**Bioinformatics Group**
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# Master Thesis

# Evaluation of Mass Spectrometry Peak Detection Algorithms

Metabolites are in the focus of pharmaceutical industries for drug discovery. Various plants and other organisms are screened for active compounds in the cure for various diseases. The most sensitive methodology available for the detection of the analytical composition of plants is mass spectrometry. At our institute, an efficient peak border detection algorithm was developed that is able to discern overlapping MS signals caused by different metabolite species. This algorithm was successfully applied in the analysis of lipids (Hartler et al., 2011), a subgroup of metabolites. However, this algorithm requires a list of compounds including their chemical composition to search for which is not feasible for the detection of completely unknown metabolites.

The aim of this diploma thesis is to integrate a peak detection algorithm for the software Lipid Data Analyzer. The algorithm shall look for candidate peak summits, which are then further verified by the LDA algorithm.

In a first step, the performance of three common peak detection algorithm should be compared based on already evaluated metabolomics data. The best performing algorithm shall then be implemented in Java and integrated in the LDA software package.

This diploma thesis will be accomplished in cooperation with the Core Facility for Mass Spectrometry at the Center for Medical Research of the Medical University of Graz.

Applicants should have skills in programming in object oriented languages, especially Java is beneficial. Basic knowledge about mass spectrometry is an advantage.

Duration of the master thesis: 6 months
Start date: as from now

## References

1. Hartler J, Trötzmuller M, Chitraju C, Spener F, Köfeler HC, Thallinger GG (2011) Lipid Data Analyzer: unattended identification and quantitation of lipids in LC-MS data. Bioinformatics 27(4):572-577.