Thesis topics of Organic Chemistry Department for the 2nd semester of the 2026/2027 academic year

Dr. Éva Bokor, PhD

Institute of Chemistry
Chemical Glycobiology Research Group
Chemistry Building E-422
e-mail: bokor.eva@science.unideb.hu

1 student/Chemistry BSc/MSc or Chemical Engineering BSc/MSc

Synthesis of new glycosyl heterocycles and their half-sandwich platinum metal complexes

Platinum complexes (e. g. cisplatin, oxaliplatin) are widely used chemotherapeutic agents for the treatment of cancer. However, these drugs frequently cause serious side effects. Thus, there is a continuing search for other platinum metal complexes with better anticancer properties. In this regard, the half-sandwich type complexes of platinum-group metals (e. g. Ru, Os, Rh, Ir) represent a promising compound class. Recently, we have synthesized a series of such type of complexes incorporating heterocyclic monosaccharides as N,N-bidentate ligands. Several of these derivatives have been shown to be active against different cancer cells. For a detailed structure-activity relationship the aim of the diploma work will be the synthesis of new glycopyranosyl heterocycles and their half-sandwich type complexes.

Dr. Krisztina Kónya, PhD

Institute of Chemistry
Heterocyclic and Stereochemical Research Group
Chemistry Building E-407
e-mail: konya.krisztina@science.unideb.hu

2 students/ BSc or MSc Thesis

Synthesis of chiral dimeric biaryls with axial and central chirality elements

Stereoselective biaryl coupling reactions are to be studied to prepare bis-flav(an)one and other heterocyclic derivatives containing a chiral biaryl axis and central chirality elements for pharmacological studies. The stereochemistry of the target molecules is to be analyzed by chiroptical measurements supported with calculations. **(2 students)**

Dr. Sándor Kun, PhD

Institute of Chemistry
Chemical Glycobiology Research Group
Chemistry Building E-422
e-mail: kun.sandor@science.unideb.hu

2 students (Chemistry BSc/MSc or Chemical Engineering BSc/MSc)

Synthesis of galactopyranosyl heterocycles for the inhibition of galectins

Galectins are a class of proteins that bind structures containing β-galactosides. Their role can be observed in many processes; therefore, they are considered as therapeutic targets. Inhibition of galectins may open up opportunities for the treatment of cancer, inflammation, fibrotic and infectious diseases. The aim of the research is the synthesis of new, potentially galectin inhibiting C-galactopyranosyl heterocycles (tetrazoles, oxadiazoles, 1,2,4-triazoles). The studies will include the exploration of possible synthesis routes, the verification of the structure of the prepared compounds (using NMR and MS techniques) and, within the framework of an international collaboration, the determination of the affinity and selectivity of the inhibitors towards galectins.

Dr. Juhászné Dr. Tóth Éva, PhD

Institute of Chemistry
Chemical Glycobiology Research Group
Chemistry Building E-409
e-mail: toth.eva@science.unideb.hu

1 student/BSc Thesis

Synthesis of novel glycomimetics for galectin inhibition

Galectins are β-galactoside-specific carbohydrate-binding proteins that play a key role in immunomodulation, the regulation of cell-cell interactions, and several pathological processes, particularly tumor progression and pathogen-host cell interactions. To date, 19 galectins have been identified in the animal kingdom, 13 of which are found on the surface of human cells. Some galectins, such as galectin-3, play a role in a number of pathological conditions, such as cancer metastasis, fibrosis, and diabetes, and are therefore key biological targets for pharmaceutical research aimed at developing drug molecules for the treatment of these diseases.

Dr. Attila Mándi, PhD

Institute of Chemistry
Chemistry Building E-412
e-mail: mandi.attila@science.unideb.hu

BSc thesis (1 chemistry BSc or chemical engineering BSc student), MSc thesis (1 chemistry MSc or chemical engineering MSc student)

Stereochemical investigations of organic derivatives by computational chemistry and spectroscopic methods

Determination of the absolute configuration of optically active synthetic and natural derivatives of variable flexibility using TD-DFT (ECD, OR) and DFT (VCD) calculations. Study of the conformational distribution by comparison and calculation of measured solid and liquid chiroptical parameters. In the case of racemic mixtures or a small excess of enantiomers/diastereomers (scalemic mixtures), HPLC-ECD analysis of the compounds is also possible. If the relative configuration is not or only partially known, 13C- and 1H-NMR shift values are also calculated in order to determine the structure. There are also cases where methods based on classical conformational analysis do not give good results. In such cases, structures obtained from explicit solvent molecular dynamics trajectories, or by calculating the stable complexes formed with solvent molecules will be used to investigate the stereochemistry of the target compounds. Requirements: basic knowledge of informatics (Excel, Word, PowerPoint, Linux), programming (bash), spectroscopics (OR, UV, ECD, IR, VCD, NMR) and molecular modeling (MM, MD, QM, DFT).

Dr. István Timári, PhD

Institute of Chemistry
Structural Chemistry, Molecular Recognition and Interaction Research Group (https://debnmr.unideb.hu/en)
Chemistry Building E-27
email: timari.istvan@science.unideb.hu

Application of advanced NMR methods for the structure elucidation of biologically active molecules

The biological activity of any molecule is primarily determined by the structure of the given molecule. Nuclear magnetic resonance (NMR) spectroscopy is one of the most powerful techniques for investigation of molecular structure in atomic detail. Due to the growing number of regulatory requirements for example in drug development, and consequently the increasing number of measurements required, there is a continuous demand for innovative methods that can provide maximal information in the shortest time possible. We will apply advanced NMR experiments to determine the structure of biologically active compounds, such as carbohydrates and peptides.

Prof. Tibor Kurtán

Professor of chemistry, department chair

Synthesis and Stereochemical Analysis of Heterocycles Research Group

Institute of Chemistry

Chemistry Building E-405

e-mail: kurtan.tibor@science.unideb.hu

Research topics for BSc. and MSc. students

5) **Synthesis of chiral biaryls with axial and central chirality elements.**

Stereoselective biaryl coupling reactions are to be studied to prepare bioactive bis-isochroman and other benzene-condensed heterocyclic derivatives containing a chiral biaryl axis and central chirality elements for pharmacological studies. Antiproliferative and antimicrobial activities are to be tested for the target compounds having a novel heterocyclic skeleton. The stereochemistry of the target molecules is to be analyzed by chiroptical measurements supported with calculations to suppport exploring stereochemistry-activity relationships. (3 student)

6) **Domino Knoevenagel-cyclization reactions for the preparation of condensed heterocycles.**

Stereoselective domino Knoevenagel-cyclization reactions are to be performed to prepare chiral condensed hetereocycles for pharmacological studies. The stereoselectivity is analyzed by NMR and chiroptical spectroscopic methods and X-ray diffraction and DFT calculations. Antiproliferative activity, specifically against human gliloblastoma cell lines, is to be identified for the novel heterocyclic scaffolds. Novel domino cyclization mechanisms will be explored to prepare condensed and bridged chiral *O,N,S*-heterocycles with a novel heterocyclic skeleton. Previous results have been patented and there are on-going *in vivo* studies to identify efficient candidates with antiproliferative activcity against glioblastoma. (3 student)