



Agilent ChemStation for GC, LC, LC/MSD, CE, CE/MSD and A/D Systems and ChemStation OpenLAB Option

Revision B.04.01

Specifications

Introduction

This document summarizes the new and changed functions of the ChemStation version B.04.01 and B.04.01 Service Pack 1. To use this document the specifications for ChemStation revision B.03.01, publication number 5989-6959EN is required. The following sections are not changed with respect to the ChemStation specifications for revision B.03.01 and are therefore omitted in this document:

- Maximum Number of Supported Instruments
- Maximum Number of Supported Modules Guidelines
- IEEE-488 GP-IB Support Matrix
- USB/GP-IB Interface Support Matrix
- Printers
- Data Model
- Software User Interface
- Data Acquisition
- Data Analysis – Specialized Reporting
- Networking

Additional information and some ChemStation screens are available in the ChemStation B.04.01 product brochure, Agilent publication number 5989-9790EN.



Agilent Technologies

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What is new in Revision B.04.01?

Agilent ChemStation B.04.01 is a new revision of the ChemStation improving the overall integration with OpenLAB ECM and customer IT infrastructure as part of Agilent's Lab Informatics strategy, while retaining proven concepts for user interaction and thus minimizing the impact on day to day operations induced by the update. The following main new features are introduced with revision B.04.01:

- New installation procedure for easier system deployment.
- Support for Windows Vista.
- Manual rubber band integration now saved with chromatogram.
- New support for custom fields per sample and per compound.
- Enhanced overlay capabilities in data analysis.
- Stopped partially executed sequences can be resumed and data can be acquired into the same existing data container (partial acquisition sequence).

For Users of the Agilent GC ChemStation

- New eMethods to allow easy application sharing.

- Numerous user interface enhancements and new features for the 7890 GC control

For Users of the Agilent LC ChemStation

- New instrument drivers for the Agilent 1200 Rapid Resolution LC system.

For Users of the Agilent ChemStation OpenLAB Option

- Better integration with OpenLAB Enterprise Content Manager (ECM) than with previous revisions
- Configurable and transparent data flow.
- Direct access to OpenLAB ECM information such as object properties and file location.
- Easy update of selected or all local methods and sequences with OpenLAB ECM data.
- Batch review functionality is removed.

For Users in Regulated Environments using the Agilent ChemStation OpenLAB Option

The G2189BA Agilent ChemStation OpenLAB option in combination with

the Agilent OpenLAB ECM data management solution enables the operation of the Agilent ChemStation in full support of all compliance requirements mandated by 21CFR part 11 for a closed system. In particular it ensures

- accurate and complete copies of records.
- versioning of all relevant records for traceability.
- no alteration of records between their creation and their automatic transfer to Agilent OpenLAB ECM immediately after acquisition, reprocessing or interactive modifications.
- no uncontrolled copies of the data.
- a mandatory login to Agilent OpenLAB ECM before getting access to the ChemStation.
- that all changes are captured in user-independent time-stamped audit trails.

For further details on the 21CFR part 11 compliance please refer to the technical note "Integration of the Agilent ChemStation for GC, LC, LC/MSD, CE, CE/MSD and A/D with Agilent OpenLAB ECM - Compliance with 21 CFR Part 11", publication number 5990-3590EN.

What is new in Revision B.04.01 Service Pack 1?

Agilent ChemStation B.04.01 Service Pack 1 is a service release of the ChemStation revision B.04.01 introducing the new 7693 automatic liquid sampler system for GC improving the OpenLAB integration and migration functions. The following main new features are introduced with revision B.04.01 Service Pack 1:

- Time based and manual session

locking now configurable.

- Enhanced Queue Management.
- Utility to create sequence containers from previous data acquired in simple sequence format.
- PDF printing support for Windows Vista.
- Support for the 7693 automatic liquid sampler system for GC.

Note: 7693 support with the 6850/90 GC is added with another service pack. Please contact your local customer contact center for details.

General Description

The general description for the Agilent ChemStations for GC, LC, LC/MSD, CE, CE/MSD and A/D systems revision B.03.01 (publication number 5989-6959EN) is still valid for the ChemStation revision B.04.01 and B.04.01 Service Pack 1 with the exception of the changes listed in this section.

ChemStation Data Analysis Only Software

For ChemStation B.04.01 the following change with respect to version B.03.01 is introduced: The ChemStation Data Analysis software license for GC (G2090BA) is no longer available. It is now included in the ChemStation Data Analysis software license for LC (G2190BA). Existing licenses remain valid regardless of the data analysis type.

ChemStation Plus Add-On Software Modules

No changes were made in this section with respect to the specifications for ChemStation Version B.03.01 as defined in document 5989-6959EN.

Dedicated Solutions for Specific Applications

In addition to the modules listed in the specification for ChemStation Version B.03.01 the modules listed in this section are available.

ChemStation GPC Data Analysis Software (G2182BA)

The ChemStation GPC Data Analysis Software allows calculating molecular weight averages and molecular weight distributions from Gel Permeation chromatography (GPC) or Size Exclusion Chromatography (SEC) measurements.

Analytical Studio Reviewer Software (G3772AA)

The Analytical Studio Reviewer (ASR) provides fast, flexible and accurate analysis of LC/MS data for small compound characterization, to expedite the development process.

ChemStation Method Scouting Wizard (G2196AA)

The ChemStation Method Scouting Wizard software is part of the Agilent 1200 Series LC method development solution for complex method scouting campaigns.

Enterprise Add-On Software Modules *Agilent ChemStation OpenLAB Option (G2189BA)*

The ChemStation OpenLAB option provides centralized secure data organization and storage, centralized user management and all features required for compliance with regulatory guidelines such as the FDA's 21 CFR part 11. In addition full utilization of all other OpenLAB modules like the Business Process Manager and the OpenLAB Intelligence Reporter is possible.

Agilent OpenLAB Intelligence Reporter (G4635AA)

The OpenLAB Intelligence Reporter Option adds functions for cross sequence reporting, trend charting, calculations and statistics to the ChemStation. It requires the ChemStation OpenLAB option.

Healex ChemLaunch Option (R2064A)

With the ChemLaunch Option the ChemStation can be operated on a central Citrix server, minimizing validation and operating costs. Thin clients can be used to operate the on-line and off-line ChemStation.

Computer Hardware

No changes were done in this section with respect to the Agilent ChemStation specifications for revision B.03.01 [publication number 5989-6959EN].

Minimum PC Configuration

General

- SXGA display (1280x1024 resolution)
- MS Windows compatible pointing device

- ATAPI CD, CD-RW or DVD drive
- 10/100 baseT LAN interface card.

Windows XP Service Pack 3

- Hewlett-Packard Compaq PC with Pentium V, 1.5 GHz
- 512 MB RAM
- 40 GB hard disk

Windows Vista Service Pack 1

- Hewlett-Packard Compaq PC with Pentium V, 3.4 GHz single core
- 1 GB RAM
- SXGA display (1280x1024 resolution)
- 160 GB hard disk

LAN-MIO Support Matrix

The following minor changes were done in this section with respect to the Agilent ChemStation specifications for revision B.03.01 [publication number 5989-6959EN].

- The current 1100/1200 LC firmware update tool version changed from 2.1 to 2.6
- Current 1100/1200 LC firmware revision is A.06.1x

Exceptions are:

- G1315C, G1365C, G1315D, G1365D: firmware revision B.06.1x
- G1314D, G1314E: firmware revision B.06.2x
- The 7890A does support a fixed IP address setting

Operating System

The Agilent 32-Bit ChemStation Version B.04.01 requires Microsoft

Windows XP Service Pack 3 or Microsoft Windows Vista Service Pack 1.

Methods and Sequences

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 template and holds the individual sample information, as well as references

to the appropriate methods, user setting up and executing data acquisition, data analysis and automatic recalibration specifications.

When the acquisition based on the sequence template is finished, a copy of this sequence template, all data files, result data and copies of all required methods are stored in the sequence container, creating a transportable

data unit. For more details please refer to the current ChemStation product brochure [publication number 5989-9790EN] or user manuals.

Changes to methods within the sequence container can be applied to the original master methods with the new update functions. This will make current changes directly available for future sequences.

System Configuration

Instrument Configuration

The configuration of the instrument system is done by the "ChemStation 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 Handling and User Access Configuration

With the ChemStation OpenLAB Option the "ChemStation Administration Tool"

is used for secure configuration of login, data handling and audit trail for all instruments on a PC. Alternatively these settings can be defined per instrument in the ChemStation.

Data Analysis – Display

The following functions are added to this section with respect to the Agilent ChemStation specifications for revision B.03.01 [publication number 5989-6959EN].

- Overlay of chromatograms from different data sets. This function allows to use reference chromatograms from any sequence container.

- Automated continuous overlay of selected chromatograms. This function allows loading one or more reference chromatograms to be used for visual comparison during single run data or sequence review.

Data Analysis – Integration

The integrator capability for “graphical manual or rubber band integration.” has been changed with respect to the Agilent ChemStation specifications for revision B.03.01 [publication number 5989-6959EN] as defined below.

- Graphical manual or rubber band integration of chromatograms added by the user can be stored with each

individual chromatogram or with the method. Traditionally ChemStation stored manual Baseline drawing (rubber band integration) events only in the method. This new function allows storing a manually created baseline in the data file. Manually integrated chromatograms can now more easily be used in sequence reprocessing and for calibration runs.

- Further, the new functionality allows to consecutively apply both types of manual events during review or reprocessing – first, the manual events stored in the sequence method are used for all sequence data (when enabled), in a second step, manually-drawn baselines stored with the individual chromatograms are applied.

Data Analysis – Quantification

The following section was missing in the Agilent ChemStation specifications for revision B.03.01 [publication number 5989-6959EN]. The specification itself did not change with respect to ChemStation Revision B.03.01:

Calibration Curve Types

Calibration curves are constructed for each compound by using the calibration levels to define the curve. The algo-

rithm used to generate the calibration curve may be selected as

<i>Piecewise</i>	a point-to-point extrapolation
<i>Linear</i>	a linear regression fit of the data points
<i>Quadratic</i>	a quadratic fit of the data points
<i>Cubic</i>	a cubic fit of the data points

<i>Exponential</i>	an exponential fit of the data points
<i>Logarithmic</i>	a natural logarithmic fit of the data points
<i>Power</i>	a power fit of the data points
<i>Average Resp/Amt</i>	single response factor is calculated from the average of the response factors.

Data Analysis – Standard Reporting

In addition to the Agilent ChemStation specifications for revision B.03.01 [publication number 5989-6959EN] the following functions are new:

Report File Formats

.PDF – With revision B.04.01 the Report file format PDF is available only for the Windows XP operating system. This function creates an Adobe PDF file

version 1.4 using the novaPDF Professional Server Ver 5.4 printer that is installed together with the ChemStation. With version B.04.01 Service Pack 1 this function is available for both, Windows XP and Windows Vista operating system. The PDF-XChange 4.0 from Tracker Software Products LTD replaces the novaPDF Professional Server Ver 5.4

printer. Version B.04.01 Service Pack 1 now allows to generate PDF report files with unique names.

Result Calculation

The option to use multiplier, amount, dilution factor and ISTD correction was moved from the Calibration Settings dialog into the Specify Report dialog. No change to internal data structures and functionality was done.

Utilities and Compatibilities

The following section is added, no changes were done in this section with respect to the Agilent ChemStation specifications for revision B.03.01 [publication number 5989-6959EN].

Migration to Sequence Containers

With B.04.01 Service Pack 1 a built-in utility to convert old style sequences into sequence containers is available.

The sequence container was introduced with ChemStation B.02.01 and without the utility a manual conversion to the sequence container was required.

XML Interface

The new part number of the ChemStation XML Connectivity guide

is G2170-90229. No further changes were done in this section with respect

to the Agilent ChemStation specifications for revision B.03.01 [publication number 5989-6959EN].

Customization

Programming

The section heading “Programming” is added to the existing text in the Agilent ChemStation specifications for revision B.03.01 [publication number 5989-6959EN].

The following additional section is new:

Custom Fields

Per sample and per compound custom fields are now available and can be used to enter and export additional information for advanced reporting, data evaluation and calculations (for example with the OpenLAB Intelligence Reporter).

Custom fields are configured in the method and values are entered via the sequence table. They can be flagged as mandatory to prohibit running samples without completion of the custom field values, and default values can be set to allow fast and easy sequence execution for fields that do not change frequently.

Automation

The paragraph on Batch Review is extended with respect to the existing text in the Agilent ChemStation specifications for revision B.03.01 [publication number 5989-6959EN]. Additions are:

Without the ChemStation OpenLAB option Batch Review is available as an additional mode of data analysis. It 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

Generally Agilent recommends using the G2189BA ChemStation OpenLAB option in regulated environments. The functions as described in the Agilent ChemStation specifications for revision B.03.01 [publication number

5989-6959EN] were not changed with the following exception:

- The Method Change History log is renamed to Method Audit Trail. With the Agilent ChemStation OpenLAB option installed this functionality is extended with an automatically

generated, detailed listing of data analysis changes, see also the audit trail section in chapter “Compatible Software Modules”, section “Agilent ChemStation OpenLAB Option (G2189BA)”.

Instrument Control

No changes were made in this section with respect to the Agilent ChemStation specifications for revision B.03.01 [publication number 5989-6959EN].

Agilent ChemStation for GC Systems

The following functions listed in this section in document 5989-6959EN are now also available for the 7890 GC system:

- Graphical User Interface for easy access to all method areas
- Method resolution
- Graphical display of time table entries
- Sampling Diagram window

- Column Compensation
- Digital auto zero
- Extended GC parameters for GC readiness determination
- Runtime event editing enhancements
- Highlighted out of limit values

With ChemStation version B.04.01 Service Pack 1 the following new functions are available:

- Support for the new Agilent 7693 automatic liquid sampler system
- Note: 7693 support with the 6850/90 GC is added with another service pack. Please contact your local customer contact center for details.*

- New Agilent MultiMode Inlet (MMI) for 7890 GC system

Agilent ChemStation for LC Systems

In addition to the Agilent ChemStation specifications for revision B.03.01 [publication number 5989-6959EN] the following instrument modules are now controlled.

Sampling Systems

- Agilent G1367D High Performance Autosampler SL Plus

Instrument Control

Detectors

- Agilent 1200 G1314D VWD
- Agilent G1314E VWD SL Plus
- Agilent 1200 G4218A Evaporative Light Scattering Detector (ELSD)

Column Compartments

- Agilent G1316C Thermostatted Column Compartment SL Plus

Agilent ChemStation for LC/MSD Systems

No changes were made in this section with respect to the specifications for ChemStation Version B.03.01 as defined in document 5989-6959EN.

Agilent ChemStation for A/D systems

No changes were done in this section with respect to the Agilent ChemStation specifications for revision B.03.01 [publication number 5989-6959EN].

Additional Data Evaluation Modules

The section “Agilent ChemStore sample organization and results database module (G2181BA)” was moved to the chapter Compatible Software Modules.

The specification for the “LC Diode-Array Detector (DAD) Spectral Evaluation Module (G2180BA)” is not changed with respect to the Agilent

ChemStation specifications for revision B.03.01 [publication number 5989-6959EN].

Compatible Software Modules

This is a new section that lists compatible software modules for the ChemStation revision B.04.01. For some Software Modules the specifications are also included.

The compatible software modules are

- High Throughput Purification Software Module (G2262AA)
- ChemStation GPC Data Analysis software module (G2182BA)
- Agilent ChemStation Method Scouting Wizard (G2196AA)
- Analytical Studio Reviewer Software (G3772AA)
- Agilent ChemStore C/S Database Client Software (G2181BA)
- Agilent ChemStation Plus Security pack (G2183AA)
- Agilent ChemStation OpenLAB Option (G2189BA)
- Agilent OpenLAB Intelligence Reporter (G4635AA)

Analytical Studio Reviewer Software (G3772AA)

For detailed specifications please refer to the document with the publication number 5989-8027EN

ChemStation Method Scouting Wizard (G2196AA)

The ChemStation Method Scouting Wizard is an ideal add-on to the ChemStation B.04.01 to support the new Agilent 1200 Series LC Method Development solution based on the G1316C Thermostatted Column Compartment SL plus. It allows to easily generate all required methods and a sequence table for up to four dimensional method scouting campaigns using multiple columns, solvents, pre-defined gradients and temperatures.

The following functions are available to allow for easy design of complex method scouting campaigns:

- Setup wizard for guidance through all required setup steps.
- Automatic generation of scouting methods and a ChemStation sequence.
- Procedures for automatic flushing and column equilibration.
- Experiment setups for multiple samples and injections.
- Settings and results are stored for re-use.

Further details can be found in publication number 5989-8695EN.

High Throughput Purification Software Module (G2262AA)

No changes were done in this section with respect to the Agilent ChemStation specifications for revision B.03.01 [publication number 5989-6959EN].

ChemStation GPC Data Analysis Software Module (G2182BA)

For detailed specifications please refer to the document with the publication number 5988-2265EN.

Agilent ChemStore C/S Database Client Software (G2181BA)

The Agilent ChemStation specifications for revision B.03.01 [publication number 5989-6959EN] is extended with the following information:

- The Agilent ChemStore C/S Database Client Software Pack is not compatible with the ChemStation OpenLAB Option.

Agilent ChemStation Plus Security Pack (G2183AA)

The Agilent ChemStation specifications

Compatible Software Modules

for revision B.03.01 [publication number 5989-6959EN] is extended with the following information:

- The Agilent ChemStation Plus Security Pack is not compatible with the ChemStation OpenLAB option.

Agilent ChemStation OpenLAB Option (G2189BA)

The ChemStation OpenLAB option integrates the ChemStation revision B.04.01 with the OpenLAB Enterprise Content Manager (OpenLAB ECM) for central data handling.

Compatibility

The ChemStation OpenLAB Option is compatible with the following OpenLAB versions:

- OpenLAB ECM Version 3.3.2
- OpenLAB ECM version 3.3.1
- OpenLAB ECM workgroup

User Access Control

- User authentication is done using OpenLAB built-in user and group management or active directory user and groups management.
- ChemStation access levels are replaced with 35 ChemStation privileges. Privileges are grouped in configurable roles. Users and user groups are assigned to the roles. A user or user group can be assigned to multiple roles, the privileges are additive.
- The ChemStation Administration tool is used to configure the logon. Access to the tool is controlled by a local operating system group to allow for PC-wide configuration.
- Logon can be configured to be mandatory or non-mandatory. Revision B.04.01 Service Pack 1 adds a configurable emergency mode to allow operation in case of a network or server failure.
- Sessions can be locked non-privately or privately. A time based private lock is available.

- The configurable "break session lock" option provides access to a locked ChemStation when the server is unavailable.
- Version B.04.01 Service Pack 1 adds a time based non-private lock and a configurable lock button for one click ChemStation locking.

Data Handling

- The ChemStation Administration tool is used to set Data transfer options for all instruments connected to a PC. Alternatively they can be configured for each instrument individually. Access to the ChemStation Administration tool is controlled by a local operating system group. Access to data transfer options configured per individual instrument session (2nd alternative) is controlled by a ChemStation privilege.
- The configuration of the target OpenLAB ECM data storage location is protected by ChemStation privileges. Version B.04.01 Service Pack 1 adds a quick selection of the last 10 upload locations.
- An upload and download queue is used to ensure reliable data transfer to and from OpenLAB ECM. revision B.04.01 Service Pack 1 adds a queue status display and the ability to view more detailed information on the data packets in the queue for users that have been assigned appropriate privileges for this task.
- The data transfer can be configured to allow for the following workflows:
 - Enforced direct upload after data acquisition,
 - enforced direct upload after a full sequence reprocess,
 - enforced upload after each data modification,
 - enforced upload for sequences not yet transferred to OpenLAB, or
 - manual upload.
- To allow for working in regulated environments, local queue operation is configurable. Revision B.04.01 Service Pack 1 adds the option to analyze and clean individual items from the local queue in case of problems.
- Local method and sequence templates can be synchronized with OpenLAB ECM. Revision B.04.01 Service Pack 1 adds visible display of synchronization status for each item and update of selected or all local methods and sequences in a single action.
- OpenLAB ECM file properties can directly be accessed and set from the ChemStation.
- Review and evaluation already acquired data during a running acquisition sequences is possible. To ensure traceability the acquired data will become version 1 of the record in OpenLAB ECM, the reviewed data set will become Version 2 of the same record after the acquisition and review is finished.

Audit Trail

- Data analysis method changes are audited individually including previous and current value in the method audit trail.
- The method audit trail can be enabled per method or globally (per PC or per instrument).
- Result calculations are audited in the ChemStation run logbook. This includes manual integration changes. The report history function allows checking for previously generated results from a data file directly in the ChemStation.
- The ChemStation Administration tool is used to configure an enforced audit trail for all methods and results.
- Once enabled audit trails can't be switched off

Compatible Software Modules

Agilent OpenLAB Intelligence Reporter (G4635AA)

The OpenLAB Intelligence Reporter Option adds functions for cross sequence reporting, trend charting, calculations and statistics to the ChemStation. It requires the ChemStation OpenLAB option.

Further details on the OpenLAB Intelligence Reporter functions can be

found in the respective functional overview, publication number 5989-8045EN. The ChemStation integration includes the following functions:

- Start OpenLAB Intelligence Reporter for the currently loaded sequence.
- Version B.04.01 Service Pack 1 adds the automatic preview of a pre-selected report at the end of a sequence to the OpenLAB Intelligence reporter functionality.

Healex ChemLaunch Option (R2064A)

With the ChemLaunch option the ChemStation can be operated on a central Citrix server, minimizing validation and operating costs. Thin clients can be used to operate the on-line and off-line ChemStation.

Further details can be found at <http://www.chemlaunch.com/>

Documentation

The following section is added with respect to the Agilent ChemStation specifications for revision B.03.01 [publication number 5989-6959EN]:

Integration with OpenLAB ECM

The concepts guide for the G2189BA Agilent ChemStation OpenLAB option, includes information on how to configure and use the ChemStation OpenLAB option ("Agilent G2189BA ChemStation OpenLAB Option – Concepts Guide", part number G2170-90033 for revision B.04.01 or G2170-90034 for revision B.04.01 service pack 1).

In depth information on how to configure the ChemStation to conform with 21 CFR part 11 is provided. In the section "Interfacing" the part number of the "Agilent ChemStation Plus XML Connectivity Guide" has changed to G2170-90229.

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