Introducing

Xevo TQ-XS

Jan Bohuslivek, PhD
October 25, 2016
Waters Technology Day
Vienna, Austria
Overview

- Introduction
- What’s new in Xevo TQ-XS
- Ease of use – new features
- Wider Ionization Coverage – UniSpray
- Benefits of the Xevo TQ family
- Summary
EXPAND YOUR CAPABILITIES

Xevo TQ-XS
ULTIMATE SENSITIVITY AND RELIABILITY

Xevo TQ-S micro
SENSITIVE, RELIABLE, AND COMPACT

Xevo C2-XS QTof
COMPREHENSIVE, QUANTITATIVE, AND QUALITATIVE INFORMATION

Xevo TQD
ACCESSIBLE, RELIABLE, AND PROVEN
- Sensitivity
Xevo TQ-XS

- Most sensitive MS we have ever produced with market-leading performance
  - Ultimate sensitivity from **StepWave XS**
  - Wider and potentially more sensitive ionization coverage with **UniSpray**
- Same principle as original StepWave ion guide

Ions (yellow) actively moved upwards and on-axis relative to the MS analyser.

Neutrals and gas flow (blue) off-axis relative to the MS analyser and are passively removed.
Key improvements to optimise performance for challenging compounds

- RF voltage constant improving robustness while mass switching
- Segmented quadrupole second stage – focussed ion beam
- Wider profile first stage, more space for ion cloud
- Horizontal plates provide more controlled extraction of ions from gas flow – less energetic collisions
StepWave XS ion guide

- Original ring-shaped StepWave occasionally caused fragmentation of labile compounds
- StepWave XS uses horizontal plates rather than rings.
- Requires less overall potential difference to extract the ions.
- No fragmentation of labile compounds
Expanding scope of ultimate sensitivity analysis

- Best sensitivity for challenging compounds - UPLC/MRM ESI mode

**Area improvements vs Xevo TQ-S**

```
<table>
<thead>
<tr>
<th>Compound</th>
<th>Improvement</th>
</tr>
</thead>
<tbody>
<tr>
<td>Aldosterone</td>
<td>7</td>
</tr>
<tr>
<td>Amphetamine</td>
<td>3</td>
</tr>
<tr>
<td>Chloramphenicol</td>
<td>7</td>
</tr>
<tr>
<td>Chloropham</td>
<td>29</td>
</tr>
<tr>
<td>Dicamba</td>
<td>11</td>
</tr>
<tr>
<td>MDA</td>
<td>4</td>
</tr>
<tr>
<td>MDEA</td>
<td>5</td>
</tr>
<tr>
<td>MDMA</td>
<td>3</td>
</tr>
<tr>
<td>Methionine</td>
<td>2</td>
</tr>
<tr>
<td>Omeprazole</td>
<td>10</td>
</tr>
</tbody>
</table>
```

**S/N improvements vs Xevo TQ-S**

```
<table>
<thead>
<tr>
<th>Compound</th>
<th>Improvement</th>
</tr>
</thead>
<tbody>
<tr>
<td>Aldosterone</td>
<td>5</td>
</tr>
<tr>
<td>Amphetamine</td>
<td>13</td>
</tr>
<tr>
<td>Chloramphenicol</td>
<td>3</td>
</tr>
<tr>
<td>Chloropham</td>
<td>7</td>
</tr>
<tr>
<td>Dicamba</td>
<td>6</td>
</tr>
<tr>
<td>MDA</td>
<td>4</td>
</tr>
<tr>
<td>MDEA</td>
<td>2</td>
</tr>
<tr>
<td>MDMA</td>
<td>1</td>
</tr>
<tr>
<td>Methionine</td>
<td>2</td>
</tr>
<tr>
<td>Omeprazole</td>
<td>1</td>
</tr>
<tr>
<td>Vancomycin</td>
<td>1</td>
</tr>
</tbody>
</table>
```

Xevo TQ-S data acquired using standard settings
Data for a diverse mix of compounds
Xevo TQ-XS versus Xevo TQ-S

<table>
<thead>
<tr>
<th>Compound</th>
<th>Mode</th>
<th>Peak Area</th>
<th>S/N</th>
</tr>
</thead>
<tbody>
<tr>
<td>Amphetamine</td>
<td>ESI+</td>
<td>54.3</td>
<td>13.3</td>
</tr>
<tr>
<td>MDA</td>
<td>ESI+</td>
<td>11.4</td>
<td>4.4</td>
</tr>
<tr>
<td>MDMA</td>
<td>ESI+</td>
<td>5.2</td>
<td>1.4</td>
</tr>
<tr>
<td>MDEA</td>
<td>ESI+</td>
<td>4.3</td>
<td>1.7</td>
</tr>
<tr>
<td>Methylon</td>
<td>ESI+</td>
<td>3.5</td>
<td>1.5</td>
</tr>
<tr>
<td>Omeprazole</td>
<td>ESI+</td>
<td>1.6</td>
<td>1.5</td>
</tr>
<tr>
<td>Aldosterone</td>
<td>ESI-</td>
<td>7.0</td>
<td>5.0</td>
</tr>
<tr>
<td>Fluticasone</td>
<td>ESI+</td>
<td>2.2</td>
<td>2.2</td>
</tr>
<tr>
<td>Formoterol</td>
<td>ESI+</td>
<td>1.5</td>
<td>1.6</td>
</tr>
<tr>
<td>Nefazodone</td>
<td>ESI+</td>
<td>1.4</td>
<td>1.4</td>
</tr>
<tr>
<td>Salmeterol</td>
<td>ESI+</td>
<td>2.1</td>
<td>2.1</td>
</tr>
<tr>
<td>Reserpine</td>
<td>ESI+</td>
<td>1.1</td>
<td>1.1</td>
</tr>
<tr>
<td>Angiotensin II</td>
<td>ESI+</td>
<td>1.7</td>
<td>1.6</td>
</tr>
<tr>
<td>Desmopressin</td>
<td>ESI+</td>
<td>1.3</td>
<td>1.2</td>
</tr>
<tr>
<td>Oxytocin 504 - 285</td>
<td>ESI+</td>
<td>1.5</td>
<td>1.3</td>
</tr>
<tr>
<td>Oxytocin 1007 - 723</td>
<td>ESI+</td>
<td>1.6</td>
<td>1.5</td>
</tr>
<tr>
<td>Vasopressin</td>
<td>ESI+</td>
<td>1.3</td>
<td>1.3</td>
</tr>
<tr>
<td>Vancomycin</td>
<td>ESI+</td>
<td>10.0</td>
<td>5.0</td>
</tr>
<tr>
<td>Chloramphenicol</td>
<td>ESI-</td>
<td>3.2</td>
<td>2.6</td>
</tr>
<tr>
<td>Chlorpropham</td>
<td>ESI-</td>
<td>6.9</td>
<td>7.3</td>
</tr>
<tr>
<td>Dicamba</td>
<td>ESI-</td>
<td>29.0</td>
<td>6.2</td>
</tr>
<tr>
<td>Dinocap</td>
<td>ESI-</td>
<td>1.2</td>
<td>1.2</td>
</tr>
<tr>
<td>Bentazon</td>
<td>ESI-</td>
<td>1.2</td>
<td>1.2</td>
</tr>
<tr>
<td>Triforin</td>
<td>ESI-</td>
<td>1.1</td>
<td>1.1</td>
</tr>
<tr>
<td>Ioxynil</td>
<td>ESI-</td>
<td>1.0</td>
<td>1.0</td>
</tr>
<tr>
<td>Fludioxonil</td>
<td>ESI-</td>
<td>1.2</td>
<td>1.1</td>
</tr>
<tr>
<td>Dithianon</td>
<td>ESI-</td>
<td>1.2</td>
<td>1.1</td>
</tr>
<tr>
<td>Fluazinam</td>
<td>ESI-</td>
<td>1.1</td>
<td>1.1</td>
</tr>
<tr>
<td>Hexaflumuron</td>
<td>ESI-</td>
<td>1.2</td>
<td>1.1</td>
</tr>
</tbody>
</table>

- UPLC/MRM ESI mode
- Analyte dependent
- Area improvements range from 1x to >50x
- S/N improvements range from 1x to >10x
Aldosterone frequently monitored in clinical research

- Can inject less sample volume with same precision

Exceptional sensitivity for endogenous steroids (ESI neg)

UPLC/MRM in ESI negative with 50 fg on column

>5x increase S/N
Sensitivity is nothing without Robustness...

- 2,000 consecutive injections (over 85 hours)
- Sulphadimethoxine in protein-precipitated plasma (100 fg on column)
- Mass switching, 5 ms dwell time to simulate real experiment

2.55% RSD
Improved Customer Experience
Xtended Dynamic Range detector

- Long-life photomultiplier technology
- Accessible sensitivity
  - data for peptide Val-Tyr-Val
  - UPLC/MRM ESI+, 6 orders linear dynamic range

Easy method transfer to a more sensitive instrument (calibration curves can still overlap)
Additional Hardware Features
Minimized maintenance time and effort: Tool-free ESI and APCI probes

- New design:
  - Completely tool-free
  - Based on QDa design
  - Takes <2 min to change the probe assembly
  - Minimized maintenance time, maximized ease-of-use
Improved new ESI probe spray stability with UPC²

- New ESI probe for UPC² shows better spray stability leading to improved peak reproducibility

Old ESI probe:
- Peak height: 13% RSD
- S/N: 18% RSD

New ESI probe:
- Peak height: 4% RSD
- S/N: 9% RSD
New Rough Pump - Ebara EV-SA30

- Totally clean multi-stage Roots technology
  - No oil or tip seal dust contamination risk
- No annual service required
- 80% lower power consumption*
- 50% smaller footprint*
- 4 dB(A) quieter*

* Compared with two rotary vane pumps giving a similar combined pumping speed
New Software Features
New features: Software updates

- **MassLynx v4.2**
- **LIMS v3.0 interface** now available for all TQ
  - More results uploaded, easier configuration, better regulation compliance
- Key improvements for **TargetLynx XS/Quanpedia**
  - Ensure best possible experience for method update and results review
    - Improved R.T. update in Quanpedia
    - R.T. tolerance in TargetLynx either absolute or %
    - Report results above cut-off without calibration
    - Improved manual peak edit capability
- Instrument control updates
  - Full implementation of UniSpray throughout the quantitative workflow
  - “Soft ionization mode” option for labile compounds
MRM Method Development

Streamlining the workflow: Quanpedia

Quanpedia™

©2016 Waters Corporation
Xevo TQ-XS Quanpedia

- 23 Analysis methods
- 400 + compounds
- Method creation in only minutes
- LC, MS and TargetLynx methods

Antibiotics
- Pesticides
- Bisphenol
- PFAAS
- Pigments
- Clenbuterol
- Paraquat

Paralytic shellfish toxins

Methylamino alanine

Neurotoxins
- Binding agents
  - PFCAS
  - Pyrrolizidine alkaloids
  - Imidazole and phenicols
  - Parabens
  - Veterinary drugs

Indoleamine neurotransmitters

Mycotoxin

Paralytic shellfish toxins

©2016 Waters Corporation
UniSpray™
A novel ionization source for broader compound coverage
What is UniSpray?

- A novel ion source exclusive to Waters
- Wider compound coverage
- Potential for greater sensitivity
- All results in a single data stream
- Greater ionization efficiency
- Comparable robustness and linearity to ESI
- Spectra comparable with current ionization modes
How does UniSpray work?

- Increased ionisation efficiency
  - Creation of small volume secondary droplets through impact and shear stress
  - Enhanced desolvation and droplet evaporation

Grounded Probe

Sample Cone

Target (High Voltage)
UniSpray with Xevo TQ-XS
Pesticides in Green Tea Extract

<table>
<thead>
<tr>
<th></th>
<th>UniSpray S:N Improvement</th>
<th>UniSpray Peak Area Improvement</th>
</tr>
</thead>
<tbody>
<tr>
<td>Methamidophos</td>
<td>1.9</td>
<td>5.7</td>
</tr>
<tr>
<td>Acephate</td>
<td>1.3</td>
<td>1.7</td>
</tr>
<tr>
<td>Methomyl</td>
<td>0.9</td>
<td>1.5</td>
</tr>
<tr>
<td>Dicrotophos</td>
<td>1.4</td>
<td>3.5</td>
</tr>
<tr>
<td>Atrazine desethyl</td>
<td>0.8</td>
<td>4.6</td>
</tr>
<tr>
<td>Metoxuron</td>
<td>1.6</td>
<td>4.1</td>
</tr>
<tr>
<td>Cyanazine</td>
<td>1.1</td>
<td>4.4</td>
</tr>
<tr>
<td>Simazine</td>
<td>1.5</td>
<td>3.6</td>
</tr>
<tr>
<td>Hexazinone</td>
<td>0.4</td>
<td>2.8</td>
</tr>
<tr>
<td>Monolinuron</td>
<td>1.5</td>
<td>3.6</td>
</tr>
<tr>
<td>Chortoluron</td>
<td>2.5</td>
<td>4.1</td>
</tr>
<tr>
<td>Metobromuron</td>
<td>1.9</td>
<td>3.8</td>
</tr>
<tr>
<td>Atrazine</td>
<td>3.0</td>
<td>4.3</td>
</tr>
<tr>
<td>Diuron</td>
<td>1.7</td>
<td>4.7</td>
</tr>
<tr>
<td>Linuron</td>
<td>1.9</td>
<td>4.0</td>
</tr>
<tr>
<td>Sebuthylazine</td>
<td>3.1</td>
<td>4.4</td>
</tr>
<tr>
<td>Terbutylazine</td>
<td>2.4</td>
<td>3.9</td>
</tr>
<tr>
<td>Buprofenzin</td>
<td>1.8</td>
<td>3.2</td>
</tr>
<tr>
<td>Fenpropimorph</td>
<td>2.5</td>
<td>2.4</td>
</tr>
</tbody>
</table>
UniSpray with Xevo TQ-XS UPC$^2$ for triazole fungicide separation

(R)-Tebuconazole  (S)-Tebuconazole

stereogenic center *
Xevo TQ-XS with UniSpray Robustness

- Preliminary robustness data:
  - Caffeine spiked in precip. plasma
  - RSD = 2.93%
Receptor-based high-throughput screening and identification of estrogens in dietary supplements using bioaffinity liquid-chromatography ion mobility mass spectrometry

Payam Aqai & Natalia Gómez Blesa & Hilary Major & Mattia Pedotti & Luca Varani & Valentina E. V. Ferrero & Willem Haasnoot & Michel W. F. Nielen

**Anal Bioanal Chem**
**DOI 10.1007/s00216-013-7384-1**
Enhanced performance for the analysis of prostaglandins and thromboxanes by liquid chromatography-tandem mass spectrometry using a new atmospheric pressure ionization source

Arnaud Lubin, Suzy Geerinckx, Steve Bajic, Deirdre Cabooter, Patrick Augustijns, Filip Cuyckens, Rob J. Vreeken

*Journal of Chromatography A, 1440 (2016) 260–265*

- Human plasma
- Pig colon
- Mouse colon
UniSpray Summary

- Novel ionisation source, developed by Waters.
- Compatible with Xevo TQ-XS
- Optional purchase for additional capability
  - Increased Compound Coverage
  - Potential for Increased Performance
- Simple to use and maintain
  - One piece probe similar to QDa probe design
Compatibility across the board

- Universal Source platform
  - ESI
  - APCI
  - ESCi™
  - APPI
  - APCI
  - APGC
  - ionKey/MS
  - ASAP
  - NanoESI
  - UniSpray

- Chromatographic versatility
  - H-Class and I-Class
  - M-Class
  - UPC²
Xevo TQ- XS Summary

- Ultimate sensitivity
- Low maintenance, increased ease-of-use
- Easier method transfer (XDR detector)
- Wider compound coverage with optional UniSpray source
QUESTIONS

?