TRAINING PROGRAMME AND RESEARCH AREAS OF THE DOCTORAL SCHOOL OF CHEMISTRY

The Hungarian Qualifications Framework

The **MKK8 level** (Workplace Skills Requirement Level 8) is one of the highest levels of the Hungarian Qualifications Framework (MKKR), typically associated with a doctoral degree or equivalent scientific or artistic achievement. This level describes knowledge and skills that go beyond master's level and require the acquisition and independent, creative application of the most advanced and current expertise in the given field.

Competencies associated with MKK8 include generating new scientific results, methodological rigour in research, complex problem solving, and the ability to develop new theories and solutions. At this level, the professionals can contribute independently and in a leading role to the advancement of science, technology or the arts, and can engage in professional discourse at an international level.

In short: the MKK8 level represents independent, innovative, responsible, and internationally recognised research and professional activity.

Introduction

Modern chemical research in Debrecen has a history of nine decades. The chemical departments operating at various faculties of the University of Debrecen, along with academic research groups, study some of the most current and exciting questions of the discipline. Internationally recognised results have been achieved in several fields, such as nonlinear chemical dynamics, organometallic catalysis in aqueous media, kinetics of redox reactions, metal complexes of amino acids and peptides, biologically active and pharmaceutically applicable metal complexes, natural organic compounds (alkaloids, antibiotics, flavonoids, carbohydrates) and their synthetic derivatives, mechanisms of various enzymes, and cationic polymerisation. Significant research also focuses on developing methods in structural chemistry, structural biology, and environmental instrumental analytics.

The "Chemistry" Doctoral Programme, 1993–2000

Following accreditation in 1993, Lajos Kossuth University, and later the University of Debrecen, was authorised to award the PhD degree in chemistry. The "Chemistry" doctoral programme, overseen by **Dr. András Lipták** (academician and professor, 1993–1996) and, from 1997, by **Dr. Ferenc Joó** (academician and professor), comprised the following sub-programmes:

- **K/1** Reaction Kinetics and Catalysis (Leaders: Dr. Mihály Beck, Dr. Ferenc Joó)
- **K/2** Coordination Chemistry (Leader: Dr. Ernő Brücher)
- **K/3** Environmental and Instrumental Analytical Chemistry (Leaders: Dr. Lajos Papp, Dr. József Posta)
- **K/4** Macromolecular and Surface Chemistry (Leader: Dr. Miklós Zsuga)
- **K/5** Chemistry, Biochemistry and Structural Study of Natural and Synthetic Carbohydrate-Containing Compounds (Leader: Dr. Ferenc Sztaricskai)
- **K/6** Synthesis and Structural Investigation of Natural Heterocycles and their Analogues (Leader: Dr. Sándor Antus)

The Doctoral School of Chemistry, 2000–2013

Based on the decision of the Hungarian Accreditation Committee, the Chemistry Doctoral School of the University of Debrecen received accreditation in autumn 2000. The School was led by **Dr. Ferenc Joó**, academician and professor, until 2009, and from September 2009 by **Dr. Vilmos Gáspár**, professor. The Doctoral School began its work with a renewed personnel base but following the structure of the earlier programme. Accordingly, between 2000 and 2013 the Doctoral School operated with six programmes:

- **K/1** Reaction Kinetics and Catalysis (Leader: Dr. Ferenc Joó)
- **K/2** Coordination Chemistry (Leader: Dr. Imre Sóvágó)
- **K/3** Environmental and Instrumental Analytical Chemistry (Leaders: Dr. József Posta, Dr. István Fábián)
- **K/4** Macromolecular and Surface Chemistry (Leaders: Dr. Miklós Zsuga, Dr. Sándor Kéki)
- **K/5** Chemistry and Biochemistry of Carbohydrates (Leaders: Dr. Ferenc Sztaricskai, Dr. Pál Herczeg, Dr. László Somsák)

- **K/6** Synthesis and Structural Investigation of Natural Heterocycles and their Analogues (Leader: Dr. Sándor Antus)

The Doctoral School of Chemistry, 2013–2024

Based on a decision of the Council of the Doctoral School of Chemistry on 13 March 2013, and with the aim of improving efficiency while considering changes in staff, programmes **K/2 and K/3**, as well as **K/5 and K/6**, were merged. The restructuring did not affect the status or training programme of doctoral students, and the course structure and its documentation in the Neptun system remained unchanged. The changes were introduced in the 2013/14 academic year.

The School was led by **Dr. Katalin Kövér**, academician and professor, from June 2016 to April 2023. Since April 2023, the Head of the Doctoral School has been **Dr. István Fábián**, professor.

Programmes (2013–2024):

- **K/1** Reaction Kinetics and Catalysis (Leader: Dr. Ferenc Joó)
- **K/2** Coordination and Analytical Chemistry (Leader: Dr. István Fábián)
- **K/4** Macromolecular and Surface Chemistry (Leader: Dr. Sándor Kéki)
- **K/5** Chemistry and Chemical Biology of Carbohydrates and Heterocycles (Leader: Dr. László Somsák)

The Doctoral School of Chemistry, 2024 – Present

Following the proposal of the Council of the Doctoral School, the core members' assembly held on **16 January 2024** approved the new division of programmes and the nomination of new programme leaders. The restructuring did not affect the students' status, training programme, or the documentation of courses in the Neptun system. The new structure was implemented on **1 February 2024**.

Since **1 August 2025**, the Head of the Doctoral School has been **Dr. Tibor Kurtán**, professor.

Current programmes:

- **K/1** Reaction Mechanisms and Catalysis (Leader: Dr. István Fábián)
- **K/2** Coordination Chemistry (Leader: Dr. Gyula Tircsó)
- **K/3** Analytical Chemistry (Leader: Dr. Attila Gáspár)
- **K/4** Macromolecular and Surface Chemistry (Leader: Dr. Sándor Kéki)

- **K/5** Chemistry and Chemical Biology of Carbohydrates and Heterocycles (Leader: Dr. Tibor Kurtán)

In the following, we present the individual programmes of the Doctoral School in their current form, together with their scope of activities and research topics.

Description of the programmes of the Doctoral School of Chemistry

K/1 Reaction Mechanisms and Catalysis (Head: Dr. István Fábián)

Teaching staff involved in the programme

György Bazsa, Attila Bényei, Csilla Enikő Czégéni, Zoltán Dudás, István Fábián, Attila Forgács, Oldamur Hollóczki, Henrietta Horváth, Ferenc Joó, József Kalmár, Ágnes Kathó, Adél Len, Norbert Lihi, Nóra May, Gábor Papp, Mária Szabó, Zoltán Tóth, Antal Udvardy

Research topics

Organometallic catalysis in aqueous media and its application in organic synthesis. Mechanisms of catalytic solution reactions. Mechanisms of redox reactions with complex kinetics. Synthesis and characterisation of functionalised aerogels. Heterogenisation of molecular catalysts. Solid-state reactions. Application of X-ray diffraction in supramolecular chemistry. Structure determination from powder diffraction data. Investigation of the polymorphism of pharmaceutical active ingredients. Computer-aided molecular modelling.

Description of the Doctoral Programme

The program is based on the achievements of the traditionally strong research activity in reaction kinetics and materials science at the Institute of Chemistry, University of Debrecen.

In the field of homogeneous catalysis, we investigate the chemical features and applications of metal-organic catalyzed reactions in aqueous media (e.g., hydrogenation, deuteration, redox isomerization, carbon-carbon cross-couplings), as well as the homogeneous catalytic transformations of carbon dioxide and nitrogen oxides. As soluble catalysts, we primarily use platinum metal complexes containing tertiary phosphines, N-heterocyclic carbenes, and hydrogenated salen (salan) ligands, the synthesis and characterization of which are of fundamental importance in our studies. We prepare stabilized metal colloids and study their use as efficient hydrogenation catalysts in aqueous solution. Using a microfluidic hydrogenation reactor and employing microwave activation, we explore the possibilities for new types of organic syntheses. Solid-phase reactions are mainly applied to produce new ligands and catalytically active metal complexes, as well as to develop simple and fast methods for the preparation of known catalysts. Based on these results, we develop new chemical hydrogen

storage systems. Using planetary and vibratory ball mills, we design standardized grinding programs for mechanochemical reactions.

Our studies on the kinetics and mechanisms of complex redox reactions focus on the following topics: redox reactions of chlorine, sulfur(IV), oxychlorine and peroxo compounds; the reactions of reactive oxygen species (ROS); the synthesis, characterization, and coordination chemistry of substituted 1,10-phenanthroline N-oxides; the activation of O_2; and the models of metalloenzymes that regulate ROS concentrations in biological systems. This research activity is based on the following tasks: i) identification and characterization of reactive intermediates; ii) thorough investigation of the kinetics of the reactions and determination of the rate equation for each step; iii) recognition of the dominant reaction paths; iv) exploring the kinetic couplings between competing reaction paths; and v) developing detailed models for the interpretation of the kinetic and stoichiometric properties by evaluating all experimental data simultaneously. The results can be useful in practical applications related to environmental chemistry, drinking and wastewater treatment technologies, greywater recycling, disinfection, bleaching, high-efficiency industrial oxidation processes, etc., and facilitate understanding the chemical background of various in vivo redox processes.

Over the course of our studies on aerogels, we develop optimized methods for synthesizing high-porosity materials suitable for various applications, including removal of toxic metal ions from water and air; creation of special thermal insulation systems, also applicable in space technology; high-efficiency heterogeneous catalysis; artificial active bone replacement; designing new drug carriers; enzyme immobilization; and the production of photocatalytic aerogel hybrid systems. We explore the relationships between the composition, structure, and various physical and chemical properties of aerogels. The results make it possible to design and produce new functionalized materials with special properties.

The structural investigation of new compounds, heterogeneous catalysts and aerogels is closely related to the previously mentioned research areas. For this purpose, single crystal X-ray diffraction structure analysis method is used. Other topics of studying solid state materials include supramolecular chemistry, structure determination from powder diffraction data, and the investigation of the polymorphism of active ingredients in pharmaceutical products.

Computational chemistry is extensively used to support experimental data in all research areas of the program. In addition, the impact of nanomaterials on the environment and human health is investigated using computational molecular modelling methods. This research area

contributes to understanding of how nanomaterials interact with biomolecules and how they change the secondary structure of proteins and cell membranes. The results will be used to clarify how these interactions may contribute to the development of various neurodegenerative diseases.

The Council of the Doctoral School of Chemistry has decided that research on didactical issues in the teaching of chemistry at primary, secondary and tertiary level is to be carried out within this program. The significance of education in the development of the chemical knowledge and attitudes of the youth and adult population is extensively analyzed. These studies are highly relevant in training and supplying chemistry teachers. Regular surveys are conducted among primary and secondary school students to understand the impact and role of various factors (textbook, teaching methods, everyday experiences, etc.) that determine their conceptual development. We aim to identify the knowledge structure that mostly characterizes students using knowledge space theory and word association methods.

K/2 Coordination Chemistry (Head: Dr. Gyula Tircsó)

Teaching staff involved in the programme

Zsolt Baranyai, Ernő Brücher, Péter Buglyó, Éva Dóka, Etelka Farkas, Zoltán Garda, István Jószai, Csilla Kállay, Ferenc Krisztián Kálmán, Nigel John Mason, Péter Nagy, Imre Sóvágó, Dezső Szikra, Gyula Tircsó, Imre Tóth, Katalin Várnagy

Research topics

Coordination chemistry research in bioinorganic chemistry. Complexes of metal ions of importance in medical diagnosis and therapy formed with oxygen- and nitrogen-donor polyfunctional ligands. Organometallic chemistry. Investigation of redox reactions that play a pivotal role in living organisms.

Description of the Doctoral Programme

Within the framework of the program, the largest area of the coordination chemistry research is dedicated to topics motivated by bioinorganic chemistry. One of the most extensive research fields involves the equilibrium and structural (UV–Vis, CD, ESR, NMR, MS) studies of complexes formed between essential trace elements (Fe, Cu, Zn, Ni, Co, Mn, Mo), as well as certain toxic elements (Cd, Pb, Pd), and amino acids, peptides, and their derivatives. In addition,

the research also focus on the redox properties of the formed complexes, and on the metal ion–catalyzed oxidation and hydrolysis of peptides. The primary aim of these studies is to uncover potential relationships between metal ions and neurodegenerative disorders.

Another major area of coordination chemistry research concerns the thermodynamic, kinetic (formation, dissociation, solvent exchange, etc.) and structural characterization of complexes formed by oxygen- and nitrogen-donor polyfunctional ligands with metal ions used in medical diagnostics (e.g., Gd(III), Mn(II), Fe(II/III)) and in therapeutic applications, particularly metal isotopes (^{47}Sc, ^{67}Cu, ^{90}Y, ^{177}Lu, ^{212}Bi, ^{223}Ra, ^{225}Ac, etc.), as well as isotope pairs applicable in theragnostic procedures, combining diagnostic and therapeutic modalities (e.g., $^{44/47}$Sc, $^{64/67}$Cu, $^{86/90}$Y, ^{89}Zr/^{90}Y, ^{89}Zr/^{177}Lu, etc.). Based on the results of intensive research in these areas, our objectives also include the application-oriented design and synthesis of chelators and the characterization of their complexes - steps that are indispensable precursors to clinical applications. Recently, we have also turned our attention to the design and synthesis of "smart" probes (e.g., pH- or Zn(II)-responsive systems), organ-specific (e.g., liver-specific), and bimodal (MRI–PET, MRI–optical, etc.) contrast agent candidates. Techniques applied include pH-potentiometry (equilibrium studies), UV–visible spectrophotometry (equilibrium and kinetic measurements), spectrofluorimetry (equilibrium and kinetic studies), one- and multidimensional and TD NMR spectroscopy (using conventional nuclei such as ^{1}H, ^{13}C, ^{17}O, ^{19}F and ^{31}P, as well as more exotic nuclei such as ^{45}Sc, ^{67}Ga, ^{89}Y, ^{115}In, ^{195}Pt, $^{203/205}$Tl, etc. for equilibrium, structural, kinetic, and dynamic studies), along with HPLC (analytical and preparative purification) and MS techniques supporting preparative organic chemistry (ligand synthesis).

Redox reactions play a fundamental role in living organisms. A substantial shift in the redox balance toward oxidative processes leads to oxidative distress, which is cell-damaging and may contribute to, among other things, the development of cancer. Reactive oxygen species (ROS), such as the superoxide radical anion ($O_2^{\bullet -}$) and hydrogen peroxide (H_2O_2), are primarily responsible for oxidative stress. Therefore, the program places special emphasis on studying the oxidative processes induced by ROS on the thiol side chain of proteins containing cysteine (Cys-SH) amino acid residues (Protein–Cys–SH). These include investigating the effects of thiol-group redox reactions on protein function (inhibition or activation), protein–protein interactions, intracellular localization of proteins, and transcription-level regulation. Redox regulation - regulation via oxidation - affects numerous key proteins within cells, such as phosphatases, kinases, and various transcription factors. In this context, and from the

perspective of redox signaling, H_2O_2 is the most important and widely studied oxidant. Consequently, our research objectives also include the detailed investigation of the enzymes responsible for its degradation, particularly the peroxiredoxin protein family. The study of reactive sulfur species (RSS) has become a significant field in redox biology in recent decades; their investigation is also within our scope, as are the persulfidation processes of redox-active proteins, given that reactive sulfur species play key roles both in tumor development and in the response to cancer therapy.

K/3 Analytical Chemistry (Head: Dr. Attila Gáspár)

Teaching staff involved in the programme

Melinda Pokoraczkiné Andrási, Edina Baranyai, Ildikó Bodnár, Mihály Braun, Attila Gáspár, Róbert Huszánk, Zoltán Juhász, Zsófia Kertész, József Posta

Research topics

Developments and applications of analytical and environment monitoring methods for pharmaceutical, clinical, proteomic, food and environment chemistry. Development, hyphenation and application of different spectrometric methods (mostly mass, UV, atomic and X-ray spectrometric) and separation methods (chromatography and electrophoresis). Ion-beam spectrometry. Determination of environment pollutants in (human) biological and envrironmental samples. Study of atmospheric aerosols. Analysis of elemental species. Development of microfludic, lab-on-a-chip devices. Study of chemical structures of molecules.

Description of the Doctoral Programme

Fundamental, bioanalytical and proteomic research and applications of capillary electrophoresis. In these studies after the high efficiency separation of components (mostly pharmaceuticals, proteins, monoclonal antibodies, biologicums), their sensitive detection and elucidation of their structure are performed with tandem mass spectrometry. The study of the posttranslational modifications of proteins is received special emphasis.

In environmental analyses the components of gas, liquid and solid environmental samples are determined with elemental analytical instruments, often coupled with separation methods. These studies aim at the determinations of pollutants with natural or antropogenic origin in environmental biological and food samples (drinking water, surface and grey waters,

atmospheric aerosols, dusts, soil extracts, sediments, honey and oher food samples, pharmaceuticals, blood, hair, EDC materials (endocrine desrupting chemicals), etc). An important research topic is the reconstruction and monitoring of the change of the environment in our region which is getting more and more industrialized (pharmaceutical, battery and car industry).

The goal of the microfluidic research to develop analytical systems based on the lab-on-a-chip conception, which can be fast, efficient and still cheap tools to analyse environmental or clinical samples.

K/4 Macromolecular and Surface Chemistry (Head: Dr. Sándor Kéki)

Teaching staff involved in the programme

István Bányai, Katalin Czifrák, Sándor Kéki, Mónika Kéri, Ákos Kuki, István Lázár, Noémi M. Nagy, Lajos Nagy, Tibor Nagy, Levente Novák, Zoltán Szűcs, Nóra Vajda, Miklós Zsuga

Research topics

Synthesis of polymers and copolymers with tailored properties. Preparation of light-emitting and shape-memory polymers. Characterization of natural and synthetic polymers by soft ionization mass spectrometry. Investigation of interfacial reactions on clay minerals using radioindication. Macromolecular colloids and their metal complexes. Synthesis and study of aerogels and aerogel nanocomposites. Application of high- and low-resolution NMR to the study of porous materials, gels and sols.

Description of the Doctoral Programme

Our research topics include the preparation of new functional homo- and copolymers and their transformation via polymer-analogous reactions, as well as the synthesis of linear and star-shaped amphiphilic copolymers and polymer networks with designed segment lengths, and the study of phase separation by transmission electron microscopy and by light-scattering photometry in different solvents. During the programme, students can learn the basics of dry-box techniques while studying living cationic polymerization.

With a view to green chemistry, we work on the following topics: the synthesis of new, partially biodegradable thermoplastic materials; the use of recycled polyurethanes; the preparation and investigation of synthetic macromolecular hydrocarbons with lubricant and lubricant-additive properties; and the synthesis of biopolymers. Our topics related to the medical applications

include e.g. development of sustained- and controlled-release dosage forms and investigation of the release process; study of the micro- and macrostructure of the resulting dosage forms, the behavior of membranes, and diffusion and osmotic conditions; investigation of the solution structure and dynamics of PAMAM dendrimers with a view to controlled and delayed drug release; improvement of the bioavailability of poorly soluble active ingredients; and beyond the methods known so far, exploration of new possibilities for improving solubility by extrusion of polymers and active ingredients and the study of molecularly dispersed systems formed in the resulting “solid solutions” after solidification.

Further research areas include the synthesis and investigation of aerogels and aerogel nanocomposites with particular emphasis on their chemical, engineering, optical and biomedical applications as well as the synthesis and study of new macrocyclic complexing agents.

We also conduct extensive research on smart polymer-based systems, such as the preparation and characterization of compounds, polymers and composites with light-emitting and shape-memory properties. Our goal is to produce materials that emit light of different wavelengths in solvents of different polarity, i.e. that exhibit solvatochromic effects. This property can be used to determine the polarity of the microenvironment (e.g. biological systems) and can also extend their applicability to molecular detection.

In the field of shape-memory polymers, our topics include the preparation of chemically cross-linked shape-memory di- and triblock copolymers based on polyurethanes. As flexible blocks, we incorporate well-defined functional polyisobutylene and/or polyethylene oxide prepared by living polymerization. The mechanical properties of the cross-linked systems are investigated, and possibilities are explored for their biomedical applications and composite formation. The shape-memory behavior of interpenetrating polymer networks (semi-IPN), e.g. polyurethane/epoxy (PU/EP) systems is also studied including the incorporation of reinforcing agents to increase the force generated during recovery.

Our analytical research focuses on the characterization of natural and synthetic polymers by modern soft ionization mass spectrometric methods, and on uncovering relationships between the properties and structures of polymers/copolymers using artificial intelligence.

The main objectives of our research on macromolecular colloids include the following: the synthesis and functionalization of poly(amino acid)-type polymers and their partial hydrophobization to modify their tertiary structure; characterization of the resulting ligands and

investigation of their solution structure using multinuclear and multidimensional NMR spectroscopy; study of the equilibria, structure and dynamics of metal complexes of macromolecular ligands in solution; and exploration of possible applications of these metal complexes in environmental protection, catalysis and medicine.

In the field of interfacial reactions, we primarily use radioindication methods to investigate the binding of microelements essential for plants, environmentally relevant cations, and radioactive contaminant ions on the surface of clay minerals. We also study the mechanisms of catalytic reactions occurring at the surface of clay minerals.

The three types of solution-state NMR spectroscopy are suitable for studying solid materials, gels and sols. Using NMR cryoporometry, the pore size of both soft and hard porous materials can be determined if it is smaller than 100 nm. Our PhD students can study the swelling of macromolecular colloids and the pore size of carbon nanoparticles and carbon-based gels using this technique. NMR diffusometry is an important tool for investigating larger pore sizes and pore structures and through this our students can gain insight into certain aspects of the structure and adsorption behavior of solid materials and gels. Low- and high-resolution NMR relaxometry is suitable for studying the size and dynamics of colloids; with this method, PhD students can characterize carbon nanoparticles and dilute polymer solutions. Involving quadrupolar NMR nuclei (^{23}Na, ^{17}O) opens up new perspectives in this field.

In the future, it will also be possible to study solid-state NMR within the Doctoral School. The necessary hardware has been installed, and experiments are beginning to integrate this method into the programme's portfolio.

K/5 Chemistry and Chemical Biology of Carbohydrates and Heterocycles

(Head: Dr. Tibor Kurtán)

Teaching staff involved in the programme

Ilona Bakai-Bereczki, Teréz Barna, Gyula Batta, Éva Bokor, Anikó Borbás, Magdolna Csávás, Anikó Fekete, Erzsébet Fekete, Gyöngyi Gyémánt, Mihály Herczeg, Pál Herczegh, László Juhász, Éva Juhászné Tóth, Levente Karaffa, János Kerékgyártó, Attila Kiss, Krisztina Kónya, Tibor Kurtán, Attila Mándi, László Somsák, László Szilágyi, István Timári, Marietta Vágvölgyiné Tóth

Research topics

Synthesis, selective transformations and structural analysis of condensed chiral O- and O,N-heterocycles with potential pharmacological activity. Application of domino cyclization reactions to prepare condensed and spirocyclic bioactive heterocycles having novel skeleton and containing condensed benzene and/or heteroaromatic subunits. Stereoselective synthesis and pharmacological investigation of benzene-fused homo- and heterodimeric heterocycles containing central and axial chirality elements. Application of chiroptical and in silico methods to study the absolute configuration and conformation of natural and synthetic derivatives.

Synthesis of carbohydrate-containing, carbohydrate-based natural compounds, their analogues and building blocks. Design and synthesis of glycomimetics and enzyme inhibitors. Study of the mechanisms of action of glycoenzymes. Study of carbohydrate-protein interactions using modern instrumental methods.

Description of the Doctoral Programme

More than half of the known organic compounds are considered heterocycles, and in the vast majority of them, the heteroatom is nitrogen, sulphur and oxygen. Heterocyclic derivatives provide the skeleton of numerous natural pharmacologically important groups of compounds such as flavonoids, alkaloids, antibiotics, and play a fundamental role in biochemical processes of living organisms. The majority of naturally occurring and synthetic pharmaceuticals and agrochemicals contain at least one heterocycle, the efficient and stereoselective preparation of which is a major challenge for organic synthetic chemistry.

The most abundant and widespread carbohydrates on earth usually exists in (hetero)cyclic form. The study of carbohydrates is a more or less separate field of organic and biochemistry, due to the large number of functional groups and stereogenic centers, as well as their biological properties. However, due to the mutual influence with other scientific fields (e.g. analytics, biomedicine, materials science), we can now speak of an independent carbohydrate science.

Glycobiology, the study of the biological role, biosynthesis and transformation of carbohydrates, has demonstrated the key role of sugar derivatives and their conjugates, e.g. glycoproteins and glycolipids, in several fundamental recognition processes. The rapid development of this field and of carbohydrate science continues today, progressing synergistically with improvements in separation techniques and structural elucidation methods.

Like other "omics" fields (e.g. genomics, proteomics), the systematic study of the carbohydrate content of a cell or organism (glycan, glycome) is now part of the subject of glycomics.

The biological roles of heterocycles and carbohydrate derivatives are mediated by their interactions with macromolecules, most often with proteins (receptors/lectins, (glyco)enzymes, antibodies) that recognise, transform or induce immune responses to (small) molecules. These interactions can also be studied using chemical biology methods. This involves 'perturbing' biological systems *in vitro* or *in vivo* with small molecules and inferring the essential properties of the system from the response to these perturbations. This information can be used, among other things, in drug design.

The above gives rise to important areas of research for both synthetic carbohydrate chemistry and heterocyclic chemistry: the preparation of natural compounds (e.g. oligosaccharides, glycoproteins, glycolipids, alkaloids, antibiotics) and/or their essential constituents (e.g. *N*- and *O*-glycosylated amino acids, peptides, heterocyclic scaffolds); the synthesis of mimetics (compounds structurally and/or functionally analogous to naturally occurring substances: e.g. *C*-glycosyl derivatives, neoglycoconjugates, glycodendrimers, vaccines, bioisostere compounds); the design and synthesis of inhibitors that may provide the possibility to interfere with biochemical processes.

Our doctoral program offers training and research opportunities in these areas:

Development of carbohydrate protective groups and their application to the synthesis of biologically active oligosaccharides; use of cyclodextrins for the preparation of linear glycoside derivatives; synthesis of *N*-glycans and *N*-glycopeptides; transformations of the anomeric centre of carbohydrates by radical, anionic, carbenic reactions; design and preparation of glycomimetics (e.g. carbohydrate sulphonic acids, derivatives containing non-classical glycosidic bonds, *C*-glycosyl compounds, neoglycoproteins, carbohydrate-amino acid hybrids).e. g. carbohydrate sulphonic acids, derivatives with non-classical glycosidic bonds, *C*-glycosyl compounds, neoglycoproteins, carbohydrate-amino acid hybrids); design and preparation of glycoenzyme inhibitors (e.g. glycoside hydrolase, neuraminidase, glycosyltransferase, glycogen phosphorylase); design and synthesis of SGLT inhibitors; investigation of transformation possibilities of unsaturated carbohydrate derivatives; preparation of platinum metal complexes containing a carbohydrate moiety; Glycoenzyme binding site mapping, active site and mechanism of action studies; enzyme catalysed syntheses;

lectin inhibitor design and synthesis; carbohydrate-protein interaction studies using mass spectrometry, ITC and NMR methods.

Stereoselective synthesis of chiral heterocycles condensed with benzene or heteroaromatic units by domino ring closure reactions and their further transformations; elucidation of the stereochemistry of chiral targets and exploration of the stereoselectivity of the reactions by combined structural (chiroptical spectroscopy, X-ray diffraction, 2D NMR) and in silico (DFT mechanism calculations, OR, ECD, VCD calculations) methods; investigation of the efficient production of polycyclic, condensed or bridged heterocycles by domino reactions; specific ring-closure reactions (e.g. oxa-Pictet-Spengler, intramolecular oxa-Michael, hetero Diels-Alder) for the formation of heterocyclic systems. Stereoselective preparation of biaryl-type homo- and heterodimeric heterocycles containing central and axial chirality elements for pharmacological and stereochemical studies. Investigation of antiproliferative, neuroprotective and antimicrobial activity on chiral heterocyclic target compounds.

OR, ECD (HPLC-ECD) and VCD characterisation of natural and synthetic heterocycles and DFT calculation of the chiroptical data. DFT calculation of NMR chemical shift values and coupling constants for the determination of relative configuration. DFT calculation of ring-closure reaction mechanisms and determination of activation parameters.

Study of metal-free and metal-catalysed cross-coupling reactions (C-C and C-N bond formation), elucidation of their selectivity (e.g. Suzuki-Miyaura, Heck-Mizoroki, Sonogashira, Buchwald-Hartwig and Ullman couplings); study of cross-coupling reactions of *O*-heterocyclic compounds based on C-H activation; synthesis of heterocyclic compounds with biological activity. Closely linked to the above is the provision and development of the necessary analytical background (GC, HPLC, SCF-LC, GC-MS, HPLC-MS).

The actual research topics from these areas change annually and are generally characterised by the fact that they include chemical, biochemical, structural and chemical-biological aspects of the areas under investigation.

List of courses of the Doctoral School of Chemistry, University of Debrecen

Instructor	Course Title	Tárgy kód
Zoltán Tóth	Methodology of Didactic Research	T_PK6131
Anikó Borbás	Chemical Biology	T_PK5305
Attila Mándi	Asymmetric Syntheses	T_PK6202
Katalin Várnagy, Péter Buglyó	Coordination Chemistry of Transition Metals	T_PK2110
József Posta	Atomic Absorption Spectrometry	T_PK3214
László Somsák	Carbohydrate chemistry	T_PK6117
Levente Novák	Biocolloid Systems	T_PK4502
Katalin Várnagy, Csilla Kállay	Bioinorganic Chemistry	T_PK2109
Péter Buglyó	Organometallic Chemistry	T_PK2010
Melinda Pokoraczkiné Andrási	Gel Electrophoresis	T_PK4123
Teréz Barna	Glycoenzymes	T_PK5301
István Fábián, Mária Szabó	Kinetics of Fast Reactions	T_PK2105
József Kalmár	Advanced Chemometrics	T_PK2113
Tibor Kurtán	Advanced Chiroptical Spectroscopy	T_PK5304
Noémi Nagy, József Kónya	Interfacial reactions on rocks and soils	T_PK4130
Mihály Braun	ICP-MS	T_PK4122
Sándor Kéki	Smart Plastics	T_PK4132
Ildikó Bodnár	Ionchromatography	T_PK4124
Ilona Bakai-Bereczki	Chemistry and Medicinal Use of Drugs of Abuse	T_PK5312
Attila Gáspár	Capillary zone electrophoresis	T_PK4121
Gábor Papp	Organometallic Catalysis in Organic Synthesis	T_PK1108
Ferenc Kálmán, Norbert Lihi	Coordination Chemistry	T_PK2104
Zoltán Garda	Modern Chromatographic Procedures	T_PK3206
István Timári	Application of Modern NMR Methods	T_PK5315
Gyula Tircsó	Complexes of macrocyclic ligands	T_PK2107
László Juhász	Chemistry and synthesis of secondary natural compounds	T_PK5316
Antal Udvardy	Mechanochemical synthesis	T_PK1124
Attila Gáspár	Microfluidics, Lab-on-a-chip	T_PK3220
Lajos Nagy	Modern Liquid Chromatographic Methods	T_PK4127
Gyula Batta	Theory of Modern NMR Methods	T_PK5101
Tibor Nagy	Modern Mass Spectrometric Methods	T_PK4129
Katalin Czifrák	Plastics	T_PK4113
Krisztina Kónya	High throughput synthetic methods	T_PK5307
Gyula Batta	NMR Operator Training I (Practical)	T_PK5201
István Timári	NMR Operator Training II (Practical)	T_PK5203
István Timári	Multidimensional NMR	T_PK6110
Nóra May	Structural investigation of paramagnetic transition metal complexes by EPR spectroscopy	T_PK2116
Noémi Nagy	Nuclear and radioanalysis; its applications	T_PK3301
Krisztina Kónya, Marietta Vágvölgyiné Tóth	Reaction Mechanisms	TTKME0311
Péter Nagy	Redox Chemistry in Biological Systems	T_PK2112
István Bányai	Relaxation Methods in Chemistry	T_PK1101

Attila Bényei	Structure determination by X-ray diffraction	T_PK1115
Éva Bokor	Carbohydrate-Based Drug Design	TTKME4303
Attila Kiss, Gyula Batta	Carbohydrate Analysis and Structural Studies	T_PK5309
Attila Mándi	In silico conformational analysis and spectrum calculation of organic compounds	T_PK5311
Tibor Kurtán	Stereochemical structural elucidation methods	T_PK6201
Oldamur Hollóczki	Selected Topics in Theoretical Chemistry	T_PK1125
Anikó Borbás	Protective Group Manipulations in Carbohydrate Chemistry	T_PK5310
Ákos Kuki	Simulation of Chemical Industry Processes	T_PK4131
Mihály Herczeg	Chemistry of Anticoagulant Compounds	T_PK5126

List of subjects for the complex (comprehensive) examination of the Doctoral School of Chemistry, University of Debrecen

Major subjects

1. Reaction kinetics
2. Catalysis
3. Research in chemical education
4. Coordination chemistry of transition metals
5. Coordination chemistry of main-group elements
6. Instrumental analytics
7. Macromolecular chemistry
8. Colloid and surface chemistry
9. Radiochemistry
10. Modern NMR methods
11. Medicinal chemistry
12. Chemistry and biochemistry of carbohydrates
13. Chemistry of heterocyclic compounds
14. Chemistry of antibiotics
15. Chemistry of non-metallic elements
16. Molecular modelling

Minor subjects

1. Nonlinear chemical dynamics
2. Activation of small molecules
3. Catalysis in green chemistry
4. Relaxation kinetic methods
5. Transition-metal complex catalysis
6. Teaching of chemistry
7. Bioinorganic chemistry
8. Analytical chemistry of environmental protection

9. Kinetics and mechanisms of reactions of complexes
10. Macrocyclic ligands and their complexes
11. Chemistry of complex equilibria
12. Organoelement chemistry
13. Coordination chemistry of non-metallic elements
14. Atomic and molecular spectroscopy
15. Electrochemical analytical methods
16. Electrophoretic methods
17. Chromatographic analytical methods
18. Surface analytical chemical methods
19. Radioanalytical methods
20. Synthesis and structure of macromolecules
21. Plastics
22. Colloid chemistry of macromolecules
23. Interfacial chemistry
24. Spectroscopic methods in structural elucidation
25. Synthetic methods for carbon–carbon bond formation
26. Structural studies of peptides and proteins
27. Glycoenzymes
28. Mechanisms of organic reactions
29. Synthons and retrosynthesis
30. Analytical chemistry of carbohydrates
31. Chemistry of enantio- and diastereoselective reactions
32. Materials chemistry
33. Application of theoretical chemical methods in elucidating reaction mechanisms and in structural studies

Other essential elements of the training programme

Personal and infrastructural conditions of the doctoral training

In the "Chemistry" doctoral programme and in the Chemistry Doctoral School that developed from it, internationally recognised, highly qualified and experienced lecturers and researchers have worked and continue to work, which has always guaranteed that doctoral students receive up-to-date, high-level training.

The infrastructural conditions of the doctoral training and the technical and instrumental background of the research—despite known difficulties—are adequate by international standards and outstandingly good in a national comparison. As a result of the coordinated development programme of the Institute of Chemistry and the Doctoral School of Chemistry (KTDI), modern instrumental laboratories have been established. The most important instruments in the central institutional facility include: Avance II 400 and Avance II 500 MHz and Avance Neo 700 NMR spectrometers, a Bruker Nonius MACH3 single-crystal X-ray diffractometer, Bruker MALDI-TOF, ESI-QTOF and CE-QTOF-MS and Pfeiffer quadrupole mass spectrometers, a MicroCal ITC200 titration calorimeter, an AR550 advanced rheometer, a Beckman J2-21M ultracentrifuge, Paragon 1000 and Spectrum One FT-IR spectrometers, a J-810 Jasco CD spectropolarimeter with a coupled chiral HPLC system, a J-715 Jasco CD spectropolarimeter, a Chiral-IR2X VCD spectrometer, a Perkin Elmer Polarimeter 341, an Elementar Vario Microcube elemental analyser, continuous-flow reactors (H-cube, Phoenix reactor, ASIA flochem reactor system), and a Liberty 1 peptide synthesiser. The continuously expanding instrument park has created and ensures the possibility that individual subject areas can be taught and demonstrated at the highest scientific level, with a realistic chance of direct practical implementation.

International relations of the Doctoral School

The Doctoral School of Chemistry has extensive international relations. These have primarily developed through the scientific work of the School's academic staff, but there are also contractual international collaborations that apply to the School as a whole or to the participating teaching and research units. We make use of the opportunities offered by the Erasmus programme and Marie Curie fellowships, and there have also been examples of French–Hungarian joint PhD training. In addition to the above, almost all forms of international

cooperation have occurred (TéT collaborations, COST programmes, MTA–NSF, MTA–DAAD, MTA–CNRS and other international relations and scholarships, e.g. Stipendium). Our aim is that, during the four years of doctoral training, as many PhD students as possible participate in a study visit abroad, as we consider this to be an important element of the training.

Aim of the doctoral training

Our doctoral program primarily attracted students with degrees in chemistry, chemistry teaching, and pharmacy, but we also admitted students with degrees in bioengineering and biotechnology, both from Hungary and from abroad. Through theoretical and practical training, doctoral students become familiar with key questions in a particular subfield of chemistry. They carry out experimental and theoretical research to explore known problems in the field and to achieve new research goals. In this way, they acquire the most important methodological knowledge of scientific research.

Training competences

Upon completion of the program, doctoral students will be able to conduct independent research and plan and execute research based on scientific literature. They will be familiar with and able to apply modern research methods and interpret measurement results in a well-founded manner. They will publish their research findings in international journals. They will apply their knowledge in the fields of basic and applied research, while also protecting the environment.

Forms and requirements of the doctoral training

In accordance with the Higher Education Act, the duration of doctoral training is four years. During this period, doctoral students must obtain 241 credits, of which full-time students must earn 196 research, 13 study and 32 teaching credits. For part-time students, 228 research credits and 13 study credits are compulsory.

A weekly 2-hour doctoral lecture course running for one semester (with examination) generally corresponds to 2 credits. In the Chemistry Doctoral School, apart from the course “Ethics of Scientific Research”, there are no compulsory courses. Taking into account the recommendation of their supervisor, doctoral students are free to choose from the announced courses. To assist

in this choice, the list of available doctoral courses can be found in the database compiled on the website of the Doctoral School of Chemistry: https://chemistryphd.unideb.hu/en/elective-subjects-doctoral-school-chemical-sciences

The research topics, which are renewed annually, can be found on the website of the National Doctoral Council: https://doktori.hu/doktori-kepzes/temakiirasok/ (The ID of the Doctoral School of Chemistry of the University of Debrecen is: 59). Our experience of more than two decades is that many prospective applicants find exciting research opportunities matching their professional goals among the topics offered by the Doctoral School of Chemistry.

Over eight semesters, doctoral students carry out the experimental and/or theoretical work forming the basis of their dissertation. The Doctoral School of Chemistry expects that, in the field of the dissertation topic, at least two papers will be published in peer-reviewed journals with an impact factor (with a DOI number, or available as a proof, or accepted for publication with written confirmation from the journal editor). A basic requirement is that at least one of these should be based on the candidate's substantial contribution.

In a given semester, typically close to thirty full-time, state-funded scholarship students and a few self-financed part-time and individual-track doctoral (PhD) students study and conduct research within the framework of the School. The tuition fees of the latter are often paid by their workplace (typically a pharmaceutical company or an academic institute). Under an agreement between the University and Richter Gedeon Plc., over the past ten years one of our full-time students each year has received their doctoral scholarship (supplemented by research support) from the pharmaceutical company.

Concluding remarks

In this document, we aimed to provide a comprehensive overview of the establishment, structure, development, and key research areas of the Doctoral School of Chemistry. This also serves as our training programme. As the most important general characteristic, we highlight that from the start of organised doctoral (PhD) training until 2025, **285 doctoral degrees** have been awarded to students who completed their studies within the framework of the Chemistry Doctoral Programme, and later the Doctoral School of Chemistry, or who prepared individually with the support of our faculty members.

The website of the Doctoral School of Chemistry is available at: https://chemistryphd.unideb.hu/en

Debrecen, 20 November 2025

Dr. Tibor Kurtán
professor
Head of the Doctoral School
of Chemistry