ABSTRACT

In the early phases of drug design and development, scientists must overcome many challenges involved in identifying potential drug-like or lead-like compounds. This has led to the need of creating large sets of chemical data which will aid in improving the identification of pharmacophores and active compounds. Various scientific fields especially pharmacology, medicinal chemistry and biochemistry have begun to employ the use of computer sciences to aid in the screening for potential leads with more specificity with regards to drug-like compounds' or substances' bioactivity. The emphasis of this project was to create a database containing a collection of pyrazine compounds synthesized overtime in the Faculty of Pharmacy (Charles University, Hradec Kralove) with the aim of having anti-mycobacterium (and possible antibacterial and antifungal) activity, and further utilize this database to predict certain pharmacokinetic and bioavailability properties. This project seeks to demonstrate how certain molecular descriptors can be used as reliable chemoinformation to determine the likeliness or possibility of developing a lead-like or drug-like compound by utilizing computer software. An in-house database of 623 compounds saved in SMILES format was created and used in demonstrating quantitative structure-activity relationships (QSAR) and in evaluating and analyzing whether optimal lead-like or drug-like compounds are being produced. The database can be used to guide future synthesis with regards to CADD (Computer aided drug design).