

COMPREHENSIVE SCREENING OF AN ENVIRONMENTAL WATER SAMPLE WITH HRMS COUPLED WITH IMS AND AN INTEGRATED SCIENTIFIC INFORMATION SYSTEM

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INTRODUCTION

Companies and environmental regulatory authorities are looking toward High Resolution Mass Spectrometry (HRMS) to expand the scope of their screening methods. Improvements in mass spectrometer sensitivity and highly selective acquisition techniques allow users to find more compounds in a single injection than ever before, whether by a targeted analysis or via elucidation of unknown, or non-targeted masses of interest. Advancements in the Informatics used to process, interact and review non-targeted HRMS datasets have also increased markedly. Here we demonstrate how the use of modern informatics (UNIFI) can be used to comprehensively screen environmental samples for a range of contaminants in a given target list, as well as look for non-targeted or unknown compounds of interest. A typical experiment workflow is shown in the diagram below. We focus on the steps highlighted in green, typically the rate determining steps in getting from injection to report. Coupling ion picking and componentization¹ not only enables a user to process data beyond the Chromatogram (XIC) approach and (HDMSE)² without the need to reprocess data. injection to result bottleneck and quickly get



Non-Targeted Acquisition

Ion mobility experiments occur on a convenient timescale (msec) between MS scan times (s) and ToF pusher frequencies (µs). A user gets orthogonal separation of compounds with 12-15 points across a UPLC peak (4-6 s) for precursor ions and products ions in a single injection (HDMSE). There is no compromise.

IMS - Separation of ionic species as they drift through a gas under the influence of an electric field. Mobility is dependent on mass, charge and Interaction Cross Section.

CCS values are calculated for every molecular ion. CCS is a robust and precise physicochemical property

System peak capacity 50% higher with IMS. An IMS 7 min gradient delivers comparable peak capacity to a non-IMS 12 min gradient.

Apex Peak Picking

UNIFI uses a sophisticated apex peak picking algorithm which selects mass spectral data using the apex of chromatographic and drift peaks for ion mobility data. This results in spectra being generated that only include masses with the same apex, thus reducing the background interferences and bringing clarity to the data.

Following Apex peak picking these spectra are then processed further, grouping masses into components by identifying potential isotopes, adducts and fragment ions. The resulting component table is what a user will interrogate for answers, not individual raw data files.

Cleaner observed Low Energy (LE) and High Energy (HE) Spectra in MS^E and "ridiculously" cleaner LE and HE Spectra for HDMSE^E compared to a traditional 2D XIC approach

Automatic removal of spectral peaks (background) with no apex

Data Review

Binary Compare - Component Plot

Common Fragment Search for Microcystins

Non-Targeted "Unknown" Screening
Binary Compare, Halogen Match, Common Fragment, Mass Defect, Neutral Loss and Multivariate

Targeted Screening
Match componentized data by Retention Time, Theoretical Accurate Mass Fragment Ions, Isotope Scores, CCS.

HDMSE^E Componentized Data
Process Data Once – Interrogate Many Times

Elucidation Toolset
A comprehensive selection of tools for elucidation of unknown masses of interest. Batch elucidation tool results are shown below for the highlighted masses in the binary compare plot above.

Discovery Tool - Batch Elucidation

Transformations List

Degradation Studies/Metabolite ID
Potential metabolites of Atrazine discovered by interrogating componentized data for transformations. Localization of the transformation is predicted based on fragmentation data shifts from control and analyte samples

CONCLUSIONS

- The collection of a non-targeted comprehensive dataset incorporating UPLC and ion mobility separations (HDMSE) in combination with a sophisticated apex peak algorithm maximizes peak capacity for a given injection.
- Componentization of data following Apex peak picking enables a user to process data and interrogate it in many ways, without the need for reprocessing.
- Interrogation of data for targeted, non-targeted and unknown masses of interest is possible within a single integrated scientific information system (UNIFI).

REFERENCES

- Componentization White Paper <http://www.waters.com/webassets/cms/library/docs/720004597en.pdf>
- MS^E White Paper: <http://www.waters.com/webassets/cms/library/docs/720004036en.pdf>

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