Thesis topics of Organic Chemistry Department for the 1st semester of the 2025/2026 academic year

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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.

Prof. Tibor Kurtán

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

Stereoselective biaryl coupling reactions are to be studied to prepare bis-isochroman 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 student)

2) 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. (2 student)

Dr. Juhászné Dr. Tóth Éva, PhD and Vágvölgyiné Dr. Tóth Marietta, PhD

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BSc thesis topic (Biochem. Eng. or Chem. Eng. or Chemistry BSc students)

Synthesis of anhydro-aldimines and their half-sandwich platinum-group metal complexes as potential anticancer agents

Carbohydrates are the most common natural compounds, which, in addition to playing a significant role as skeletal and nutritional functions, are also involved in the structural construction of the cell surface and in the vital cell recognition processes taking place there. These compounds are a relatively unexploited source of drugs and therefore offer exciting new therapeutic opportunities. The results achieved in the functional understanding of carbohydrate-protein interactions enabled the development of a new class of small molecule drugs. Glycomimetics imitate the biological functions of carbohydrates, so the investigation of their structure-effect relationship is essential, which opened a new path in pharmaceutical research.
In the Chemical Glycobiology Research Group (Department of Organic Chemistry, University of Debrecen) a large number of bioactive monosaccharide derivatives have been designed and synthesized for many years. During this work sugar containing half-sandwich platinum metal complexes have been synthesized and patented. Some have shown (sub)micromolar cytostatic activity against carcinoma, lymphoma and sarcoma cancer cells as well as antibacterial activity against multiresistant Gram positive bacteria.
Based on these preliminaries the aim of this research work to extend the SAR (structure – activity relationships) studies for different anhydro-aldose and aldonolactone (thio)semicarbazones, benzoylhydrazones and amidrazones by preparing of a diverse set of their new platinum metal complexes. Investigation of their antineoplastic activity will be performed in collaboration with Institute of Medical Chemistry, University of Debrecen.

Dr. Krisztina Kónya, PhD

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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

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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. Attila Mándi, PhD

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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

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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.