

Fast Multiplexing of Analytical Parameters for Performance Improvements in Time-of-Flight Mass Spectrometry

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Outline

- Background to multiplexing in TOF MS
- Tandem Ionisation (TI)
 - What is it?
 - How does it work?
- How can TI help with environmental analyses?
 - Case study: Quantitation of organotins



What is multiplexing?

And how is it accommodated?



• TOF parameters can be accessed remotely during runtime

What parameters would we change?

- Ionisation energy
- Select-eV soft electron ionisation
 - No source-switching
 - No additional variables
 - Isomer identification, e.g.
 - Branched alkanes
 - Terpenes





- At 70 eV, electrons are readily pulled into the ion chamber = high sensitivity
- But also results in a high degree of fragmentation



- At <70 eV, electrons are not pulled efficiently into the ion chamber
- Low density electron beam = very poor sensitivity

Soft electron ionisation

By Select-eV



- Prevents electron clustering at the filament
- Soft EI spectra obtained with high sensitivity

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Previous limitations

- An analytical run per ionisation energy
- Potential peak alignment issues



Tandem Ionisation



- Acquire soft and hard EI simultaneously
- Full sample characterisation in a single run

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Multiplexing of ionisation energy

What does it actually look like?



- Separate .lsc datafiles are created for the two eV settings automatically
- Near-real time data processing can still be applied

What does it actually look like?



- Analogous to SIM/scan
- Raw data is hidden as default



Effect on sensitivity?



Minimal

- IDL <50 fg OFN for Tandem Ionisation at 70/16 eV
- Benefit from reduced background at low eV

70 eV 2800000-7 119 2600000-5.97118E+ 2400000-70 eV Lower baseline 2200000-CO₂ molecular 4.8E+ 2000000ion at m/z 44 1800000-1600000-3.6E+0 1400000-1200000-2.4E+06 1000000-800000-134 1.2E+06 600000-12 eV 117 400000-120 115 77 200000-65 0.0 1.05 Retention Time (mins) 1.15 1.2 1.25 0-20 40 60 80 100 120 140 160 180 m/z

Sensitivity enhancement at low eV

Reduced chemical background

Ionisation potential of common gases in GC–MS

The details

- Any two eV values can be used in a single run
 - 70/12 eV, 16/14 eV, 20/12 eV...
 - Unlockable from the method for even faster workflow
 - Fully automated
- Switching speeds up to 100 Hz
 - i.e. two 50 Hz data files
 - Compatible with GCxGC



Integrates into lab workflow

- TOF-DS data processing for both 70 eV and soft EI in real time
- Two complementary datasets in a single workflow

TI for environmental analyses

Extended detection limits for organotins





- Water samples, spiked with four organotins
- Derivatised prior to extraction



Enhanced quantitation ions



Enhanced quantitation ions

Improving LoQ for organotins EIC m/z 263 + 291



Comparison of LoQ

Derivatised tributyltin



Comparison of LoQ

Derivatised tributyltin



Comparison of LoQ



Summary

- Soft EI acquired simultaneously with referencequality 70 eV spectra
- Complementary data for improved compound identification
- Extended detection limits
- Perfect peak alignment
- Multiplexing speeds of up to 100 Hz



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Thank you for listening!





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