



« The 6520 Accurate-Mass quadrupole time-of-flight (Q-TOF) liquid chromatography/mass spectrometry (LC/MS) system from Agilent

» The SYNAPT MS system from Waters



Massive Potential

Updates in Mass Spec

From pharmacokinetics to space exploration, mass spectrometers help us analyze and identify virtually anything that can be made into a liquid or gas, using a very small minimum sample size. Read below to learn about the newest improvements to this most useful tool.

Waters announces the **SYNAPT MS** system, a next-generation quadrupole orthogonal acceleration, time-of-flight (OA-TOF) mass spectrometry (MS) platform. The SYNAPT MS system is the only platform which provides an upgrade pathway to the SYNAPT High Definition MS system, uniquely enabling researchers to analyze samples differentiated by size, shape and charge, as well as mass, ultimately providing new capabilities that can help them meet and exceed future requirements. "Confident sample identification, detailed characterization and increased productivity are primary requirements for intelligent mass spectrometry based solutions in key biomedical applications such as proteomics, metabolomic profiling, biomarker discovery/validation and pharmaceutical R&D," said Brian W. Smith, Vice President, Mass Spectrometry Operations for the Waters Division. "The new SYNAPT MS meets these demands through application specific system solutions designed to help our customers accelerate and improve the quality of laboratory analysis with the goal of advancing research and reducing time-to-market," he adds. **More information:** www.waters.com

Agilent introduces the **6220 Accurate-Mass time-of-flight (TOF)** and **6520 Accurate-Mass quadrupole time-of-flight (Q-TOF) liquid chromatography/mass**

spectrometry (LC/MS) systems, delivering superior mass accuracy, mass resolution, sensitivity and speed for proteomics, metabolomics, product degradation and other complex experiments. The new 6220 TOF and 6520 Q-TOF have added proprietary 32 Gbit/second high-speed data acquisition electronics that improve mass resolution to 20,000. Additionally, the new products incorporate proprietary dual-gain analog to digital (ADC) time-of-flight electronics for a tenfold improvement of dynamic range – now approaching up to five orders of magnitude. "We set out to deliver exceptional analytical performance for MS and MS/MS analyses for experiments demanding the highest accurate-mass measurements, and these two instruments have achieved this," said Ken Miller, Agilent marketing director, LC/MS Division. "These improvements will enable scientists in metabolomics, proteomics and complex qualitative analyses to find and identify more lower-abundance compounds faster than ever. All of this performance is achieved without significantly compromising rapid analysis time for higher-quality data," he adds. The new Agilent 6520 Q-TOF performs at its best in the most important categories: attomole sensitivity; better than 2 ppm MS mass accuracy – approaching FTMS mass accuracy; better than 5 ppm MS/MS mass accuracy – much

better than FTMS mass accuracy at fast spectral acquisition rate; tenfold improvement in in-spectra dynamic range without loss of sensitivity; mass resolution to 20,000 – not dependent on spectral acquisition rate; fast data acquisition (greater than or equal to 10 MS/MS spectra/sec) compatible with fast LC chromatography; and, broad mass range from m/z 25 to 20,000. Similarly, when operating in MS mode only, the Agilent 6220 TOF incorporates the same high-speed electronics and ADC TOF technology to deliver the same benefits as when operating in MS/MS mode. Targeted applications include product degradation studies, biomarker discovery, metabolomics and confirmation of compounds in synthetic chemistry labs. **More information:** www.agilent.com

Answering researchers' need for improved accuracy and speed in identification of unknown components, **Shimadzu** has developed a system featuring the **LCMS-IT-TOF** mass spectrometer. Using information-rich MSn data, the patent-pending Formula Predictor software takes advantage of multiple levels of fragmentation, isotope pattern verification, and unique fragment-ion filtering techniques to accurately determine the correct formula for unknown components. Traditional approaches for deducing empirical formulae from mass spec data often depend on very high mass accuracy,

» The PerkinElmer Clarus 600



which carries a correspondingly high cost, and considerable time input from the user to eliminate low-probability structures. Shimadzu's new system reduces or eliminates this need for tedious, manual processing of target candidates. In many cases, the software can reduce the collection of target compounds from a high number of possible candidates to predicting the most likely empirical formula with just a simple mouse click. The LCMS-IT-TOF addresses the needs of biomarker discovery, trace amount impurity identification, and natural products research. Features of the LCMS-IT-TOF include: high mass accuracy MSn analysis; high level of accuracy in database searching enabling workflows and data interpretation to greater precision; high-sensitivity, full-spectrum TOF analyzer providing low femtomole/picogram detection of multiple components in a single analysis; constant mass accuracy and mass resolution in all MS modes; fast data acquisition, up to 10 spectra per second, for efficient peak detection and compatibility with ultrafast HPLC separations; and, high-speed polarity switching (switching time of 100 milliseconds). **More information:** www.shimadzu.com

PerkinElmer introduces the Clarus 600 Gas Chromatograph/Mass Spectrometers (GC/MS) with superior oven performance, delivering quick combined heat-up and cool-down rates for a conventional GC. It also provides state-of-the-art electronics, enhanced software and a choice of three different pumps to meet the diverse performance demands and budget requirements of a range of laboratories. This precise and accurate system for both routine and high-performance analy-

ses offers reliable performance for a variety of markets and applications - environmental, forensic, petrochemical, chemical, food and fragrances, among others. While other manufacturers OEM or partner to provide a complete system, PerkinElmer is unique in offering customers a single source for a complete and fully integrated system based on its performance and throughput requirements. The Clarus 600 MS, combined with the new Clarus 600 GC, is designed for a variety of laboratory requirements to ensure increased throughput and improved detection limits and to provide significant return on investment. Hardware improvements include state-of-the-art electronics, providing fast scanning and increased productivity, multiple pumping options to meet every lab's needs, a compact footprint to maximize laboratory bench space, the PreVent suite of column flow controls for increased uptime and productivity, and industry-leading sensitivity for both electron ionization and chemical ionization. **More information:** www.perkinelmer.com

Thermo Fisher Scientific announces **MetWorks 1.1.0 Metabolite Identification Software**, an updated version of its established metabolite identification software. Thermo Scientific MetWorks 1.1.0 software facilitates automated acquisition, processing and reporting of LC/MSn data in support of biotransformation studies. MetWorks software is compatible with all Thermo Scientific mass spectrometers capable of performing MS/MS and MSn fragmentation. In addition, MetWorks allows high resolution accurate mass data from the Thermo Scientific LTQ Orbitrap and LTQ FT instruments to be fully

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—**Brian W. Smith**
Vice President
Mass Spectrometry Operations
Waters Division

leveraged. MetWorks 1.1.0 Software features enhanced tools that facilitate distinguishing xenobiotic components from endogenous biological matrix interferences in LC/MSn chromatograms and spectra. New features include: automatic generation of a Data-Dependent Parent Mass Table (DDPT); component filtering to exclude duplicates originating from adducts and isotopic contributions; and flexibility to apply up to six multiple mass defect filters (MMDF's), which are based on high-resolution, exact mass and mass deficiencies of the parent-drug and its putative metabolites. The structure column in the MetView table can be used to attach a molecular structure drawing (.mol file) to a potential putative candidate. **More information:** www.thermofisher.com ■

Companies Mentioned in this Product Spotlight:

Agilent - www.agilent.com

PerkinElmer - www.perkinelmer.com

Shimadzu - www.shimadzu.com

Thermo Fisher Scientific - www.thermofisher.com

Waters - www.waters.com

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