Abstract

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Title of Diploma Thesis: **Creation of a virtual library of synthetic compounds for practical use in a molecular modelling study**

Drug development is a process requiring the analysis of a large amount of data. Creating a virtual library of synthesized compounds provides access to primary data concerning structure, results of biological activity studies, and molecular descriptors necessary for drug-like prediction. Chemical databases are usually used in virtual screening, which is a modern strategy of Computer Assisted Drug Design (CADD). Molecular docking is one of the methods.

Microsoft Excel was used to create the database, which includes different structural types, e.g., pyrazine, rhodanine, thiazolidin-2,4-dione, and 1,2,4-oxadiazole derivatives prepared in the research group Design and Development of New Antimicrobial Agents. Molecules are available in a spreadsheet containing all compounds in a line-notation ready-to-dock format.

To demonstrate this database's actual usage, a molecular modelling study was performed using the software Molecular Operating Environment (MOE). This study included molecular docking with three selected potential drug targets (human aldose reductase, mycobacterial β-hydroxyacyl-ACP dehydratase and mycobacterial phosphotyrosine phosphatase B). The aim of the study was to examine interactions and score of individual small molecules. Results emphasized compounds that could be of interest to upcoming real screening.

The virtual library of total 317 compounds was created and can be used for academical and scientific use, e.g., for a future molecular modelling study or for other CADD approaches.