

[P136] Mass Spectrometry Imaging visualization tools developed during the Computis European project

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The Computis European project (2006-2009) was aimed at developing innovative experimental mass spectrometry imaging (MSI) techniques and software tools for data treatment and visualization, and at validating them in key biological applications (neurobiology, pharmaceutical drug development). The project succeeded in defining a specific standard format for MSI, imzML, in collaboration with the HUPO consortium. The four main MSI software tools developed by the project all handle the imzML format.

Data Cube Explorer provides an easy spectral and spatial exploration of MS images: spectrum zooming, scrolling through the dataset masses with a manual contrast tuning for images, selection of Regions Of Interest with the display of the associated spectra. The self-organizing map functionality classifies images according to the intensity of all pixel places and automatically selects images as different as possible.

Mirion is a simple visualization module displaying spectra by pixel and for the total image, with zooming and scrolling functions. Histogram of the total ion count of each pixel can be calculated, using different input parameters. Images are displayed for each peak of the total spectrum, with a manual intensity tuning and a comparison of the intensity distributions by pixel between several images.

EasyMSI enables spatial and spectral visualization of mass spectrometry imaging datasets (spectrum and image display, peak and pixel picking, zooming on spectra and images, ROI selection), as well as an assistance for the interpretation of data: This assistance includes indicators (relative variance, Moran index, m/z correlation) to highlight peaks that bring interesting information, peak list for molecule identification, spectrum denoising or structure analysis by clustering methods (K-means, fuzzy, hierarchical clustering, diffusion map). EasyMSI offers the advantage of processing and displaying the original data (i.e. without binning).

BioMap is an image analysis platform for MSI and Magnetic Resonance Imaging. It includes viewing functions (spectrum and image display, intensity adjustment, zoom, treatment of multiple ROIs, geometrical transformations and operations), and spectrum treatment (spatial or temporal filtering, baseline correction, detrending). More elaborated functions enable a simultaneous view of all dataset images, creation of a movie, statistical and histogram analysis, co-registration of images of one or two dataset(s), and realignment of images.

The use and capacities of these tools are presented through a comparative analysis of a rodent urinary bladder dataset in imzML format.

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