

# 20<sup>th</sup> International Mass Spectrometry Conference

August 24-29, 2014 Geneva, Switzerland

ABSTRACT BOOK

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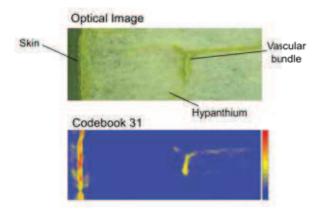


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#### Conclusions

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. This co-localization can be used to improve the chemical selectivity of imaging experiments, giving important tissue-specific information.

#### **Novel Aspect**

With the proposed algorithm, SOMs are used to associate the thousands of signals collected over the tissue to a limited number of characteristic spatial distributions. The ions belonging to the same spatial class are co-localized and they can be used in combination to mass spectra libraries and in-silico fragmentation engines to perform (partial) chemical annotation.

P.Franceschi, R Wehrens, PROTEOMICS Special Issue: Tissue Proteomics and Imaging Mass Spectrometry Volume 14, Issue 7-8, pages 853–861

# MPS07-17 / Tissue Surface Properties Jeopardize Quantitative DESI Imaging of Organic Acids in Grapevine Stem

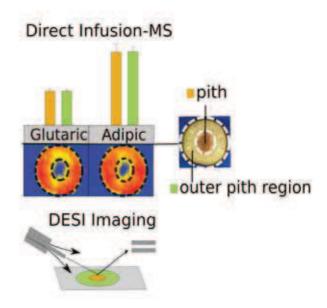
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### Introduction

DESI imaging has recently gain popularity as a tool to assess spatially resolved biological processes and to assist biomarker identification over unmodified sample surfaces, but how surface properties affect the output of DESI imaging experiments has not been investigated to date. We addressed this issue in a series of experiments which studied the distribution of small organic acids in grapevine stems. In our investigation, we compared the spatial distribution of endogenous and xenobiotic compounds obtained by DESI with the one resulting from the conventional analysis of the sections. The specific effects of the surface properties on the DESI detection of this class of compounds was also investigated by DESI profiling on different PTFE surfaces.

## Methods

DESI imaging of endogenous and xenobiotic organic acids in grapevine stem was performed using a Thermo-Fisher Scientific LTQ Orbitrap XL mass spectrometer equipped with an OmniSprayTM ion source under negative ion mode with spatial resolution of 200 µm. Ion chromatography and direct infusion-MS were used to quantify the endogenous and xenobiotic organic acids in grapevine stems, respectively. DESI profiling of a mixture of organic acid standards was done with the same instrument on 3 PTFE surfaces with different pore size and porosity.



#### Results

DESI imaging showed that the distribution of malic (endogenous), glutaric (xenobiotic) and adipic (xenobiotic) acid were significantly different between pith and out pith region. This specific distribution was not confirmed by IC and direct infusion, which indicated a rather uniform distribution over the tissue section. DESI profiling results on the PTFE surfaces suggest that the local physical properties of the tissue surfaces strongly affect the ionization process as well as their relative quantitative detection.

#### **Conclusions**

Different surface properties within a structurally/biologically heterogeneous tissue can affect the quantitative detection of analytes resulting in MS images misrepresenting the true distribution of the analytes.

# **Novel Aspect**

As in the case of MALDI, the outcomes of DESI imaging experiments could be affected by the local properties of the tissue sample. Experimental results, then, have to be carefully validated.

# MPS07-19 / Development of new stigmatic imaging mass spectrometer and its application for surface analysis of high functional organic materials

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#### Introduction

Measurement methods of spatial distribution of molecules such as proteins and drugs at cellular-scale are required in many fields including pathology, pharmacology, etc. Recently, scanning type imaging mass spectrometry (IMS) with matrix-assisted laser desorption/ionization (MALDI) is intensively used for biomolecular analysis. However, the spatial resolution of scanning MALDI-IMS is limited by the laser focus diameter to about 10 - 100  $\mu m$ . Therefore, we are developing a stigmatic MALDI imaging mass spectrometer, in which spatial resolution of sub-micron can be achieved irrespectively to the laser focus diameter.

#### Methods

The experimental apparatus for stigmatic imaging consists of MALDI ion source, a multi-turn time-of-flight mass spectrometer (MULTUM-IMG) and a time and position sensitive delay line detector. Ion distributions at the sample plate are magnified and