ISOQuant, Installation Guide

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8. Dezember 2011

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1 Description

One of the main bottlenecks in the evaluation of label-free quantitative proteomics experiments is the often cumbersome data export for in-depth data evaluation and analysis. Data-independent, alternate scanning LC-MS peptide fragmentation data can currently only be processed by Waters PLGS software.
PLGS performs absolute quantification only on a run-to-run level, it does not afford absolute quantification of protein isoforms and label-free relative quantification of peptides and proteins based on clustered accurate mass-retention time pairs on a complete experiment basis.
`ISOQuant` , a java based application, directly accesses xml files from the PLGS root folder and browses for relevant data from a label-free Expression Analysis project (quantification analyses, sample descriptions, search results) for fully automated import into a MySQL database. EMRTs are subjected to multidimensional Lowess-based intensity normalization and annotated by matching exact masses and aligned retention times of detected features with highest scoring peptide identification data from associated workflows. Based on the annotated cluster table, `ISOQuant` calculates absolute in-sample amounts with an integrated protein isoform quantification method, utilizing average intensities of proteotypic peptides for the partitioning of non-unique peptide intensities between protein isoforms.
All data is stored in a local MySQL based database that can be queried directly by experienced users.
`ISOQuant` is an integrated solution for in-depth evaluation and statistical analyses, allowing easy data access and export to third party analysis software.

2 System requirements

Operating System	Windows (2k/XP/Vista/7), Mac OS X Linux
Memory	minimum of 2GB RAM
Java Virtual Machine	Java™2 Platform Standard Edition (J2SE) Runtime Environment 1.6.0 or newer
Database	MySQL 5.2

3 Installation steps

ISOQuant is distributet as a single JAR file. JAR file is an executable java archive package.

3.1 Java Installation

To be able to execute a JAR file Java Virtual Machine has to be installed. Please install last available Java version from http://www.java.com/download/. Now you should be able to execute JAR files by doubleclicking them or by using the command line e.g.

```
>java -jar ISOQuant.jar
```

3.2 MySQL Installation

ISOQuant uses MySQL databases for storing data. Please install last version of MySQL from http://dev.mysql.com/downloads/mysql/ or the XAMPP package from http://www.apachefriends.org/en/xampp.html.
ISOQuant uses the ability of MySQL to handle large in memory tables to speed up data import. For this reason please edit MySQL's configuration file *my.ini* (or *my.cnf* depending on MySQL version) and append to the section *[mysqld]* the following attributes

```
max_heap_table_size = 2048M
tmp_table_size = 2048M
```

(or change values if these attributes are already defined) You will find this configuration file in [MySQL-Installation-Folder]/bin (alternative locations are possible depending on your operating system and MySQL distribution of your choice.)

3.3 Application folder

After you have successfully installed Java and MySQL you may execute ISOQuant first time. After first execution ISOQuant will place a configuration file **isoquant.ini** into directory where ISOQuant.jar is placed. So the moving ISOQuant.jar file in a separate folder of your choice will be a good idea before executing it.

4 Usage

Read built-in application help or help.pdf for details.

5 About developers

`ISOQuant` is developed by

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March 2011

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