Agilent 5977B Series MSD with MassHunter

Quick Start
Notices

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CAUTION

A CAUTION notice denotes a hazard. It calls attention to an operating procedure, practice, or the like that, if not correctly performed or adhered to, could result in damage to the product or loss of important data. Do not proceed beyond a CAUTION notice until the indicated conditions are fully understood and met.

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Welcome to the Agilent MSD System

Your system includes:

• The **Agilent 5977B MSD** featuring advanced technology, increased analytical abilities, and reduced maintenance requirements.

• An **Agilent 8890, 9000, or 7890B GC** built on a legacy of robust excellence and unparalleled, gold-standard performance.

• The **Agilent MassHunter Workstation Software**, a comprehensive portfolio of software, for your GC/MS.

• A comprehensive collection of manuals, videos, eFamiliarization, user applications, and method development tools. You will find these on the:

  - **Agilent GC/MS Software Information and Manuals memory stick**

  - **Agilent GC and GC/MS User Manuals and Tools DVD** for the standard 5977B model

This Quick Start guide provides a brief summary of what is included on the DVDs and memory stick supplied with your system.
Agilent 5977B MSD and Agilent 8890, 9000, or 7890B GC

The Agilent 5977B is a stand-alone mass selective detector for use with an Agilent 8890, 9000, or 7890B Gas Chromatograph.

Included with your system is a full library of reference material. See “Your Hardware Library” on page 6 for how to install and access this wealth of information.
The Agilent MassHunter Workstation

The MassHunter Workstation provides dedicated software modules for quantitation, compound confirmation, target compound screening, degradant and unknown identification, characterization of biomolecules, and protein and metabolite identification.

Be sure to see the full library of information available for your MassHunter Workstation software on the Agilent GC/MS Software Information and Manuals memory stick. See “Your Software Library” on page 8 for how to install and access this vast library.
Your Hardware Library

Along with your system comes a complete library of Learning Products (in HTML and PDF formats) with manuals and videos that explain how to install, operate, maintain, and troubleshoot your system plus valuable user applications, and method development tools.

For the 5977B, standard model, use the Agilent GC and GC/MS User Manuals and Tools DVD. Insert Disk 2 into your DVD drive, and follow the system prompts to install these tools on your computer. Similar to the example shown below. Once installed, icons will be placed on your desktop for quick access to your material.
Parts Finder Tool

Included with your system is the Agilent Parts Finder tool. This interactive software features an intuitive search with image-based inventory for quick identification of needed parts and supplies for your Agilent instruments.

Using Parts Finder, rather than thumbing through a paper catalog, you can click on nested photos to quickly locate parts you need.

The Parts Finder tool is installed on your PC along with MassHunter Workstation. Also, it is included with the Agilent GC and GC/MS User Manuals and Tools DVD set, and can be installed on any PC from there. See “Your Hardware Library” on page 6.

To open Parts Finder, click the Parts Finder desktop icon.
Your Software Library

Use the Agilent GC/MS Software Information and Manuals memory stick (G1701-60175) to install the extensive library of software Manuals, Tutorials, online Help, Videos, and more for your system.

Here you will find manuals, Help, videos, familiarization guides, and more for the:

- MassHunter 5975/5977 Series GC/MSD
- MassHunter 7000/7010 Series Triple Quad GC/MS
- MassHunter 7200 Accurate-Mass Q-TOF GC/MS System
- 8860/8890 GC System
- Intuvo 9000 GC System
- 7890 Series GC System
- MassHunter Data Analysis

Insert the memory stick into a USB port, and follow the system prompts to install these manuals on your computer. Once installed, icons will be placed on your desktop for quick access to your manuals.
Online Help

The online Help files contain extensive information and tutorials about instrument control, data acquisition, data analysis, methods, sequencing, tuning, troubleshooting, and how to use system commands and variables. In Help, the following features are available:

- Enter a search term, and click **Search** to search the Help content.
- Click ✦ **Set as favorite** to save the current topic to your favorites list.
- Click ☰ **Favorites** to view the topics you have set as a favorite topic.
- Click ⌁ **Filter** to filter the Help content or search results based on your selection.
- Click Ⓟ **Print** to print the current topic or save it as a PDF.
- Click ⓦ **Expand** or ⓧ **Minimize** to show or hide the Table of Contents.

Press F1, use the Help menu, the Help icon, or the Help button on any dialog box to access Online Help for MassHunter Data Acquisition software.

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**Overview - Acquisition**

This MassHunter Workstation controls acquisition of GC/MS data.

This section covers the acquisition of sample data using stored methods created by a method developer. The method developer creates and saves the more complicated sequences involving calibration updates. The help found in the Method Development and Sequences sections cover the details needed by the method developer.

The lab associate running the workstation software normally loads and runs multiple sample vials using an ALS. This person must be able to perform simple edits to stored sequences for vial numbers, sample names, data file names and storage locations, and bar codes. This person must also be able to pause and restart a sequence to edit the order or other sequence details of future samples to be processed.
Familiarization and Workflow Guides

There are several familiarization and workflow guides included on the GC/MS Software Information and Manuals memory stick, including:

- Getting Started
- DrugQuant Workflow
- EnviroQuant Workflow
- Data Acquisition
- Quantitative Analysis
- Qualitative Analysis
- Unknowns Analysis
- Reporting

These and other manuals provide detailed step-by-step instructions on how to prepare your system for data acquisition, how to create acquisition methods, qualitative methods, and quantitative methods, how to use the Unknowns Analysis software, and how to use the MassHunter reporting features.

Once installed, you may access Familiarization Guides through the desktop icon, online Help, or the Windows Start menu.
Data Acquisition Software

From one screen in the MassHunter Data Acquisition software you can:

- Start and stop the instrument
- Download instrument settings in real time
- Load, edit, create, or run a method
- Load, edit, create, check, or run a sequence
- Evaluate the MS parameters
- Autotune the MS parameters
- Monitor the real-time conditions of the instrument parameters
- View the instrument logs
- View and print the real-time plot for chromatograms and instrument spectra
- Select and label the total ion chromatograms (TIC) or extracted ion chromatograms (EIC) that you want to appear in the real-time plot
Quantitative Analysis Software

The MassHunter Quantitative Analysis software will quantify very low amounts of sample.

From one screen in the MassHunter Quantitative Analysis software you can:

- Import information directly from the acquisition method
- Use the curve-fit assistant to test all fits and statistics on the calibration curve quality
- Use the **Compounds at a Glance** feature to review all the chromatograms in your batch at once, side-by-side
- Quickly scan the batch table and see your quality metrics such as high outliers (in red) or low outliers (in blue)
- Press F1 to access context sensitive online Help

Once installed, you may access **Familiarization Guides** for this software through the desktop icon, online Help, or the Programs/Start... menu.
Qualitative Analysis Software

The MassHunter Qualitative Analysis software uses advanced data mining and processing tools, including integrated deconvolution algorithms, to rapidly and accurately find all detectable compounds in your samples and easily confirm targets or identify unknowns.

This software presents large amounts of data for review in one central location. From one screen you can:

- Extract chromatograms
- View and extract peak spectra
- Subtract background
- Integrate the chromatogram
- Find compounds and generate formulas
- Press F1 to see context sensitive online Help

You can also set up methods to automatically do the tasks in the above list, as well as others, when you open the data files.

Once installed, you may access Familiarization Guides for this software through the desktop icon, online Help, or the Programs/Start... menu.
Compliance and Security Mode

Both MassHunter Data Acquisition and MassHunter Quantitative Analysis Software can be installed in one of three modes: **Standard Workflow**, **User Management and Audit Trail** mode, or the **Compliance** mode.

- In the **Standard Workflow** mode, all users have the same privileges, and data are saved to a designated drive. Records are not treated as regulated records.
- In the **User Management and Audit Trail** mode, similar to the Standard Workflow mode, records are not treated as regulated records. However, this mode includes four security user groups, each with its own set of privileges, plus a detailed audit trail that tracks all changes to method files, sequence files, data files, and the instrument configuration.
- The **Compliance** mode is designed to support the requirements of the U.S. Food and Drug Administration (FDA) regulations and the handling of electronic records and electronic signatures published as 21 CFR Part 11. Records are treated as regulated records. This mode includes the four security user groups, an audit trail of all activity, similar to the User Management and Audit Trail mode, plus a secure ECM storage location. All regulated records are stored in ECM, with digital signatures being applied using ECM. This option requires that the computer is connected to an ECM server, and that the ECM client is installed and operational.

For details on the Compliance and Security features, see the online Help in the software, and the Administrator Guide and Quick Start Guide on the GC/MS Software Information and Manuals memory stick.

For details on setting roles and responsibilities for security groups:
- For MassHunter Data Acquisition, see the Configuration Editor’s online Help
- For MassHunter Quantitative Analysis, see the Audit Trail Map’s (ATM) configuration window online Help
Report Designer Add-in

MassHunter stores all results in XML format and uses Microsoft Excel and the Report Designer Add-in for reporting. Many application-specific templates and customized reports, including custom calculations for your specific application needs, are available in the familiar Excel environment.

Using these preconfigured templates, you can easily create reports in the Data Acquisition software, the Qualitative Analysis software, and the Quantitative Analysis software.

You can also customize many of the application-specific templates, including the custom calculations, with the Report Designer Add-in.

Once installed, you may access Familiarization Guides for this software through the desktop icon, online Help, or the Programs/Start... menu.

Add tables and graphics using tool buttons

Drag and drop columns from XML source

Print preview

Format headers and footers using Excel

Use Excel number formatting

Use conditional formatting for outlier flagging
Unknown Analysis Software

The MassHunter Unknowns Analysis software identifies compounds that may be present in a sample batch beyond those that have been identified in the MassHunter Quantitative Analysis software.

From one screen in the MassHunter Unknowns Analysis you can:

- Import data directly from the MassHunter Quantitative Analysis software
- Use optimized deconvolution and library match algorithms to identify target and non-target hits
- View chromatograms, component lists, spectrums, ion peaks, and molecular structures side-by-side
- Easily review library match and peak shape metrics of unknown components in table and spectrum formats

Once installed, you may access **Familiarization Guides** for this software through the desktop icon, online **Help**, or the **Programs/Start...** menu.
Library Editor Software

The MassHunter Library Editor software customizes libraries used to identify compounds and components in the MassHunter Qualitative and Quantitative Data Analysis software.

From one screen in the MassHunter Library Editor you can:

- Add compounds to a library
- Copy spectral data from your data analysis software to a library
- Add a structure to your custom library
- Import JCAMP files into a custom library
- Create a reference pattern library

Once installed, you may access Familiarization Guides for this software through the desktop icon, online Help, or the Programs/Start... menu.
To learn how your Agilent 5977B MSD works in conjunction with the MassHunter software, take a look at the Concepts Guide. This document includes:

- Conceptual models
- Illustrations
- Screen captures
- An overview of how the 5977B MSD works
- Concepts behind the design of the Agilent MassHunter Data Acquisition software
- The theory behind Chemical Ionization in GC/MS

Once installed, you may access this guide through the desktop icon, or the Programs/Start... menu.
Your Agilent 5977B MSD is extremely powerful and flexible. Refer to the Operation Manual for extensive information on operating the instrument and performing routine maintenance on it. Included are step-by-step instructions and videos on installing GC columns, operating in electron impact (EI) mode, general maintenance procedures, and more.

Once installed, you may access this guide through the desktop icon, or the Programs/Start... menu.

Any topic with the camera icon is linked to a video. Watch these videos to learn more.
The Agilent 5977B MSD system consists of a 5977B MSD, and an 8890, 9000, or 7890 Gas Chromatograph (GC).

The Troubleshooting and Maintenance Manual for your system includes step-by-step instructions along with videos, IPBs, and annotated high-resolution photos to help you identify the cause of problems in your system. Also included are detailed procedures for completing common maintenance tasks, sections on the components of the GC/MS vacuum system and analyzer system, and a listing of parts.

Once installed, you may access this guide through the desktop icon, or the Programs/Start... menu.

Any topic with the camera icon is linked to a video. Watch these videos to learn more.
Hydrogen Safety Manual

Hydrogen presents a number of dangers. Some are general, others are unique to GC or GC/MS operation. Review this document for details on the use of Hydrogen with the GC/MS.

Once installed, you may access this guide through the desktop icon, or the Programs/Start... menu.