Agilent MSD Productivity ChemStation for GC and GC/MSD Systems

Brochure Brief

General Information

The Agilent mass selective detector (MSD) Productivity ChemStation is a full-featured 32-bit integrated gas chromatography/mass spectrometry (GC/MS) software application for all the tasks associated with GC/MS analysis, data processing, and reporting. Supported on the Windows® 2000 and Windows XP®, the MSD Productivity ChemStation software controls multiple GC/MSs and GCs and consists of software modules that include the following functionality:

- Integrated instrument control (of the GC, MSD, and automatic liquid sampler)
- Data analysis (for GC, MS, and combined GC and MS data)
- Integrated system automation
- Custom reports
- Macroprogramming
- User-defined security
- Software validation tools

From sample introduction to final report, the MSD Productivity ChemStation integrates and simplifies the analytical process and provides the tools needed to maximize laboratory productivity (Figure 1).

With enhanced 21 CFR Part 11 compliance capabilities, Agilent MSD Security ChemStation (G1732AA) takes data integrity, advanced security, audit trails, and reporting to an unparalleled level.

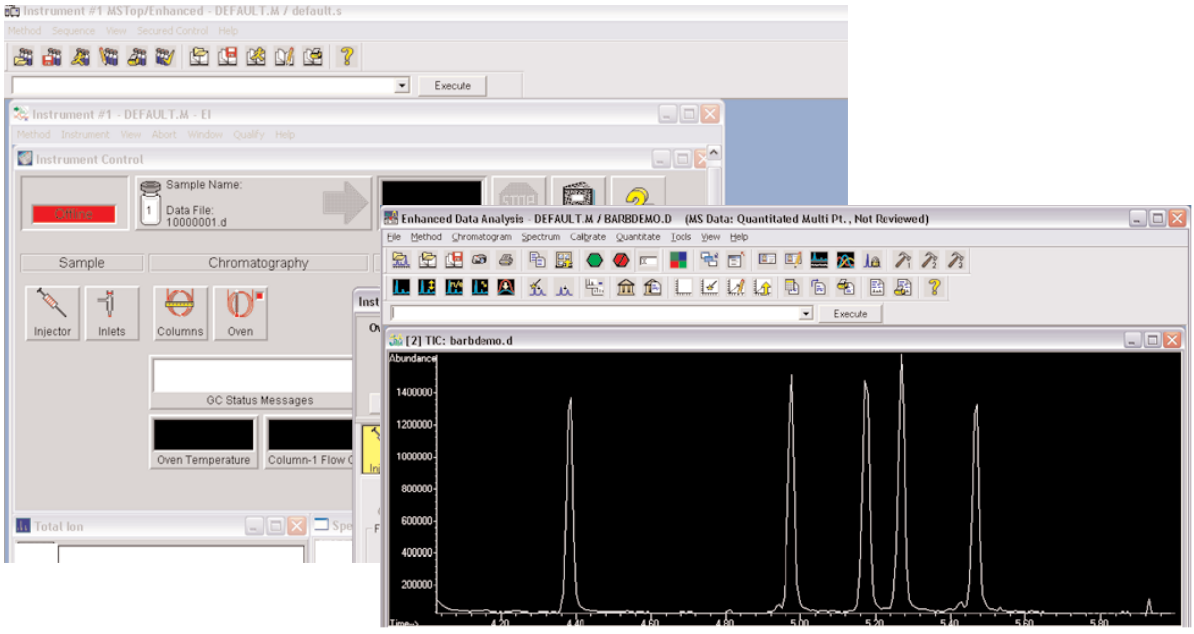


Figure 1. The MSD Productivity software is many applications in one - from sample introduction to the final report - the software operates seamlessly to meet your application requirements.

Agilent Technologies

Multi-Instrument, Multi-User Operation

The software is suitable for multi-user laboratories with customizable supervisor and user capability levels. Methods can be secured so that they cannot be changed. Maintenance tasks are often forgotten in multi-user operations. Early Maintenance Feedback notifies the users when a certain level of use is reached. Videos show how to perform maintenance tasks.

The software is designed for automation and high production operations. Laboratory information management systems (LIMS) sample lists can be downloaded to create the autosampler sequence. Automated prerun and postrun procedures simplify data evaluation and review. Custom reports can be created. A macro language is available for expert users to automate processes, change menu selections, or perform other customization.

The software is available with interface and help in English and Japanese. A Chinese help version is also available.

Advanced Automation

The software incorporates tools to simplify operations beyond the use of wizards and automation capabilities. Complex tasks that require extensive data input were simplified with advanced automation.

Automatic Set Up of the Calibration Table (AutoQuant Setup)

AutoQuant Setup allows the user to quickly establish a GC/MS calibration with minimal knowledge of 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 (Figure 2).

Automated Selected Ion Monitoring (SIM) Method

Complex SIM methods are difficult to set up manually. Retention times (RTs) and ions must be entered for each compound. The MSD Productivity

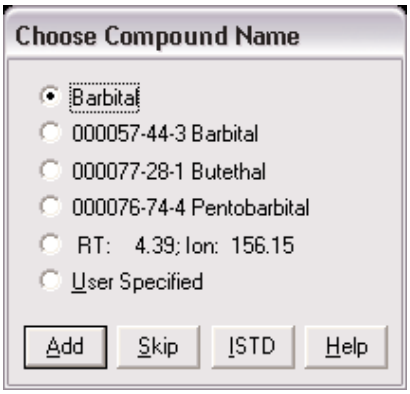


Figure 2. AutoQuant Setup makes it easy to establish a GC/MS calibration table.

ChemStation simplifies the process. From an injected standard, the software can create a SIM method with RTs, selected ions, and identification ratios (Figure 3).

Retention Time Locking (RTL)

RTL methods will maintain constant RTs - eliminating the need to edit method RTs after maintenance or when transferring a method to another instrument.

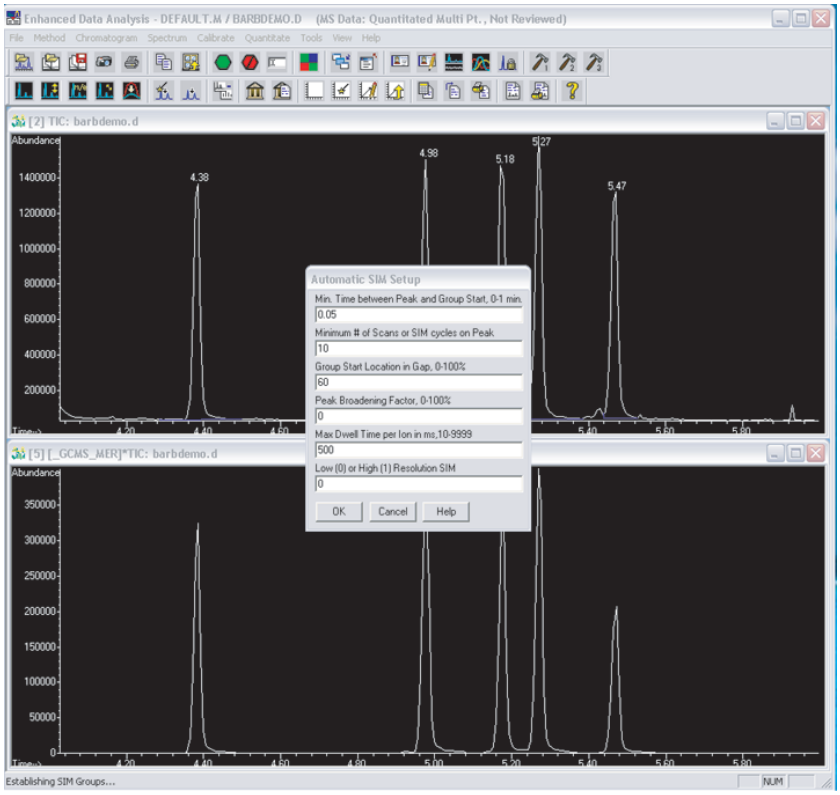
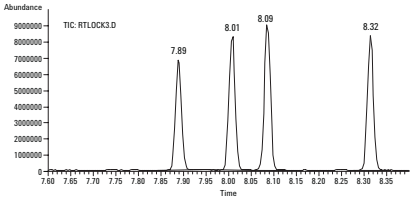


Figure 3. The "Automatic SIM Setup" function lets you automatically generate a SIM acquisition method from a quantitation method.

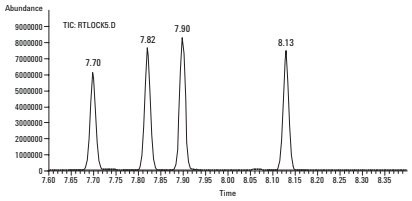
Because RTs are constant, it is possible to create databases of RTs and spectral data to screen for classes of compounds. RTL databases with mass spectra and RT data are available for pesticides, polynuclear aromatics, flavors, fatty acid methyl ester (FAME), forensic toxicology and other compound classes. The user can create RTL databases and methods for sharing.

RTL allows user to retain the RTs after column trimming or match very closely the RTs on one system to those in 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 figure below shows how the shifts in RT are fixed by RTL when a column is changed.

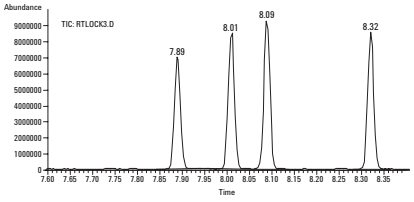
Before



After column trimming



After relocking with RTL



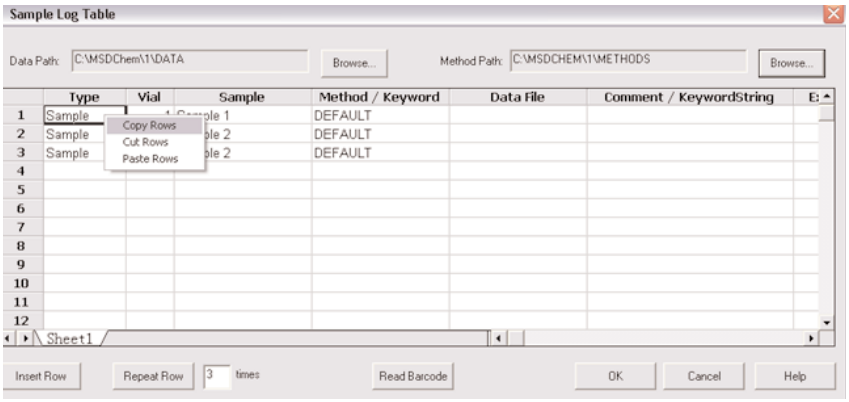


Figure 4. The new spreadsheet-like Sample Log Table makes it easy to create or edit big sequences; the right mouse click provides quick access to copy, cut, and paste rows in the Sample Log Table.

Results Screener

A retention time-locked acquisition can be screened for a large number of compounds in the database without searching every peak against a spectral library. The identifications are of a higher certainty because both RTs and spectral characteristics are used.

Intelligent Sequencing

In drugs-of-abuse testing, extensive quality control procedures encompass checks on the calibration, chromatography, and spectral results. The MSD Productivity ChemStation software can automatically make these checks and alter the autosampler sequence of injections (Figure 4).

Application-Tuned Software

As the world's most popular GC/MS software for over a decade, Agilent receives significant input from users around the world. The software is configurable for the special requirements of key applications. It can be configured for general enhanced quantitation, EnviroQuant, DrugQuant, and aromatics in gasoline modes. Each of these modes provides additional entries or reports specific to these applications.

Regulatory Compliance

The software meets the productivity and regulatory requirements of different applications. Drug testing laboratories can use Intelligent Sequencing to automate injects based on the results of prior injections. Pharmaceutical labs can add the 21 CFR Part 11 compliance package (Agilent MSD Security ChemStation, G1732AA) and IQ/OQ services. Environmental laboratories can use autotune to meet DFTPP/BFB requirements, the single-sample, and multisamples QC reports. Using a single software for both GC and GC/MS simplifies laboratory operations and reduces costs.

Environmental Applications

- Autotune for DFTPP/BFB compliance
- Pesticide and Endocrine disruptor RTL spectral and RT database
- Polynuclear aromatic hydrocarbons (PAH) RTL spectral and RT database
- Volatile organic compound (VOC) RTL spectral and RT database
- Polychlorinated biphenyls (PCB) congener RTL spectral and RT database
- USEPA CLP-like reports including tentatively identified compounds, multi-sample, spike, and other QC reports

Food Applications

- FAME RTL spectral and RT database
- Flavors RTL spectral and RT database
- Pesticide and endocrine disruptor RTL spectral and RT database

Drugs of Abuse/Forensic Applications

- Forensic toxicology RTL spectral and RT database
- Intelligent sequencing

Petrochemical Applications

- Reformulated gasoline analyses via ASTM - D5769-95

Pharmaceutical Applications

- Weighted calibration based on concentration
- Optional 21 CFR Part 11 compliance software (Agilent MSD Security ChemStation, G1732AA)
- Optional IQ/OQ/PV services

Instrument Control

- Up to two GC/MS per data system
- Up to four GC detectors
- Connect to both LAN and GP-IB 5973x instruments.
- Autotunes for electron impact (EI), positive chemical ionization (PCI), NCI, DFTPP, BFB, max sensitivity
- Autosampler batch list can be downloaded as a file
- Barcode operation supported
- Prerun and postrun macros can be part of sequence
- Results-driven sampling available in DrugQuant mode
- Timed start/stop events to operate other samplers or devices

Qualititative Analysis

- Peak purity software can detect overlapping peaks
- Probability based matching (PBM) search algorithm standard with NIST search optional
- Optional libraries include: NIST02, Wiley 7th, PMW drug, and Stan pesticide
- Molecular structures (optional)
- RT and spectral database for pesticide and endocrine disruptor (optional).

Quantitative Analysis

- Capacity for over 2000 compounds
- Twenty levels of calibration
- GC-optimized and MS-optimized integrators
- Extensive curve fitting: Linear, quadratic, average response factor, weighted (some options for forced zero intercept)
- Quant editor displays extracted ion chromatography (EIC), spectra, quant results on a single screen.

Automated Setup

- Target Compound Method
- Automated SIM Method
- RTL

Customization

- On-screen monitors of key instrument readings
- Drop-down menu items
- Maintenance reminders for injectors, pump oil changes, and other items
- Custom reports integrating text and graphics
- Process automation through a macro language designed for chromatographic and spectral data

User-Defined Security

- Manager and user levels
- Optional 21 CFR Part 11 compliance software (Agilent MSD Security ChemStation, G1732AA)

User Assistance

- MS Basics computer based training
- English, Japanese or Chinese online help depending on version
- Videos and text for maintenance processes
- Software patches on web site
- Contributed software on web site

For More Information

For more information on our products and services, visit our Web site at www.agilent.com/chem

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