🌐 Supporting protocol for use-case 1: Dimensionality reduction in "M2aia - Interactive, fast and memory efficient analysis of 2D and 3D multi-modal mass spectrometry imaging data" V.2

Version 2 ▼

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1	Works for me		⌒ₒ Share

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ABSTRACT

M²aia is able to apply dimensionality reduction methods to 2D/3D MSI images. To demonstrate the DR methods we load a single peptide brain slice MS image, select multiple peaks from a peak list and start a PCA and t-SNE.

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EXTERNAL LINK

https://jtfcordes.github.io/M2aia

PROTOCOL CITATION

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protocols.io
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MANUSCRIPT CITATION please remember to cite the following publication along with this protocol

WHAT'S NEW

DR is now integrated into the Peak Picking utilities view.

KEYWORDS

Mass spectrometry imaging, MSI, MALDI, M2aia

LICENSE

CREATED

Jul 28, 2021

BEFORE STARTING

a) Download and install M²aia

M²aia 2021.07.00 🔗
Windows/Linux
source by Jonas Cordes

b) Download the data set

APP_NL-G-F_67weeks_3D_maldi_lipid_slice_all (GigaDB) [3]

Load Data into M²aia

1   Open the *Data* view and define the signal processing:
- set your normalization strategy (e.g. TIC)
- set your smoothing strategy (e.g. Gaussian)
- set your baseline correction strategy (e.g. Median)

Load at least one continuous profile *.imzML image file into M²aia: *File > Open File* or *Ctrl + O.*
Ensure, that the corresponding *.ibd file is available at the same directory level.
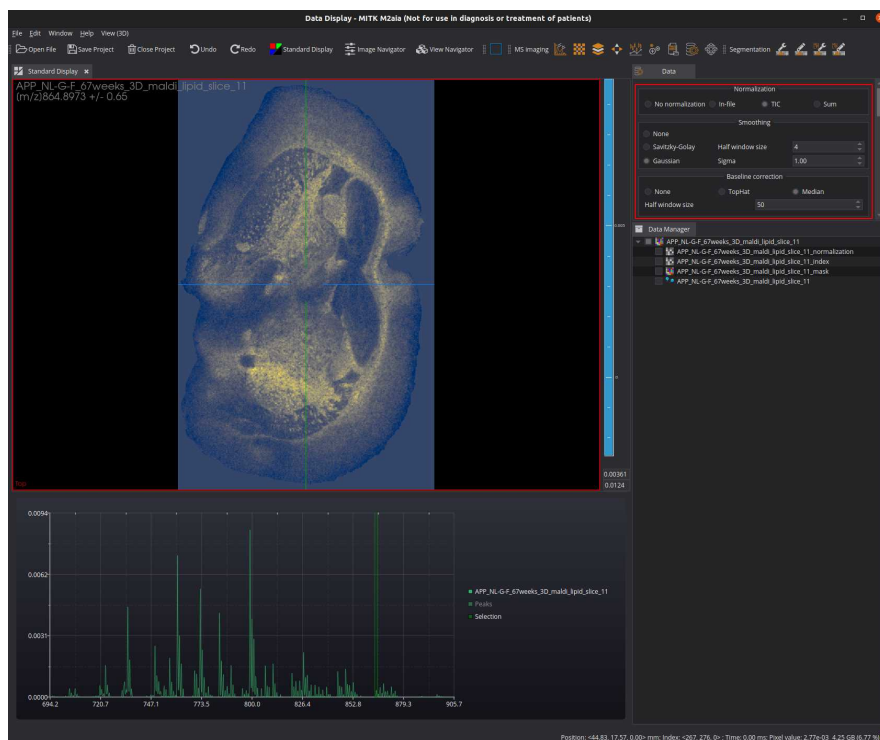
M²aia application with selected ion image at m/z 864.89 +/- 0.65 Da.

Peak picking

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

> The peak picking utilities of the *Peak Picking* view are designed for handling overview spectra. Pixel-wise peak picking is not realized within the graphical user interface of M²aia.

Select an overview spectrum type in the drop-down menu (e.g. Mean).

> The drop-down menu selection is not synced to the overview spectrum shown in the *Spectrum* view. You can change the overview spectrum shown in the *Spectrum* view using the right click context menu while hovering the overview spectrum.

Set the peak picking parameters (example):
- set the SNR to 2
- enable monoisotopic peak harvesting
- set the min correlation to 0.6

Start the peak picking.
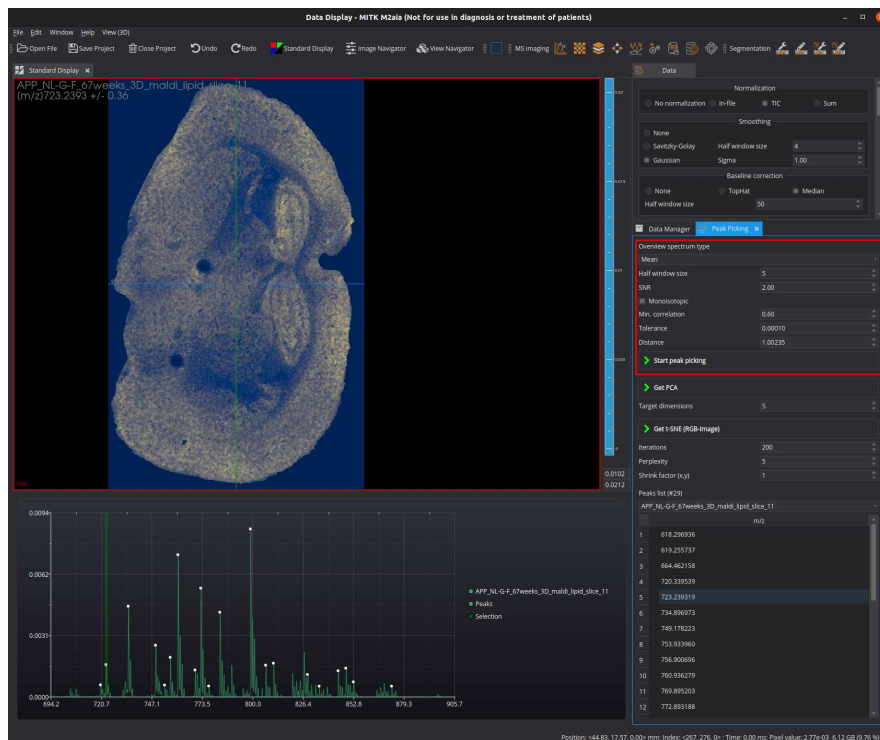
M²aia application with selected ion image at peak-of-interest (POI) m/z 723.23 +/- 0.36 Da.

Peak selection and PCA

3 Select peaks of interest (red annotations).

> You can select/deselect all peaks by clicking on the upper left corner button (red arrow). Double click on individual rows will perform an imaging request according to the given *m/z* value of this row and tolerance specified in the *Imaging* tab of the *Data* view.

Select the target dimensionality and start the PCA (blue annotation).

> The image generated by the PCA serves as the input for the t-SNE.
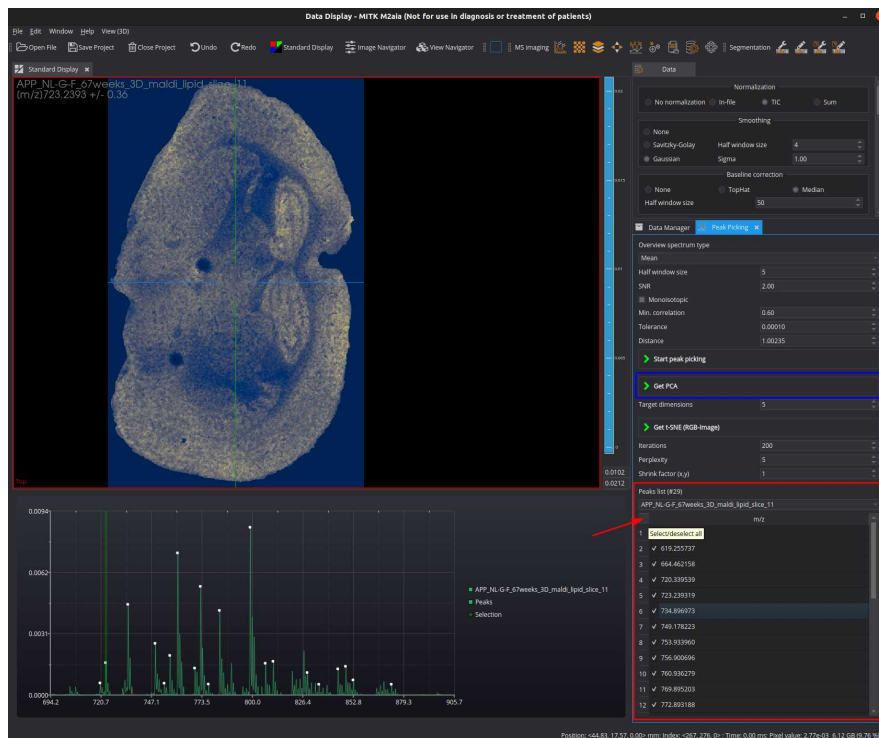
The result image is now available in the *Data Manager* view. You can change the currently displayed projected image by using the right click menu of the "PCA"-datanode and the *Component* slider.
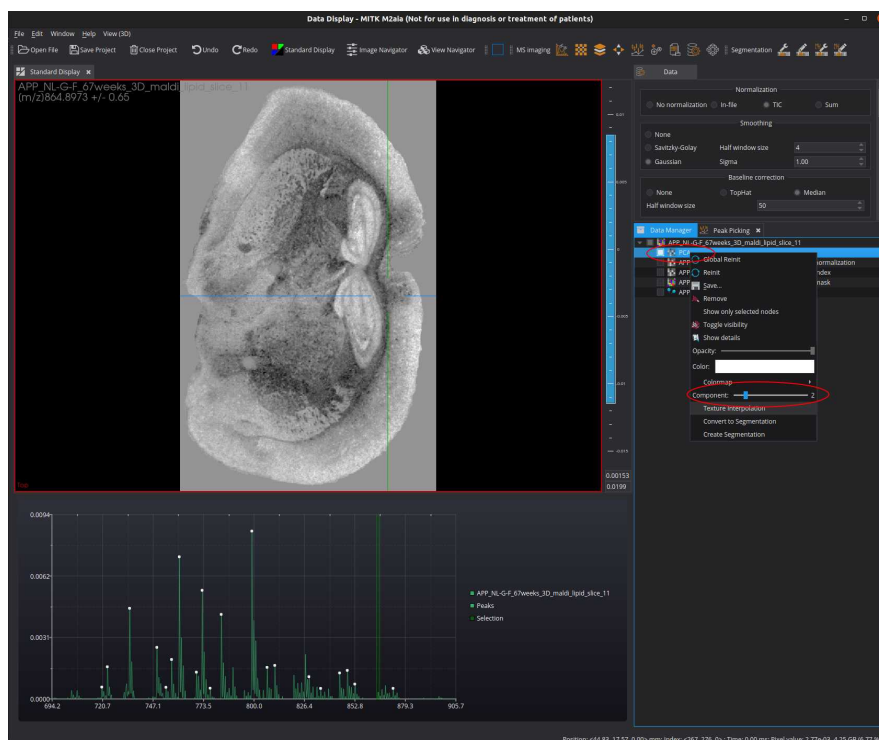
M²aia application with selected 3rd component of the PCA image.

t-SNE

4   Set the t-SNE parameters (example):

- set iterations to 200
- set perplexity to 10
- set shrink factor to 2

Make sure that a "PCA" named datanode is available as derived node of the MSI datanode. Start the t-SNE.

To find good parameters for the t-SNE please check the FQA of Laurens van der Maaten's github.io page.

The calculation of the t-SNE may take some time. The status can be tracked within the console window of M²aia.

If the image has many pixels (as in the example shown >140k pixels), the calculation time can be very long. This can be reduced e.g. by decreasing the lateral resolution. For this purpose the shrinkage factor can be adjusted. The image is reduced in resolution by dividing the lateral dimensions by the specified factor. This reduces the t-SNE calculation time. After successful application of the t-SNE, the image is resampled to restore the original image geometry.
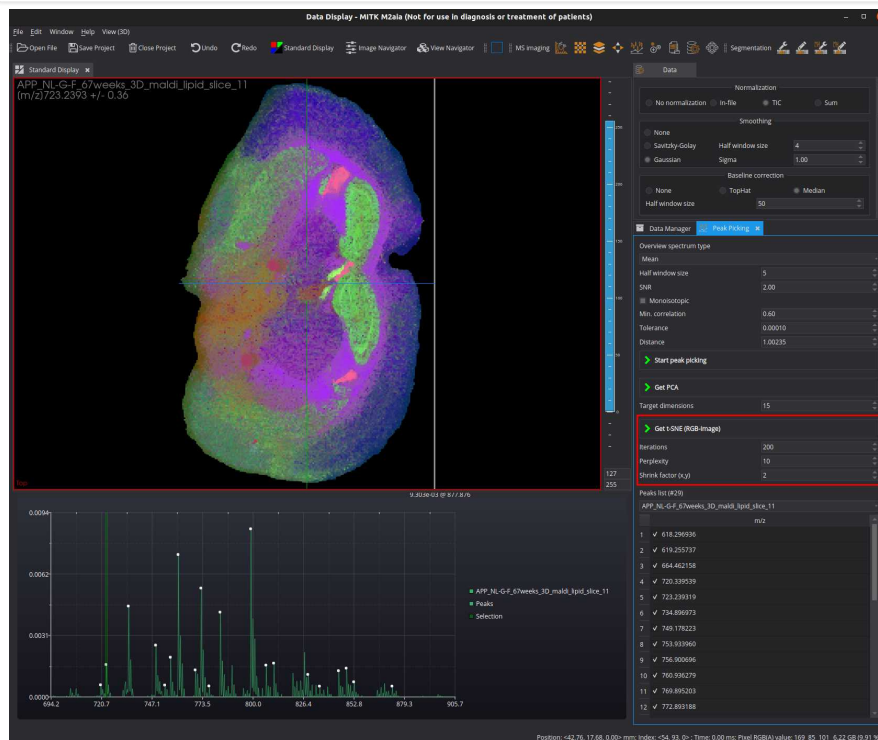
M²aia application with t-SNE image.