

SIMULTANEOUS COMPOUND QUANTIFICATION AND IDENTIFICATION USING HIGH RESOLUTION MS: THE AB SCIEX TRIPLETOF™ 5600 SYSTEM

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Increasing productivity in discovery and development continues to be a primary goal not only in pharmaceutical research but in many other scientific disciplines. One of the most promising approaches to improving productivity is combining quantitative and qualitative analysis in a single analytical run (Quant / Qual). Quantitative information can be obtained on the parent compound while simultaneously acquiring qualitative information on metabolites in a completely automated fashion.

Triple quadrupole instruments have been the workhorse instrument for the quantitative portion of this application due to their excellent sensitivity and high throughput. Accurate mass instruments such as Time of Flight (TOF) and orbital trapping analyzers have been used for metabolite identification due to their high mass accuracy and resolution. Unfortunately, orbital trapping involves a compromise between resolution and speed. Traditional TOF technology has shown limitations in linearity and requires internal calibration to maintain mass accuracy. Modifying study designs, sample preparation procedures, or chromatography in order to accommodate instrument limitations is not acceptable.

Here we introduce a new technology, The AB SCIEX TripleTOF™ 5600 System, which combines the best attributes of triple quadrupoles and accurate mass analyzers in a single instrument. The highly innovative design of the TripleTOF™ 5600 System, combines a proven high performance triple quadrupole front end with the Accelerator TOF™ Analyzer, a state of the art accurate mass analyzer with unprecedented performance and stability. This results in linearity and sensitivity of a high performance triple quadrupole, combined with speed, high mass accuracy (2 ppm or less) and high resolution (35,000) of an accurate mass instrument, even at low mass for small molecules.