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## Bioinformatics Thesis

# Elucidation of Lipid Structure by Mass Spectrometry

Lipids are not just important players in the metabolism but are involved in the pathogenesis of various diseases. The elucidation of the composition of the lipidome in a sample is therefore a key step in the understanding of health and disease. The most sensitive methodology available for the identification and quantification of lipids is mass spectrometry (MS), whereupon MS identifies the intact lipid and MS/MS provides detailed information about the lipid composition and structure. However, available software solutions cannot exploit this information or are restricted to a specific experimental setup.

The aim of this diploma thesis is to develop a generic extension for the analysis of MS/MS data to an existing software package.

The first step encompasses the development of generic means for characterization of MS/MS spectra and classification algorithms working on them, which shall be compared to conventional algorithms in the field.

In the second step, the applicant shall implement the generic solution on the most common lipid classes and the experimental setup applied by our partners at the Center for Medical Research.

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 of object oriented languages, especially Java is beneficial. Basic knowledge about mass spectrometry and lipid structure is an advantage.

Duration of the master thesis: 6 months

Start date: as from now

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