

**November 2, 2011 (13:15-14:15)**



**VENDOR SEMINAR:**

**WATERS TODAY. FEATURED: SCIENTIFIC INNOVATION, FOOD AUTHENTICITY, PROFILING & QUANTITATION**

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*Chair: Dr Sandra Rontree, European Headquarters, Waters Corporation*

**Use of the Xevo TQ-S as applied to the routine and not so routine analysis of animal tissues for residues of veterinary medicines**

Guest speaker: Dr Simon Hird, FERA, UK

Even with approved use, it is expected that residues will usually turn up in food supplies. Conditions of use are set to ensure that these residues are not at levels that may cause harm. For many of these compounds, legal action limits/levels in food have been established or their use is banned. Fera delivers two separate UK surveillance programs: the statutory plan covers > 30,000 samples of UK produce each collected for a different analysis, whereas the non-statutory program is much smaller (1400 samples) and focuses mainly on imports. The latter requires multiple tests on each sample for which a multi-residue approach is essential.

We have been using three Xevo TQ-S instruments with UPLC to deliver much of the above programs. Case studies will be presented to show how the enhanced sensitivity and additional capabilities is helping us deliver determination of a range of different classes of analytes and many combined as a multi-residue suite.

**Profiling of Highly Complex Citrus Juice Samples using UPLC Ion Mobility Time of Flight Mass Spectrometry**

Ramesh Rao, Director Strategic Marketing, Waters Corporation

Flavonoids are one of the largest and most wide spread classes of compounds and possess diverse pharmacological and biological properties. Such attributes mean many flavonoid-containing plant species may be used as functional foods or phytomedicines. The presence of flavonoids in Citrus juices has attracted attention because of their biological and physiological importance. The use of HPLC-MS and HPLC-MS/MS based methods to profile flavonoids has become more routine. The role of flavonoids compounds as markers is important and is a challenge due to sample complexity. HDMS can provide a route to specific and unambiguous identification. As well as enable the unequivocal distinction of flavonoid isomers.

High definition mass spectrometry has been utilised to profile citrus juice products and this technique offers some unique advantages to profiling complex mixtures. It is a combination of high resolution mass spectrometry and high efficiency ion mobility based measurements and separations. Ion mobility (IM) mass spectrometry is a rapid orthogonal gas separation phase technique that technique which allows another dimension of separation to be obtained within an LC timeframe. Compounds can be differentiated based on size, shape and charge, as well as mass. The study undertaken investigates the use of Ion Mobility separation in combination with UPLC (Ultra High Performance Chromatography).

The profiling study undertaken clearly shows the benefits of using HDMS. The results obtained show that isomer/conformational analysis can be performed. It is possible to separate co-eluting analytes and increase peak capacity. This enables single component accurate mass spectra of chromatographic co-eluting components to be obtained. These were used to generate elemental composition information. The enhanced peak capacity enables more

information to be extracted from fragmentation studies and the individual MSe fragmentation spectra have been obtained for flavonoid isomers which are co-eluting, from which structural elucidation has been performed.

The enhanced peak capacity brought about by profiling using UPLC HDMS can be visualised rapidly using the MSe data viewer. Co-eluting compounds and unknown isomers can to be resolved rapidly.