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Data Processing and Preparation of MALDI IMS data

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1 Works for me dx.doi.org/10.17504/protocols.io.bed3ja8n

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ABSTRACT

Scope:
How to process a mass spectrometry imaging data into a final imzML file.

1 For each spectrum in the data set, apply total ion current normalization by dividing the intensity values in the spectrum by the sum of the spectrum's intensity values.

2 Generate a mean spectrum for the dataset by taking the mean of each mass bin of the dataset.

3 Internally recalibrate the mean spectrum using well-known, spectrally ubiqitious lipid species, retaining the calibration equation.

4 Extract peak intensity data for every pixel using the provided identified mass list generated here (Lipid Annotation of MALDI IMS Datasets) by inverting the calibration coefficients to get the mass values in the original calibration and pulling intensity values from the Bruker .sqlite file that match these mass values.

5 Process the extracted peak list into a data table of columns: x, y, m/z 1, m/z 2, m/z 3... where 1, 2, and 3 are placeholders for the identified lipid species.

6 Read this table into R and create a *Cardinal* **MSImagingExperiment** object from the pixel coordinates and peak intensity values.
https://cardinalmsi.org

7 Use *Cardinal's* writeImzML() function to write the **MSImagingExperiment** object to an imzML file.

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