

Agilent MSD Productivity ChemStation for GC and GC/MSD Systems

The Agilent MSD Productivity ChemStation is a full-featured 32-bit integrated GC/MS software application for all the tasks associated with GC/MS data acquisition, data analysis, and reporting. Supported on Windows Vista and XP®, the MSD Productivity ChemStation software controls multiple GC/MSs and GCs and consists of the following functionality (Figure 1):

- Integrated instrument control (of the GC, MSD, ALS, head-space samplers, and PAL autosamplers)
- Data analysis (for GC, MS, and combined GC/MS data)
- Integration with Agilent OpenLAB Enterprise Content Manager (ECM)
- High-performance synchronous SIM/Scan and Automatic SIM/Scan Setup
- Gain Normalized Autotune
- SemiQuant
- eMethods
- Custom reports
- Enhanced data analysis tools
- Macro programming
- User-defined security
- Software validation tools

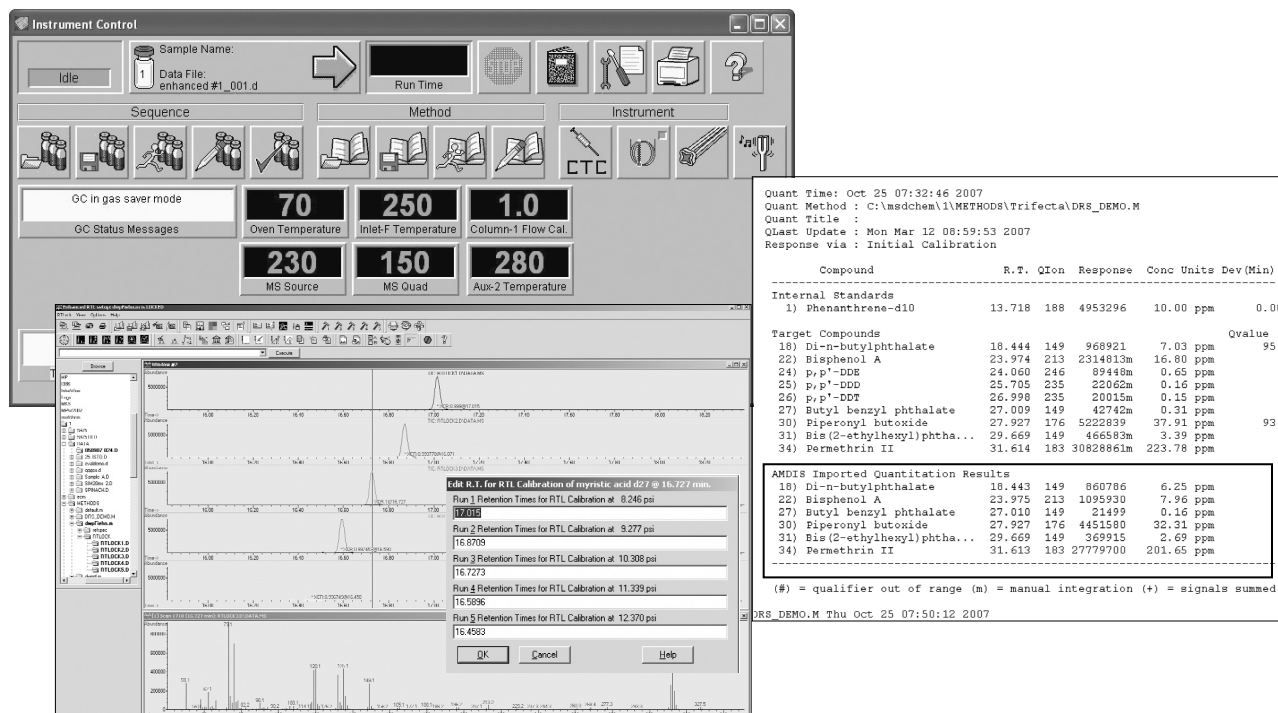


Figure 1. The MSD Productivity ChemStation is many applications in one. From sample introduction to the final report — the software operates seamlessly to meet your application requirements.



Agilent Technologies

Integration with Agilent OpenLAB ECM

Data archival and retrieval is enabled seamlessly through the integration of GC/MSD ChemStation and Agilent OpenLAB ECM. The GC/MSD ChemStation integrates common ECM functions within its user interface, allowing organizations to store and organize data from multiple instruments in one central secure repository without disrupting current workflow (Figure 2).

Improve Every Analysis with Gain!

An important feature of the GC/MSD Productivity ChemStation is Gain Normalized Methods. Setting GAIN in your methods (Figure 3) provides:

- Better signal reproducibility in your analyses!
- Simple “Tune and Use” methods!
- Better consistency between every MSD instrument in your lab!
- Better method optimization for sensitivity and linearity!
- More benefits from the new Triple-Axis Detector!

High-Performance Synchronous SIM/Scan

High-Performance Synchronous SIM/Scan is an acquisition mode possible on the 5975C Series MSD that enables collection of both SIM data and full scan data in a single run. SIM dwell time as low as 1 millisecond allows extremely narrow 600 millisecond chromatographic peaks to be acquired in SIM/Scan.

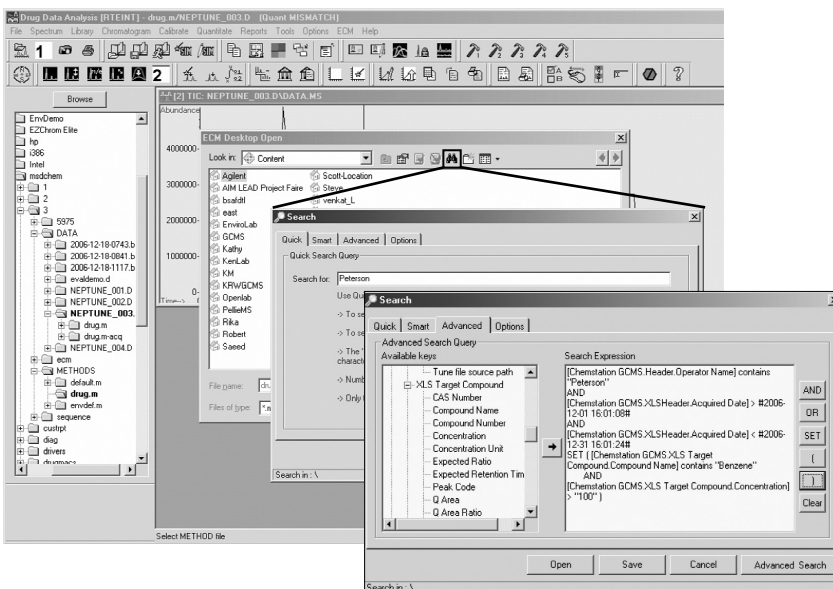


Figure 2. Access common ECM functionality, like open, save, and search data, directly from the GC/MSD ChemStation.

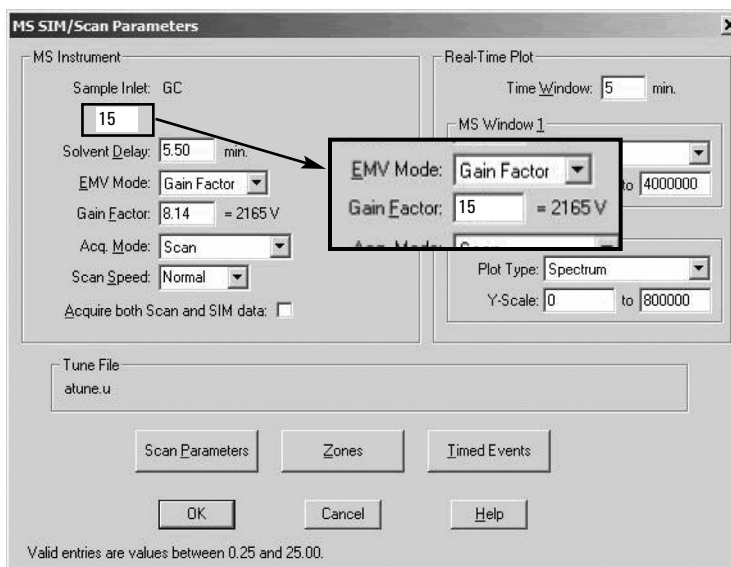


Figure 3. Setting GAIN in your methods will provide optimized and consistent performance from instrument to instrument.

Automated Selected Ion Monitoring (SIM) and SIM/Scan Setup

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

The AutoSIM Setup simplifies this process for you by creating an acquisition method with RTs, selected ions or ion ranges, and identification ratios from an existing quantitation method (Figure 4).

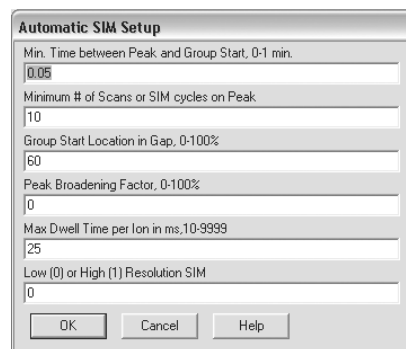


Figure 4. AutoSIM setup creates a SIM or SIM/Scan method automatically from any existing full scan method.

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 can be easily converted to SemiQuant by using *Global SemiQuant*, while *Specific SemiQuant* allows you to add SemiQuant compounds to any method (Figure 5). Quantitation reports handle the SemiQuant compounds separately from target compounds for easy identification within reports (Figure 1).

Four Application Modes: Enhanced, EnviroQuant, DrugQuant, and AIG

The Agilent MSD Productivity ChemStation 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.

eMethods

eMethods is short for electronic methods – a quick and easy way to obtain packaged application solutions from Agilent or to share and distribute your own personal applications.

eMethods allow you to easily package and transfer methods between the Agilent 5973 Series and 5975C Series MSDs.

You may also download any new Agilent eMethod from the Agilent Web site and import that method to your Agilent 5975C or 5973 Series MSD and receive the entire method without any manual editing errors.

The screenshot shows the 'Compound #4 - Page 1' window. It contains several sections: 'Retention Time Information' with Ret Time 9.779 and RRT 1.853; 'Extract signals from' with a range of 0.500 to 0.500; 'This is' with a range of 9.279 to 10.279; 'Ref Spec Name' field; 'Signals to Be Used for Quantitation' table; 'Quantitation Parameters' with 'Semi-Quant Compound' selected; 'Measure response by' set to 'Area'; 'Ident by' set to 'Best RT Match'; 'Maximum number of hits' set to 1; 'Subtraction Meth.' set to 'External'; 'Calibration Information' with 'Linear Regression' selected; 'Curve Fit' set to 'Linear Regression'; 'Weight' set to 'Equal weighting'; 'Linear term' 1.93e+000; 'Constant term' 0.00e+000; 'Coef of Det (r^2)' 1.000000. A small inset window shows the same 'Quantitation Parameters' section.

Tgt	m/z	Relative Response	% Uncertainty
Q1	87.05	67.70	35.00
Q2	143.15	20.30	35.00
Q3	75.10	19.00	35.00

Figure 5. SemiQuant: a novel way to estimate compound concentration without the hassle of calibration.

RTL

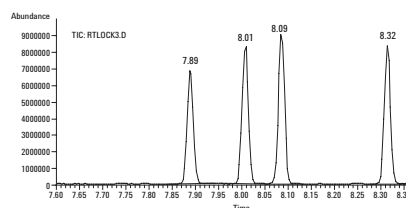
RTL methods will maintain constant RTs – eliminating the need to edit method RTs after maintenance or when transferring a method to another instrument.

By making an adjustment in the inlet pressure, the RTs on a given system can be closely matched to those on another system. Figure 6 shows how the shifts in RT are fixed by RTL when a column is changed.

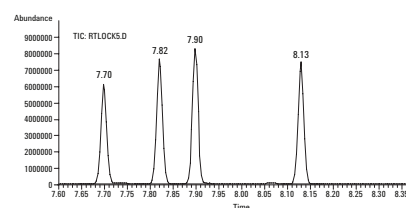
Chinese and Japanese Languages

In addition to English, the MSD Productivity ChemStation software, and online help for Enhanced Mode, as well as the hardware and software manuals are available in Japanese and Simplified Chinese.

Before



After column trimming



After relocking with RTL

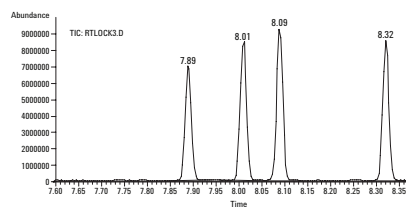


Figure 6. RTs remain constant with RTL.

Environmental Applications

- Autotune for DFTPP/BFB compliance
- Hazardous chemical RTL database
- 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, multisample, 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

System Requirements

The MSD Productivity ChemStation supports the following products:

- 5973 (LAN only) and 5975 Series MSDs
- 7890A Series GCs, 6890 Series GCs, and 6850 GC
- 7683 Series ALS
- G1888 Headspace Samplers
- PAL Autosamplers

The MSD Productivity ChemStation supports the following operating systems:

- Windows XP Pro SP2
- Windows Vista Business

Instrument Control

- Up to four instruments (maximum two MSDs)
- Controls instruments via standard LAN communications
- Autotunes for EI, PCI, NCI, DFTPP, BFB, and max sensitivity
- Sample list can be downloaded from LIMS
- Integrated control of the headspace samplers and PAL autosamplers

Qualitative Analysis

- PBM search algorithm with NIST search optional
- Optional libraries include NIST05, Wiley 8th, PMW drug, and Stan pesticide
- Molecular structures (optional)
- RT and spectral database for pesticide and endocrine disruptor (optional)

Quantitative Analysis

- Capacity for more than 2,000 compounds
- Twenty levels of calibration

- GC-optimized and MS-optimized integrators
- Extensive curve fitting: linear, quadratic, average response factor, and weighted

Optional Software

Deconvolution Reporting Software (G1716AA)

An application for target compound analyses that utilizes Agilent MSD Productivity ChemStation, NIST AMDIS_32, and the NIST MS Search Program.

Headspace Software Control for MSD (G2923AA) Provides integrated software control of the headspace samplers.

PAL Autosampler Control for MSD ChemStation (G3384AA) Provides integrated software control for the PAL autosampler.

MSD Security ChemStation (G1732AA)

A secured software system for data acquisition, data processing, and reporting of GC/MS data in laboratories regulated by FDA 21 CFR Part 11.

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