

# Agilent 32-Bit ChemStation for GC, LC, LC/MSD, CE, and A/D Systems - Rev. B.01.03

## Specifications

July 2005

### What's New in Rev. B.01.03

Revision B.01.03 completes the two-step port of ChemStation to a new 32-Bit globalised software platform. The new platform offers increased performance and stability and forms the basis for active development of ChemStation in the future. This is the first 32-Bit ChemStation software release to provide support for existing CE and CEMS instruments, existing 1046 FLD and the 1049 ECD detectors, the new Agilent 1100 chip cube interface and the new 1100 DAD and MWD detectors (G1315C and G1365C).

The existing 16-Bit ChemStation Rev A.10.02 will remain available in parallel in the short term to

allow sufficient time to plan to upgrade to the new 32-Bit platform. Customers can take advantage of the new features offered by this release by upgrading their software. A ChemStation software upgrade product, G1656B, is available for customers who do not currently have an active ChemStation software upgrade contract.

*Note: Rev. B.01.03 Agilent ChemStation software release does not relate to UV-VIS or GC/MSD instrumentation. These instruments are controlled and supported by separate Agilent ChemStation software products.*

The following new features are included in Revision B.01.03:

#### For LC Systems

- Support for USB-GPIB interface (PN 82357A) for GPIB communication based LC and CE systems (HP 1090, HP 1046, HP 1049, CE, CE/MS)
- Software support for new G4240A Agilent 1100 Series chip cube, designed for LC systems using an Agilent Ion Trap MSD as detector.
- Software support for new G1315C Agilent 1100 Series diode-array detector (DAD)
- Software support for new G1365C Agilent 1100 Series multiple wavelength detector (MWD)

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- Support for HP 1046 (FLD) and HP 1049 (ECD) detectors
- Eight signals available using the G1315C DAD/G1365C MWD detectors
- Additional instrument curves using the G1315C DAD/G1365C MWD detectors
- Support of high data rate (80 Hz) using the G1315C DAD/G1365C MWD detectors
- Run buffering allows data recovery after a power/network failure using the G1315C DAD/G1365C MWD detectors
- ID-tags for UV-lamp and cell for G1315C DAD/G1365C MWD detectors

*Important firmware information for Agilent 1100 Series systems:*

- For Agilent 1100 Series modules the minimum firmware revision is A.06.01
- The new G1315C/G1356C DAD/MWD require firmware B.01.01.
- Firmware Rev. A.06.01 and B.01.01 are *not* compatible with Rev. A.05.xx or earlier.

#### **For CE/CEMS systems**

- Support for CE systems using GPIB or USB communication
- Wildcard definition of method vials for easier method development
- Enhanced productivity for CE ChemStation customers due to instrument set points modifications directly in the sequence table for each sequence line

#### **For LC/MS systems**

- Support for Multimode Source
- Support for multiple method FIA
- Support for latest version of NIST library search algorithm
- Support for NETCDF protocol for data exchange

*Note: Peptide Tools is not supported with Rev B.01.03.*

#### **For all users: (\* available since Rev B.01.01)**

- Support for Microsoft Windows® XP Professional with Service Pack 2
- Support for Microsoft Windows 2000 Professional with Service Pack 4\*
- Support for the use of hyper-threading on Pentium IV or higher PC's running Windows XP\*
- Conversion to 32-Bit architecture provides increased system performance and stability\*
- Support for long file names for data files, methods, sequences, logbook entries and reports\*
- Extension of the automatic file naming function which names raw data files with a prefix and counter to allow for generation of filenames with a total of 17 characters\*
- Support for long file names in user interfaces and dialog boxes\*
- Optimization of screens and windows to use 1024x768 resolution\*
- New Chem32 integrator provides improved integration result accuracy\*

- New 'Baseline Correction' integration event allows treatment of noisy or drifting baselines\*
- Four new integration events allow selection of skimming mode for tailing or fronting peaks\*
- New Sequence Editor dialog allows the user to define the columns to be displayed in the Sequence Table and define the width (in characters) of each column shown\*
- Quality and defect fixes

#### **For users with ChemStore software add-on module:**

**(\* available since Rev B.01.01)**

*Note: These features will only be seen if ChemStore is installed.*

- Improved integration with ChemStore\*
- Two new ChemStore related icons in 'Method and Run Control' and 'Data Analysis' views\* - ChemStore Lock Session
- Launch ChemStore Review Client
- Display of ChemStore 'Study' name in status bar in 'Method and Run Control' view\*
- Inclusion of new ChemStore 'Study' column in the Sequence Table\*
- New ChemStore custom field set-up dialog which can be opened via a button and is automatically called whenever a new line is appended in the Sequence Table\*
- Incorporation of ChemStore transfer settings in the Sequence Parameters dialog\*

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## General Description

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The Agilent 32-Bit ChemStations for GC, LC, LC/MSD, CE and A/D systems are instrument control, data acquisition and data evaluation systems for:

- Agilent 6890N, 6890 Plus and 6890A gas chromatographs,
- Agilent 6850 Series II and 6850 gas chromatographs,
- Agilent 5890 Series II and 4890D gas chromatographs,
- Agilent 1100 Series modules and systems for HPLC, including the Agilent 1100 Series LC/MSD,
- HP 1090 Series liquid chromatographs,
- Agilent 35900E dual channel analog-to-digital interfaces, and
- Agilent capillary electrophoresis systems.

The software is designed to run on IBM compatible personal computers with a PCI interface under Microsoft Windows operating environments.

### Core ChemStation 2D Software

Four core 32-Bit ChemStation 2D software products are available. Each core software product provides data acquisition, instrument control, data analysis (integration, quantification and reporting), automation and customization for a single analytical instrument. A single instrument may collect data from a number of different detec-

tors simultaneously. The four core 2D software products are:

- Agilent 32-Bit ChemStation for 2D Liquid Chromatography (LC) systems (G2170BA)
- Agilent 32-Bit ChemStation for Gas Chromatography (GC) systems (G2070BA)
- Agilent 32-Bit ChemStation for Liquid Chromatography / Mass Selective Detector (LC/MSD) systems (G2710BA)
- Agilent 32-Bit ChemStation for Capillary Electrophoresis (CE) systems (G1601BA)
- Agilent 32-Bit ChemStation for 35900E Analog to Digital Converter (A/D) systems, (G2072BA)

### ChemStation 3D Software Module

The capabilities of the core 2D LC software may be expanded to allow for 3D data through the purchase of the additional LC 3D Spectral Module (G180BA).

### ChemStation Additional Instrument Control Software

The instrument control capabilities of the core Agilent ChemStation software may be extended to allow for multiple instrument systems by purchasing additional instrument control software. It is possible to configure up to four chromatography instruments per ChemStation PC. The

four additional instrument control software products are:

- Additional LC Instrument Control and Data Acquisition software, (G2171BA).
- Additional GC Instrument Control and Data Acquisition software (G2071BA)
- Additional LC/MS Instrument Control, Data Acquisition and data evaluation software, (G2715BA).
- Additional CE Instrument Control, Data Acquisition and data evaluation module (G2172BA)
- CE/MS Add-on software (G2201BA) for G1946X.
- Additional 35900E Analog to Digital Converter (A/D) Instrument Control and Data Acquisition software (G2073BA)

### ChemStation License to use software on another PC

Once an initial core ChemStation software product has been purchased it is possible to purchase licenses to use that software on another PC. The available license products are:

- License to use 2D LC ChemStation software on another PC (G2175BA)
- License to use 3D LC ChemStation software on another PC (G2185BA)
- License to use GC ChemStation software on another PC (G2075BA)

- License to use CE ChemStation software on another PC (G2205BA)
- License to use A/D ChemStation software on another PC (G2077BA)

### **ChemStation Data Analysis Only Software**

There are three data analysis only ChemStation software products. These products are designed for data evaluation only purposes, for example in an office environment, and should not have instruments configured. The three data analysis only software products are:

- ChemStation Data Analysis software for LC (G2190BA)
- ChemStation Data Analysis software for GC (G2090BA)
- ChemStation Data Analysis software for LC/MSD (G2730BA)

### **ChemStation Plus Add-On Software Modules**

Agilent provides a range of add-on software modules which extend the capabilities of the ChemStation base software. The modular architecture ensures that you can control your enhanced system from the same, familiar user interface. ChemStation Plus is a fully scalable solution that enables you to expand your data system

from single PC to instrument configurations right through to distributed, multi-technique configurations and client-server functionality. Users, instruments and applications can be added without disruption.

- **Agilent ChemStore, Standalone/Client (G2181BA) ChemStore Server (G1410A)**  
ChemStore provides centralized data organization and storage, custom calculations, review and approval as well as powerful report generation capabilities such as control charting. It is available as either a Standalone or Client/Server configuration.
- **Agilent ChemStation Plus Security Pack, (G2183AA)**  
Compliance with regulatory guidelines such as the FDA's 21 CFR Part 11
- **Agilent Method Validation Pack (G2184AA)**  
Provides automated validation of analytical methods

### **Dedicated Solutions for Specific Applications**

- **High Throughput Purification (Purify) software modules**  
Advanced, high-capacity preparative LC for large numbers of samples.

- **Agilent ChemStation Companion**

Provides a simple single-screen user interface for GC routine analysis. Automatically installed with ChemStation GC software.

- **Retention Time Locking (G2080BA)**

Retention Time Locking software for the 32-Bit GC ChemStation.

- **Integrated Headspace Control Software (G2924AA)**

Requires 32-Bit GC ChemStation software.

- **Analyst Software (G2731AA)**

For LC/MSD data analysis. Requires LC/MSD ChemStation software.

- **Peptide Tools (G2720AA)**

LC/MSD Deconvolution & Bioanalysis SW. For determination of molecular weight from multiply charged API-ES mass spectra & for evaluation of MS data from proteins/peptides/oligonucleotides. Requires G2710AA LC/MSD ChemStation Software or G2715AA LC/MSD Add-on Software module to operate. *Note: Only Deconvolution is supported with Rev B.01.03 ChemStation.*

- **TOF Software (G3300AA)**  
For CE-MS TOF.

## Computer Hardware

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The 32-Bit ChemStation consists of Hewlett-Packard personal computer hardware and ChemStation software. The hardware is an IBM compatible personal computer with an ISA or PCI interface bus.

The personal computer is interfaced to the analytical instruments through a LAN card, a GP-IB internal card, a USB/GP-IB interface, or a combination of one GP-IB card and a LAN card. All cards plug directly into the computer's PCI or interface. Third-Party instruments can be connected via the Agilent 35900E A/D-Converter interface. The separate hardware components that comprise a particular instrument configuration, including third party instrumentation, may need to be coordinated through a remote cabling system

for time critical events such as injection.

### Non HP / Compaq Computers

The Agilent ChemStation has been designed to successfully run on a wide range of compatible personal computers equipped with accessories and peripherals that adhere to the programming standards for the Intel PC platform and Microsoft Windows operating systems. Agilent Technologies has tested the Agilent ChemStation software mainly on Hewlett Packard/Compaq equipment. All configuration information listed in this manual applies to Hewlett-Packard/Compaq Kayak, Vectra and EVO computers and may not be optimized for other vendor's PCs. The standard configuration

of the GPIB interface, for instance, may conflict with the memory configuration of a non-HP /Compaq computer. Additional accessory interface boards may cause conflicts of hardware related resources (I/O ports, interrupt settings, DMA channels). For a non-HP/Compaq computer, use the setup utility program supplied by the manufacturer to configure your computer and check the supplied documentation to eliminate resource conflicts in your PC's setup, especially regarding the configuration of the GPIB interface. Although the software is also designed to be run on other compatible hardware Agilent Technologies will not necessarily accept responsibility for defects solely observed and reported on third party hardware.

## Minimum PC Configuration (for all systems excluding the G1315C Diode-Array Detector)

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### Windows XP and Windows 2000 based systems:

- Hewlett-Packard / Compaq PC with Pentium III\*, 800 MHz
- XGA display (1024x768 resolution)
- 8 GB hard disk

- MS Windows compatible pointing device
- ATAPI CD, CD-RW or DVD drive
- 10/100 baseT LAN interface card.

### Minimum memory specifications:

- 256 MB RAM

\* Agilent supports the use of hyperthreading on Pentium IV or higher PC's running Windows® XP.

## Minimum PC Configuration (for systems with the G1315C Diode-Array Detector)

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### Windows XP and Windows 2000 based systems:

- Hewlett-Packard / Compaq PC with Pentium IV\*, 1.5 GHz
- XGA display (1024x768 resolution)
- 40 GB hard disk

- MS Windows compatible pointing device
- ATAPI CD, CD-RW or DVD drive
- 10/100 baseT LAN interface card.

### Minimum memory specifications:

- 256 MB RAM

\* Agilent supports the use of hyperthreading on Pentium IV or higher PC's running Windows® XP.



## Recommended PC Configuration

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### Windows XP and Windows 2000 based systems:

- Hewlett-Packard / Compaq Vectra VL420 or Evo D510 or comparable Intel based PC model Pentium IV or higher\*, 1.5 GHz or higher
  - XGA display (1024 x 768 resolution)
  - 256 MB RAM or higher
  - 20 GB hard disk or higher
  - MS Windows compatible pointing device
  - ATAPI CD, CD-RW or DVD drive
  - 10/100 baseT LAN interface card
- \* Agilent supports the use of hyper-threading on Pentium IV or higher PC's running Windows XP.

## LC/MSD ChemStation Minimum PC Configuration

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A distinct set of hardware specifications and requirements exists for LC/MS ChemStation systems running an SL MSD and using the fast scanning feature. The software requires data system components with the following minimal specifications for Windows XP or Windows 2000 based systems:

- Hewlett-Packard / Compaq PC with Pentium III\*, 800MHz
  - XGA display (1024x768 resolution)
  - 15 GB hard disk
  - MS Windows compatible pointing device
  - ATAPI CD, CD-RW or DVD drive (minimum 4x speed)
  - A 10/100 baseT LAN interface card
  - 256 MB RAM
  - A PCI interface bus for the data acquisition interface
  - A 10/100 baseT LAN interface card
  - Audio card or integrated audio capability
- \* Agilent supports the use of hyper-threading on Pentium IV or higher PC's running Windows XP.

## Agilent 1100 Series Diode-Array Detector (G1315C) Minimum PC Specifications

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### Windows XP and Windows 2000 based systems:

- Hewlett-Packard/Compaq PC with Pentium IV\*, 1.5 GHz
  - XGA display (1024 x 768 resolution)
  - 512 MB RAM
  - 40 GB hard disk
  - MS Windows compatible pointing device
  - ATAPI CD, CD-RW or DVD drive
  - A 10/100 baseT LAN interface card.
- \* Agilent supports the use of hyperthreading on Pentium IV or higher PC's running Windows XP.

## Maximum Number of Supported Instruments

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A maximum of four instruments may be configured per Agilent ChemStation PC. The following instrument/module specific limitations exist:

- A maximum of two diode-array detector instruments may be configured per PC. If two diode-array detector instruments are configured in addition to ChemStore the configuration requires a PC with at least 512 MB RAM and a 1 GHz Pentium processor.
- A maximum of one variable wavelength detector (VWD), one pump module, one autosampler module and one thermostated column compartment (TCC) module are allowed per instrument on a PC with four instruments configured.
- A maximum of three instruments are supported per PC when ChemStore is installed.
- A maximum of three instruments are supported per PC when spectroscopy instruments are configured.
- An Agilent 1100 Series LC/MSD system only allows one additional Agilent 1100 or 1090 Series II HPLC instrument to be configured.
- Only one CE instrument may be configured per PC.
- A maximum of one CE/MS (including the DAD on the instrument) may be configured per PC. No additional instruments are supported on the CE/MS ChemStation system.
- CE ChemStation can co-reside with a second system (either LC or CE ChemStation), however coexecution of the software is not supported.

## Maximum Number of Supported Modules Guidelines

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The guideline for the maximum number of modules that may be configured per Agilent ChemStation PC is 18.

Approximately 12 analytical modules can be configured but this depends on the exact configuration.

The following modules are counted as 2 modules in this calculation: Agilent 1100 Series DAD, Agilent 1100 Series FLD and the Agilent 1100 Series VWD.

*Note: Please contact your Agilent Technologies representative to confirm whether configurations approaching this 12 module limit are possible.*

Additionally 6 CAN-slave modules can also be configured, e.g. values or UIB interfaces. For correct configuration of specific instruments and modules please contact your Agilent Technologies representative. The ChemStation Plus Ordering Guide provides additional details on supported configurations.

## IEEE-488 GP-IB Support Matrix

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### Instruments Supported on GP-IB

Agilent 6890 Gas Chromatograph  
Agilent 5890 Gas Chromatograph  
Agilent 1090 Series LC systems  
Agilent Capillary Electrophoresis (CE)  
Agilent Capillary Electrophoresis Mass Spectrometry (CE/MS)  
HP 1046 FLD  
HP1049 ECD

### 82350A/B GP-IB Interface Cards

Analytical instruments can communicate with the Agilent ChemStation via GPIB using a GPIB board installed in the computer. Agilent 82350A or 82350B PCI high-performance GPIB interface cards can be used on Windows 2000 and Windows XP Professional systems. For both

cards a PCI slot is required on the PC. The Agilent 82350 is a PCI GPIB interface card and no additional settings such as changing the I/O base address are required. Please note that GPIB communication requires installation of the SICL I/O library version L.02.01. Please ask your local Agilent representative for additional details.



## USB/GP-IB Interface Support Matrix

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### Instruments supported on USB/GP-IB (USB port on PC is used):

- Agilent Capillary Electrophoresis (CE)
- Agilent Capillary Electrophoresis Mass Spectrometry (CE/MS)
- HP 1046 FLD
- HP1049 ECD
- HP 1090 LC

### USB/GP-IB Interface

A USB/GPIB interface allows you to directly connect from the USB port on your PC to GPIB instruments. The interface is small, portable, flexible, uses industry standards and is easy to connect. The interface can be used on both Windows 2000 and Windows XP Professional systems. The USB/GPIB cable is available as an option against the CE PC bundle

(G1602BA Option 720) or as an internal support part (G1680-63200) from the Support Organisation. Please ask your local Agilent Technologies representative for additional details.

*Note: USB/GPIB interfaces are only supported with legacy LC and CE instruments.*

## LAN-MIO Support Matrix

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### G1369A Agilent LAN Interface Card

The firmware of the card must be revision A.01.05 or higher. For non-LC systems (35900E ADC, 6890 GC and 6850 GC) a minimum Firmware Revision of C.03.00 is required. Please refer to Service Note G1369-003.

### J2552B/C JetDirect Internal Printer Servers (MIO)

The firmware of the JetDirect card has to be revision A.08.32 or higher.

### J4100A JetDirect N Internal Printer Servers (MIO)

The firmware of the JetDirect card has to be revision K.08.32 or higher.

#### Note:

- LAN communication with the Agilent 6890A requires firmware revision A.03.08 or higher. This is available in an electronic chip format from Agilent Technologies (Please ask your local Agilent Technologies representative for

details). The 6890N requires firmware revision N.05.04 or higher and LAN board firmware revision 04.7B3.

- LAN communication with the Agilent 1100 Series requires a minimum firmware revision of A.06.01. The new G1315C DAD and G1356C MWD detectors require a minimum firmware revision of B.01.01. A new LAN/RS-232 Firmware Update Tool 2.00 is available for updating firmware quickly and easily. Please ask your local Agilent Technologies representative for details.

*Note: Firmware Rev. A.06.01 & B.01.01 are NOT compatible with Rev. A.05.xx or earlier.*

### Instruments / Modules Supported on LAN

Agilent 1100 Series LC systems  
Agilent 6890 Gas Chromatograph  
Agilent 6850 Gas Chromatograph  
Agilent 1100 Series LC/MS systems  
Agilent 35900E A/D systems  
Agilent 1100 G1315C diode-array-detector  
Agilent 1100 G1365C multiple

wavelength detector  
Agilent 1100 Chip Cube interface (G4240A for Ion Trap systems)

### G1369A LAN Interface Card

LAN interface cards are used to connect analytical instruments to the LAN. Jet Direct or G1369A LAN cards are required. The minimum firmware required for LC systems used with the G1369A LAN card is Rev. A.01.05 or higher. For non-LC systems (35900E ADC, 6890 GC and 6850 GC) a minimum Firmware Revision of C.03.00 is required. Additional details are available in the Agilent G1369A LAN Interface manual.

### Communication Protocols

Instruments are controlled over LAN using industry standard TCP/IP (Transmission Control Protocol / Internet Protocol). It is necessary to verify correct communication between the PC and analytical instruments connected over the LAN. The Microsoft TCP/IP protocol needs to be installed and configured as a network protocol on the PC.

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The boot strap protocol is used to configure the JetDirect or G1369A LAN card. The Boot strap protocol requires a BootP server. The Agilent BootP Server Program uses the LAN communication parameters specified in the Configuration Editor to establish communication. The Agilent BootP Server Program can be used for central administration and distribution of IP addresses and settings.

#### **Fixed IP Addresses for Communication**

IP addresses can be stored in the non-volatile RAM of the modules. It is possible to assign fixed IP address to the Agilent 1100 Series modules, using either a handheld Control Module or Telnet to assign IP addresses.

#### **Additional Hardware Required for LAN Instrument Control**

An industry standard LAN PC card is shipped with all Agilent ChemStation 32-Bit PC bundles.

An instrument LAN card can also be ordered from Agilent Technologies as an option to the instrument or as an individual part. Please ask your Agilent Technologies representative for details.

Industry standard LAN cabling using twisted pair or coaxial cabling:

- Twisted pair –10/100 baseT twisted pair cabling with RJ45 connectors can be used together with an Agilent G2402A 8-port 10/100 auto sensing switch for the ability to connect one or more instrument to a PC.

A twisted pair 'crossover' cable can be used to make a single connection from one PC to one instrument. This configuration is only suitable for single instrument configurations. This configuration is not supported on Agilent 1100 Series LC/MSD systems.

- BaseT coaxial cabling with the appropriate tee connectors and terminators can also be used to configure single and multi-instrument systems.

#### **LAN Transmission Rates**

Traffic on the LAN from each instrument is approximately 100KB per second for a 2D instrument at maximum data rate.

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## **Printers**

The Agilent ChemStation has been designed to work with printers that are compatible with the operating system. The software operates with any Microsoft Windows compatible printer capable of interpreting an escape code language (e.g. PCL) or page description language (e.g. PostScript). The printer may be directly connected to the computer through a parallel or serial interface or connected through a Local Area Network. Serial port printers are supported by the operating system but may exhibit speed performance limitations.

Networked printers must be shared by a network server running a network protocol supported by the Microsoft operating system.

Recommended black and white printers are the HP LaserJet family using PCL 5e or 6. For lower performance applications it is possible to use the HP DeskJet family. Please note that the HP DeskJet printer family is not recommended for high throughput applications.

Recommended color printers are the HP LaserJet 2500TN or an HP DeskJet family printer. Agilent Technologies has not tested all printer and printer driver combinations that are supported in the Windows environment. Print performance and results may vary on other manufacturer's printers and appropriate drivers. Please note that host-based printers (e.g. GDI or PPA printers) impose more processing tasks on the CPU and are not recommended for use with the Agilent ChemStation on-line sessions.

## Operating System

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The Agilent 32-Bit ChemStation requires Microsoft Windows 2000 Professional with Service Pack 4

or Windows XP Professional with Service Pack 2.

## Methods and Sequences

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The Agilent ChemStation analytical method fully describes how a particular separation is performed. It contains all the parameters for instrument control, data acquisition and evaluation, including

integration, quantification and reporting. The system may be set up to acquire data from a number of samples by different methods. The control file for this operation is called a sequence and holds the

individual sample information, references to the appropriate methods and automatic recalibration specifications.

## System Configuration

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The configuration of the instrument system is done through the configuration editor program.

It allows users to define their instruments, GP-IB addresses, IP LAN addresses, the directories for

data, sequences and methods, and the color definition for the ChemStation software.

## Data Model

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The ChemStation software is designed around a data model based on a memory structure called a register. Registers are multi-purpose structures that can hold analytical data and information for both two dimensional (e.g., time/intensity) and three dimensional (e.g. time/intensity/wavelength) analyses.

The ChemStation provides, commands and functions to construct, expand, extract and, where it does not alter primary data, edit registers.

Registers hold information about their contents in register headers. The registers are further subdivided into one or more objects. Typically an object holds data that describes an analytical measurement, such as a chromatogra-

phy signal. Each of these objects have their own header with information about the analytical measurement such as the data file name, injection date and time, sample name, and tables. Tables are used to hold different types of data as one block of information. For example, the quantification process in a calibrated method constructs a quantification table that contains peak numbers, compound names, compound amounts and retention times.

Like other parts of the registers, tables may be user-defined and have the functionality of database tables with the additional benefit of being directly associated with the base piece of analytical information from which they were derived.

Each register may hold information for different purposes. As well as analytical data, the register data model is used for holding configuration information and analytical methods. They may be saved as files on non-volatile storage and reloaded into the ChemStation memory, printed and plotted to the screen or a hard-copy device. Their binary format means they are not editable outside the ChemStation and each data item may also be protected by assigning access attributes to it when it is created.

Their design fits extremely well to modern database technology enabling systems to be developed to map analytical results or data directly to a relational database system.

## Software User Interface

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The Agilent ChemStation user interface is designed into Views that group software functionality according to typical analytical tasks. Three standard views are present in all software configurations:

- The *Method and Run Control* view for controlling and acquiring data from the instrument.
- The *Data Analysis* view for reviewing and re-evaluating data that has been acquired.
- The *Report Layout* view for designing specific report layouts.

Additional views are present if additional data evaluation modules have been installed or for certain instrument configurations that support instrument diagnostics and verification procedures. The ChemStation Companion view offers an easy to use interface specifically designed for the production operator and routine labs. Instrument operators can run samples from an easy to use, preconfigured table.

Each view consists of a set of standard user elements including menus and toolbars.

The standard toolbar provides rapid access to the common system specification information such as methods and sequences.

The *Method and Run Control* view additionally incorporates a system status bar, a sample information area, that may be configured for single runs or automated runs, and a schematic instrument interface diagram for GC, LC, LC/MSD, CE and CE/MSD configurations. The schematic instrument interface diagram uses hot spots to allow rapid access to instrument parameters and an animated graphical overview of the status of each analysis as it proceeds. The schematic instrument diagram may be turned off if it is not required, to save memory and other Windows resources.

The *Data Analysis* view extends the standard toolbar to specific data analysis modes including integration, calibration, reporting, annotation, signal comparison and additional specialized modes if the appropriate modules are installed. Each of these separate data analysis modes are supported with a mode-specific toolset.

The *Report Layout* view allows the user to graphically define the layout of a specific report style in a graphical object orientated fashion. It too uses a set of toolbars specific to this task.

## Data Acquisition

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The status of the instrument is continually monitored and updated on the display, along with the elapsed run time of the analysis, both when the software is a visible window and when it is iconized. The transactions that occur during the analysis, including any errors and the instrument conditions at the start and the end of the analysis, are recorded in the system's logbook, an extract of which is stored with every data file.

The instrument conditions, such as flow, temperature, pressure and solvent composition for liquid chromatographs may be recorded and stored with each data file. These instrument parameters can be displayed and plotted to testify to the quality of each analysis. The exact nature of the parameters recorded depends both on the technique and the capabilities of the configured instrument.

One or more display windows may be used to monitor the data being acquired by the instrument in real time. The data are displayed in real measurement units such as mAU, Volts, degrees or bar. The windows may each show multiple overlaid chromatographic signals or instrument parameters, such as pressure. The display default settings may be adjusted and are remembered by the system so users can set their own

preferred settings as the instrument default. The window has zoom capability and the cursor may be used to display a specific signal's response at any point in time.

The complete functionality of the ChemStation can be used during an analysis with an off-line copy of the software.

A snapshot command is available for users who wish to start processing data before the analysis is completed.

The layout of the signal and status information windows, including the components of the schematic instrument interface diagram, is saved automatically.

## Data Analysis - Display

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The data analysis view extends the standard tool bar with task-grouped data analysis functions including integration, calibration, reporting, annotation and signal comparison toolsets. The following key graphical operations are possible:

- Single or multi-signal displays selectable when loading the chromatogram.
  - Overlays of chromatograms from different samples.
  - Subtraction of one chromatogram from another.
  - Graphical vertical and horizontal alignment of signals to help visual comparison.
  - Signal inversion or mirroring to help visual comparison.
  - Graphical zoom and scrolling functions.
  - Adjustment of display attributes including selection of tick marks, baselines, axes, retention times and compound names. The user can also select the font for the RT and compound labels, adjust the size and orientation of the display, select the display as overlaid or separated and select scaling factors.
- The chromatogram display may include graphical overlays of instrument parameters depending on the capability of the configured instrument.
  - User defined annotations may be interactively added to the display, with the selection of font, size, text rotation and color. Once defined, the annotations may be graphically moved, edited or deleted.
  - Copy the display to the Windows clipboard in both metafile and bitmap format.
  - A *Pick Mode* function to display the values of individual data points in detector units.
  - Export of time/intensity digitized points to the Microsoft Windows clipboard.
  - Display of fraction results in graphics and table format



## Data Analysis - Integration

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The Chem32 integration algorithm used in the 32-Bit ChemStation is the second revision of a new generation integrator offering improved ruggedness, reliability and ease-of-use.

### Integrator Capabilities

The integrator algorithms include the following key capabilities:

- an autointegrate capability used to set up initial integrator parameters,
- the ability to define individual integration event tables for each chromatographic signal if multiple signals or more than one detector is used,
- interactive definition of integration events that allows users to graphically select event times,
- graphical manual or rubber-band integration of chro-

matograms requiring human interpretation (these events may also be recorded in the method and used as part of the automated operation),

- display and printing of integration results,
- the ability to integrate at least 1000 peaks per chromatogram.
- integrator parameter definitions to set or modify the basic integrator settings for area rejection, height rejection, peak width and slope sensitivity,
- baseline control parameters, such as force baseline, hold baseline, baseline at all valleys, baseline at the next valley, fit baseline backwards from the end of the current peak,
- area summation control,
- negative peak recognition,
- tangent skim processing

including solvent peak definition commands,

- the ability to define individual front/tail tangent skim calculations event tables for all chromatographic signals,
- the ability to use baseline correction parameters (non signal related),
- integrator control commands defining retention time ranges for the integrator operation.
- peak shoulder allocation through the use of second derivative or degree of curvature calculations, and
- improved sampling of non-equidistant data points for better performance with DAD LC data files that are reconstructed from DAD spectra

## Data Analysis - Quantification

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The Agilent ChemStation's calibration mode of the data analysis view allows simultaneous display of

- the signal or signals being calibrated with an indication of the current compound's retention time window,
- the calibration table whose display may be configured from a comprehensive selection of calibration parameters, and
- the calibration curve for the compound being calibrated.

All the calibration mode windows are linked so that changes in one

are automatically reflected in all the others. This mode allows graphical selection and modifications of the calibration data.

Quantification is based on %, Normalized %, External standard, External standard %, Internal standard and Internal standard % calculations calculated on either peak area or height. Calibrations may be multilevel and include multiple internal standard definitions. Calibration histories are automatically saved and can be used to weight the recalibration calculations.

The following calibration point weighting options are available:

**Equal** – All calibration points have equal weight in the curve.

**Linear (Amnt)** – A calibration point with the amount  $x$  has the weighting  $1/x$  normalized to the smallest amount so that the largest weight factor is 1. Normalization is done by multiplying the weight with the smallest amount. For example the weight of a calibration point with the amount  $x$  is  $(1/x) \times a$  where  $a$  is the smallest amount of the cali-

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brated compound prepared in the calibration standards. If the origin is included it is assigned the mean of the weightings of the other calibration points.

**Linear (Resp)** – A calibration point with the response  $y$  has the weighting  $1/y$  normalized to the smallest response so that the largest weight factor is 1. Normalization is done by multiplying the weight with the smallest response. For example the weight of a calibration point with the amount  $y$  is  $(1/y) \times b$  where  $b$  is the response corresponding to the smallest amount of the calibrated compound prepared in the calibration standards. If the origin is included it is assigned the mean of the weightings of the other calibration points.

**Quadratic (Amnt)** – A calibration point with the amount  $x$  has the weighting  $1/x^2$  normalized to the smallest amount so that the largest weight factor is 1. Normalization is done by multiplying the weight with the smallest amount. For example the weight of a calibration point with the amount  $x$  is  $(1/x^2) \times a^2$  where  $a$  is the smallest amount of the calibrated compound prepared in the calibration standards.

**Quadratic (Resp)** — A calibration point with the response  $y$  has the weighting  $1/y^2$  normalized to the smallest response so that the largest weight factor is 1. Normalization is done by multiplying the weight with the smallest

response. For example the weight of a calibration point with the response  $y$  is  $(1/y^2) \times b^2$  where  $b$  is the response corresponding to the smallest amount of the calibrated compound prepared in the calibration standards.

**# Calibrations** – A calibration point is weighted according to the number of recalibrations of the point. No normalization is done.

The origin of the calibration curve may be specified as

- ignored — the origin (0,0) is not used in the curve calculations,
- included — the origin is used as one of the calibration points,
- forced — the curve is forced through the origin, and
- connected — the linear segment is constructed between the origin and lowest calibration point on the curve.

Compound identification may be refined by defining individual retention time windows' 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 retention times.

Each calibrated compound may have individual absolute limits for the amount, peak area, peak height, symmetry, efficiency in plates, resolution and  $k'$ . Results lying outside any defined limits

are indicated on the appropriate analysis report. They may be used in conjunction with the control samples that can be defined as part of the automation setup, to verify the performance of the system running automatically. The ChemStation can calibrate methods with up to 1000 peaks and 2000 calibration points. This means, for example, with 1000 calibrated peaks only two calibration levels may be defined for each peak. With fewer peaks more levels may be defined in proportion to these limits (for example, 100 compounds could have 20 levels each).

The group calibration capability allows the user to group calibrated peaks into a named group and report quantitative results for both the individual group members and the group itself.

## Data Analysis - Standard Reporting

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A standard set of user definable report styles for sample reporting are selectable from the report specification screen. Every standard report type contains standard information groups and a series of optional information groups.

The standard groups include

- A header with the originating data file and sample name.
- A footer with the instrument name, operator name, print time and page number in 'page x of y' format.
- A sample information block that includes sample name, vial number, method and sequence information, operator and instrument name and sample information text.
- A quantification results table containing retention times and the integration or quantification table depending on the calculation scheme chosen. This table can be formatted either by retention time or by signal.

Users may select from a series of optional information groups by specifying a particular style for the analytical report. These groups include

- A front page that can include user-defined text.
- Repetition of the sample information block on every page.
- Instrument conditions.
- The analytical column for LC and LC/MSD systems.
- The run logbook.
- The chromatogram with annotation options that include selection from peak retention times, compound names, tick marks, baselines and axes. The user

may also select the annotation fonts, graphical orientation, size and whether the graphics are overlaid or separated. If the ChemStation is connected to instruments that can record instrument parameters as a signal, such as temperature, flow and pressure, the user may also select to include these graphics in the report.

- Calibration table and calibration graphics.

Reports may be output to either the screen, printer or to file.

If the screen is selected as the report destination, the report together with graphics will be displayed in the Report Preview window from which it can be printed.

### Report File Formats

A report can be saved in four different formats. Each format has a specific extension. It is possible to select more than one format for a report.

**.TXT** – The report text is printed as an ASCII text file.

**.WMF** – Each report graphic (signal or calibration curve) is saved in a Microsoft Windows metafile (WMF). Several .WMF files for one report are possible. The generated file format adheres to the Microsoft standard metafile format as defined in the Windows software development documentation. These files are compatible with the Aldus Placeable Metafile (APM) format used by a number of proprietary software packages.

**.DIF** – The tabular report data is saved in Data Interchange Format (DIF). This format is accepted by spreadsheet programs such as

Microsoft Excel. Independent from the report style selected, only the information contained in the report style Short will be saved.

**.CSV** – The report is in Comma Separated Values (CSV) format. This is a very simple format for tabular data that is accepted by many spreadsheet programs and databases. Independent from the report style selected, only the information contained in the report style "Short" will be saved. There can be several .DIF and .CSV files for a single report. For each report block, the first file, for example, REPORT00.CSV, contains the report header information. Subsequent files contain the tabular results. If the results are sorted by retention time, only one file is required for the complete table, for example, REPORT01.CSV. If the results are sorted by signal, a separate table is required for each signal. In this case, the files are named Report01.CSV through ReportNN.CSV, where NN is the number of the signal.

**.XLS** – The report is exported to a Microsoft Excel spreadsheet in (XLS) format. The

data generally requires additional processing.

**.HTML** – Results are saved in Hypertext markup language for viewing in web browsers.

The Agilent ChemStation for CE has an additional mobility report that uses the voltage signal and the electropherogram to compensate for the velocity of the compounds migrating through the detector cell.

## Data Analysis - Specialized Reporting

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Advanced reporting capabilities are also included in the 32-Bit ChemStation for users who require a more specialized set of reports. These include statistics on separation quality, reports that include trend analyses between samples and user-defined report layouts.

### System Suitability Reports

System suitability reports enable users to report system performance parameters for individual analyses. There are three variations, or styles of these reports.

The *Standard Performance* report prints parameters for uncalibrated methods that include

- retention time,
- capacity factor,  $k'$ ,
- peak area,
- peak height,
- symmetry,
- true peak width at half height,
- efficiency in plates,
- resolution, and
- selectivity.

For calibrated methods the compound name and amount replace the peak area, height and selectivity columns.

The report header includes the standard header and footer, sample information block, the analytical column parameters and optionally a plot of the chromatogram.

The *Performance and Noise* style adds an evaluation of the signal noise, in up to seven user-defined evaluation ranges, to the data from the performance report style.

The noise parameters are reported as a signal-to-noise ratio for each peak or calibrated compound and a noise table for each signal. Each noise table includes noise calculated by the six times standard deviation, peak to peak and ASTM methods as well as the wander and drift.

The *Extended Performance* style adds plots of each individual peak showing graphically the peak start and stop times, half width and baseline. This style includes the following parameters in addition to the ones reported by the standard performance reports:

- area, height and amount,
- skew,
- excess,
- USP tailing factor,
- time interval between data points and number of data points over the peak,
- statistical moments (M0 to M4),
- peak width at half height calculated by the true, five sigma, tangent and tailing methods, and
- plate/column and plates/meter calculated by the peak width at half height, five sigma, tangent and statistical methods.

Users may define their own noise evaluation ranges and acceptable limits for these performance criteria. Values lying outside the user-defined acceptable limits are indicated on the report.

### Sequence Summary Reports

Sequence summary reports are produced at the end of a series of automated analyses. Their range of application is from a brief sum-

mary of the samples analyzed to a detailed graphical repeatability or trend analysis of user-selectable parameters between different samples analyzed by the same method. The reports are built up from nine optional categories of information:

- a header page that may be user defined,
- the instrument configuration including revision numbers and analytical column or capillary specifications for LC, CE and LC/MSD systems,
- the list of samples scheduled for analysis; the sequence,
- the logbook printout which states what was analyzed and documents the data acquisition and processing steps as well as any unexpected events,
- a printout of the analytical methods,
- individual sample reports,
- statistics on calibration samples,
- statistics on unknown samples, and
- a summary page that may be either a sample summary, one line of information per analysis, or a compound summary with a short compound summary table in addition to the sample summary.

The statistical reports may be selected as standard or extended styles. The *Standard Style* is text-based and includes the mean, standard deviation (SD), relative standard deviation (RSD) and standard error for the following parameters tabulated by compound:

- retention time,
- area,
- height,
- peak width, and
- peak symmetry.

The *Extended Style* includes graphical trend analyses based on a selection of parameters for statistical evaluation. The parameters that can be selected include

- retention time,
- area,
- height,
- amount,
- peak width at half height, by the sigma, tangent and tailing methods,
- peak symmetry,
- tailing factor,
- capacity factor,  $k'$ ,
- theoretical plates by the peak width at half height, sigma, tangent and statistic methods ,
- resolution by the peak width at half height, sigma, tangent and statistic methods,
- selectivity,
- skew, and
- excess.

Technique specific parameters for liquid chromatography include:

- peak purity evaluation factors (with the diode-array spectral evaluation module only), and
- spectral library comparison factor (with the diode-array spectral evaluation module only).

The report includes a separate graphical trend analysis for each selected parameter. Sequence summary reports may be output to the printer, to file or both. The user may select to either print or suppress individual analysis reports together with the sequence summary.

#### Customized Reports

A customized reporting design view is included in the ChemStation for users who want to define the exact content of their own reports. The user graphically defines a report layout which may include general sample information, signal, integration and quantitative analytical result information. The user may define individual elements, such as text, tables and graphics, organize them in sections and graphically adjust the relative position, size and orienta-

tion of each defined element. The individual sections may be added, deleted, re-ordered and nested.

The user may define headers and footers to appear on every page, time stamps for the report and page numbering in the 'page x of y' format. The information included in the report may be any ChemStation or user-defined parameter.

Once the report has been designed it may be associated with a particular method to make it the default report format for that particular type of analysis.

Customized reports may be output to the screen, a printer or a file. Reports to the screen include graphics.

#### Control Chart Reports

A Control Chart feature is included with the ChemStation software. Once this feature is installed and selected, the user may automatically track a selected parameter of a compound each time a method is run. These parameters include: Amount, Response Factor, Retention Time, and Area.

## Utilities and Compatibilities

### General

The ChemStation can import and export data files in the ANDI (Analytical Data Interchange) chromatography format of the Analytical Instrument Association (AIA), revision 1.0, copyright 1992. Data import is supported at com-

pliance level one (sample information and signal data) and data export at compliance level two (sample information, signal data and integration results).

The ChemStation includes commands and functions to support the Dynamic Data Exchange

(DDE) standard of the Microsoft Windows platform as both a DDE client and a DDE server. The command set includes commands to establish and terminate connections, transfer information in both directions and execute remote functions.



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### Data Analysis - Integration

All files (data files, methods, sequences, log files etc) created on previous ChemStation Rev A.xx.xx systems can be loaded and used in the new 32-Bit Rev B.01.0x ChemStation. The Rev B.01.0x system converts Rev A.xx.xx files to a new structure during saving. The new structure

is not compatible for use with older Rev A.xx.xx systems and the system will warn users to save files with a new name when performing the one-time conversion in the new system. To maintain backwards compatibility it is recommended to save converted files with a different name to the original Rev A.xx.xx file. This pre-

serves the original Rev A.xx.xx file which can continue to be used with ChemStation Rev. A.xx.xx systems if desired.

## XML Interface

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XML (eXtensible Markup Language) is a protocol for structuring data in pure text format; the XML file contains data with embedded structural information and, being pure text, it can be edited with a simple editor like Notepad. XML has become a very flexible and portable format especially for exchanging data between different systems.

To connect the ChemStation to a Laboratory Information Management System (LIMS) or Knowledge Management System (KMS) the ChemStation offers an interface based on the standardized XML format. The interface allows manual import of sample data into the ChemStation sequence. This process can be automated using the ChemStation macro language. In addition the

interface allows manual or fully automated export of sample and result information. The XML schema files provided with the software allow an easy adaptation of the interface for a specific LIMS or knowledge Management system. More information is available in the Agilent ChemStation XML interface users guide (Agilent Part Number G2170-90223).

## Customization

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The ChemStation can be customized using a powerful command set. These commands may be grouped to automatically execute a specific function; such a group is called a macro. Users writing macros may define their own variables, build in conditional or looping constructs, perform physical I/O including file handling and

user interaction, nest their macros and schedule and exchange data with other MS-DOS or Microsoft Windows applications.

More information on customization is available in the *Macro Programming Guide* within the Agilent ChemStation online help.



## Automation

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The ChemStation can execute multi-method sequences.

The sequence parameter set may be defined to use automatically generated files or sequentially numbered files with a user-defined prefix of up to fifteen characters. The user may select to run full analyses or data reprocessing only sequences and can also select one of a series of technique specific shutdown commands or a user-defined shutdown macro that runs when the sequence terminates either by error or after all the analyses are completed.

The sequence 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, sample quantification parameters including sample amount, a multiplier and dilution factor, calibration specification, a data exchange parameter (LIMSID) and the number of repeat injections. Depending on the configured instruments and modules, additional fields will be accessible. For example if an Agilent 1100 LC system includes a fraction collector the "Fract. Start" column will appear in the sequence table. The user can configure the columns to be displayed in the sequence table as well as the individual column widths. 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. A sequence table can easily be created or changed using the fill-down wizard function. The sequence import wizard allows the import of sequences from any kind of delimited text file.

Samples may be identified in the sequence table as unknowns, calibration or control sample types. The sample type determines any special data evaluation treatment of the sample:

- Unknown samples are evaluated and reported according to the method specification,
- Calibration samples are used to recalibrate the quantification component of the method as described below, and
- Control samples are evaluated against the limits for each component defined in the method. If the results lie outside any specified parameter range the execution of the sequence will be halted.

Calibration samples may be defined as simple, cyclic or bracketed. Simple recalibrations mean a recalibration occurs each time a calibration sample is defined in the sequence. Cyclic recalibrations occur at defined intervals during analysis of a series of unknowns. In bracketing a series of unknown samples are analyzed between two calibration sets. The quantitative reports for the

unknown samples are then calculated using a calibration table averaged between the two calibration sets.

The partial sequence functionality allows users to see the order of execution of the sequence and also select individual sample entries to rerun or re-evaluate. When re-evaluating data already acquired users can specify whether reprocessing uses the original sample quantification data or new data entered in the sequence's sample table.

Sequences may be paused to run single injection priority samples by another method then restarted without disrupting the automation. Samples can be added to the sequence table while the sequence is executing.

Both the sequence and partial sequence tables may be printed.

Batch Review is an additional mode of data analysis that provides automation by allowing a fast and easy first-pass review of a batch of samples. The batch consists of all or a selection of runs from a sequence. You can check the calibration accuracy and the individual integrations before approving the results. All chromatogram-specific modified integration parameters can be saved for data traceability. Once data is accepted the entire batch can be reprocessed to generate reports with one keystroke.

## Good Laboratory Practice

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The 32-Bit ChemStation is developed to internationally recognized design and development standards and has a number of features specifically to help users operating in a regulated environment. These features help users validate and specify methods, verify that methods are fit for their intended use, verify system performance and operation and ensure the traceability, integrity and security of the data.

### Development Process

The Agilent Certificate of Validation shipped with each software package documents the software development and testing steps executed as part of the development cycle. The development process is registered to the ISO 9001 quality standard. It is documented together with on-site revalidation protocols in the validation CD-ROM.

### Method Specification and Use

- Global methods — the complete instrument and data analysis specification is stored in one place. Methods include individual compound range specifications to check that quantification results are not applied outside the calibrated range.
- The method change history log allows users of a validated method to automatically record how and when a method was changed. Users may add a reason for the change to the

change history log. The change history log is automatically stored as part of the method. To prevent unauthorized access to the records it is protected by the user access scheme, described below. The change history log may be viewed and printed.

- Limits may be assigned on a compound-by-compound basis in each method for a number of chromatographic and system performance parameters, as described in the data analysis quantification section. Results exceeding these parameter ranges are used to control the execution of automated sequences as described in the automation section. They are indicated on the appropriate analysis report.
- System performance or suitability reports (see 'Reporting' sections ) provide detailed analysis of the separation quality.
- The ChemStation may be configured for restricted access through two user access levels, an operator and manager level. The manager level may be password protected and allows access to the complete ChemStation functionality. The operator level restricts the user to key functionality and to executing defined analytical methods. The operator level is intended for use in routine laboratories and specifically prevents users from modifying and creating new methods.

### Method Robustness

Sequence summary reports (see section "Data Analysis - Specialized Reporting" provide a means to test methods for robustness. The extended format reports for user-selected criteria are reported as trend charts and may be used to determine the realistic operation limits. These limits can then be incorporated in the method to ensure, through the analysis of control samples, that the method is operating within specifications.

### System Operation

The ChemStation software verification kit, that is part of the standard software, automatically checks for the correct operation of the data evaluation parts of the software by comparing results generated when a test is executed against pre-recorded known values. The verification test allows users to define their own data files and methods to be the basis of the test.

### Data Traceability, Integrity and Security

- The run-time logbook provides a transaction log of the complete system. It also records any unusual events (such as errors or parameter changes made during a run), as well as the instrument conditions before and after each analysis. A copy of the relevant logbook extract is saved with each data file.

- 
- The actual instrument conditions, such as pressure, flow, and temperature, that occurred during each analysis are also recorded if the configured instrument supports this capability. This data can be subsequently displayed graphically with the chromatogram to show the actual instrument conditions during that particular analysis. These graphics may be included on each report.
  - Methods saved with the data file record the actual method at the time of the analysis and allow the complete reconstruction of the reported data at a later date. The method is saved at the completion of all the analytical steps.
  - All reports have time stamps and traceable page numbering ('page x of y' style). The user may select the level of detail in each report ranging from simple summary reports to complete system details (see Reporting section).
  - GLP save register files, specified as part of the method configuration, save all the original data including sample information, data analysis method, chromatographic signals, instrument conditions, integration and quantification results, report data and the run logbook in one checksum protected binary file. This is an uneditable binary format that ensures the integrity of the results. The file includes a revisioning scheme that indicates if data has been reprocessed.
  - Control sample types may be defined in the sequence table and used to automatically check the instrument performance against quality control sample results when the instrument is running unattended. Results that are outside the user-specified acceptable range will stop the automatic execution of the instrument.
  - Data security is achieved in the PC environment through password protected PCs, software locks built into both Microsoft operating systems and secure (password-protected) networks.

## Instrument Control

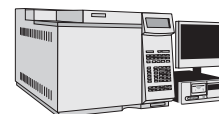
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The instrument control capabilities of the Agilent ChemStation may be expanded through the purchase of additional instrument

modules to allow multiple instrument, mixed technique configurations.

The instrument control capabilities

are documented in the following sections, each relating to a specific technique.



## Agilent ChemStation for GC

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### **Instrument Control and Data Acquisition with the Agilent ChemStation for GC (G2070BA) and the Additional GC Instrument Module (G2071BA)**

The Agilent ChemStation for GC combines instrument control, data acquisition, and data analysis software for the Agilent 6890, 6850, 5890 Series II, and 4890D gas chromatographs and the Agilent 35900E A/D converter.

The Agilent ChemStation is interfaced to the GC via GP-IB, or LAN and collects full range digital data from detectors. Depending on the detector type, data can be acquired at rates up to 20 Hz from the Agilent 5890 and Agilent 4890D Series and up to 200 Hz from the Agilent 6890 and Agilent 6850 Series.

When interfaced to an Agilent gas chromatograph, the Agilent ChemStation can control GC parameters for heated zones, oven temperatures, detectors, inlets, cryogenic cooling, signals, electronic pressure and flow control, and cool on-column temperature programming.

In addition to GC control the following features are noted:

- Graphical user interface for easy access to all method areas for all Agilent GCs
- Table driven system scheduler which permits clock time programming for all Agilent GCs. Quick Method allows the Agilent Series 6890 and Agilent 6850 GC user to enter a limited number of setpoints from which the Agilent ChemStation will create a method.
- Method resolution in the Agilent ChemStation (Agilent 6890 and Agilent 6850 Series only) will verify and alert the operator of potential problems if a method was created on a different GC system or if the configuration has changed.
- Capillary columns can be calibrated from the ChemStation

The Agilent ChemStation can display graphically the oven temperature, inlet temperature, inlet pressure, auxiliary channel pressure and column flow programs. The Agilent ChemStation also can con-

trol, through a timetable, a maximum of eight valves or relays.

### **Sampling**

The Agilent 7673 and Agilent 7683 Series automatic samplers allow for complete automation of sample introduction in single front, single rear or dual-injector configurations.

Dual-injector configurations (Agilent 6890 Series, 5890 II, and 4890D GCs) allow individual or synchronous injections. Each automatic sampler allows a 3-vial turret, 8-vial turret, or 100-vial access if a sample tray is fitted. (6890 and 5890 Series only). The 6850 GC also supports the G2880A 22/27 positions tray. The Agilent ChemStation allows random sample access and priority sample injection.

The following autosampler parameters may be controlled:

- number of syringe pumps
- number of syringe washes
- the injection volume
- the bottle number for each injection

- a viscosity delay
- on-column injection setup
- syringe size
- depth of needle penetration
- multiple injections per run in cooperation with PTV for large volume injection
- For the Agilent 7683 Series, plunger speed may be controlled from a maximum of 100 µl/sec to a minimum of 5 µl/sec when using a 10 µl syringe.
- For the Agilent 7683B, larger turret for 2x increase in solvent and waste capacity (6890, 6850 only).
- For the Agilent 7683B, solvent saver made for 4x increase in solvent usage (6890, 6850 only).
- For large volume injections a 100-µl syringe can be used with the Agilent 7683 Series.

The Agilent ChemStation allows the user to optionally display a Sampling Diagram window containing a graphical display of the one hundred vial tray, indicating which samples have already run, which sample is currently running, and which samples will be run.

The G1926A bar code reader attachment is supported in the 100-vial tray configuration of the autosampler. The bar code reader can be used to help build automation sequences and verify that the identity of the injected sample matches the name in the sequence table at injection time.

The new G2615A bar code reader is used with the 7683 automatic liquid sampler tray.

The Agilent ChemStation can acquire a third and fourth signal

from external detectors in a single run by adding the 35900E A/D converter.

### **Agilent GC ChemStation Companion**

The Agilent ChemStation Companion provides the user with a simple single-screen user interface for GC routine analysis. In the Companion View, the user is limited to selecting pre-programmed samples, methods, vial numbers, and run control. Users cannot modify or create any methods or run any methods or samples not assigned to them by their lab manager. The Agilent ChemStation Companion is installed automatically during the GC ChemStation installation.

### **Retention Time Locking Software**

Retention Time Locking (RTL) software, product number G2080BA, is an add-on to the G2070BA.

Retention Time Locking (RTL), is a useful technique developed by Agilent Technologies to match analyte retention times between and among Agilent GC systems. RTL is essentially based on void-time matching through an empirically determined pressure-retention time calibration curve. RTL calibration curves are specific to the analyte chosen (pick one analyte in your standard, the best choice is a peak well separated from other peaks and in the middle portion of the chromatogram), type of column used (stationary phase type, phase ratio, and column dimensions), carrier gas type,

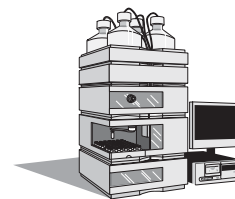
and oven temperature program used in the method. Once the calibration has been done for an initial ("original") method, the method and its associated RTL calibration can be transferred to another instrument with the same column type and carrier gas type. RTL software in Agilent ChemStations assists with the process of determining and using RTL calibrations.

To lock a new system to the original system, carrier gas head pressure is adjusted using the RTL calibration curve. The retention time of a target compound (same one used to generate the RTL calibration) can be locked onto the desired retention time value. All other analyte retention times will then also match those of the original.

RTL software also provides the capability to search retention timetables. Searching unknowns is based primarily on retention times and may also include element information (such as one might get from selective detectors) to narrow search results further. Users can create, edit, import and export RTL libraries.

The RTL Pesticide Library, product number G2081AA, includes the retention times for pesticides and suspected endocrine disrupters. To use this library, the RTL software product G2080BA must be installed. Peak identification is performed by comparing the retention time of the unknown peak with that of a standard included in the library table.





## Agilent ChemStation for LC Systems

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### Instrument Control and Data Acquisition with the Agilent ChemStation for LC Systems (G2170BA) and the Additional LC Instrument Module (G2171BA).

The Agilent ChemStation for LC and additional LC instrument module controls and acquires data from the Agilent 1100 Series modules and systems for LC, the HP 1090 Series liquid chromatography systems with either the filter photometric detector (FPD) or built-in diode-array detector (DAD), the stand-alone HP 1040 diode-array detector (DAD), the HP 1046A fluorescence detector (FLD), the HP 1049A Electrochemical Detector (ECD) and the Agilent 35900E dual channel interfaces. All the sampling, pumping and detector options of the Agilent 1100 Series modules and systems for LC, and the HP 1090 Series liquid chromatographs can be controlled.

### Sampling Systems

The injection systems may be manual or automated with an autosampler or well-plate autosampler. All automatic injectors may be programmed for different injection volumes, the speed of injection and the injector wash procedure. The user may also specify a complete injector program for sample dilution, standard addition or sample derivatization. The commands available for the injector program include draw, eject, mix, wait, inject, sampler valve and column switch control. These can be defined in conjunction with the sample, a vial/well-plate offset from the sample, a number

red vial/well, waste and air.

The Agilent bar code reader (G2256A) is available for selected autosampler configurations. It can be used to help build automation sequences and verify the identity of the injected sample matches the name in the sequence table at injection time. In LC configurations it can also be used to mix liquid samples as a step in an injection program.

The following Agilent 1100 injection systems are supported:

- Standard autosampler (G1313A / G1329A)
- Thermostatted standard autosampler (G1327A)
- Well-plate autosampler (G1367A)
- Thermostatted well-plate autosampler (G1368A)
- Micro well-plate autosampler (G1377A)
- Thermostatted micro well-plate autosampler (G1378A)
- Thermostatted micro autosampler (G1387A)
- Preparative autosampler (G2260A)
- Thermostatted preparative autosampler (G2261A)
- Agilent sample capacity extension (G2257A) for the 1100 Series well-plate sampler G1367A and micro well-plate sampler G1377A
- Agilent dual loop autosampler (G2258A)
- Agilent thermostat option (G1330A / B)
- Agilent fraction collectors (G1364A / B / C / D)
- Agilent 1100 Series barcode reader (G2256A) for the sample capacity extension G2257A

### Solvent Delivery Systems

All the solvent delivery systems have a set of initial parameters, including pressure limits, initial flow and composition, that are complemented by a time-table for programming changes in flow, composition and pressure limits. These parameters can be viewed graphically. Users can define a post-run time for column equilibration.

The following Agilent 1100 solvent delivery systems are supported:

- Isocratic pump (G1310A)
- Binary pump (G1312A)
- Quaternary pump (G1354A / G1311A)
- Preparative pump (G1361A / G1391A with gradient extension)
- Capillary pump (G1376A pump only / G1382A with degasser)
- Agilent 1100 nanoflow pump (G2226A pump only / G2225A with degasser)

### Column Compartments

The Agilent 1100 Series thermostatted column compartment can be set between 10 °C below ambient and 80 °C. The temperature is programmable during the run through a timetable. The HP 1090 column oven temperature can be set to a constant temperature (20 °C above ambient to 100 °C without external cooling). Column switching valves are programmable from the software.



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## Valves

The Agilent ChemStation supports external valves as well as thermostatted valves built into the column compartment.

The following external Agilent valves are supported:

- Agilent 1100 Series 6-position/7-port valve (G1156A)
- Agilent 1100 Series 2-position/10-port valve (G1157A)
- Agilent 1100 Series 2-position/6-port (standard) valve (G1158A)
- Agilent 1100 Series 6-position selection valve (G1159A)
- Agilent 1100 Series 12-position/13-port selection valve (G1160A)
- Agilent 1100 Series 2-position/6-port (micro) valve (G1162A)
- Agilent 1100 Series 2-position/10-port (micro) valve (G1163A)

The following thermostatted valves built into the column compartment are supported:

- 2-position/6-port valve option (G1316A # 055)
- 2-position/6-port micro valve option (G1316A # 056)
- 2-position/10-port valve option (G1316A # 057)

The maximum number of external valves connected to one Agilent 1100 Series HPLC system is limited to 5 or less, depending on the system configuration. For details please contact your Agilent representative.

## Detectors

Spectral data from all diode-array detectors may be acquired in a peak-controlled or full acquisition mode.

The ChemStation software can simultaneously acquire five chromatographic and reference signals each with an independent bandwidth from the *Agilent 1100 Series diode-array detector (G1315A or G1315B)*.

The system can simultaneously acquire up to a total of eight chromatographic and reference signals from the *HP 1090* with an independent bandwidth.

The detectors have a graphical test for signal intensity and wavelength calibration. All DADs may have the initial parameters changed during a run by a time-based program. Users can program wavelength and spectral acquisition mode changes in the time table.

Initial parameters that may be set for the DADs include signal wavelengths and reference wavelengths, spectral acquisition mode, signal sampling rate and autobalance.

The Agilent 1100 Series diode-array detector (DAD), G1315C, and the Agilent 1100 Series multiple wavelength detector (MWD), G1365C, support 80Hz full spectral Data Acquisition. The G1315C and G1365C support up to 80Hz data acquisition of up to 8 Signals and offer data buffering on a built-in

Compact Flash Card to provide 'data never lost' insurance. The cells and UV lamp utilize RFID tags to capture and store lamp and cell information. The improved Temperature Management System provides ambient rejection and stable cell temperature.

The *HP 1090 filter photometric detector (FPD)* may be programmed with parameters to set the lamp current, response time and the filter. The filter may be changed during an analysis through events in the detector's time table. The ChemStation includes a diagnosis screen for testing the reference and sample photo diode light paths in the detector. The FPD is interfaced to the ChemStation through the digital GP-IB interface for control and through a dual channel A/D interface for the data acquisition (see below).

The excitation and emission wavelengths of the *HP 1046A Fluorescence Detector (FLD)* can be set from 190 to 800nm, in steps of 1nm. Gain, response time, gate, delay and lamp frequency may also be set. Gain and changes in the emission and excitation wavelength may be time-programmed. The excitation and emission wavelengths may be optimized by analyzing scans. The range and speed may be specified for each scan during the optimization process. The scans taken during an analysis are stored in a ChemStation spectral file format that allows them to be displayed and used in a spectral library.

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The *HP 1049A Electrochemical Detector (ECD)* may be used in amperometry, pre-treatment, sweep, pulse and differential mode. The voltage potential and limits may be defined between -2.0V and +2.0V in steps of 0.001V. A voltage potential increment between analysis may be defined from -2.0V and +2.0V in steps of 0.001V and the number of repeat analyses at a given increment may be set. Drift limits for the detector not ready condition may be specified from 0.1 nA to 500 nA in steps of 0.1 nA. The user may also specify auto-zero control, based on the prepare or stop signal or a user defined drift value, full scale detector output at 0.05ma or 500ma, the signal polarity and the temperature of the solvent thermostat (20 to 60°C).

The Agilent 1100 Series variable wavelength detector (VWD) may be programmed with a single detection wavelength. Data acquisition rates may be programmed for peak widths from <0.12 up to 8.00 seconds. The VWD can be programmed with a timetable to change the wavelength and perform wavelength scans during the course of an analysis.

The *Agilent 1100 Series multiple wavelength detector (MWD)* (G1365A or G1365B) can simultaneously acquire up to five chromatographic signals each with inde-

pendent reference wavelengths and bandwidths. The signal acquisition rate may be set for peak widths between 0.1 and 16 seconds. During the course of an analysis the MWD can be programmed with a timetable to change wavelengths, bandwidths and peak-widths for all five wavelengths.

The *Agilent 1100 Series multiple wavelength detector (MWD)*, G1365C, can simultaneously acquire up to 8 Signals at an 80Hz data acquisition rate. Data Buffering is possible on a built-in Compact Flash Card providing 'data never lost' insurance. The cells and UV lamp utilize RFID tags to capture and store lamp and cell information. The improved Temperature Management System provides ambient rejection and stable cell temperature.

The optical unit temperature of the *Agilent 1100 Series refractive index detector (RID)* can be set between 20 and 55°C. The signal acquisition rate may be adjusted for peak widths from <0.12 up to 8 seconds. During the course of an analysis the RID can be programmed with a timetable to change Polarity and Peakwidth of the acquired chromatographic signal. For diagnostic and troubleshooting purposes, it is possible to store Diode Signal 1, Diode Signal 2, Optical Unit Temperature, Polarity and the Balance Signal in addition to the chromatographic signal.

The *Agilent 1100 Series fluorescence detector (FLD)* may be programmed for single wavelength or simultaneous multiple wavelength detection and spectra acquisition. Up to four signals at different excitation or different emission wavelengths may be obtained. Within a timetable initial excitation or emission wavelengths, response time, PMT Gain and baseline behaviour as well as spectral parameters may be changed. Excitation or emission spectra can be watched online and stored and analyzed as described for DAD spectra. For a single compound trapped in the flow cell, complete information on excitation and emission spectra is available in a single task with the fluorescence scan and can be watched as an iso-plot or as 3D-graphics.

The *Agilent 35900E dual channel interface* allow the system to acquire data from detectors that are not interfaced for data acquisition through GP-IB or LAN, such as the FPD, the HP 1047A refractive index detector or a third party detector. One or two analog signals per instrument may be configured; if only one is used the other is available for use with another instrument. Data rates up to 100 Hz per signal may be defined. The user may also define the units for acquisition and their relationship to the voltage signal (units/volt).

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The Agilent 35900E interfaces offer external event control through digital TTL (transistor-transistor logic) signals, each of which are given specific state (high and low) names, that may be time-programmed before, during and after an analysis. The Agilent 35900E can be configured for up to eight signals for each independent channel.

### **Fraction collectors**

All different versions of the Agilent 1100 Series fraction collectors (G1364A, G1364B, G1364C, G1364D) can be fully controlled from Agilent ChemStation. Fraction data can be reviewed in the fraction task of the data analysis screen. The maximum number of fraction collectors connected to one Agilent 1100 Series Purification system is limited to 3 (with the possibility for one additional recovery fraction collector). Depending on the system configuration up to two Purification systems can be controlled from single ChemStation system (without purification related software add on). Optional add-on software, e.g. High/Throughput Purification software (G2262AA, G2263AA, G2265AA) or Easy Access (G2725AA) provides advanced functionalities.

### **Agilent 1100 Series Instrument Verification**

The Agilent ChemStation for LC includes an instrument operational qualification and performance verification (OQ/PV) view in which users of the Agilent 1100 Series of modules and systems may select a series of semi or fully-automated tests to test the operational suitability of the LC instrument.

To perform instrument verification it is first necessary to purchase the relevant service from Agilent Technologies. The required method and sequence files will be installed at the time of service delivery by an authorised Agilent service provider. Please contact your local Agilent Technologies representative for more details.

### **Agilent 1100 Series Diagnostics**

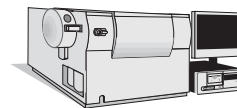
The Agilent 1100 Series of systems and modules for LC have an additional ChemStation diagnosis view.

The diagnosis view is designed to help users identify instrument malfunctions starting from a particular symptom. A failure of a

particular instrument verification test will automatically identify the appropriate symptom for the user or the user may select the symptom interactively.

One or more possible causes is listed for each symptom. Each possible cause is associated with a series of diagnostic measurements, with limits, and a series of diagnostic tests. Users observe the measurements and carry out the tests in order to confirm or dismiss the possible cause of the instrument malfunction.

Once identified, the cause of the instrument malfunction may be repaired by using the repair procedures given on the Agilent 1100 Series Maintenance and Repair CD-ROM. The repair procedures include parts and materials breakdowns and clear animated step-by-step graphics or video with a sound track for each repair procedure. The procedures are called directly from the Agilent ChemStation diagnostics view.



## Agilent ChemStation for LC/MSD Systems

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### **Instrument Control, Data Acquisition, and Data Evaluation with the Agilent ChemStation for LC/MSD Systems (G2710BA) and the LC/MSD ChemStation Add-on Module (G2715BA)**

The Agilent ChemStation for LC/MSD systems (G2710BA) and the LC/MSD ChemStation Add-on module (G2715BA) provide control, data acquisition, and data evaluation capabilities for Agilent 1100 Series LC/MSD systems. The G2710BA and G2715BA LC/MS software includes the G2170BA LC ChemStation and G2180AA diode-array detector (DAD) spectral evaluation module. Add-on module. Together, these software components provide integrated control with a common graphical user interface for all of the Agilent 1100 Series LC modules and systems, including the Agilent 1100 Series DAD as well as the Agilent 1100 Series LC/MSD. In addition to the Agilent 1100 Series family of modules and systems, the HP 1090 Series II liquid chromatography system, as well as the Agilent 35900E A/D interface can be controlled by G2710BA as part of LC/MSD systems. The Agilent ChemStation for LC/MSD system supports a single Agilent 1100 Series LC/MSD system.

### **LC/MSD System Control**

The software provides digital control of the LC/MSD API ion source and ion optics, dynamic ramping of ion optics element voltages, and

control for spraying and drying gases. Method-specific LC/MSD parameters include spectral acquisition mode (scan/SIM), signal sampling rate, LC/MSD tune file, ionization mode (APCI, APPI or API-ES mode) and polarity (positive or negative ion detection). Within a LC/MSD method, LC/MSD-timed events include mass range, SIM ion groups, mass analyzer stepsize, fragmentor voltage, electron multiplier gain, MS on/off, and API ion source parameters. Fragmentor voltage settings may be dynamically ramped within a scan to optimize response for various  $m/z$  values. LC/MSD operating parameters such as fragmentor voltage, drying gas temperature, and EMV gain can be acquired and saved with a data file. These instrument parameters can be displayed and plotted as a record of the exact values associated with the acquired data.

In addition to the standard ChemStation automation capabilities for single run methods and multiple method sequences, an FIA (Flow Injection Analysis) Series automation mode is available through software selection. In this mode, which requires the Agilent 1100 Series LC autosampler, the Agilent 1100 Series LC/MSD system can be programmed to make multiple injections from a single or multiple sample vials, storing all data in a single datafile. Up to two LC/MSD method parameters can be programmatically varied with each injection.

The system includes the ability to do fast scanning of up to 5250 amu/sec and includes autotune for fast scanning. Also included is support of the Agilent Analog Output Accessory which provides up to 12 SIM signals directly to a customer LIMS system.

### **LC/MSD Tuning**

The Agilent ChemStation for LC/MSD systems includes a LC/MSD tune view in which users of the Agilent 1100 Series LC/MSD may select to either automatically, or manually tune the instrument. The Agilent 1100 Series LC/MSD integrated calibrant delivery system is software-controlled, and together with the software autotune provides fully automated tuning of the Agilent 1100 Series LC/MSD for API-electrospray (API-ES), atmospheric pressure chemical ionization (APCI) and atmospheric pressure photo ionization (APPI) modes of operation. An extensive set of manual tune capabilities is also provided for users who wish to manually tune the Agilent 1100 Series LC/MSD.

### **Agilent 1100 Series LC/MSD Instrument Verification**

Computer-aided operational qualification and performance verification (OQ/PV) tests and procedures can be used to verify that system performance is acceptable on an ongoing basis. Early maintenance feedback (EMF) tracks the status

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of system maintenance items and provides notification when a preventive maintenance procedure is due. On-line diagnostics enable system troubleshooting using integrated tests. System logbooks provide date- and time-stamped records of runs, errors, and maintenance events.

To perform instrument verification it is first necessary to purchase the relevant service from Agilent Technologies. The required method and sequence files will be installed at the time of service delivery by an authorised Agilent service provider. Please contact your local Agilent Technologies representative for more details.

### **Diagnostics/Early Maintenance Feedback**

The Agilent 1100 Series LC/MSD software extends the diagnosis view of the existing LC ChemStation to include tests for the Agilent 1100 Series LC/MSD. The diagnosis view is designed to help users identify instrument malfunctions starting from a particular symptom. Maintenance and repair procedures for the Agilent 1100 Series LC/MSD can be called directly within the diagnosis view from the Agilent 1100 Series LC/MSD Maintenance and Repair CD-ROM. The procedures include parts and materials breakdowns and clear animated step-by-step graphics and multimedia clips for each repair procedure.

Early Maintenance Feedback

(EMF) automatically notifies the user when maintenance is required for key system components such as rough pumps, calibrant delivery system, spray chamber, and electron multiplier.

### **LC/MS Technical Primer**

The Agilent ChemStation for LC/MSD includes an on-line multimedia LC/MS technical primer. The primer includes information to assist users of the Agilent 1100 Series LC/MSD system with a variety of LC/MS technical topics, including API-LC/MS theory, method development and solution chemistry for API-LC/MS, and CID (collision induced dissociation).

### **LC/MSD Data Evaluation**

The LC/MSD ChemStation includes all of the data evaluation capabilities of the Agilent 3D ChemStation for LC, including data evaluation for UV-visible spectra acquired from a supported diode-array detector (DAD). In addition, the LC/MSD ChemStation includes capabilities for evaluation of mass spectral data acquired from the Agilent 1100 Series LC/MSD module.

Both UV-visible and LC/MSD data can be viewed, compared, and printed. Chromatograms from the separate detectors may be simultaneously displayed, aligned, and resized to correlate peaks from one chromatogram to the other. Mass spectra and UV-visible spectra can be simultaneously

reviewed using a common spectral toolset. Reports can include either UV-visible or mass spectral data, or both.

### **Interactive Data Processing**

The data from the mass selective detector may be displayed in a number of ways. The total ion chromatogram (TIC) is the summation of all mass signals ( $m/z$  values) over the entire acquired data range. An extracted ion chromatogram (EIC) displays the signals of individual ions ( $m/z$  values) or a range of  $m/z$  values.

The mass selective detector signals (TIC and/or EICs) may be displayed along with those from other LC detectors. The software permits peak alignment for chromatograms from different detectors connected in series. Full, comparative mass and UV-visible spectra manipulation are available including selection of spectra by:

- individual spectrum,
- peak apex spectrum,
- average spectrum over a graphically defined retention time range
- range of spectra, and
- all spectra over a peak.

The user may also select how the spectra are processed when they are displayed. The available options include:

- background subtracted spectra,
- limiting the  $m/z$  range,



- smoothing,
- normalization, and
- continuous curves or histogram mode.

## Quantification

All of the standard ChemStation quantification capabilities are available for use with mass spectral data. TIC or EIC signals can be used for quantification. For target compound analysis, retention time windows, quantification ion signals, and qualifier ion signals/ratios can be defined on a per-compound basis.

## Peak Purity

The LC/MSD ChemStation includes all the UV-visible peak purity data evaluation capabilities of the Agilent diode-array detector (DAD) spectral evaluation module. Capability for peak purity determination using LC/MSD mass spectral data is also included. Peak purity may be determined interactively on either a peak by peak basis, for all the peaks from a certain data file, or automatically at the end of an analysis as part of the method.

The user can select to interactively evaluate peak purity for data sets that include both DAD spectral data and LC/MSD spectral data in either a single or dual mode. In single mode, the software configures the purity user interface for evaluation of data

types at a time. The user can toggle between the data types if desired. The dual mode user interface permits simultaneous evaluation of spectral purity using both DAD and LC/MSD data.

In interactive operation, the LC/MSD peak purity function examines the most significant ions across a user-selected chromatographic peak to determine if more than one compound is present. The software automatically overlays extracted ion chromatograms for the selected peak, with each extracted ion chromatogram displayed in a separate color. A table of the number of components located and the two most significant ions used to resolve each component is displayed. The next/previous peak or the next/previous impure peak can be selected by simple mouse actions. A purity report that includes peak purity assessment for all peaks in a chromatogram can also be specified and displayed/printed.

## Iso-abundance Plot and Three Dimensional Plot

In addition to iso-absorbance and three dimensional plots for UV-visible spectral data, the LC/MSD ChemStation also provides equivalent capabilities for mass spectral data.

The MS iso-abundance plot displays acquired mass spectra as a color-contoured map of m/z against retention time together with areas for display of m/z sig-

nals and mass spectra defined by the position of cross-hairs on the iso-abundance plot. In the iso-abundance plot, a color scale is used to represent signal intensity. Users can define the contour color schemes and retention time and m/z ranges for the display.

Acquired mass spectra can also be displayed as a three dimensional plot of m/z against retention time and abundance. The display can be graphically adjusted by the user in the time, m/z, and intensity domains. The resolution of the plot is selectable, and the orientation of the plot can be adjusted graphically. The plot may be printed, and the color scheme adjusted.

## Agilent 1100 Chip Cube Interface (G4240A)

The Agilent 1100 Chip Cube interface is designed for LC systems using an Agilent Ion Trap MSD as detector and Bruker Software for Data Analysis. The ChemStation provides software support for this interface.





## Agilent ChemStation for A/D

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### **Acquisition with the Agilent ChemStation for A/D (G2072BA) and the Additional A/D Instrument Module (G2073BA)**

The A/D ChemStation and additional A/D interface acquisition module controls and acquires data from Agilent 35900E dual channel interface. These interfaces allow the ChemStation to acquire data from instruments that are not capable of being interfaced for data acquisition through the GP-IB system or LAN. One or two analog signals per instrument may be configured; if only one is used the other is available for use with another instrument running on another timebase. Data may be acquired at up to 100 Hz per signal.

The user may also define the units for acquisition and their relationship to the voltage signal (units/volt). The Agilent 35900E interfaces offer external event control through digital TTL (transistor-transistor logic) signals, each of which are given specific state (high and low) names, that may be time-programmed before, during and after an analysis. The Agilent 35900E can be configured for up to eight TTL signals for each independent channel.

## Additional Data Evaluation Modules

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The data processing capability of the ChemStation may also be expanded through the purchase of additional data processing modules for specific applications:

- LC diode-array detector (DAD) spectral evaluation module (G2180BA)
- Agilent ChemStore sample organization and results database module (G2181BA)

### LC Diode-Array Detector (DAD) Spectral Evaluation Module (G2180BA)

UV-visible spectra, acquired using a diode-array detector, may be graphically selected from a chromatogram signal for visual inspection and comparison or may be used for peak purity determinations, wavelength optimization and component identification through spectral libraries. The spectral library functionality can be extended to automatic identification of components in up to four user-defined spectral libraries based on peak or target compound identification.

### Interactive Spectral Processing

Users may graphically select spectra from a chromatographic signal for visual inspection and printing. The spectra are displayed in a separate spectral window and may be overlaid for comparisons. The user can select spectra in the following modes:

- individual spectrum,

- peak apex spectrum,
- average spectrum over a graphically defined retention time range,
- range of spectra, and
- all spectra over a peak

The user may also select how the spectra are processed when they are extracted. The available options include:

- setting the subtracted reference spectrum or spectra,
- limiting the extracted wavelength range,
- customizing the spectral and reference display, and
- setting the spectral processing. Options include setting a smoothing and splining factor, logarithmic processing and derivative order.

### Peak Purity Determinations

Peak purity may be determined interactively on a peak by peak basis, for all the peaks from a certain data file, or automatically at the end of each analysis as part of the method. Users may optimize peak purity processing for accuracy or performance by setting preferences relating to:

- the number of spectra used over a peak,
- the wavelength range used for the purity determination,
- the reference spectra,
- the purity threshold,
- spectral processing including logarithmic, smoothing and splining factors and derivative order.

The purity components are calculated and displayed. These include the spectra, the spectral differences, the signals, a signals-based ratiogram, similarity and threshold curves.

Similarity curves give the most detailed information about a peak's purity. User selected or average spectra are compared with all the other spectra acquired during the peak's elution and the resulting spectral comparison factors are plotted as the similarity curve. For a perfectly pure peak the similarity curve will be a straight line corresponding to a theoretically pure compound. Impurities will cause a deviation from this ideal line. The similarity curves are plotted with reference to the theoretically pure line and the user-defined purity threshold. The similarity curve gives the best indication of any impurities that occurred in the peak as it eluted. The deviation of the similarity curve from the ideal theoretically pure value is influenced by both compound impurities and spectral noise. The user-defined purity threshold may be replaced by a system calculated threshold curve based on the signal-to-noise ratio of the peak in question. The noise sample may be user selected and, if truly representative of the spectral noise when the peak eluted, compensates for any deviation of the similarity curve, from the theoretically pure value, attributable to spectral noise.

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### Wavelength Optimization using the Iso-absorbance Plot

UV-visible spectra, acquired continuously during an analysis, can be used to determine the optimum signal wavelengths and bandwidths for routine detection by a signal-based method. The iso-absorbance plot displays the acquired spectra as a color-contoured map of wavelength against retention time together with areas for the display of both signals and spectra defined by the position of the cross-hairs on the iso-absorbance plot.

The iso-absorbance map can be used in four modes:

- Quick view mode allows users to view and compare spectra and signals by moving a cross-hair over the area of the contour map. Spectra and signals are continuously extracted and updated in the display areas. The extracted spectra and signals may be frozen in the display areas for comparison purposes.
- Zoom mode allows users to zoom into areas of interest on the iso-absorbance map.
- Signals mode allows users to extract a particular signal, with a graphically determined bandwidth, into the chromatographic window for routine data processing such as integration and quantification.
- Spectral mode allows users to extract spectra into the spectral window for further processing.

The iso-absorbance plot is typically used during method development to explore the sample's response at different UV-visible wavelengths in order to determine the optimal detection wavelengths and bandwidths through experimentation with the integration and quantification processes.

Users can define the contour color schemes and retention time and wavelength ranges for display.

### Three Dimensional Plot

UV-visible spectra acquired continuously during an analysis, can be displayed as a three-dimensional plot. The display may be graphically adjusted by the users in the time, intensity and wavelength domains. The resolution of the plot is selectable.

- The orientation of the plot can be adjusted graphically. The orientation of the display is not restricted in any dimension.
- The plot may be printed.
- The color scheme used in the plot may be selected from a number of choices.

### Spectral Libraries

Spectral libraries allow users to positively identify compounds by comparing the spectra of peaks in the sample to libraries of spectra derived from analytical standards.

The ChemStation allows users to use libraries both interactively and automatically. The ChemStation

can manage an unlimited number of spectral libraries each with up to as many entries as there is available system memory (typically hundreds of entries). Libraries may be loaded and searched by selecting individual spectra from a chromatogram and searching the library for the best matches. The library search may be constrained by specifying a search template that allows the user to define a retention time window and include the informational data associated with each library entry. For example, the applicable retention time can be constrained to  $\pm 5\%$  of the library retention time and the entry names must start with the letter 'B'. The search results may be displayed on the screen and printed.

Users may build their own libraries by analyzing known substances under defined analytical conditions, creating a new library and entering the individual spectra and the information fields to describe the entry into the library. Library entries may be added, deleted, edited, viewed or printed. Details of each spectrum in a library including absorbance and wavelength data may be examined.

### Automated Spectral Library Search Reports

Automated spectral library search reports allow users to automatically identify and quantify unknown samples based on the positive identification from up to

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four separate spectral libraries. Search criteria may be specified for each library separately through a library search template that allows users to constrain the search both in the retention time and library entry identification parameters.

One of three search modes may be selected :

- Standard search mode identifies each integrated peak in the chromatogram from the library.
- Target analysis from the calibration table limits the library search to those library entries identically named in the calibration table. Identification may be further constrained through the use of the library template to restrict other search criteria such as the retention time window. After positive identification, quantification proceeds according to the data in the calibration table
- Target analysis from the library uses the library entries to identify peaks in the chromatogram that are within the RT window specified for the particular library entry. This mode differs from the standard search mode in that it excludes peaks whose retention times are not covered by library entry time windows.

Consequently it is typically faster than the Standard search, especially if there are many more peaks in the sample than there are entries in the library. After positive identification, quantification proceeds according to the data in the calibration table.

The calculation of the peak purity factor may be included as part of the library search.

Report styles can be selected to produce simple library search reports or a combination of library search and standard performance reports described above.

### **Spectral Data Import and Export**

The ChemStation spectral module can import spectra stored in Agilent's .WAV format files, from the HP 8452 and Agilent 8453 spectrophotometers, and industry standard JCAMP spectrum files.

The ChemStation is data file compatible with Agilent's ChemStation for UV-visible spectroscopy running in the Windows environment. Both DAD and UV-visible spectra may be exchanged between the two systems either as ChemStation register files or through the Windows clipboard.

## High Throughput Purification Software Module (Purify)

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The High Throughput/Purification software module (G2262AA) is designed for the needs of preparative HPLC. It offers utmost flexibility for purification of large numbers of samples. For efficient data review the graphical user interface provides an easy way for sample and fraction tracking. Sophisticated import and export functionality allows smooth integration of the system in the purification workflow.

In addition, the MS-based fraction collection add on software package G2263AA allows fraction triggering based on up to 16 masses. And/Or fraction logic on UV and MS or other signal offers highest flexibility for complex purification tasks.

## Agilent ChemStore C/S Database Client Software

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The Agilent ChemStore C/S database client software G2181BA may be added to any Agilent ChemStation configuration. The

specifications for this product may be found in the dedicated “Agilent ChemStation Plus Specifications” document.

## Agilent ChemStation Plus Security Pack

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The ChemStation Plus Security Pack (G2183AA) is a module of the Agilent Plus Series designed to support the requirements of 21 CFR Part 11. In the Agilent ChemStation the ChemStation Plus Security Pack modifies data analysis and provides advanced data management with regard to

supporting the requirements for electronic records and electronic signature. The specifications for this product can be found in the "Agilent ChemStation Plus Specifications"

## Agilent ChemStation Plus Method Validation Pack

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The Method Validation Pack (G2184AA) is an add-on software module for ChemStation Plus and provides a fully validated, off-the-shelf software solution that supports labs in performing the entire method validation process from

planning through to presentation of the final report – without the problems associated with data transfer. The specifications for this product can be found in the "Agilent ChemStation Plus Specifications" document.

## Networking

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The software has been successfully tested for compatibility with the standard networking components of the Windows environment. The software will run at the same time as other network software and computer applications written for, and adhering to, the recommended programming practices of the Microsoft Windows operating environments.

These products enable the ChemStation to share physical devices such as plotters and printers with other laboratory computers as well as sharing information such as data files and methods.

The Agilent ChemStation software may be installed on a suitable network server and

downloaded onto the client PCs as required. Each client specific configuration ensures a suitable environment for different techniques and individual users while the centralized software installation relieves the burden of managing many copies of the same Agilent ChemStation installation in one work environment.



## Documentation

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The documentation set has specific components designed for:

- installing the Agilent ChemStation software,
- using the Agilent ChemStation software,
- understanding the principles of how the software works, and
- customizing the Agilent ChemStation.
- interfacing the Agilent ChemStation with LIMS

### Installing and Learning

Each Agilent ChemStation software product comes with an installation manual that includes details of the key steps in PC hardware and software requirements, instrument interface installation, Agilent ChemStation installation and installation qualification. The installation manual is specific to the purchased configuration and includes troubleshooting, system records and system maintenance advice.

Each Agilent ChemStation includes a task-based tutorial that is built into the software. This tutorial is the primary learning aid and is designed to let users learn what they want at their own pace. Each analytical task is divided into a number of clear, guided steps each of which the users may see executed automatically by the software and then practice themselves.

### Using

Two additional categories of on-line information are designed for the routine user.

The ChemStation includes comprehensive, Windows-style, context sensitive and indexed on-line help. This system gives detailed explanations of every screen and the meaning of the parameters on that screen. The detailed explanations are backed up by graphics where appropriate, and may be copied to the Windows clipboard for incorporation in the users own documentation, or printed.

The online help also includes check lists of the more complex technique-specific and common chromatography tasks to help less frequent users who want to be sure they set up the system correctly. These checklists are directly linked to the detailed on-line help information.

### Understanding

The *Understanding Your ChemStation* manual documents the principals of the software operation and the algorithms used in the data manipulations.

### Customization

Sophisticated users who wish to customize the operation of the ChemStation, or who want to build in additional features, may

do so by writing macros using the command set.

The primary reference manual, *A Guide to Macro Programming* (available as online help), has a comprehensive set of functional examples backed up by a complete description of the internal data types and structures.

The Commands Help file, accessed directly from the ChemStation's Help menu or the Show command dialog box, is the programmer's function reference. It includes syntax and parameter explanations with example macros illustrating the use of many of the commands. By virtue of being on-line, the users can copy the examples and command syntax directly into their own macro source files.

### Interfacing

The Agilent ChemStation Plus XML Connectivity Guide (Agilent Publication Number: G2170-90223) includes installation and reference information for implementing an XML interface between the Agilent ChemStation and a LIMS (Laboratory Information Management System). The guide contains examples of the XML files and the schemas used to generate them. XML (eXtensible Markup Language) is a protocol for structuring data in pure text format. XML is a highly flexible and portable format for exchanging data between different

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