



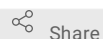
Version 2 ▾

Jun 11, 2021

# Supporting protocol for use-case 2: Multi-modal 3D image reconstruction in "M2aia - Interactive, fast and memory efficient analysis of 2D and 3D multi-modal mass spectrometry imaging data" V.2

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1 Works for me



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[dx.doi.org/10.17504/protocols.io.bvq8n5zw](https://dx.doi.org/10.17504/protocols.io.bvq8n5zw)

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## ABSTRACT

We provide 10 consecutive brain slices of an APP NL-G-F mouse model [1], imaging both lipid and peptide features. The objective of use-case described in the following is to demonstrate the applicability of M<sup>2</sup>aia v2021.01.01 [2,3] for mono- and multi-modal 3D image reconstructions by showing how to embed the peptide information into the lipid structural context in three dimensions using M<sup>2</sup>aia.

To demonstrate mono-modal 3D reconstruction, all 10 slices of the lipid dataset are loaded into M<sup>2</sup>aia and used for slice-wise reconstruction of 3D image stack. For multi-modal 3D-reconstruction, the peptide dataset will be pair-wise registered with the respective lipid slices of the previously reconstructed 3D lipid image stack.

[1] Cordes J; Enzlein T; Marsching C; Hinze M; Engelhardt S; Hopf C; Wolf I (2021): Supporting data for "M<sup>2</sup>aia - 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>

[2] <http://github.com/jtfcordes/m2aia>

[3] M<sup>2</sup>aia (RRID:SCR\_019324): MSI applications for interactive analysis in MTK

## DOI

[dx.doi.org/10.17504/protocols.io.bvq8n5zw](https://dx.doi.org/10.17504/protocols.io.bvq8n5zw)

## EXTERNAL LINK

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

## PROTOCOL CITATION

Jonas Cordes 2021. Supporting protocol for use-case 2: Multi-modal 3D image reconstruction in "M<sup>2</sup>aia - 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.bvq8n5zw>

Version created by Jonas Cordes

## KEYWORDS

Mass spectrometry imaging, MSI, MALDI, M2aia, 3D reconstruction

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## CREATED

Jun 11, 2021

LAST MODIFIED

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PROTOCOL INTEGER ID

50688

BEFORE STARTING

a) Download and install M<sup>2</sup>aia

**M<sup>2</sup>aia 2021.01.01** [↗](#)

Windows/Linux

[source](#) by Jonas Cordes

b) Extract the elastix binaries

**elastix 5.0.0** [↗](#)

Windows/Linux/Apple Mac

[source](#) by © by Stefan Klein & Marius Staring

c) Download the dataset

APP NL-G-F 3D MALDI Mouse Brain (GigaDB) [1]

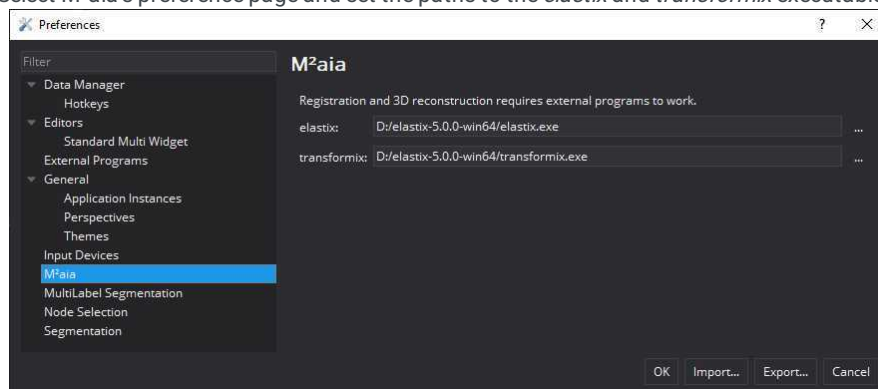
d) Start M<sup>2</sup>aia

3D reconstruction

8m

1m

- 1 Open the Preferences of M<sup>2</sup>aia, e.g. from the menu: *Window > Preferences* or *Ctrl+P*.  
Select M<sup>2</sup>aia's preference page and set the paths to the *elastix* and *transformix* executables, respectively.

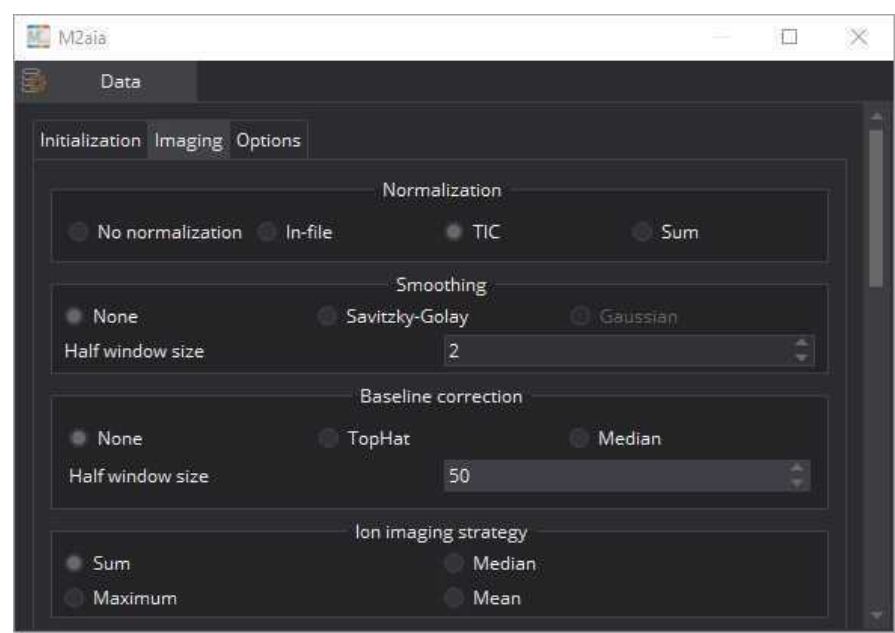


- 2 Open the *Data* view, e.g. from the menu: *Window > Show View > Data*

Open the *Imaging* tab in the *Data* view.

- enable TIC normalization
- disable smoothing

- disable baseline correction



3 Load the dataset into M<sup>2</sup>aia: *File > Open File* or *Ctrl + O*.

2m

Open all lipid files at once:

Name	Änderungsdatum	Typ	Größe
lipid_area_04.ibd	19.01.2021 10:06	IBD-Datei	4.956.562 KB
lipid_area_05.ibd	19.01.2021 10:08	IBD-Datei	4.867.294 KB
lipid_area_06.ibd	19.01.2021 10:11	IBD-Datei	5.018.326 KB
lipid_area_07.ibd	19.01.2021 10:13	IBD-Datei	5.028.608 KB
lipid_area_08.ibd	19.01.2021 10:16	IBD-Datei	4.964.482 KB
lipid_area_09.ibd	19.01.2021 10:18	IBD-Datei	4.825.875 KB
lipid_area_10.ibd	19.01.2021 10:21	IBD-Datei	5.052.769 KB
lipid_area_11.ibd	19.01.2021 10:23	IBD-Datei	4.960.049 KB
lipid_area_12.ibd	19.01.2021 10:26	IBD-Datei	5.092.589 KB
lipid_area_13.ibd	19.01.2021 10:29	IBD-Datei	4.882.190 KB
lipid_area_04.imzML	19.01.2021 10:06	IMZML-Datei	176.229 KB
lipid_area_05.imzML	19.01.2021 10:09	IMZML-Datei	173.052 KB
lipid_area_06.imzML	19.01.2021 10:11	IMZML-Datei	178.427 KB
lipid_area_07.imzML	19.01.2021 10:14	IMZML-Datei	178.793 KB
lipid_area_08.imzML	19.01.2021 10:16	IMZML-Datei	176.515 KB
lipid_area_09.imzML	19.01.2021 10:19	IMZML-Datei	171.577 KB
lipid_area_10.imzML	19.01.2021 10:22	IMZML-Datei	179.659 KB
lipid_area_11.imzML	19.01.2021 10:24	IMZML-Datei	176.358 KB
lipid_area_12.imzML	19.01.2021 10:27	IMZML-Datei	181.071 KB
lipid_area_13.imzML	19.01.2021 10:30	IMZML-Datei	173.577 KB
lipid_area_04.nrrd	28.08.2020 10:01	NRRD-Datei	3 KB
lipid_area_05.nrrd	25.02.2020 15:23	NRRD-Datei	6 KB
lipid_area_06.nrrd	25.02.2020 15:16	NRRD-Datei	6 KB
lipid_area_07.nrrd	25.02.2020 15:09	NRRD-Datei	6 KB
lipid_area_08.nrrd	25.02.2020 15:02	NRRD-Datei	6 KB
lipid_area_09.nrrd	25.02.2020 14:57	NRRD-Datei	6 KB
lipid_area_10.nrrd	25.02.2020 14:20	NRRD-Datei	6 KB
lipid_area_11.nrrd	25.02.2020 14:01	NRRD-Datei	6 KB
lipid_area_12.nrrd	25.02.2020 13:53	NRRD-Datei	6 KB
lipid_area_13.nrrd	25.02.2020 13:47	NRRD-Datei	6 KB

Ensure, that all \*.nrrd and \*.ibd files are available at the same directory level.

#### 4 Load the dataset into M<sup>2</sup>aia: *File > Open File* or *Ctrl + O*.

2m

Open all peptide files at once:

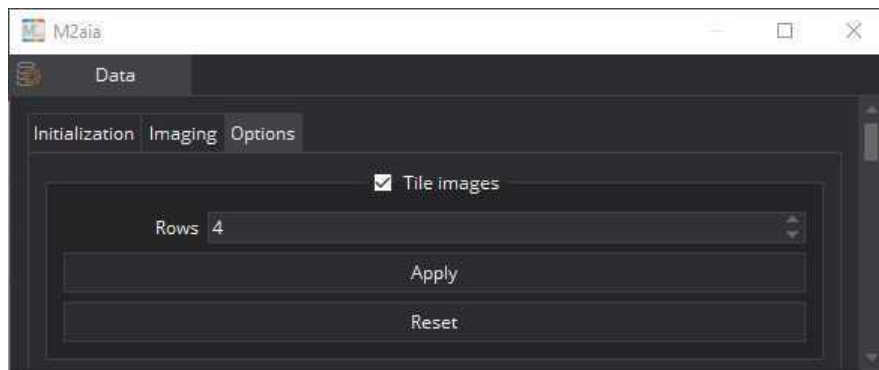
Name	Änderungsdatum	Typ	Größe
peptide_area_04.ibd	19.01.2021 11:13	IBD-Datei	2.760.964 KB
peptide_area_05.ibd	19.01.2021 11:15	IBD-Datei	2.690.495 KB
peptide_area_06.ibd	19.01.2021 11:17	IBD-Datei	2.821.581 KB
peptide_area_07.ibd	19.01.2021 11:19	IBD-Datei	2.885.469 KB
peptide_area_08.ibd	19.01.2021 11:21	IBD-Datei	2.833.231 KB
peptide_area_09.ibd	19.01.2021 11:23	IBD-Datei	2.769.691 KB
peptide_area_10.ibd	19.01.2021 11:25	IBD-Datei	2.893.337 KB
peptide_area_11.ibd	19.01.2021 11:27	IBD-Datei	2.860.760 KB
peptide_area_12.ibd	19.01.2021 11:28	IBD-Datei	2.927.121 KB
peptide_area_13.ibd	19.01.2021 11:31	IBD-Datei	2.784.753 KB
peptide_area_04.imzML	19.01.2021 11:14	IMZML-Datei	174.487 KB
peptide_area_05.imzML	19.01.2021 11:15	IMZML-Datei	170.024 KB
peptide_area_06.imzML	19.01.2021 11:18	IMZML-Datei	178.320 KB
peptide_area_07.imzML	19.01.2021 11:19	IMZML-Datei	182.366 KB
peptide_area_08.imzML	19.01.2021 11:21	IMZML-Datei	179.064 KB
peptide_area_09.imzML	19.01.2021 11:23	IMZML-Datei	175.040 KB
peptide_area_10.imzML	19.01.2021 11:25	IMZML-Datei	182.865 KB
peptide_area_11.imzML	19.01.2021 11:27	IMZML-Datei	180.805 KB
peptide_area_12.imzML	19.01.2021 11:29	IMZML-Datei	185.002 KB
peptide_area_13.imzML	19.01.2021 11:31	IMZML-Datei	175.989 KB
peptide_area_04.nrrd	04.09.2020 18:55	NRRD-Datei	5 KB
peptide_area_05.nrrd	04.09.2020 18:55	NRRD-Datei	5 KB
peptide_area_06.nrrd	04.09.2020 18:55	NRRD-Datei	5 KB
peptide_area_07.nrrd	04.09.2020 18:55	NRRD-Datei	5 KB
peptide_area_08.nrrd	04.09.2020 18:55	NRRD-Datei	5 KB
peptide_area_09.nrrd	04.09.2020 18:55	NRRD-Datei	5 KB
peptide_area_10.nrrd	04.09.2020 18:55	NRRD-Datei	5 KB
peptide_area_11.nrrd	04.09.2020 18:55	NRRD-Datei	5 KB
peptide_area_12.nrrd	04.09.2020 18:55	NRRD-Datei	5 KB
peptide_area_13.nrrd	04.09.2020 18:55	NRRD-Datei	5 KB

Ensure, that all \*.nrrd and \*.ibd files are available at the same directory level.

#### 5 Setup *Standard Display* for 2D visualization (optional).

When the export utility saves the original world coordinate origin (with respect to the MSI acquisition device), the image origin is available in world coordinates. If several such datasets were loaded at the same time, they may appear stacked or may be offset.

Open the *Options* tab in the *Data* view. Set Rows to 4 in the *Tile images* box and hit *Apply*.



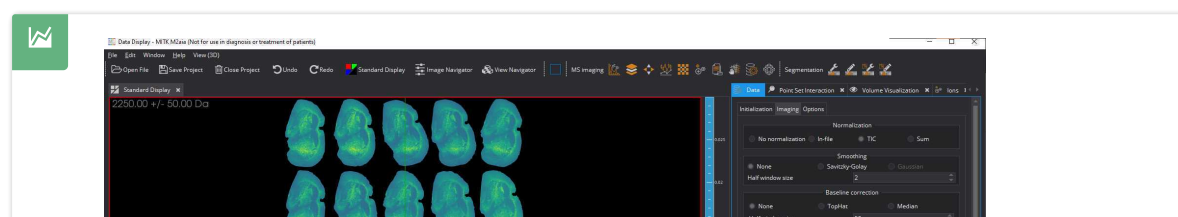
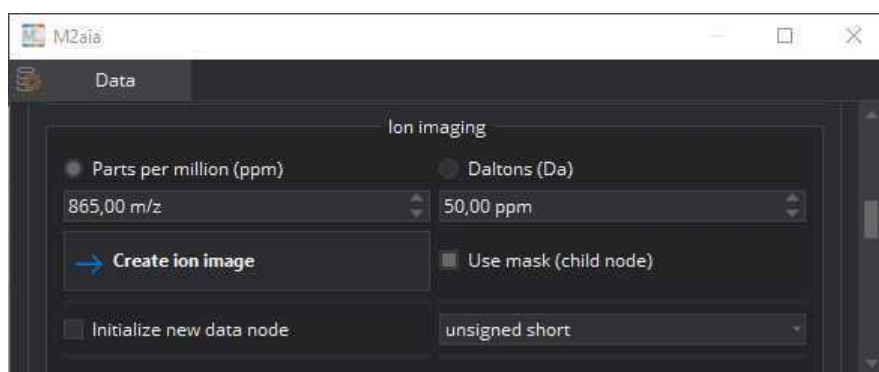
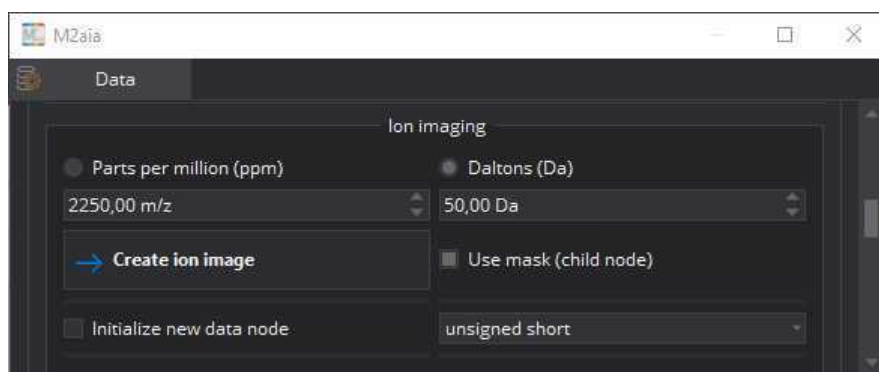
Maximize the top view display by pressing the blue square at the top right of the display menu.

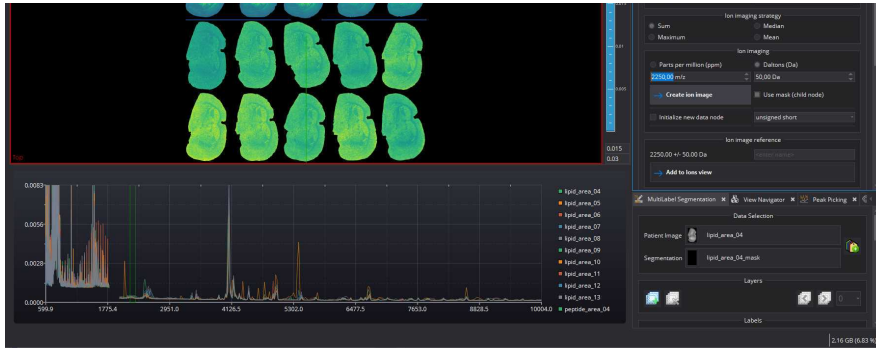
6

2m

Open the *Data* view, e.g. from the menu: *Window > Show View > Data* or click on the *Data* view tab.

Navigate to the *Ion imaging* box and create ion images at  $m/z$  2250  $\pm$  50 Da. and  $m/z$  865  $\pm$  50 ppm.



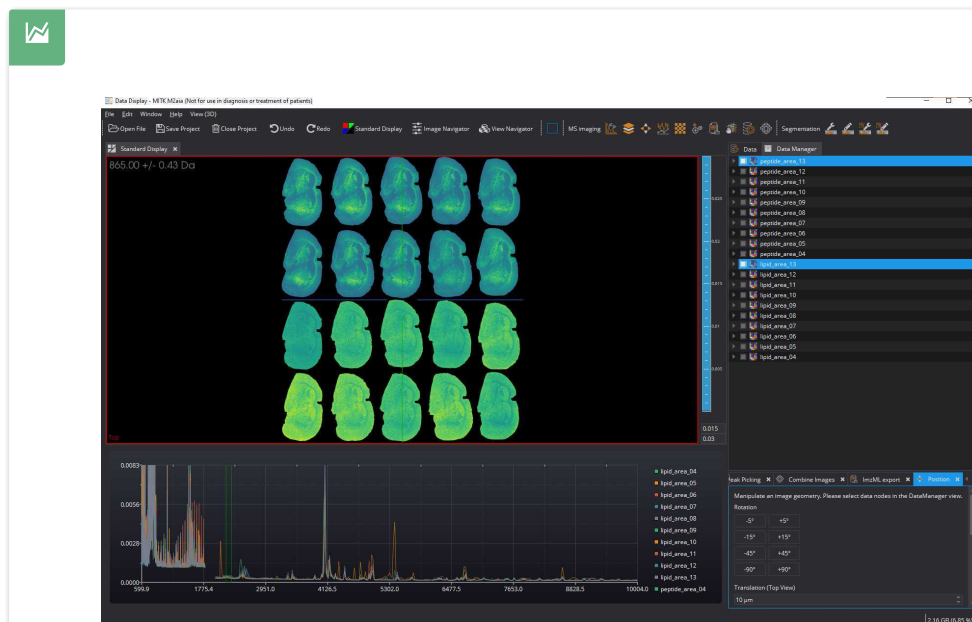


## 7 Pre-align images (optional). This can increase the registration accuracy.

Open the *Position* view: *Window > Show View > Position*.

Open the *Data Manager* view: *Window > Show View > Data Manager*.

Select image nodes in the Data Manager and use the Position view to align the images.



## 8

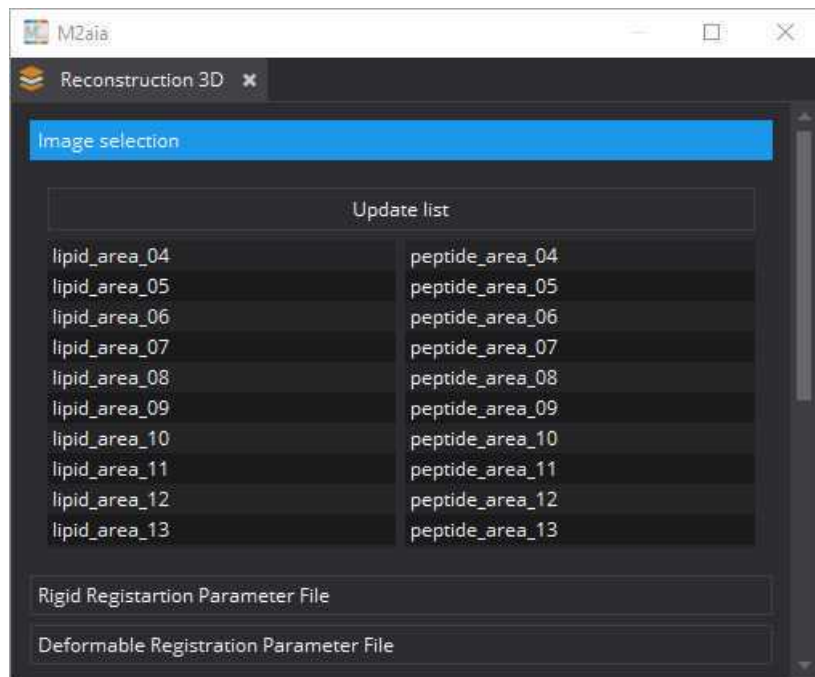
Open the *Reconstruction 3D* view, e.g. from the menu: *Window > Show View > Reconstruction 3D*

Select the *Image selection* tab.

Drag&Drop all peptide images to the right table.

1m



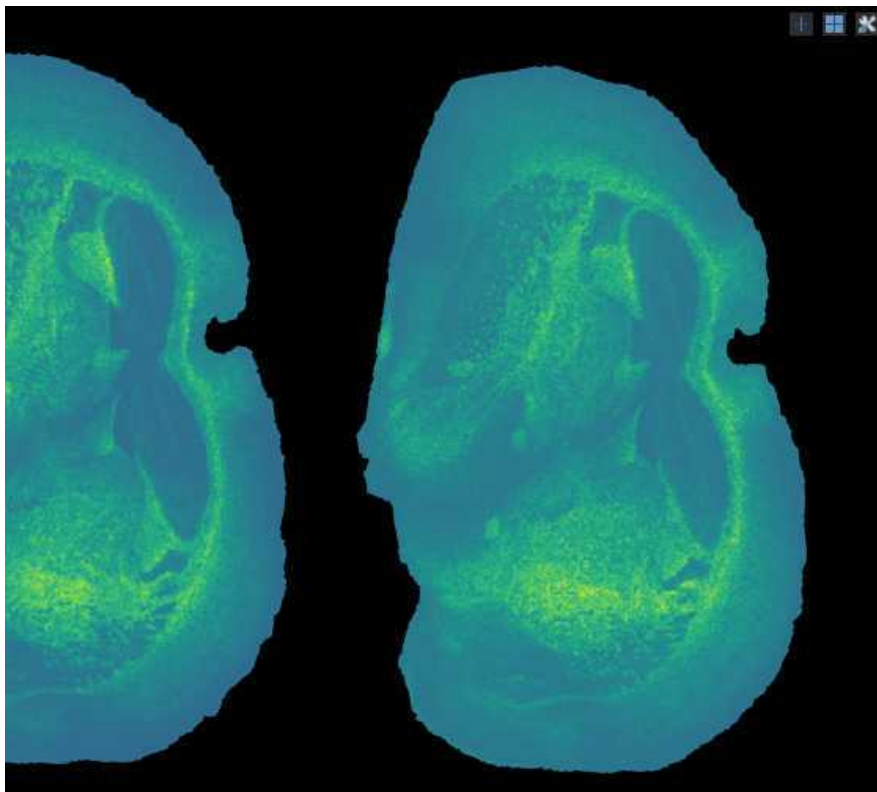


Select a reference slice in the left table (with lipid images) and click "Start stacking". Progress can be traced in the console window.

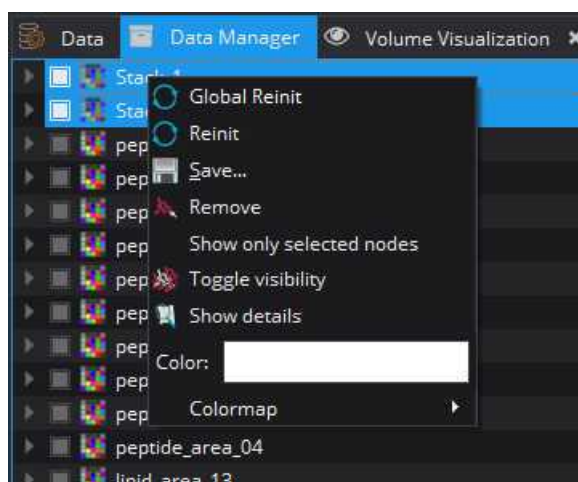


Two new nodes are listed in *Data Manager* (Stack\_0 -> lipids, Stack\_1 -> peptides).

- 9 Minimize the top view again to see all render windows by pressing the blue square at the top right of the display menu.<sup>2m</sup>



- 10 Select one or both nodes of the image stacks in the Data Manager and perform a *Reinit* and "*Show only selected nodes*"<sup>1m</sup> by right-clicking on the node(s).



- 11 In the *Data* view, select the *Initialization* tab and enable *Only visible*.<sup>1m</sup>  
Now perform 3D ion imaging by using the Spectrum view or the Ion imaging utilities (see step 6.).



