

PHARMA-IT

Student Research Project with the Pharma-IT Platform

www.pharma-it.net

Suitable for Bachelor's and Master's level, for student with a chemical/biological/life science as well as a computer science / machine learning background

*Leiden / Amsterdam Center for Drug Research (LACDR, www.lacdr.nl) and
Leiden Institute for Advanced Computer Science (LIACS, www.liacs.nl)*

Development of Methods to Analyze High-Dimensional Data Using Barrier Trees and Applications to Drug Design

The exploration of high-dimensional spaces, such as for the detection of minima and maxima, is by no means trivial – the spaces are usually too large for a systematic exploration, and often also characterized by ruggedness which makes the application of simple descent methods impossible. One possibility to understand high-dimensional problems better is to simplify them, by reducing their dimensionality, and to make them easier accessible to the human way of thinking, and to visualize them in 2 or 3 dimensions. Well-known approaches of this type are PCA or Factor Analysis. Another very interesting way to visualize the characteristics of functions in high-dimensional spaces are 'Barrier Trees' where, in a phylogenetic tree, branch lengths of the tree correspond to energy barriers between two adjacent minima or maxima of a function. Thus, the structure of the function value landscape can be understood easier and the underlying structure of extrema of the function can be detected and visualized.

In this work, the student would implement an algorithm to generate barrier trees and in the second part apply it to a typical drug design task, namely the detection of underlying structures from ligand-target docking tasks and from ligand-based molecular optimization algorithms. Due to the necessity to develop programming code in the first part of the project good command of a common programming language such as C would be an advantage.

Requirements

Projects within the Pharma-IT Platform are usually concerned with the analysis of life science data using novel computational techniques, thus our research is interdisciplinary and we have both life scientists and computer scientists working in our group. Accordingly, most projects advertised in the context of the Pharma-IT Platform are suitable for undergraduate (BSc) as well as graduate (MSc) student with either a chemical/biological/life science or a computer science/machine learning background. **No previous experience in the other field is required**, but interest to either get familiar with life science data, or with computational methods, would clearly be an advantage. We strongly support students to publish their results if possible and the project results are suitable. For discussing individual projects, or to suggest your own ideas, please contact either Andreas or Michael directly.

Contact:

For more information and to discuss details of the project contact Andreas Bender (Andreas.Bender@pharma-it.net) or Michael Emmerich (Michael.Emmerich@pharma-it.net). We are looking forward to hearing from you!

More information about the Pharma-IT Platform, currently ongoing research projects and people involved can be found on the Internet at www.pharma-it.net.