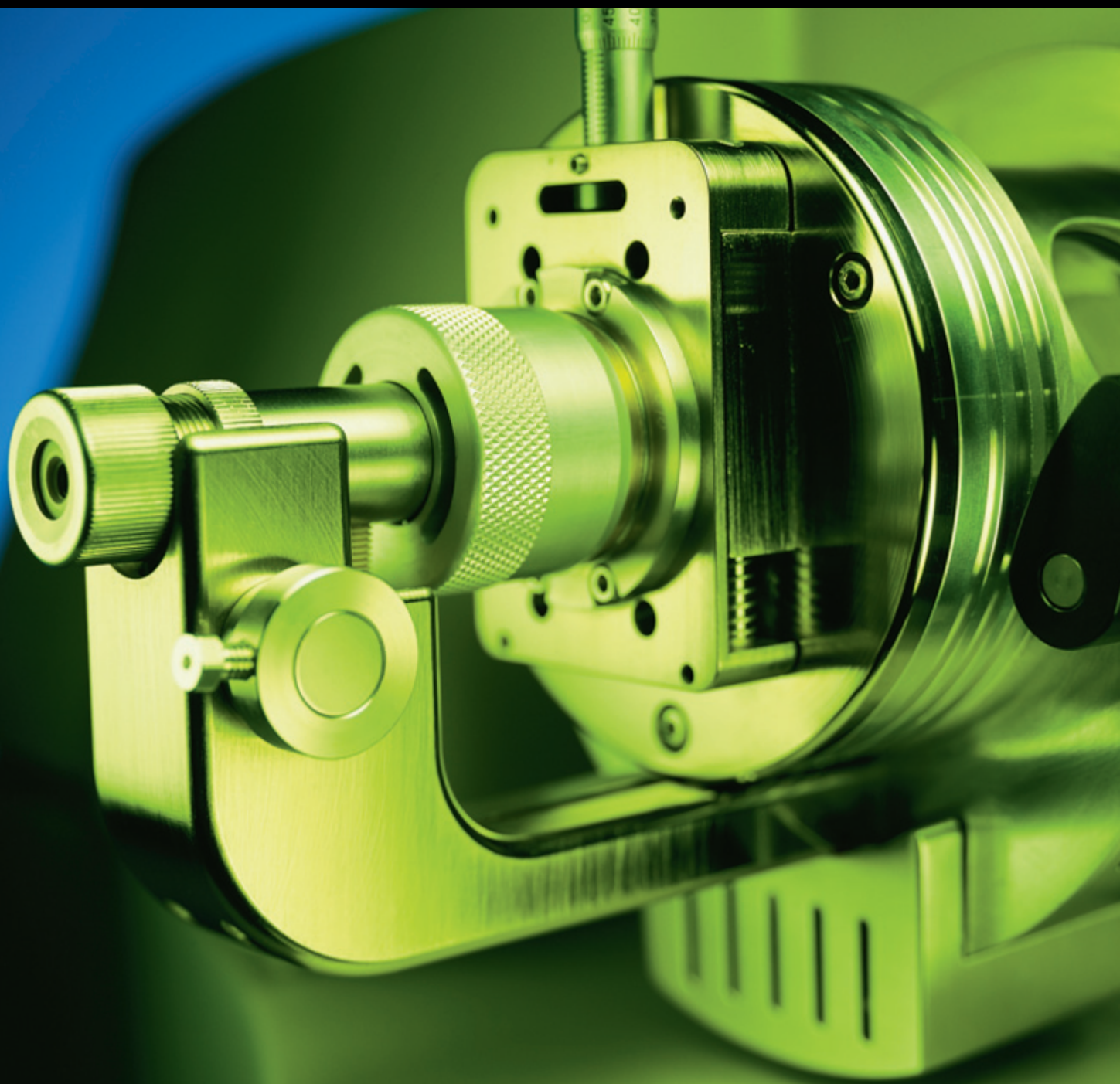


More metabolites, more proteins, more confidence in your results

AB Applied Biosystems | **MDS SCIEX**

Q TRAP™

LC/MS/MS System



more per

Now you can go straight

Introducing the Applied Biosystems/MDS SCIEX Q TRAP™ LC/MS/MS System. How's this for straight thinking? A linear, hybrid mass spectrometer that outperforms any conventional ion trap *and* delivers all the functionality of a high-performance triple quadrupole.



Patented linear ion trap technology delivers superior sensitivity, resolution, and mass accuracy—significantly enhancing efficiency, productivity, and confidence in results.

The new Q TRAP LC/MS/MS System, the latest innovation from the leaders in mass spectrometry, features new, patented linear ion trap technology that considerably extends ion trap capabilities. It offers unmatched qualitative performance for drug discovery and proteomics, as well as the wide dynamic range required for accurate quantitation.

The compact benchtop system, with intuitive application-specific software, is a powerful, easy-to-use tool that's rugged enough for continuous-duty high-throughput operation. With a full complement of automation features, it fits seamlessly into your lab's workflows and boosts your discovery productivity.

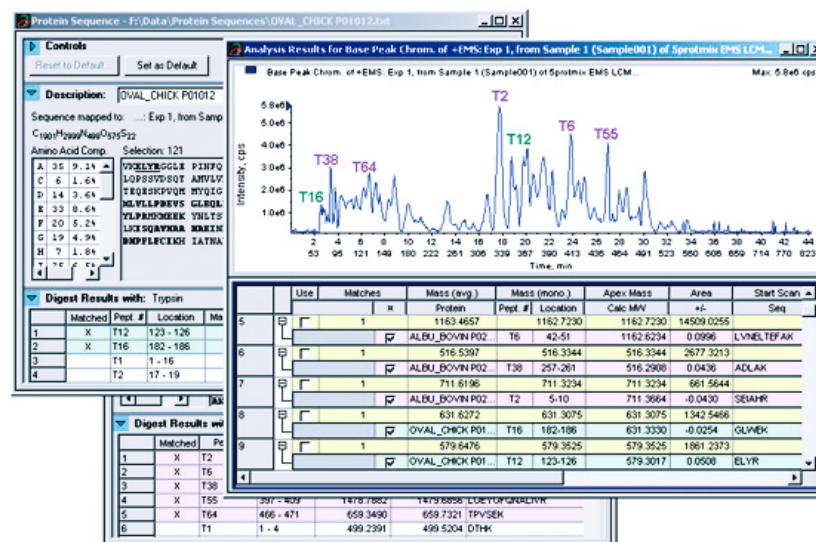
Performance to the answers.

Powerful, industry-leading software.

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

Integrated system approach combines unmatched performance and ease of use.

The combination of advanced linear ion trap technology and versatile Analyst software offers a total system solution that's a perfect fit for any busy DMPK or proteomics laboratory. The extended productivity features of the application-specific software—Metabolite ID and Pro ID—complement the Q TRAP system's superior performance, to give you more useful information per sample.

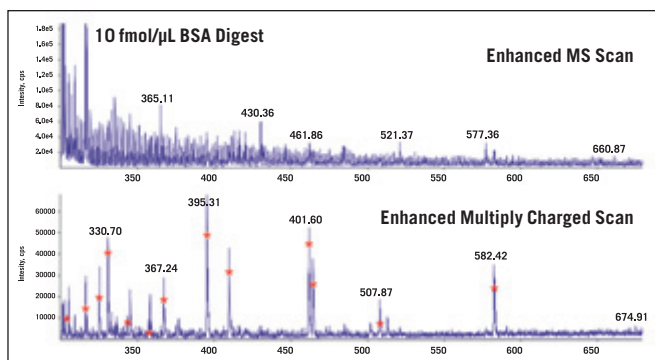


Peptide mapping tools in BioAnalyst™ software.

more co

The advantages of straight

Performance you won't find in any other ion trap.



Enhanced multiply charged scan preferentially reduces singly charged ions and highlights the peptide ions of interest.

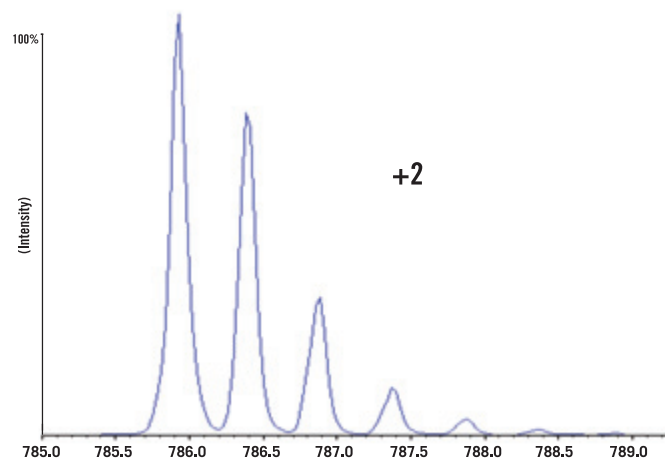
ADVANCED SCANNING CAPABILITIES

Information Dependent Acquisition (IDA) provides the framework for deriving maximum benefit from your experiments. When used with the Q TRAP™ system's powerful mixed scan modes, IDA lets you focus on your specific ions of interest—and not waste time collecting irrelevant information.

Multiply charged scans, neutral loss scans, and precursor ion scans can be used in flexible combinations to give you more answers in fewer experiments, saving valuable time.

EXCEPTIONAL SENSITIVITY

Patented collisional focusing and linear ion trap technologies combine to optimize full scan MS and MS/MS sensitivity, enabling you to identify low abundance metabolites and proteins with a high degree of confidence.

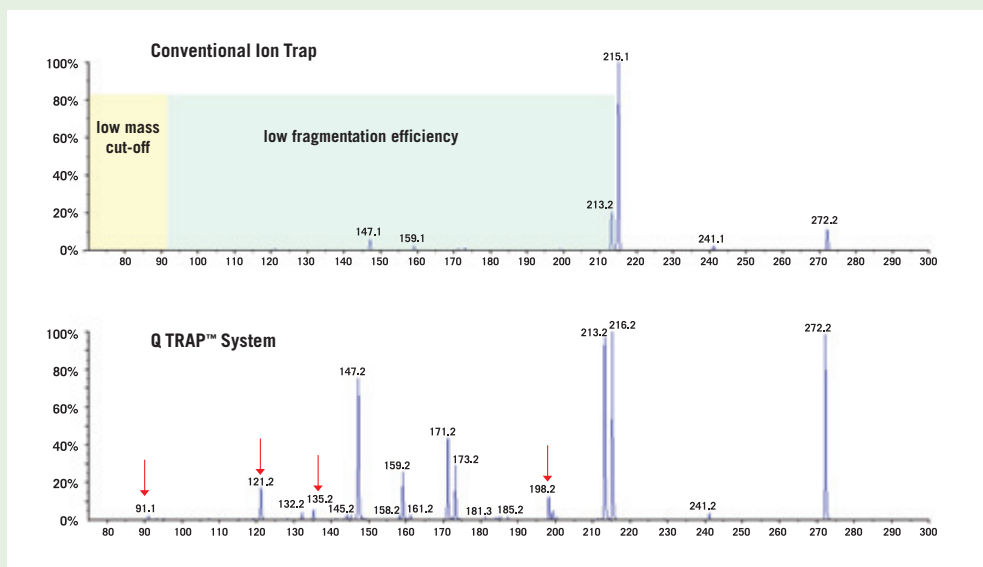


HIGHER RESOLUTION, IMPROVED MASS ACCURACY

The increased resolution of Q TRAP linear ion trap technology provides real-time charge state determination and superior mass accuracy across the entire mass range. The higher mass accuracy greatly increases the specificity and speed of database searches to give you better confidence in all identification results.

Confidence

thinking.



Triple quadrupole fragmentation patterns and no inherent low mass cut-off result in more fragment ion information.

NO LOW MASS CUT-OFF

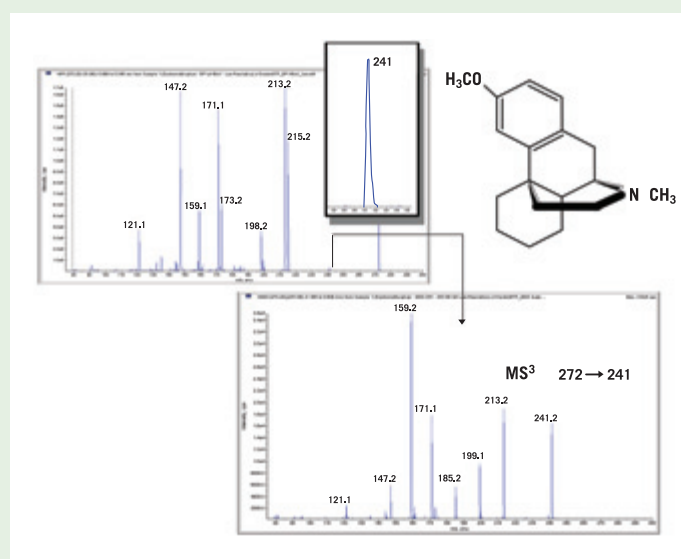
With the Q TRAP system, you get the information-rich MS/MS spectra you expect from a high-performance triple quadrupole. Because the Q TRAP system doesn't suffer from the low mass cut-off and low fragmentation efficiencies observed in conventional ion trap systems, you don't lose important structural information.

BROAD LINEAR DYNAMIC RANGE

The Q TRAP system provides true triple quadrupole multiple reaction monitoring (MRM) performance for accurate quantitation. The extended dynamic range also enhances identification of ions in complex matrices.

MS³ CAPABILITY

Advanced MS³ functionality, together with triple quadrupole fragmentation patterns, gives you the maximum amount of information in fewer experiments—including detailed structural information and insight into metabolic pathways.



MS³ combines with triple quadrupole fragmentation to provide detailed structural information.

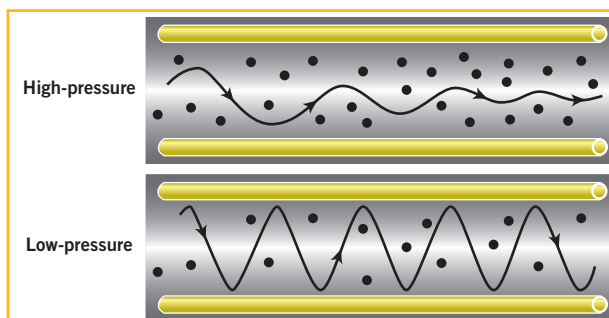
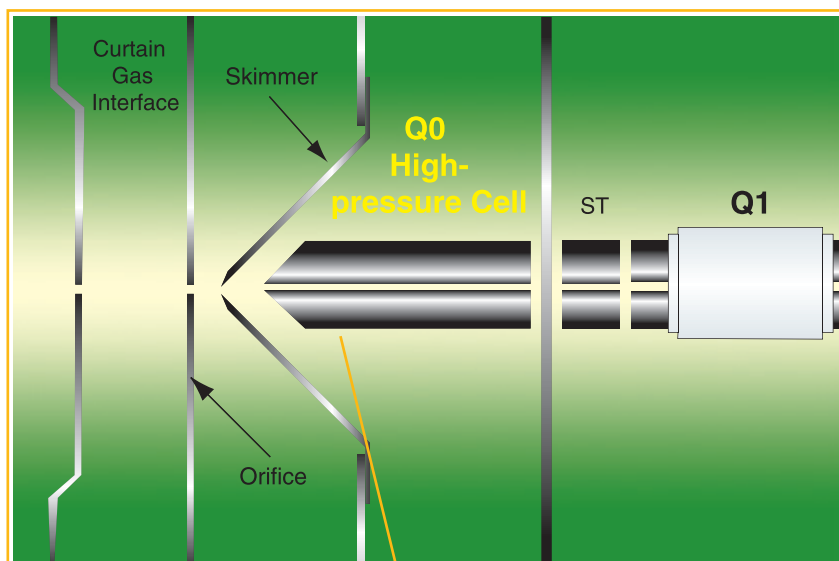
more Straight talk on linear ion t

The Applied Biosystems/MDS SCIEX Q TRAP™ LC/MS/MS System is the product of a number of technological breakthroughs, and is built around several unique, patented technologies. The linear design provides considerably enhanced ion trap capabilities, including significantly higher injection and trapping efficiency, greater ion capacity, and higher duty cycle. At the same time, the hybrid instrument delivers full triple quadrupole functionality and performance.



Plug-and-play sources

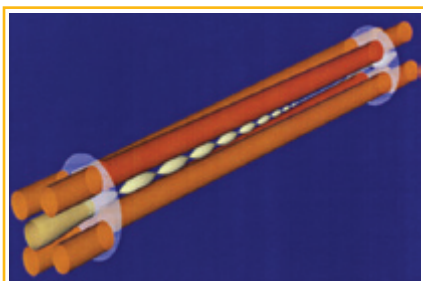
Rugged and reliable interchangeable ion sources, including the new Flow Nanospray™ source, are available for a wide range of flow rates to suit your application needs.



Collisional focusing Q0

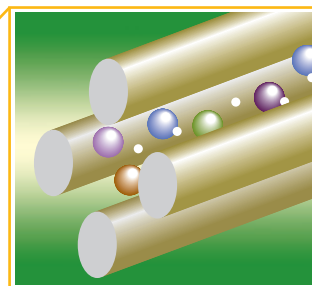
Unique, patented, high-pressure collisional focusing technology maximizes transmission of ions for superior sensitivity.

power rap technology.



Patented LINAC™ collision cell technology

The patented LINAC high-pressure collision cell accelerates ions through the collision quadrupole, providing increased sensitivity at greatly reduced dwell times.



Patented Q3 linear ion trap

Greater ion capacity.

The larger, linear ion trap can accommodate up to 45X more ions, providing greater sensitivity before the onset of space charge effects.

Improved injection and trapping efficiency.

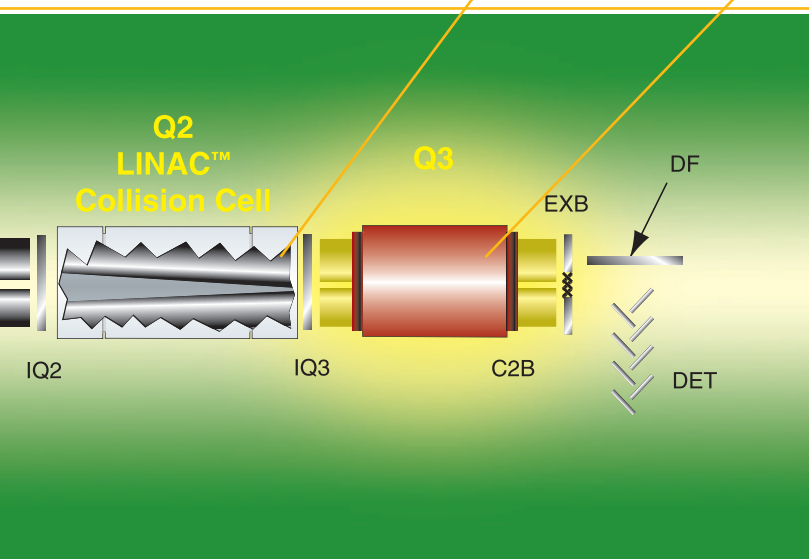
With an ion path 20X longer than a 3D ion trap, ions have more time to lose energy, promoting capture and further enhancing sensitivity.

Higher duty cycle.

Faster scan times provide 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.

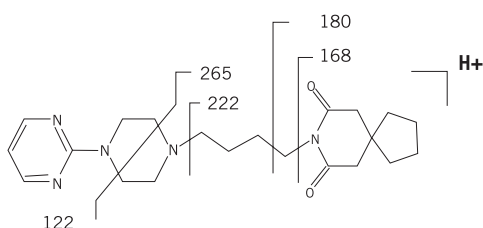
The fragmentation step (LINAC collision cell) and the trapping step (Q3) are spatially separated, making capture and analysis of lower mass ions possible.



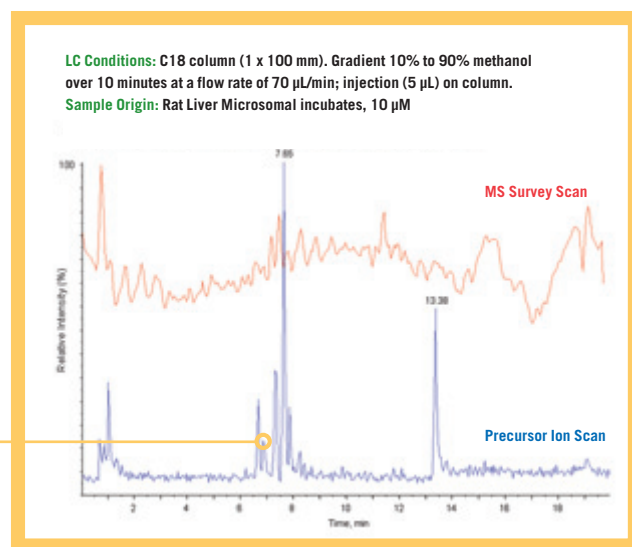
more meta

Quickly identify more met And quantitate them, too.

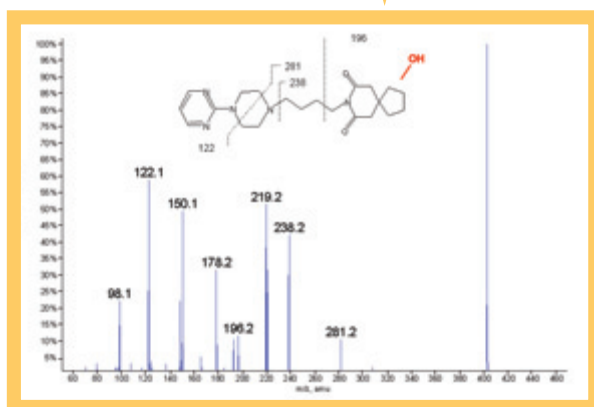
Phase I and Phase II metabolites. The specificity of precursor ion and neutral loss as IDA survey scans (or as a combination of survey scans) improves the detection of metabolites per injection for both in vitro and in vivo samples. Combining IDA with Metabolite ID on a Q TRAP™ system leads to faster identification of more metabolites with increased confidence.



Identifying metabolites of a drug candidate, such as buspirone, from complex in vitro and in vivo samples presents a challenge. Based on the chemical structure and fragmentation pattern, the site of modification that may occur on the rings from the A or B side can be identified using a precursor ion scan of mass 122 or 168, respectively. Data were acquired using precursor ion scans 122 and 168, the major fragments of buspirone, as the survey scans.



The precursor scan of mass 122 demonstrates well-defined peaks that can be easily identified; nine metabolites were directly identified and confirmed.



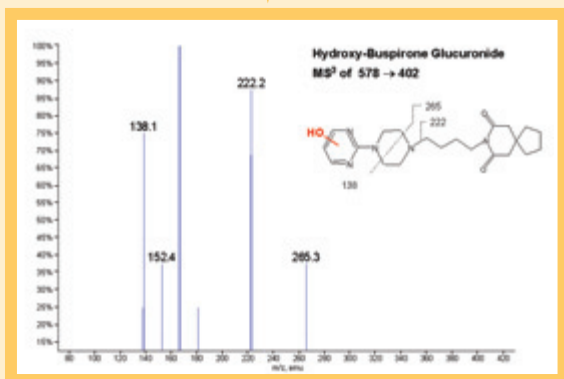
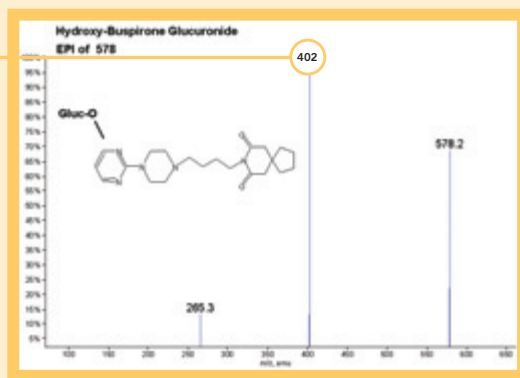
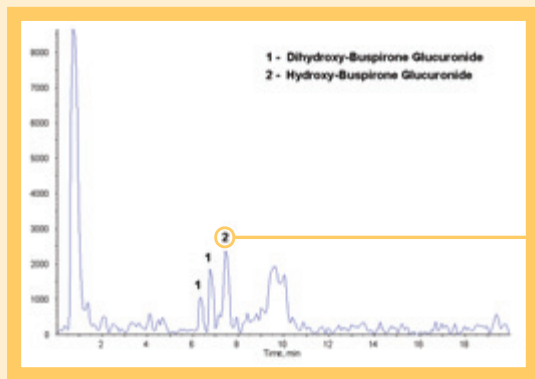
The enhanced product ion spectrum reveals the major fragment hydroxy-buspirone, providing information on the site of modification. In all cases, the use of a precursor ion scan as the survey scan resulted in the identification and confirmation of more metabolites than the single MS survey scan approach. Using Analyst® software with IDA, up to two precursor ion scans can be combined in the survey step, minimizing the number of injections required while improving the detection specificity of ions of interest.

bolites

abolites.



For the detection of Phase II metabolites, IDA was used with a neutral loss of 176 to specifically identify the glucuronide species of buspirone. As expected, the microsomal incubates resulted in low-level glucuronides. Since the MS/MS of glucuronide species typically yields the aglycon as the major fragment ion, IDA was set to provide further structural information by adding an MS³ experiment following the enhanced product ion scan step. A total of three glucuronide metabolites were identified and confirmed.



The MS³ experiment on the aglycon fragment clearly indicates the site of hydroxylation. This approach is useful in the detection of expected and non-expected metabolites.

Metabolite ID Software Application

- Identifies predefined and user-defined transformations
- Triggers automatic acquisition of MS/MS structural information
- Detects unexpected metabolites by recognition of isotope ratio patterns
- Compares sample to control for identification confirmation
- Includes library search function

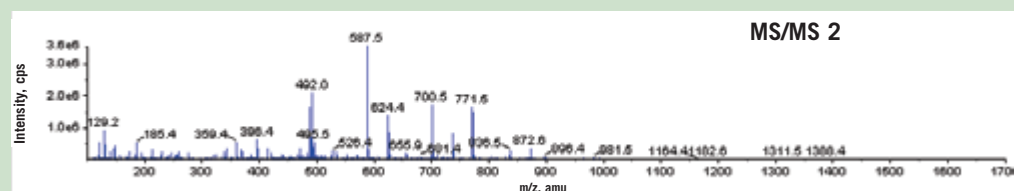
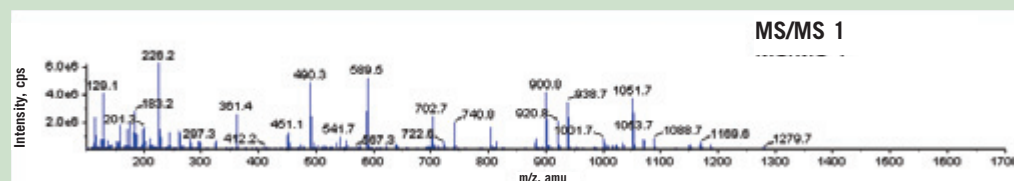
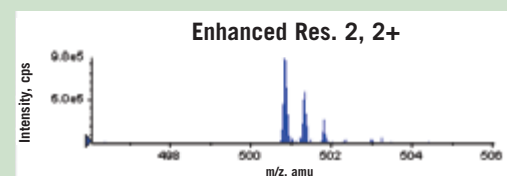
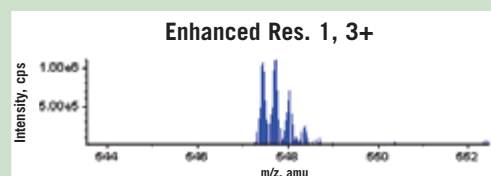
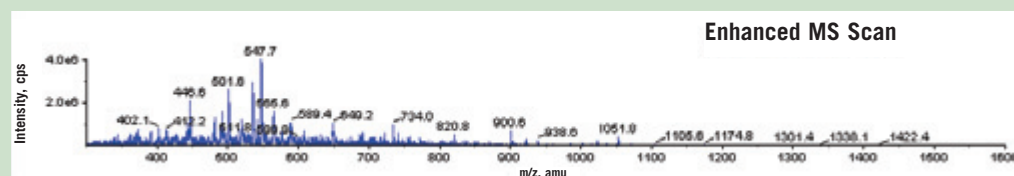
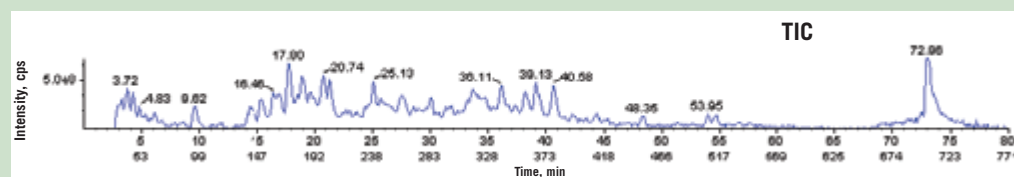


More of the info

Pro ID Software Application

- Specifically designed for *high-throughput* protein identification
- Interrogator™ search algorithm performs extremely fast database searches
- Powerful zone modification feature identifies unexpected modifications
- All results are stored in a back-end relational database for easy and flexible access
- Single mouse-click to view protein sequences and compare ID evidence

Fast, positive protein identification



A mixture of twelve enzymatically digested proteins, representative of a common complex proteomics sample, was analyzed on the Q TRAP™ LC/MS/MS System using IDA. High sensitivity data were acquired using the Enhanced MS (EMS) scan as the IDA survey scan. The most intense EMS peaks are automatically selected for an Enhanced Resolution scan to determine charge state and assign an accurate monoisotopic mass. Subsequently, each of the precursor ions

is subjected to a high sensitivity Enhanced Product Ion (EPI) scan, to acquire fragmentation data. Pro ID software automatically processes the complex IDA data to accurately determine peptide molecular weights using the calculated charge state. The Interrogator™ search algorithm then uses this information, along with the superior mass accuracy of the fragment ion data, for high-confidence identification of proteins from complex mixtures.

Want some straight answers?

If your research involves metabolism studies or proteomics, Applied Biosystems/MDS SCIEX Q TRAP™ LC/MS/MS System can make your efforts more productive by helping you identify more metabolites and proteins, faster and easier.

For more information, call the Applied Biosystems sales office nearest you, or go straight to <http://www.appliedbiosystems.com/qtrap>

Worldwide Sales Offices

Applied Biosystems vast distribution and service network, composed of highly trained support and applications personnel, reaches 150 countries on six continents. For international office locations, please call the division headquarters or refer to our Web site at www.appliedbiosystems.com

Applera Corporation is committed to providing the world's leading technology and information for life scientists. Applera Corporation consists of the Applied Biosystems and Celera Genomics businesses. Applied Biosystems/MDS SCIEX is a joint venture between Applera Corporation and MDS Inc.

Headquarters

850 Lincoln Centre Drive
Foster City, CA 94404 USA
Phone: 650.638.5800
Toll Free: 800.345.5224
Fax: 650.638.5884

For Research Use Only.
Not for use in diagnostic procedures.

Q TRAP system products are covered by U.S. patents 4,963,736; 5,847,386; and 6,177,668.

AB (Design), Applera, BioAnalyst, Interrogator, and Nanospray are trademarks, and Applied Biosystems and Analyst are registered trademarks of Applera Corporation or its subsidiaries in the US and certain other countries. Q TRAP is a trademark of Applied Biosystems/MDS SCIEX.

LINAC, MDS, and SCIEX are trademarks of MDS Inc.

© 2002 Applied Biosystems. All rights reserved.

Printed in the USA, 6/02, P+s
Publication 114BR11-01

drug discovery/proteomics