Data processing for LCMS-based metabolomics

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Aim: To get meaningful metabolic information from LCMS raw data
Existing applications for LCMS-based metabolomics

(Sieve)
MzMine
Maven
Metalign
XCMS

Data requires improved:
- Filtering
- Identification
- Visualisation

~90% false identifications
IDEOM Pipeline

Data processing pipeline: Main Functions

- Peak Picking
- Group samples
- Noise filtering (reproducibility, peak shape, intensity)
- Gap filling
- Related peaks annotation
- Additional filtering (contaminants, isotopes/adducts)
- Metabolite Identification (mass and RT)
- Univariate statistics and visualisation
- Biological network/pathway analysis
- Multivariate statistics

# PEAKS

- XCMS: ~50,000
- mzMatch: ~20,000
- IDEOM: ~500
- Metexplore: ~20
IDEOM Pipeline

Data processing pipeline: Graphical User Interface (in Excel)
Definitions

Terminology

- **PPM**: mass error \( \frac{1,000,000 \times (\text{detected mass} - \text{theoretical mass})}{\text{theoretical mass}} \)
- **EIC (XIC)**: Extracted Ion Chromatogram (single mass window)
- **TIC**: Total Ion Chromatogram (all masses)
- **RT**: Chromatographic Retention Time
- **RSD**: Relative Standard Deviation \( \frac{\text{standard deviation (of peak intensities)}}{\text{mean (of peak intensities)}} \)
- **Feature or Peak**: Single mass/RT window usually corresponding to a chemical entity
- **Related Peak**: Detected peak that doesn’t correspond to the MH+ ion for the metabolite (e.g., isotope, adduct, fragment)
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# PEAKS
~50,000
~20,000
~500
~20
Peak Picking: XCMS (Centwave)

- Finds peaks and creates a list of peaks

Parameters:

- **PPM**: mass deviation from scan to scan
- **Peakwidth**: range for baseline peakwidth
- **S/N threshold**: Signal to Noise ratio
- **Prefilter**: number of scans greater than a given intensity threshold
Pipeline

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- IDEOM: ~500
- Metabolist: ~20
mzMatch: Group Samples

- Matches peaks from each sample to produce a single dataset

Parameters:

• PPM window: mass deviation from sample to sample

• RT window: RT deviation from sample to sample

NOTE: RT alignment is not performed because it is both difficult and unnecessary. Data-driven methods are not suitable because RT shift is not consistent across metabolite classes. If major shifts are apparent the signal intensity will not be comparable, so no point trying to make sense of datasets with large RT variability.
Data processing pipeline:

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# PEAKS
- ~50,000
- ~20,000
- ~500
- ~20
mzMatch: Noise Filtering

RSD filter:
• Peak reproducibility is assessed by the RSD of peak intensities for each group of replicates

Noise filter:
• Peak shape is assessed by CoDA-DW score (0-1)

Intensity filter:
• Features are removed if no sample has a peak above the intensity threshold

Detections filter:
• Peaks must be present in a minimum number of samples
Data processing pipeline:

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# PEAKS

- ~50,000
- ~20,000
- ~500
- ~20
Related Peaks

Related Peaks include:
- Isotopes
- Adducts (Na\(^+\), K\(^+\), Cl\(^-\), ACN)
- Fragments
- Multiply-charged species
- Dimers, trimers etc
- Complex adducts
- FT or ringing signals
- Combinations of the above
mzMatch: Related Peaks

Related Peaks determined by:
- Retention time (window)
- Peak shape correlation
- Peak intensity correlation

Annotation:
- Every peak in a related set is given the same relation.id number
- The largest peak is denoted the ‘Basepeak’
- Other peaks are annotated if possible according to the mass difference to the basepeak
Pipeline

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- Noise filtering (reproducibility, peak shape, intensity)
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- Related peaks annotation

**Additional filtering (contaminants, isotopes/adducts)**

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# PEAKS

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IDEOM: Additional Filters - Noise

Samples are allocated to study groups

Blank (contaminant) filter:
• All intensities in a study group must be greater than all intensities in the solvent blanks

Repeat RSD, Intensity and Detections filters:
• Only applies filters to ‘included’ study groups
• RSD filter can be applied at 3 levels:
  • STRICT: all groups must pass
  • GENEROUS: 1 group must pass
  • TECHNICAL: QC group must pass
IDEOM: Additional Filters - Chromatography

Shoulder peak filter
- Smaller isomeric peaks:
  - Within given RT window AND
  - Less than X-fold lower intensity

Duplicate peak filter
- Smaller isomeric peaks:
  - Within given RT window OR
  - Very low intensity (<1%) OR
  - Very highly correlated intensity (r>0.95)
IDEOM: Additional Filters – Mass Spec

Very common related peaks
- Within RT window (<10 seconds)
- Mass difference from ‘Fragments’ sheet
  - Less than intensity threshold

Specific fragments
Fragments from specific metabolites
- Within RT window (<10 seconds)
- Mass difference from experimental data (standards)

Likely fragments or adducts
- Within RT window (<10 seconds)
- mzMatch annotation as ‘related peak’
- Annotated as common fragment/adduct in IDEOM

<table>
<thead>
<tr>
<th>Common related peak</th>
<th>mzdiff</th>
<th>maxheight</th>
<th>* mass</th>
</tr>
</thead>
<tbody>
<tr>
<td>xMSnoise</td>
<td>1</td>
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<tr>
<td>xC13</td>
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<tr>
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</tr>
<tr>
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<tr>
<td>x3+</td>
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<tr>
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<tr>
<td>x3-mer</td>
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# IDEOM: Additional Filters – Mass Spec

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<th>Mass Difference</th>
<th>Neutral Loss</th>
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<td>H2O</td>
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<td>H2O</td>
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<td>H2O</td>
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<td>H2O</td>
</tr>
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<td>H2O</td>
</tr>
<tr>
<td>25-aminobutyric acid</td>
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<td>H2O</td>
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<td>27-aminobutyric acid</td>
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<td>H2O</td>
</tr>
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<td>H2O</td>
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<tr>
<td>33-aminobutyric acid</td>
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<td>C4H7NO</td>
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<td>H2O</td>
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<tr>
<td>39-aminobutyric acid</td>
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<td>H2O</td>
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<td>C4H7NO</td>
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<td>42-aminobutyric acid</td>
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<td>C4H7NO</td>
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<td>H2O</td>
</tr>
</tbody>
</table>
Data processing pipeline:

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# PEAKS

- **XCMS**: ~50,000
- **mzMatch**: ~20,000
- **IDEOM**: ~500
- **Metaboanalyst**: ~20
IDEOM: Metabolite Identification
Mass and retention time

Exact mass – mass error < 3 ppm suitable for formula identification from biochemical database

<table>
<thead>
<tr>
<th>mass accuracy (ppm)</th>
<th>Unique entries in DB</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>99%</td>
</tr>
<tr>
<td>2</td>
<td>97%</td>
</tr>
<tr>
<td>3</td>
<td>95%</td>
</tr>
<tr>
<td>5</td>
<td>92%</td>
</tr>
<tr>
<td>10</td>
<td>80%</td>
</tr>
</tbody>
</table>

Assumption: all peaks are corrected by H⁺ (in mzMatch)

If no formula match for a specific mass: search other adducts
  • Default = 2+
  • other adducts optional
IDEOM: Metabolite Identification

Mass and retention time

Exact mass

Retention time
- Accurate: Authentic standards analysed in same batch
- Approximate: Predicted retention time

Beware isomers...
Retention time prediction (QSRR)

100-200 authentic standard RT's

Calculated physico-chemical properties (JChem)

Multiple Linear Regression

Online metabolite databases

Calculated physico-chemical properties (JChem)

QSRR model

Database of 30,000 predicted Retention Times

R² = 0.81

Creek et al. 2011. Anal Chem
Automated isomer selection: based on RT and existing biological knowledge

- Your Preferred Database
- KEGG Central Pathways
- KEGG and Biocyc Identifiers
- Other Database Identifiers

1. Get formula from mass
2. Select most likely metabolite
3. Check Retention time
4. (Putative) Identification
Automated isomer selection: based on RT and existing biological knowledge

<table>
<thead>
<tr>
<th>Searchmass</th>
<th>Formula</th>
<th>Metabolite</th>
<th>sRT</th>
<th>cRT</th>
<th>Yeastycyc</th>
<th>Map</th>
<th>DB</th>
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</thead>
<tbody>
<tr>
<td>132.05349</td>
<td>C4H8N2O3</td>
<td>L-Asparagine</td>
<td>18.62</td>
<td>18.71</td>
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<td>Amino Acid Metabolism</td>
<td>KEGG_Metacyc_HMDB</td>
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<tr>
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<td>N-Carbamoylsarcosine</td>
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<td>KEGG_Metacyc_HMDB</td>
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<td>C4H8N2O3</td>
<td>3-Ureidopropionate</td>
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<td>D-Asparagine</td>
<td>18.71</td>
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<td>2-Ureido-propionate</td>
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<td>Metacyc</td>
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</table>
IDEOM: Metabolite Identification

Mass and retention time

Exact mass

Retention time

Confidence assignment

- Every ‘metabolite’ is assigned a confidence level from 0 to 10 (10 = most confident)
- Confidence <5 is rejected as false identification
- Metabolites with authentic standards are highlighted yellow

<table>
<thead>
<tr>
<th>CONFIDENCE ASSIGNMENTS:</th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>Confidence levels</td>
<td>arbitrary</td>
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<tr>
<td>sRT within 5%</td>
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<td>cRT within 35%</td>
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<tr>
<td>ID-dependent rejection</td>
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<tr>
<td>Xenobiotics</td>
<td>4.5</td>
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<td>RT outside window</td>
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<td>Peak-dependent rejection</td>
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<td>Below intensity filter</td>
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<td>RSD filter</td>
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<td>not more that blank control</td>
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<tr>
<td>Related peak (mzMatch)</td>
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</tbody>
</table>
Data processing pipeline:
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- Related peaks annotation
- Additional filtering
- Metabolite Identification
- Univariate statistics and visualisation
- Biological network/pathway analysis
- Multivariate statistics
Mass accuracy: Improving Orbitrap calibration from 3 to 1 ppm

Ideom
Data processing pipeline:

- Peak Picking
- Group samples
- Noise filtering (reproducibility, peak shape, intensity)
- Gap filling
- Related peaks annotation
- Additional filtering (contaminants, isotopes/adducts)
- Metabolite Identification (mass and RT)
- Statistics and visualisation
- Biological network/pathway analysis
- Multivariate statistics

### # PEAKS

- XCMS: ~50,000
- mzMatch: ~20,000
- IDEOM: ~500
- Metaboanalyst: ~20
- Metexplore: ~
- Pathos: ~
Visualisation

Sort or autofilter results by:

- Intensity differences
- Statistical significance (t-test, fisher ratio, rank products)
- Intensity correlation (eg. time series)
- Identification confidence
- Metabolite class
- Metabolic pathway

Clickable links to:

- Intensity graphs (by sample, by group, bubble, volcano)
- Identity confidence information (isomers, related peaks, RT)
- Metabolite-specific websites (Chemspider, KEGG, BioCyc)
- Raw data (raw: Xcalibur, peakml: mzMatch.R)
Data export options:

Biochemical analysis
- **Metexplore**: maps metabolite levels to a MetaCyc network
- **Pathos**: maps metabolites to individual KEGG pathways

Statistical analysis
- **R**: Automatic PCA, HCA and heatmap
- **Metaboanalyst**: Multivariate stats

Analytical confirmation
- MSMS ‘include list’
Running the Pipeline

Data processing pipeline:

- XCMS
  - mzMatch
    - R
  - IDEOM
    - IDEOM (MS Excel)
    - MS Excel
    - Web Browsers

- Metexplore
  - Metaboanalyst
  - Pathos
Ideom requirements

• Basic Requirements
  • Microsoft Excel 2007 or higher (2003 not sufficient, Mac not fully functional)
  • No installation required. Simply open the file and enable macros.

• Requirements for full function
  • R Statistical Software: for xcms & mzmatch pre-processing
    R packages: XCMS (BioC), mzMatch.R (Rforge), rJava and dependencies
    R package: rCDK: for FormulaGenerator
    Installation instructions and commands are located in the IDEOM help section
  • Msconvert (or ReAdW): for conversion of .RAW to .mzXML files
  • Web browser: for Hyperlinks to online databases
  • Thermo Xcalibur: for EIC lookup

http://mzmatch.sourceforge.net/ideom.php
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Dave Watson & lab members
• Morning
  • Visualizing and interpreting pre-processed data in IDEOM

• Lunch

• Afternoon
  • Processing raw data with IDEOM (and mzMatch)
  • Additional features in IDEOM
  • New features and discussion of future directions

Tutorial Agenda