

Target Quantitation and Non-Target Suspect Screening using High Resolution Mass Spectrometry on the Agilent 6546 Q-TOF.

Gordon Ross, Agilent Technologies, Cheadle UK

High Resolution Mass Spectrometry (HRMS) provides for multiple avenues of investigation in Forensic and Toxicological investigations. In comparison with triple quadrupole analyses where compound identity is confirmed using retention time and two MRM transitions (one for quantification and the other for qualification), HRMS can deliver equally as robust confirmation, using co-eluting compound derived fragments as qualifiers, with the additional confidence of providing isotope pattern and accurate mass information exemplified in the performance of the Agilent 6546 Q-TOF. The quantitative performance of the 6546 compares very well regarding linearity, reproducibility and sensitivity but can also provide the means for investigative non-target or suspect screening and historical investigation.

The MassHunter family of powerful software tools, allows the investigation of NPS and large suites of drug substances using proprietary Personal Compound Databases and Libraries even in the absence of available standards. The nature of the HRMS data generated allows retrospective interrogation of any sample should additional information come to light, allowing the analyst to 'look back' into historical cases. We will present data demonstrating the quantitative performance of the 6546 Q-TOF and highlight those software tools and workflows which turn high resolution mass spectrometric data into useful, insightful qualitative information.

For Forensic Uses.