Advanced Linear Ion Trap technology at the highest level of sensitivity
The highest performance ion trap and the highest sensitivity triple quad. All in one system.

Introducing the Applied Biosystems/MDS SCIEX 4000 Q TRAP™ LC/MS/MS System. Innovative Linear Ion Trap (LIT) technology from the leaders in mass spectrometry brings together fast, sensitive qualitative analysis with the proven, high sensitivity quantitation of the industry’s premier triple quadrupole.

Exciting new application possibilities.
Delivering maximum sensitivity quantitative and qualitative performance in one instrument, the new 4000 Q TRAP™ LC/MS/MS System opens up a whole new class of application workflows for proteomics, drug discovery, and drug development. By combining true triple quadrupole scan modes with sensitive ion trap scans in a single LC/MS/MS run, you can achieve results that previously required multiple analyses on multiple MS platforms. And in many cases, you can acquire data that is not easily obtainable by any other means.

A complete, integrated system.
The rugged, robust 4000 Q TRAP system sets a new standard of dependability for the high throughput laboratory. With a full complement of automation features, it fits seamlessly into your lab’s workflow and boosts your discovery productivity. The system includes intuitive application-specific software with all the controls required for 21 CFR Part 11 compliance; we’ll also help with any validation support you may need. In addition to the mass spectrometer, Applied Biosystems/MDS SCIEX can also supply the chromatography front end through our LC partners.

Powerful, industry-leading software.
Powerful Analyst™ and BioAnalyst™ software puts all of the 4000 Q TRAP system’s sophisticated performance features right at your fingertips, and simplifies every aspect of methods development, data acquisition and processing. Advanced, built-in automation capabilities make it easy to get meaningful results, and the flexible control software supports most popular LC platforms.

A single solution for discovery and development.
The combination of the highest sensitivity triple quad with the most sensitive linear ion trap technology, coupled with versatile Analyst™ software, offers a total system solution that’s a perfect fit for any busy laboratory. The extended productivity features of the application-specific software—Metabolite ID, Pro ID, and Pro ICAT with links to Celera Discovery System™ (CDS) software—complement the 4000 Q TRAP system’s superior sensitivity and performance, to give you more useful information per sample than any other single system.
Unequalled triple quad and ion trap sensitivity
Superior triple quad performance, plus patented collisional focusing and linear ion trap technologies combine to maximize full scan MS and MS/MS sensitivity, enabling you to identify more low abundance metabolites, proteins and post-translational modifications with a high degree of confidence.

Highest sensitivity MRM
The 4000 Q TRAP™ system provides true triple quadrupole multiple reaction monitoring (MRM) at the highest level of sensitivity, as well as extended dynamic range, ensuring superior quantitation performance for both small molecules and peptides.

MS² capability
Advanced MS² functionality, together with triple quadrupole fragmentation patterns, gives you more useful information in fewer experiments—including detailed structural information and insight into metabolic pathways.

Advanced scanning capabilities
The highest sensitivity neutral loss and precursor ion scans and enhanced multiply charged scan can be used in flexible combinations to enable information-rich, high throughput workflows.

Automated LC/MS/MS workflows using Information Dependent Acquisition (IDA) provide the framework for deriving maximum information from every experiment. When used with the 4000 Q TRAP system’s powerful mixed scan modes, IDA lets you focus on specific ions of interest for increased productivity.

Higher resolution, improved mass accuracy
Next generation linear ion trap technology provides enhanced resolution for reliable real-time charge state and isotope pattern determination, plus superior mass accuracy across the entire mass range.

Plug-and-play sources
Rugged, reliable ion sources are easily interchanged for a wide range of applications and flow rates to suit your lab’s needs. Choices include the exclusive Turbo V™ source with TurboIonSpray® probe and APCI probe, the new DuoSpray™ ion source—a combined software-selectable ESI/APCI ionization source—and a new NanoSpray™ source and interface for nanoflow applications.

Dynamic Fill Time (DFT)
The system dynamically calculates the time required to fill the linear ion trap. For abundant compounds, a short fill time reduces the space charge effects by limiting the number of ions in the ion trap, while a longer fill time increases weak signals by allowing ions to accumulate.

Ones ystem not only does it all. It does it better.

Superior resolution and higher mass accuracy greatly increase the specificity and speed of database searches to give you better confidence in all identification results.

Dynamic Fill Time capability ensures high quality data over a wide dynamic range.

Enhanced Multiply Charged Scan
Enhanced Multiply Charged Scan preferentially reduces singly charged ions and highlights the peptide ions of interest.
Taking Linear Ion Trap technology to new levels of performance and sensitivity.

The 4000 Q TRAP™ LC/MS/MS System takes advantage of a number of mass spectrometry innovations to deliver unmatched quantitative and qualitative performance within a single system. The instrument combines the advanced features of Applied Biosystems/MDS SCIEX Linear Ion Trap (LIT) technology—including significantly higher injection and trapping efficiencies, greater ion capacity, and higher duty cycle—with the unequalled sensitivity of the leading triple quadrupole system for drug development.

Patented Q3 linear ion trap
Use of a quadrupole as a linear ion trap significantly enhances ion trap performance while maintaining complete triple quadrupole functionality:
- Greater ion capacity. The larger, linear ion trap can accommodate up to 70X more ions than a 3D ion trap, providing greater sensitivity before the onset of space charge effects.
- Improved injection and trapping efficiencies. With an ion path 30X longer than a 3D ion trap, ions have more time to lose energy, promoting capture and further enhancing sensitivity.
- New Dynamic Fill Time (DFT). Ensures high quality data for a wide range of analyte concentrations.
- Higher duty cycle. Faster scan time provides more information in less time for any given experiment; more scans over a given chromatographic peak result in more thorough investigation of your complex samples.
- No low mass cut-off. The fragmentation step (LINAC collision cell) and the trapping step (Q3) are spatially separated, making capture and analysis of lower mass ions possible.

“The 4000 Q TRAP™ system is really more than just a hybrid instrument. It gives you all the capabilities of the world’s most sensitive triple quad and the world’s largest capacity linear ion trap, without sacrificing performance on either side.”

Dr. Jim Hager, Senior Research Scientist, MDS SCIEX
Automated metabolite identification and confirmation.

The 4000 Q TRAP™ system’s highest quantitative (MRM) sensitivity and highly specific scan functions, along with the ability to trigger MS/MS and MS3 from MRM transitions, enables rapid, single-run identification, characterization and confirmation of Phase I and II metabolites.

In complex biological matrices, the added selectivity of triple quadrupole scan functions such as precursor ion (PI) and neutral loss (NL) scans can identify expected as well as unexpected metabolites based on basic knowledge of the drug and its MS/MS fragments. The superior triple quadrupole performance—with the highest sensitivity PI and NL scans available—assures detection of even low abundance metabolites; the highest sensitivity ion trap guarantees superb product ion spectra for confirmation, all in the same run.

Parent Drug MS/MS

For targeted Phase I and II metabolite analysis, MRM provides an extremely sensitive and selective approach. In this example, potential Phase I metabolites were screened based on a list of 26 theoretical MRM transitions automatically compiled from the mass shifts of six potential common biotransformations of the parent drug, together with two fragment ion masses determined from the parent drug MS/MS fragmentation pattern.

With the LINAC™ collision cell, up to 100 MRM transitions can be monitored in a single experiment. In order to eliminate erroneous metabolite identifications from the MRM transitions, the system has the ability to trigger MS/MS and MS3 to generate a spectrum that can be used to confirm the presence and structure of the metabolite.

Six Phase I transformations yield 26 MRM transitions

Comparison of EMS vs. MRM

In a single 15-minute run, targeted MRM analysis significantly increased the number of identified and confirmed metabolites compared to traditional full scan enhanced MS analysis, a standard 3D ion trap scan mode.

Now extremely sensitive metabolite identification can be performed with theoretical MRM transitions and verified with IDA triggered MS/MS to confirm the identity of each metabolite in a single, quick experiment.
Fast, automated workflow lets you quickly identify PTMs in complex protein samples.

A novel single-run 4000 Q TRAP™ system workflow enables the automated investigation of post-translational modifications. By taking advantage of the system’s sensitive, highly specific precursor ion and neutral loss scan functions, and linking them to the highest sensitivity ion trap MS/MS scans, in a single experiment you can achieve fast, definitive results that previously required multiple runs on multiple instruments.

Precursor Ion of 79 (-)  
Enhanced Resolution (+)  
Acquire MS/MS Spectra (+)  
Add to Exclusion List  

In the automated PTM workflow, Information Dependent Acquisition (IDA) links advanced scan functions to identify phosphopeptides and determine specific phosphorylation sites.

A highly sensitive and specific negative ion precursor ion scan for m/z 79 determines which peptide ions are releasing a phosphate ion (PO₃⁻). The most intense ions from the negative ion survey scan are automatically selected for a positive ion, Enhanced Resolution (ER) scan to determine charge state and assign an accurate monoisotopic mass. Subsequently, these ions are subjected to a high sensitivity, Enhanced Product Ion (EPI) scan to acquire fragmentation data. This fragmentation data is used to determine the sequence and phosphorylation site on the phosphopeptide.

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Add to Exclusion List  

Automated PTM discovery workflow using Information Dependent Acquisition (IDA)  
- Negative ion precursor ion (PD) scan for m/z 79 as a survey scan  
- Switch polarity to positive ion  
- Positive ion enhanced resolution (ER) scan for charge state determination and accurate mass  
- Positive ion enhanced product ion (EPI) scan  
- Database search using Pro ID software or de novo sequencing to identify protein and phosphorylation site

A tryptic digest of reduced and alkylated standard glycoprotein, fetuin, was analyzed using the automated PTM discovery workflow on the 4000 Q TRAP™ LC/MS/MS System. An overlay of the negative ion precursor ion (PI) scan (red trace) with a corresponding positive ion full scan (blue trace) demonstrates the specificity of the precursor ion experiment and the ability to identify the elution time of the phosphopeptides in an LC/MS experiment.

The most intense negative ion PI peaks are automatically selected for an ER scan. The IDA software automatically adjusts the mass for the polarity switch from negative ion to positive ion, and assigns a more accurate monoisotopic mass. In this case, the negatively charged precursor ion at 1098.4 was assigned a more accurate positive ion m/z value of 1100.4 and a charge state of 2.

Each of the ions identified by the PI scan is subjected to a high sensitivity EPI scan to acquire fragmentation data. This fragmentation data is used by BioAnalyst™ and Pro ID software to identify the protein source of the phosphopeptide, as well as the site of phosphorylation on the phosphopeptide.

Using the ion matching features in BioAnalyst software, the theoretical fragment ion coverage matched to the experiment fragment ions in the spectrum can be displayed, including the phosphorylation-specific ions where phosphoric acid is lost from the b and y ions.

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Explore the advantages of new Linear Ion Trap technology.

If your research involves proteomics, drug discovery, or drug development studies, Applied Biosystems/MDS SCIEX 4000 Q TRAP™ LC/MS/MS system can make your efforts more productive by giving you a powerful, single-system solution for a wide range of applications. For more information, call the Applied Biosystems sales office nearest you, or visit http://www.appliedbiosystems.com/4000qtrap