Other software for metabolomics data analysis

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Software

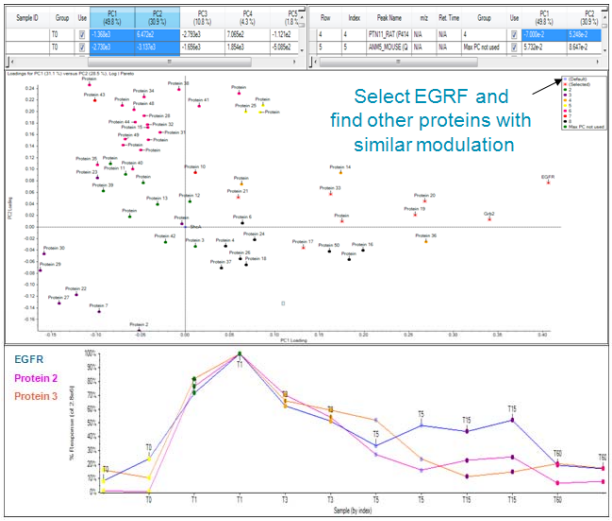
- MarkerView™ - AB Sciex
- Progenesis CoMet – Nonlinear Dynamics
- TransOmics – Waters
- Mass Hunter – Agilent
- Molfind – downloadable – free
- metAlign
- MZmine
- XCMS 2
- metaXCMS
- MAVEN

MarkerView™ Software (AB Sciex)

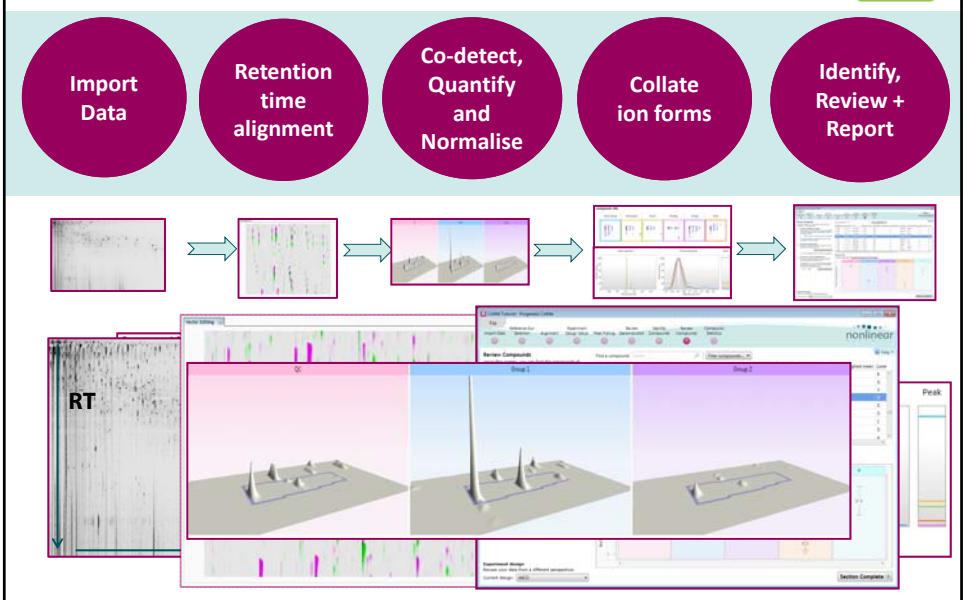
- Designed for metabolomics and protein/peptide biomarker profiling applications
  - Allows rapid and easy data review to determine up- and down-regulation of endogenous compounds in complex samples.
  - Mass and retention time alignment
  - Classified and non-classified workflows - PCA, T-tests, etc.
  - Powerful PCVG analysis for immediate recognition of groups and biological trends
- Supports the AB SCIEX TripleTOF™ 5600 System, QTRAP® Systems, and TOF/TOF Systems

MarkerView™ Software (AB Sciex)

- PCVG analysis color-codes groups of identifications that demonstrate similar behaviors
- Easily pick out trends by profiling the response across the samples
- Links PCA analysis back to protein or peptide identification results

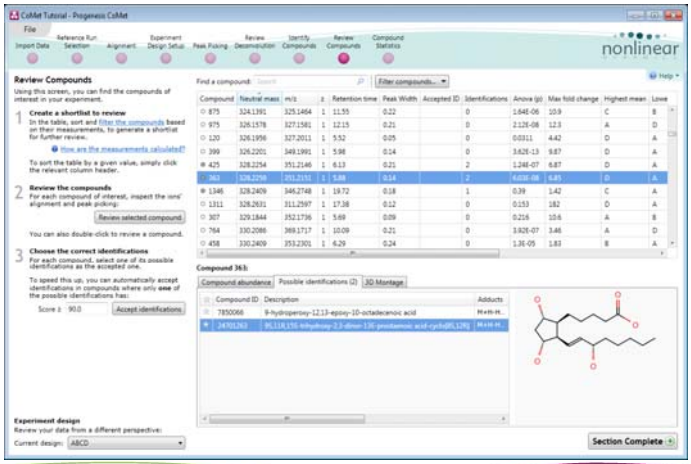


Progenesis CoMet workflow schematic



Identification

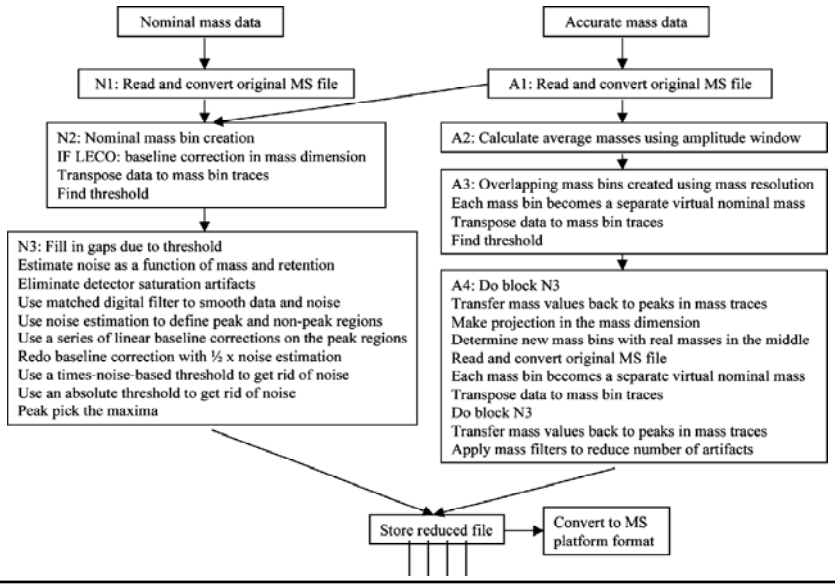
- MetaScope, our search tool, is integrated into the software
  - Search your own data and return compound identifications, **including chemical structures** from SDF databases



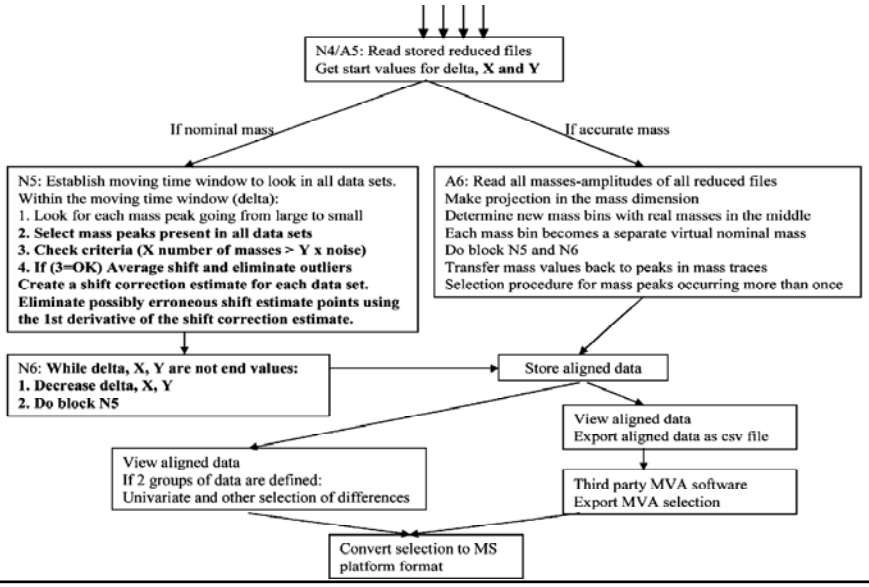
metAlign (I)

- **Features:**
  - Format conversion
  - accurate mass calculations
  - baseline corrections
  - peak picking
  - saturation and mass peak artifact filtering
  - alignment
- **Availability**
  - Free
  - www.metalign.nl

metAlign (II)

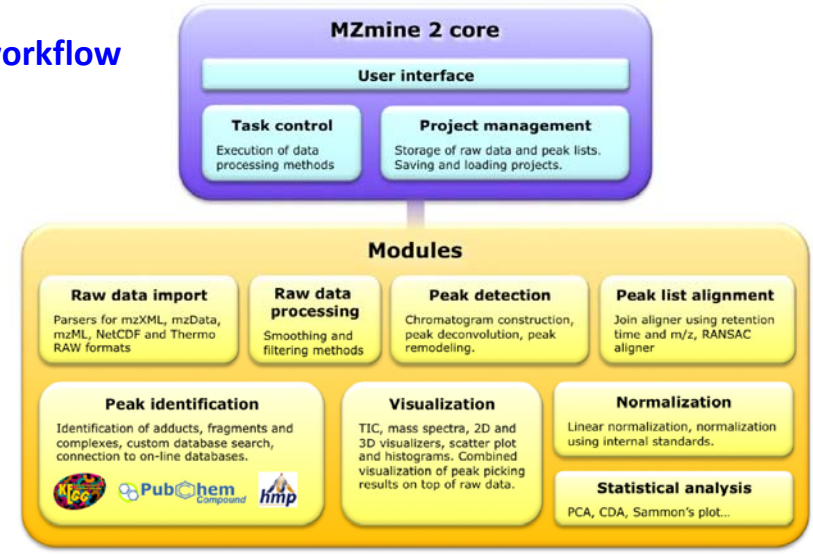


metAlign (III)



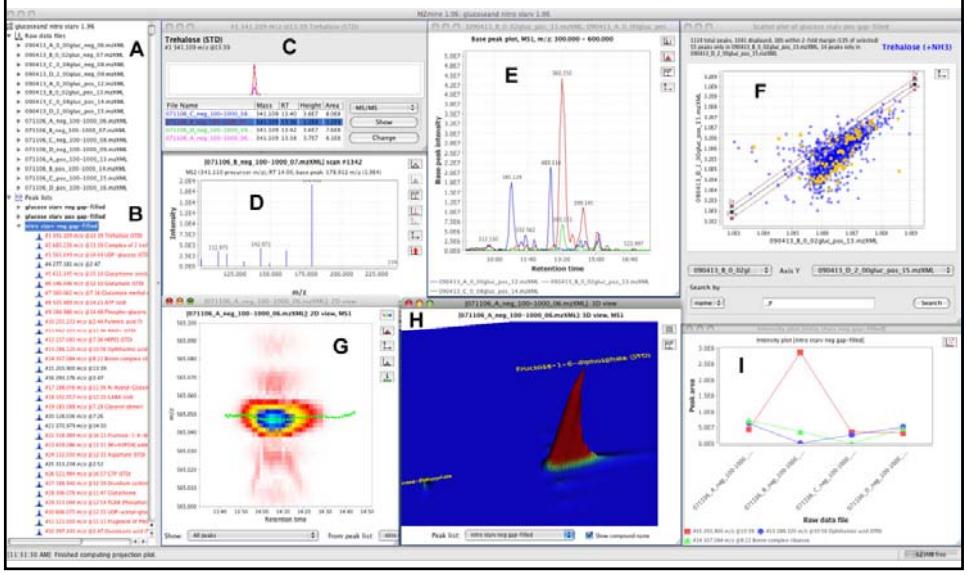
MZmine (I)

workflow



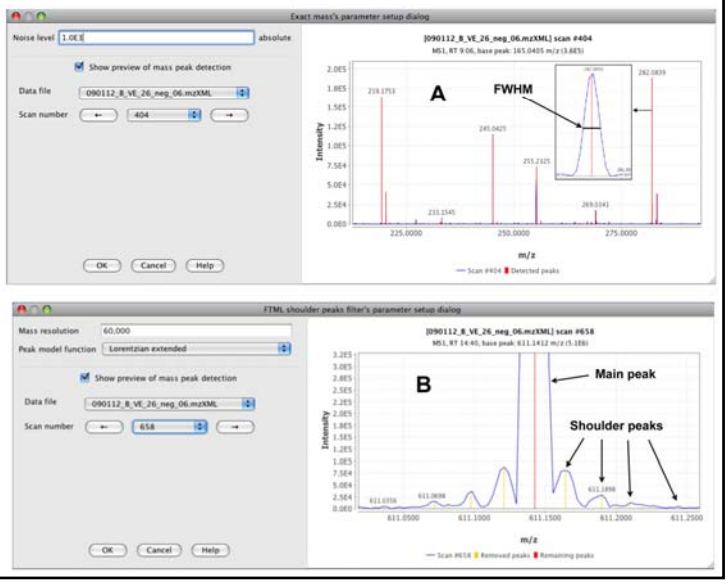
visualization

MZmine (II)



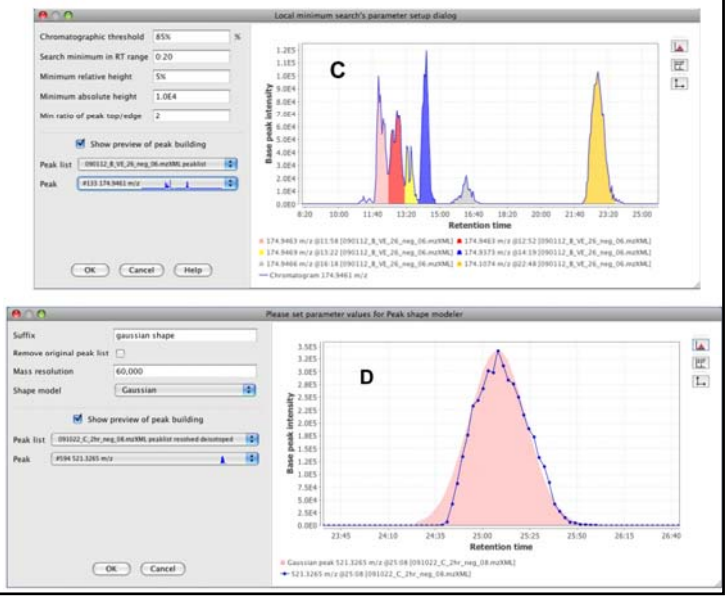
MZmine (III)

peak detection (I)



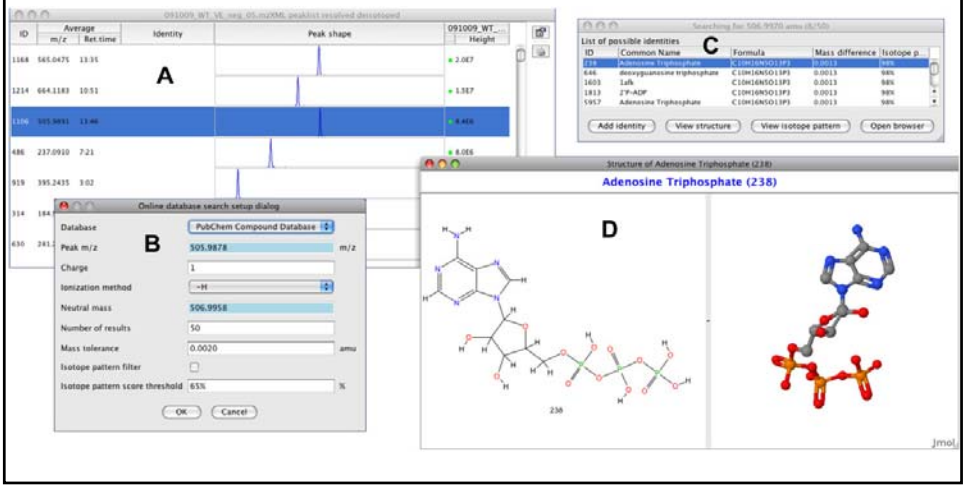
MZmine (IV)

peak detection (II)



MZmine (V)

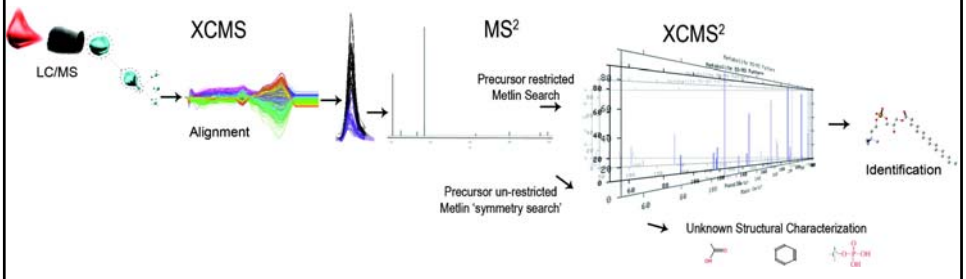
peak identification



MZmine (VI)

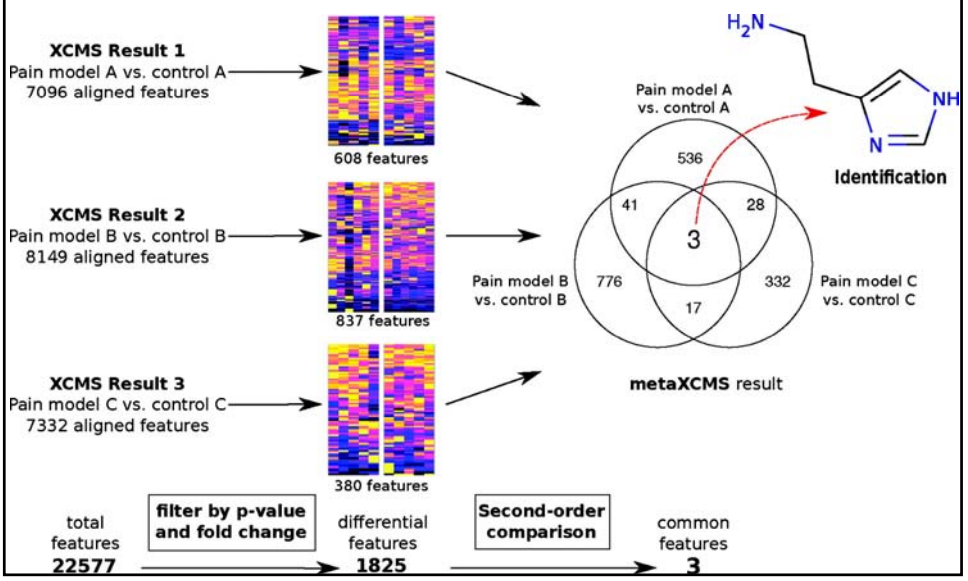
- **Availability**
  - Free
  - http://mzmine.sourceforge.net/index.shtml

XCMS 2



- **Availability**
  - Open source

metaXCMS (I)



metaXCMS (II)

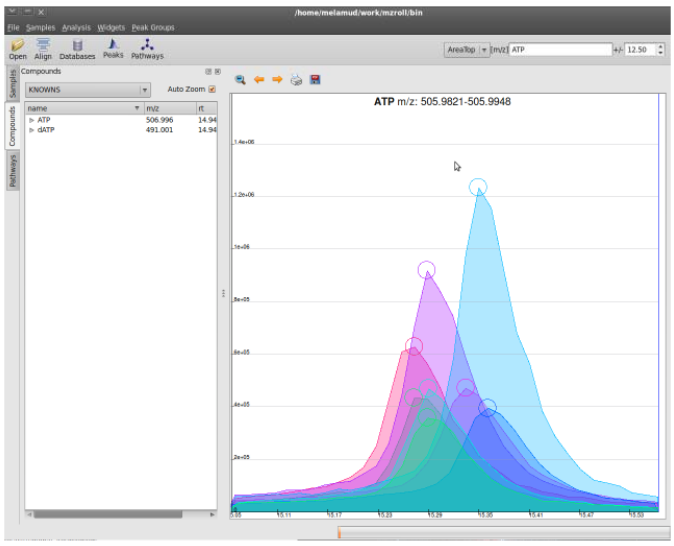
- **Availability**
  - Free
  - http://metlin.scripps.edu/metaxcms/index.php

MAVEN (I)

- **Features**
  - chromatographic alignment
  - peak feature detection
  - isotope and adduct calculator
  - formula predictor
  - pathway visualization
- **Availability**
  - Free
  - http://genomics-pubs.princeton.edu/mzroll/index.php?show=index

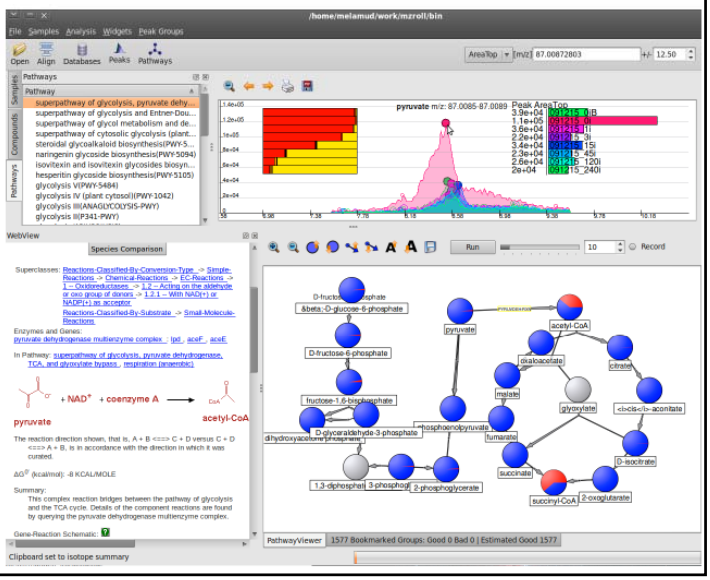
MAVEN (II)

multi-file EIC view



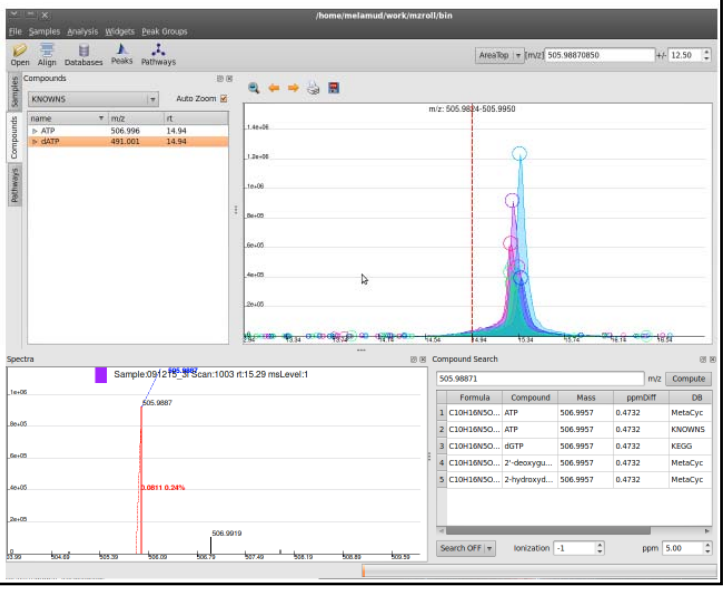
MAVEN (III)

pathway view



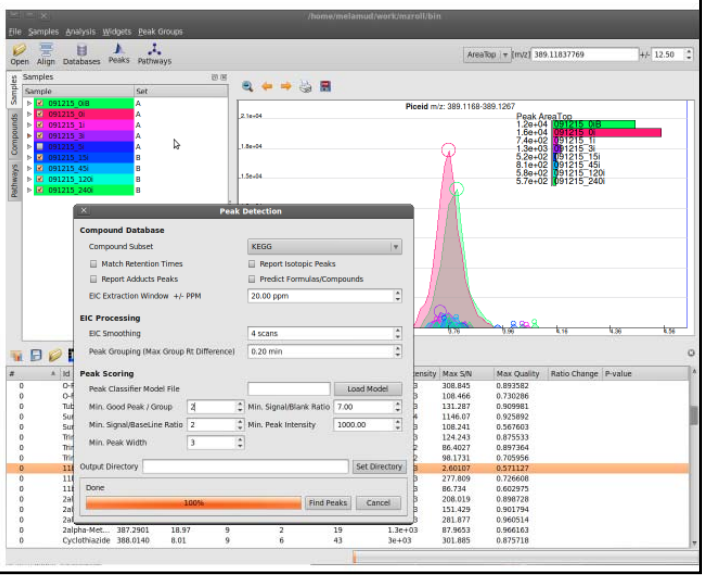
MAVEN (IV)

compound identification



MAVEN (V)

peak detection



Other useful links

- **Metabonews**
  - **http://www.metabonews.ca/archive.html**
  - **You can subscribe to get monthly newsletter**
- **Metabolomics Society**
  - **http://www.metabolomicssociety.org/**
- **Regional Comprehensive Metabolomics Research Centers**
  - **RTI Intl – ssumner@rti.org**
  - **UC-Davis – ofienh@ucdavis.edu**
  - **U. Michigan – burantc@med.umich.edu**
  - **U. Florida – aedison@ufl.edu**
  - **Mayo – nair@mayo.edu**
  - **U Kentucky – rickhigashi@me.com**