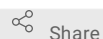Jun 11, 2021

🌐 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"

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| 1 | Works for me | | Share | dx.doi.org/10.17504/protocols.io.brw4m7gw |

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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 MITK
[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

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EXTERNAL LINK

http://github.com/jtfcordes/m2aia

PROTOCOL CITATION

KEYWORDS

Mass spectrometry imaging, MSI, MALDI, M2aia

LICENSE

CREATED

Jan 29, 2021

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Jun 11, 2021

PROTOCOL INTEGER ID

46780

a) Download and install M²aia

M²aia 2021.01.01 🔗
Windows/Linux
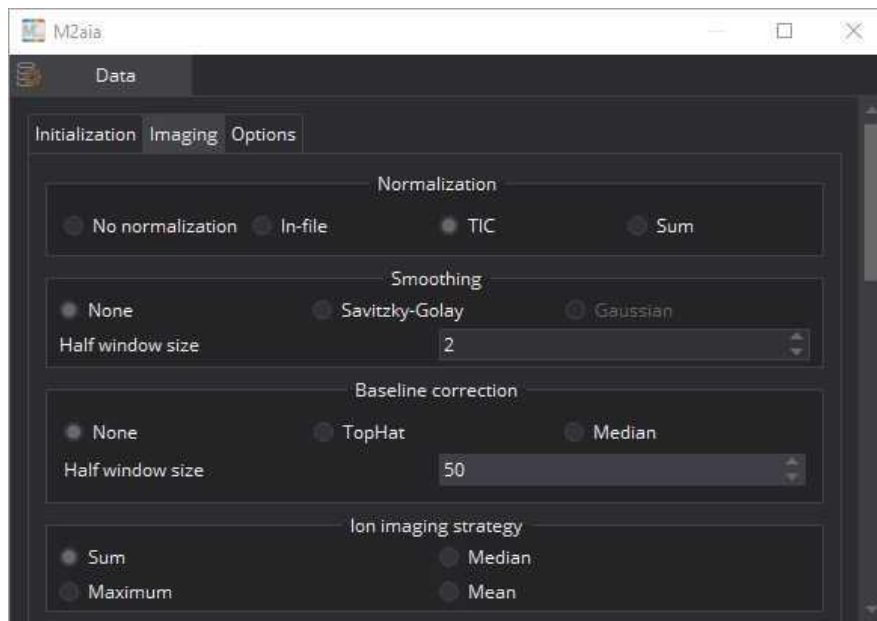source by Jonas Cordes

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.*   1m
Ensure, that the *.ibd files are available at the same directory level.

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.

4   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.

4.1   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 s*pectr*al view.
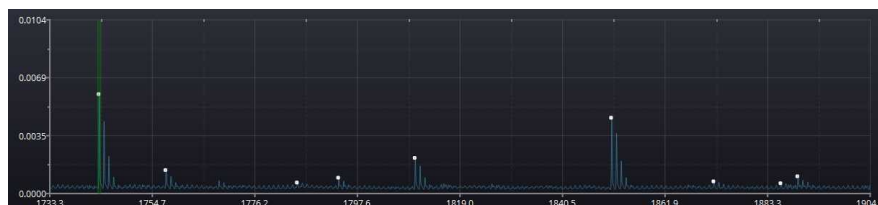
Right-click context menu available. Mouse Wheel + Scrolling: zoom. Mouse Wheel + Press: drag

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

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


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.

5   Return to the *Ions* view and select ion image references that should be used for the dimension reduction method.
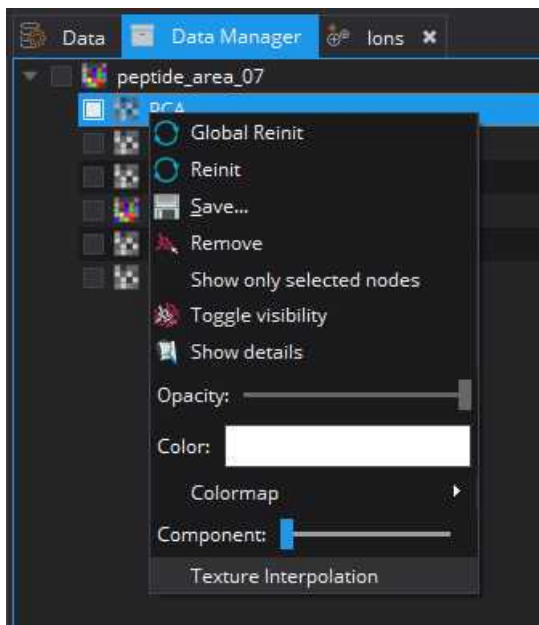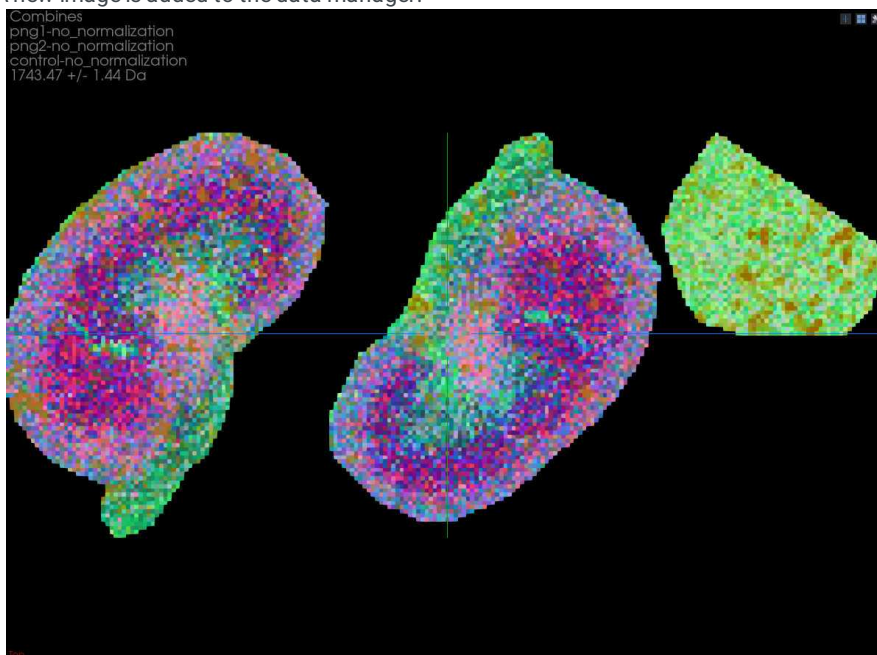
6   *Right-click* the selection and choose PCA or t-SNE as dimension reduction method.
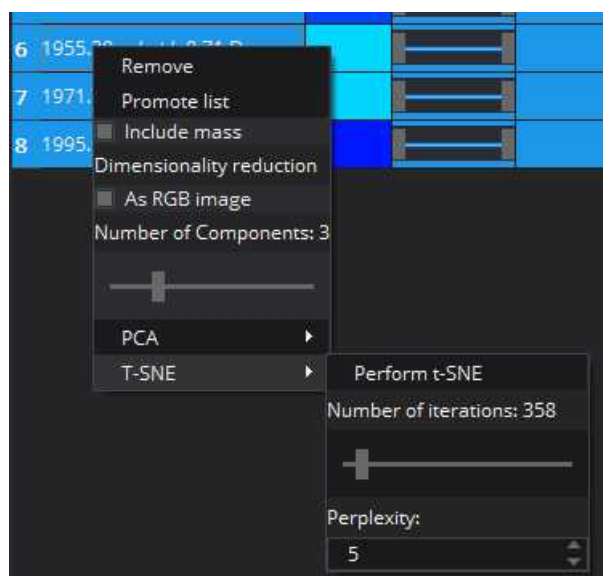
If the RGB check box is unchecked (step 6), a vector image is created with the desired number of components. A component slider is displayed in the right-click menu of the corresponding data node.

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).