

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

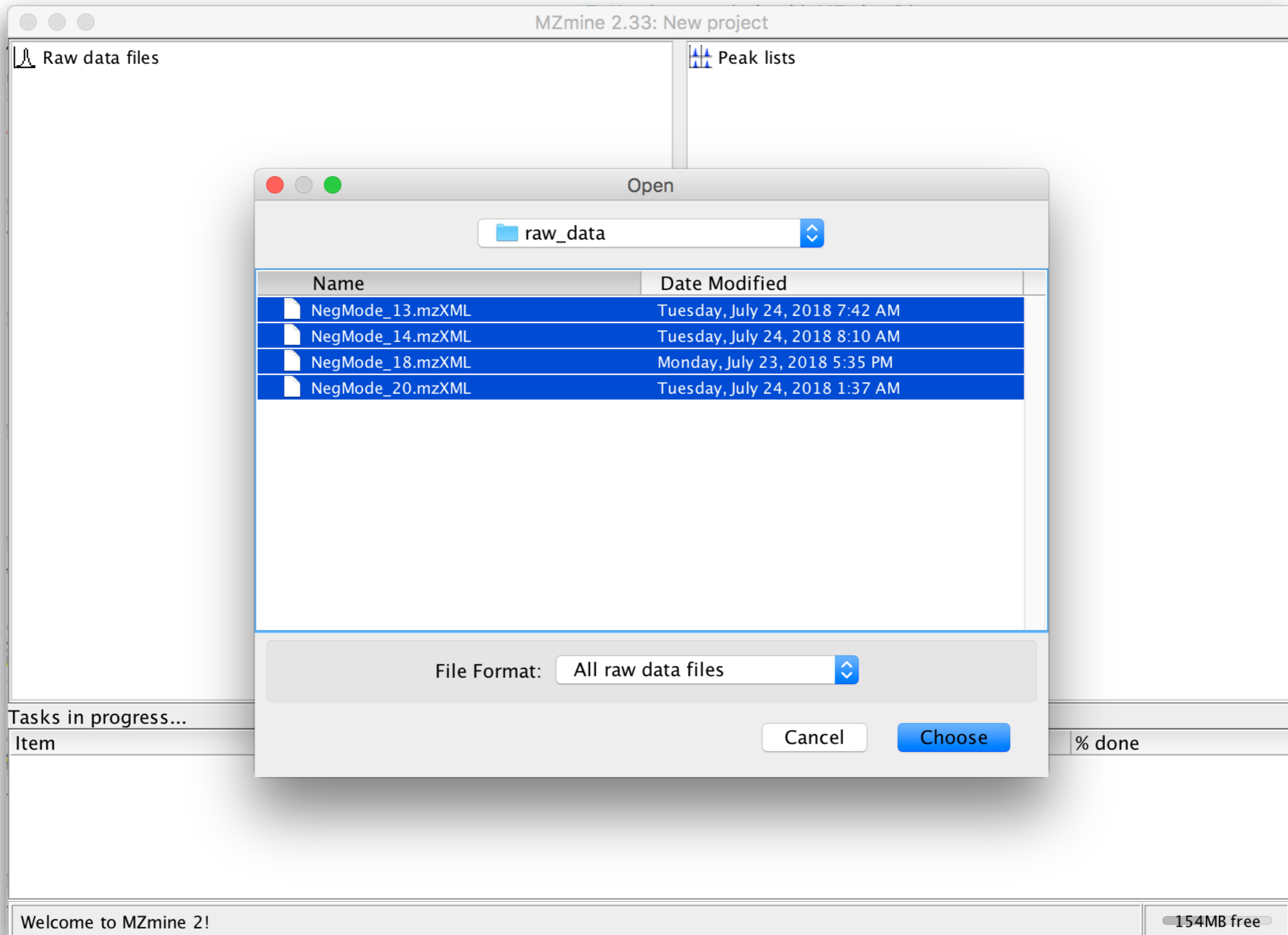
Data import

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 'Raw data methods' menu is open, showing options: 'Raw data import' (highlighted), 'Raw data export', 'Order raw data files', 'Filtering', and 'Peak detection'. The main workspace is split into two panes: 'Raw data files' on the left and 'Peak lists' on the right. A tooltip above the 'Peak lists' pane reads 'This module imports raw data into the project.' At the bottom, there is a 'Tasks in progress...' table and a status bar.

Tasks in progress...			
Item	Priority	Status	% done

Welcome to MZmine 2! 220MB free

Data import



Data import

The screenshot shows the MZmine 2.33: New project window. The interface is split into two main panels. The left panel, titled 'Raw data files', contains a list of four mzXML files: NegMode_18.mzXML, NegMode_20.mzXML, NegMode_14.mzXML, and NegMode_13.mzXML. The right panel, titled 'Peak lists', is currently empty. Below these panels is a 'Tasks in progress...' section with a table. The table has four columns: 'Item', 'Priority', 'Status', and '% done'. The table is currently empty. At the bottom of the window, a status bar shows the time [9:24:51 AM], the current task 'Processing of task Opening file /Users/xdu4/Documents/Duxiuxia/Analysis/UAB_workshop_2018/raw_data/NegMod...', and a memory usage indicator showing 839MB free.

Item	Priority	Status	% done
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[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

The screenshot displays the MZmine 2 software interface. The top menu bar includes 'MZmine 2', 'Project', 'Raw data methods', 'Peak list methods', 'Visualization', 'Windows', and 'Help'. The 'Visualization' menu is open, showing 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'. The left sidebar shows 'Raw data files' with four files: 'NegMode_18.mzXML', 'NegMode_20.mzXML', 'NegMode_14.mzXML', and 'NegMode_13.mzXML'. The bottom status bar shows a task in progress: '[9:24:51 AM]: Processing of task Opening file /Users/xdu4/Documents/Duxiuxia/Analysis/UAB_workshop_2018/raw_data/NegMod...' with a progress indicator for '494MB free'.

Item	Priority	Status	% done

Data visualization: BIC

MZmine 2.33: New project

Raw data files

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

Peak lists

Please set the parameters

Raw data files 4 selected As selected in main window

Scans MS level: 1 Set filters Clear filters

Plot type Base peak intensity

m/z 49.9907 - 800.0076 Auto range From mass From formula

Peaks All Clear

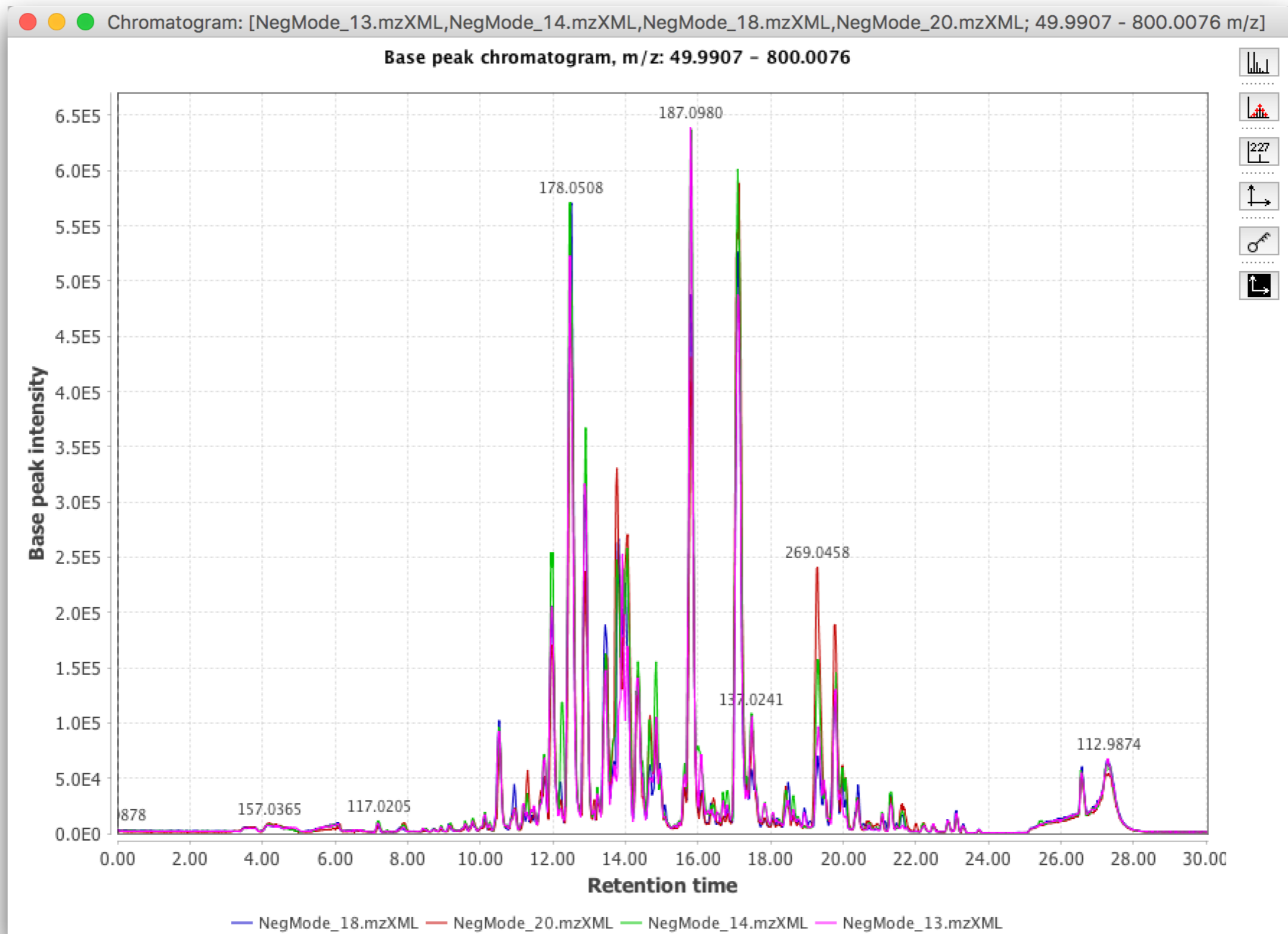
OK Cancel Help

Tasks in progress...

Item	Priority	Status	% done
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[9:24:51 AM]: Processing of task Opening file /Users/xdu4/Documents/Duxiuxia/Analysis/UAB_workshop_2018/raw_data/NegMod... 368MB free

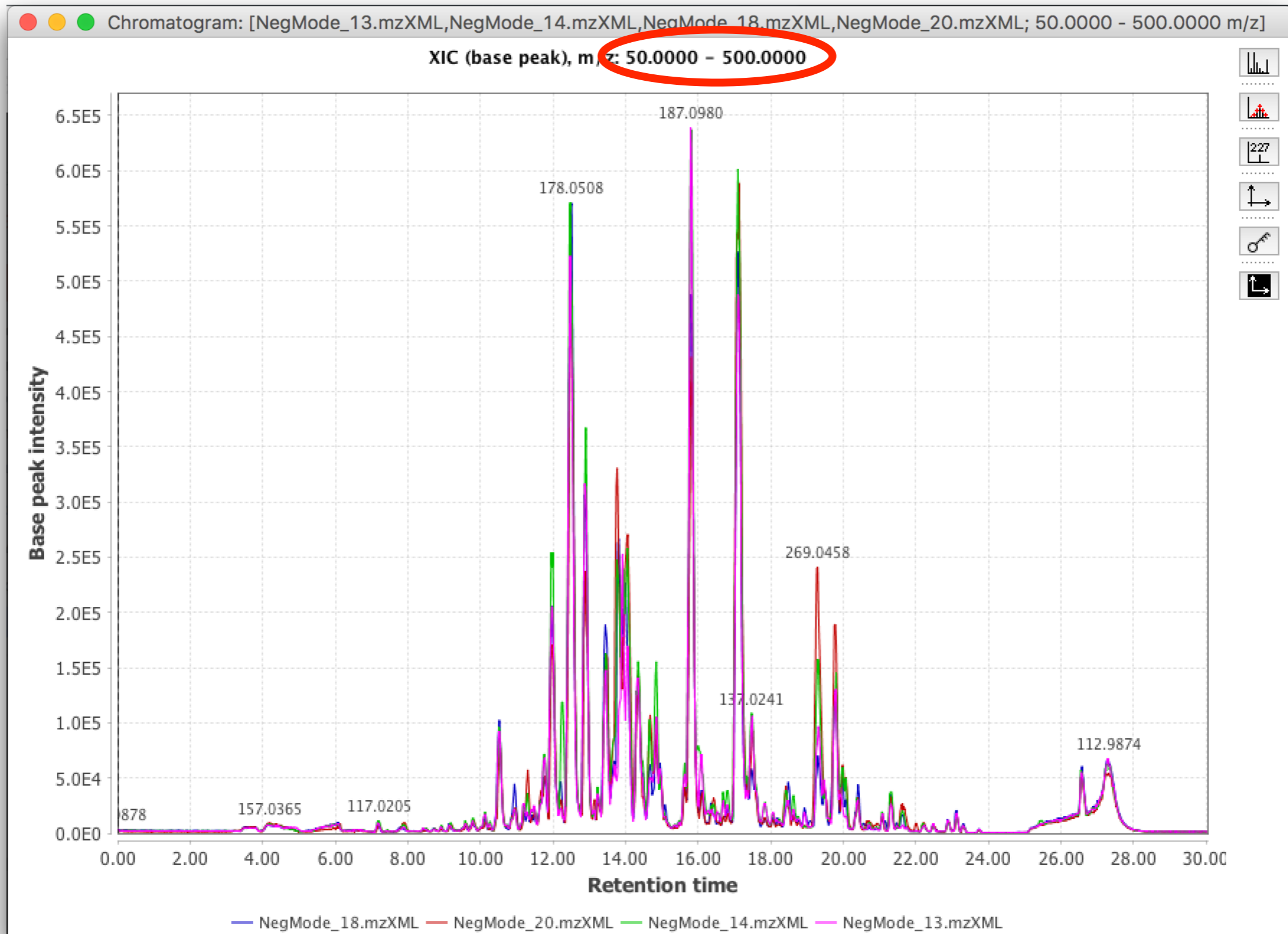
Data visualization: BIC



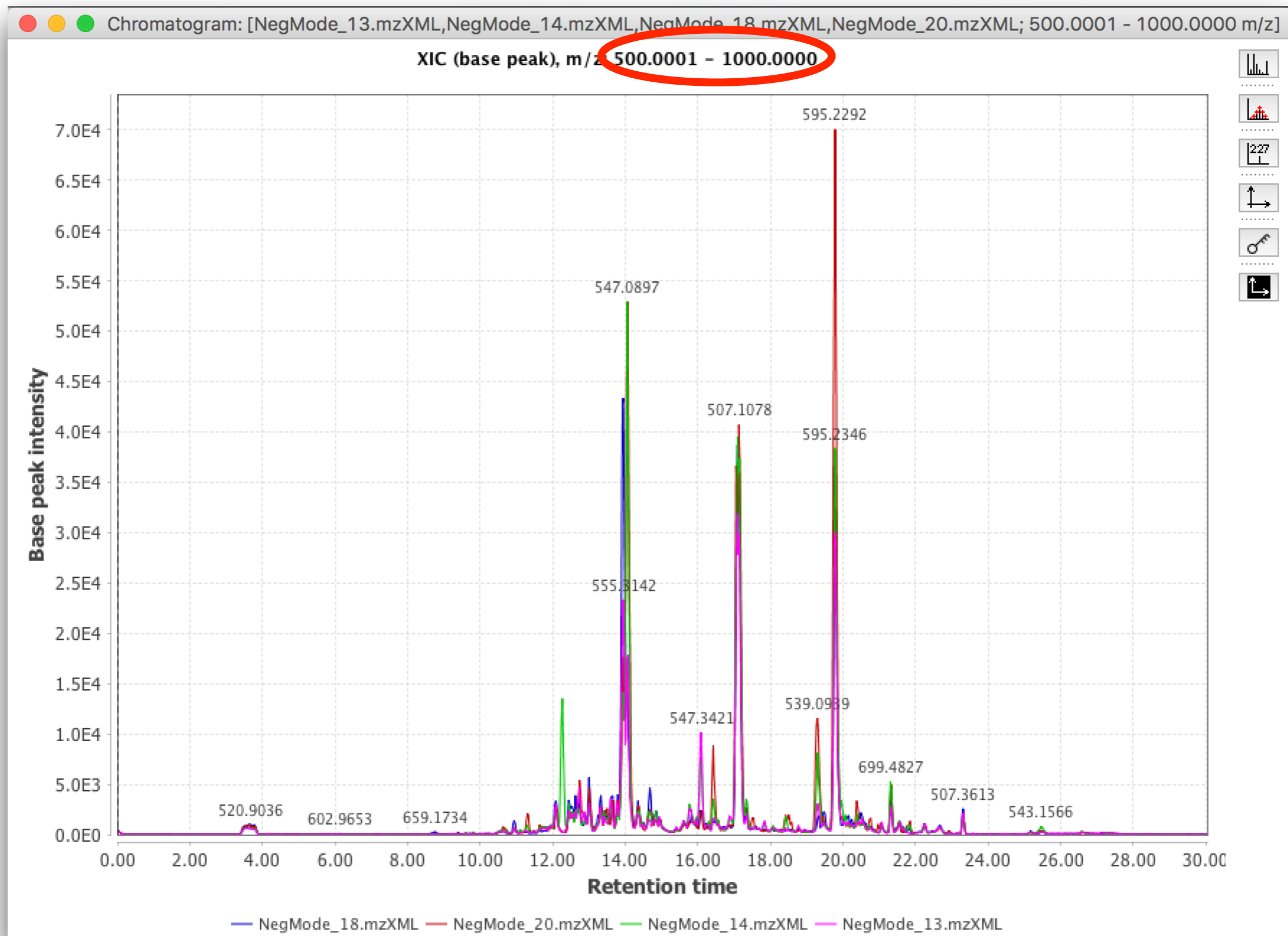
Data visualization: BIC

You can zoom in the BICs and examine them.

Data visualization: BIC



Data visualization: BIC



Data visualization: TIC

The screenshot displays the MZmine 2 software interface. The top menu bar includes 'MZmine 2', 'Project', 'Raw data methods', 'Peak list methods', 'Visualization', 'Windows', and 'Help'. The 'Visualization' menu is open, showing 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'. The 'TIC/XIC visualizer' option is highlighted. On the left, a file explorer shows 'Raw data files' with four files: 'NegMode_18.mzXML', 'NegMode_20.mzXML', 'NegMode_14.mzXML', and 'NegMode_13.mzXML'. The 'NegMode_14.mzXML' file is selected. At the bottom, a task progress table is visible, and a status bar at the very bottom shows a log message: '[10:47:01 AM]: Processing of task Updating TIC visualizer of NegMode_14.mzXML done, status FINISHED' and a memory indicator '8699MB free'.

Tasks in progress...			
Item	Priority	Status	% done

[10:47:01 AM]: Processing of task Updating TIC visualizer of NegMode_14.mzXML done, status FINISHED

8699MB free

Data visualization: TIC

MZmine 2.33: New project

Raw data files

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

Peak lists

Please set the parameters

Raw data files 4 selected As selected in main window

Scans MS level: 1 Set filters Clear filters

Plot type **Total ion current (TIC/XIC)**

m/z 49.9907 - 800.0076 Auto range From mass From formula

Peaks All Clear

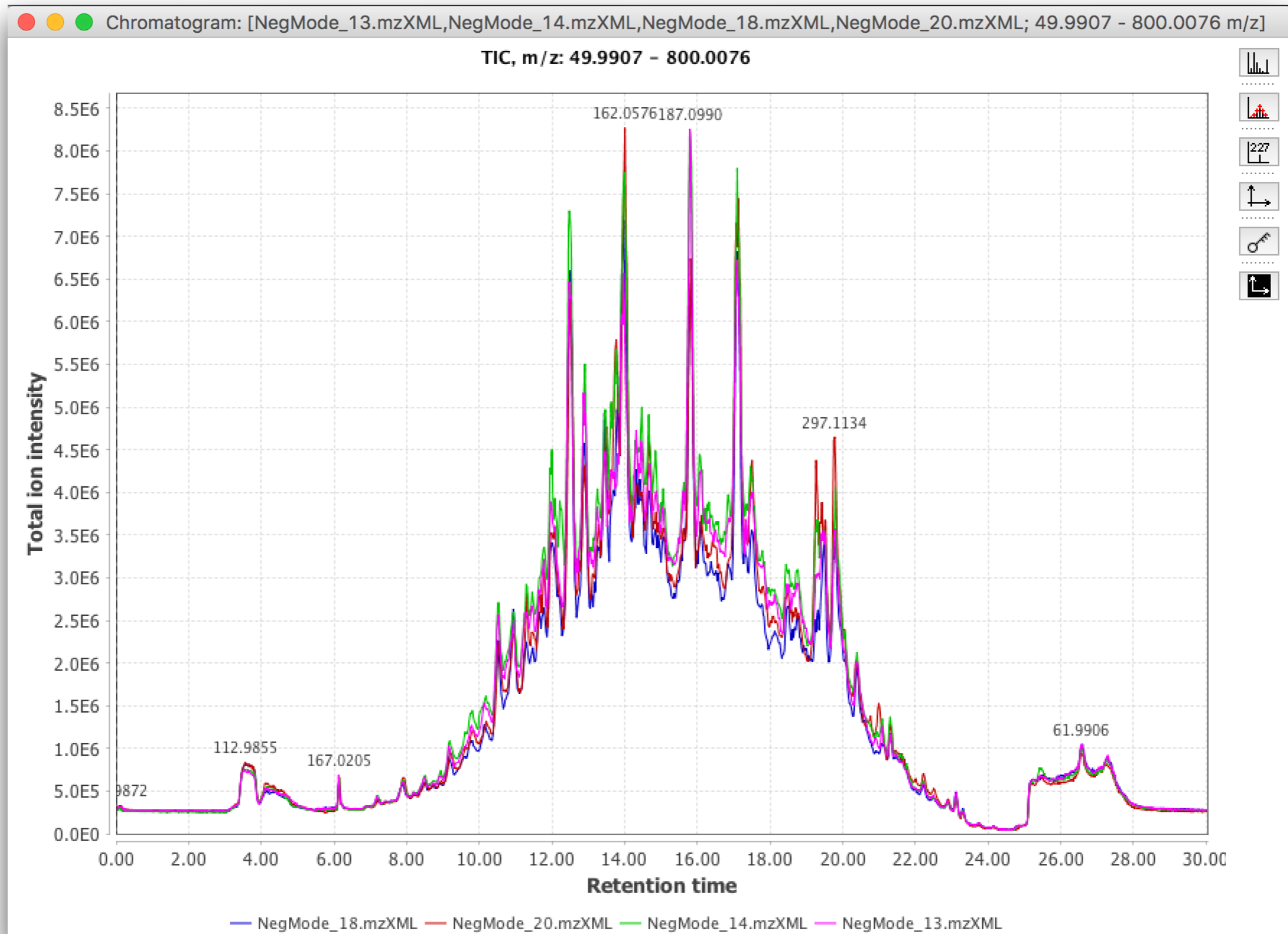
OK Cancel Help

Tasks in progress...

Item	Priority	Status	% done
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[11:00:08 AM]: Processing of task Updating TIC visualizer of NegMode_13.mzXML done, status FINISHED 4679MB free

Data visualization: TIC



Data visualization: 2D

The screenshot shows the MZmine 2 software interface. The menu bar includes 'MZmine 2', 'Project', 'Raw data methods', 'Peak list methods', 'Visualization', 'Windows', and 'Help'. The 'Visualization' menu is open, listing options: 'TIC/XIC visualizer', 'Spectra visualizer', '2D visualizer' (highlighted), '3D visualizer', 'MS/MS visualizer', 'Neutral loss visualizer', 'Scatter plot', 'Histogram plot', 'Peak intensity plot', 'Kendrick mass plot', and 'Van Krevelen Diagram'. The main window displays a file tree under 'Raw data files' with four files: 'NegMode_18.mzXML', 'NegMode_20.mzXML', 'NegMode_14.mzXML', and 'NegMode_13.mzXML'. A status bar at the bottom shows a task log entry: '[9:30:21 AM]: Processing of task Updating TIC visualizer of NegMode_13.mzXML done, status FINISHED' and a memory indicator '501MB free'.

Item	Priority	Status	% done
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Data visualization: 2D

MZmine 2.33: New project

Raw data files

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

Peak lists

Please set the parameters

Type of plot: **Resampled data**

Raw data files: NegMode_18.mzXML As selected in main window

Scans: MS level: 1 Set filters Clear filters

m/z: [] - [] Auto range From mass From formula

OK Cancel Help

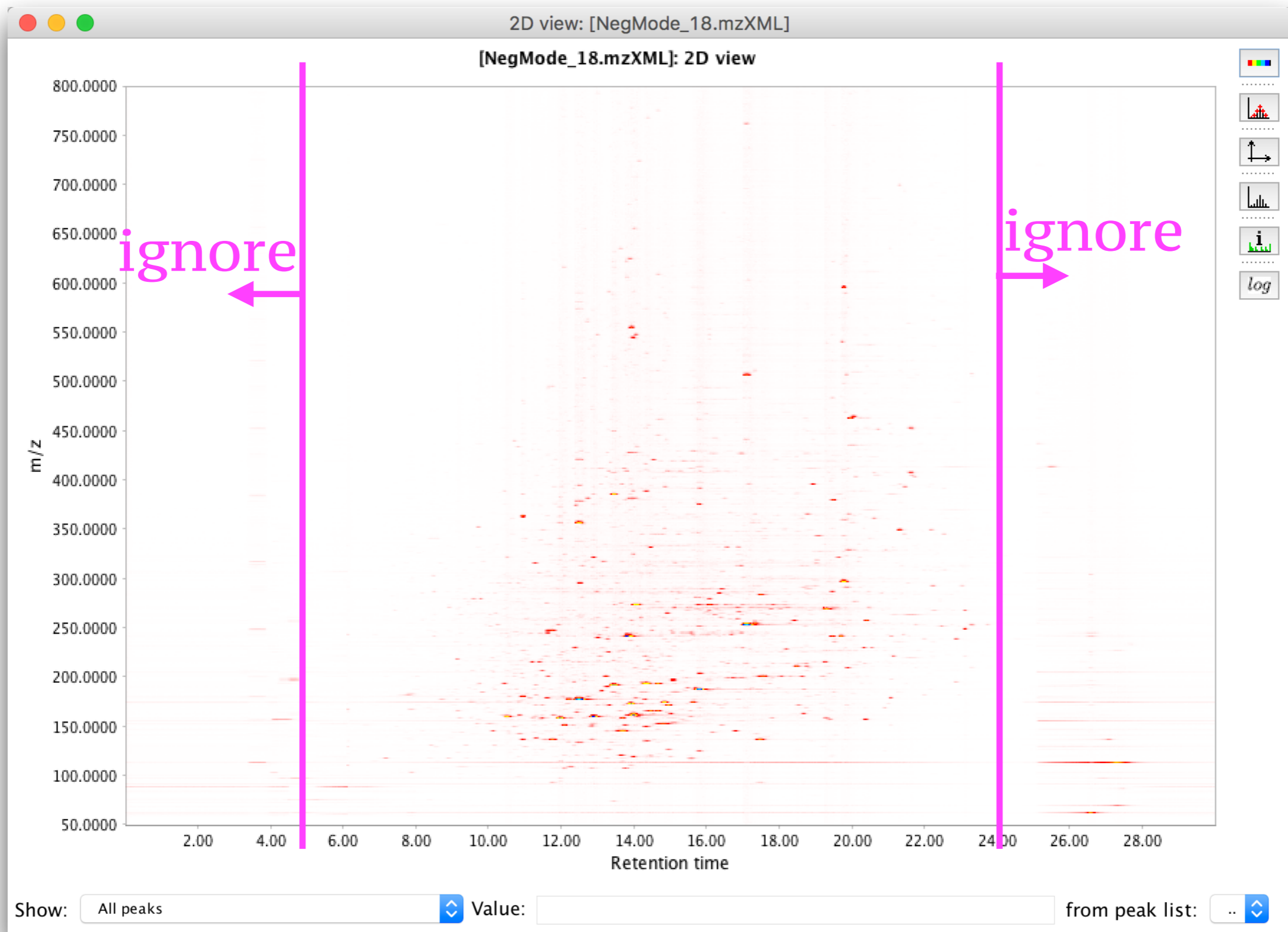
Tasks in progress...

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

616MB free

Data visualization: 2D



Data visualization: 2D

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 'Visualization' menu is open, listing options: TIC/XIC visualizer, Spectra visualizer, 2D visualizer (highlighted), 3D visualizer, MS/MS visualizer, Neutral loss visualizer, Scatter plot, Histogram plot, Peak intensity plot, Kendrick mass plot, and Van Krevelen Diagram. The main window displays a file tree under 'Raw data files' with 'NegMode_13.mzXML' selected. A task progress table is visible at the bottom, and a status bar at the very bottom shows a task completion message and memory usage.

Tasks in progress...			
Item	Priority	Status	% done

[9:42:27 AM]: Processing of task Updating 2D visualizer of NegMode_20.mzXML done, status FINISHED

4911MB free

Data visualization: 2D

MZmine 2.33: New project

Raw data files

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

Peak lists

Please set the parameters

Type of plot: Use raw data points

Raw data files: NegMode_13.mzXML As selected in main window

Scans: MS level: 1 Set filters Clear filters

m/z: 49.9915 - 800.0070 Auto range From mass From formula

OK Cancel Help

Tasks in progress...

Item	Priority	Status	% done
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[9:42:27 AM]: Processing of task Updating 2D visualizer of NegMode_20.mzXML done, status FINISHED

5413MB free

Data visualization: 2D

The image shows the MZmine 2.33 interface for setting parameters for a 2D data visualization. The main window displays a list of raw data files under 'Raw data files', with 'NegMode_13.mzXML' selected. The 'Please set the parameters' dialog is open, showing various settings:

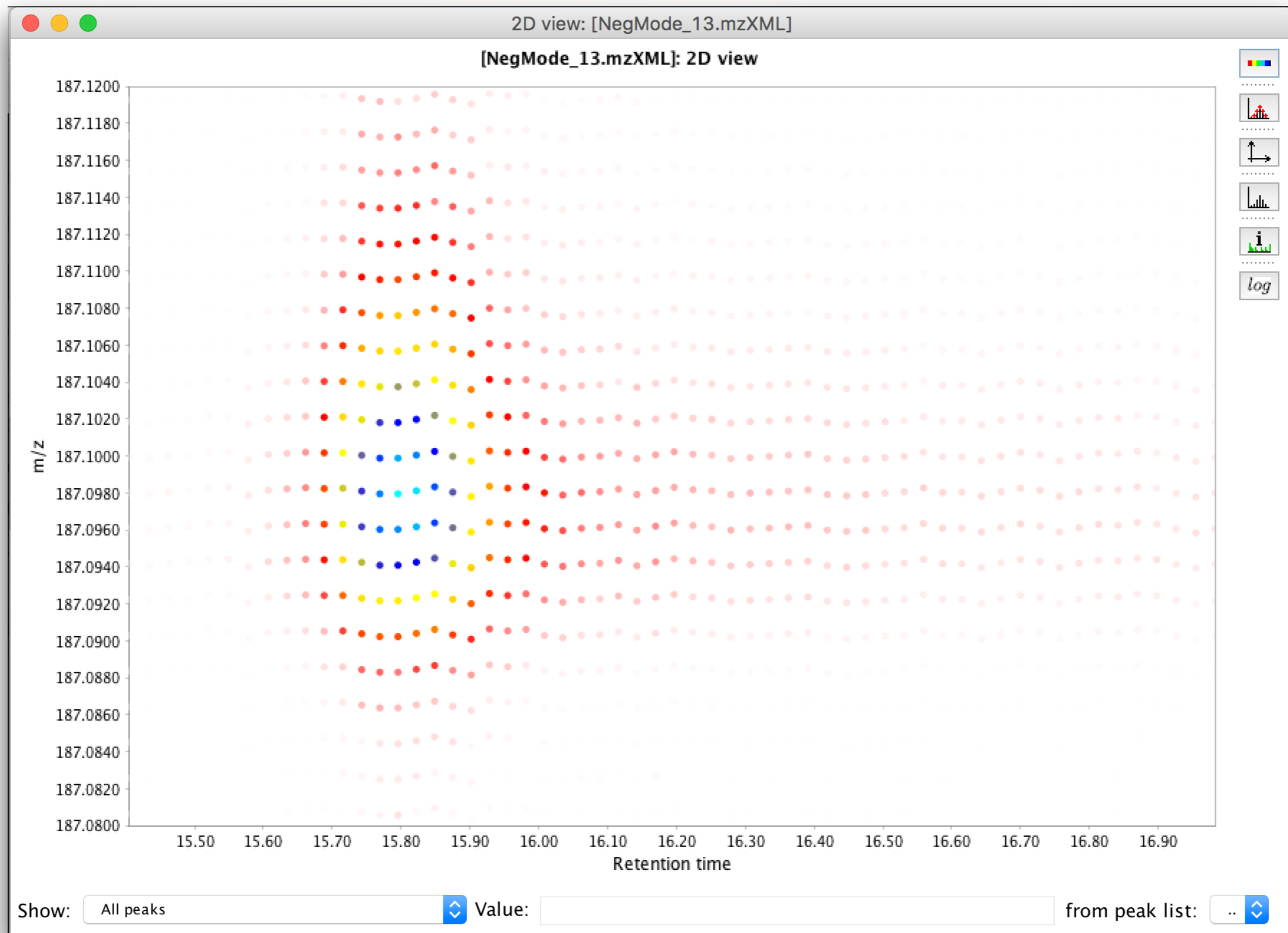
- Scan number: [] - []
- Base Filtering Integer: []
- Retention time: 15.4 - 17.0 min. [Auto range]
- MS level: 1
- Scan definition: []
- Polarity: Any
- Spectrum type: Any

The foreground dialog, also titled 'Please set the parameters', shows the following settings:

- Type of plot: Use raw data points
- Raw data files: NegMode_13.mzXML (As selected in main window)
- Scans: MS level: 1 [Set filters] [Clear filters]
- m/z: 187.0800 - 187.1200 (circled in red) [Auto range] [From mass] [From formula]

Buttons at the bottom include OK, Cancel, and Help. A red arrow points from the circled m/z range to the 'Scan number' field in the background dialog.

Data visualization: 2D



Data visualization: EIC

The screenshot displays the MZmine 2 software interface. The top menu bar includes 'MZmine 2', 'Project', 'Raw data methods', 'Peak list methods', 'Visualization', 'Windows', and 'Help'. The 'Visualization' menu is open, showing 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'. The 'TIC/XIC visualizer' option is highlighted. On the left, a file browser shows 'Raw data files' with four files: 'NegMode_18.mzXML', 'NegMode_20.mzXML', 'NegMode_14.mzXML', and 'NegMode_13.mzXML'. The 'NegMode_14.mzXML' file is selected. At the bottom, a task progress table is visible, and a status bar at the very bottom shows a log message: '[10:47:01 AM]: Processing of task Updating TIC visualizer of NegMode_14.mzXML done, status FINISHED' and '8699MB free'.

Tasks in progress...			
Item	Priority	Status	% done

[10:47:01 AM]: Processing of task Updating TIC visualizer of NegMode_14.mzXML done, status FINISHED

8699MB free

Data visualization: EIC

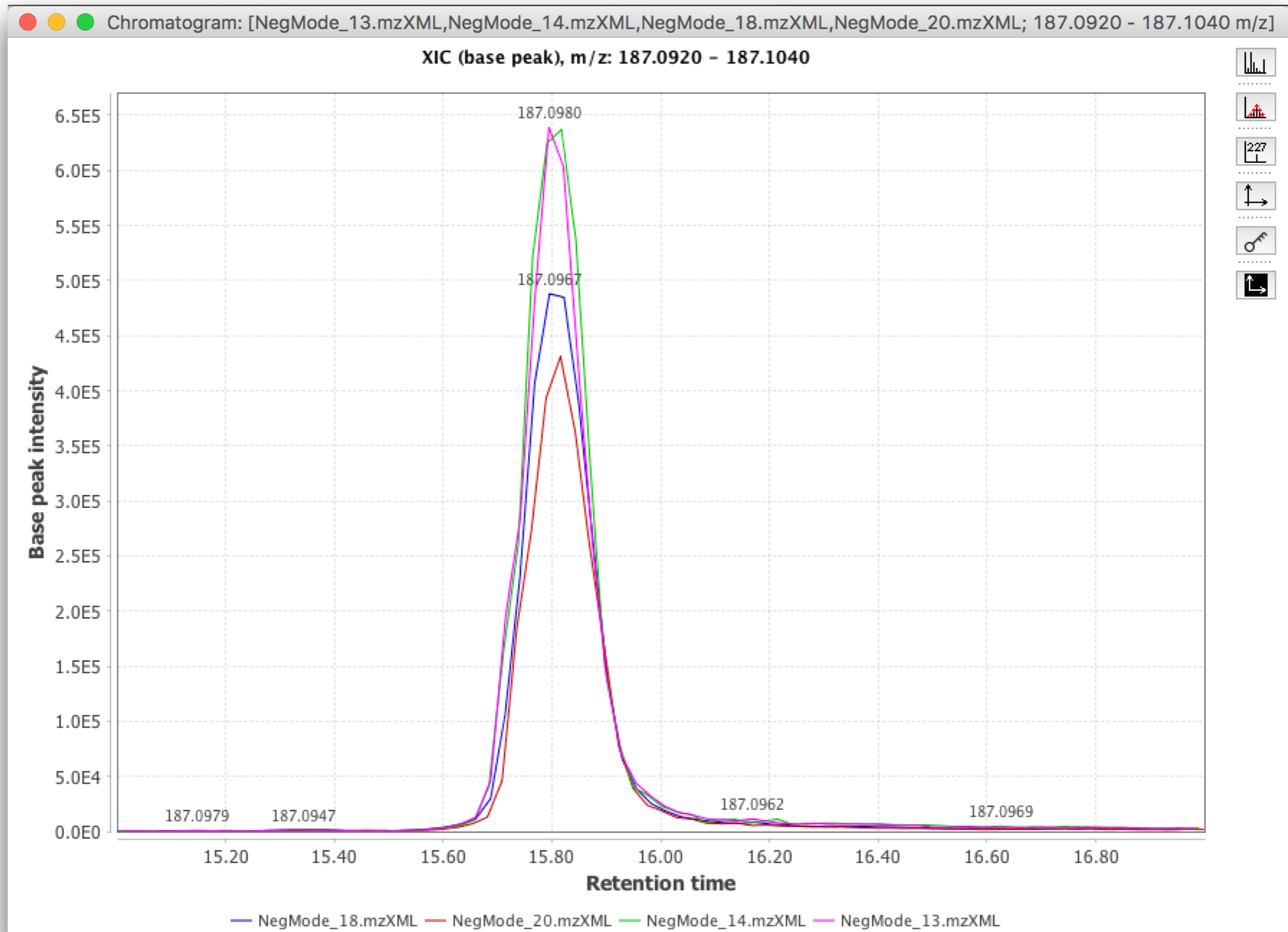
The image shows a software interface for data visualization, specifically for EIC (Extracted Ion Chromatogram). The interface is divided into several sections:

- Raw data files:** A list of files is shown, including NegMode_18.mzXML, NegMode_20.mzXML, NegMode_14.mzXML, and NegMode_13.mzXML. The files are selected, and the selection is reflected in the "Raw data files" field of the "Please set the parameters" dialog.
- Please set the parameters (Main):** This dialog allows users to set various parameters for the visualization:
 - Scan number: [] - []
 - Base Filtering Integer: []
 - Retention time: 15 - 17 min. (with an "Auto range" button)
 - MS level: 1
 - Scan definition: []
 - Polarity: Any (dropdown)
 - Spectrum type: Any (dropdown)
- Please set the parameters (Secondary):** This dialog provides more detailed settings:
 - Raw data files: 4 selected (As selected in main window)
 - Scans: MS level: 1 (with "Set filters" and "Clear filters" buttons)
 - Plot type: Base peak intensity (circled in red)
 - m/z: 187.0920 - 187.1040 (circled in red, with "Auto range", "From mass", and "From formula" buttons)
 - Peaks: [] (with "All" and "Clear" buttons)
 - Buttons: OK, Cancel, Help

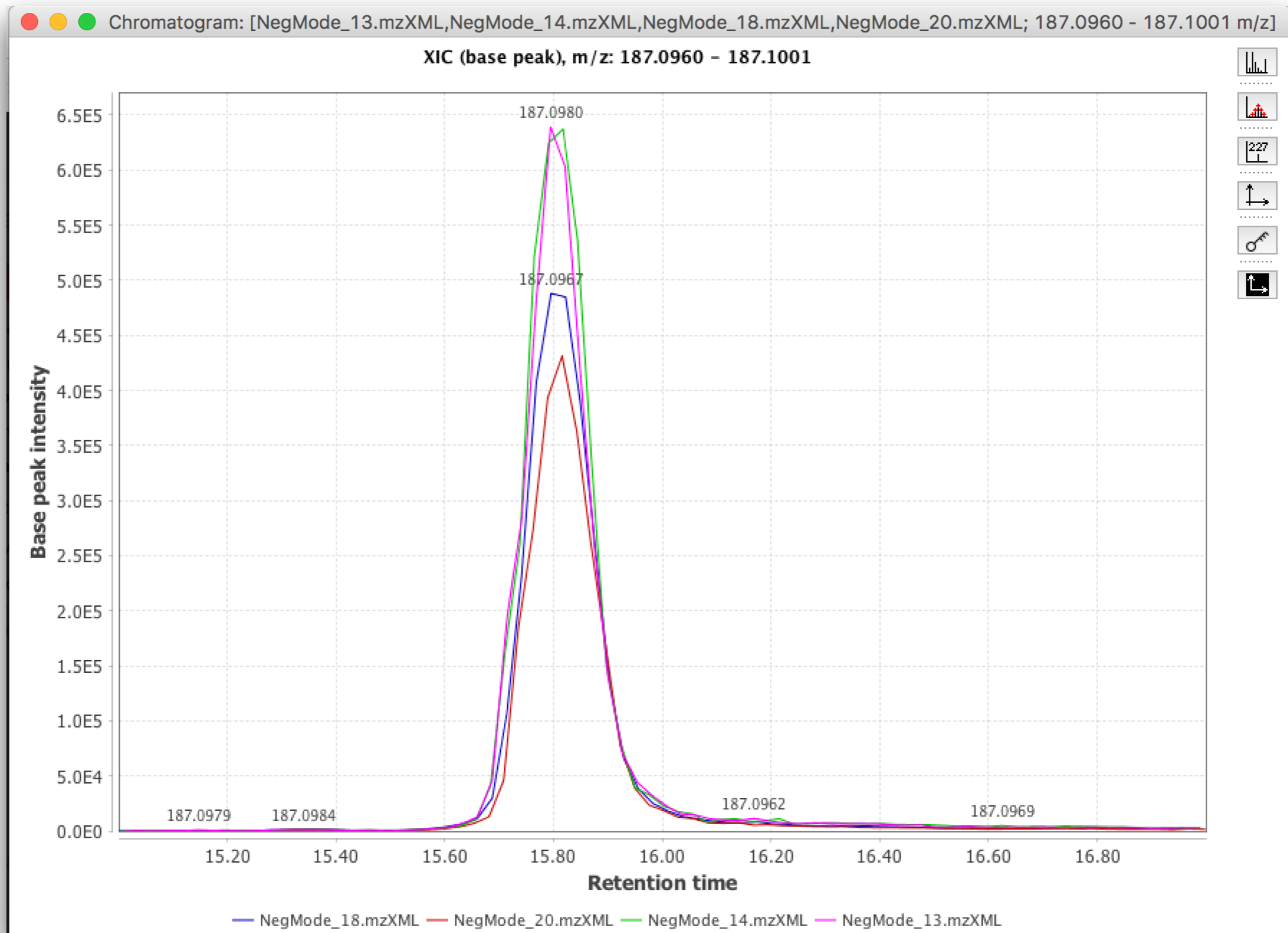
A red arrow points from the "Base peak intensity" dropdown in the secondary dialog to the "Spectrum type" dropdown in the main dialog, indicating a relationship between the two settings.

Tasks in progress
Item
[11:01:22 AM]:

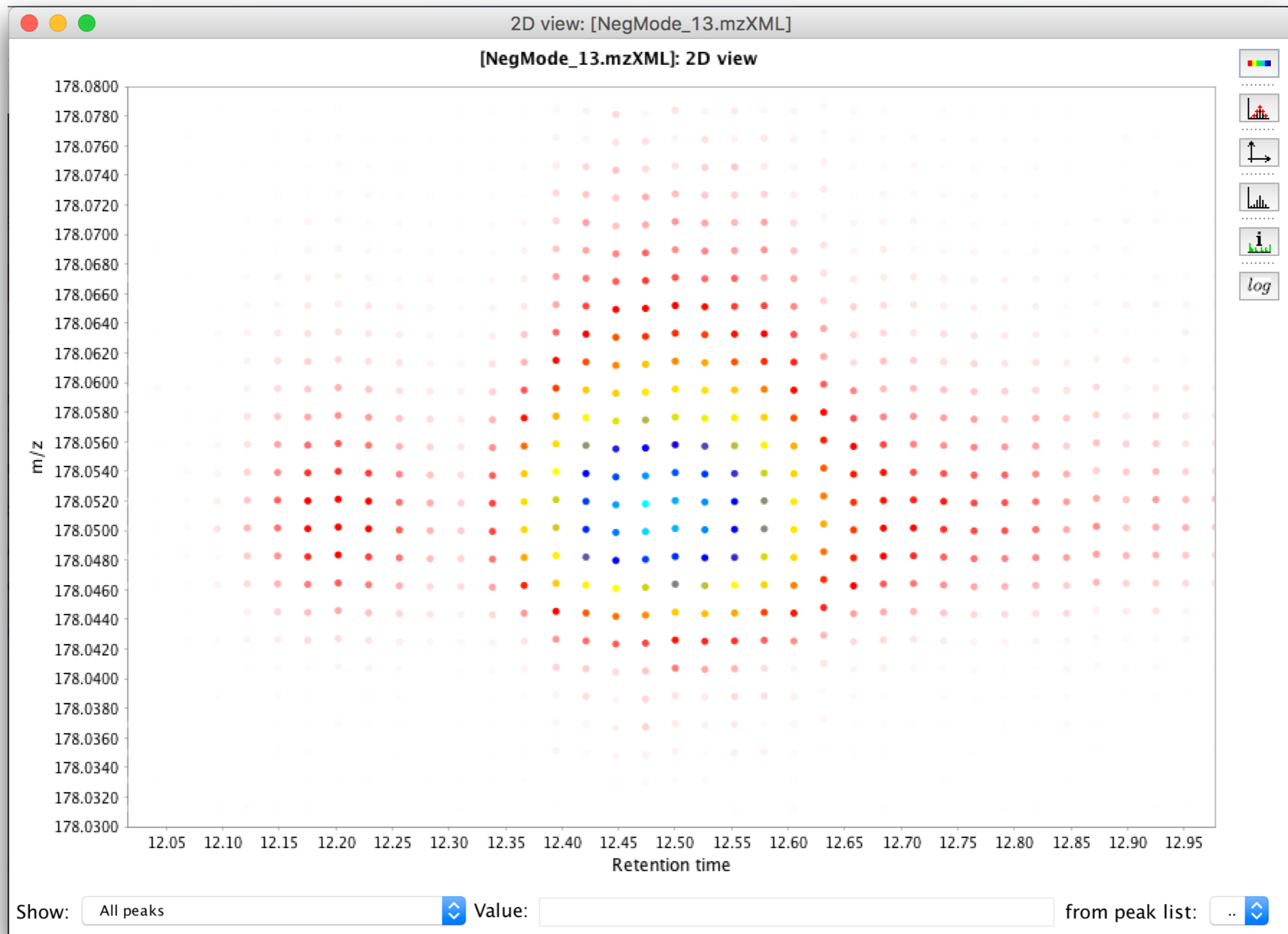
Data visualization: EIC



Data visualization: EIC



Data visualization: 2D



Data visualization: EIC

MZmine 2.33: New project

Raw data files

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

Peak lists

Please set the parameters

Raw data files: NegMode_13.mzXML (As selected in main window)

Scans: Retention time: 12.00 - 13.00 min., MS level: 1

Plot type: Base peak intensity

m/z: 178.04 - 178.06

Peaks: [Empty list]

Buttons: Set filters, Clear filters, Auto range, From mass, From formula, All, Clear, OK, Cancel, Help

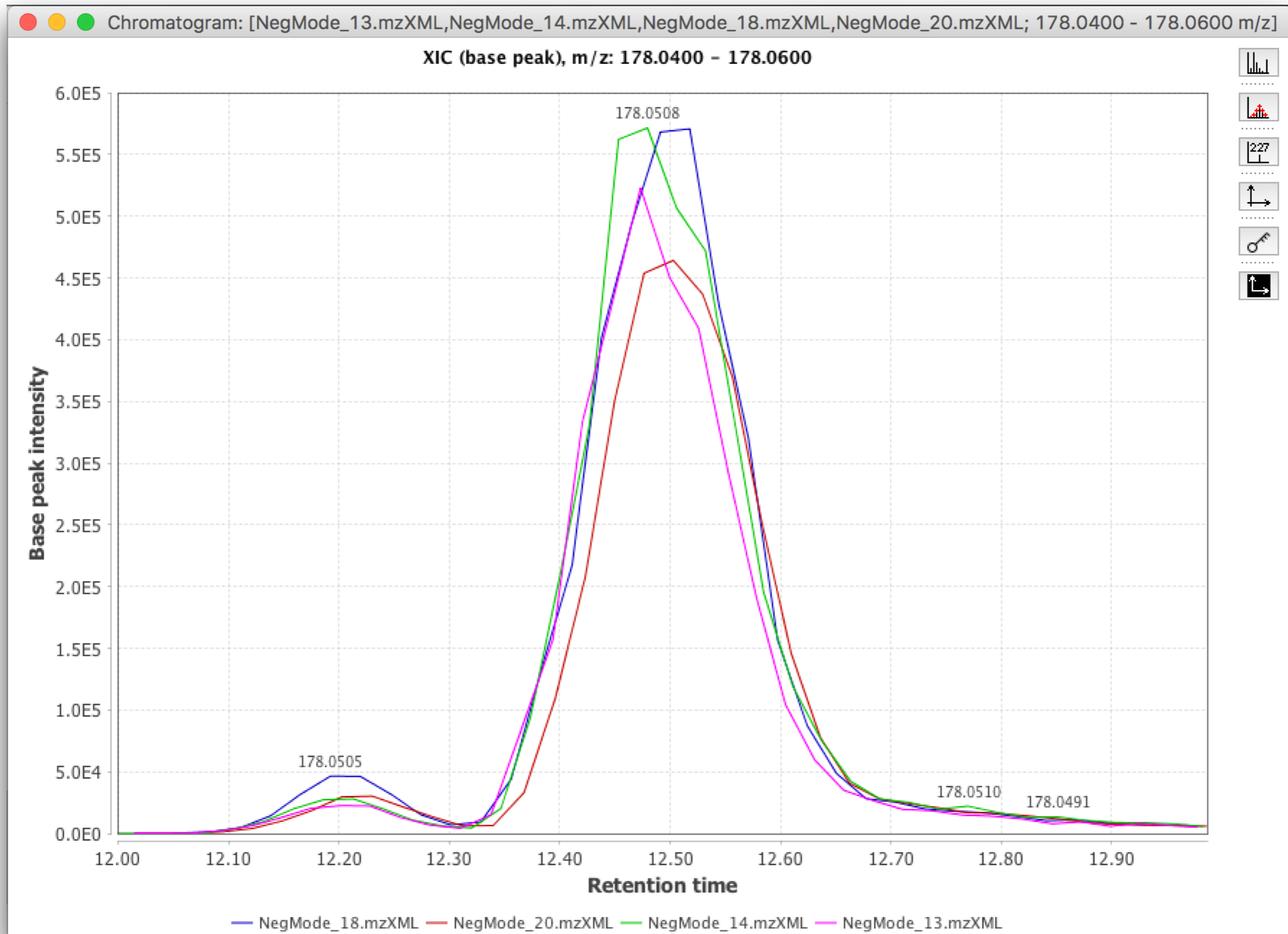
Tasks in progress...

Item	Priority	Status	% done
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[11:19:58 AM]: Processing of task Updating 2D visualizer of NegMode_13.mzXML done, status FINISHED

5425MB free

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

Raw data files

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

Raw data methods

- 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

Peak lists

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

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

The screenshot displays the MZmine 2.33 software interface. The main window, titled "MZmine 2.33: New project", shows a file browser on the left with four raw data files selected: NegMode_18.mzXML, NegMode_20.mzXML, NegMode_14.mzXML, and NegMode_13.mzXML. The right pane is titled "Peak lists".

Two "Please set the parameters" dialog boxes are overlaid. The larger one in the foreground has the following settings:

- Raw data files: 4 selected, As selected in main window
- Scans: Retention time: 5.00 - 24.00 min., MS level: 1. Buttons: Set filters, Clear filters
- Mass detector: Wavelet transform
- Mass list name: masses
- CDF Filename (optional): [empty field] ...
- Buttons: OK, Cancel, Help

A smaller dialog box is partially visible behind it, showing:

- Noise level: 1.0E2
- Scale level: 5
- Wavelet window size (%): 30.0 %
- Show preview
- Buttons: OK, Cancel, Help

At the bottom, a "Tasks in progress..." table is visible:

Item	Priority

The status bar at the bottom shows: [11:28:52 AM]: Processing of task Detecting masses in NegMode_18.mzXML done, status CANCELED. 2688MB free

Mass detection


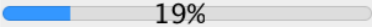


MZmine 2.33: New project

Raw data files

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

Peak lists

Tasks in progress...

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%

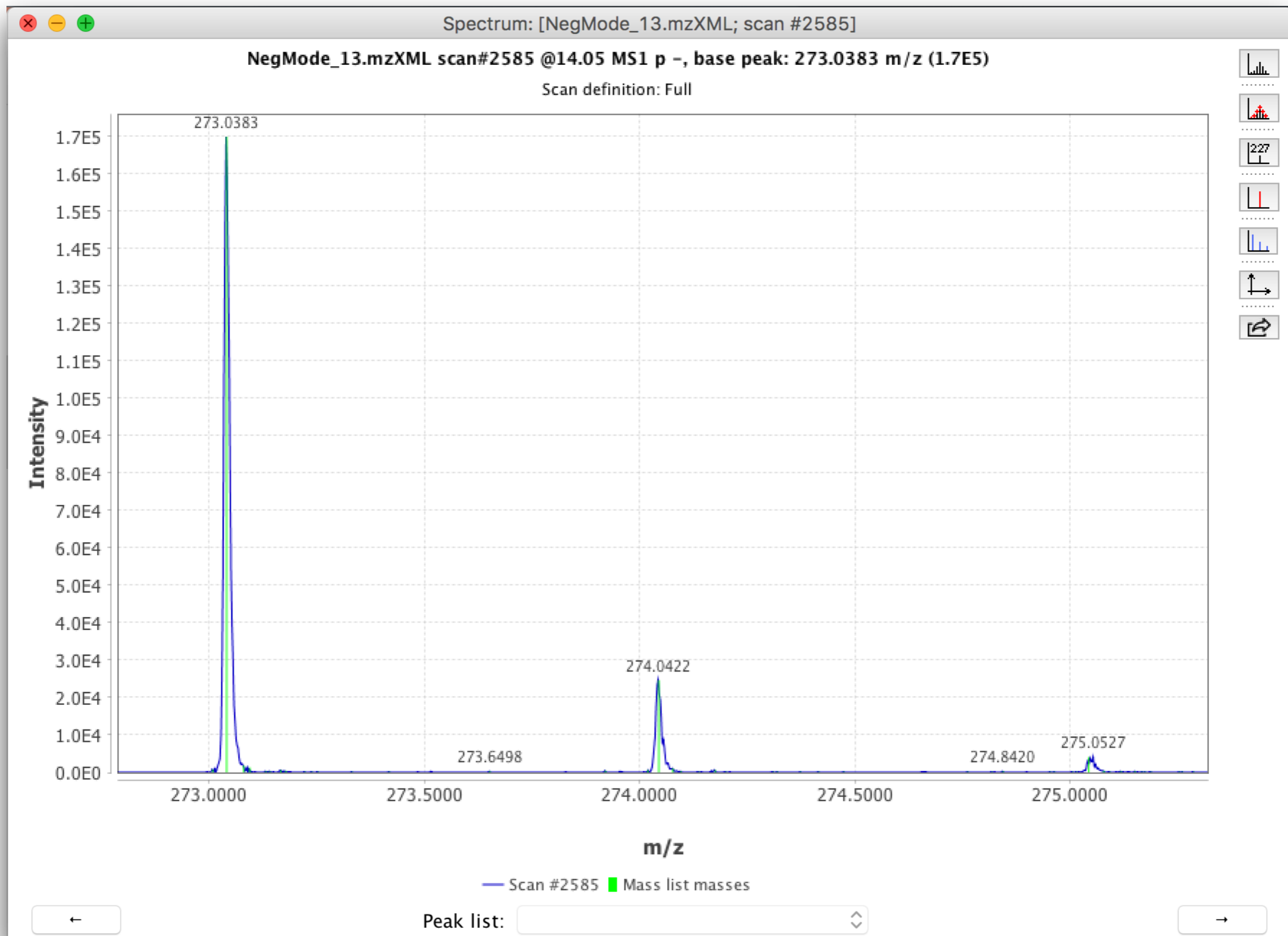
[11:30:17 AM]: Started mass detector on NegMode_13.mzXML

8768MB free

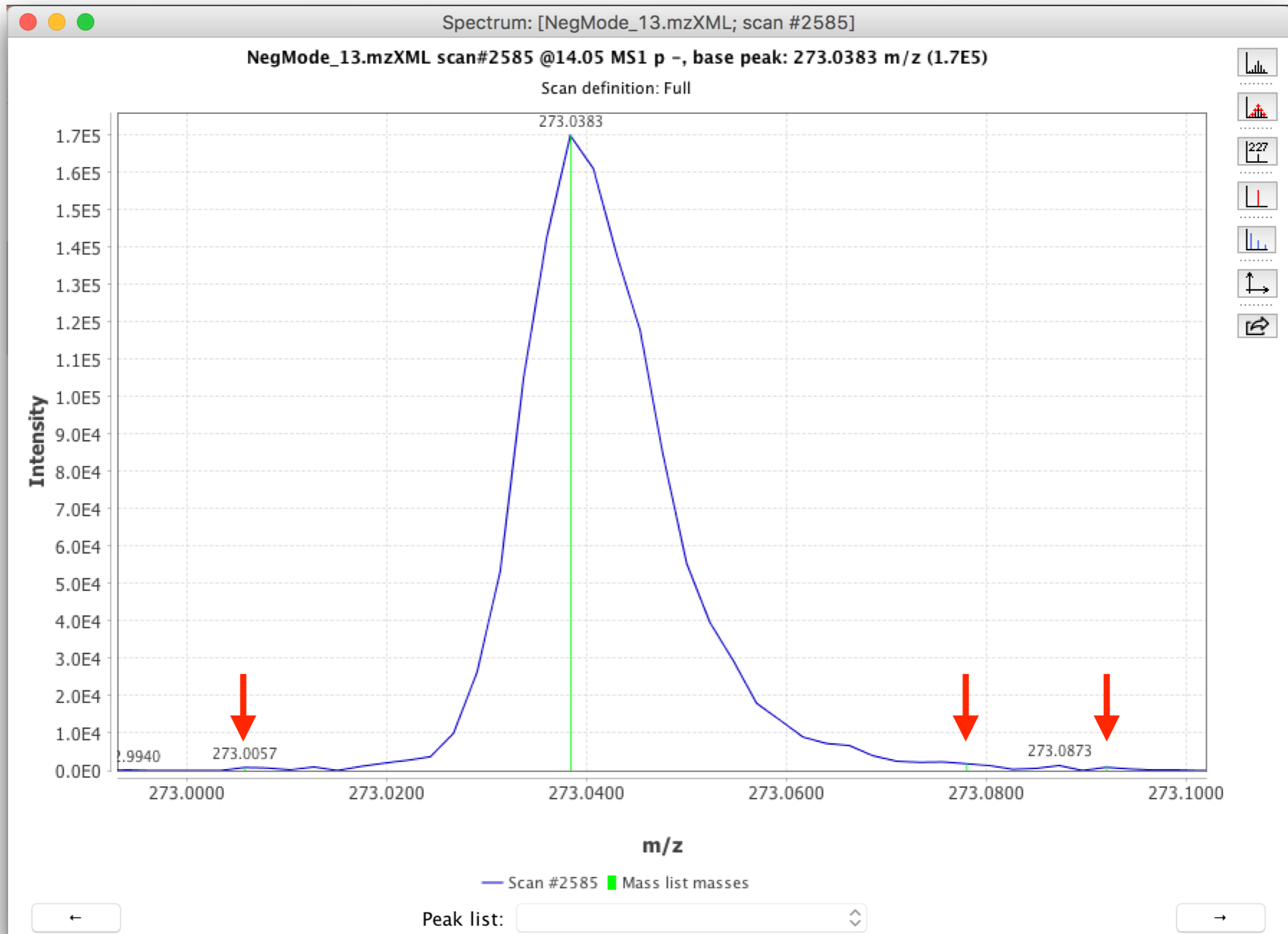
Mass detection



Mass detection



Mass detection



EIC construction

The screenshot shows the MZmine 2 software interface. The 'Raw data methods' menu is open, and the 'Peak detection' option is selected. A sub-menu is displayed, listing several methods, with 'ADAP Chromatogram builder' highlighted. The interface also shows a file list on the left, a task progress table at the bottom, and a status bar at the very bottom.

Raw data files

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

Raw data methods

- 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

Tasks in progress...

Item	Priority	Status	% done
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[11:31:40 AM]: Processing of task Detecting masses in NegMode_13.mzXML done, status FINISHED

7837MB free

EIC construction

The screenshot shows the MZmine 2.33: New project dialog box. The main window displays a file tree with 'Raw data files' and 'Peak lists'. A modal dialog box titled 'Please set the parameters' is open, allowing configuration of EIC construction settings. The parameters are as follows:

Parameter	Value
Raw data files	4 selected As selected in main window
Scans	Retention time: 5.00 - 24.00 min. MS level: 1
Mass list	masses
Min group size in # of scans	5.00
Group intensity threshold	1.0E3
Min highest intensity	2.0E3
m/z tolerance	0.029 m/z or 0.0 ppm
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 pro
Item

OK Cancel Help

[12:32:14 PM]: Error of task Detecting chromatograms in NegMode_13.mzXML: Scan NegMode_13.mzXML #101 does not have a ... 7222MB free

EIC construction

MZmine 2.33: New project

Raw data files

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

Peak lists

Tasks in progress...

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%

[12:33:17 PM]: Started chromatogram builder on NegMode_13.mzXML

8335MB free

EIC construction

The screenshot displays the MZmine 2.33 software interface. The main window, titled "MZmine 2.33: New project", is divided into two panes. The left pane, titled "Raw data files", shows a list of files: NegMode_18.mzXML, NegMode_20.mzXML, NegMode_14.mzXML, and NegMode_13.mzXML. The right pane, titled "Peak lists", shows a list of chromatograms: NegMode_18.mzXML chromatograms, NegMode_13.mzXML chromatograms, NegMode_20.mzXML chromatograms, and NegMode_14.mzXML chromatograms. Below the panes is a "Tasks in progress..." section with a table. The table has columns for "Item", "Priority", "Status", and "% done". The table is currently empty. At the bottom of the window, there is a status bar with a log entry: "[12:33:28 PM]: Processing of task Detecting chromatograms in NegMode_14.mzXML done, status FINISHED" and a memory indicator showing "8066MB free".

MZmine 2.33: New project

MZmine 2.33: New project

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

Tasks in progress...

Item	Priority	Status	% done
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[12:33:17 PM]: S

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

8066MB free

EIC construction

The screenshot displays the MZmine 2.33 software interface with three overlapping windows. The top window shows the 'Raw data files' panel with a list of files: NegMode_18.mzXML, NegMode_20.mzXML, NegMode_14.mzXML, and NegMode_13.mzXML. The middle window shows the 'Peak lists' panel for 'NegMode_18.mzXML chromatograms', listing 22 peaks with their retention times and m/z values. The bottom window shows a 'Tasks in progress' table with columns for Item, Priority, Status, and % done. A task 'Detecting chromatograms in NegMode_14.mzXML' is shown as 'FINISHED'.

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_14.mzXML		FINISHED	

[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

MZmine 2.33: New project

Raw data files

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

#95 179.1070 m/z @21.09

#96 180.0545 m/z @12.44

#97 181.0504 m/z @10.94

#98 181.0849 m/z @14.95

#99 182.0450 m/z @7.82

#100 183.0657 m/z @13.57

#101 184.0599 m/z @9.83

#102 184.0967 m/z @15.14

#103 185.0269 m/z @14.32

#104 185.0806 m/z @13.44

#105 185.1170 m/z @19.51

#106 186.1133 m/z @13.14

#107 186.5159 m/z @15.80

#108 187.0598 m/z @10.18

#109 187.0967 m/z @15.80

#110 188.0342 m/z @11.27

#111 188.0982 m/z @15.80

#112 189.0403 m/z @13.25

#113 189.0728 m/z @13.98

#114 189.1120 m/z @15.69

#115 190.0491 m/z @13.27

#116 190.1150 m/z @15.71

#117 191.0525 m/z @13.25

#118 192.0666 m/z @13.44

Tasks in progress...

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

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

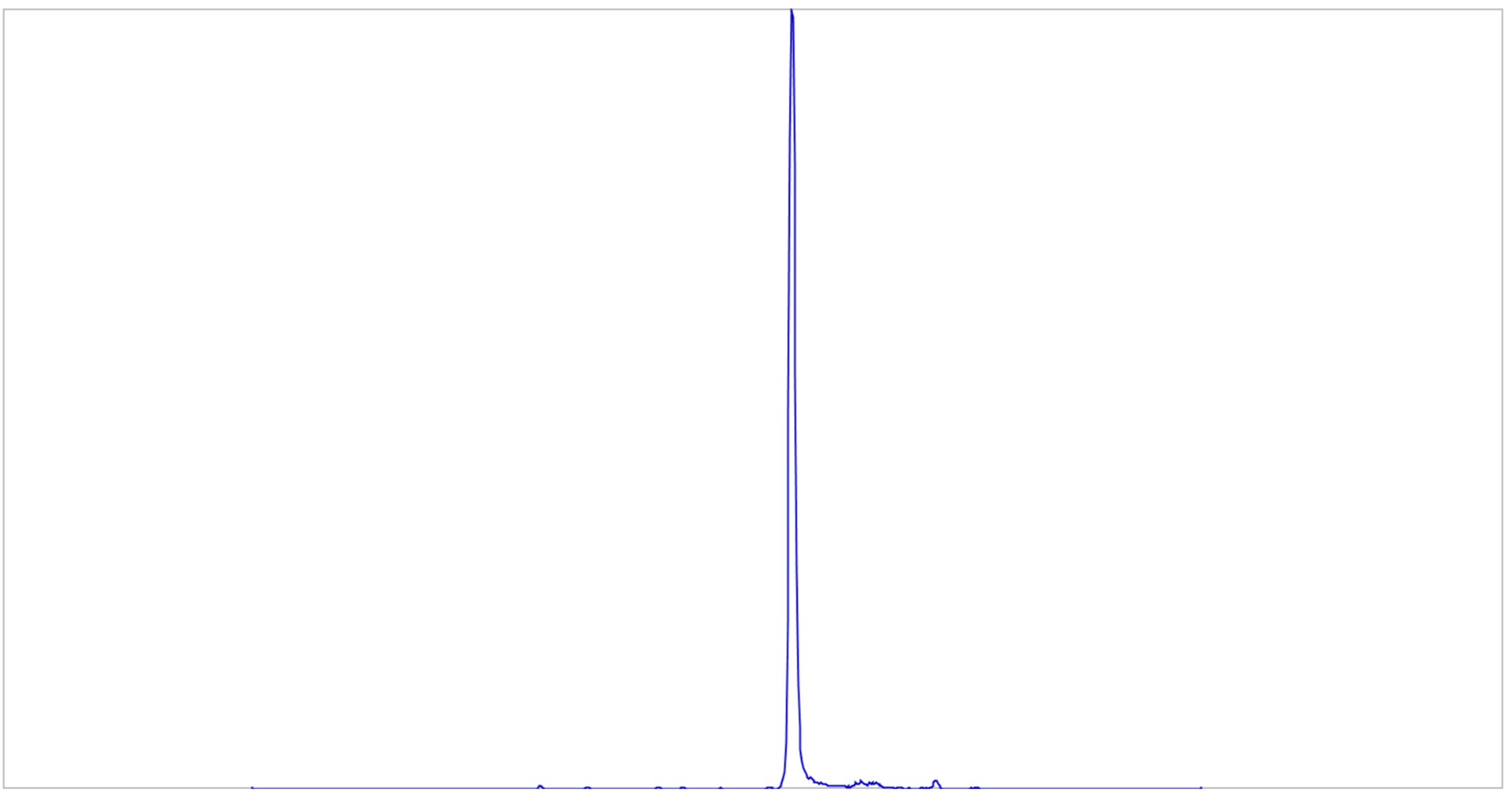
8217MB free

EIC construction

MZmine 2.33: New project

Raw data files #109 187.0967 m/z @15.80

#109 187.0967 m/z @15.80



Tasks in progress: Item

File Name	Mass	RT	Height	Area
NegMode_18.mzXML	187.0967	15.80	4.9E5	5.2E6

[12:33:28 PM]: P

Chromatogram

EIC construction



EIC peak detection

The screenshot shows the MZmine 2 software interface. The 'Peak list methods' menu is open, and 'Chromatogram deconvolution' is selected. The left sidebar shows a list of raw data files: NegMode_18.mzXML, NegMode_20.mzXML, NegMode_14.mzXML, and NegMode_13.mzXML. The bottom status bar shows a task log entry: '[12:40:56 PM]: Processing of task Updating TIC visualizer of NegMode_18.mzXML done, status FINISHED' and a system tray icon indicating 7030MB free.

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

The screenshot displays the MZmine 2.33 interface. The main window shows a project titled "MZmine 2.33: New project" with two panes: "Raw data files" and "Peak lists". The "Raw data files" pane contains four files: NegMode_18.mzXML, NegMode_20.mzXML, NegMode_14.mzXML, and NegMode_13.mzXML. The "Peak lists" pane contains four corresponding chromatogram files. A dialog box titled "Please set the parameters" is open, showing the following settings:

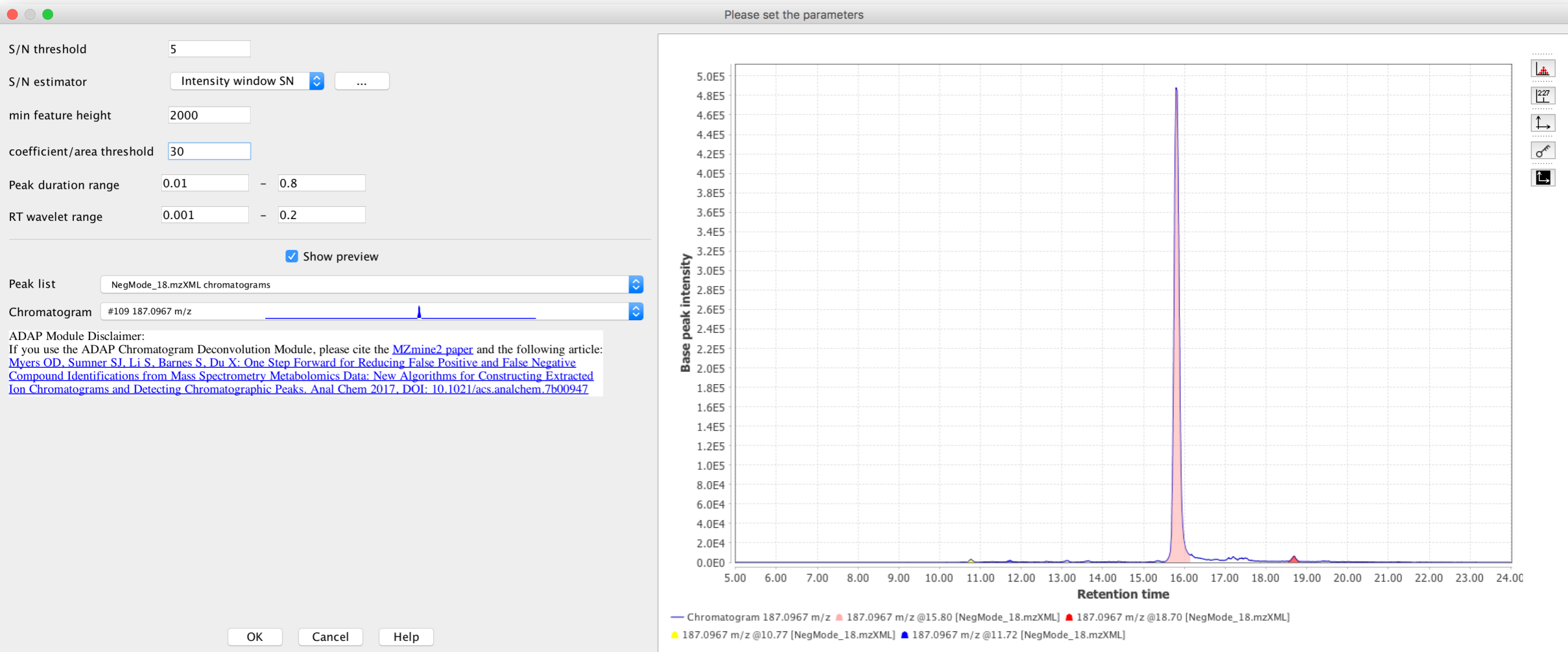
- Peak lists: 4 selected, As selected in main window
- Suffix: deconvoluted
- Algorithm: Wavelets (ADAP) (selected from a dropdown menu that also includes Baseline cut-off, Noise amplitude, Savitzky-Golay, and Local minimum search)
- m/z range for MS2 scan pairing (Da):
- RT range for MS2 scan pairing (min):
- Remove original peak list:

Buttons for OK, Cancel, and Help are visible at the bottom of the dialog. At the bottom of the main window, a task list table is partially visible:

Item	Priority	Status	% done

The status bar at the bottom indicates: [12:40:56 PM]: Processing of task Updating TIC visualizer of NegMode_18.mzXML done, status FINISHED. 6872MB free.

EIC peak detection



EIC peak detection

MZmine 2.33: New project

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

Tasks in progress...

Item	Priority	Status	% done
Peak recognition on NegMode_18.mzXML chromatograms	NORMAL	PROCESSING	19%
Peak recognition on NegMode_13.mzXML chromatograms	NORMAL	PROCESSING	18%
Peak recognition on NegMode_20.mzXML chromatograms	NORMAL	PROCESSING	17%
Peak recognition on NegMode_14.mzXML chromatograms	NORMAL	PROCESSING	16%

[12:53:27 PM]: Started peak deconvolution on NegMode_14.mzXML chromatograms

6229MB free

EIC peak detection

MZmine 2.33: New project

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 'Peak list methods' menu is open, with 'Isotopes' and 'Isotopic peaks grouper' highlighted. A tooltip for 'Isotopic peaks grouper' reads: 'This module detects isotopic peak them together into isotope pattern'. The 'Raw data files' panel on the left shows four files: NegMode_18.mzXML, NegMode_20.mzXML, NegMode_14.mzXML, and NegMode_13.mzXML. The 'Tasks in progress...' table at the bottom is empty. The status bar at the bottom shows a task completion message and a memory usage indicator.

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

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

7405MB free

Isotopic grouper parameters

The screenshot displays the MZmine 2.33 interface with a 'Please set the parameters' dialog box open. The background window shows 'Raw data files' and 'Peak lists' panels. The dialog box contains the following settings:

- Peak lists: 4 selected, As selected in main window
- Name suffix: deisotoped
- m/z tolerance: 0.01 m/z or 0 ppm
- Retention time tolerance: 30 relative (%)
- Monotonic shape:
- Maximum charge: 3
- Representative isotope: Most intense
- Remove original peaklist:

Buttons at the bottom of the dialog: OK, Cancel, Help.

Tasks in progress table:

Item	Progress
Peak recognition on NegMode_14.mzXML chromatograms	done, status FINISHED

System tray: 7177MB free

Isotopic grouper parameters

The screenshot displays the MZmine 2.33 software interface. The top menu bar includes 'MZmine 2', 'Project', 'Raw data methods', 'Peak list methods', 'Visualization', 'Windows', and 'Help'. The window title is 'MZmine 2.33: New project'. The interface is divided into two main panels: 'Raw data files' on the left and 'Peak lists' on the right. The 'Raw data files' panel shows four files: 'NegMode_18.mzXML', 'NegMode_20.mzXML', 'NegMode_14.mzXML', and 'NegMode_13.mzXML'. The 'Peak lists' panel shows a list of processed files, including 'chromatograms' and 'deconvoluted' versions for each of the four raw data files. The 'deconvoluted' files are highlighted in blue. At the bottom, there is a 'Tasks in progress...' section with a table showing the progress of tasks. The table has columns for 'Item', 'Priority', 'Status', and '% done'. The status bar at the bottom indicates that the task 'Isotopic peaks grouper on NegMode_14.mzXML chromatograms deconvoluted' is done, with a status of 'FINIS...' and 5819MB free.

Item	Priority	Status	% done

[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 As selected in main window ...

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