

Thesis topics of Organic Chemistry Department for the 2nd semester of the 2021/2022 academic year

Dr. Kun Sándor

Institute of Chemistry
Chemical Glycobiology Research Group
Chemistry Building E-422
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 development 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 (β 4GalT7) 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. István Timári, assistant professor

email: timari.istvan@science.unideb.hu
Structural Biology, Molecular Recognition and Interaction Research Group
NMR Facility
website: <https://debnmr.unideb.hu/>

BSc and 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) ^1H NMR is still the most frequently applied experiment due to its simplicity and good sensitivity. However, 1D ^1H 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.