

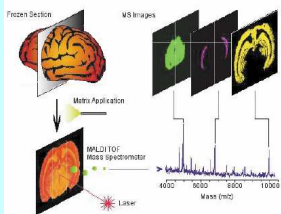
COMPUTIS:

A SOFTWARE PLATFORM FOR MULTIMODE IMAGING MASS SPECTROMETRY

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INTRODUCTION

Molecular imaging mass spectrometry



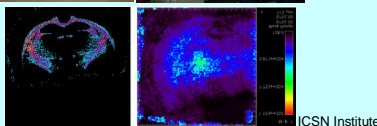
Access to the spatial distribution of chemical compounds in biological tissue samples^{1,2}:

- with no a priori
- in only one scan

Proteomics and metabolomics applications^{2,3}:

- biomarker discovery (tumor profiling)
- drug metabolism

SIMS and MALDI: metabolite or protein ionization



Modality	SIMS	MALDI
Mass range (Da)	10 ²	10 ³
Molecules	Metabolites	Proteins
Resolution (µm)	1	10
Matrix	No	Yes
Depth of analysis	10 nm	10 µm

Computis project

(<http://www.computis.org>)



STREP (coordinator: S. Haan)
 3.5 years
 Kick-off: January 27th, 2006



Innovative methods for:

- 1) sample preparation
- 2) instrumentation
- 3) data processing
- 4) industrial applications

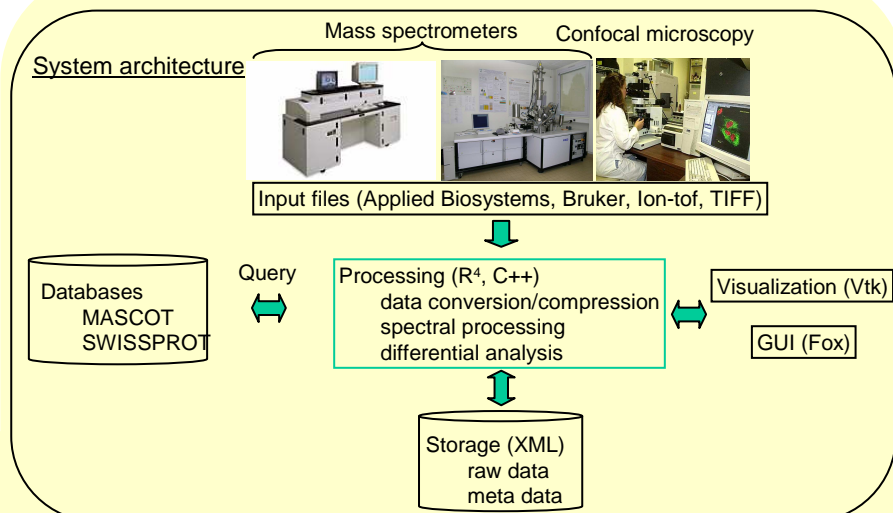


OBJECTIVES

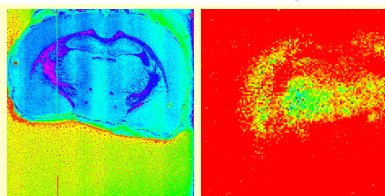
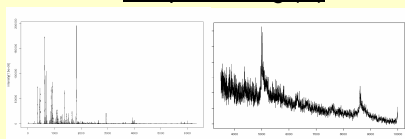
Development of a dedicated software

- 1) high performance massive data acquisition and processing:
 - high size of images (Go): 10⁴ spectra with 10⁴ m/z intensities each
 - noise processing
 - peak detection
- 2) superpositioning information from various analytical techniques:
 - SIMS
 - MALDI
 - confocal
- 3) connection to existing databases

PRELIMINARY RESULTS

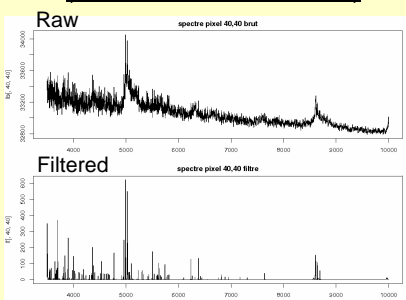


Pre-processing (R)

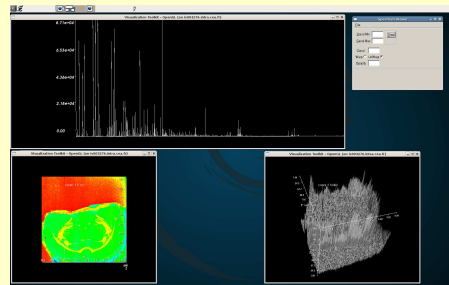


Modality	SIMS	MALDI
Nb of pixels	256 × 256	114 × 114
Pixel size (µm)	62.5	115
Nb of channels	10 ⁶	10 ⁴

Baseline correction (wavelet transform, R, C++)

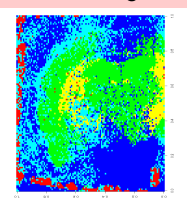


Visualization (Vtk)

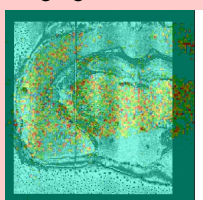


PERSPECTIVES

Clustering



Merging modalities



BrainVISA/Anatomist (T. Delzescaux, SHFJ)

REFERENCES

1. Stoeckli M, *et al.* (2001). Imaging mass spectrometry: a new technology for the analysis of protein expression in mammalian tissues. *Nature Medicine*, 7:493-6
2. Brunelle A, *et al.* (2005). Biological tissue imaging with time-of-flight secondary ion mass spectrometry and cluster ion sources. *Journal of Mass Spectrometry*, 40:985-999
3. Rubakhin S, *et al.* (2006). Imaging mass spectrometry: fundamentals and applications to drug discovery. *Drug Discovery Today*, 10:823-837.
4. The R project for statistical computing [<http://www.R-project.org>]

ABBREVIATIONS

MALDI: matrix-assisted laser desorption/ionization, SIMS: secondary ion mass spectrometry, TOF: time-of-flight, XML: extensible markup language

