Agilent 1100 Series LC/MSD

New standards for value and performance

Agilent Technologies

Innovating the HP Way

The advantages of mass spectral data—made easy and reliable

The Agilent 1100 Series LC/MSD offers you the sensitivity, selectivity, and depth of molecular information inherent in mass spectrometry—in a package that is rugged, reliable, and surprisingly easy to learn, operate, and maintain.

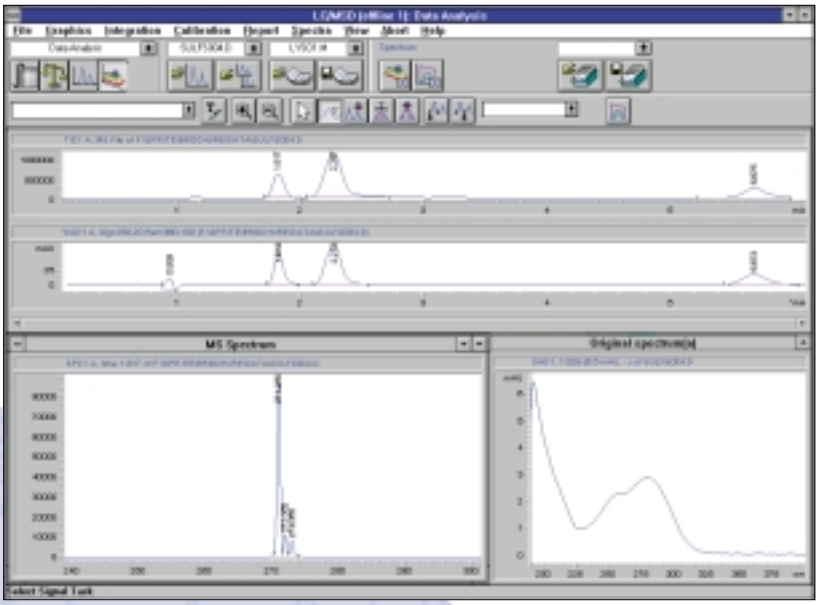
Analyze a wide variety of samples

Standard positive and negative ionization modes, and a choice of electrospray ionization (ESI) or atmospheric-pressure chemical ionization (APCI), allow you to analyze a wide variety of compounds such as:

- Drugs and drug metabolites
- Proteins and peptides
- Pesticides and herbicides

Increase confidence in results and shorten analysis times

The LC/MSD provides molecular weight and structural information that complements the spectral information from a diode-array UV-Visible detector. These orthogonal sets of data provide confident compound identification from a single chromatographic run—in one report.



These results from the analysis of a sulfa drug mixture show the complementary combination of mass chromatograms, UV chromatograms, and spectral information.

- You do not need to derivatize analytes lacking chromophores to obtain data
- Mass spectral data make it easy to detect and identify low-level impurities
- The ability to quantitate using unique masses means quantitative performance is less affected by matrix interference and unresolved chromatographic peaks
- Fully-resolved peaks are not required for mass spectral analysis; allowing you to shorten chromatographic runs and reduce sample preparation
- Reproducible in-source fragmentation can confirm sample identity

Use existing HPLC methods

With its patented orthogonal-spray ion source and high-capacity drying gas system, the LC/MSD provides excellent sensitivity and reproducibility over a wide range of LC operating conditions. This minimizes the need to alter established LC methods for LC/MS analyses.

Flow Rates

Up to 1.0 ml/min ESI
Up to 1.5 ml/min APCI

Solvent Composition

100% aqueous to 100% organic

Save time with fast, easy system setup

Automated tuning and a built-in calibrant delivery system make system setup fast and easy, while ensuring the highest sensitivity and reproducibility.

- Calibrant delivery is automatic, without replumbing
- Pre-made calibrants save time and avoid mistakes
- Easy-to-use software allows you to manually tune the instrument when desired

Autotune and automated calibrant delivery shorten system setup time and ensure the highest sensitivity and day-to-day reproducibility.

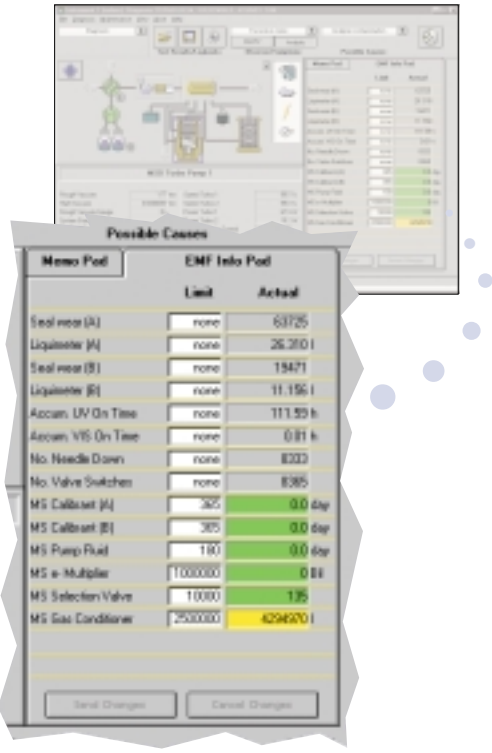
Automated switching improves performance

The LC/MSD's automated switching valve simplifies plumbing and provides a single LC connection. This reduces leakage, minimizes extra-column band broadening, and allows you to divert the void volume as part of a method.

An optional, integrated manual injection valve gives you a way to quickly introduce samples that do not require separation.

Switch from ESI to APCI in just a few minutes

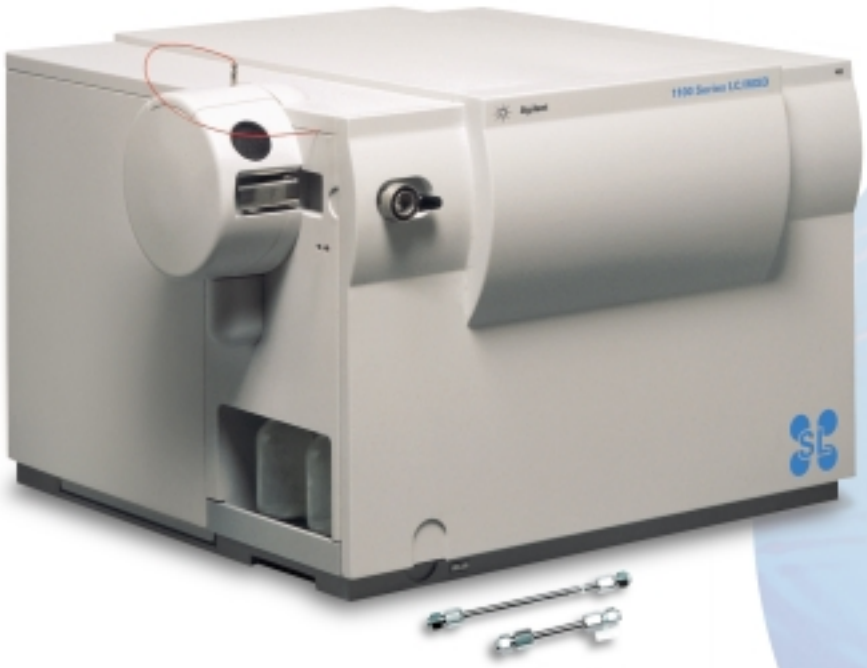
A hinged, swing-out spray chamber speeds switching between modes and makes cleaning easier.



Improve uptime with easy maintenance

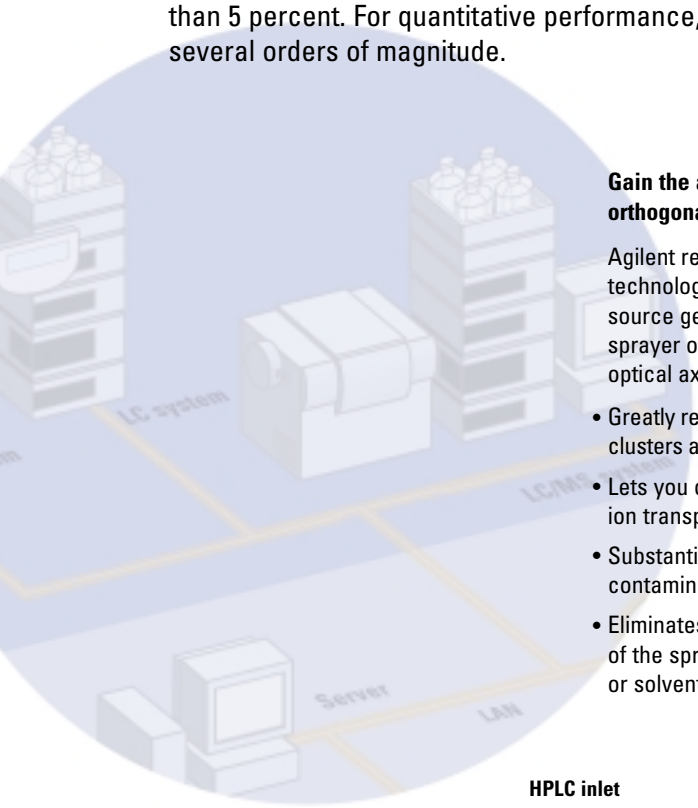
The LC/MSD is designed to minimize maintenance requirements and make what maintenance is required fast and easy.

- Orthogonal spray orientation keeps the capillary and ion optics cleaner
- Large sampling orifice prevents capillary plugging
- Slide-out, self-aligning components such as the sprayer make maintenance easier
- Diagnostic software can log the hours of system use and prompt you when key components are due for servicing



Achieve the highest sensitivity and reproducibility

Analyses at low picogram levels are common thanks to Agilent's patented orthogonal-spray ion source design and high-capacity drying gas system. Data are exceptionally reproducible, with RSDs of less than 5 percent. For quantitative performance, response is linear over several orders of magnitude.



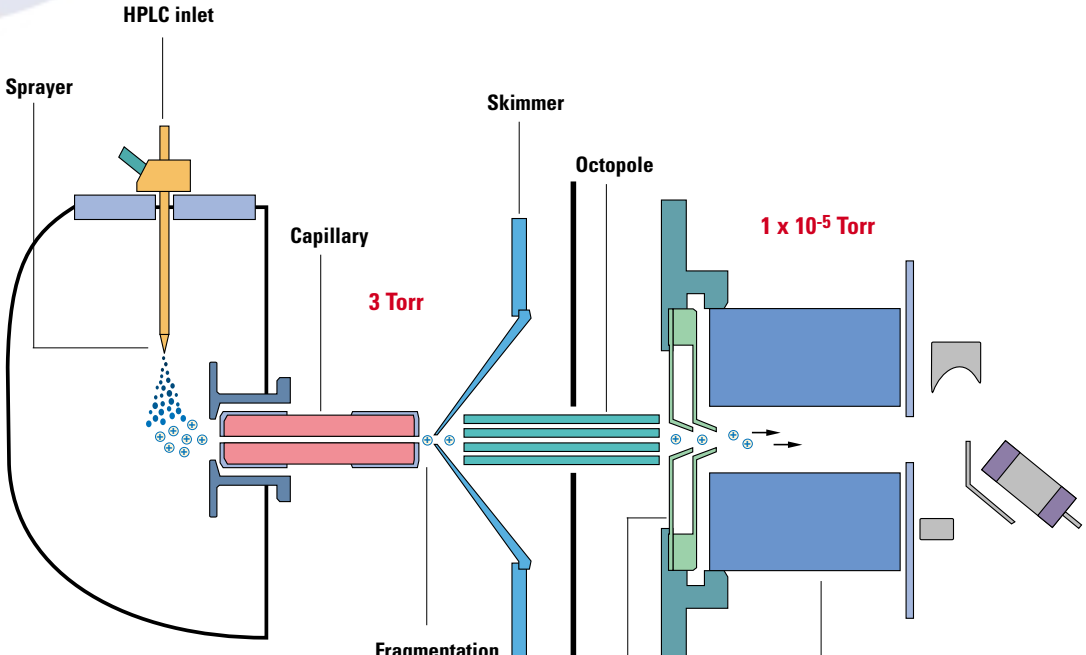
Gain the advantages of orthogonal spray...

Agilent revolutionized electrospray technology, replacing traditional in-line source geometry with a fixed-position sprayer orthogonal to the mass analyzer's optical axis. This approach:

- Greatly reduces background from solvent clusters and mobile-phase adducts
- Lets you optimize both desolvation and ion transport for improved sensitivity
- Substantially reduces ion source contamination and the need for cleaning
- Eliminates the need to adjust the position of the sprayer—even when the flow rate or solvent composition changes

Orthogonal-spray ion source is very tolerant of non-volatile components in samples or mobile phase. This ion source was still generating useful data.

Swing-out spray chamber makes maintenance easier.

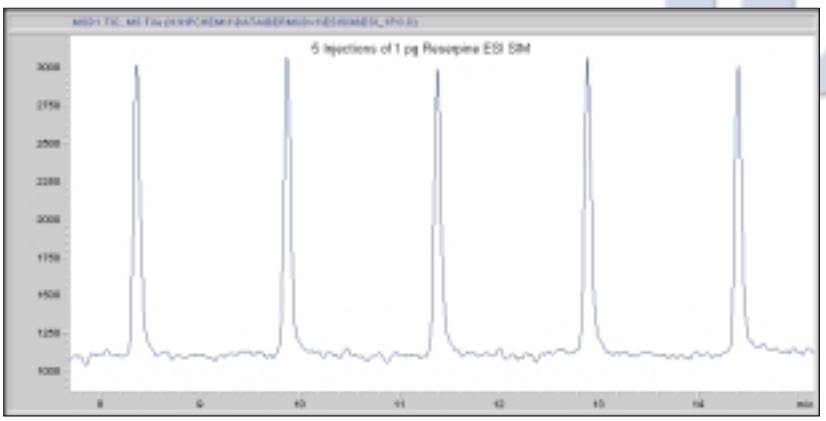


Orthogonal spray orientation and high-capacity drying gas system improve instrument performance and decrease maintenance requirements.

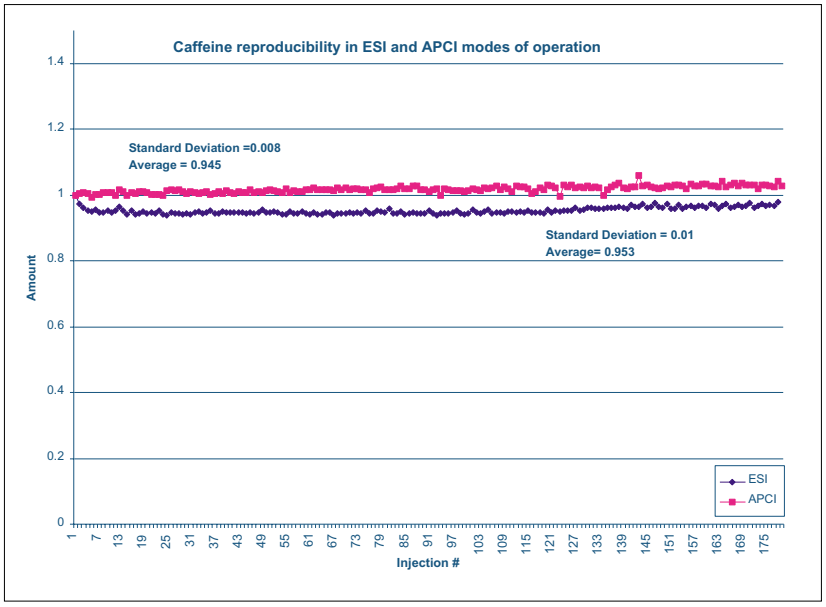
...excellent sensitivity...

The LC/MSD delivers excellent sensitivity in all operating modes. And the extra specificity provided by mass spectral data makes that sensitivity more useful.

- When scanning a range of masses, LC/MSD sensitivity is comparable to the sensitivity of a good diode array UV detector
- Sensitivity is enhanced 5 to 100 times when the LC/MSD is set to monitor only selected masses characteristic of the compounds being analyzed (selected ion monitoring mode)
- With its improved ion optics, sensitivity of the LC/MSD SL model is 10 times greater than the sensitivity of previous LC/MSDs



Five replicate injections of 1 picogram of reserpine on column in ESI mode (SL model).

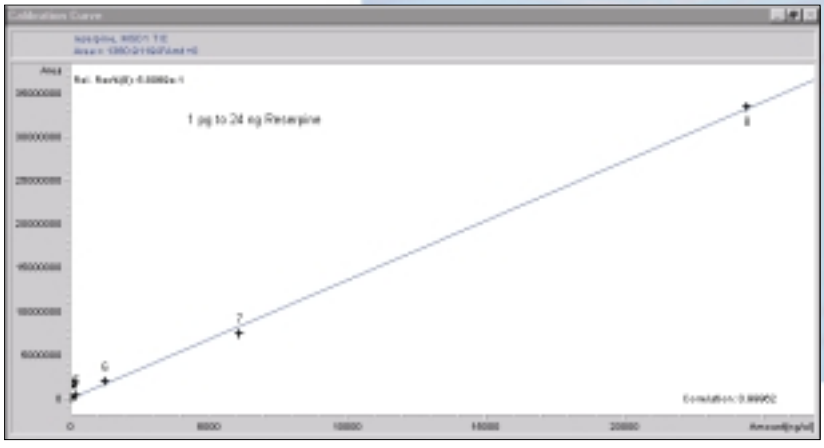


Reproducible data increase confidence in methods and results.

...and enhanced stability and reproducibility

Good reproducibility yields better qualitative and quantitative results. The LC/MSD exhibits exceptional stability and reproducibility, giving you more confidence in the validity of your methods and data.

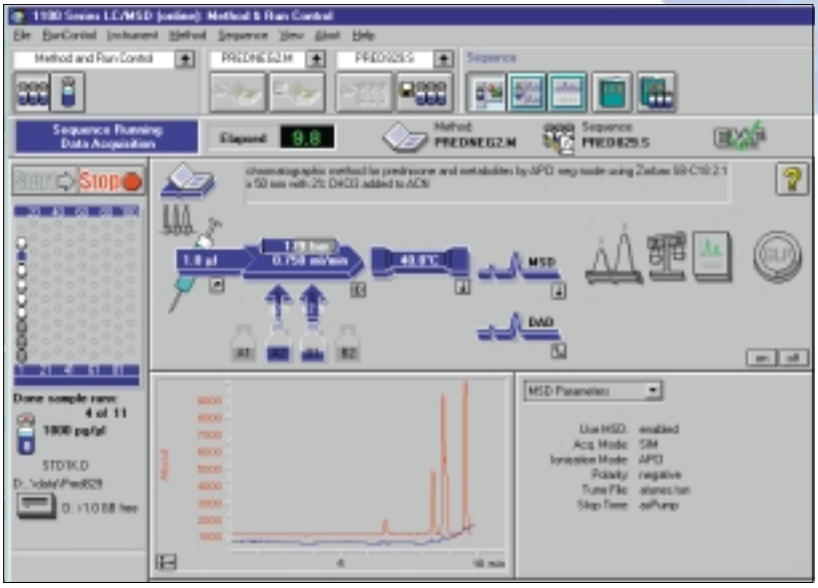
The VL model can provide linear quantitation results over three orders of magnitude. The SL model is even better: it can provide linear quantitation results over four orders of magnitude.



Added sensitivity extends linear range to improve quantitation results.

Acquire more data quickly and easily

The LC/MSD ChemStation software is fully integrated with our LC 3D ChemStation software. Thanks to an easy-to-use graphical user interface and powerful automation features, both new and experienced users can quickly take advantage of the LC/MSD's capabilities.



The software is fully integrated with the Agilent LC 3D ChemStation software.

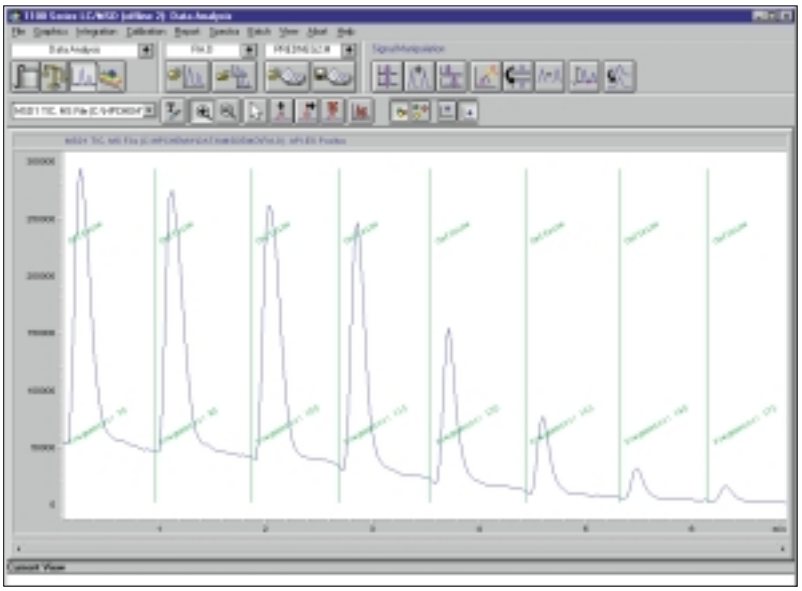
Simplify operation

The Microsoft® Windows® -based user interface makes the software easy to learn and operate.

- System control and data acquisition parameters require only two windows
- Some parameters are calculated automatically. For example, if you provide the chromatographic peak width, the system automatically optimizes the data acquisition rate
- Other parameters are preset or reliable defaults are provided
- Online help includes tutorials to lead you through tasks. Digital videos show you how to perform common maintenance tasks

Speed analyses

Automated flow-injection analysis (FIA) allows you to quickly analyze samples that do not require separation. When you are developing methods, FIA can help you find the best settings for MS parameters. Setup is easy using the FIA series table.

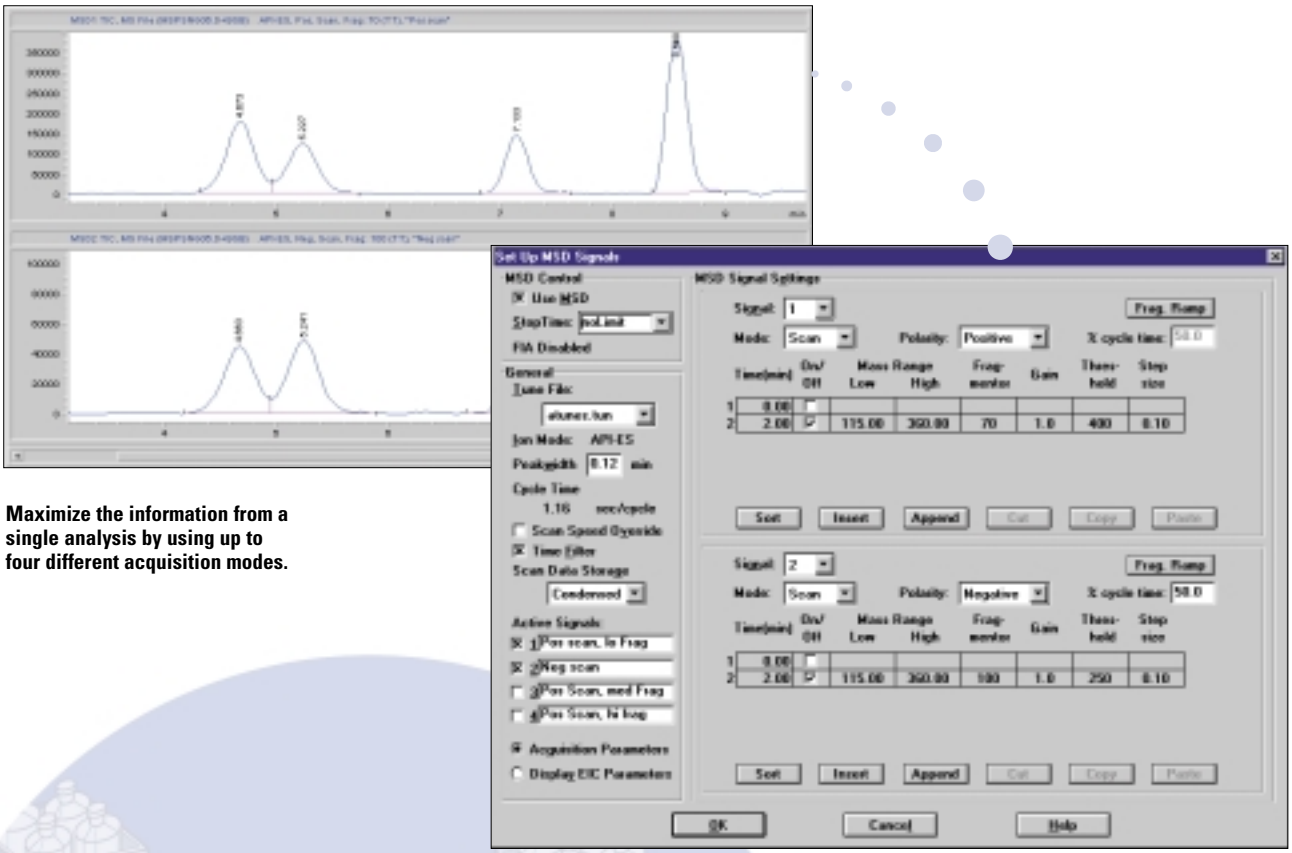


In this example, the FIA series table was used to make repeated flow injections of a caffeine standard while the fragmentor voltage was varied.

Maximize the information from each analysis

The multisignal analysis found in the LC/MSD SL model gives you the power to acquire up to four separate signals, each using a different acquisition mode, from a single sample injection. Choose positive or negative ionization, selected ion monitoring (SIM) or scanning, and fragmentor voltage.

- Acquiring positive and negative ions helps you determine which mode produces the best response for a particular compound. And seeing both $[M+H]^+$ and $[M-H]^-$ ions can confirm molecular weight
- Combining SIM and scan data means that, from the same run, you get the utmost sensitivity for quantitation of low-level target compounds and complete spectra for other high-level compounds and unknowns
- Acquiring data with low and high fragmentor voltages can provide you with molecular ion information to confirm mass and fragmentation information to determine structure
- And multisignal data acquired together can be linked for easier processing



Maximize the information from a single analysis by using up to four different acquisition modes.

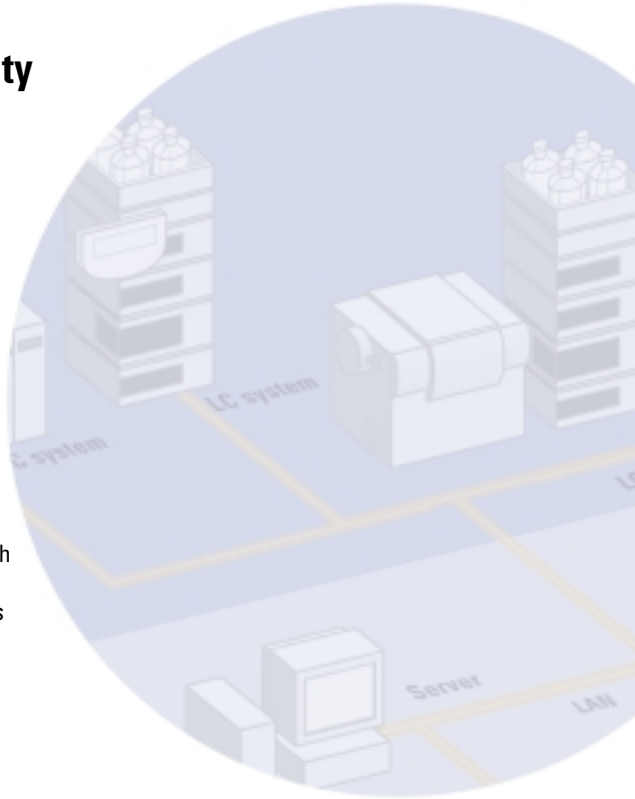
Combine the power of LAN and the Intranet

The Agilent ChemStation software is compatible with the latest in networking technologies.

- Instruments can be controlled, and their operating status checked, from any PC—even if it is not in the laboratory
- Complete web-page-ready reports can be sent directly to your desktop

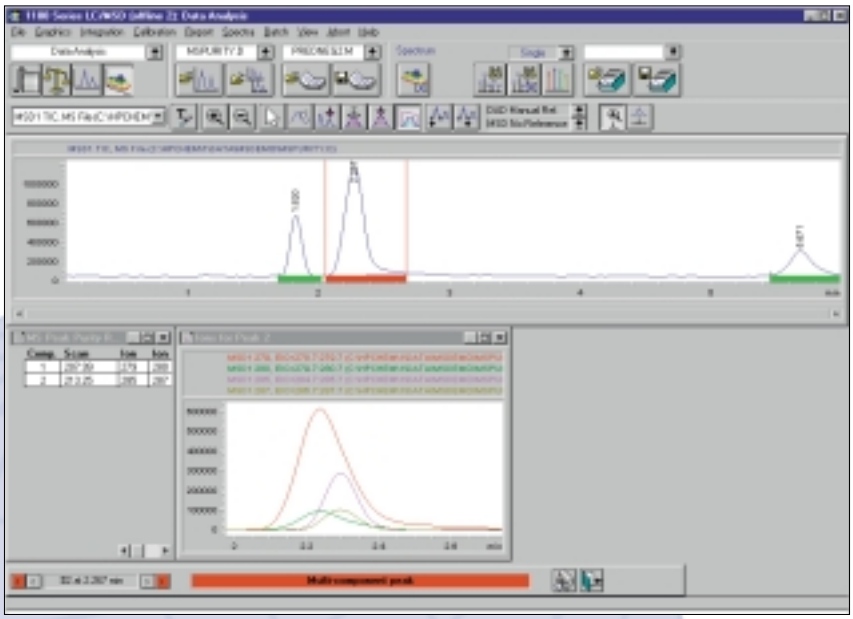
Speed up data processing for greater productivity

Powerful, easy-to-use software speeds processing of qualitative and quantitative data. UV and mass-spectral data can be processed together using the same software tools. Data processing can be automated and included as part of a method.



Speed peak identification

Automatic alignment of UV and mass-spectral data allows rapid visualization and peak-to-peak data comparisons. Each peak in the MS and UV chromatograms is integrated and labeled with a retention time. In mass spectra, major ions are automatically labeled with mass information.



Peak purity software with a multi-component peak in red. The software draws the extracted ion chromatograms below to identify components.

Identify coeluting compounds quickly

Peak purity software uses UV data or mass-spectral data or both to identify chromatographic peaks with incompletely-resolved compounds. This is useful for developing separation methods or for choosing quantitation ions without further refinement of the separation.

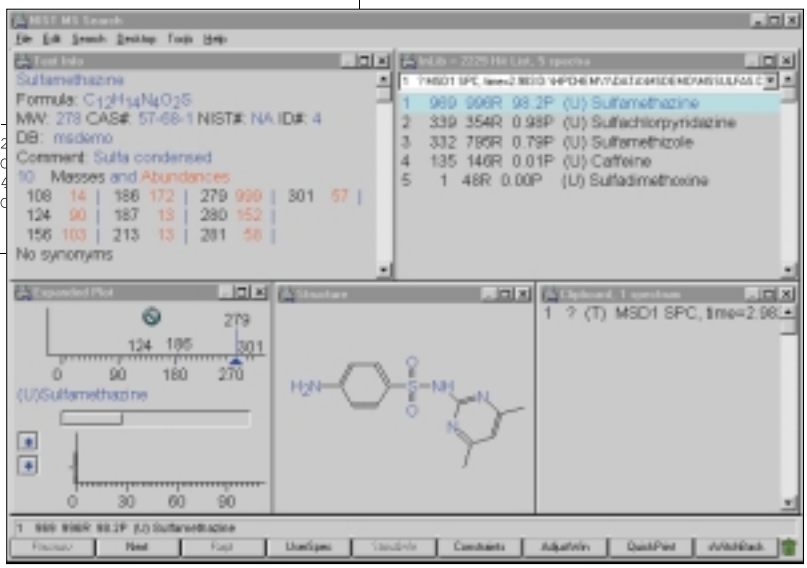
- Toggle buttons make it possible to quickly move from one impure peak to the next across a chromatogram
- The peak purity report displays the retention time, number of possible peak components, and characteristic ions for each peak in a chromatogram

Visualize complex data rapidly

Isoabundance plots of mass-spectral data allow rapid visualization of complex data. This feature is useful for detecting patterns of specific functional groups.

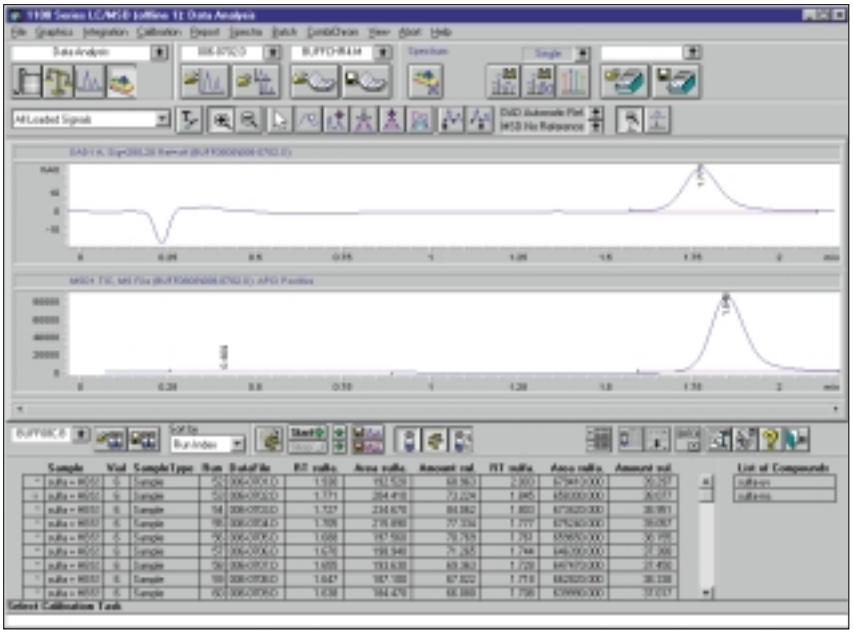
```
Meas.   Library CalTbl
RetTime RetTime RetTime Sig   Area      Purity Library  Name
 [min]   [min]   [min]          %      Factor # Match
-------|-------|-------|---|----------|------|-|------|--------------------
  2.584   2.589     -     1  1.32737e-3   -     1 1000   Sulfamethizole
  2.819   2.815     -     1  1.49818e-3   -     1 1000   Sulfamethazine
  3.410   3.415     -     1  1.11062e-3   -     1 1000   Sulfachlorpyridazine
  5.971   5.975     -     1  1.40215e-3   -     1 1000   Sulfadimethoxine
=====================================================================
NIST MS library search mode:    Automatic library search

NIST MS library file No.  : 1
NIST MS library file name : msdemo

RetTime Sig  MW    Library Match Formula
 [min]          #   Id
-------|---|----|-|-------|-----|---------
  2.746  2   270 1  3       967  C9H10N4O2
  2.987  2   278 1  4       915  C12H14N4O
  3.571  2   284 1  5       938  C10H9ClN4
  6.143  2   310 1  6       978  C12H14N4O
```

Quickly identify compounds with optional library search software.



Identify compounds fast

Optional NIST mass-spectral library searching quickly identifies compounds by matching MS spectra with user-created library spectra. You can combine UV and mass-spectral searching and reporting. The software is optimized for both ESI and APCI data.



Batch review software helps you evaluate and, if necessary, reprocess the results for large batches of samples.

Speed quantitation through automation

Instrument control, data analysis, and reporting can be automated and included as part of your method.

- You can quantitate using both UV and MS signals in a single calibration table
- Quantitation methods can include peak area or peak height, external standards (ESTD), internal standards (ISTD), peak ratios, and multi-point calibration curves
- Batch review software provides rapid, interactive user evaluation of results for large batches of samples. You can quickly review a set of calibration compounds, controls, and samples; and, only if necessary, manually reintegrate peaks and recalculate the calibration curves and sample results
- Automated report options are available. Or the drag-and-drop report builder provides an easy way to customize reports

Increase uptime with validation tools, diagnostics, and support

The Agilent 1100 Series LC/MSD includes an array of integrated validation tools to help you meet the most demanding regulatory requirements. High reliability, easy-to-use diagnostics, and support services increase instrument uptime.

ChemStation Security Pack software supports 21 CFR Part 11 compliance

OQ/PV software helps assess ongoing system performance quickly.

System-wide validation

Because the LC/MSD is a member of the Agilent 1100 Series family of LC and MS modules and systems, you get a complete system approach to installation qualification (IQ) and operational qualification/performance verification (OQ/PV).

- The Declaration of System Validation qualifies the Agilent LC/MSD design according to documented procedures
- IQ and OQ/PV software and services qualify system installation and operation. The ChemStation software includes online standard operating procedures (SOPs) for performing OQ/PV, maintenance, and repairs
- The Declaration of Conformity for performance verifies that the LC/MSD met specifications prior to its shipment from Agilent
- Software, test files, and methods help the system manager assess the functionality of the system
- For data integrity and traceability, the software saves instrument conditions, together with raw data, in checksum-protected binary files
- Two password-protected levels of system access ensure operators have only the access they need

Maximize uptime

Built-in diagnostics and remote access maximize uptime and make maintenance easier.

- Early maintenance feedback (EMF) software tracks operating time and alerts you when components are due for maintenance
- Built-in diagnostic software makes system troubleshooting easy
- If maintenance is required, multimedia tools, including digital videos, show you how to do it
- Remote access enables remote operation and troubleshooting

Enjoy a range of support services

Agilent offers a broad range of support services designed to improve instrument uptime and to help you comply with regulatory requirements.

- Industry-specific service bundles are designed to meet the needs of pharmaceutical, hydrocarbon processing, chemical, and environmental laboratories
- ISO-registered training courses are available at selected locations world wide. On-site courses can be tailored to meet special needs

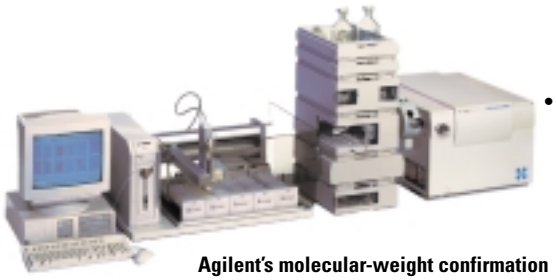
Complete analytical solutions

Agilent offers complete analytical solutions with fully-integrated hardware and software. All components are supplied and supported by Agilent.

Combinatorial libraries solution

This molecular-weight confirmation solution is for the rapid molecular-weight confirmation of combinatorial libraries—from sample analysis to reporting. Using this system, you can rapidly identify the products of combinatorial syntheses and estimate their purities. The products can then be purified as necessary before screening.

Mass-based fraction collection lets you monitor specific masses and their adducts to trigger fraction collection, thereby collecting the compounds of interest.



Agilent's molecular-weight confirmation system for combinatorial libraries.

Protein and peptide analysis solutions

Optional software tools make the analysis of proteins and peptides easier.

- Protein and peptide analysis software eliminates the tedious manual calculations required to match the masses of peptide digest fragments to those predicted by digest conditions
- Deconvolution software automatically deconvolutes mass-spectral data from multiply-charged ions and assigns molecular weights to the mass peaks
- Protein database search software searches protein databases against mass-spectral information generated by peptide maps

Capillary electrophoresis with tandem UV and MS detection

The LC/MSD can be directly coupled to the Agilent 3D CE system to assist with the analysis of complex mixtures. An optional capillary sprayer optimizes performance for CE/MS analyses.

Agilent's capillary electrophoresis (CE) system with tandem UV and MS detection.

MS/MS and MS^n solutions

The Agilent 1100 Series LC/MSD Trap system provides the multiple stages of MS data required to solve challenging research questions faster and with more confidence.

Multiple stages of MS deliver the information needed to unambiguously characterize compounds and elucidate structures.

MS/MS provides greater specificity and sensitivity and therefore faster, more accurate quantitation—even when chromatographic peaks are not completely resolved or sample matrices are complex.

Agilent's 1100 Series LC/MSD Trap system for MS/MS and MS^n analyses.

High-performance design features

- Orthogonal-flow sprayer with pneumatic nebulizer – enhances sensitivity over a wide range of LC conditions and reduces maintenance requirements
- High-capacity solvent drying system with user control of gas flow rate and gas temperature – reduces chemical noise and permits the analysis of thermally-sensitive compounds
- Dielectric platinum-plated capillary – permits independent optimization of spray chamber and ion optics
- User-adjustable in-source fragmentation
- Air-cooled vacuum system with dual turbomolecular pumps – eliminates the need for cooling water
- Fraction collection capability – can monitor and trigger the collection of fractions based on mass, an analog signal input, or time. For mass-based determination, up to 16 *m/z* values can be monitored. Requires optional I/O Accessory Module.

Specifications

Mass range
VL – *m/z* 50 - 1500
SL – *m/z* 50 - 3000

Mass accuracy
± 0.13 u within the calibrated mass range in scan mode

Mass axis stability
± 0.13 u over 8 hours

SIM sensitivity

- **API-electrospray** at 400 µl/min or **APCI** at 1000 µl/min
- Selected ion monitoring of *m/z* 609.3
- Positive ionization

	Quantity	Signal-to-Noise Ratio
VL	10 pg reserpine	50:1 RMS (10:1 peak-to-peak)
SL	1 pg reserpine	50:1 RMS (10:1 peak-to-peak)

Scan sensitivity

- **API-electrospray** at 400 µl/min or **APCI** at 1000 µl/min
- Scan range *m/z* 100 - 650
- Extracted ion at *m/z* 609.3
- Positive ionization

	Quantity	Signal-to-Noise Ratio
SL	50 pg reserpine	50:1 RMS (10:1 peak-to-peak)

Multiple signal acquisition (SL model only)
Ability to cycle through four different acquisition modes on a scan-by-scan basis within a single run.

For more information

For more information about the Agilent 1100 Series LC/MSD, call toll free: 1-800-227-9770 (in the U.S.) or 1-800-341-2477 (in Canada).

In other countries, please call your local Agilent Technologies analytical sales office or authorized Agilent Technologies distributor.

You can also visit our site on the World Wide Web at:

http://www.agilent.com/chem

The Agilent 1100 Series LC/MSD has been designed and manufactured under a quality system that has been registered to ISO 9001.

Certificate no. FS25109

Printed in the USA 3/00
5968-9804E

Agilent Technologies
Innovating the HP Way