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RESEARCH AREA

Development and application of computer-aided drug design 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. Computational analysis of target-drug interactions: Computational docking is an indispensable tool in drug design and is widely used by pharmaceutical companies. This project focuses on the prediction of the structure and energy of drug-target interactions by computer docking. The capabilities and limitations of the method will be investigated.

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

Horváth, I., Jeszenői, N., Bálint, M., Paragi, G, **Hetényi, C.** (2019) A fragmenting protocol with explicit hydration for calculation of binding enthalpies of targetligand complexes at a quantum mechanical level. **Int J Mol Sci 20:** 4384