

Hands-on Data Analysis with MZmine 2

Xiuxia Du

Department of Bioinformatics and Genomics
University of North Carolina at Charlotte

About MZmine 2

- LC/MS and GC/MS metabolomics data processing, analysis, and visualization
- Where to get it? <http://mzmine.github.io/>

About MZmine 2

The screenshot shows the 'About MZmine 2' page of the MZmine 2 website. At the top, there's a header bar with a 'Not Secure | mzmine.github.io' message and a star icon. Below the header is the MZmine 2 logo, featuring a red and blue stylized peak icon followed by the text 'MZmine 2'. A navigation menu with links for 'HOME' (highlighted in blue), 'FEATURES', 'DOWNLOAD', 'DEVELOPMENT', 'SUPPORT', and 'CONTRIBUTORS' is visible. A large black banner below the menu contains the word 'MZmine' in white. The main content area has a light gray background and features the title 'About MZmine 2' in bold black font. To the right of the title are two buttons: 'Download' (blue) and 'Report issue' (red). Below the title, a paragraph explains that MZmine 2 is an open-source software for mass-spectrometry data processing, based on the original MZmine toolbox from 2006. It mentions that the software has been redesigned and rewritten, aiming for a user-friendly, flexible, and extendable tool. It also encourages users to check the development page if interested in implementing their own methods. A citation for the 2010 publication is provided, along with a 'Donate' button for supporting the development of MZmine.

Not Secure | mzmine.github.io

MZmine 2

HOME FEATURES DOWNLOAD DEVELOPMENT SUPPORT CONTRIBUTORS

MZmine

About MZmine 2

Download Report issue

MZmine 2 is an open-source software for mass-spectrometry data processing, with the main focus on LC-MS data. It is based on the original MZmine toolbox described in the [2006 Bioinformatics publication](#), but has been completely redesigned and rewritten since then. Our main goal is to provide a user-friendly, flexible and easily extendable software with a complete set of modules covering the entire LC-MS data analysis workflow.

If you are interested in implementing your own data processing methods or help improve MZmine 2 then please check the [development page](#).

Please cite the following publication if you use MZmine 2 to analyze your data:

T. Pluskal, S. Castillo, A. Villar-Briones, M. Orešič, MZmine 2: Modular framework for processing, visualizing, and analyzing mass spectrometry-based molecular profile data, BMC Bioinformatics 11:395 (2010). PMID: 20650010

Donate to support MZmine development

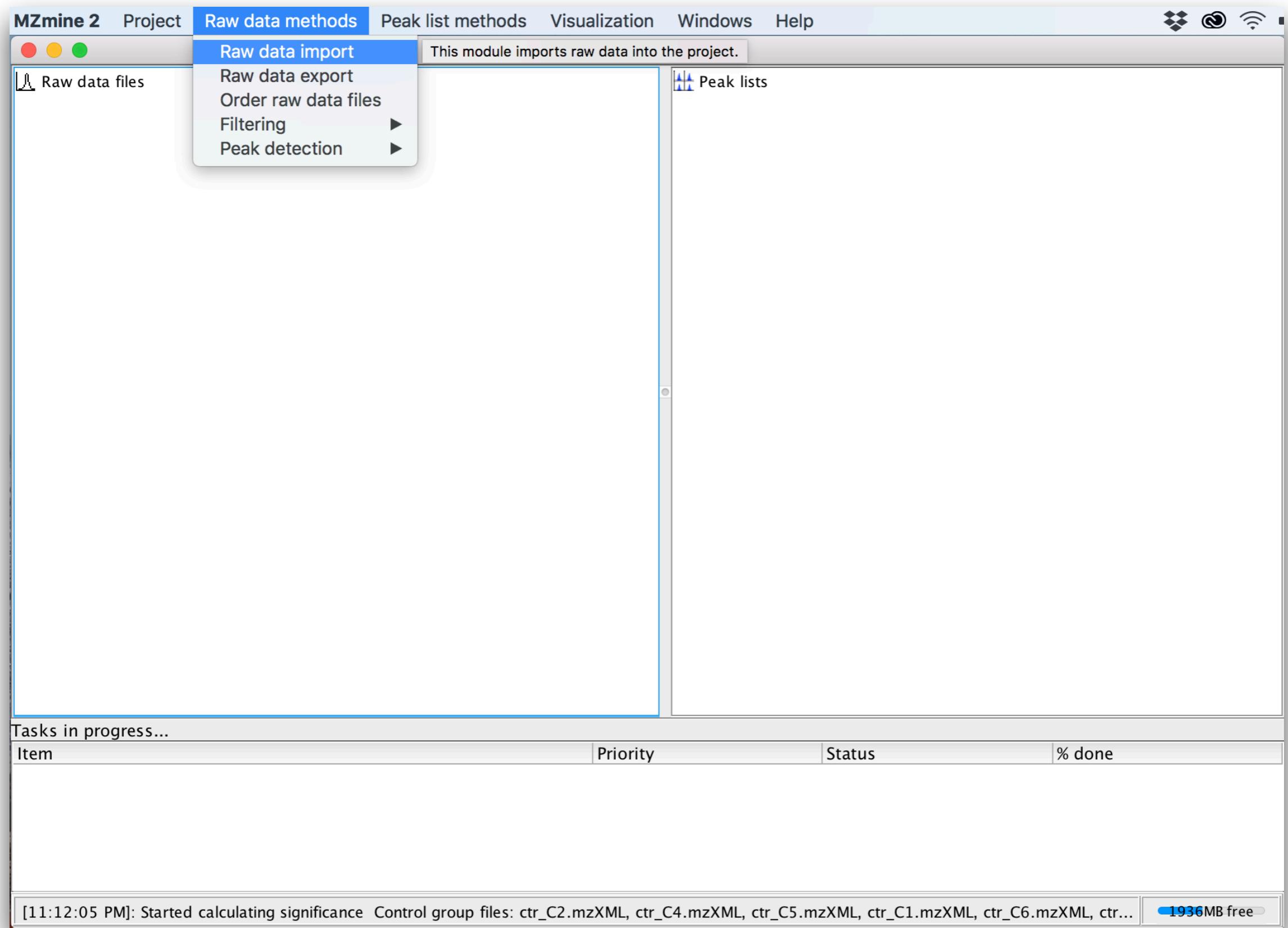
If you wish to support further open-source development of MZmine, you can do so via this button: [Donate](#)

LC-MS

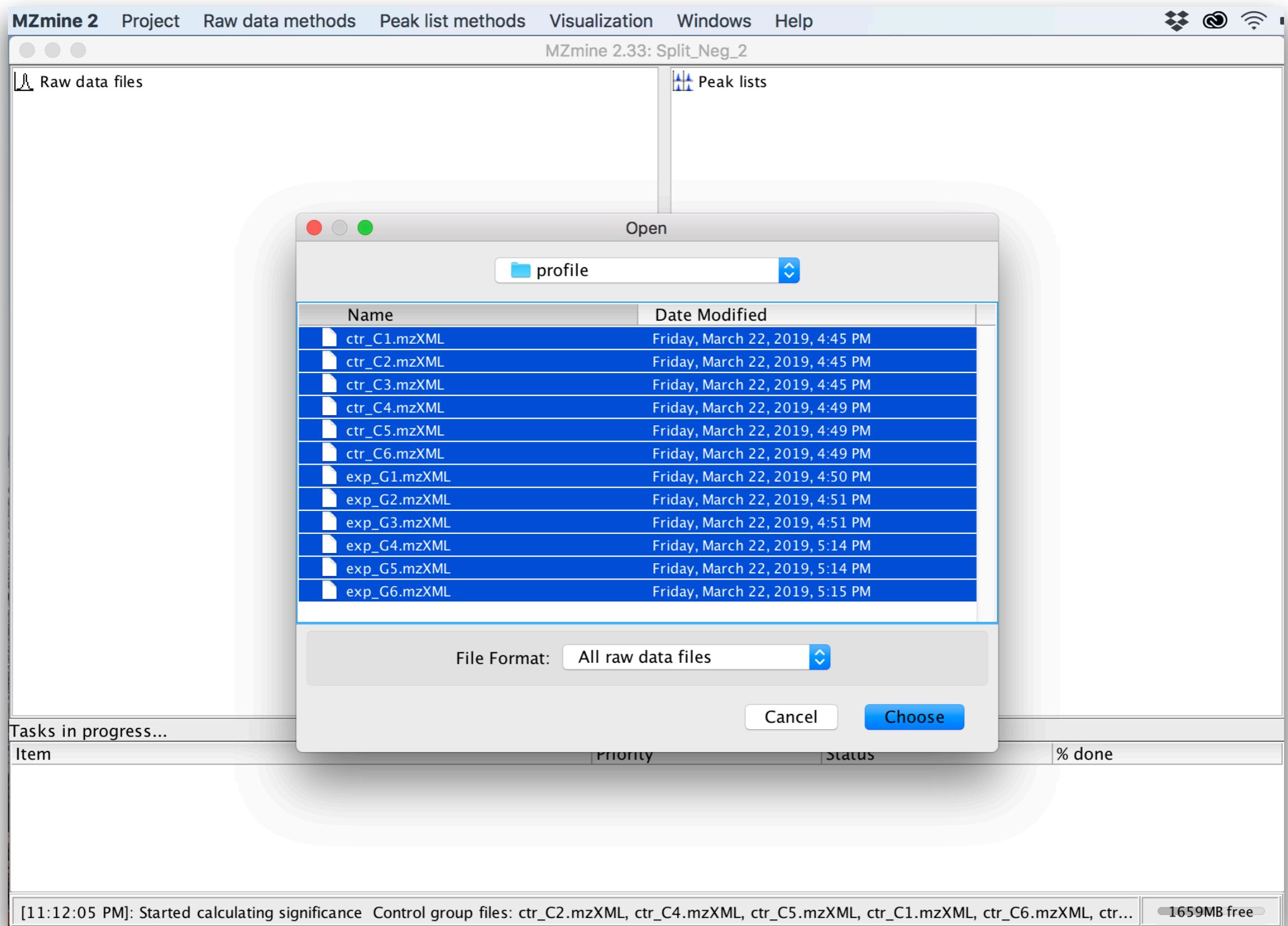
Workflow

- Raw data import
- Data visualization
- Mass detection
- Chromatogram building
- Deconvolution / Peak detection
- Peak alignment
- Mummichog
- Results export

Data import



Data import



Data import

MZmine 2 Project Raw data methods Peak list methods Visualization Windows Help

MZmine 2.33: Split_Neg_2

Raw data files Peak lists

Tasks in progress...

Item	Priority	Status	% done
Opening file /Users/xdu4/Documents/Duxiuxia/my_projects/MCBIOS_2019/raw...	NORMAL	PROCESSING	41%
Opening file /Users/xdu4/Documents/Duxiuxia/my_projects/MCBIOS_2019/raw...	NORMAL	PROCESSING	39%
Opening file /Users/xdu4/Documents/Duxiuxia/my_projects/MCBIOS_2019/raw...	NORMAL	PROCESSING	30%
Opening file /Users/xdu4/Documents/Duxiuxia/my_projects/MCBIOS_2019/raw...	NORMAL	PROCESSING	40%
Opening file /Users/xdu4/Documents/Duxiuxia/my_projects/MCBIOS_2019/raw...	NORMAL	WAITING	0%
Opening file /Users/xdu4/Documents/Duxiuxia/my_projects/MCBIOS_2019/raw...	NORMAL	WAITING	0%

[11:12:05 PM]: Started calculating significance Control group files: ctr_C2.mzXML, ctr_C4.mzXML, ctr_C5.mzXML, ctr_C1.mzXML, ctr_C6.mzXML, ctr... 2892MB free

Data import

MZmine 2 Project Raw data methods Peak list methods Visualization Windows Help

MZmine 2.33: Split_Neg_2

The screenshot shows the MZmine 2 software interface. The top menu bar includes 'MZmine 2', 'Project', 'Raw data methods', 'Peak list methods', 'Visualization', 'Windows', and 'Help'. The title bar reads 'MZmine 2.33: Split_Neg_2'. The main window has two main panes: 'Raw data files' on the left and 'Peak lists' on the right. The 'Raw data files' pane contains a list of mzXML files: ctr_C1.mzXML, ctr_C4.mzXML, ctr_C2.mzXML, ctr_C3.mzXML, ctr_C6.mzXML, exp_G1.mzXML, ctr_C5.mzXML, exp_G2.mzXML, exp_G3.mzXML, exp_G4.mzXML, exp_G5.mzXML, and exp_G6.mzXML. The 'Peak lists' pane is currently empty. At the bottom, a 'Tasks in progress...' section shows a table with columns 'Item', 'Priority', 'Status', and '% done'. A status bar at the bottom displays the message '[11:12:05 PM]: Started calculating significance Control group files: ctr_C2.mzXML, ctr_C4.mzXML, ctr_C5.mzXML, ctr_C1.mzXML, ctr_C6.mzXML, ctr...' and '1957 MB free'.

Raw data files

- ctr_C1.mzXML
- ctr_C4.mzXML
- ctr_C2.mzXML
- ctr_C3.mzXML
- ctr_C6.mzXML
- exp_G1.mzXML
- ctr_C5.mzXML
- exp_G2.mzXML
- exp_G3.mzXML
- exp_G4.mzXML
- exp_G5.mzXML
- exp_G6.mzXML

Peak lists

Tasks in progress...

Item	Priority	Status	% done
------	----------	--------	--------

[11:12:05 PM]: Started calculating significance Control group files: ctr_C2.mzXML, ctr_C4.mzXML, ctr_C5.mzXML, ctr_C1.mzXML, ctr_C6.mzXML, ctr... 1957 MB free

Data import

MZmine 2 Project Raw data methods Peak list methods Visualization Windows Help

MZmine 2.33: New project

Raw data files

- ctr_C2.mzXML
 - #1320 @10.01 MS1 p -
 - #1321 @10.02 MS1 p -
 - #1322 @10.03 MS1 p -
 - #1323 @10.03 MS1 p -
 - #1324 @10.06 MS2 (145.9328) p -
 - #1325 @10.06 MS1 p -
 - #1326 @10.08 MS2 (678.2014) p -
 - #1327 @10.09 MS2 (717.1485) p -
 - #1328 @10.09 MS1 p -
 - #1329 @10.10 MS2 (145.9325) c -
 - #1330 @10.11 MS2 (180.9752) p -
 - #1331 @10.11 MS2 (322.0795) p -
 - #1332 @10.11 MS2 (594.2857) p -
 - #1333 @10.12 MS2 (678.1998) p -
 - #1334 @10.12 MS2 (717.1486) p -
 - #1335 @10.12 MS1 p -
 - #1336 @10.14 MS2 (180.9748) p -
 - #1337 @10.14 MS2 (322.0789) p -
 - #1338 @10.15 MS2 (594.2857) p -
 - #1339 @10.15 MS1 p -
 - #1340 @10.16 MS1 p -
 - #1341 @10.17 MS1 p -
 - #1342 @10.18 MS1 p -
 - #1343 @10.19 MS1 p -
 - #1344 @10.21 MS2 (739.2846) n -

Peak lists

list of scans in raw files

- MS scans in blue
- MS/MS scans in red
- # sequential number
- @ retention time
- MS level
- type of spectrum
 - p = profile
 - c = centroid
 - t = thresholded
- polarity of ionization
 - + = positive
 - = negative
 - ? = unknown

Tasks in progress...

Item	Priority	Status	% done

[8:35:54 AM]: Processing of task Detecting masses in exp_G6.mzXML done, status FINISHED

2960MB free

Data visualization

The screenshot shows the MZmine 2 software interface. The main window displays a list of raw data files in the left panel, including various control (ctr) and experimental (exp) mzXML files. The top navigation bar includes tabs for Project, Raw data methods, Peak list methods, Visualization (which is currently selected and highlighted in blue), Windows, and Help. A sub-menu for 'Visualization' is open, listing several data visualization options: TIC/XIC visualizer, Spectra visualizer, 2D visualizer, 3D visualizer, MS/MS visualizer, Neutral loss visualizer, Scatter plot, Histogram plot, Peak intensity plot, Kendrick mass plot, and Van Krevelen Diagram. At the bottom of the interface, there is a 'Tasks in progress...' section and a status bar indicating system activity and memory usage.

MZmine 2 Project Raw data methods Peak list methods **Visualization** Windows Help

Raw data files

- ctr_C1.mzXML
- ctr_C4.mzXML
- ctr_C2.mzXML
- ctr_C3.mzXML
- ctr_C6.mzXML
- exp_G1.mzXML
- ctr_C5.mzXML
- exp_G2.mzXML
- exp_G3.mzXML
- exp_G4.mzXML
- exp_G5.mzXML
- exp_G6.mzXML

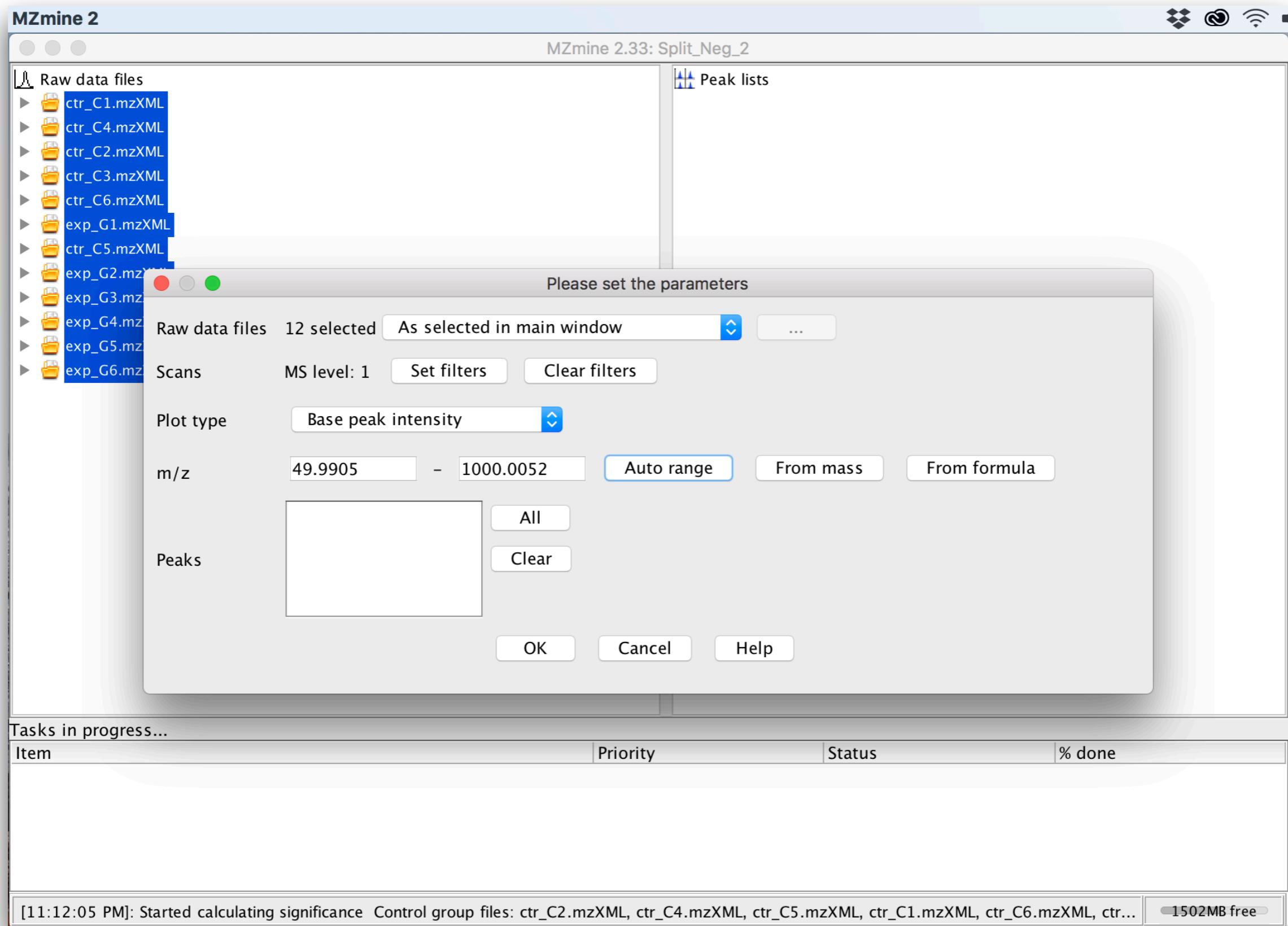
TIC/XIC visualizer
Spectra visualizer
2D visualizer
3D visualizer
MS/MS visualizer
Neutral loss visualizer
Scatter plot
Histogram plot
Peak intensity plot
Kendrick mass plot
Van Krevelen Diagram

Tasks in progress...

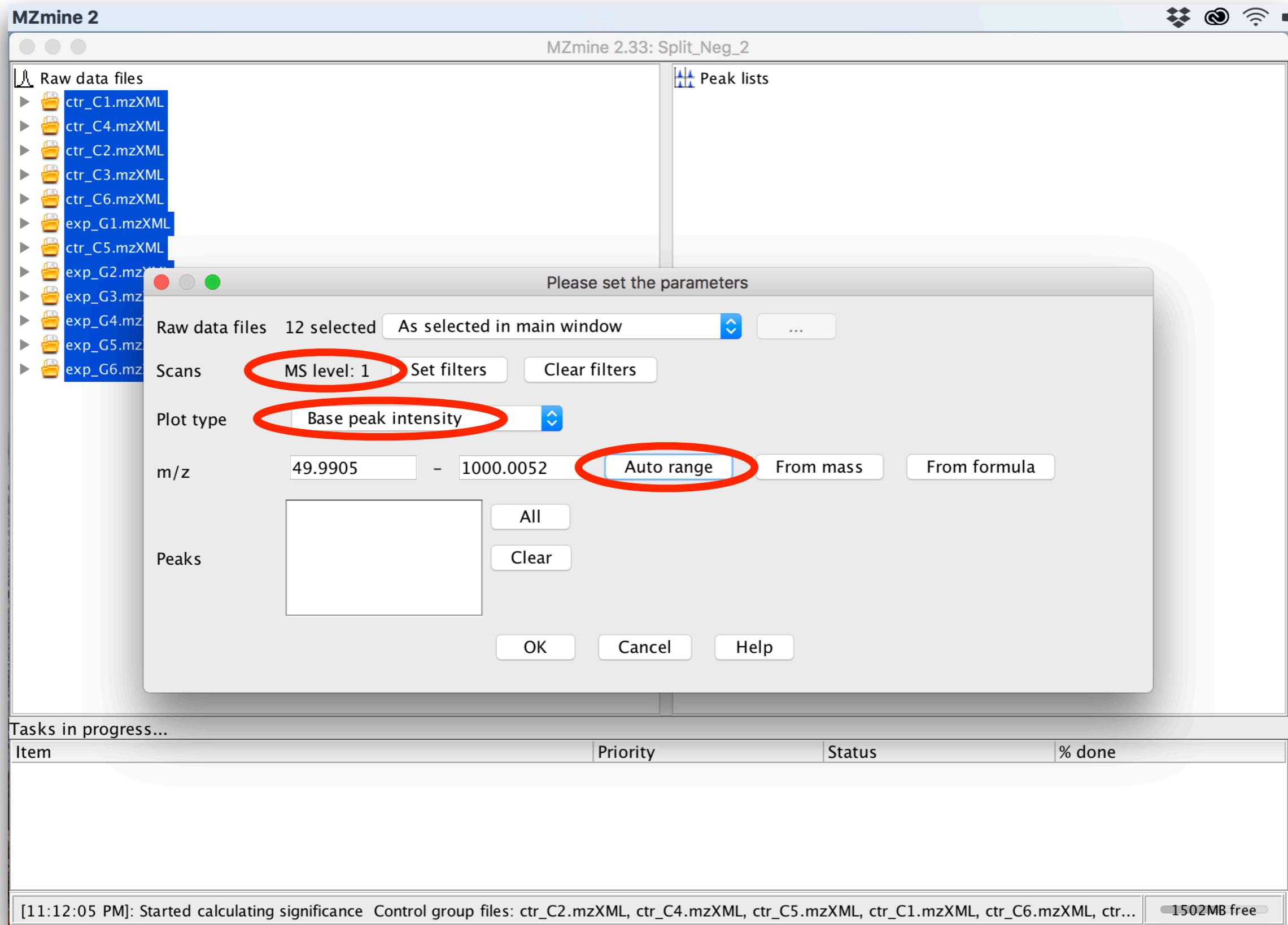
Item	Priority	Status	% done
------	----------	--------	--------

[11:12:05 PM]: Started calculating significance Control group files: ctr_C2.mzXML, ctr_C4.mzXML, ctr_C5.mzXML, ctr_C1.mzXML, ctr_C6.mzXML, ctr... 1694MB free

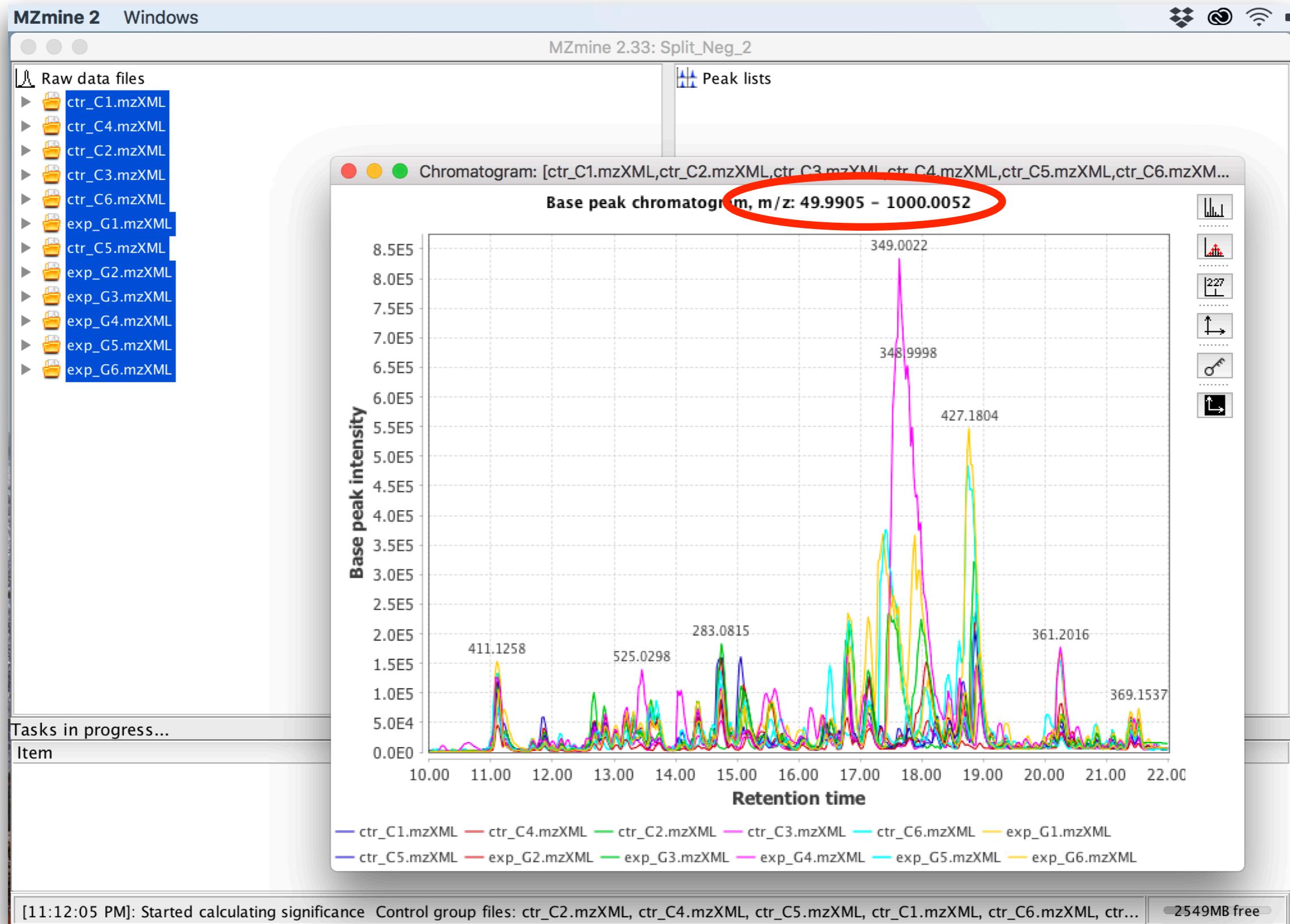
Data visualization



Data visualization: BIC



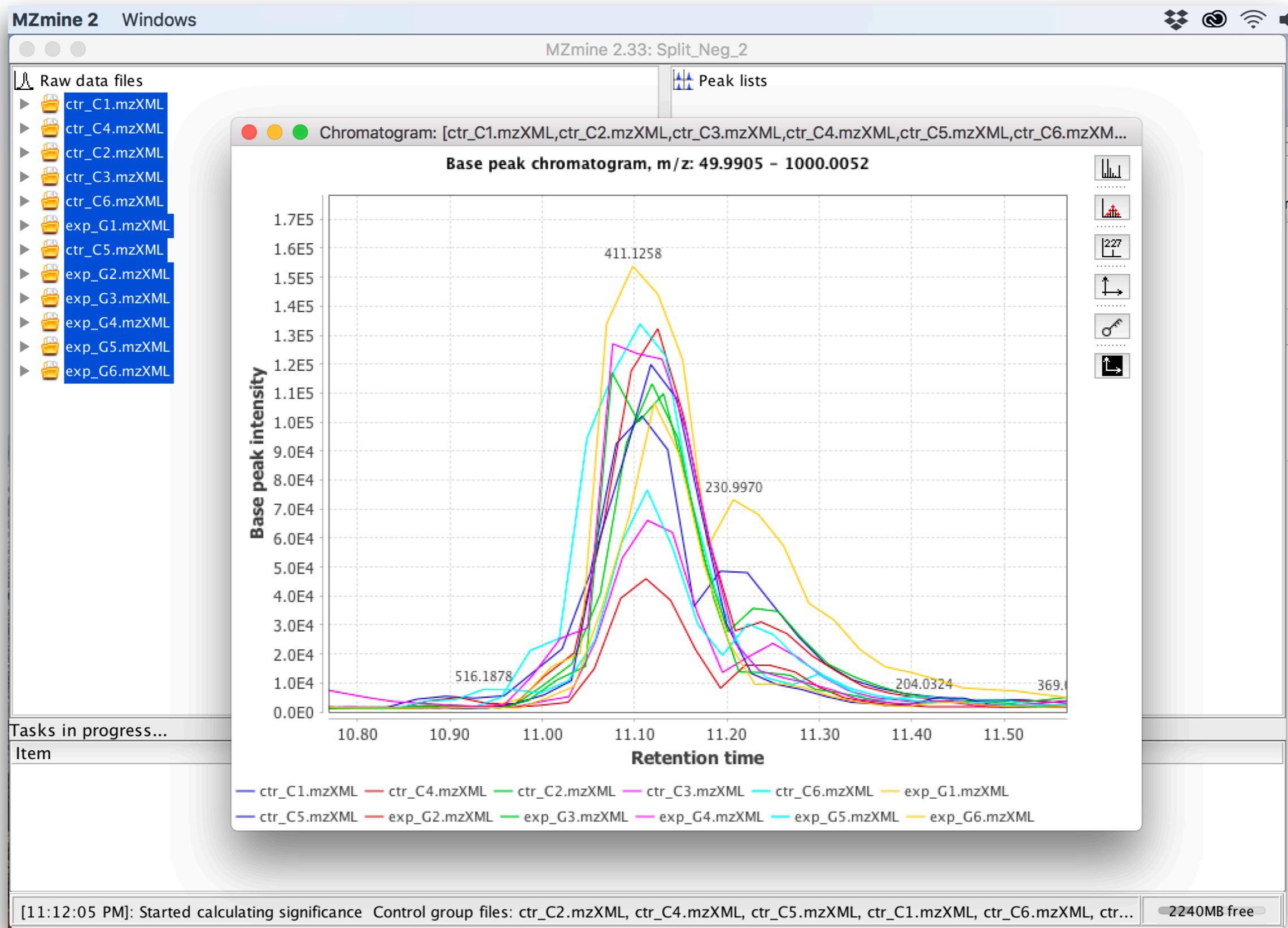
Data visualization: BIC



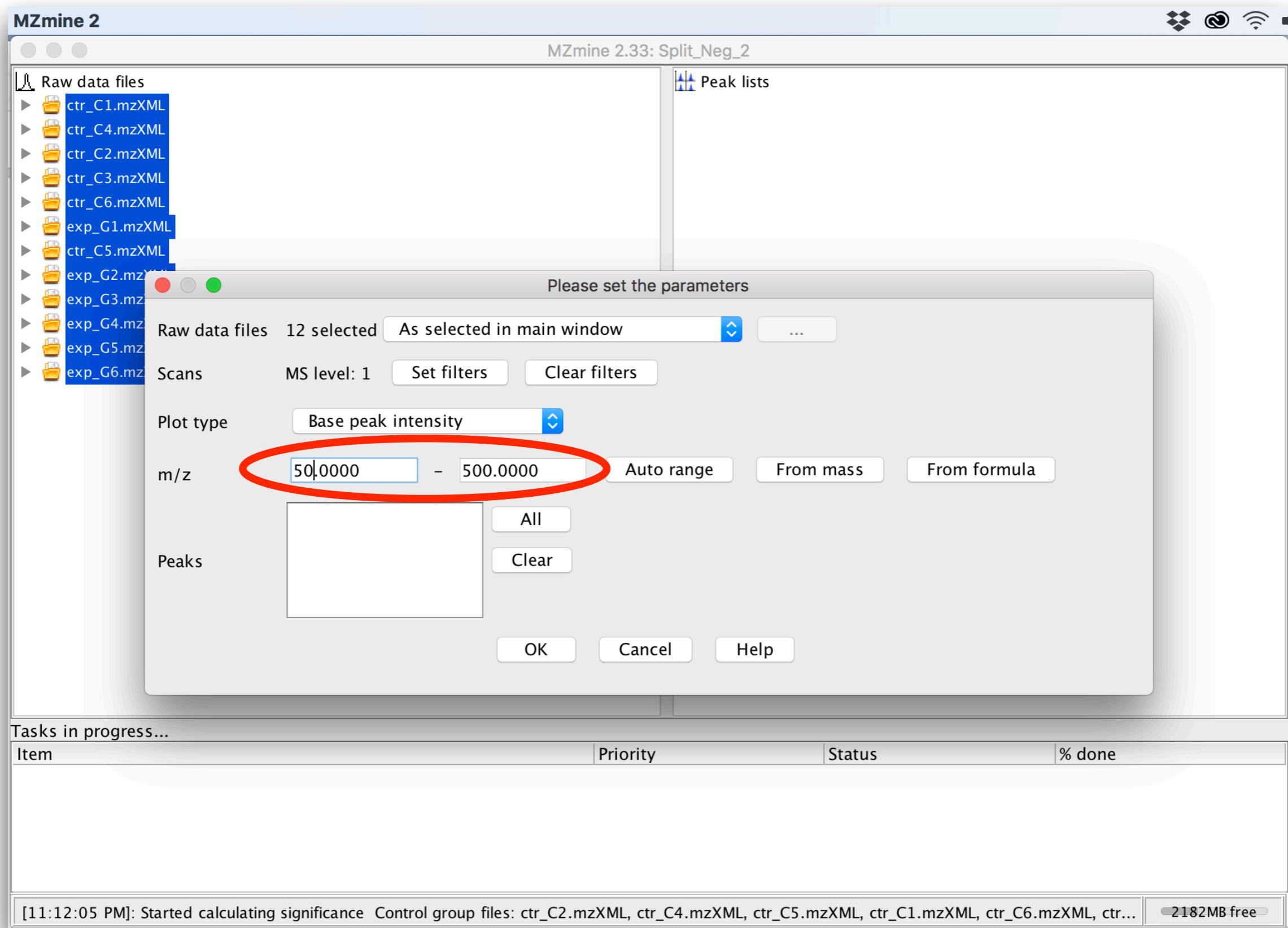
Data visualization: BIC

You can zoom in the BICs and examine them.

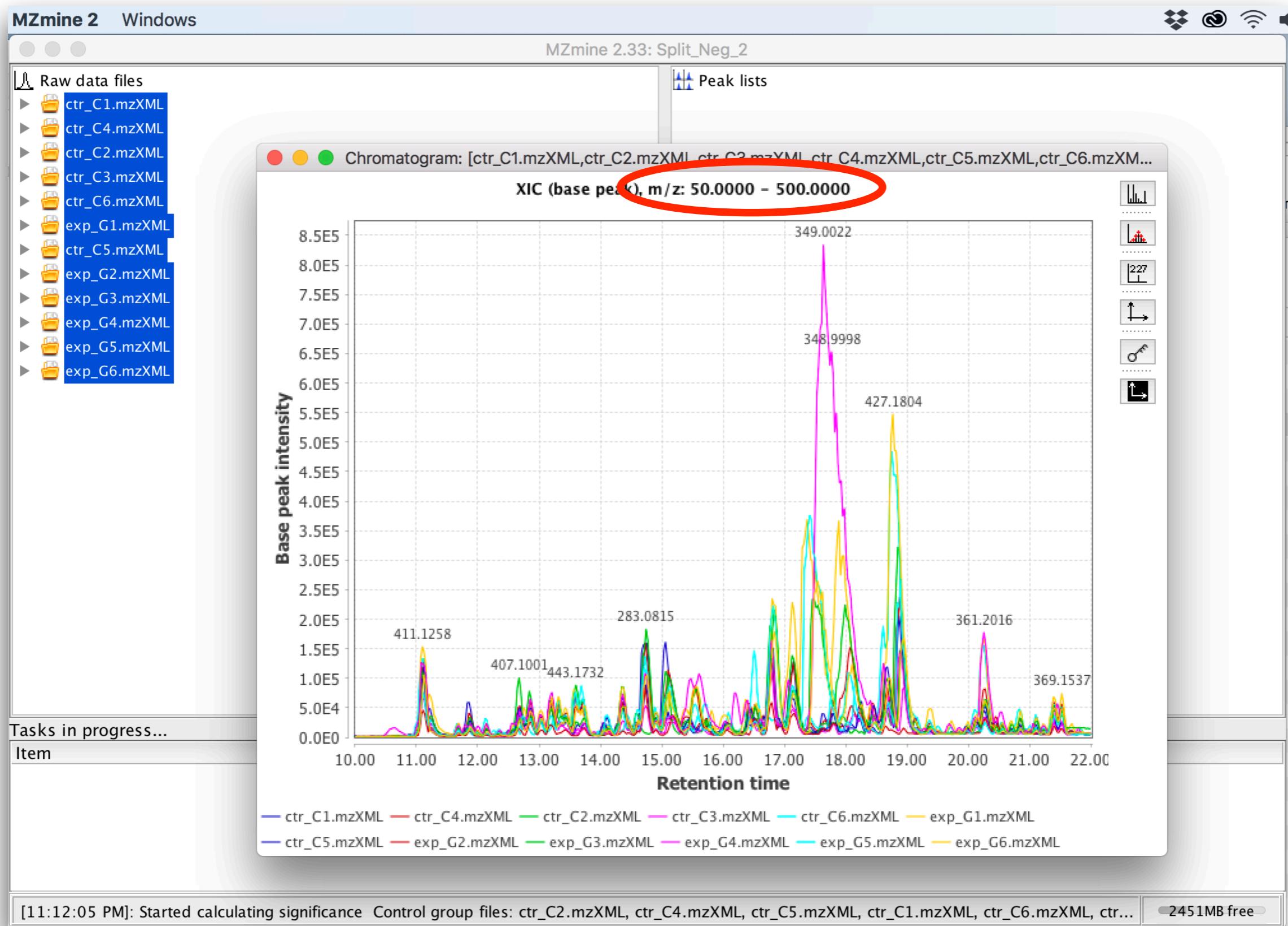
Data visualization: BIC



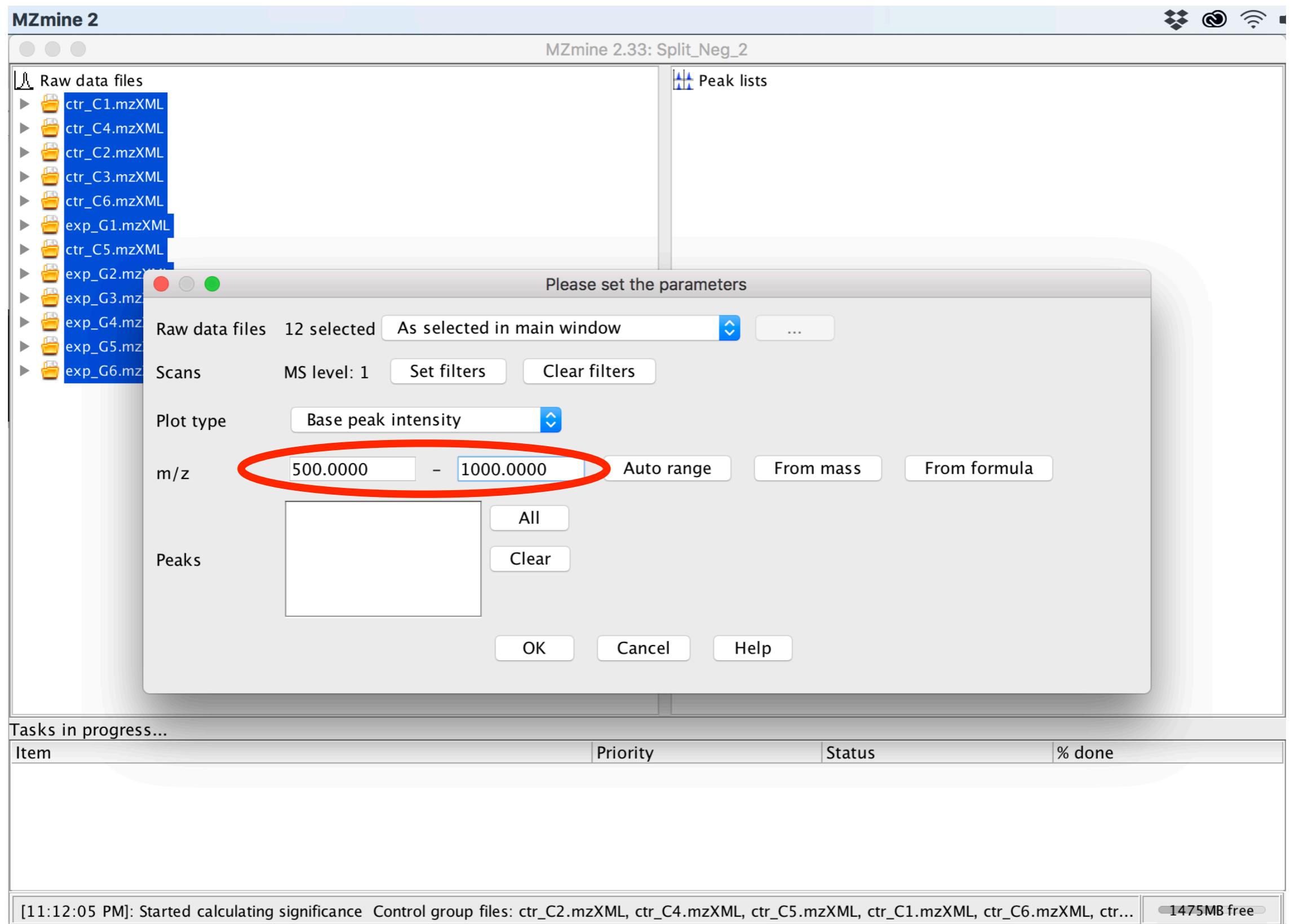
Data visualization: BIC



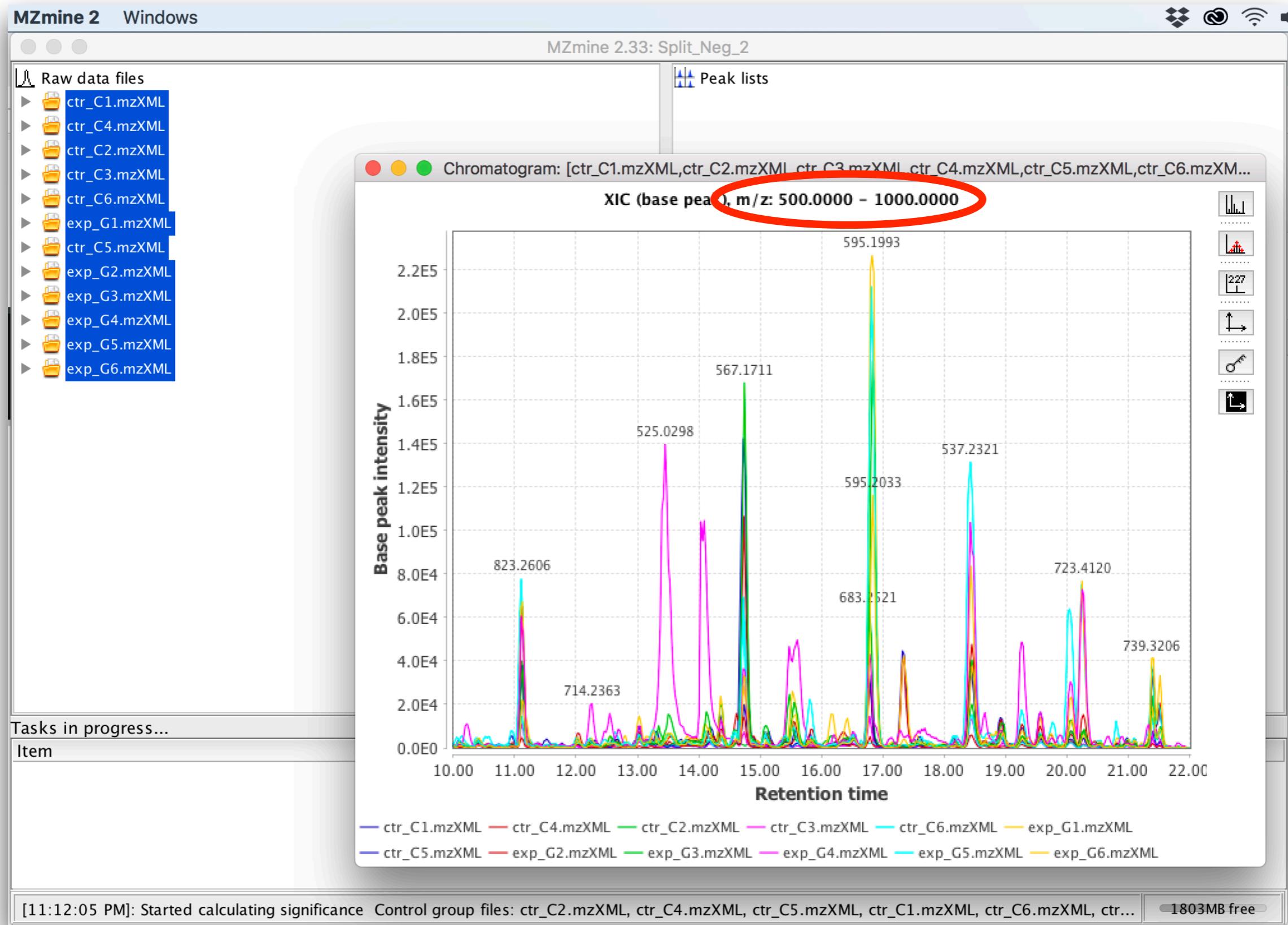
Data visualization: BIC



Data visualization: BIC



Data visualization: BIC



Data visualization: TIC

The screenshot shows the MZmine 2 software interface. The main window displays a list of raw data files in the left panel, including various control (ctr) and experimental (exp) mzXML files. The top navigation bar includes tabs for Project, Raw data methods, Peak list methods, Visualization, Windows, and Help. A context menu is open over the 'Visualization' tab, listing several data visualization options. The 'TIC/XIC visualizer' option is highlighted with a blue selection bar. The right panel contains a placeholder text 'TIC/XIC visualizer.' and a list of other plot types: Spectra visualizer, 2D visualizer, 3D visualizer, MS/MS visualizer, Neutral loss visualizer, Scatter plot, Histogram plot, Peak intensity plot, Kendrick mass plot, and Van Krevelen Diagram. At the bottom of the interface, there is a 'Tasks in progress...' section and a status bar indicating system activity and free memory.

MZmine 2 Project Raw data methods Peak list methods **Visualization** Windows Help

Raw data files

- ctr_C1.mzXML
- ctr_C4.mzXML
- ctr_C2.mzXML
- ctr_C3.mzXML
- ctr_C6.mzXML
- exp_G1.mzXML
- ctr_C5.mzXML
- exp_G2.mzXML
- exp_G3.mzXML
- exp_G4.mzXML
- exp_G5.mzXML
- exp_G6.mzXML

TIC/XIC visualizer

Spectra visualizer
2D visualizer
3D visualizer
MS/MS visualizer
Neutral loss visualizer

Scatter plot
Histogram plot
Peak intensity plot
Kendrick mass plot
Van Krevelen Diagram

Tasks in progress...

Item	Priority	Status	% done
------	----------	--------	--------

[11:12:05 PM]: Started calculating significance Control group files: ctr_C2.mzXML, ctr_C4.mzXML, ctr_C5.mzXML, ctr_C1.mzXML, ctr_C6.mzXML, ctr... 1377MB free

Data visualization: TIC

MZmine 2

MZmine 2.33: Split_Neg_2

Raw data files

- ctr_C1.mzXML
- ctr_C4.mzXML
- ctr_C2.mzXML
- ctr_C3.mzXML
- ctr_C6.mzXML
- exp_G1.mzXML
- ctr_C5.mzXML
- exp_G2.mzXML
- exp_G3.mz
- exp_G4.mz
- exp_G5.mz
- exp_G6.mz

Peak lists

Please set the parameters

Raw data files 12 selected As selected in main window

Scans MS level: 1 Set filters Clear filters

Plot type Total ion current (TIC/XIC)

m/z 49.9905 - 1000.0052 Auto range From mass From formula

Peaks All Clear

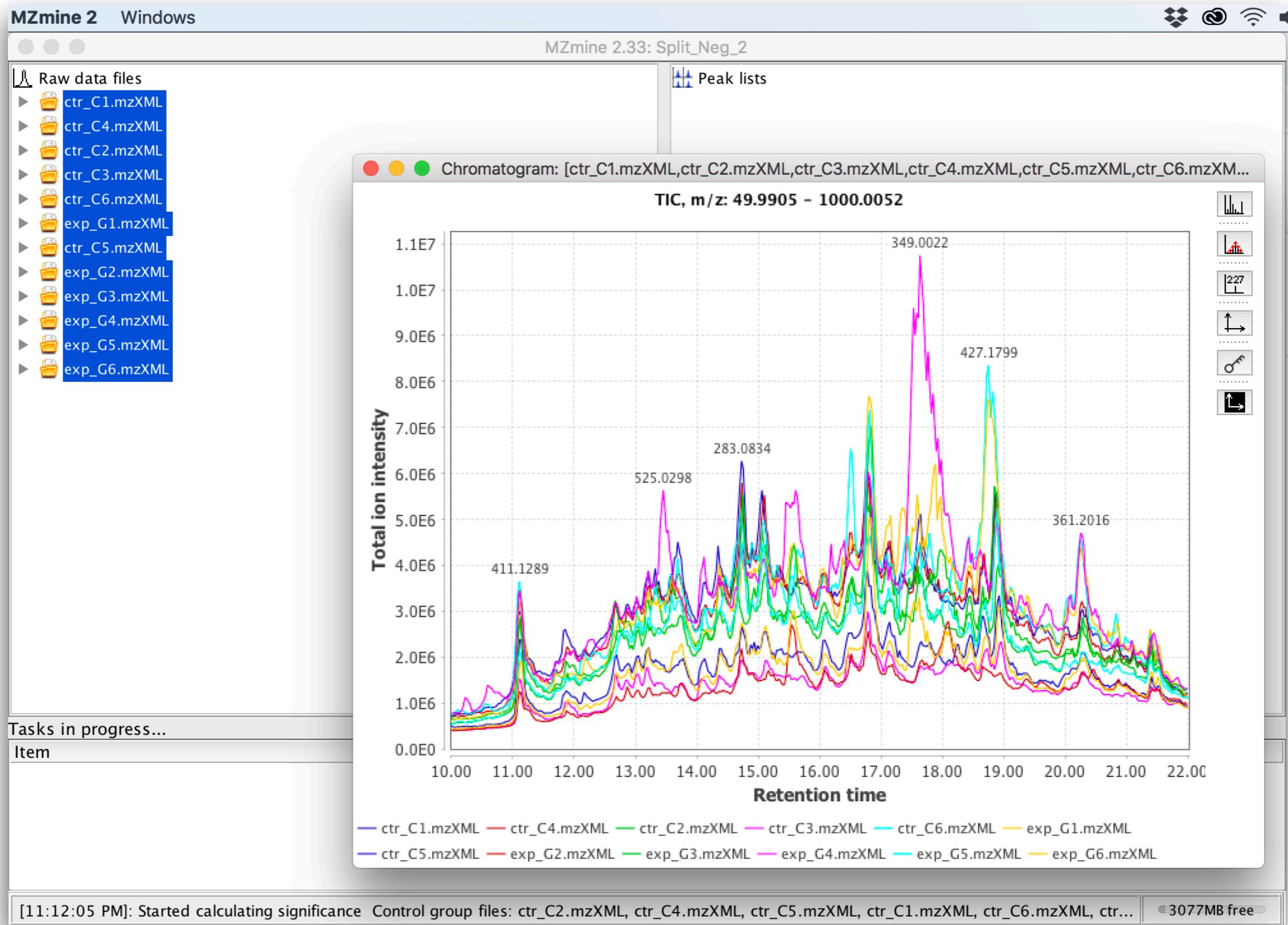
OK Cancel Help

Tasks in progress...

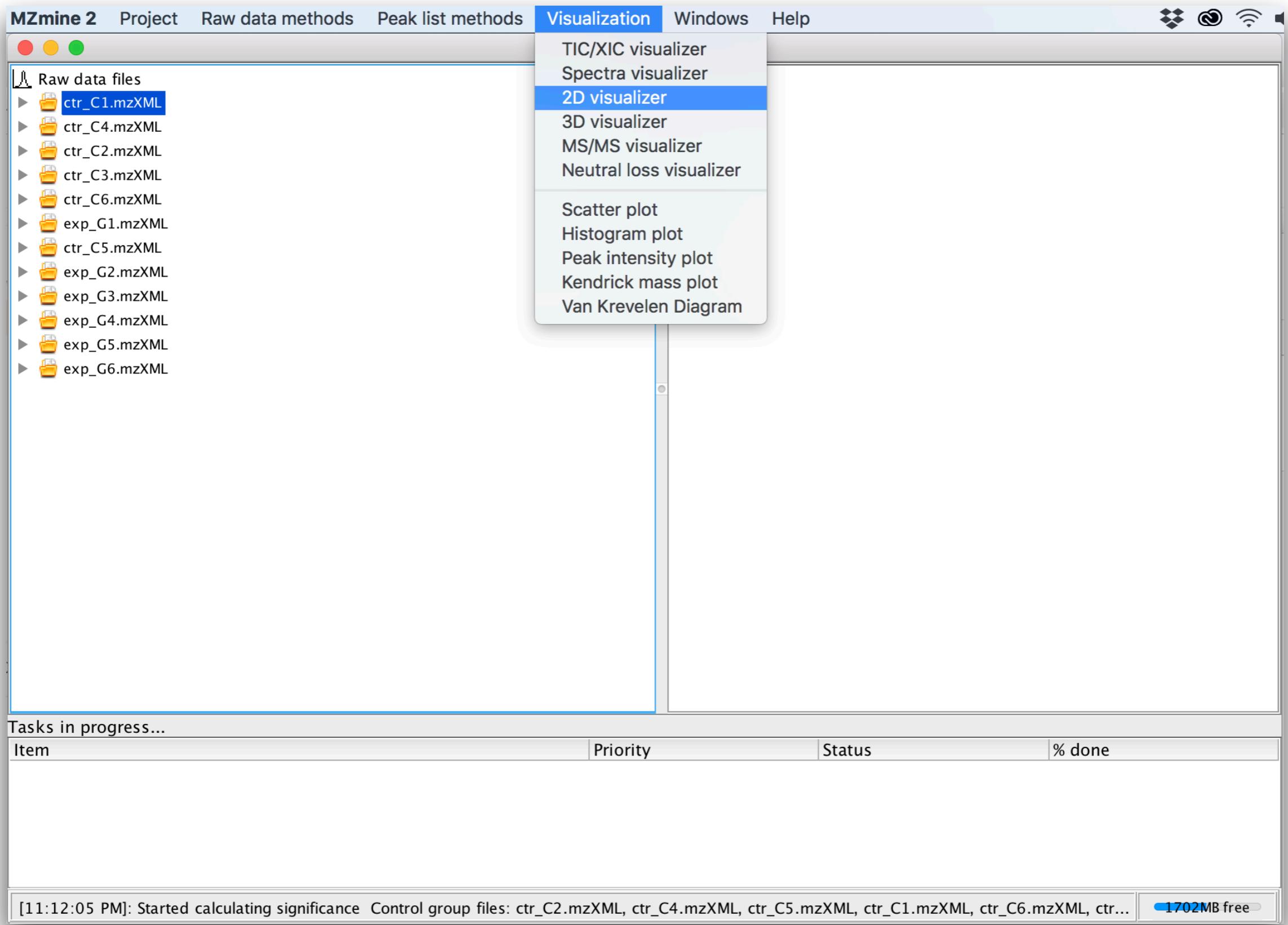
Item	Priority	Status	% done

[11:12:05 PM]: Started calculating significance Control group files: ctr_C2.mzXML, ctr_C4.mzXML, ctr_C5.mzXML, ctr_C1.mzXML, ctr_C6.mzXML, ctr... 1260MB free

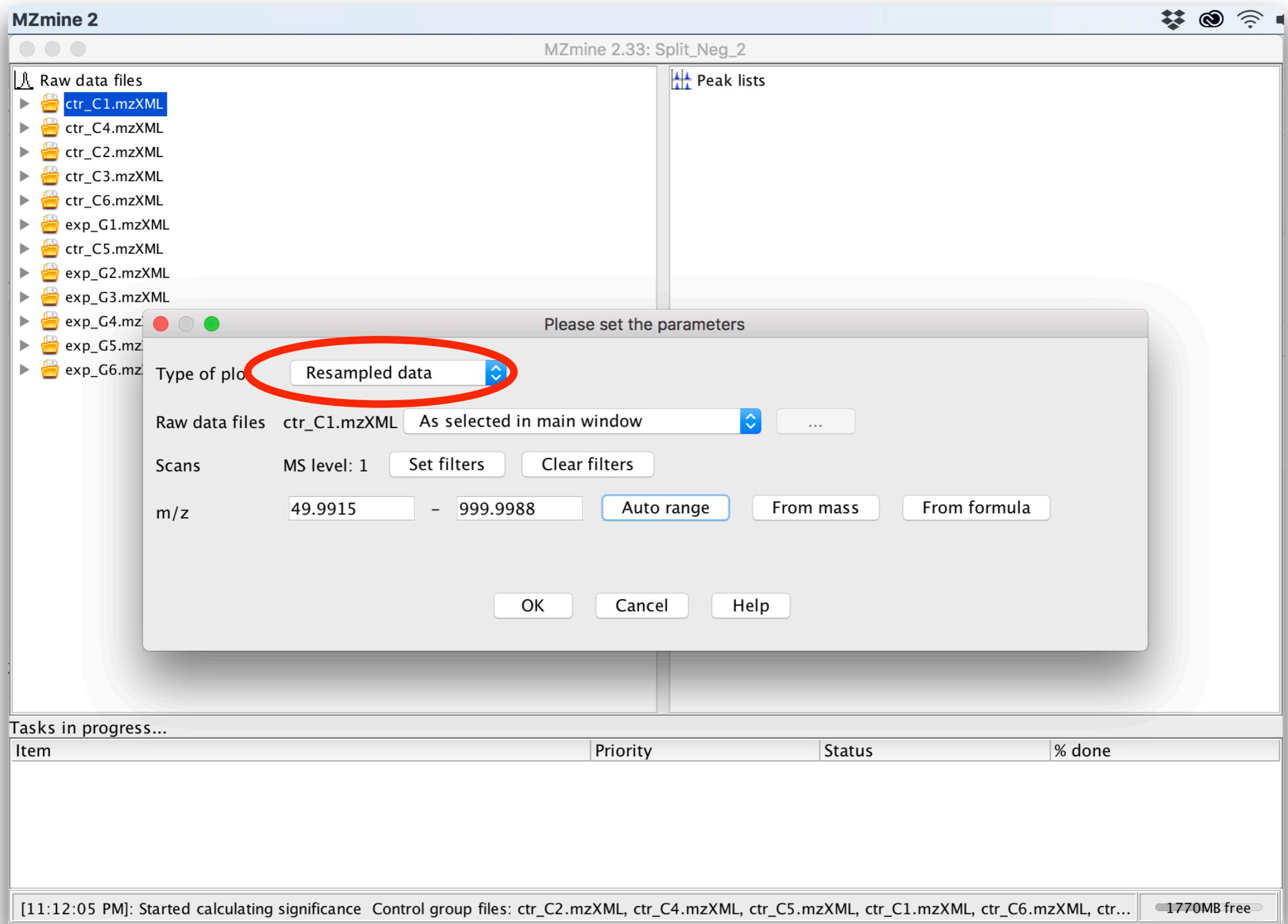
Data visualization: TIC



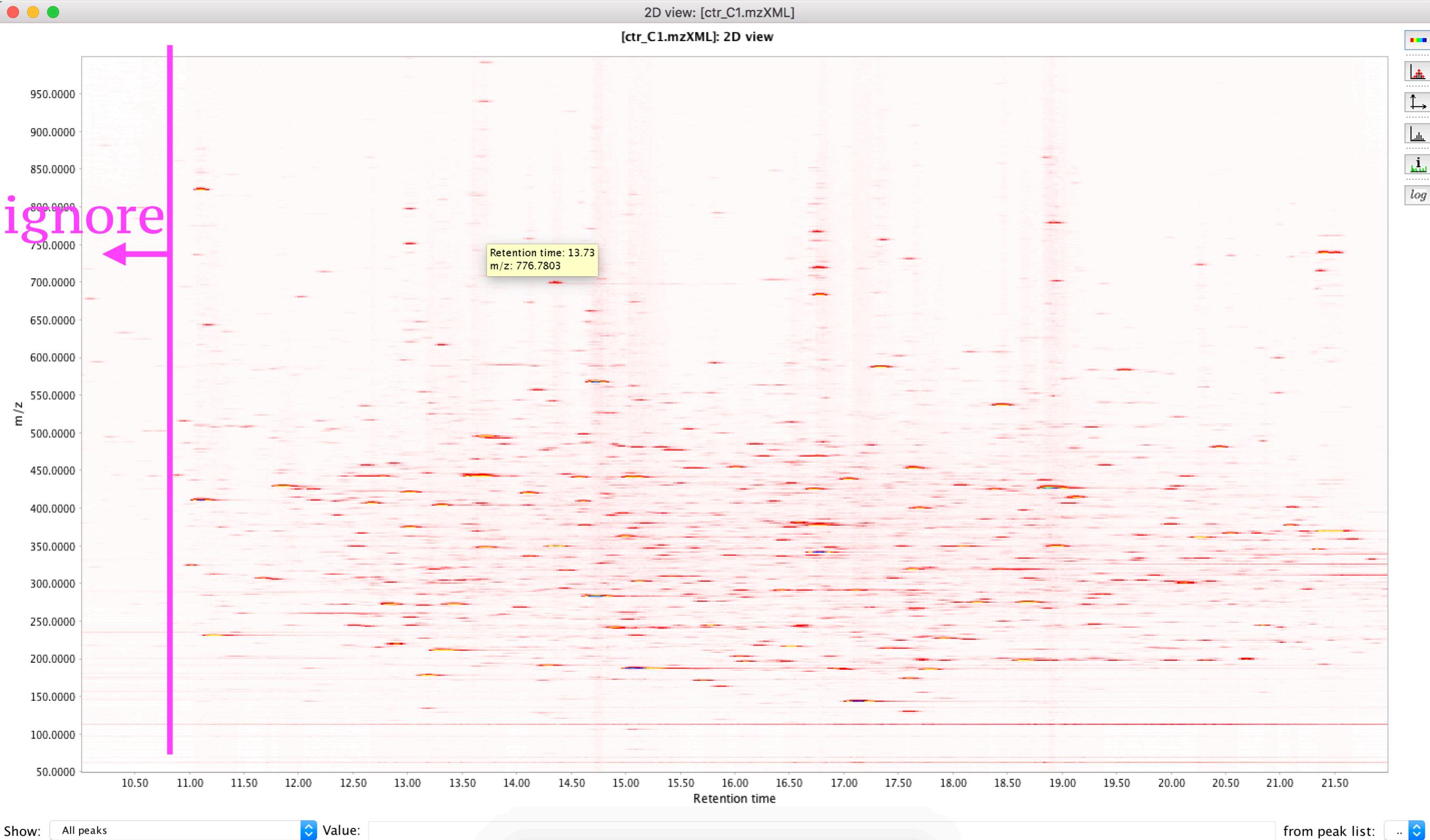
Data visualization: 2D



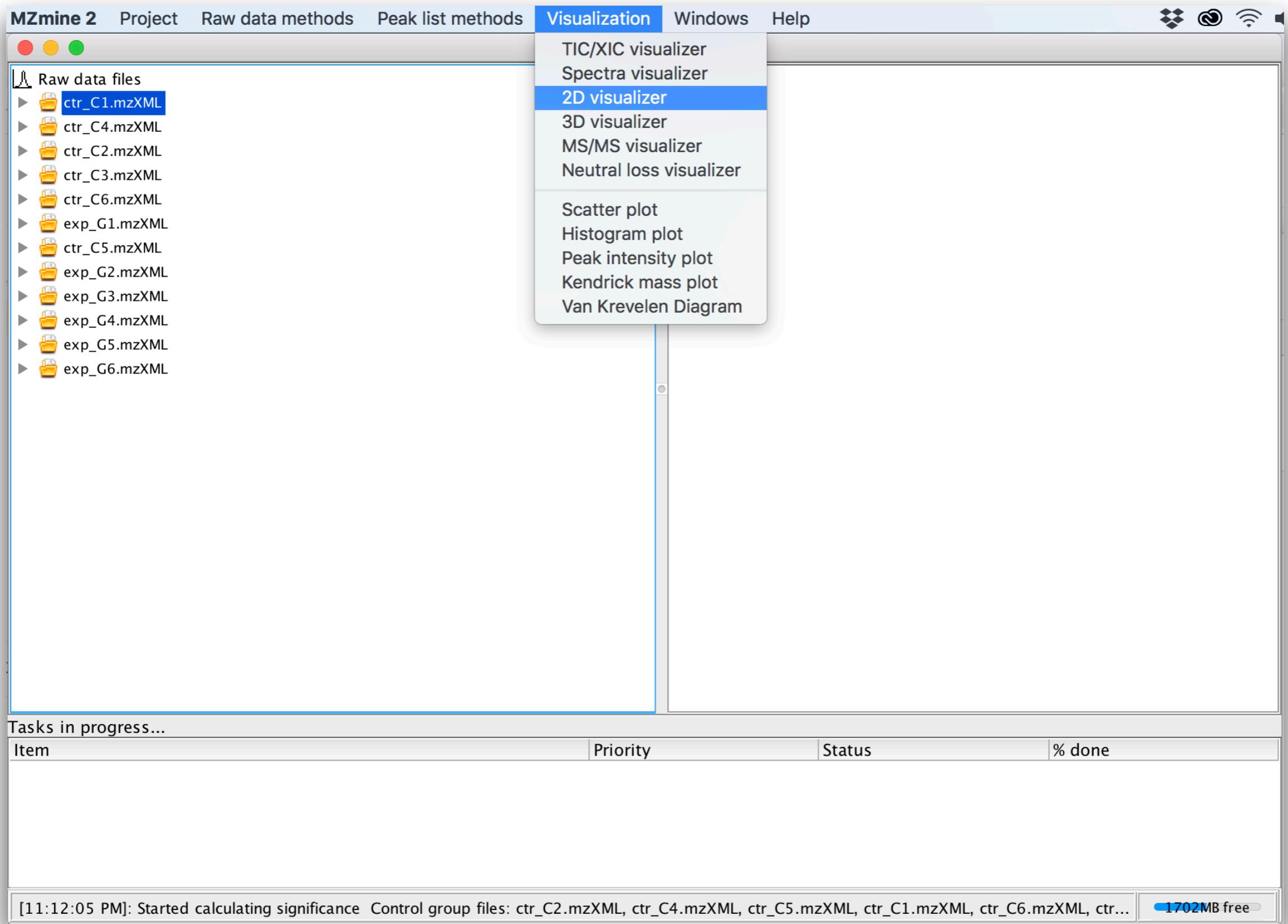
Data visualization: 2D



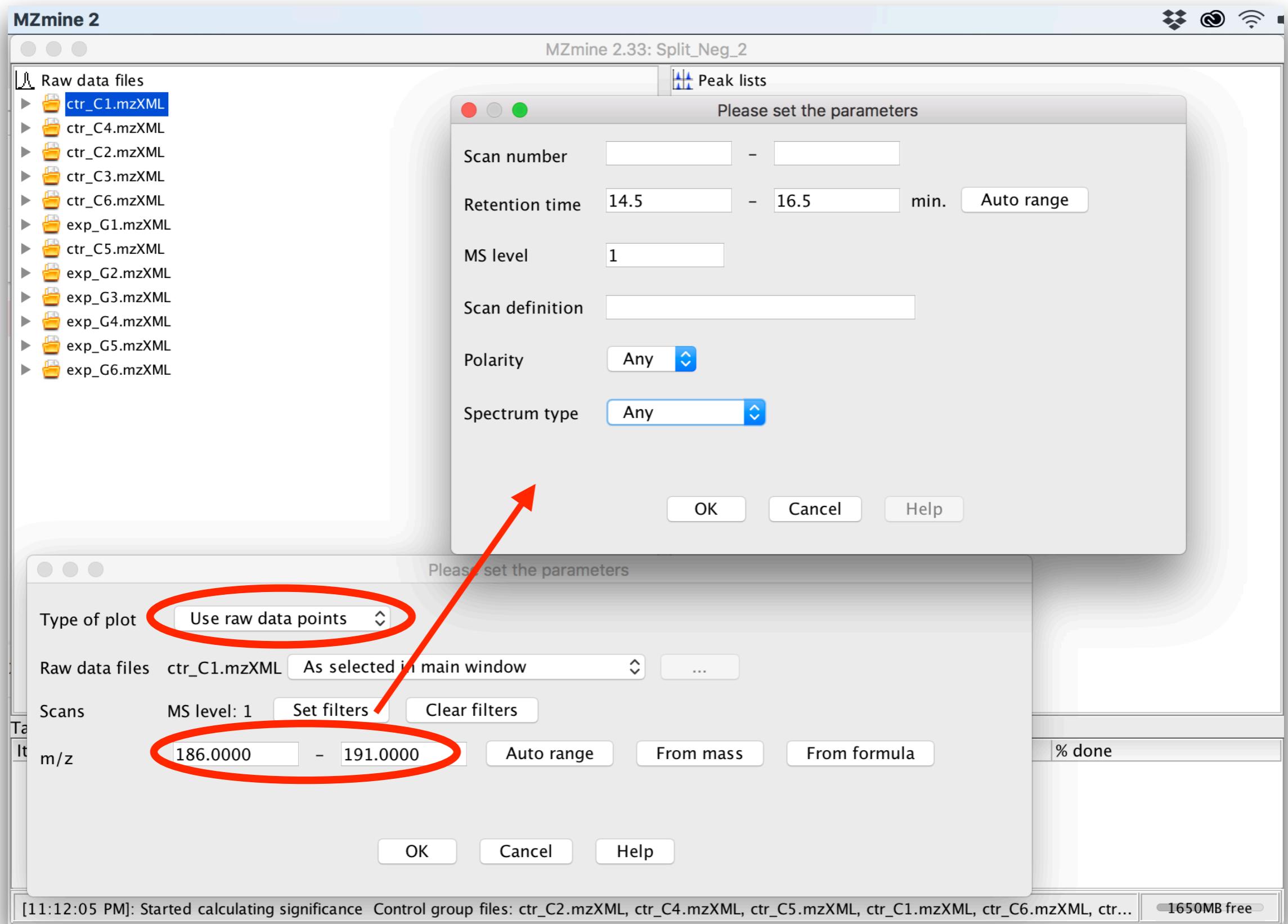
Data visualization: 2D



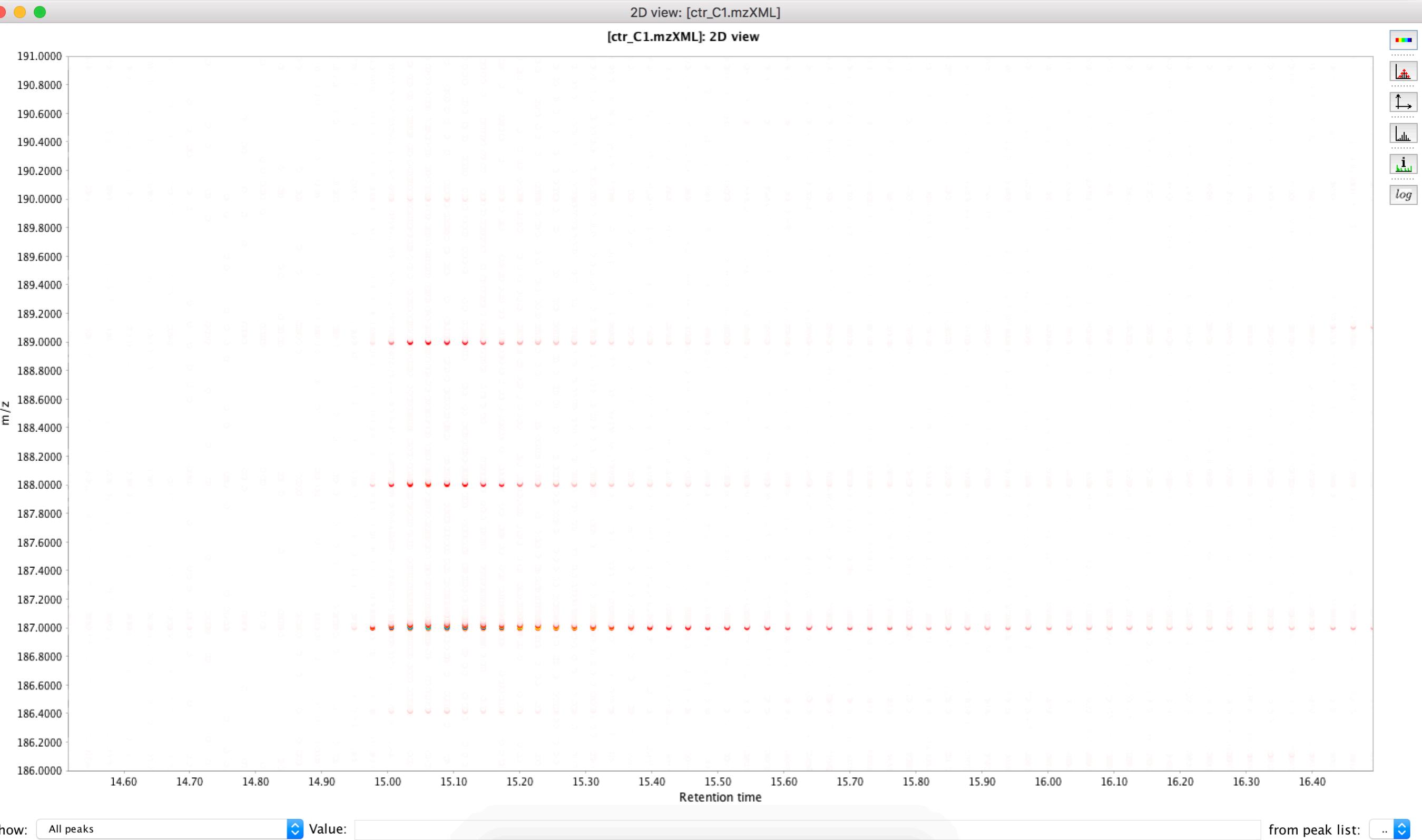
Data visualization: 2D



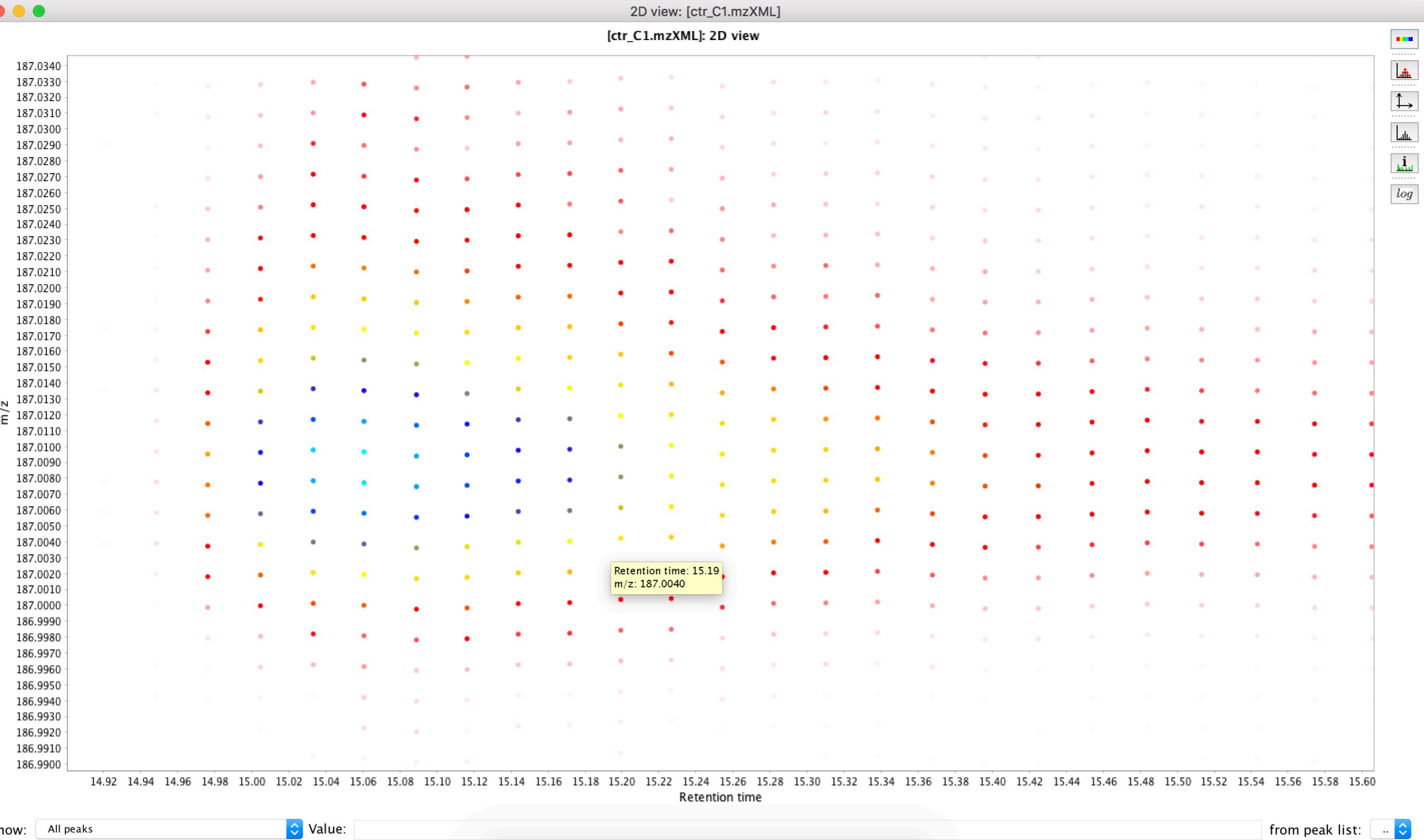
Data visualization: 2D



Data visualization: 2D



Data visualization: 2D



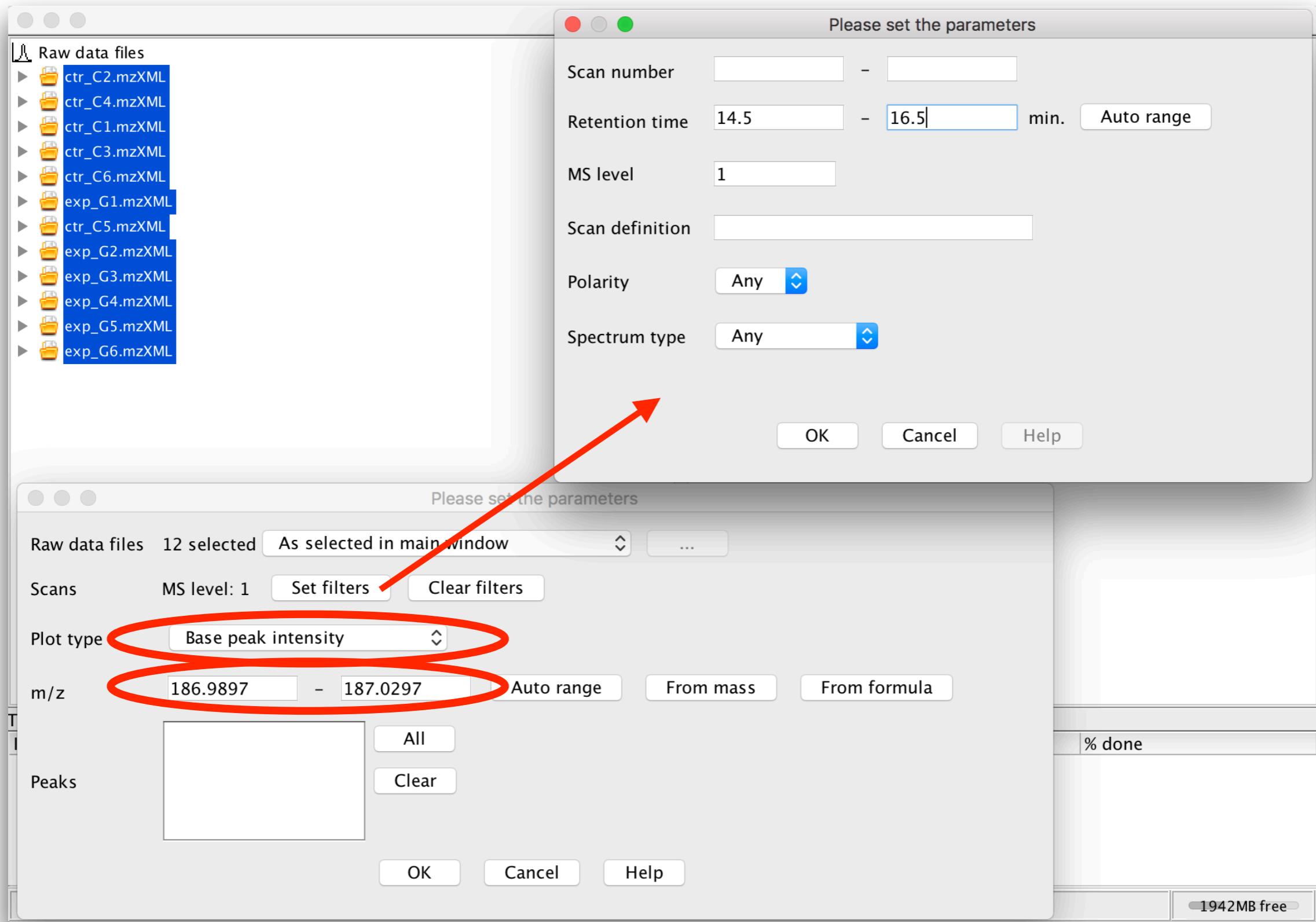
Data visualization: EIC

The screenshot shows the MZmine 2 software interface. The top menu bar includes "MZmine 2", "Project", "Raw data methods", "Peak list methods", "Visualization" (which is highlighted in blue), "Windows", and "Help". The "Visualization" menu is open, displaying various plotting options:

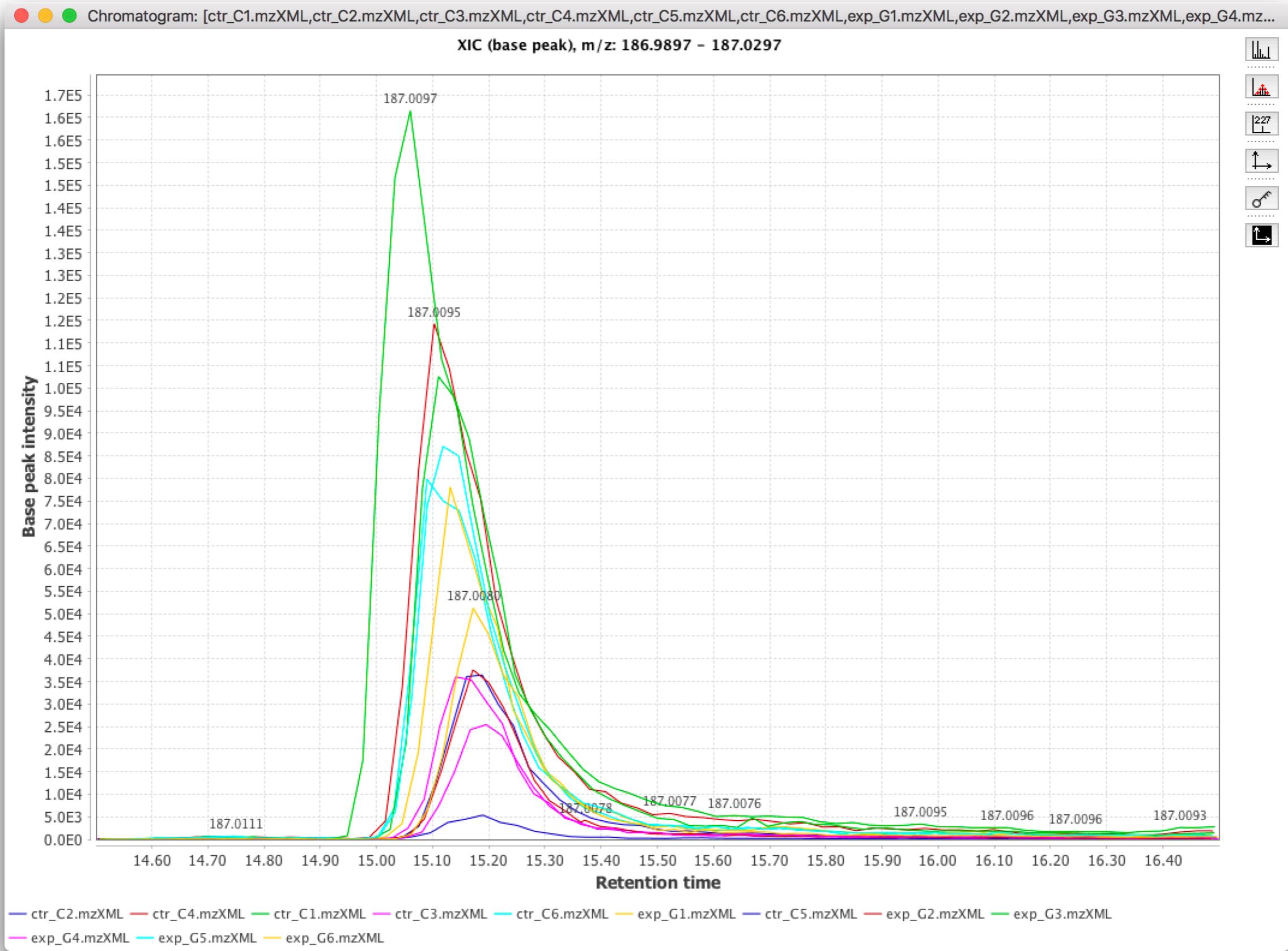
- TIC/XIC visualizer (selected)
- Spectra visualizer
- 2D visualizer
- 3D visualizer
- MS/MS visualizer
- Neutral loss visualizer
- Scatter plot
- Histogram plot
- Peak intensity plot
- Kendrick mass plot
- Van Krevelen Diagram

The main workspace on the left lists "Raw data files" with entries for "ctr_C1.mzXML" through "ctr_C6.mzXML" and "exp_G1.mzXML" through "exp_G6.mzXML". A "Tasks in progress..." section at the bottom indicates no active tasks. The status bar at the bottom shows the message "[11:12:05 PM]: Started calculating significance Control group files: ctr_C2.mzXML, ctr_C4.mzXML, ctr_C5.mzXML, ctr_C1.mzXML, ctr_C6.mzXML, ctr..." and "1377MB free".

Data visualization: EIC



Data visualization: EIC



Mass detection

- Mass detection: detect masses from mass spectra
 - Centroid
 - Exact mass
 - Local maxima
 - Recursive threshold
 - Wavelet transform

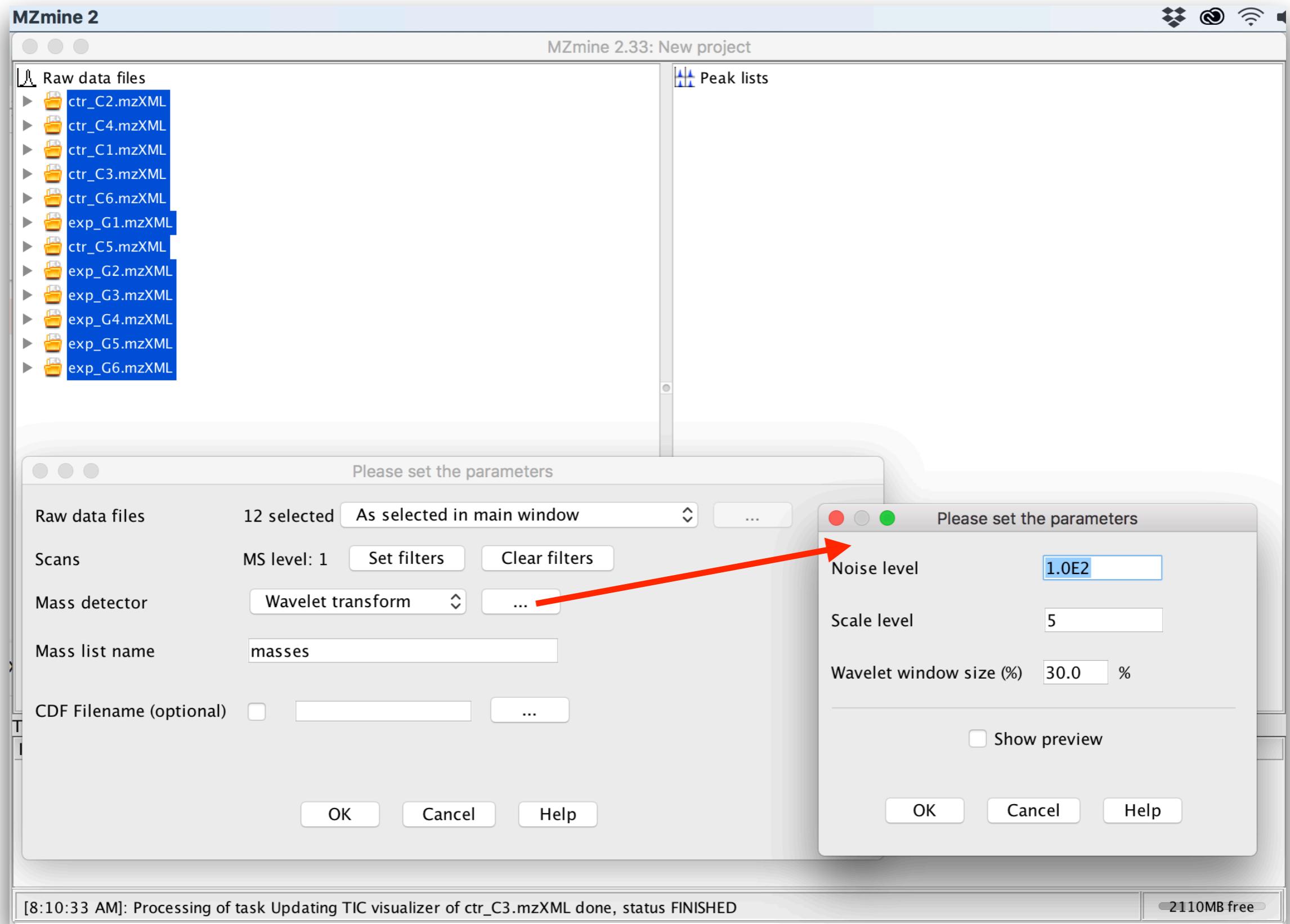
Mass detection

- Mass detection: detect masses from mass spectra
 - Centroid
 - Exact mass
 - Local maxima
 - Recursive threshold
 - Wavelet transform

Mass detection

The screenshot shows the MZmine 2 software interface. The menu bar includes 'MZmine 2', 'Project', 'Raw data methods' (which is selected), 'Peak list methods', 'Visualization', 'Windows', and 'Help'. The 'Raw data methods' menu is open, showing sub-options: 'Raw data import', 'Raw data export', 'Order raw data files', 'Filtering', 'Peak detection' (selected), and 'Mass detection'. A tooltip for 'Mass detection' states: 'This module detects individual ions in each scan and builds a mass list for each scan.' The main workspace displays a list of raw data files on the left: 'ctr_C2.mzXML', 'ctr_C4.mzXML', 'ctr_C1.mzXML', 'ctr_C3.mzXML', 'ctr_C6.mzXML', 'exp_G1.mzXML', 'ctr_C5.mzXML', 'exp_G2.mzXML', 'exp_G3.mzXML', 'exp_G4.mzXML', 'exp_G5.mzXML', and 'exp_G6.mzXML'. Below the workspace, a table titled 'Tasks in progress...' shows four columns: 'Item', 'Priority', 'Status', and '% done'. At the bottom of the screen, a status bar indicates '[8:10:33 AM]: Processing of task Updating TIC visualizer of ctr_C3.mzXML done, status FINISHED' and '2268MB free'.

Mass detection



Mass detection

MZmine 2 Project Raw data methods Peak list methods Visualization Windows Help

MZmine 2.33: New project

Raw data files

- ctr_C2.mzXML
- ctr_C4.mzXML
- ctr_C1.mzXML
- ctr_C3.mzXML
- ctr_C6.mzXML
- exp_G1.mzXML
- ctr_C5.mzXML
- exp_G2.mzXML
- exp_G3.mzXML
- exp_G4.mzXML
- exp_G5.mzXML
- exp_G6.mzXML

Peak lists

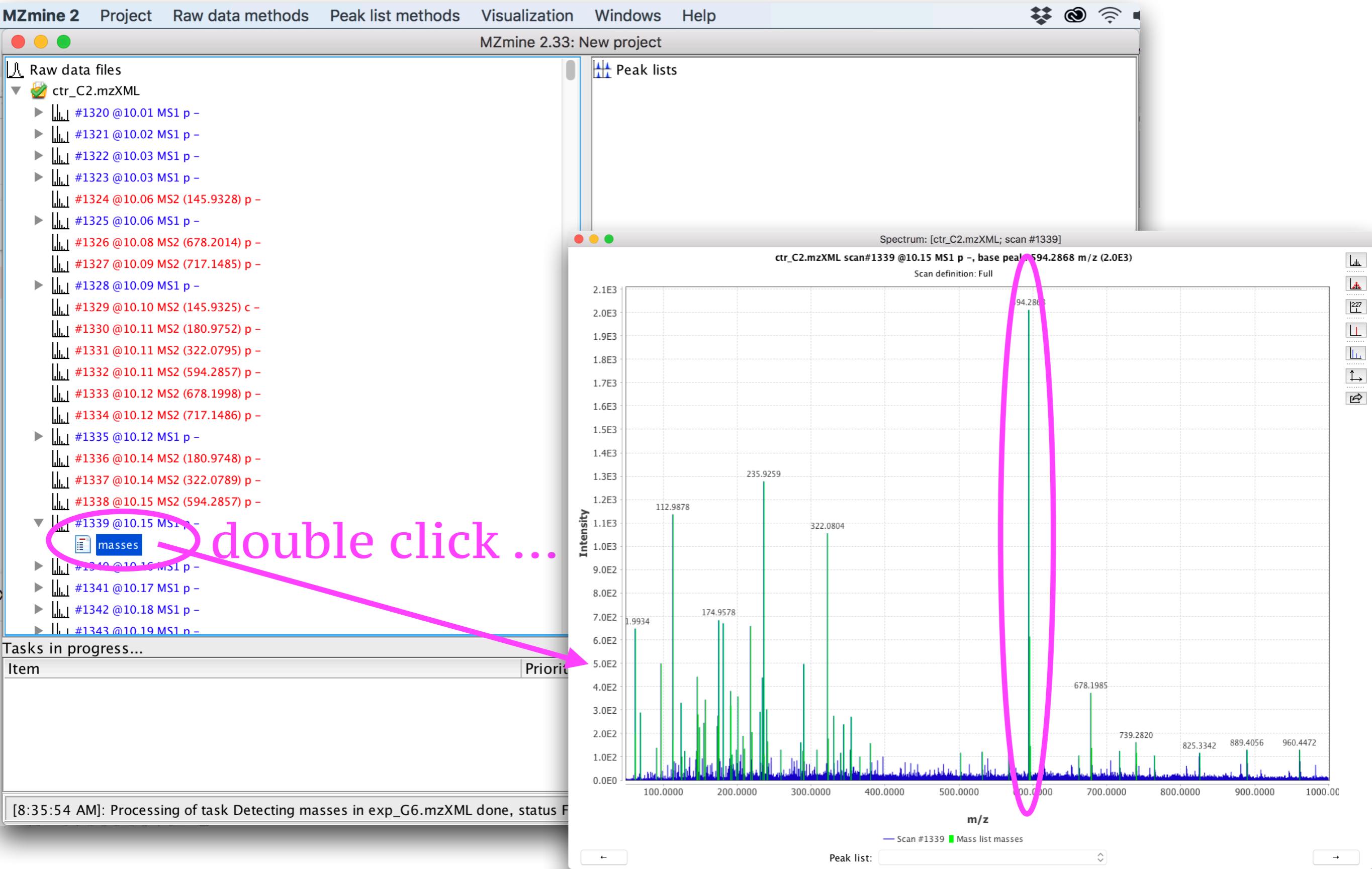
Tasks in progress...

Item	Priority	Status	% done
Detecting masses in ctr_C2.mzXML	NORMAL	PROCESSING	32%
Detecting masses in ctr_C4.mzXML	NORMAL	PROCESSING	32%
Detecting masses in ctr_C1.mzXML	NORMAL	PROCESSING	32%
Detecting masses in ctr_C3.mzXML	NORMAL	PROCESSING	30%
Detecting masses in ctr_C6.mzXML	NORMAL	WAITING	0%
Detecting masses in exp_G1.mzXML	NORMAL	WAITING	0%

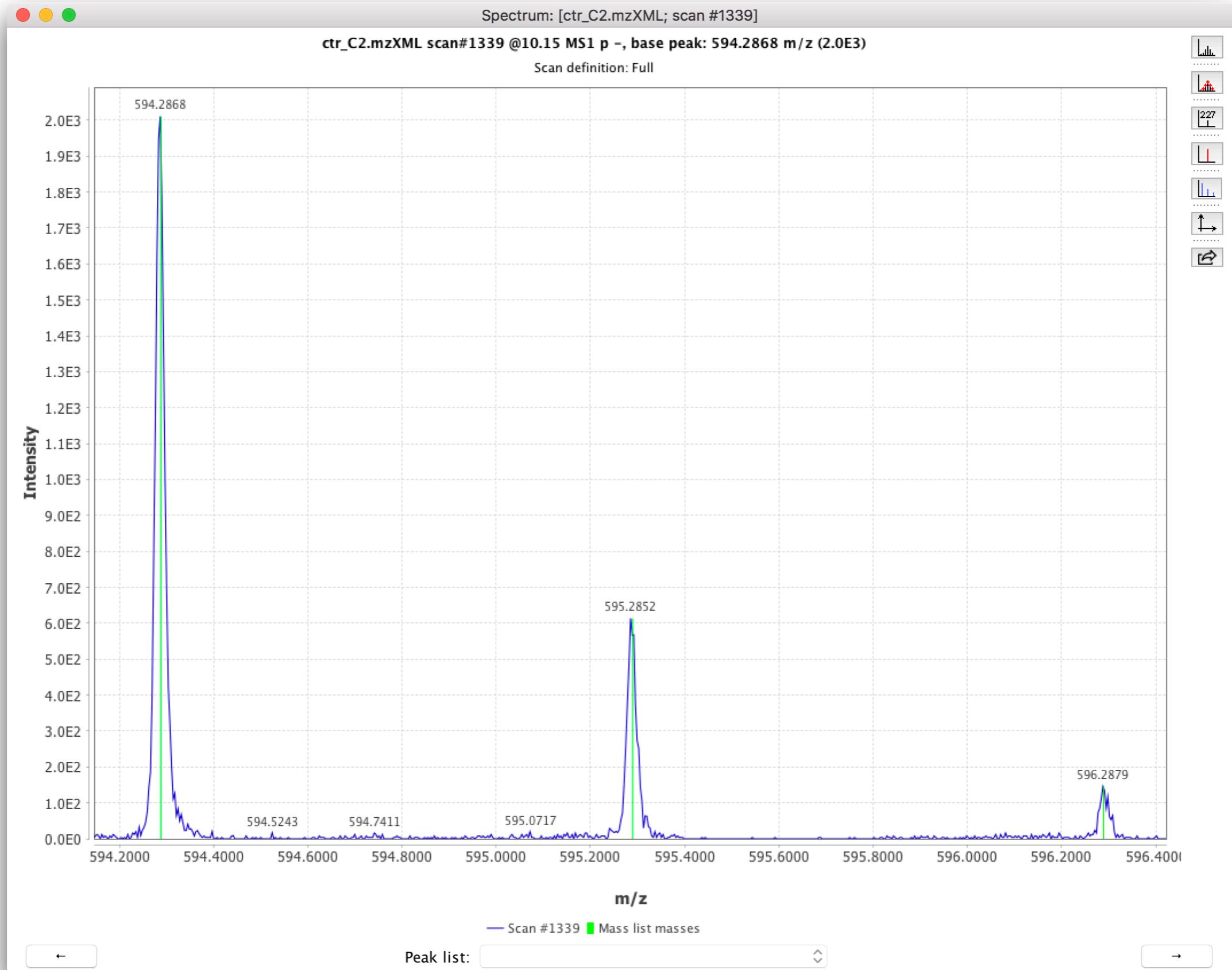
[8:34:47 AM]: Started mass detector on ctr_C3.mzXML

1312MB free

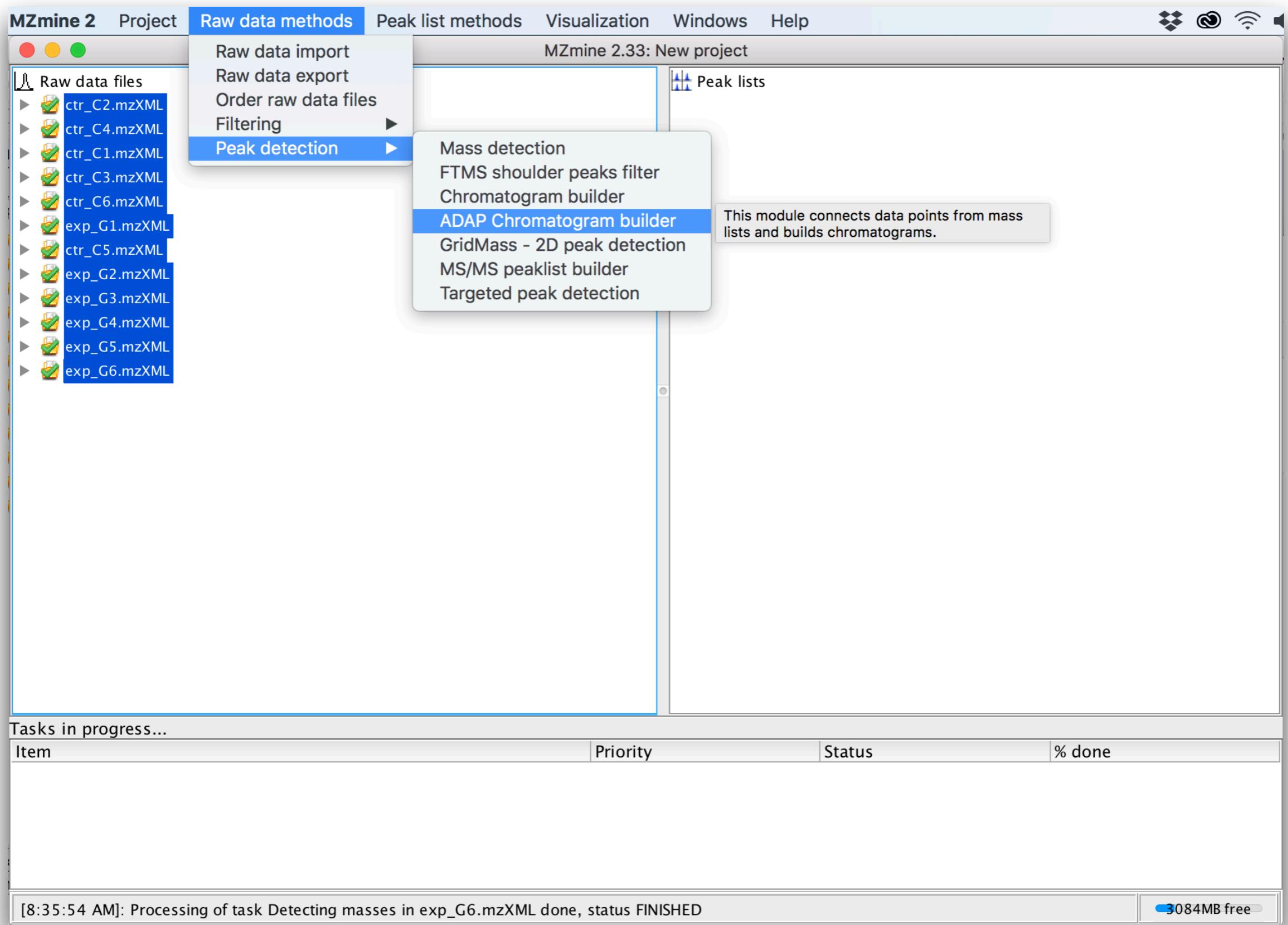
Mass detection



Mass detection



EIC construction



EIC construction

MZmine 2

MZmine 2.33: New project

Raw data files

- ctr_C2.mzXML
- ctr_C4.mzXML
- ctr_C1.mzXML
- ctr_C3.mzXML
- ctr_C6.mzXML
- exp_G1.mzXML
- ctr_C5.mzXML
- exp_G2.mzXML
- exp_G3.mzXML
- exp_G4.mzXML
- exp_G5.mzXML
- exp_G6.mzXML

Peak lists

Please set the parameters

Raw data files 12 selected As selected in main window

Scans MS level: 1 Set filters Clear filters

Mass list masses Choose...

Min group size in # of scans 5.00

Group intensity threshold 1.0E2

Min highest intensity 1.0E3

m/z tolerance 0.01 Points below this intensity will not be considered in starting a new chromatogram

Suffix chromatograms

ADAP Module Disclaimer:
If you use the ADAP Chromatogram Builder Module, please cite the [MZmine2 paper](#) and the following article:
[Myers OD, Sumner SJ, Li S, Barnes S, Du X: One Step Forward for Reducing False Positive and False Negative Compound Identifications from Mass Spectrometry Metabolomics Data: New Algorithms for Constructing Extracted Ion Chromatograms and Detecting Chromatographic Peaks. Anal Chem 2017, DOI: 10.1021/acs.analchem.7b00947](#)

Tasks in progress...

Item

OK Cancel Help

[8:35:54 AM]: Processing of task Detecting masses in exp_G6.mzXML done, status FINISHED

2810MB free

EIC construction

MZmine 2 Project Raw data methods Peak list methods Visualization Windows Help

MZmine 2.33: New project

The screenshot shows the MZmine 2 software interface. The left panel displays a list of 'Raw data files' containing 12 entries: ctr_C2.mzXML, ctr_C4.mzXML, ctr_C1.mzXML, ctr_C3.mzXML, ctr_C6.mzXML, exp_G1.mzXML, ctr_C5.mzXML, exp_G2.mzXML, exp_G3.mzXML, exp_G4.mzXML, exp_G5.mzXML, and exp_G6.mzXML. The right panel displays a list of 'Peak lists' containing 12 chromatogram entries: ctr_C3.mzXML chromatograms, ctr_C2.mzXML chromatograms, ctr_C1.mzXML chromatograms, ctr_C4.mzXML chromatograms, exp_G2.mzXML chromatograms, ctr_C6.mzXML chromatograms, ctr_C5.mzXML chromatograms, exp_G3.mzXML chromatograms, exp_G1.mzXML chromatograms, exp_G5.mzXML chromatograms, exp_G6.mzXML chromatograms, and exp_G4.mzXML chromatograms. A central message 'Tasks in progress...' is visible. At the bottom, a status bar indicates '[8:57:53 AM]: Processing of task Detecting chromatograms in exp_G4.mzXML done, status FINISHED' and '5263MB free'.

Raw data files

- ctr_C2.mzXML
- ctr_C4.mzXML
- ctr_C1.mzXML
- ctr_C3.mzXML
- ctr_C6.mzXML
- exp_G1.mzXML
- ctr_C5.mzXML
- exp_G2.mzXML
- exp_G3.mzXML
- exp_G4.mzXML
- exp_G5.mzXML
- exp_G6.mzXML

Peak lists

- ctr_C3.mzXML chromatograms
- ctr_C2.mzXML chromatograms
- ctr_C1.mzXML chromatograms
- ctr_C4.mzXML chromatograms
- exp_G2.mzXML chromatograms
- ctr_C6.mzXML chromatograms
- ctr_C5.mzXML chromatograms
- exp_G3.mzXML chromatograms
- exp_G1.mzXML chromatograms
- exp_G5.mzXML chromatograms
- exp_G6.mzXML chromatograms
- exp_G4.mzXML chromatograms

Tasks in progress...

Item	Priority	Status	% done

[8:57:53 AM]: Processing of task Detecting chromatograms in exp_G4.mzXML done, status FINISHED

5263MB free

EIC construction

MZmine 2 Project Raw data methods Peak list methods Visualization Windows Help

MZmine 2.33: New project

Raw data files

- ctr_C2.mzXML
- ctr_C4.mzXML
- ctr_C1.mzXML
- ctr_C3.mzXML
- ctr_C6.mzXML
- exp_G1.mzXML
- ctr_C5.mzXML
- exp_G2.mzXML
- exp_G3.mzXML
- exp_G4.mzXML
- exp_G5.mzXML
- exp_G6.mzXML

Peak lists

- ctr_C3.mzXML chromatograms
 - #1 61.9909 m/z @18.96
 - #2 68.9962 m/z @20.30
 - #3 96.9607 m/z @18.08
 - #4 112.9850 m/z @19.04
 - #5 121.0298 m/z @14.42
 - #6 130.0664 m/z @17.61
 - #7 134.0604 m/z @13.20
 - #8 144.0455 m/z @17.12
 - #9 145.0486 m/z @17.12
 - #10 146.0243 m/z @14.50
 - #11 155.1069 m/z @17.73
 - #12 164.0352 m/z @15.87
 - #13 169.0667 m/z @20.16
 - #14 171.0665 m/z @14.24
 - #15 172.0982 m/z @15.72
 - #16 173.0828 m/z @14.94
 - #17 174.0557 m/z @17.61
 - #18 174.9563 m/z @10.97
 - #19 175.0594 m/z @17.58
 - #20 178.0509 m/z @13.20
 - #21 179.0545 m/z @13.20
 - #22 181.0530 m/z @17.37
 - #23 183.0664 m/z @14.50
 - #24 184.0973 m/z @16.70
 - #25 185.0812 m/z @14.30

double click ...

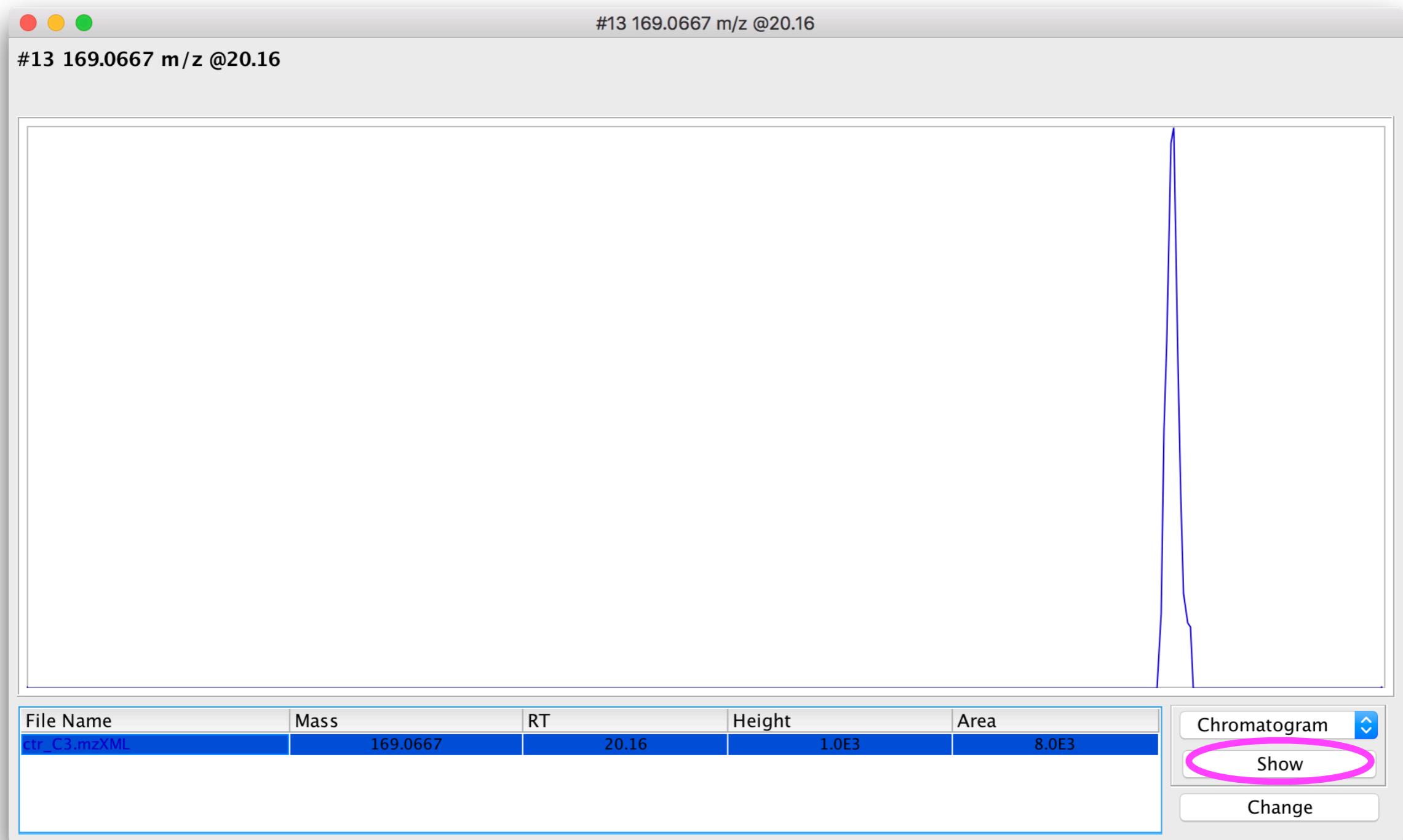
Tasks in progress...

Item	Priority	Status	% done
------	----------	--------	--------

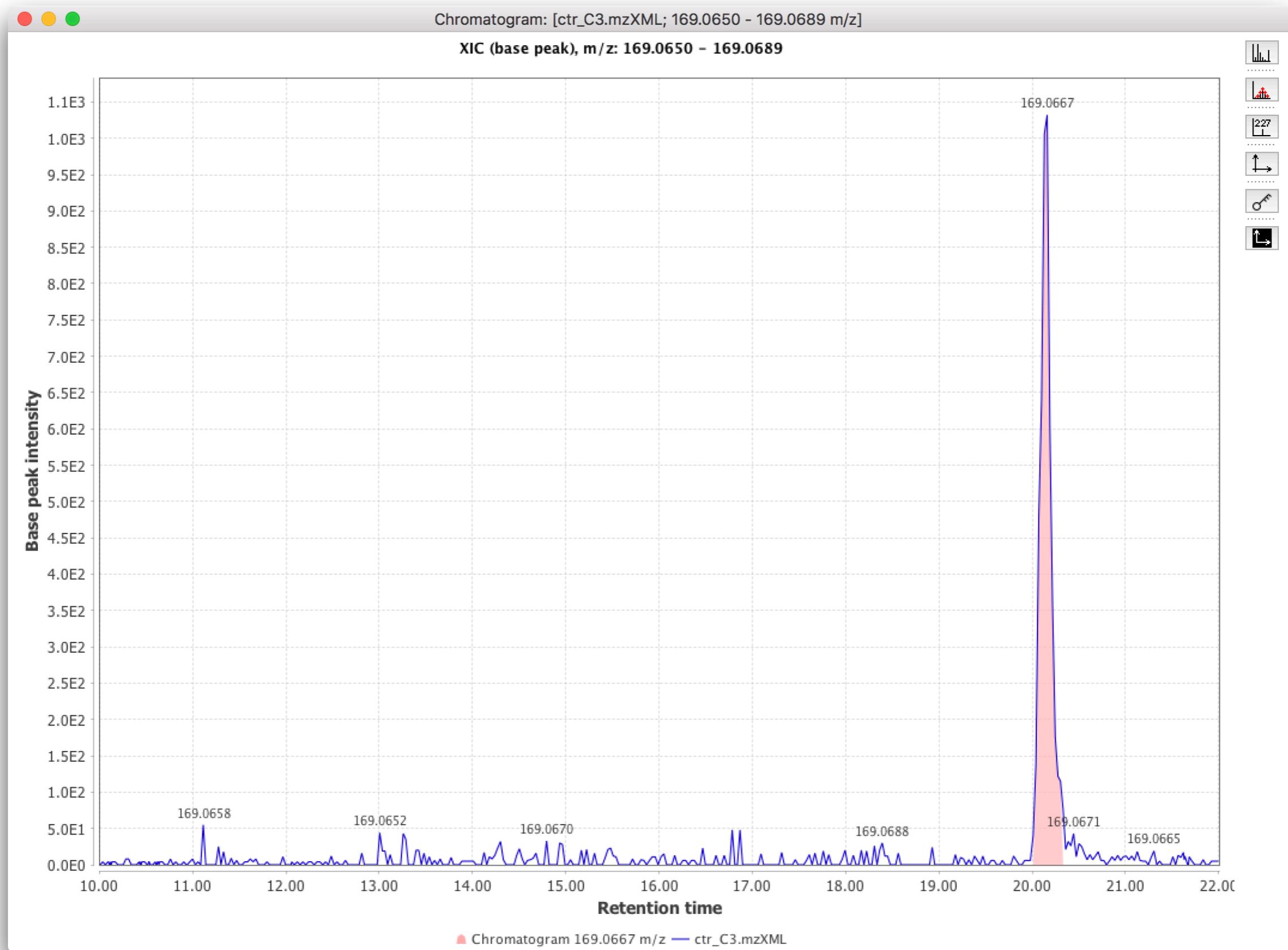
[8:59:28 AM]: Processing of task Updating TIC visualizer of ctr_C3.mzXML done, status FINISHED

5343MB free

EIC construction



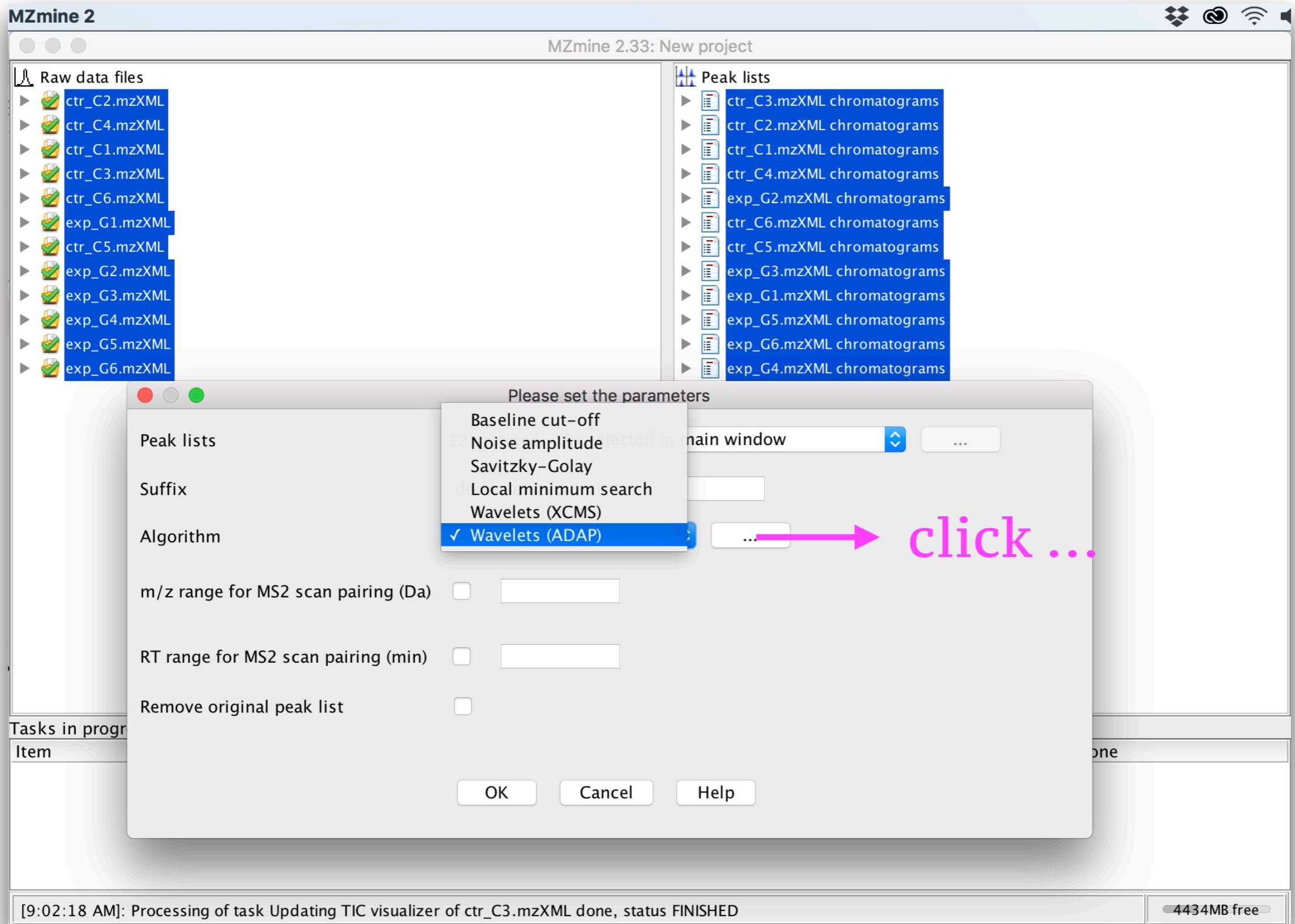
EIC construction



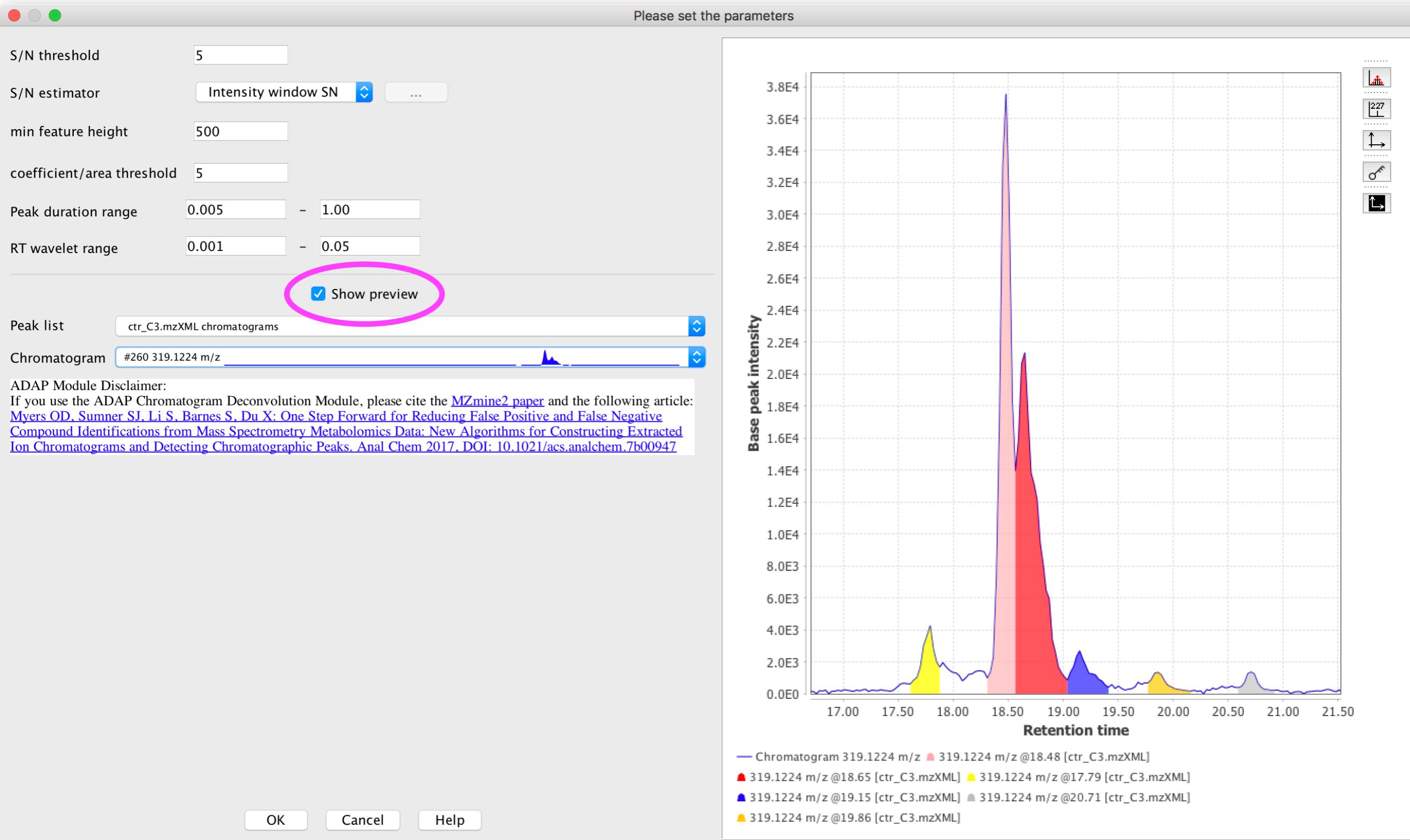
EIC peak detection

The screenshot shows the MZmine 2 software interface. The menu bar includes Project, Raw data methods, Peak list methods (which is currently selected), Visualization, Windows, and Help. The Peak list methods menu is open, displaying various processing steps: Order peak lists, Peak detection, Spectral deconvolution, Gap filling, Isotopes, Filtering, Alignment, Normalization, Identification, Data analysis, and Export/Import. The 'Peak detection' option is expanded, showing sub-options: New project, Smoothing, Chromatogram deconvolution, Peak shape modeler (experimental), and Peak extender. The 'Chromatogram deconvolution' option is highlighted with a blue selection bar. A tooltip for this option states: "This module separates each detected chromatogram into individual peaks." On the left, a sidebar lists raw data files: ctr_C2.mzXML, ctr_C4.mzXML, ctr_C1.mzXML, ctr_C3.mzXML, ctr_C6.mzXML, exp_G1.mzXML, ctr_C5.mzXML, exp_G2.mzXML, exp_G3.mzXML, exp_G4.mzXML, exp_G5.mzXML, exp_G6.mzXML, and exp_G6.mzXML. Below the sidebar, a message says "Tasks in progress...". At the bottom, a status bar shows "[9:02:18 AM]: Processing of task Updating TIC visualizer of ctr_C3.mzXML done, status FINISHED" and "4814MB free".

EIC peak detection



EIC peak detection



EIC peak detection

MZmine 2 Project Raw data methods Peak list methods Visualization Windows Help

MZmine 2.33: New project

The screenshot shows the MZmine 2 software interface. The left panel displays a list of raw data files (ctr_C2.mzXML, ctr_C4.mzXML, ctr_C1.mzXML, ctr_C3.mzXML, ctr_C6.mzXML, exp_G1.mzXML, ctr_C5.mzXML, exp_G2.mzXML, exp_G3.mzXML, exp_G4.mzXML, exp_G5.mzXML, exp_G6.mzXML) and peak lists (ctr_C3.mzXML chromatograms, ctr_C2.mzXML chromatograms, ctr_C1.mzXML chromatograms, ctr_C4.mzXML chromatograms, exp_G2.mzXML chromatograms, ctr_C6.mzXML chromatograms, ctr_C5.mzXML chromatograms, exp_G3.mzXML chromatograms, exp_G1.mzXML chromatograms, exp_G5.mzXML chromatograms, exp_G6.mzXML chromatograms, exp_G4.mzXML chromatograms, ctr_C3.mzXML chromatograms deconvoluted). The right panel shows a table of tasks in progress:

Item	Priority	Status	% done
Peak recognition on ctr_C3.mzXML chromatograms	NORMAL	FINISHED	100%
Peak recognition on ctr_C2.mzXML chromatograms	NORMAL	PROCESSING	60%
Peak recognition on ctr_C1.mzXML chromatograms	NORMAL	PROCESSING	44%
Peak recognition on ctr_C4.mzXML chromatograms	NORMAL	PROCESSING	48%
Peak recognition on exp_G2.mzXML chromatograms	NORMAL	PROCESSING	36%
Peak recognition on ctr_C6.mzXML chromatograms	NORMAL	WAITING	0%

[9:25:48 AM]: Started peak deconvolution on exp_G2.mzXML chromatograms

4101MB free

EIC peak detection

MZmine 2 Project Raw data methods Peak list methods Visualization Windows Help

MZmine 2.33: New project

The screenshot shows the MZmine 2 software interface. The left panel displays a list of 'Raw data files' containing 12 entries: ctr_C2.mzXML, ctr_C4.mzXML, ctr_C1.mzXML, ctr_C3.mzXML, ctr_C6.mzXML, exp_G1.mzXML, ctr_C5.mzXML, exp_G2.mzXML, exp_G3.mzXML, exp_G4.mzXML, exp_G5.mzXML, and exp_G6.mzXML. The right panel displays a list of 'Peak lists' containing 24 entries, which are the same 12 raw data files followed by their deconvoluted versions: ctr_C3.mzXML chromatograms, ctr_C2.mzXML chromatograms, ctr_C1.mzXML chromatograms, ctr_C4.mzXML chromatograms, exp_G2.mzXML chromatograms, ctr_C6.mzXML chromatograms, ctr_C5.mzXML chromatograms, exp_G3.mzXML chromatograms, exp_G1.mzXML chromatograms, exp_G5.mzXML chromatograms, exp_G6.mzXML chromatograms, exp_G4.mzXML chromatograms, ctr_C3.mzXML chromatograms deconvoluted, exp_G2.mzXML chromatograms deconvoluted, ctr_C2.mzXML chromatograms deconvoluted, ctr_C4.mzXML chromatograms deconvoluted, ctr_C1.mzXML chromatograms deconvoluted, ctr_C5.mzXML chromatograms deconvoluted, ctr_C6.mzXML chromatograms deconvoluted, exp_G3.mzXML chromatograms deconvoluted, exp_G5.mzXML chromatograms deconvoluted, exp_G6.mzXML chromatograms deconvoluted, exp_G1.mzXML chromatograms deconvoluted, and exp_G4.mzXML chromatograms deconvoluted. A blue box highlights the first 12 entries in the peak lists list. At the bottom, a 'Tasks in progress...' section shows a table with columns: Item, Priority, Status, and % done. The status column shows 'Processing' for all items. A message at the bottom left says '[9:26:21 AM]: Processing of task Peak recognition on exp_G4.mzXML chromatograms done, status FINISHED'. A memory usage indicator at the bottom right shows '2645MB free'.

Item	Priority	Status	% done
ctr_C2.mzXML		Processing	
ctr_C4.mzXML		Processing	
ctr_C1.mzXML		Processing	
ctr_C3.mzXML		Processing	
ctr_C6.mzXML		Processing	
exp_G1.mzXML		Processing	
ctr_C5.mzXML		Processing	
exp_G2.mzXML		Processing	
exp_G3.mzXML		Processing	
exp_G4.mzXML		Processing	
exp_G5.mzXML		Processing	
exp_G6.mzXML		Processing	

[9:26:21 AM]: Processing of task Peak recognition on exp_G4.mzXML chromatograms done, status FINISHED

2645MB free

Peak alignment

MZmine 2 Project Raw data methods Peak list methods Visualization Windows Help

Raw data files

- ctr_C2.mzXML
- ctr_C4.mzXML
- ctr_C1.mzXML
- ctr_C3.mzXML
- ctr_C6.mzXML
- exp_G1.mzXML
- ctr_C5.mzXML
- exp_G2.mzXML
- exp_G3.mzXML
- exp_G4.mzXML
- exp_G5.mzXML
- exp_G6.mzXML

Peak list methods

- Order peak lists
- Peak detection
- Spectral deconvolution
- Gap filling
- Isotopes
- Filtering
- Alignment**
- Normalization
- Identification
- Data analysis
- Export/Import

New project

Peak lists

- ctr_C3.mzXML chromatograms
- ctr_C2.mzXML chromatograms
- ctr_C1.mzXML chromatograms
- ctr_C4.mzXML chromatograms
- exp_G1.mzXML chromatograms
- exp_G5.mzXML chromatograms
- exp_G6.mzXML chromatograms
- exp_G4.mzXML chromatograms
- ctr_C3.mzXML chromatograms deconvoluted
- exp_G2.mzXML chromatograms deconvoluted
- ctr_C2.mzXML chromatograms deconvoluted
- ctr_C4.mzXML chromatograms deconvoluted
- ctr_C1.mzXML chromatograms deconvoluted
- ctr_C5.mzXML chromatograms deconvoluted
- ctr_C6.mzXML chromatograms deconvoluted
- exp_G3.mzXML chromatograms deconvoluted
- exp_G5.mzXML chromatograms deconvoluted
- exp_G6.mzXML chromatograms deconvoluted
- exp_G1.mzXML chromatograms deconvoluted
- exp_G4.mzXML chromatograms deconvoluted

Join aligner

This method aligns detected peaks using a match score. This score is calculated based on the mass and retention time of each peak using preset tolerance.

Hierachical aligner (GC)
RANSAC aligner
ADAP Aligner

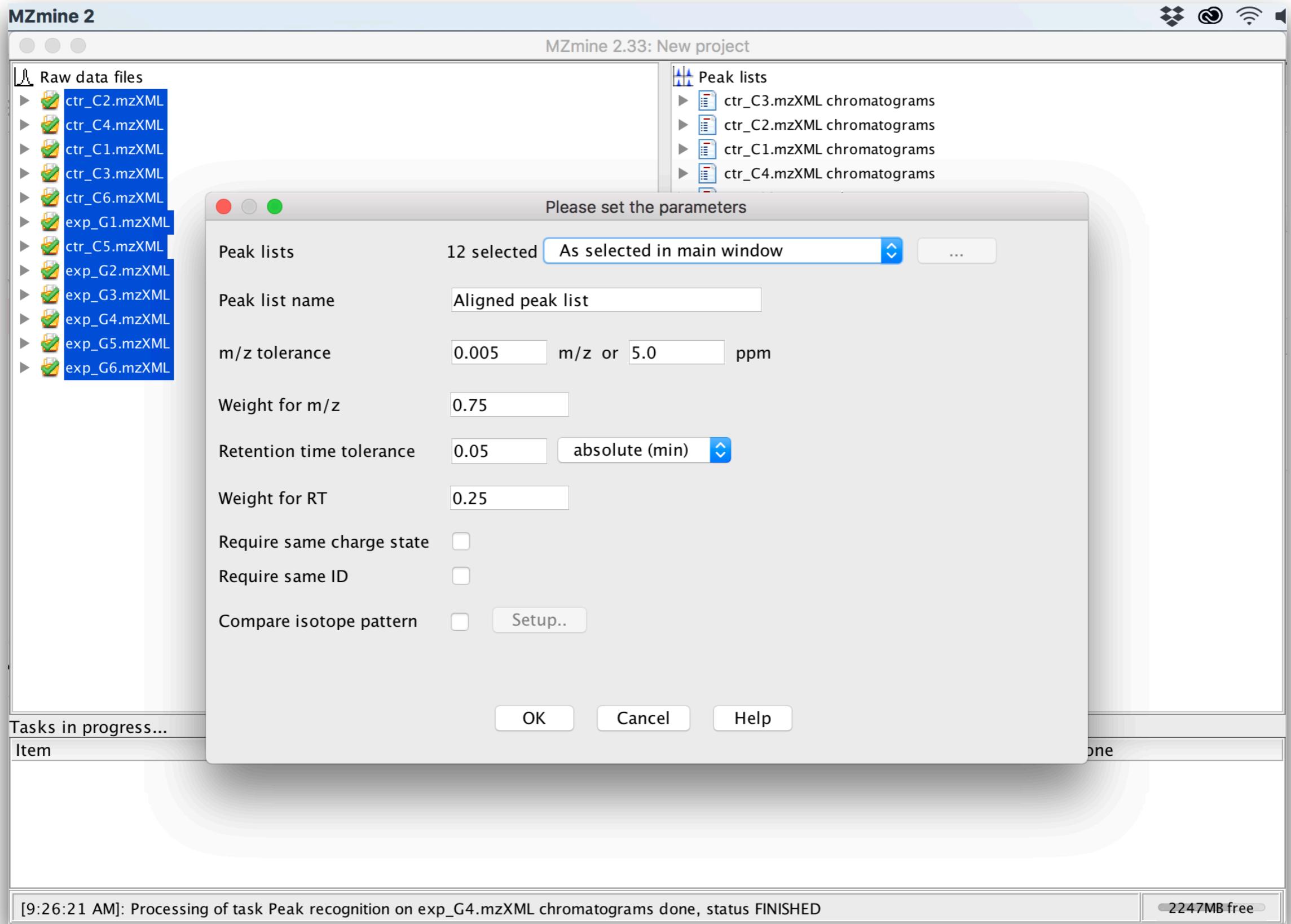
Tasks in progress...

Item	Priority	Status	% done

[9:26:21 AM]: Processing of task Peak recognition on exp_G4.mzXML chromatograms done, status FINISHED

2426MB free

Peak alignment



Peak alignment

MZmine 2 Project Raw data methods Peak list methods Visualization Windows Help

MZmine 2.33: New project

The screenshot shows the MZmine 2 software interface with two main panels: 'Raw data files' on the left and 'Peak lists' on the right. Both panels list chromatogram files. The 'Raw data files' panel contains 12 entries: ctr_C2.mzXML, ctr_C4.mzXML, ctr_C1.mzXML, ctr_C3.mzXML, ctr_C6.mzXML, exp_G1.mzXML, ctr_C5.mzXML, exp_G2.mzXML, exp_G3.mzXML, exp_G4.mzXML, exp_G5.mzXML, and exp_G6.mzXML. The 'Peak lists' panel contains 24 entries, including deconvoluted versions of the raw data and an 'Aligned peak list' at the bottom. A 'Tasks in progress...' section at the bottom shows an empty table with columns for Item, Priority, Status, and % done. A status bar at the bottom indicates '[9:34:36 AM]: Processing of task Join aligner, Aligned peak list (12 peak lists) done, status FINISHED' and '4251MB free'.

Raw data files

- ctr_C2.mzXML
- ctr_C4.mzXML
- ctr_C1.mzXML
- ctr_C3.mzXML
- ctr_C6.mzXML
- exp_G1.mzXML
- ctr_C5.mzXML
- exp_G2.mzXML
- exp_G3.mzXML
- exp_G4.mzXML
- exp_G5.mzXML
- exp_G6.mzXML

Peak lists

- ctr_C3.mzXML chromatograms
- ctr_C2.mzXML chromatograms
- ctr_C1.mzXML chromatograms
- ctr_C4.mzXML chromatograms
- exp_G2.mzXML chromatograms
- ctr_C6.mzXML chromatograms
- ctr_C5.mzXML chromatograms
- exp_G3.mzXML chromatograms
- exp_G1.mzXML chromatograms
- exp_G5.mzXML chromatograms
- exp_G6.mzXML chromatograms
- exp_G4.mzXML chromatograms
- ctr_C3.mzXML chromatograms deconvoluted
- exp_G2.mzXML chromatograms deconvoluted
- ctr_C2.mzXML chromatograms deconvoluted
- ctr_C4.mzXML chromatograms deconvoluted
- ctr_C1.mzXML chromatograms deconvoluted
- ctr_C5.mzXML chromatograms deconvoluted
- ctr_C6.mzXML chromatograms deconvoluted
- exp_G3.mzXML chromatograms deconvoluted
- exp_G5.mzXML chromatograms deconvoluted
- exp_G6.mzXML chromatograms deconvoluted
- exp_G1.mzXML chromatograms deconvoluted
- exp_G4.mzXML chromatograms deconvoluted
- Aligned peak list

Tasks in progress...

Item	Priority	Status	% done

[9:34:36 AM]: Processing of task Join aligner, Aligned peak list (12 peak lists) done, status FINISHED

4251MB free

Export for MetaboAnalyst

The screenshot shows the MZmine 2 software interface. The window title is "MZmine 2.33: New project". The menu bar includes "Project", "Raw data methods", "Peak list methods", "Visualization", "Windows", and "Help". The "Project" menu is open, displaying the following options:

- Open project ^O
- Save project ^S
- Save project as ^W
- Close project
- Batch mode
- Set sample parameters** (highlighted in blue)
- Set preferences
- Save MZmine parameters
- Load MZmine parameters
- Exit ^X

The main workspace on the right lists chromatograms and deconvoluted chromatograms for various samples, including control (ctr) and experimental (exp) groups. The list includes:

- Peak lists
 - ctr_C2.mzXML chromatograms
 - ctr_C4.mzXML chromatograms
 - ctr_C1.mzXML chromatograms
 - ctr_C4.mzXML chromatograms
 - exp_G2.mzXML chromatograms
 - ctr_C6.mzXML chromatograms
 - ctr_C5.mzXML chromatograms
 - exp_G3.mzXML chromatograms
 - exp_G1.mzXML chromatograms
 - exp_G5.mzXML chromatograms
 - exp_G6.mzXML chromatograms
 - exp_G4.mzXML chromatograms
 - ctr_C3.mzXML chromatograms deconvoluted
 - exp_G2.mzXML chromatograms deconvoluted
 - ctr_C2.mzXML chromatograms deconvoluted
 - ctr_C4.mzXML chromatograms deconvoluted
 - ctr_C1.mzXML chromatograms deconvoluted
 - ctr_C5.mzXML chromatograms deconvoluted
 - ctr_C6.mzXML chromatograms deconvoluted
 - exp_G3.mzXML chromatograms deconvoluted
 - exp_G5.mzXML chromatograms deconvoluted
 - exp_G6.mzXML chromatograms deconvoluted
 - exp_G1.mzXML chromatograms deconvoluted
 - exp_G4.mzXML chromatograms deconvoluted
- Aligned peak list

At the bottom left, there is a "Tasks in progress..." section. At the bottom right, a status bar shows the time [9:37:51 AM], the message "Started calculating significance Control group files: ctr_C4.mzXML, ctr_C3.mzXML, ctr_C5.mzXML, ctr_C6.mzXML, ctr_C2.mzXML, ctr...", and free disk space "2175MB free".

Export for MetaboAnalyst

MZmine 2 Project Raw data methods Peak list methods Visualization Windows Help

MZmine 2.33: New project

Raw data files

- ctr_C2.mzXML
- ctr_C4.mzXML
- ctr_C1.mzXML
- ctr_C3.mzXML
- ctr_C6.mzXML
- exp_G1.mzXML
- ctr_C5.mzXML
- exp_G2.mzXML
- exp_G3.mzXML
- exp_G4.mzXML
- exp_G5.mzXML
- exp_G6.mzXML

Peak lists

- ctr_C3.mzXML chromatograms
- ctr_C2.mzXML chromatograms
- ctr_C1.mzXML chromatograms
- ctr_C4.mzXML chromatograms
- exp_G2.mzXML chromatograms
- ctr_C6.mzXML chromatograms
- ctr_C5.mzXML chromatograms
- exp_G3.mzXML chromatograms
- exp_G1.mzXML chromatograms
- exp_G5.mzXML chromatograms
- exp_G6.mzXML chromatograms

Setup project parameters and values

Raw data

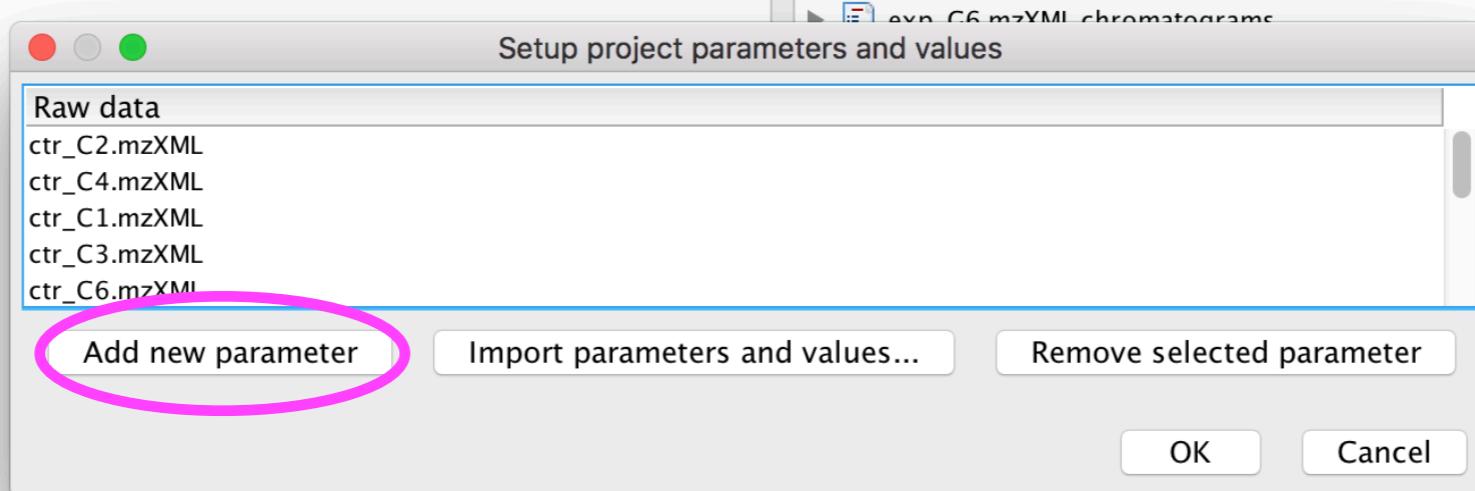
- ctr_C2.mzXML
- ctr_C4.mzXML
- ctr_C1.mzXML
- ctr_C3.mzXML
- ctr_C6.mzXML

Add new parameter Import parameters and values... Remove selected parameter OK Cancel

Tasks in progress...

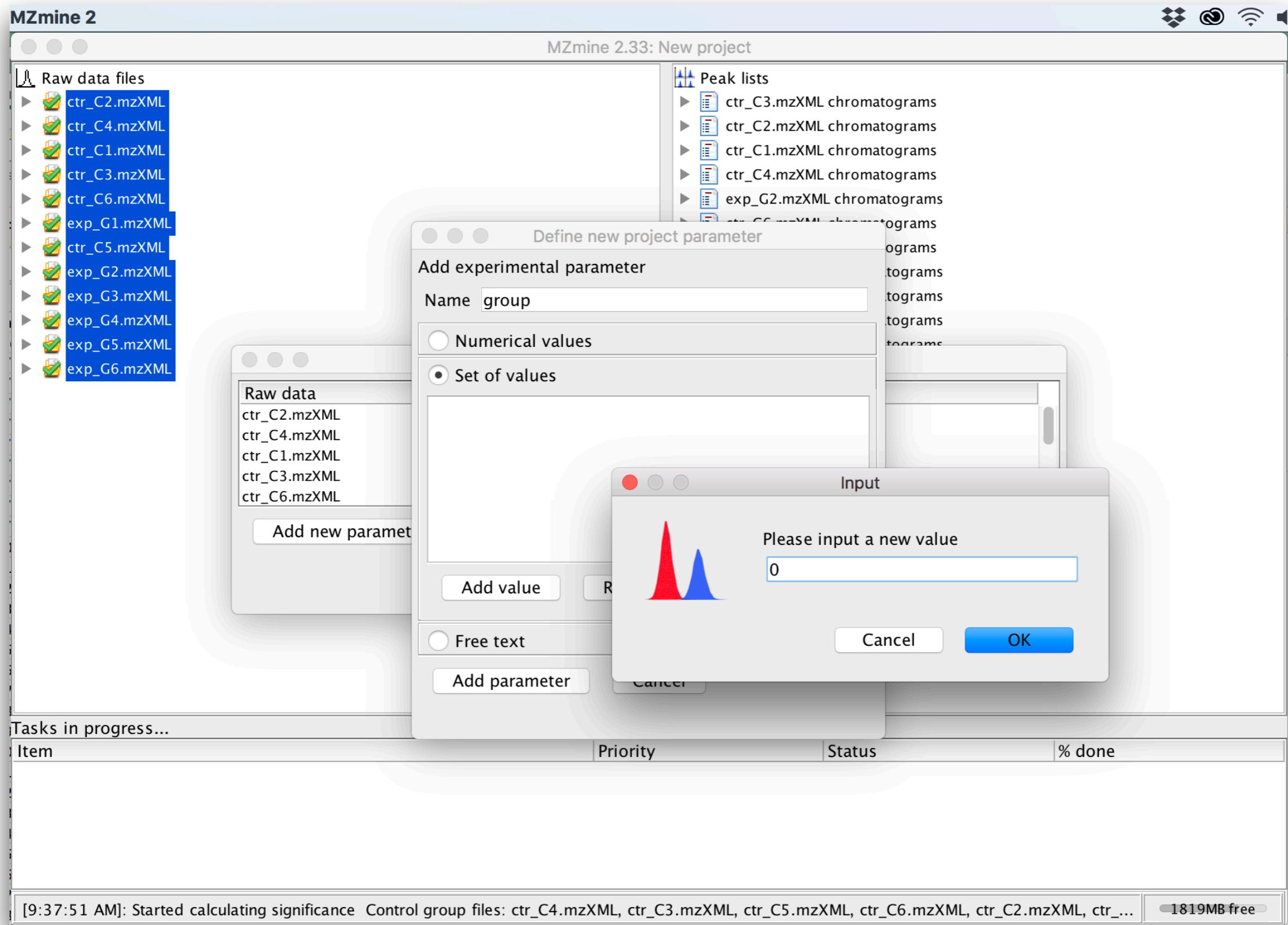
Item	Priority	Status	% done

[9:37:51 AM]: Started calculating significance Control group files: ctr_C4.mzXML, ctr_C3.mzXML, ctr_C5.mzXML, ctr_C6.mzXML, ctr_C2.mzXML, ctr... 1968MB free

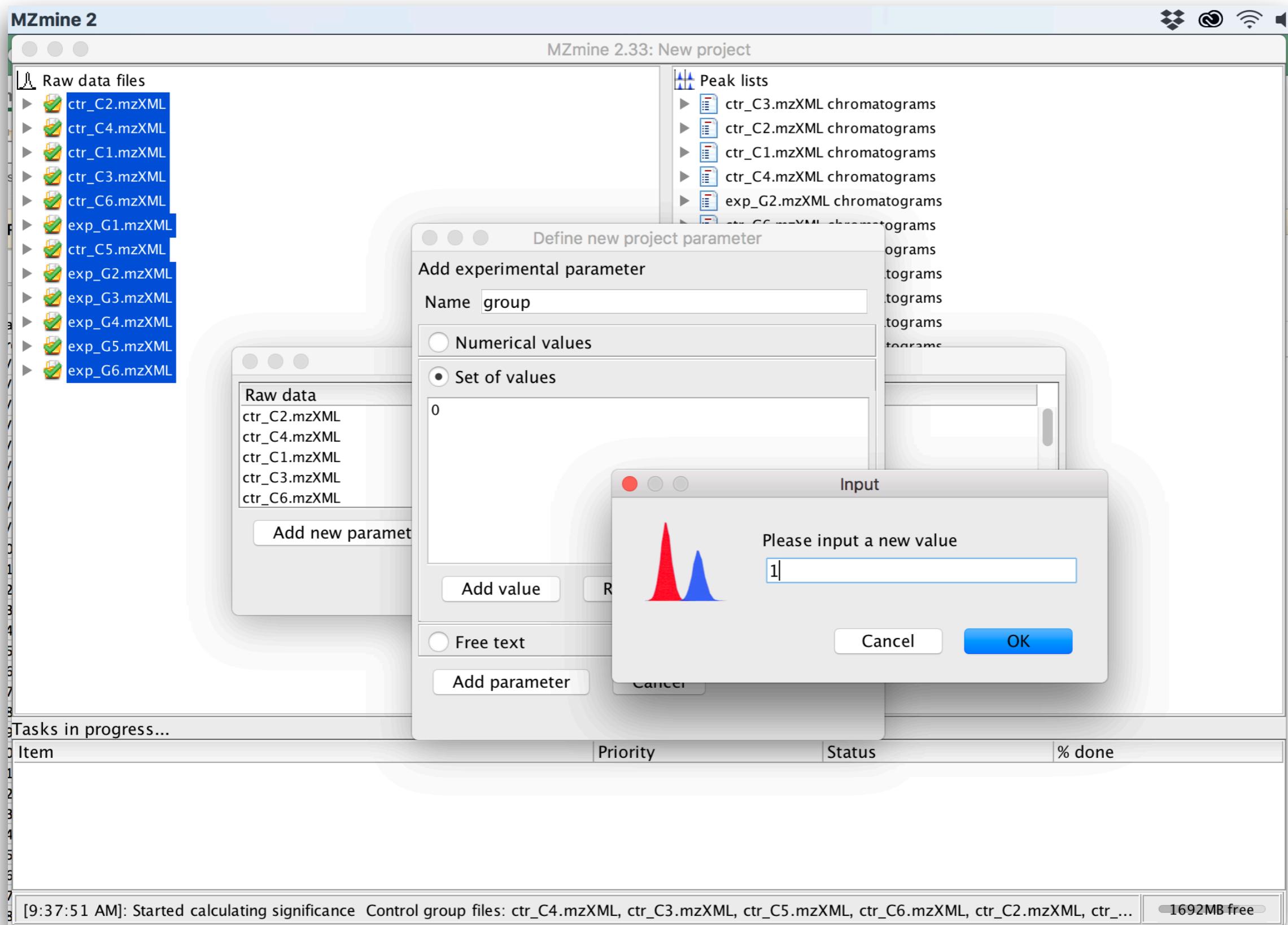


- exp_G2.mzXML chromatograms deconvoluted
- exp_G1.mzXML chromatograms deconvoluted
- exp_G4.mzXML chromatograms deconvoluted
- Aligned peak list

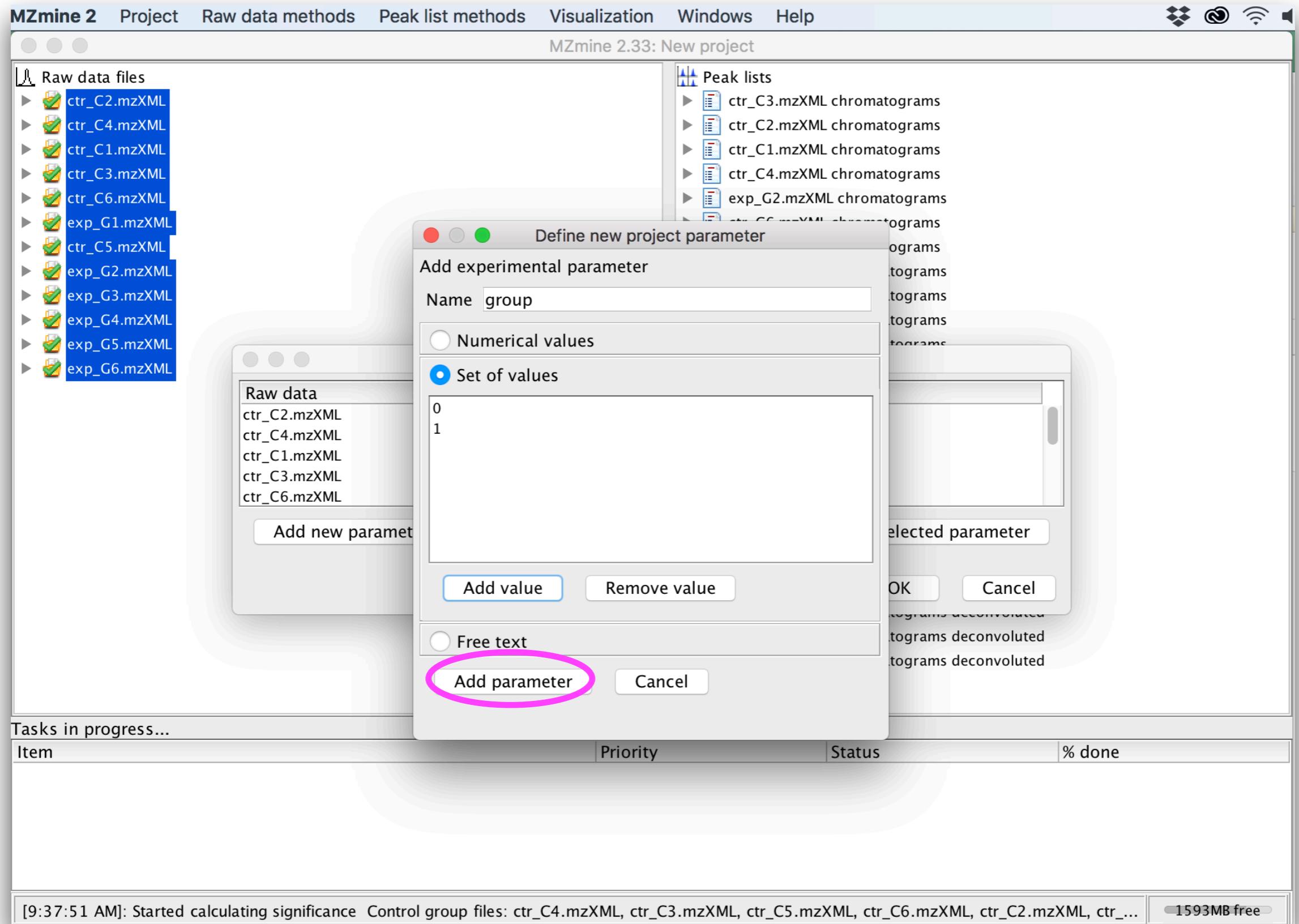
Export for MetaboAnalyst



Export for MetaboAnalyst



Export for MetaboAnalyst



Export for MetaboAnalyst

MZmine 2 Project Raw data methods Peak list methods Visualization Windows Help

MZmine 2.33: New project

Raw data files

- ctr_C2.mzXML
- ctr_C4.mzXML
- ctr_C1.mzXML
- ctr_C3.mzXML
- ctr_C6.mzXML
- exp_G1.mzXML
- ctr_C5.mzXML
- exp_G2.mzXML
- exp_G3.mzXML
- exp_G4.mzXML
- exp_G5.mzXML
- exp_G6.mzXML

Peak lists

- ctr_C3.mzXML chromatograms
- ctr_C2.mzXML chromatograms
- ctr_C1.mzXML chromatograms
- ctr_C4.mzXML chromatograms
- exp_G2.mzXML chromatograms
- ctr_C6.mzXML chromatograms
- ctr_C5.mzXML chromatograms
- exp_G3.mzXML chromatograms
- exp_G1.mzXML chromatograms
- exp_G5.mzXML chromatograms
- exp_G6.mzXML chromatograms

Setup project parameters and values

Raw data	group
ctr_C2.mzXML	0
ctr_C4.mzXML	0
ctr_C1.mzXML	0
ctr_C3.mzXML	0
ctr_C6.mzXML	0
exp_G1.mzXML	1
ctr_C5.mzXML	0
exp_G2.mzXML	1
exp_G3.mzXML	1
exp_G4.mzXML	1
exp_G5.mzXML	1
exp_G6.mzXML	1

Add new parameter Import parameters and values... Remove selected parameter

OK Cancel

Tasks in progress...

Item

done

[9:37:51 AM]: Started calculating significance Control group files: ctr_C4.mzXML, ctr_C3.mzXML, ctr_C5.mzXML, ctr_C6.mzXML, ctr_C2.mzXML, ctr...

5273MB free

Export for MetaboAnalyst

MZmine 2 Project Raw data methods Peak list methods Visualization Windows Help

MZmine 2.33: New project

Raw data files

- ctr_C2.mzXML
- ctr_C4.mzXML
- ctr_C1.mzXML
- ctr_C3.mzXML
- ctr_C6.mzXML
- exp_G1.mzXML
- ctr_C5.mzXML
- exp_G2.mzXML
- exp_G3.mzXML
- exp_G4.mzXML
- exp_G5.mzXML
- exp_G6.mzXML

Peak lists

- ctr_C3.mzXML chromatograms
- ctr_C2.mzXML chromatograms
- ctr_C1.mzXML chromatograms
- ctr_C4.mzXML chromatograms
- exp_G2.mzXML chromatograms
- ctr_C6.mzXML chromatograms
- ctr_C5.mzXML chromatograms
- exp_G3.mzXML chromatograms
- exp_G1.mzXML chromatograms
- exp_G5.mzXML chromatograms
- exp_G6.mzXML chromatograms

Setup project parameters and values

Raw data	group
ctr_C2.mzXML	0
ctr_C4.mzXML	0
ctr_C1.mzXML	0
ctr_C3.mzXML	0
ctr_C6.mzXML	0
exp_G1.mzXML	1
ctr_C5.mzXML	0
exp_G2.mzXML	1
exp_G3.mzXML	1
exp_G4.mzXML	1
exp_G5.mzXML	1
exp_G6.mzXML	1

Tasks in progress...

Item

Add new parameter Import parameters and values... Remove selected parameter

OK Cancel

[9:37:51 AM]: Started calculating significance Control group files: ctr_C4.mzXML, ctr_C3.mzXML, ctr_C5.mzXML, ctr_C6.mzXML, ctr_C2.mzXML, ctr_... 2466MB free

Export for MetaboAnalyst

The screenshot shows the MZmine 2 software interface. The menu bar includes 'MZmine 2', 'Project', 'Raw data methods', 'Peak list methods' (which is currently selected), 'Visualization', 'Windows', and 'Help'. The 'Peak list methods' menu is open, showing various processing steps: 'Order peak lists', 'Peak detection', 'Spectral deconvolution', 'Gap filling', 'Isotopes', 'Filtering', 'Alignment', 'Normalization', 'Identification', 'Data analysis', and 'Export/Import'. The 'Export/Import' option is also expanded, listing 'Export to CSV file', 'Export to MetaboAnalyst file' (which is highlighted in blue), 'Export to mzTab file', 'Export to SQL database', 'Export to XML file', 'Export to MSP file', 'Export to MGF file', 'Export for GNPS', 'Export for SIRIUS', 'Import CASMI challenge task', 'Import mzTab file', and 'Import from XML file'. A tooltip for 'Export to MetaboAnalyst file' explains: 'This method exports the peak list contents into a CSV (comma-separated values) file that is formatted for easy processing by the MetaboAnalyst service (<http://www.metaboanalyst.ca>).'. On the left, a tree view shows 'Raw data files' with numerous entries like 'ctr_C2.mzXML' through 'exp_G6.mzXML'. At the bottom, a 'Tasks in progress...' section is empty, and a status bar at the bottom right shows '[9:37:51 AM]: Started calculating significance Control group files: ctr_C4.mzXML, ctr_C3.mzXML, ctr_C5.mzXML, ctr_C6.mzXML, ctr_C2.mzXML, ctr_C1.mzXML' and '3724MB free'.

Export for MetaboAnalyst

A	B	C	D	E	F	G	H	I	J	K	L	M
Sample	ctr_C3.mzXML	exp_G2.mzXML	ctr_C2.mzXML	ctr_C4.mzXML	ctr_C1.mzXML	ctr_C5.mzXML	ctr_C6.mzXML	exp_G3.mzXML	exp_G5.mzXML	exp_G6.mzXML	exp_G1.mzXML	exp_G4.mzXML
group	0	1	0	0	0	0	0	1	1	1	1	1
1/61.9912mz/17.18min	19791.665		26254.13								30670.955	27264.04
2/61.9916mz/13.20min	6392.365	8110.552	23863.063					21747.0475	21215.892			
3/61.9912mz/18.77min	30071.145						46088.65					
4/61.9909mz/16.08min	18982.158											
5/61.9909mz/17.31min	18301.895											
6/61.9909mz/18.96min	24567.695											
7/61.9909mz/19.83min	21855.27											
8/61.9914mz/11.10min	7837.0175			3390.073				2423.3625				
9/61.9913mz/11.97min	5749.1325			8127.692								
10/68.9978mz/20.34min	18204.745		14709.5		5314.985							
11/68.9979mz/17.25min	10706.445	14951.04										
12/68.9962mz/16.47min	6223.2405											
13/68.9962mz/21.45min	11545.54											
14/68.9978mz/18.86min	12856.26		8589.115					3853.525				
15/68.9976mz/15.19min	8177.21		6953.218									
16/68.9972mz/18.19min	8247.03			5935.355								
17/68.9984mz/18.73min	3834.82	19078.34				7471.455				6503.58		
18/96.9619mz/18.10min	6402.455							8408.145				
19/96.9621mz/13.22min	9371.182		7490.63	9168.4035				7103.832	5149.4665	7748.895		
20/96.9607mz/16.17min	8094.678											
21/96.9607mz/17.09min	4992.205											
22/96.9613mz/14.93min	7390.656								3115.6735			
23/96.9624mz/11.32min	2432.392		4147.493					5368.547				
24/96.9613mz/14.44min	2368.26			2217.982						7181.124		
25/112.9850mz/12.73min	10250.853											
26/112.9864mz/19.02min	33460.61				44701.095	30452.04						
27/112.9850mz/12.84min	15876.685											
28/121.0303mz/14.43min	12463.765		11641.832	20921.7005	14455.189			15657.002		12163.3055	10619.15	
29/130.0673mz/17.61min	52245.175	48118.915	115715.315	91814.365	93542.675	66928.67	57733.805	44086.305	52622.545	41445.88	110309.475	13191.19
30/134.0616mz/13.21min	34553.834	12071.18	39661.5765	30153.01	35701.028	37647.1625		28839.2715	21552.653	37375.9235	34707.502	43489.649
31/144.0472mz/17.13min	501336.94	436492.73	1495367.435	1228207.23	1216160.72	704572.755	880038.73	807635.48	796327.245	737482.015	2089051.41	494894.68
32/144.0472mz/12.11min	6812.6115	4676.799	13566.149	18030.4955	14622.933	10284.6185	32001.4535	10608.084	22337.46	11084.1755	31259.001	12573.2635

Pathway analysis using mummichog

MZmine 2 Project Raw data methods Peak list methods Visualization Windows Help

Raw data files

- ctr_C2.mzXML
- ctr_C4.mzXML
- ctr_C1.mzXML
- ctr_C3.mzXML
- ctr_C6.mzXML
- exp_G1.mzXML
- ctr_C5.mzXML
- exp_G2.mzXML
- exp_G3.mzXML
- exp_G4.mzXML
- exp_G5.mzXML
- exp_G6.mzXML

Peak list methods

- Order peak lists
- Peak detection
- Spectral deconvolution
- Gap filling
- Isotopes
- Filtering
- Alignment
- Normalization
- Identification
- Data analysis
- Export/Import

New project

Peak lists

- ctr_C3.mzXML chromatograms
- ctr_C2.mzXML chromatograms
- ctr_C1.mzXML chromatograms
- ctr_C4.mzXML chromatograms
- exp_G2.mzXML chromatograms
- ctr_C6.mzXML chromatograms
- ctr_C5.mzXML chromatograms

CV plot

Logratio analysis

Principal component analysis (PCA)

Curvilinear distance analysis (CDA)

Sammon's projection

Clustering

Heat map plot

Significance calculation

Mummichog calculation

ctr_C1.mzXML chromatograms deconvoluted

ctr_C5.mzXML chromatograms deconvoluted

ctr_C6.mzXML chromatograms deconvoluted

exp_G3.mzXML chromatograms deconvoluted

exp_G5.mzXML chromatograms deconvoluted

exp_G6.mzXML chromatograms deconvoluted

exp_G1.mzXML chromatograms deconvoluted

exp_G4.mzXML chromatograms deconvoluted

Aligned peak list

Tasks in progress...

Item	Priority	Status	% done

[9:34:36 AM]: Processing of task Join aligner, Aligned peak list (12 peak lists) done, status FINISHED

4072MB free

Pathway analysis using mummichog

MZmine 2

MZmine 2.33: New project

Raw data files

- ctr_C2.mzXML
- ctr_C4.mzXML
- ctr_C1.mzXML
- ctr_C3.mzXML
- ctr_C6.mzXML
- exp_G1.mzXML
- ctr_C5.mzXML
- exp_G2.mzXML
- exp_G3.mzXML
- exp_G4.mzXML
- exp_G5.mzXML
- exp_G6.mzXML

Peak lists

- ctr_C3.mzXML chromatograms
- ctr_C2.mzXML chromatograms
- ctr_C1.mzXML chromatograms
- ctr_C4.mzXML chromatograms
- exp_G2.mzXML chromatograms
- ctr_C6.mzXML chromatograms
- ctr_C5.mzXML chromatograms
- exp_G3.mzXML chromatograms
- exp_G1.mzXML chromatograms
- exp_G5.mzXML chromatograms

Please set the parameters

Peak lists Aligned peak list As selected in main window

Experimental Group Name exp

Control Group Name ctr

OK Cancel Help

Tasks in progress...

Item	Priority	Status	% done

[9:34:36 AM]: Processing of task Join aligner, Aligned peak list (12 peak lists) done, status FINISHED

3959MB free

Pathway analysis using mummichog

MZmine 2 Project Raw data methods Peak list methods Visualization Windows Help

Raw data files

- ctr_C2.mzXML
- ctr_C4.mzXML
- ctr_C1.mzXML
- ctr_C3.mzXML
- ctr_C6.mzXML
- exp_G1.mzXML
- ctr_C5.mzXML
- exp_G2.mzXML
- exp_G3.mzXML
- exp_G4.mzXML
- exp_G5.mzXML
- exp_G6.mzXML

Peak list methods

- Order peak lists
- Peak detection
- Spectral deconvolution
- Gap filling
- Isotopes
- Filtering
- Alignment
- Normalization
- Identification
- Data analysis
- Export/Import

New project

- Peak lists
- ctr_C3.mzXML chromatograms
- ctr_C2.mzXML chromatograms
- ctr_C1.mzXML chromatograms
- ctr_C4.mzXML chromatograms
- exp_G2.mzXML chromatograms
- ctr_C6.mzXML chromatograms
- ctr_C5.mzXML chromatograms

CV plot

Logratio analysis

Principal component analysis (PCA)

Curvilinear distance analysis (CDA)

Sammon's projection

Clustering

Heat map plot

Significance calculation

Mummichog calculation

Builds an Activity Network after doing pathway and modular analysis

- ctr_C1.mzXML chromatograms deconvoluted
- ctr_C5.mzXML chromatograms deconvoluted
- ctr_C6.mzXML chromatograms deconvoluted
- exp_G3.mzXML chromatograms deconvoluted
- exp_G5.mzXML chromatograms deconvoluted
- exp_G6.mzXML chromatograms deconvoluted
- exp_G1.mzXML chromatograms deconvoluted
- exp_G4.mzXML chromatograms deconvoluted
- Aligned peak list

Tasks in progress...

Item	Priority	Status	% done
------	----------	--------	--------

[9:37:51 AM]: Started calculating significance Control group files: ctr_C4.mzXML, ctr_C3.mzXML, ctr_C5.mzXML, ctr_C6.mzXML, ctr_C2.mzXML, ctr_C1.mzXML 4351MB free

Pathway analysis using mummichog

MZmine 2

MZmine 2.33: New project

Raw data files

- ctr_C2.mzXML
- ctr_C4.mzXML
- ctr_C1.mzXML
- ctr_C3.mzXML
- ctr_C6.mzXML
- exp_G1.mzXML
- ctr_C5.mzXML
- exp_G2.mzXML
- exp_G3.mzXML
- exp_G4.mzXML
- exp_G5.mzXML
- exp_G6.mzXML

Peak lists

- ctr_C3.mzXML chromatograms
- ctr_C2.mzXML chromatograms
- ctr_C1.mzXML chromatograms
- ctr_C4.mzXML chromatograms
- exp_G2.mzXML chromatograms
- ctr_C6.mzXML chromatograms
- ctr_C5.mzXML chromatograms

Please set the parameters

Peak lists Aligned peak list ...

Significance Cutoff

Metabolic Network

Primary Ion Mandate

Distrition Estimator

Output Directory ...

OK Cancel Help

Tasks in progress...

Item	Priority	Status	% done

[9:37:51 AM]: Started calculating significance Control group files: ctr_C4.mzXML, ctr_C3.mzXML, ctr_C5.mzXML, ctr_C6.mzXML, ctr_C2.mzXML, ctr... 4511MB free

Pathway analysis using mummichog

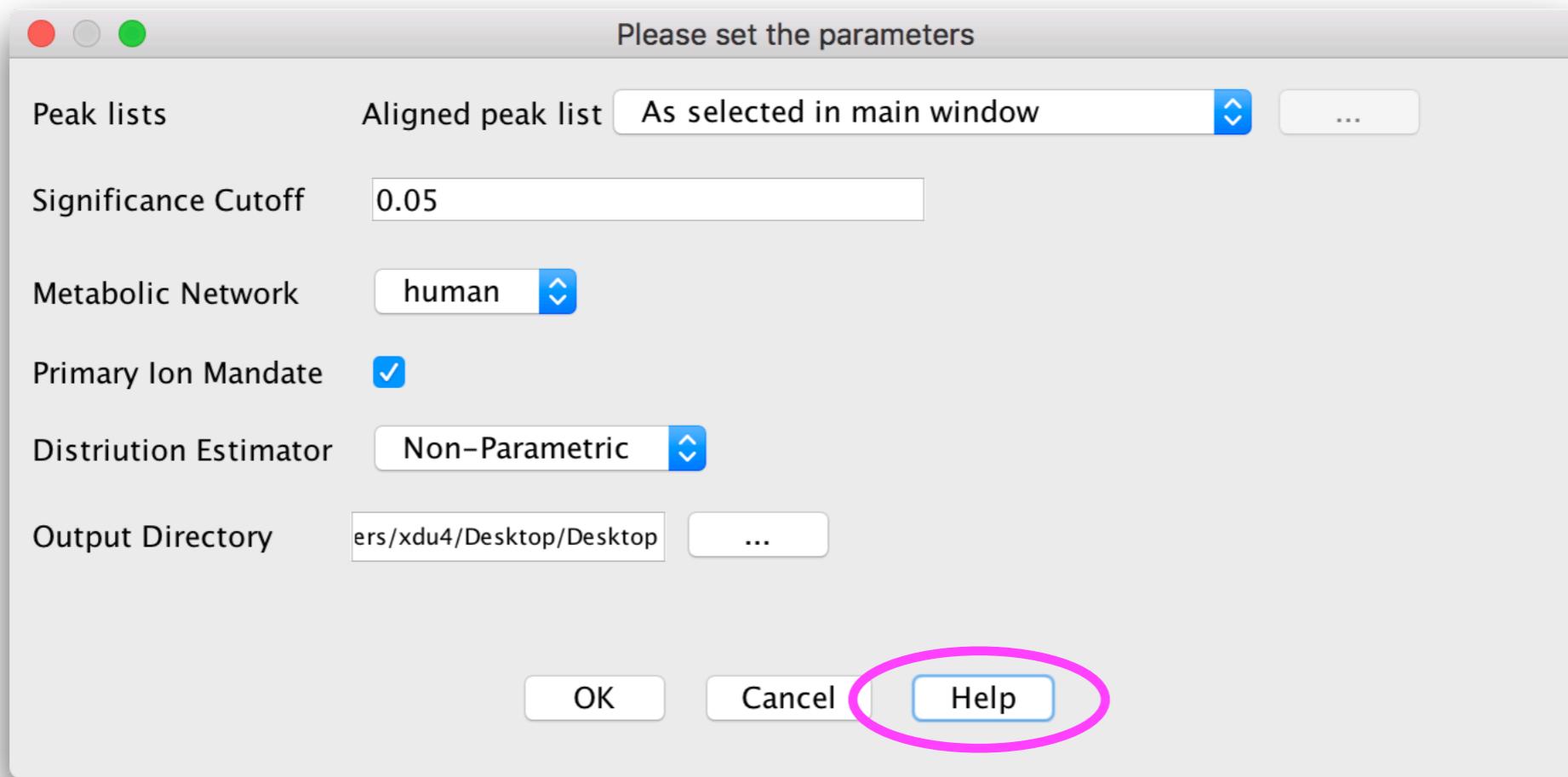
MCGResults_1553785464215	
	modular_analysis.csv
	pathway_analysis.csv
	empirical_compounds.csv

Empirical compounds.csv

	A	B	C	D	E	F	G	H	I	J	K	L
1	EID	massfeature_rows	rows_mz_retention_time	str_row_ion	compounds	compound_names						
2	E3	row2287;row89	(row2287;569.1720825195313;1 row2287_M+H[1+]; C11376			"SN38 glucuronide; SN-38G"						
3	E5	row160	(row1605;392.1644973754883;1 row1605_M+Na[1+ 5adrostestrones;CE6			"5alpha-Dihydrotestosterone sulfate";"androsterone sulfate"						
4	E9	row200	(row2003;300.1097412109375;1 row2003_M+Na[1+ C01449			"Queuine; Base Q"						
5	E15	row220	(row2202;447.204842703683;14 row2202_M+H[1+]; C11133;estroneglc			"Estrone glucuronide; Estrone 3-glucuronide; Estrone beta-D-glucuronide";"estrone glucuronide"						
6	E18	row16	(row160;232.08099873860678;1 row160_M+H[1+]; C05932			"N-Succinyl-L-glutamate 5-semialdehyde; (2S)-2-(3-Carboxypropanoylamino)-5-oxopentanoic acid"						
7	E26	row171;row192	(row171;240.12429555257162;1 row171_M[1+];row C01262			"beta-Alanyl-N(pi)-methyl-L-histidine; Anserine"						
8	E28	row2	(row21;175.06000033291903;17 row21_M+Na[1+]; CE5276			"dopamine o-quinone"						
9	E32	row1332;row202	(row1332;308.0973423549107;1 row1332_M+H[1+]; C14798;C14797;C1			"null";"null";"null"						
0	E33	row44	(row448;310.1048980712891;14 row448_M+Na[1+]; C06350			"null"						
1	E34	row24	(row247;259.1190376281738;12 row247_M+H[1+]; C00670			"sn-Glycero-3-phosphocholine"						
2	E36	row544;row54	(row544;340.05411529541016;1 row544_M+H[1+];C04751			"5-amino-1-(5-phospho-D-ribosyl)imidazole-4-carboxylate"						
3	E39	row7	(row73;200.12984339396158;19 row73_M+H[1+]; C12448;egme			"Ecgonine methyl ester; Methyl ecgonine";"ecgonine methyl ester"						
4	E45	row84	(row845;447.204928588672;12 row845_M+H[1+]; C11133;estroneglc			"Estrone glucuronide; Estrone 3-glucuronide; Estrone beta-D-glucuronide";"estrone glucuronide"						
5	E48	row1760;row84	(row1760;448.20692952473956 row1760_M(C13)+;C11133;estroneglc			"Estrone glucuronide; Estrone 3-glucuronide; Estrone beta-D-glucuronide";"estrone glucuronide"						
6	E50	row47	(row473;319.12325286865234;1 row473_M+Na[1+]; C16609			"Didemethylcitalopram"						
7	E54	row157	(row1574;379.15892028808594 row1574_M+H[1+]; C01007			"Reduced riboflavin"						
8	E58	row114	(row1145;232.08080836704798 row1145_M+H[1+]; C05932			"N-Succinyl-L-glutamate 5-semialdehyde; (2S)-2-(3-Carboxypropanoylamino)-5-oxopentanoic acid"						
9	E60	row132	(row1325;307.0313232421875;2 row1325_M+H[1+]; C02355			"2',3'-Cyclic UMP"						
0	E61	row9	(row93;208.0618659125434;13. row93_M+H[1+]; C14876;C14801;C0			"null";"1-Nitro-5,6-dihydroxy-dihydronaphthalene; 1,2-Dihydro-5-nitro-1,2-naphthalenediol";"4-(2-Aminoph						
1	E63	row2	(row23;179.05465952555338;13 row23_M+Na[1+]; CE2026			"3-methylcrotonoylglycine"						
2	E64	row2	(row29;185.08246959339488;16 row29_M+H[1+]; C00588;C05594			"Choline phosphate";"3-Methoxy-4-hydroxyphenylethyleneglycol"						
3	E67	row62	(row624;363.2163798014323;20 row624_M+H[1+]; C00735;C05469;C0			"Cortisol; Hydrocortisone; 11beta,17alpha,21-Trihydroxy-4-pregnene-3,20-dione; Kendall's compound F; Re						
4	E69	row1096;row7	(row1096;201.1330784388951;2 row1096_M(C13)+;C12448;egme			"Ecgonine methyl ester; Methyl ecgonine";"ecgonine methyl ester"						
5	E70	row195	(row1955;271.0474802652995;1 row1955_M+Na[1+ C00647			"Pyridoxamine 5'-phosphate"						
6	E73	row136	(row1362;319.12235260009766 row1362_M+Na[1+ C16609			"Didemethylcitalopram"						

Where to go from here?

Help files in MZine 2



Help files in MZmine 2

MZmine 2

The screenshot shows the MZmine 2 software interface. On the left is a vertical toolbar with various icons and a list of help topics. The main window title is "MZmine 2". The current help topic is "Mummichog Calculation". Below the title, there is a section titled "Description" which contains a detailed text about the Mummichog algorithm. At the bottom of the main window, there is a link to the algorithm's website: <http://mummichog.org/>. A modal dialog box titled "Please set the parameters" is open in the center. It contains several input fields and dropdown menus:

- Peak lists: "Aligned peak list" dropdown set to "As selected in main window".
- Significance Cutoff: Text input field containing "0.05".
- Metabolic Network: Dropdown menu set to "human".
- Primary Ion Mandate: Checkmark input field checked.
- Distribution Estimator: Dropdown menu set to "Non-Parametric".
- Output Directory: Text input field and browse button.

At the bottom of the dialog are "OK", "Cancel", and "Help" buttons.

Method parameters

Significance Cutoff

MZmine 2 website

ⓘ Not Secure | mzmine.github.io/documentation.html



[HOME](#) [FEATURES](#) [DOWNLOAD](#) [DEVELOPMENT](#) [SUPPORT](#) [CONTRIBUTORS](#)

[Support](#) / [Documentation](#)

User Documentation

The following documentation is available for getting familiar with MZmine 2 and its architecture. If you have further questions regarding the usage or development of MZmine 2 please contact the [developers](#).

- [MZmine 2 manual](#)

This manual covers the general functionality of MZmine 2 including installation, batch mode and data processing.

- [ADAP feature detection manual](#)

This manual covers the ADAP feature detection method.

- [Video Tutorial](#)

This animated tutorial created by Sandra Castillo introduces the basic features of MZmine 2, including raw data import, peak detection, visualization of results etc.

- [Usage tutorial](#)

This tutorial written by Mark Earll covers the data processing features of MZmine 2.

- [Manual for the Lipid Search module](#)

This manual covers in detail the Lipid Search module developed by Ansgar Korf.

Thank you!