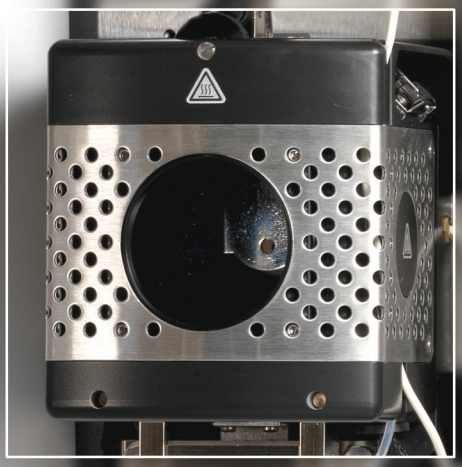
Agilent 500 Ion Trap LC/MS

LC/MS PERFORMANCE AND PRODUCTIVITY THROUGH INNOVATION

The Measure of Confidence

Agilent Technologies

LC/MS Performance and Productivity through Innovation



The Agilent 500 Ion Trap LC/MS is the instrument of choice for high-throughput LC/MS analysis where sensitivity, reliability, and productivity are essential.

The Agilent 500 Ion Trap LC/MS is a new and innovative system that provides a robust platform for demanding LC/MS/MS applications. The system sensitivity, mass resolution, and scan speed reflect the inherent advantages of the ion trap, while the new Enhanced Charge Capacity (ECC) extends the number of ions that can be stored. The results are greater sensitivity and reduced background noise for reliable quantitation.

By delivering excellent sensitivity over the entire mass range in full scan mode, and exceptional MS/MS and MS^n capabilities, the Agilent 500 Ion Trap LC/MS quickly provides superior qualitative information, for even the most complex sample matrices.

Unique sensitivity enhancements include SelecTemp, the temperature programmable API (Atmospheric Pressure Ionization), for the optimum analysis of thermally labile compounds. These innovations lead to the remarkable performance and capabilities of the Agilent 500 Ion Trap LC/MS.

The Agilent 500 Ion Trap LC/MS features a patented “tilted” capillary inlet and ion gating optics to ensure the lowest possible chemical noise while, delivering premium detection levels.

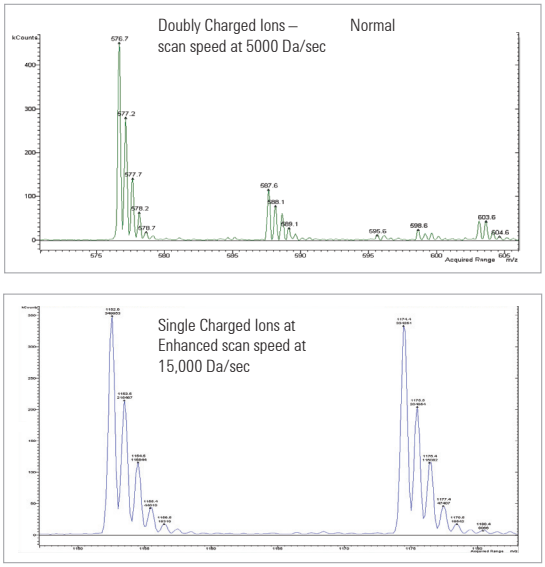
500 Ion Trap LC/MS
With SelecTemp and Enhanced Charge Capacity

State-of-the-art API interface

The Agilent 500 Ion Trap LC/MS delivers increased sensitivity and selectivity for all analytes. Even highly thermally labile compounds can be reliably analyzed, using Agilent's patented temperature programmable SelecTemp API interface. Maintaining sample integrity is no longer a concern.

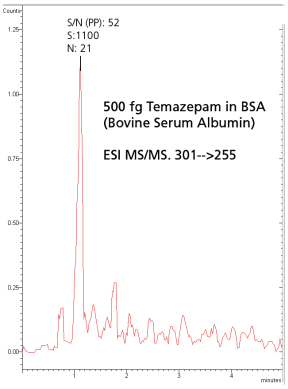
SelecTemp's programmable temperature control delivers optimum drying gas temperatures at every time point throughout a complex analysis. Additional SelecTemp API benefits include reduced interface contamination, improved throughput, simplified setup, and automatically recorded parameters for GLP purposes.

The rugged yet elegant design of the SelecTemp API and its unique capabilities will improve the performance of routine, high sample throughput applications reliably, consistently, and easily while increasing accuracy and productivity.



The Agilent 500 Ion Trap LC/MS delivers superior resolution at normal and enhanced scan speeds.

ECC, triple resonance, and the power of MS^n



ECC ensures the reliable detection of trace amounts in the presence of high concentrations of coeluting compounds and heavy matrices. Patented triple resonance scanning allows scan speeds up to 15,000 Da/sec and preserves chromatographic spectral resolution. The fast scan speed is complemented by rapid ion polarity switching of 200 ms to accommodate optimum detection of ion polarity for every analyte in the sample. Enhanced qualitative information is delivered by the 500 Ion Trap LC/MS with MS^n operation to n=10, expanding the spectral information content for structure elucidation.

Agilent 1220 Infinity LC

Simply more in tune with your lab's needs

Take a close look at the Agilent 1220 Infinity LC System and you'll find everything you need for first-class results and rewarding day-after-day productivity. Choose from three standard configurations to fit your LC workflow and rest assured that you have made an investment that is truely future-proof.

With a range of future options available, you can choose an upgrade path that meets your lab's requirements today and tomorrow. Move from isocratic to gradient solvent delivery, from manual injector to autosampler, or add a click-in column oven.

- Extend your detection capabilities with any 1200 Infinity Series detector such as diode array (DAD), evaporative light scattering (ELSD), fluorescence (FLD) or refractive index (RID)
- Upgrade your Agilent CDS software from a single workstation to a client/server installation for enhanced system control and data handling

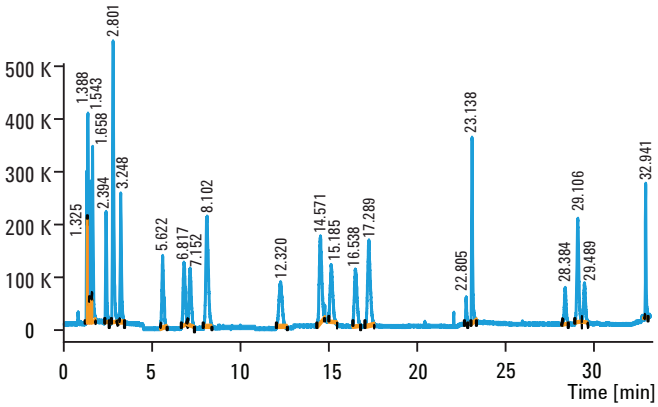
Solvent delivery

Based on the design used in the Agilent 1260 Infinity LC, the pumping module ensures stable, virtually pulse-free solvent flow up to 10 mL/min. Servo-controlled, dual floating pistons enable variable stroke volume optimized for the selected flow rate, and keeps maintenance to a minimum. The pressure range up to 600 bar lets you discover the power and advantages of columns with smaller particles for optimization of resolution and faster run times. Choose from different configurations, including either an isocratic pump or a gradient pump with up to two solvents and integrated two-channel degassing unit.

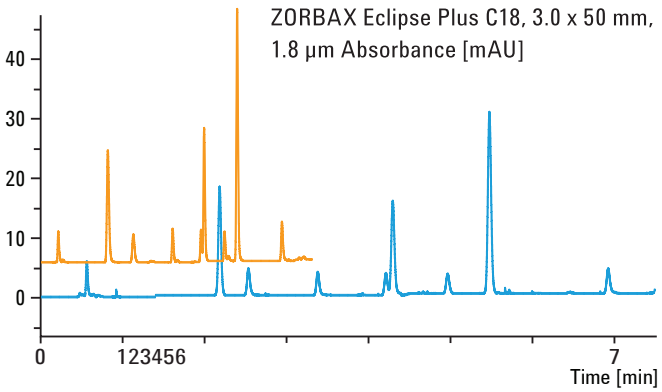
Pump options include:

- Automated solvent selection valve for gradient pump, combining two-out-of-four solvents for gradient formation or for column flushing with different solvents
- Continuous seal wash kit – based on the design of the Agilent 1260 Infinity pumps – to prevent corrosion for applications running buffer solutions with high salt concentrations (> 0.1 M)

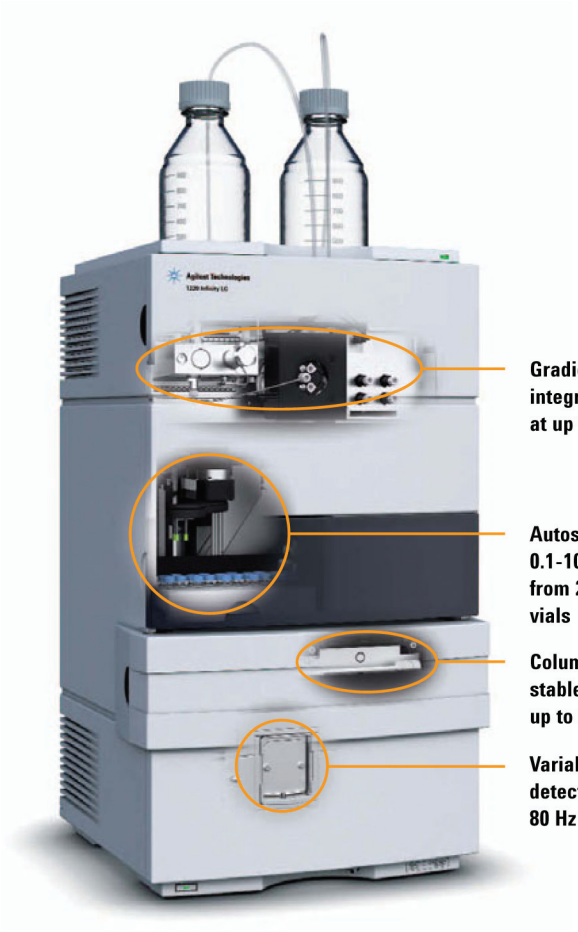
The gradient pump includes an integrated dual-channel degassing unit that creates continuous vacuum using the same Teflon AF technology used in the 1290 Infinity Binary Pump. With low internal volumes of 1.5 mL per channel, the degassing unit eliminates baseline fluctuations and shortens equilibration times.



LC/MS screening for EU-banned dyes in textiles. Total ion chromatogram (TIC) of a mixture of 22 aromatic amines operated in time programmed SIM mode.



Easy transfer of an HPLC method to RRLC by deploying a shorter column with sub-2-micron particles. Both shorter analysis times and improved resolution are the result.



Isocratic Configuration	Gradient Configurations	
Isocratic Pump	Gradient Pump	Gradient Pump
Manual Injector	Manual Injector	Autosampler
—	—	Column Oven
Variable Wavelength	Variable Wavelength	Variable Wavelength
Detector	Detector	Detector

Choose from three standard configurations to fit your LC workflow – then upgrade as required to meet your lab's future needs.

Manual injector

An easy to use, easy to maintain solution for low throughput sampling, the manual injector includes a long-life Rheodyne 2-position, 6-port sample injection valve and standard 20 µL loop. Front access to the valve facilitates easy sample injection and straightforward exchange of sample loops.

Autosampler

The integrated autosampler is designed for reliability, safety, and easy maintenance, and facilitates reliable injections from 0.1 to 100 µL. The unit delivers high precision as well as excellent linearity over a wide volume range. The autosampler's flow-through design ensures that there is no loss of sample; the entire sample drawn from the vial is injected. The standard configuration offers a sample capacity of 100 2-mL vials; alternatively, two half-trays each with 40 2-mL vials or 15 6-mL vials can be used.

Column oven

The optimized column oven houses a single column, and provides accurate, stable column temperature from 10 degrees above ambient to 60 °C, for applications where retention time reproducibility and separation quality improve above ambient temperatures.

Variable wavelength detector

Featuring simplified optics for high sensitivity, low baseline drift, wide linear range, and 80 Hz data rate, Agilent's variable wavelength detector not only lowers your detection limits and expands your capabilities – it lowers your cost of ownership with easy front access for fast lamp and flow cell replacement.

Agilent's MS Workstation Software

More power with Agilent MS Workstation software

Intuitive instrument control and data processing are simple yet powerful with the Agilent MS Workstation software

- Effortless detector optimization and control
- Superior data transfer rate with dual processors
- Simple navigation while reviewing and processing results
- Full featured network compatibility for file management, printing, and remote access
- Extensive reporting for complete analyses

Analyze, identify, and confirm with TurboDDS data dependent scanning

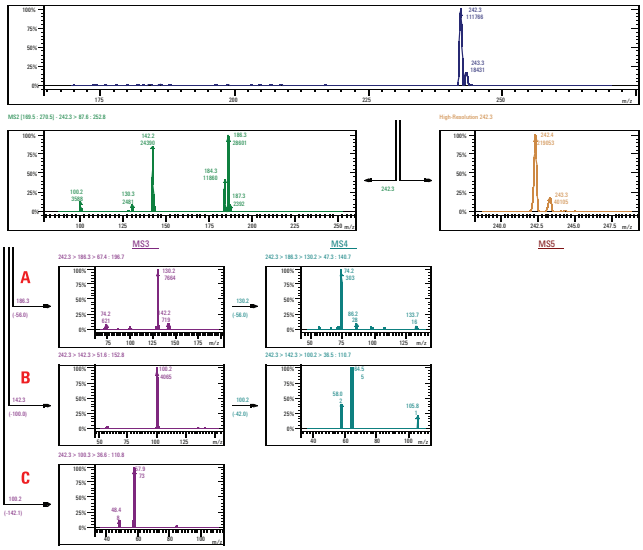
TurboDDS is an advanced scanning form of the 500 Ion Trap LC/MS. TurboDDS can be used to automatically gain qualitative information based on simple operator-specified criteria. The system performs MS/MS and MS^n experiments in a single analytical run.

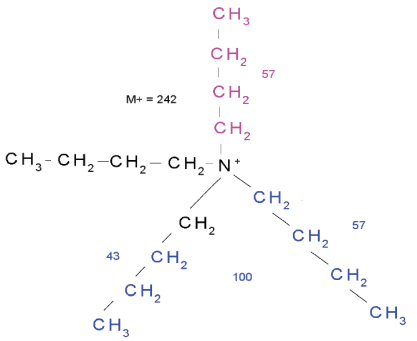
Key Benefits include:

- Data dependent scanning. Accelerate and simplify information capture from unknown samples.
- Extended mass range. Analyze large molecules up to 3500 *m/z*.
- High resolution scanning. Accurately determine charge state of multiply-charged ions — up to charge state 6.
- Rapid auto CID-scan. Optimize CID up to 5 times faster than existing instruments to provide more comprehensive identification of unknowns.
- Easy-to-use, data review software. Discover informative links between related data points. Generate user libraries effortlessly.
- Fast calculation. Mass Ruler software tool measures mass difference between peaks with two mouse clicks.
- Easy data export. Transfer results to third party databases (such as Mascot and Phenyx) to enhance information derived from the sample.

TurboDDS Data dependent scanning

A simple structural elucidation with TurboDDS





Tetrabutylammonium bromide salt, tetrabutyl-ammonium ion M^+=*m/z* 242. Each side chain is 57 Da.

Survey & High-resolution Scan

The survey scan is the starting point of the TurboDDS process. The tetra-n-butylammonium (TBA) ion was identified as the only target ion, *m/z* 242.3, to further analyze. The tree report shows the high resolution MS spectrum (in brown) of the analyte, confirming the single charge state for the target ion, *m/z* 242.3.

MS2 Spectrum

From the survey scan, the precursor ion, *m/z* 242.3, is identified for MS/MS (MS^2) analysis. The MS^2 spectrum (in green) includes several product ions; the most abundant is *m/z* 186.3. This is TBA minus one butyl side chain (-56.0). The ion intensity values (displayed below the peak *m/z* values on the spectra) indicate that "Path A" is the predominant breakdown pathway.

MSn Path "A"

From the MS/MS analysis the *m/z* 186.3 ion is isolated and the MS^3 analysis generates the product ion (*m/z* 130.2). This represents the loss of another butyl side chain group (-56.0). The *m/z* 130.2 ion is isolated and the MS^4 analysis produces a product ion (*m/z* 74.2), representing the loss of the third butyl side chain group (-56.0). An MS^5 analysis is not performed because the scan of the MS^4 product ions fails to meet the ion intensity threshold defined in the method.

MSn Path "B"

The second most abundant product ion in the MS/MS spectrum is *m/z* 142.2. This is TBA minus one butyl side chain and one propyl group (-100.0). The *m/z* 142.2 ion is isolated and the MS^3 analysis produces a product ion (*m/z* 100.2). This represents the loss of another propyl group (-42.0). The *m/z* 100.2 ion is isolated and the MS^4 analysis creates a product ion (*m/z* 58.0), representing the loss of yet another propyl group (-42.0). The intensity of the MS^3 product ions meets the threshold requirement and the MS^4 analysis proceeds. However, the generated product ions have extremely low ion intensities — with limited significance.

MSn Path "C"

The third most abundant product ion in the MS/MS spectrum is *m/z* 100.2. This is TBA minus one butyl side chain and two propyl groups (-142.0). The *m/z* 100.2 ion is isolated and the MS^3 analysis produces a product ion (*m/z* 57.9), representing the loss of yet another propyl group (-42.1). An MS^4 analysis is not performed because the intensity of the MS^3 product ions falls below the ion intensity threshold defined in the method.

NIST 08 and the MS Search Program

New Features in NIST 08 and the MS Search Program: Version 2.0 of the MS Search Program

The basic software of the NIST MS Search Program for Windows Version 2.0 is unchanged. A number of new features have been added.

- A new spectrum search for MS/MS spectra in MS/MS libraries, including the NIST MS/MS library.
- Five new Constraints have been added; Tags in Comment, Peptide Sequences, Peptide Mobile Protons, Peptide Charge, and Peptide Number of Residues. Tags in comment, for example, allows searching for the name of the contributor in the EI library.
- A search for information in the Contributor/Comment field which may be particularly useful for certain types of information relevant to MS/MS.
- Flexibility has been added to searches using a Name Fragment in Constraints. It is now possible to specify the presence or absence of any arbitrary part or parts of a name.
- The program does not use or require the installation of NIST fonts.

Column Options

Maximize system performance and reliability for all your separation needs by combining your 1200 Infinity Series LC system with Agilent ZORBAX and Poroshell LC columns and LC supplies. Designed with the same attention to detail, quality and superior performance you have come to expect from Agilent instruments and backed by over 40 years of chromatography experience, you can count on Agilent's columns and supplies to deliver the high quality results you need and expect, time after time.

Unparalleled quality and flexible choices within the ZORBAX LC column family

- Wide selection of chemistries – Eclipse Plus, Eclipse XDB, StableBond, Extend, Bonus-RP, HILIC and more
- Superior flexibility and product scalability with a wide range of particle sizes (1.8, 3.5, 5, 7 µm and superficially porous 2.7 µm) and column dimensions
- Individual column performance reports to document column-to-column and lot-to-lot reproducibility
- Superior particle strength for even the most demanding high pressure applications

Column technology to help you get the most from your 1260 Infinity LC

Agilent Poroshell 120 Columns have a solid 1.7 µm core and a 0.5 µm porous outer layer, so you get the resolving power of a 2.7 µm particle, at the speed of a sub-2-micron particle, with significantly lower backpressure. And, they are manufactured with a proprietary single-step porous shell process that has been designed by Agilent to improve reproducibility.

Poroshell 120 columns offer:

- Up to two times the number of theoretical plats compared to conventional 3.5 µm columns
- Improved resolving power, even as you take advantage of speed gains
- Improved ability to handle dirty samples, due to their standard 2 µm frit

Polaris and Pursuit

- Polaris columns provide unique bonded phases that maximize polar retention and selectivity, while virtually eliminating silanol activity. Polaris' ability to outperform the competition on challenging separations sets the standards for peak symmetry, selectivity, and reproducibility
- Pursuit diphenyl columns deliver faster separations without sacrificing resolution. Moving through the analytical development process and into production, Pursuit materials meet requirements for resolution critical analytical methods and high quality preparative chromatography

Infinitely better together with MS

The 1260 Infinity Binary LC sets higher standards in performance and value to give you more confidence in your results. The 600 bar power range combines with 80 Hz UV detector speeds and up to 10 times higher sensitivity. Its scalable delay volume makes it ideally suited for standard bore columns and as a front-end for MS detection. Further, it comes at the price of a typical binary system for conventional HPLC!

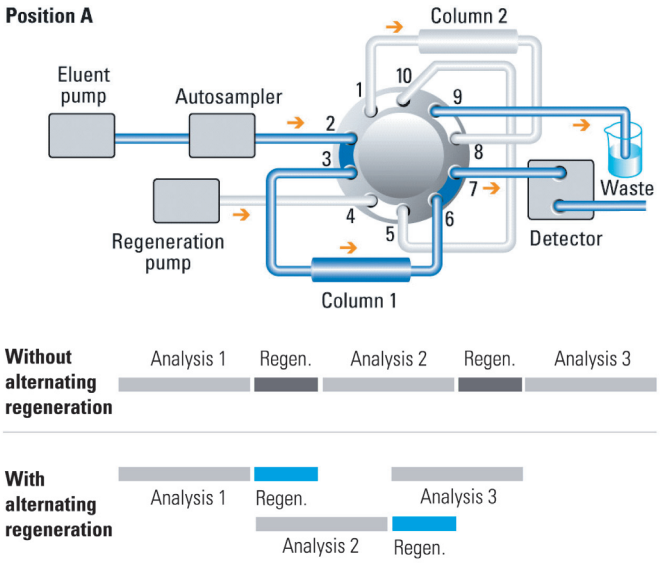
Higher throughputs

A special high throughput configuration of the 1260 Infinity Binary LC enables maximized productivity for laboratories with high sample loads. While one column is used for the analysis the second column is washed and regenerated by a regeneration pump. With this high throughput configuration, you can reduce cycle times by up to 50 percent.

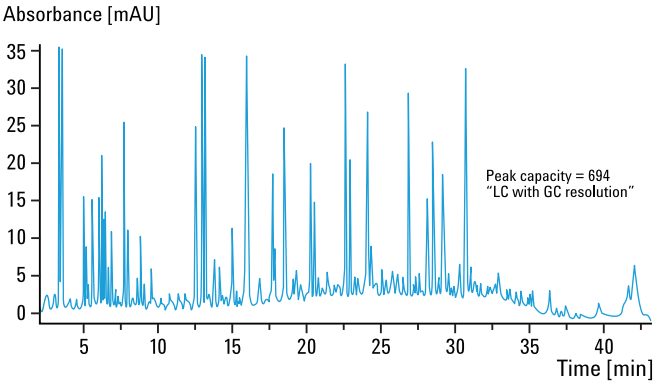
Use an 1290 Infinity LC Injector HTS or HTS for highest sample capacity and benefit from the full mix-and-match capabilities of the 1200 Infinity Series!

Full mix-and-match capabilities of the 1200 Infinity Series

A wide range of autosamplers are available for a variety of tasks, ranging from general HPLC needs up to dedicated solutions for high sample throughput. UV-visible detectors are offered with up to 10x higher UV sensitivity – from programmable single wavelength to high speed multi-wavelength and full spectral detection. A range of special detection techniques, including fluorescence, refractive index or evaporative light scattering, are also available for applications where non-UV absorbing chromophores are analyzed.



Higher throughputs can be achieved through alternating column regeneration (ACR).



Peak capacities of more than 700 can be achieved using a ZORBAX RRHT SB-C18 column (2.1 x 150 mm, 1.8 µm) to analyze a tryptic digest of BSA.

1200 Infinity system	Standard HPLC	Poroshell columns	Sub-2-µm columns	4.6 mm columns	3.0 mm columns	2.1 mm columns	Fast LC	High resolution	MS frontend	Semi-prep
1260 Infinity Binary LC										

Unequaled ownership advantages

The Agilent 500 Ion Trap LC/MS versatility and distinctive features allow easy adjustment to accommodate a wide variety of analytical requirements. The standard electrospray ionization source (ESI) of the 500 Ion Trap LC/MS can easily be replaced with an optional atmospheric pressure chemical ionization (APCI) source in less than a minute.

LC flow rates from microliters to milliliters can be used with our fully adjustable electrospray ion source and the vortex atmospheric pressure chemical ionization source. The novel design of the ion sources means the 500 Ion Trap LC/MS requires less cleaning, leading to returns in up-time and productivity. The built in syringe pump, diverter valve, and Electronic Gas Control (EGC) provide ease-of-use benefits enhancing productivity even more. Clearly, the performance-driven Agilent 500 Ion Trap LC/MS delivers increased selectivity, sensitivity, and accuracy while reducing contamination and downtime. The resounding capabilities of the Agilent 500 Ion Trap LC/MS ultimately translate into value through exceptional results, unparalleled economy, and cost of ownership advantages second to none.

Agilent 500
Ion Trap LC/MS

For more information on Agilent Technologies' 500 Ion Trap please visit our website at: www.agilent.com

U.S. and Canada
1-800-227-9770
agilent_inquiries@agilent.com

Europe
info_agilent@agilent.com

Asia Pacific
adinquiry_aplsca@agilent.com

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Agilent Technologies