Version 1

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Supporting protocol for use-case 1: N-linked glycan m/z candidate detection in "M2aia - Interactive, fast and memory efficient analysis of 2D and 3D multi-modal mass spectrometry imaging data" V.1

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ABSTRACT

An N-glycan MALDI-MSI dataset (treated and untreated sections) [1,2] is preprocessed in M²aia [3], resulting in an intermediate result in the form of a combined continuous centroid-imzML file. In this protocol, the M²aia-based processing steps are demonstrated.

[1] Gustafsson et al. 2018; Data in Brief
[2] Gustafsson et al. 2018: PRIDE repository; N-linked glycan dataset page
[3] M²aia (RRID:SCR_019324): MSI applications for interactive analysis in MITK

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PROTOCOL CITATION

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BEFORE STARTING

a) Download and install M²aia

M²aia v2021.01.01
Windows/Linux
source by Jonas Cordes

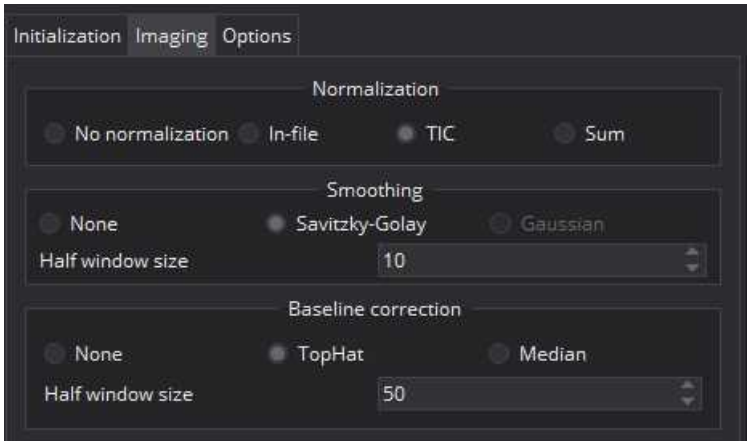
b) Download the dataset

N-glycan MALDI MSI data (PRIDE repository)

c) Start M²aia

1 Open the Data view, e.g. from the menu: Window > Show View > Data

Open the Imaging tab in the Data view.
- enable TIC normalization
- enable Savitzky-Golay smoothing with half-window-size of 10
- enable TopHat baseline correction with half-window-size of 50



2 Load the dataset: File > Open File or Ctrl + O

Open the files:
- png1-no_normalization.imzML
- png2-no_normalization.imzML
- control-no_normalization.imzML

During the initialization of the datasets, the in step 1 defined signal processing steps will be applied.

Setup Standard Display for 2D visualization (optional).

By default, images lacking the position of the image origin in the world space will be initialized at (x=0mm, y=0mm).If several of such datasets were loaded simultaneously and they will appear stacked.

Open the Options tab in the Data view. Apply the Tile images with 1 row and hit Apply.

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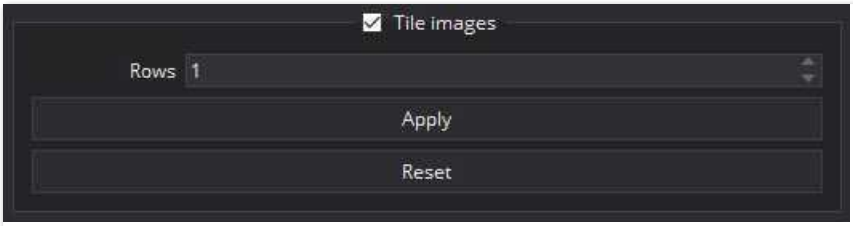
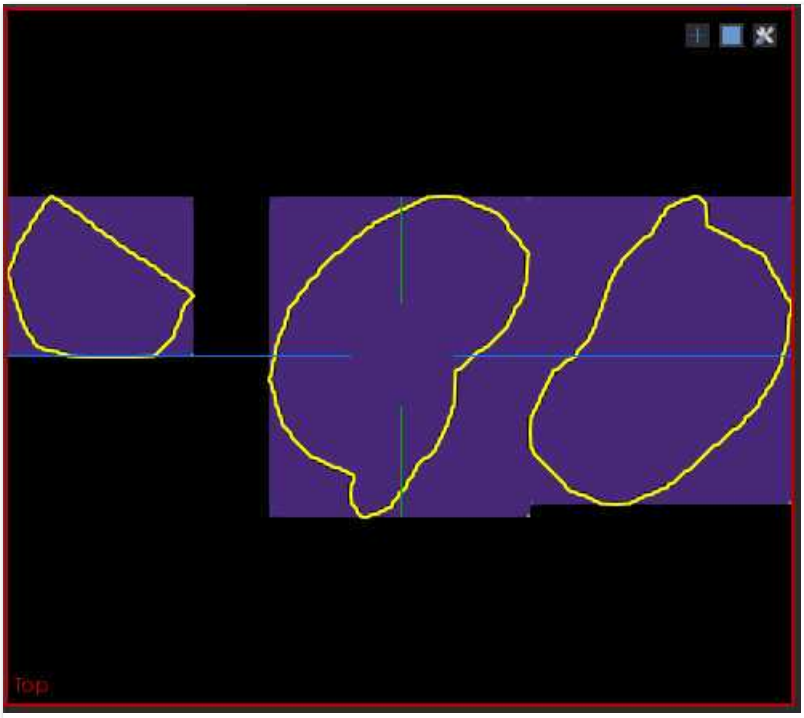


Maximize the top view display by pressing the blue square at the top right of the display menu.

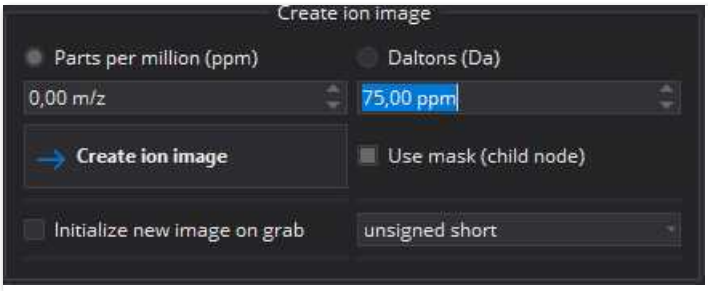


o

Explore the dataset by creating ion images using the Spectrum view (optional).

Ion images can be created by:

- Double click any position in the value-area of the Spectrum view. Ion image tolerance can be specified (in parts per million (ppm) or Daltons (Da)) in the Data view in the Create ion image property box.



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- Alt + Click&Drag

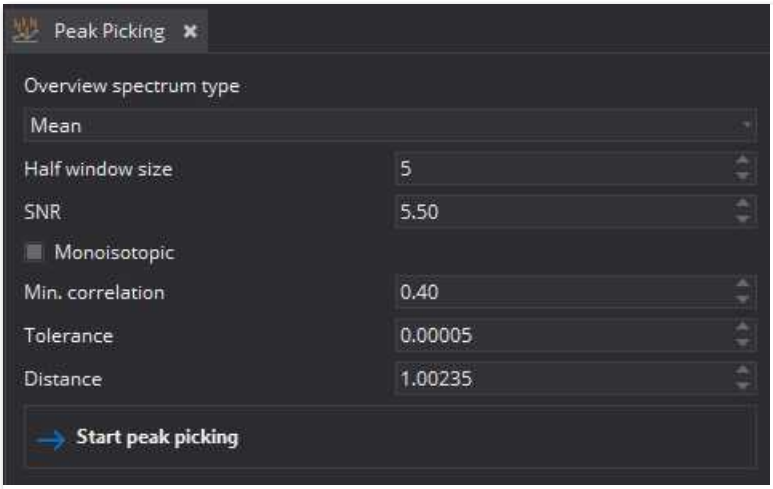
Spectrum view interactions:
- Zoom x-axis: turn the mouse wheel while hovering over the plotting area or x-axis.
- Zoom y-axis: turn the mouse wheel while hovering over the y-axis.
- Zoom isotrop: turn the mouse wheel while hovering over the plotting area and holding Ctrl.

While hovering over the Spectrum view, explore the right click menu.

3 Open the Peak Picking view, e.g. from the menu: Window > Show View > Peak Picking

Setup peak picking
1. Set Overview spectrum type Skyline to Mean.
2. Enable Monoisotopic peak detection.
3. Set SNR to 5.5.
4. Set Min. correlation to 0.4.
5. Click the Start peak picking button.

Peak picking is applied for each dataset.



4 Open the Combine Images view: Window > Show View > Combine Images
Select images (the order is important!):

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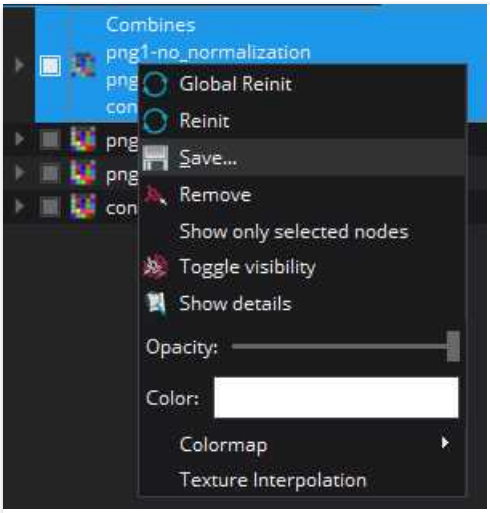
Click Combine images.

5 Open the imzML export view: Window > Show view > imzML export
Select Continuous Centroid in the drop-down menu.

6 Open the Data Manager view: Window > Show view > Data Manager
Right-click on the combined-result-node and click save.



In the Save File Dialog, select the file-format type "*.imzML" from the drop-down menu.
Change the name and target file location.
Save the file!

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