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ABSTRACT BOOK

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SFSM
Société Française de Spectrométrie de Masse

Conclusion
Desorption nanoelectrospray can analyze plant materials without sample preparation. New moving device for nanoDESI imaging allowed lateral resolution bellow 100 µm.

Novel Aspect
The new version of nanoDESI ionization allows mass spectrometry imaging and is useful for analysis of plant material without sample preparation.

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MPS07-15 / Dependence of mass peak shape on r/r0 ratio in quadrupole mass analyser

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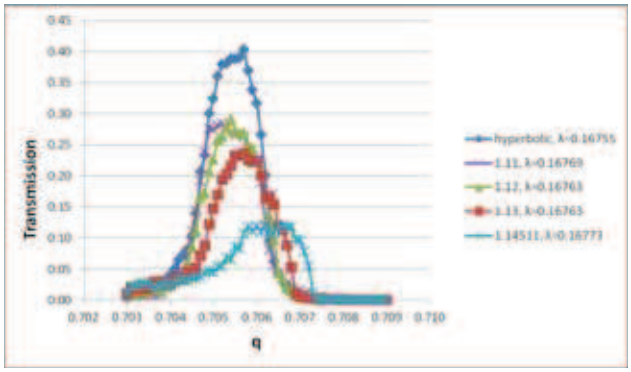
Introduction
The use of round rods in quadrupole mass analysers (QMA) arise a task of rods radius determination, to make best substitution of hyperbolic electrodes.

Earlier [1-4], a number of most successful QMA field radius to round rods radius (r/r0) ratios was indicated. In this work, a new view on peak shape vs. r/r0 ratio dependence, and possible ways to choose r/r0 ratio based on mass peak shape analysis are presented.

Methods
Using Boundary Element Method, potential distribution in electrode configurations of four rods inside round shield with various r/r0 ratios were calculated. After it, QMA spatial harmonics coefficients for each configuration were computed.
Peak shapes were determined by calculating ions trajectories considering realistic number of RF-field cycles and thirty calculated harmonic coefficients.
Trajectory calculations were performed by solving Mathieu equation, using Runge-Kutta–Nustrom–Dormand-Prince method.
It was proposed to assess field quality by harmonic coefficient a2, as a factor of "quadrupolarity", and k=sqrt(a12+a22+a32+...+aNmax2), as a factor of field "purity".
Harmonic coefficient a2 have nearest to 1 value at r/r0=1.112, while k reaches minimum at r/r0=1.1447. Consequently, the best r/r0 value should lie between these boundaries.



Results
Mass peak profiles for a number of r/r0 ratios were plotted. λ=a/(2q) parameter was chosen individually for each r/r0 ratio to obtain equal peak width at half height. Resulted profiles were overlapped at one drawing.
It was discovered, that approaching to lower boundary of r/r0 range increases transmission and improves peak low-mass boundary, but deteriorates peak high-mass boundary.
On the other hand, approaching to higher boundary of r/r0 range deteriorates transmission and peak low-mass boundary, but improves peak high-mass boundary. Peak tip shape becomes best at the middle of the range.

Conclusions
The choice of r/r0 ratio in the range from 1.112 to 1.1447 should be determined by tasks, which is to be solved by QMA, and by specified mass peak shape requests.
A simple averaging of high and low range boundaries gives compromise value of r/r0=1.12835, which agrees with previously obtained results [3-4].

Novel Aspect
Factors, that determine a choice of r/r0 ratio, were proposed. The influence of r/r0 ratio on peak boundaries and peak tip was considered.

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MPS07-16 / Self-organizing maps: A versatile tool for the automatic analysis of untargeted imaging datasets

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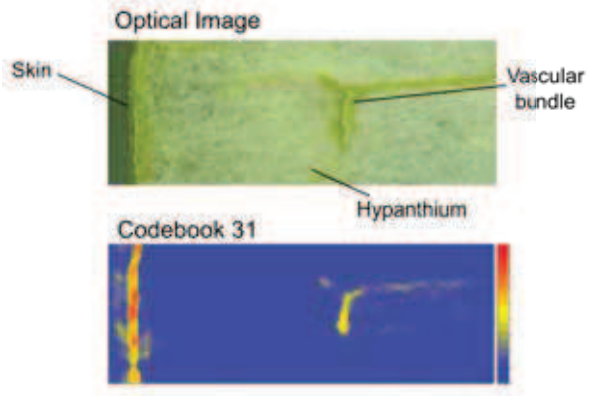
Introduction
Mass Spectrometry Imaging (MSI) experiments constitute the ideal complement to metabolomics to investigate the spatial distribution of key metabolites. In spite of their caveats and limitations, they generate highly informative datasets, which are difficult to mine mainly due to their sheer size. In this contribution we illustrate how self-organising maps (SOMs) could be efficiently used to automatically analyze spatial information in MSI untargeted metabolomics datasets. In our approach, SOMs are used to identify a shortlist of m/z signals sharing a common, characteristic and interesting spatial distribution, thus labeling them as "biomarkers" for an area of the section. Additionally, the proposed algorithm can be used to process the raw data and extract high-resolution information on interesting ions.

Methods
Untargeted full scan (m/z 120 - m/z 700) imaging experiments were performed on apple (Golden Delicious) sections with a MALDI LTQ Orbitrap XL mass spectrometer with a resolution of 60.000. The CHCA matrix was deposited by using an ImagePrep station. Raw data were converted into the open CDF format and analyzed with a set of algorithms developed in R.

Results
The proposed algorithm has been applied to the imaging dataset collected on the apple section (Figure) to identify 42 characteristic spatial distributions. The one grouping the ions which show a high concentration in the region below the apple skin and in correspondence of one of the apple bundles is shown in Figure. The SOM algorithm associates to this spatial class a list of 35 ions. For 17 of these ions, it was possible to to associate them to secondary metabolites known to be present in apple in this specific area.



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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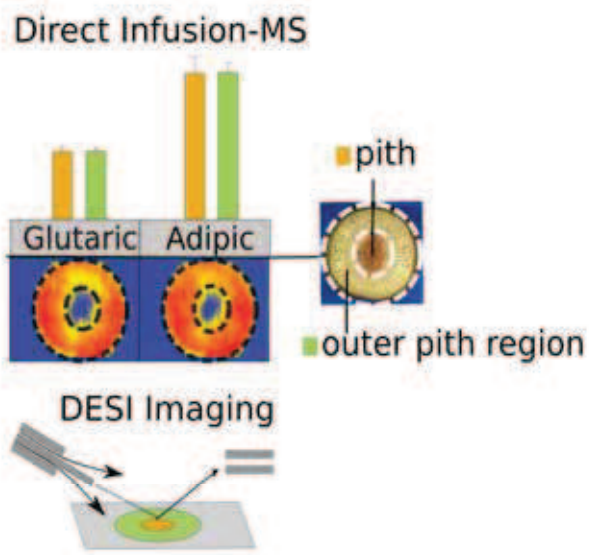
Introduction
DESI imaging has recently gain popularity as a tool to assess spatially resolved biological processes and to assist biomarker identification over unmodified sample surfaces, but how surface properties affect the output of DESI imaging experiments has not been investigated to date. We addressed 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 µm. 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