

Student Research Project with the Analytical Biosciences Department and the Pharma-IT Platform

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

Analytical Biosciences Department (<http://www.analyticalbiosciences.leidenuniv.nl/>)

Leiden / Amsterdam Center for Drug Research (LACDR, www.lacdr.nl)

Leiden Institute for Advanced Computer Science (LIACS, www.liacs.nl)

Development of Methods to Analyze Mass Spectrometry Data for Metabolomics Compound Identification

The newly emerging field of 'Metabolomics' employs analytical chemical techniques such as mass spectrometry (MS) to detect a large number of metabolites in body fluids which characterize the state of a living system - for example, a certain disease a person may have. While the analytical detection methods have been refined in recent years, chemical structural characterization using mass spectrometry still remains the largest bottleneck. Mass spectral data used for identification purposes are acquired not as a single spectrum but as a spectral tree. A spectral tree contains information of the fragmentation process of a certain chemical structure. One common approach is to 'look up' a given set of spectral data and compare it to an existing reference library. However, due to the relational nature of the data, the matching between them is not straightforward. The development and evaluation of methods to compare MS trees, which is an important cornerstone for the chemical annotation of MS data, would be the task of the prospective research student. Currently the data are stored as text files and the practical work would involve devising and implementing algorithms in a common programming language such as C or Java, as well as the development of benchmarks to find which graph comparison method performs 'best' in a given situation. Given the amount of programming the work involves we suggest this project either for a computer science student or a life science student with previous programming experience.

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..

Contact:

For more information and to discuss details of the project contact Miguel Rojas Cherto (m.rojas@lacdr.leidenuniv.nl), Theo Reijmers (t.reijmers@lacdr.leidenuniv.nl), Andreas Bender (Andreas.Bender@pharma-it.net) or Michael Emmerich (Michael.Emmerich@pharma-it.net). We are looking forward to hearing from you!