



Agilent MSD Productivity ChemStation for GC and GC/MSD Systems Rev. D.03.00

Specification

July 2006

General Description

The Agilent Mass Selective Detector (MSD) Productivity ChemStation controls data acquisition, performs data review, library searches, and quantitation, and generates selected reports via methods or sequences. It offers a number of productivity tools for data processing, as well as two levels of access control to the system.

The MSD ChemStation software is designed to run on IBM-compatible personal computers with the Microsoft® Windows® operating environments.

The MSD ChemStation software is supplied on CD-ROM and contains extensive online help with both task and reference information about system operation. The example methods and data files supplied with the software can be used to practice and learn the MSD ChemStation software.

The software user interface, online help, and manuals are supplied in English, Japanese, and Chinese languages.

The user operation manuals are also available in French, German, Italian, Spanish, and Russian.

The MSD ChemStation software can be configured to support a maximum of four instruments, (maximum of two MSDs). The following Agilent instruments are supported:

- 5973 Series MSDs (GPIB and LAN)
- 5975 Series MSDs (LAN only)
- 6890 Series GCs (GPIB and LAN)
- 6850 GC
- 7683 automatic liquid samplers (ALS)
- G1888A, G1289B, and G1290B headspace samplers (with G2923AA add-on headspace software)
- G650x-CTC CTC Autosamplers (with G3384AA CTC Control for MSD ChemStation)

The software controls 5973N, 5973 inert, and 5975 Series MSDs with 6890 or 6850 Series GCs using standard local area network (LAN) communications, while GPIB communication is used for 5973A MSDs with 6890 Series GCs.

It is possible to simultaneously acquire GC data and GC/MS data. It is also possible to acquire and review mixed mode (GC and GC/MS) data.



Agilent Technologies

What's New in D.03.00

Hardware

- Support for the new 5975B Series MSDs
- Support for the CTC autosamplers with the G3384AA CTC Control for MSD Chemstation (available for Enhanced, DrugQuant, and EnviroQuant modes of operation only)

Operating Systems

- Support for Windows 2000 Professional SP4 and Windows XP Professional SP2 in English versions
- Support for Windows XP Professional SP2 in Japanese and Chinese versions

SemiQuant

- SemiQuant allows you to estimate a compound's concentration based on the response for a similar compound, such as a homolog or congener.
- Entire methods are easily converted by using *Global SemiQuant* while *Specific SemiQuant* allows you to add SemiQuant compounds to any method.
- SemiQuant reports are available to handle the SemiQuant compounds separately from target compounds for easy identification within the report.
- For more details, download the SemiQuant Technical Note 5989-4997EN from the Agilent Web site.

Instrument Control Enhancements

- High performance SIM/scan functionality is available for the 5975B Series MSDs. The MSDs now have 1-millisecond SIM dwell time capability for SIM and SIM/scan modes of operation.
- Integrated control for the G650x-CTC PAL autosamplers (with G3384AA add-on CTC control software)

Data Analysis Enhancements

- Easy Extracted Ion Chromatograms (Easy EICs) allows the user to add multiple EICs to the chromatogram window with only a few clicks of the mouse.
- AutoSIM Setup converts a full scan method to a high sensitivity SIM or SIM/Scan acquisition methods automatically.
- Quantitation mass assignments can be quickly updated with the new Update Calibration dialog.
- The snapshot feature can now display data being acquired during a SIM, Scan, or SIM/Scan run.
- The new Reprocessing menu allows easy analysis of previously run sequences.

Enhanced Data Analysis Tools

- This collection of enhancements designed for the Enhanced and Aromatics data analysis modes offer a deeper, more detailed view of your data.
- The Analyze Multiple Data Files view is designed for qualitative investigation of groups of data files.
- The ability to export numerous reports in HTML, XLS, and XML formats enables a new level of reporting flexibility. Exporting to an XLS file requires Microsoft Excel.
- The data file viewer/manager allows viewing, keyword searching, and moving of multiple data files via a unique interface.
- PBM library search results are viewable graphically as chromatogram annotations.
- Linking of multiple data files' total chromatograms is available.
- Correlation Chromatograms allow an efficient comparison of a total ion chromatogram with any mass spectrum.
- Smoothing of chromatograms is enabled via the Savitsky-Golay smoothing algorithm or the splining feature.
- The new Performance Report gives the user a powerful and comprehensive chromatography evaluation tool.
- A new Peak Purity chromatogram annotation is available to quickly detect multicomponent peaks.

Specifications - At a Glance

Supported Operating Systems

The MSD ChemStation software is supported with the following operating software:

- Windows 2000 Professional SP4 and Windows XP Professional SP2 in English versions
- Windows XP Professional SP2 in Japanese and Chinese versions

The ChemStation software is **not** supported on Windows 2000 Professional Server software, Windows XP Professional Server software, or Windows NT®.

Supported Instruments

Current compatible hardware products include the following:

- 5973 Series MSDs (GPIO and LAN)
- 5975 Series MSDs
- 6850 GC
- 6890 Series GCs (GPIO and LAN)
- 7683 autosamplers
- G1512A and G2612A ALS controllers
- G1888A, G1289B, G1290B headspace samplers (with G2923AA add-on headspace software)
- G3163A and G3164A real-time gas analyzers
- G650x-CTC CTC PAL autosamplers (with G3384AA add-on CTC control software)

Minimum PC Requirements

The minimum requirements for operation of the MSD ChemStation software are:

- Pentium® III computer, 1.0 GHz or faster
- SVGA color monitor
- 128 MB of RAM
- 20 GB of hard disk storage
- CD-ROM drive
- Sound card and speakers or headphones for viewing avi files
- Windows-supported mouse

Recommended PC Requirements

For optimum system performance, the following PC capacity is recommended:

- Pentium 4 computer, 2.8 GHz (or faster)
- 512 MB (or greater) of RAM
- 80 GB of hard disk storage (or greater)

MSD Communication Card

The interface from the ChemStation PC to the analytical instruments is through a LAN card or a GPIO internal card depending on the configuration:

Supported Printers

- HP LaserJet 2200d or 2300dn, Post Script, revision 5.02
- HP LaserJet 4050 or 4100, PCL 5e or 6, revision 5.02
- HP LaserJet 4020, PCL 6
- Not all DeskJet printers are supported

Supported Spectral Libraries

- G1033A NIST MS Library Bundle
- G1036A NIST Chemical Structures
- G1035B Wiley Registry 7th Edition with NIST MS Spectra

- G1038A Stan Pesticide Library
- G1039C Pflieger Drug Library
- G1671AA Hazardous Chemical RTL Library
- G1672AA Pesticide and Endocrine Disruptor Library

File Compatibility

- Virtually every file format used by the software supports long file names. Any programmatic access of ChemStation files may require updating.
- Data and sequence files created on previous versions of the MSD ChemStation are compatible.
- Macros, methods, and Quant databases prepared on earlier versions of the MSD ChemStation software (prior to G1034C, revision C.03.04) must be modified.
- Report templates created with Excel-based Custom Reports software are not compatible. The .CRT files from the Custom Reports software may be saved as .XLS files and used in Excel.

Validation Tools

- Certificate of Validation, IQ/OQ services are available using built-in software functionality.

Computer Hardware and Printers

Computer Hardware

The MSD ChemStation consists of Hewlett-Packard/Compaq personal computer hardware and MSD ChemStation software. The hardware is an IBM-compatible personal computer with a PCI interface bus.

The personal computer is interfaced to the analytical instruments through a LAN card or a GPIB internal card. All cards plug directly into the computer's PCI interface bus.

Note: *The MSD ChemStation software was tested on Agilent Technologies ChemStation (PC) hardware that conforms to the above specifications. Although the software is also designed to run on other IBM-compatible PCs, Agilent is not responsible for defects reported on third-party hardware.*

Computer Hardware Considerations

The minimum PC configuration required to use the G1701DA MSD ChemStation software is shown below. Multiple instrument control, multiple sessions of data analysis, extensive custom reporting, and additional application software products will require additional RAM and hard disk resources.

Minimum PC Configuration

- A Pentium III computer (1.0 GHz or faster recommended)
- An SVGA color monitor
- 1024 × 800 × 65,536 colors video display resolution (maximum supported resolution is 1600 × 1200 × 16,000,000 colors)
- 128 MB (or more) of RAM
- 256 MB of RAM for quad GC acquisition
- At least 20 GB of hard disk storage (MSD ChemStation program files use approximately 115 MB)
- A CD-ROM drive
- A sound card and speakers or headphones
- A Windows 2000- or XP-supported mouse
- A data backup device is strongly recommended
- BIOS, which supports Windows 2000 with Service Pack 3 (or later) or Windows XP with Service Pack 1a (or later)
- All power-saving features of the BIOS disabled
- All power-saving programs removed
- MSD communication card. Depending upon required communications, either
 - a Network Interface Card for LAN-based systems, or
 - an HP 82350B Control Card for GPIB-based systems

Printers

The ChemStation software can print to any Microsoft Windows compatible printer directly connected to the computer through a parallel interface or connected through a LAN.

The ChemStation is designed to use the Windows default local printer. The typical system is sold with an HP LaserJet printer, which is intended to be the local printer on the parallel port of the ChemStation computer.

- HP LaserJet 2200d or 2300dn printers are fully tested and supported. Supported drivers are Post Script, revision 5.02.
- HP LaserJet 4050 or 4100 printers, although not tested with this release, are supported due to testing on older revisions. Supported drivers include PCL 5e or 6, revision 5.02.
- HP LaserJet 4020 printers are fully tested and are supported. The supported drivers are PCL 6.
- HP DeskJet printers are not tested or supported.

Service engineers are not trained to configure and support network printers. Network printers work very well if the correct printer drivers are installed; however, analytical instrumentation may produce long graphical reports which can overburden a shared network printer. In most cases, local printers are recommended.

System Configuration

The configuration of the GC or GC/MSD system is done through the system configuration program. It allows users to define their instruments, GPIB addresses or LAN IP addresses, and the analysis mode to use.

The MSD Productivity ChemStation can be configured in four Data Analysis modes. In all modes, the ChemStation lets you evaluate standards, set up calibrations, quantify samples, search industry standard and custom spectral databases, produce reports, and reprocess batches of samples.

Enhanced Quantitation Mode

This mode combines ease of use and simplicity with powerful processing tools that help to increase your productivity. This is the default mode of operation and is used for routine or complex samples. This is the only mode in which mixed mode quantitation (MS detector and GC detector) is supported.

EnviroQuant Mode

This mode is specifically designed to meet the needs of laboratories performing analyses compliant with USEPA methodology.

Drug Analysis Mode

This mode is specifically designed to meet the needs of laboratories performing analyses for drugs of abuse, sports doping, and forensic applications. The Drug Analysis mode includes predefined methods for analyzing amphetamines, cocaine, opiates, PCP, and THC.

Aromatics in Gasoline Mode

This mode is very similar to the Enhanced mode except that it contains modifications that make it compliant with ASTM protocols. Specifically, the sequencing editor (sample log table) permits the weight and density of the sample (gasoline) to be entered on a per sample basis as well as the precise (gravimetric) weight of the internal standard (ISTD). Once this data is entered, the quantitation report will calculate the total concentration of aromatics in gasoline. This mode should be used only when it is necessary to comply with ASTM-D5769-95.

Offline Operation

In the system configuration program it is also possible to configure a system to operate the software in an offline mode. In this mode, the system is not actually connected to the GC/MS system and cannot acquire data or access some of the features that require online operation. This mode is useful, however, for learning the software, data review, or method development.

Software User Interface

The MSD Productivity ChemStation user interface is designed into Views that group software functionality according to typical analytical tasks. Each view consists of a set of standard user elements including menus and toolbars. The toolbars provide rapid access to the common system tasks such as loading a method or sequence.

Instrument Control View

Instrument Control is where most of your work will originate. You can edit a method, set up and start a single run, and perform an autotune of the MSD. You can also fine-tune and monitor discrete parts of the GC and/or MSD control and display various status monitors.

In addition, the laboratory manager can set up two levels of security to control access to the ChemStation through Secured Control.

Note: *The Secured Control feature is not a solution for laboratories needing to comply with 21 CFR Part 11 regulations. Customers that need to comply with 21 CFR Part 11 regulations should purchase the G1732AA MSD Security ChemStation.*

Data Analysis View

Data Analysis is an offline "view" that runs independently of the other views. This view is used for interactive data review.

The menus and productivity tools available to you in Data Analysis

will vary depending on which analysis mode you selected during system configuration.

The View menu in Enhanced Data Analysis mode lets you access the following productivity tools:

- **EasyID** – Lets you update expected RTs and ion ratios for MS data in an existing quantitation database on a compound-by-compound basis.
- **QEdit** – Lets you review and edit quantitation results once a data file is quantitated.
- **Edit Non-Target Peaks** – Lets you edit the results of the Non Target Peak search by visually comparing the mass spectra from the data with the mass spectra of possible matches in the library.
- **Parametric Retrieval** – Lets you access the Parametric Retrieval view which helps you locate compounds in a mass spectral library.
- **Align GC** – Accesses the Alignment view where you can align chromatographic peaks from a mixed mode data file.
- **Review Peak Purity** – Helps you detect overlapping peaks (multiple-component peaks) in your chromatogram.
- **Results Screener** – The Results Screener is used to evaluate the expected RT/ions (MS only) for the locked compounds in any data file that was acquired under locked conditions.

- **Analyze Multiple Data Files** – The Multiple Data File view is designed for qualitative investigation of groups of data files.

- **Analyze Multiple Spectra** – The Multiple Spectra view allows qualitative investigation of groups of spectra.

- **RTL Lock Setup** – Accesses the RTL Lock Setup view which is used for retention time locking (RTL) tasks.

Tune and Vacuum Control View

This view provides tools for tuning and maintaining your MSD. The user can select from several autotuning options (including tuning for DFTPP or BFB specifications), use the tune wizard for target tuning, or access the software's manual tuning capabilities.

Tuning is a process for optimizing the performance of the MSD. The goal of tuning is to maximize sensitivity while maintaining acceptable resolution, ensuring accurate mass assignment, and providing the desired relative abundances across the mass spectrum. As electron impact mass spectrometry provides a fingerprint for a compound, the relative abundances of a mass spectrum will affect the quality of a library search.

Methods and Sequences

The MSD Productivity ChemStation analytical method fully describes how a particular analysis is performed. It contains all the parameters for instrument control, data acquisition, and data analysis, including integration, quantitation and reporting.

A sequence allows you to automate the analysis of one or more samples using one or more methods. When an ALS is installed, the entire analysis, from injection of the sample through reporting of results, can be automated. A barcode reader can be used for further automation.

Example methods and sequences are supplied with the ChemStation software. The example methods can be edited and used as a starting point for a particular application (such as drug analysis). It is also possible to create RTL methods.

eMethod

eMethods is short for electronic methods – a quick and easy way to obtain packaged application solutions from Agilent or to share your own personal applications. It's a process that can greatly improve your laboratory's productivity. eMethod enables you to:

- *Electronically export existing methodologies to new instrumentation* – Agilent's eMethod process allows you to package any 5973 Series MSD method and export it to an Agilent 5975 Series MSD, thus enabling you to bring a new GC/MS instrument online in the shortest possible time.
- *Maximize instrument productivity* – Whether you have multiple GC/MS systems in the same laboratory or across the world, the Agilent eMethod process makes sharing and standardizing methodologies across your organization as easy as e-mailing an attachment. Analytical separation can be easily duplicated on multiple systems thus maximizing the productivity of each GC/MS.
- *Electronically import new Agilent application solutions* – No more manual entering of method parameters. Agilent's integrated eMethod process allows you to download any new Agilent eMethod application solution from the Agilent Web site and import that method to your Agilent 5975 Series MSD or 5973 Series MSD and receive the entire method without any manual editing errors.

For a complete list of available Agilent eMethods, please visit the eMethod home page on the Agilent Web site.

Acquisition and Instrument Control

The Instrument Control view has an easy-to-use graphical user interface. Each instrument control option is represented by buttons on the icon bar of the Instrument Control screen. These buttons let you control, set, and monitor parameters for the:

- 6850, 6890A, 6890 Plus, and 6890N GCs
- 5973 and 5975 Series MSDs
- 7683 Family Autosampler
- G2612A ALS controllers
- G1888A, G1289B, and G1290B headspace samplers
- G650X-CTC CTC Autosamplers

Acquisition

The ChemStation allows the control of and data acquisition from multiple GC and MSD detectors. Up to four detectors can be controlled by one MSD ChemStation (a maximum of two MS detectors).

Data may be acquired in scan, selected ion monitoring (SIM), or synchronous SIM/Scan modes.

Synchronous SIM/Scan

Synchronous SIM/Scan is an acquisition mode that enables collection of both SIM (Selected Ion Monitoring) data and full scan data in a single run.

In many laboratories, full scan is the most common form of data collection due to the ease of set-up and the availability of spectral libraries for compound confirmation. SIM mode, on the other hand, offers significant improvement in sensitivity over full-scan. The Agilent SIM/Scan mode combines the best of both SIM and full scan from a single sample injection to improve productivity.

Agilent MSD ChemStation's AutoSIM feature allows you to create a SIM or SIM/Scan method automatically from ANY existing full scan method. Once you create the SIM or SIM/Scan method you can run synchronous SIM/Scan.

The Agilent Synchronous SIM/Scan offers the following benefits:

- Confirmatory information - full-scan data for library search capability
- Maximum sensitivity - SIM data enables trace analysis
- Automated setup conversion - The AutoSIM feature automatically processes full-scan data of chemical standards into SIM or SIM/Scan acquisition parameters for use in the SIM/Scan method

Combined Signals

Combined GC and MS signals can be acquired from a single sample. Signals from GC and MS detectors can be aligned, calibrated, quantified, and the results reported in a combined report.

Select and Display Monitors

The Instrument Control panel lets you select which system monitors you want to display. These monitors include GC and MSD [total ion chromatogram (TIC), extracted ion chromatogram (EIC), spectra] detector signals, system temperatures, and flow and pressure set points.

Easy Tuning

Tuning the MSD is easy; you can select from several existing Autotune algorithms (including tuning for DFTPP or BFB specifications) or tune manually. All tune results can be viewed, printed, and saved for review and later evaluation.

Early Maintenance Feedback

The EMF (early maintenance feedback) utilities in the Instrument Control view are used to select or reset various limits and counters. These values are used to alert you when a limit is reached and a maintenance task needs to be performed, such as changing the GC septum. These utilities are only available in an online configuration.

Data Analysis - Integration

The MSD ChemStation includes two integration algorithms: the RTE integrator and the ChemStation integrator.

Integration is controlled by integration parameters which can be reviewed and edited. These parameters can be saved in an integration parameter (.P) file which can be used to integrate the target or qualifier ions for a particular compound or as the default integration for an entire method.

ChemStation Integrator

The ChemStation integrator can satisfactorily integrate all types of chromatograms, including those with difficult baselines and negative peaks. You can control the integration process by setting integration parameters, usually referred to as "integration events".

The ChemStation integrator allows you to AutoIntegrate using initial integration events. If the results are not suitable, you can make changes to the integration parameters and then reintegrate manually or automatically.

RTE Integrator

The RTE integrator is a fast peak detector and integrator for GC/MS data. It is well suited for target compound analyses. The default parameters assume that the data to be integrated is a total ion current (TIC) of scanned data from capillary column chromatography over the entire chromatographic range. If the appropriate integration parameters are selected, the RTE integrator can handle SIM acquisition and integration objectives such as detecting ISTDs within a small RT window.

Data Analysis - Quantification

Quantification is based on external standard or internal standard calculations calculated on either peak area or height. Calibrations may be multilevel and include multiple internal standards. Calibration histories are automatically saved and can be used to weight the recalibration calculations based on running averages.

Calibration curves are constructed for each compound by using the calibration levels to define the curve. The algorithm used to generate the calibration curve may be selected as:

- Linear – a linear regression fit of the data points
- Linear, force – a linear regression fit forcing origin
- Quadratic – a quadratic fit of the data points
- Quadratic, force – a quadratic fit forcing origin
- Average response/amount

In addition, for linear and quadratic curves, point weighting can be applied as equal, inverse of concentration, or inverse square of concentration.

Compound identification may be refined by defining individual RT window parameter limits and qualifier peaks.

Qualifier peaks are usually the same compound detected on a different signal with a predictable response ratio. They are used as a further check on peak identification rather than just relying on RTs.

The MSD ChemStation allows 20 individual levels of calibration for each target compound your analytical method requires. While actual and practical limits are different, the quantitation database can handle compound lists in excess of 2,000 entries.

Data Analysis - Quantitative Analysis

Two stages are involved in quantitative analysis:

- Calibration, in which you set up a quantitation database from the analysis of calibration standards. This analysis is used to generate a calibration curve for every compound you plan to quantitate.
- Quantitation, in which you run unknown samples and generate reports on how much of a particular compound is present in a sample.

The ChemStation software produces a quantitative report in two stages: first the quantitation calculation and then the report generation.

Quantitation Database

A quantitation database is a collection of information and data needed to perform quantitative analysis. For each compound, the database includes the calibration table and the information required to extract and integrate the ion chromatograms. Calibration curves from the calibration tables are used to quantitate target compounds.

Quantitation Calculations

Two sets of parameters are used to maximize the effectiveness of the quantitation calculations: peak integration parameters and peak identification parameters.

The steps the software performs during quantitation are shown in *Quantitation Flow*.

At each stage of the calculations, the two steps the quantitation process uses to determine the presence or absence of a compound are **Integrate** and **Analyze**.

The quantitation procedure creates a **<methodname>.res** results file in the data file directory. Report generation software reads the results file and formats a report.

AutoQuant Setup

Setting up a GC/MS calibration table often requires knowledge of the sample and software. For new users, or occasional or routine operators who are not familiar with the software, setting up the MS calibration may be difficult and time-consuming.

The AutoQuant Setup feature allows the user to quickly establish a GC/MS calibration with minimal knowledge of either the sample or the software.

When AutoQuant Setup is selected, it steps through each integrated compound in the total ion chromatogram, searches the selected MS spectral database compound name, and provides the first four hits as possible names. The user selects the compound name of interest or enters a user-defined name, and the software automatically selects the target ion and three qualifier ions. Additional compounds and calibration edits are also easily performed.

Quantitation Flow

Process external standards

1. Retrieve information about first compound from the quantitation database. If not an ISTD, process as an external standard.
2. Extract the quantitation (target) and qualifier ions signals over the expected RT range.
3. **Integrate** the extracted ion chromatograms.
4. **Analyze** the integrated peaks.
5. Repeat steps 1-4 until an ISTD is encountered.

Process ISTD and target compounds

6. Retrieve information about first ISTD from the quantitation database.
7. Extract the quantitation (target) and qualifier ion signals over the corrected expected RT range. If the compound is an ISTD, then the correction factor is 1 (value not corrected).
8. **Integrate** extracted ion chromatograms.
9. **Analyze** the integrated peaks.
10. Calculate RT correction factor if the compound is a time-reference ISTD.
11. Repeat steps 7-9 for each target compound until the next ISTD is retrieved.
12. Repeat steps 7-11 until the end of the quantitation database is reached.
13. Generate quantitation report.

Data Analysis - Reporting

Each of the Data Analysis mode configurations use common report types (for example, area percent or quantitation reports) as well as report types that are specific to that particular application. These report types are described in the online help for each application mode.

Enhanced Mode Reports

The following reports are available from the Enhanced Data Analysis:

- Area Percent Report
- Library Search Report
- Quantitation Report
- Classic Quantitation Report
- Non-Target Peaks Report
- Integration Results Report
- Calibration Report
- Compound List Report
- Quant Database Report
- Area Percent Report with Chromatogram
- Performance Report
- Multiple Library Search Report
- Quant Report with Compound Groups

EnviroQuant Reports

The following reports are available from the EnviroQuant Data Analysis:

- Integration Results Report
- Area Percent Report
- Tune Evaluation Report
- Compound List Report
- Calibration Status Report
- Response Factor Report
- Continuing Calibration Report

- Evaluate Continuing Calibration Report
- Quantitation Report
- Library Search Compound Report
- LibSearch Report
- Locate All Compounds Report
- Matrix Spike/Duplicate Recovery Report
- Chromatographic Resolution Report

Drug Analysis Reports

The following reports are available from the Drug Analysis mode:

- Area Percent report by RT
- Area Percent report by signal
- Batch Log File
- Batch Summary Report
- Express Report
- DOD Express Report
- Mass Spectrum Tabulation
- PBM (Library Search) Report
- Prebatch verification report
- Post-batch verification report
- QC Summary Report
- Scan Drug Report
- SIM Drug Report
- Sequence Log File

Custom Reports

The ChemStation software includes the ability to let you create custom report formats. The Custom Reports software lets you transfer quantitative results from Data Analysis into the Custom Reports spreadsheet program where you can create your own custom report templates. You can also set up databases of

quantitative results from multiple samples, then view and print charts of the data.

The Custom Reports software uses a Report Wizard which lets the user select the content they want to use for their custom reports. The user can define which elements to include in the header: general information about the data file (such as date acquired and method name), single-compound information and calibration information. Next you can select the compound-specific information (such as compound name or number) for all compounds in the quantitation database.

Once the report content is selected, the software formats the report automatically into the spreadsheet program. You can then further customize the report using the formatting features available from the menus and toolbar. Up to 240 graphic elements can be added to the report template. Any formatting changes you make are saved with the report template.

Once a report template or database is created and linked to a method, you can print the report or update the database automatically whenever the method is run.

Data Analysis - Spectral Data Evaluation

Data Processing Tools

The Data Analysis software is a complete mass spectral data processing application. Mass spectra can be viewed, tabulated, added, subtracted, and printed with just a click of the mouse. Mass spectra from the GC/MS systems of other manufacturers can be imported in tabular or AIA formats and processed.

Export 3-D Data

Data acquired with the MSD ChemStation can be exported (into the CSV file format) to third party applications using the Export 3-D Data feature.

Mass Spectral Libraries

Commercial mass spectral libraries can be searched using the probability-based matching algorithm (PBM) included with the software.

You can also create your own custom library. These can be created and edited using mass spectra acquired on other instruments or from other library sources.

Up to three libraries may be selected for sequential searching of unknown spectra. Default search criteria provide quality search results for most applications. However, in those cases where default values are not applicable, the MSD ChemStation software allows the operator to define the parameters used in the search.

The mass spectral PBM search result list returns the "hits" with the highest quality as defined by the search criteria.

About PBM

The PBM algorithm uses a reverse search to verify that peaks in the reference spectrum are present in the unknown spectrum. Extra peaks in the unknown are ignored, thus allowing the analysis of a spectrum resulting from a mixture of compounds.

Since not all mass-to-charge (m/z) values of a mass spectrum are equally likely to occur, the PBM algorithm uses both the mass and abundance values to identify the most significant peaks in the reference spectrum. When a spectrum is added to a library, these peaks are used to generate a condensed reference spectrum that is used by the PBM search routine.

A prefilter within the search routine then assigns a significance to each of the peaks in the unknown spectrum and uses these to find the most probable matches in the condensed reference library. The selected condensed spectra are then compared, using the reverse search described above, with the complete unknown spectrum. The prefilter immediately eliminates approximately 95% of the compounds in the database and greatly speeds up the search (when using the default strategy parameters).

Chemical Structures

Chemical structures provide additional information that helps in detailed evaluation of the mass spectrum. The MSD ChemStation software supports chemical structure libraries in the .MOL format. Chemical structures with valid CAS numbers are automatically recalled and displayed with each searched spectrum.

Parametric Retrieval

The Parametric Retrieval feature in Data Analysis allows you to locate compounds in a spectral library based on specific criteria. The retrieval produces a list of compounds in the library that satisfy the specified criteria. You may then view the spectra of these compounds and compare them with the spectra from your samples.

Peak Purity

The peak purity tool helps you detect overlapping peaks (multiple-component peaks) in your chromatogram. Overlapping peaks can interfere with library searches or quantitation.

Good chromatography is essential for the peak purity tool to function correctly. If chromatography is poor, the peak purity tool may identify single-component peaks as having multiple components.

Secured Access Control

The Secured Control feature allows the laboratory manager to set up two modes of security for operation of the MSD ChemStation. Both modes use an accounts system that requires an operator to be logged in before using the instrument. The first mode is the normal ChemStation environment, which gives the operator complete access to method development, instrument tuning and data processing. The

second mode restricts the operator to running samples with a predefined set of methods using an autosampler. The first mode is typically used to ensure that only trained and qualified individuals access the ChemStation. The second mode is used to permit untrained individuals to submit samples for analysis, but not to have access to the full capability of the ChemStation.

Note: *The Secured Control feature is not a solution for laboratories needing to comply with 21 CFR Part 11 regulations.*

Customers that need to comply with 21 CFR Part 11 regulations should purchase the G1732AA MSD Security ChemStation.

Customization

You can greatly extend the power and convenience of your MSD ChemStation software by using and writing macro programs. Macro programming gives you the power to automate and customize ChemStation operation. Since all methods, sequences, and most menu items are actually implemented as calls to macros, you can customize ChemStation operation by writing new custom macros or by editing and using modified versions of existing macros.

A macro, or macro program, is a series of instructions written in the ChemStation macro language. A macro is given a name and stored in a text file, which may contain more than one macro.

The purpose of most instructions in a macro is to execute MSD ChemStation commands or functions. Information about the use and effects of these

commands and functions is available in the online help which can be accessed from any ChemStation application window.

Macros that are part of the original MSD ChemStation software are called system macros. The command processor (CP) responsible for each major MSD ChemStation application (Top, Instrument Control, and Data Analysis) loads a set of system macros when the application starts up. All methods and many menu choices are implemented as system macros.

Macros that MSD ChemStation users create to automate or customize some aspect of ChemStation operation are called user macros.

The command lines of the ChemStation application windows give the user a way to submit commands to the CP for

execution. A macro is basically just a series of ChemStation commands that are stored in a file. They can also be executed from the command line.

Macros are useful for automating tasks you frequently perform on the MSD ChemStation that otherwise require you to make many mouse actions, menu choices, panel entries, or command line entries. They can also be used to customize operation of the MSD ChemStation, such as to print a report in a special format.

Automation

Methods

With the MSD Productivity ChemStation, you can edit or create methods that completely automate tuning the MSD, sample introduction, signal acquisition, data processing, searching mass spectral databases, and creating/printing custom reports.

Sequences

The ChemStation uses sequences to run batches of samples automatically, using one or more methods. The sequence information is entered into the Sample Log Table where there must be a line for each injection to be made.

A sequence is saved on disk and is automatically designated by .S at the end of the file name. Once a sequence is created and saved, it may be recalled again as a starting point for running another batch of samples.

The sequence may be defined to use automatically generated or user-defined file names. The user may select to run full analyses or data reprocessing only sequences.

The Sample Log Table, or list of analyses to run, is built in a spreadsheet-like user interface that allows users to specify vial numbers and sample names, analysis methods, and sample quantification parameters.

While entering information, the user can jump between individual cells in the table and copy, cut, or paste individual cells or entire rows or series of rows in order to build sequences efficiently and quickly.

Once started, the sequence will proceed with the analysis of all the samples until completed or paused for priority samples. If paused, changes can be made to the sample list and the sequence restarted.

Importing LIMS Sample Work Lists

Sample work lists can be imported directly from a LIMS into the MSD ChemStation software. When selected, the user may select a sample work list file in the .CSV or .TAB format. The user may include additional information such as data file, method and sample names, miscellaneous information, vial number, and sample multiplier. Once the sample work-list file is imported, the MSD ChemStation software will build the sequence and then process (simulate) the sequence. Simulating the sequence ensures that the imported sample work list was done successfully.

Intelligent Sequencing in Drug Analysis Mode

Intelligent Sequencing is a feature of the Drug Analysis mode that makes "programmed" decisions based on the quantitative and qualitative results of sample analysis. Some of the parameters checked are RTs, ion ratio values, calculated concentrations for controls, calibrators, and cutoff specimens, and quality of blanks and negative specimens. The "programming" is done by editing the intelligent sequencing portion of a method to set up the intelligent sequencing parameters and then setting up a batch analysis using the Sample Log Table. The decisions may be based on NIDA (National Institute on Drug Abuse) regulations, the instrument operator's discretion, or simply good laboratory practices.

Intelligent Sequencing reduces the number of batches that have to be run. Quality guidelines in the methodologies can be followed without an operator constantly monitoring the run. This is accomplished by saving a method of interest with preset decisions that are carried out depending on the result of each sample.

Retention Time Locking (RTL)

RT is the fundamental qualitative measurement of chromatography. Most peak identification is performed by comparing the RT of the unknown peak to that of a standard. It is much easier to identify peaks and validate methods if there is no variation in the RT of each analyte.

However, shifts in RT occur frequently. Routine maintenance procedures such as column trimming alter RTs. In a multi-instrument laboratory running duplicate methods, the RTs for each instrument will differ from each other, even when run under nominally identical conditions. These differences in RTs mean that each instrument must have a separate calibration and integration event table, making it time-consuming to transfer methods from one instrument to another. Differences in RT also complicate comparison of data between instruments over time.

The ChemStation's RTL feature gives you the ability to very closely match RTs on one system to those on another system with the same nominal column. By making an adjustment in the inlet pressure, the RTs on a given system can be closely matched to those on another system.

The process of RTL is to determine what adjustment in inlet pressure is necessary to achieve the desired match in RTs.

To establish and maintain a locked method, RTL should be performed whenever:

- The column is changed or trimmed
- The method is installed on a

new instrument

- A detector of different outlet pressure is used
- System performance is validated
- Troubleshooting chromatographic problems

To lock a given method for the first time or for the reasons below, you must first develop a retention time versus pressure (RT versus P) calibration. Even when using columns with the same part number (same id, stationary phase type, phase ratio, and same nominal length), separate/different locking calibration curves are needed when using:

- Systems with different column outlet pressures
- Columns differing from the "nominal" length by more than 15% (for example, due to trimming)
- Systems where the predicted locking pressure falls outside the range of the current calibration

A specific solute (usually one found in the normal method calibration standard) must be chosen and then used for both developing the locking calibration and locking all future systems. The solute, or target peak, should be easily identifiable, symmetrical, and should elute in the most critical part of the chromatogram. Solutes that are very polar or subject to degradation should be avoided.

Once the target solute is chosen and all other chromatographic parameters of the method are determined, five calibration runs

are performed. The runs are made at conditions identical to the nominal method except that four of the runs are made at different pressures. The pressures used are typically:

- Target pressure -20%
- Target pressure -10%
- Target pressure (nominal method pressure)
- Target pressure +10%
- Target pressure +20%

The RT of the target compound is determined for each run. The resulting five pairs of inlet pressures and corresponding RTs are generated by the ChemStation software and an RTL calibration is generated.

This calibration need only be generated once. Subsequent users of the method can use this calibration when running the method on a similar instrument setup, regardless of location.

Documentation

Using the Online Help

The MSD ChemStation software comes with extensive online help which includes both task and reference information about the system. The four main help files include application-specific topics tailored to the configured analysis mode:

- Enhanced Quantitation Mode
- EnviroQuant Mode
- Drug Analysis Mode
- Aromatics in Gasoline Mode

The online help for each analysis mode is comprehensive and context-sensitive, with full text-search capabilities. There is a Help menu in every view of the software which gives you access to the help topics.

The information in the online help can be viewed on the screen, printed as an individual topic, printed as a set of topics, or copied to the Windows clipboard for incorporation into the user's documentation.

Japanese and Chinese Languages

In addition to English, the online help as well as hardware and software manuals are supplied in Japanese and Simplified Chinese languages.

The user operation manuals are also available in French, German, Italian, Spanish, and Russian.

Learning the Software

The online help is the primary source of information on how to use the MSD ChemStation software. It provides information about instrument control, data acquisition, data analysis, methods, sequencing, tuning, troubleshooting the MSD, and system commands. It also includes an online book on using and writing macros.

The example methods and data files supplied with the software can be used to practice and learn the MSD ChemStation software features described in the online help.

Example (demo) files are particularly useful when learning about the EnviroQuant and Drug Analysis modes:

- The EnviroQuant online help includes data analysis tutorials that use demonstration files created specifically for learning about environmental analysis.
- The Drug Analysis mode includes special drug methods and report formats which can be used as a starting point for performing drug analysis. The example methods, reports, and data files are described fully in the online help.

Software User Information CD

A Software User Information CD-ROM is supplied with the MSD ChemStation software. This CD can be used to learn more about your GC/MS system.

The Software User Information CD contains the following information:

- An MS Fundamentals tutorial. This tutorial explains the basics of GC/MS principals, and includes graphics, animations, and video files.
- A glossary that defines common MS terms.
- A collection of manuals in PDF format:
 - G1701DA Software Installation Manual
 - G1701 Software Getting Started
 - Drug Analysis Software Getting Started
 - EnviroForms User's Guide

MSD ChemStation Revision History

MSD ChemStation			Supported instruments		
Revision	Description	Operating system	MSD	GC/ALS	Interface
G1701DA D.03.00 7/2006	Supports all 5973 and 5975 series MSDs, Fast SIM/Scan SemiQuant, and EDA Plus tools.	Windows 2000 Pro SP4 & Windows XP Pro SP2	5973 Series 5975 Series	6850 6890 Series 7683 ALS, H1888x HSS CTC Autosamplers	LAN 82350B GPIB
G1701DA D.02.00 SP1 8/2005	Supports Japanese and Simplified Chinese languages	Same as D.02.00	Same as D.02.00	Same as D.02.00	Same as D.02.00
G1701DA D.02.00 6/2005	Supports 5975 inert MSDs, High Mass, eMethods, SIM/Scan, and DA enhancements	Windows 2000 SP4 Windows XP SP2	5973A 5973N 5973 inert 5975 inert 5975 inert XL	6850 6890A 6890N 6890 Plus-LAN 7683 ALS H1888 HSS	LAN 82350B GPIB
G1701DA D.01.00-SP2 8/2004	Supports Smart Card III & III+	Windows 2000 SP3 Windows XP SP1a	5973A 5973N 5973 inert	6890A 6890N 6890 Plus-LAN 7683 ALS H1888 HSS	LAN 82350B GPIB
G1701DA D.01.00 SP1 11/03	Supports Smart Card III & III+	Windows 2000, SP 3 or later Windows XP, SP 1a or later	5973A 5973N 5973 inert	6890A 6890N 6890 Plus-LAN 7683	LAN 82350B GPIB
G1701DA D.01.00 9/03	Adds toolbars, long file names, spreadsheet-like interface for sample log table, simplified Tune and Vacuum Control view, and GPIB support for 5973A	Windows 2000, SP 3 or later Windows XP, SP 1a or later	5973A 5973N 5973 inert	6890A 6890N 6890 Plus-LAN 7683	LAN 82350A/B GPIB
G1701DA D.00.01 12/02	Adds features to the Drug Analysis mode: intelligent sequencing, reports	Windows 2000, SP 2 Windows NT 4.0, SP 6a	5973N	6890N 6890 Plus-LAN 7683	LAN
G1701DA D.00.00 11/01	Incorporates patches from G1701CA and adds AutoSIM setup and integrated intelligent sequencing in Drug Analysis mode	Windows 2K, SP 2 Windows NT 4.0, SP 6a	5973N	6890N 6890 Plus-LAN 7683	LAN

MSD ChemStation			Supported instruments		
G1701CA C.00.00 12/99	Adds LAN support for 5973N, dual MSD control for 5973N, software validation tools, sample names for secured control, closed-loop RTL, intelligent sequencing for drug analysis mode, and AutoQuant setup	Windows NT 4.0, SP 4	5972 5973 5973N	6890 6890 Plus 18594B G1512A G2612A	LAN 82341C/D GPIB
G1701BA B.01.00 8/98	Adds Y2K compliance, RTL, real-time plot, and reference chromatogram comparison	Windows NT 4.0	5972 5973 G1801C	5890 II 6890 6890 Plus	82341C/D GPIB
G1701BA B.00.00 11/97	Adds Windows NT, 5973 CI, Drug Analysis mode, AIA data files, graphics in custom reporting	Windows NT 4.0	5972 5973 G1801C	5890 II 6890 6890 Plus	82341C/D GPIB

Note: All revisions prior to D.01.00 are obsolete. It is strongly recommended that customers owning 5973 Series MSDs upgrade to D.01.00 or later for the best support.

Ordering Information

Description	Product no.
MSD Productivity ChemStations	
Require but do not include Windows 2000 (SP4) or XP (SP2).	
MSD Productivity ChemStation Software	G1701DA
MSD Data Analysis Software	G1710DA
Upgrades MSD Productivity ChemStation Software from G1701XA	G1617DA
Upgrades MSD Data Analysis Software from G1710XA	G1618DA
MSD Productivity ChemStation Bundles	
Include PC, monitor, printer, LAN communications, LAN cable, LAN hub, and Windows XP.	
Data Analysis Bundle	G1717DA
Includes G1710DA data analysis software. Pentium PC with 512 MB RAM, DVD/CD-RW, 17-inch LCD monitor, and printer equivalent to HP 2300 LaserJet. Installation and familiarization are not included.	
High-performance MSD ChemStation	G1729DA
Includes G1701DA MSD Productivity ChemStation, Pentium PC with 512 MB RAM, DVD/CD-RW, 17-inch LCD monitor, printer equivalent to HP 2300 LaserJet, installation, and familiarization.	
Academic MSD ChemStation Data System	G1740DA
Includes G1701DA, MSD Productivity ChemStation, 20 DA licenses, a training CD-ROM, Pentium PC with 512 MB RAM, DVD-RW, 17 inch LCD monitor, printer equivalent to HP 2300 LaserJet. Installation and familiarization and one year of software upgrade. (For Academic accounts only.)	
Optional Software	
Deconvolution Reporting Software	G1716AA
Requires but DOES NOT include G1701DA MSD ChemStation, NIST MS Library Bundle, and one of the Agilent RTL Libraries. Installation and familiarization NOT included.	
Deconvolution Reporting Software Upgrade	G1638AA
Headspace SW for MSD ChemStation	G2923AA
Requires but DOES NOT include G1701DA MSD ChemStation. Installation and familiarization NOT included.	
Headspace Control SW for MSD Upgrade	G1639AA
MSD Security ChemStation	G1732AA
21 CFR Part 11 compliant GC/MS software, includes installation and familiarization, and one year of software upgrade, and 5975B firmware upgrade.	
CTC Control for MSD ChemStation	G3384AA
Requires but DOES NOT include the MSD Productivity ChemStation. Installation and Familiarization included.	
MSD Security ChemStation Upgrade	G1742AA
Migrates SW from G1701xx to G1732AA.	
MSD Security ChemStation Upgrade	G1652AA
Upgrades from A.01.xx to A.02.00	

MSD Libraries

All require a PC with CD-ROM drive.

NIST Chemical Structures Library	G1036A
NIST05 MS Library Bundle Includes NIST 05 MS library, NIST 05 Mass Spectral Search and Deconvolution programs, and NIST 05 Chemical Structures Library (G1036A). Requires 145 MB of free disk space.	G1033A
NIST 05 MS Library Bundle Upgrade	G1041A
Wiley 7th Edition/NIST 05 MS Spectra Includes 461K Spectra, 1,372K unique chemical names, 222K CAS RNs, and 240K Structures (MS-Search).	G1035B
Stan Pesticide MS Library Requires 1 MB of free disk space.	G1038A
Pfleger/Maurer/Weber MS Drug Library, 3rd Edition Requires 4.5 MB of free disk space.	G1039C
Hazardous Chemical RTL Library	G1671AA
Pesticide and Endocrine Disruptor RTL Library	G1672AA
Pesticide RTL library upgrade from G1049A to G1672AA	G1692AA

www.agilent.com/chem

For More Information

For more information about ChemStation products and services, go to our Web site at: www.agilent.com/chem.

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