Hands-on Data Analysis with MZmine 2

Xiuxia Du, Stephen Barnes

About MZmine 2

- LC/MS and GC/MS metabolomics data processing, analysis, and visualization

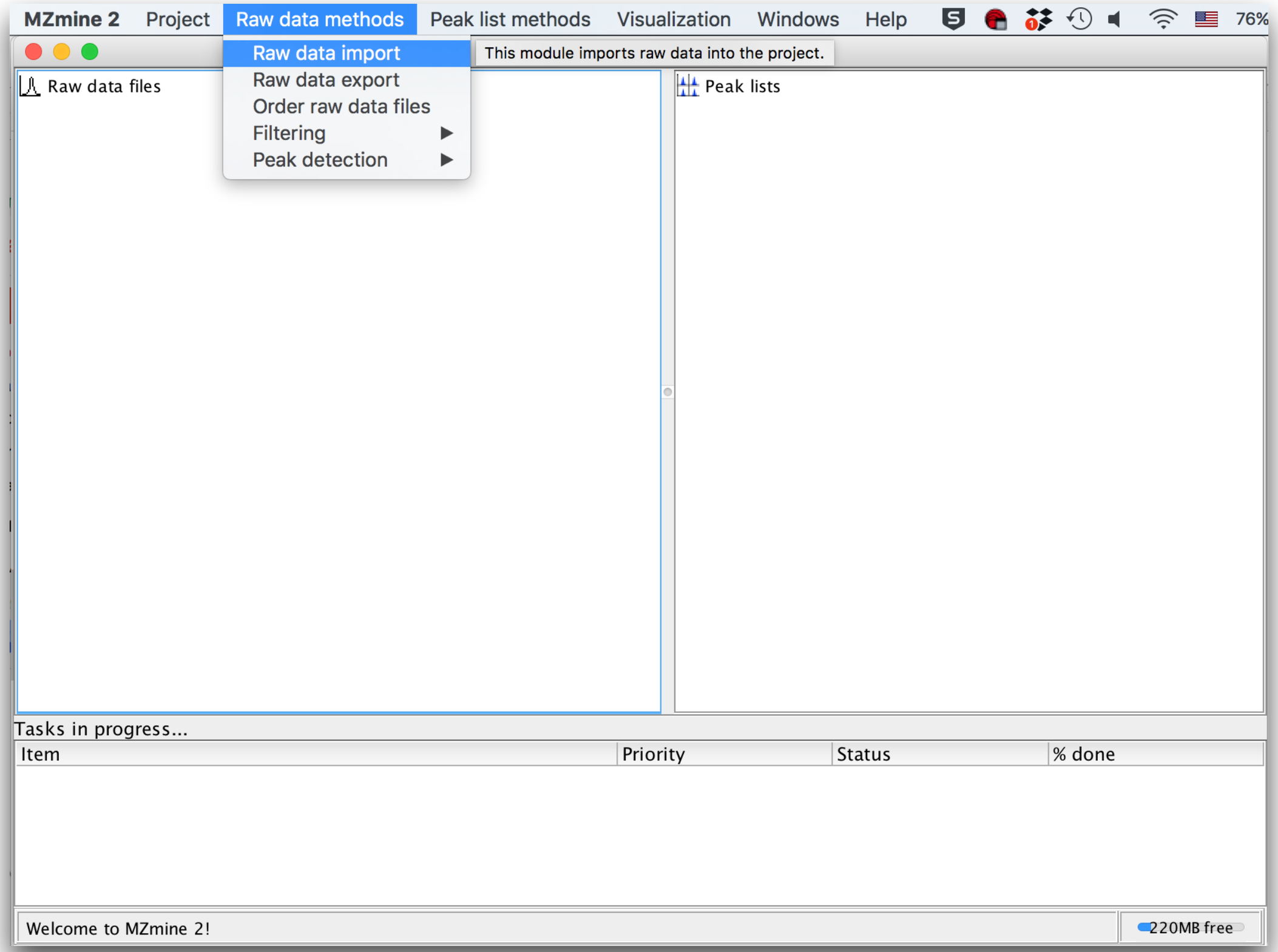
- Supported open data formats
  - mzXML
  - mzML
  - mzData
  - NetCDF

LC-MS

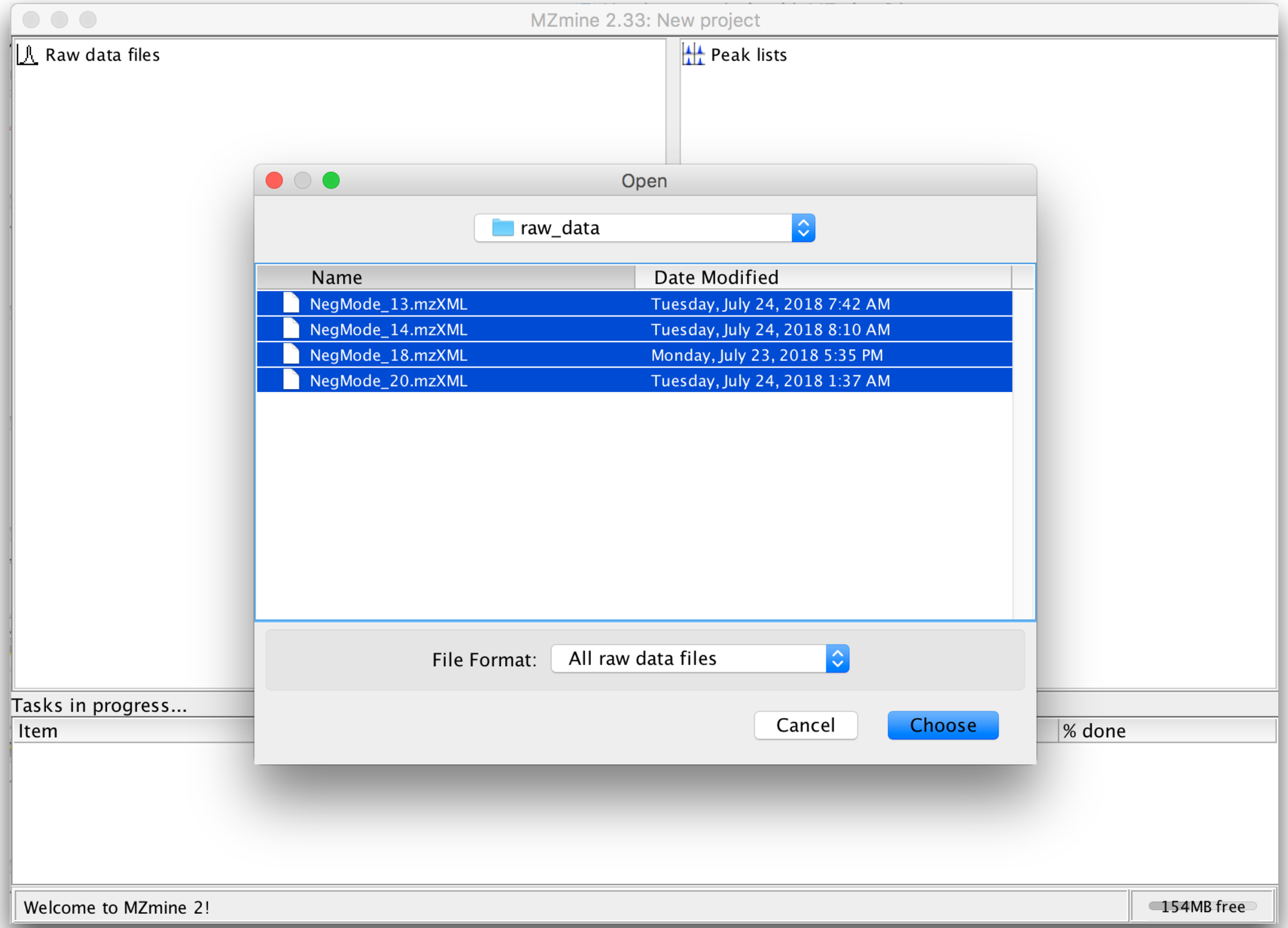
Workflow

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

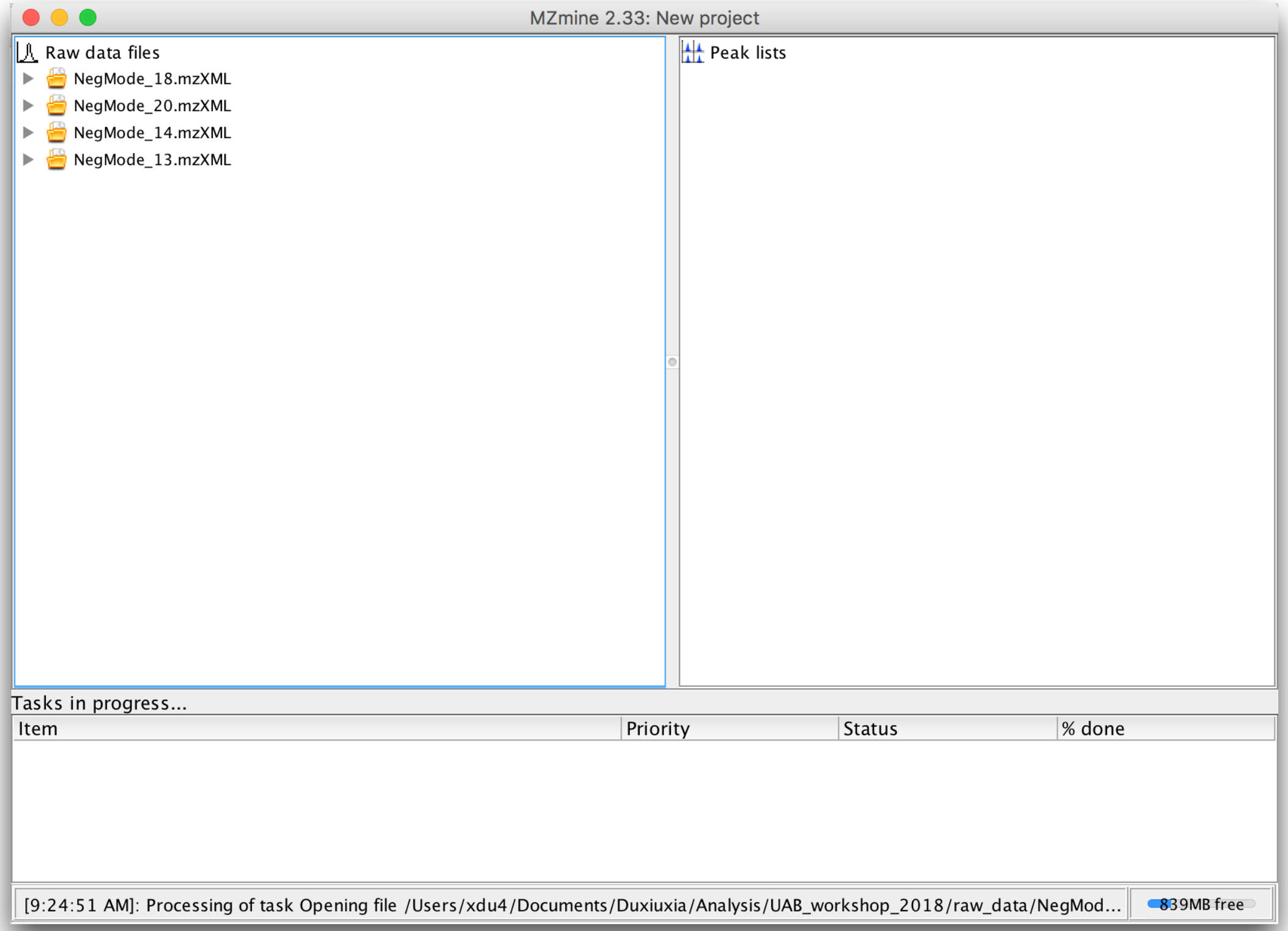
Data import


MZmine 2
Project
Raw data methods
Peak list methods
Visualization
Windows
Help
76%
Raw data import
Raw data export
Order raw data files
Filtering
Peak detection
This module imports raw data into the project.
Raw data files
Peak lists
Tasks in progress...
Item
Priority
Status
% done
Welcome to MZmine 2!
220MB free

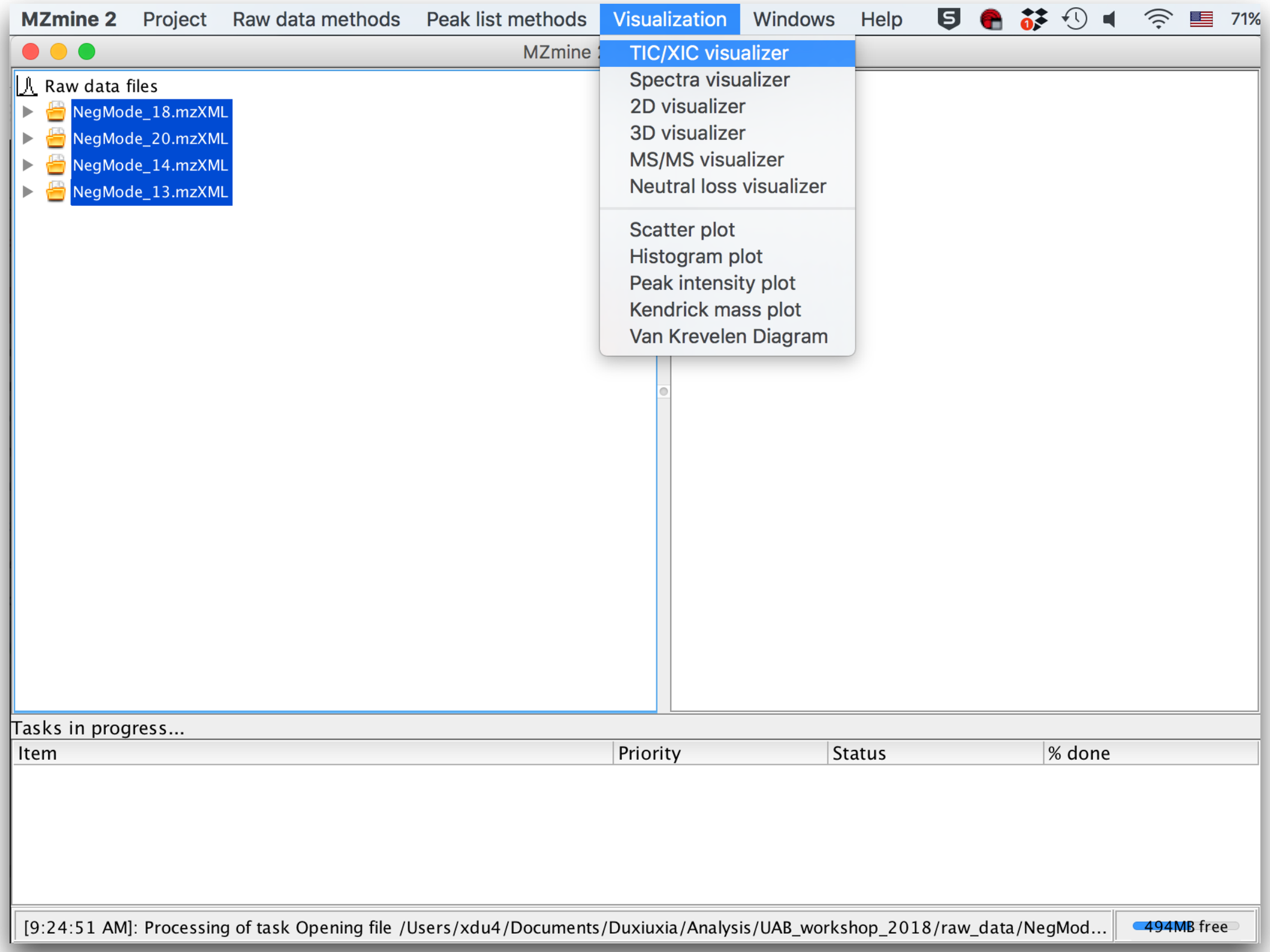
Data import


MZmine 2.33: New project
Raw data files
Peak lists
Open
raw_data
Name
Date Modified
NegMode_13.mzXML
Tuesday, July 24, 2018 7:42 AM
NegMode_14.mzXML
Tuesday, July 24, 2018 8:10 AM
NegMode_18.mzXML
Monday, July 23, 2018 5:35 PM
NegMode_20.mzXML
Tuesday, July 24, 2018 1:37 AM
File Format:
All raw data files
Cancel
Choose
Tasks in progress...
Item
% done
Welcome to MZmine 2!
154MB free

Data import


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
[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



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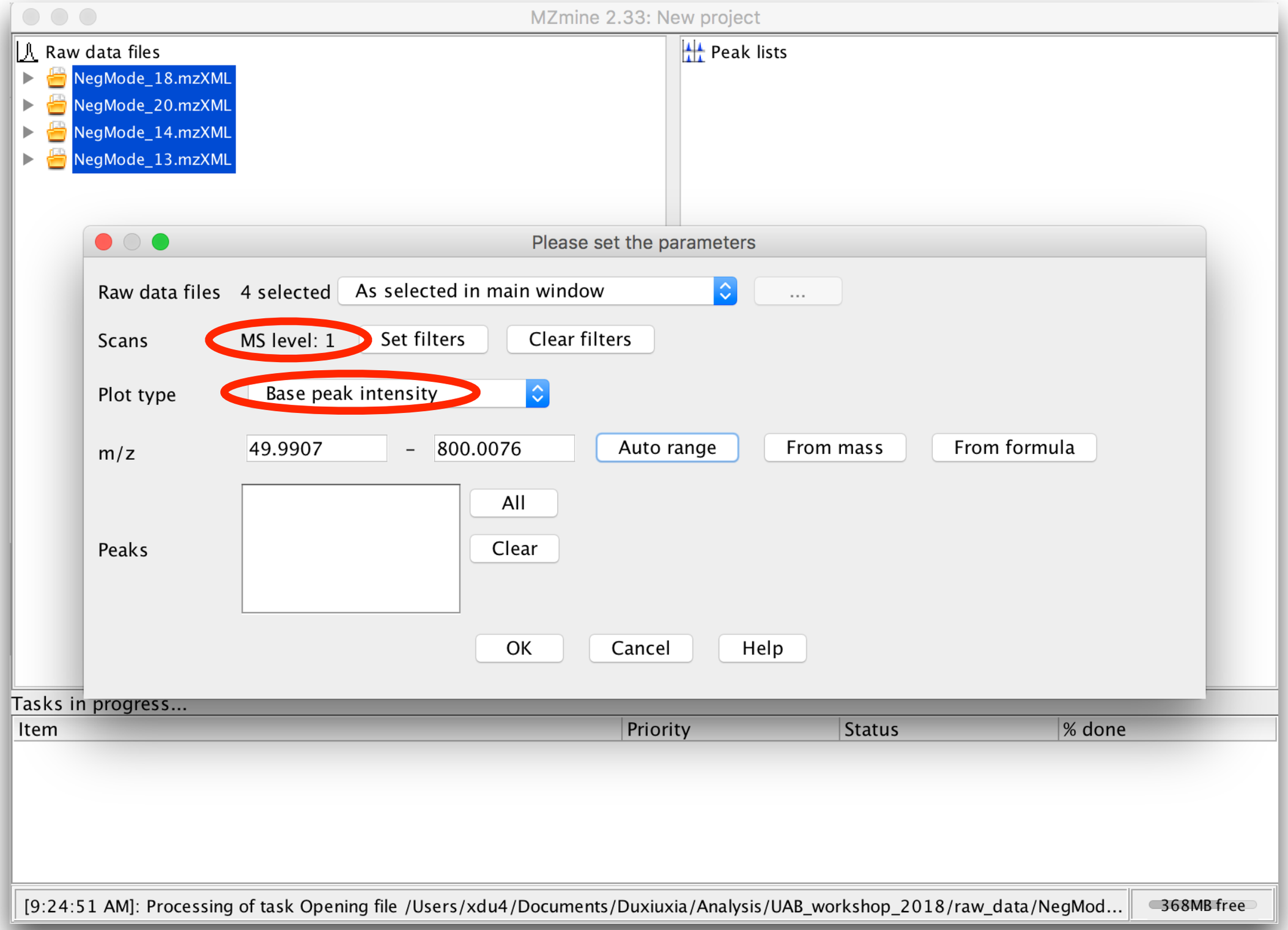
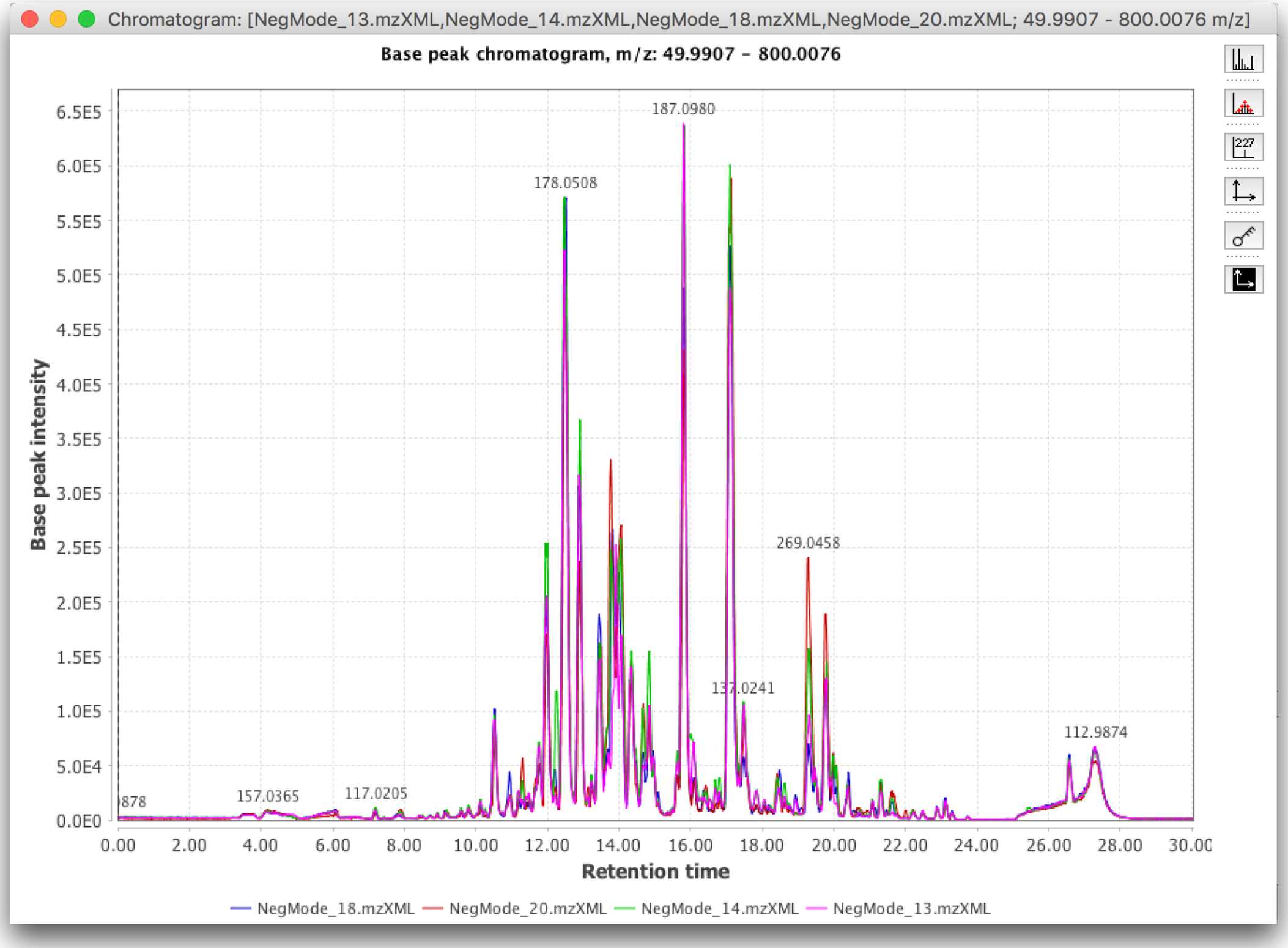


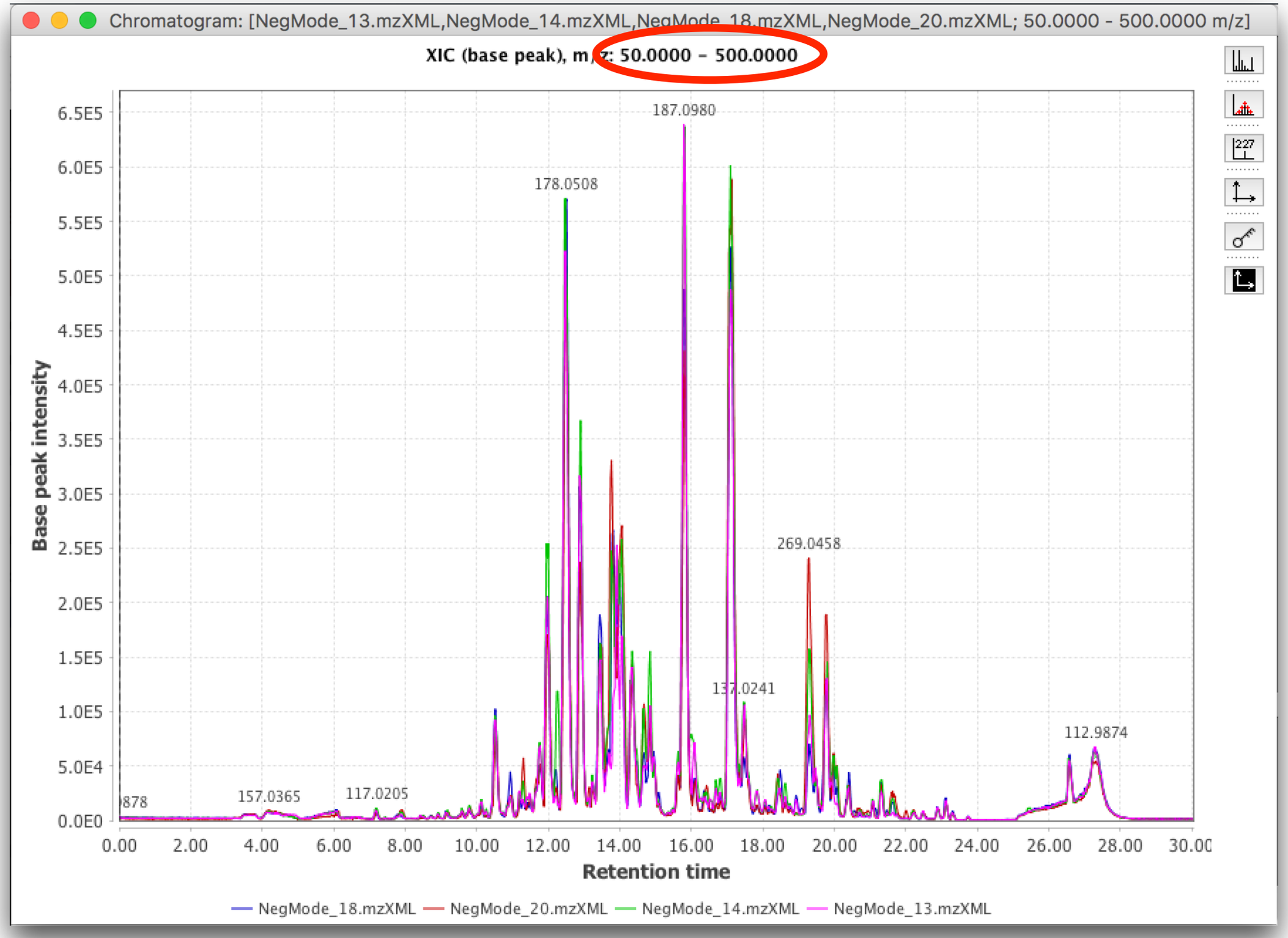
Data visualization: BIC



Data visualization: BIC

You can zoom in the BICs and examine them.

Data visualization: BIC



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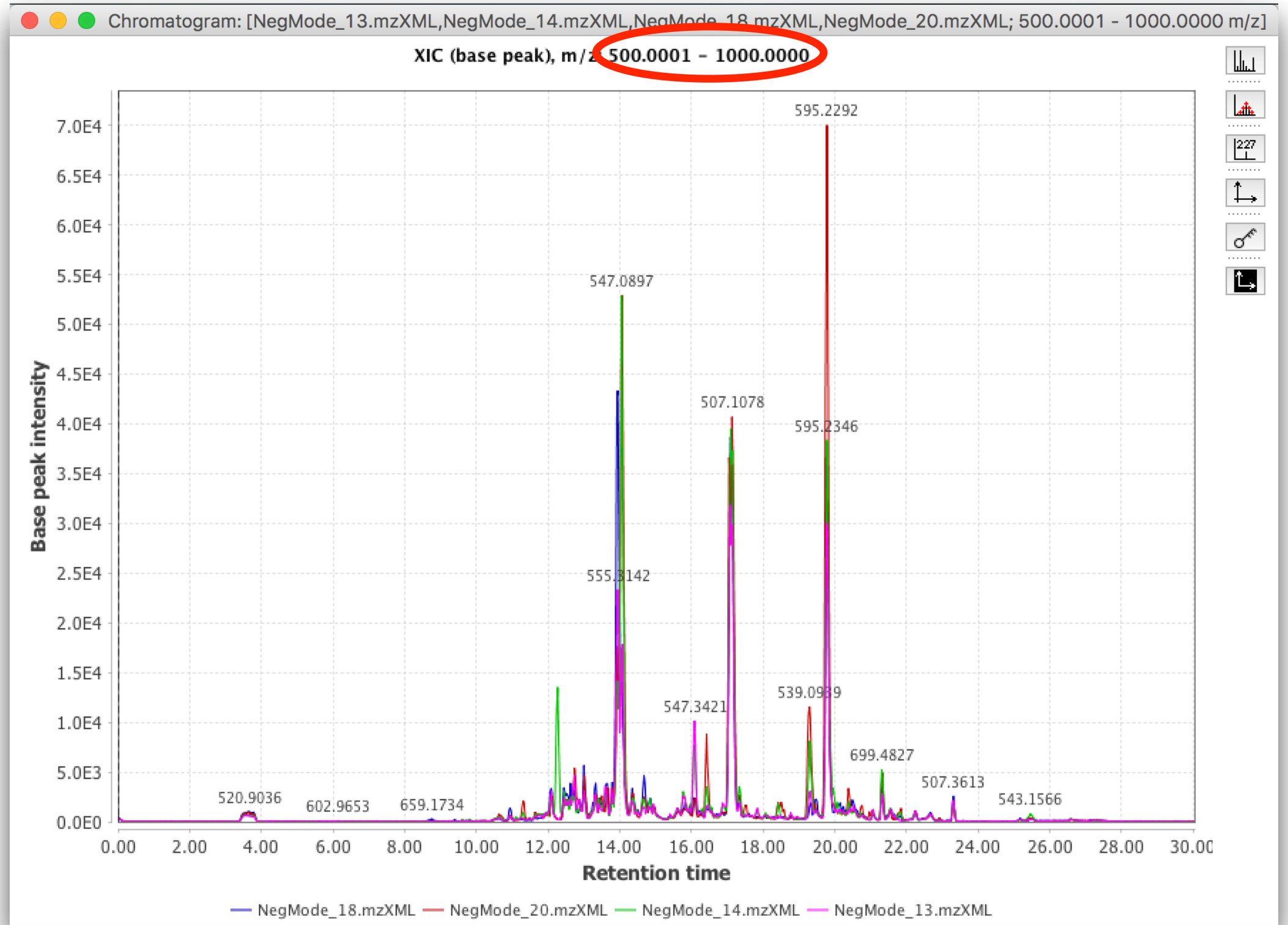
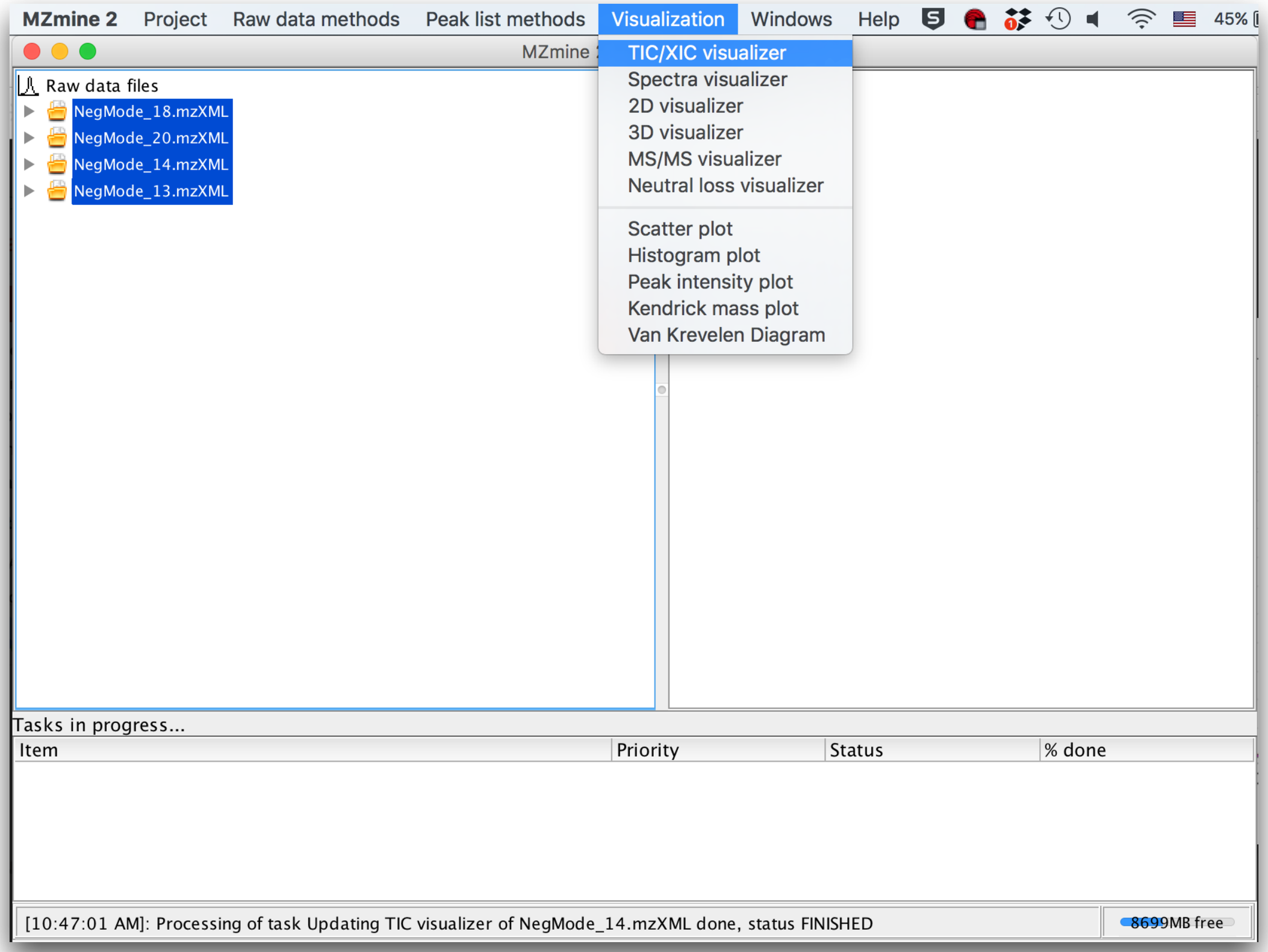
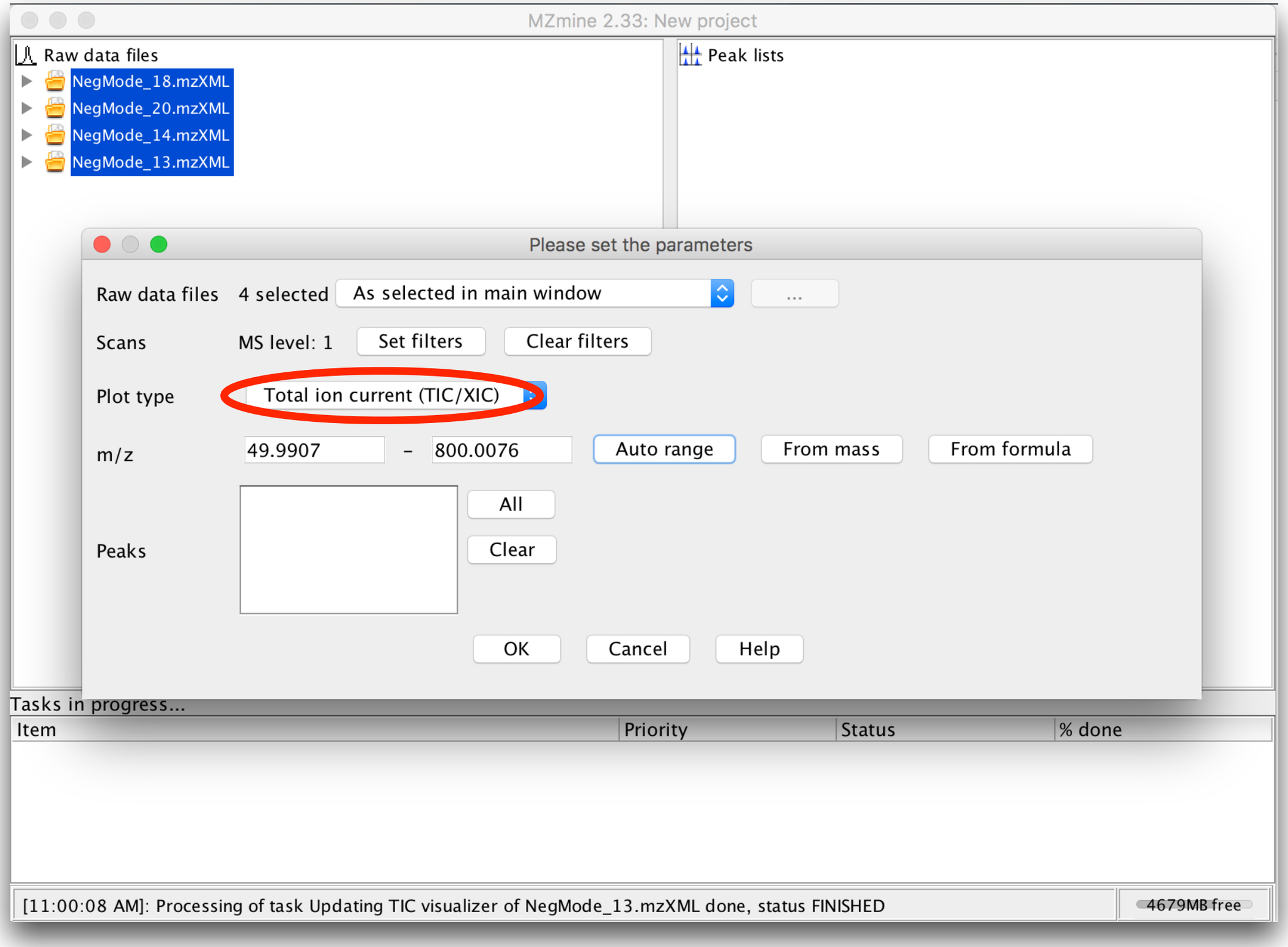


Data visualization: TIC



Data visualization: TIC



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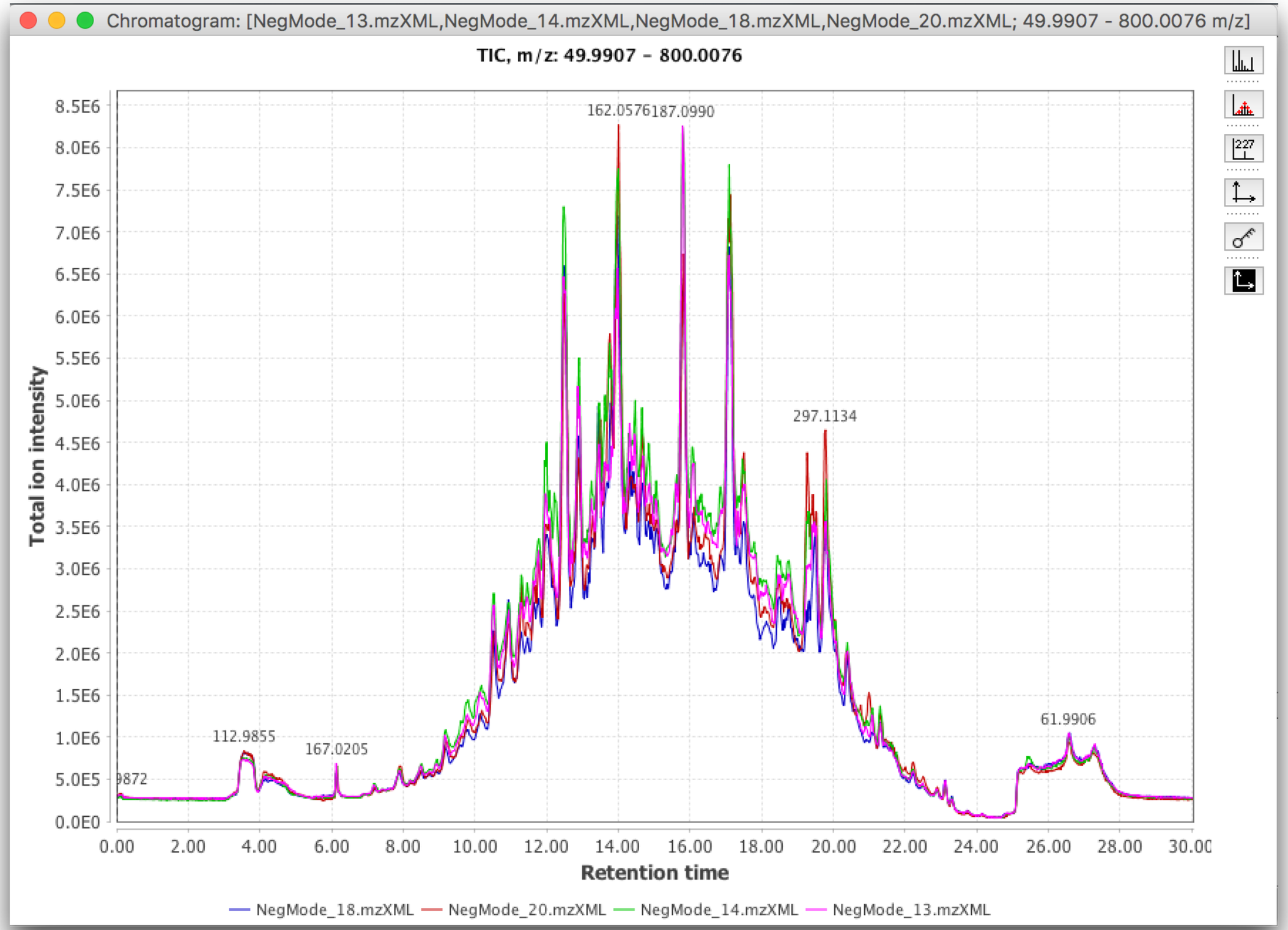
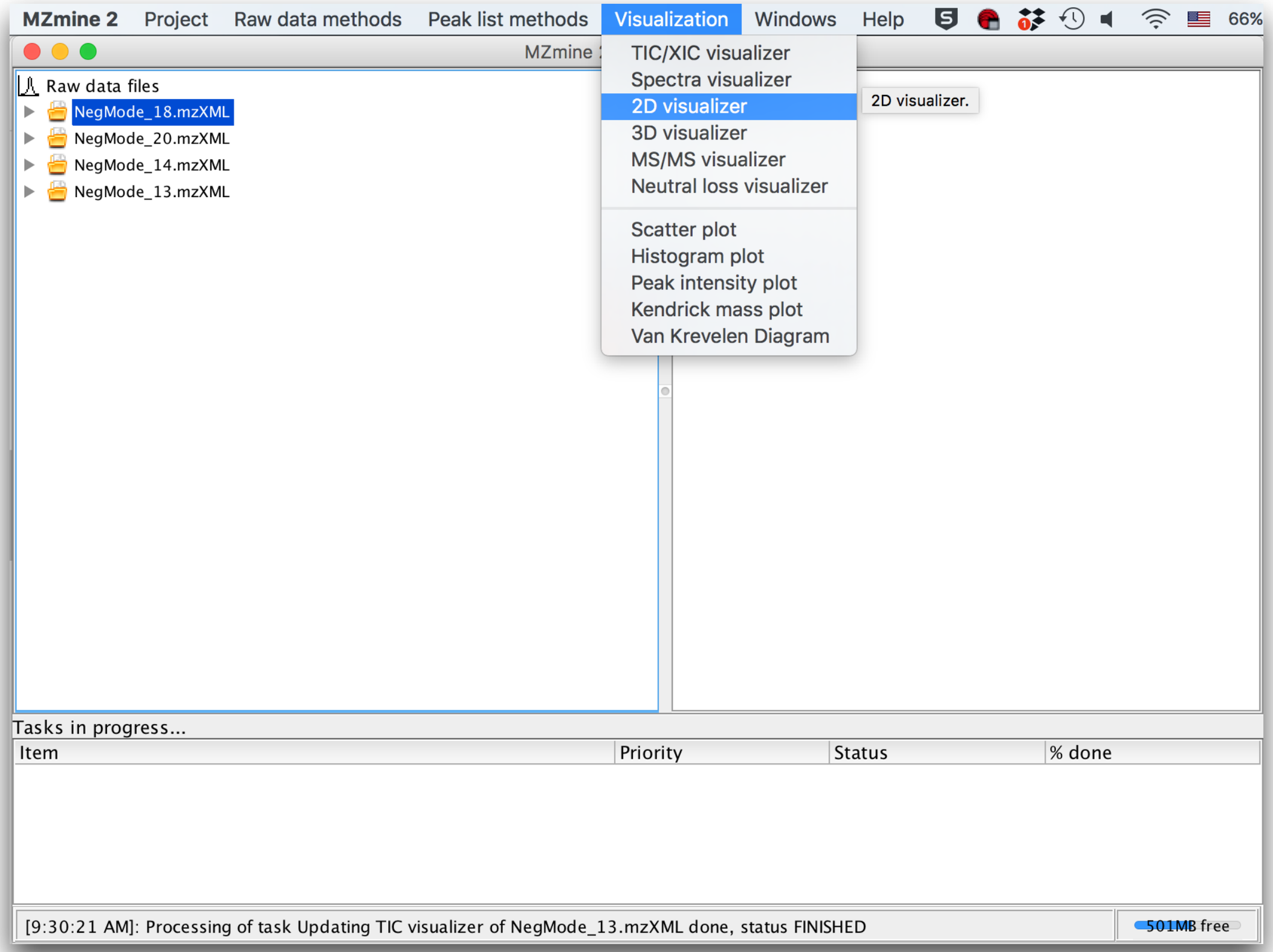


Data visualization: 2D



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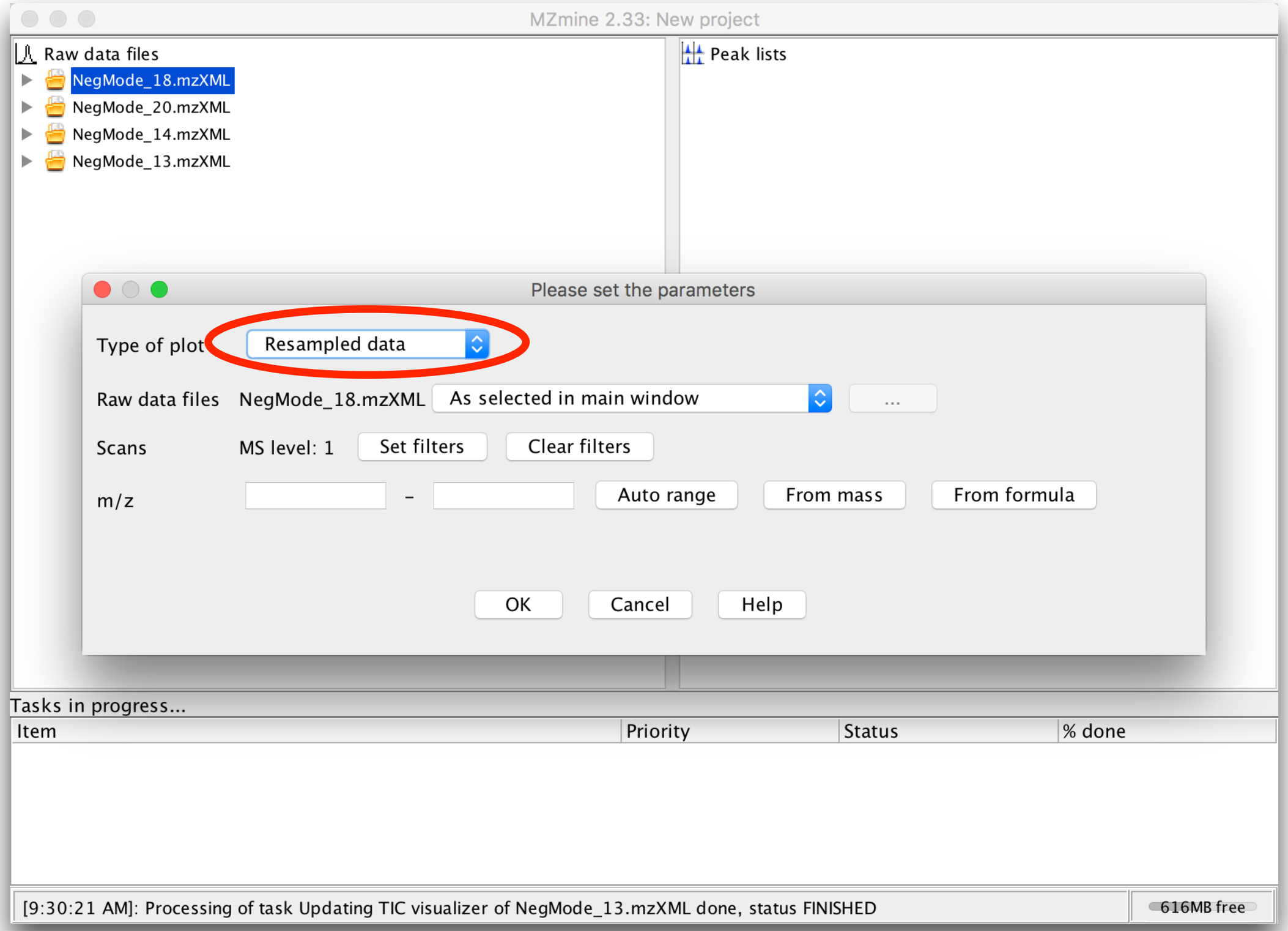

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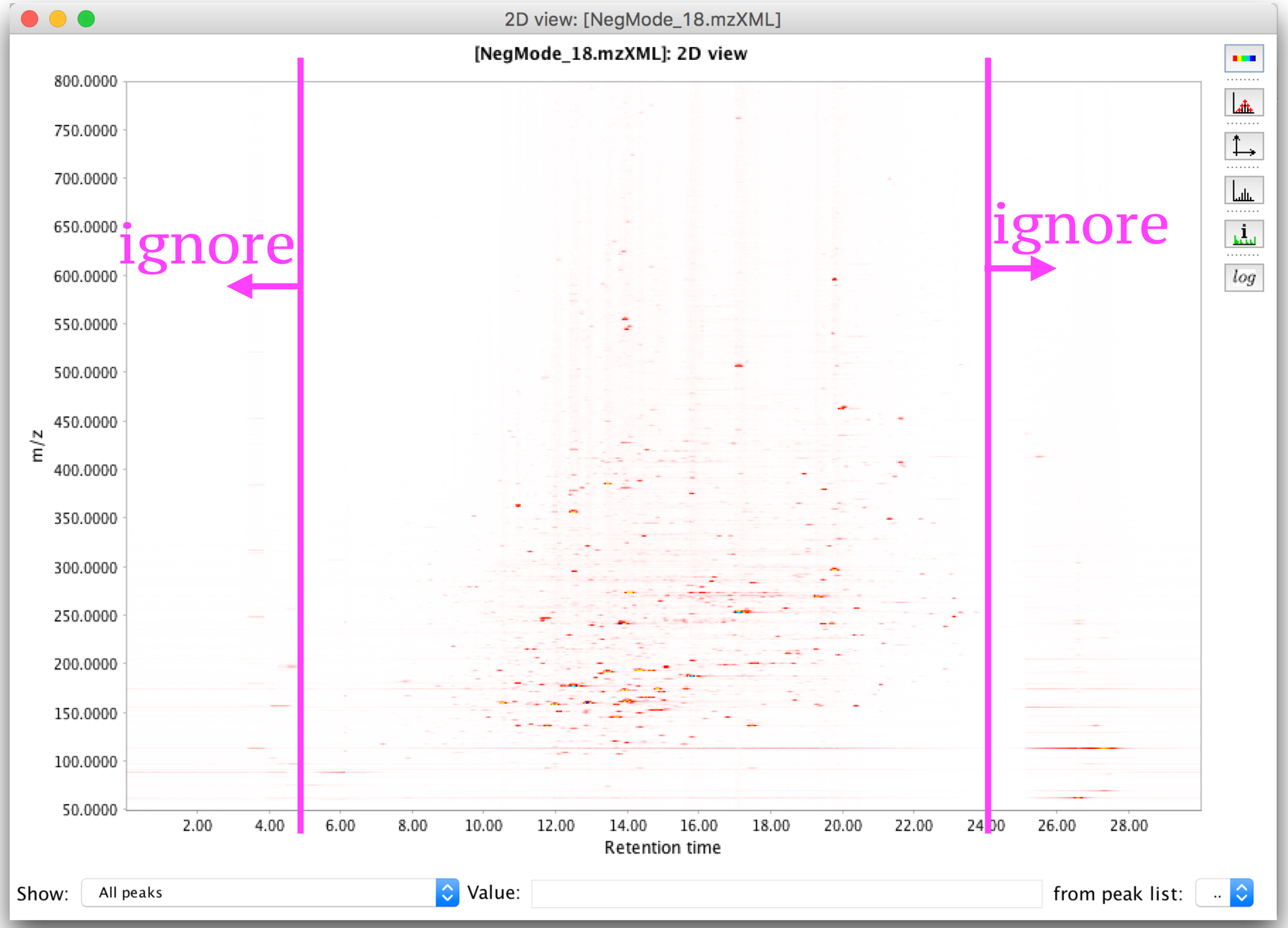

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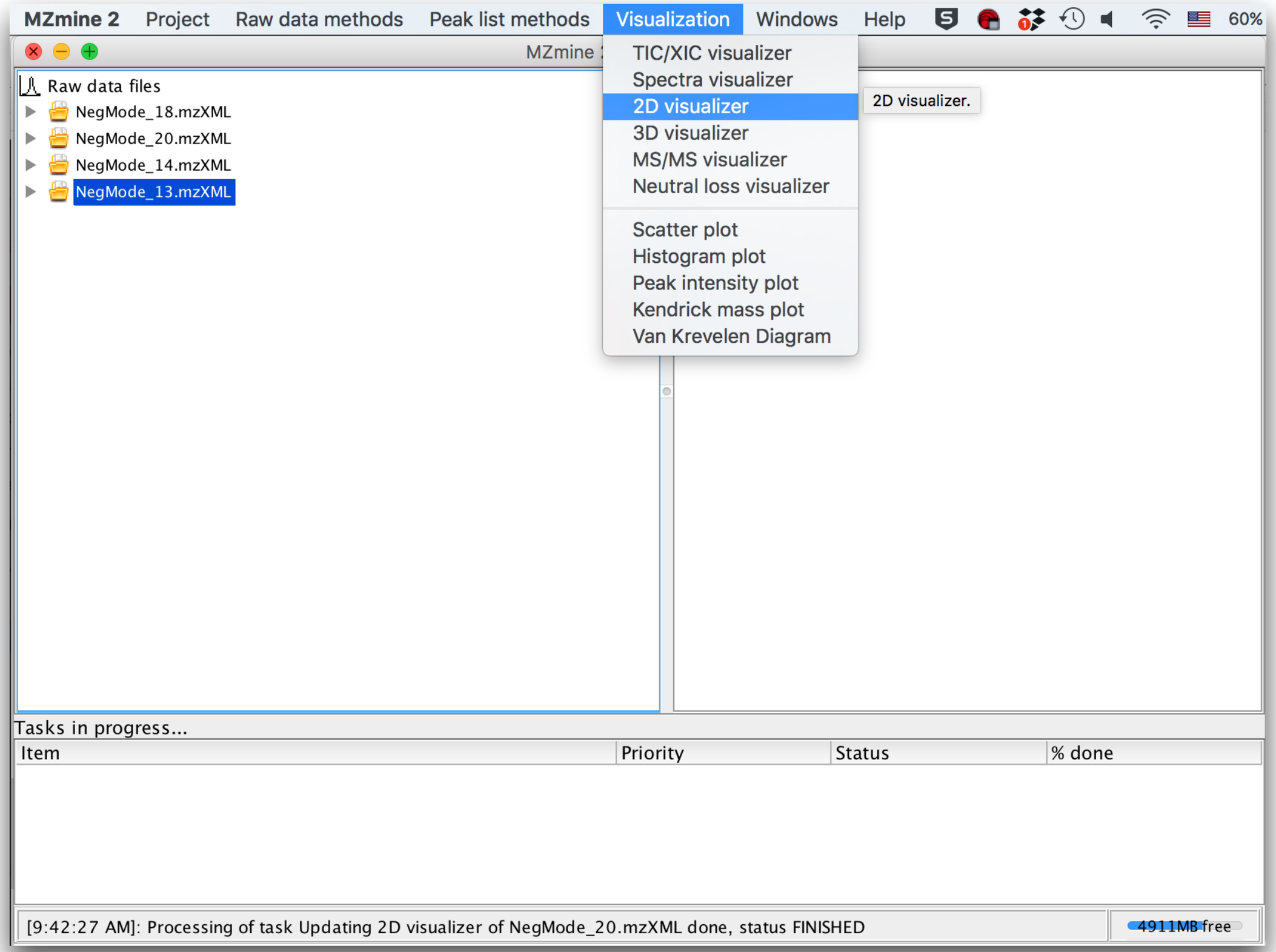

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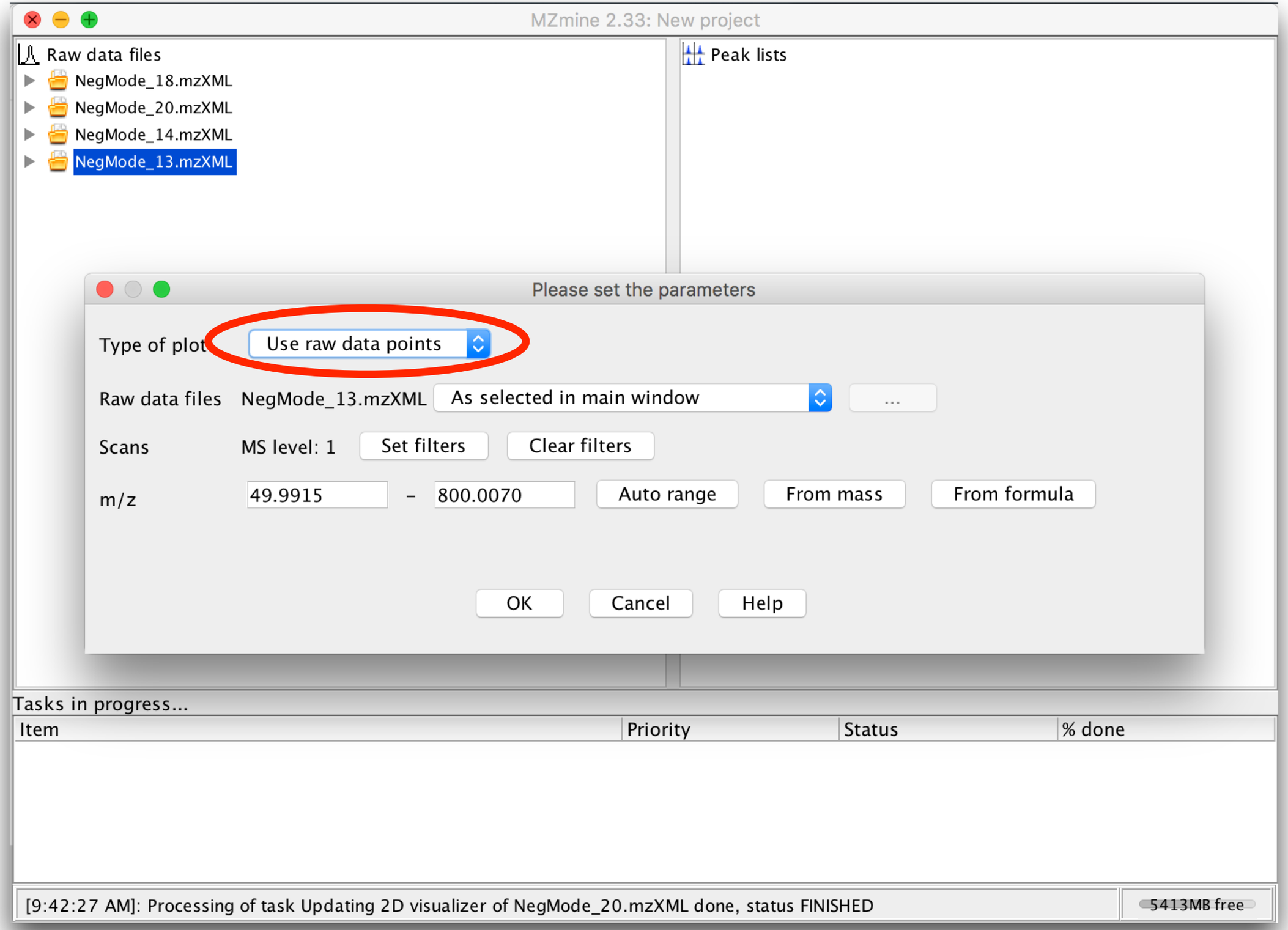

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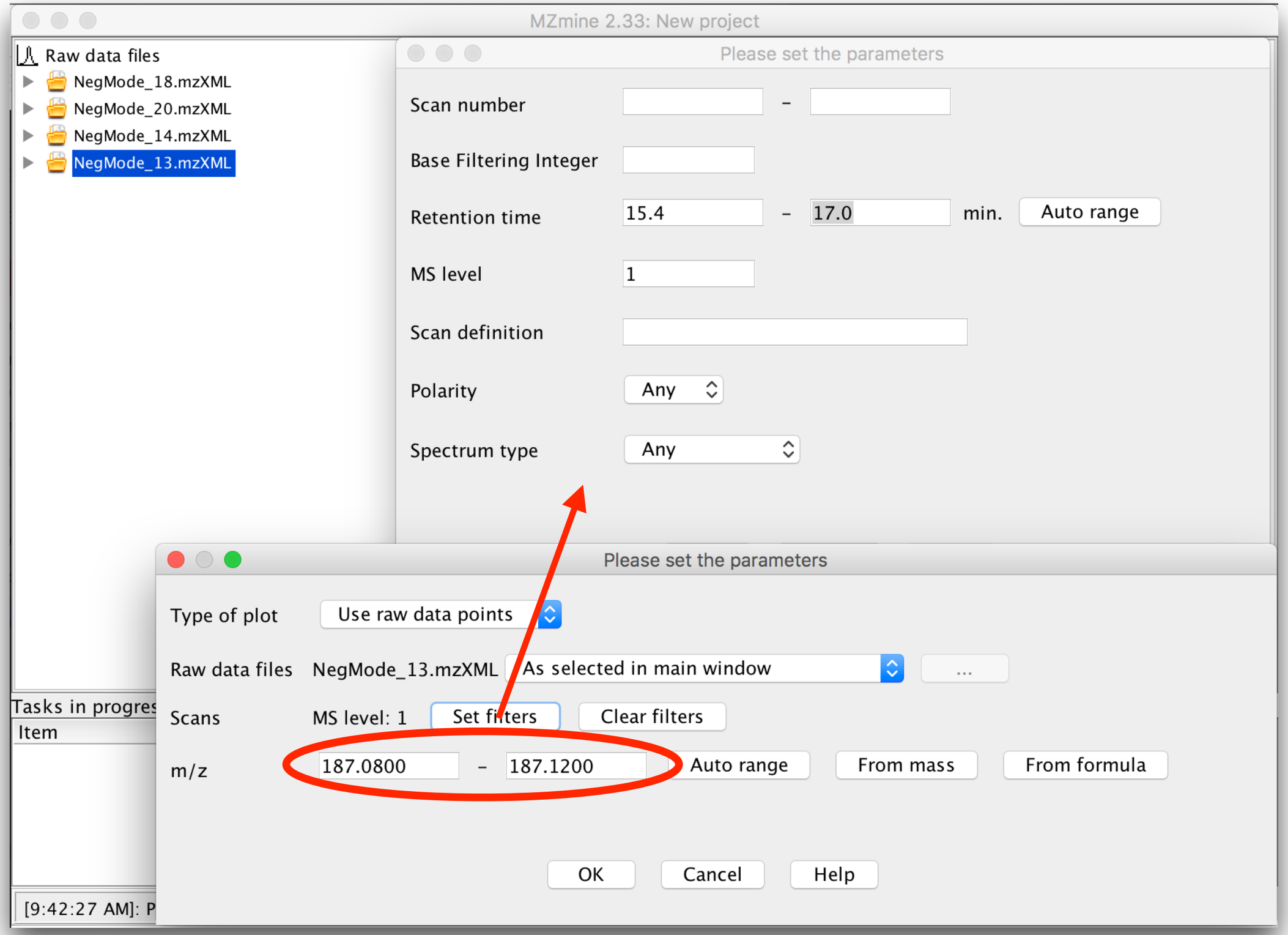

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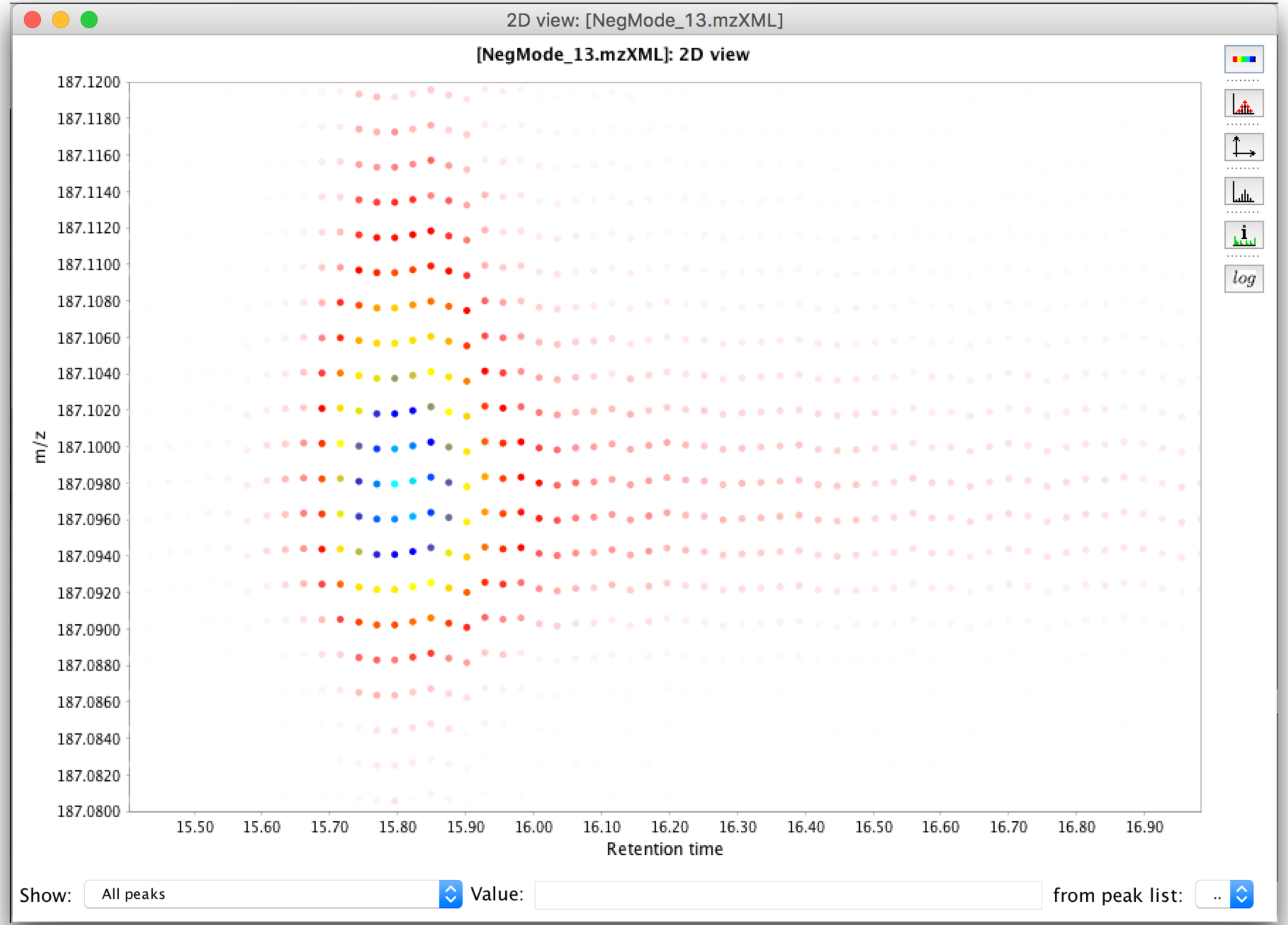
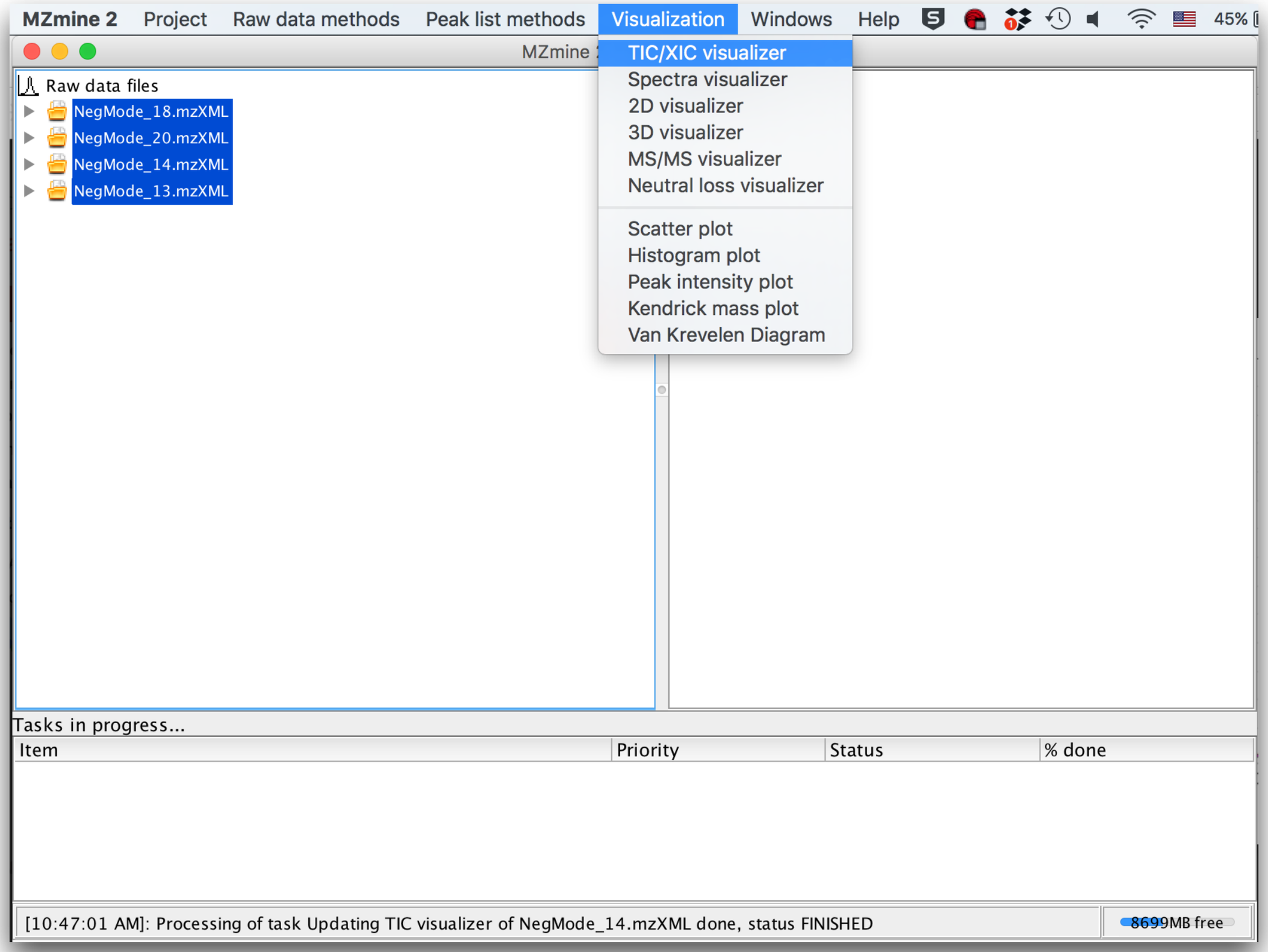


Data visualization: EIC



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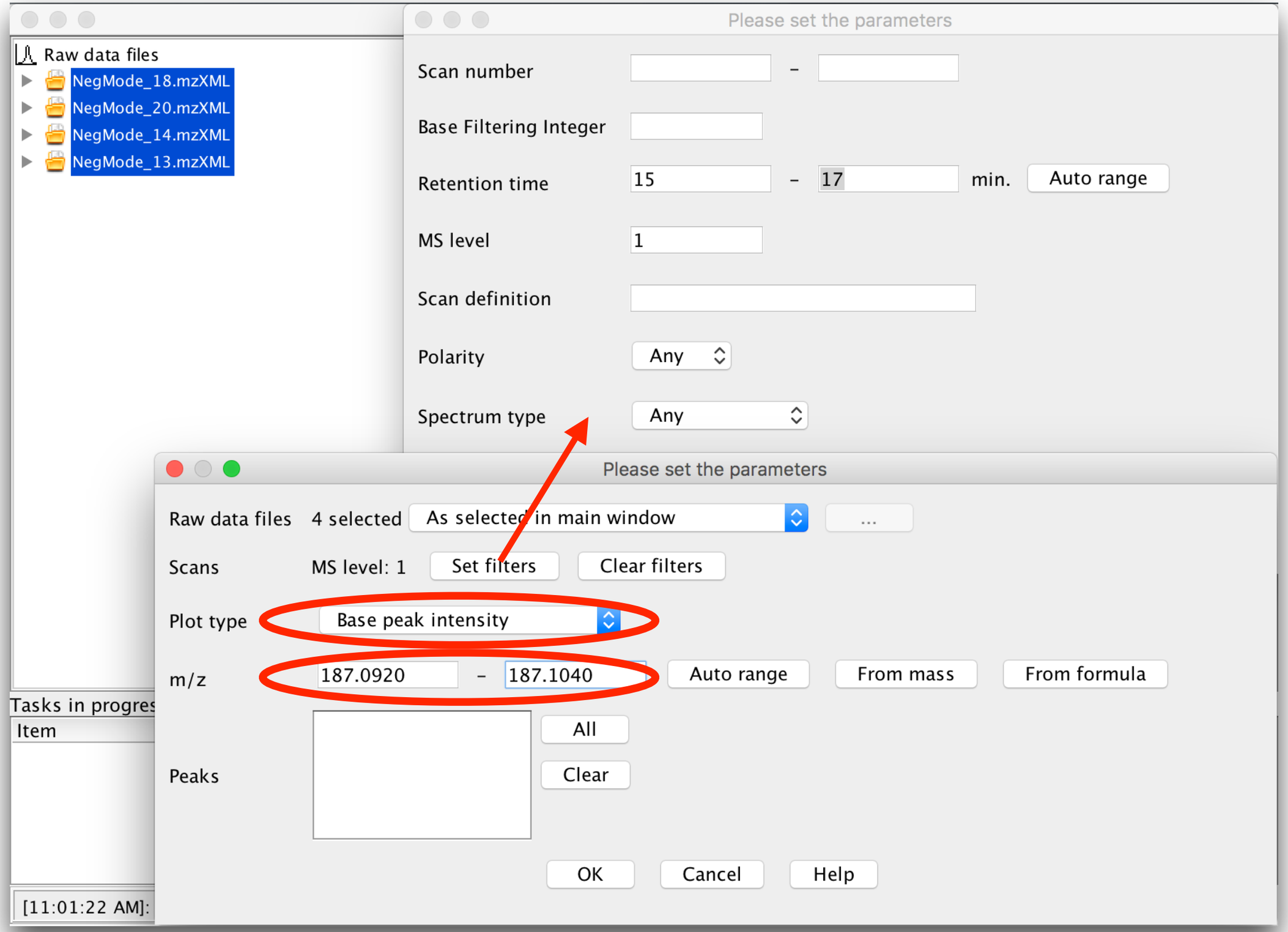

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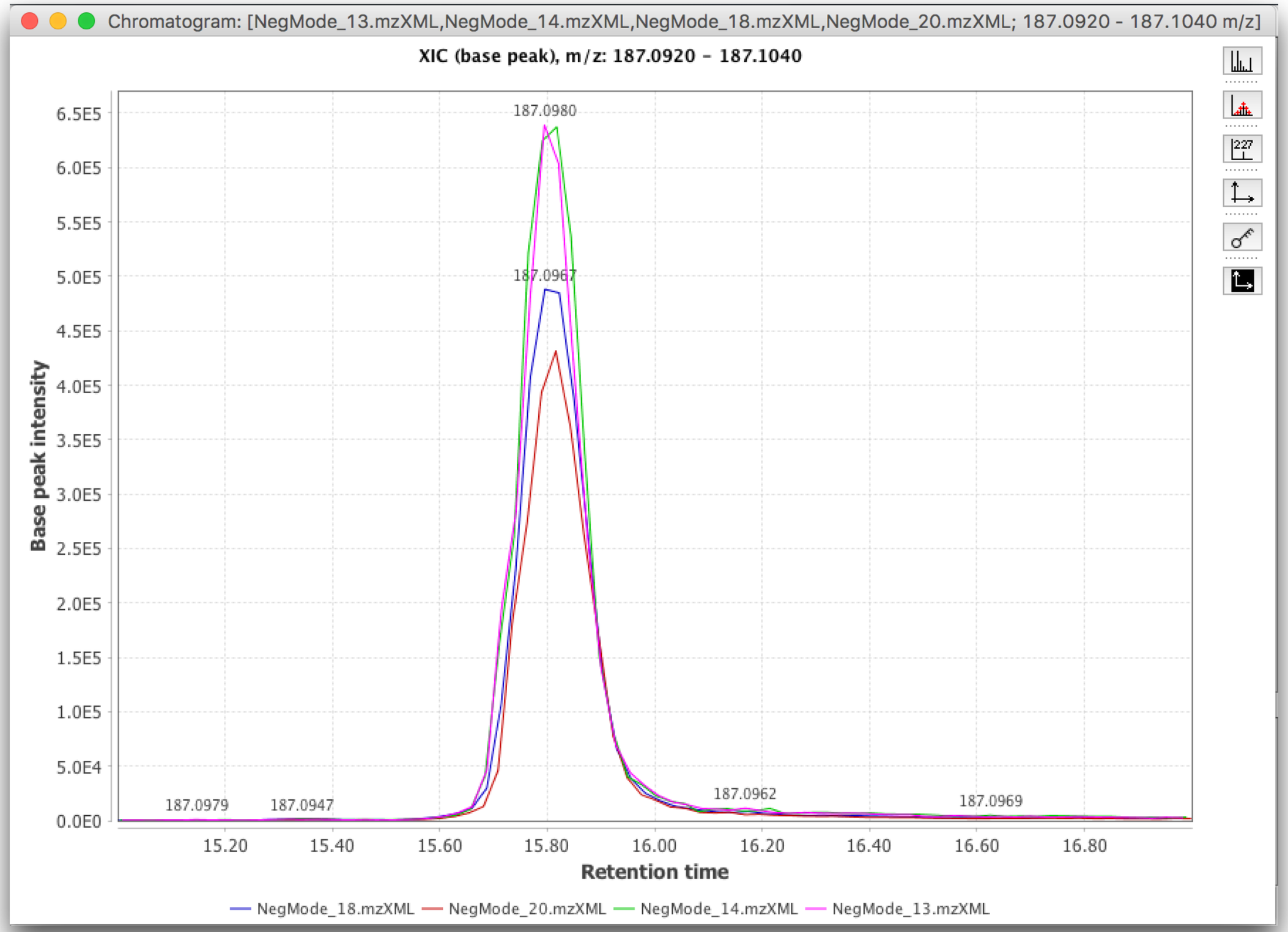

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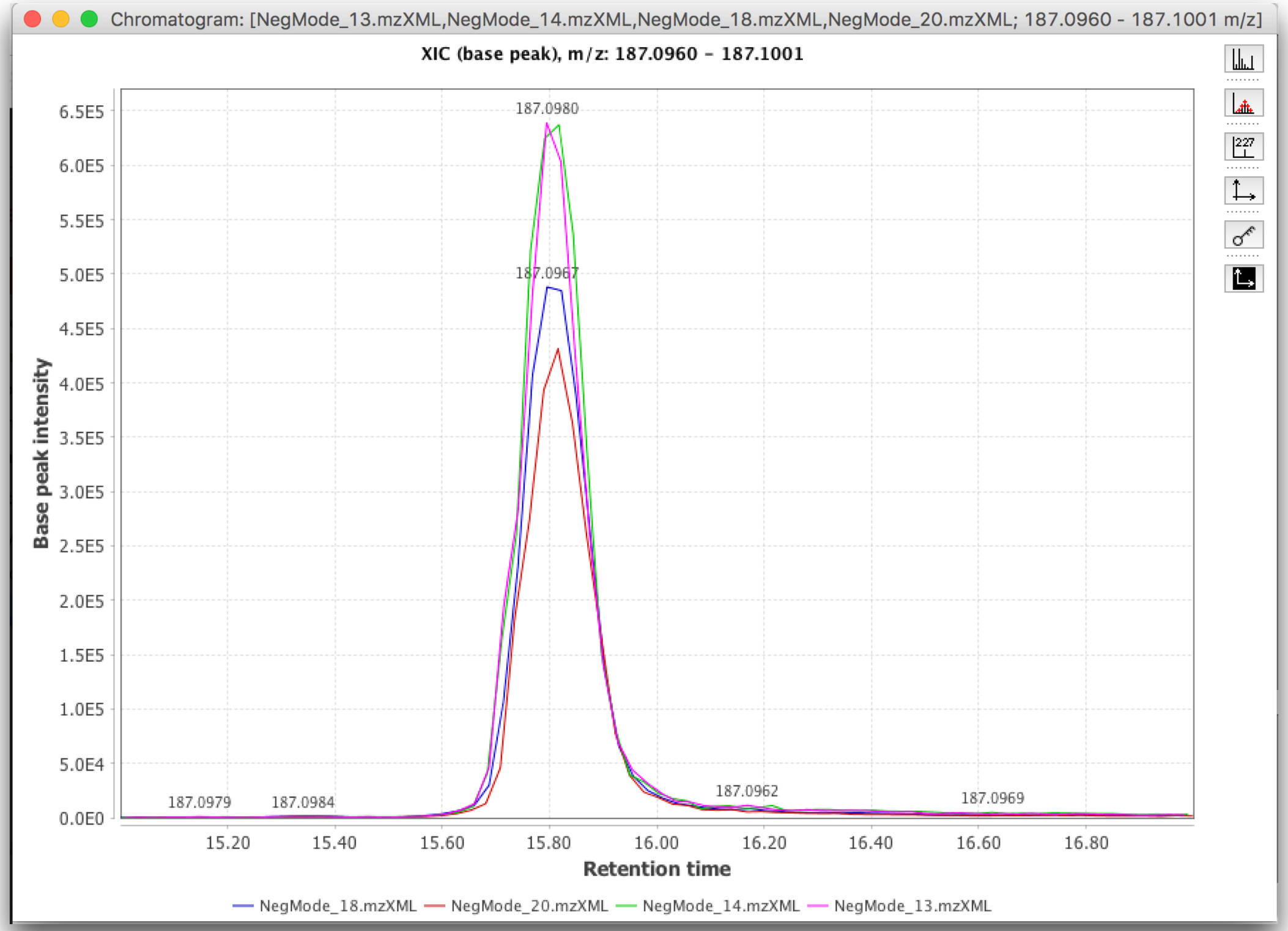

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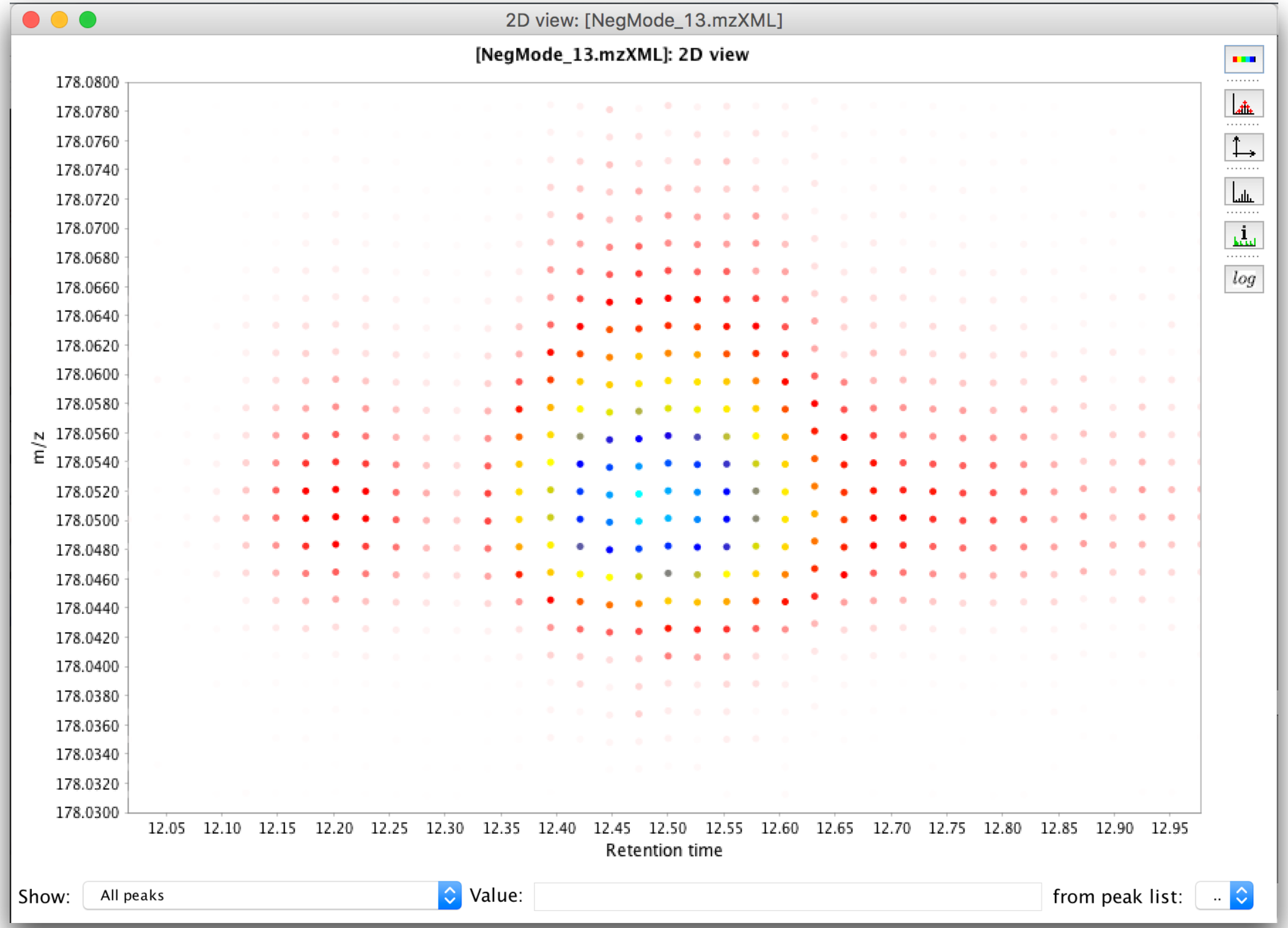

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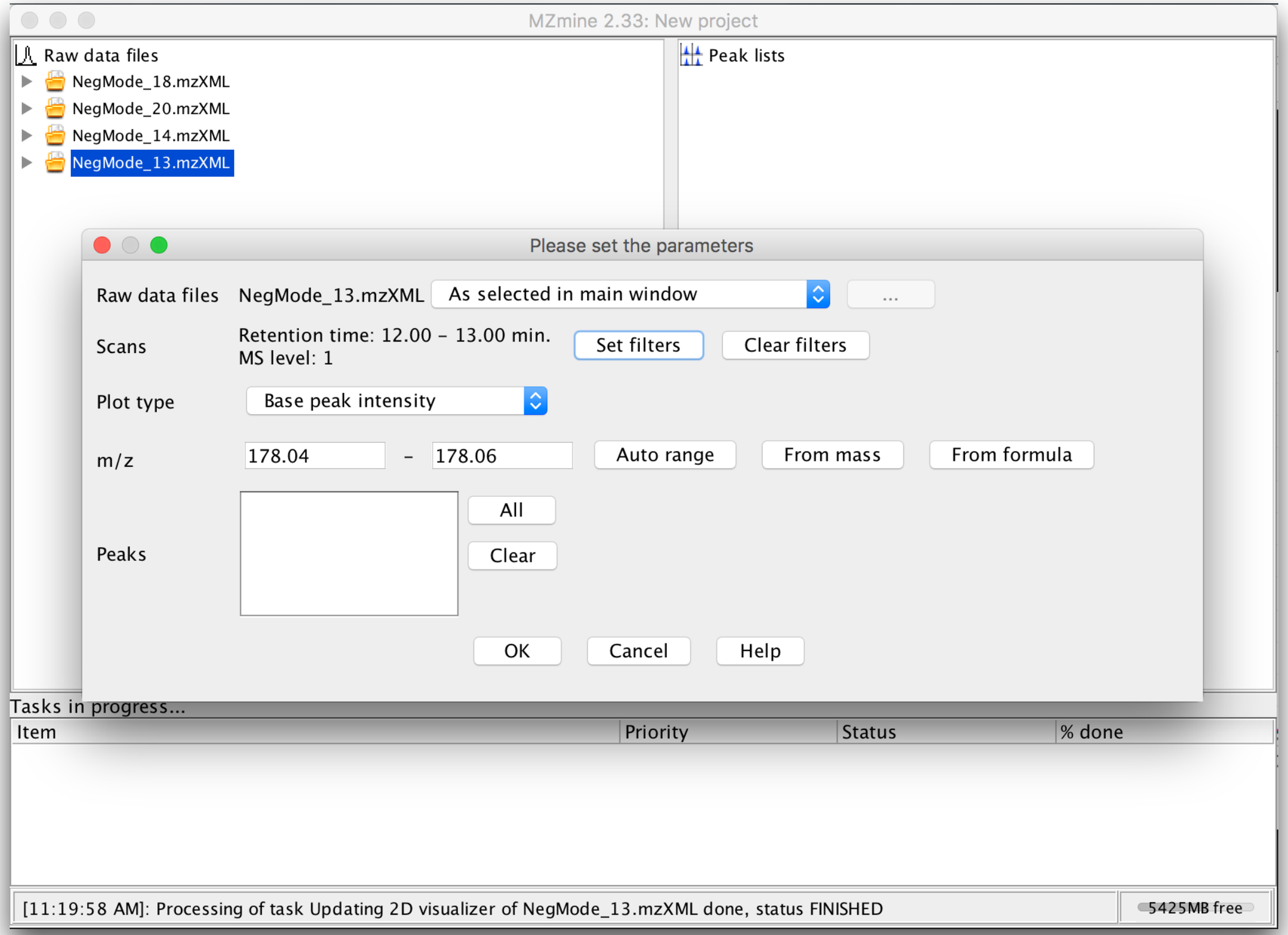

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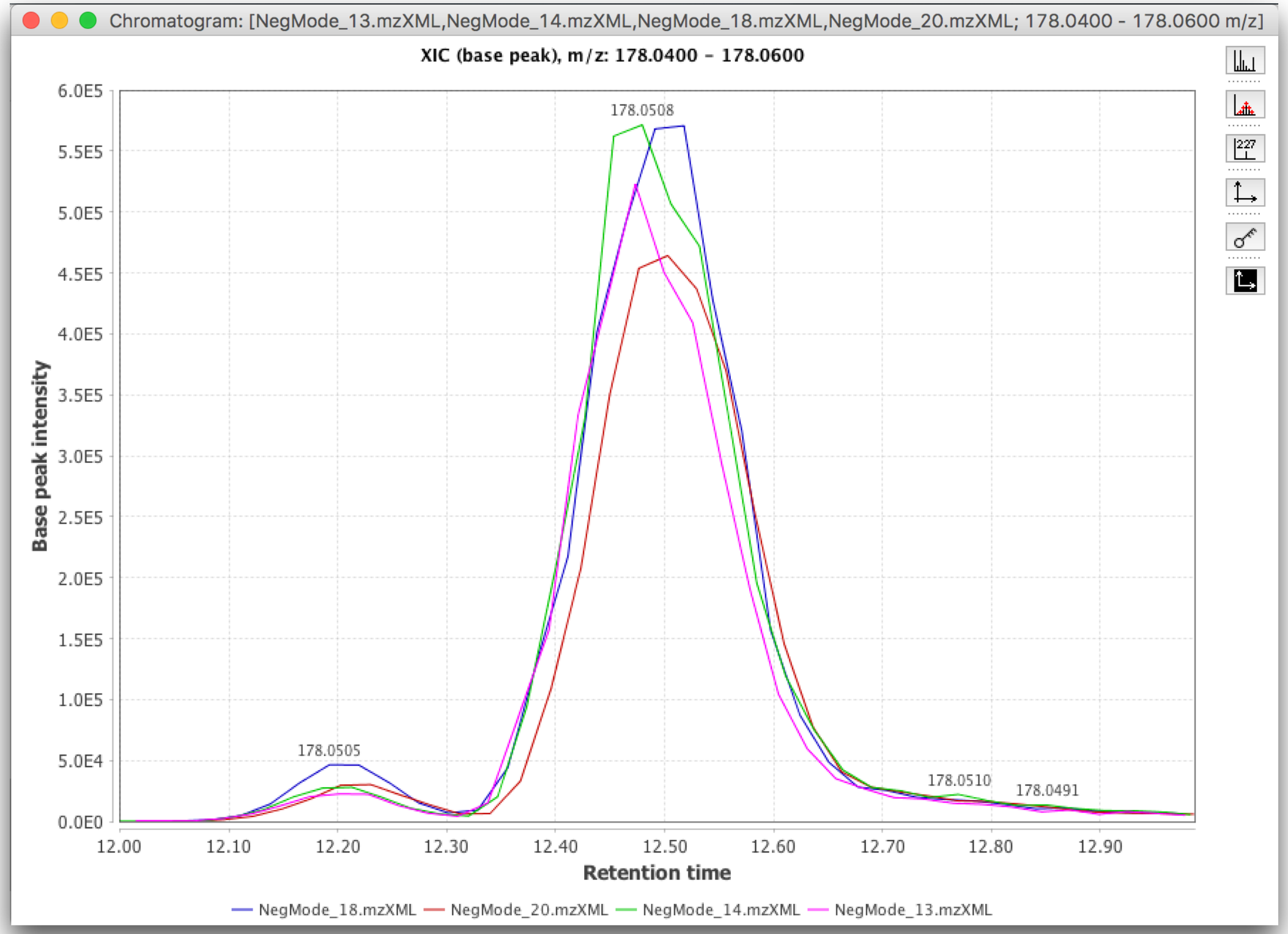

Mass detection

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

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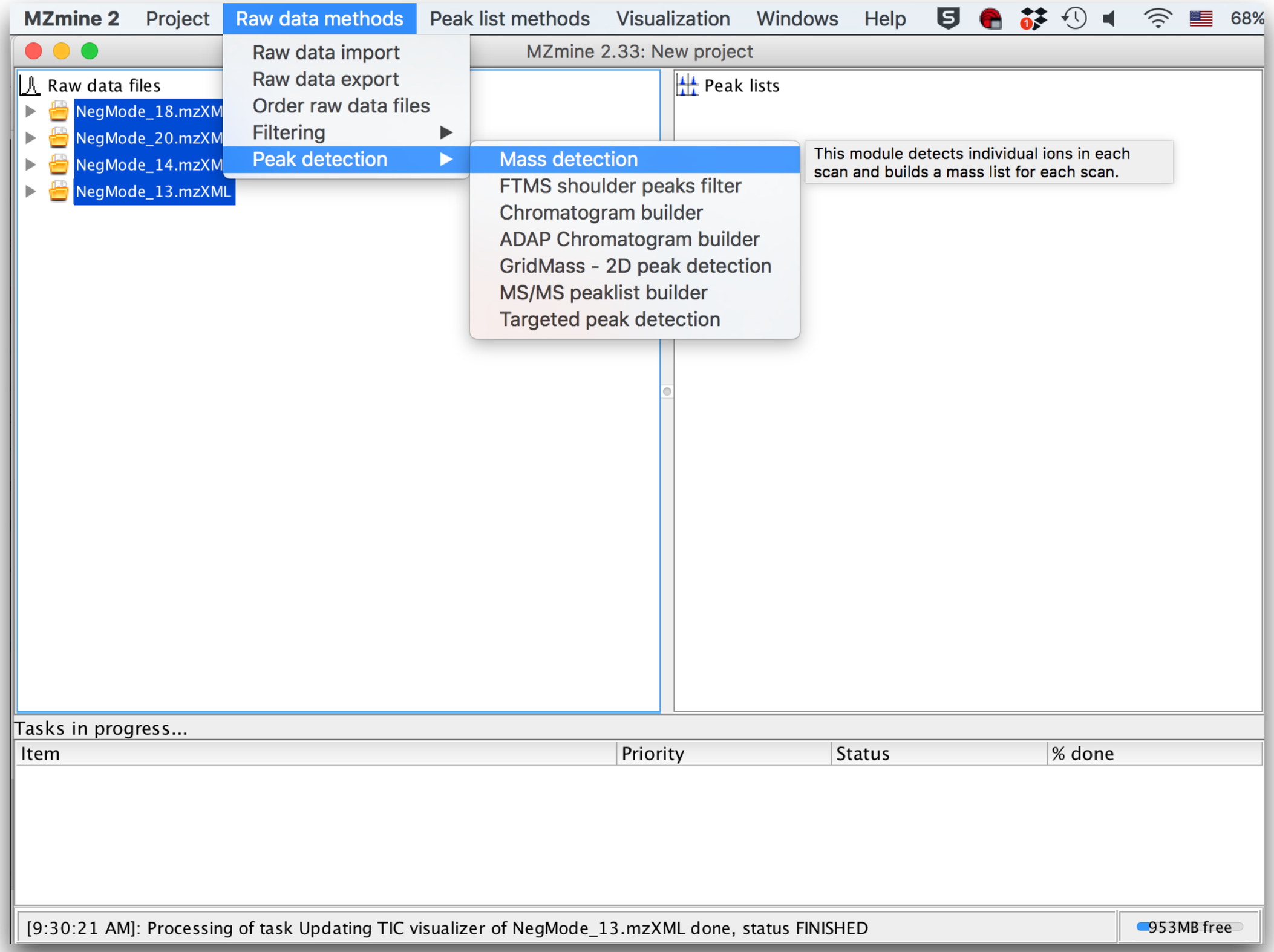

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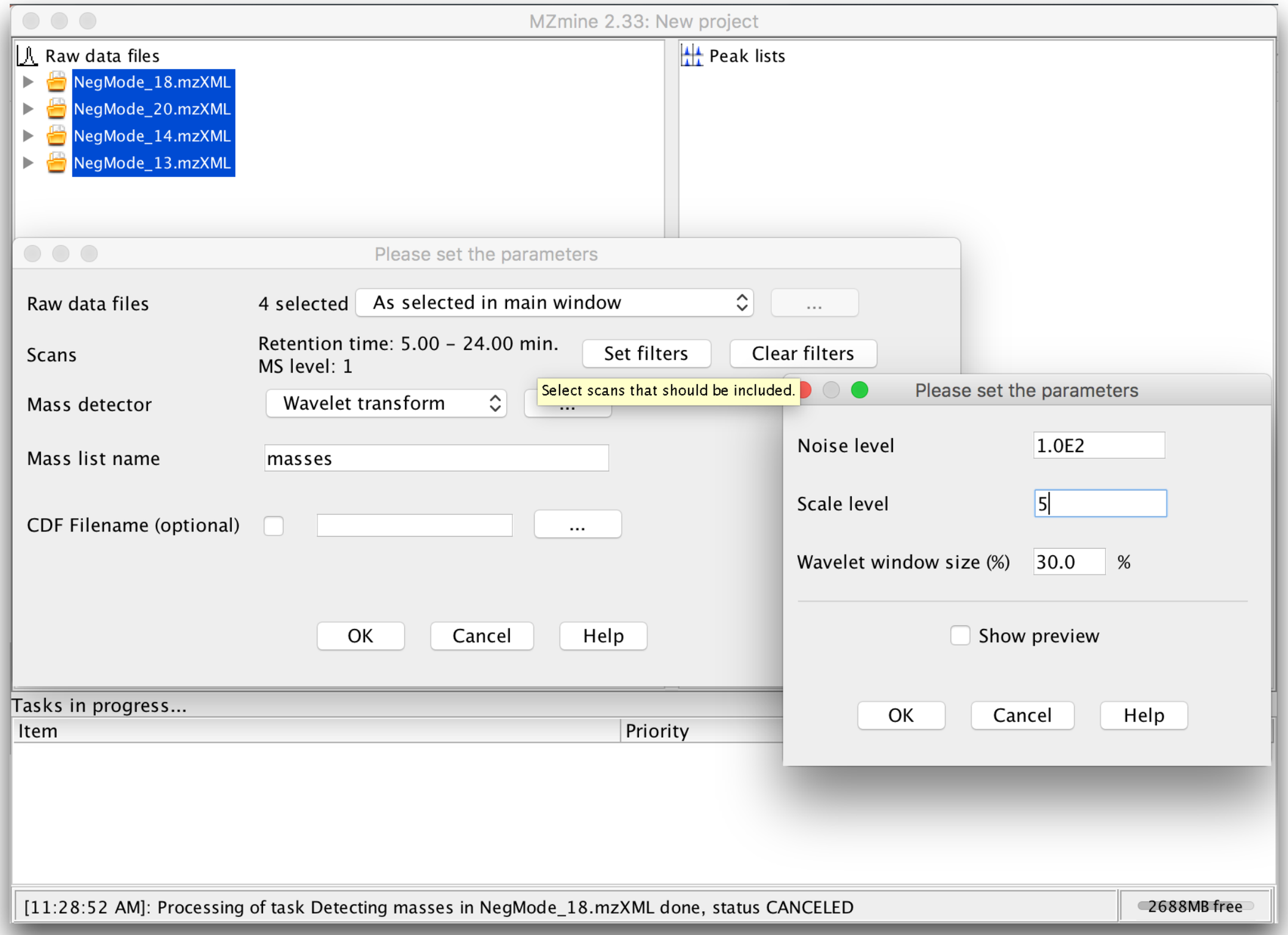
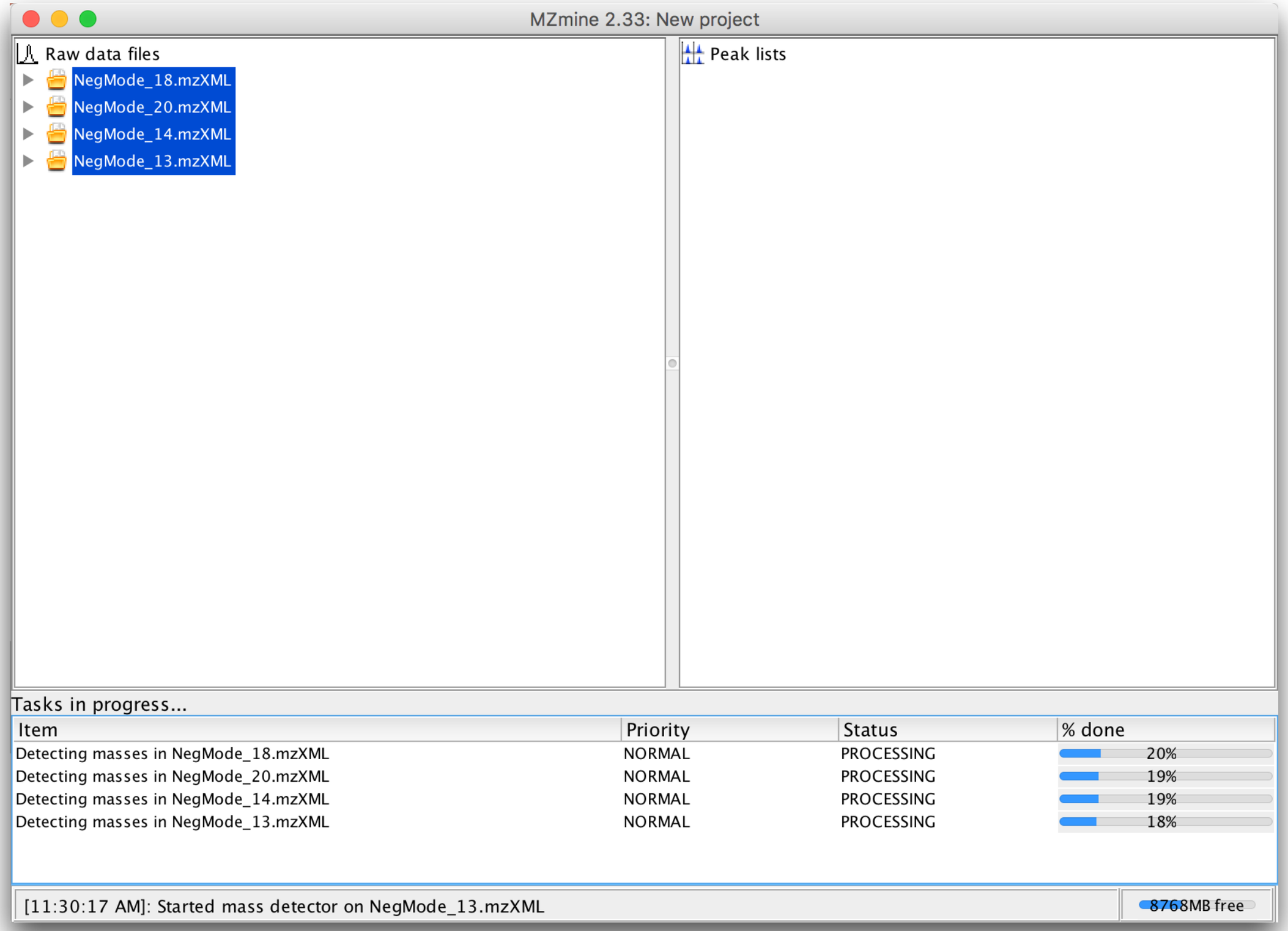


Mass detection



Mass detection

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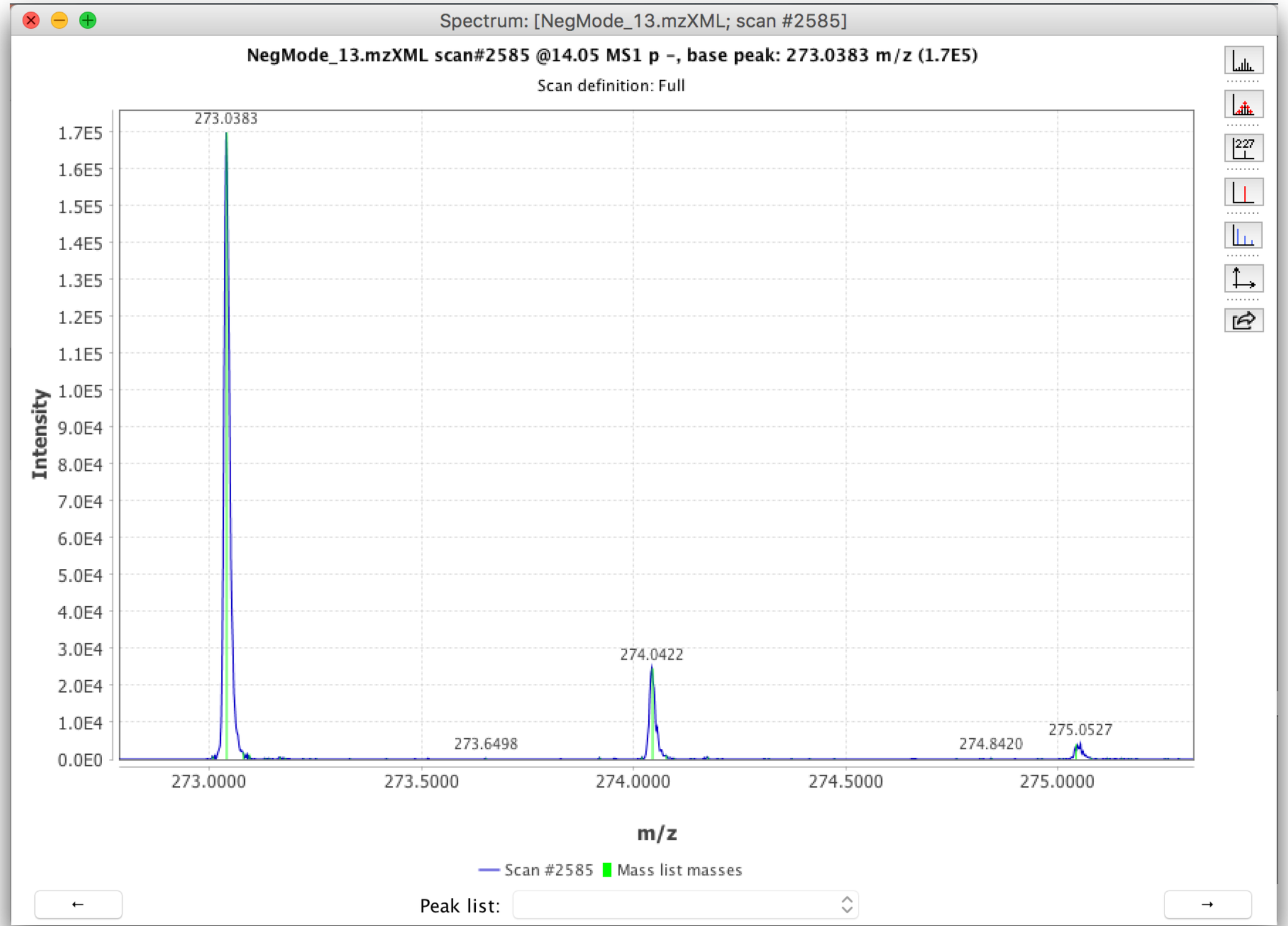
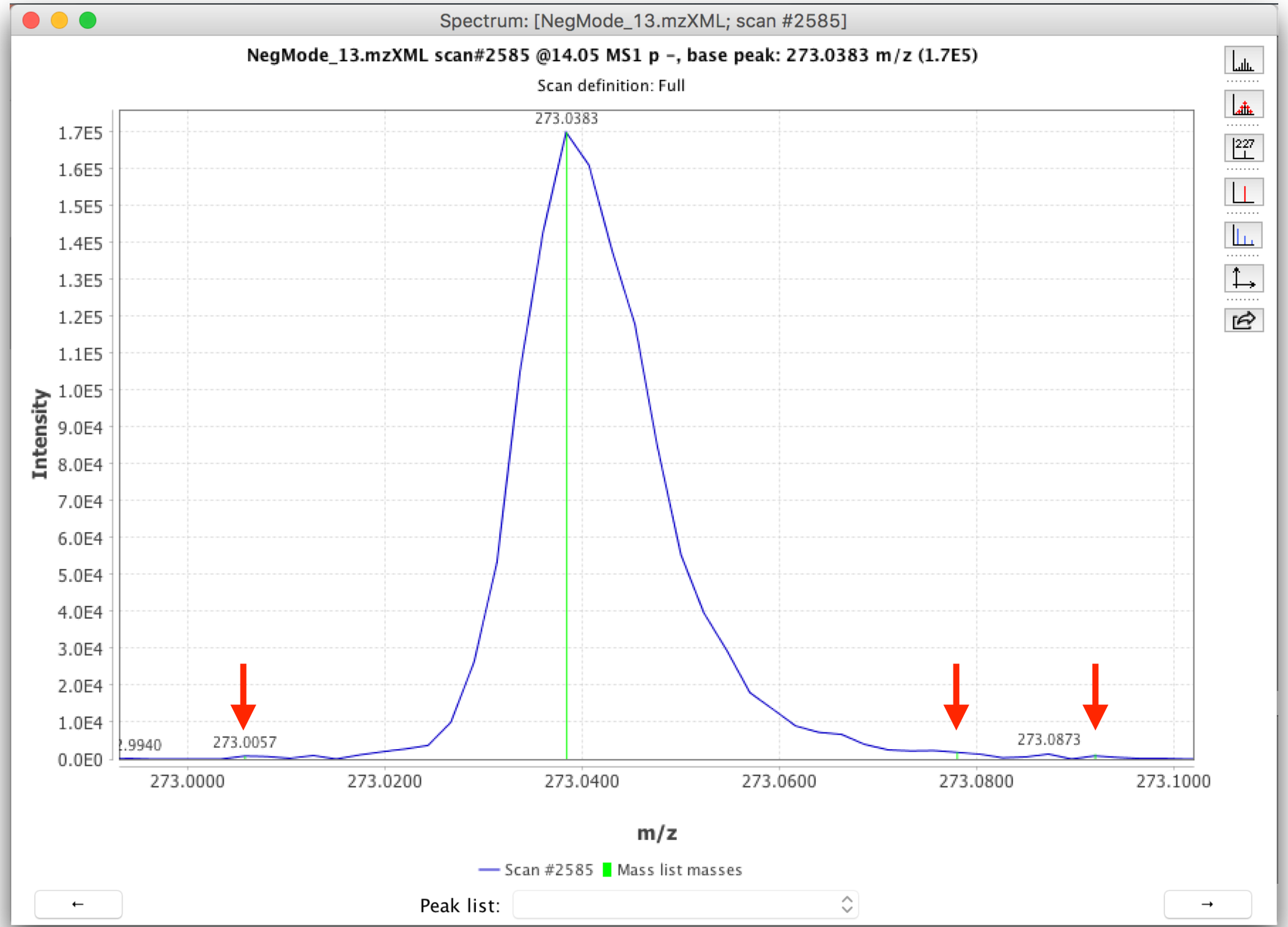
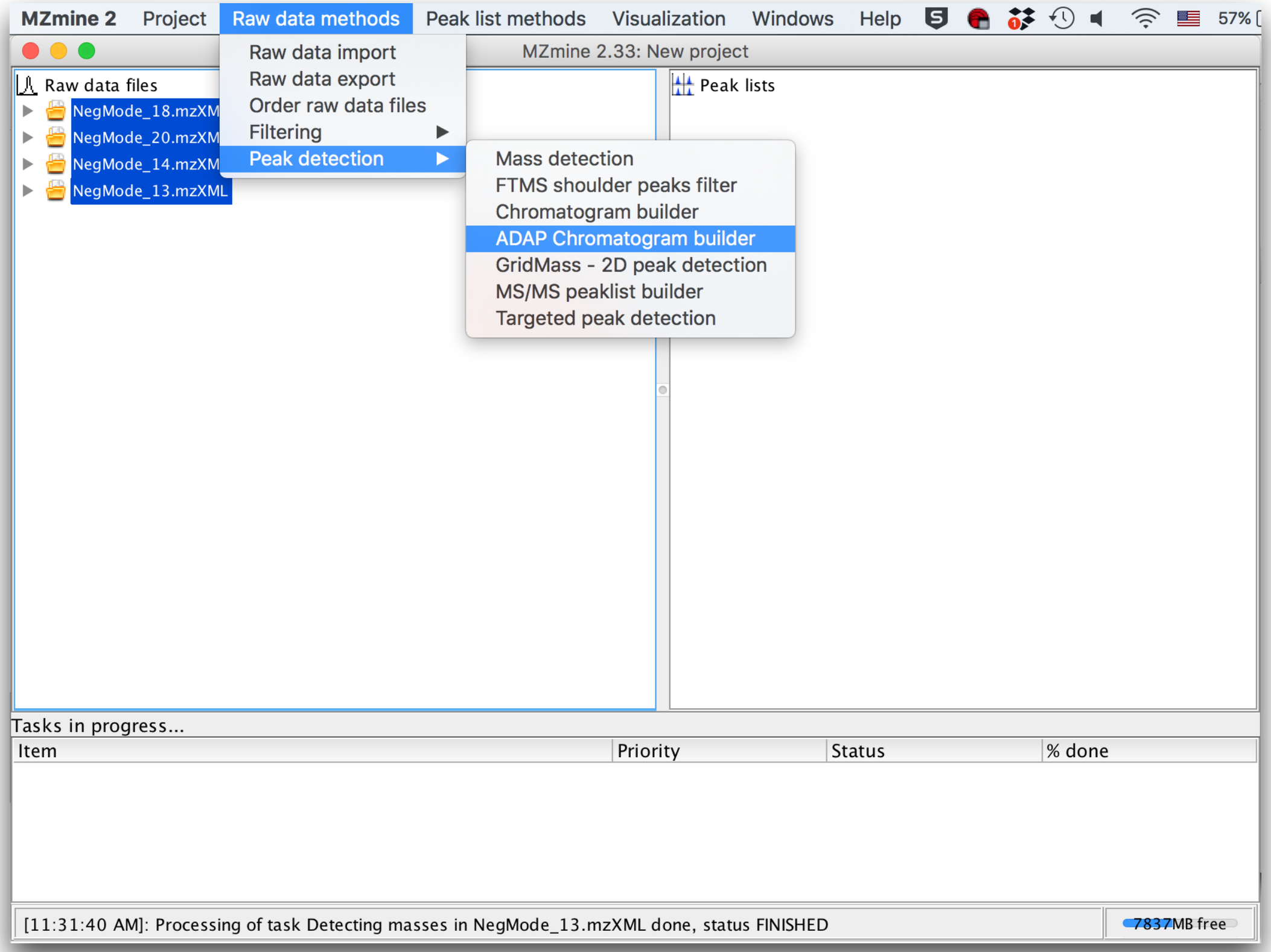


Mass detection



EIC construction



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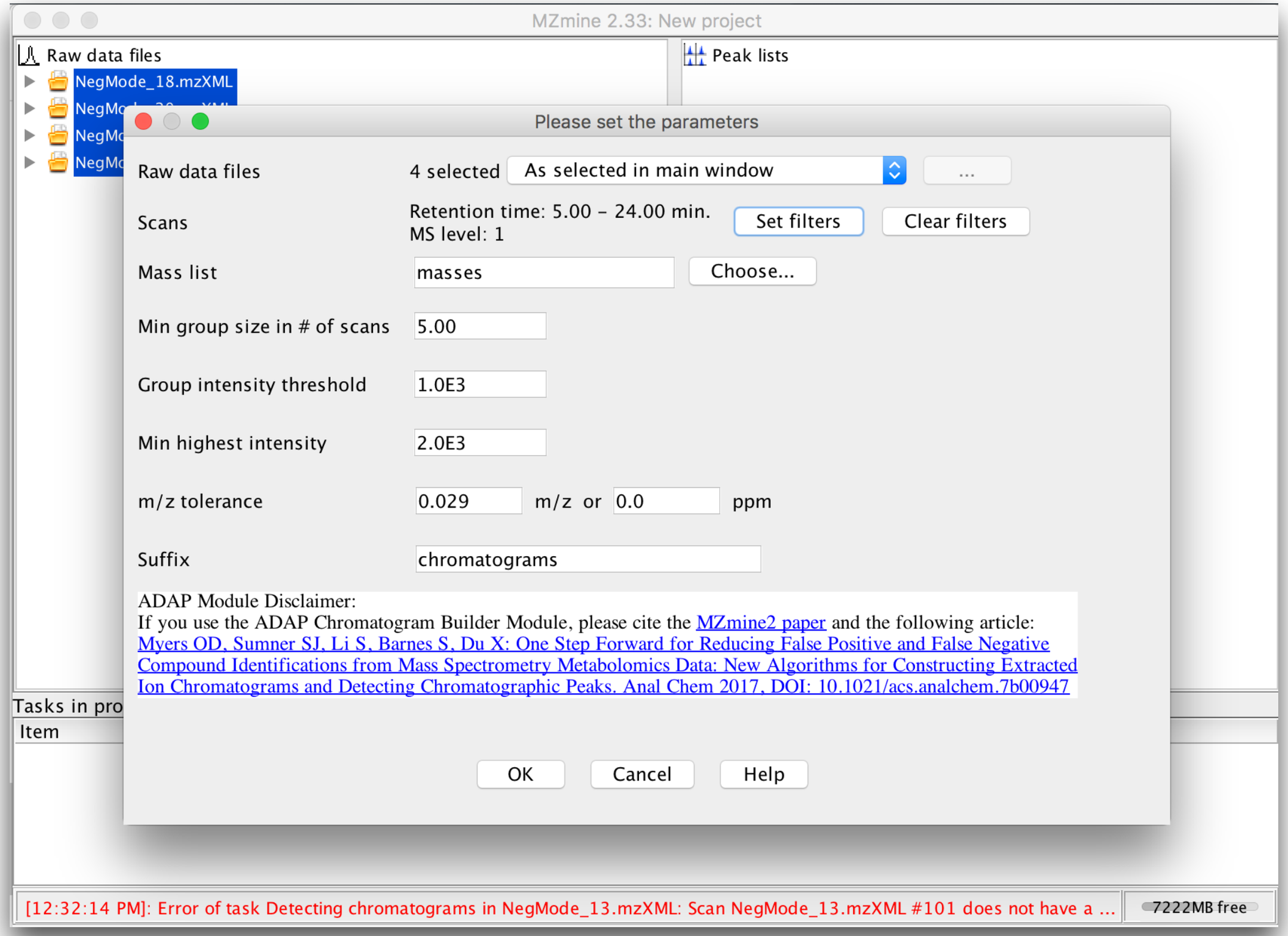
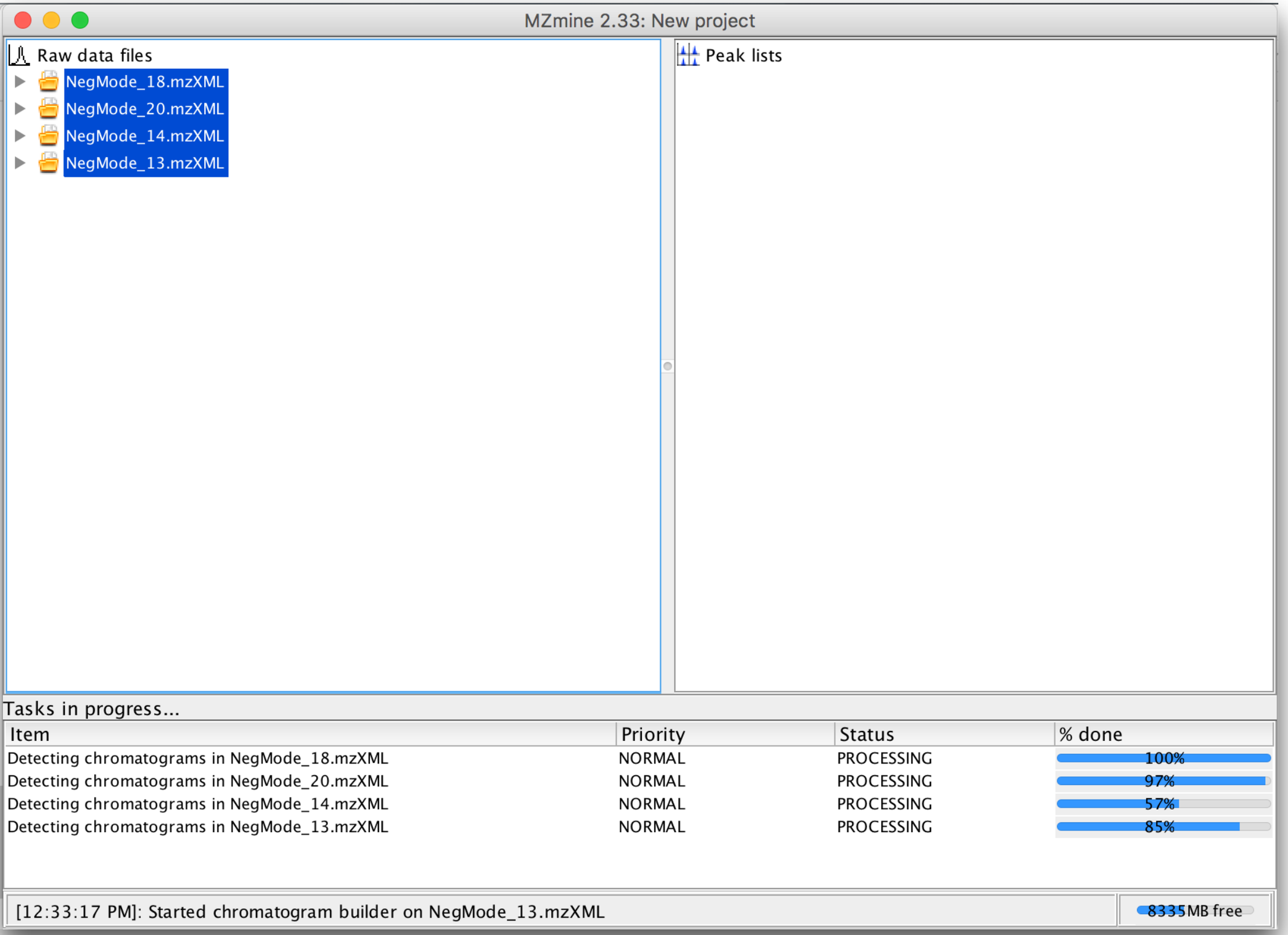
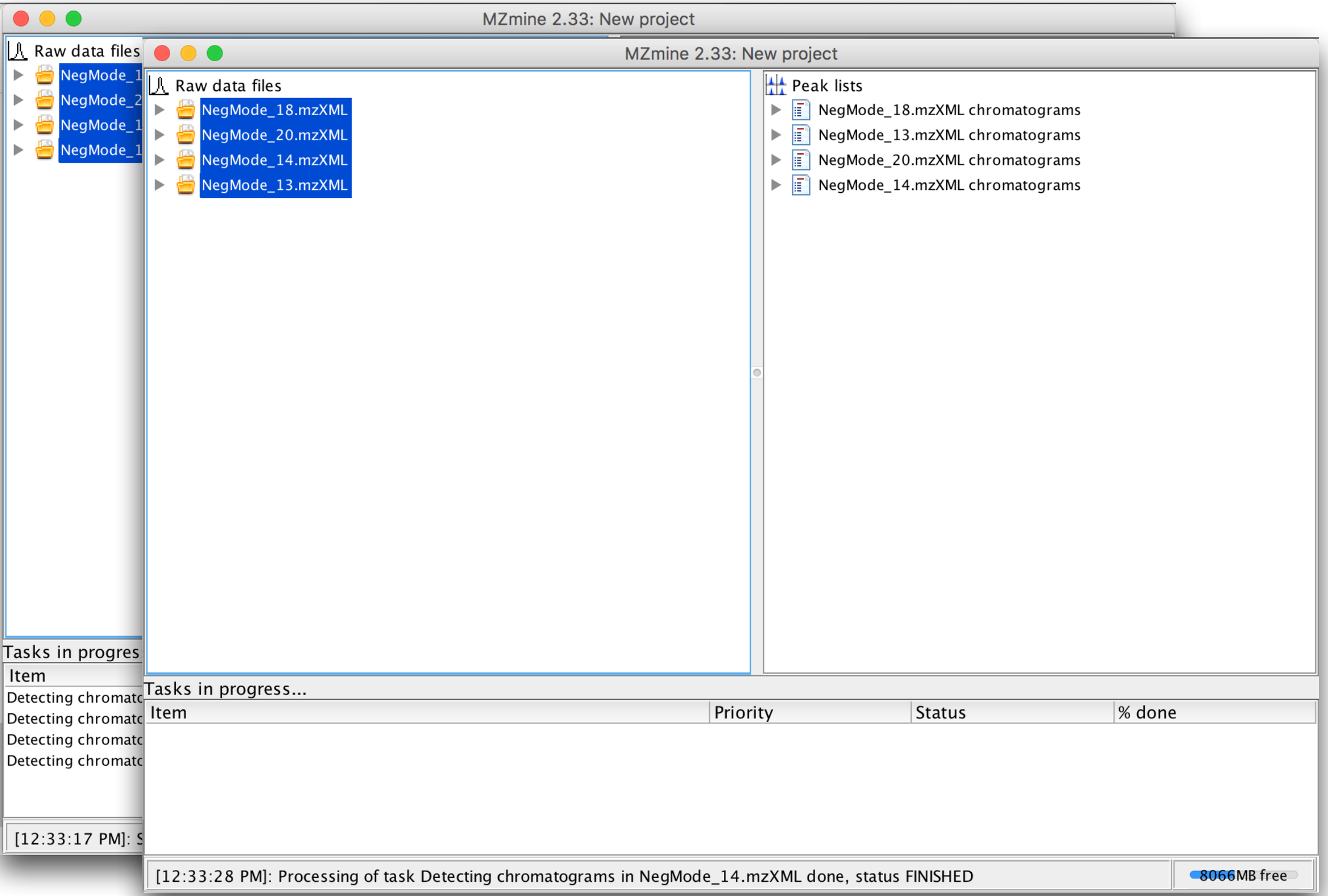


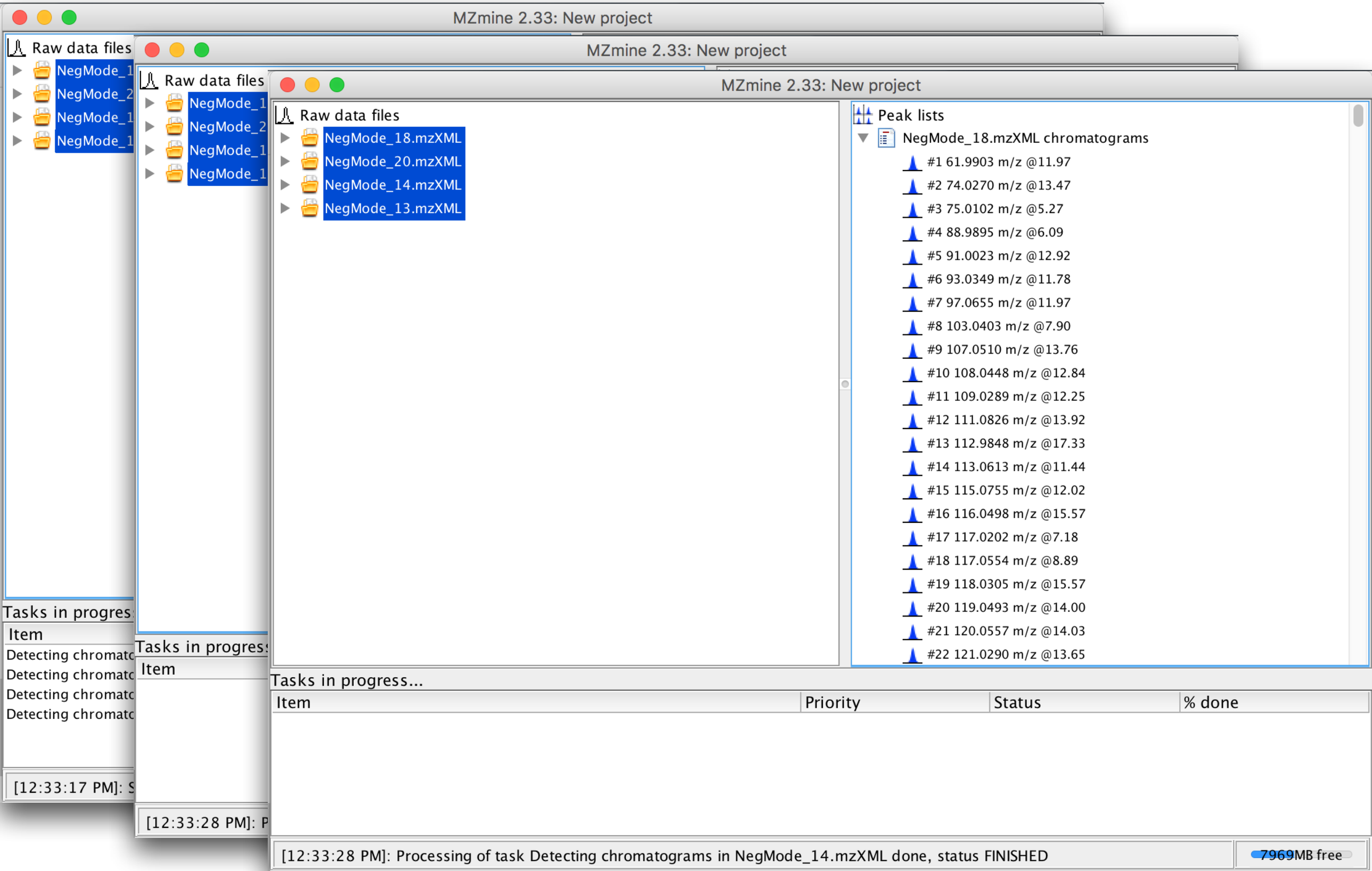
EIC construction



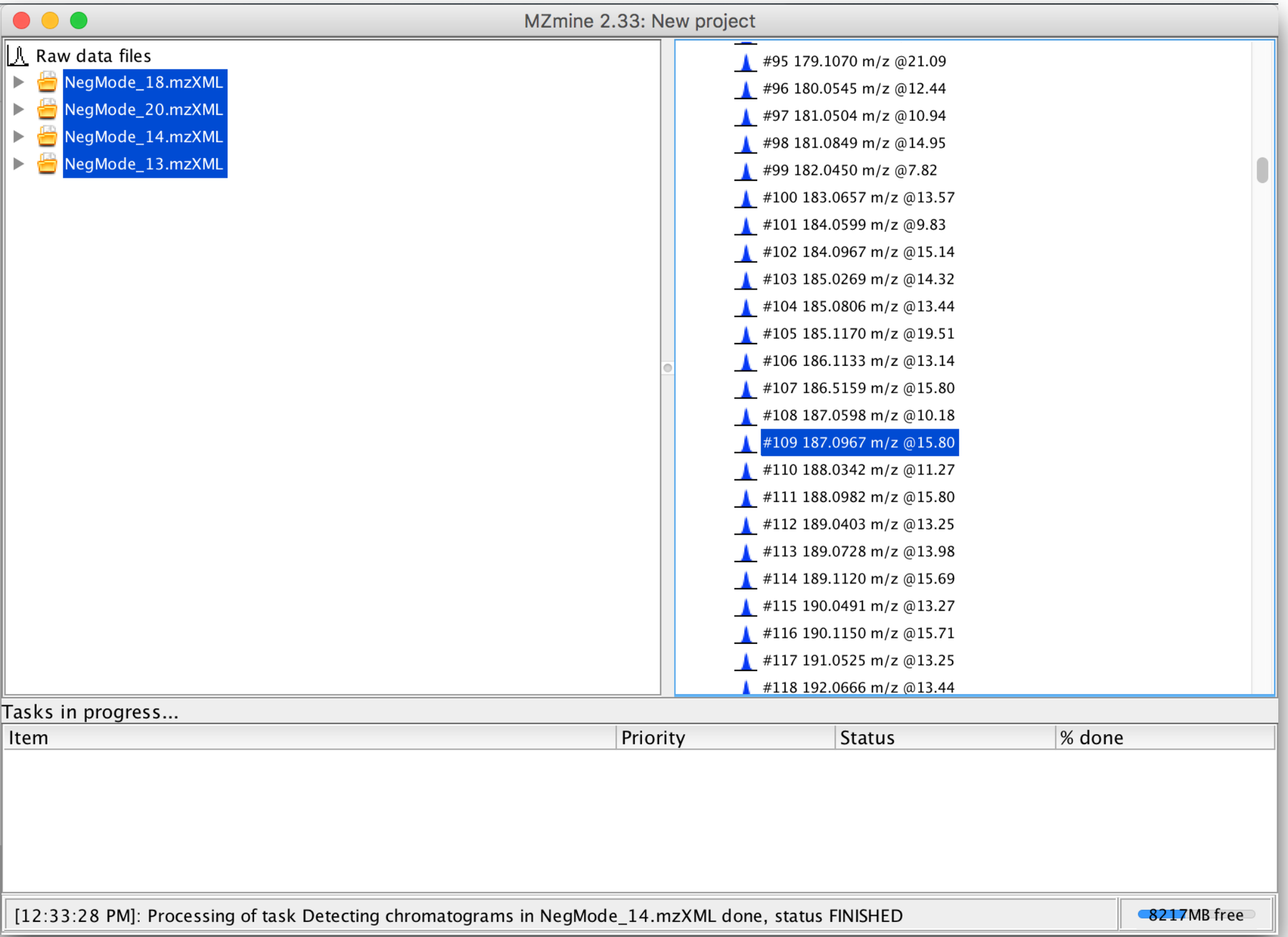
EIC construction



EIC construction



EIC construction



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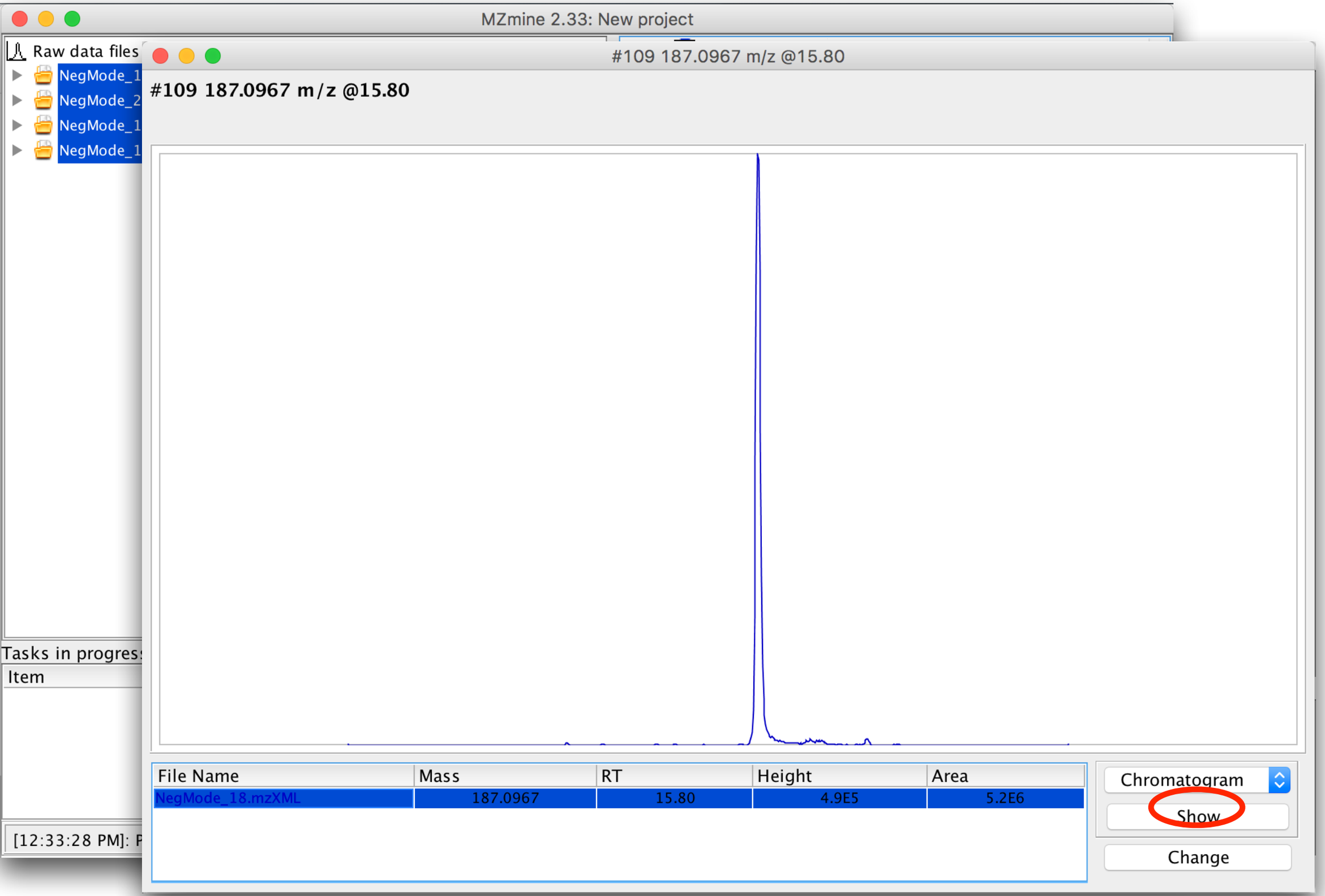

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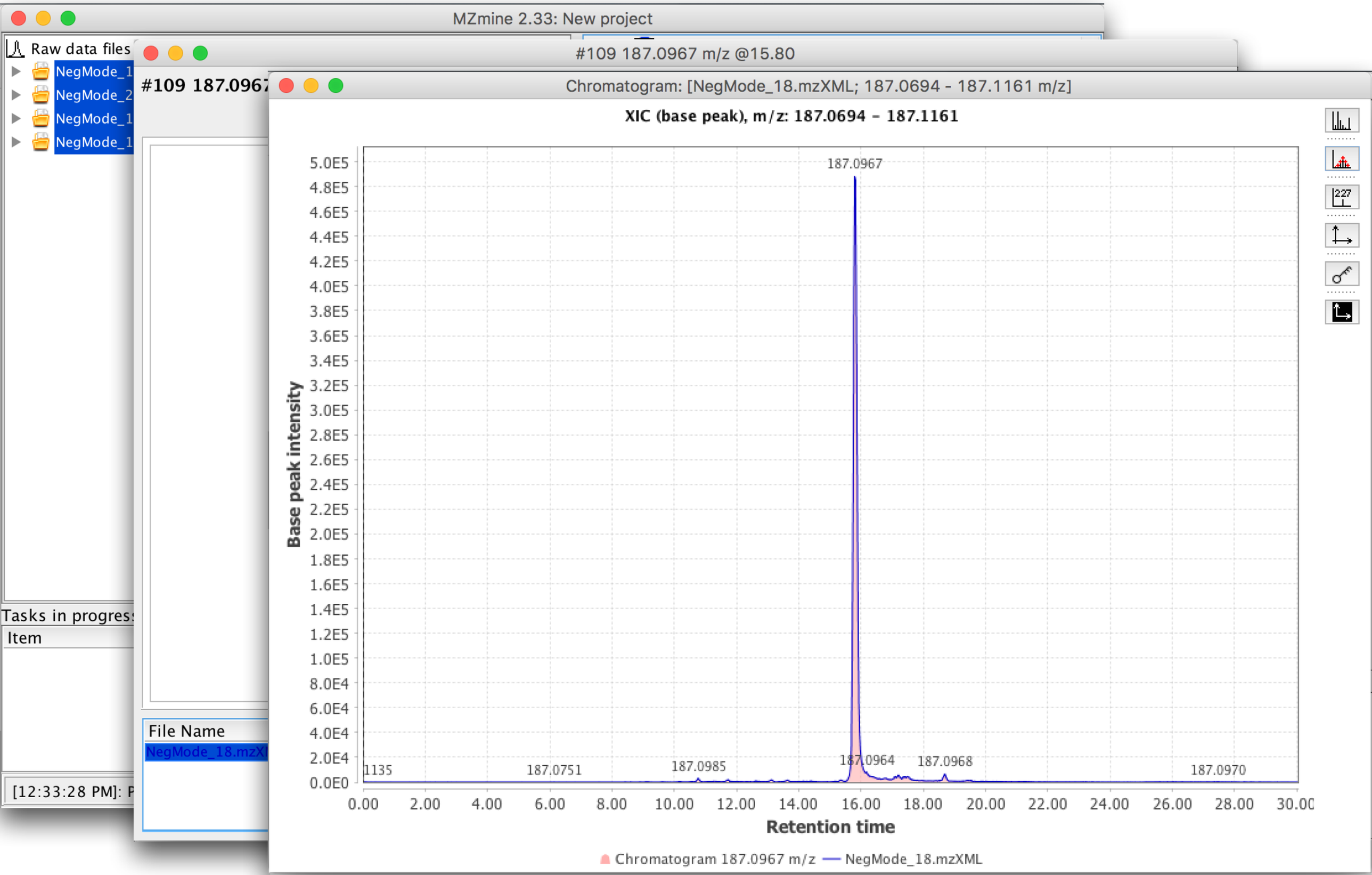
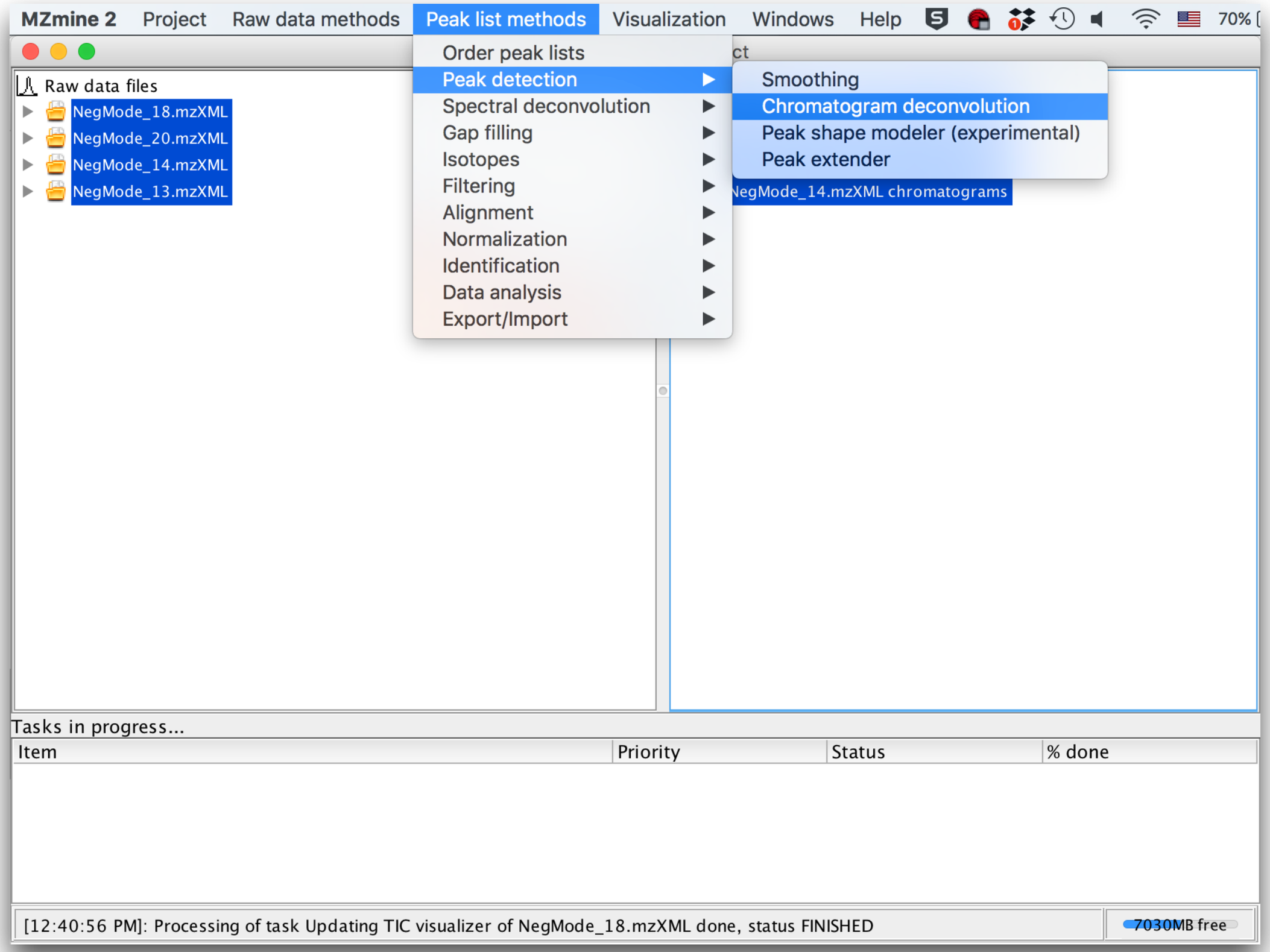
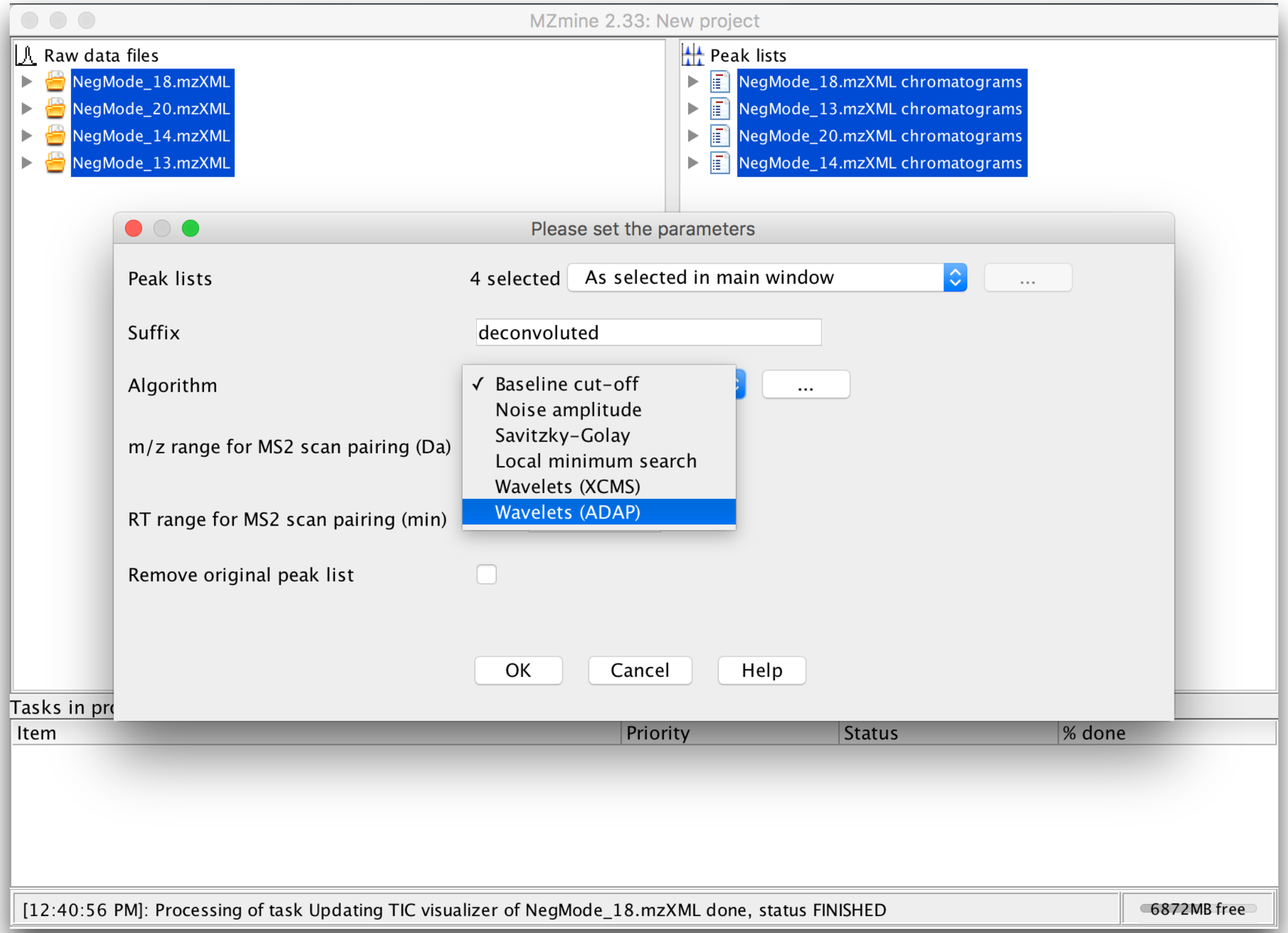


EIC peak detection



EIC peak detection



EIC peak detection

Please set the parameters

S/N threshold 5

S/N estimator Intensity window SN ...

min feature height 2000

coefficient/area threshold 30

Peak duration range 0.01 – 0.8

RT wavelet range 0.001 – 0.2

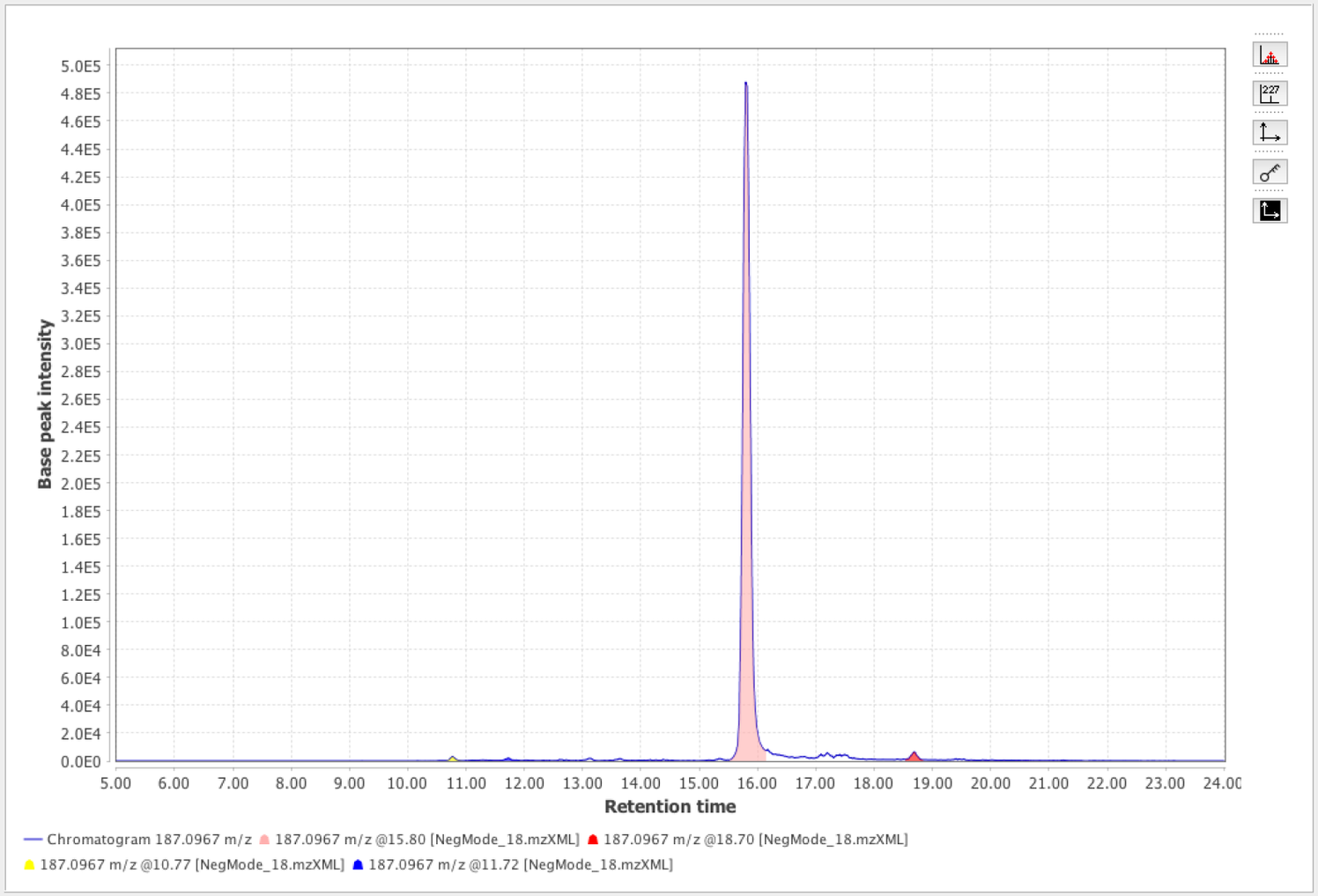
Show preview

Peak list NegMode_18.mzXML chromatograms

Chromatogram #109 187.0967 m/z

ADAP Module Disclaimer:
If you use the ADAP Chromatogram Deconvolution 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

OK Cancel Help



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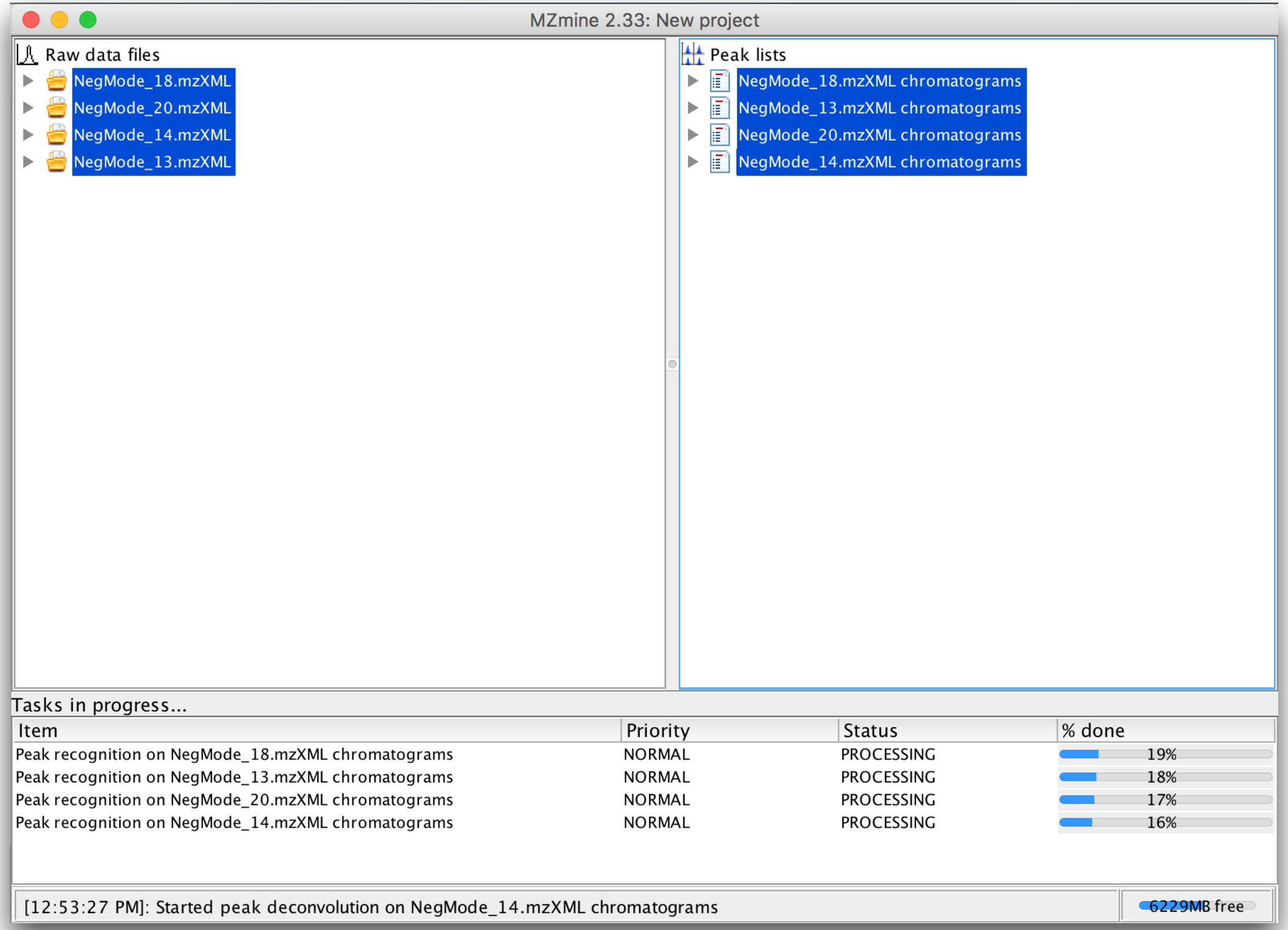

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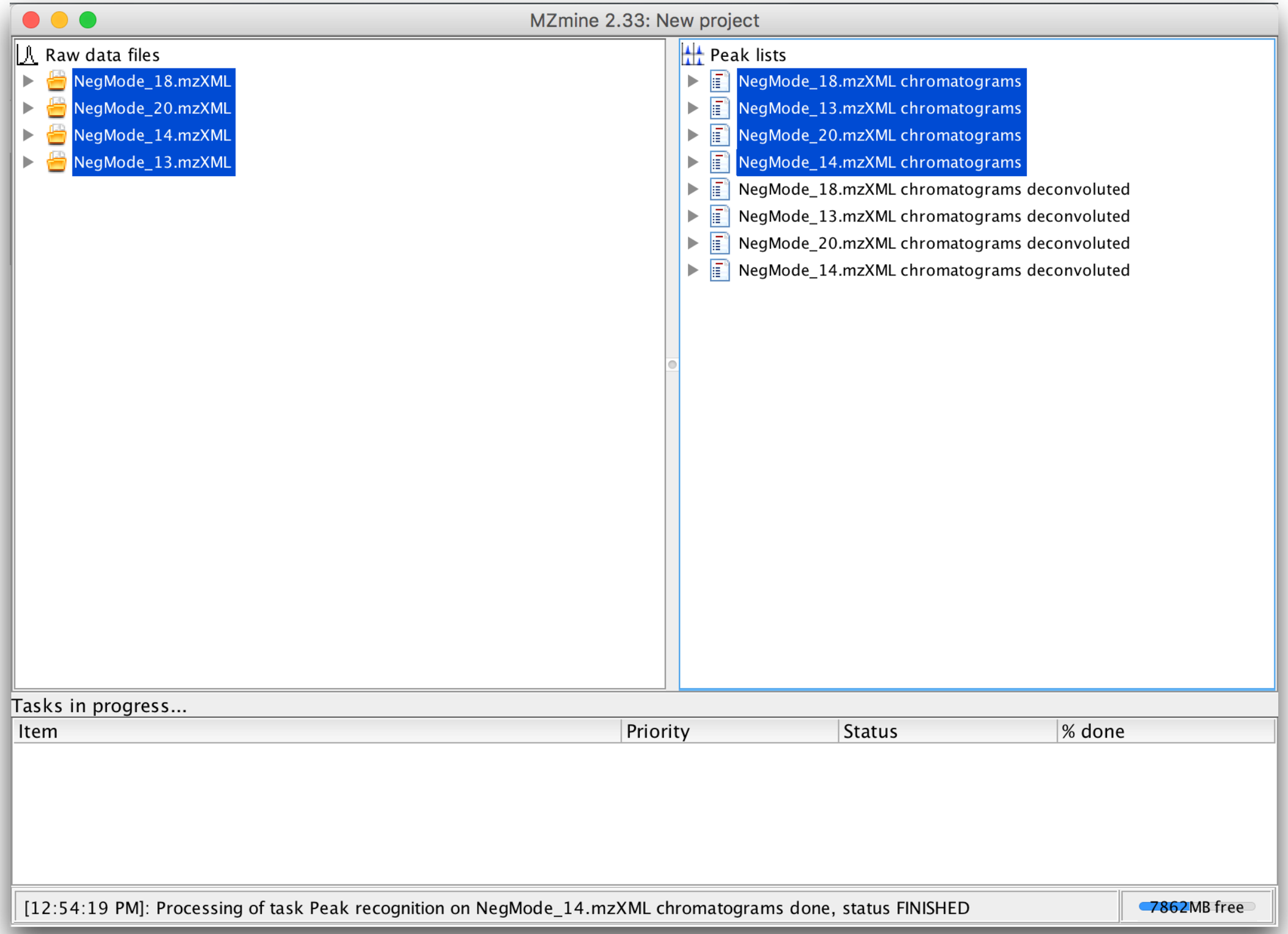
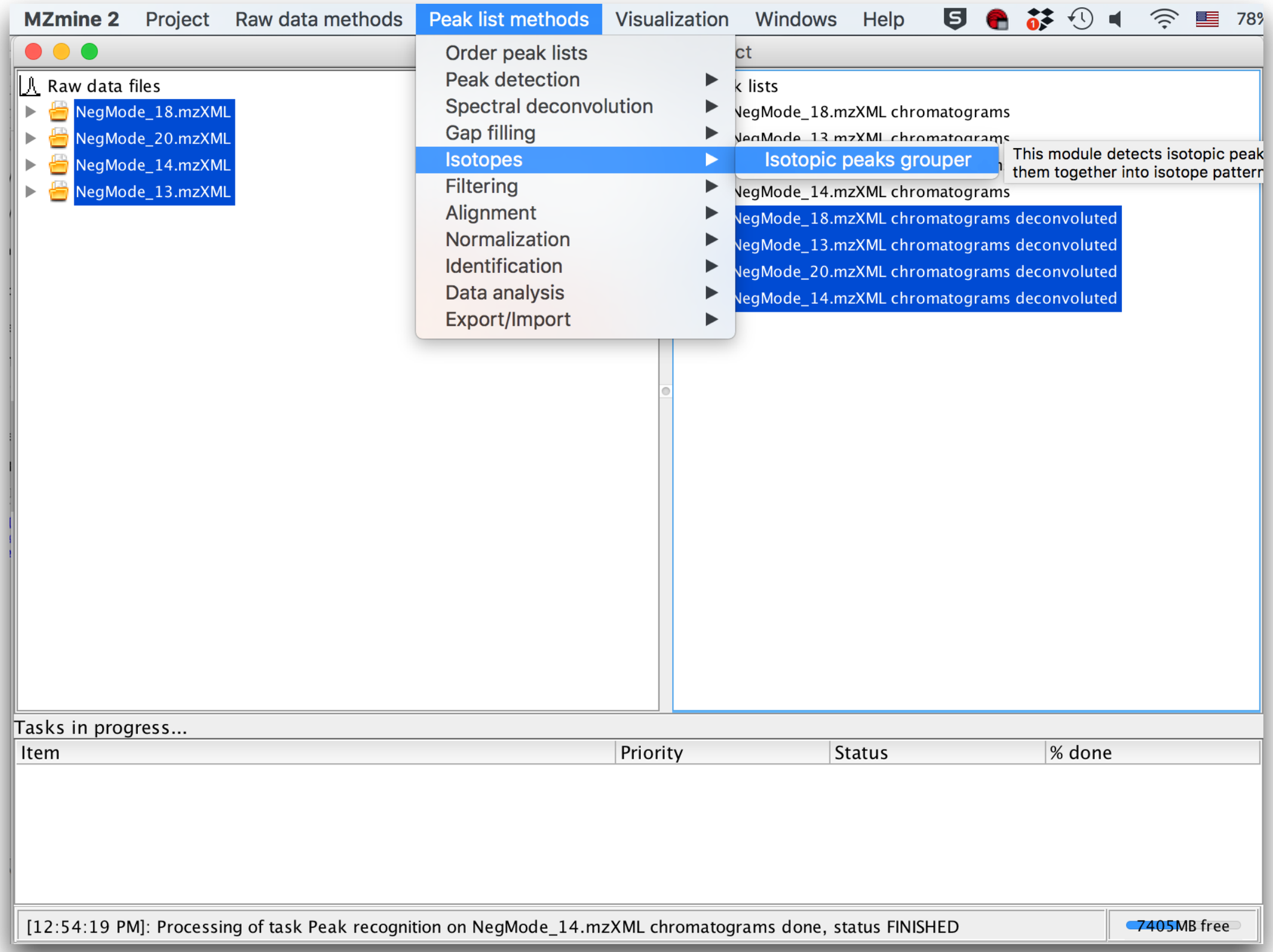


Isotopic grouper parameters



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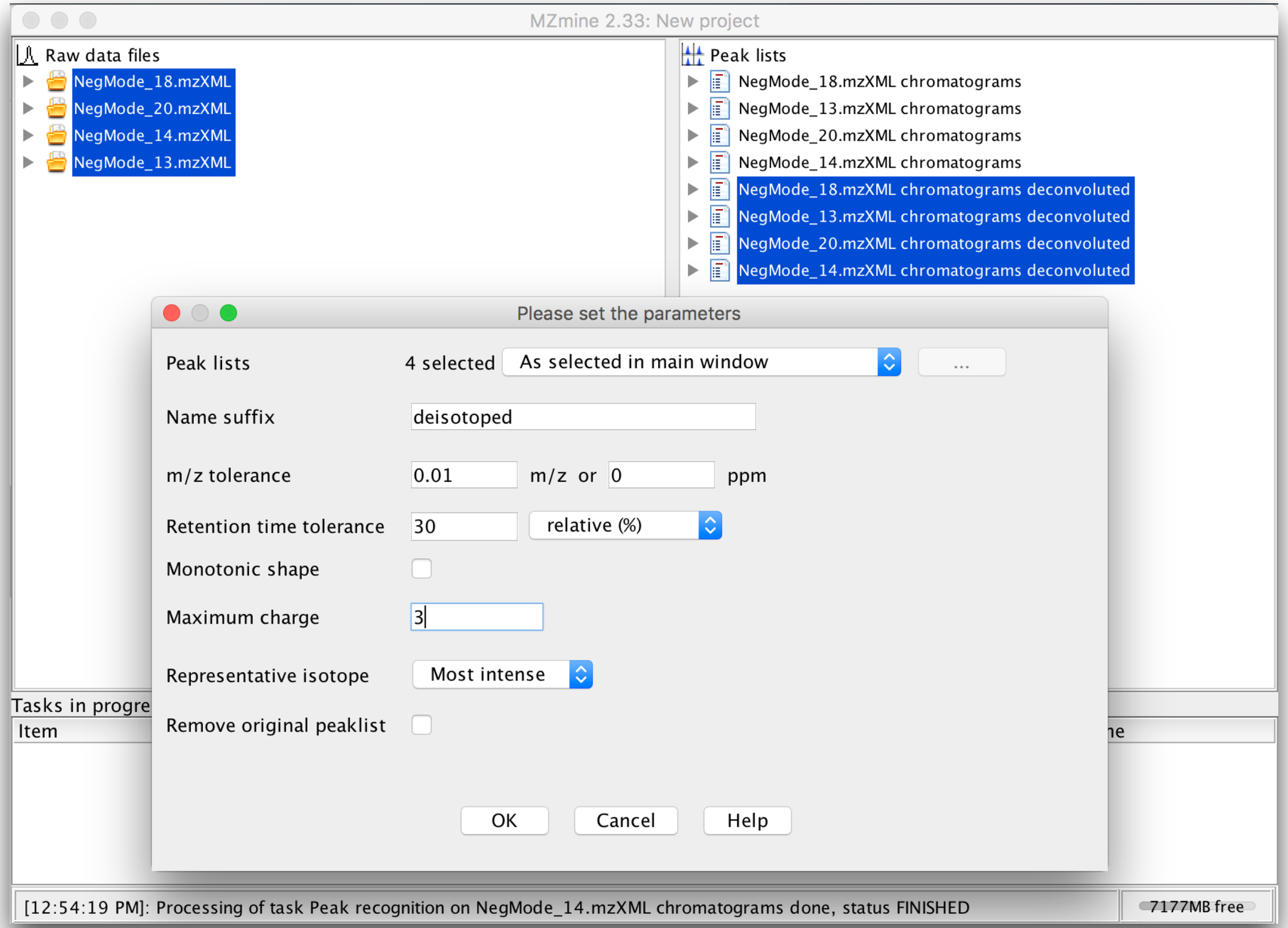
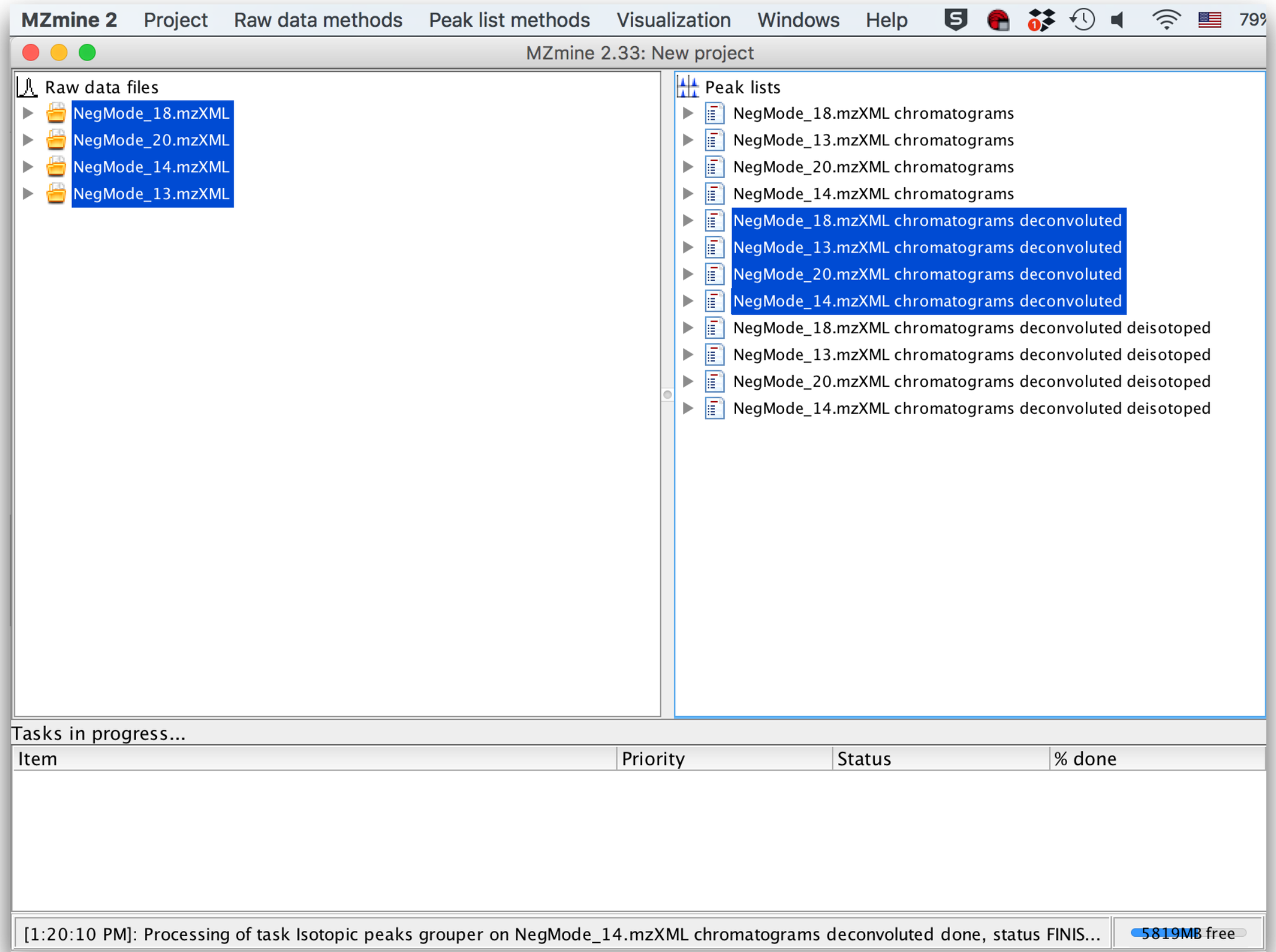
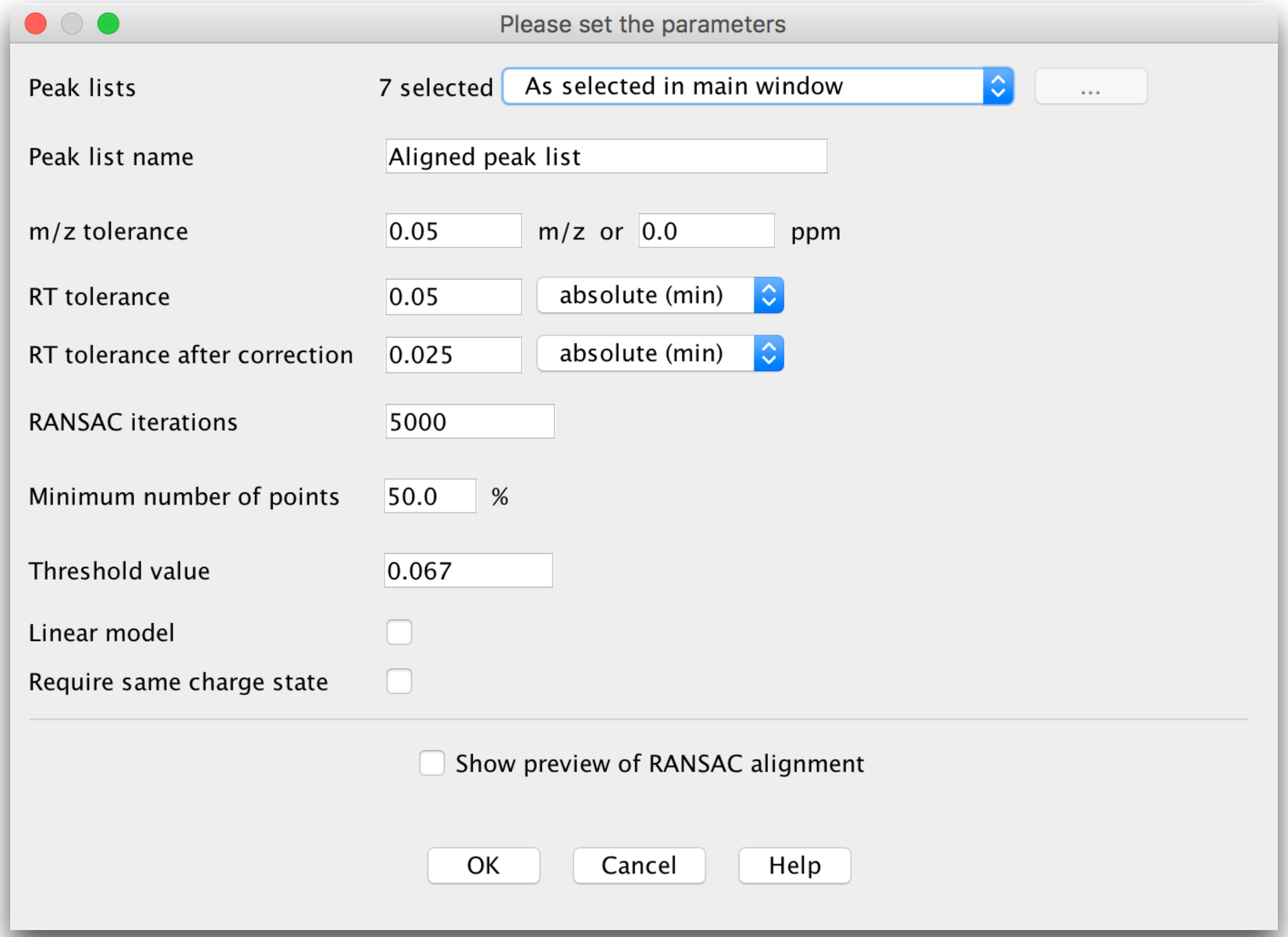


Isotopic grouper parameters



Alignment parameters