

Mass Spectrometry Imaging visualization tools developed during the Computis European project

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Mass spectrometry imaging visualization tools developed during the Computis European project

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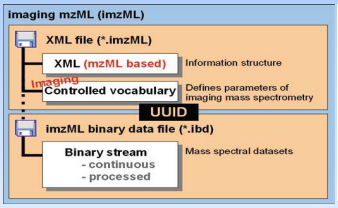
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b NOVARTIS, Lichstraße 35, WSJ-507.1101, CH-4002 Basel, Switzerland
c Justus Liebig University, Schubertstraße 60, Building 16, D-35392 Giessen, Germany
d FOM/AMOLF, Kruislaan 407, NL-1098 SJ, Amsterdam, The Netherlands

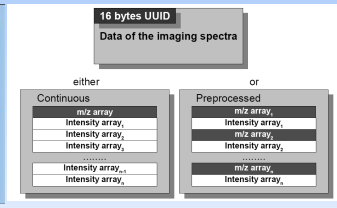
Mass spectrometry imaging technology is an operational and matured technology.
The goal of the Computis European project was to develop a standard format and efficient tools for processing and visualization of large size and complex datasets to answer the users' needs.
www.computis.org

imzML standard data format

XML file based on mzML format and validated by HUPO-PSI, including an extension of the mzML vocabulary for imaging specific parameters
+ Binary file for mass spectral data (external file for faster access and processing time)

Version 1.1.0 RC1 developed by the COMPUTIS project (2006-2009) and announced on 31 August 2009 at the IMSC conference in Bremen





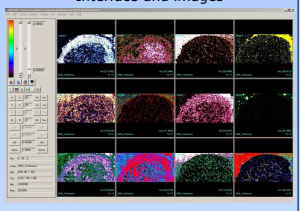
imzML enables reading data from all MSI equipments by external post-processing software.

Comparison of the functionalities of 4 software tools developed or upgraded during the COMPUTIS project on a rodent urinary bladder image.

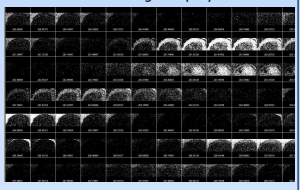
BioMap

- A well-known free platform for MALDI MSI and MRI analysis, adapted to the needs of proteomic and biologist teams.
  Running under Windows and Linux.
  IDL virtual machine free setup necessary.
- Export/Import of multiple formats including DICOM, Analyze, imzML, jpg, tiff, mp4, avi and text.
- Visualization based on multiplanar analysis.
  Spectrum and image display with numerous colour tables, zooming and intensity adjustment.
  Multi-image display (simultaneous view of all images of a dataset, display of an image stack shifted and partially overlaid).
  Geometrical transformations (translation, rotation, flipping and resizing of images).
- Possibility to download and process only part of a dataset to manage large datasets with limited memory.
  Selection and processing of multiple ROIs with annotation of images.
  Statistical and histogram analysis.
  Geometrical operations.
  Movie creation.
  Co-registration to superimpose several images and compare the position of patterns appearing at different m/z.

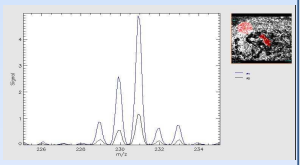
Interface and images



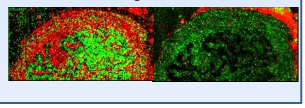
Multi-image display



Region Of Interest and spectrum



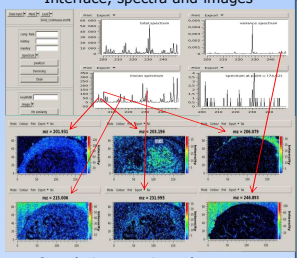
Co-registration



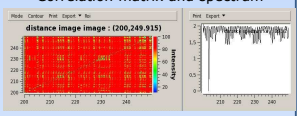
Easy MSI

- A platform for visualization and interpretation of MALDI and SIMS images.
  Full raw data loading and processing
  Running under Windows and Linux.
- Import of Analyze, GRD, Bruker Flex and imzML formats.
  Export in jpg, tiff, bmp, csv, postscript and svg formats.
- Spectrum and image display with several colour tables, zooming, peak and pixel picking, intensity tuning.
- Spectrum processing (wavelet denoising, baseline subtraction).
  Data reduction (binning, subimage).
  Selection of Region Of Interest (ROI) with display of the associated spectrum.
  Indicators highlighting peaks of interest in the spectra to guide data interpretation (relative variance, Moran index).
  Correlation matrix of the image, and correlation spectrum of a given m/z with the other m/z.
  Spatial and spectral classification with 4 clustering methods (K-means, fuzzy, hierarchical, diffusion map).
  Parametric peak extraction for faster interrogation of biological databases
  Image registration with EasyReg2D software.

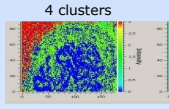
Interface, spectra and images



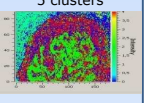
Correlation matrix and spectrum



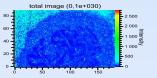
4 clusters



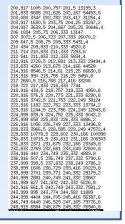
5 clusters



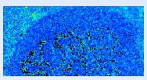
Total image



Peak list



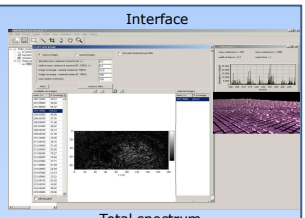
Residual image after peak extraction



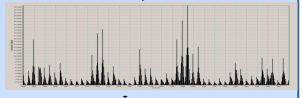
Mirion

- A software for combining MS^n measurements with MALDI, SIMS and DESI techniques, and processing high mass resolution images under Windows.
  Xcalibur installation necessary.
- Import of imzML , JLU internal and Thermo Fisher raw formats.
  Export in bmp, tif and jpeg formats.
- Display with zooming of pixel spectrum and total spectrum as histogram.
  Total ion count display as rotating hypercube.
  Image display with an automatic selection of the best images, based on general image criteria, mass lists and individually given parameters.
  Manual intensity adjustment and legend options for images.
- Data management and processing organized as projects with saving.
  Analysis guided by the user-interface.
  Comparison of MS images with complementary imaging techniques (optical, PCA, …) through arithmetic operations.
  Masks to keep aside unwanted data (m/z, regions, shots, runs) and process larger datasets.

Interface



Total spectrum



Images

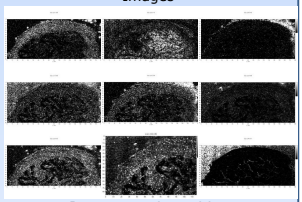


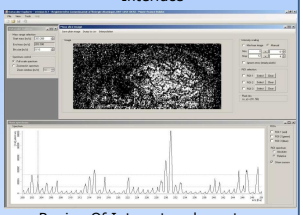
Image superimposition



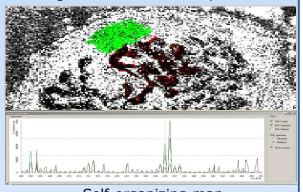
Data Cube Explorer

- A user-friendly tool to provide an easy spectral and spatial exploration of imaging MALDI and SIMS datasets under Windows.
- Import of imzML and FOM internal formats.
  Export in png and csv formats.
- Total spectrum display with zooming
  Image display with a manual greyscale tuning to improve image contrast.
- Selection of Regions Of Interest (ROI) with the display of the associated spectra.
  "Self-organizing map" function to classify images according to pixel intensity and to select automatically a given number of images as different as possible. The classification method used is unsupervised competitive learning, also known as the Kohonen neural network.

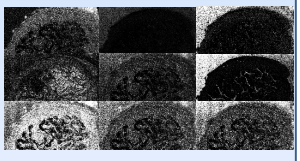
Interface



Region Of Interest and spectrum



Self-organizing map



Several offline software tools are at users' disposal for processing mass spectrometry images.
Next step is molecular characterization and quantification.
imzML specifications, imzML converters and MSI software are available on www.maldi-msi.org

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