UPPSALA UNIVERSITET

Bioinformatics Engineering Program

Uppsala University School of Engineering

UPTEC X 12 021	Date of issue 2012-09

Author

Niklas Malmqvist

Title (English)

Building a standard operating procedure for the analysis of mass spectrometry data

Title (Swedish)

Abstract

Mass spectrometry (MS) is used in peptidomics to find novel endogenous peptides that may lead to the discovery of new biomarkers. Identifying endogenous peptides from MS is a time-consuming and challenging task; storing identified peptides in a database and comparing them against unknown peptides from other MS runs avoids re-doing identification. MS produce large amounts of data, making interpretation difficult. A platform for helping the identification of endogenous peptides was developed in this project, including a library application for storing peptide data. Machine learning methods were also used to try to find patterns in peptide abundance that could be correlated to a specific sample or treatment type, which can help focus the identification work on peptides of high interest.

Keywords

Mass spectrometry, database, spectra, peptide annotation, pattern recognition

Supervisors

Claes Andersson
Uppsala University

Scientific reviewer

Mats Gustafsson
Uppsala University

Project name	Sponsors
Language **English**	Security
ISSN 1401-2138	Classification
Supplementary bibliographical information	Pages **68**

Biology Education Centre Biomedical Center Husargatan 3 Uppsala
Box 592 S-75124 Uppsala Tel +46 (0)18 4710000 Fax +46 (0)18 471 4687