THE XS COLLISION CELL FROM WATERS

Increased sensitivity and resolution for Time-of-Flight mass spectrometry

Waters®' Quadrupole Time-of-Flight (Q-Tof™) mass spectrometers are fast, sensitive, high resolution, accurate mass instruments that integrate fully with fast separation techniques and are capable of generating the information scientists need to detect, identify, and quantify trace level compounds in complex and difficult samples. Since the first commercial Q-Tof instrument was introduced by Waters in 1996, they have served to expand the analytical capabilities of laboratories around the world, across a range of scientific disciplines. From health science research to industrial manufacturing, from pharmaceutical discovery to consumer protection, the impact of these instruments has been significant over the last 18 years.

Since 1996, improvements in technology have significantly enhanced the dynamic range, mass accuracy, sensitivity and resolving power of Waters' Q-Tof instruments. The XS Collision Cell is the latest technological advance that delivers increased sensitivity and allows the Q-Tof to match the quantitative performance of many tandem quadrupole instruments without compromising mass resolution.

TECHNOLOGY DESCRIPTION

A schematic of the Xevo G2-XS QTof is shown in Figure 1, where the position of the XS Collision Cell can be seen within the instrument. The XS Collision Cell is a segmented quadrupole as shown in Figure 2. The segmented nature of the quadrupole rods allows a DC gradient to be applied in order to draw ions through the device rapidly and enables fast switching between multiple MS/MS experiments. An RF field applied between opposing rods confines the ions so that they pass down the device and into the Tof mass analyser. The net average RF field experienced by the ions drives them towards the central axis and confines them to a narrow beam.

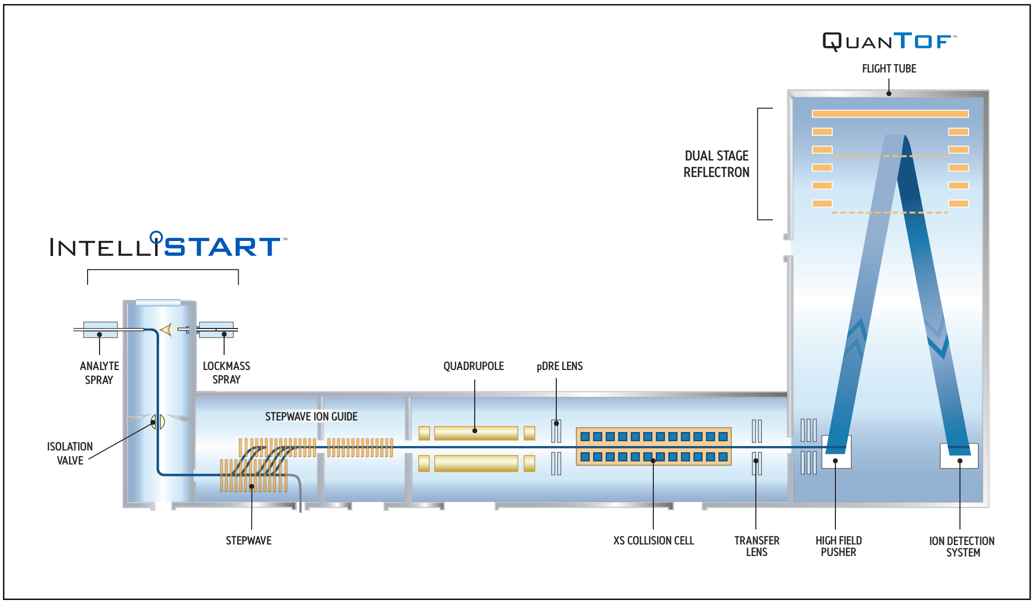

Figure 1. Schematic diagram of the Xevo G2-XS QTof, showing the location of the XS Collision Cell in the central part of the instrument.

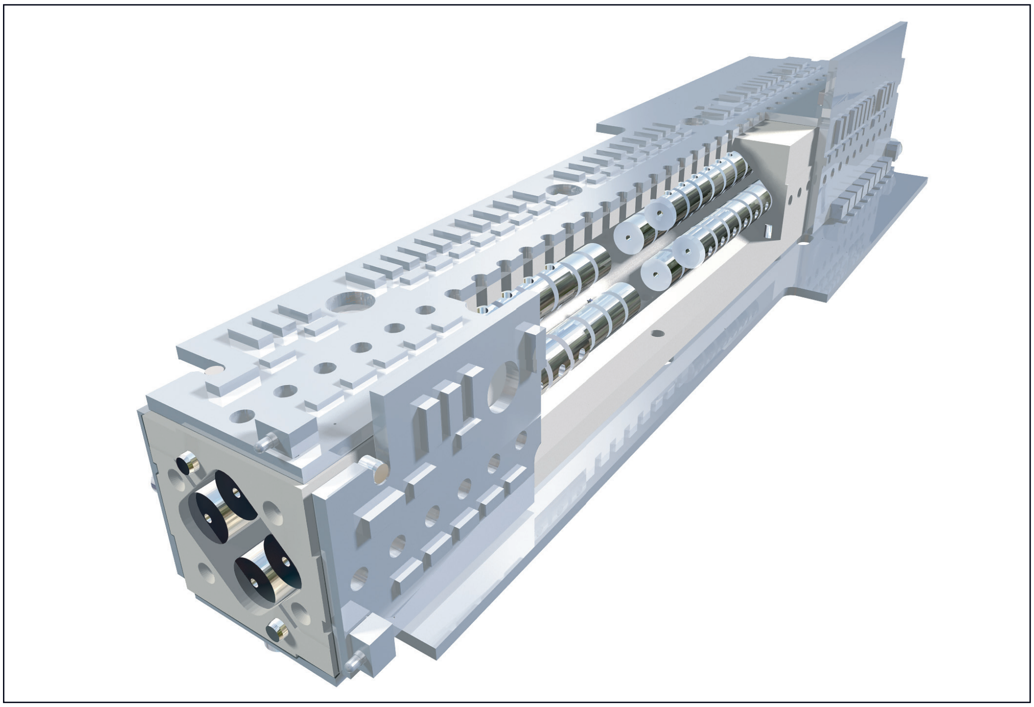

Figure 2. A cutaway drawing of the XS Collision Cell that shows the segmented quadrupole design.

In order to achieve good mass resolution, the beam of ions exiting a Q-Tof collision cell must be conditioned and focused by a series of lenses before it is allowed into the pusher region of the Tof. Figure 3 shows the ion beam as it exits a standard collision cell and passes through the final focusing slit before the Tof region. In order to achieve good resolution from the Tof mass analyser, the width and velocity spread of the ion beam entering the Tof must be tightly controlled. The initial broad width of the ion beam means that only about 30% of the beam leaving the focusing region can be allowed into the pusher region. Around 70% of the beam is lost as it strikes the final slit and is not transmitted.

Figure 4 shows the ion beam as it exits the XS Collision Cell. Since the beam has a significantly narrower profile to begin with, the whole of it is able to pass through the final focusing slit into the pusher region of the Tof. Since effectively 100% of the beam is transmitted, the overall sensitivity of the instrument is increased by a factor of 3 to 4 with no reduction in mass resolution.

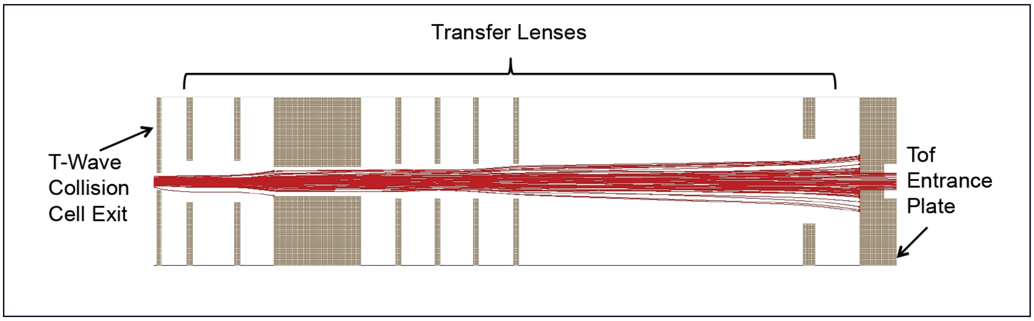

Figure 3. A mathematical simulation of the trajectories taken by ions as they emerge from a standard collision cell and pass through the focusing lenses prior to entering the Tof mass analyzer. Approximately 30% of the ion beam passes through the final slit.

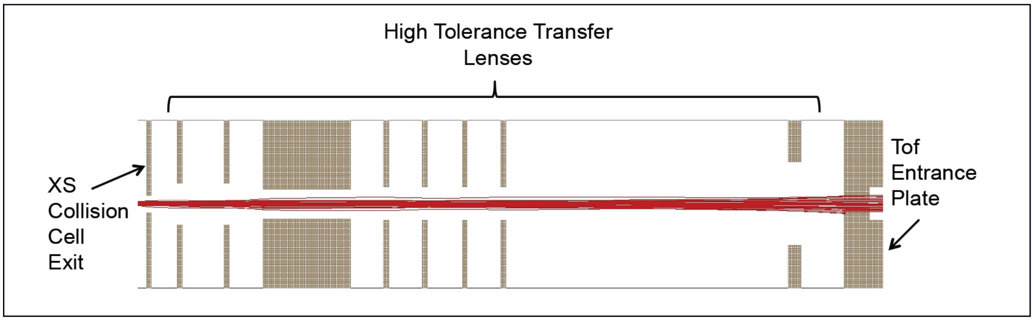

Figure 4. A mathematical simulation of the trajectories taken by ions as they emerge from an XS Collision Cell and pass through the focusing lenses prior to entering the Tof mass analyzer. Approximately 100% of the ion beam passes through the final slit.

For increased flexibility and versatility, Waters Xevo Time-of-Flight mass spectrometers have two modes of operation that can be chosen as appropriate. Sensitivity Mode provides maximum ion transmission and high sensitivity, whereas Resolution Mode gives increased resolving power at lower ion transmission. Figure 5 shows a graph of sensitivity versus resolution. The two modes of operation are plotted for Xevo G2-S QTof (standard collision cell) and Xevo G2-XS QTof (XS Collision Cell). When measured at equivalent resolution settings of 30,000, it can be seen that the XS Collision Cell delivers a 15 fold increase in overall sensitivity.

IMPACT ON DATA QUALITY

Figure 6 shows two extracted ion chromatograms of equivalent amounts of caffeine on column, obtained using a Xevo G2-S QTof with an ordinary collision cell and Xevo G2-XS with the new XS Collision Cell. Both instruments were operated at equivalent mass resolution. The significant increase in signal intensity can be clearly seen. The XS Collision Cell is one of the cutting edge technologies that enable the Xevo G2-XS QTof to achieve levels of quantitative performance equivalent to many tandem quadrupole instruments and extends the effectiveness and usefulness of Q-Tof mass spectrometers for all those laboratories that depend on them for routine, high-resolution, accurate-mass, quantitative assays.

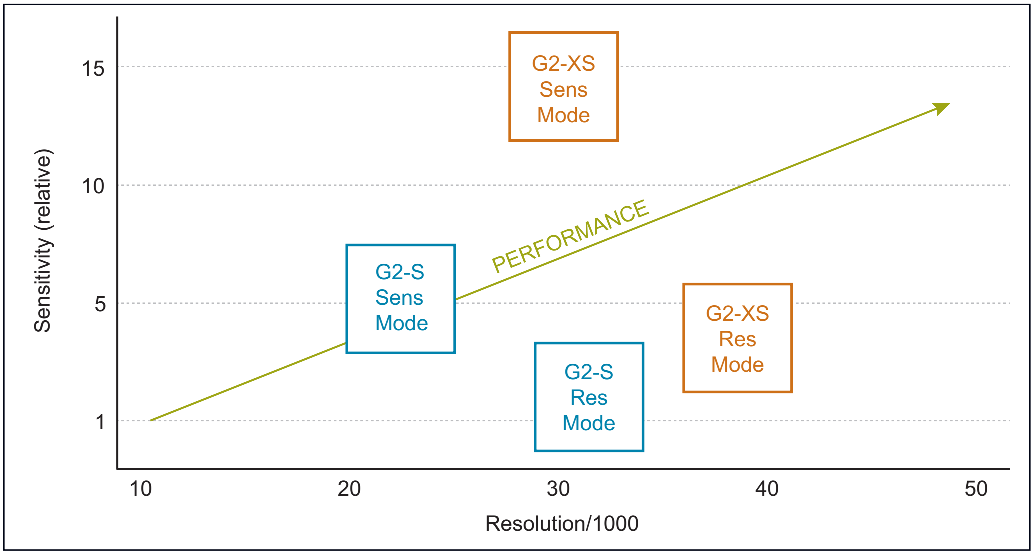

Figure 5. Graph of resolution versus sensitivity. The relative performance of Sensitivity and Resolution Modes of operation is shown for Waters' Xevo G2-S and Xevo G2-XS QTof mass spectrometers.

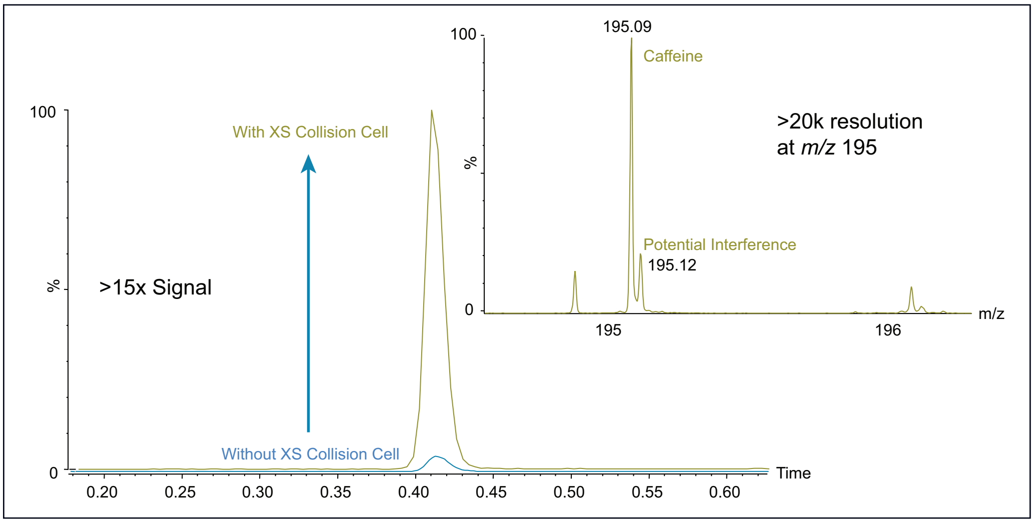

Figure 6. UPLC/MS chromatograms acquired on Xevo G2-S QTof (standard collision cell) and Xevo G2-XS QTof (XS Collision Cell) at equivalent resolution settings. The XS Collision Cell delivers a significant increase in signal, whilst maintaining the fast data acquisition rate necessary for narrow UPLC peaks and the mass resolution required to separate potential interferences.

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