



## Mass Spectrometry Imaging visualization tools developed during the Computis European project

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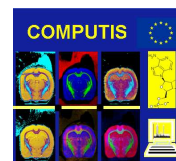
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# Mass spectrometry imaging visualization tools developed during the Computis European project



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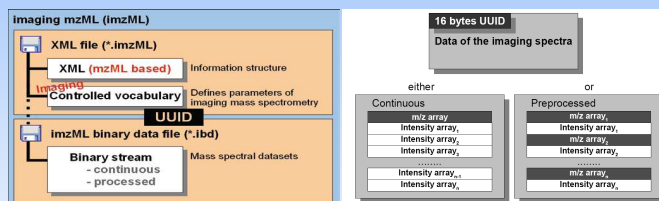
**Mass spectrometry imaging technology is an operational and matured technology. The goal of the Computis European project was to develop a standard format and efficient tools for processing and visualization of large size and complex datasets to answer the users' needs.**

[www.computis.org](http://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.

**NOVARTIS 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.

**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.

**JUSTUS-LIEBIG-UNIVERSITÄT GIESSEN Mirion**

- A software for combining MS<sup>n</sup> 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.

**AMOLF FOM 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 grayscale 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.

**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](http://www.maldi-msi.org)**

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