

## Video Article

# The Waters Xevo™ TQ-S Equipped With New StepWave™ and ScanWave™ Technology - ADVERTISEMENT

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## Abstract

## Video Link

The video component of this article can be found at <http://www.jove.com/video/2268/>

## Protocol

### I.Xevo™ TQ-S StepWave technology

The Xevo TQ-S Mass Spectrometer is equipped with a new StepWave ion guide: a revolutionary new off-axis, ion-source technology, delivering the most sensitive LC/MS/MS performance of any available tandem quadrupole system. The StepWave technology dramatically increases the efficiency of ion transfer from the ion source to the quadrupole MS analyzer, while efficiently eliminating undesirable neutral contaminants.

The new ion optics consists of two ion transfer stages, which are differentially pumped. Both stages are T-Wave-enabled, stacked-ring RF devices. The first stage is revolutionary in its design, constructed from two stacked-ring electrode devices that are conjoined to give a single, off-axis ion transfer lens with unique properties.

As the ion beam passes through the source sampling orifice, it undergoes expansion. The entrance of the StepWave is designed to be large enough to efficiently capture all of the ions in this expanded ion cloud.

The design of the first stage ensures that all the ions are efficiently focused and directed up into the second stage. The off-axis design ensures that any neutral materials entering the source sampling orifice are actively extracted from the system.

This increased ion sampling efficiency and noise removal produces a significant improvement in the limits of detection, allowing scientists to detect compounds at levels they could only dream of before. This is not only true for quantitative multiple reaction monitoring, or MRM, analysis, but also for qualitative full scan analysis.

### II.Xevo™ TQ-S Applications

LC/MS/MS analysis plays a key role in ensuring food safety, water quality, and the quantification of pharmaceuticals in biological fluids to support drug development and discovery. High sensitivity performance facilitates lower levels of sensitivity, allowing researchers to measure drugs at even lower dose levels or with reduced sample volumes. This becomes applicable when using genetically-engineered rodents or in dried blood spot bioanalysis.

The sensitivity benefits of the new StepWave ion guide can be seen for the analysis of desmopressin, a modified form of the normal human hormone arginine vasopressin (Figure 1). This compound is present in the circulatory system at very low levels. Thus, a high sensitivity assay is required to accurately measure its pharmacokinetics. In this example, the Xevo TQ-S produces a response 20 times greater than of the Xevo TQ. This increase in signal-to-noise response is exhibited for many other compounds as well (Table 1).

#### a. Spectral Sensitivity

In many analytical environments, regulators are demanding more than quantification alone; they require confirmation of identity. The increased sensitivity of the Xevo TQ-S StepWave technology produces the highest quality spectra at lower levels. For example, the new StepWave technology gives a 20 fold increase in signal to noise response for the MS/MS spectra of the glucuronide metabolite of ibuprofen (Figure 2).

#### **b. ScanWave Technology:**

Spectral quality is dependent upon the ions sampled to produce the spectrum. The Xevo TQ family of instruments uses ScanWave, a novel patented collision cell design to increase full scan MS/MS sensitivity. ScanWave technology allows scientists to get both the very best quantitative data as well as superior spectral MS/MS information.

With ScanWave enabled, ions within the collision cell accumulate and then separate according to their mass-to-charge ratio. Synchronizing the release of these ions with the scanning of the second quadrupole mass analyzer simplifies the confirmation of the identities and structure of analytes.

#### **c. UPLC® Compatibility and RADAR™:**

One of the unique features of the Xevo TQ-S is the fast data acquisition rate and an information rich acquisition mode called RADAR. This functionality is made possible by the novel, high speed transfer optics and collision cell design. The specialized design allows both full scan MS and MRM data to be simultaneously acquired in the time scale of a narrow, 1-2 second wide, LC peak and still obtain greater than 12 points across the peak (Figure 3).

RADAR is particularly useful in methods development when dealing with a complex matrix, for monitoring for the presence of new components in the sample during routine analysis, or troubleshooting an assay. The data in Figure 4 shows the simultaneous collection of quantitative data and metabolite information in a bioanalysis assay.

#### **d. Versatility and Flexibility:**

One of the biggest advantages of the new Xevo platform is the flexibility afforded by the source design of the instrument. The new universal source platform in the Xevo TQ and TQ-S allows the scientist to easily and rapidly switch between electrospray, APPI, nanospray, atmospheric solid analysis probe and even GC-MS/MS to name a few.

This flexibility allows the core facility laboratories to make better use of in house instrumentation, minimizing the need for duplicate instruments and maximizing Xevo utilization and productivity.

### **III. Xevo™ TQ-S Complete Workflow**

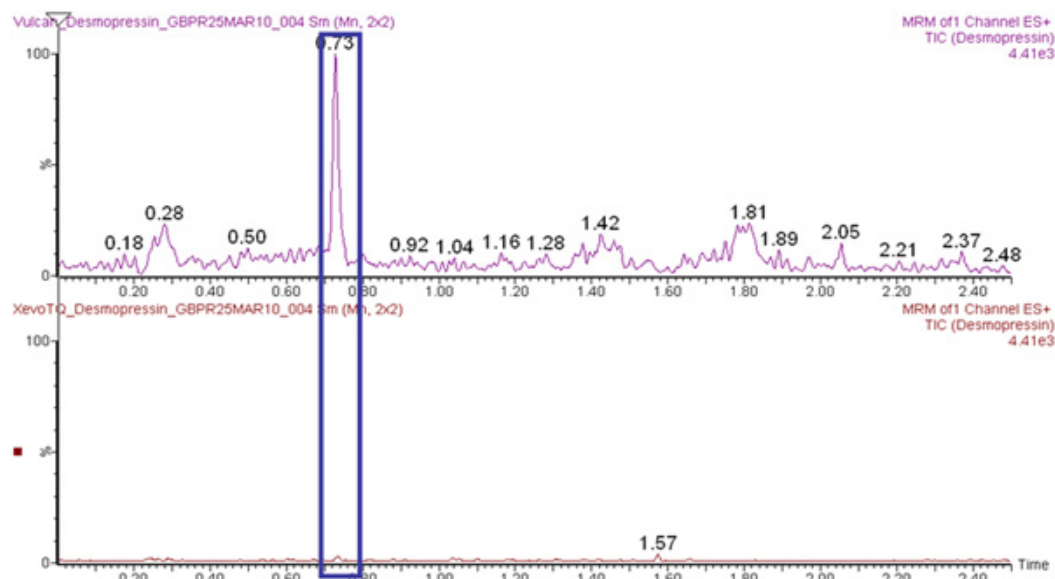
The acquisition of data is an important part of sample analysis but the process of deriving meaningful information from a sample involves multiple steps, including sample preparation, data acquisition, data analysis, and reporting. Supporting the Xevo TQ-S is a comprehensive software and informatics suite which simplifies the whole process of methods development, data acquisition, analyte quantification, structural analysis and data management.

The process of MS method development is simplified using the IntelliStart™ functionality which ensures that the instrument is performing correctly, and then develops the MRM method automatically in just a few minutes (Figure 5). Methods can be developed for larger batches of compounds in an open access mode using the QuanOptimize™ functionality (Figure 6). This quickly develops the MRM methods for tens of compounds at a time. Analyte quantification is simplified with TargetLynx™ which allows one or hundreds of analytes to be quantified in one simple applications browser (Figure 7). Turning to structural analysis and data interpretation are a range of market-leading MassLynx™-enabled applications management solutions for tasks such as metabolite ID with MetaboLynx™, ADME compound screening with ProfileLynx™, statistical data mining with MarkerLynx™, and newborn screening with NeoLynx™, to name a few. All of this data can be easily archived, stored, re-processed, and reported using the NuGenesis SDMS® scientific data management system, which allows compliant, fast, and simple data archival and retrieval (Figure 8).

### **IV. Summary**

The Xevo TQ-S MS delivers unprecedented levels of sensitivity and data quality. This is derived from the new StepWave technology and advanced ion transfer optics. The overall full scan data sensitivity and quality is further enhanced by the ScanWave collision cell design. Uniquely, these two features of MRM sensitivity and full scan information content can be applied simultaneously via the Xevo TQ-S's RADAR functionality, simplifying methods development and troubleshooting. When combined with superior UPLC separations and the versatility of Waters informatics, the system solution delivers new levels of productivity and information.

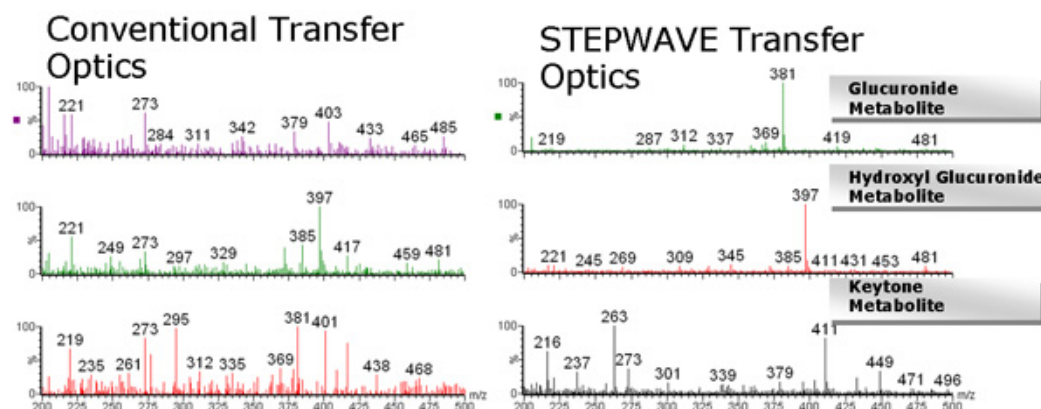
## V.Figures



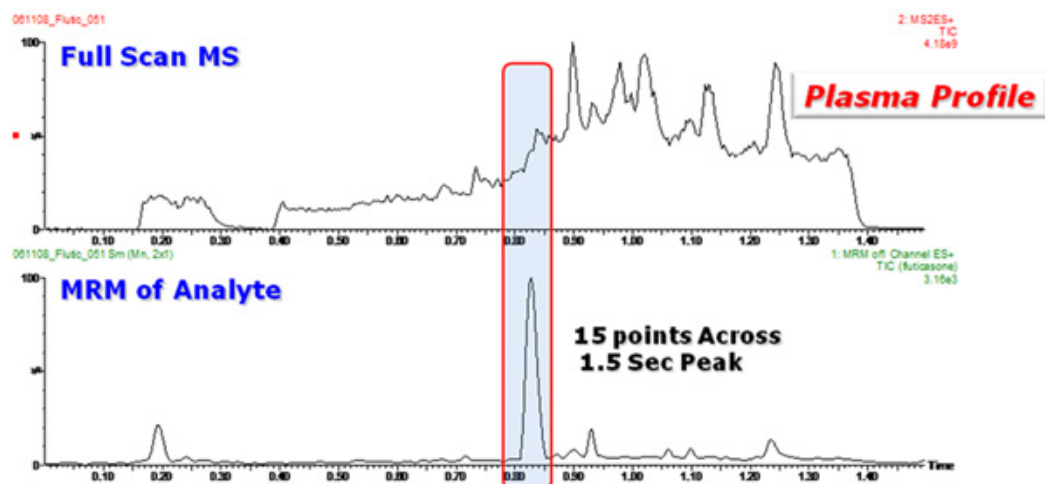
**Figure 1:** Spectral analysis of desmopressin, a modified form of the normal human hormone arginine vasopressin. The Xevo TQ-S StepWave ion guide provides high sensitivity, producing a response 20 times greater than achieved with the Xevo TQ.

Compound	Compound Class	Increase In Response
Fluticasone Propionate	Steroid	12
Salmeterol Succinate	B2-Agonist	15
Alprazolam	Benzodiazepine	13
Formoterol	B2-Agonist	20
Desmopressin	Peptide	25
Nefazodone	Antidepressant	16

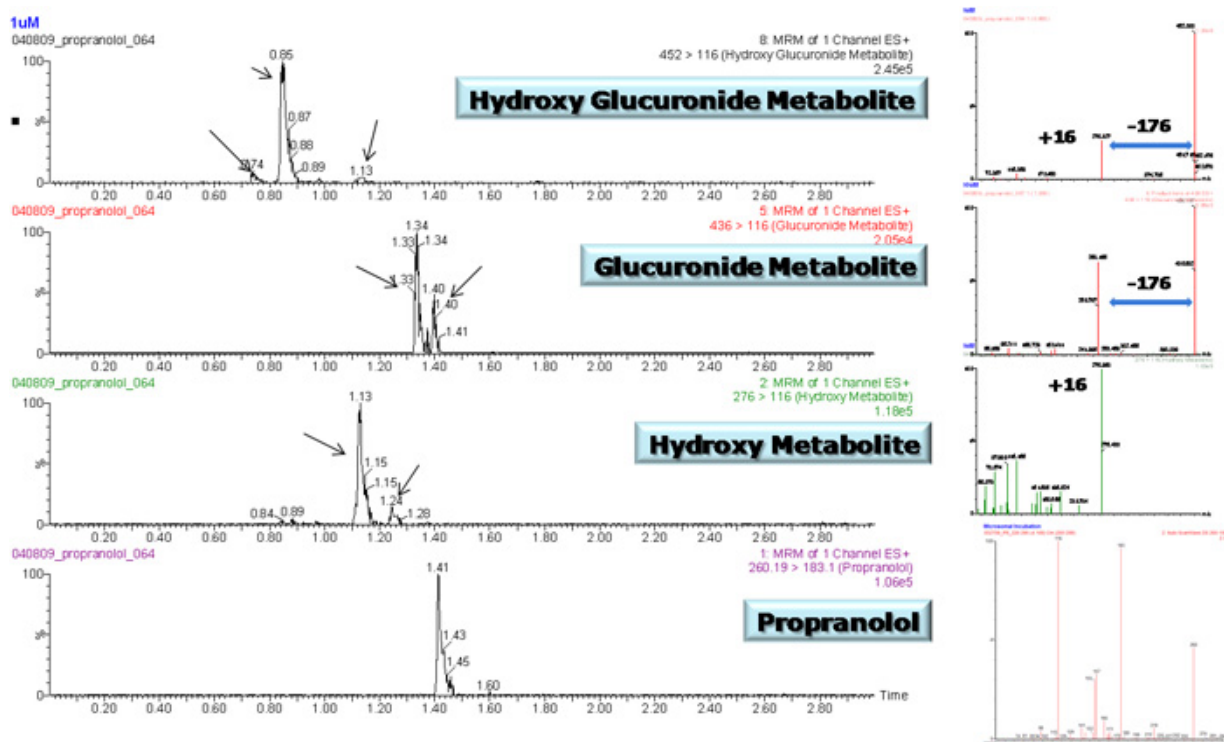
**Table 1:** This increase in signal-to-noise response afforded by the Xevo TQ-S is exhibited for many other compounds as well.



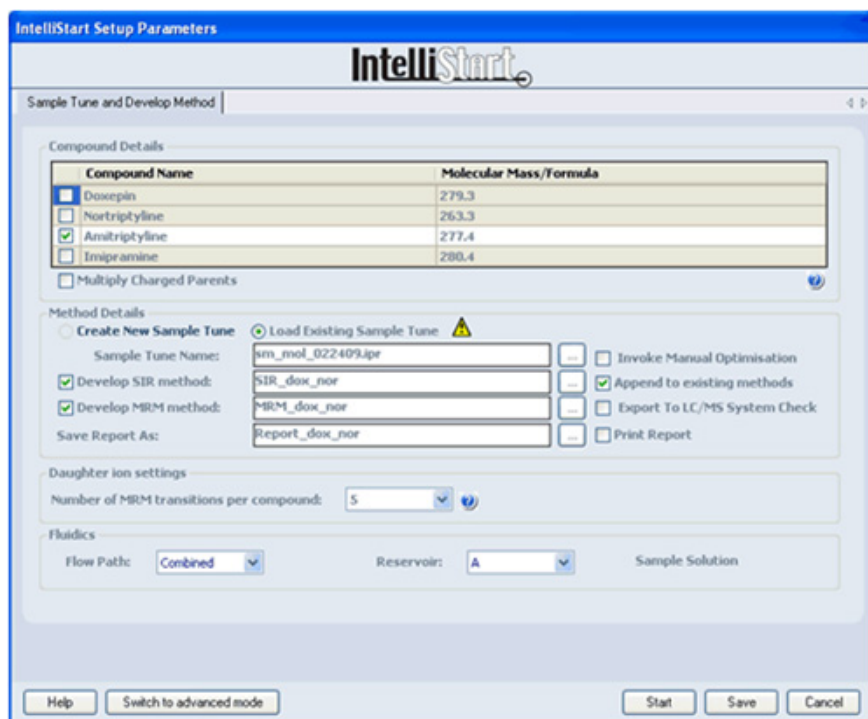
**Figure 2:** StepWave technology gives a 20 fold increase in signal to noise response for the MS/MS spectra of the glucuronide metabolite of ibuprofen.



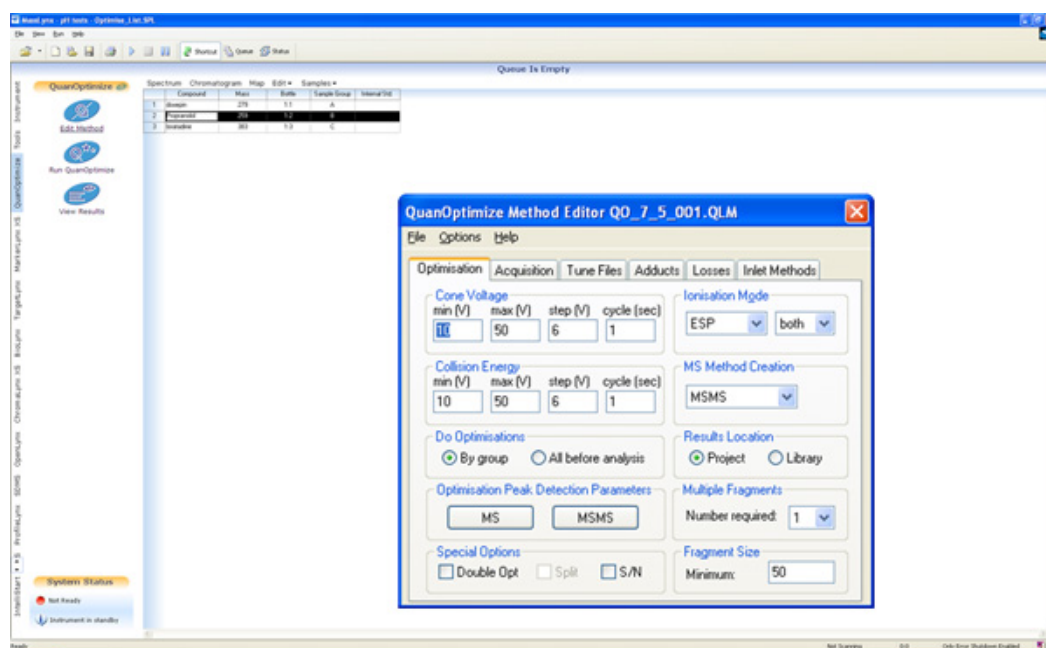
**Figure 3:** RADAR acquisition mode allows both full scan MS and MRM data to be simultaneously acquired in the time scale of a narrow, 1-2 second wide, LC peak and still obtain greater than 12 points across the peak.



**Figure 4:** RADAR mode allows for the simultaneous collection of quantitative data and metabolite information in a bioanalysis assay.



**Figure 5:** IntelliStart functionality ensures that the instrument is performing correctly, and then develops the MRM method automatically in just a few minutes.



**Figure 6:** Methods can be developed for larger batches of compounds in an open access mode using the QuanOptimize functionality.

