

## **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**

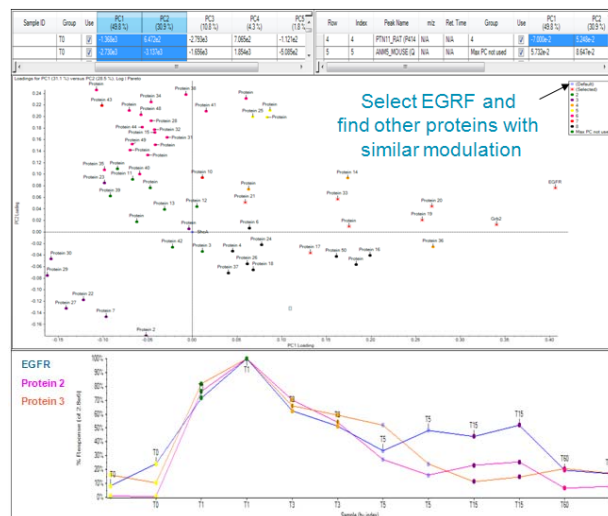
## MarkerView™ Software (AB Sciex)

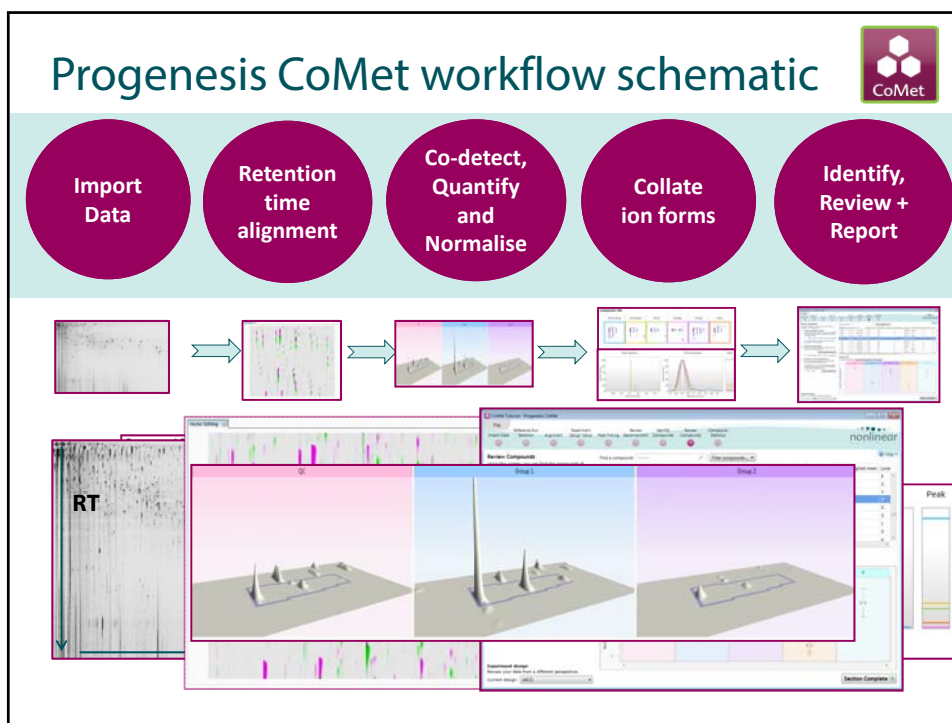
- Designed for metabolomics and protein/peptide biomarker profiling applications
  - Allows rapid and easy data review to determine up- and down-regulation of endogenous compounds in complex samples.
  - Mass and retention time alignment
  - Classified and non-classified workflows - PCA, T-tests, etc.
  - 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





## Identification

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

The screenshot shows the 'Review Compounds' section of the Progenesis CoMet software. The interface includes a 'Find a compound' search bar and a table of compounds. The table has the following columns: Compound, Neutral mass, m/z, Retention time, Peak Width, Accepted ID, Identifications, Anova (p), Max fold change, Highest mean, and Locus.

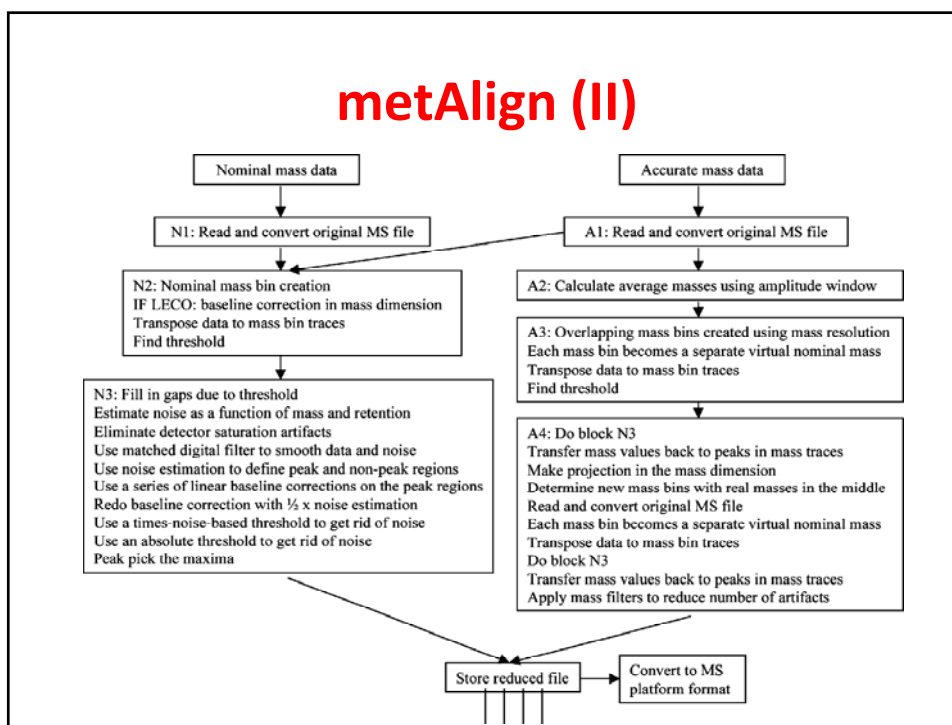
Compound	Neutral mass	m/z	Retention time	Peak Width	Accepted ID	Identifications	Anova (p)	Max fold change	Highest mean	Locus
875	324.1361	325.1464	11.555	0.22	0	0	1.046-06	10.9	C	B
975	326.1578	327.1581	12.115	0.21	0	0	2.126-06	12.3	A	D
120	326.1596	327.2011	5.52	0.05	0	0	0.0112	1.42	D	A
390	326.2201	348.1261	5.58	0.14	0	0	3.628-13	6.87	D	A
425	328.2254	351.2146	6.53	0.21	2	1	1.246-07	6.87	D	A
360	328.2259	351.2151	5.89	0.14	2	1	4.656-06	6.85	D	A
1346	328.2409	346.2748	19.72	0.18	1	0	0.39	1.42	C	A
1211	328.2621	311.2997	17.38	0.12	0	0	0.153	1.82	D	A
367	329.1844	352.1756	5.69	0.09	0	0	0.218	1.64	A	B
764	330.2086	349.1717	10.09	0.21	0	0	3.826-07	3.48	A	D
458	330.2409	352.2301	6.29	0.24	0	0	1.36-05	1.81	B	A

Below the table, the 'Compound 363' section is expanded, showing 'Compound abundance', 'Possible identifications (2)', and '3D Montage'. The chemical structure of 3-hydroxyundecanoic acid is displayed, along with its molecular weight (328.34) and other identifiers.

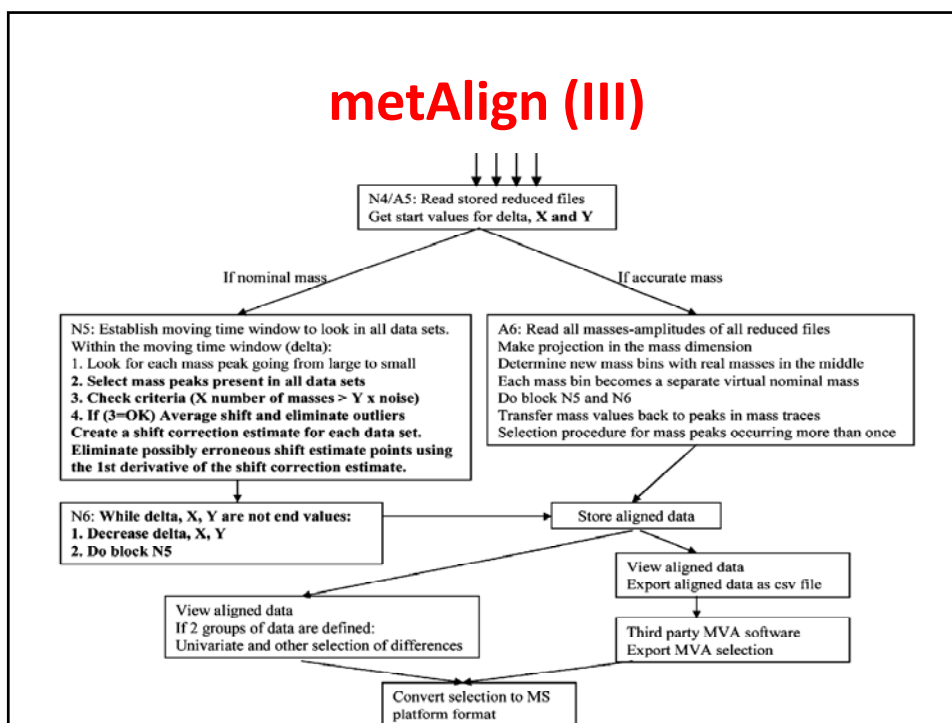
## metAlign (I)

- **Features:**
  - Format conversion
  - accurate mass calculations
  - baseline corrections
  - peak picking
  - saturation and mass peak artifact filtering
  - alignment
- **Availability**
  - Free
  - [www.metalalign.nl](http://www.metalalign.nl)

## metAlign (II)

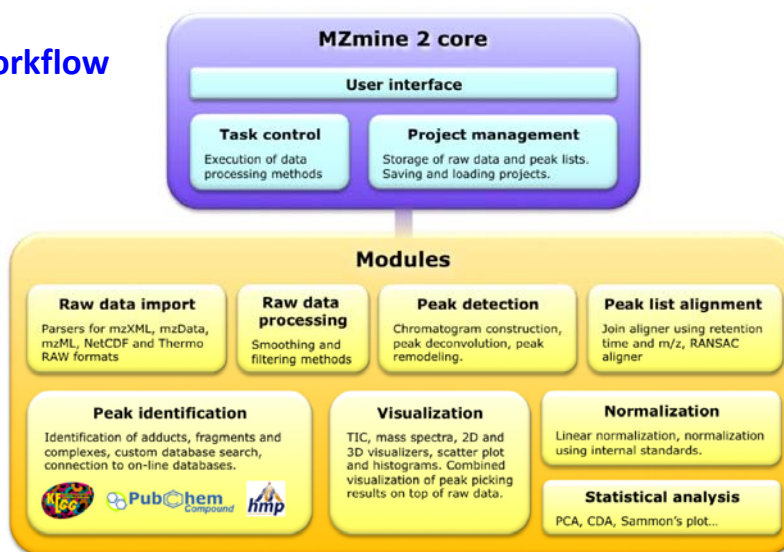


## metAlign (III)



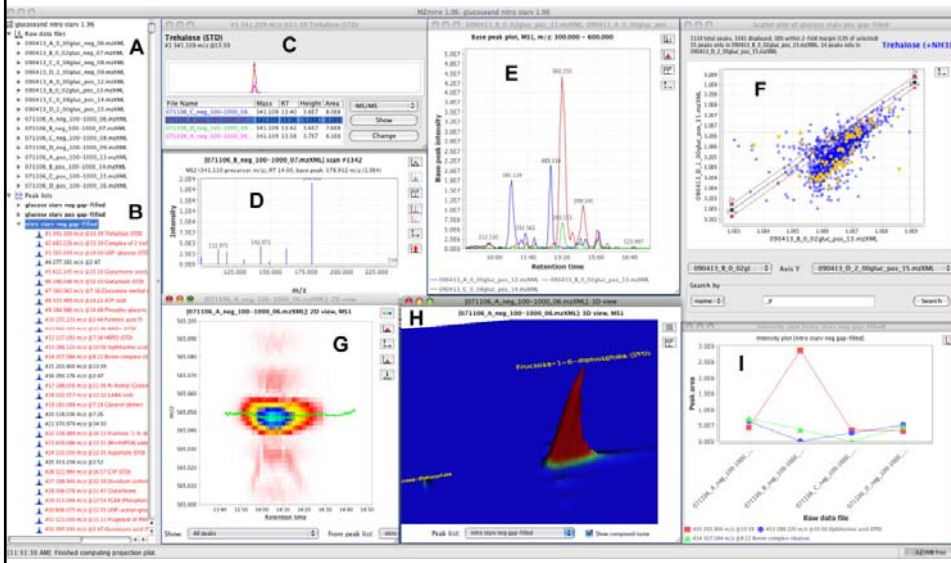
## MZmine (I)

workflow



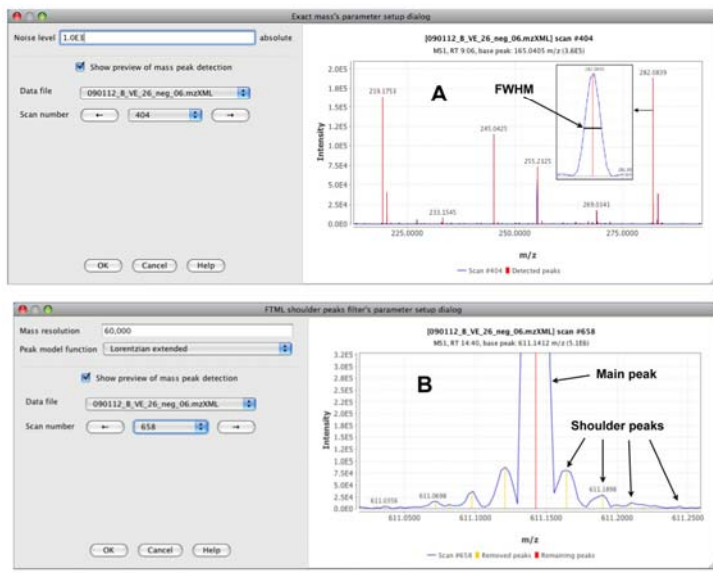
visualization

# MZmine (II)



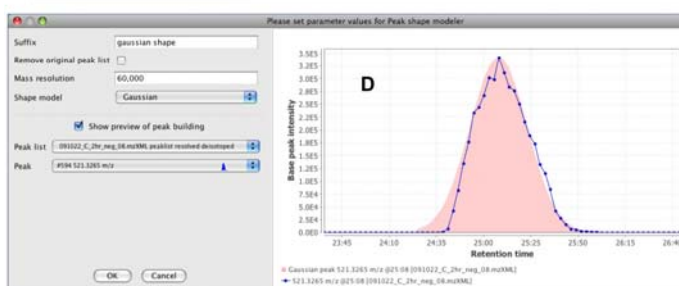
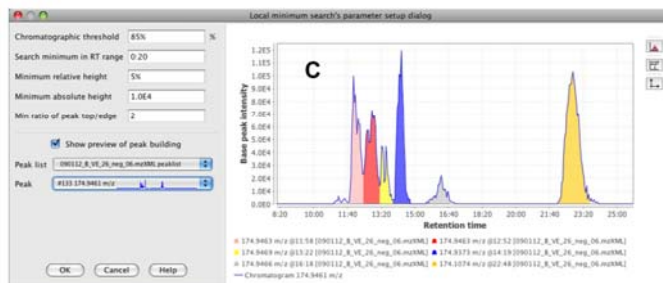
peak detection (I)

# MZmine (III)



# MZmine (IV)

peak detection (II)



# MZmine (V)

peak identification

The composite screenshot illustrates the peak identification workflow. Panel A shows a table of peaks with columns for ID, Average m/z, Ret. time, Identity, Peak shape, and Height. The peak at m/z 106.9051 is highlighted. Panel B is the 'Online database search setup dialog' with 'PubChem Compound Database' selected and 'Peak m/z' set to 106.9051. Panel C is the 'List of possible identities' table:

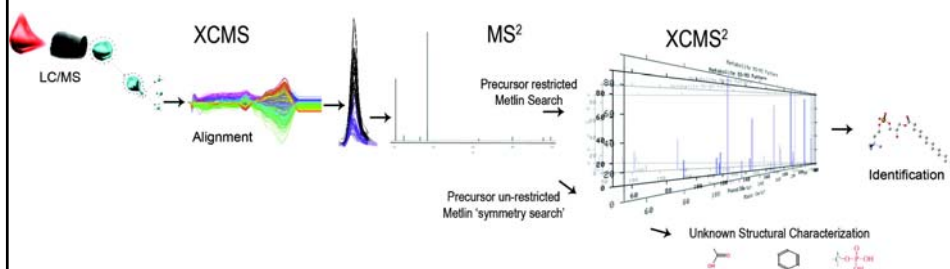
ID	Common Name	Formula	Mass difference	Isotope p.
117	Adenosine Triphosphate	C <sub>10</sub> H <sub>16</sub> N <sub>5</sub> O <sub>13</sub> P <sub>3</sub>	0.0013	98%
446	deoxyguanosine triphosphate	C <sub>10</sub> H <sub>16</sub> N <sub>5</sub> O <sub>13</sub> P <sub>3</sub>	0.0013	98%
1463	IdA	C <sub>10</sub> H <sub>16</sub> N <sub>5</sub> O <sub>13</sub> P <sub>3</sub>	0.0013	98%
1813	2'-P-ADP	C <sub>10</sub> H <sub>16</sub> N <sub>5</sub> O <sub>13</sub> P <sub>3</sub>	0.0013	98%
1967	Adenosine Triphosphate	C <sub>10</sub> H <sub>16</sub> N <sub>5</sub> O <sub>13</sub> P <sub>3</sub>	0.0013	98%

Panel D shows the chemical structure of Adenosine Triphosphate (238) in both 2D and 3D ball-and-stick models.

## MZmine (VI)

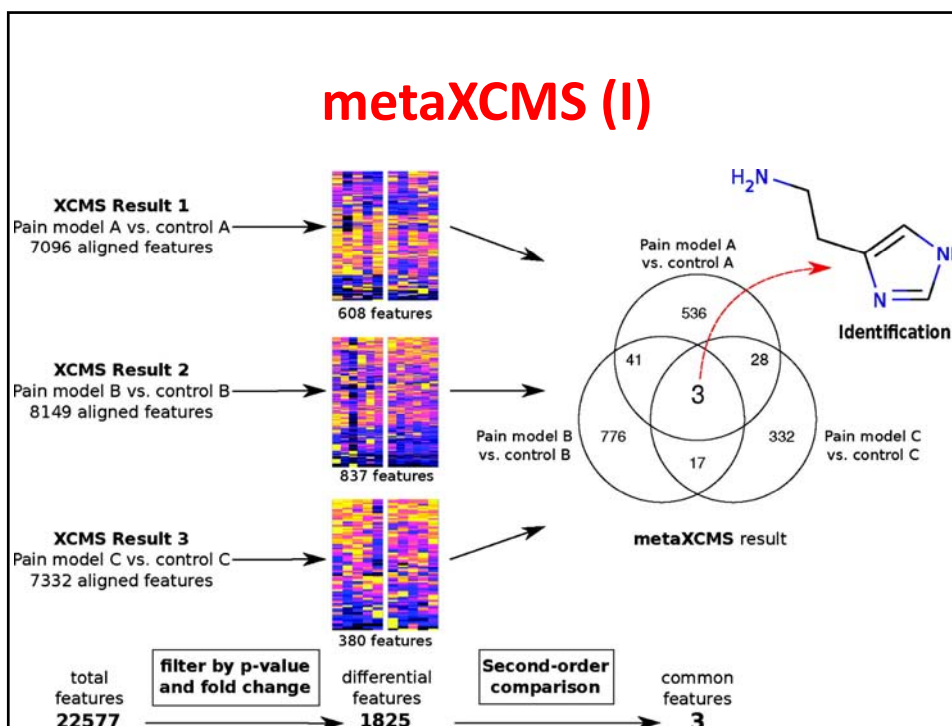
- **Availability**
  - Free
  - <http://mzmine.sourceforge.net/index.shtml>

## XCMS 2



- **Availability**
  - Open source





## metaXCMS (II)

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

## MAVEN (I)

- **Features**

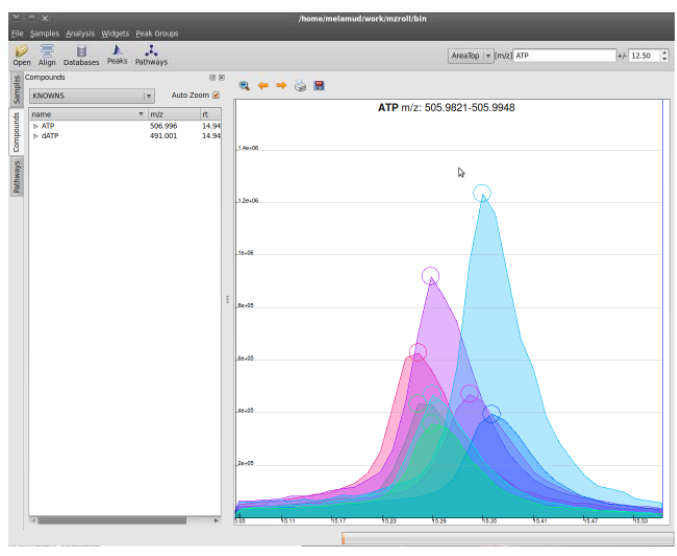
- chromatographic alignment
- peak feature detection
- isotope and adduct calculator
- formula predictor
- pathway visualization

- **Availability**

- Free
- <http://genomics-pubs.princeton.edu/mzroll/index.php?show=index>

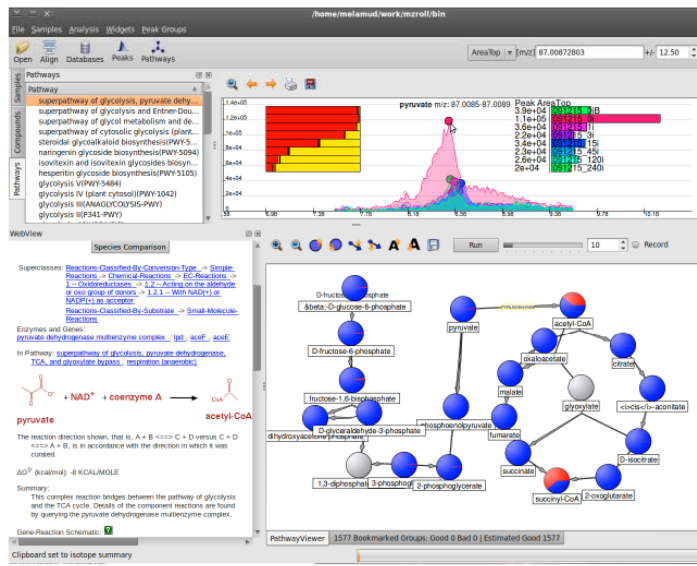
## MAVEN (II)

multi-file  
EIC view



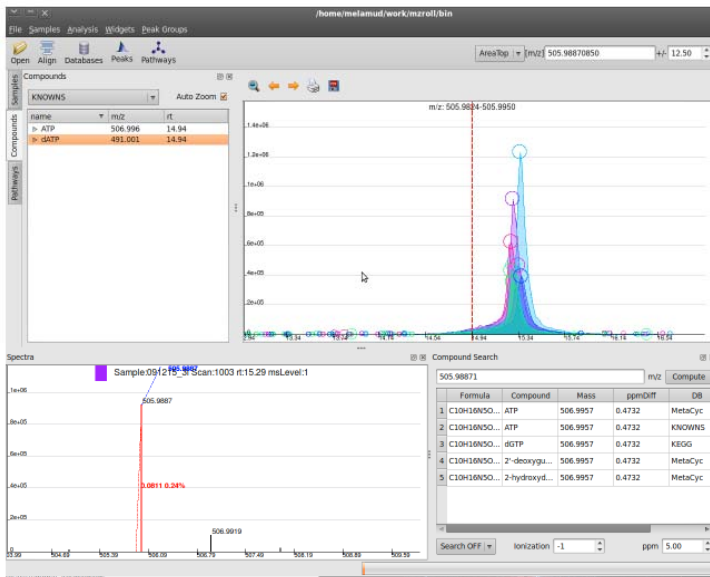
pathway view

# MAVEN (III)



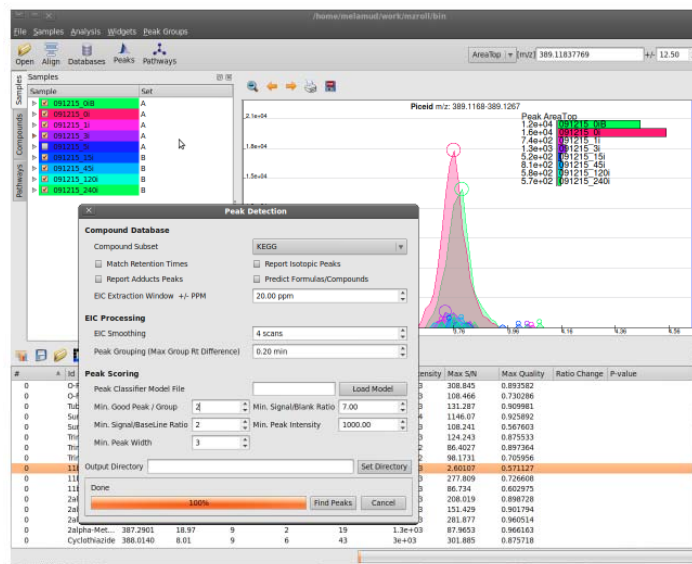
compound identification

# MAVEN (IV)



## 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](mailto:ssumner@rti.org)
  - UC-Davis – [ofienh@ucdavis.edu](mailto:ofienh@ucdavis.edu)
  - U. Michigan – [burantc@med.umich.edu](mailto:burantc@med.umich.edu)
  - U. Florida – [aedison@ufl.edu](mailto:aedison@ufl.edu)
  - Mayo – [nair@mayo.edu](mailto:nair@mayo.edu)
  - U Kentucky – [rckhigashi@me.com](mailto:rckhigashi@me.com)