Thesis topics of Organic Chemistry Department for the first semester of the 2021/2022 academic year

Prof. Tibor Kurtán
Institute of Chemistry
e-mail: kurtan.tibor@science.unideb.hu

BSc or MSc thesis topics

Domino cyclization methods for the synthesis of condensed chiral *O,N*-heterocycles

From readily available heterocyclic or acyclic starting materials, domino Knoevenagel-intramolecular hetero Diels-Alder and imine formation-cyclization reactions are planned for the synthesis of condensed chiral *O,N*-heterocycles. We are to examine how the structures of the substrate and reagent and the reaction condition influence the mechanism and outcome of the cyclization step. We aim to study the bioactivity and stereochemistry-activity relationship of the prepared target heterocycles containing new scaffolds.

two students, chemist-chemical engineer, B.Sc., M.Sc.

Dr. Bokor Éva
Institute of Chemistry
Chemical Glycobiology Research Group
Chemistry Building E-423
e-mail: bokor.eva@science.unideb.hu

BSc or MSc thesis topics

Synthesis of *C*-glycopyranosyl 1,2,4,5-tetrazines and study of their aza-Diels-Alder cycloadditions

1,2,4,5-Tetrazines are widely used as azadienes in Diels-Alder cycloaddition reactions. These types of reactions belong to the so called „click" reactions. The potential application of these transformations is intensively studied, e.g. for labeling of biomolecules. *C*-Glycosyl 1,2,4,5-tetrazines are unknown compounds, therefore the aim of the diploma work will be the synthesis

of such type of molecules. In addition, the study of the inverse elctron-demand [4+2] cycloaddition reactions of these heterocycles is also planned.

Synthesis of *C*-galactopyranosyl heterocycles as potential inhibitors of galectins

C-Glycopyranosyl heterocycles are among the important group of carbohydrate-based small molecules, whose biological effects are extensively studied. Numerous biologically active representatives of this compound class – e.g inhibitors of carbohydrate binding proteins – have been discovered. Recently, some *C*-β-D-galactopyranosyl azoles were shown to have galectin inhibitory activities. In the course of the diploma work the syntheses of new *C*-β-D-galactopyranosyl heterocycles are planned for the inhibition of galectins.

Dr. Kun Sándor
Institute of Chemistry
Chemical Glycobiology Research Group
Chemistry Building E-423
e-mail: kun.sandor@science.unideb.hu

BSc or MSc thesis (2 chemistry or chemical engineering students)

Synthesis of new spirocyclic glycomimetics

Carbohydrates involved in countless biological processes which motivates the developement of carbohydrate based therapeutics. In spite of this fact only a few carbohydrate based drugs are on the market.

The aim of the research is to design and synthesize potentially bioactive spirocyclic carbohydrates focusing on one of these areas:

a) Study of alternative pathways for the synthesis of sugar-spiro-morpholines, since there is no efficient and general method to get these compounds. These antioxidant spiroalkaloids and their analogs are promising therapeutics for the treatment of diabetic nephropathy, cardiovascular diseases and several other pathologies in which reactive oxygen species are involved.

b) Synthesis of xylopyranosylidene-spirocyclic substrates for a galactosyl transferase enzyme (β4GalT7) involved in glycosaminoglycan (GAG) biosynthesis. The planned derivatives may be applied against tumors by the inhibition GAG synthesis and forming cytotoxic xylose primed GAGs.

c) Synthesis of ribofuranosylidene-spiro derivatives against Helicobacter pylori infection, which is connected with a risk of gastric diseases, such as gastric cancer. The aim of this topic is to synthesize selective hybrid inhibitors of H. pylori adenylosuccinate synthase (AdSS) to impede purine supply of the bacterium.

Dr. Timári István
Institute of Chemistry
Chemistry Building B-12
e-mail: timari.istvan@science.unideb.hu

BSc or MSc thesis topics

1. Application of advanced NMR methods for 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 our advanced NMR experiments to enhance the structure determination procedure of biologically active compounds, such as carbohydrates, peptides and metal ion complexes.

2. Analysis of metabolomic samples by multi-dimensional NMR methods

In metabolomics (the systematic study of metabolites), one-dimensional (1D) ^{1}H NMR is still the most frequently applied experiment due to its simplicity and good sensitivity. However, 1D ^{1}H spectra of complex mixtures are often overcrowded, which makes the identification of many metabolites impossible causing a loss of potentially important information. Modern, multi-dimensional NMR methods can overcome many of these issues making the characterization of metabolomics samples more accurate.

Dr. Juhász László és Dr. Juhászné Dr. Tóth Éva
Institute of Chemistry
Chemical Glycobiology Research Group
Chemistry Building E-409
e-mail: juhasz.laszlo@science.unideb.hu
e-mail: toth.eva@science.unideb.hu

BSc thesis topic (1 student)

Study of functionalization reactions of glycal and exo-glycal derivatives

Glycals are derivatives in which there is a double bond between the C-1 and C-2 atoms of the carbohydrate backbone. In the case of exo-glycals, an exocyclic double bond is attached to the anomeric center. These compounds are important starting materials for many organic chemical syntheses, so the investigation and extension of their transformation possibilities are an important area of our research. We plan to prepare haloglycals (1- and 2-haloglycals and haloglycals with a halogen substituent on exomethylene) and their use in cross-coupling reactions (e.g. Suzuki, Sonogashira, Heck, Buchwald-Hartwig coupling).