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Introduction

MALDI-imaging is a mass spectrometry technique for studying thin spatial samples (e.g. a tissue section).

MALDI-imaging is modern and fast growing technology with spatial resolution upto 10 μm used to localized proteins and small molecules for many purposes.

For a spatial point with coordinates (x,y) a high-dimensional mass spectrum is measured.

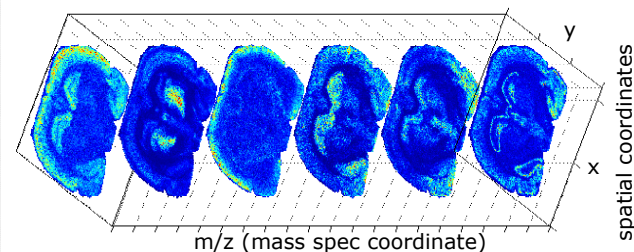


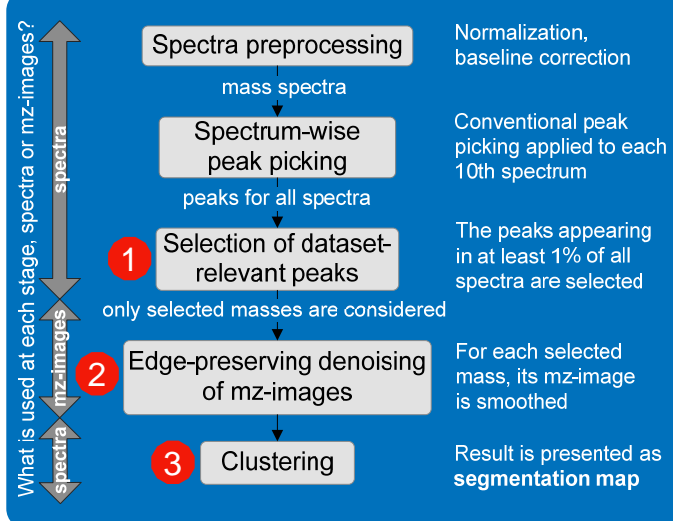
Fig. 1 Schematic representation of a MALDI-imaging data set (data cube).

We propose a new procedure for spatial segmentation of MALDI-imaging data which clusters all spectra into different groups based on their similarity.

The partition is represented by a segmentation map which explains the full data set with one image.

The key point of this procedure is the edge-preserving denoising of images corresponding to specific masses (m/z-images).

Our approach to spatial segmentation



Pipeline steps

1 Selection of dataset-relevant peaks

Reduces dimensionality ($\times 100$)

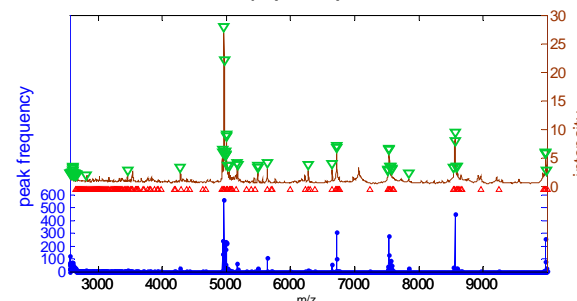


Fig. 2 Mean spectrum (brown), frequencies of peaks (blue) and selected dataset-relevant peaks (green triangles).

2 Edge-preserving denoising of m/z-images

Diminishes pixel-to-pixel variation

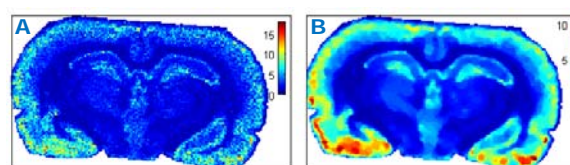


Fig. 3 A. Original m/z-image for 6648 Da; B. its denoised version.

3 Clustering

Splits spectra (pixels) into groups

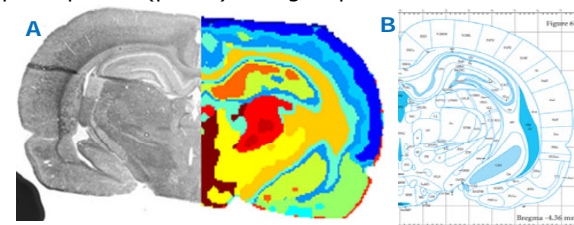


Fig. 4 A. Halves of optical image and the segmentation map. B. Schematic of the anatomical structure of the rat brain atlas (Elsevier). Anatomical structure is highlighted.

Interpretation of a cluster

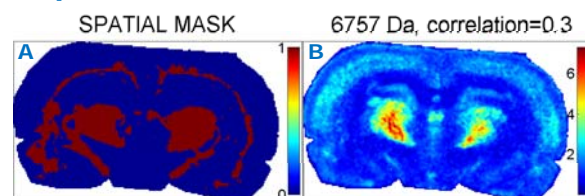


Fig. 5 A. Cluster as a spatial mask; B. The most co-localized m/z-image.

Importance of denoising

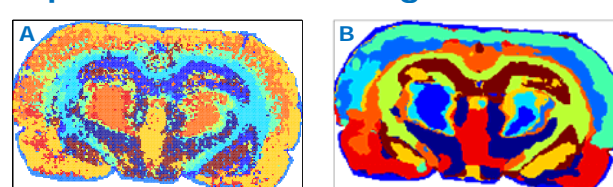


Fig. 6 Segmentation maps without (A) and with (B) edge-preserving denoising of m/z-images.

Applications

Neuroendocrine tumor

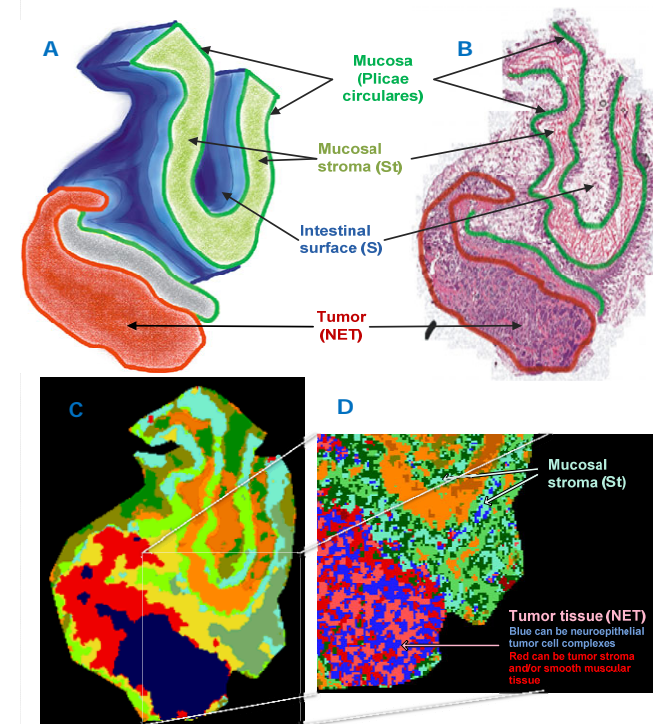


Fig. 7 A. 3D-structure of the tissue; B. optical image of the H&E stained section; C. Segmentation map, strong denoising. Tumor area is found (blue and red clusters). D. A part of the segmentation map, weak denoising. Tumor area shows the heterogenous composition.

Bacteria interactions

Study of natural products in zones of interactions of bacteria colonies.

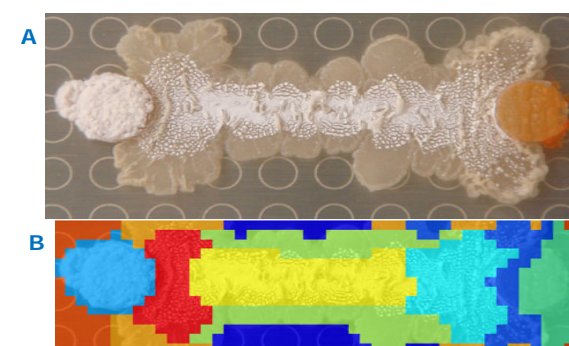


Fig. 8 A. Optical image of bacteria colonies; B. Segmentation map. Zones of interactions are found (light blue and red).

Conclusions

- New pipeline for spatial segmentation of MALDI-imaging data is proposed
- Potential of the approach is proven
- Segmentation maps highlight morphological/histological structures
- University of Bremen-Bruker patent application 20100225\267