of approx. (give total number): 29* *Author(s): Ferencz S., Szegi K., Winkler Zs., Barna T. and Kovacs K.* *Title: Oligomannan Prebiotic Attenuates Immunological, Clinical and Behavioral Symptoms in Mouse Model of Inflammatory Bowel Disease.* *Any other information:* *Publisher, place of publication, date of publication or*

	name of periodical, volume, issue, page numbers: *SCIENTIFIC REPORTS, (2016)* *Volume: 6 Article Number: 34132.* *Author(s): Tóth Á., Barna T., Szabó E., Elek R., Hubert Á., Nagy I., Kriszt B.,Táncsics A. and Kukolya J.* *Title: Cloning, Expression and Biochemical Characterization of Endomannanases from Thermobifida Species Isolated from Different Niches.* *Any other information:* *Publisher, place of publication, date of publication or name of periodical, volume, issue, page numbers: PLoS ONE, (2016) 11(5): e0155769. doi:10.1371/ journal.pone.0155769.* *Author(s): Fizil Á., Gáspári Z., Barna T., Marx F. and Batta Gy.,"* *Title:* ."Invisible" Constrained Cold and Heat Unfolding, CEST-NMR Experiments, and Molecular Dynamics Calculations., *Any other information:* *Publisher, place of publication, date of publication or name of periodical, volume, issue, page numbers: Chemistry A European Journal, (2015) 21(13): 5136–5144.* *Author(s): Ferenczi S., Cserháti M., Krifaton C., Szoboszlay S., Kukolya J., Szőke Z., Kőszegi B., Albert M., Barna T., Mézes M., Kovács K.J.* *Title:* A New Ochratoxin A Biodegradation Strategy Using *Cupriavidus basilensis Őr16 Strain.* *Any other information:* *Publisher, place of publication, date of publication or name of periodical, volume, issue, page numbers: PLoS ONE (2014)* *9(10): e109817. doi:10.1371/journal.pone.0109817.*
Activities in specialist bodies over the last 5 years	*Organisation - Role – Period* *Membership without a specific role need not be mentioned.*

Name	*Prof. Dr. Gyula Batta*
Position	*Professor, Structural Chemistry and Biology*
Academic career	*Initial academic appointment (UD, 1980)* Habilitation *(UD, 2002)*
	doctoral qualification (MTA DSc., 2001) *Doctorate, Chemistry (MTA CSc. 1987)* *MSc., physics (Institution, 1976)*
Employment	*Professor - UD – from 2007*
Research and development projects over the last 5 years	*Name of project or research focus: Antifungal proteins: structure and dynamics, Glycopeptide Antibiotics* *2013-2018* *Partners, if applicable: Innsbruck Medical University, Institute of New Antibiotics, Moscow* *Amount of financing: 33M HUF (NKFI 110821) , ca. 150M HUF(GINOP)*
Industry collaborations over the last 5 years	*Project title: NMR Structure determination* *Partners: TEVA, CF Pharma, GLYCOM*
Patents and proprietary rights	*N/A*
Important publications over the last 5 years	*Selected recent publications from a total of approx. (200):* **1.** Anna Huber, Dorottya Hajdu, Doris Bratschun-Khan, Zoltán Gáspári, Mihayl Varbanov, Stéphanie Philippot, Ádám Fizil, András Czajlik, Zoltán Kele, Christoph Sonderegger, László Galgóczy, Andrea Bodor, Florentine Marx, **Gyula Batta** *New antimicrobial potential and structural properties of PAFB: a cationic, cysteine-rich protein from Penicillium chrysogenum Q176* **SCIENTIFIC REPORTS** 8: Paper 1751. 16 p. (2018) **2.** Sándor Boros, Zoltán Gáspári, **Gyula Batta** *Accurate NMR determinations of proton–proton distances* **ANNUAL REPORTS ON NMR SPECTROSCOPY** 94: pp. 1-39. (2018) **3.** Christoph Sonderegger, Ádám Fizil, Laura Burtscher, Dorottya Hajdu, Alberto Muńoz, Zoltán Gáspári, Nick D Read, **Gyula Batta**, Florentine

	Marx: *D19S mutation of the cationic, cysteine-rich protein PAF: novel insights into its structural dynamics, thermal unfolding and antifungal function* **PLOS ONE** 12:(1) Paper e0169920. 21 p. (2017) **4.** Fizil Á, Gáspári Z, Barna T, Marx F, **Batta G**: *"Invisible" Conformers of an Antifungal Disulfide Protein Revealed by Constrained Cold and Heat Unfolding, CEST-NMR Experiments, and Molecular Dynamics Calculations*.**CHEMISTRY-A EUROPEAN JOURNAL** 21:(13) pp. 5136-5144. (2015) **5.** Váradi Györgyi, Tóth Gábor K., Kele Zoltán, Galgóczy László, Fizil Ádám, **Batta Gyula**: *Synthesis of PAF, an Antifungal Protein from P. chrysogenum, by Native Chemical Ligation: Native Disulfide Pattern and Fold Obtained upon Oxidative Refolding,* **CHEMISTRY-A EUROPEAN JOURNAL** 19:(38) pp. 12684-12692. (2013)
Activities in specialist bodies over the last 5 years	*Hungarian NMR Society http://www.nmrmb.hu/ - President – from 2018* *Journal of Antibiotics, Member of Editorial Board*

Name	*Attila Bényei*
Position	*Associate Professor, teaching physical chemistry, X-ray diffraction, polymorphismn*
Academic career	Habilitation *(University of Debrecen, 2011)*
	Doctor of University (University of Debrecen, 1990) *PhD in Chemistry (University of Debrecen, 1995)* *Chemist, English translator (University of Debrecen, 1986)*
Employment	*Head of Laboratory for X-ray Diffraction, University of Debrecen, from 1995*
Research and development projects over the last 5 years	*Name of project or research focus: Single crystal X-ray diffraction studies. Determination of solid state structures of organic and organometallic compounds.* *GINOP-2.3.2-15-2016-00008 and GINOP-2.3.3-15-2016-00004, Participant scientist.* *Period and any other information: 2015-2019*

	Partners, if applicable: *Amount of financing:*
Industry collaborations over the last 5 years	*Project title: Single crystal X-ray diffraction studies* *Partners: Alkaloida Research and Development Ltd.*
Patents and proprietary rights	--
Important publications over the last 5 years	*Selected recent publications from a total of approx. (110):* *Author(s): Buglyó P., Kacsir I., Kozsup M., Nagy I., Nagy S., Bényei A.C., Kováts É., Farkas E.* *Title: Tuning the redox potentials of ternary cobalt(III) complexes containing various hydroxamates* *Any other information:* *Publisher, place of publication, date of publication or name of periodical, volume, issue, page numbers* *INORGANICA CHIMICA ACTA 472: pp. 234-242. (2018)* *2. Author(s): Buglyo P, Parajdi-Losonczi PL, Benyei AC, Lihi N, Biro L, Farkas E* *Title: Versatility of Coordination Modes in Complexes of Monohydroxamic Acids with Half-Sandwich Type Ruthenium, Rhodium, Osmium and Iridium Cations* *Any other information:* *Publisher, place of publication, date of publication or name of periodical, volume, issue, page numbers* *CHEMISTRYSELECT 2:(26) pp. 8127-8136. (2017)* *3. Author(s): Farkas G, Császár Z, Stágel K, Nemes E, Balogh S, Tóth I, Bényei A, Lendvay G, Bakos J* *Title: Efficient stereochemical communication in phosphine-amine palladium-complexes: exploration of N-substituent effects in coordination chemistry and catalysis* *Any other information:* *Publisher, place of publication, date of publication or name of periodical, volume, issue, page numbers* *JOURNAL OF ORGANOMETALLIC CHEMISTRY 846: pp. 129-140. (2017)* *4. Author(s): Matyuska F, Szorcsik A, May NV, Dancs Á, Kováts É, Bényei A, Gajda T* *Title: Tailoring the local environment around metal ions:*

	A solution chemical and structural study of some multidentate tripodal ligands *Any other information:* *Publisher, place of publication, date of publication or name of periodical, volume, issue, page numbers* *DALTON TRANSACTIONS 46:(26) pp. 8626-8642. (2017)* *5. Author(s): Illyés TZ, Balla S, Bényei A, Kumar AA, Timári I, Kövér KE, Szilágyi L* *Title: Exploring the Syntheses of Novel Glycomimetics. Carbohydrate Derivatives with Se-S- or Se-Se- Glycosidic Linkages* *Any other information:* *Publisher, place of publication, date of publication or name of periodical, volume, issue, page numbers* *CHEMISTRYSELECT 1:(10) pp. 2383-2388. (2016)* *6. Author(s): Rodríguez-Rodríguez A, Regueiro-Figueroa M, Esteban-Gómez D, Tripier R, Tircsó G, Kálmán FK, Bényei AC, Tóth I, de Blas A, Rodríguez-Blas T, Platas-Iglesias C* *Title: Complexation of Ln3+ Ions with Cyclam Dipicolinates: A Small Bridge that Makes Huge Differences in Structure, Equilibrium, and Kinetic Properties* *Any other information:* *Publisher, place of publication, date of publication or name of periodical, volume, issue, page numbers* *INORGANIC CHEMISTRY 55:(5) pp. 2227-2239. (2016)*
Activities in specialist bodies over the last 5 years	*Organisation - Role – Period* *International Union of Crystallography, individual member, 2004-* *European Crystallographic Association, SIG13 member 2000-*

Name	*Éva Bokor PhD*
Position	*Assistant professor*
Academic career	
	Doctoral qualification: PhD in Chemistry, University of Debrecen, Hungary, 2010

	Undergraduate degree, subject: MSc in Chemistry, University of Debrecen, Hungary, 2006
Employment	Department of Organic Chemistry, University of Debrecen, Hungary: 2009–2010: Assistant lecturer 2010–2011: Research assistant 2011–2012: Research associate 2012–2015: Postdoctoral research fellow supported by the Hungarian Scientific Research Fund 2012 – : Assistant professor
Research and development projects over the last 5 years	*Name of project or research focus:* Grant OTKA, PD 105808, supported by the National Research, Development and Innovation Office of Hungary (Hungarian Scientific Research Fund): Synthesis of *C*-glycosyl heterocycles for glycogen phosphorylase inhibition. *(*Principal investigator) *Period and any other information: 2012-2015* *Name of project or research focus:* GINOP-2.3.2-15-2016-00008, supported by the EU co-financed by the European Regional Development Fund: Chemistry for better life: strategic R&D center at the University of Debrecen, Chemistry of carbohydrates and heterocycles subproject. (Participant) *Period and any other information: 2016-2020* *Name of project or research focus:* Grant OTKA, FK 125067, supported by the National Research, Development and Innovation Office of Hungary: New types and new biological applications of C-glycopyranosyl heterocycles. (Principal investigator) *Period and any other information: 2017-2021*
Industry collaborations over the last 5 years	*Project title: -* *Partners: -*
Patents and proprietary rights	László SOMSÁK, Éva BOKOR, Marietta VÁGVÖLGYINÉ TÓTH, László JUHÁSZ, Katalin CZIFRÁK, Bálint KÓNYA, Sándor KUN, András PÁHI, Béla SZŐCS, Gergely VARGA, Pál GERGELY, Tibor DOCSA, Lászlóné KÓDER, Károlyné NAGY. *Title:* Glycogen phosphorylase inhibitors / Glikogén

	foszforiláz inhibitorok P1100602/P1200475, 2012, Hungarian patent application *Title:* Preparation of imidazolyl and triazolyl glycosides as glycogen phosphorylase inhibitors and antitumor agents. WO2013061105A2, 2013, International patent application.
Important publications over the last 5 years	*Selected recent publications from a total of approx. (give total number): 33* *Author(s):* Éva BOKOR, Attila FEKETE, Gergely VARGA, Béla SZŐCS, Katalin CZIFRÁK, István KOMÁROMI, László SOMSÁK: *Title:* *C*-(β-D-Glucopyranosyl)formamidrazones, formic acid hydrazides and their transformations into 3-(β-D-glucopyranosyl)-5-substituted-1,2,4-triazoles: a synthetic and computational study *Any other information:* *Publisher, place of publication, date of publication or name of periodical, volume, issue, page numbers:* Tetrahedron, **2013**, 69, 10391-10404. *Author(s):* Éva BOKOR, Sándor KUN, Tibor DOCSA, Pál GERGELY, László SOMSÁK: *Title:* 4(5)-Aryl-2-*C*-glucopyranosyl-imidazoles as new nanomolar glucose analogue inhibitors of glycogen phosphorylase *Any other information:* *Publisher, place of publication, date of publication or name of periodical, volume, issue, page numbers:* ACS Med. Chem. Lett., **2015**, 6, 1215-1219. *Author(s):* Anastassia L. KANTSADI, Éva BOKOR, Sándor KUN, George A. STRAVODIMOS, Demetra S.M. CHATZILEONTIADOU, Demetres D. LEONIDAS, Éva JUHÁSZ-TÓTH, Andrea SZAKÁCS, Gyula BATTA, Tibor DOCSA, Pál GERGELY, László SOMSÁK: *Title:* Synthetic, enzyme kinetic, and protein crystallographic studies of *C*-β-D-glucopyranosyl pyrroles and imidazoles reveal and explain low nanomolar inhibition of human liver glycogen

	phosphorylase *Any other information:* *Publisher, place of publication, date of publication or name of periodical, volume, issue, page numbers Eur. J. Med. Chem.,* **2016**, 123, 737-745. *Author(s):* Éva BOKOR, Sándor KUN, **David GOYARD, Marietta TÓTH, Jean-Pierre PRALY, Sebastien VIDAL, László SOMSÁK:** *Title: C*-Glycopyranosyl arenes and hetarenes: synthetic methods and bioactivity focused on antidiabetic potential *any other information:* *Publisher, place of publication, date of publication or name of periodical, volume, issue, page numbers: Chem. Rev.*, **2017**, 117, 1687-1764. *Author(s):* Éva BOKOR, Efthimios KYRIAKIS, Theodora G. A. SOLOVOU, Csenge KOPPÁNY, Anastassia L. KANTSADI, Katalin E. SZABÓ, Andrea SZAKÁCS, George A. STRAVODIMOS, Tibpr DOCSA, Vassiliki T. SKAMNAKI, Spyros E. ZOGRAPHOS, P. Gergely, Demetres D. LEONIDAS, László SOMSÁK: *Title:* Nanomolar inhibitors of glycogen phosphorylase based on β-D-glucosaminyl heterocycles: a combined synthetic, enzyme kinetic, and protein crystallography study *Any other information:* *Publisher, place of publication, date of publication or name of periodical, volume, issue, page numbers: J. Med. Chem.*, **2017**, 60, 9251-9262.
Activities in specialist bodies over the last 5 years	*Organisation - Role – Period* Chemistry BSc State Exam Committee – Secretary – 2013 – 2017

Name	*Péter Buglyó*
Position	*associate professor*
Academic career	*1989 research fellow, Dept. of Inorg. and Anal. Chem., L. Kossuth University* *1990 research fellow, Hungarian Academy of Sciences* *1992 assistant professor, Dept. of Inorg. and Anal. Chem., L. Kossuth University*

	1996 postdoctoral fellow, University of British Columbia *1998 assistant professor, Dept. of Inorg. and Anal. Chem., L. Kossuth University* *2000 assistant professor, Dept. of Inorg. and Anal. Chem., L. Kossuth University* *2006 associate professor, Dept. of Inorg. and Anal. Chem., University of Debrecen*
	M.Sc. Chemistry, 1989 Lajos Kossuth University, Debrecen *Ph.D. Chemistry, 1993 Lajos Kossuth University, Debrecen* *Dr.Habil. Chemistry, 2003 University of Debrecen*
Employment	*1989 research fellow, Dept. of Inorg. and Anal. Chem., L. Kossuth University* *1990 research fellow, Hungarian Academy of Sciences* *1992 assistant professor, Dept. of Inorg. and Anal. Chem., L. Kossuth University* *1996 postdoctoral fellow, University of British Columbia* *1998 assistant professor, Dept. of Inorg. and Anal. Chem., L. Kossuth University* *2000 assistant professor, Dept. of Inorg. and Anal. Chem., L. Kossuth University* *2006 associate professor, Dept. of Inorg. and Anal. Chem., University of Debrecen*
Research and development projects over the last 5 years	*Chemistry for better life: strategic R&D center at the university of Debrecen (DECHEM), 01/10/2016-30/09/2020, GINOP-2.3.2-15-2016-00008, 1 984 M HUF, subproject leader* *Synthesis and Characterization of bimetallic complexes as potential hypoxia-activated prodrugs with dual anticancer activity, OTKA 112317, 2015-2018, 24.3 M HUF, principal investigator* *Synthesis and Characterization of Novel Ruthenium-Hydroxamate Complexes, OTKA 76142, 2009-2013 11.8 M HUF, principal investigator*
Industry collaborations over the last 5 years	-

Patents and proprietary rights	-
Important publications over the last 5 years	*Selected recent publications from a total of approx. 81:* J. Patalenszki, L. Bíró, A. C. Bényei, T. R. Muchova, J. Kasparkova, *P. Buglyó,* **Half-sandwich complexes of ruthenium, osmium, rhodium and iridium with DL-methionine or S-methyl-L-cysteine: A solid state and solution equilibrium study,** *RSC Advances*, **2015**, *5,* 8094-8107 P. L. Parajdi-Losonczi, A. C. Bényei, É. Kováts, I. Timári, T. R. Muchova, J. Kasparkova, *P. Buglyó,* **[(η^6-*p*-cym)Ru(H_2O)$_3$]$^{2+}$ Binding Capability of Aminohydroxamates – A Solution and Solid State Study,** *J. Inorg. Biochem.,* **2016**, *160,* 236–245 Zs. Bihari, F. Vultos, C. Fernandes, L. Gano, I. Santos, J. D. G. Correia, *P. Buglyó,* **Synthesis, characterization and biological evaluation of a ^{67}Ga-labeled (□^{6}-Tyr)Ru(□^{5}-Cp) peptide complex with the HAV motif,** *J. Inorg. Biochem.,* **2016**, *160,* 189–197 E. Farkas, *P. Buglyó,* **Lead(II) Complexes of Amino Acids, Peptides, and Other Related Ligands of Biological Interest**, in Lead: Its Effects on Environment and Health, *Met. Ions Life Sci*. **2017**, *17*, 201–240 D. Sanna,V. Ugone, G. Sciortino, *P. Buglyó*, Zs. Bihari, P. L. Parajdi-Losonczi, E. Garribba, **Complexes of $V^{IV}O^{2+}$ ion with antibacterial quinolones ligands and their interaction with serum proteins,** *Dalton Trans.,* **2018,** *47*, 2164-2182
Activities in specialist bodies over the last 5 years	*Secretary of the Chemical Institute, University of Debrecen, 2010-2017* *Advisory Board member, COST CM1115, 2013-2016* *Elected member of the Physical Chemistry Scientific Comittee of the Hungarian Academy of Sciences 2014-2017* *Elected secretary of the Physical Chemistry Scientific Comittee of the Hungarian Academy of Sciences 2018-*

Name	*Dr. András Csehi*
Position	*Senior lecturer (Dept. Theor. Phys., University of Debrecen)*

Academic career	*Initial academic appointment: Faculty of Informatics, University of Debrecen, 2013* Habilitation: –
	doctoral qualification: Faculty of Informatics, UD, 2014 *Doctorate: physics & informatics, Faculty of Informatics, UD, 2014* *Undergraduate degree: physics MSc, Department of Theoretical Physics, UD, 2010*
Employment	*Senior lecturer – Department of Theoretical Physics, UD, 2015-present* *Assistant lecturer – Department of Theoretical Physics, UD, 2014-2015* *Research fellow – Faculty of Informatics, UD, 2013-2014*
Research and development projects over the last 5 years	*Name of project or research focus: EFOP-3.6.2-16-2017-00005 EU projekt: Ultrafast processes in atoms, molecules, nanostructures and biological systems* *Period and any other information: 2017-2020* *Partners, if applicable: University of Szeged & University of Debrecen* *Amount of financing:*
Industry collaborations over the last 5 years	*Project title: –* *Partners: –*
Patents and proprietary rights	–
Important publications over the last 5 years	*Selected recent publications from a total of approx. 23:* [1] A. Csehi, G. J. Halász, L. S. Cederbaum and Á. Vibók: Light-induced conical intersections. in Attoseond Molecular Dynamics, (Eds.: M. J. J. Vrakking, F. Lépine) Theoretical and Computational Chemistry Series, Royal Society of Chemistry (2018) [2] A. Csehi, G. J. Halász, L. S. Cederbaum, Á. Vibók: Competition between Light-Induced and Intrinsic Nonadiabatic Phenomena in Diatomics. *J. Phys. Chem. Lett.*, 8 (7), 1624 (2017). [3] G. J. Halász, A. Csehi, Á. Vibók, L. S. Cederbaum: Influence of Light-Induced Conical Intersection on the Photodissociation Dynamics of D_2^+ Starting from Individual Vibrational Levels. *J. Phys. Chem. A 118, 11908, (2014).*

Activities in specialist bodies over the last 5 years	*Organisation - Role – Period* –

Name	*Lajos Daróczi*
Position	*associate professor*
Academic career	Habilitation *University of Debrecen 2016*
	PhD degree University of Debrecen 1997 Physicist Lajos Kossuth University 1989
Employment	*2016- associate professor, Department of Solid State Physics, University of Debrecen* *1997-2016 senior lecturer University of Debrecen* *1992-1997 assistant lecturer Lajos Kossuth University* *1989-1992 Phd student Lajos Kossuth University*
Research and development projects over the last 5 years	**GINOP-2.3.2-15-2016-00041** Regionális Anyagtudományi Kiválósági Műhely – Kutatási Program és Infrastruktúra 2017- **TÁMOP-4.2.2.A-11/1 KONV-2012-0036** Intelligens funkcionális anyagok: Mechanikai , kémiai, elektromágneses, optikai tulajdonságok és alkalmazásaik 2013-2015 **OTKA K 084065** Termomechanikus kezelések hatására végbemenő termoelasztikus és nem termoelasztikus martenzites átalakulások 2011-2014
Industry collaborations over the last 5 years	*Project title: Oxidation induction time measurements* *Partners: Texor Kft,Partium40 Kft.*
Patents and proprietary rights	*Titanát polimer nanokompozitok és eljárás előállításukra 2007*
Important publications over the last 5 years	Bolgár MK, Tóth LZ, Szabó S, Gyöngyösi S, Daróczi L, Panchenko EY, Chumlyakov YI, Beke DL: Thermal and acoustic noises generated by austenite/martensite transformation in NiFeGaCo single crystals, J ALLOY

	COMPD 658: 29-35, 2016 Daróczi L, Gyöngyösi S, Tóth LZ, Beke DL: *Effect of the martensite twin structure on the deformation induced magnetic avalanches in Ni2MnGa single crystalline samples*, SCRIPTA MATER 114: 161-164, 2016 Tóth LZ, Daróczi L, Szabó S, Beke DL: Simultaneous investigation of thermal, acoustic, and magnetic emission during martensitic transformation in single-crystalline Ni2MnGa, PHYS REV B CONDENS MATTER MATER PHYS 93: (14) , 2016 Daróczi Lajos, Gyöngyösi Szilvia, Tóth László Zoltán, Szabó Sándor, Beke Dezső László: *Jerky magnetic noises generated by cyclic deformation of martensite in Ni2MnGa single crystalline shape memory alloys*, APPL PHYS LETT 106: (4) 041908, 2015 Tóth LZ, Szabó S, Daróczi L, Beke DL: *Calorimetric and acoustic emission study of martensitic transformation in single-crystalline Ni2 MnGa alloys*, PHYSICAL REVIEW B CONDENS MATTER MATER PHYS 90: (22) 224103, 2014
Activities in specialist bodies over the last 5 years	*Lorand Eötvös Physical Society, member of Hajdu Bihar County presidency.*

Name	Gábor Dobosi, DSc
Position	*Professor, Geology*
Academiccareer	*Professor (UD, Department of Mineralogy and Geology, 2014-)* Habilitation *(UD, 2012)*
	Doctoral qualification: *DSc, Hungarian Academy of Sciences, 2004* *PhD (CSc), Hungarian Academy of Sciences, 1994* *Doctorate, subject (Institution, year)* *Undergraduate degree: (subject (Institution, year):* *Chemistry MSc, ELTE 1975* *Geology MSc, ELTE 1979*

Employment	*From assistant research fellow to scientific advisor - Hungarian Academy of Sciences - 1975 - 2014* *Professor, UD Department of Mineralogy and Geology, 2014 - present*
Research and development projects over the last 5 years	*Name of project or research focus:* *Period and any other information:* *Partners, ifapplicable:* *Amount of financing:*
Industry collaborations over the last 5 years	*Project title:* *Partners:*
Patents and proprietary rights	*Title (Year)*
Important publications over the last 5 years	*Selected recent publications from a total of approx. (give total number): 14* Jankovics MÉ, Taracsák Z, Dobosi G, Embey-Isztin A, Batki A, Harangi Sz, Hauzenberger CA Clinopyroxene with diverse origins in alkaline basalts from the western Pannonian Basin: implications from trace element characteristics LITHOS 262: pp. 120-134 (2016) Dobosi G, Harangi Sz Hungarian National Report on IAVCEI (2011-2014) GEOMATIKAI KÖZLEMÉNYEK 18:(1) pp. 137-145. (2015) Downes H, Carter A, Armstrong R, Dobosi G, Embey-Isztin A Lower crustal zircons reveal Neogene metamorphism beneath the Pannonian Basin (Hungary) OPEN GEOSCIENCES 7:(1) pp. 223-233. (2015) Batki A, Pál-Molnár E, Dobosi G, Skelton A Petrogenetic significance of ocellar camptonite dykes in the Ditrău Alkaline Massif, Romania LITHOS 200-201: pp. 181-196. (2014) Embey-Isztin A, Dobosi G, Bodinier J-L, Bosch D, Jenner G A, Pourtales S, Bruguier O Origin and significance of poikilitic and mosaic peridotite xenoliths in the western Pannonian Basin: geochemical and petrological evidences

	CONTRIBUTIONS TO MINERALOGY AND PETROLOGY 168:(3) pp. 1-16. (2014)
Activities in specialist bodies over the last 5years	*Central European Geology (AK journals), member of the Editorial Board, 2012 - present*

Name	*Katalin E. Kövér, PhD, DSc*
Position	*Full Professor of Chemistry*
Academic career	*Member of Hungarian Academy of Sciences (HAS, 2013)* *Habilitation (UD, 2007)*
	Doctor of the Hungarian Academy of Sciences (D.Sc.), *Chemistry,* 2002 *Candidate degree, Chemistry, Hungarian Academy of Sciences, 1988* *Doctoral qualification, University Doctor, Chemistry, Lajos Kossuth University, 1984* *Undergraduate degree, chemistry, Lajos Kossuth University, 1979*
Employment	*Professor of Chemistry*, Department of Inorganic and Analytical Chemistry, University of Debrecen, 2008- *Distinguished Research Scientist*, Department of Inorganic and Analytical Chemistry, University of Debrecen, 2003-2008 *Senior Research Scientist*, Department of Inorganic and Analytical Chemistry, University of Debrecen, 1996-2003*Senior Research Associate*, BIOGAL Pharmaceutical Works - Department of Organic Chemistry, Lajos Kossuth University, Debrecen, 1988-1996 *Postdoctoral Fellow*, Department of Chemistry, University of Arizona, Tucson, Arizona, USA, 1991-1993 *Research Associate*, BIOGAL Pharmaceutical Works - Department of Organic Chemistry, Lajos Kossuth University, Debrecen, 1991-1993 *Postdoctoral Fellow*, Department of Biochemistry, University of Illinois, Chicago, Illinois, USA, 1987 *Research Fellow*, BIOGAL Pharmaceutical Works - Department of Organic Chemistry, Lajos Kossuth University, Debrecen, 1979-1984
Research and development projects over the last 5 years	*Name of project or research focus:* GINOP-2.3.2-15-2016-00008, EU project, Chemistry for better life:

	strategic R&D Center at the University of Debrecen (DECHEM) *Period and any other information: 2016-2020* *Name of project or research focus:* GINOP-2.3.3-15-2016-00004, EU project, Integrated Instrumental Infrastructure for Research in Molecular Science and Molecular Medicine (I2M2) *Period and any other information: 2016-2019*
Industry collaborations over the last 5 years	*Project title: Structure verification based on NMR and other analytical measurements* *Partners: TEVA Pharmaceutical Company, Debrecen*
Patents and proprietary rights	*Title (Year)*
Important publications over the last 5 years	*Selected recent publications from a total of approx. (give total number): 220* *Author(s):* K Fehér, I Timári, K Rákosi, J Szolomajer, TZ Illyés, A Bartok, Z Varga, G Panyi, GK Tóth, **KE Kövér** *Title:* Probing pattern and dynamics of disulfide bridges using synthesis and NMR of an ion channel blocker peptide toxin with multiple diselenide bonds *Any other information:* *Publisher, place of publication, date of publication or name of periodical, volume, issue, page numbers* Chemical Science 7 (4), 2666-2673, 2016. *Author(s):* A Bartok, K Fehér, A Bodor, K Rákosi, GK Tóth, **KE Kövér**, G Panyi, Z Varga *Title:* An engineered scorpion toxin analogue with improved Kv1.3 selectivity displays reduced conformational flexibility *Any other information:* *Publisher, place of publication, date of publication or name of periodical, volume, issue, page numbers* Scientific reports, 5:18397, DOI: 10.1038/srep18397, 2015 *Author(s):* I Timári, TZ Illyés, RW Adams, M Nilsson, L Szilágyi, GA Morris, **KE Kövér**

	Title: Precise Measurement of Long-Range Heteronuclear Coupling Constants by a Novel Broadband Proton–Proton-Decoupled CPMG-HSQMBC Method *Any other information:* *Publisher, place of publication, date of publication or name of periodical, volume, issue, page numbers* Chemistry–A European Journal 21 (8), 3472-3479, 2015 *Author(s):* I Timári, L Kaltschnee, A Kolmer, RW Adams, M Nilsson, CM Thiele, GA Morris, **KE Kövér** *Title:* Accurate determination of one-bond heteronuclear coupling constants with "pure shift" broadband proton-decoupled CLIP/CLAP-HSQC experiments *Any other information:* *Publisher, place of publication, date of publication or name of periodical, volume, issue, page numbers* Journal of Magnetic Resonance 239, 130-138, 2014 *Author(s):* L Kaltschnee, A Kolmer, I Timári, V Schmidts, RW Adams, M Nilsson, **KE Kövér** *Title:* "Perfecting" pure shift HSQC: full homodecoupling for accurate and precise determination of heteronuclear couplings *Any other information:* *Publisher, place of publication, date of publication or name of periodical, volume, issue, page numbers* Chemical Communications 50 (99), 15702-15705, 2014
Activities in specialist bodies over the last 5 years	Member of the International Evaluation Panel of iNEXT: Infrastructure for NMR, EM and X-rays for Translational Research, 2015 - Member of the International Evaluation Panel of Instruct research infrastructure project, 2016 - Member of the Corbel, Shared Services for Life-Science, Scientific Review Panel tagja, 2017- MMCE and EUROMAR Conferences – Member of the International Scientific Board, 2016-2017.

Name	*István Fábián*
Position	*Analytical chemistry*
Academic career	*Initial academic appointment Kossuth Lajos University 1980* *Habilitation: Kossuth Lajos University, 1998*
	doctoral qualification: NA *Doctorate: coordination chemistry, Kossuth Lajos University, 1982* *Undergraduate degree: chemistry, Kossuth Lajos University, 1980*
Employment	*Professor (current), University of Debrecen, from 1980*
Research and development projects over the last 5 years	*Name of project or research focus: reaction kinetics and mechanisms; aerogels; environmental chemistry;* *Period and any other information: NA* *Partners, if applicable: NA* *Amount of financing: Annually HUF 50000000*
Industry collaborations over the last 5 years	*Project title: Hypochlorous acid decomposition under industrial condition* *Partners: AkzoNobel Pulp and Performance Chemicals, Bohus, Sweden*
Patents and proprietary rights	*Method for the preparation of composite silica alcogels, aerogels and xerogels, apparatus for carrying out the method continuously, and novel composite silica alcogels, aerogels and xerogels, 2013*
Important publications over the last 5 years	*Selected recent publications from a total of approx. (give total number): 139* 1. J. Kalmár, M. Szabó, N. Simic, M. Wildlock, **I. Fábián** **Kinetics and mechanism of the chromium(VI) catalyzed decomposition of hypochlorous acid at elevated temperature and high ionic strength** *Dalton Transactions* **2018**, *47, in press* DOI: 10.1039/C8DT00120K. [Q1, IF.: 4.029, Cit.: 0/1] 2. F. Najóczki, G. Bellér, M. Szabó, **I. Fábián** **Substituent effect on the N-oxidation of 1,10-phenanthroline derivatives by peroxomonosulfate ion** *New J. Chem.* **2017**, *41*, 9947-9953. DOI: 10.1039/C7NJ01860F [Q1, IF.: 3.269, Cit.: 0/0] 3. M. Szabó, G. Bellér, J. Kalmár, **I. Fábián**

	The Kinetics and Mechanism of Complex Redox Reactions in Aqueous Solution: The Tools of the Trade *In Adv. Inorg. Chem.: Inorganic Reaction Mechanisms*, **2017**, *70*, 1-61. DOI 10.1016/bs.adioch.2017.02.004 [Q1, IF.: 4.250, Cit.: 0/0] 4. G. Bellér, M. Szabó, G. Lente, **I Fábián** **Formation of 1,10-Phenanthroline-N,N′-dioxide under Mild Conditions: The Kinetics and Mechanism of the Oxidation of 1,10-Phenanthroline by Peroxomonosulfate Ion (Oxone)** *J. Org. Chem.* **2016,** *81*, 5345-5353 DOI: 10.1021/acs.joc.6b00641 [D1, IF.: 4.785, Cit.: 1/3] 5. J. Kalmár, G. Lente, **I. Fábián** **Kinetics and mechanism of the adsorption of methylene blue from aqueous solution on the surface of a quartz cuvette by on-line UV-Vis spectrophotometry** ***Dyes and Pigments*** **2016,** *127*, 170-178. DOI: 10.1016/j.dyepig.2015.12.025 [Q1, IF.: 4.055, Cit.: 1/3]
Activities in specialist bodies over the last 5 years	*Organisation - Role – Period* *Membership without a specific role need not be mentioned.*

Name	*Krisztina Fehér*
Position	*Research Fellow*
Academic career	*Research Fellow (Chemistry Institute, 2014)*
	PhD, Debrecen University 2003) *Diploma, University of Lajos Kossuth, 1998*
Employment	*Doctor Assistant, Ghent University, Belgium, 2012-2017* *Research Scientist, INFAI GmbH, Germany, 2011* *Senior Researcher, Vernalis R&D, UK, 2008-2010* *Research Scientist - Visiting Scientist, Max-Planck Institute for Medical Research – European Molecular Biology, Laboratory, Germany, 2006-2007* *Research Scientist, Bayer AG, Germany, 2003-2004* *Max Planck Fellow, Max-Plank Institute for Biophysical Chemistry, Germany, 2002*
Research and development	*Name of project or research focus:* GINOP-2.3.2-15-

projects over the last 5 years	2016-00044 “A gyógyszerkutatás újabb irányai: peptid-fehérje kölcsönhatások a magasabbrendű fehérjeszerveződések szabályozásában” – PHARMPROT teaming *Period and any other information: 2017-2021* *Partners, if applicable:* PI : Prof. Fuxreiter Mónika, Debrecen University, Hungary *Amount of financing:* *Name of project or research focus: Marie Curie Career Integration Grant*, (Project No: 303917, PGN-INNATE), “Molecular recognition of bacterial cell wall peptidoglycans and related molecules by innate immune receptors”, *Period and any other information:* 2014-2018 *Partners, if applicable: -* *Amount of financing:* *Name of project or research focus: Research Grant by the Research Foundation – Flanders* (Project ID: 1525517N)., for the project of “NMR and molecular modelling investigations of hydroxyl apatite –DNA immune stimulator nanoplatforms for improved vaccine delivery” *Period and any other information:* 01.01.2017-12.31.2019 *Partners, if applicable:* Prof. Jose Martins, Ghent University, Belgium *Amount of financing:* *Name of project or research focus: : Research Grant by the Research Foundation – Flanders* (Project ID: 1508414N), “Study of the molecular recognition of natural and derivatised peptidoglycan by immune receptors for the design of improved immunomodulators” *Period and any other information:* 01.01.2014 – 31.12.2017 for the project *Partners, if applicable: Prof. Srjdanka Tomic, Zagreb University, Croatia* *Amount of financing:*

	Name of project or research focus: International Collaboration by the Hungarian Scientific Research Foundation (OTKA), (Project Nr. 109671), "Novel carbohydrate derivatives as potential anti-trypanosomal agents: chemical and parasitological investigations" *Period and any other information:* 2014-2018 *Partners, if applicable:* PI: Prof. Szilágyi László, Debrecen University, Hungary *Amount of financing:* *Name of project or research focus: Social Renewal Operational Programme* by the European Regional Development Fund (TÁMOP-4.2.2.A-11/1/KONV-2012-0025.), "Molecular oncology: identification of targets in Signal transduction processes for the development of novel tumortherapeutics." *Period and any other information:* 2014-2018 *Partners, if applicable:* PI: Prof. György Panyi, Debrecen University, Hungary *Amount of financing:*
Industry collaborations over the last 5 years	*Project title: -* *Partners: -*
Patents and proprietary rights	-
Important publications over the last 5 years	*Selected recent publications from a total of approx. (give total number): 43* Kaltner H, Szabó T, Fehér K, André S, Balla S, Manning JC, Szilágyi L, Gabius H-J Bivalent O-glycoside mimetics with S/disulfide/Se substitutions and aromatic core: Synthesis, molecular modeling and inhibitory activity on biomedically relevant lectins in assays of increasing physiological relevance BIOORGANIC & MEDICINAL CHEMISTRY 25:(12) pp. 3158-3170. (2017)

	Feher Krisztina, Timari Istvan, Rakosi Kinga, Szolomajer Janos, Illyes Tunde Zita, Bartok Adam, Varga Zoltan, Panyi Gyorgy, Toth Gabor, Kover Katalin E Probing pattern and dynamics of disulfide bridges using synthesis and NMR of an ion channel blocker peptide toxin with multiple diselenide bonds. CHEMICAL SCIENCE 7:(4) pp. 2666-2673. (2016) Bartok A, Feher K, Bodor A, Rakosi K, Toth GK, Kover KE, Panyi G, Varga Z An engineered scorpion toxin analogue with improved Kv1.3 selectivity displays reduced conformational flexibility. SCIENTIFIC REPORTS 5: Paper 18397. (2015) Buyst D, Gheerardijn V, Feher K, Van Gasse B, Van Den Begin J, Martins JC, Madder A Identification of a pKa-regulating motif stabilizing imidazole-modified double-stranded DNA NUCLEIC ACIDS RESEARCH 43:(1) pp. 51-62. (2015) Fehér K, Groves P, Batta G, Jiménez-Barbero J, Muhle-Goll C, Kövér K E Competition Saturation Transfer Difference Experiments Improved with Isotope Editing and Filtering Schemes in NMR-Based Screening JOURNAL OF THE AMERICAN CHEMICAL SOCIETY 130:(50) pp. 17148-17153. (2008)
Activities in specialist bodies over the last 5 years	-

Name	*László Galuska MD*
Position	*Nuclear Medicine, Professor emeritus*
Academic career	University of Debrecen **2001 Habilitation**
	D.Sc*. Hungarian Academy of Sciences* ***2016*** *doctoral qualification (Institution, year)* ***PhD*** *Medical University of Szentgyörgyi-Albert* ***1996*** *subject (Institution, year)* ***MD****, University of Szeged* ***1972***
Employment	*Professor emeritus, University of Debrecen from* ***2016***
Research and development projects over the last 5 years	*Name of project or research focus:* **Comparison of different smoking customs on pulmonary demage. Smoking and e-cigar**
	Period and any other information: 2015 09 10 - 2016 12 30
	Partners, if applicable: *Amount of financing:*
Industry collaborations over the last 5 years	*Project title:* *Partners:*
Patents and proprietary rights	*Title (Year)*
Important publications over the last 5 years	Total:232 1. Palatka K, Kacska S, Lovas S, Garai I, Varga J, Galuska L The potential role of FDG PET-CT in the characterization of the activity of Crohn's disease, staging follow-up and prognosis estimation: a pilot study ***SCANDINAVIAN JOURNAL OF GASTROENTEROLOGY*** **53:**(1) *pp. 24-30.* (2018) 2. Galuska L, Barna S, Varga J, Garai I, Nagy EV The role of 99mTc-DTPA retrobulbar SPECT in staging and follow-up of Graves' orbitopathy. ***NUCLEAR MEDICINE REVIEW: CENTRAL AND EASTERN EUROPE*** **21:**(1) Paper 51. (2018) 3. Gellén E, Sántha O, Janka E, Juhász I, Péter Z, Erdei I,

	Lukács R, Fedinecz N, Galuska L, Remenyik É, Emri G Diagnostic accuracy of 18F-FDG-PET/CT in early and late stages of high-risk cutaneous malignant melanoma ***JOURNAL OF THE EUROPEAN ACADEMY OF DERMATOLOGY AND VENEREOLOGY* 29:**(10) pp. 1938-1944. (2015) 4. Gábor Máté, Dezső Szikra, Jakub Šimeček, Szandra Szilágyi, György Trencsényi, Hans-Jürgen Wester, István Kertész, László Galuska Multiparametric labeling optimization and synthesis of 68Ga-labeled compounds applying a continuous-flow microfluidic methodology ***JOURNAL OF FLOW CHEMISTRY* 6:**(2) *pp. 86-93.* (2016) 5. Erdei A, Paragh G, Kovacs P, Karanyi Z, Berenyi E, Galuska L, Lenkey A, Szabados L, Gyory F, Ujhelyi B, Berta A, Boda J, Berta E, Bodor M, Gazdag A, Nagy EV Rapid response to and long-term effectiveness of anti-CD20 antibody in conventional therapy resistant Graves' orbitopathy: A five-year follow-up study. ***AUTOIMMUNITY* 47:**(8) *pp. 548-555.* (2014)
Activities in specialist bodies over the last 5 years	*Organisation - Role – Period* *Membership without a specific role need not be mentioned.*

Name	Attila Gáspár
Position	Professor
Academic career	Doctor of Science (HAS, 2015) Habilitation (UD, 2005) PhD (UD, 1997) chemist, chemistry teacher, translator of English (UD, 1994)
Employment	University of Debrecen, Dept. of Inorganic and Analytical Chemistry (1997-)
Research and development projects over the last 5 years	„Chemistry for better life: strategic R&D center at the University of Debrecen” GINOP-2.3.2-15-2016-00008 project Support: 1.983.995.445 Ft Number of participants: 139

	Duration: 2016.10.01-2020.09.30 website for further information: www.dechem.unideb.hu „Integrated Instrumental Infrastructure for Research in Molecular Science and Molecular Medicine (I2M2)" GINOP-2.3.3-15-2016-00004 project Support: 807 759 930 Ft Number of participants: 71 Duration: 2016.09.01-2019.06.30. website for further information: www.i2m2.unideb.hu OTKA K75286, 2008-10-01 2013-10-31 9 Title: Fabrication of new types of microfluidic devices and the study of their capabilities for liquid chromatographic, electrophoretic and electrochromatographic separation OTKA K111932, 2015-01-01 2018-12-31 Title: Analytical separations in microfluidic chips 19701000 HUF
Industry collaborations over the last 5 years	Project title: Capillary electrophoretic analysis of monoclonal antibodies Partner: Richter G. Plc.
Patents and proprietary rights	A.Gáspár, H.Berndt: "Vorrichtung zum Atomisieren von flüssigen Proben", German patent, DE 19944650.4 Gomez, F.A, Gaspar, A., Piyasena, M.E., Magnetically controlled valve for flow manipulation in polymer microfluidic devices, US Patent application, #44,228 2006. Patent No. 2008/0163,946
Important publications over the last 5 years	A.Kiss, A.Gaspar: Fabrication of a Microfluidic Flame Atomic Emission Spectrometer: a Flame-on-a-Chip, Anal.Chem., 2018, 90, 5995-6000 A.Kecskemeti, A.Gaspar: Particle based liquid chromatographic separations in microfluidic devices, Anal.Chim.Acta, 2018, 1021, 1-19 A.Kecskemeti, A.Gaspar: Particle-based immobilized enzymatic reactors in microfluidic chips, Talanta, 2018,

	180, 211-228 A.Kecskemeti, C.N.Nagy, G.Kallo, E.Csosz, A.Gaspar: The application of a microfluidic reactor including spontaneously adsorbed trypsin for rapid protein digestion of human tear samples, Proteomics Clin. Appl., 2017, 11, 1700055 A.Kecskemeti, J.Bako, I.Csarnovics, E.Csosz, A.Gaspar: The application of non-covalently immobilized trypsin in a poly(dimethylsiloxane) microfluidic device for rapid protein digestion, Anal. Bioanal. Chem., 2017, 409, 3573-3585 A.Kecskemeti, A.Gaspar: Preparation and characterization of a packed bead immobilized trypsin reactor integrated into a PDMS microfluidic chip for rapid protein digestion, Talanta, 2017, 166, 275–283
Activities in specialist bodies over the last 5 years	MTA Work Commitee for Analysis of Organic Materials and Pharmaceuticals (2005-) Hungarian Society for Separation Sciences (2005-) CEEPUS H-076 program (2001-)

Name	*Dr. Gyöngyi Gyémánt*
Position	*Teaching area and designation* *Biochemistry for pharmacists and chemical engineers. Biochemistry practicals for biologists and chemists. Bioanalytical courses: Chromatography, MS, Carbohydrate analysis*
Academic career	*Associate Professor of Analytical Chemistry (UD, 2011-)* *Habilitation (UD, 2009)*
	PhD in Chemistry, 2002, University of Debrecen ***MSc. in Chemistry, 1983, University of Lajos Kossuth, Debrecen*** ***High School Gárdonyi Géza Gimnázium, Eger, 1978***
Employment	*Assistant Professor of Analytical Chemistry,(UD, 2009-2011)* *Assistant Professor of Biochemistry, (UD, 2002-2009)* *Assistant Lecturer, University of Lajos Kossuth, 1994-2002* *Analytical engineer, BIOGAL Pharm. Wor,k 1983-1994*
Research and development projects over the last 5 years	*Structure and Function of the Antifungal Proteins PAFB and NFAP, OTKA 2014-2017 33M HUF, participant*

	Analitical separations on microchip, OTKA, 2015-2018, 19.7 M HUF, participant
Industry collaborations over the last 5 years	*Project title: Structure and interaction of CD derivatives and complexes* *Partners: Cyclolab 2015-*
Patents and proprietary rights	*Use of siderophores in prevention of vascular diseases, production of siderophores and qualifying siderophore containing meat-products 2008* *Novel preparation. of polyvinyl-pyrrolidone-iodine complex - and surgical hand cleanser containing it 1988* *.*
Important publications over the last 5 years	*Selected recent publications from a total of approx. 80* *Gábor Lehoczki, Lili Kandra, Gyöngyi Gyémánt The use of starch azure for measurement of alpha-amylase activity Carbohydrate Polymers, 183 (2018) 263-266. IF:4,811* *Lehoczki G, Szabó K, Takács I, Kandra L, Gyémánt G Simple ITC method for activity and inhibition studies on human salivary α-amylase, JOURNAL OF ENZYME INHIBITION AND MEDICINAL CHEMISTRY 31:(6) (2016) 1648-1653. IF: 4,293* *Judit R. Homoki, Andrea Nemes, Erika Fazekas, Gyöngyi Gyémánt, Péter Balogh, Ferenc Gál, Jamil Al-Asri, Jérémie Mortier, Gerhard Wolber, László Babinszky and Judit Remenyik, Anthocyanin composition, antioxidant efficiency, and α-amylase inhibitor activity of different Hungarian sour cherry varieties (Prunus cerasus L.), Food Chemistry, 194, (2016) 222-229. IF: 3,391* *Jamil Al-Asri, Erika Fazekas, Gábor Lehoczki, Andrej Perdih, Cornelia Görick, Matthias F. Melzig, Gyöngyi Gyémánt, Gerhard Wolber, Jérémie Mortier From Carbohydrates to Drug-Like Fragments: Rational Development of Novel α-Amylase Inhibitors, Bioorganic and Medicinal Chemistry, 23 (2015) 6725-6732., IF: 2,793* *B Bécsi, D Dedinszki, G Gyémánt, C Máthé, G Vasas, B Lontay, F Erdődi, Identification of protein phosphatase interacting proteins from normal and UVA-irradiated HaCaT cell lysates by surface plasmon resonance based binding technique using biotin-microcystin-LR*

	as phosphatase capturing molecule, Journal of Photochemistry and Photobiology B: Biology 138 (2014) 240-248. IF:3,11 *E. Fazekas, K. Szabó, L. Kandra, G. Gyémánt, Unexpected mode of action of sweet potato β-amylase on maltooligomer substrates, Biochimica et Biophysica Acta (BBA) - Proteins and Proteomics, 1834, (2013),1976-1981, IF: 3,73*
Activities in specialist bodies over the last 5 years	*Ad hoc reviewer for the following journals and organizations:* *Journals.* • *Acta Biologica Hungarica* • *Enzyme and Microbial Technology* • *Fitoterapia* • *Carbohydrate Research* • *Reaction Kinetics, Mechanisms and Catalysis.* *Organisations* • *Hungarian Scientific Research Fund (OTKA)* • *NKTH*

Name	*Henrietta Győrvári Horváth PhD*
Position	*Associate Research Professor*
Academic career	*Associate Research Professor (MTA-DE Redox and Homogeneous Catalytic Reaction Mechanisms Research Group, UD, Department of Physical Chemistry **2017**. July 1-)* Habilitation *(Institution, year): -*
	2011: English-Hungarian translator of natural science ***2006***: **PhD. degree** (Summa Cum Laude) (*Synthesis and catalytic properties of new water-soluble Ru(II)-phosphine complexes*) ***2002***:**Chemist, M. Sc. degree** ***1998***: **Chemistry-biology teacher** ***1994***: **General certification of education** *Doctorate, subject (Institution, year)* *Undergraduate degree, subject (Institution, year)*
Employment	*Position - Employer – Period* ***2016** - Associate Research Professor, MTA-DE Redox and Homogeneous Catalytic Reaction Mechanisms Research Group* ***2015** - Associate Research Professor, MTA-DE Homogeneous*

	Catalysis and Reaction Mechanisms Research Group, Debrecen ***2012 -2015*** *Scientific associate, MTA-DE Homogeneous Catalysis and Reaction Mechanisms Research Group, Debrecen* ***2008 -2011*** *Scientific associate, MTA-DE Homogeneous Catalysis Research Group, Debrecen* ***2005 -2007*** *Research assistant, MTA-DE Homogeneous Catalysis Research Group, Debrecen*
Research and development projects over the last 5 years	*Name of project or research focus:* NKFI-FK128333, *Efficient reversible chemical hydrogen storage – towards a viable practical device* *Period and any other information:* ***2018-2021*** *Partners, if applicable:* *Amount of financing:* *Name of project or research focus:* GINOP-2.3.2- 15-2016-00008, EU project: *Chemistry for better life: strategic R&D center at the University of Debrecen* *Period and any other information:* ***2016-2020*** *Partners, if applicable:* *Amount of financing:* *Name of project or research focus:* TÁMOP-4.2.2.A-11/1/KONV-2012-0043, EU project: *ENVIKUT - Basic Chemical and Biological Research for Elimination of Environmentally Hazardous Chemicals* *Period and any other information:* ***2013-2015*** *Partners, if applicable:* *Amount of financing:* *Name of project or research focus:* OTKA K101372, *Aqueous organometallic catalysis - molecular mechanisms and new applications* *Period and any other information:* ***2012-2017*** *Partners, if applicable:* *Amount of financing:*
Industry collaborations over the last 5 years	-
Patents and proprietary rights	*Title (Year)* CATALYST, HYDROGENATION OF HYDROGEN CARBONATE,

	HYDROGEN STORAGE SYSTEM – **2013** (WO 2015/040440) PROCESS FOR THE ACTIVATION OF THE C-H BOND OF ORGANIC COMPOUNDS AND A REACTIONS SYSTEM SERVING THE PROCESS – **2012** (WO 2014/006433)
Important publications over the last 5 years	*Selected recent publications from a total of approx. (give total number):* **20** *Author(s):* Péter, Pál FEHÉR, Henrietta HORVÁTH, Ferenc JOÓ, Mihály PURGEL *Title*: DFT Study on the Mechanism of Hydrogen Storage Based on the Formate-Bicarbonate Equilibrium Catalyzed by an Ir-NHC Complex: An Elusive Intramolecular C–H Activation *Any other information:* *INORGANIC CHEMISTRY.* **2018** 57**,** 5903-5914 *Author(s): Natália* MAROZSÁN, Henrietta HORVÁTH, Éva KOVÁTS, Antal UDVARDY, Anikó ERDEI, Mihály PURGEL, Ferenc JOÓ *Title*: Catalytic racemization of secondary alcohols with new (arene)Ru(II)-NHC and (arene)Ru(II)-NHC-tertiary phosphine complexes *Any other information:* *MOLECULAR CATALYSIS* **2018**, *445*, 248-256. *Author(s):* Gábor PAPP, Gábor ÖLVETI, Henrietta HORVÁTH, Ágnes KATHÓ, Ferenc JOÓ *Title:* Highly efficient dehydrogenation of formic acid in aqueous solution catalysed by an easily available water-soluble iridium(III) dihydride *Any other information:* *DALTON TRANSACTIONS* **2016***, 45,* 14516-14519 *Author(s):* Henrietta HORVÁTH, Gábor PAPP, Roland SZABOLCSI, Ágnes KATHÓ, Ferenc JOÓ *Title:* Water-Soluble Iridium-NHC-Phospine Complexes as Catalysts for Chemical Hydrogen Batteries Based on Formate *Any other information:* *CHEMSUSCHEM* **2015***, 8,* 3036-3038 *Author(s):* Henrietta HORVÁTH, Ágnes KATHÓ, Antal UDVARDY, Gábor PAPP, Dorina SZIKSZAI, Ferenc JOÓ *Title:* New water-soluble iridium(I)-N-heterocyclic carbene-

	tertiary phosphine mixed-ligand complexes as catalysts of hydrogenation and redox isomerization *Any other information:* *ORGANOMETALLICS* **2014**, *33,* 6330-6340
Activities in specialist bodies over the last 5 years	*Organisation - Role – Period* *Membership without a specific role need not be mentioned.*

Name	*István Hajdu PhD.*
Position	*Chemist,* *University of Debrecen, Faculty of Medicine,* *Medical Imaging Department,* *Division of Nuclear Medicine and Translational Imaging*
Academic career	*Chemist (University of Debrecen, 2016-)* *Postdoctoral Fellow (University of Saskatchewan, 2014-2016)* *PhD student (University of Debrecen, 2011-2014)*
	doctoral qualification: PhD (University of Debrecen, 2014) *Doctorate, subject: Preparation, and in vitro, in vivo investigation of nanoparticles as tumor specific MR contrast agents. (University of Debrecen, 2014)* *Undergraduate degree: Chemist MSc (University of Debrecen, 2008)*
Employment	*Chemist (University of Debrecen, 2016-)* *Postdoctoral Fellow (University of Saskatchewan, 2014-2016)* *Senior Researcher, Team leader of contrast agent group. Head of Biopolymer Lab and Cell Lab, Quality*

	Assurance Manager (BBS Nanotechnolgy Ltd., 2008-2014) *Research Assistant (University of Debrecen, 2011-2012)*
Research and development projects over the last 5 years	*Investigation of the pharmacokinetics and siRNA delivery properties of cyclodextrin derivatives. NKFI-6: 124634 (OTKA)* *Duration: 48 (2017-10-01 - 2021-09-30)* *Budget plan: 23 950 000 Ft* *Imaging gene delivery nanoparticles targeted to melanoma.* *Duration: 2014-2016* *Sylvia Fedoruk Centre for Nuclear Innovation (Canada)* *Total Funding - 196,650 (Canadian dollar)* *Developing a new nanotechnology-based drug formulation process for targeting targeted contrast agents and chemotherapies.* *Duration: 2012-2014* *JEREMIE - Joint European Resources for Micro to Medium Enterprises*
Industry collaborations over the last 5 years	*Project title:* *Partners:*
Patents and proprietary rights	***Cancer Cell Diagnosis by Targeting Delivery of Nanodevices*** *U. S. Patent, Patent No.: US 7,976,825 B2 Date of Patent: Jul. 12, 2011* ***Self-assembled Nanoparticles for Targeted Drug Delivery of Methotrexate.*** *U. S. Patent Application, Application Number: US 61/918,005 (Field: 12/19/2013)* ***Tumorspecific SPECT/MR and SPECT /CT contrast agent*** *U. S. Patent Application, Application Number: US*

	14/133,975 (Field: 06/28/2013) ***Tumorspecific PET/MR and PET/CT contrast agent*** *U. S. Patent Application, Application Number: US 14/133,766 (Field: 06/28/2013)* ***Self-assembled Nanoparticles for Targeted Drug Delivery of Epirubicin*** *U. S. Patent Application, Application Number: US 14/228,852 (Field: 03/28/2013)* ***Magnetic Fluid Nanosystem*** *U. S. Patent Application, Application Number: US 13/944,742 (Field: 10/9/2012)* ***Novel Targeted Paramagnetic Contrast Agent*** *U. S. Patent Application, Application Number:US 13/888,675 (Field: May. 9. 2012)* ***Polymeric nanoparticles by ion-ion Interactions*** *U. S. Patent Application, Application Number:US 12/005,643 (Field: Dec. 27. 2007)*
Important publications over the last 5 years	*Gábor Nagy, Noémi Dénes, Adrienn Kis, Judit P. Szabó, Ervin Berényi, Ildikó Garai, Péter Bai, István Hajdu, Dezső Szikra, György Trencsényi* ***Preclinical evaluation of melanocortin-1 receptor (MC1-R) specific ^{68}Ga- and ^{44}Sc-labeled DOTA-NAPamide in melanoma imaging*** *European Journal of Pharmaceutical Sciences (2017) Vol. 106, Pages 336-344* *IF: 3.756 (2016)* ***<u>Istvan Hajdu</u>***, *Deborah Michel, Mays Al-Dulaymi, Kishor M. Wasan, Humphrey Fonge, Ildiko Badea* ***A ^{89}Zr-labeled lipoplex nanosystem for image-guided gene delivery: design and initial characterization*** *Molecular Pharmaceutics Manuscript ID: mp-2016-*

	002759 *IF: 4.342 (2015)* *András Polyák, **<u>István Hajdu</u>**, Magdolna Bodnár, Gabriella Dabasi, Róbert P. Jóba, János Borbély, Lajos Balogh* ***Folate receptor targeted self-assembled chitosan-based nanoparticles for SPECT/CT imaging: demonstrating a preclinical proof of concept*** *International Journal of Pharmaceutics (**2014**) Vol. 474, Pages 91-94.* *IF: 3.650 (2014)* ***<u>István Hajdu</u>**, György Trencsényi, Magdolna Bodnár, Miklós Emri, Gáspár Bánfalvi, Judit Sikula, Teréz Márián, József Kollár, György Vámosi, János Borbély* ***Tumor-specific Localization of Self-assembled Nanoparticle PET/MR Modalities*** *Anticancer Research (**2014**) Vol. 34, Pages 49-59* *IF: 1.826 (2014)* *Magdolna Bodnár, **<u>István Hajdu</u>**, Eszter Rőthi, Nóra Harmati, Zsuzsanna Csikós, John F. Hartmann, Csaba Balogh, Béla Kelemen, János Tamás, János Borbély* ***Biopolymer-based Nanosystem for Ferric Ion Removal from Water*** *Separation and Purification Technology (**2013**) Vol. 112, Pages 26-33* *IF: 3.065 (2013)* *András Polyák, **<u>István Hajdu</u>**, Magdolna Bodnár, György Trencsényi, Zita Pöstény i, Veronika Haász, Gergely Jánoki, Győző A. Jánoki, Lajos Balogh, János Borbély* ***^{99m}Tc-labeled Nanosystem as Tumor Imaging Agent for SPECT and SPECT/CT Modalities*** *International Journal of Pharmaceutics (**2013**) Vol. 449, Pages 10-17* *IF: 3.785 (2013)*

	<u>István Hajdu</u>**, Magdolna Bodnár, György Trencsényi, Teréz Márián, György Vámosi, József Kollár, János Borbély* ***Cancer Cell Targeting and Imaging with Biopolymer – based Nanodevices *International Journal of Pharmaceutics (**2013**) Vol. 441, Pages 234-241* *IF: 3.785 (2013)*
Activities in specialist bodies over the last 5 years	*European Association of Nuclear Medicine (EANM) Member 2017-* *Hevesy György Magyar Orvostudományi Nukleáris Társaság (MONT) Member 2017-* *American Association of Pharmaceutical Scientists (AAPS) Member 2015*

Name	*Katalin Illyés Czifrák PhD*
Position	*Assistant Professor*
Academic career	
	doctoral qualification: PhD, University of Debrecen, Hungary, 2005 *Doctorate, subject: University of Debrecen, Hungary, Preparation of oligopeptides incorporating anomeric α-amino acids* *Undergraduate degree, subject: MSc in chemistry* *Qualification: chemist, 2001*
Employment	*Assistant Professor, University of Debrecen, Department of Applied Chemistry - 2015-* *Postdoctoral, University of Debrecen, Department of Applied Chemistry - 2013-2015* *Scientific Associate, University of Debrecen, Department of Organic Chemistry - 2006-2012* *Research Assistant, University of Debrecen, Department of Organic Chemistry - 2005*
Research and development projects over the last 5 years	*Name of project or research focus* participant in GINOP-2.3.2-15-2016-00041, EU project: Regional Material Science Excellence Workshop - Research Program and Infrastructure

	Period and any other information: 2016- *Partners, if applicable:* *Amount of financing:* *Name of project or research focus: participant in* TÁMOP-4.2.2.A-11/1/KONV-2012-0036, EU project: Intelligent Functional Materials: Their mechanical, thermal, electromagnetic, optical properties and their applications, *Period and any other information: 2013-2015* *Partners, if applicable:* *Amount of financing:*
Industry collaborations over the last 5 years	*Project title:* *Partners:*
Patents and proprietary rights	*Title (Year)*
Important publications over the last 5 years	*Selected recent publications from a total of approx. (give total number): 63 (journal:33 + conference publication: 30)* *Author(s):* ***Czifrák K.****; Lakatos Cs.; Karger-Kocsis, J.; Daróczi L, Zsuga, M.; Kéki, S.* *Title: One-pot synthesis and characterization of novel shape-memory poly(-caprolactone) based polyurethane-epoxy conetworks with Diels-Alder couplings* *Any other information: Polymers, 10, 504, 2018, (p:1-9), IF: 3.364 (2016)* *Author(s): Lakatos, Cs.;* ***Czifrák, K.****; Papp, R.; Karger-Kocsis, J.; Zsuga, M.; Kéki, S.* *Title: Shape Memory Crosslinked Polyurethanes Containing Thermoreversible Diels-Alder Couplings* *Any other information: J. Appl. Polym. Sci. 26,* ***2016****;133, 44145(9)* *Author(s): Lakatos, Cs.;* ***Czifrák, K.;*** *Papp, R.; Karger-Kocsis, J.; Zsuga, M.; Kéki, S.* *Title: Segmented linear shape memory polyurethanes*

	with thermoreversible Diels-Alder coupling: effects of polycaprolactone molecular weight and diisocyanate type *Any other information: Express Polym. Lett. 10(4), **2016**, 324-336.* *Author(s): Kuki, Á.; **Czifrák, K**.; Karger-Kocsis, J.; Zsuga M.; Kéki, S.* *Title: An approach to predict the shape-memory behavior of amorphous polymers from Dynamic Mechanical Analysis (DMA) data.* *Any other information: Mechanics of Time-Dependent Materials. 19, **2015**;87-93.* *IF:1.587 (2014)* *Author(s): **Czifrák, K**.; Karger-Kocsis, J.; Daróczi, L.; Zsuga, M.; Kéki, S.* *Title: Poly(-caprolactone) and Pluronic Diol Containing Segmented Polyurethanes for Shape Memory Performance* *Any other information: Macromol. Chem. Phys., 215, **2014**, 1896-1907.* *IF: 2.39 (2013)*
Activities in specialist bodies over the last 5 years	*Organisation - Role – Period* *Membership without a specific role need not be mentioned.*

Name	*Ferenc Joó*
Position	*Physical chemistry; professor*
Academic career	*Initial academic appointment : Lajos Kossuth University, Debrecen, 1972* *Habilitation: None (DSc accepted)*
	Member of the Hungarian Academy of Sciences, 2001- *Doctor of Chemical Sciences (Hungarian Academy of Sciences) 1991-* *doctoral qualification: dr. rer. nat, summa cum laude, Lajos Kossuth University, Debrecen, 1975* *Doctorate, subject: Physical chemistry, Lajos Kossuth*

	University, Debrecen, 1975 *Undergraduate degree, subject : Diplome chemist, Lajos Kossuth University, Debrecen, 1972*
Employment	*Position - Employer – Period:* *Assistant lecturer, assistant professor, associate professor, full professor: Lajos Kossuth University, Debrecen, 1972-2000* *Full professor: University of Debrecen, 2000 -*
Research and development projects over the last 5 years	*TÁMOP-4.2.2.A-11/1/KONV-2012-0043 (ENVIKUT): Basic chemical and biological research for elimination of environmentally hazardous chemicals, 2013-2015, 899.6 million HUF* *GINOP-2.3.2-15-2016-00008 (DECHEM): Chemistry for improving quality of life, 2016-2020, 1 984.0 million HUF* *OTKA K 101372: Organometallic catalysis in aqueous media – molecular mechanisms and new applications, 2011-2017, 29.983 million HUF*
Industry collaborations over the last 5 years	*Project title: -----* *Partners:*
Patents and proprietary rights	*Title (Year) -----*
Important publications over the last 5 years	*Total number of publications: 190* *Marozsán N, Horváth H, Kováts É, Udvardy A, Erdei A, Purgel M, Joó F:* *Catalytic racemization of secondary alcohols with new (arene)Ru(II)-NHC and (arene)Ru(II)-NHC-tertiary phosphine complexes* *MOLECULAR CATALYSIS 445: pp. 248-256. (2018)* *Kovacs Z, Papp G, Horvath H, Joo F, Guttman A:* *A novel carbohydrate labeling method utilizing transfer hydrogenation-mediated reductive amination.* *JOURNAL OF PHARMACEUTICAL AND BIOMEDICAL ANALYSIS 142: pp. 324-327. (2017)* *Papp G, Ölveti G, Horváth H, Kathó Á, Joó F:*

	Highly efficient dehydrogenation of formic acid in aqueous solution catalysed by an easily available water-soluble iridium(III) dihydride *DALTON TRANSACTIONS 45: pp. 14516-14519. (2016)* *Horváth H, Papp G, Szabolcsi R, Kathó Á, Joó F:* *Water-Soluble Iridium-NHC-Phospine Complexes as Catalysts for Chemical Hydrogen Batteries Based on Formate* *CHEMSUSCHEM 8:(18) pp. 3036-3038. (2015)* *Voronova K, Purgel M, Udvardy A, Bényei A Cs, Kathó Á, Joó F:* *Hydrogenation and Redox Isomerization of Allylic Alcohols Catalyzed by a New Water-Soluble Pd-Tetrahydrosalen Complex* *ORGANOMETALLICS 32:(15) pp. 4391-4401. (2013)*
Activities in specialist bodies over the last 5 years	*Organisation - Role – Period:* *Hungarian Academy of Sciences – President, Chemistry Section – 2011-2017*

Name	*István Jószai PhD*
Position	*chemist*
Academic career	*doctoral qualification: PhD, University of Debrecen, Hungary, 2008* *Doctorate, subject: Homogeneous catalytic hydrogenation of* *poorly water-soluble carbonates with transition metal complexes, 2007*
Employment	*chemist, head of QC - University of Debrecen, Department of Nuclear Medicine – 2006-* *chemist - University of Debrecen, PET Center – 2004-2006*
Important publications over the last 5 years	*Selected recent publications from a total of approx. (give total number): 20* *Author(s):* Joszai I, Papreti N, Szikra D, Miklovicz T, Mikecz P: *Title:* Radiochemical stability study of [methyl-C-11]choline by HPLC method *Any other information:*

	Publisher, place of publication, date of publication or name of periodical, volume, issue, page numbers: JOURNAL OF LABELLED COMPOUNDS & RADIOPHARMACEUTICALS 58:(1) p. S350. 1 p. (2015) *Author(s):* Lajtos I, Czernin J, Dahlbom M, Daver F, Emri M, Farshchi-Heydari S, Forgacs A, Hoh CK, Joszai I, Krizsan AK, Lantos J, Major P, Molnar J, Opposits G, Tron L, Vera DR, Balkay L: *Title:* Cold wall effect eliminating method to determine the contrast recovery coefficient for small animal PET scanners using the NEMA NU-4 image quality phantom. *Any other information:* *Publisher, place of publication, date of publication or name of periodical, volume, issue, page numbers:* PHYSICS IN MEDICINE AND BIOLOGY 59:(11) pp. 2727-2746. (2014) *Author(s):* Joszai I, Svidro M, Potari N, Mikecz P, Laszlo G: *Title:* Effective suppression of radiolytic decomposition of [F-18]FDG using hydroxyl radical scavengers *Any other information:* *Publisher, place of publication, date of publication or name of periodical, volume, issue, page numbers:* JOURNAL OF LABELLED COMPOUNDS & RADIOPHARMACEUTICALS 56:(1) p. S478. 1 p. (2013) *Author(s):* Joszai I, Hamori C, Balogh B, Potari N, Mikecz P: *Title:* Simultaneous analysis of FDG, ClDG and radiochemical components in [F-18]FDG preparation by a new NP-HPLC method *Any other information:* *Publisher, place of publication, date of publication or name of periodical, volume, issue, page numbers:* JOURNAL OF LABELLED COMPOUNDS & RADIOPHARMACEUTICALS 56:(1) p. S479. 1 p. (2013) *Author(s):* Mikecz P, Potari N, Miklovicz T, Nemeth E,

	Zakota G, Joszai I: *Title:* Investigation of the usability of SOLA AX columns for separation and concentration of F-18 isotopes *Any other information:* *Publisher, place of publication, date of publication or name of periodical, volume, issue, page numbers:* JOURNAL OF LABELLED COMPOUNDS & RADIOPHARMACEUTICALS 56:(1) p. S125. 1 p. (2013)

Name	*László Dr. Juhász Ph.D., dr. habil*
Position	*associate professor, in charge of organic chemistry of chemist, chemical engineer and bioengineer BSc*
Academic career	education leader of the Chemistry Institute (oct. of 2008. – jan. of 2013.) Habilitation *(University of Debrecen, 2015)*
	doctoral qualification: Ph.D.: (University of Debrecen, 2001) *Undergraduate degree, subject: Chemist M.Sc. (Lajos Kossuth University, 1996)*
Employment	*Research assistant, University of Debrecen; Jan. of 2000. – Aug. of 2000.* *Assistant lecturer, University of Debrecen; Sept. of 2000. -June. of. 2007.* *Assistant professor, University of Debrecen; July of 2007. – Aug.of 2015.* *Associate professor, University of Debrecen; from Sept. of 2015*
Research and development projects over the last 5 years	*Name of project or research focus: New transformations of monosaccharide derivatives at and around the anomeric centre - researcher* *Period and any other information: 08. of 2013. – 08 of 2018.* *Partners, if applicable:* *Amount of financing: 43 852 000 HUF* *Name of project or research focus: Chemistry for better life: strategic R &D center at the University of Debrecen (DECHEM; GINOP-2.3.2- 15-2016- 00008) - researcher* *Period and any other information: oct. of 2016. – sept of 2020.* *Partners, if applicable:* *Amount of financing: 1 983 995 445 HUF*

Industry collaborations over the last 5 years	*Project title: -* *Partners: -*
Patents and proprietary rights	*L. Somsák, É.,Bokor, M. Tóth, L. Juhász, K. Czifrák, B. Kónya, S. Kun, A. Páhi, B. Szőcs, G. Varga, L. Kóder, K. Nagy, P. Gergely, T. Docsa: Glikogén foszforiláz inhibitorok. P1100602/P1200475 Hungarian patent application. 2011.PCT/HU2012/000116*
Important publications over the last 5 years	*Selected recent publications from a total of approx. (give total number): 26* ***L. Lázár; L. Juhász;Gy. Batta, A. Borbás, L. Somsák; Unprecedented β-manno type thiodisaccharides with a C-glycosylic function by photoinitiated hydrothiolation of 1-C-substituted glycals, New Journal of Chemistry,*** 2017, *41*, **1284-1292** J. József, L. Juhász, T. Z. Illyés, M. Csávás, A. Borbás, L. Somsák; Photoinitiated hydrothiolation of pyranoid exo-glycals: the D-galacto and D-xylo cases, *Carbohydrate Research*, **2015**, *413*, 63-69 *J. Begum, G. Varga, T. Docsa, P. Gergely, J.M. Hayes, L. Juhász, L. Somsák; Computationally motivated synthesis and enzyme kinetic evaluation of N-(β-D-glucopyranosyl)-1,2,4-triazolecarboxamides as glycogen phosphorylase inhibitors* *MedChemComm*, **2015**, 6(1), 80-89 *L. Juhász, G. Varga, A. Sztankovics, Ferenc Béke, T. Docsa, A. Kiss-Szikszai, P. Gergely, J. Kóňa, I. Tvaroška, L. Somsák; Structure-activity relationships of glycogen phosphorylase inhibitor FR258900 and its analogues: a combined synthetic, enzyme kinetic and computational study. ChemPlusChem*, **2014**, 79(11), 1558 – 1568 *M. Polyák, G. Varga, B. Szilágyi, L. Juhász, T. Docsa, P. Gergely, J. Begum, J. M. Hayes, L. Somsák; Synthesis, enzyme kinetics and computational evaluation of N-(β-D-glucopyranosyl) oxadiazolecarboxamides as glycogen phosphorylase inhibitors; Bioorganic and Medicinal Chemistry*, **2013**, 21, 5738 – 5747.

Activities in specialist bodies over the last 5 years	*Organisation - Role – Period* *Membership without a specific role need not be mentioned.*

Name	Dr. Éva Juhász Tóth, PhD
Position	Senior lecturer
Academic career	
	Doctoral qualification: PhD in Chemistry, University of Debrecen, Hungary, 2002 Undergraduate degree, subject: MSc in Chemistry Chemist and Chemistry teacher and English-Hungarian translator Kossuth Lajos University, Debrecen, Hungary, 1998
Employment	Department of Organic Chemistry, University of Debrecen, Hungary: 2016– : Senior lecturer 2003–2016: Assistant lecturer 2001–2003: Assistant research fellow
Research and development projects over the last 5 years	*Name of project or research focus:* Grant OTKA, K75806, supported by the National Research, Development and Innovation Office of Hungary (Hungarian Scientific Research Fund): Development and application of modern amination methodologies in the field of oxygen heterocycles. (Participant) *Period and any other information: 2009-2013* *Name of project or research focus:* GINOP-2.3.2-15-2016-00008, supported by the EU co-financed by the European Regional Development Fund: Chemistry for better life: strategic R&D center at the University of Debrecen, Chemistry of carbohydrates and heterocycles subproject. (Participant) *Period and any other information: 2016-2020* *Name of project or research focus:* Grant OTKA, FK 125067, supported by the National Research, Development and Innovation Office of Hungary: New types and new biological applications of C-glycopyranosyl heterocycles. (Participant)

	Period and any other information: 2017-2021
Industry collaborations over the last 5 years	*Project title: -* *Partners: -*
Patents and proprietary rights	-
Important publications over the last 5 years	*Selected recent publications from a total of approx. (give total number): 7* *Author(s):* Anastassia L. KANTSADI, Éva BOKOR, Sándor KUN, George A. STRAVODIMOS, Demetra S.M. CHATZILEONTIADOU, Demetres D. LEONIDAS, Éva JUHÁSZ-TÓTH, Andrea SZAKÁCS, Gyula BATTA, Tibor DOCSA, Pál GERGELY, László SOMSÁK: *Title:* Synthetic, enzyme kinetic, and protein crystallographic studies of *C*-β-D-glucopyranosyl pyrroles and imidazoles reveal and explain low nanomolar inhibition of human liver glycogen phosphorylase *Any other information:* *Publisher, place of publication, date of publication or name of periodical, volume, issue, page numbers Eur. J. Med. Chem.,* **2016**, 123, 737-745. *Author(s):* Juhász-Tóth, É.; Favi, G.; Attanasi, O. A.; Bényei, A. C.; Patonay, T.; *Title:* α-Azido ketones, part 8: base-induced coupling of α-azido ketones with a 1,2-diaza-1,3-diene as a Michael acceptor *Any other information:* *Publisher, place of publication, date of publication or name of periodical, volume, issue, page numbers: Synlett* (**2014**), 25(14), 2001-2004.
Activities in specialist bodies over the last 5 years	*Organisation - Role – Period* Education organizer of the Organic Chemistry Department 2016-

Name	*Ferenc Krisztián Kálmán PhD*
Position	*Assistant professor*
Academic career	

	Doctoral qualification: PhD, University of Debrecen (UD), Hungary, 2008 *Undergraduate degree: Chemist MSc, UD, 2002*
Employment	2006-2007: Research assistant (UD, Department of Inorganic and Analytical Chemistry) 2010-2013: Postdoctor (UD, Department of Inorganic and Analytical Chemistry, PD-OTKA 83253) 2013-2014: Researcher (UD, Department of Inorganic and Analytical Chemistry) 2014-2018: Researcher (UD, Department of Inorganic and Analytical Chemistry) 2018-: Assistant professor (UD, Department of Physical Chemistry)
Research and development projects over the last 5 years	*Name of project or research focus:* OTKA 109029 *Period and any other information: 2013-2017* *Partners, if applicable: -* *Amount of financing: -* *Name of project or research focus:* OTKA 120224 *Period and any other information: 2016-2020* *Partners, if applicable: -* *Amount of financing: -* *Name of project or research focus:* TÁMOP-4.2.2.A-11/1/KONV-2012-0043 *Period and any other information: 2013-2015* *Partners, if applicable: -* *Amount of financing: -* *Name of project or research focus:* GINOP-2.3.2-15-2016-00008 *Period and any other information: 2016-2020* *Partners, if applicable: -* *Amount of financing:-*
Industry collaborations over the last 5 years	*Project title: -* *Partners: -*

Patents and proprietary rights	Botár Richárd, Garda Zoltán, Fodor Tamás, Kálmán Ferenc Krisztián, Nagy Viktória, Tircsó Gyula, Tóth Imre: Triaza-ciklononán alapú vegyületek és alkalmazásuk ligandumként Mn(II)-tartalmú MRI kontrasztanyagban: Triaza-cyclononane derivatives and their use as ligands in Mn(II)-based MRI contrast agents Patent number: HU2015000563A2 (2017) Botár Richárd, Garda Zoltán, Fodor Tamás, Kálmán Ferenc Krisztián, Nagy Viktória, Tircsó Gyula, Tóth Imre: New 3,6,9,15-tetraaza-bicyclo [9.3.1]pentadeca-1(14), 11(15), 12-triene based compounds and their application as ligands of essential metal ion based MRI and ^{52}Mn based PET contrast agents Patent number: WO2017089847A1 (2017) Botár Richárd, Garda Zoltán, Fodor Tamás, Kálmán Ferenc Krisztián, Nagy Viktória, Tircsó Gyula, Tóth Imre: New 2,11-diaza-[3.3](2,6)pyridinophane compounds and their application as ligands of essential metal ion based MRI contrast agents and ^{52}Mn based PET contrast agents Patent number: WO2017089848A1 (2017) Botár Richárd, Garda Zoltán, Fodor Tamás, Kálmán Ferenc Krisztián, Nagy Viktória, Tircsó Gyula, Tóth Imre: New 6-oxa-3,9,15-triaza-bicyclo[9.3.1]pentadeca-1(14),11(15),12-triene derivatives based compounds and their application as ligands of essential metal ion based MRI and ^{52}Mn based PET contrast agents Patent number: WO2017089849A1 (2017) Baranyai Zsolt, Garda Zoltán, Kálmán Ferenc Krisztián, Krusper László, Tircsó Gyula, Tóth Imre, Ghiani Simona, Maiocchi Alessandro: Ethylenediaminetetraacetic acid bis(amide) derivatives and their respective complexes with Mn(II) ion for use as MRI contrast agent Patent number: WO2016135234 (2016)
Important publications over the last 5 years	*Selected recent publications from a total of approx. (give total number): 30* *Author(s):* Ferenc Krisztián Kálmán, Andrea Végh, Martín Regueiro-Figueroa, Éva Jakab Tóth, Carlos

	Platas-Iglesias, and Gyula Tircsó *Title:* H_4octapa: Highly Stable Complexation of Lanthanide(III) Ions and Copper(II) *Publisher, place of publication, date of publication or name of periodical, volume, issue, page numbers: Inorg. Chem., 2015, 54(5), 2345–2356.* *Author(s):* Edit Farkas, Tamás Fodor, Ferenc K. Kálmán, Gyula Tircsó and Imre Tóth *Title:* Equilibrium and Dissociation Kinetics of [Al(1,4,7-triazacyclononane-1,4,7-triacetate)] ([Al(NOTA)]) Complex *Publisher, place of publication, date of publication or name of periodical, volume, issue, page numbers: Reaction Kinetics, Mechanisms and Catalysis, 2015, 116(1), 19-33.* *Author(s):* Zoltán Garda, Attila Forgács, Quyen N. Do, Ferenc K. Kálmán, Sarolta Timári, Imre Tóth, Zsolt Baranyai, Lorenzo Tei, Zoltán Kovács and Gyula Tircsó *Title:* Physico-chemical properties of Mn^{2+} complexes formed with cis- and trans-DO2A: thermodynamic, electrochemical and kinetic studies *Publisher, place of publication, date of publication or name of periodical, volume, issue, page numbers:* J. Inorg. Biochem., 2016, 163, 206–213. *Author(s):* Christian Vanasschen, Enikő Molnár, Gyula Tircsó, Ferenc K. Kálmán, Éva Tóth, Marie Brandt, Heinz H. Coenen, and Bernd Neumaier *Title:* Novel CDTA-based, Bifunctional Chelators for Stable and Inert Mn^{II} Complexation: Synthesis and Physicochemical Characterization *Publisher, place of publication, date of publication or name of periodical, volume, issue, page numbers:* Inorg. Chem., 2017, 56(14), 7746–7760. *Author(s):* Gyula Tircsó, Zsolt Baranyai, Ferenc Krisztián Kálmán, Zoltán Kovács, Ernő Brücher and Imre Tóth *Title:* Stability of metal complexes, chapter 1.3 in

	Contrast Agents for MRI: Physical Methods Lability of metal complexes, chapter 1.4 in Contrast Agents for MRI: Physical Methods *Publisher, place of publication, date of publication or name of periodical, volume, issue, page numbers:* Eds Valerie C. Pierre and Matthew J. Allen RSC publishing, UK, 2018, pp. 40-74.
Activities in specialist bodies over the last 5 years	*Organisation - Role – Period* *Membership without a specific role need not be mentioned.*

Name	József Kalmár, Ph.D.
Position	Assistant Professor, Department of Inorganic and Analytical Chemistry
Academic career	from 2016: assistant professor, Department of Inorganic and Analytical Chemistry, University of Debrecen, Hungary 2014 – 2016: research fellow, MTA-DE Homogeneous Catalysis and Reaction Mechanisms Research Group, University of Debrecen, Hungary 2010 – 2011: junior research fellow, Department of Chemistry and Biochemistry, University of Oklahoma, USA 2009 – 2012: graduate student, Doctoral School of Chemistry, University of Debrecen, Hungary
Employment	2012 – 2014: R&D Chemist, Active Pharmaceutical Ingredients R&D, TEVA Pharmaceutical Works, Hungary
Research and development projects over the last 5 years	*Project:* Principal Investigator in “Structure and Application of Micro- and Mesoporous Materials” National Research, Development and Innovation Fund of Hungary – FK-17_124571 *Period:* 2017 – 2021 *Amount of financing:* 84 100 EUR *Project:* Principal Investigator in “Functionalized and Hybrid Aerogels as Heterogeneous Catalysts” University of Debrecen Research Fund

<table>
<tr><td></td><td>Period: 2015 – 2016
Amount of financing: 20 200 EUR

Project: Project Leader in “Chemistry for Better Life: Strategic R&D Center at the University of Debrecen (DECHEM)” GINOP-2.3.2- 15-2016- 00008
Period: 2016 – 2020
Amount of financing: 6 104 600 EUR</td></tr>
<tr><td>Industry collaborations over the last 5 years</td><td>Project: “Decomposition of OCl^- into ClO_3^-.”
Partners: AkzoNobel N.V.</td></tr>
<tr><td>Important publications over the last 5 years</td><td>Total number of international publications: 22
Total impact factor of publications: 81.43
Total number of independent citations: 158
<table>
<tr><td>1</td><td>Péter Veres, Dániel Sebők, Imre Dékány, Pavel Gurikov, Irina Smirnova, István Fábián, <u>József Kalmár*</u>
A redox strategy to tailor the release properties of Fe(III)-alginate aerogels for oral drug delivery
CARBOHYDRATE POLYMERS 188: pp. 159-167. (2018)</td></tr>
<tr><td>2</td><td><u>József Kalmár</u>, Mária Szabó, Nina Simic, István Fábián*
Kinetics and mechanism of the chromium(VI) catalyzed decomposition of hypochlorous acid at elevated temperature and high ionic strength
DALTON TRANSACTIONS 47: DOI: 10.1039/C8DT00120K. (2018)</td></tr>
<tr><td>3</td><td>Péter Veres, Gábor Király, Gábor Nagy, István Lázár, István Fábián, <u>József Kalmár*</u>
Biocompatible silica-gelatin hybrid aerogels covalently labeled with fluorescein
JOURNAL OF NON-CRYSTALLINE SOLIDS 473: pp. 17-25. (2017)</td></tr>
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		4	Péter Veres, Mónika Kéri, István Bányai, István Lázár, István Fábián, Concepción Domingo, József Kalmár* *Mechanism of drug release from silica - gelatin aerogel – Relationship between matrix structure and release kinetics* **COLLOIDS AND SURFACES B: BIOINTERFACES** 152: pp. 229-237. (2017)
		5	József Kalmár*, Gábor Lente, István Fábián *Kinetics and mechanism of the adsorption of methylene blue from aqueous solution on the surface of a quartz cuvette by on-line UV-Vis spectrophotometry* **DYES AND PIGMENTS** 127: pp. 170-178. (2016)
		6	József Kalmár*, Mónika Kéri, Zsolt Erdei, István Bányai, István Lázár, Gábor Lente, István Fábián *The Pore Network and the Adsorption Characteristics of Mesoporous Silica Aerogel: Adsorption Kinetics on a Timescale of Seconds* **RSC ADVANCES** 5:(130) pp. 107237-107246. (2015)
		7	István Lázár, József Kalmár*, Anca Peter, Anett Szilágyi, Enikő Győri, Tamás Ditrói, István Fábián *Photocatalytic performance of highly amorphous titania–silica aerogels with mesopores: The adverse effect of the in situ adsorption of some organic substrates during photodegradation* **APPLIED SURFACE SCIENCE** 356: pp. 521-531. (2015)
		8	József Kalmár*, Gábor Lente, István Fábián *Detailed kinetics and mechanism of the oxidation of thiocyanate ion (SCN–) by peroxomonosulfate ion (HSO5–). Formation and subsequent oxidation of hypothiocyanite ion (OSCN–).* **INORGANIC CHEMISTRY** 52:(4) pp. 2150-2156. (2013)
		9	József Kalmár, Shawna B Ellis, Michael T Ashby, Ronald R Halterman* *Kinetics of Formation of the Host-Guest Complex of a Viologen with Cucurbit[7]uril* **ORGANIC LETTERS** 14:(13) pp. 3248-3251. (2012)

		10	József Kalmár, Kelemu L Woldegiorgis, Bernadett Biri, Michael T Ashby* *Mechanism of Decomposition of the Human Defense Factor Hypothiocyanite Near Physiological pH* **JOURNAL OF THE AMERICAN CHEMICAL SOCIETY** 133:(49) pp. 19911-19921. (2011)

Name	*Prof. Sándor Kéki, PhD, DSc*
Position	*Full Professor, in charge of Chemical Engineering BSc and MSc*
Academic career	*Head of Department (University ofDebrecen Department of Applied Chemistry, 2010-)* *DSc, Hungarian Academy of Sciences (2008)* *Habilitation (University of Debrecen, 2004)*
	Doctoral qualification: PhD, Kossuth Lajos University, Hungary, 1996 *Doctorate, subject:Oscillation reactions* *Undergraduate degree, subject: Chemistry MSc, Kossuth Lajos University, Hungary, 1989*
Employment	*Full Professor, University of Debrecen, Department of Applied Chemistry (2010-)* *Associate Professor, University of Debrecen, Department of Applied Chemistry (2004-2010)* *Assistant Professor, University of Debrecen, Department of Applied Chemistry (1998-2004)* *Research assistant, Kossuth Lajos University, Department of Applied Chemistry (1994-1998)* *Research assistant, Kossuth Lajos University, Department of Physical Chemistry (1992-1994)* *TMB fellow, Kossuth Lajos University, Department of Physical Chemistry (1989-1992)*
Research and development projects over the last 5 years	*Name of projects:* participant in EFOP-3.6.1-16-2016-00022, EU project: Debrecen Venture Catapult Program *Period: 2017-* group leader in GINOP-2.3.2-15-2016-00041, EU project: Regional Material Science Excellence Workshop - Research Program and Infrastructure

	Period: 2016- project leader in NKFI K-116465, Hungarian project: Synthesis and characterization of smart fluorescent polymers *Period: 2016-* project leader in NKFI K-101850, Hungarian project: Mass spectrometry of non-polar polymers *Period: 2012-2016* project leaderin TÁMOP-4.2.2.A-11/1/KONV-2012-0036, EU project: Intelligent Functional Materials: Their mechanical, thermal, electromagnetic, optical properties and their applications, *Period: 2013-2015*
Industry collaborations over the last 5 years	*Project title: Characterization of low molecular weight pharmaceuticals* *Partner: Teva Pharmaceutical Works Ltd.* *Project title: Characterization of polymers* *Partner: MOL Petrochemicals* *Project title: Characterization of isocyanates* *Partner: BorsodChem* *Project title: Investigation and characterization of polyisobutylenes* *Partner: Infineum Ltd.*
Patents and proprietary rights	*Dynamic star polymers and a method for the synthesis thereof (2000)*
Important publications over the last 5 years	*Selected recent publications from a total of approx. (give total number): 154* *Authors:* Miklós Nagy, Dávid Rácz, Zsolt László Nagy, Péter Pál Fehér, József Kalmár, István Fábián, Alexandra Kiss, Miklós Zsuga, Sándor Kéki *Title:* Solvatochromic isocyanonaphthalene dyes as ligands for silver (I) complexes, their applicability in silver (I) detection and background reduction in biolabelling *Publisher, place of publication, date of publication or*

	name of periodical, volume, issue, page numbers: SENSORS AND ACTUATORS B: CHEMICAL, **255**, 2555-2567 (2018) *Authors:* Nagy T, Kuki A, Zsuga M, Keki S *Title:* Mass-Remainder Analysis (MARA): a New Data Mining Tool for Copolymer Characterization *Publisher, place of publication, date of publication or name of periodical, volume, issue, page numbers:* ANALYTICAL CHEMISTRY, **90,** 3892-3897 (2018) *Authors:* Borbála Antal, Ákos Kuki, Lajos Nagy, Tibor Nagy, Miklós Zsuga, Sándor Kéki *Title:* Rapid detection of hazardous chemicals in textiles by direct analysis in real time mass spectrometry (DART-MS) *Publisher, place of publication, date of publication or name of periodical, volume, issue, page numbers:* ANALYTICAL AND BIOANALYTICAL CHEMISTRY, **408**, 5189-5198 (2016) *Authors:* Lajos Nagy, Ákos Kuki, György Deák, Mihály Purgel, Ádam Vékony, Miklós Zsuga, Sándor Kéki *Title:* Gas-Phase Interaction of Anions with Polyisobutylenes: Collision Induced Dissociation Study and Quantum Chemical Modeling *Publisher, place of publication, date of publication or name of periodical, volume, issue, page numbers:* JOURNAL OF PHYSICAL CHEMISTRY B, **120**, 9195-9203 (2016) *Authors:* Katalin Czifrák, Csilla Lakatos, József Karger-Kocsis, Lajos Daróczi,Miklós Zsuga,Sándor Kéki *Title:* One-Pot Synthesis and Characterization of Novel Shape-Memory Poly(ε-Caprolactone) Based Polyurethane-Epoxy Co-networks with Diels–Alder Couplings *Publisher, place of publication, date of publication or name of periodical, volume, issue, page numbers:* POLYMERS, **10**, 504 (2018)

Activities in specialist bodies over the last 5 years	Hungarian Academy of Sciences, Member of the Committee of Inorganic Chemistry and Materials Science (2011-) Hungarian Academy of Sciences, Chairman of the Regional Committee of Polymer Chemistry (2005-) Faculty of Chemical and Biochemical Engineering, Budapest University of Technology and Economics, Member of the Doctoral and Habilitation Committee (2006-) University of Debrecen, Leader of the Macromolecular and Surface Chemistry program of the Chemistry Doctoral School, (2011-) University of Debrecen, Supervisor of the Chemical Engineering BSc major (2010-)

Name	*János Kerékgyártó, PhD, CSc*
Position	*Senior research fellow, in charge of Biology BSc*
Academic career	*CSc, Hungarian Academy of Sciences, Budapest, 1994*
	Doctoral qualification: PhD, University of Debrecen, 1994 *Doctorate, subject: „Chemical synthesis of biologically active oligosaccharides”, 1994* *Undergraduate degree, subject: Chemistry MSc, Debrecen, 1981*
Employment	*Senior research fellow, Department of Botany, Faculty of Sciences and Technology, University of Debrecen, 2009-present* *Senior research fellow, Institute of Biochemistry, Faculty of Sciences and Technology, University of Debrecen, 2000-2009* *Senior research fellow, Institute of Biochemistry, Faculty of Sciences, Lajos Kossuth University, Debrecen, 1995-2000* *Postdoctoral fellow, Bijvoet Center, Department of Bio-Organic Chemistry, Utrecht University, Utrecht, The Netherlands, 1995* *Scientific fellow, Institute of Biochemistry , Faculty of Sciences, Lajos Kossuth University, Debrecen, 1988-1994*

	Post Graduate Scholarship Student of the Hungarian Academy of Sciences, Institute of Biochemistry, Faculty of Sciences, Lajos Kossuth University, Debrecen, 1985-1988 *Young investigator, Bijvoet Center, Department of Bio-Organic Chemistry, Utrecht University, Utrecht, The Netherlands, 1986-1987* *Junior research assistant, Institute of Biochemistry, Faculty of Sciences, Lajos Kossuth University, Debrecen, 1981-1984*
Research and development projects over the last 5 years	*Name of project or research focus: Functional glycomics* *Period and any other information: 2012-present* *Partners, if applicable:* *MTA-PE Translational Glycomics Group, MUKKI, University of Pannonia, Veszprém, Hungary* *Horváth Laboratory of Bioseparation Sciences, University of Debrecen, Hungary*
Industry collaborations over the last 5 years	*Partners: GlycOptim Ltd., Debrecen, 2018* *Cyclolab Ltd., Budapest, 2016-2017*
Patents and proprietary rights	*„Procedure for the synthesis of glycosides of aromatic amines"* *Hungarian patent: HU 203 896 (1988)* *„Procedure for the synthesis of amino-benzoicacid-N-glycoside derivatives"* *Hungarian patent: HU 208 146 (1989)*
Important publications over the last 5 years	*Selected recent publications from a total of 37:* *1. L. Kalmár, Z. Szurmai, J. Kerékgyártó, A. Guttman, M. Bojstrup, K. Ágoston* *Phenyl-2-O-acetyl-3-O-allyl-4-O-benzyl-1-thio-β-D-glucopyranoside, a versatile, orthogonally protected building block* *Carbohydr. Chem. Proven Methods, 24, (2015) 187-192.*

	2. K. Ágoston, Gy. Gyémánt, L. Kalmár, J. Kerékgyártó, Z. Szurmai, B. Döncző, A. Guttman *Synthesis and MALDI-TOF analysis of protected oligosaccharide components of N-glycoproteins* *J. Carbohydr. Chem., 33, (2014) 326-343* *3. B. Döncző, J. Kerékgyártó, Z. Szurmai, A. Guttman* *Glycan microarrays: new angels and strategies* *Analyst, 139, (2014) 2650-2657* *4. B. Döncző, L. Kalmár, J. Kerékgyártó, Z. Szurmai, A. Guttman* *Combinatorial glycomics 1: Synthesis options* *Chem. Listy 107, s352-s354 (2013)* *5. M. Kerékgyártó, A. Fekete, Z. Szurmai, J. Kerékgyártó, L. Takács, I. Kurucz, A. Guttman* *Neoglycoproteins as carbohydrate antigens: synthesis, analysis, and polyclonal antiboday response* *Electrophoresis, 34, (2013) 2379-2386*
Activities in specialist bodies over the last 5 years	*Head of the Asklepios Scientific Foundation, 1995-2017*

Name	*Mónika Kéri*
Position	*Colloid and environmental chemistry* *Assistant professor*
Academic career	*Assistant lecturer (University of Debrecen, UD, 2013)*
	PhD in chemistry (UD, 2015), The behavior of PAMAM dendrimers in aqueous solution and their interaction with small molecules *Environmental scientist with specification in chemistry and English-Hungarian special translator (UD, 2008)*
Employment	*Assistant lecturer and assistant professor - UD, Department of Physical Chemistry – 2013-present* *Environmental Scientist - DTMP (Debreceni Tudományos Műszaki Park) Kht. and Aquaprofit Zrt. - 2008-2009*
Research and development projects over the last 5 years	*-Structures and applications of micro- and mesoporous materials, 2017-21, NKFI 124571, 27.3 M HUF* *- Preparation and physical chemistry of doped carbon*

	nanoparticles, 2013-18, NKFI 109558, 27.9 M HUF *- NMR study of porous materials of environmental importance, 2013-2014, Jedlik Ányos Fellowship, 2.4 M HUF* *- Study of porous adsorbents with NMR cryoporometry, relaxometry and diffusiometry, 2013, ENVIKUT project TÁMOP-4.2.2.A-11/1/KONV-2012-0043* *- The interaction of functionalized dendrimers with metal ions and small molecules, 2011-2013, Chinese-Hungarian Science and Technology Program, TÉT_10-1-2011-0145* *- Vanadium-dendrimer catalysts for the oxidation of trichloroethylene (TCE), 2010-2011, CHEMIKUT project TÁMOP-4.2.2.-08/1-2008-0012*
Industry collaborations over the last 5 years	*- Elimination method for arsenic sludge from drinking water treatment, Aquaprofit Zrt.* *- Structure study of colloidal drug carriers by NMR, Nangenex Inc.*
Patents and proprietary rights	*Elimination method for arsenic sludge from drinking water treatment (2015)*
Important publications over the last 5 years	*Selected recent publications from a total of approx.: 8* *– Kéri M, Nagy Z et.al. Beware of phosphate: evidence of dendrimer—phosphate interactions* *Phys. Chem. Chem. Phys. 19: pp. 11540-11548 (2017)* *– Veres P, Kéri M, et. al.* *Mechanism of drug release from silica - gelatin aerogel – Relationship between matrix structure and release kinetics* *Colloids And Surfaces B : Biointerfaces 152: pp. 229-237. (2017)* *–Kalmár J, Kéri M, et.al. The Pore Network and the Adsorption Characteristics of Mesoporous Silica Aerogel: Adsorption Kinetics on a Timescale of Seconds* *RSC Advances 5:(130) pp. 107237-107246. (2015)* *–Kéri M , Peng C , Shi X , Bányai I.* *NMR characterization of PAMAM-G5.NH2 entrapped atomic and molecular assemblies* *Journal of Physical Chemistry B 119:(7) pp. 3312-3319.(2015)*

	–Bányai I , Kéri M , Nagy Z , Berka M , Balogh LP *Self-diffusion of water and poly(amidoamine) dendrimers in dilute aqueous solutions* *Soft Matter 9:(5) pp. 1645-1655. (2013)*
Activities in specialist bodies over the last 5 years	-

Name	*István Kertész PhD*
Position	*College Professor, in charge of Mechanical Engineering BSc*
Academic career	*Research fellow (2004-2018) Medical Imaging Department* *Division of Nuclear Medicine and Translational Imaging* *Faculty of Medicine, University of Debrecen*
	Szent-Györgyi Albert Medical University, Szeged (1997-2000) *PhD.* *József Attila University, Faculty of Science, Szeged (1991-1993) Chemistry Teacher* *József Attila University, Faculty of Science, Szeged (1985-1990) Chemist MSc*
Employment	*Postdoc (2016-2017)* *University of Antwerp, MICA, Antwerp, Belgium* *Research Fellow(2004-to date)* *University of Debrecen,Debrecen* *Head of the radiochemical laboratory (part time) (2011-2013)* *Scanomed Ltd., Debrecen* *Postdoc (2002-2004)* *University of Antwerp, Dep. of Medicinal Chemistry, Antwerp, Belgium* *Project leader (2001-2002)* *Institute of Isotopes Co. Radiopharmaceutical Business*

	Line, Budapest *PhD. student/research assistant(1995-2001)* *Biological Research Centre of the Hungarian Academy of Sciences, Dep. of Biochemistry, Szeged* *Research assistant(1993-1995)* *University of Szeged, Dep. of Colloid Chemistry, Szeged* *Chemistry teacher (1993-1993)* *Primary school of Csikéria, Csikéria* *Quality controller (1990-1993)* *Cannery of Szeged, Szeged*
Research and development projects over the last 5 years	*Hungarian Scientific Research Fund (2010-2014)* *Luteinizing hormone-releasing hormone receptors as potential molecular targets for cancer visualization by positron emission tomography* *Hungarian Scientific Research Fund (2012-2016)* *Development of anticancer drug-peptide bioconjugates for combination targeted cancer chemotherapy* *National Research, Development and Innovation Office (2016-2020)* *Development of bioconjugates for targeted tumor therapy of cancer types leading to high mortality*
Industry collaborations over the last 5 years	*Project title: Partners:*
Patents and proprietary rights	*Title (Year)*
Important publications over the last 5 years	*Number of articles and impacts: 21/46,432* *Cited (Based on Google Scholar): 460* *Hirsch-index: 10* Kertész, I., Vida, A., Nagy, G., Emri, M., Farkas, A., Kis, A., Angyal, J., Dénes, N., Péli-Szabó, J., Kovács, T., Bai, P., Trencsényi, G.: In Vivo Imaging of Experimental Melanoma Tumors Using The Novel Radiotracer 68Ga-NODAGA-Procainamide (PCA). J. Cancer 8 (5), 774-785., 2017. Trencsényi, G., Dénes, N., Nagy, G., Kis, A., Vida, A.,

	Farkas, F., Péli-Szabó, J., Kovács, T., Berényi, E., Garai, I., Bai, P., Hunyadi, J., Kertész, I.: Comparative preclinical evaluation of 68Ga-NODAGA and 68Ga-HBED-CC conjugated procainamide in melanoma imaging. J. Pharmaceut. Biomed. Anal 139 54-64., 2017. Simecek, J., Máté, G., Szikra, D., Szilágyi, S., Trencsényi, G., Wester, H., Kertész, I., Galuska, L.: Multiparametric labeling optimization and synthesis of 68Ga-labeled compounds applying a continuous-flow microfluidic methodology. Journal of Flow Chemistry 6 (2), 86-93., 2016. Máté, G., Kertész, I., Enyedi, K., Mező, G., Angyal, J., Vasas, N., Kis, A., Szabó, É., Emri, M., Bíró, T., Galuska, L., Trencsényi, G.: In vivo imaging of Aminopeptidase N (CD13) receptors in experimental renal tumors using the novel radiotracer 68Ga-NOTA-c(NGR). Eur. J. Pharm. Sci 69 61-71., 2015. Simecek, J., Máté, G., Pniok, M., Kertész, I., Notni, J., Wester, H., Galuska, L., Hermann, P.: The Influence of the Combination of Carboxylate and Phosphinate Pendant Arms in 1,4,7-Triazacyclononane-Based Chelators on Their 68Ga Labelling Properties. Molecules 20 (7), 13112-13126., 2015.
Activities in specialist bodies over the last 5 years	*Organisation - Role – Period* *Membership without a specific role need not be mentioned.*

Name	*Attila Kiss PhD*
Position	*Assistant Professor*
Academic career	*Laboratory Manager (University of Debrecen, 2008)* Habilitation *(University of Debrecen, 2018)*
	doctoral qualification: PhD (University of Debrecen, 2005) *Undergraduate degree, Chemistry (University of Debrecen, 1999)*
Employment	*Assistant Professor - University of Debrecen – 2011-* *Research fellow - University of Debrecen – 2009-2011* *Analytical research scientist – Teva Pharmaceuticals Ltd.-2008-2009*

	Postdoctoral research Fellow - University of North Texas Health Science Center, Forth Worth, Texas – 2006-2007
Research and development projects over the last 5 years	*Name of project or research focus: (GINOP-2.3.2-15-2016-00008, DECHEM) supported by the EU and co-financed by the* *European Regional Development Fund.* *Period and any other information: 2016-2020* *Partners, if applicable:* *Amount of financing:*
Industry collaborations over the last 5 years	*Project title: Analytical Development and sample measurment projects in varied fields* *Partners: Teva Pharmaceuticals Ltd, Debrecen; KisChemicals Ltd, Sajóbábony; Coloplast Ltd, Nyírbátor; Korax Ltd, Leányvár; Robert Bosch Elektronika Ltd, Hatvan*
Patents and proprietary rights	*The use of compounds showing heat shock protein (hsp) co-inducing properties to enhance the insulin sensitizing effect in the treatment of type 2 diabetes (2015)*
Important publications over the last 5 years	*Selected recent publications from a total of 40:* *Dócs K, Mészár Z, Gonda S, Kiss-Szikszai A, Holló K, Antal M, Hegyi Z* *The Ratio of 2-AG to Its Isomer 1-AG as an Intrinsic Fine Tuning Mechanism of CB1 Receptor Activation* *FRONTIERS IN CELLULAR NEUROSCIENCE 11:(Art 39) pp. 1-13. (2017)* *Sándor Gonda, Attila Kiss-Szikszai, Zsolt Szűcs, Borbála Balla, Gábor Vasas* *Efficient biotransformation of non-steroid anti-inflammatory drugs by endophytic and epiphytic fungi from dried leaves of a medicinal plant, Plantago lanceolata L.* *INTERNATIONAL BIODETERIORATION & BIODEGRADATION 108: pp. 115-121. (2016)* *Krisztina Kónya, Dávid Pajtás, Attila Kiss-Szikszai, Tamás Patonay*

	Buchwald–Hartwig Reactions of Monohaloflavones *EUROPEAN JOURNAL OF ORGANIC CHEMISTRY 2015:(4) pp. 828-839. (2015)* *Szőcs Béla, Bokor Éva, Szabó Katalin E, Kiss-Szikszai Attila, Tóth Marietta, Somsák László* *Synthesis of 5-aryl-3-C-glycosyl- and unsymmetrical 3,5-diaryl-1,2,4-triazoles from alkylidene-amidrazones* *RSC ADVANCES 5:(54) pp. 43620-43629. (2015)* *Juhász L, Varga G, Sztankovics A, Béke F, Docsa T, Kiss-Szikszai A, Gergely P, Kona J, Tvaroska I, Somsák L* *Structure-activity relationships of glycogen phosphorylase inhibitor FR258900 and its analogues: a combined synthetic, enzyme kinetics, and computational study* *CHEMPLUSCHEM 79:(11) pp. 1558-1568. (2014)*
Activities in specialist bodies over the last 5 years	*Hungarian Chemical Society - Head of Hajdú-Bihar County Division – 2015-*

Name	Ákos Kuki
Position	associate professor
Academic career	college assistant lecturer, Teachers' Training College Nyíregyháza, 1992 Habilitation: University of Debrecen, 2015
	PhD, Material Sciences, University of Miskolc, 2002 MSc. (electrical engineer, Technical University of Budapest, 1991), MSc (teacher of electrical engineering, Technical University of Budapest, 1994)
Employment	college assistant lecturer, Teachers' Training College Nyíregyháza, 1992-1996 college senior lecturer, Teachers' Training College Nyíregyháza, 1996-2002 college associate professor, Teachers' Training College Nyíregyháza, 2002-2008 college associate professor, University of Debrecen, 2008-2016

	associate professor, University of Debrecen, 2016-
Research and development projects over the last 5 years	OTKA K116465, OTKA K101850, OTKA K109006, TÁMOP-4.2.2.A-11/1/KONV-2012-0036, Smart functional materials, 2012-2015 GINOP-2.3.2-15-2016-00041, Regional Workshop for Excellence in Materials Science, 2017-2020 EFOP-3.6.1-16-2016-00022, Debrecen Venture Catapult Program, 2018-
Industry collaborations over the last 5 years	
Patents and proprietaryrights	
Important publications over the last 5 years	*Selected recent publications from a total of approx. 40:* [1] Nagy L, Nagy L, Deák Gy, Kuki Á, Purgel M, Narmandakh M, Iván B, Zsuga M, Kéki S, Can non-polar polyisobutylenes be measured by electrospray ionization mass spectrometry? Anion-attachment proved to be an appropriate method, *J. Am. Soc. Mass Spectrom.,* **2016**, *27*, 432. [2] Nagy, L; Kuki, A; Deak, G; Purgel, M; Vekony, A; Zsuga, M; Keki, S, Gas-Phase Interaction of Anions with Polyisobutylenes: Collision-Induced Dissociation Study and Quantum Chemical Modeling, *J. Phys. Chem. B*, **2016**, *120*, 9195. [3] Antal, B; Kuki, A; Nagy, L; Nagy, T; Zsuga, M; Keki, S, Rapid detection of hazardous chemicals in textiles by direct analysis in real-time mass spectrometry (DART-MS), *Anal. Bioanal. Chem.*, **2016**, *408*, 5189. [4] Kuki, A; Nagy, L; Nagy, T; Zsuga, M; Keki, S., Screening of additives and other chemicals in polyurethanes by direct analysis in real time mass spectrometry (DART-MS), *Anal. Bioanal. Chem.*, **2017**, *409*, 6149-6162. [5] Nagy, T; Kuki, A; Zsuga, M; Keki, S, Mass-Remainder Analysis (MARA): a New Data Mining Tool for Copolymer Characterization, *Anal. Chem.*, **2018**, 90, 3892-3897.
Activities in specialist bodies over the last 5years	Member of the Committee of Physical Chemistry of the Hungarian Academy of Sciences

Name	*Tibor Kurtán*
Position	*professor of chemistry, in charge of chemistry M.Sc. (synthetic chemistry major), vice-head of Department of Organic Chemistry*
Academic career	*DSc (Chemistry) 2014* *Habilitation (UD) 2010*
	Ph.D (chemistry, UD) 2001 *M.Sc. in Chemistry and specialized English translator (UD, 1996)*
Employment	*full professor, UD, 2016-* *associate professor, UD, 2011-2016* *assistant professor, UD, 2006-2010* *assistant lecturer, UD, 2001-2006*
Research and development projects over the last 5 years	1) application identifier: GINOP-2.3.2-15-2016-00008 Title: Chemistry for improving living conditions: fundamental R&D center at the University of Debrecen status: running project, participant Applied financial support: 1 983 995 445 HUF Time frame: 2016.10.01-2020.09.30. 2) application identifier: GINOP-2.3.3-15-2016-00004 Title: Integrated instrumental infrastructure for the research of molecular science and pharmacology (I2M2) status: running project, participant Applied financial support: 810 015 130 HUF Time frame: 2016.07.01-2020.06.30. 3) application identifier: K120181 Title: Stereochemistry and stereoselective synthesis of bioactive heterocycles status: running project, principle investigator financial support: 31 680 000 HUF Time frame: 2016 .10.01-2020 .09.30.
Industry collaborations over the last 5 years	*Project title: N/A* *Partners: N/A*
Patents and proprietary rights	*Title (Year) N/A*
Important publications over the last 5 years	1) Ling-Hong Meng, Chen-Yin Wang, Attila Mándi, Xiao-Ming Li, Xue-Yi Hu, Matthias U Kassack, Tibor Kurtán, Bin-Gui Wang; ORG LETT 18: (20) 5304-5307, 2016

	2) Attila Mándi, I Wayan Mudianta, Tibor Kurtán, Mary J Garson: J NAT PROD 78: (8) 2051-2056, 2015 3) Zhang P, Meng LH, Mandi A, Li XM, Kurtan T, Wang BG: RSC ADV 5: (62) 49904, 2015 4) Peng Zhang, Attila Mándi, Xiao-Ming Li, Feng-Yu Du, Jia-Ning Wang, Xin Li, Tibor Kurtán, Bin-Gui Wang: ORG LETT 16: (18) 4834-4837, 2014 5) Liang LF, Kurtan T, Mandi A, Yao LG, Li J, Zhang W, Guo YW: ORG LETT 15: (2) 274-277, 2013 160 scientific SCI publications and 2 book chapters with *ca* 1900 citations, Hirsch index: 30
Activities in specialist bodies over the last 5 years	-HAS Working Committee for Alkaloid and Flavonoid Chemistry, secretary, (2012-) -HAS Working commettee for Heterocyclic Chemistry (2012-) -Hungarian Chemical Society, member, (2007-) -HAS, Organic and Biomolecular Chemistry Committee (2015) -Chirality journal, editorial board member (2016-) -HAS, Chemical Science Board, non-academician member (2016-)

Name	István Lázár, PhD
Position	Associate Professorof Chemistr, Department of Inorganic and Analytical Chemistry
Academic career	
	Candidate of Science (C.Sc.) degree: 1994, Hungarian Academy of Scienc, Coordination Chemistry Doctorate, subject: Kossuth Lajos University, 1987, Boron organic chemistry Undergraduate degree, subject: Chemist, MSc, 1984
Employment	PhD scholarship: Hungarian Academy of Science, 1984-1987 Assistant lecturer – Associate professor from 1987 to present: University of Debrecen (formerly Kossuth Lajos University) Research Associate, 1989-1991, 26 months; 1994, 5 months, – The University of Texas at Dallas, US
Research and development	Role: researcher

projects over the last 5 years	Name of project or research focus: TÁMOP-4.2.2.A-11/1/KONV-2012-0036; Intelligent Functional Materials: Mechanical, thermal, electromagnetic and optical properties and applications Period and any other information: 2012-2016 Role: researcher GINOP-2.2.1-15-2017-00068, Gel-based biomatrices for human tissue replacements, and the development of their production technologies Period and any other information: 2017-2021 Role: researcher GINOP-2.3.2-15-2016-00041, Regionális Anyagtudományi Kiválósági Műhely - Kutatási Program és Infrastruktúra Period and any other information: 2017-2021
Industry collaborations over the last 5 years	L'Oréal Co.,France: Material Transfer, and Evaluation, 2015, L'Oréal Co.,France: Material Production, and Evaluation, 2016
Patents and proprietary rights	Using polyazamacrocyclic compounds for intracell ular measurement of metal ions using MRS; U.S. (1993), US 5188816: Polyazamacrocyclic compounds for complexation of metal ions; U.S. (1994), US 5342606 ELJÁRÁS KOMPOZIT SZILIKA ALKOGÉLEK, AEROGÉLEK ÉS XEROGÉLEK ELŐÁLLÍTÁSÁRA, VALAMINT AZ ELJÁRÁS FOLYAMATOS MEGVALÓSÍTÁSÁRA ALKALMAS BERENDEZÉS; Hung. Pat. Appl. (2013), HU 2011000060 A2 20130628 Method for the preparation of composite silica alcogels, aerogels and xerogels, apparatus for carrying out the method continuously, and novel composite silica alcogels, aerogels and xerogels; PCT Int. Appl. (2013), WO 2013061104 A2 20130502.

Important publications over the last 5 years	Selected recent publications from a total of: 16 1) Author: István Lázár Helga Fruzsina Bereczki Sándor Manó Lajos Daróczi György Deák István Fábián Zoltán Csernátony Title: Synthesis and study of new functionalized silica aerogel poly(methyl methacrylate) composites for biomedical use Polym. Compos. (2015) Volume36, Issue2 Pages 348-358 2) Author: István Lázár, József Kalmár, Anca Peter, Anett Szilágyi, Enikő Győri, Tamás Ditrói, István Fábián Title: Photocatalytic performance of highly amorphous titania–silica aerogels with mesopores: The adverse effect of the in situ adsorption of some organic substrates during photodegradation Applied Surface Science 356 (2015) 521–531 3) Author: I. Lázár, A. Szilágyi, G. Sáfrán, A. Szegedi, S. Stichlautner, K. Lázár Title: Iron oxyhydroxide aerogels and xerogels by controlled hydrolysis of FeCl3.6H2O in organic solvents: stages of formation RSC Adv., 2015, 5, 72716 4) Author: H. F. Bereczki, L. Daróczi, I.Fábián, I. Lázár Title: Sol-gel synthesis, characterization and catalytic activity of silica aerogels functionalized with copper(II) complexes of cyclen and cyclam Microporous and Mesoporous Materials 234 (2016) 392e400 5) Author: P. Veres, M. Kéri, I. Bányai, I. Lázár, I. Fábián, C. Domingo, J. Kalmár Title: Mechanism of drug release from silica-gelatin aerogel—Relationship between matrix structure and release kinetics Colloids and Surfaces B: Biointerfaces 152 (2017) 229–

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Activities in specialist bodies over the last 5 years	

Name	*Attila Mándi PhD*
Position	*researcher / assistant professor (organic chemistry, stereochemistry, chemical informatics, molecular modeling)*
Academic career	Habilitation: -
	Ph.D. degree in chemistry, University of Debrecen, 2012; Title of dissertation: Quantum chemical and dynamic investigations on acetal derivatives of carbohydrates and cycloaddition reactions of antibiotic derivatives (supervisor: Prof. Dr. András Lipták) *Master's degree in English-Hungarian translation (minor), University of Debrecen, 2009* *Master's degree in chemistry (major) and German-Hungarian translation (minor), University of Debrecen, 2005*
Employment	Assistant research fellow, researcher, postdoc and assistant professor at the Department of Organic Chemistry, University of Debrecen, 2010 - Assistant research fellow at the Research Group for Carbohydrates of the Hungarian Academy of Sciences at University Debrecen, 2009-2010.
Research and development projects over the last 5 years	*Name of project or research focus: GINOP-2.3.2-15-2016-00008* *Period and any other information: 2016 -* *Partners, if applicable:* *Amount of financing:* *Name of project or research focus: NKFI K120181* *Period and any other information: 2016 -* *Partners, if applicable: Prof. Tibor Kurtán* *Amount of financing:* *Name of project or research focus: TÉT_12_CN-1-2012-0023*

	Period and any other information: 2013 -2015 *Partners, if applicable: Prof. Tibor Kurtán* *Amount of financing:* *Name of project or research focus: OTKA K106294* *Period and any other information: 2013 -2015* *Partners, if applicable: Dr. István Komáromi* *Amount of financing:* *Name of project or research focus: OTKA K105871* *Period and any other information: 2012 -2016* *Partners, if applicable: Prof. Tibor Kurtán* *Amount of financing:* *Major international cooperation partners:* *Prof. Peter Proksch, Heinrich-Heine-Universität, Düsseldorf* *Prof. Yue-Wei Guo, SIMM, Chinese Academy of Sciences, Shanghai* *Prof. Yang Ye, SIMM, Chinese Academy of Sciences, Shanghai* *Prof. Wen Zhang, Second Military Medical University, Shanghai* *Prof. Changsheng Zhang, South China Sea Institute of Oceanology, Guangzhou* *Prof. Bingui Wang, Institute of Oceanology, Chinese Academy of Sciences, Qingdao* *Prof. Dehai Li, Ocean University of China, Qingdao* *Prof. Mary J. Garson, University of Queensland, Brisbane* *Prof. Kenji Monde, Hokkaido University, Sapporo* *Dr. Valentin Paul Nicu, Vrije Universiteit Amsterdam & University of Sibiu*
Industry collaborations over the last 5 years	*Project title: -* *Partners:*
Patents and proprietary rights	-

Important publications over the last 5 years	*Selected recent publications from a total of approx. (give total number): 113* *Author(s): P. Sun, D. X. Xu, A. Mándi, T. Kurtán, T. J. Li, B. Schulz, W. Zhang* *Title: Structure, Absolute Configuration, and Conformational Study of 12-Membered Macrolides from the Fungus Dendrodochium sp. Associated with the Sea Cucumber Holothuria nobilis Selenka* *Any other information:* *Publisher, place of publication, date of publication or name of periodical, volume, issue, page numbers: J. Org. Chem. 2013, 78, 7030-7047.* *Author(s): Y. Ye, A. Minami, A. Mándi, C. Liu, T. Taniguchi, T. Kuzuyama, K. Monde, K. Gomi, H. Oikawa* *Title: Genome mining for sesterterpenes using bifunctional terpene synthases reveals a unified intermediate of di/sesterterpenes* *Any other information:* *Publisher, place of publication, date of publication or name of periodical, volume, issue, page numbers: J. Am. Chem. Soc. 2015, 137, 11846-11853.* *Author(s): A. Mándi, I. W. Mudianta, T. Kurtán, M. J. Garson* *Title: Absolute Configuration and Conformational Study of Psammaplysins A and B from the Balinese Marine Sponge Aplysinella strongylata* *Any other information:* *Publisher, place of publication, date of publication or name of periodical, volume, issue, page numbers: J. Nat. Prod. 2015, 78, 2051-2056.* *Author(s): Z. Tian, P. Sun, Y. Yan, Z. Wu, Q. Zheng, S. Zhou, H. Zhang, F. Yu, X. Jia, D. Chen, A. Mándi, T. Kurtán, W. Liu* *Title: An Enzymatic [4+2] Cyclization Cascade Creates the Pentacyclic Core of Pyrroindomycins*

	Any other information: *Publisher, place of publication, date of publication or name of periodical, volume, issue, page numbers: Nat. Chem. Biol. 2015, 11, 259-265.* *Author(s): L. F. Liang, T. Kurtán, A. Mándi, L. G. Yao, J. Li, W. Zhang, Y. W. Guo* *Title: Unprecedented Diterpenoids as a PTP1B Inhibitor from the Hainan Soft Coral Sarcophyton trocheliophorum Marenzeller* *Any other information:* *Publisher, place of publication, date of publication or name of periodical, volume, issue, page numbers: Org. Lett. 2013, 15, 274-277.*
Activities in specialist bodies over the last 5 years	-

Name	*Dr. Mihály Molnár*
Position	*Senior Research Fellow*
Academic career	*PhD in Environmental Physics (Univ. Debrecen, 2003)*
	Physcis-Chemistry Teacher, MSc Diploma (Univ. Kossuth Lajos, 1997)
Employment	*Oct 2011-today:* Senior Research Associate/ Assistant Head of Hertelendi Laboratory Institution: Institute of Nuclear Research of the Hungarian Academy of Science, Debrecen, Hungary *Jul 2010- Mar 2011* Position: Postdoc Fellow, Hungarian NSF/ Swiss Sciex Institution: Laboratory of Ion Beam Physics, ETHZ, Zürich, Switzerland *Oct 2009- Jul 2010* Senior Research Associate/ Assistant Head of Hertelendi Laboratory Institute of Nuclear Research of the Hungarian

	Academy of Science, Debrecen, Hungary *Feb 2008 – May 2008* Fulbright Researcher Scholar NSF-Arizona AMS Facility, Tucson, Arizona, USA. *Sep 2000 - Sep 2009* Research Assistant/Research Fellow Institute of Nuclear Research of the Hungarian Academy of Science, Debrecen, Hungary
Research and development projects over the last 5 years	*2012. Participating Researcher in an HU NSF Grant (OTKA NF 101362): „PROLONG: Providing long environmental and genetic records of glacial and interglacial climatic oscillations and human impact in the Carpathian Basin"* *2015 Organizer of the IAEA training related to the IAEA's TC project RER/0/039: Extending and Diversifying the Application of nuclear Technology in Cultural Heritage (Oracle Project Nr: 1060285).*
Industry collaborations over the last 5 years	*NA*
Patents and proprietary rights	*NA*
Important publications over the last 5 years	*Selected recent publications from a total of approx. 134:* *Janovics R, Kern Z, Güttler D, Wacker L, Barnabás I, MolnárM. Radiocarbon impact on a nearby tree of a light-water VVER-type nuclear power plant, Paks, Hungary. Radiocarbon, Vol 55, Nr 2–3, 2013, p 826–832* *Molnár M, Janovics R, Major I, Orsovszki J, Gönczi R, Veres M, Leonard AG, Castle SM, Lange TE, Wacker L, Hajdas I, Jull AJT. Status report of the new AMS 14C sample preparation lab of the Hertelendi Laboratory of Environmental Studies (Debrecen, Hungary) Radiocarbon, Vol 55, Nr 2–3, 2013, p 665–676* *Molnár M, Rinyu L,Veres M, Seiler M, Wacker L, Synal H-A. EnvironMICADAS: a mini 14C AMS with enhanced*

	Gas Ion Source Interface in the Hertelendi Laboratory of Environmental Studies (HEKAL), Hungary. Radiocarbon, Vol 55, Nr 2 *Sümegi, P., Magyari, E., Dániel, P., Molnár, M., TörőTcsik, T., 2013. Responses of terrestrial ecosystems to Dansgaard–Oeshger cycles and Heinrich-events: a 28,000-year record of environmental changes from SE Hungary. Quaternary International, 293, 34–50.* *G Újvári, M Molnár, Á Novothny, B Páll-Gergely, J Kovács, A Várhegyi. AMS 14C and OSL/IRSL dating of the Dunaszekcső loess sequence (Hungary): chronology for 20 to 150 ka and implications for establishing reliable age–depth models for the last 40 ka. Quaternary Science Reviews 106, 140-154* *Harangi S, Lukács R, Schmitt AK, Dunkl I, Molnár K, Kiss B, Seghedi I, Novothny Á, Molnár M. Constraints on the timing of Quaternary volcanism and duration of magma residence at Ciomadul volcano, east–central Europe, from combined U–Th/He and U–Th zircon geochronology. Journal of Volcanology and Geothermal Research 301: pp. 66-80. (2015).* *Major I., Furu E., Haszpra L, Kertész Zs., Molnár M.: One-year-long continuous and synchronous data set of fossil carbon in atomspheric PM2.5 and carbon dioxide in Debrecen, Hungary. Radiocarbon 57 (2015)5:991-1002. IF: 2.228* *Rinyu L, Orsovszki G., Futó I., Veres M., Molnár M.: Application of zinc sealed tube graphitization on sub-milligram samples using EnvironMICADAS. Nuclear Instruments and Methods in Physics Research Section B: Beam Interactions with Materials and Atoms 361 (2015)406-413. IF: 1.124* *Janovics R., Kelemen D. I., Kern Z., Kapitány S., Veres M., Jull A. J. T., Molnár M.: Radiocarbon signal of a low and intermediate level radioactive waste disposal facility in*

	nearby trees. Journal of Environmental Radioactivity 153 (2016)10-14. IF:2.483 *Demény A, Czuppon G, Kern Z, Leél-Ossy S, Németh A, Szabó M, Tóth M, Wu C-C, Shen C-C, Molnár M, Németh T, Németh P, Óvári M. Recrystallization-induced oxygen isotope changes in inclusion-hosted water of speleothems - Paleoclimatological implications Quaternary International 415: pp. 25-32. (2016)* *Újvári G, Molnár M, Páll-Gergely B. Charcoal and mollusc shell 14C-dating of the Dunaszekcso loess record, Hungary. Quaternary Geochronology 35: pp. 43-53. (2016)* *PP Povinec, L Liong Wee Kwong, J Kaizer, M Molnár, H Nies, L Palcsu, L Papp, MK Pham, P Jean-Baptiste. Impact of the Fukushima accident on tritium, radiocarbon and radiocesium levels in seawater of the western North Pacific Ocean: A comparison with pre-Fukushima situation. Journal of Eenvironmental Rradioactivity, Volume 166, Part 1, January 2017, Pages 56–66* *Turi M, Palcsu L, Papp L, Horváth A, Futó I, Molnár M, Rinyu L, Janovics R, Braun M, Hubay K, Kis BM, Koltai G. Isotope Characteristics of the water and sediment in volcanic lake Saint Ana, East-Carpathians, Romania. Carpathian Journal oOf Earth aAnd Environmental Sciences 11:(2) pp. 475-484. (2016)* *Ilona Pál, Enikő Katalin Magyari, Mihály Braun, Ildikó Vincze, József Pálfy, Mihály Molnár, Walter Finsinger and Krisztina Buczkó. Small-scale moisture availability increase during the 8.2-ka climatic event inferred from biotic proxy records in the South Carpathians (SE Romania). The Holocene, 2016, Vol. 26(9) 1382–1396* *Újvári G, Stevens T, Molnár M, Demény A, Fabrice L, Varga G, Jull AJT, Páll-Gergely B, Buylaert JP, Kovács J. Coupled European and Greenland last glacial dust*

	activity driven by North Atlantic climate. Proceedings of the National Academy of Sciences of The United States of America (PNAS) 114:(50) pp. 10632-10638. (2017) *Major István, Gyökös Brigitta, Túri Marianna, Futó István, Filep Ágnes, Hoffer András, Furu Enikő, Timothy Jull A J, Molnár Mihály. Evaluation of an automated EA-IRMS method for total carbon analysis of atmospheric aerosol at HEKAL. Journal of Atmospheric Chemistry Online First: pp. 1-12. (2017), https://doi.org/10.1007/s10874-017-9363-y* *Saadi R, Túri M, Palcsu L, Marah H, Oum Keltoum Hakam, Rinyu L, Molnár M, Futó I. A potential groundwater aquifer for palaeoclimate reconstruction: Turonian aquifer, Tadla basin, Morocco. Journal of African Earth Sciences 132: pp. 64-71. (2017)* *Salma I, Németh Z, Weidinger T, Maenhaut W, Claeys M, Molnár M, Major I, Ajtai T, Utry N, Bozóki Z. Source apportionment of carbonaceous chemical species to fossil fuel combustion, biomass burning and biogenic emissions by a coupled radiocarbon–levoglucosan marker method. Atmospheric Chemistry and Physics 17:(22) pp. 13767-13781. (2017)*
Activities in specialist bodies over the last 5 years	*NA*

Name	*Miklós Nagy PhD*
Position	*Associate Professor*
Academic career	Habilitation *(UD, 2017)*
	doctoral qualification: PhD, University of Debrecen, Hungary, 2005 *Doctorate, subject: University of Debrecen, Synthesis and characterization of functionalized polymers* *Undergraduate degree, subject: Chemistry MSc* *Qualification: Chemist, 2000*
Employment	*Associate Professor, University of Debrecen, Department of Applied Chemistry 2018-*

	Assistant Professor, University of Debrecen, Department of Applied Chemistry 2007-2018 *Teaching Assistant, University of Debrecen, Department of Applied Chemistry - 2002-2007*
Research and development projects over the last 5 years	*Name of projects:* participant in GINOP-2.3.2-15-2016-00041, EU project: Regional Material Science Excellence Workshop - Research Program and Infrastructure *Period: 2016-* participant in TÁMOP-4.2.2.A-11/1/KONV-2012-0036, EU project: Intelligent Functional Materials: Their mechanical, thermal, electromagnetic, optical properties and their applications, *Period: 2013-2015* participant in NKFI K-116465, Hungarian project: Synthesis and characterization of smart fluorescent polymers *Period: 2016-*
Industry collaborations over the last 5 years	*Project title: Photopolymrerization of epoxidated plant oils* *Partners: Polinvent Zrt.*
Patents and proprietary rights	*Title (Year)*
Important publications over the last 5 years	*Selected recent publications from a total of approx. (give total number): 11* *Authors:* Miklós Nagy, Dávid Rácz, Zsolt László Nagy, Péter Pál Fehér, József Kalmár, István Fábián, Alexandra Kiss, Miklós Zsuga, Sándor Kéki *Title:* Solvatochromic isocyanonaphthalene dyes as ligands for silver (I) complexes, their applicability in silver (I) detection and background reduction in biolabelling Sensors and Actuators B: Chemical, **255**, 2555-2567 (2018) *Authors:* Miklós Nagy, Dávid Rácz, Zsolt László Nagy, Tibor Nagy, Péter Pál Fehér, Mihály Purgel, Miklós Zsuga, Sándor Kéki *Title:* An acrylated isocyanonaphthalene based solvatochromic click reagent: Optical and biolabeling

	properties and quantum chemical modeling. Dyes and Pigments, **133**, 445-457 (2016) *Authors:* Miklós Nagy, Dávid Rácz, Sándor Lajos Kovács, László Lázár, Péter Pál Fehér, Mihály Purgel, Miklós Zsuga, Sándor Kéki *Title:* New blue light-emitting isocyanobiphenyl based fluorophores: Their solvatochromic and biolabeling properties Journal of Photochemistry and Photobiology A: Chemistry, **318**, 124-134 (2016) *Authors:* Miklós Nagy, Dávid Rácz, László Lázár, Mihály Purgel, Tamás Ditrói, Miklós Zsuga, Sándor Kéki *Title:* Solvatochromic study of highly fluorescent alkylated-isocyanonaphthalenes, their pi-stacking, hydrogen bonding complexation and quenching with pyridine. ChemPhysChem, **15**, 3614-3625 (2014). *Authors:* Dávid Rácz, Miklós Nagy, Attila Mándi, Miklós Zsuga, Sándor Kéki *Title:* Solvatochromic properties of a new isocyanonaphthalene based fluorophore Journal of Photochemistry and Photobiology A: Chemistry, **270**, 19-27 (2013).
Activities in specialist bodies over the last 5 years	

Name	*Noémi M. Nagy*
Position	*professor, Nuclear and radiochemistry*
Academic career	*2009 DSc, Hungarian Academy of Sciences* *2003 habilitation, environmental science, University of Debrecen* *1993 candidate of chemical science, Hungarian Academy of Sciences, Budapest* *1987 PhD, Kossuth Lajos University, Debrecen* *1984 Master of Science (MSc) as a chemist and English-Hungarian translator, Kossuth Lajos University,*

	Debrecen
Employment	*2013- Professor* *2004- Head of Isotope Laboratory* *2004-2013 Associate professor, University of Debrecen, Dep. Colloid and Environmental Chemistry, Isotope Laboratory* *1995-2004 Senior research fellow, Kossuth Lajos University, Isotope Laboratory, Debrecen* *1988-1994 Research fellow, Kossuth Lajos University, Isotope Laboratory, Debrecen* *1985-1988 Junior research fellow, Kossuth Lajos University, Isotope Laboratory, Debrecen* *1984 - 1985 Junior research fellow, Kossuth Lajos University, Dep. Colloid Chemistry, Debrecen*
Research and development projects over the last 5 years	1. EU and co-finan*ced by the European Regional Development Fund under the project GINOP-2.3.2-15-2016-00008, 2016-2020. (within the Chemical Institute)* *2. Hungarian National Research, Development, and Innovation Office (NKFIH K 120265), Study of phosphate transport of soils by radioisotopic labeling, 2016-2020. 48 MFt*
Industry collaborations over the last 5 years	-
Patents and proprietary rights	-
Important publications over the last 5 years	*1. Kónya J., N.M. Nagy: Nuclear and radiochemistry, Elsevier, Oxford, 2nd edition, 2018, eBook* *ISBN: 9780128136447, Paperback* *ISBN: 9780128136430, pp 480 o.* *2. Kovács E.M. , Baradács E.E. , Kónya P. , Kovács-Pálffy P. , Harangi S. , Kuzmann E. , Kónya J. , Nagy N.M.* *Preparation and structure's analyses of lanthanide (Ln) -exchanged bentonites* *COLLOIDS AND SURFACES A : PHYSICOCHEMICAL AND ENGINEERING ASPECTS 522: pp. 287-294. (2017)* *3. Nagy N.M. , Kovács E.M. , Kónya J.* *Ion exchange isotherms in solid: electrolyte solution systems* *JOURNAL OF RADIOANALYTICAL AND NUCLEAR CHEMISTRY 308:(3) pp. 1017-1026. (2016)* *4.Kuzmann E. , Garg V.K. , Singh H. , de Oliveira A.C. , Pati S.S. , Homonnay Z. , Rudolf M. , Molnár Á.M. , Kovács E.M. , Baranyai E ., Kubuki S. , Nagy N.M ., Kónya J.* *Mössbauer study of pH dependence of iron-*

	intercalation in montmorillonite *HYPERFINE INTERACTIONS 237:(1) Paper 106. (2016)* *5. Kónya J. , Nagy N.M.* *Determination of water-soluble phosphate content of soil using heterogeneous exchange reaction with 32P radioactive tracer* *SOIL & TILLAGE RESEARCH 150: pp. 171-179. (2015)*
Activities in specialist bodies over the last 5 years	*Working Committee of Isotope Application, Hungarian Academy of Sciences, chair, 2018-* *EuCheMS Division of Nuclear and Radiochemical Division, Hungarian representative 2016-* *Bolyai Grant Committee, Hungarian Academy of Sciences, member of jury, 2014-*

Name	Levente Novák
Position	assistant professor
Academic career	*Initial academic appointment:* Research Associate, University of Debrecen, 1998-2006 Assistant Professor from 2006
	doctoral qualification: PhD in Molecular and Cellular Biology, Genetics and Biotechnology, Institut National des Sciences Appliquées (INSA) de Toulouse, France, 1998 *Doctorate, subject (Institution, year):* The metabolic network of *Lactococcus lactis* NCDO2118: *i*nteractions between carbon and nitrogen metabolism, INSA de Toulouse, France, 1994-1997 *Undergraduate degree, subject:* DEA in Microbiology, INSA, Toulouse, France, 1994 Biologist (specialization in Biotechnology), Lajos Kossuth University (later University of Debrecen), 1993
Employment	Natural History Museum, Budapest, Hungary, 1986-1987 Fontesz Ltd., Budapest, Hungary, 1997-1998 University of Debrecen, 1998-present
Research and development projects over the last 5 years	1. GINOP-2.3.2- 15-2016- 00008, EU project: Chemistry for better life: strategic R&D centre at the University of Debrecen

	Period and any other information: 2016-2020 Partners, if applicable: Amount of financing: 1 983 995 445 HUF 2. Hungarian-Chinese Bilateral Cooperation (2013-2015, Hungarian-Chinese TÉT-2012) Period and any other information: 2013-2015 Partners, if applicable: Donghua University, Sghanghai, China Amount of financing: 5 464 000 HUF 3. TÁMOP-4.2.2.A-11/1/KONV-2012-0043, EU project: ENVIKUT - Basic Chemical and Biological Research for Elimination of Environmentally Hazardous Chemicals Period and any other information: 2013-2015 Partners, if applicable: Nuclear Research Institute of the Hungarian Academy of Sciences Amount of financing: 899 600 000 HUF
Industry collaborations over the last 5 years	TEVA Ltd., Hungary, 2017. Rheological measurements
Patents and proprietary rights	1. Borbély J., Fleischer É., Novák L., Borbély Zs.: Hydrogels from biopolymers. US20050238678A1, Application number: US11074314, Publication date: 2005-10-27 2. Novák L., Fleischer É., Borbély J.: Nanoparticles from biopolymers. US20060246096A1, Application number: US11406208, Publication date: 2006-11-02 3. Novák L., Serra B., Bányai I.: Széles pH tartományban stabilis emulgeátorok és emulgeátorkeverékek, eljárás azok előállítására és alkalmazásuk: Process for preparation and application of emulgeator and mixture of it appliea in a wide range of pH. Lajstromszám: HU2012000589A2, Ügyszám: P1200589, Benyújtás éve: 2012., Közzététel éve: 2014, Benyújtás helye: Magyarország
Important publications over the last 5 years	*Selected recent publications from a total of 19:* 1. Kéri M., Palcsu L., Túri M., Heim E., Czébely A., Novák L., Bányai I.: 13C NMR analysis of cellulose samples

	from different preparation methods. *Cellulose* **22** (4): 2211-2220. (2015) 2. Kerékgyártó M., Járvás G., Novák L., Guttman A.: Activation energy associated with the electromigration of oligosaccharides through viscosity modifier and polymeric additive containing background electrolytes. *Electrophoresis* **37** (4): 573-578 (2016) 3. Németh Z., Molnár Á. P., Fejes B., Novák L., Karaffa L., Keller N. P., Fekete E.: Growth-phase sterigmatocystin formation on lactose is mediated via low specific growth rates in Aspergillus nidulans. *Toxins* **8** (12): 354 14 p. (2016) 4. Tóth I. Y., Nesztor D., Novák L., Illés E., Szekeres M., Szabó T., Tombácz E.: Clustering of carboxylated magnetite nanoparticles through polyethylenimine: Covalent versus electrostatic approach. *J. Magnetism Magn. Mater.* **427**: 280-288 (2017) 5. Kéri M., Nagy Z., Novák L., Szarvas E., Balogh P L., Bányai I.: Beware of phosphate: evidence of specific dendrimer— phosphate interactions. *Phys. Chem. Chem. Phys.* **19**: 11540-11548 (2017)
Activities in specialist bodies over the last 5 years	

Name	*Mihály Purgel PhD*
Position	*Senior lecturer; Teaching in Chemistry BSc, Chemistry MSc, Chemical Engineering BSc and Chemical Engineering MSc*
Academic career	*Research fellow (MTA-DE Homogeneous Catalysis and Reaction Mechanisms Research Group, 2014)* *Assistant research fellow (MTA-DE Homogeneous Catalysis Research Group, 2009)*
	PhD, Structural and dynamic study of the aluminium(III)-, thallium(III)- and lanthanide(III) complexes using DFT calculations and NMR

	spectroscopy (University of Debrecen, 2011) *Chemistry MSc, Study of the intramolecular rearrangement of aluminium(III)-edta by NMR and DFT calculations; Study of Pt-Tl compounds with direct metal-metal bond (University of Debrecen, 2006)*
Employment	*Senior lecturer – University of Debrecen – 2017 - present*
Research and development projects over the last 5 years	*Name of project or research focus: GINOP-2.3.2-15-2016-00008* *Period and any other information: 2016 – 2020* *Partners, if applicable: -* *Amount of financing: -* *Name of project or research focus: TÁMOP-4.2.2.A-11/1/KONV* *Period and any other information: 2013 –2015* *Partners, if applicable: -* *Amount of financing: -*
Important publications over the last 5 years	*Selected recent publications from a total of approx. (give total number): 20* *Author(s): P. P. Fehér, H. Horváth, F. Joó, <u>M. Purgel</u>* *Title: DFT Study on the Mechanism of Hydrogen Storage Based on the Formate-Bicarbonate Equilibrium Catalyzed by an Ir-NHC Complex: An Elusive Intramolecular C–H Activation* *Any other information:* *Publisher, place of publication, date of publication or name of periodical, volume, issue, page numbers: ACS, Inorg. Chem. 2018, 57:(10), 5903-5914.* *Author(s): N. Marozsán, H. Horváth, É. Kováts, A. Udvardy, A. Erdei, <u>M. Purgel</u>, F. Joó* *Title: Catalytic racemization of secondary alcohols with new (arene)Ru(II)-NHC and (arene)Ru(II)-NHC-tertiary phosphine complexes* *Any other information:* *Publisher, place of publication, date of publication or*

	name of periodical, volume, issue, page numbers: Elsevier, Mol. Catal. 2018, 445, 248-256. *Author(s): T. Fodor, I. Banyai, A. Benyei, C. Platas-Iglesias, M. Purgel, G.L. Horvath, L. Zekany, G. Tircso, I. Toth* *Title: An Extraordinarily Robust Macrocyclic Complex* *Any other information:* *Publisher, place of publication, date of publication or name of periodical, volume, issue, page numbers: ACS, Inorg. Chem. 2015, 54:(11), 5426-5437* *Author(s): P. P. Fehér, F. Joó, M. Purgel* *Title: Performance of exchange-correlation functionals on describing ground state geometries and excitations of Alizarin Red S: Effect of complexation and degree of deprotonation* *Any other information:* *Publisher, place of publication, date of publication or name of periodical, volume, issue, page numbers: Elsevier, Comp. Theor. Chem. 2014, 1045, 113-122.*

Sheet of staff handbook

Name	*László SOMSÁK*
Position	*Full professor, Head of the Department of Organic Chemistry, Responsible for Chemistry BSc*
Academic career	*University of Debrecen (UD) 1978* *Habilitation (UD, 1997)* *Doctor of the Hungarian Academy of Sciences 2002*
	doctoral qualification (UD, 1983) *Undergraduate degree, subject (UD, 1978, MSc in Chemistry)*
Employment	*Full professor at the Department of Organic Chemistry of UD since 2003, head of the department since 2015*
Research and development projects over the last 5 years	**2013-2017** **Alexander von Humboldt Stiftung – Institutspartnerschaft (Universität Rostock, Prof. P.**

	Langer – University of Debrecen, Prof. L. Somsák) – (53.990 Euro) Untersuchungen zur Anwendbarkeit moderner Synthesemethoden für die Herstellung pharmakologisch relevanter Kohlenhydrat-Derivate **2013-2018** **OTKA K-109450 – PI of research project (43.852 kHUF)** New transformations of monosaccharide derivatives at and around the anomeric centre **2016-2020** **GINOP-2.3.2-15-2016-00008 – participant (1.984 MHUF)** Chemistry for better life quality **2017-2021** **OTKA FK-125067 – participant (35.664 kHUF)** **New types and new biological applications of *C*-glycopyranosyl heterocycles**
Industry collaborations over the last 5 years	*Project title: Custom synthesis of carbohydrate derivatives* *Partners: Carbosynth Ltd, Oxford, UK* *Project title: Custom synthesis of cyclodextrin derivatives* *Partners: Cylolab Ltd, Budapest, Hungary*
Patents and proprietary rights	SOMSÁK L.; BOKOR É.; TÓTH M.; JUHÁSZ L.; CZIFRÁK K.; KÓNYA B.; KUN S.; PÁHI A.; SZŐCS B.; VARGA G.; KÓDER L.-NÉ; NAGY K.-NÉ; GERGELY P.; DOCSA T. Glikogén foszforiláz inhibitorok P1100602 alapszámú magyar szabadalmi bejelentés, 2011. PCT/HU2012/00116 WO2013061105 A3 PATONAY T.; SZILVÁSSY Z.; PEITL B.; VÍGH L.; TÖRÖK ZS.; BERÉNYI S.; HORVÁTH I.; BALOGH G.; SOMSÁK L.; KISS A.; DRIMBA L.; MOLNÁRNÉ HATVANI I. Hő-sokk protein (HSP) ko-inducer

	sajátosságot mutató vegyületek alkalmazása 2-es típusú cukorbetegség kezelésében inzulin-érzékenyítő hatás fokozására P1100709 alapszámú magyar szabadalmi bejelentés, 2011. ANTUS, S.; SOMSÁK, L.; CZAKÓ, Z.; KÓNYA, B.; GERGELY, P.; DOCSA, T.; KÓDER, L.-NÉ; MAGYAR, L.-NÉ Glükóz és oxigéntartalmú heterociklusok antidiabetikus hatású konjugátumai P1200626 alapszámú magyar szabadalmi bejelentés, 2012.
Important publications over the last 5 years	*Selected recent publications from a total of 167:* KUN, S.; BEGUM, J.; KYRIAKIS, E.; STAMATI, E. C. V.; BARKAS, T. A.; SZENNYES, E.; BOKOR, É.; SZABÓ, E. K.; STRAVODIMOS, G. A.; SIPOS, Á.; DOCSA, T.; GERGELY, P.; MOFFATT, C.; PATRASKAKI, M. S.; KOKOLAKI, M. S.; GKERDI, A.; SKAMNAKI, V. T.; LEONIDAS, D. D.; SOMSÁK, L.; HAYES, J. M. A multidisciplinary study of 3-(β-D-glucopyranosyl)-5-substituted-1,2,4-triazole derivatives as glycogen phosphorylase inhibitors: computation, synthesis, crystallography and kinetics reveal new potent inhibitors *Eur. J. Med. Chem.*, **2018**, *147*, 266-278. BOKOR, É.; KYRIAKIS, E.; SOLOVOU, T. G. A.; KOPPÁNY, CS.; KANTSADI, A. L.; SZABÓ, K. E.; SZAKÁCS, A.; STRAVODIMOS, G. A.; DOCSA, T.; SKAMNAKI, V. T.; ZOGRAPHOS, S. E.; GERGELY, P.; LEONIDAS, D. D.; SOMSÁK, L. Nanomolar inhibitors of glycogen phosphorylase based on β-D-glucosaminyl heterocycles: a combined synthetic, enzyme kinetic and protein crystallography study *J. Med. Chem.*, **2017**, *60*, 9251-9262. KASZÁS, T.; TÓTH, M.; SOMSÁK, L. A new synthesis of *C*-β-D-glycopyranosylmethyl sulfides by metal-free coupling of anhydro-aldose tosylhydrazones with thiols *New J. Chem.*, **2017**, *41*, 13871-13880. BOKOR, É.; KUN, S.; GOYARD, D.; TÓTH, M.; PRALY, J.-P.; VIDAL, S.; SOMSÁK, L. *C*-Glycopyranosyl arenes and hetarenes: Synthetic methods and bioactivity focused on

	antidiabetic potential *Chem. Rev.*, **2017**, *117*, 1687−1764. BOKOR, É.; KUN, S.; DOCSA, T.; GERGELY, P.; SOMSÁK, L. 4(5)-Aryl-2-*C*-glucopyranosyl-imidazoles as new nanomolar glucose analog inhibitors of glycogen phosphorylase *ACS Med. Chem. Lett.*, **2015**, *6*, 1215-1219.
Activities in specialist bodies over the last 5 years	*European Chemistry Thematic Network (representative of the University of Debrecen) since 1999* *Chair of the Working Committee on Carbohydrate Chemistry of the HAS since 2006* *European Carbohydrate Organization (Hungarian representative) since 2006* *Chair of Organic Chemistry Panel of the Hungarian Scientific Research Fund since 2016*

Name	*Gyula Tircsó PhD*
Position	*Associate Professor (University of Debrecen, Department of Physical Chemistry, **2018-**).*
Academic career	
	*Doctoral qualification (Institution, year): PhD, University of Debrecen, Hungary, **2008*** *Doctorate, subject (Institution, year): Synthesis and complexation properties of some diamino-polycarboxilate type ligands having „in-chain" phosphinate and alcoholic OH groups, **2008.*** *Undergraduate degree, subject (Institution, year): Chemist and chemistry teacher, **1999,** Uzhgorod National University Uzhgorod, Ukraine*
Employment	***2018-,** associate professor at the Department of Physical Chemistry, University of Debrecen, Hungary* ***2017-2018,** associate professor at the Department of Inorganic and Analytical Chemistry, University of Debrecen, Hungary* ***2010-2017,** assistant professor at the Department of Inorganic and Analytical Chemistry, University of Debrecen, Hungary* *meanwhile **in 2015**, Le Studium Research Fellow at the Center of Molecular Biophysics, Oreléans, France.*

	2008-2010, *junior assistant professor at the Department of Inorganic and Analytical Chemistry, University of Debrecen, Hungary* ***2004-2008,*** *research associate at the Chemistry Department, University of Texas at Dallas, Richardson, USA* ***2003-2004,*** *chemist at the Department of Inorganic and Analytical Chemistry Faculty of Science, University of Debrecen, Hungary*
Research and development projects over the last 5 years	*Name of project or research focus:* GINOP-2.3.2- 15-2016- 00008, EU project: *Chemistry for better life: strategic R&D centre at the University of Debrecen* *Period and any other information:* ***2016-2020*** *Partners, if applicable:* *Amount of financing:* *Name of project or research focus:* TÁMOP-4.2.2.A-11/1/KONV-2012-0043, EU project: *ENVIKUT - Basic Chemical and Biological Research for Elimination of Environmentally Hazardous Chemicals* *Period and any other information:* ***2013-2015*** *Partners, if applicable:* *Amount of financing:* *Name of project or research focus:* OTKA K-84920, *Rational design of new ligands for biomedical applications* *Period and any other information:* ***2011-2016*** *Partners, if applicable:* *Amount of financing:* *Name of project or research focus:* OTKA K- 109029, *Preparation and chemical characterisation of metal complexes for theragnostic applications* *Period and any other information:* ***2013-2017*** *Partners, if applicable:* *Amount of financing:* *Name of project or research focus:* OTKA K- 120224, *Design, synthesis and chemical characterization of new rigid macrocyclic ligand based Magnetic Resonance*

	imaging probes: the safe way in diagnosis with manganese(II) complexes *Period and any other information:* ***2016*-*2020*** *Partners, if applicable:* *Amount of financing:*
Industry collaborations over the last 5 years	*Project title: Development of „In vivo" Ca2+-sensitive MRI contrast agents for following/detecting brain activity* *Period and any other information:* ***2011*-*2014*** *Partners: Richter Gedeon NyRT* *Project title: Synthesis and physico-chemical characterization of ten new ligands based on bisamide derivatives of CDTA (trans-1,2-Diaminocyclohexane-N,N,N',N'-tetraacetic acid) and their respective Mn(II) complexes* *Period and any other information:* ***2016*-*2018*** *Partners: Bracco Imaging SpA*
Patents and proprietary rights	*6. Botár Richárd, Garda Zoltán, Fodor Tamás, Kálmán Ferenc Krisztián, Nagy Viktória, Tircsó Gyula, Tóth Imre:* *Triaza-cyclononane derivatives and their use as ligands in Mn(II)-based MRI contrast agents* *(HU2015000563A2 - 2017)* *5. Botár Richárd, Garda Zoltán, Fodor Tamás, Kálmán Ferenc Krisztián, Nagy Viktória, Tircsó Gyula, Tóth Imre* *New 3,6,9, 15-tetraaza-bicyclo [9.3.1]pentadeca- 1(14), 11(15), 12-triene based compounds and their application as ligands of essential metal ion based MRI and 52Mn based PET contrast agents (WO2017089847A1 –* ***2017****)* *4. Botár Richárd, Garda Zoltán, Fodor Tamás, Kálmán Ferenc Krisztián, Nagy Viktória, Tircsó Gyula, Tóth Imre* *New 2,11-diaza-[3.3](2,6)pyridinophane compounds and their application as ligands of essential metal ion based MRI contrast agents and 52Mn based PET contrast agents.* *(WO2017089848A1 –* ***2017****)*

	3. Botár Richárd, Garda Zoltán, Fodor Tamás, Kálmán Ferenc Krisztián, Nagy Viktória, Tircsó Gyula, Tóth Imre: *New 6-oxa-3,9,15-triaza-bicyclo[9.3.1]pentadeca-1(14),11(15),12-triene derivatives based compounds and their application as ligands of essential metal ion based MRI and 52Mn based PET contrast agents.* *(WO2017089849A1 – **2017**)* *2. Baranyai Zsolt, Garda Zoltán, Kálmán Ferenc Krisztián, Krusper László, Tircsó Gyula, Tóth Imre, Ghiani Simona, Maiocchi Alessandro:* *Ethylenediaminetetraacetic acid bis(amide) derivatives and their respective complexes with Mn(II) ion for use as MRI contrast agent.* *(WO2016135234 – **2016**)* *1. Zoltán Kovács, Garry E. Kiefer, C. Bensimon, A. Dean Sherry Gyula Tircsó:* *Bifunctional polyazamacrocyclic chelating agents (WO 2007104135 - **2007**)*
Important publications over the last 5 years	*Selected recent publications from a total of approx. (give total number): 55* *5. Mariane Le Fur, Enikő Molnár, Maryline Beyler, Ferenc K. Kálmán, Olivier Fougère, David Esteban-Gómez, Olivier Rousseaux, Raphaël Tripier, <u>Gyula Tircsó,*</u> Carlos Platas-Iglesias*:* *A Coordination Chemistry Approach to Fine-Tune the Physicochemical Parameters of Lanthanide Complexes Relevant to Medical Applications* *Chem. Eur. J., **2018,** 24(13), 3127-3131.* *4. Lei Zhang, André F. Martins, Piyu Zhao, Yunkou Wu, <u>Gyula Tircsó,</u> and A. Dean Sherry:* *Lanthanide-based T2ex and CEST complexes provide new insights into the design of pH sensitive MRI agents* *Angew. Chem. Int. Ed. **2017,** 56 (52), 16626–16630.* *3. Mariane Le Fur, Maryline Beyler, Enikő Molnár, Olivier Fougère, David Esteban-Gómez, <u>Gyula Tircsó,</u> Carlos Platas-Iglesias, Nicolas Lepareur, Olivier*

	Rousseaux, Raphaël Tripier: *The role of the capping bond effect on pyclen $^{nat}Y^{3+}/^{90}Y^{3+}$ chelates: full control of the regiospecific N-functionalization makes the difference* *Chem. Commun.,* ***2017,*** *53(69), 9534-9537.* *2. Gyula Tircsó,* Martín Regueiro-Figueroa, Viktória Nagy, Zoltán Garda, Tamás Garai, Ferenc Krisztián Kálmán, David Esteban-Gómez, Éva Tóth, and Carlos Platas-Iglesias*:* *Approaching the Kinetic Inertness of Macrocyclic Gd3+-based MRI Contrast Agents with Highly Rigid Open-Chain Derivatives* *Chem. Eur. J.,* ***2016,*** *22(3), 896-901.* *1. Aurora Rodríguez-Rodríguez, David Esteban-Gómez, Raphaël Tripier,* Gyula Tircsó*, Zoltán Garda, Imre Tóth, Andrés de Blas, Teresa Rodríguez-Blas and Carlos Platas-Iglesias,** *Lanthanide(III) Complexes with a Reinforced Cyclam Ligand Show Unprecedented Kinetic Inertness* *J. Am. Chem. Soc.,* ***2014,*** *136 (52), 17954–17957.*
Activities in specialist bodies over the last 5 years	*Association of Hungarian Chemists (**2008-**)* *Coordination Chemistry Committee of the Hungarian Academy of Science, Physical and Inorganic Chemistry Committee (**2008-**)* *The Society of Biological Inorganic Chemistry (**2013-2015**)* *The Royal Society of Chemistry (**2014-2016**)*

Name	*Dr. György Trencsényi*
Position	*associate professor*
Academic career	Habilitation *(University of Debrecen, Faculty of Medicine, 2018)*
	Ph. D. in Clinical Medicine, University of Debrecen, 2010 „Establishment and characterization of new cell lines derived from chemically induced experimental tumors”

	M.Sc. in Biology, University of Debrecen, 2006 *M.Sc. in Biology Teacher, University of Debrecen, 2004*
Employment	*2018- University of Debrecen, Faculty of Medicine, Department of Medical Imaging; associate professor* *2009-2018 University of Debrecen, Faculty of Medicine, Department of Medical Imaging; senior lecturer* *2015- Scanomed Ltd., Translational Center; Head of preclinical imaging*
Research and development projects over the last 5 years	*- LIFEVALVE - Living autologous heart valves for minimally invasive implantable procedures (*FP7-HEALTH) 2014 - Development of bio-conjugates suitable for the directed tumor-therapy treatment of high-mortality malignant diseases (NKFI-6: 119552) 2015-2020 - Mapping the behavior of micro-scalarization biomarkers using targeted nanostructures using imaging diagnostics in an expert system (GINOP-2.1.1-15-2015-00609) 2016-2018
Industry collaborations over the last 5 years	*Project title: Labeling and imaging of new radiopharmaceuticals* *Partners: BRACCO IMAGING SPA., Italy*
Patents and proprietary rights	*Title (Year)*
Important publications over the last 5 years	*Selected recent publications from a total of 42* *Trencsényi G, Dénes N, Nagy G, Kis A, Vida A, Farkas F, Szabó JP, Kovács T, Berényi E, Garai I, Bai P, Hunyadi J, Kertész I. Comparative preclinical evaluation of 68Ga-NODAGA and 68Ga-HBED-CC conjugated procainamide in melanoma imaging. JOURNAL OF PHARMACEUTICAL AND BIOMEDICAL ANALYSIS 139: pp. 54-64. (2017) IF: 3.169* *Kertész I, Vida A, Nagy G, Emri M, Farkas A, Kis A, Angyal J, Dénes N, Szabó PJ, Kovács T, Bai P, Trencsényi Gy. In Vivo Imaging Of Experimental Melanoma Tumors Using The Novel Radiotracer 68Ga-NODAGA-Procainamide (PCA). JOURNAL OF CANCER 2017; 8(5): 774-785. doi: 10.7150/jca.17550 (2017) IF: 3.609*

	Nagy G, Szikra D, Trencsenyi G, Fekete A, Garai I, Giani AM, Negri R, Masciocchi N, Maiocchi A, Uggeri F, Toth I, Aime S, Giovenzana GB, Baranyai Z. AAZTA: An Ideal Chelating Agent for the Development of 44 Sc PET Imaging Agents. ANGEWANDTE CHEMIE-INTERNATIONAL EDITION 56:(8) pp. 2118-2122. (2017) IF: 11.709 *Kocsis T, Trencsenyi G, Szabo K, Baan JA, Muller G, Mendler L, Garai I, Reinauer H, Deak F, Dux L, Keller-Pinter A. Myostatin propeptide mutation of the hypermuscular Compact mice decreases the formation of myostatin and improves insulin sensitivity. AMERICAN JOURNAL OF PHYSIOLOGY: ENDOCRINOLOGY AND METABOLISM 8:(5) pp. 744-785. (2017) IF: 3.825* *Gábor Máté, Dezső Szikra, Jakub Šimeček, Szandra Szilágyi, György Trencsényi, Hans-Jürgen Wester, István Kertész, László Galuska. Multiparametric labeling optimization and synthesis of 68Ga-labeled compounds applying a continuous-flow microfluidic methodology. JOURNAL OF FLOW CHEMISTRY 6:(2) pp. 86-93. (2016) IF: 1.878* *L. Naszályi Nagy, A. Polyak, J. Mihály, Á. Szécsényi, I. Cs. Szigyártó, Zs. Czégény, E. Jakab, P. Németh, B. Magda, P. Szabó, Zs. Veres, K. Jemnitz, I. Bertóti, R. P. Jóba, Gy. Trencsényi, L. Balogh and A. Bóta. Silica@zirconia@poly(malic acid) nanoparticle: a promising nanocarrier for theranostic applications. JOURNAL OF MATERIALS CHEMISTRY B (2016) IF: 4.872* *Tekes K, Pöstényi Z, Faigl EB, Magyar K, Polyák A, Trencsényi G, Balogh L, Kalász H. Distribution of N-methyl-14C-labeled selegiline in the rat. JOURNAL OF PHARMACEUTICAL AND BIOMEDICAL ANALYSIS. 2015 Mar 30;111:147-152. (2015)* *IF: 3.169* *Araki N , Trencsenyi G , Krasznai ZT , Nizsaloczki E ,*

	Sakamoto A , Kawano N , Miyado K, Yoshida K , Yoshida M. Seminal vesicle secretion 2 acts as a protectant of sperm sterols and prevents ectopic sperm capacitation in mice. BIOLOGY OF REPRODUCTION 92:(1) p. 8. (2015) IF: 3.451 *Trencsényi G, Kertész I, Krasznai ZT, Máté G, Szalóki G, Szabó Judit P, Kárpáti L, Krasznai Z, Márián T, Goda K. 2'[18F]-fluoroethylrhodamine B is a promising radiotracer to measure P-glycoprotein function. EUROPEAN JOURNAL OF PHARMACEUTICAL SCIENCES 10;74:27-35. (2015) IF: 3.773* *Mate G, Kertesz I, Enyedi KN, Mezo G, Angyal J, Vasas N, Kis A, Szabo E, Emri M, Biro T, Galuska L, Trencsenyi G. In vivo imaging of Aminopeptidase N (CD13) receptors in experimental renal tumors using the novel radiotracer Ga-NOTA-c(NGR). EUROPEAN JOURNAL OF PHARMACEUTICAL SCIENCES 69: pp. 61-71. (2015) IF: 3.773* *Trencsenyi G, Bako F, Nagy G, Kertai P, Banfalvi G. Methotrexate induced apoptotic and necrotic chromatin changes in rat myeloid leukemia cells. INFLAMMATION RESEARCH 64: pp. 1-11. (2015) IF: 2.557* *Trencsényi G, Márián T, Lajtos I, Krasznai Z, Balkay L, Emri M, Mikecz P, Goda K, Szalóki G, Juhász I, Németh E, Miklovicz T, Szabó G, Krasznai ZT. 18FDG, [18F]FLT, [18F]FAZA and 11C-methionine are Suitable Tracers for the Diagnosis and In Vivo Follow Up the Efficacy of Chemotherapy by MiniPET both in Multidrug Resistant and Sensitive Human Gynecologic Tumor Xenografts. BIOMED RESEARCH INTERNATIONAL 2014: Paper 787365. 10 p. (2014) IF: 2.706* *Krasznai, Z.T., Trencsényi, G., Krasznai, Z., Mikecz, P., Nizsalóczki, E., Szalóki, G., Szabó, J.P., Balkay, L., Márián, T., Goda, K., 18FDG a PET tumor diagnostic tracer is not a substrate of the ABC transporter P-glycoprotein. EUROPEAN JOURNAL OF*

	PHARMACEUTICAL SCIENCES 64: pp. 1-8. (2014) IF: 3.350 *Trencsenyi G, Marian T, Bako F, Emri M, Nagy G, Kertai P, Banfalvi G. Metastatic Hepatocarcinoma He/De Tumor Model in Rat. JOURNAL OF CANCER 2014; 5(7): 548-558. (2014) IF: 2.639* *Trencsenyi G, Nagy G, Kahlik B, Nemeth E, Kertai P, Kiss A, Banfalvi G. Lymphoid metastasis of rat My2/De leukemia. LEUKEMIA RESEARCH. 2014 May;38(5):586-593. (2014) IF: 2.764* *Szalóki G, Krasznai ZT, Tóth Á, Vízkeleti L, Szöllősi AG, Trencsényi G, Lajtos I, Juhász I, Krasznai Z, Márián T, Balázs M, Szabó G, Goda K. The strong in vivo anti-tumor effect of the UIC2 monoclonal antibody is the combined result of Pgp inhibition and antibody dependent cell-mediated cytotoxicity. PLOS ONE 19;9(9):e107875. (2014) IF: 3.534* *Hajdu I, Trencsényi G, Bodnár M, Emri M, Bánfalvi G, Sikula J, Márián T, Kollár J, Vámosi G, Borbély J. Tumor-specific Localization of Self-assembled Nanoparticle PET/MR Modalities. ANTICANCER RESEARCH Jan;34(1):49-59. (2014) IF: 1.713*
Activities in specialist bodies over the last 5 years	*European Association of Nuclear Medicine, 2010-* *Hungarian Society of Nuclear Medicine, 2009-* *Hungarian Society of Laboratory Animals, 2009-*

Name	*Katalin Várnagy, DSC, PhD*
Position	*Full Professor*
Academic career	*Chairwoman of the Educational Committee of Institute of Chemistry (2013-2017)* *Director of Chemsitry Institute (2017-)* *Habilitation: 1999*
	doctoral qualification: Univ dr. 1987 (PhD: 1995), Lajos Kossuth University, Debrecen (University of Debrecen) *Doctorate, subject: Transition metal complexes of sulfur*

	containing dipeptides *Undergraduate degree: Teacher of chemistry and mathematics, Lajos Kossuth University Debrecen, 1985, Translator in Chemistry (German-Hungarian) Lajos Kossuth University Debrecen, 1996,* *subject: Complexes of amino acid derivatives containing thiocarbonyl group.*
Employment	*1985-92: Junior research fellow, Lajos Kossuth University* *1992-2000: Research fellow, University of Debrecen (Lajos Kossuth University)* *2000-2016: Assistant professor (University of Debrecen)* *2016- : Full professor (University of Debrecen)*
Research and development projects over the last 5 years	*Name of project or research focus:* OTKA72956 Project Studies on the redoxi properties of copper(II)-oligopeptides and peptide-derivatives systems (principal investigator): *Period and any other information: 2008-2013* *Name of project or research focus:* OTKA115480 Project Coordination and electrochemical background of role of metal ions in neurodegenerative disorders (principal investigator): *Period and any other information: 2016-2019* *Name of project or research focus:* TÁMOP-4.2.2.A-11/1/KONV-2012-0043, EU project: Basic chemical and biological research for elimination of environmentally hazardous chemicals *Period and any other information: 2013-2015* *Partners, if applicable:* *Amount of financing:* *Name of project or research focus:* GINOP-2.3.2-15-2016-00008, EU project: Chemistry for Quality of Life: Strategic R & D Workshop at the University of Debrecen *Period and any other information: 2016-2020* *Partners, if applicable:* *Amount of financing:*

Industry collaborations over the last 5 years	*Project title:* *Partners:*
Patents and proprietary rights	*Title (Year)*
Important publications over the last 5 years	*Selected recent publications from a total of approx. (give total number): 68* *Author(s):* David A, Kallay C, Sanna D, Lihi N, Sovago I, Varnagy K: *Title:* Potentiometric and spectroscopic studies on the copper(ii) complexes of rat amylin fragments. The anchoring ability of specific non-coordinating side chains. *Any other information:* *Publisher, place of publication, date of publication or name of periodical, volume, issue, page numbers:* DALTON TRANSACTIONS 44:(39) pp. 17091-17099. (2015) *Author(s):* Sóvágó I, Várnagy K, Lihi N, Grenács Á: *Title:* Coordinating properties of peptides containing histidyl residues *Any other information:* *Publisher, place of publication, date of publication or name of periodical, volume, issue, page numbers:* COORDINATION CHEMISTRY REVIEWS 327-328: pp. 43-54. (2016) *Author(s):* Grenács Á, Lihi N, Sóvágó I, Várnagy K: *Title:* The influence of penicillamine/cysteine mutation on the metal complexes of peptides *Any other information:* *Publisher, place of publication, date of publication or name of periodical, volume, issue, page numbers:* DALTON TRANSACTIONS 46:(39) pp. 13472-13481. (2017) *Author(s):* Csire G, Timári S, Asztalos J, Király JM, Kiss M, Várnagy K: *Title:* Coordination, redox properties and SOD activity of Cu(II) complexes of multihistidine peptides

	Any other information: *Publisher, place of publication, date of publication or name of periodical, volume, issue, page numbers:* JOURNAL OF INORGANIC BIOCHEMISTRY 177: pp. 198-210. (2017) *Author(s):* Ágnes Dávid, Éva Tünde Hartman, Norbert Lihi, Imre Sóvágó, Katalin Várnagy: *Title:* Complex formation of nickel(II) and zinc(II) ions with peptide fragments of rat amylin *Any other information:* *Publisher, place of publication, date of publication or name of periodical, volume, issue, page numbers:* NEW JOURNAL OF CHEMISTRY 42:(10) pp. 8131-8136. (2018)
Activities in specialist bodies over the last 5 years	*Organisation - Role – Period* *Membership without a specific role need not be mentioned.* 2014- Member of the Physical chemistry scientific committee of the Hungarian Academy of Sciences 2011- Chairwoman of the Division of Coordination Chemistry 2013- Chairwoman of the Educational Committee of Institute of Chemistry 2013- Member of the Educational Committee of Faculty of Science and Technology

Name	*Zékány András Dr., PhD*
Position	*Honorary Associate Professor*
Academic career	*Head of External Department of Pharmaceutical Industry since 2017.*
	doctoral qualification: Candidate of chemical sciences, Institute of Organic Chemistry of Academy ofSciences of Ukraine, Kiev, USSR, 1979. *PhD University of Kossuth Lajos, Debrecen, Hungary. 1996.* *Doctorate, subject: Synthesis and study of pentabromopyridine. Institute of Organic Chemistry, 1975-1978.* *Undergraduate degree, subject: Chemist and teacher of chemistry, MsC. 1975.*

Employment	*Scientific researcher – 1978-1980.Institute of Organic Chemistry.* *Research engineer, head of synthetic Development group, Biogal/Teva Pharmeciutical Works Ltd. 1980-2016.* *Heas of External Department of Pharmaceutical Industry 2017 – , Debrecen University/Teva Pharmaceutical Works*
Research and development projects over the last 5 years	*Runing projects of development of lead compounds, life cycle investment of some drugs and QA support of new drugs.*
Industry collaborations over the last 5 years	*Teva Pharmaceutical Industries Co. Ltd.*
Patents and proprietary rights	*Teva Pharmaceutical Industries Co. Ltd.*
Important publications over the last 5 years	*Teva in-house reports*
Activities in specialist bodies over the last 5 years	*Member of working comitee of Heterocyclic Chemistry of Hungarian Academy of Sciences.* *Member of working comitee of Medicinal Chemistry and Pharmaceutical Techologies of Hungarian Academy of Sciences.* *Head of Hajdú-Bihar County Organisation of Chemical Society.*