IMSC 2014

20th International Mass Spectrometry Conference

August 24-29, 2014
Geneva, Switzerland

ABSTRACT BOOK

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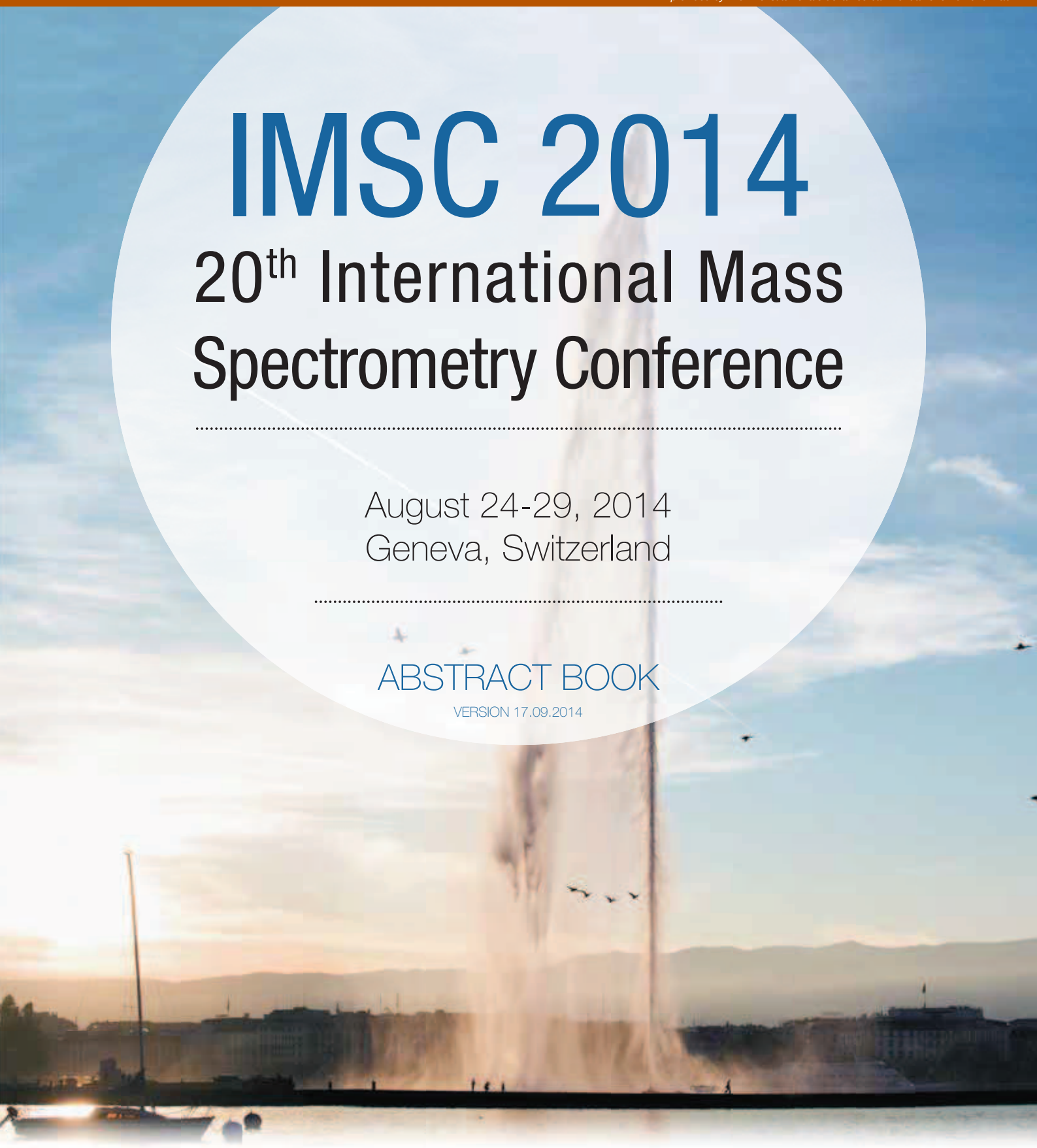

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candidate metabolites were analyzed using LC-MS. The results demonstrated that the amino acid profiles of urine and serum were changed when mice were treated with tt-DDE. Ten amino acids were found to be significantly reduced in the serum of mice treated with tt-DDE at the 8 weeks after tt-DDE was instilled.

Conclusions
LC-MS method has been proved to be powerful and reliable analytic platform for urine and serum metabolites screening with relative high sensitivity. The main conclusion of our study is related to the identification of the metabolic profiling in urine and serum of mice treated to tt-DDE. The results demonstrated that the amino acid profiles of urine and serum were changed when mice were treated with tt-DDE.

Novel Aspect
The objective of this study was to identify any changes in metabolite profiles associated with the development of tt-DDE-induced lung lesions.

WPS26-35 / Analysis of untargeted MS-based metabolomics data: the metaMS package for R
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Introduction
Untargeted MS metabolomics data provide a wealth of data on the presence and abundance of metabolites in biological samples. The extraction of relevant information can be difficult, and many software platforms have been proposed. One of the most popular tools for analysing LCMS and GCMS data is XCMS, written in the R language. An add-on to XCMS, developed specifically in the context of untargeted metabolomics, is metaMS, providing facilities for building in-house databases of chemical standards geared towards specific organisms or groups of metabolites, automatic annotation, and quantification. MetaMS, like XCMS, is publicly available from the Bioconductor repository.

Methods
For LCMS, the main part of the metaMS pipeline is similar to the XCMS pipeline. The additions from metaMS focus on improved annotation using in-house databases, an m/z and intensity-dependent mass accuracy window and an explicit definition of minimal support for annotation. The outcome is a matrix summarizing for all samples the intensities of the aligned peaks. The GCMS pipeline is different, working on so-called pseudospectra rather than individual peaks; here, the output is a relative intensity measure for chemical compounds rather than individual peaks (Wehrens et al., 2014). The compounds may be annotated (when there is a match with the database), or labelled as Unknowns.

Results
A web-based pipeline has been built using the metaMS package, which now is in daily use by the metabolomics platform at FEM. Processing hundreds of samples takes only a couple of hours on a regular four-core linux desktop computer. The generated tables can be immediately be used for subsequent statistical analysis. A common application is Quality Control: a score plot from a Principal Component Analysis can be inspected to see whether the quality control samples do not show a trend with injection order.

Conclusions
Open-source software like metaMS provides ultimate control over data processing, which is of utmost importance when analysing data as complex as GCMS or LCMS data. In addition, the large user base of the underlying XCMS package guarantees rapid adaptation to new developments, timely bug reporting and on-line user feedback. MetaMS provides a top layer over XCMS, specifically geared to untargeted metabolomics.

Novel Aspect
The novel aspects of metaMS are found at several levels: at the most abstract level the functionality of XCMS is extended and geared towards untargeted metabolomics data. At more detailed levels this includes tools for setting up in-house databases, doing annotation in a principled way, and a completely new approach to handle GCMS metabolomics data.

R. Wehrens, G. Weingart and F. Mattivi: J. Chrom. B DOI: 10.1016/j.jchromb.2014.02.051

WPS26-36 / The potential of two-dimensional chromatography in non-targeted metabolome analysis
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Introduction
Non-targeted metabolomic approaches have received more and more attention during the past years. Nowadays, many laboratories rely on the selectivity and resolving power of mass spectrometry based systems to identify the individual metabolites and create metabolic fingerprints via non-targeted analysis. This strategy has clear shortcomings for unstable metabolites and those that occur as multiple isomers. Moreover, peak capacity and sufficient retention of both polar and apolar compounds are the limiting factors in LC-MS based non-targeted analysis. Metabolic fingerprints obtained by such methods might therefore be biased and have to be evaluated carefully.

Methods
In this work, the potential of two-dimensional (2D) chromatography in non-targeted metabolomic approaches with a special focus on isomeric metabolites is explored exemplarily for sugar phosphates. Aiming at the establishment of an online combination in a 2DLC-TOFMS setup, different modes of chromatography including hydrophilic interaction liquid chromatography (HILIC), reversed-phase chromatography (RPLC) as well as ion chromatography techniques were evaluated.

Results
A comparison between data sets generated using conventional non-targeted LC-MS methods and employing a 2DLC-MS approach in non-targeted analysis will show if the application of the latter increases the amount of extractable isomer information from the resulting metabolic fingerprints.

Conclusions
LC-MS based non-targeted analysis in metabolomics requires a comprehensive approach that takes the high chemical variability of intracellular metabolites into account. If left unassessed, a potential methodological bias might result in misleading metabolic fingerprints and wrong biological interpretations. Especially the determination of sugar phosphates and their isomeric forms demands for method optimization even in non-targeted analysis.

Novel aspect
To the authors' knowledge, it is the first time that different modes of chromatography are systematically evaluated in a 2DLC-MS setup in terms of their potential beneficial effects on the