

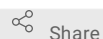


Jun 11, 2021

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"

Jonas Cordes¹¹Mannheim University of Applied Sciences

1 Works for me



Share

dx.doi.org/10.17504/protocols.io.brw4m7gw

 Jonas Cordes
Mannheim University of Applied Sciences

ABSTRACT

M²aia [1,2] 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 ion images and start a PCA and t-SNE. Example data available [3].

[1] <https://github.com/jtfcordes/m2aia>

[2] [M²aia \(RRID:SCR_019324\): MSI applications for interactive analysis in MTK](#)

[3] Cordes J; Enzlein T; Marsching C; Hinze M; Engelhardt S; Hopf C; Wolf I (2021): Supporting data for "M²aia - Interactive, fast and memory efficient analysis of 2D and 3D multi-modal mass spectrometry imaging data" GigaScience Database. <http://dx.doi.org/10.5524/100909>

DOI

dx.doi.org/10.17504/protocols.io.brw4m7gw

EXTERNAL LINK

<http://github.com/jtfcordes/m2aia>

PROTOCOL CITATION

Jonas Cordes 2021. 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".

protocols.io<https://dx.doi.org/10.17504/protocols.io.brw4m7gw>

KEYWORDS

Mass spectrometry imaging, MSI, MALDI, M2aia

LICENSE

————— This is an open access protocol distributed under the terms of the [Creative Commons Attribution License](#), which permits unrestricted use, distribution, and reproduction in any medium, provided the original author and source are credited

CREATED

Jan 29, 2021

LAST MODIFIED

Jun 11, 2021

PROTOCOL INTEGER ID

46780

BEFORE STARTING

a) Download and install M²aia

M²aia 2021.01.01 [↗](#)

Windows/Linux

[source](#) by Jonas Cordes

b) Download the dataset

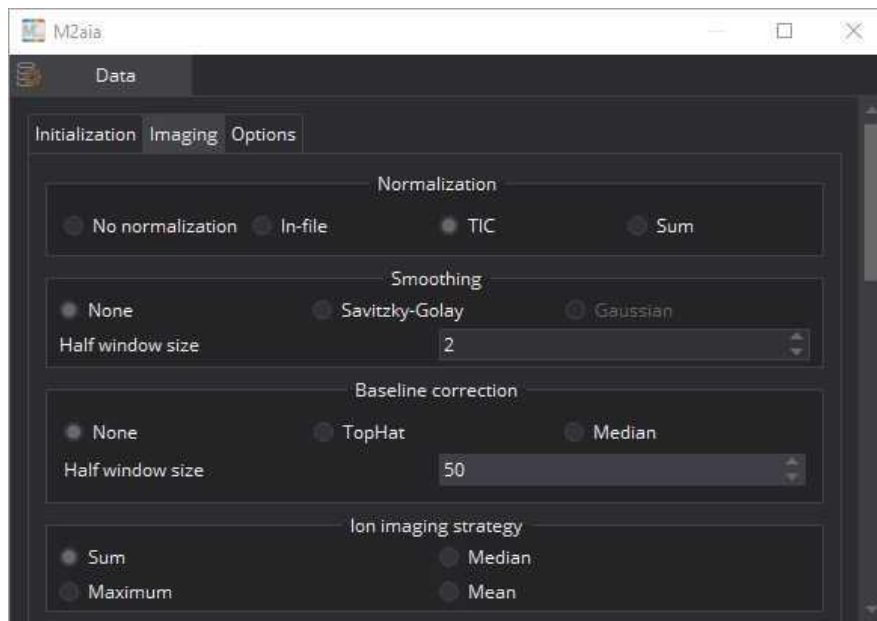
N-glycan MALDI Mouse Kidney Combined Dataset (GigaDB) [3]

d) 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
- disable smoothing
- disable baseline correction



- 2 Load at least one imzML image into M²aia: *File > Open File* or *Ctrl + O*.
Ensure, that the *.ibd files are available at the same directory level.

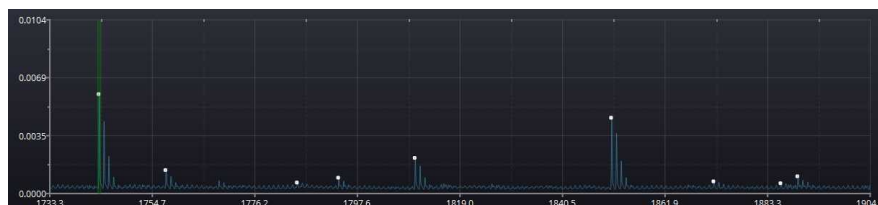
1m

- 3 Open the *Ions* view at least once, e.g. from the menu: *Window > Show View > Ions*

This view must stay open but not in focus (it can be a background tab).
For the upcoming actions the *Data* view tab has to stay in the foreground.

- Now we can start selecting multiple ion images by using the Spectrum view interactively (step 4.1) or the Data view by typing ion image m/z-ranges (step 4.2). You can use both approaches simultaneously and interchangeable.

- Create ion images by interactive select an m/z range using *Alt+Left Click+Dragging* the mouse over the *Spectrum* view. Alternatively, *double-click* in the plot area of the *spectral* view.



Right-click context menu available. Mouse Wheel + Scrolling: zoom. Mouse Wheel + Press: drag

If the selection is satisfactory, press *Ctrl+I*, and a corresponding ion image reference s generated and added to the *Ions* view.

- Create ion images by manually defining m/z ranges using the *Data* view's *Ion imaging* group box.

The screenshot shows two panels from a software interface. The top panel, titled 'Ion imaging strategy', has radio buttons for 'Sum', 'Maximum' (selected), 'Median', and 'Mean'. Below it is the 'Ion imaging' panel, which has radio buttons for 'Parts per million (ppm)' (selected) and 'Daltons (Da)'. It contains input fields for '1743,47 m/z' and '75,00 ppm', a 'Create ion image' button with a blue arrow, a 'Use mask (child node)' checkbox, an 'Initialize new data node' checkbox, and a dropdown menu set to 'unsigned short'. The bottom panel, titled 'Ion image reference', lists 'Combines' with three entries: 'png1-no_normalization', 'png2-no_normalization', and 'control-no_normalization'. Below these is the text '1743.47 +/- 1.44 Da' and a button labeled 'Add to Ions view' with a blue arrow.

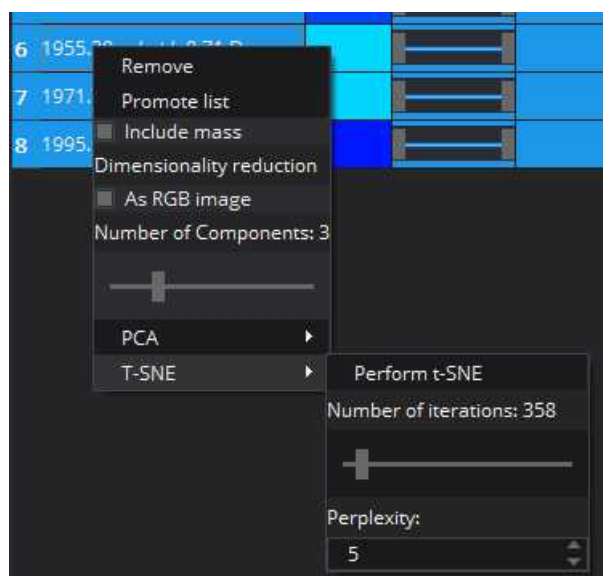
If the selection is satisfactory, use the "Add to Ions view" button of *Data* view's *Ion image reference* group box, and a corresponding ion image reference s generated and added to the *Ions* view. A name for the ion image m/z range can be specified.

- Return to the *Ions* view and select ion image references that should be used for the dimension reduction method.

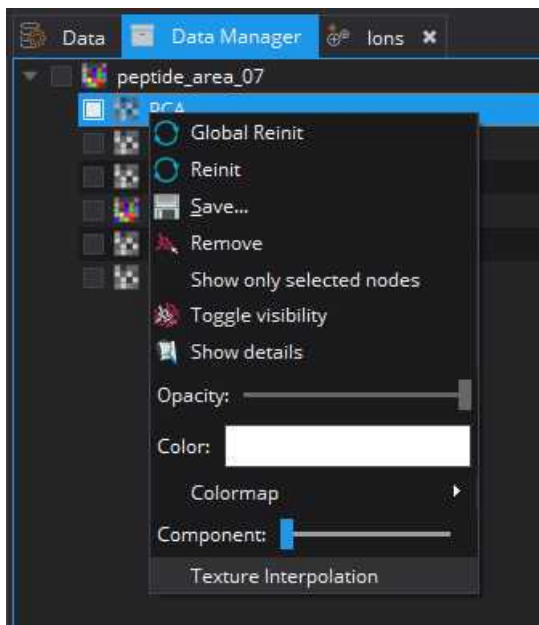
☐ Enable visualization

	m/z value	color	scale	name
1	1743.47 m/z +/- 1.44 Da	blue		
2	1793.23 m/z +/- 1.91 Da	green		
3	1851.08 m/z +/- 0.91 Da	orange		
4	1889.24 m/z +/- 0.91 Da	blue		
5	1905.16 m/z +/- 1.83 Da	blue		
6	1955.39 m/z +/- 0.71 Da	cyan		
7	1971.72 m/z +/- 0.81 Da	cyan		
8	1995.96 m/z +/- 1.50 Da	blue		

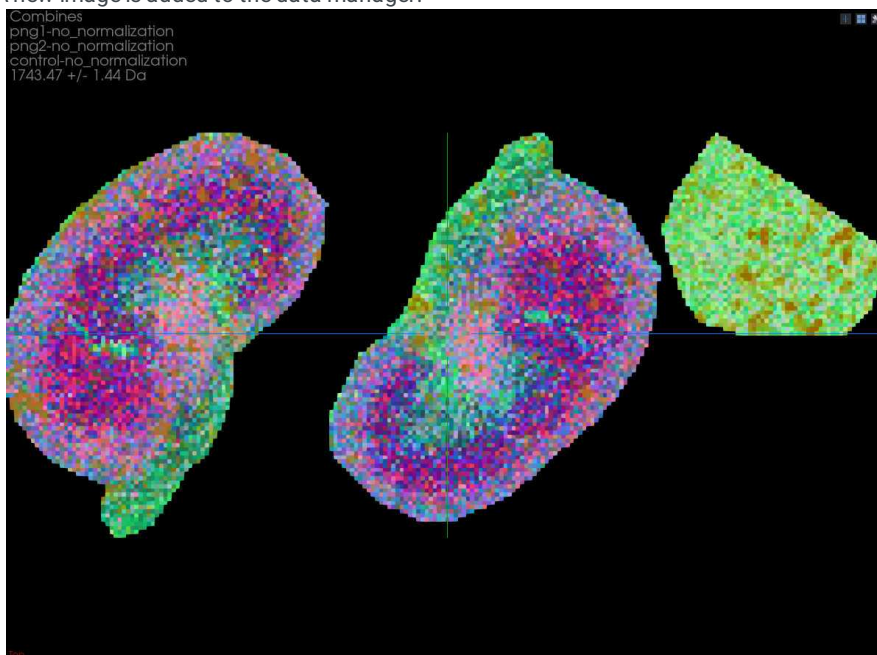
6 *Right-click* the selection and choose PCA or t-SNE as dimension reduction method.



If the RGB check box is unchecked (step 6), a vector image is created with the desired number of components. A component slider is displayed in the right-click menu of the corresponding data node.



A new image is added to the data manager.



t-SNE applied to the in step 5 promoted ion image references. Output dimension = 3 (RGB).