



Web interface for Quantitative Structure-Activity Relationship modelling

(Bachelor-/ Studienarbeit)

Quantitative Structure-Activity Relationship (QSAR) aims at predicting the biological activity of chemical compounds from their structure. If done reliably, this can be especially useful for rational drug design. Thus, the number of drug candidates to be examined by further computational and experimental tests can be drastically reduced and insight into which properties of compounds are important for the desired biological action might be attained.

The goal of this project is to create a web interface to our QSAR library which is part of the BALL [1,2] (Biochemical Algorithms Library) package. The constructed website should allow interactive, user-friendly creation of regression and classification models and application of feature selection and validation procedures. Furthermore an interface to the molecular descriptor calculator program DRAGON [3] is to be implemented and included into the web page.

Some experience with web programming (html, php, etc) and some basic C++ skills would thus be helpful for this project.

[1] Kohlbacher, O, and Lenhof, H (2000). BALL - Rapid Software Prototyping in Computational Molecular Biology. *Bioinformatics* 16(9):815–824.

[2] www.ball-project.org

[3] www.taletе.mi.it

Kontakt:

Marcel Schumann
Div. for Simulation of Biological Systems
WSI/ZBIT, Sand 14
schumann@informatik.uni-tuebingen.de