Self-organizing maps: A versatile tool for the analysis of untargeted imaging datasets

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Objective

Mass Spectrometry Imaging (MSI) experiments can be used to complement metabolomics and investigate the spatial distribution of metabolites generating highly informative datasets. We propose to apply self-organising maps (SOMs) to analyze spatial information in MSI untargeted metabolomics datasets and identify a shortlist of m/z signals sharing a common spatial distribution, thus labeling them as "biomarkers" for an area of the section.

Methods

Untargeted full scan (m/z 120 - m/z 700) imaging experiments were performed on apple sections with a MALDI LTQ Orbitrap XL. CHCA was used as matrix and it was deposited by a Bruker ImagePrep station. Raw data were converted and analyzed in R.

Results

The proposed algorithm has been applied to the imaging dataset collected on an apple section (Figure) to identify 42 characteristic spatial distributions. The one grouping the ions which show a high concentration in the region below the apple skin and in correspondence of one of the apple bundles is shown in Figure. The SOM algorithm assign to this spatial class a list of 35 ions. 17 of these ions, were associated to secondary metabolites known to be present in apple in this specific area.

Conclusions

SOMs form a versatile tool for the untargeted analysis of high-resolution and high-accuracy MSI metabolomics datasets where they can be used to automatically identify spatial patterns and assess co-localization among different ions. Co-localization can be used to improve the chemical selectivity of imaging experiments, giving important tissue-specific information.

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