

Hands-on Data Analysis with MZmine 2

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About MZmine 2

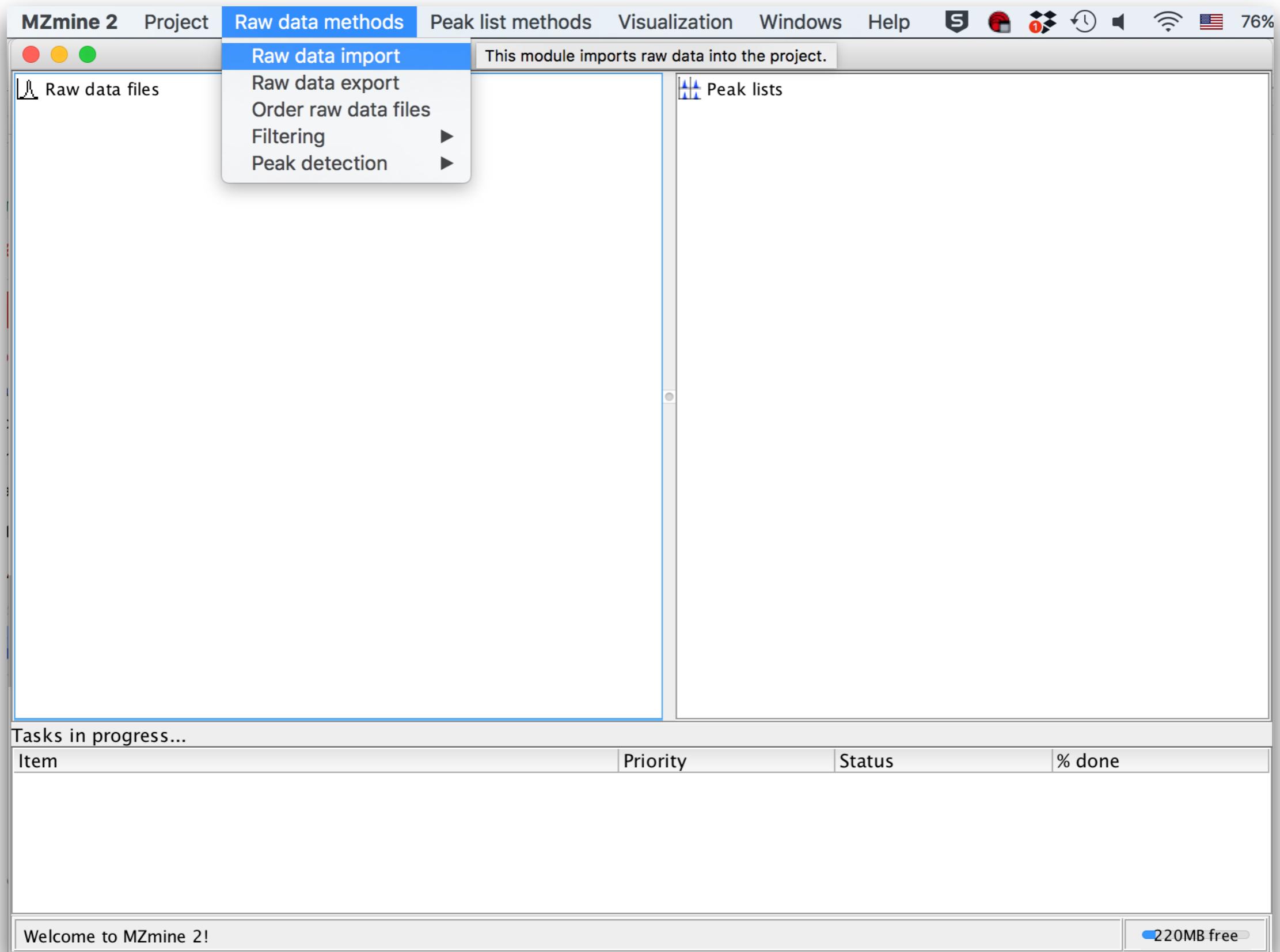
- LC/MS and GC/MS metabolomics data processing, analysis, and visualization
- Supported open data formats
 - mzXML
 - mzML
 - mzData
 - NetCDF

LC-MS

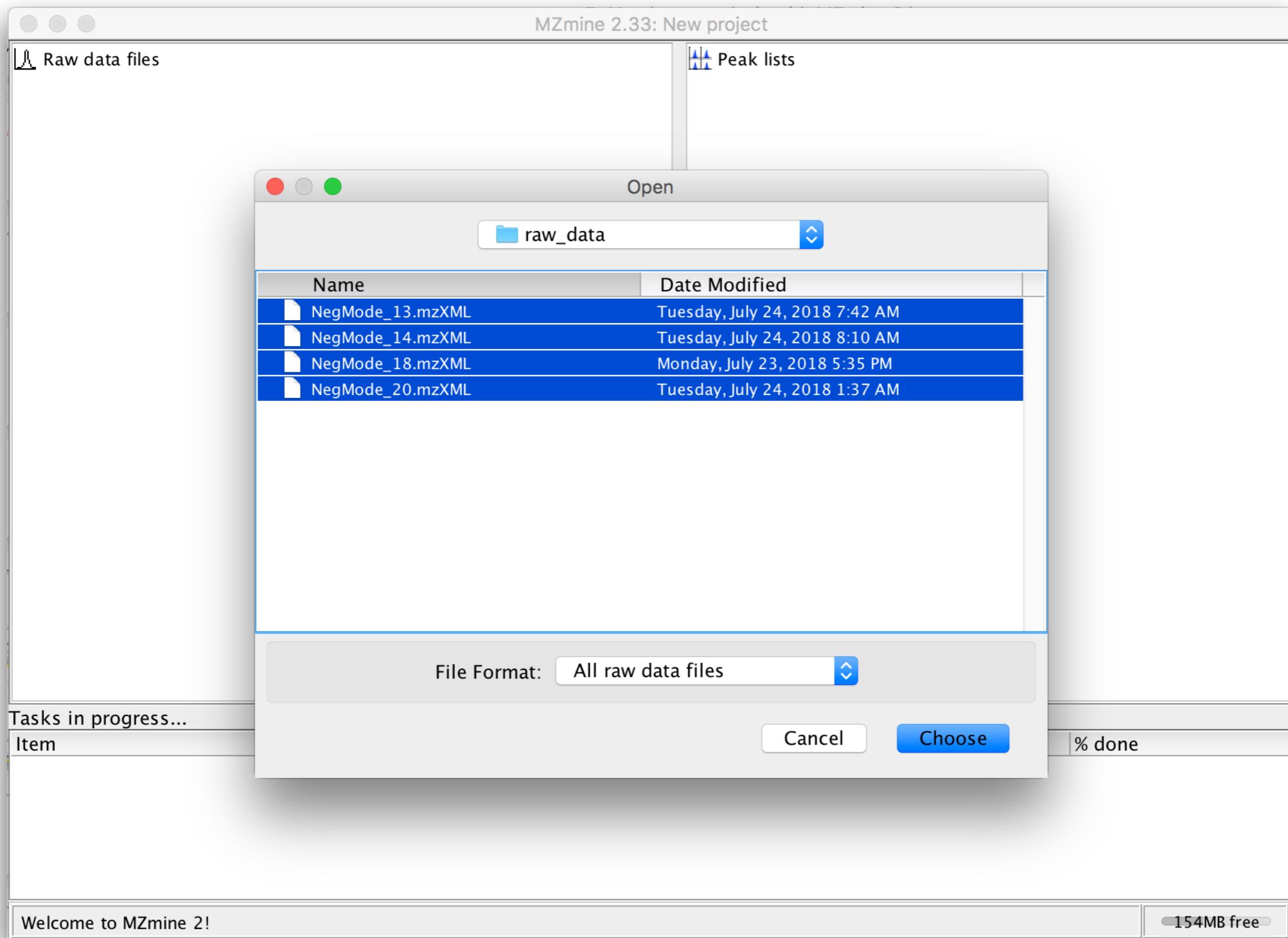
Workflow

- Raw data import
- Data visualization
- Mass detection
- Chromatogram building
- Deconvolution / Feature detection
- Feature alignment
- Feature identification
- Export

Data import



Data import



Data import

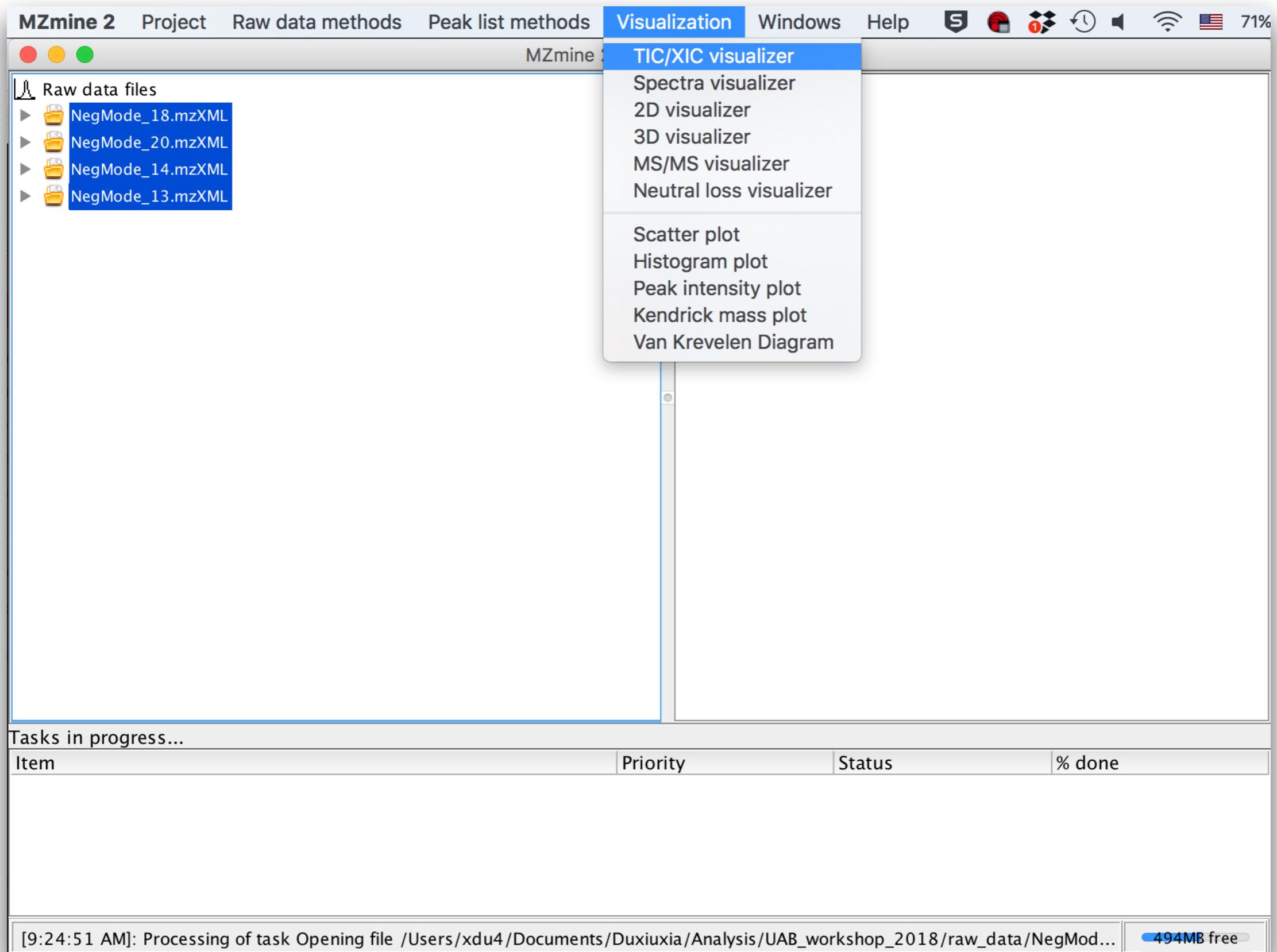
MZmine 2.33: New project

The screenshot shows the MZmine 2.33 software interface. At the top, there are three colored window control buttons (red, yellow, green). The title bar reads "MZmine 2.33: New project". The main area is divided into two sections: "Raw data files" on the left and "Peak lists" on the right. The "Raw data files" section contains four entries: "NegMode_18.mzXML", "NegMode_20.mzXML", "NegMode_14.mzXML", and "NegMode_13.mzXML", each represented by a folder icon. The "Peak lists" section is currently empty. Below these sections is a table titled "Tasks in progress...". The table has four columns: "Item", "Priority", "Status", and "% done". There are no items listed in the table. At the bottom of the screen, a status bar displays the message "[9:24:51 AM]: Processing of task Opening file /Users/xdu4/Documents/Duxiuxia/Analysis/UAB_workshop_2018/raw_data/NegMod..." and shows "839MB free" with a small disk icon.

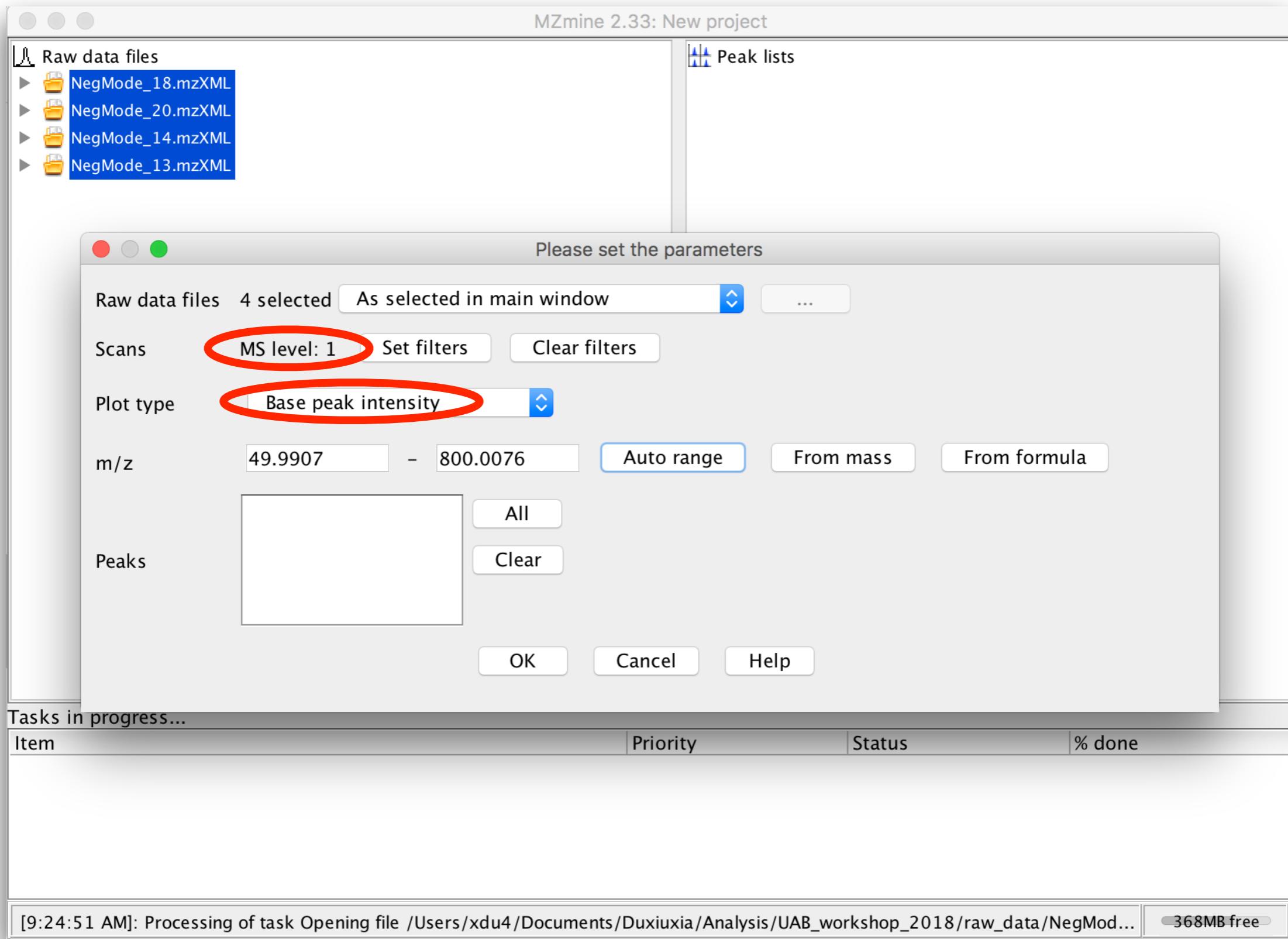
Item	Priority	Status	% done

[9:24:51 AM]: Processing of task Opening file /Users/xdu4/Documents/Duxiuxia/Analysis/UAB_workshop_2018/raw_data/NegMod... 839MB free

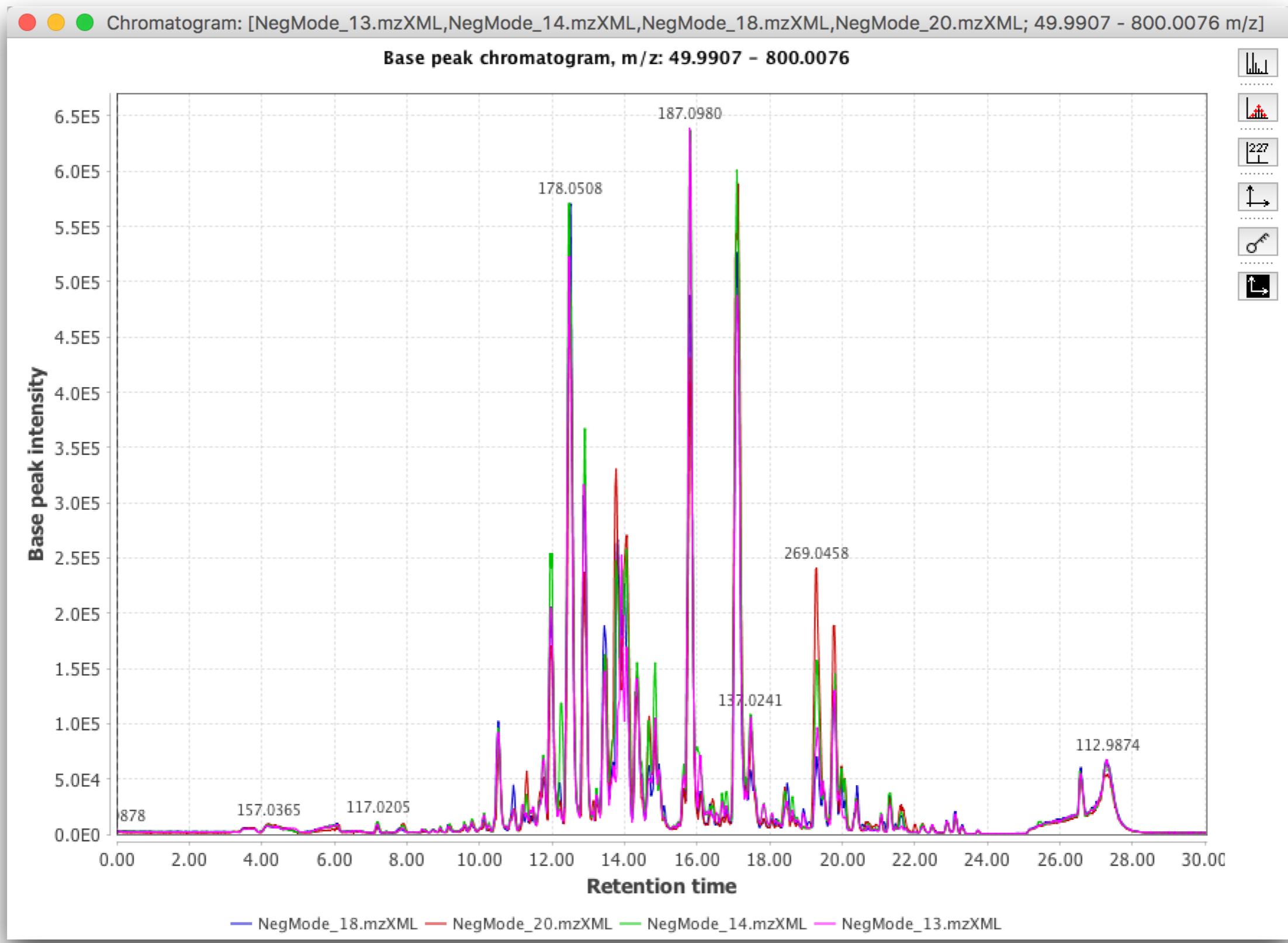
Data visualization: BIC



Data visualization: BIC



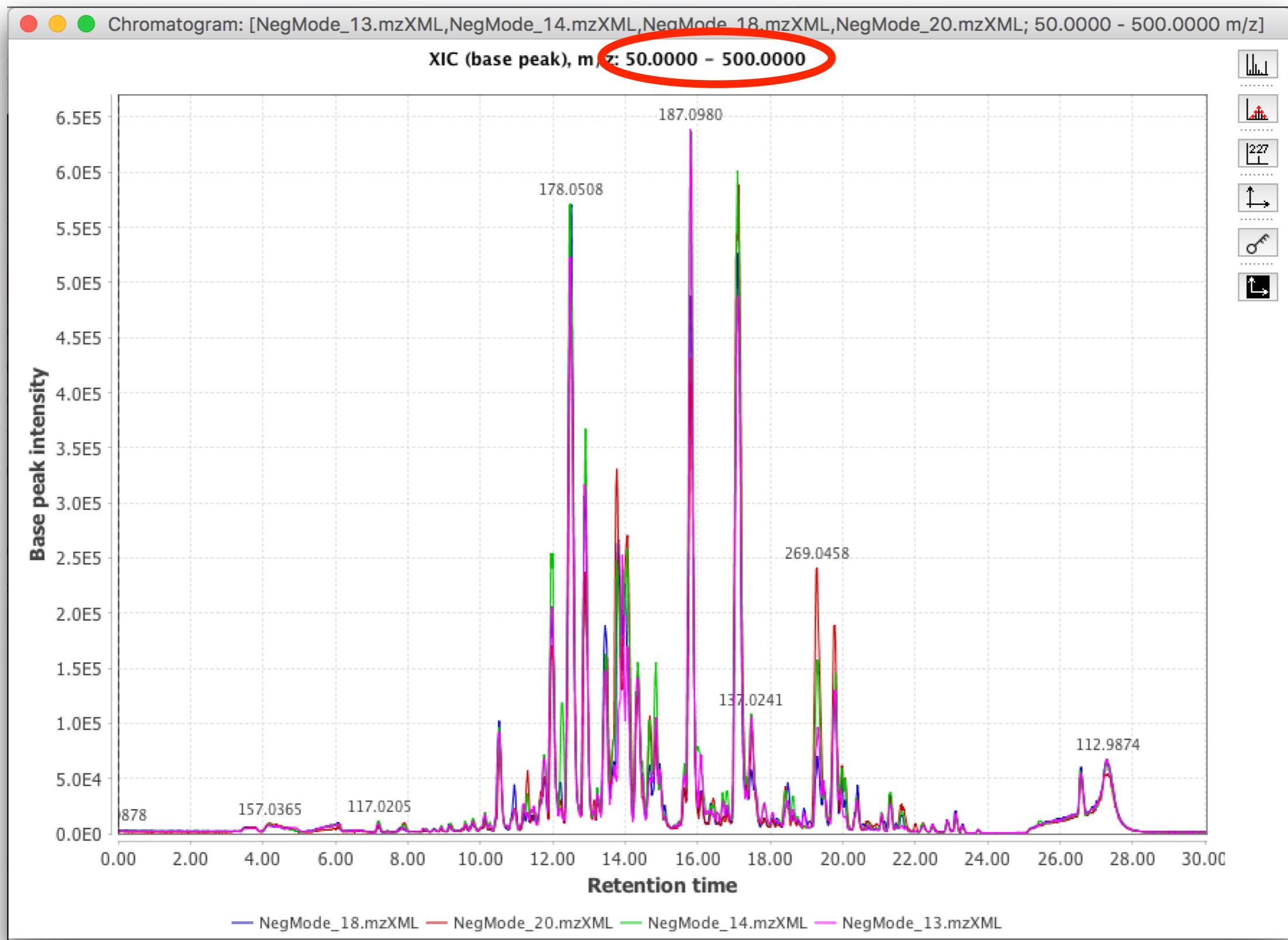
Data visualization: BIC



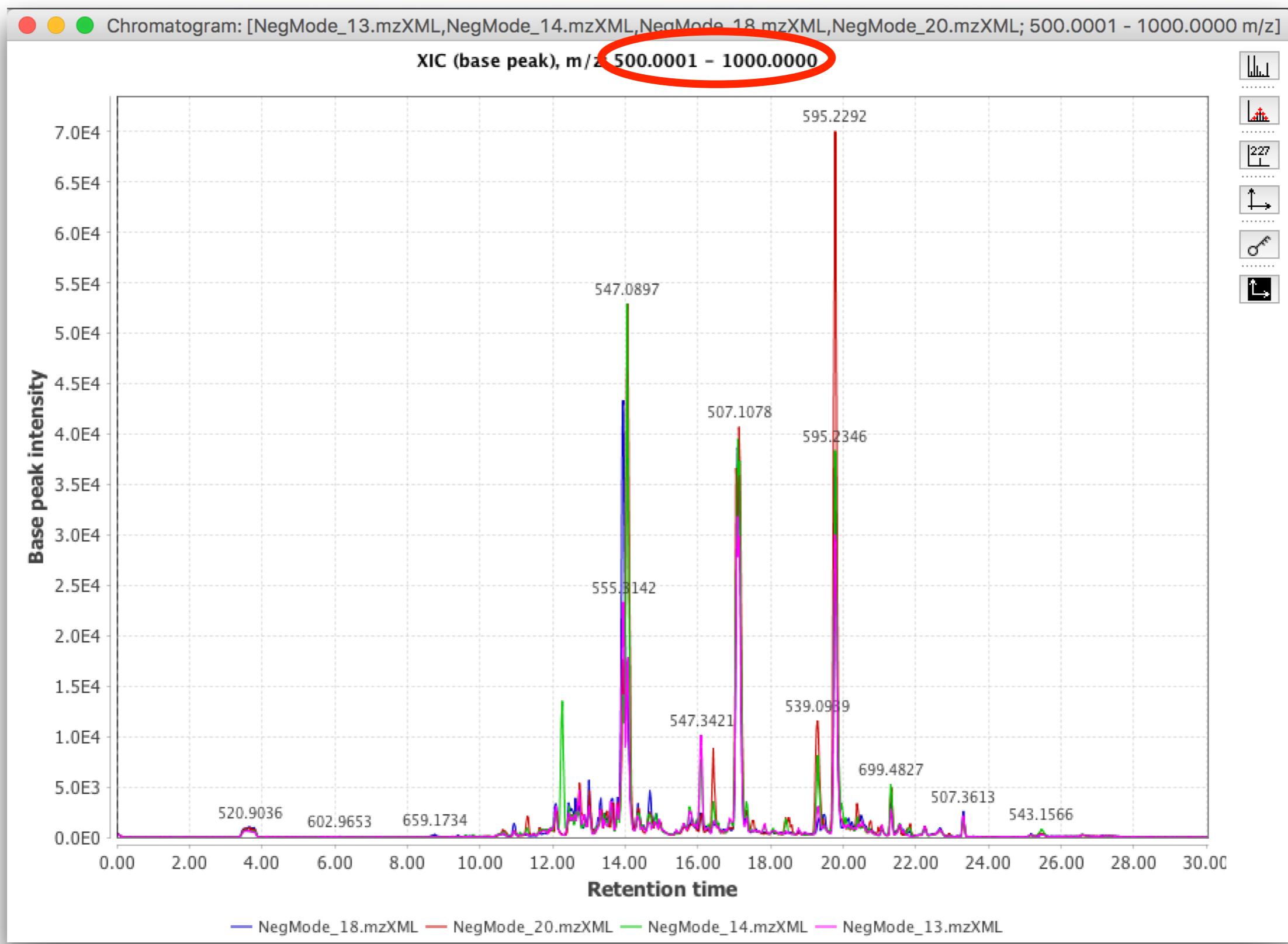
Data visualization: BIC

You can zoom in the BICs and examine them.

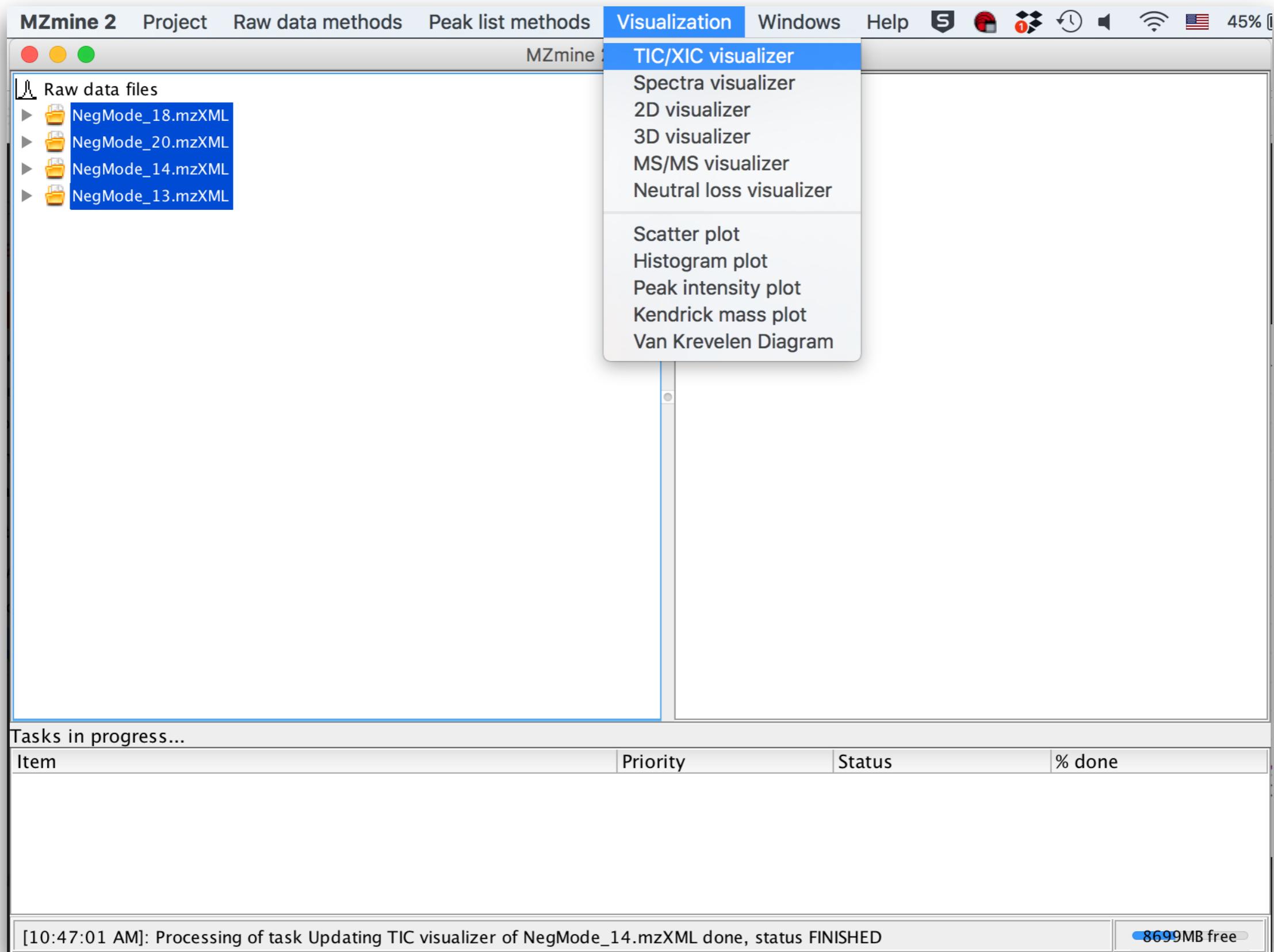
Data visualization: BIC



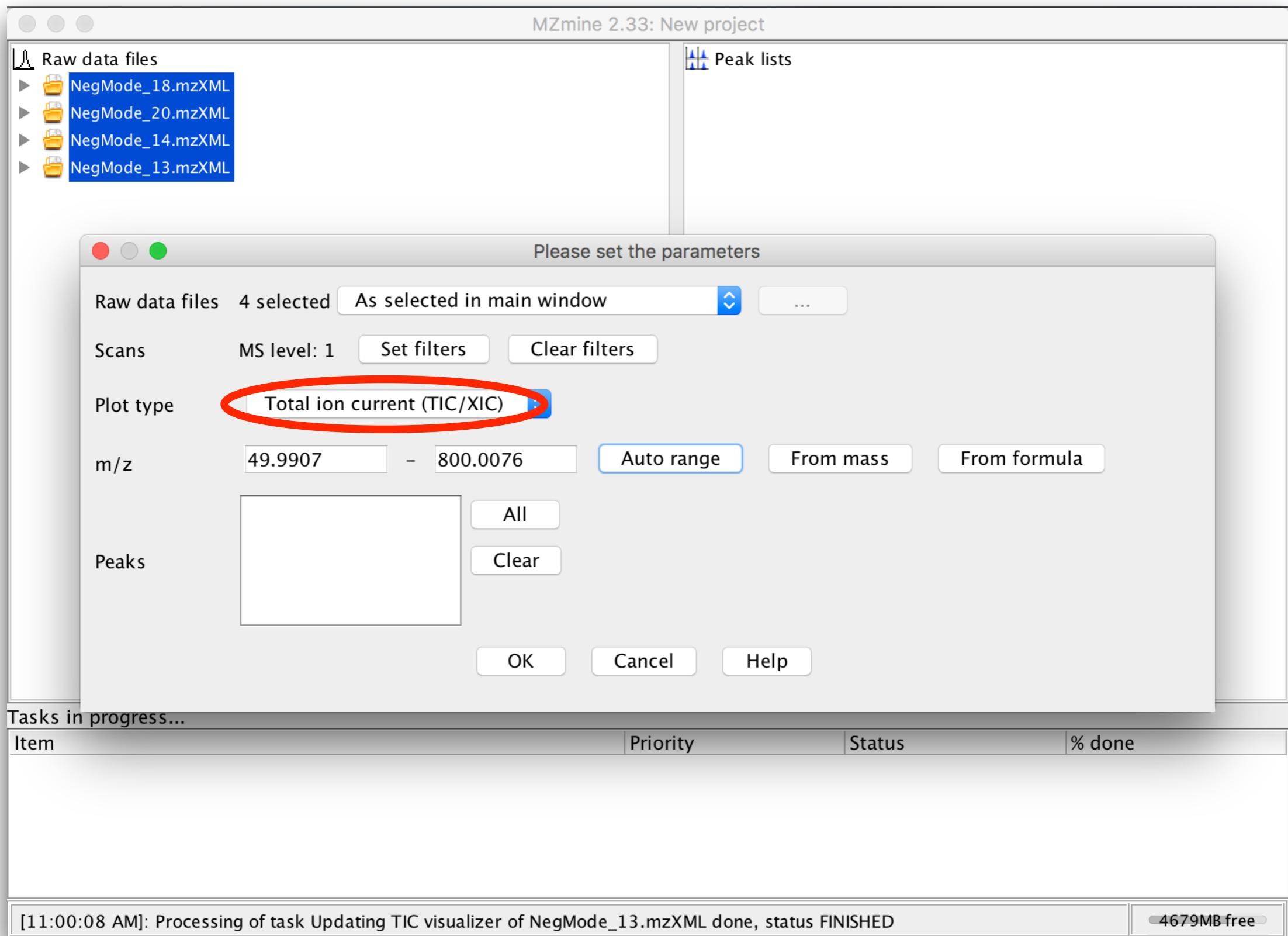
Data visualization: BIC



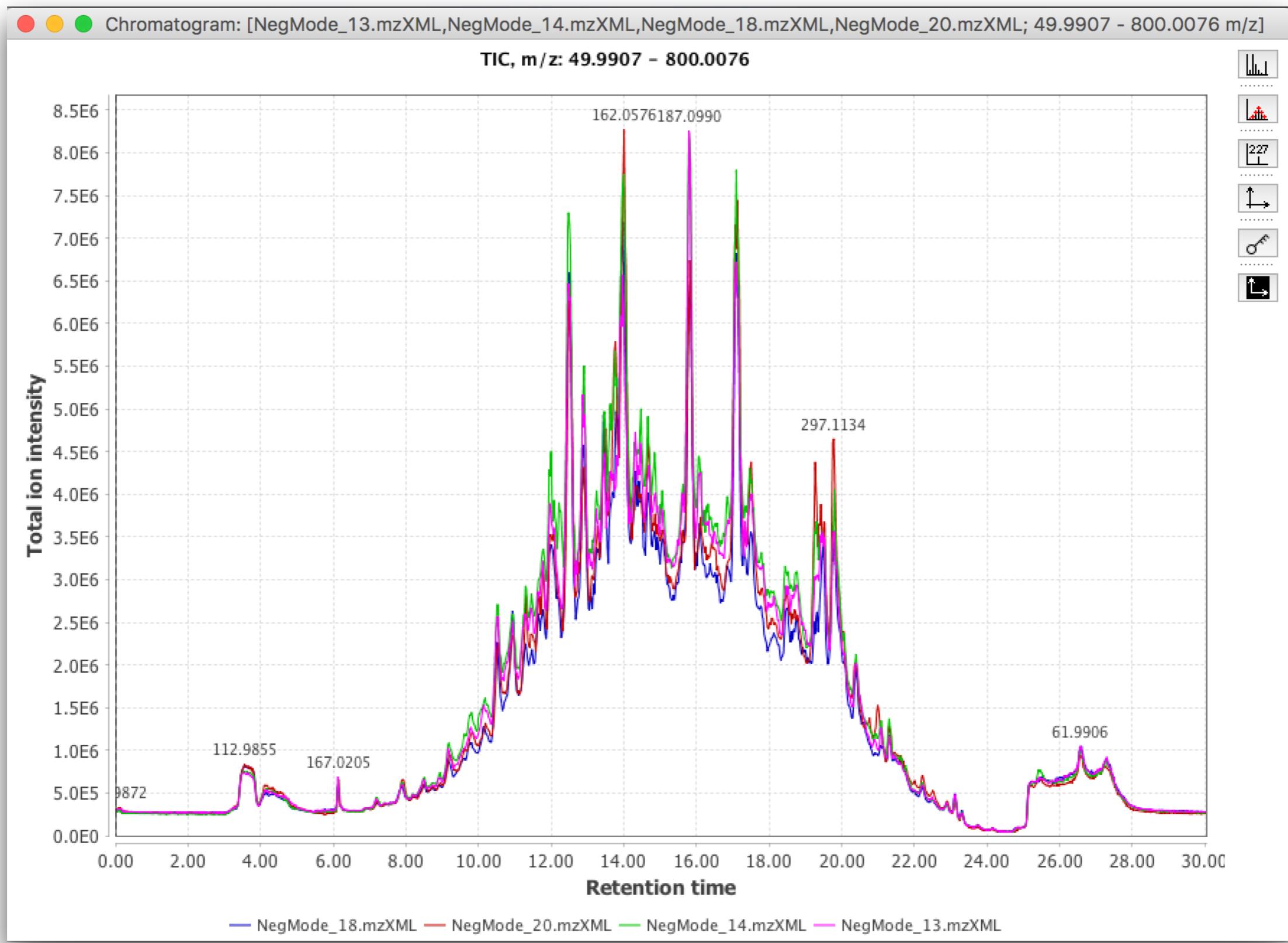
Data visualization: TIC



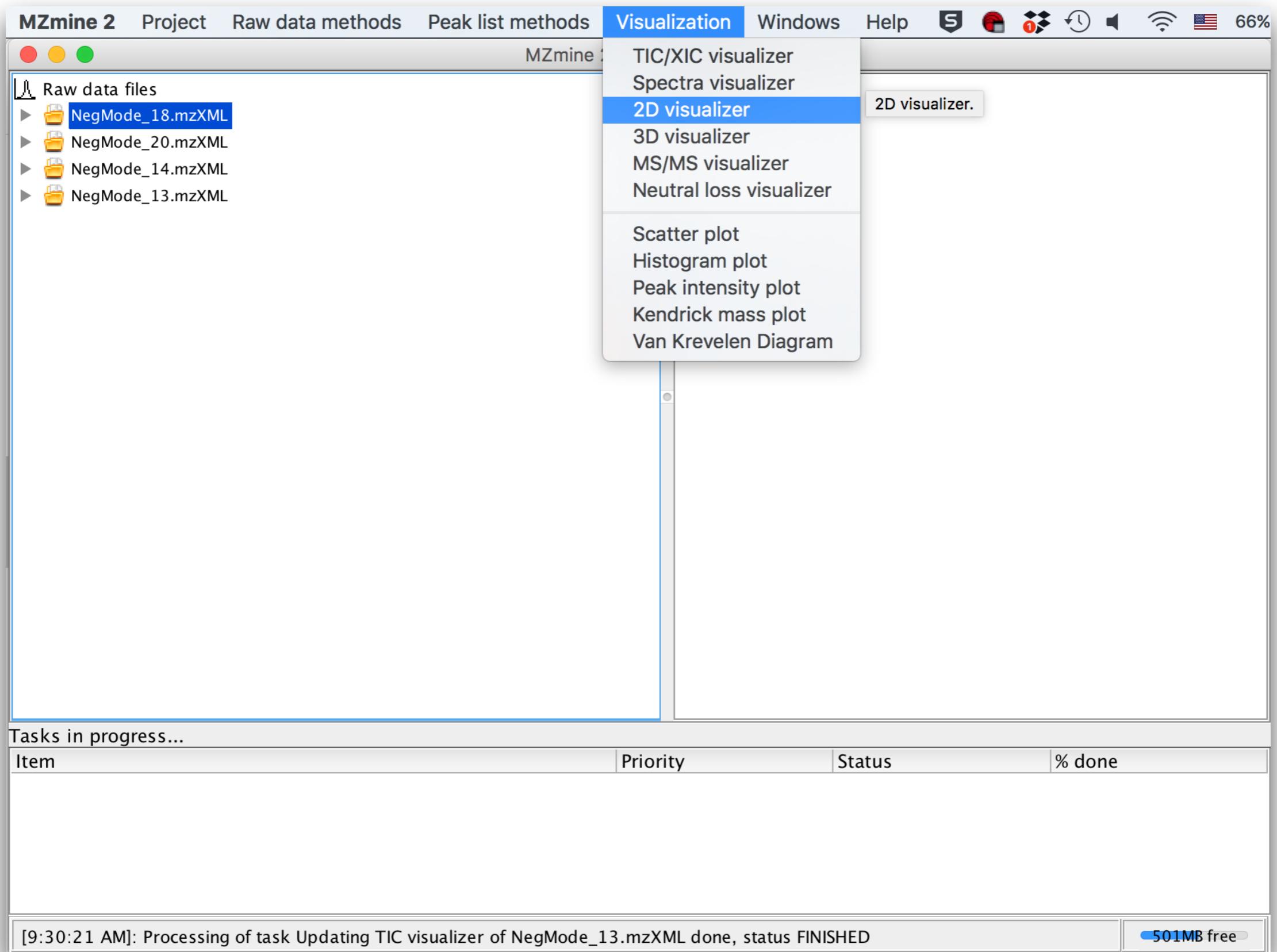
Data visualization: TIC



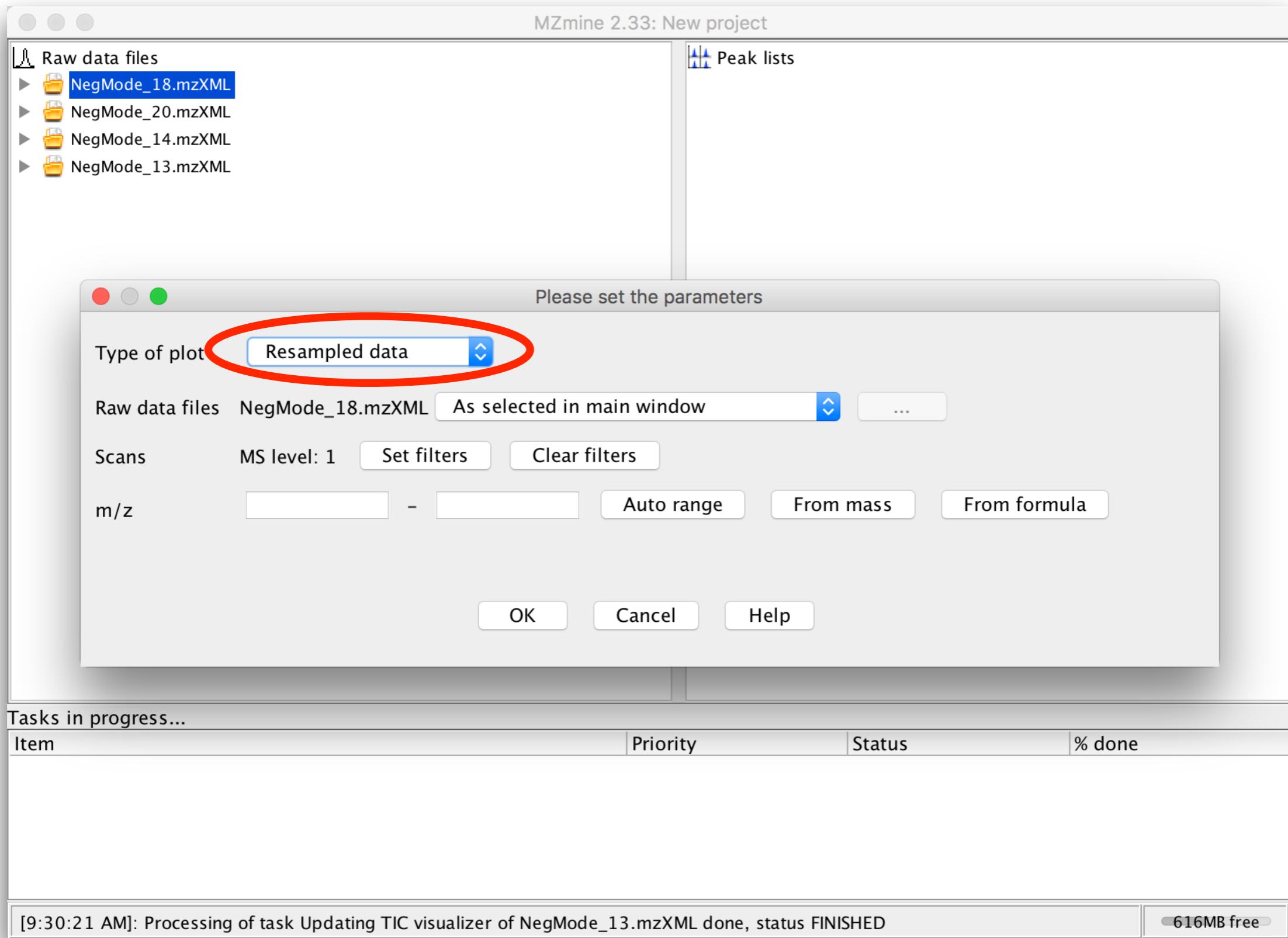
Data visualization: TIC



Data visualization: 2D



Data visualization: 2D

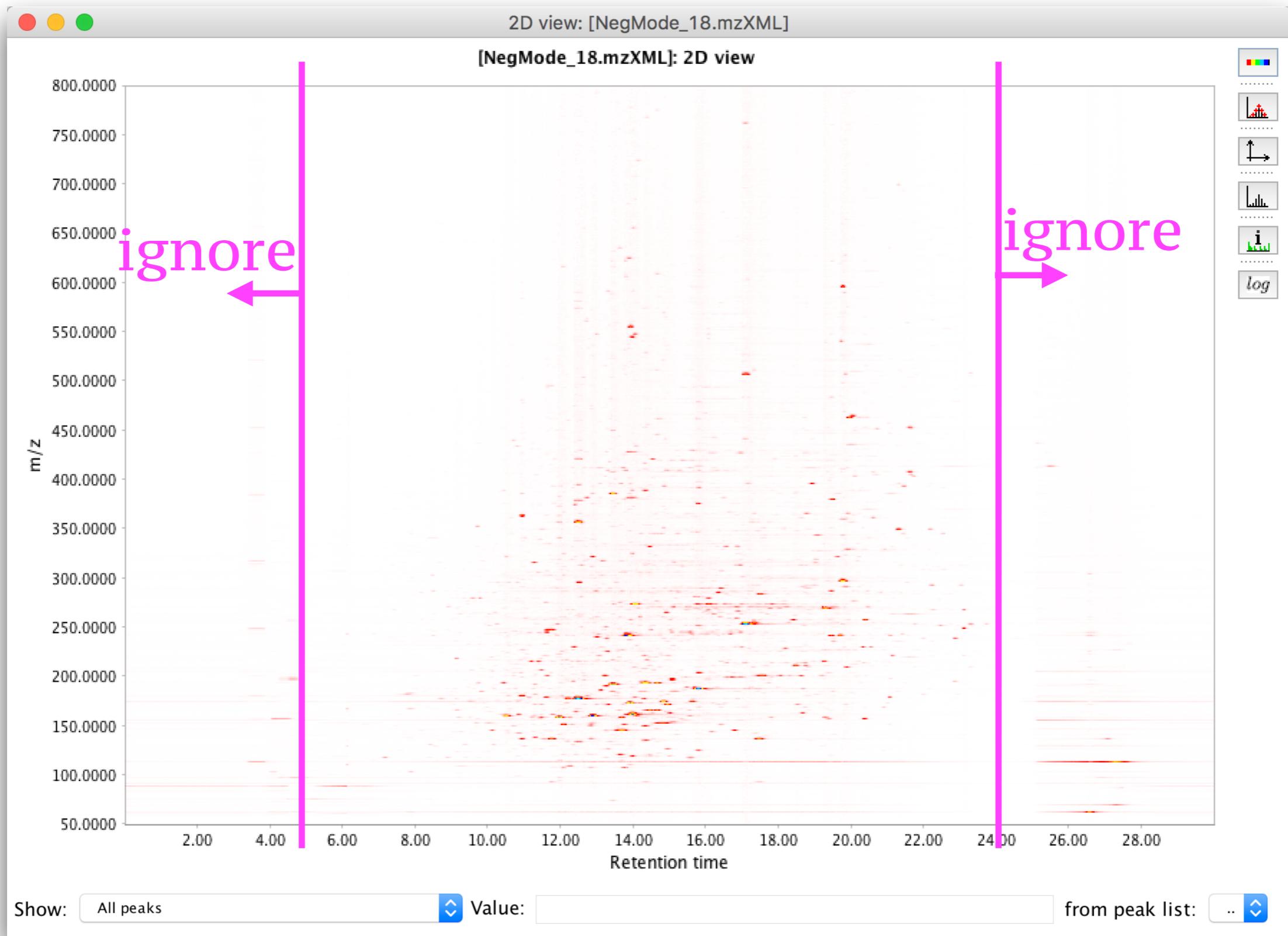


Item	Priority	Status	% done

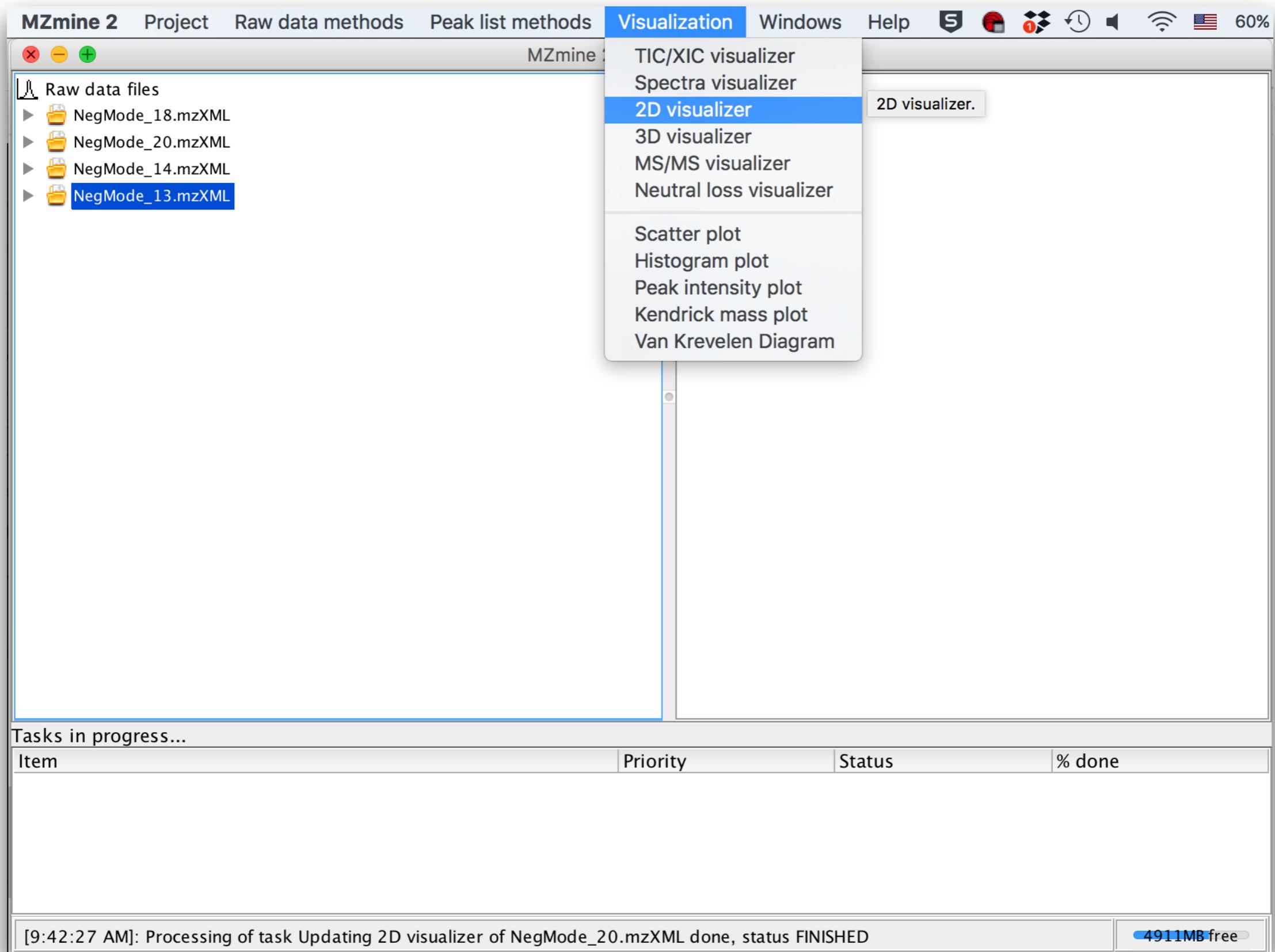
[9:30:21 AM]: Processing of task Updating TIC visualizer of NegMode_13.mzXML done, status FINISHED

616MB free

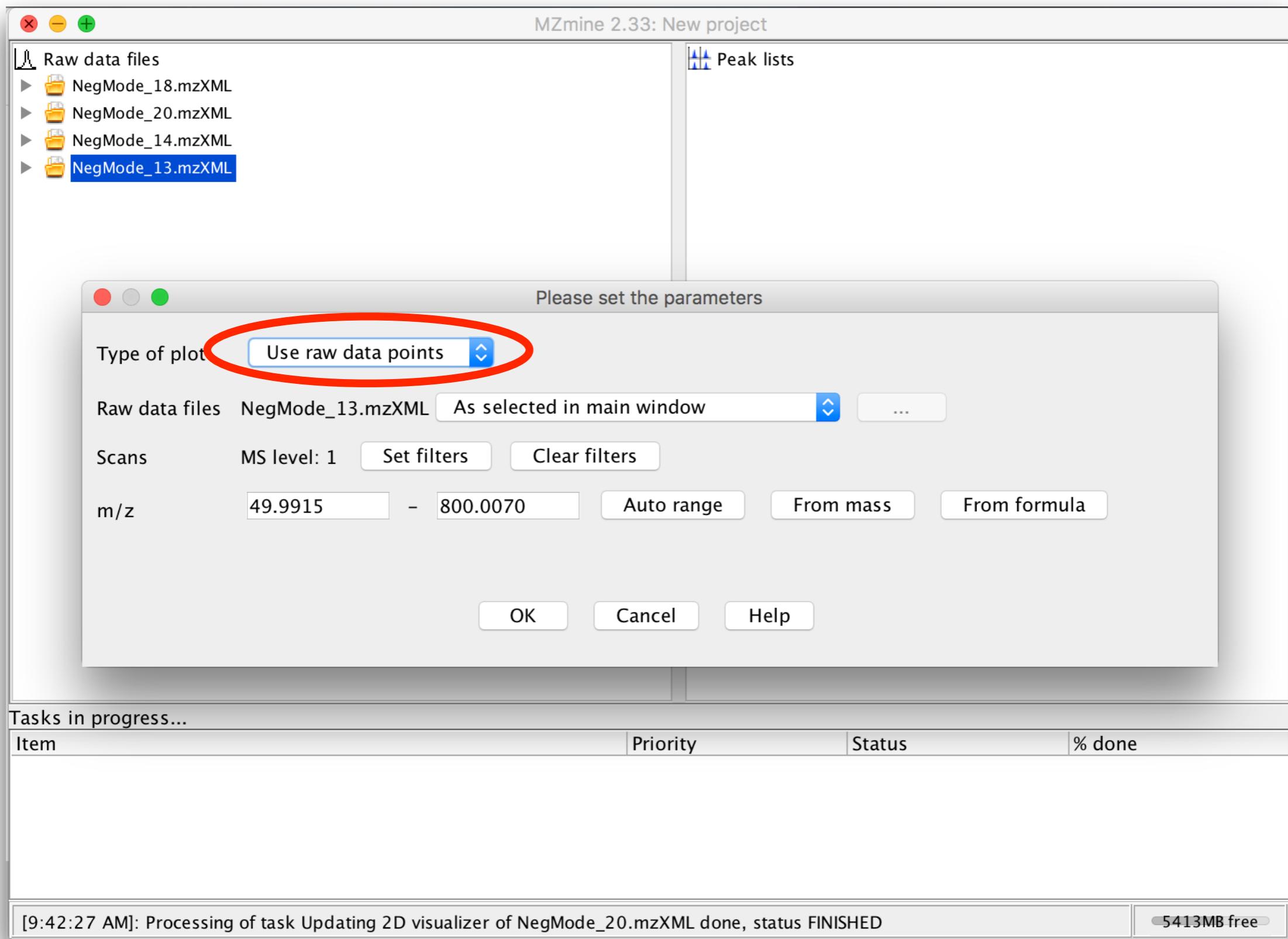
Data visualization: 2D



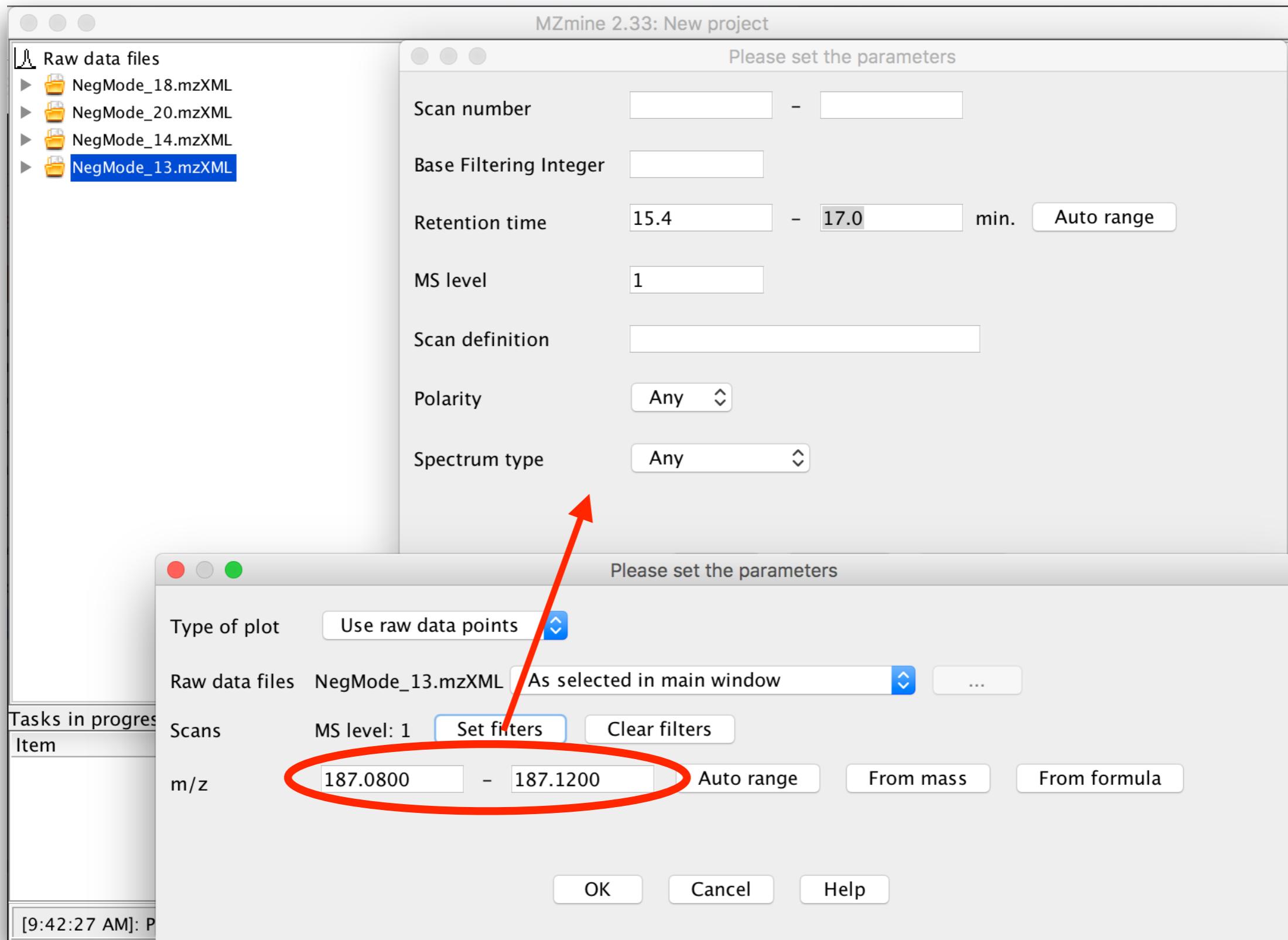
Data visualization: 2D



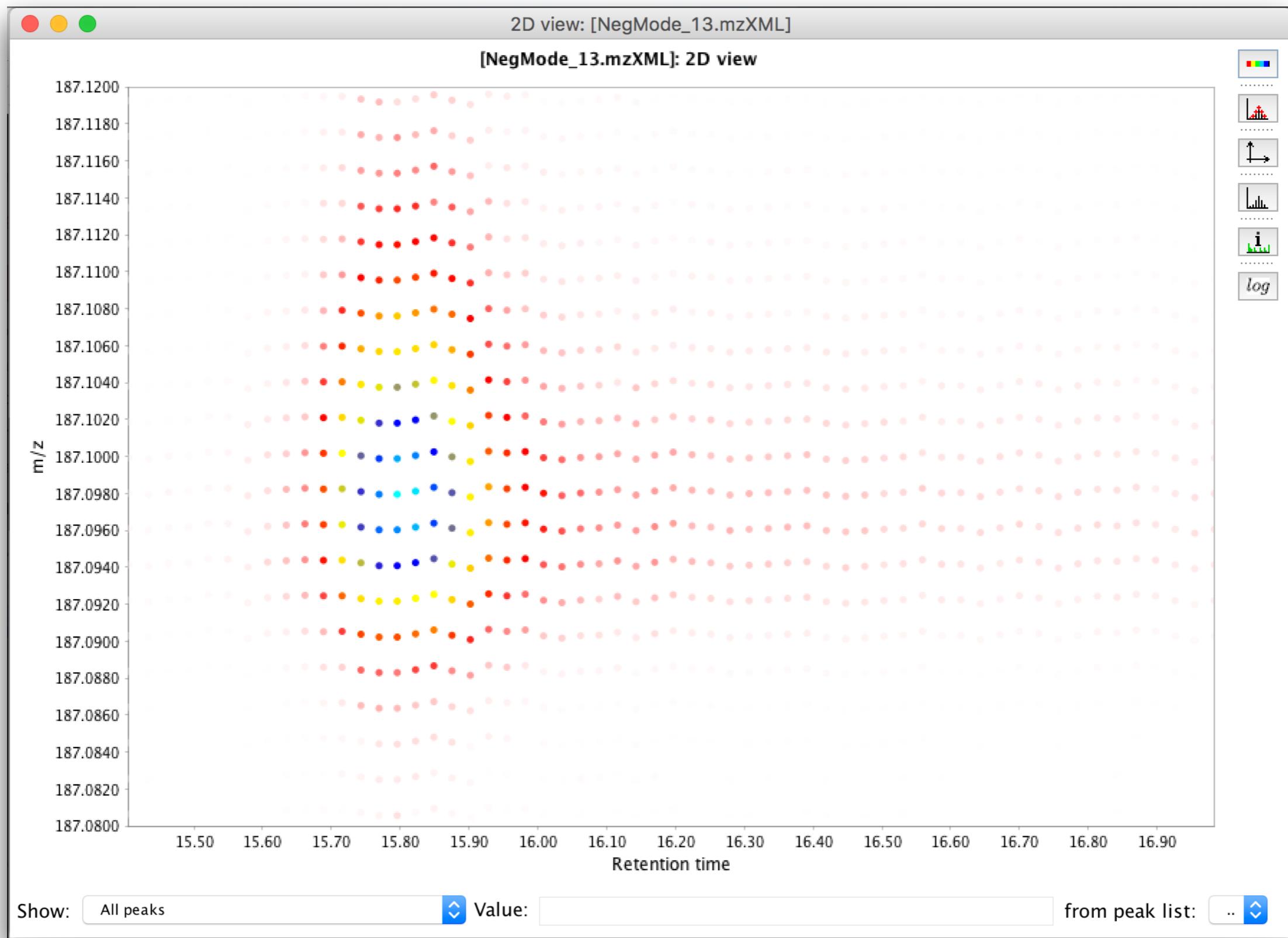
Data visualization: 2D



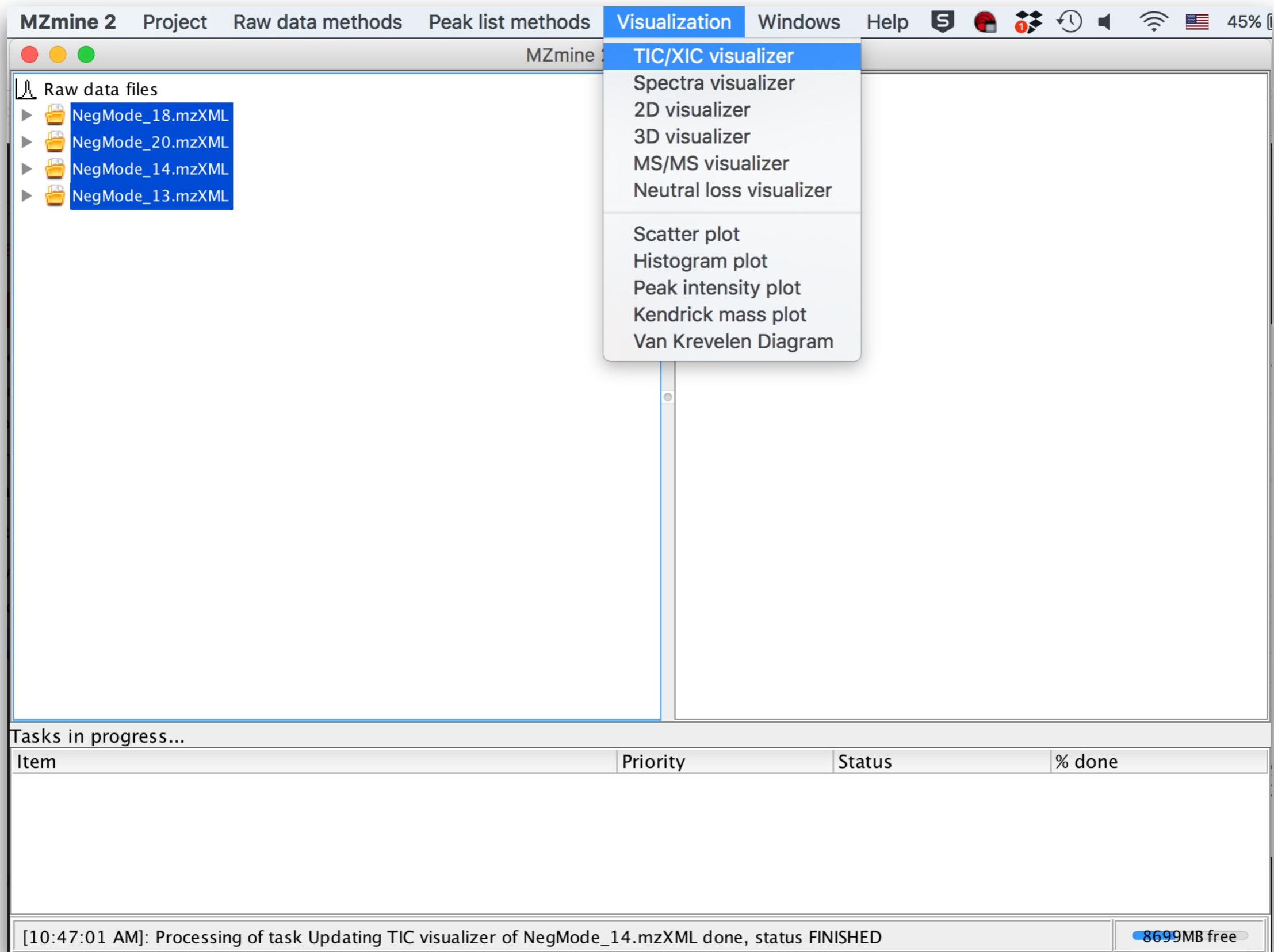
Data visualization: 2D



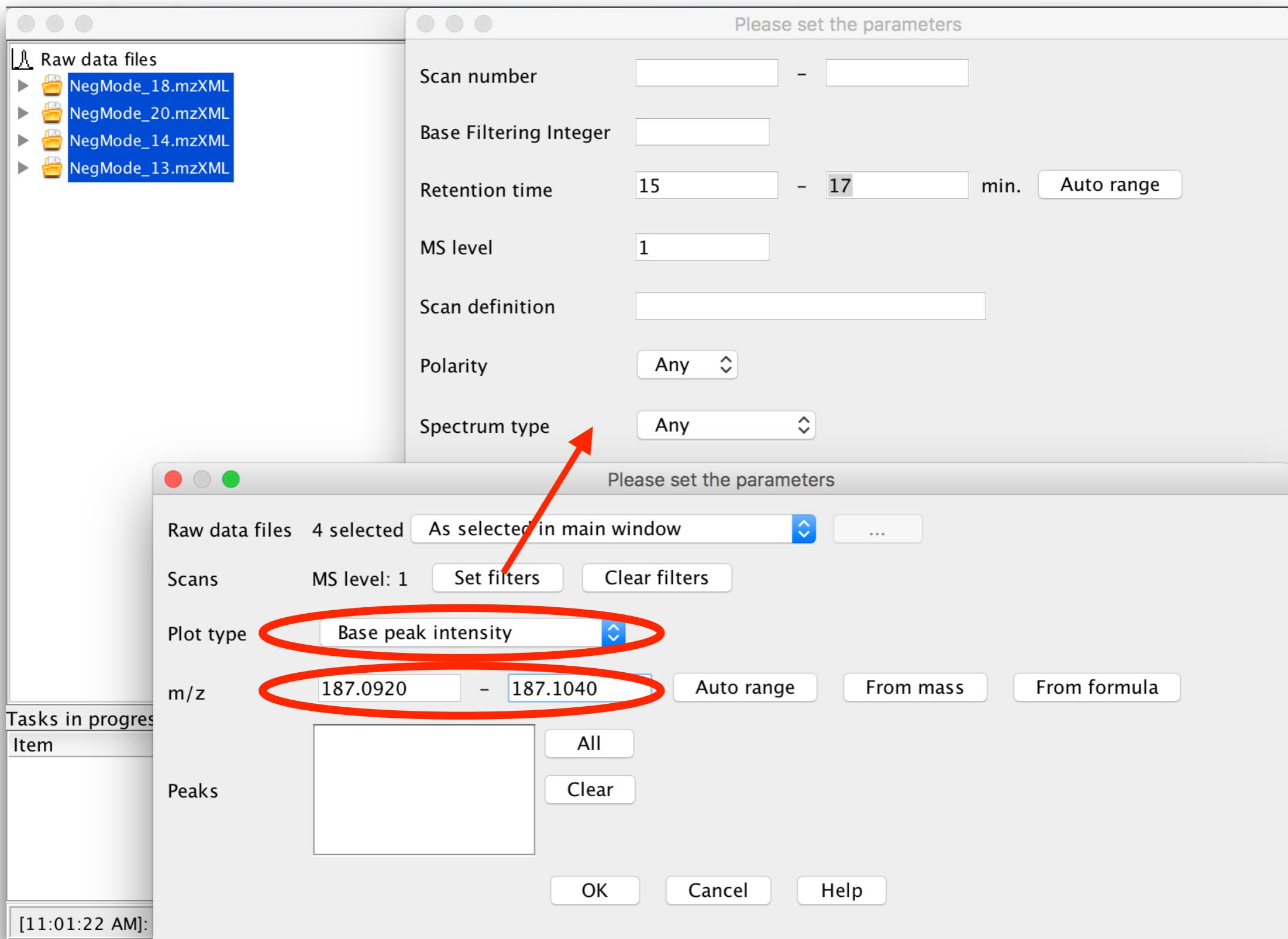
Data visualization: 2D



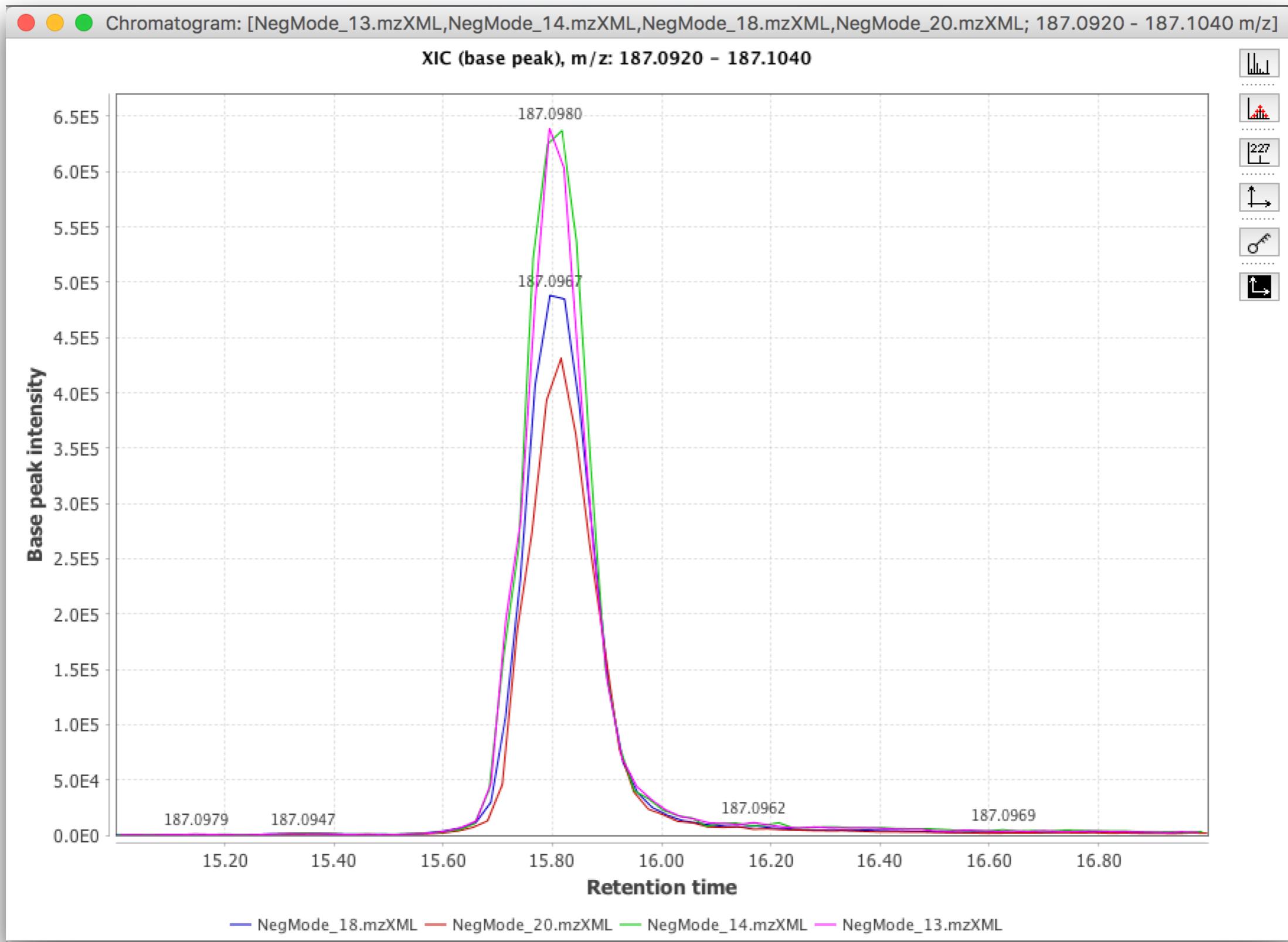
Data visualization: EIC



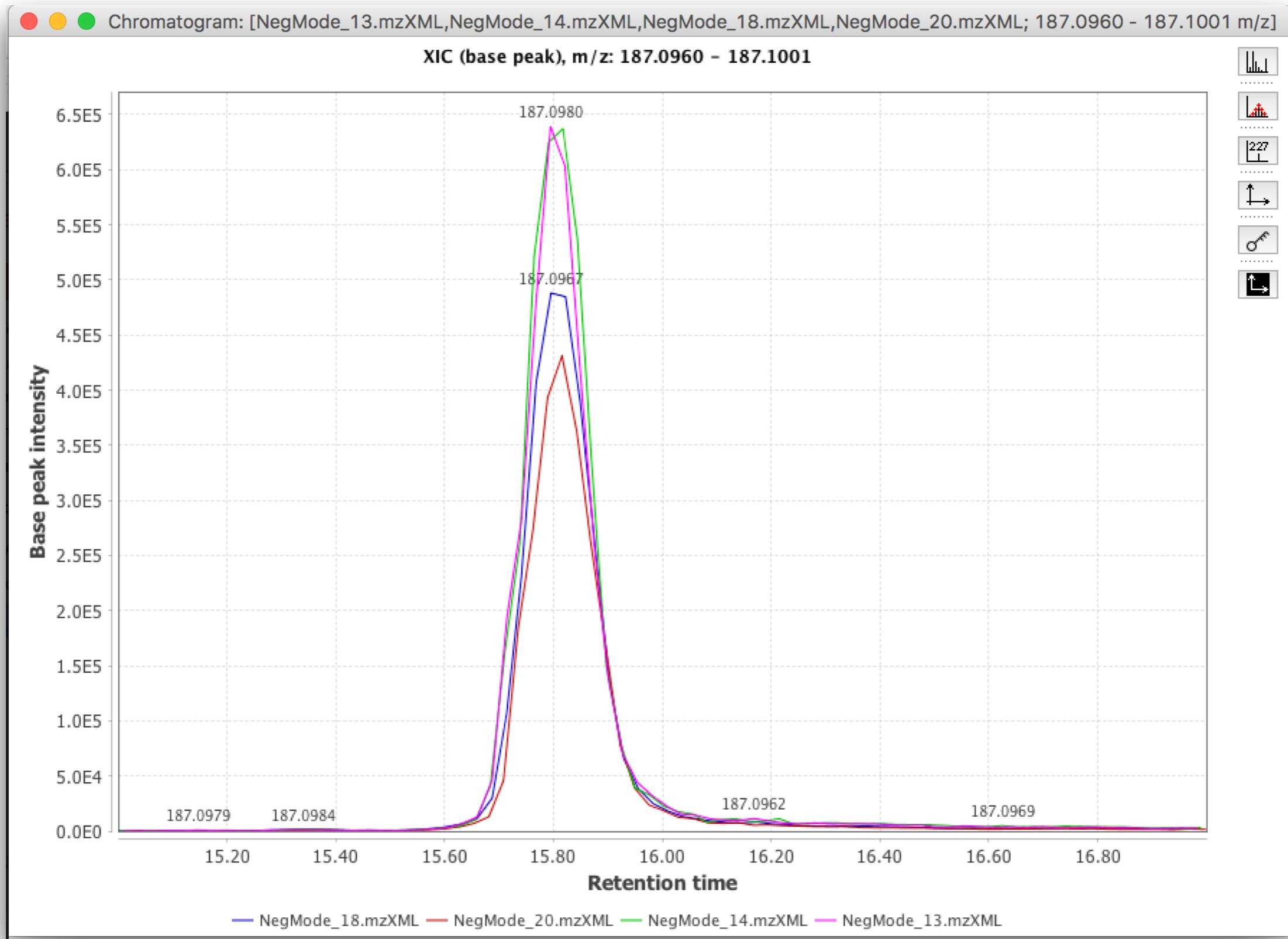
Data visualization: EIC



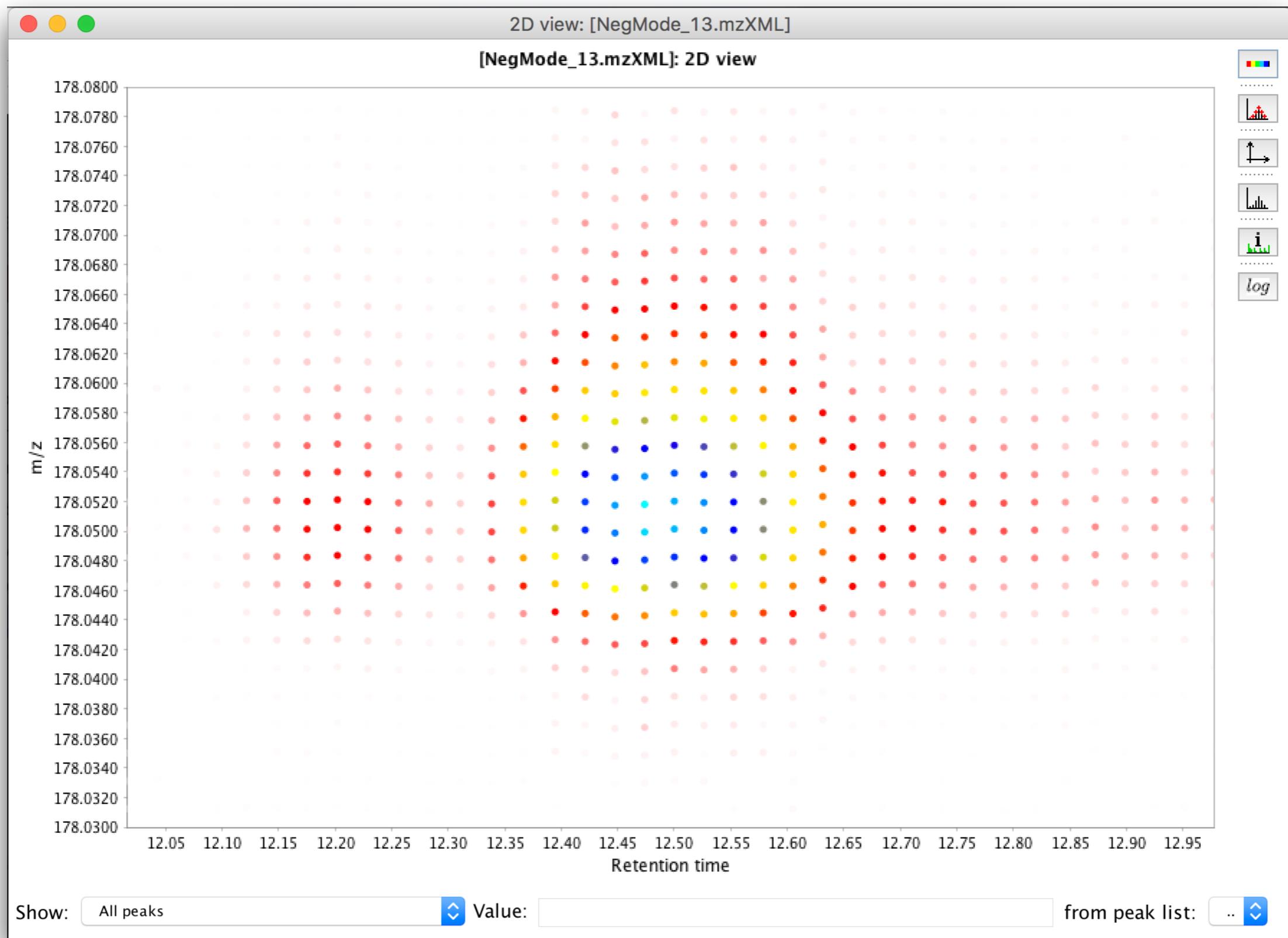
Data visualization: EIC



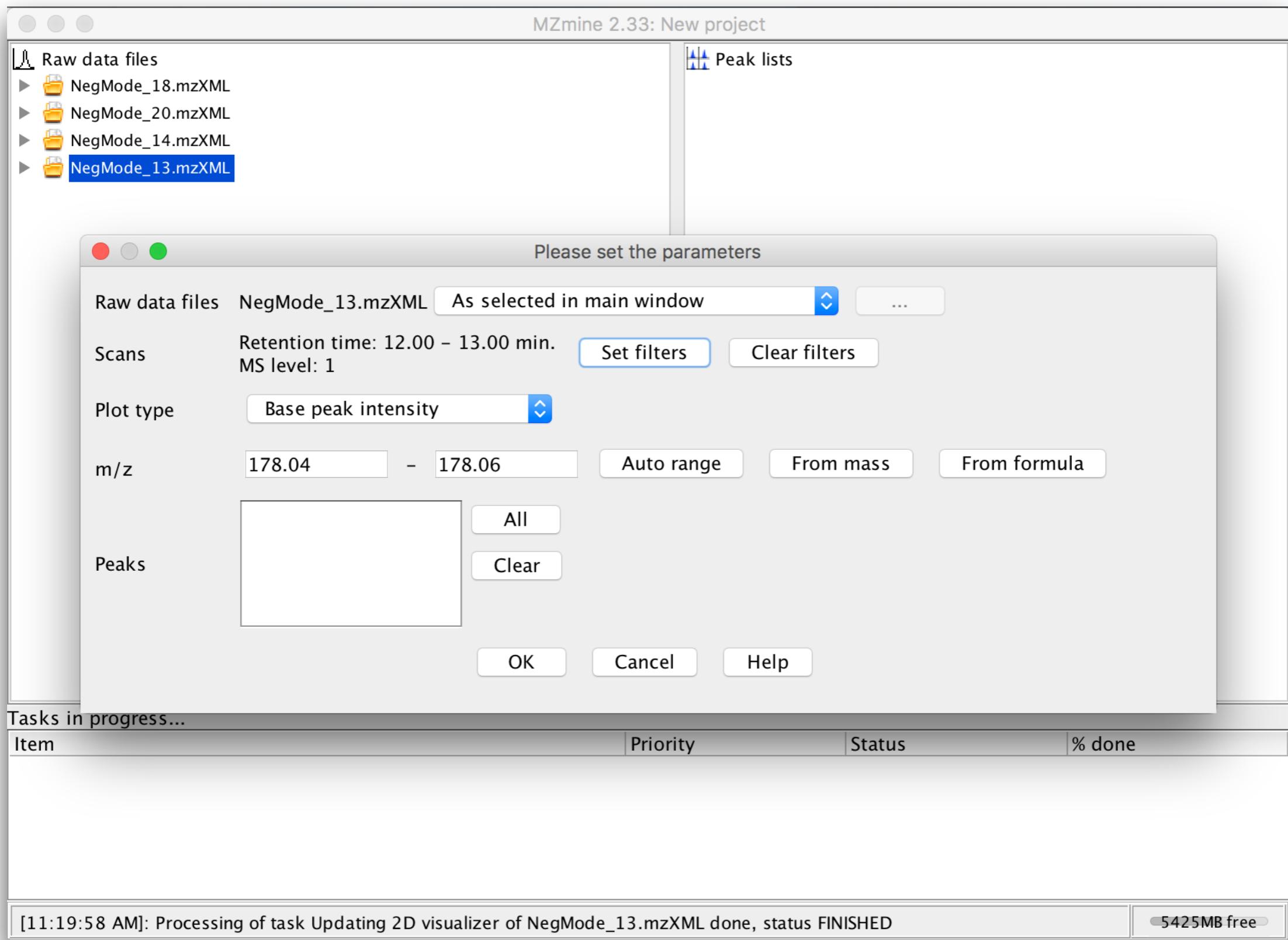
Data visualization: EIC



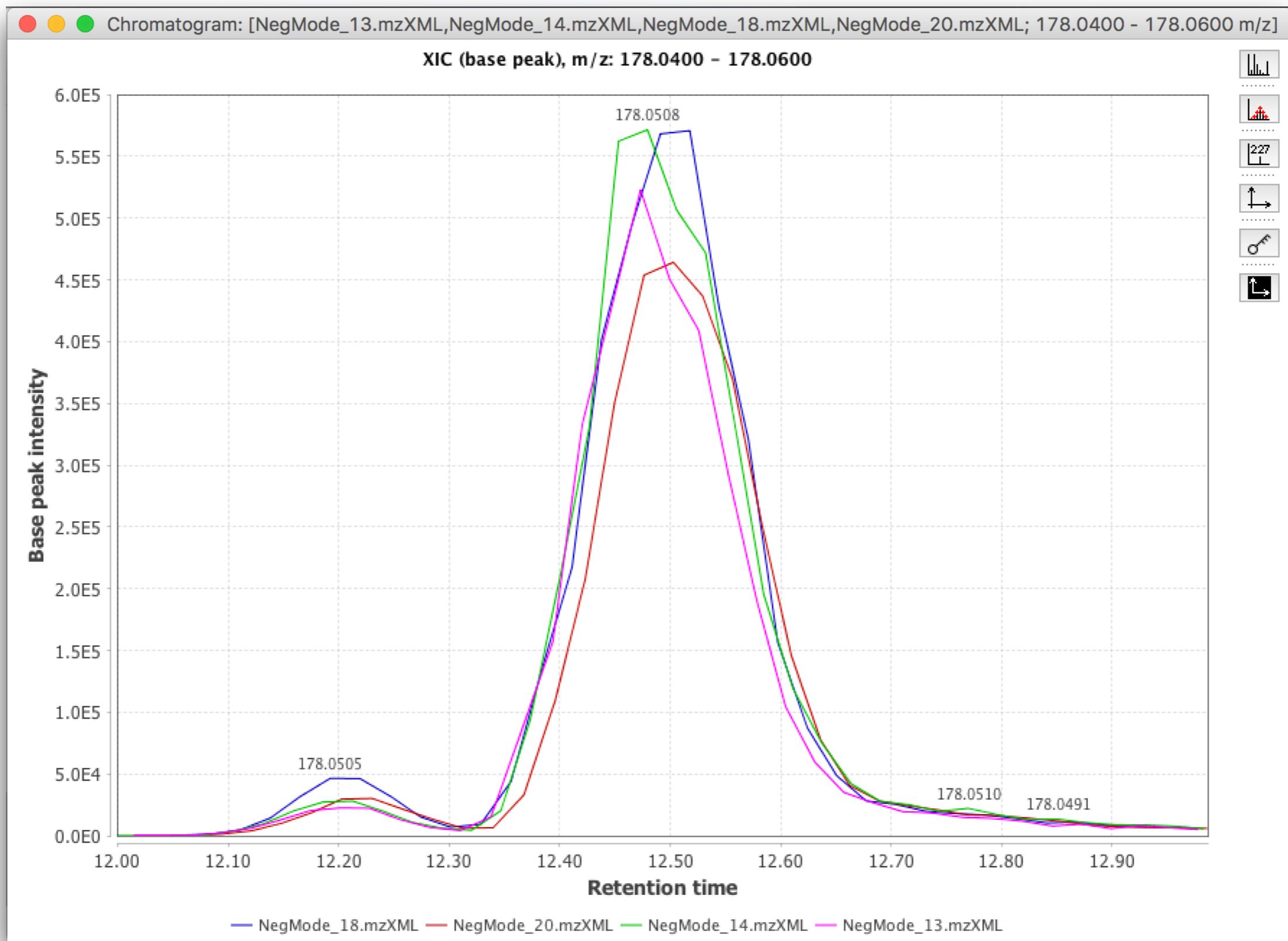
Data visualization: 2D



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 top menu bar includes Project, Raw data methods, Peak list methods, Visualization, Windows, Help, and various system icons. The 'Raw data methods' menu is open, showing options like Raw data import, Raw data export, Order raw data files, Filtering, Peak detection, and Mass detection. The 'Mass detection' option is highlighted with a blue selection bar. A tooltip for 'Mass detection' states: "This module detects individual ions in each scan and builds a mass list for each scan." On the left, a sidebar lists 'Raw data files' with entries: NegMode_18.mzXML, NegMode_20.mzXML, NegMode_14.mzXML, and NegMode_13.mzXML. At the bottom, a status bar shows the message "[9:30:21 AM]: Processing of task Updating TIC visualizer of NegMode_13.mzXML done, status FINISHED" and a free memory indicator of 953MB.

MZmine 2 Project Raw data methods Peak list methods Visualization Windows Help S 68%

Raw data files

- NegMode_18.mzXML
- NegMode_20.mzXML
- NegMode_14.mzXML
- NegMode_13.mzXML

Raw data import
Raw data export
Order raw data files
Filtering
Peak detection
Mass detection

FTMS shoulder peaks filter
Chromatogram builder
ADAP Chromatogram builder
GridMass - 2D peak detection
MS/MS peaklist builder
Targeted peak detection

This module detects individual ions in each scan and builds a mass list for each scan.

MZmine 2.33: New project

Peak lists

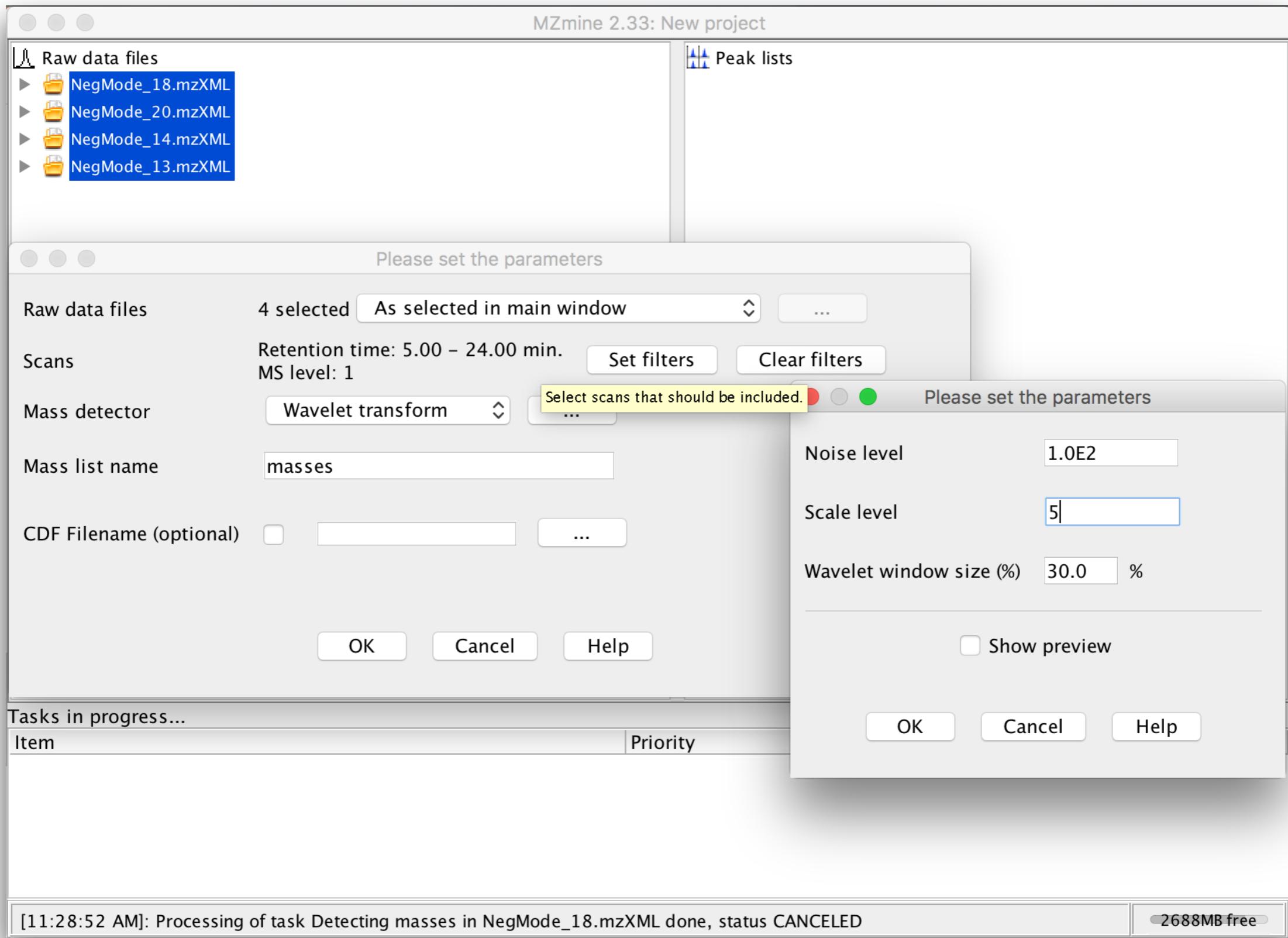
Tasks in progress...

Item	Priority	Status	% done
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[9:30:21 AM]: Processing of task Updating TIC visualizer of NegMode_13.mzXML done, status FINISHED

953MB free

Mass detection



Mass detection

MZmine 2.33: New project

The screenshot shows the MZmine 2.33 software interface. At the top, there are three colored window control buttons (red, yellow, green). The title bar reads "MZmine 2.33: New project". The main workspace is divided into two sections: "Raw data files" on the left and "Peak lists" on the right. The "Raw data files" section contains four entries, each with a folder icon and a file name: "NegMode_18.mzXML", "NegMode_20.mzXML", "NegMode_14.mzXML", and "NegMode_13.mzXML". The "Peak lists" section is currently empty. Below the main workspace is a "Tasks in progress..." panel. This panel has a table with four columns: "Item", "Priority", "Status", and "% done". The table lists four tasks, all of which are "NORMAL" priority and in the "PROCESSING" status. Each task also includes a progress bar indicating its completion percentage: NegMode_18.mzXML is at 20%, NegMode_20.mzXML is at 19%, NegMode_14.mzXML is at 19%, and NegMode_13.mzXML is at 18%. At the bottom of the screen, a status bar displays the message "[11:30:17 AM]: Started mass detector on NegMode_13.mzXML" on the left and "8768MB free" on the right.

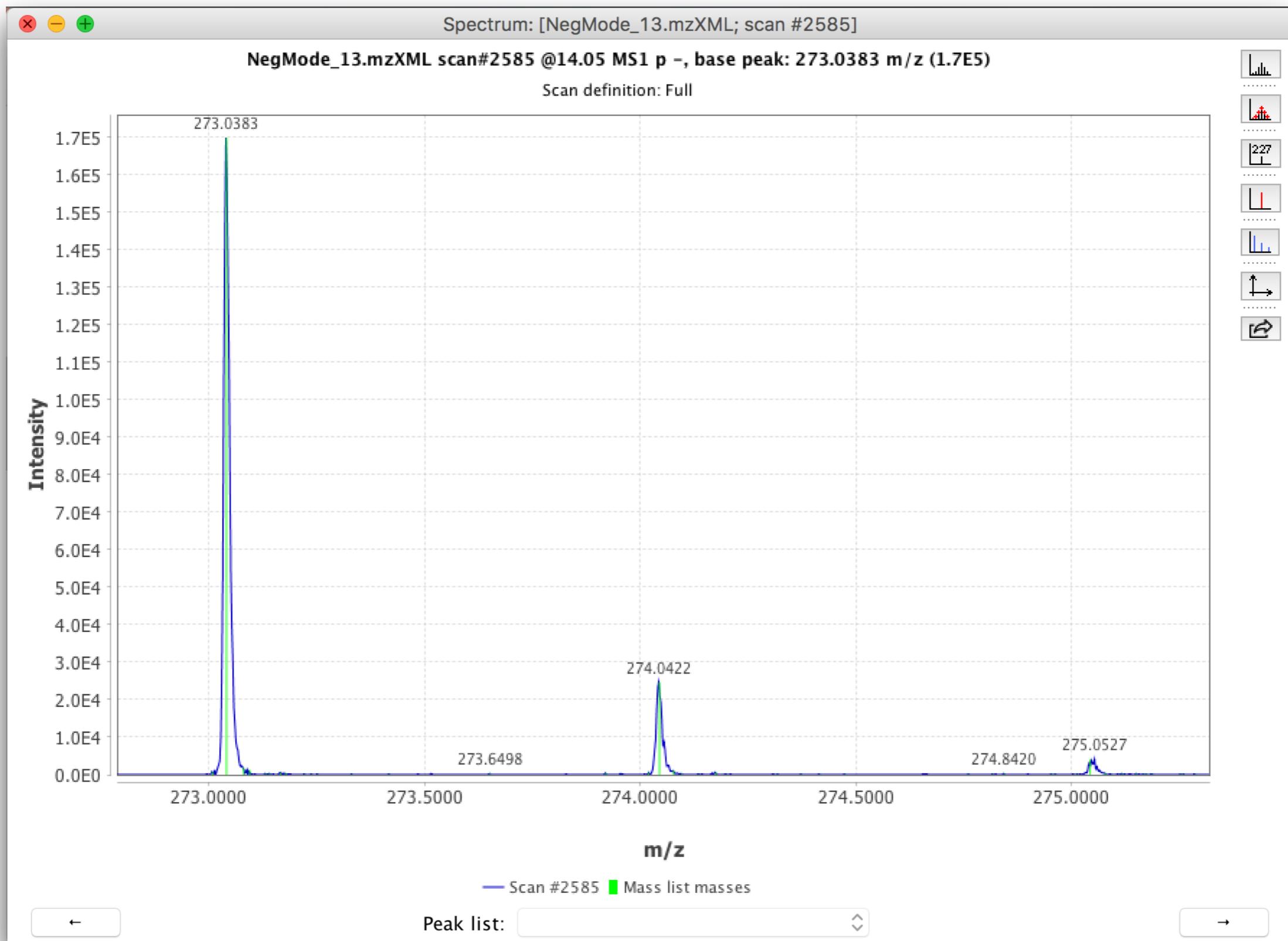
Item	Priority	Status	% done
Detecting masses in NegMode_18.mzXML	NORMAL	PROCESSING	20%
Detecting masses in NegMode_20.mzXML	NORMAL	PROCESSING	19%
Detecting masses in NegMode_14.mzXML	NORMAL	PROCESSING	19%
Detecting masses in NegMode_13.mzXML	NORMAL	PROCESSING	18%

[11:30:17 AM]: Started mass detector on NegMode_13.mzXML 8768MB free

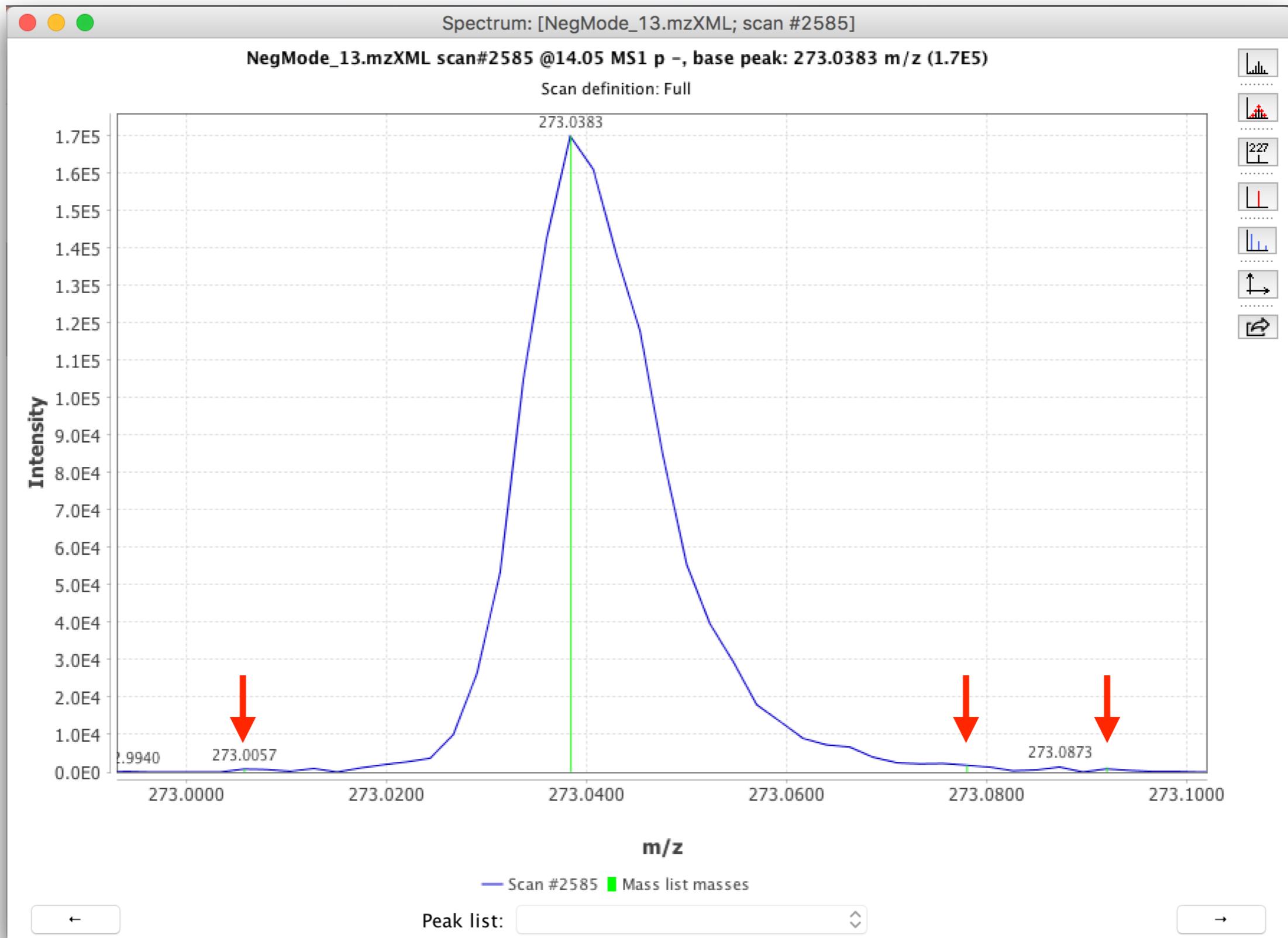
Mass detection



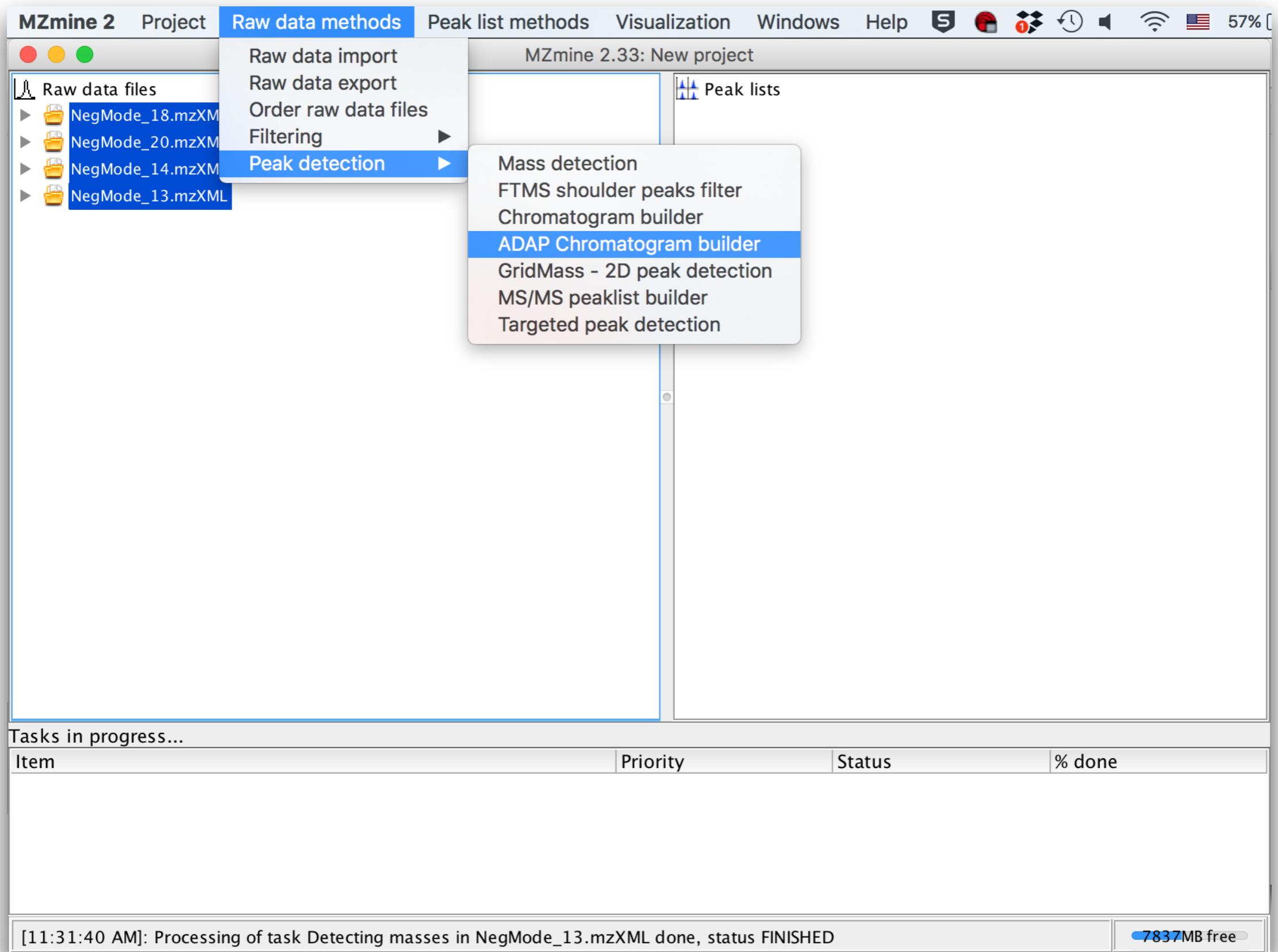
Mass detection



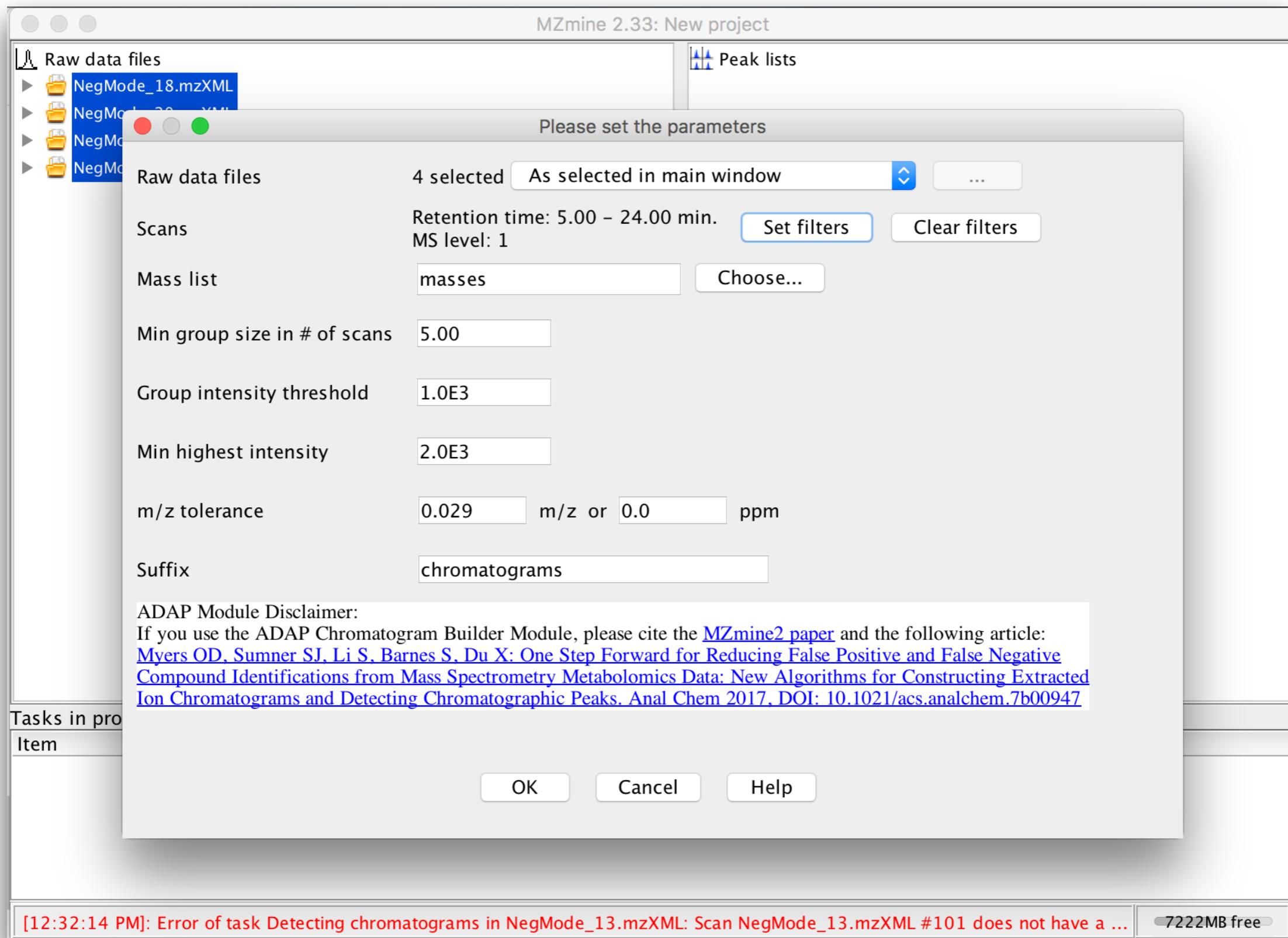
Mass detection



EIC construction



EIC construction



EIC construction

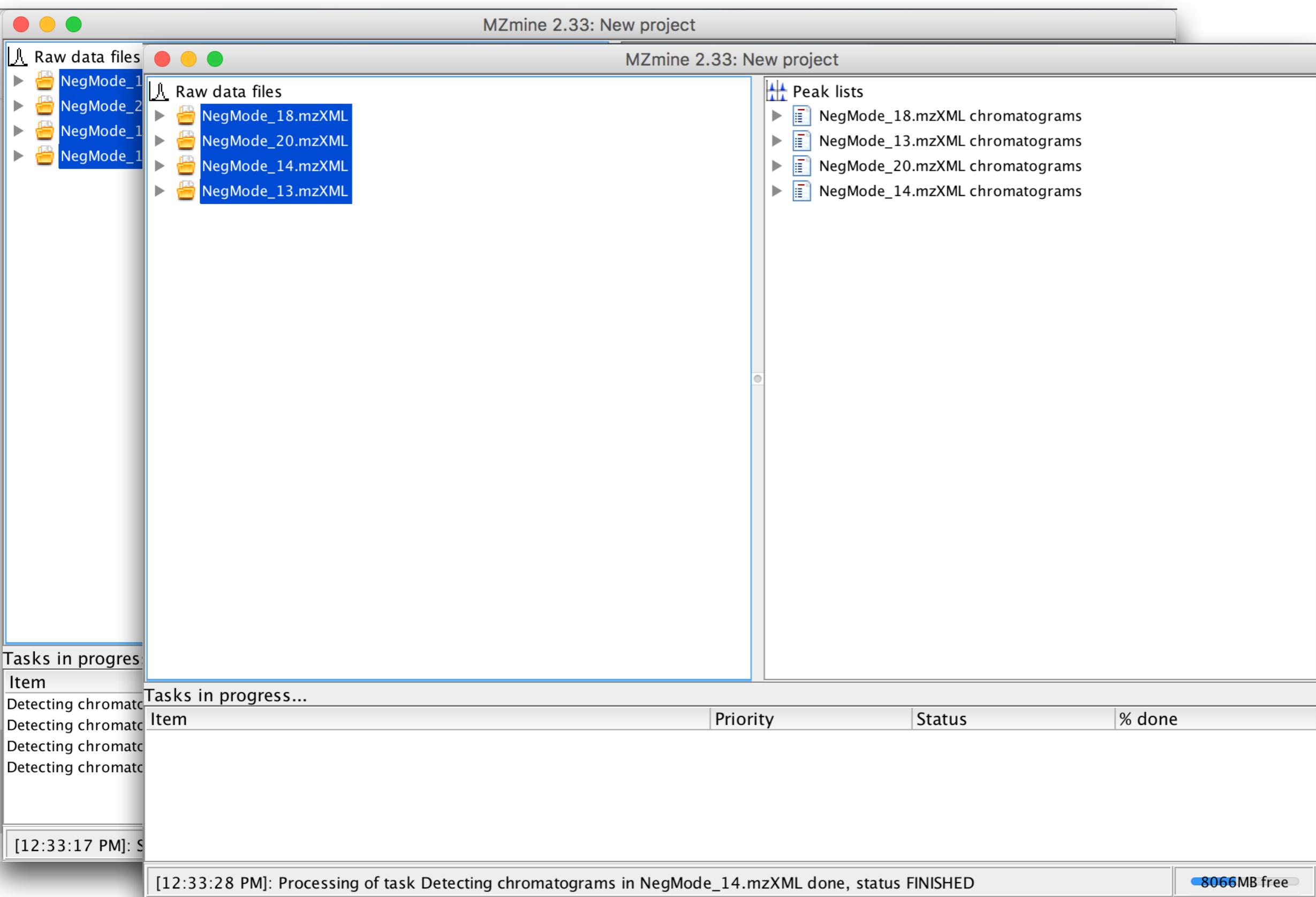
MZmine 2.33: New project

The screenshot shows the MZmine 2.33 software interface with the following sections:

- Raw data files:** Contains four entries: NegMode_18.mzXML, NegMode_20.mzXML, NegMode_14.mzXML, and NegMode_13.mzXML.
- Peak lists:** An empty list.
- Tasks in progress...** A table showing the status of chromatogram detection for each file:

Item	Priority	Status	% done
Detecting chromatograms in NegMode_18.mzXML	NORMAL	PROCESSING	100%
Detecting chromatograms in NegMode_20.mzXML	NORMAL	PROCESSING	97%
Detecting chromatograms in NegMode_14.mzXML	NORMAL	PROCESSING	57%
Detecting chromatograms in NegMode_13.mzXML	NORMAL	PROCESSING	85%
- System status:** Shows the message "[12:33:17 PM]: Started chromatogram builder on NegMode_13.mzXML" and a free memory indicator of 8335 MB.

EIC construction



EIC construction

MZmine 2.33: New project

MZmine 2.33: New project

MZmine 2.33: New project

Raw data files

- NegMode_1
- NegMode_2
- NegMode_1
- NegMode_1

Raw data files

- NegMode_1
- NegMode_2
- NegMode_1
- NegMode_1

Raw data files

- NegMode_18.mzXML
- NegMode_20.mzXML
- NegMode_14.mzXML
- NegMode_13.mzXML

Peak lists

- NegMode_18.mzXML chromatograms
 - #1 61.9903 m/z @11.97
 - #2 74.0270 m/z @13.47
 - #3 75.0102 m/z @5.27
 - #4 88.9895 m/z @6.09
 - #5 91.0023 m/z @12.92
 - #6 93.0349 m/z @11.78
 - #7 97.0655 m/z @11.97
 - #8 103.0403 m/z @7.90
 - #9 107.0510 m/z @13.76
 - #10 108.0448 m/z @12.84
 - #11 109.0289 m/z @12.25
 - #12 111.0826 m/z @13.92
 - #13 112.9848 m/z @17.33
 - #14 113.0613 m/z @11.44
 - #15 115.0755 m/z @12.02
 - #16 116.0498 m/z @15.57
 - #17 117.0202 m/z @7.18
 - #18 117.0554 m/z @8.89
 - #19 118.0305 m/z @15.57
 - #20 119.0493 m/z @14.00
 - #21 120.0557 m/z @14.03
 - #22 121.0290 m/z @13.65

Tasks in progress:

Item	Priority	Status	% done
Detecting chromatograms in NegMode_18.mzXML			
Detecting chromatograms in NegMode_20.mzXML			
Detecting chromatograms in NegMode_14.mzXML			
Detecting chromatograms in NegMode_13.mzXML			

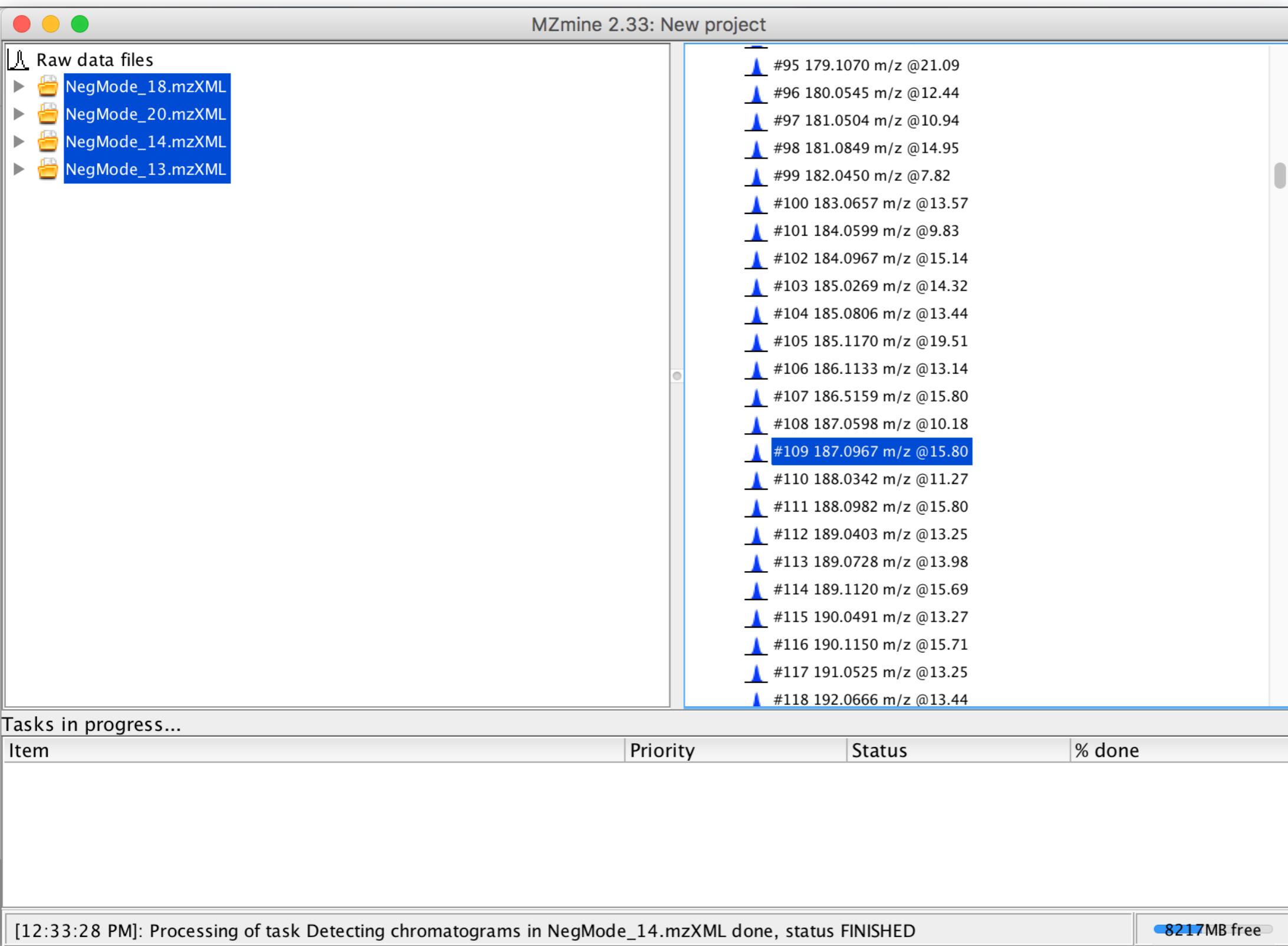
[12:33:17 PM]: S

[12:33:28 PM]: P

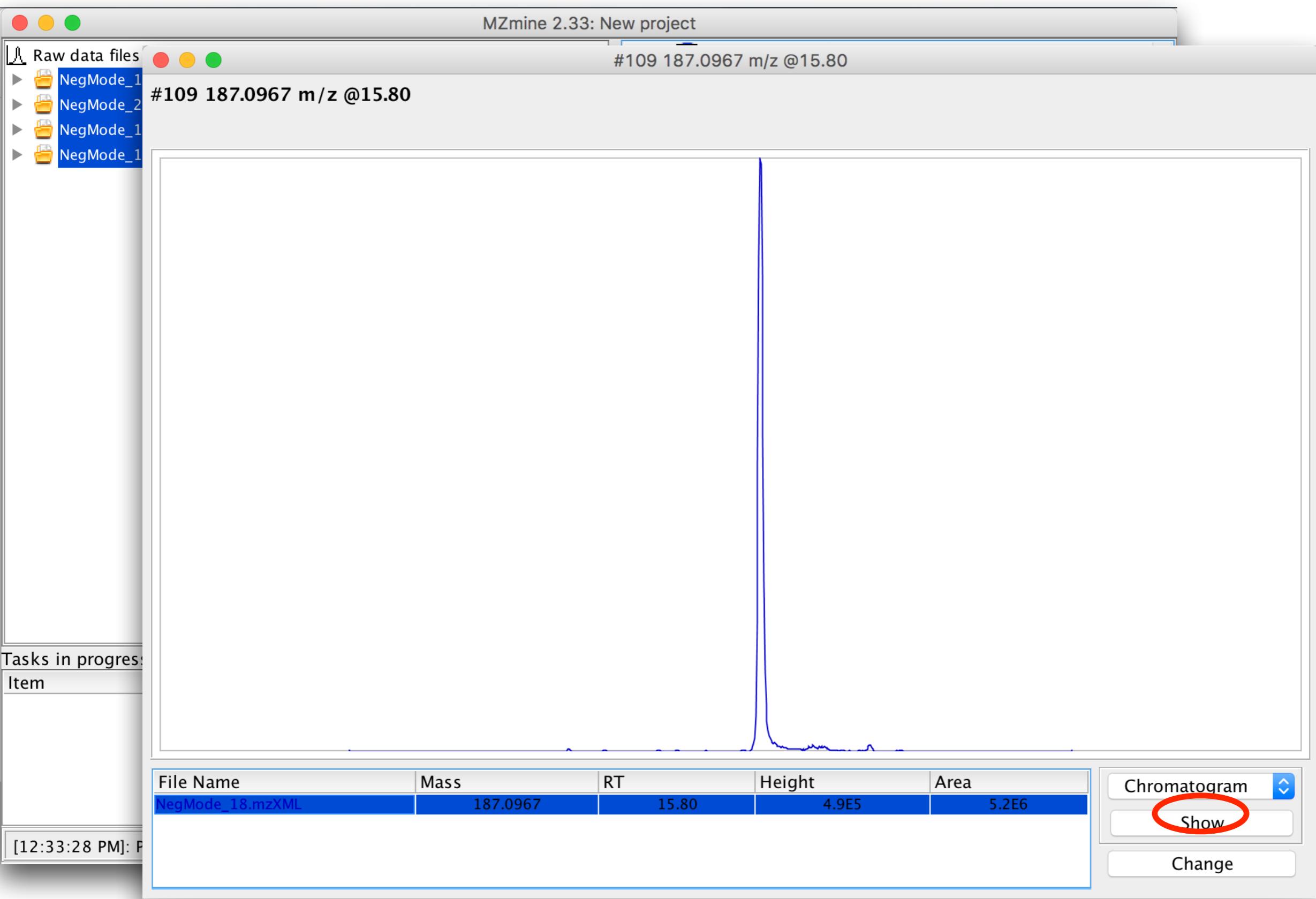
[12:33:28 PM]: Processing of task Detecting chromatograms in NegMode_14.mzXML done, status FINISHED

7969MB free

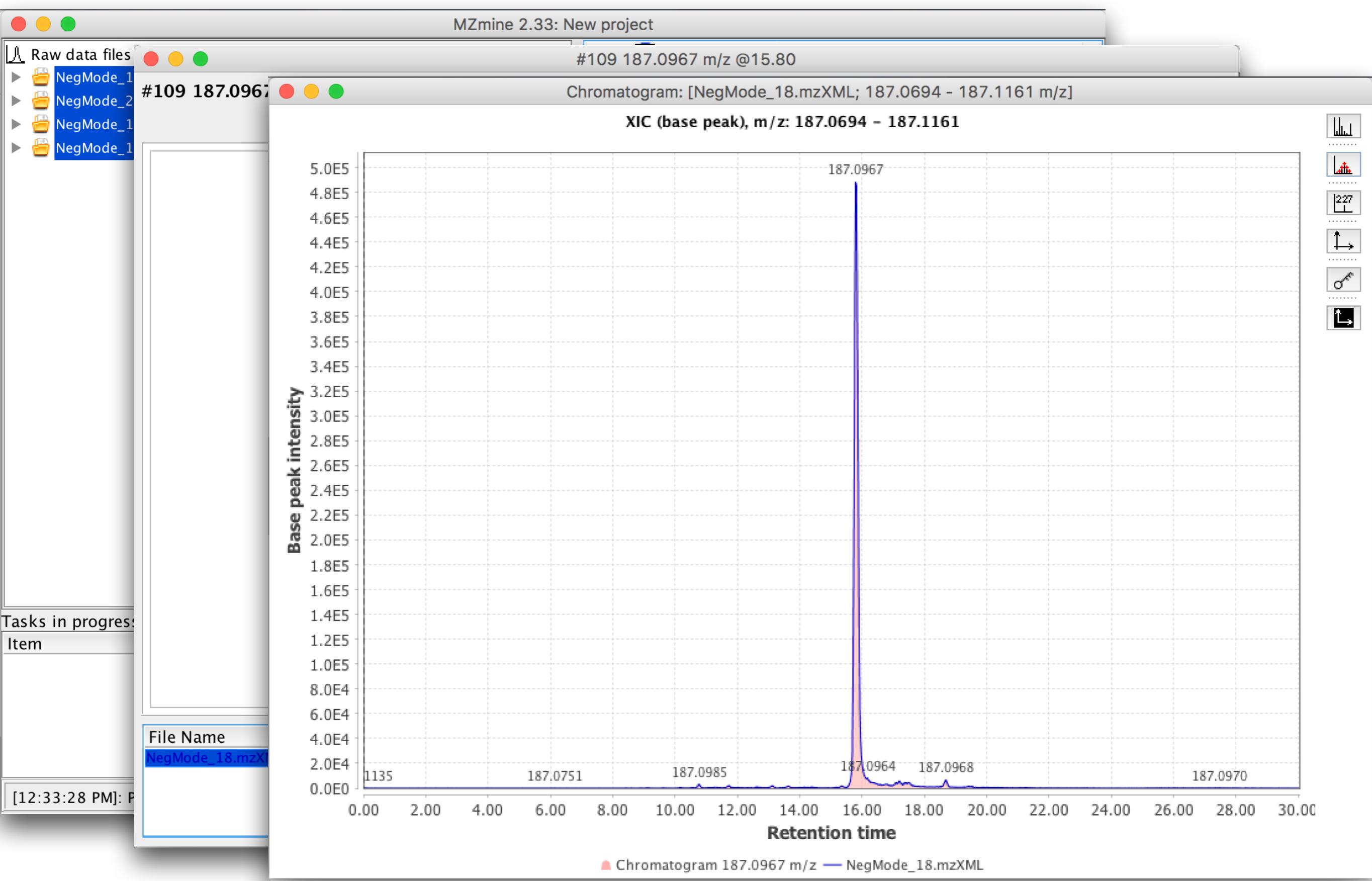
EIC construction



EIC construction



EIC construction



EIC peak detection

MZmine 2 Project Raw data methods Peak list methods Visualization Windows Help S 70% [

Raw data files

- NegMode_18.mzXML
- NegMode_20.mzXML
- NegMode_14.mzXML
- NegMode_13.mzXML

Peak list methods

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

Peak detection

- Smoothing
- Chromatogram deconvolution
- Peak shape modeler (experimental)
- Peak extender

NegMode_14.mzXML chromatograms

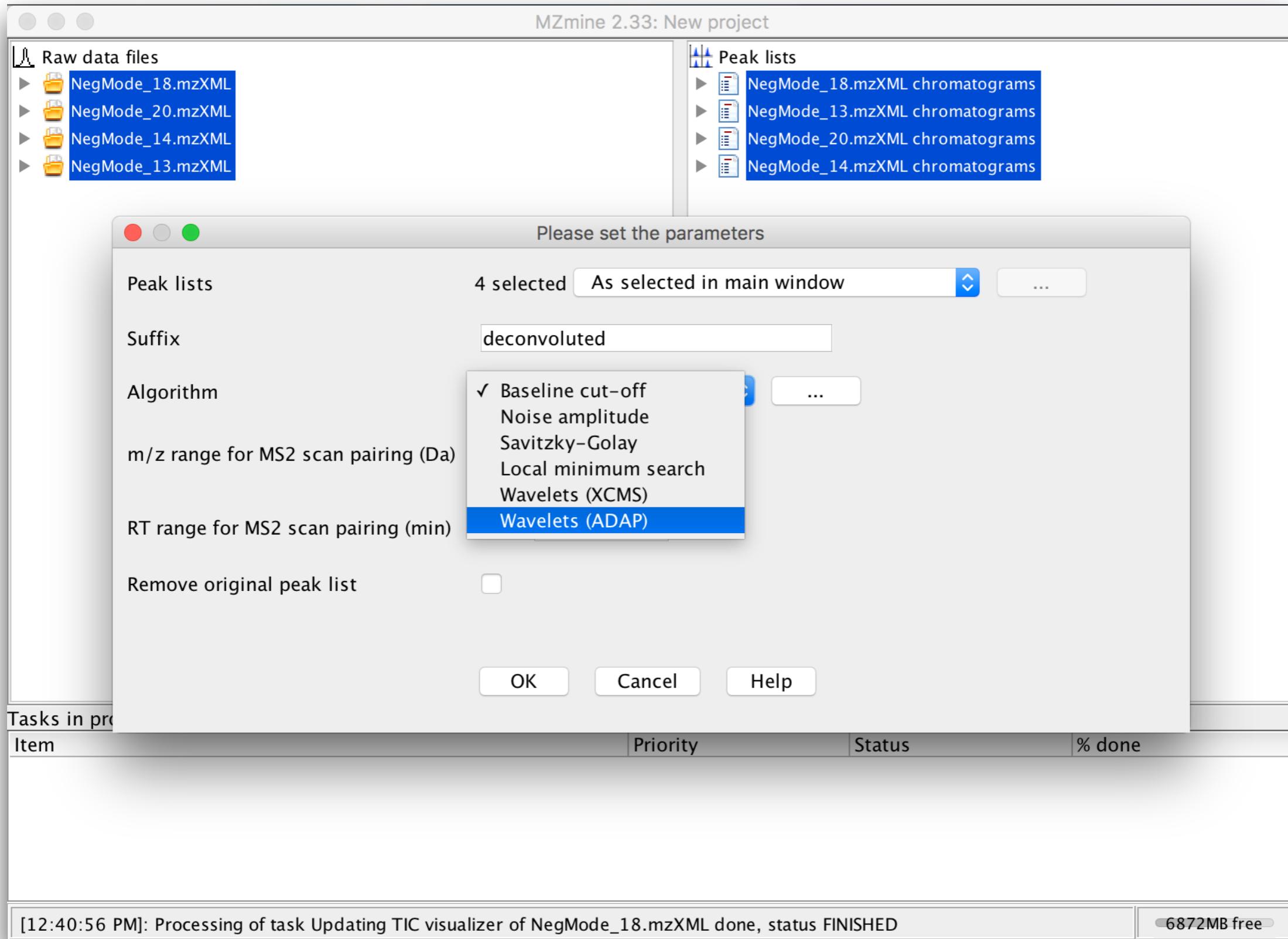
Tasks in progress...

Item	Priority	Status	% done

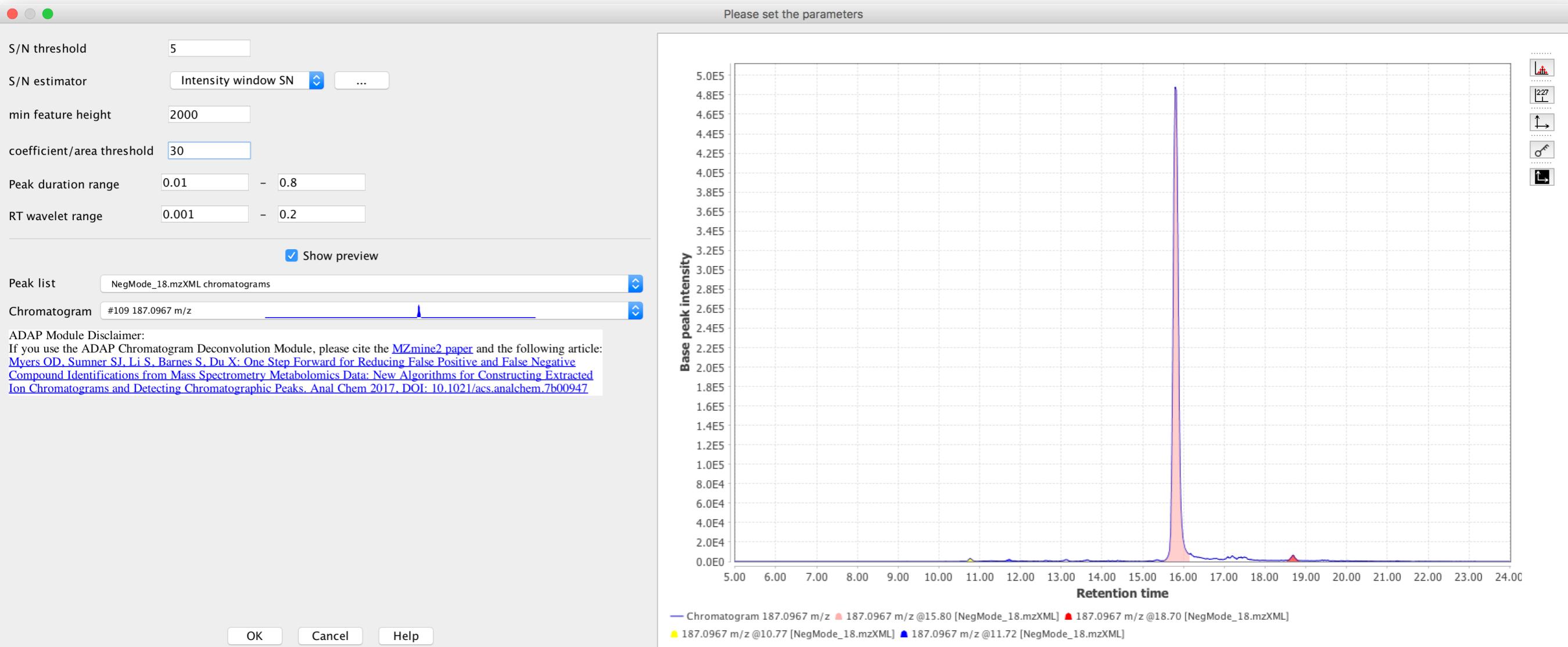
[12:40:56 PM]: Processing of task Updating TIC visualizer of NegMode_18.mzXML done, status FINISHED

7030MB free

EIC peak detection



EIC peak detection



EIC peak detection

MZmine 2.33: New project

The screenshot shows the MZmine 2.33 software interface with the following sections:

- Raw data files:** Contains four entries: NegMode_18.mzXML, NegMode_20.mzXML, NegMode_14.mzXML, and NegMode_13.mzXML.
- Peak lists:** Contains four entries: NegMode_18.mzXML chromatograms, NegMode_13.mzXML chromatograms, NegMode_20.mzXML chromatograms, and NegMode_14.mzXML chromatograms.
- Tasks in progress...**: A table showing four tasks, all labeled "Peak recognition on ... chromatograms" and set to "NORMAL" priority, all in "PROCESSING" status with a progress bar indicating completion percentages of 19%, 18%, 17%, and 16% respectively.
- System status:** At the bottom, it says "[12:53:27 PM]: Started peak deconvolution on NegMode_14.mzXML chromatograms" and shows "6229MB free".

EIC peak detection

MZmine 2.33: New project

The screenshot shows the MZmine 2.33 software interface. On the left, under 'Raw data files', there are four entries: NegMode_18.mzXML, NegMode_20.mzXML, NegMode_14.mzXML, and NegMode_13.mzXML. On the right, under 'Peak lists', there are eight entries: NegMode_18.mzXML chromatograms, NegMode_13.mzXML chromatograms, NegMode_20.mzXML chromatograms, NegMode_14.mzXML chromatograms, NegMode_18.mzXML chromatograms deconvoluted, NegMode_13.mzXML chromatograms deconvoluted, NegMode_20.mzXML chromatograms deconvoluted, and NegMode_14.mzXML chromatograms deconvoluted. The last four items in each list are highlighted with a blue border. At the bottom, a 'Tasks in progress...' section is empty. A status bar at the bottom indicates '[12:54:19 PM]: Processing of task Peak recognition on NegMode_14.mzXML chromatograms done, status FINISHED' and '7862MB free'.

Raw data files

- NegMode_18.mzXML
- NegMode_20.mzXML
- NegMode_14.mzXML
- NegMode_13.mzXML

Peak lists

- NegMode_18.mzXML chromatograms
- NegMode_13.mzXML chromatograms
- NegMode_20.mzXML chromatograms
- NegMode_14.mzXML chromatograms
- NegMode_18.mzXML chromatograms deconvoluted
- NegMode_13.mzXML chromatograms deconvoluted
- NegMode_20.mzXML chromatograms deconvoluted
- NegMode_14.mzXML chromatograms deconvoluted

Tasks in progress...

Item	Priority	Status	% done
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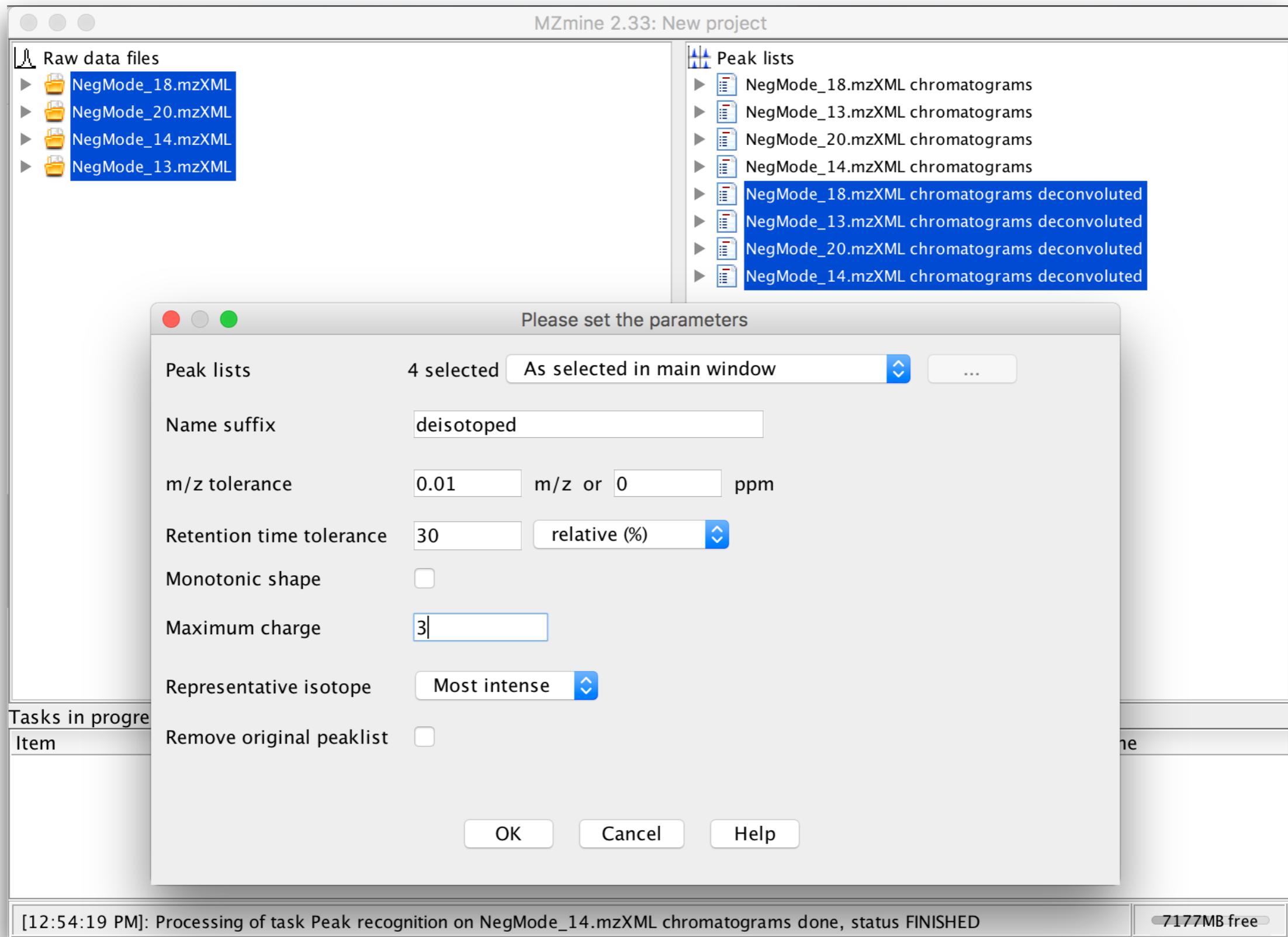
[12:54:19 PM]: Processing of task Peak recognition on NegMode_14.mzXML chromatograms done, status FINISHED

7862MB free

Isotopic grouper parameters

The screenshot shows the MZmine 2 software interface. The top 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, displaying various sub-modules: Order peak lists, Peak detection, Spectral deconvolution, Gap filling, Isotopes (selected), Filtering, Alignment, Normalization, Identification, Data analysis, and Export/Import. A tooltip for the 'Isotopes' module states: 'This module detects isotopic peak lists and groups them together into isotope patterns'. On the left, a sidebar shows 'Raw data files' with four entries: NegMode_18.mzXML, NegMode_20.mzXML, NegMode_14.mzXML, and NegMode_13.mzXML. Below the main window, a 'Tasks in progress...' section is shown, which is currently empty. At the bottom, a status bar displays the message '[12:54:19 PM]: Processing of task Peak recognition on NegMode_14.mzXML chromatograms done, status FINISHED' and '7405MB free'.

Isotopic grouper parameters



Isotopic grouper parameters

MZmine 2 Project Raw data methods Peak list methods Visualization Windows Help S ⚡ ⏱ 🔍 79%

MZmine 2.33: New project

The screenshot shows the MZmine 2 software interface. The top menu bar includes Project, Raw data methods, Peak list methods, Visualization, Windows, Help, and various system icons. The main window title is "MZmine 2.33: New project". On the left, under "Raw data files", there are four entries: NegMode_18.mzXML, NegMode_20.mzXML, NegMode_14.mzXML, and NegMode_13.mzXML. On the right, under "Peak lists", there are several chromatogram and deconvoluted chromatogram entries for each raw data file, with the last one for NegMode_14.mzXML highlighted. A "Tasks in progress..." section at the bottom shows a table with columns for Item, Priority, Status, and % done, which is currently empty. The status bar at the bottom indicates "[1:20:10 PM]: Processing of task Isotopic peaks grouper on NegMode_14.mzXML chromatograms deconvoluted done, status FINIS... 5819MB free".

Raw data files

- NegMode_18.mzXML
- NegMode_20.mzXML
- NegMode_14.mzXML
- NegMode_13.mzXML

Peak lists

- NegMode_18.mzXML chromatograms
- NegMode_13.mzXML chromatograms
- NegMode_20.mzXML chromatograms
- NegMode_14.mzXML chromatograms
- NegMode_18.mzXML chromatograms deconvoluted
- NegMode_13.mzXML chromatograms deconvoluted
- NegMode_20.mzXML chromatograms deconvoluted
- NegMode_14.mzXML chromatograms deconvoluted**
- NegMode_18.mzXML chromatograms deconvoluted deisotoped
- NegMode_13.mzXML chromatograms deconvoluted deisotoped
- NegMode_20.mzXML chromatograms deconvoluted deisotoped
- NegMode_14.mzXML chromatograms deconvoluted deisotoped

Tasks in progress...

Item	Priority	Status	% done
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[1:20:10 PM]: Processing of task Isotopic peaks grouper on NegMode_14.mzXML chromatograms deconvoluted done, status FINIS... 5819MB free

Alignment parameters

Please set the parameters

Peak lists 7 selected ...

Peak list name

m/z tolerance m/z or ppm

RT tolerance absolute (min)

RT tolerance after correction absolute (min)

RANSAC iterations

Minimum number of points %

Threshold value

Linear model

Require same charge state

Show preview of RANSAC alignment