Introducing
The Xevo TQ MS

- A tandem quadrupole mass spectrometer
- For high performance LC/MS/MS applications
- But its not a conventional tandem quadrupole mass spectrometer!

Outstanding quantitative LC/MS/MS performance &
Enhanced qualitative LC/MS/MS capabilities
Common Challenges Facing Laboratories

Common challenges:
- Complex technologies
- Inefficient work-flow
- Challenging/complex samples
- Productivity & return on investment
- More experimental choices needed

Designed for simplified user access
Innovative technology
Superior quantification & enhanced qualitative capabilities
Latest innovative high performance ion source technology
Rapid data acquisition/ UPLC compatible by design
New tools streamline method creation & data quality monitoring
Intelligent work flow
More experimental choices
Enhanced qualitative capabilities
Access to complex test simplified
High Productivity & return on investment
High sensitivity
Efficient work-flow
Simple access
Inefficient work-flow
More experimental choices
Why Xevo TQ MS?
The Accelerated Evolution Of MS Technology

Xevo TQ MS

Simple access
Efficient work-flow
More experimental choices
High sensitivity
High Productivity

Why Xevo TQ MS?
Simple Access

Non-expert users

1920 1940 1960 1980 2000 2020

Simple Access

IntelliStart

Set up  Create methods  Analysis
IntelliStart

- On-board fluidics
- Advanced LC/MS/MS
  - More Accessible
  - More Reliable
  - More Productive

Simple Access

LC/MS System check: Run 1
Peak area = 4351.6

LC/MS System check: Run 6
Peak area = 4435.2

LC/MS System Check
**Why Xevo TQ MS?**

- Simple access
- Efficient work-flow
- More experimental choices
- Higher sensitivity
- High Productivity

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**Efficient Work-Flow**

- A central data base for quantitative LC/MS methods
- Based on compound name
- A tool to aid MS method creation
  - Automatically creates data acquisition methods
  - Automatically creates data processing methods
Efficient Work-Flow

Select compounds from database
Create LC/MS methods
Ready to Acquire & Process

Use Predefined Analysis
Use Predefined Compounds

- Pro-active quantification data monitoring
  - Blanks
  - Quality Control Standards
  - Internal standards

- Action on failure:
  - Re-inject
  - Terminate sample run

Prevents precious samples from being injected if the LC/MS system is not performing appropriately.
Efficient Work-Flow

- Correct RT and ion ratios
- Analytes above RL/MRL
- Recoveries OK
- Calibrations OK
- RL standards satisfy S/N within RT tolerance
- Ion ratios OK
- Effort Work

A tool to plot TargetLynx data
- Intra and inter-batch data

Monitor long term data trends/system performance
**Efficient Work-Flow**

- Plot trends in results: TrendPlot
- Process, qualify & report results: TargetLynx
- Monitor data pro-actively: QCMonitor
- Create LC/MS/MS methods: Quanpedia
- Setup instrumentation: IntelliStart

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**Why Xevo TQ MS?**

- Simple access
- Efficient work-flow
- More experimental choices
- High Productivity
- High sensitivity

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High Sensitivity

- Zspray™
  - Robust performance in the face of complex biological samples
  - Zspray, a proven geometry (many years experience & 1000’s in use daily).

- Designed to be compatible with all your HPLC and UPLC needs

- Innovative, Ergonomic Engineering
  - Performance, usability & serviceability
  - Tool free maintenance
  - Novel tool free source exchange
  - Integrated gases
  - Plug and play probes

New High Performance AP Ion Source

High Sensitivity

- Optimized gas flow dynamics

- High temperature desolvation (650°C)

- Thermally regulated ionisation chamber

- Highly efficient ionisation
  - High LC flow rates
  - High aqueous solvents

Designed for Performance, Usability & Serviceability
**Evaluation of UPLC/MS/MS Performance**

- **Xevo TQ MS vs. Quattro Premier XE**
  - Mixture of pesticides
  - Back to back comparisons made
  - Same UPLC, mobile phases & standards
  - Enhancement in ESI response measured

- **Effect of UPLC flow rate**
  - UPLC/MS/MS repeated at different flow rates
    - 0.45mL/min
    - 0.6mL/min
    - 0.8mL/min

**UPLC/MRM analysis of a pesticide mixture (ESI+)**

- **Enhanced Peak Area Response at different UPLC flow rates**

**Xevo TQ MS**

- 0.4mL/min - Up to X6 (Ave X3) > QPXE
- 0.6mL/min - Up to X7 (Ave X4) > QPXE
- 0.8mL/min - Up to X8 (Ave X5) > QPXE

**UPLC/MS/MS (ESI -)**

- **Enhanced Peak Area Response at different UPLC flow rates**

**Xevo TQ MS**

- 0.4mL/min - Up to X3 (Ave X2) > QPXE
- 0.6mL/min - Up to X2.5 (Ave X2) > QPXE
- 0.8mL/min - Up to X3.5 (Ave X2.5) > QPXE
High Sensitivity

**Enhanced SIGNAL (Peak Area)**
- Xevo TQ MS
- Up to X4 (Ave X3) > QPXE
- Up to X30 (Ave X20) > TQD

**Enhanced SIGNAL/NOISE**
- Xevo TQ MS
- Up to X7 (Ave X3) > QPXE
- Up to X16 (Ave X9) > TQD
Why Xevo TQ MS?

Simple access
Efficient work-flow
High sensitivity
More experimental choices
High Productivity

High Productivity

HPLC-MS/MS

UPLC-MS/MS

Time
0 0.5 1.0 1.5 2.0 2.5 3.0

%
High Productivity

- Fully compatible with ACQUITY UPLC by design

- High speed data acquisition
  - T-Wave\textsuperscript{TM} enabled collision cell*
  - Rapid polarity switching (20ms)

- A winning combination that provides:
  - The lowest limits of detection
  - The very best chromatographic resolution
  - Unmatched speed of analysis
  - Highest productivity

*The traveling wave described here is similar to that described by Kirchner in US Patent 5,206,506 (1993).

High Productivity

- Tested as UPLC/MS systems
  - Multi component test mix
  - UPLC column
  - Gradient conditions
  - At 0.8mL/min

- UPLC/MRM system sensitivity specifications
  - To ensure complete confidence in total system performance
Why Xevo TQ MS?

Simple access
Efficient work-flow
High sensitivity
High Productivity
More experimental choices

More Experimental Choices

- A New Collision Cell
  - A unique patented design
  - Novel use of proven T-Wave technology*

- Enhances spectral data
  - MS
  - Product ion

- Xevo TQMS is different
  - Unlike conventional tandem quadrupole MS instruments

*The traveling wave described here is similar to that described by Kirchner in US Patent 5,206,506 (1993).
- Standard tandem quadrupole MS
  - Very sensitive in MRM mode
  - Significantly less sensitive when acquiring in spectral mode

- ScanWave operation
  - Ions are accumulated in the collision cell
  - Ions released according to their mass to charge ratio (m/z).
  - Release of these ions is synchronised with the scanning of MS2
  - Greatly improves duty cycle
  - Enhancing sensitivity in the scanning acquisition mode.

- Xevo TQ MS
  - operates in either standard or ScanWave enhanced modes

Product ion spectrum of Glu-fibrinopeptide
(Scan speed = 5,000 amu/second)
More Experimental Choices

- Scan Wave compatible with UPLC requirements
  - Rapid full scan acquisition rates
  - Rapid polarity switching

- Operates at standard gas cell pressures
  - Operates in ScanWave and T-wave modes

- Performance
  - No loss of sensitivity
  - No loss of speed
  - No loss of functionality

Providing a more versatile LC/MS System

Xevo TQ MS provides more experimental choices
- Switches rapidly between MS and MS/MS acquisition modes
- Collision gas on in all acquisition modes

Unknown Screening (survey scanning)
- Automatically generates ScanWave enhanced product ion spectra for any components found in a complex sample
- Various triggers can be used
  - MS full scanning
  - Parent ion scanning
  - Neutral loss scanning
More Experimental Choices

- Acquire **qualitative** (spectral) data & **quantification** (MRM) data in a single injection.

- MS spectral data at the same time as MRM data.
  - Valuable aid to method development
  - See all of the background interferences while developing your targeted MRM method.

- Use MRM data to trigger the acquisition of product ion spectra
  - spectral data provides useful extra information about a suspect MRM quantification result

Why Xevo TQ MS?

- High productivity & return on investment
- Efficient work-flow
- Simple technologies
- More experimental choices needed
- High sensitivity, challenging samples
Thank You For Your Attention

Any Questions?