

Accepted Manuscript

Title: Increasing selectivity and coverage in LC-MS based metabolome analysis

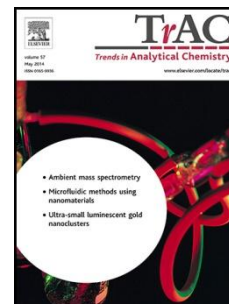
Author: Karin Ortmayr, Tim J. Causon, Stephan Hann, Gunda Koellensperger

PII: S0165-9936(16)30108-X

DOI: <http://dx.doi.org/doi: 10.1016/j.trac.2016.06.011>

Reference: TRAC 14783

To appear in: *Trends in Analytical Chemistry*



Please cite this article as: Karin Ortmayr, Tim J. Causon, Stephan Hann, Gunda Koellensperger, Increasing selectivity and coverage in LC-MS based metabolome analysis, *Trends in Analytical Chemistry* (2016), <http://dx.doi.org/doi: 10.1016/j.trac.2016.06.011>.

This is a PDF file of an unedited manuscript that has been accepted for publication. As a service to our customers we are providing this early version of the manuscript. The manuscript will undergo copyediting, typesetting, and review of the resulting proof before it is published in its final form. Please note that during the production process errors may be discovered which could affect the content, and all legal disclaimers that apply to the journal pertain.

Increasing selectivity and coverage in LC-MS based metabolome analysis

Karin Ortmayr^{a,b,§}, Tim J. Causon^{b,§}, Stephan Hann^b, Gunda Koellensperger^{a,*}

^a Institute of Analytical Chemistry, Faculty of Chemistry, University of Vienna, Waehringer Strasse 38, 1090 Vienna, Austria

^b Division of Analytical Chemistry, Department of Chemistry, University of Natural Resources and Life Sciences (BOKU) Vienna, Muthgasse 18, 1190 Vienna, Austria

* Corresponding author, E-mail address: gunda.koellensperger@univie.ac.at, Tel.: +43 664 6027752303, Fax: +43 1 42779523

[§] These authors contributed equally to this review.

HIGHLIGHTS

- Maximizing selectivity is crucial towards matching metabolome diversity.
- Structural isomers and in-source fragments challenge high-resolution mass spectrometry.
- The separation power of one-dimensional separations limits metabolome coverage.
- On-line combinations of orthogonal separations enhance coverage and throughput.
- Ion mobility separation can further supplement chromatographic selectivity.

ABSTRACT

The term non-targeted metabolomics implies a global and unbiased analysis. This involves the complex (and yet not routine) task of correct alignment and eventually annotation of statistically grouped ions as known metabolites according to accurate mass and chromatographic parameters. The comprehensiveness is practically compromised by the enormous chemical diversity of the metabolome. As solutions involving multiple methods are practically unfeasible for many extensive non-targeted metabolomics studies, increasing selectivity to yield a higher coverage of the metabolome considered (preferably within one analytical run) remains a crucial aspect for throughput, affordability and data processing considerations. This contribution presents an overview on proposed novel LC-MS-based workflows aiming to increase selectivity for maximizing metabolome coverage within a single analytical run. We suggest that analytical strategies involving on-line combinations of orthogonal liquid chromatographic separations with mass spectrometry or ion mobility-mass spectrometry are key to addressing this pursuit.

Keyword

non-targeted metabolomics; two dimensional liquid chromatography; heart-cut two dimensional liquid chromatography; comprehensive two dimensional liquid chromatography
high resolution mass spectrometry; ion mobility; collisional cross section

Download English Version:

<https://daneshyari.com/en/article/7688471>

Download Persian Version:

<https://daneshyari.com/article/7688471>

[Daneshyari.com](https://daneshyari.com)