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RESEARCH AREA

A key step in the early stages of drug design is the design of potent drug molecules. This process is now mostly carried out using computer (pharmaco-informatics) methods, which are capable of handling both large amounts of structural data and complex energy calculations. The pharmacoinformatics toolbox will be used in both target-based and ligand-based design and will be extended with new procedures in the course of the PhD work. The methods will be tested and applied in curricular areas of pharmacology such as pain management, regulation of signalling, antiviral and epigenetic-based therapies.

TECHNIQUES AVAILABLE IN THE LAB

Computational molecular modeling, statistical methods of quantitative structure-activity relationships, programming in C, shell scripting

SELECTED PUBLICATIONS

Zsidó, B. Z., Börzsei, R., Pintér, E., Hetényi, C. (2021) Prerequisite Binding Modes Determine the Dynamics of Action of Covalent Agonists of Ion Channel TRPA1. *Pharmaceuticals* **14**: 988.

Zsidó, B. Z., Hetényi, C. (2021) The role of water in ligand binding. *Curr Opin Struct Biol* **67**: 1-8.

Zsidó, B. Z., Börzsei, R., Szél, V., Hetényi, C. (2021) Determination of Ligand Binding Modes in Hydrated Viral Ion Channels to Foster Drug Design and Repositioning. *J Chem Inf Model* **61**: 4011-4022.

Zsidó, B. Z., Hetényi, C. (2020) Molecular Structure, Binding Affinity, and Biological Activity in the Epigenome. *Int J Mol Sci* **21**: 4134.