Thesis topics of Organic Chemistry Department for the 2nd semester of the 2024/2025 academic year

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 and Vágvölgyiné Dr. Tóth Marietta

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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

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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. Attila Mándi

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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).