Overview

We developed an OpenSource, platform-independent software framework and user interface for interactive visualization and analysis of large datasets from metabolomics experiments with the following features:

- definition and curatation of experiments, sample groups and individual normalization factors
- editing and execution of MalTcms processing pipelines
- import and cureation of mass spectral data in msf format (NIST) as custom databases
- visualization of raw and processed GC-MS data
- export of aligned and normalized peak areas with Anova results

Method 2: Maui

Maui, the MalTcms user interface, is an application based on the NetBeans Rich Client Platform for interactive visualization and analysis of large datasets from metabolomics experiments. Maui can be opened immediately to view processing results (bottom). Individual mass spectra can be selected and added to the MS plot (bottom) for manual inspection.

Results

Maui and MalTcms are implemented using the Java programing language allowing them to be extended and adapted easily to custom requirements. Extensions can be developed either in Java or in scripting languages like Groovy. Both projects welcome active contribution.

Maui and MalTcms are freely available under the LGPL v3 license at http://maltcms.sf.net.

References