Rapid identification of chemically-related compounds produced by bacteria by Kendrick mass defect filtering to high resolution imaging mass spectrometry


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Introduction

Over the last years, lots of progress have been done in the development of mass spectrometry imaging, making the technique more and more accessible for various applications, such as biomarkers discovery or bioactive compounds identification. However, the progresses made in terms of spatial and instrumental resolution has for consequences the dramatic increase of dataset size, shifting the burden from data production to data analysis.

We propose here to use a semi-targeted method based on Kendrick mass defect (KMD) analysis to immediately identify the chemistry-related compounds in mass spectrometry imaging applied to microbiology samples. In that aim, we developed an in-house software to simplify the analysis of high resolution MS spectra that we then applied to mass spectrometry imaging.

Results

1) In vivo assay

Strains of two different bacteria were inoculated on a semi-solid agar-based PDA medium (Potato Dextrose Agar) at different distances from each other (0.5cm and 2cm) and incubated overnight at 30°C

2) Sample preparation for MALDI-MS imaging

3) Data acquisition

- High resolution FT-ICR MS Solarix 9.4T (Bruker Daltonics, Bremen, Germany)
- Calibration from 200m/z to 2000m/z with red Phosphorous (err. >0.5 Ppm)
- Stable TIC was obtained for MS imaging with the following conditions: Laser power 50% - Laser shots per pixel: 10 - Frequency: 200 Hz
- Pixel step set to 80 μm

4) Kendrick principle

Kendrick mass defect analysis is a powerful tool for compounds identification in complex spectra, by plotting the data according to the contribution of a repeated mass unit (here: CH₃), then, the measured masses are first converted into Kendrick mass = measured m/z × [(14.00000)/(14.01565)]

Then, the Kendrick mass defect is calculated based on the difference between the Kendrick nominal mass (the integer) and the Kendrick mass.

Kendrick mass defect = nominal Kendrick mass – Kendrick mass

5) Kendrick application to imaging mass spectrometry

Conclusions and prospects

- Kendrick mass defect filtering is particularly adapted for mass spectrometry imaging enabling:
  - Rapid compound screening and identification of chemically related compounds based on their repeating unit
  - Immediate visualization of the different adducts
- Our in-house software enables to reconstruct the images according to a specific group of molecules selected on their Kendrick values. This software can be used with any type of data (HPLC, IM-MS, IMS).
- This method can be applied on many different types of compounds with a repeated unit : lipids, sugars, polymers, lipopeptides.

Methods

- Rapid data filtration by Kendrick mass defect plot
- Lipopeptides detection based on Kendrick mass defect plot
- Rapid visualization of lipopeptides distribution using Kendrick

Literature