Agilent ChemStation

Upgrade Preparation Guide for ChemStation Rev. B.03.01

Agilent Technologies

Notices

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Software Revision

This guide is valid for the B.03.0x revision of the Agilent ChemStation software.

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In This Guide...

This guide describes the upgrade of Agilent ChemStation B.01.03 software and the steps to configure your analytical system. The documentation should be used as resource prior to a ChemStation upgrade.

1 Introduction

This chapter provides an overview about the changes in Agilent ChemStation Rev. B.03.01 with respect to the previous revision and information regarding the content of this guide.

2 Prerequisites to Upgrade to Agilent ChemStation Rev. B.03.01

This chapter lists the minimum requirements for successful operation of the Agilent ChemStation software.

It provides detailed information about the requirements that must be met to ensure proper operation of the Agilent ChemStation. Requirements include PC type and performance, network protocol, printer type, GPIB/LAN cards, USB-GPIB interface, operating systems and firmware revisions of the analytical instruments.

3 How to Upgrade to Agilent ChemStation Rev. B.03.01

This chapter describes how to upgrade to Agilent ChemStation Rev. B.03.01. inclusive the Add-On Solution during the upgrade.

4 The First Time You Start Up Your ChemStation Rev. B.03.01

The chapter covers most of the recognizable changes compared to previous revisions, e.g. graphical and design changes due to long filenames. New functionality is explained in detail in the additional manuals coming along with the upgrade package, e.g. “Understanding your ChemStation” for new integration parameters.

For Updates of Rev. A system, the upload process and modifications for 16-bit files into the 32-bit ChemStation are described in addition.

5 Compliance Information

This chapter gives a general statement about Software Upgrade Qualification and describes the modifications regarding the OQ/PV usage.

6 Impact on Customized Solutions

The chapter informs about using and writing customized solutions and the necessary actions to adapt the Unicode format.

7 Upgrade Impact on Quantification Methods (relevant for Rev. A Upgrades only)

This chapter outlines the differences and impacts on methods using the various possibilities of different integrators in Rev. A.xx.xx ChemStation (e.g. G2070AA, G2170AA, etc.): Standard Integrator, Enhanced Integrator, Enhanced Integrator with Advanced Baseline Option.

8 Spectra/Purity Options using ChemStation Rev. B.03.0x. (relevant for Rev. A Upgrades only)

This chapter outlines the differences between the two available spectra/purity tool sets in ChemStation Rev. A. With ChemStation Rev. B.0x.0x the spectra tool introduced with Rev. A.04.02 becomes the standard tool set, the older spectra tool is not available anymore.

9 Appendix

Contents

1 Introduction

Introduction to Agilent ChemStation Rev. B.03.01

Agilent Technologies is pleased to announce the introduction of the new version of the LC, GC, A/D, CE, CE/MS and LC/MS Multi-Technique ChemStation. The Multi-Technique ChemStation family is a widely used system, providing both instrument control and data acquisition and management. Modular in design, the system can be extended and scaled up as laboratory needs grow. The system offers a new design and tree-based navigation, together with new flexible data management features.

New and Changed Technology in ChemStation Rev. B.03.01/B.02.01/B.01.03/B.01.01

The following changes and new functionality are included in ChemStation Revision B.03.01:

- ChemStation Software is Dual Core Processor compatible
- ChemStation introduces two data storage modes, to enable users to choose the data storage that match their workflow:
  - Mode 1: Unique Folder Creation ON - for consistency of sample data
  - Mode 2: Store all data in one directory, like in previous ChemStation revisions (Unique Folder Creation OFF)
- Performance parameters available for customization in the report layout
- Performance parameters can be calculated based on Japanese Pharmacopoeia (JP)
- Easy Review of Acquisition parameters in the Navigation Table
- Customization of the “Table of contents” in online help
- Enhanced XML Interface for result data
- GC Specific
  - Introduction and full support of the new Agilent 7890A GC System
  - Method transfer from Agilent 6890 to Agilent 7890A GC
  - GC overlapped injection supported with the Agilent 7890A GC
  - User interface supports entry of negative flow setpoints for columns connected to second pressure source for backflushing with the Agilent 7890A GC System. The negative flow indicates change of flow direction.
  - Integration of Retention Time Locking (RTL) into GC ChemStation Software
  - Support of the new Agilent Lab Monitor & Diagnostic Software
- LC Specific
  - Support for the G1315D Agilent 1200 Diode Array Detector
  - Support for the G1365D Agilent 1200 Multi Wavelength Detector
  - Support for the G1329B Agilent 1200 Autosampler SL

- LC/MS Specific
  - Introduction and full support of the new Agilent 6100 Single Quad Series LC/MS G6110A, G6120A, G6130A, and G6140A LC/MS
  - Localized LC/MS Sofware in Chinese and Japanese

The following changes and new functionality are included in ChemStation Revision B.02.01:

- New and improved ChemStation User Interface design
- New tree- and table-based navigation, providing fast and flexible data handling within various ChemStation views
- Flexible storage locations for data, methods, and sequences
- Improved data review and reprocessing capabilities using the Data Analysis Navigation Table
- New packaging concept guarantees consistency for sequence and single run sample data
- Additional Signal Options give the possibility to assign method-specific signal options to improve data review
- Possibility to save manual integration events in the Data Analysis method along with newly acquired data files
- Online help integrated ChemStation tutorial, to enable you to learn the software while working on your own methods and data
- Enhanced utilization of high resolution monitor and available screen estate
- Support for the G1312B Agilent 1200 Binary Pump SL (incl. Degasser)
- Support for the G1367C Agilent 1200 High Performance Autosampler SL
- Support for the G1314B Agilent 1200 Variable Wavelength Detector SL
- Support for the G1316B Agilent 1200 Thermost. Column Compartment SL
- Support for the Agilent 1200 LC series
- Support for the GPC Add-On software G2182BA
- Direct Software Link to the new Agilent LC Diagnostic tool

The following changes and new functionality have been introduced with ChemStation Revision B.01.03:

- Software support for the new G4240A Agilent 1100 Chip Cube, designed for LC systems using an Agilent Ion Trap MSD as detector
- Software support for the new G1315C Agilent 1100 Diode Array Detector (DAD) and the new G1365C Agilent 1100 Multi Wavelength Detector (MWD)
- Support added for CE, CE/MS, HP 1046 and HP 1049 ECD
- Support for USB-GPIB interface (PN 82357A) for GPIB communication based LC and CE systems (HP 1090, HP 1046, HP 1049, CE, CE/MS)
- Enhanced productivity for CE ChemStation customers due to instrument set points modifications directly in the sequence table for each sequence line
- 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

For ChemStation Plus

- Improved integration with ChemStore (available only if ChemStore is installed)
- All ChemStation Plus applications available via a common program group

The following changes and new functionality have been introduced with ChemStation Revision B.01.01:

- Support for long file names
- Enhanced integrator, as well as enhanced integration events and new integration parameters
- Faster software installation, software start up and switching between views
- User-configurable columns in the Sequence Editor
- Software screens and windows optimized for 1024 × 768 display resolution
- Simplified uninstall via “Add/Remove” dialog from the operating system
- New overlap injection mode for the Dual Loop Autosampler (HPLC 1100)
- Direct control of CTC/Leap autosampler for LC and LC/MS systems
- Support for the 6850 Series GC enhancements

- Support for Agilent G1888A, G1289B/G1290B Headspace Samplers with the G2924AA integrated Headspace control software
- Automatic installation of Companion software during GC ChemStation installation

About this Document

NOTE The "Upgrade Preparation Guide for Agilent ChemStation Rev. B.03.01" is applicable only for customers upgrading an existing ChemStation. The document refers only to *changes* in comparison to previous ChemStations Revisions.

NOTE ChemStation B.03.01 is supported on Windows XP only. ChemStation A.09.03 had been supported on either Windows NT 4.0 or Windows 2000, in order to upgrade to ChemStation B.03.01 the operating system needs to be updated PRIOR the ChemStation upgrade. Please check as well the PC minimum requirements, Chapter 2, "Minimum PC Hardware Requirements for the Agilent ChemStation," starting on page 19.

The document guides you through the update phase of an existing Agilent ChemStation system

A.09.03 or higher to Agilent ChemStation Rev. B.03.01

B.0x.0x to Agilent ChemStation Rev. B.03.01

The document outlines the technical part of the update as well as the impact of certain new functionality and changes to your system. If a chapter is only relevant for upgrades from Rev. A to Rev. B, the information is added in the header.

New functionality is described in detail in the user manuals and in the online help.

The manuals "Installing your ChemStation" and "Understanding your ChemStation" have been updated accordingly and are delivered with the new software revision.

Available User Documentation

The Agilent ChemStation product documentation consists of handbooks containing reference information, and online documentation for task-orientated topics. The hardcopy manuals are also located in the *manuals* directory on the CD-ROM (CD 2 - User Documentation and Accessories), together with the required Adobe Acrobat reader.

For detailed information regarding installing additional analytical instruments (e.g. cabling, connecting to an analytical instrument), refer to the appropriate *Installing your ChemStation* manual of your system.

2 Prerequisites to Upgrade to Agilent ChemStation Rev. B.03.01

Agilent ChemStation PC Hardware Details

This section states the PC hardware and operating system requirements that must be met for successful installation and operation of the Agilent ChemStation.

The Agilent ChemStation B.03.01 and greater is supported on personal computers with an Intel Pentium IV 1.5 GHz (or higher).

Using a GPIB interface, one PCI slot is required. For details about GPIB and the USB-GPIB interface requirements, refer to the LC or CE installation manual.

If a LAN connection is used for the analytical equipment, a LAN interface supported by the operating system is required, and the Microsoft TCP/IP protocol must be installed.

All PC hardware and peripherals must be listed in the Microsoft Hardware Compatibility List (HCL) which is available from the Microsoft home page on the world wide web (http://www.microsoft.com). If your PC hardware is not listed in the HCL, the system may not work correctly with the Agilent ChemStation software.

Minimum PC Hardware Requirements for the Agilent ChemStation

Table 1 Minimum PC Hardware Requirements for Windows XP-based systems

Processor	Pentium IV, 1.5 GHz
Screen resolution	Super VGA (1280 × 1024)
Mass storage	40 GB Hard-Disk and CD-ROM
Minimum Memory for Single Instrument 2D/3D	512 MB of RAM
Minimum Memory for Multi Instruments	512 MB of RAM
Instrument configuration with Agilent ChemStore C/S database module (Rev. B.03.03 SR2)	512 MB of RAM

Non-HP Computers

The Agilent ChemStation has been designed to run successfully 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 equipment. All configuration information listed in this manual has been optimized for Hewlett-Packard/Compaq Kayak, Vectra and EVO computers. Described configurations have not necessarily been optimized for other vendors' PCs. The standard configuration of the GPIB interface, for instance, may potentially conflict with the memory configuration of a non-HP computer.

Additional accessory interface boards may cause conflicts of hardware-related resources (I/O ports, interrupt settings, DMA channels).

For a non-Hewlett-Packard computer, use the setup utility program supplied by the manufacturer to configure your computer and accessories. Check the supplied documentation to eliminate potential resource conflicts in the setup, especially regarding the configuration of the GPIB interface.

Printers for the Agilent ChemStation

The Agilent ChemStation has been designed to work with operating system-compatible printers. Agilent Technologies does not test all printer and printer driver combinations that are supported in the Windows environment. Print performance and results may vary on other manufacturers' printers and appropriate drivers.

Agilent supports printers successfully tested with Agilent ChemStation Rev. A B.03.01. The complete list of successfully tested printers is listed in the "readme.txt" document on the ChemStation CD-ROM in the support, drivers folder (CD 2 -User Documentation and Accessories) . The printers listed in Table 2 have been successfully tested at the time this handbook was printed.

Table 2 Printers Successfully Tested with Agilent ChemStation Rev. B.03.01

Printer Model	Driver comment
HP LaserJet 4050 and HP LaserJet 4100	HP PCL 5e Driver or PCL 6
HP LaserJet 4200	HP PCL 5e Driver or PCL 6
HP LaserJet 4250	PCL 6 Driver
HP LaserJet P3005D	PCL 6 Driver
HP Color LaserJet 2500TN	PCL 6 Driver
OfficeJet Pro K550DTWN	PCL 3 Driver

NOTE Please note that this list is not comprehensive and does not include printers and printer drivers made available after the release of this handbook. If your printer is not listed here, it does not mean that it will not work with the Agilent ChemStation. It has simply not been tested.

NOTE

We recommend that you use Hewlett-Packard LaserJet printers.

Due to limited print performance (< 8 pages per minute) and paper tray capacity (less than 150 pages), some low-end printers may not be suitable for unattended high data-throughput operation of the Agilent ChemStation, for example, multi-instrument configurations, or when running large sequences with many injections and relatively short run-times (e.g. less than 5 minutes), even if listed in Table 2, “Printers Successfully Tested with Agilent ChemStation Rev. B.03.01,” on page 20.

Advanced Power Management (Not Supported with Analytical Hardware)

The BIOS and operating systems of many modern PCs support Advanced Power Management (APM). After a specified idle time, the BIOS switches the system to a stand-by mode by turning off the computer display, hard disk and other devices. This reduces the PC power consumption and the internal clock frequency to save energy.

The reduction in internal clock speed and hard disk slow down can render a PC incapable of handling the real-time requirements of instrument control and data acquisition. Typically, this results in overflows of the internal instrument buffers, or, in other words, loss of data. Agilent Technologies recommends that you switch off APM for systems running on-line operation of analytical hardware.

Operating System Requirements

ChemStation Rev. B.03.01 is available in English, as well as localizate versions for Japanese and Chinese. Depending of your choice of ChemStation, you will need the corresponding Microsoft Windows XP Professional *(Service Pack 2)* operating system:

- English Microsoft Windows XP Professional *(Service Pack 2)*
- Japanese Microsoft Windows XP Professional *(Service Pack 2)*
- Chinese Microsoft Windows XP Professional *(Service Pack 2)*

NOTE Agilent cannot give a support statement for other non-english operating systems.

Windows XP Professional is the only supported operating system for the Agilent ChemStation data acquisition and analysis software.

For up-to-date information on supported operating systems please contact your local service and support center.

NOTE ChemStation Rev. B.03.01 is NOT supported on Windows 2000 Professional.

If you use a LAN to connect to the analytical instruments, the Microsoft TCP/IP protocol must be installed and configured.

LC Instrument Firmware Requirements

The LC ChemStation software will require **minimum** firmware revisions in order to work with the following devices shown in Table 3.

NOTE Using 1100/1200 modules in one instrument, the firmware of the whole module stack needs to run on the minimum required firmware mentioned in the table below. Mixed firmware versions are not supported.

Table 3 LC 1100/1200 Series Instrument Firmware Requirements

LC Instrument	Product Number	Firmware Revision	Part Number
Samplers			
Agilent 1100/1200 Automation Interface	G2254A	A.06.02 or newer	n.a.*
Agilent 1100 Autosampler	G1313A	A.06.02 or newer	n.a.*
Agilent 1100/1200 Thermo. Autosampler	G1329A	A.06.02 or newer	n.a.*
Agilent 1200 Thermo. Autosampler SL	G1329B	A.06.04 or newer	n.a.*
Agilent 1100 Micro Sampler	G1389A	A.06.02 or newer	n.a.*
Agilent 1100/1200 Preparative Autosampler	G2260A	A.06.02 or newer	n.a.*
Agilent 1100 Well Plate Autosampler	G1367A	A.06.02 or newer	n.a.*
Agilent 1200 High Performance Autosampler	G1367B	A.06.02 or newer	n.a.*
Agilent 1200 High Performance Autosampler SL	G1367C	A.06.02 or newer	n.a.*
Agilent 1100 Thermo. Well Plate Autosampler	G1368A	A.06.02 or newer	n.a.*
Agilent 1100/1200 Micro Well Plate Autosampler	G1377A	A.06.02 or newer	n.a.*
Agilent 1100/1200 Thermo. Micro Well Plate Autosampler	G1378A	A.06.02 or newer	n.a.*

Table 3 LC 1100/1200 Series Instrument Firmware Requirements (continued)

LC Instrument	Product Number	Firmware Revision	Part Number
Agilent 1100/1200 Dual Loop Autosampler PS	G2258A	A.06.02 or newer	n.a.*
Column Compartments			
Agilent 1100/1200 Thermostated Column Compartment	G1316A	A.06.02 or newer	n.a.*
Agilent 1200 Thermostated Column Compartment SL	G1316B	A.06.02 or newer	n.a.*
Agilent 1100/1200 Chip Cube Interface	G4240A	A.06.02 or newer	n.a.*
Pumps			
Agilent 1100/1200 Isocratic Pump	G1310A	A.06.02 or newer	n.a.*
Agilent 1100/1200 Quaternary Pump	G1311A	A.06.02 or newer	n.a.*
Agilent 1100/1200 Binary Pump	G1312A	A.06.02 or newer	n.a.*
Agilent 1200 Binary Pump SL	G1312B	A.06.02 or newer	n.a.*
Agilent 1100/1200 Capillary Pump	G1376A	A.06.02 or newer	n.a.*
Agilent 1100/1200 Preparative Pump	G1361A	A.06.02 or newer	n.a.*
Agilent 1100/1200 Nano Pump	G2226A	A.06.02 or newer	n.a.*
Detectors			
Agilent 1100 DAD	G1315A	A.06.02 or newer	n.a.*
Agilent 1100/1200 DAD	G1315B	A.06.02 or newer	n.a.*
Agilent 1100/1200 DAD SL	G1315C	B.01.02 or newer**	n.a.*
Agilent 1200 DAD	G1315D	B.01.04 or newer***	n.a.*
Agilent 1100 MWD	G1365A	A.06.02 or newer	n.a.*
Agilent 1100/1200 MWD	G1365B	A.06.02 or newer	n.a.*
Agilent 1100/1200 MWD SL	G1365C	B.01.02 or newer**	n.a.*

Table 3 LC 1100/1200 Series Instrument Firmware Requirements (continued)

LC Instrument	Product Number	Firmware Revision	Part Number
Agilent 1200 MWD	G1365D	B.01.04 or newer***	n.a.*
Agilent 1100/1200 FLD	G1321A	A.06.02 or newer	n.a.*
Agilent 1100 VWD	G1314A	A.06.02 or newer	n.a.*
Agilent 1200 VWD	G1314B	A.06.02 or newer	n.a.*
Agilent 1200 VWD SL	G1314C	A.06.02 or newer	n.a.*
Agilent 1100/1200 RID	G1362A	A.06.02 or newer	n.a.*
Agilent 1100/1200 UIB	G1390A	A.06.02 or newer	n.a.*
Fraction Collectors			
Agilent 1100 Fraction Collector	G1364A	A.06.02 or newer	n.a.*
Agilent 1100/1200 Fraction Collector PS	G1364B	A.06.02 or newer	n.a.*
Agilent 1100/1200 Fraction Collector AS	G1364C	A.06.02 or newer	n.a.*
Agilent 1100/1200 Micro Fraction Collector	G1364D	A.06.02 or newer	n.a.*
Valves			
2Pos/10Port Valve	G1157A	A.06.02 or newer	n.a.*
2Pos/6 Port Valve	G1158A	A.06.02 or newer	n.a.*
2Pos/6 Port Valve SL	G1158B	A.06.02 or newer	n.a.*
6Position Selection Valve	G1159A	A.06.02 or newer	n.a.*
12Pos/13 Port Selection Valve	G1160A	A.06.02 or newer	n.a.*
2Pos/6 Port Micro Valve	G1162A	A.06.02 or newer	n.a.*
2Pos/10 Port Micro Valve	G1163A	A.06.02 or newer	n.a.*
Others			
Agilent 1100/1200 Degasser	G1322A	All Revisions	
Agilent 1100 Micro Degasser	G1379A	All Revisions	

Table 3 LC 1100/1200 Series Instrument Firmware Requirements (continued)

LC Instrument	Product Number	Firmware Revision	Part Number
Agilent 1200 Micro Degasser	G1379B	All Revisions	
Agilent 1100/1200 manual injector	G1328B	All Revisions	
Agilent 1100/1200 Thermostat f. Sampler/Frac.Collectors	G1330B	All Revisions	
Agilent 1100/1200 Thermostat f. Sampler/Frac.Collectors	G1330B	All Revisions	
Agilent 1100/1200 Thermostat f. Sampler/Frac.Collectors	G1330B	All Revisions	
Agilent 1100/1200 Thermostat f. Sampler/Frac.Collectors	G1330B	All Revisions	
Agilent 1100 Local User Interface	G1323A	A.02.10****	n.a.*
Agilent 1100/1200 Local User Interface	G1323B	B.04.02*****	n.a.*
Agilent 1100/1200 Control Module Instant Pilot	G4208A	B.01.02 or newer	n.a.*

* The Agilent 1100/1200 series of LC modules have flash ROM memory. Firmware updates are distributed electronically. The latest firmware can be downloaded from the following Agilent Technologies website: http://www.chem.agilent.com/scripts/cag_firmware.asp.
Starting with firmware A.06.0x/B.01.0x, a new firmware update tool is available and distributed along with the Agilent ChemStation Software CD-ROM (CD 1- Installation).

**)The Agilent G1315C DAD and G1365C MWD modules require minimum firmware B.01.02. This firmware is only compatible with firmware A.06.02 or higher. As soon as a G1315C/G1365C is used in an 1100/1200 stack, the whole stack needs to be compatible using firmware A.06.02 or higher.

***)The Agilent G1315D DAD and G1365D MWD modules require minimum firmware B.01.04. This firmware is only compatible with firmware A.06.02 or higher. As soon as a G1315D/G1365D is used in an 1100/1200 stack, the whole stack needs to be compatible using firmware A.06.02 or higher.

****)The Agilent 1100 local user interface G1323A is only supported in combination with the following modules: G1310A, G1311A, G1312A pumps, G1313A ALS, G1314A VWD,G1315A DAD, G1316A TCC, G1321A FLD

*****)The Agilent 1100/1200 local user interface G1323B is not supported in combination with a 1100/1200 stack that includes a Chip Cube module G4240A

Table 4 1090 and miscellaneous LC Instrument Firmware Requirements

LC Instrument	Product Number	Firmware Revision	Part Number
HP 1090L		MEM D-3321	01090-66573
HP 1090L		LIB E-3321	01090-66579
HP 1090M		MCO all revisions	01090-66542
HP 1090M		MEM D-3321	01090-66573
HP 1090 II/L		LIB E-3321	01090-66579
HP 1090 DAD	option #080	COM board firmware rev.E-3014	79880-13007
HP 1046 dual grating FLD	HP 1046A	FDC board rev. B-2630	01046-66503
HP 1046 dual grating FLD	HP 1046A	FDI board with firmware rev. B or C	01046-69509
HP 1049 Electrochemical Detector	HP 1049A	Firmware rev. E-3314	01049-13002

For detailed information regarding installing additional analytical instruments (e.g. cabling, connecting to an analytical instrument), refer to the appropriate “Installing your ChemStation“ manual of your system.

GC Instrument Firmware Requirements

The GC ChemStation software requires the following minimum firmware revisions in order to work with the devices shown in Table 5.

Table 5 GC Instrument Firmware Requirements

GC Instrument	Product Number	Firmware Revision	Part Number
GC System			
Agilent 7890A GC System	G3440A	A.01.01	n.a.*
Agilent 6890N	G1530N, G1540N	GC Firmware N.05.05 LAN assembly 04.7B3	n.a.*
Agilent 6890Plus, 6890A	G1530A, G1540A	A.03.08	G1530-61706
Agilent 6850 Series GC serial# >= US10243001	G2630A	GC firmware A.05.04 LAN assembly 04.7B3	n.a.*
Agilent 6850 Series GC serial# <= US00003200	G2630A	A.03.03	n.a.*
Handheld Control Module for the 6850	G2629A	A.05.06	n.a.*
5890 Series II	5890	A.03.02	Mainboard ROM 05890-80320; GPIB/RS232 PCB 19257-80040
4890D	G2690A	A.06.00	GPIB/RS232 PCB 19257-80040
GC Autosampler			
7683B Autoinjector	G2913A	A.11.02	n.a.*
7673C Autoinjector	G1513A	A.09.15	n.a.*
7683A/6890Plus ALS interface board	G2612A	A.02.01	n.a.*

Table 5 GC Instrument Firmware Requirements

GC Instrument	Product Number	Firmware Revision	Part Number
7683A Autoinjector Module	G2613A	A.10.07	n.a.*
6850 Automatic Liquid Sampler	G2880A	A.10.05	n.a.*
GC Tray			
7673C Tray	18596C	No Revision	
7683 ALS Tray for 5890	G2916A	A.02.01	n.a.*
7683A Tray module	G2614A	A.02.01	n.a.*
GC Controller			
7673C ALS Controller	G1512A	A.01.12	n.a.*
7683B ALS Controller for 6890A and 5890 Series II GCs	G2912A	A.02.01	n.a.*
A/D Converter			
35900E	35900E	E.01.02	n.a.*

* The Agilent 7890A GC System, 6890N, 6850, Autosampler (ALS) and 35900E instruments have flash ROM memory. The GC Firmware Update Utility is provided on the ChemStation CD-ROM under the Support directory (CD 1 - Installation). The latest firmware can be downloaded from the following Agilent Technologies website: http://www.chem.agilent.com/scripts/cag_firmware.asp

For detailed information regarding installing additional analytical instruments (e.g. cabling, connecting to an analytical instrument), refer to the appropriate “Installing your ChemStation“manual of your system.

LC/MS Instrument Firmware Requirements

The LC/MS ChemStation software requires the following minimum firmware revisions in order to work with the devices shown in Table 6.

Table 6 LC/MS Instrument Firmware Requirements

LC/MS Instrument	Product Number	Firmware Revision	Part Number
Agilent 6100 Series LC/MS	G6110A/G6120A G6130A/G6140A	3.02.18 or higher	n.a*
Agilent 1100/1200 Series LC/MSD	G1946B/C/D G1956A/B	3.01.93 or higher	n.a*

* The firmware for the Agilent 6100 Series LC/MS and Agilent 1100/1200 series LC/MSD is provided as part of the ChemStation software. To update the instrument firmware, run the program x:\chem32\ms\firmware\msupdate.exe (where 'x' is the drive letter corresponding to where the ChemStation software is installed)

CE Instrument Firmware Requirements

The CE ChemStation software requires the following minimum firmware revisions in order to work with the devices shown in Table 7.

Table 7 CE Instrument Firmware Requirements

CE Instrument	Product Number	Firmware Revision	Part Number
Built-in DAD		Rev. 1.2 or higher	n.a.
Mainframe Agilent CE G1601A	G1601A	Rev. 2.3	n.a.

Communication Components

Using LAN Communication

If you connect your instrument using a standard LAN connection, you must ensure proper communication between the PC and the analytical instruments. The communication uses the TCP/IP protocol, which needs to be installed as a network protocol on your PC. The current configuration of the LAN Assembly or Jet Direct or G1369A LAN cards that are used to connect the analytical instrument to the LAN remains during the upgrade.

When upgrading from a GPIB control instrument, you must install the required LAN communication components and reconfigure your instrument. The necessary steps are documented in the “Installing your ChemStation” Manual of the appropriate chromatographic-specific technique.

Customers using LAN communication or moving from GPIB to LAN connection have to use the Agilent BootP Service as communication component for ChemStation Rev. B.03.01. Customers currently using the CAG BootP Server need to remove this component. The Agilent BootP Service needs to be installed instead; the CAG BootP Server is no longer supported. The Agilent BootP Service Program can be found on the ChemStation CD-ROM (CD 1 - Installation).

Using GPIB and USB-GPIB Communication

Some analytical instruments that communicate with the Agilent ChemStation Rev. A.xx.xx via GPIB may continue to use GPIB connection for communication with ChemStation Rev. B.03.0x. In addition, a USB-GPIB Interface can be used. For details, please refer to Table 8 on page 34.

NOTE Agilent LC 1100 and 35900E using GPIB communication are no longer supported with ChemStation Rev. B.03.01. These systems need an upgrade to LAN connection PRIOR to the upgrade to ChemStation Rev. B.03.0x.

Table 8 GPIB and Analytical Hardware Compatibility Matrix

Instrument Type	Agilent 82350 A	Agilent 82350 B	Agilent USB-GPIB Interface 82357A
Agilent 1100/1200 LC	No	No	No
HP 1090 LC	Yes	Yes	Yes
HP 1046 FLD	Yes	Yes	Yes
HP 1049 ECD	Yes	Yes	Yes
HP 5890 GC, 4890D GC	No	Yes	No
Agilent 7890A GC System	No	No	No
Agilent 6890N GC	No	No	No
Agilent 6890A and 6890 Plus GCs	No	Yes	No
Agilent 6850 GC	No	No	No
G1600A Capillary Electrophoresis	Yes	Yes	Yes
35900E	No	No	No

CAUTION The GPIB board is electrostatic-sensitive, and should be handled with care. Be sure to hold the board by the edges and do not touch the electrical components. Use anti-static equipment, such as a grounding mat and wrist-straps, during installation.

The necessary steps to configure the GPIB card, USB-GPIB interface and the related instrument parameters are documented in the “Installing your ChemStation” manual of the appropriate chromatographic-specific technique.

A document describing the installation of the SICL libraries in order to control the GPIB systems can be found on the ChemStation CD-ROM in the Manual, Installation folder (CD 2 - User Documentation and Accessories).

3 How to Upgrade to Agilent ChemStation Rev. B.03.01

Upgrades from Previous ChemStations

General Upgrade Procedure for ChemStation Systems

NOTE Before you upgrade your system, we strongly recommend that you back up your complete system.

NOTE Before starting the upgrade, read carefully the sections regarding the general upgrade, as well as the instrument-specific upgrade information.
If you have Add-On Solution software installed, read the section Chapter 3, "Upgrade Procedure for ChemStation Systems with Add-On Solutions," starting on page 51, prior to starting the upgrade procedure. Verify that your Add-On Solution is supported on ChemStation B.03.01.
If you have used GPIB communication, read the section Chapter 2, "Communication Components," starting on page 33 prior to starting the upgrade procedure.

Licenses in ChemStation Rev. B.03.0x

ChemStation Rev. A.xx.xx License numbers in general allow the upgrade to ChemStation Rev. B.03.0x. In addition, new installations can be performed using license numbers purchased for ChemStation Rev. A.xx.xx.

Agilent Training licenses (tx0000xxxx) are not valid for ChemStation Rev. B.03.0x. If your system was installed using a training license, a valid full license needs to be installed using the "Add Licenses" utility prior to or during the upgrade.

Automatic Upgrade Rev. B.0x.0x to ChemStation Rev. B.03.01

The upgrade of an existing ChemStation revision B.0x.0x to revision B.03.01 does not need specific requirements as for upgrades of Rev. A ChemStation to Rev. B. Refer to the “Installing your ChemStation” of your appropriate instrument to perform an upgrade from Revision B.0x.0x to B.03.01.

Automatic Upgrade Rev. A.09.03 to ChemStation Rev. B.03.01

Due to the move to Unicode format within ChemStation, which has a general impact, this upgrade works slightly differently than previous upgrades.

NOTE

ChemStation B.03.01 is supported on Windows XP only. ChemStation A.09.03 had been supported on either Windows NT 4.0 or Windows 2000, in order to upgrade to ChemStation B.03.01 the operating system needs to be updated PRIOR the ChemStation upgrade. Please check as well the PC minimum requirements, Chapter 2, “Minimum PC Hardware Requirements for the Agilent ChemStation,” starting on page 19.

- The upgrade process checks for configured instruments. The system upgrades the software and communication parameters based on the configuration information. For unsupported configurations, an alert is displayed, and the upgrade process is aborted
- The Windows uninstallation shield uninstalls the current ChemStation, and a backup copy is saved under the new backup directory. The original installation directory name is used to create this directory, by default HPCHEM_BACKUP. All user-created data is filed in this directory.
  The directory structure remains the same.
  A new ChemStation directory using the same name as the previous installation is created, by default HPCHEM.

  E.g.: After a default ChemStation upgrade, the structure changes from:

  - C:\hpchem (installed by default)

  to the new structure:

  - C:\hpchem_backup (contains Rev. A. higher ChemStation)

- C:\hpchem (now contains the Rev. B.03.0x ChemStation)

NOTE Before starting the upgrade, close all programs and reboot your system. Verify the LAN communication software. The Agilent BootP Service needs to be installed in place of the CAG BootP Server, which is no longer supported.

1 Starting with Agilent ChemStation B.03.01 the Microsoft .NET Framework 2.0 is used. Microsoft. NET Framework improves security and speed of the used applications and generates a basis for programs of various programming languages. If Microsoft .NET Framework is not already installed on your computer, the Agilent ChemStation installation notice you to run the installation of Microsoft.Net Framework 2.0. Microsoft.Net Framework is available on the ChemStation CD-ROM (CD 1 - Installation),in directory dotnetFramework 2.0. The upcoming message displays the location of the file. Execute the file dotnetfx20.exe.

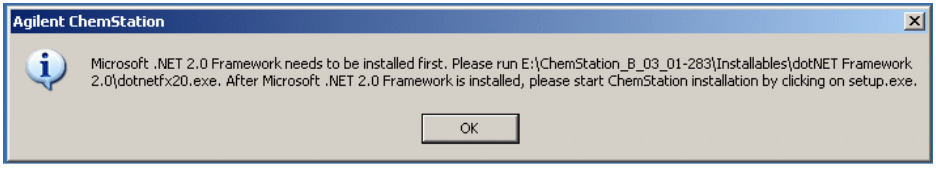


Figure 1 Microsoft .NET Framework Installation Message

2 The system needs to be rebooted after the Microsoft .NET Framework installation. After the reboot of the system, the Agilent ChemStation installation will continue.

3 Insert the Agilent ChemStation CD-ROM (CD 1 - Installation) into the CD-ROM drive.

4 From the Start menu in the Task Bar, select **Start > Run**.

5 At the command line, type *cd*:`\Setup` (e.g., `D:\Setup`), then click on **OK**. The installation wizard for Rev. B.03.0x starts and guides you through the upgrade process.

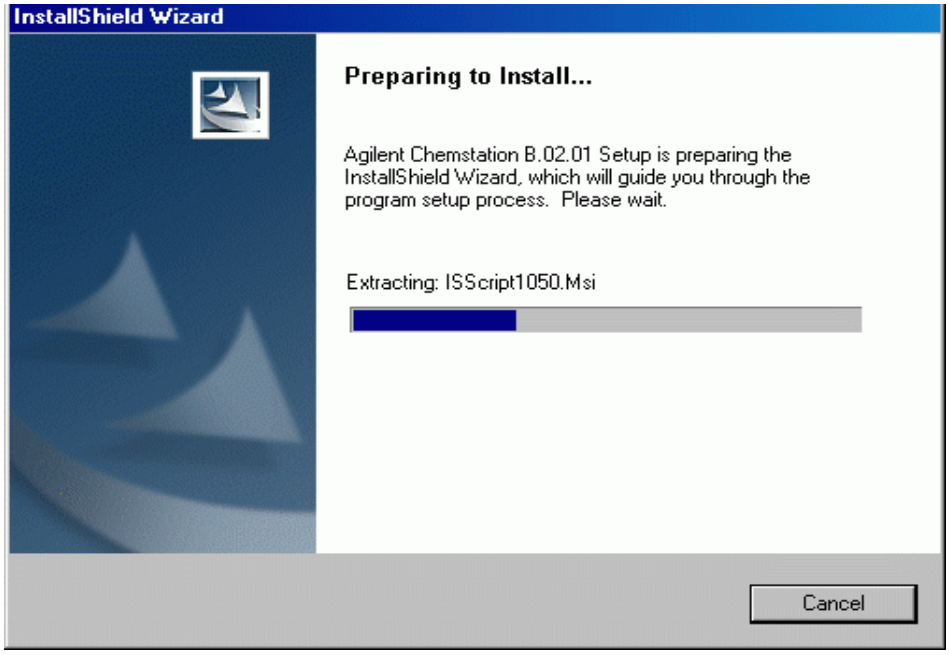


Figure 2 Installation Upgrade screen

6 If you are upgrading from ChemStation Rev. A.09.03 or higher, the system proceeds with the upgrade installation. The upgrade program analyzes your system in order to read out all necessary information to perform the upgrade.

For revisions below A.09.03, an alert is displayed and the upgrade process is aborted. See "Chapter 3, "Licenses in ChemStation Rev. B.03.0x," starting on page 38."

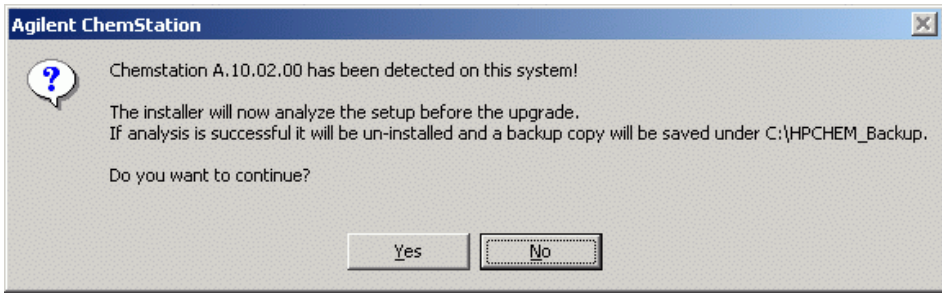


Figure 3 Installation Upgrade screen

7 Press **Yes** in order to continue the upgrade process. With the next message, you confirm the backup of the current ChemStation directory, e.g. HPCHEM, and the Win.ini file. Press **OK** to proceed with the upgrade.

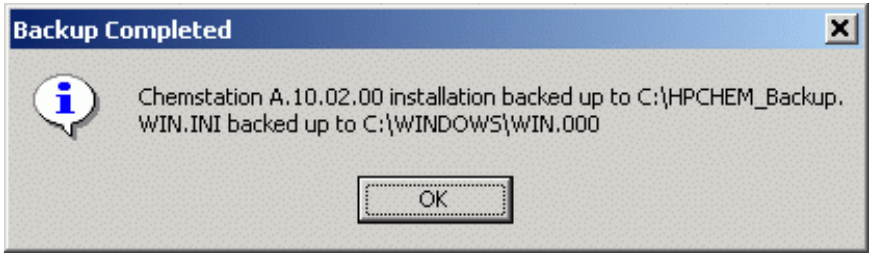


Figure 4 Backup information during Upgrade

8 The system backs up the current ChemStation into the specified backup directory. The backup directory depends on the original installed path information.

A new ChemStation directory using the same name as the previous installation is created and the ChemStation Rev. B.03.0x is installed in this new directory. This can take a few minutes.

9 At the end of the upgrade process, the system offers you the possibility to automatically move all user-created methods, sequences and datafiles to the upgraded directory. If you would like to move these files automatically, choose **Yes**, otherwise choose **No**; you then have to move the files of interest manually to the upgraded directory.

The ChemStation structure remains the same. All files in the upgraded ChemStation will be placed according to the previous ChemStation directory; for details, refer to Chapter 3, “Additional Upgrade Instructions,” starting on page 44.

(The “new” ChemStation directory has the same name as the previous installed ChemStation; this rule applies also to the backup directory.).

e.g.: Update All methods (except read-only methods) are copied from

- hpchem*instrument number*\methods

to the appropriate directory

- hpchem*instrument number*\methods

If the option for the automatic move is not selected, all files remain in their normal structure in the created backup directory

- hpchem_backup*instrument number*\methods

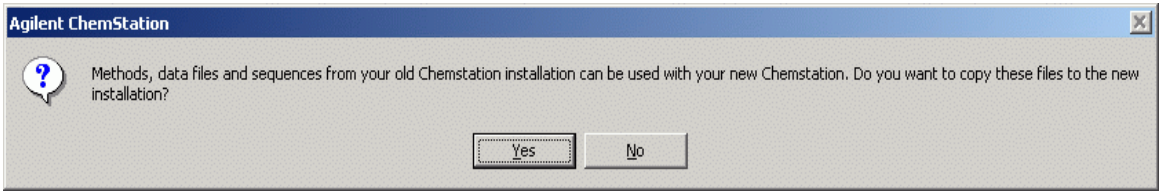


Figure 5 Automatic move of user created files during upgrade

10 Your software upgrade is now complete; press **OK** to confirm it. Remove and store your CD-ROM in a safe place. Be sure to exit Windows and reboot your system before starting the ChemStation

11 Run Installation Verification to check out the upgrade installation. Installation Verification is documented in your appropriate “Installing your ChemStation” manual.

Additional Upgrade Instructions

When you request it, the following specific files are automatically moved to the upgraded ChemStation according to their structure:

- hpchem\x\data*.d files: user-created data files
- hpchem\x\methods*.m files: user-created methods
- hpchem\x\sequences*.s files: user-created sequences
- hpchem\x\hypersequences*.hyp files: user-created hypersequences
- hpchem\speclibs*.uvl files: user-created UV library files
- hpchem\repstyles*. frp files: user-created report styles
- hpchem\core\user.mac: specially user -created macro file

The following files. if they exist, need to be moved manually to the corresponding path in ChemStation Rev. B.03.0x:

- hpchem\core*.mac, mcx files: specially user-created macro files
- hpchem\core*.xml: user-created xml files
- hpchem\chemstor*.*:
  Please refer to Chapter 5, “Upgrading ChemStation Plus Systems”
- Additional macro files if used

NOTE Customized macro solutions and the macros within the user.mac might be effected due to the move to Unicode-based encoding. Refer to Chapter 6, “Impact on Customized Solutions,” starting on page 101.

Manual Upgrade from ChemStation below Rev. A.09.03 to Rev. B.03.01

NOTE

ChemStation B.03.01 is supported on Windows XP only. ChemStation A.09.03 had been supported on either Windows NT 4.0 or Windows 2000, in order to upgrade to ChemStation B.03.01 the operating system needs to be updated PRIOR the ChemStation upgrade. Please check as well the PC minimum requirements, Chapter 2, "Minimum PC Hardware Requirements for the Agilent ChemStation," starting on page 19.

ChemStation revisions earlier than A.09.03 cannot be upgraded automatically. In order to upgrade from a lower revision than A.09.03, the PC hardware and software requirements, as well as the firmware requirements, need to be checked. If the prerequisites are met, you can upgrade any ChemStation Revision to Rev. A.09.03 or higher and then run the upgrade procedure to Rev. B.03.0x.

The other upgrade possibility is to install ChemStation Rev. B.03.0x on a supported, clean system. Then move the required user-created files of interest manually to the appropriate directories. Be sure to backup all your necessary data. If you load methods, sequences, etc. within Rev. B.03.0x, they are saved using the new file format. Files saved in ChemStation Rev. B.03.0x are not backwards-compatible with any ChemStation Rev. A.xx.xx.

Unsupported Upgrades to ChemStation Rev. B.03.01

The automatic upgrade mode is supported for ChemStation Rev. A.09.03 or higher. If your ChemStation has a lower revision than Rev. A.09.03 you must first upgrade to a ChemStation revision supporting the automatic upgrade (Rev. A.09.03 or higher). Otherwise you have to install ChemStation on a new system and move the required data manually. In this case, the new system has to match the required hardware and software specifications.

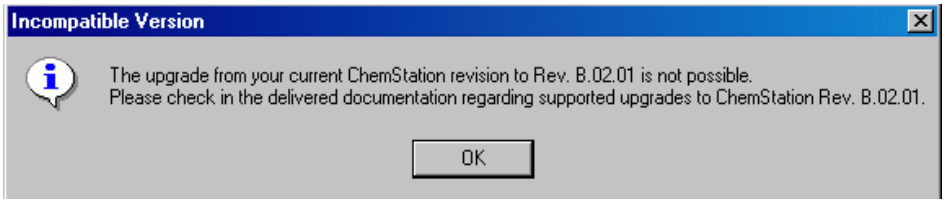


Figure 6 Alert message for unsupported upgrades

The following instruments/modules or connections types are not supported with ChemStation Rev. B.03.0x:

- all HP 1050 modules
- GPIB connection for all Agilent LC 1100/1200 modules
- GPIB connection for 35900E

For the non supported instruments/modules, an upgrade to ChemStation Rev. B.03.01 is not possible. An alert is displayed when one of these configurations is found during the upgrade:

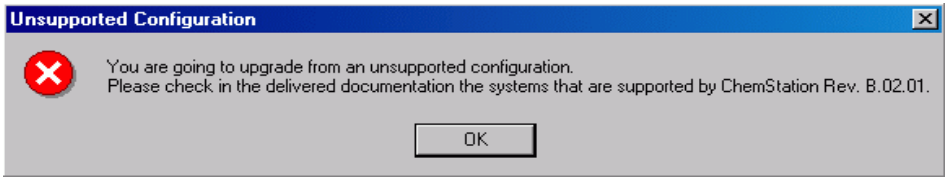


Figure 7 Alert message for unsupported upgrades

Instrument Specific Upgrade Instructions

The instrument specific upgrade instructions can differ depending if the system is upgraded from Rev A.xx.xx ChemStation or Rev. B.0x.0x ChemStation to ChemStation B.03.01. The header of the instrument specific upgrade information specify, if the information is in general valid for upgrade installation, or only for a specific upgrade, e.g. Rev. A to Rev. B.

LC-Specific Upgrade Instructions

Upgrade Rev. A.09.03/A.10.01/A.10.02 to Rev. B.03.01

LC 1100 modules communication The following HPLC 1100-specific file is moved to the upgraded ChemStation when you accept the automatic move of ChemStation files during the upgrade:

- hpchem*instrument number*\clusterx.mth: system-created configuration file for LC 1100 modules

Wellplate Configuration The following Wellplate Sampler-specific file is moved to the upgraded ChemStation when you accept the automatic move of ChemStation files during the upgrade:

- hpchem*instrument number**.wpt files: user-created Wellplate definition file

GC-Specific Upgrade Instructions

GC Column Catalog

The user-defined column entry is saved with the method and stays with the method after the upgrade. However, during the upgrade, the user-defined columns are not transferred to the GC column catalog directly. The GC Column Database Utility must be used after the upgrade from G2070AA to G2070BA ChemStation to transer user-defined GC Columns to the column catalog.

The Utility is available on the ChemStation CD-ROM (CD 2- User Documentation and Accesories) under the support directory.

35900E

The G2072BA and G2073BA A/D products require a 35900E with LAN communication.

LC/MS-Specific Upgrade Instructions

Updating LC/MSD Firmware

The firmware for the Agilent 6100 Series LC/MS and Agilent 1100/1200 series LC/MSD is included as part of the LC/MSD ChemStation software. After the LC/MSD ChemStation is upgraded to Rev. B.03.0x, the LC/MSD firmware needs to be updated.

To update the instrument firmware, first make sure the LC/MSD ChemStation is closed, then run the program x:\chem32\ms\firmware\msupdate.exe (where 'x' is the drive letter corresponding to where the ChemStation software is installed)

Tune Files

After upgrading to Rev. B.03.0x LC/MSD ChemStation, a dual polarity autotune should be performed to reestablish the tuning parameters for the instrument.

CE and CE/MS-Specific Upgrade Instructions

CE ChemStation

There are no CE specific upgrade instructions.

CE/MS ChemStation

CE/MS ChemStation consists of a G1601AA CE ChemStation including a G2201AA MS ChemStation. The G2201 is an Add-On program to the CE ChemStation; for instructions on how to handle the upgrade of a CE/MS ChemStation Rev. A to the Rev. B.03.01, please refer to "CE and CE/MS-Specific Add-On Solutions" on page 67.

Upgrade Procedure for ChemStation Systems with Add-On Solutions

NOTE Verify PRIOR to the upgrade, that your installed Add-On Solution is supported on ChemStation B.03.01. Refer to Table 9, "Supported Add-On Solution Products with ChemStation Rev. B.03.01," on page 52, to see the supported Add-On Solutions and the minimum revision.

All Add-On software products need to be uninstalled before any automatic upgrade of an existing ChemStation Rev. A.09.03 or higher to ChemStation Revision B.03.0x.
There is no automatic upgrade for Add-On products. The different behaviors regarding uninstallation are summarized in the table below. The Add-On software must be reinstalled following the ChemStation upgrade.

During the installation of an Add-On solution, certain information is written to a specific file (located in the windows directory of your system) in order to maintain the Add-On solution program:

- ChemStation Revision A: win.ini
- ChemStation Revision B: chemstation.ini

During the upgrade process, the upgrade program reads all win.ini/chemstation.ini entries and detects Add-On solutions by their entries in this file. Uninstalling the ChemStation software without previously removing the Add-On solution triggers an alert during the upgrade process.

Installed products belonging to the ChemStation Plus Family, such as ChemStore or ChemAccess, must be uninstalled using the standard Windows uninstall procedure (Start> Settings>Control Panel > Add/Remove programs). Uninstall these products using the Windows routine prior to upgrading the ChemStation.

In addition, some Add-On programs create certain entries in the win.ini/chemstation.ini file that are not removed during the uninstallation; these entries may need to be MANUALLY removed from the win.ini/chemstation.ini file AFTER the uninstallation of the Add-On solution, but PRIOR to the upgrade installation.

Supported Add-On Solution Products with ChemStation Rev. B.03.01

NOTE Verify PRIOR to the upgrade, that your installed Add-On Solution is supported on ChemStation B.03.0x. Not every Add-On Solution software is initially supported. The supported Add-On Solutions are documented in Table 9, "Supported Add-On Solution Products with ChemStation Rev. B.03.01," on page 52.

Please find below the supported Rev. of Add-On Solutions to be installed on ChemStation Rev. B.03.01:

Table 9 Supported Add-On Solution Products with ChemStation Rev. B.03.01

Add-On Solution for ChemStation Rev. B.03.01	Required Revision for ChemStation Rev. B.03.01	Uninstall from ChemStation Rev. B.03.01
G2198BA Enterprise Content Manager (ECM)	B.03.01 **only with** Data Storage Mode: Unique Data Container ON	ECM cannot be uninstalled.
G2181BA ChemStore Client/Server	B.03.03 SR2 **only with** Data Storage Mode: Unique Data Container ON	Uninstalls completely from the Add/Remove Programs in Control Panel, including entries in the chemstation.ini.
G2183BA Security Pack	B.03.03 SR2	Uninstall done by ChemStore
Purify	B.01.01	Uninstalls completely from the Add/Remove Programs in Control Panel, including entries in the chemstation.ini.
G2182BA GPC Gel Permeation Chromatography	B.01.01	Uninstalls completely from the Add/Remove Programs in Control Panel, including entries in the chemstation.ini.
G2080BA Retention Time Locking for GC	Installed with GC ChemStation	RTL cannot be uninstalled
GC Companion	Installed with GC ChemStation	Companion cannot be uninstalled
G3382AA Control for CTC PAL Autosampler for GC Systems	A.01.03	Uninstalls completely from the Add/Remove Programs in Control Panel, including entries in the chemstation.ini.

Table 9 Supported Add-On Solution Products with ChemStation Rev. B.03.01 (continued)

Add-On Solution for ChemStation Rev. B.03.01	Required Revision for ChemStation Rev. B.03.01	Uninstall from ChemStation Rev. B.03.01
G3383AA Control for CTC PAL Autosampler for LC and LC/MS Systems	A.01.02	Uninstalls completely from the Add/Remove Programs in Control Panel, including entries in the chemstation.ini.
G2924AA Integrated HeadSpace software for GC	A.01.06	Uninstalls completely from the Add/Remove Programs in Control Panel, including entries in the chemstation.ini.
Active Splitter	A.01.02.16	Uninstalls completely from the Add/Remove Programs in Control Panel, including entries in the chemstation.ini.
G1979A Multi-Signal Output Accessory	A.01.01	Uninstalls completely from the Add/Remove Programs in Control Panel, including entries in the chemstation.ini.
Analyst	1.4	Uninstalls completely from the Add/Remove Programs in Control Panel.
Easy -Access	A.04.03	Uninstalls completely from the Add/Remove Programs in Control Panel, including entries in the chemstation.ini.
Data Browser	A.03.01	Uninstalls completely from the Add/Remove Programs in Control Panel, including entries in the chemstation.ini.
G2201BA CE/MS	B.03.01	Uninstalls completely from the Add/Remove Programs in Control Panel, including entries in the chemstation.ini.

Performing an Upgrade with Add-On Solutions installed

Upgrade from ChemStation B.0x.0x Revision with Add-On Solution

Required steps for performing an upgrade of ChemStation revision B.01.0x with installed Add-On solution. e.g. Purify:

1 Uninstall the Add-On Solution software using the standard Windows uninstall procedure (Control Panel > Add/Remove programs). During this uninstallation process, the system removes the Add-On solution entries corresponding to the just uninstalled Add-On solution program. If more Add-On Solutions are installed on the system, each Add-On solution needs to be removed using the Add/Remove programs.

Table 10 ChemStation Rev. B.0x.0x Add-On-Solution Uninstall Instructions - Summary

Add-On Solutions for ChemStation B.0x.0x	Rev.	Add-On Entries in ChemStation.ini (may need to be removed manually AFTER running the Uninstallation via ADD/REMOVE programs)	Add/Remove Programs from Windows
G2198BA Enterprise Content Manager (ECM)	starting B.02.01 SR1	After installation included in ChemStation. ECM cannot be uninstalled.	No
G2181BA ChemStore Client/Server	starting B.03.02 SR1	[PCS] ChemStore C/S =C:\CHEM32\ChemStor\database [PCS, Instrument number] ADDONS=x (whereas x is the number of installed Add-Ons) ADDONx=C:\CHEM32\ChemStor\hpdbif00.mcx ChemStore C/S =C:\CHEM32\ChemStor\database	Yes, removes completely all related entries in chemstation.ini
G2183BA Security Pack	starting B.03.02 SR1	No Add-On entries in win.ini	No, will be uninstalled during ChemStore uninstallation.

Table 10 ChemStation Rev. B.0x.0x Add-On-Solution Uninstall Instructions - Summary

Add-On Solutions for ChemStation B.0x.0x	Rev.	Add-On Entries in ChemStation.ini (may need to be removed manually AFTER running the Uninstallation via ADD/REMOVE programs)	Add/Remove Programs from Windows
Purify	starting B.01.01	[PCS, Instrument number] ADDONS=x (whereas x is the number of installed Add-Ons) ADDONx=C:\Purify\bin\inl_puri.mcx [Purify] Version = xx.xx Path=c:\Purify	Yes, removes completely all related entries in chemstation.ini
Method Validation Pack	up to A.02.01	[PCS, Instrument number] ADDONS=x (whereas x is the number of installed Add-Ons) ADDONx=C:\CHEM32\CORE\hpca.mac MVPrevSeqFile=... MVPrevSeqPath=... MethodValidationMode=1	Yes, removes completely all related entries in chemstation.ini
Easy Access	starting A.04.00	[PCS, Instrument number] ADDONS=x (whereas x is the number of installed Add-Ons) ADDONx=C:\CHEM32\CORE\ezxmmain.mac	Yes, removes completely all related entries in chemstation.ini
Data Browser	starting A.02.00	[PCS, Instrument number] ADDONS=x (whereas x is the number of installed Add-Ons) ADDONx=C:\CHEM32\CORE\aevgen.mac	Yes, removes completely all related entries in chemstation.ini
G2080BA Retention Time Locking for GC	starting B.01.02	[PCS, Instrument number] ADDONS=x (whereas x is the number of installed Add-Ons) ADDONx=C:\CHEM32\RTL\RTLTOP.MAC	Yes, removes completely all related entries in chemstation.ini
GC Companion	no Rev.	Included with GC ChemStation. Companion cannot be uninstalled.	No
G3382AA Control for CTC PAL Autosampler for GC Systems	starting A.01.01	[PCS, Instrument number] ADDONS=x (whereas x is the number of installed Add-Ons) ADDONx=C:\Chem32\CTC\CTC_TOP.MAC	

Table 10 ChemStation Rev. B.0x.0x Add-On-Solution Uninstall Instructions - Summary

Add-On Solutions for ChemStation B.0x.0x	Rev.	Add-On Entries in ChemStation.ini (may need to be removed manually AFTER running the Uninstallation via ADD/REMOVE programs)	Add/Remove Programs from Windows
G3383AA Control for CTC PAL Autosampler for LC and LC/MS Systems	starting A.01.01	[PCS, Instrument number] ADDONS=x (whereas x is the number of installed Add-Ons) ADDONx=C:\Chem32\CTC\CTC_TOP.MAC	
G2924AA Integrated HeadSpace software for GC	starting A.01.04	[PCS, Instrument number] ADDONS=x (whereas x is the number of installed Add-Ons) ADDONx=C:\CHEM32\HS\HSAddon.MAC	Yes, but it is required to manually delete Add-On entries from the chemstation.ini
CTC Cycle Composer	1.5.2	[PCS, Instrument number] ADDONS=x (whereas x is the number of installed Add-Ons) ADDONx=C:\CHEM32\CORE\PALSEQ.mac	Yes, but it is required to manually delete Add-On entries from the chemstation.ini
Active Splitter	starting A.01.01	[PCS, Instrument number] ADDONS=x (whereas x is the number of installed Add-Ons) ADDONx=C:\CHEM32\CORE\actsplit.mac	Yes, removes completely all related entries in chemstation.ini
G1979A Multi-Signal Output Accessory	starting A.01.01	[[PCS, Instrument number] ADDONS=x (whereas x is the number of installed Add-Ons) ADDONx=C:\CHEM32\CORE\G1979A.mac	Yes, removes completely all related entries in chemstation.ini
Analyst	starting 1.4	No Add-On entries in win.ini	
G2201A CE/MS	starting B.01.03	[PCS, Instrument number] ADDONS=x (whereas x is the number of installed Add-Ons) ADDON1=C:\CHEM32\MS\MSTOP.MAC	Yes, but it is required to manually delete Add-On entries from the chemstation.ini

Upgrade from ChemStation Revision A.xx.xx with Add-On Solution

Required steps for performing an upgrade of ChemStations A.xx.xx with installed Add-On solution. e.g. GC Companion:

1 Uninstall the Add-On Solution software using the standard Windows uninstall procedure (Control Panel > Add/Remove programs)

2 From the Start menu in the Task Bar, select Start > Run.

3 Type Win.ini into the command line and press OK. The win.ini file opens.

4 Within the [PCS] and [PCS,x] section where x reflects the number of the instruments installed, search for the Add-On solution-related entries.
e.g. for ChemStation Companion
ADDONS=1
ADDON1=C:\HPCHEM\PUI\PUITOP.mac
When Add-On Solutions are installed on the system, the variable ADDONS=x is incremented and represents the number of installed Add-On solutions.

The win.ini entries related to the installed Add-On solutions are listed in Table 11, “ChemStation Rev. A.xx.xx Add-On-Solution Uninstall Instructions - Summary,” on page 59.

5 Delete the Add-On solution entries corresponding to the just uninstalled Add-On solution program. If more Add-On Solutions are installed on the system, the variable ADDONS=x must be decremented to represent the number of the remaining Add-On solutions, since the Add-On programs need to be deinstalled separately.

NOTE Refer to the corresponding software documentation of the Add-On Solution product for more details regarding the win.ini entries.

6 Save and close the win.ini file.

7 Verify that all Add-On programs are removed, otherwise proceed with step 1 to uninstall further Add-On solutions.

The following message during the upgrade procedure indicates that either

- there is still an Add-On solution installed on top of ChemStation

or

- the Add-On entries are not removed from the win.ini file prior the ChemStation upgrade.

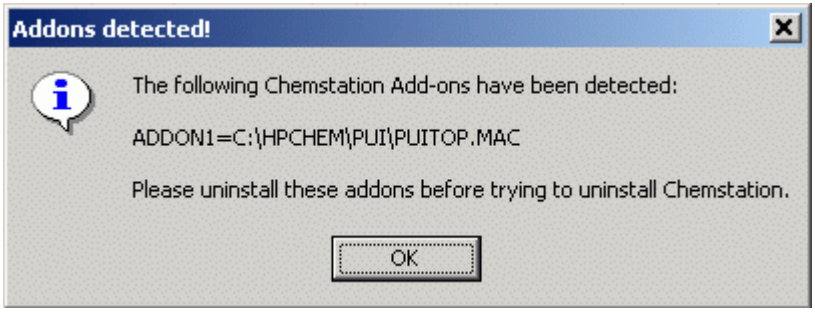


Figure 8 Alert message during upgrade with Add-On solution installed

Table 11 ChemStation Rev. A.xx.xx Add-On-Solution Uninstall Instructions - Summary

Add-On Solutions for ChemStation A.xx.xx	Rev.	Add-On Entries in Win.ini (may need to be removed manually AFTER running the Uninstallation via ADD/REMOVE programs)	Add/Remove Programs from Windows
ChemStore Client/Server	up to B.03.02	[PCS] ChemStore C/S =C:\HPCHEM\ChemStor\database [PCS, Instrument number] ADDONS=x (whereas x is the number of installed Add-Ons) ADDONx=C:\HPCHEM\ChemStor\hpdbif00.mcx ChemStore C/S =C:\HPCHEM\ChemStor\database	Yes, but it is required to manually delete Add-On entries from the win.ini
Security Pack	up to B.03.02	No Add-On entries in win.ini	No, will be uninstalled during ChemStore uninstallation.
Purify	up to A.02.01	[PCS, Instrument number] ADDONS=x (whereas x is the number of installed Add-Ons) ADDONx=C:\Purify\bin\inl_puri.mcx [Purify] Version = xx.xx Path=c:\Purify	Yes, removes completely all related entries in win.ini.
ChemAccess	up to A.02.01	[PCS, Instrument number] ADDONS=x (whereas x is the number of installed Add-Ons) ADDONx=C:\HPCHEM\CORE\hpca.mac	Yes, but it is required to manually delete Add-On entries from the win.ini
Method Validation Pack	up to A.02.01	[PCS, Instrument number] ADDONS=x (whereas x is the number of installed Add-Ons) ADDONx=C:\HPCHEM\CORE\hpca.mac MVPrevSeqFile=... MVPrevSeqPath=... MethodValidationMode=1	Yes, but it is required to manually delete Add-On entries from the win.ini
GPC	up to A.02.02	[PCS, Instrument number] ADDONS=x (whereas x is the number of installed Add-Ons) ADDONx=C:\HPCHEM\GPC\Gpc_top.mac and GPC files need to be manual removed from the installation directory, refer to the readme.txt of the GPC Software	Not possible, remove manually

Table 11 ChemStation Rev. A.xx.xx Add-On-Solution Uninstall Instructions - Summary (continued)

Add-On Solutions for ChemStation A.xx.xx	Rev.	Add-On Entries in Win.ini (may need to be removed manually AFTER running the Uninstallation via ADD/REMOVE programs)	Add/Remove Programs from Windows
Easy Access	up to A.03.00	[PCS, Instrument number] ADDONS=x (whereas x is the number of installed Add-Ons) ADDONx=C:\HPCHEM\CORE\ezxmmain.mac	Yes, removes completely all related entries in win.ini.
Data Browser	up to A.01.02	[PCS, Instrument number] ADDONS=x (whereas x is the number of installed Add-Ons) ADDONx=C:\HPCHEM\CORE\aevgen.mac	Yes, removes completely all related entries in win.ini.
G2080AA Retention Time Locking for GC	A.05.02 A.06.01 B.01.01	[PCS, Instrument number] ADDONS=x (whereas x is the number of installed Add-Ons) ADDONx=C:\HPCHEM\RTL\RTLTOP.MAC	Yes, but it is required to manually delete Add-On entries from the win.ini
GC Companion	no Rev.	[PCS, Instrument number] ADDONS=x (whereas x is the number of installed Add-Ons) ADDONx=C:\HPCHEM\PUI\PUITOP.MAC	Yes, but it is required to manually delete Add-On entries from the win.ini
G2401AA Standalone HeadSpace software for GC	A.01.01	G2401AA is not an Add-on and is not added to the win.ini file. The G2401AA is not supported with the ChemStation.	No, must be removed separately.
G2922AA Integrated HeadSpace software for GC	A.01.0x	[PCS, Instrument number] ADDONS=x (whereas x is the number of installed Add-Ons) ADDONx=C:\HPCHEM\HS\HSAddon.MAC	Yes, but it is required to manually delete Add-On entries from the win.ini
CC Mode	A.03.02	[PCS, Instrument number] ADDONS=x (whereas x is the number of installed Add-Ons) ADDONx=C:\CCMODE\bin\ccmode3.mcx [CCMODE3] Path=C:\CCMODE etc. [CCMODEIII] version=À.03.xx	Yes, but it is required to manually delete Add-On entries from the win.ini

Table 11 ChemStation Rev. A.xx.xx Add-On-Solution Uninstall Instructions - Summary (continued)

Add-On Solutions for ChemStation A.xx.xx	Rev.	Add-On Entries in Win.ini (may need to be removed manually AFTER running the Uninstallation via ADD/REMOVE programs)	Add/Remove Programs from Windows
CTC Cycle Composer	1.5.2	[PCS, Instrument number] ADDONS=x (whereas x is the number of installed Add-Ons) ADDONx=C:\HPCHEM\CORE\PALSEQ.mac	Yes, but it is required to manually delete Add-On entries from the win.ini
Active Splitter	A.01.00	[PCS, Instrument number] ADDONS=x (whereas x is the number of installed Add-Ons) ADDONx=C:\HPCHEM\CORE\actsplit.mac	Yes, removes completely all related entries in win.ini.
G1979A Multi-Signal Output Accessory	A.01.00	[[PCS, Instrument number] ADDONS=x (whereas x is the number of installed Add-Ons) ADDONx=C:\HPCHEM\CORE\G1979A.mac	Yes, removes completely all related entries in win.ini.
Analyst	1.1.1/ 1.4	No Add-On entries in win.ini	
G2201A CE/MS	A.09.03 and higher	[PCS, Instrument number] ADDONS=x (whereas x is the number of installed Add-Ons) ADDON1=C:\HPCHEM\MS\MSTOP.MAC	Yes, but it is required to manually delete Add-On entries from the win.ini

General Add-On Solutions

All Add-On software products need to be uninstalled before any upgrade of Rev. A.09.03 or higher ChemStation to ChemStation Revision B.03.0x. There is no automatic upgrade of following general Add-On products: ChemStore and ChemStation Plus Security Pack. The Add-On software must be upgraded after the ChemStation upgrade.

ChemStore (up to B.03.02)

The G2181BA ChemStore software on top of ChemStation Rev. A cannot be updated to ChemStore B.03.03 software. The software needs to be uninstalled according to the uninstallation section of the ChemStore C/S Installation Guide. In addition, the following entries need to be deleted from the win.ini file:

In the [PCS] section:

ChemStore C/S =C:\HPCHEM\ChemStor\database

In all [PCS,x] sections:

ADDONS=x (whereas x is the number of installed Add-Ons)
ADDONx=C:\HPCHEM\ChemStor\hpdbif00.mac
ADDON(x+1)= C:\HPCHEM\Core\mv.mac (for G2184A only)
ChemStore C/S =C:\HPCHEM\ChemStor\database

ChemStore (above B.03.02 SR1)

The G2181BA ChemStore software on top of ChemStation Rev. B cannot be updated to ChemStore B.03.03 software. The software needs to be uninstalled according to the uninstallation section of the ChemStore C/S Installation Guide. The deinstallation program removes in addition all related section in the chemstation.ini file.

Security Pack

The ChemStore uninstallation program removes all Security Pack-related items. A separate uninstallation is not possible.

LC-Specific Add-On Solutions

All Add-On software products need to be uninstalled before any upgrade of G2170AA/G2180AA ChemStation to G2170BA/G2180BA ChemStation Revision B.03.01. The Add-on software must be upgraded after the ChemStation upgrade.

Purify Software

The following Purification Add-On Solution Software cannot automatically be upgraded to next higher revision B.03.0x. The software needs to be uninstalled according to the uninstallation section of the appropriate manual:

G2262AAPurification/HiThruput SW module
G2263AAMass based fraction collection add-on SW (LC/MS specific)
G2265AAStandalone Purification/HiThruput DA SW

The uninstallation shield of the Purification software removes all Purification related entries from the win.ini file. For details refer to Table 11 on page 59.

GC-Specific Add-On Solutions

All Add-On software products need to be uninstalled before any upgrade of G2070AA ChemStation to G2070BA ChemStation B.03.01.
The Add-On software must be upgraded after the ChemStation upgrade.

Retention Time Locking

The G2080AA Retention Time Locking (RTL) Add-On software must be removed using the Add/Remove Programs in Control Panel. In addition, the RTL add-on entries in the win.ini file must be manually deleted before the Rev. B.03.0x GC ChemStation is installed.

Beginning with B.03.01, RTL is now integrated in the GC ChemStation.

Companion

The Companion Add-On software must be removed using the Add/Remove Programs in Control panel. In addition, the Companion add-on entries in the win.ini file must be manually deleted.

Beginning with B.01.01, the ChemStation Companion is included with the G2070BA GC ChemStation installation.

Headspace

ChemStation G2070BA supports the integrated G2924AA HeadSpace software.

The G2922AA Integrated Headspace software is supported only on G2070AA/G2071AA ChemStation and must be removed using the Add/Remove Programs in Control Panel before upgrading to GC ChemStation revision B.03.01. In addition, the HeadSpace add-on entries in the win.ini file must be manually deleted.

Be aware, that the G2922AA registration number will not load the G2924AA software. The G2924AA software will need to be purchased.

The G2401AA A.01.01 Headspace software is a separate standalone program and is not supported with G2070BA/G2071BA ChemStation.

LC/MS-Specific Add-On Solutions

All Add-On software products, except Analyst, need to be uninstalled before any upgrade of G2710AA LC/MSD ChemStation to G2710BA LC/MSD ChemStation Revision B.03.0x. The Add-on software must be upgraded after the ChemStation upgrade.

Purify Software

Following Purification Add-On Solution Software cannot automatically be upgraded to next higher revision B.03.0x:

G2262AAPurification/HiThruput SW module
G2263AAMass based fraction collection add-on SW (LC/MS specific)
G2265AAStandalone Purification/HiThruput DA SW

'The uninstallation shield of the Purification software removes all Purification related entries from the win.ini file. For details refer to Figure 11 on page 59.

Active Splitter Software

The Active Splitter Add-On software must be removed using the Add/Remove Programs in Control Panel before the Rev. B.03.0x LC/MSD ChemStation software is installed.

G1979A Multi-Signal Output Accessory Software

The G1979A Multi-Signal Output Accessory Add-On software must be removed using the Add/Remove Programs in Control Panel before the Rev. B.03.0x LC/MSD ChemStation software is installed.

Analyst Software

If Analyst Rev. 1.1.1 Add-On software is installed, it must be upgraded to Analyst Rev. 1.4 before the Rev. B.03.0x LC/MSD ChemStation is installed. The Analyst Rev. 1.4 Add-on software should not be removed before the Rev. B.03.0x LC/MSD ChemStation software is installed. The Rev. B.03.0x LC/MSD ChemStation should be installed with the Analyst Rev. 1.4 still installed.

Easy-Access Software

The Easy Access Add-on software must be removed using the Add/Remove Programs in Control Panel before the Rev. B.03.0x LC/MSD ChemStation software is installed.

CTC Cycle Composer Software

The CTC Cycle Composer Add-on software must be removed using the Add/Remove Programs in Control Panel. In addition, the CTC Cycle Composer add-on entries in win.ini must be manually deleted before the Rev. B.03.0x LC/MSD ChemStation is installed.

Data Browser Software

The Data Browser Add-On software must be removed using the Add/Remove Programs in Control Panel before the Rev. B.03.0x LC/MSD ChemStation software is installed.

CE and CE/MS-Specific Add-On Solutions

Updating CE/MSD G2201 from ChemStation Rev. A09.03/A.10.01/A.10.02

CE/MS ChemStation consists of a G1601AA CE ChemStation including a G2201AA MS ChemStation. Upgrading a CE/MS ChemStation Rev. A.09.03 or higher following steps need to be performed:

1 Verify that all programs are closed.

2 Locate and open the win.ini (C:\windows directory). Search for the following entries in the PCS section and either delete them manually or disable them by setting a semicolon (;) in front of each line.

[PCS, Instrument number]
ADDONS=x (whereas x is the number of installed Add-Ons)
ADDON1=C:\HPCHEM\MS\MSTOP.MAC

This modification disables the G2201 MS Add-On program.

3 Insert the ChemStation B.03.01 CD-ROM (CD 1 - Installation) and start setup.exe to run the upgrade to Rev. B.03.01 ChemStation (CE ChemStation G1601BA only).

4 The system follows the described upgrade process outlined in chapter "Automatic Upgrade Rev. A.09.03 to ChemStation Rev. B.03.01" on page 39.

5 At the end of the upgrade process, the system offers to open the configuration editor. In the case of a CE/MS upgrade *do not* open the configuration editor yet. Leave the screen with **No.**
The system will give you instructions on the screen.

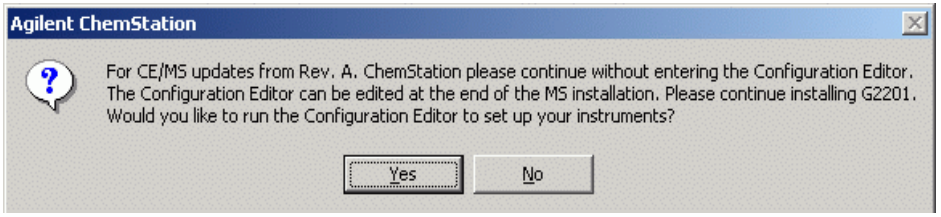


Figure 9 Alert message after upgrading CE part of a CE/MS ChemStation

6 Finish the upgrade and reboot your system.

7 Open the explorer and locate the folder G2201 on the B.03.01 ChemStation CD ROM (CD 1 - Installation). Start setup.exe to install the MS ChemStation Add-On Software for ChemStation B.03.01.

8 Select the CE ChemStation to enable MS capabilities for the system. Press **OK** to continue the upgrade.

9 At the end of the upgrade process you can access the configuration editor to check for the configured modules.

10 After the review of the readme, finish the installation of the G2201 MS ChemStation and reboot your system.

Configuring your Instruments

The upgrade process detects the configured instruments and establishes the instrument setup based on the current configuration. No additional configuration is needed, except that it may be necessary, when the upgrade is used, to move from GPIB to LAN communication. The LAN and GPIB communications, as well as the configuration of the instruments in the case of a communication change, is documented in the appropriate “Installing your ChemStation” manual.

When upgrading from a GPIB controlled instrument, you must install the required LAN communication components and reconfigure your instrument prior to the upgrade. The necessary steps are documented in the “Installing your ChemStation” manual of the appropriate chromatographic specific technique.

Customers using LAN communication or moving from GPIB to LAN connection have to use the Agilent BootP Service as communication component for ChemStation Rev. B.03.01.
Customers currently using the CAG BootP Server need to remove this component. The Agilent BootP Service needs to be installed instead, since the CAG BootP Server is no longer supported. The Agilent BootP Service Program can be found on the ChemStation CD-ROM (CD 1 -Installation).

NOTE The Agilent 82350 A/B cards are supported on Windows XP Professional using ChemStation Rev. B.03.0x, for all analytical hardware as described in Table 8, “GPIB and Analytical Hardware Compatibility Matrix,” on page 34.

NOTE Systems including Agilent LC 1100 modules or 35900E communicating via GPIB need upgrade to LAN connection PRIOR to the upgrade to ChemStation Rev. B.03.0x.

Agilent LC 1100 and 35900E using GPIB communication are no longer supported with ChemStation Rev. B.03.0x.

4 The First Time You Start Up Your ChemStation Rev. B.03.01

Startup Changes Introduced with B.03.01

Since revision B.02.01, ChemStation has introduced a new data organization scheme (as outlined below in chapter "Startup Changes Introduced with B.02.0x and B.01.0x" on page 75) that provides a number of advantages:

- Sequence data are not overwritten. Each sequence acquisition stores the resulting data files in its own sequence container with unique name.
- With the sequence container concept, the data are stored with all necessary information needed for data analysis, i.e. copies of the sequence file and of all methods employed with the sequence. These methods can be changed with sequence specific input and do not influence the original master method. The container concept thus strengthens the meaning of a sequence as a set of data files and methods belonging together for result creation.
- Data review and reprocessing are both available in Data Analysis view via the Navigation Table.
- The data container concept provides the optimal preconditions for the ChemStation Integration with the Agilent Enterprise Content Manager (ECM).

However, there may be situations where users may want to store their data as in ChemStation B.01.03 or earlier and work according to the corresponding workflows:

- During method development it may be more convenient to have only one method for both acquisition and data analysis to automatically have changes available for future acquisition and reanalysis of already acqired data.
- Data from several acquisitions have to be in one folder, e.g. in case of partial acquisition.
- Customized macro solutions on a ChemStation system that have been designed for older revisions may require the data, methods, or sequence to be stored according to the old data organization scheme.
- When ChemStation B.03.01 runs in a lab where there are also system still running on ChemStation revisions B.01.03 or earlier, it may be more convenient to use the same data organization mode on all systems.

In order to allow working with a data storage concept as in ChemStation revisions before B.02.01, the Sequence tab of the Preferences dialog box a Data Storage section. Here you can choose between “Unique Folder Creation ON” and “Unique Folder Creation OFF” (Figure 10). Per default, “Unique Folder Creation ON” is selected. “Unique Folder Creation ON” enables the data storage concept as outlined below in “Startup Changes Introduced with B.02.0x and B.01.0x” on page 75. “Unique Folder Creation OFF” allows you to store data as in ChemStation B.01.03 or earlier. More details can be found in the “Getting Started with New ChemStation Workflow” manual.

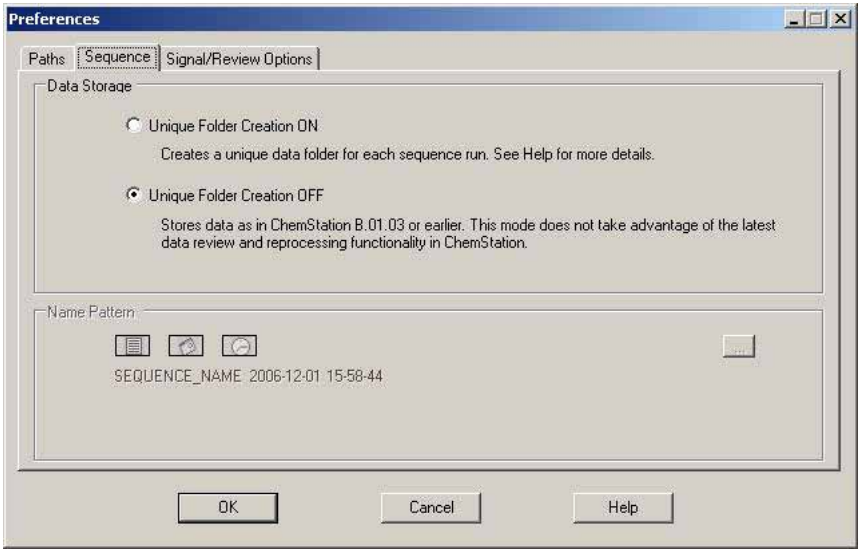


Figure 10 Preferences Dialog / Sequence Tab

NOTE Switching Unique Folder Creation on or off only affects future acquisitions, but does not change the data organization of already acquired data.

NOTE We recommend to decide between the two modes at the beginning of your work and not to switch between them.

Switching Unique Folder Creation off is not possible with the ChemStation ECM Integration or ChemStore/Security Pack installed.

The enhanced ChemStation user interface as introduced with ChemStation B.02.01 (see below in chapter "Startup Changes Introduced with B.02.0x and B.01.0x" on page 75) is also available when Unique Folder Creation is switched off. However, there are functions you can not take advantage of in this mode. The same limitations apply to any run acquired with ChemStation prior to B.02.01.

- When a sequence is loaded into the Navigation Table, the reprocessing toolset is grayed out. Sequences that have been acquired in this data storage mode can only be reprocessed in Method and Run Control view using the "Reprocessing only" option in the Sequence Parameters.
- With the method usage options "Use method from data file" and "Use sequence method", a warning message will be displayed each time a run is double-clicked in the Navigation Table that the individual method/sequence method does not exist. As outlined above, these methods are not stored with the data. In this case, the only meaningful option for data review is "Use current method".

Startup Changes Introduced with B.02.0x and B.01.0x

Starting with B.02.01, ChemStation offers a new design and tree-based navigation, together with a new flexible data management. Navigation items enable you to use right-mouse click functions for easy data handling, for example, loading data files. The graphical user interface items have been improved and reorganized to allow more flexible handling, and to make use of the tree-based navigation. The functionality of the graphical action items (icons), and the ChemStation view location of these items has not been changed. To support these graphical changes, note that the supported screen resolution is 1280x 1024.

Navigation Items

A tree-based navigation pane is available on the left side of all ChemStation views. This **Navigation Pane** includes an autohide feature, and offers standard features such as resizing and re-arranging of the navigation button area. The Navigation Pane contains the following two items:

Navigation Buttons

The Navigation Buttons allow the ChemStation view to be switched by clicking on the specific Navigation button. The Navigation Button section can be minimized, expanded or re-arranged.

ChemStation Explorer

The contents of the ChemStation Explorer are view-dependent. For Method and Run Control, Data Analysis and Report Layout, the ChemStation Explorer allows you to navigate to the different ChemStation elements. By default these elements are based on the configuration editor settings. So, as in previous ChemStation revisions, the methods and sequences are located in the chem32\n\methods and chem32\n\sequence folders (where n refers to the instrument number). Now, these paths can be expanded and new nodes for methods, sequences, data location can be specified using the newly introduced “Preferences” option in the view menu. These paths contain the master methods and sequence templates to be used for acquisition.

Table 12 Navigation Pane Items

Navigation Buttons	ChemStation Explorer Elements
Method and Run Control	Sequence templates (*.s) / Master methods (*.m)
Data Analysis	Data (*.d) / Master methods (*.m)
Report Layout	Master methods
Verification (LC and LC/MS)	Verification view specific shortcuts
Diagnosis (LC and LC/MS)	Diagnosis view specific shortcuts
Tune (LC/MS)	Tune view specific shortcuts

ChemStation Explorer elements, for example, methods and data files, can be loaded using right mouse actions or double clicks. The changes are directly reflected in the general ChemStation graphical interface. In addition, online help about the specific view items can be called by right mouse click.

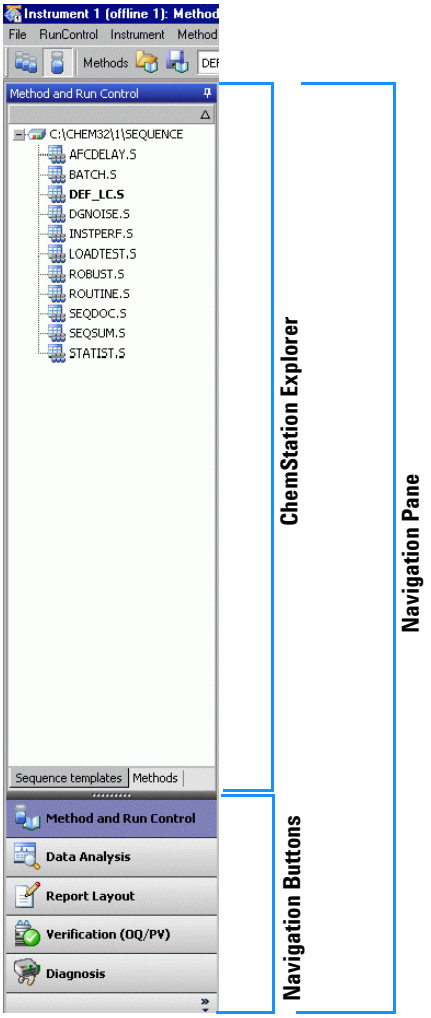


Figure 11 Navigation Pane showing ChemStation Explorer and Navigation Buttons

Enhancements using Method and Run Control View

The ChemStation Explorer for the Method and Run Control View enables methods and sequence templates to be loaded directly. The newly introduced Preferences option in the View Menu allows you to set up additional paths to be included in the ChemStation Explorer. The Preference option gives you new flexibility, for example for data storage.

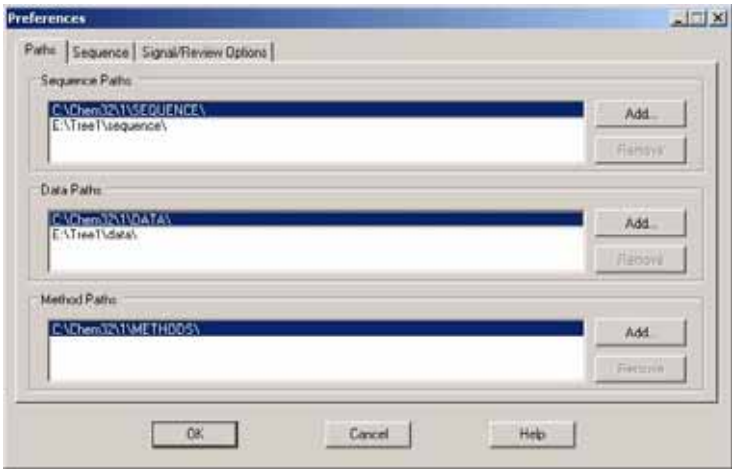


Figure 12 Paths preferences for the ChemStation Explorer

Sample Info

In the sample info dialog, it is possible to select available paths for data storage. Additional data paths can be specified using the Preferences dialog box in the View menu. After adding a data path, it is possible to select the new path via a drop-down menu in the path item of the sample info dialog box. The location of the data files is no longer limited to the chem32/n/data folder of the ChemStation (or the user defined setting in the configuration editor).

Sequence Parameters

In the sequence parameter dialog it is possible to select available paths for data storage. Additional data paths can be specified using the Preferences dialog box in the View menu. After adding a data path, it is possible to select the new path via a drop-down menu in the path item of the sequence

parameter dialog box. The location of the data files is no longer limited to the chem32/n/data folder of the ChemStation (or the user defined setting in the configuration editor).

Sequence Table

For setting up the sequence table, the system offers you the facility to browse for available methods. The location of the methods is no longer limited to the chem32/n/method folder of the ChemStation (or the user defined setting in the configuration editor). The available methods in the ChemStation Explorer are the “master” methods, the method field in the sequence table is linked to the last used “master” method folder. Master methods normally remain unchanged once the method development is finish.

The sequence table and sequence parameters, as well as the other sequence-related parameters, are stored in the sequence.s file. The sequence (*.s files) are by default located in chem32/n/sequences. Using the Preferences, it is now possible to specify additional locations for storing sequence *.s templates. These sequences are treated as sequence templates and can be used to re-run, but not to reprocess a sequence.

Acquire Sequence Data using Preferences

When you run a sequence, the loaded sequence_name.s template is taken and executed: the system performs the scheduled runs according to the defined sequence lines. Starting with ChemStation Rev. B.02.01, the sequence_name.S file is used as a sequence template and offers new flexibility in conjunction with the ChemStation Preferences.

The sequence data are stored in a sequence data container using a defined sequence container name. In the Sequence tab of the Preferences dialog box, it is possible to specify the naming conventions (Name Pattern) for these sequence containers. The Sequence Tab is only used for the data acquisition and therefore is present only for online systems.

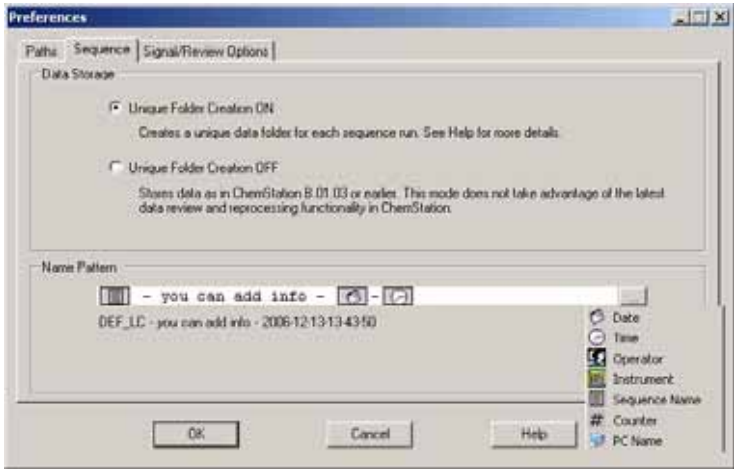


Figure 13 Preferences for sequence naming

The sequence name pattern can contain various sections; if nothing is selected, the default sequence name pattern is:

- Sequence Name Time Date

Depending on the selected sections, the system creates a name pattern for your sequence data container. All data files, methods, the sequence logbook, the sequence_name.s file and the sequence_name.b file belonging to this particular sequence are stored in the sequence data container. A new sequence data container is created each time the sequence is started.

The sequence (.S) files are now used as sequence templates, and this new concept allows you to run any sequences.s file multiple times without overwriting existing data and without changing the sequence parameters. If neither counter nor time are used in the sequence name pattern, the system introduces a counter automatically to avoid overwriting data. For the second, third and all subsequent sequences using the same sequence template, a counter is added to the sequence container name.
Because of the sequence data container concept, reprocessing of sequence data created with ChemStation Rev. B.02.01 or higher needs to be performed in the Data Analysis view. Sequence data acquired in ChemStation revisions up to B.01.03 or with Unique Folder Creation switched off in B.03.01 have to be reprocessed in the Method and Run Control view.

NOTE

Starting with ChemStation B.02.01, Data Analysis tasks needs to be executed in the offline instrument session of your instrument. It is no longer possible to switch to the Data Analysis view of an Online System while running an acquisition.

Note, therefore, that shapshot.d files need to be reviewed in the offline session of your system. Open the offline ChemStation session using the Program Group item or start the reprocess copy from within the ChemStation using View/Reprocess Copy.

Acquire Sequence Data performing Recalibration

To perform recalibration within a sequence, you need to select a calibrated method, select the sample type “calibration”, and specify the recalibration options in the sequence table.

When a sequence is recalibrated, the system creates the sequence data container based on the defined sequence name pattern. All sequence-related methods are copied to the sequence data container, and the system stores the acquired data files. As the sequence is executed line by line, the updated calibration table used to calculate the amounts for the individual data file is stored in the data analysis method (DA.M) for that data file. When the sequence is finished, the updated calibration table is stored in the sequence method. If you now want to use the updated sequence container method for data acquisition, you need to copy this method from the sequence data container to one of the defined method paths. The new/updated method is then available in the ChemStation Explorer in the method view as a master method.

Data File Structure

Starting with ChemStation B.02.01, a new data storage concept is introduced for acquired sequence data. All items belonging to an executed sequence (*.S) file are stored in the sequence data container using a unique name:

- sequence data files (*.D)
  - acquisition method ACQ.M for individual data files
  - data analysis method DA.M for individual data files

  The two individual methods stored with the data file are copies of the used method, containing the parameters exactly as they were at the time of acquisition of the data.
- all methods (*.M) files used during the sequence
- original sequence template (*.S) file
- sequence-related batch (*.B) file
- sequence related logbook (sequence_name.log) file

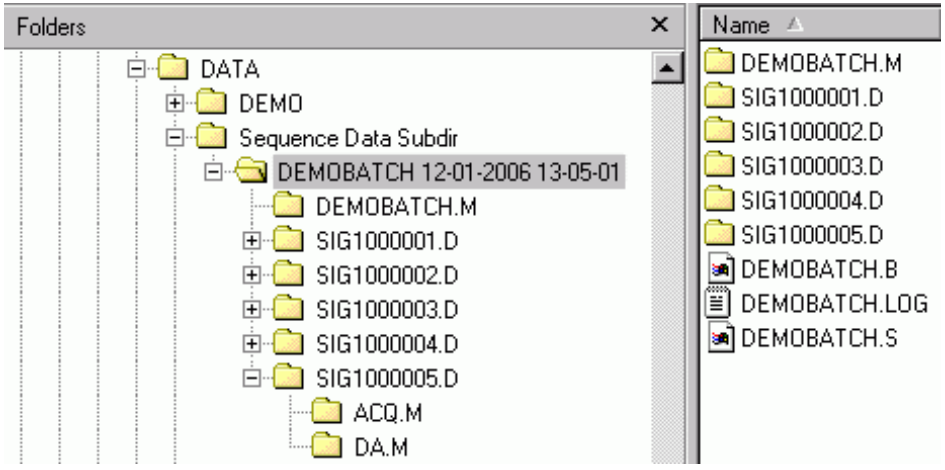


Figure 14 Sequence Data Container Content

The sequence data container files are used for review and reprocess in Data Analysis, without the need to change the master methods or master sequence template.

Available Methods

Methods have a name with up to forty alphanumeric characters followed by the extension .M. Methods are now stored in the ChemStation in up to three locations:

- The Master Method is stored in a methods subdirectory, available in a Methods node of the ChemStation Explorer, and is not directly associated with any data container. These methods are used to acquire data
- When a sequence is run, copies of all the master methods used in the sequence are stored in the sequence data container along with the sequence data files. These methods are directly linked to the sequence, and are used as well when the sequence is reprocessed. Changes to these methods are not propagated to the master methods. Changes are propagated to the sequence method as well to the individual methods during the sequence is reprocessed.
- In addition, two copies of the method used to run a sample are stored with the data files: ACQ.M is the acquisition method, DA.M is the data analysis method. DA.M is the method that is loaded along with the data file if the “Load DA method from data file” checkbox in the Signal Options tab of the Preferences dialog box is selected. Changes to this method (for example, manual integrations) are specific to the associated data file, and are not propagated to the sequence method or the master method.

Enhancements using Data Analysis View

The ChemStation Explorer for the Data Analysis View allows you to load data sets and methods. The concept of the ChemStation structure shows the available sets of sequence data containers in a particular subdirectory, as well as the sets of available single runs in a particular subdirectory. You can load a data set using the right-mouse click option “load”, by double-clicking on the data set, or by using the menu function to load a single data file.

Sequence data container

Single run data

The loaded data set is now displayed data file by data file in the Navigation Table in the top section of the Data Analysis View.

Navigation Table

The Navigation table is read-only and offers you standard table configuration features, such as sorting, drag-and-drop options to move columns to a different places, column selection etc. In addition, column-specific grouping is possible, for example, single runs of a particular operator can be displayed by grouping the loaded files by the column “operator”.

The Navigation table offers right mouse click functions to load a signal, overlay a signal, export data, print reports etc. Each Navigation Table line can be expanded by clicking the + (plus) sign at the line start to configure signal-specific options.

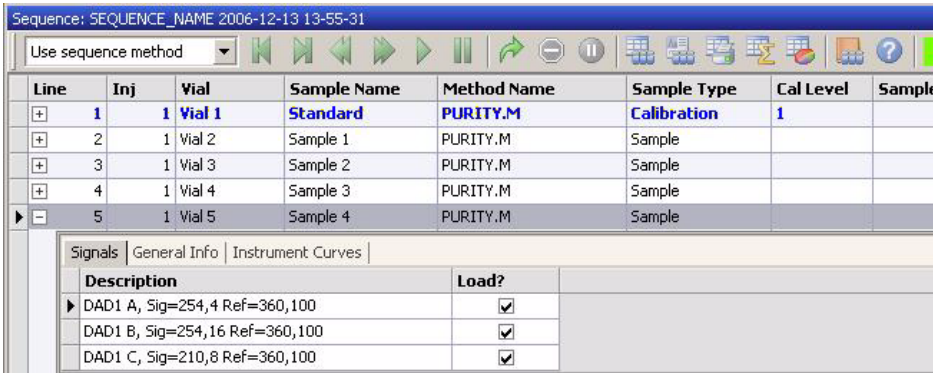


Figure 15 Navigation Table in Data Analysis

Remember, that the Preferences option allows you to set up additional paths to be displayed in the ChemStation Explorer. In addition, the Preferences dialog box contains Signal/Review Options that have a significant impact on your data review.

Preferences - Signal/Review Options Tab

The Signal Options tab in the Preferences allows you to specify the actions to be taken when a signal is loaded. The first section of this tab, “Load Signal Options”, specifies which of the signals in a run are loaded, and if the chromatograms are to be integrated and the results reported directly after loading.

In the second section, “Data Review Options”, you have the possibility to configure the interval for stepping through the runs in the Navigation Table automatically.

The remainder of this section specifies which method is loaded during data review when a run is loaded from the Navigation Table. They only apply to data review, but not to reprocessing.

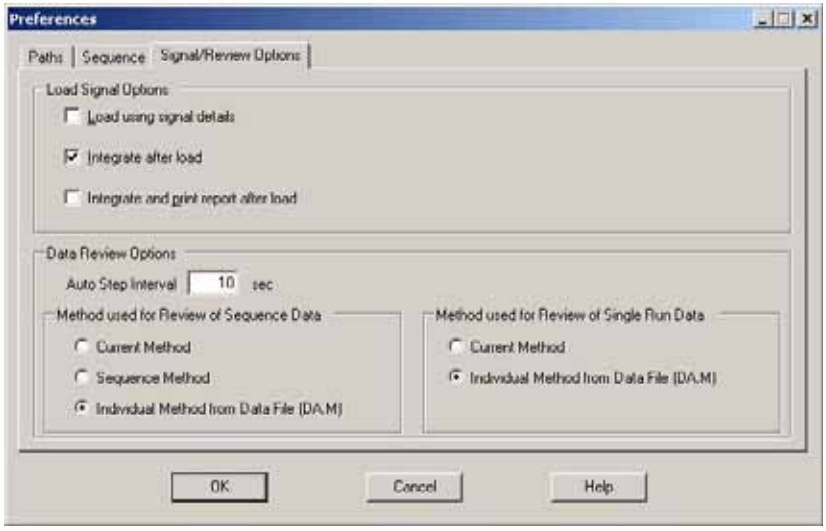


Figure 16 Preferences for Signal options

Navigation Table Review and Reprocess

Additional review and reprocessing capabilities are available in Data Analysis view for all data sets and for sequences acquired with B.02.01 and higher. This new functionality is described in detail in the “Getting Started with New

ChemStation Workflow" manual, and in the online help. Sequence data acquired with ChemStation revisions up to B.0l.03 need to be reprocessed using the reprocess option in the Method and Run Control View.

Data Review: The new review functionality of the Navigation table allows you to step automatically through the loaded signals and, depending on the specifications defined in the Preferences/ Signal/Review Options, automatically integrate the signal, for example, and print a report for each file.

If the "Use Current Method" option in Preferences/ Signal/Review Options is selected, the system uses the currently loaded method for reviewing and generating the report. The method name is visible in the Status Bar.

If the "Use Sequence Method" option is selected, the system alsways loads the sequence method that corresponds to the run that you load from the Navigation Table. The sequence methods are located in the sequence container. The method name is visible in the Status Bar with "sequence" added in brackets.

If the "Use Individual Method from Data File (DA.M)" option is selected, the system loads the individual data analysis method (DA.M) stored with the data file. For each line in the Navigation table, the linked DA.M for the selected data file is loaded and used for reviewing and generating the report. The method name is visible in the Status Bar, the system will add "from data file" in brackets to alert you that the loaded method is the individual method for the data file.

Data Reprocessing (Data acquired with ChemStation B.02.0x): Using the reprocessing functionality, it is possible to modify the sequence.s file of the data container in order to change the multiplier, dilution etc., method settings, or to use a different method for reprocessing. The sequence.s is part of the sequence data container and is opened in Data Analysis. By default, the sequence parameter "part of method to run" for a sequence.s file in Data Analysis is set to "Reprocess only", and the option "Use Sequence Table Information" is checked. These predefined default values enable you to change the sequence.s file and continue to reprocess without editing the Data Analysis sequence parameters again. During reprocessing, the individual methods DA.M for the data files are updated as well as the batch.b file.

If you have not changed the method in the sequence.s file, the system uses the methods stored in the sequence data container to reprocess the sequence. These methods are the original methods used during data acquisition. If

particular method parameters need to be changed (e.g. specify to print to a *.xls file), the methods in the sequence container need to be modified and saved. This general change is then applied to all data files during reprocessing.

If you now want to use the updated sequence container method for data acquisition, you need to copy this method from the sequence data container to one of the defined method paths. The new/updated method is then available in the ChemStation Explorer in the method view as a master method.

Manual Integration

For data files containing a DA.M individual method, it is possible to save manual integration events specific for this data file only. The newly added manual integration items needs to be copied to the DA.M and the DA.M needs to be saved.

NOTE The Navigation Table does not replace the complex batch functionality. The Batch view is available in the Data Analysis View and the batch functionality stays unchanged.

Long File Names

ChemStation Rev. B.0x.0x supports the use of long file names for following ChemStation files:

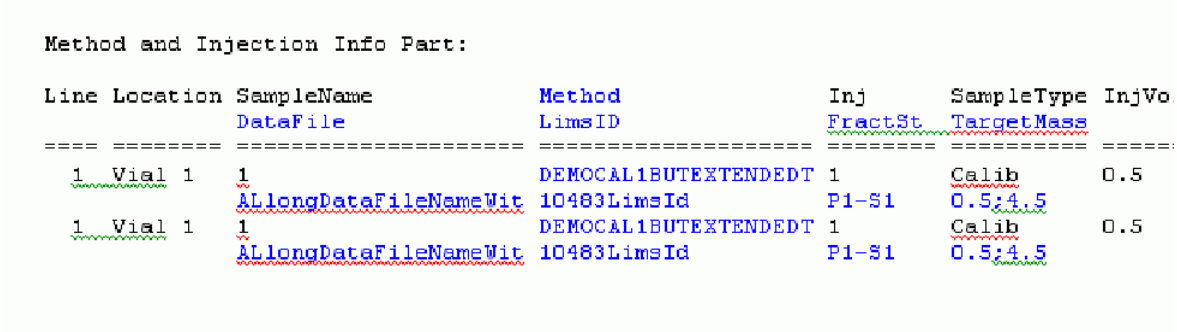
- Data
- Method
- Sequence, Hypersequences
- Batch
- Spectra Libraries
- Report Templates
- Macro Files
- Subdirectories
- Sample Names (since B.01.03)

The long file names effect the ChemStation graphical interface and the report layout.

Because of the acceptance of long file names, all ChemStation screens have been resized. The graphical elements are enlarged, and long file names for methods, sequences etc. are displayed accordingly in all ChemStation screens and input/output fields. For graphical reasons, long files names in the graphical views are limited to a maximum of 18 characters.

Figure 17 Method and Run Control screen shot

All ChemStation reports (data reports, method/sequence printouts etc.) are redesigned to support long file names. The ChemStation logbooks also use an extended format for system messages: long information strings are fully printed; if necessary, the information is printed over multiple lines. Certain reports, for example, the sequence report, may truncate long filenames to fit all information onto the report template.



Method and Injection Info Part:

Line	Location	SampleName DataFile	Method LimsID	Inj FractSt	SampleType TargetMass	InjVo
1	Vial 1	1 ALlongDataFileNameWit	DEMOCAL1BUTEXTENDEDT 10483LimsId	1 P1-S1	Calib 0.5;4.5	0.5
1	Vial 1	1 ALlongDataFileNameWit	DEMOCAL1BUTEXTENDEDT 10483LimsId	1 P1-S1	Calib 0.5;4.5	0.5

Figure 18 Sequence report extract

NOTE Nearly all screens reflect the acceptance of long filenames. The toolbars displaying datafile/sequence/method names have been resized to display a minimum of 18 characters.

Naming Conventions

The following rules enable the ChemStation to create and process valid names for files and directories:

The following characters are not allowed as part of file or directory names:

< > : " / \ | * ? blank (spaces)

The following rules apply in addition:

Table 13 Restricted characters

ChemStation parameter	Character
Method File Names:	% and . (decimal point) are not allowed
Data Subdirectory and Sequence Subdirectory:	[] + = ; , . (decimal point), blank (spaces) are not allowed

The following reserved device names cannot be used as the name of a file:

- CON, PRN, AUX, NUL
- COMx (whereas x is a number from 1 to 9)
- LPT1x (whereas x is a number from 1 to 9)

Also avoid these names followed by an extension (e.g. Nul.txt).

NOTE English, Japanese, and Chinese operating systems are used to test naming conventions. Agilent cannot give a support statement for non-English operating systems and their special characters.

Maximum Length of ChemStation File Names and Subdirectories

The Agilent ChemStation specifications for file names and subdirectories are listed below:

Table 14 Maximum Length of ChemStation file names and subdirectories

DataFile/Subdirectory/Path	Max. Input Length	Auto append	Example
Data file name	38	. D	Demodad.d
Data file name using prefix/counter	15	. D	longname000001.d
Method Sequence Hypersequence Libraries Customized Report Templates	40	. M . S . HYP . UVL . FRP	def_lc.m def_lc.s def_lc.hyp demodad.uvl areapct.frp
Data file subdirectory	40		demo (in sample info)
Data sequence subdirectory	40		demo (in sequence parameters)
Sequence Data Container Name	40		test_date_time (create using sequence preferences)
Data Path Method Path Sequence Path Hypersequence Path Libraries Path Customized Report Template Path	100	100	c:\chem32\1\data c:\chem32\1\methods c:\chem32\1\sequence c:\chem32\1\hyper c:\chem32\speclib c:\chem32\repstyle

Prefix/Counter

If you use the Prefix/Counter to name data files, the ChemStation generates a name for each analysis. For an instrument that supports dual-signal analyses, such as the GC, the ChemStation generates a name for each signal.

The prefix/counter component of a datafile and in the sequence has been extended to cater for the use of long filenames.
The datafile name defined by prefix/counter can have up to fifteen characters plus the .d extension: 17 characters in total.

The following rules apply to the prefix/counter field:

- the counter itself can have a maximum of six characters
- if a prefix provides less than nine characters, the counter is automatically extended to six digits
- the number given in the counter is the start number for incrementation

Table 15 Prefix/Counter

Prefix	Counter	Results in File Name
long	000001	long000001
longname	000001	longname000001
testwithalongna	1	testwithalongna1

Loading Data from ChemStation Rev. A.xx.xx

ChemStation Rev. B.0x.0x uses a 32-bit-based software architecture, and the character set used is Unicode. This section give an overview of the handling of uploaded data, methods, sequences, etc.

Data Files

No changes are made to an uploaded data file in Rev. B.0x.0x.
The datafile can be integrated and used within B.01x.0x, and remains backwards-compatible.
Datafiles acquired with Rev. B0x.0x are not backwards-compatible because of the modified data structure.

NOTE The import of PASCAL files and 3365 files into Rev. B.0x.0x is no longer possible. If these files are required, they need first to be imported into ChemStation Rev. A.xx.xx and converted to ChemStation files.

In general, all files (methods, sequences, logfiles, etc.) from previous ChemStation revisions using the old data structure can be loaded into B.0x.0x; the system converts these files to the new 32-bit structure during saving. Once converted to the new structure set, these files are not backwards-compatible. Therefore you are alerted to save the files under a different name, so that both 16-bit and 32-bit file sets are available (if necessary). The 16-bit files remain unchanged, and can still be used with ChemStation Rev. A.xx.xx.

Methods

All methods created with earlier ChemStation revisions can be loaded into Rev. B.0x.0x. If the method includes either the “old” spectra/purity option or integration using either “Standard integrator” or “advanced baseline” option of the enhanced integrator, an alert is displayed (see Figure 19 on page 95). These method parameters are automatically converted to the new B.0x.0x functionality. The method gets a “method modified” flag to reflect the changes. Details regarding this conversion are documented in “Chapter 7, “Upgrade Impact on Quantification Methods (relevant for Rev. A Upgrades only),” starting on page 107.

Figure 19

Methods created in Rev. B.0x.0x are not backwards-compatible because of the modified data structure.

Sequences

All sequences created with earlier ChemStation revisions can be loaded into Rev. B.0x.0x. The system detects if a sequence has the 16-bit structure, and treats the sequence accordingly. The prefix/counter and automatic naming conversion are reset to use the eight-character set. This allows uploaded sequences to be reprocessed.

When you save an uploaded sequence, you are alerted to save it under a different name. In this case, the original sequence remains with the old data structure and is backwards-compatible.

Sequences created in Rev. B.0x.0x are not backwards-compatible because of the modified data structure.

Hypersequences (only for LC ChemStation)

All hypersequences created with earlier ChemStation revisions can be loaded into Rev. B.0x.0x. The system detects if a hypersequences has the 16-bit structure, and treats it accordingly. The prefix/counter and automatic naming conversion are reset to use the eight-character set. This allows uploaded hypersequences to be reprocessed.

When you save an uploaded hypersequences, you are alerted to save it under a different name. In this case, the original sequence remains with the old data structure and is backwards-compatible.

Hypersequences created in Rev. B.0x.0x are not backwards-compatible because of the modified data structure.

Batch Files

All batch files created with earlier ChemStation revisions can be loaded into Rev. B.0x.0x. The batch can be executed, and manual integration events can be saved to the batch. If the batch file is not saved immediately, you have to save this particular batch as soon as it is reloaded.

When you save an uploaded batch file, you are alerted to save it under a different name. In this case, the original batch files remains with the old data structure and is backwards-compatible.

Report Styles

All report styles created with earlier ChemStation revisions can be loaded into Rev. B.0x.0x.

When you save an uploaded report style, you are alerted to save it under a different name. In this case, the original report styles remains with the old data structure and is backwards-compatible

UV Libraries (only for LC and CE 3D ChemStation)

All UV libraries created with earlier ChemStation revisions can be loaded into Rev. B.0x.0x. UV libraries established using the “old” spectra/purity option need to be adapted to the “new” spectra/purity set.

Details regarding this update are documented in “Upgrading to the “New” Spectra/Purity Tool Set” on page 144”.

When you save an uploaded UV library, you are alerted to save it under a different name. In this case, the original UV library remains with the old data structure and is backwards-compatible.

5 Compliance Information

General Compliance Information for Upgrade Rev. B.03.01

Overview

After installing the Agilent ChemSstation system software on your computer and configuring the analytical system, your internal validation procedure may require you to assess the correctness and completeness of the installation and to verify that the analytical system is fully operational.

Software Upgrade Qualification

As with any important upgrade to your ChemStation software, Agilent recommends that a full Installation Qualification (IQ) and Operational Qualification (OQ/PV) be performed after installation of release B.03.01. This will help in your validation needs according to your validation master plan, which should also include Design Qualification (DQ) and Performance Qualification (PQ).

The Operational Qualification service from Agilent will provide documented evidence that your new ChemStation is performing according to the accepted performance parameters. In particular, it will also verify the operation of the new integrator algorithm as part of the chromatography verification tests. Other important areas that it will cover are the instrument communication and control, as well as the data security and access controls.

A very important characteristic of Agilent's NDS qualification services is their high degree of automation and deep interactivity with the qualified system. This not only reduces system downtime, but also ensures that the process is performed reliably and consistently, so minimizing the risks before an audit.

Upgrade Verification

After upgrading the Agilent ChemStation system software on your computer and configuring the analytical system, your internal validation procedure may require you to assess the correctness and completeness of the installation and to verify that the analytical system is fully operational.

Agilent ChemStation Installation Verification utility uses factory-delivered installation reference files to verify the existence, correctness and integrity of the required Agilent ChemStation system files (executable program files, binary register files, macro files, initialization files, help files, customized report templates). This can be part of your Installation Qualification (IQ).

File integrity is verified by comparing the 32-bit cross-redundancy-check (CRC) checksum of the installed file with the checksum of the original file recorded on Agilent Technologies installation master. The file details of the installation master are delivered on so-called *reference files*. Modified or corrupted files have different checksums and are thus detected by the IQ utility.

The integrity of the reference files themselves is also tracked with the help of checksums. In case the installation verification utility is supplied with a reference file that was modified after its generation, this is flagged in the report (section *invalid reference files*).

In addition, the IQ utility checks the version code of the Agilent ChemStation executable system files (*.EXE, *.DLL).

Upgrading the HPLC 1100 OQ/PV Method and Sequence Files

Release B.03.01 of the Agilent ChemStation features the same “Verification View” present in previous versions, however it does not include sample files for 1100 OQ/PV methods and sequences, which could be used as aid to perform qualification on the 1100 Series LC system.

You can however continue to use the same sample files from release, A.10.02, as they are compatible with B.03.01. In order to do so, you must copy them after the installation of B.03.0x has been completed, from the backup HPCHEM directory onto the new ChemStation directory, using the same structure as before.

Remember that the upgrade installation uses the original installation path information of the Rev. A.09.03 or higher installation.

One OQPV folder under the “METHODS” folder, under each instrument session.

- C:\HPCHEM_backup\X\METHODS\OQPV should be copied to:
  - C:\HPCHEM\X\METHODS\OQPV, were x is the instrument number

One OQPV folder under the “SEQUENCE” folder, under each instrument session.

- C:\HPCHEM_backup\X\SEQUENCE\OQPV should be copied to:
  - C:\HPCHEM\X\SEQUENCE\OQPV, were x is the instrument number

HPLC 1100 OQ/PV Example Files for New Installations

The 1100 OQ/PV sample files can be purchased from Agilent when they are not available from previous installations. In addition the CD-ROM contains the QO/PV help file, that had been available in A.10.02 ChemStation. Please use the following reference:

P/N 01100-60050 “1100 Verification Sample Files CD-ROM”

These files are included in the Agilent OQ/PV qualification services, thus there is no need to acquire them when Agilent performs your instrument qualification.

6
Impact on Customized Solutions

Macro Solutions

Starting with ChemStation Revision B.02.01 a significantly refreshed user interface (UI) and a new navigation concept has been introduced. All elements of this concept as well as new controls in the ChemStation UI are based on the Microsof.NET Framework.

Customization of Toolbars

The Toolbar commands of the ChemStation have been changed in ChemStation Rev. B.03.01 with respect to the usage of Microsoft.NET Framework. Current customized solutions utilizing toolbar commands for ChemStations till Rev. B.01.03 will not be executable on ChemStation Rev. B.03.01 unmodified. Please check the online help for more information.

Customization of Menubars

No changes are made with respect to the use of ChemStation macro language to add/modify Menubars. In general current customized solutions should be able to run on ChemStation Rev. B.03.01 without modification.

Data Structure Impact on ChemStation Macros

Starting with ChemStation B.02.01 a new data organization concept has been introduced and ChemStation B.03.01 offers additional enhancements. Within the software it is possible to choose which data organization concept will be used to acquire data by defining “Unique Folder Creation ON” and “Unique Folder Creation OFF” in the Preferences. Per default, “Unique Folder Creation ON” is selected. “Unique Folder Creation ON” enables the data storage concept as outlined below in “Startup Changes Introduced with B.03.01” on page 72.

“Unique Folder Creation OFF” allows you to store data as in ChemStation B.01.03 or earlier. More details can be found in the “Getting Started with New ChemStation Workflow” manual.

Unique Folder Creation ON

This data storage mode makes use of the new data structure introduced with ChemStation B.02.01. Please check your ChemStation macros and adapt if necessary the new pathes items.

Unique Folder Creation OFF

This data storage mode allows to store data as in ChemStation B.01.03 or earlier. Using this mode, ChemStation macros created on ChemStation B.01.03 and earlier does not need to be reworked.

Macro Solutions (relevant for Rev. A upgrades only)

Overview

With the upgrade to ChemStation Rev. B.03.0x, the system uses Unicode Standard as encoding system to express characters. Unicode provides a unique number for every character, no matter what platform, program or language. Each file header contains the information when Unicode Encoding is used. All macro or report files generated by ChemStation are in Unicode.

Most of the available programs are able to read Unicode-based files, e.g. Word, NotePad. However, some applications are not able to open Unicode-based files.

The following text files generated by ChemStation are in Unicode:

- *.txt
- *.log
- clusterx.mth (where as x is the instrument number)
- *.ms
- *.inf
- *.dif

Any file generated by the following commands is in Unicode:

- PRINT #
- PRINT USING #
- OPEN #
- CLOSE#

User Contributed Library (UCL)

A User Contributed Library (UCL) is placed in the UCL directory of the ChemStation CD-ROM (CD 2 - User Documentation and Assessories). This library contains a set of macros and utilities for LC, GC and LC/MS ChemStations. The contents of this library are intended to help users of the ChemStation software to develop and customize their installations to their specific needs. The contents of the library come from both Agilent internal and user-contributed sources, and all contributions are welcome. Each contribution is checked for functionality, but does not necessarily go through any formal testing procedure. Therefore, Agilent Technologies supports the operation of UCL programs on a best-effort basis only.

With the move to Unicode encoding, no changes have been made to the UCL macro files. The UCL macros work within their designed environment. If you modified certain UCL macros to match your requirements, and generate files for use in other applications, it might be necessary to convert these files to ANSI format.

Customized Macros and User.mac

By automating the loading and running of a macro, you can make your ChemStation operate unattended. You can define a macro file called USER.MAC in the ChemStation executable directory. The name of this directory depends on your installation, xx:\<original installation path>\Core, for upgraded default systems c:\hpchem\Core.

In the user.mac you place commands to load and execute your own macros within the ChemStation. During an upgrade from ChemStation Rev. A.09.03 or higher to ChemStation Rev. B.01.0x, your own macros are moved to the HPCHEM_BACKUP directory, but they are NOT moved during the automatic copy process to the upgraded system. Your macro files need to be located and moved manually according to their structure. Only the User.mac is moved during the automation process.

If your custom application is not able to open Unicode-based files, a conversion to ANSI is required. Please see Chapter 6, “Converting Unicode to ANSI,” starting on page 106.

Converting Unicode to ANSI

Installed custom solutions need verification that the used program is able to read unicode-based files. If this is not the case, either the program needs to be adapted to allow unicode encoding, or the files need to be converted to ANSI standard files.

Agilent provides a conversion tool “UnicodeToAnsi.exe” which is installed automatically in following directory during installation:

x:\Chem32\sys

This tool allows easy conversion of Unicode-based files to ANSI standard files and should be executed after the Unicode-based file has been created. The following macro illustrates the use:

e.g. a= execnowait (“UnicodeToAnsiFile.exe ”+ “c:\temp”+”\ansi.txt”)

(Be aware that there must be a blank after the UnicodeToAnsiFile.exe.

DDE

The information exchange using DDE (Dynamic Data Exchange) can be used for information transfer from ChemStation.

ODBC

The use of ODBC is initially not support with Chemstation B01.01. Agilent delivers the option to use XML as data interchange format, as well as ChemStore as Data Management system.

7 Upgrade Impact on Quantification Methods (relevant for Rev. A Upgrades only)

General Aspects

With the move to 32-bit software architecture, Agilent has improved the capabilities of the familiar Enhanced ‘ChemStation Integrator’. To take advantage of the improvements in integration accuracy, as well as new integration events, we have moved forward to the improved Chem32 integrator. In ChemStation Rev. B.0x.0x, the accuracy of integration calculations and results in general are improved, and small differences in the results may be seen. Note that the ‘Standard Integrator’ and the ‘Enhanced Integrator using Advanced Baseline’ used in Rev. A.xx.xx ChemStation are not available in Rev. B.0x.0x ChemStation.

The Chem32 integrator in ChemStation Rev. B.0x.0x contains numerous enhancements and is now used across the entire Agilent Networked Data Systems (NDS) product family. The Chem32 integrator provides enhanced ruggedness and ease of use, based on higher accuracy for the determination of peak start/stop position times, and additional parameters for baseline construction. Agilent has implemented new integration events used for all signals in response to customer requests.

The new integration events provide greater flexibility in performing your integration tasks. The new ‘Baseline Correction’ integration event makes it easier to treat noisy or drifting baselines. The new integration events (marked in Figure 20 on page 110) allow selection of skimming modes for tailing or fronting peaks, as well as the specification of when this mode should be applied. The Chem32 integrator provides you with more efficient and faster integration method development and improved accuracy of the integration results.

The major elements in the graphical user interface remain unchanged. The use and selection of signal-specific integration events as well as timed integration events also remain unchanged. The new integration events are accessible on the top of the signal-specific integration events, see Figure 20 on page 110.

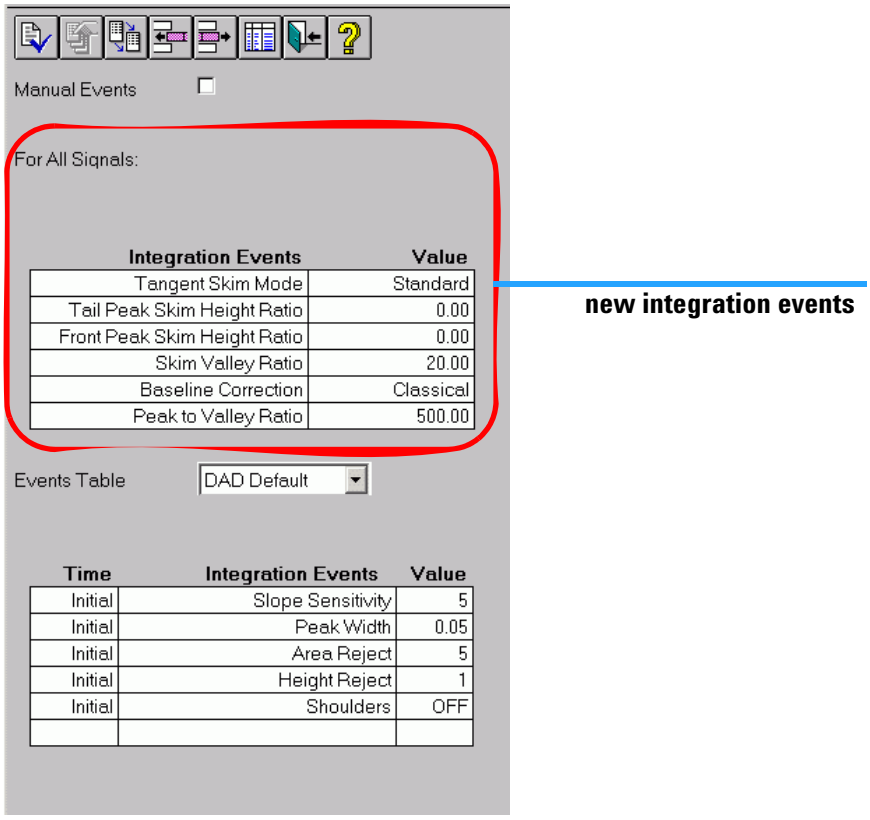


Figure 20 The default values for the new integration events

The new integration events in ChemStation Rev. B.0x.0x are:

- Tangent Skim Mode
- Tail Peak Skim Height Ratio
- Front Peak Skim Height Ratio
- Skim Valley Ratio
- Baseline Correction
- Peak to Valley Ratio

These parameters are generic for all loaded signals, while the “initial” integration events can be defined signal specific.

The use and functionality of these new integration events are described in detail in the Rev. B.0x.0x 'Understanding your ChemStation' manual as well as in the online-help.

When you load the default method DEF_xx.M, or a method from a Rev. A.xx.xx ChemStation, all new Chem32 integration events are set to default values. The default values for the new integration events are shown in Figure 20 on page 110.

The assignment of default values for the new Chem32 integration events does not interfere with any existing integration events coming from a ChemStation Rev. A.xx.xx system. When default values for the new integration events are used, the Chem32 integrator algorithm behaves in a similar manner to the 'Enhanced Integrator' from the Rev. A.xx.xx ChemStation.

The new Chem32 integration events are automatically applied to all Rev. A.xx.xx methods loaded into the Rev. B.0x.0x ChemStation. If the Rev. A.xx.xx method is saved for the first time, the new integration events are saved as part of the Rev. B.0x.0x method.

Integration Algorithms Rev. A.xx.xx ChemStation

The integration algorithms offered with ChemStation Rev. A.xx.xx are:

- Standard Integrator
- Enhanced Integrator
- Enhanced Integrator using Advanced Baseline option

Table 16 on page 112 shows the integration events tables of the different integrators. The following sections describe the changes during the update of the integration method depending on the different starting points.

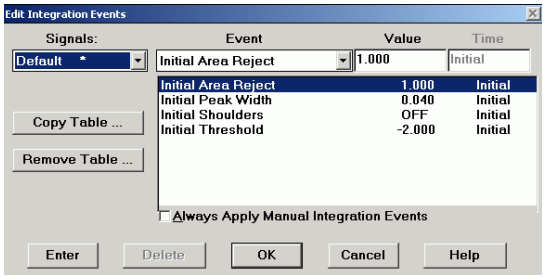
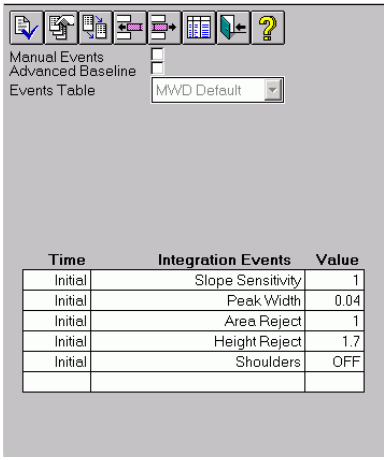
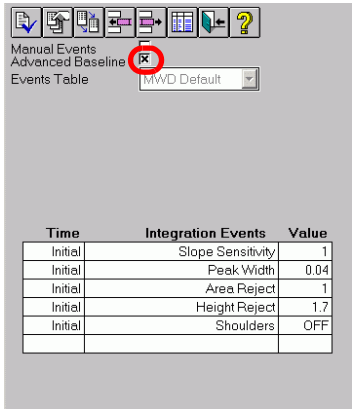
NOTE

The *Standard integrator* is not available in Rev. B.0x.0x ChemStation.

An improved version of the *Enhanced Integrator* is available in Rev. B.0x.0x ChemStation.

The *Advanced Baseline option* in the *Enhanced Integrator* is not available in Rev. B.0x.0x ChemStation. Instead the integrator offers more enhancements with the new *Baseline Correction* functionality.

Table 16 Agilent ChemStation Rev. A.xx.xx Integrators

Description	Available since	Example Screen shots
Standard Integrator Please refer to "Upgrade from Standard Integrator" on page 113	Rev. A.02.xx (1993)	
Enhanced Integrator Default integrator Please refer to "Upgrade from Enhanced Integrator" on page 118	Rev. A.04.01 (1996) A.05.01 (1997)	
Enhanced Integrator with Advanced Baseline option Please refer to "Upgrade from Enhanced Integrator with Advanced Baseline" on page 136	Rev. A.06.01 (1998)	

Upgrade from Standard Integrator

When a Rev. A.xx.xx method containing the ‘Standard Integrator’ is loaded in a Rev. B.0x.0x system, the dialog shown in Figure 21 below is displayed. The dialog advises that a method containing old integration settings has been loaded and will be automatically updated to allow its use in a Rev. B.0x.0x system.

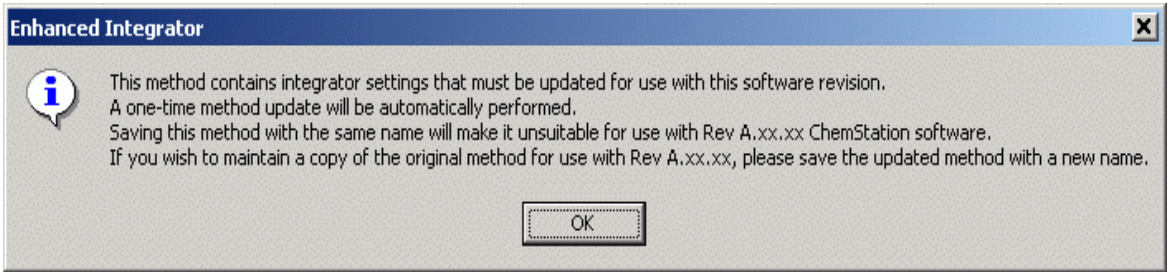


Figure 21 Automatic update of the method

You must select ‘OK’ to continue. The method is updated automatically.

NOTE

The new integration events are saved only if you save the method. If you wish to keep a copy of the original 16 bit method, save the method with a new name.

The original method remains and is backwards-compatible with ChemStation Rev. A.xx.xx. You are always prompted to change the name when saving a 16-bit method in a Rev. B.0x.0x system.

The Chem32 integrator does not use the integration events of the ‘Standard Integrator’ from a Rev. A.xx.xx ChemStation. The ‘Standard Integrator’ used integration events with slightly different functionality, e.g., the ‘Initial Threshold’ event uses the height above baseline expressed in powers of two. The Chem32 Integrator’ in Rev. B.0x.0x detects slope changes for peak recognition, using the ‘Slope Sensitivity’ event. The ’Slope Sensitivity’ value changes on a linear scale.

The Chem32 integrator uses default values for all new integration events. The integration event values are not correlated with the previously used values from the ‘Standard Integrator’ in Rev. A.xx.xx (see Table 17). Uploaded methods using the ‘Standard Integrator’ of Rev. A.xx.xx need to readjust their integration parameters accordingly.

Table 17 Integration Parameter in B.0x.0x based on ‘Standard Integrator’

Integration Events Standard Integrator A.xx.xx	Value (default)	Integration Events Enhanced Integrator A.xx.xx Chem32 Integrator B.0x.0x	Value (default)
Initial Threshold	- 2	Slope Sensitivity	5
Initial Peak width	0.04	Peak width	0.05
Initial Area Reject	1.00	Area Reject	5
Initial Shoulders	OFF	Shoulders	OFF
		Height Reject	1

Impact on Validated Systems - based on ‘Standard Integrator’

The Chem32 integrator has an impact on integration results acquired in previous revisions of ChemStation software. The integration section of methods based on the ’Standard Integrator’ needs to be reworked.

All integration events need to be adjusted for the Chem32 integrator. Be aware that updated ChemStation Rev. A.xx.xx methods used with the Chem32 integrator are affected in the following areas:

Results:	E.g. Amounts, Calibration areas, Response factors, etc.
User Requirement Specifications:	E.g. Acceptance Criteria
Functional Specifications:	E.g. Signal to Noise, Peak Symmetry, etc.

The Chem32 Integrator changes affect the following scenarios:

- You work with uploaded Rev A.xx.xx methods in Rev. B.0x.0x.
- You use defined product specifications relating to integration values.
- You need to upload ChemStation Rev. A.xx.xx data for reprocessing, exchanging data between system using different ChemStation Revisions, audit purposes or other reasons.

Continue to work with existing Methods from A.xx.xx based on ‘Standard Integrator’

After uploading methods in Rev. B.0x.0x and opening the integration events, all integration events are set to default values.

The Chem32 integrator default values are shown in Figure 20 on page 110. Integration events need to be redefined accordingly. Agilent recommends that you use the new integration events available in the Chem32 integrator to take advantage of the integration improvements.

After optimizing the integrator settings, existing calibration tables need to be updated by the recalibration/replace function to obtain an updated calibration curve in Rev. B.0x.0x. The updated calibration table contains the newly calculated areas corresponding to your updated integration settings.

The difference between the original calibration curve in Rev. A.xx.xx and the updated calibration curve in Rev. B.0x.0x needs to be evaluated for each of your methods.

You need to assess whether a partial method revalidation is necessary. Data acquisition parameters remain unchanged and as such re-validation can be based on existing data sets.

You use defined Product Specifications relating to integration values

The updated integration settings may have an impact on the following results: area, height, peak width, peak symmetry, peak start- and end times, etc. If your product specifications are based on any of these results the integration events needs to be updated accordingly.

You need to assess whether a partial method revalidation is necessary. Data acquisition parameters remain unchanged, and, as such, re-validation can be based on existing data sets.

You need to upload ChemStation Rev. A.xx.xx data for reprocessing, exchanging data

You need to upload ChemStation Rev. A.xx.xx data for reprocessing or exchanging data between system using different ChemStation Revisions, audit purposes or other reasons:

Exchanging results between ChemStation systems on different revisions

In order to compare results from systems using different ChemStation revisions, e.g. Rev. A.xx.xx and Rev. B.0x.0x, you need to document the integrator and all integration settings used, so that the variation between integrators can be taken into account and appropriately documented.

Restoring Rev. A.xx.xx ChemStation data for Audit reasons, Inspections etc.

In the case of an audit situation, where you need to restore or replay A.xx.xx results, it may be necessary to reprocess the data files in Rev. B.0x.0x.

The Chem32 integrator in Rev. B.0x.0x yields different integration results. However, the Chem32 integrator allows you to specify integration events that generate an equivalent baseline construction. If the new baseline construction visually matches the original baseline construction, the remaining result deviation is significantly lower than the analytical accuracy. A manual baseline construction should be considered if the baseline construction does not match and cannot be achieved using the Chem32 integration events. ChemStation Plus users can retrieve peak start and stop times for manual baseline reconstruction from the ChemStore database.

NOTE

This “Upgrade guide” is important for regulatory audit purposes and should be made available for inspections in case of an auditor request to reprocess data generated on ChemStation Rev. A.xx.xx using a method with “Standard Integrator“.

Upgrade from Enhanced Integrator

Loading a Rev. A.xx.xx 'Enhanced Integrator' method into a Rev. B.0x.0x system generates an additional table in the integration events dialog. This table contains new integration events introduced with ChemStation Rev. B.01.01

Saving the method updates the method to the 32-bit structure.

Once a method has been saved in Rev. B.0x.0x, it can no longer be used in a previous revision of ChemStation.

NOTE

The new integration events are saved only if you save the method. If you wish to keep a copy of the original 16 bit method – save the method with a new name (see Figure 22).

The original method remains and is backwards-compatible with ChemStation Rev. A.xx.xx. You are always prompted to change the name when saving a 16-bit method in a Rev. B.0x.0x system.

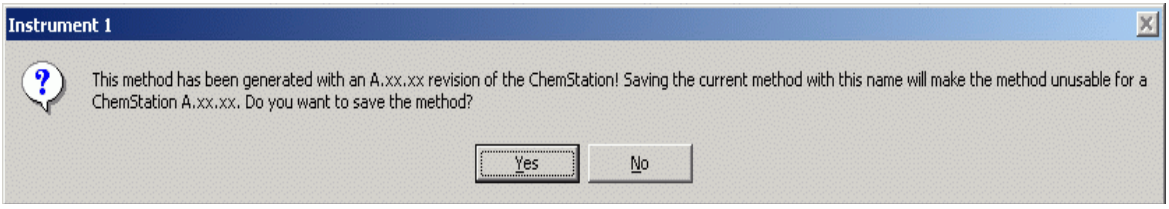


Figure 22 Prompt for changing the name

All specified signal-specific integration events (initial and timed) existing in the original method remain unchanged following the update for use with Rev. B.0x.0x. The assignment of default values for new Chem32 'For All Signals' integration events does not interfere with any existing integration events coming from a ChemStation Rev. A.xx.xx system. The new Chem32 integration events are automatically applied to all Rev. A.xx.xx methods loaded into the Rev. B.0x.0x ChemStation. The new integration events are saved as a part of the Rev. B.0x.0x method as soon as a loaded Rev. A.xx.xx method is saved for the first time in the Rev. B.0x.0x ChemStation.

The default values for the new integration events are illustrated in Figure 23.

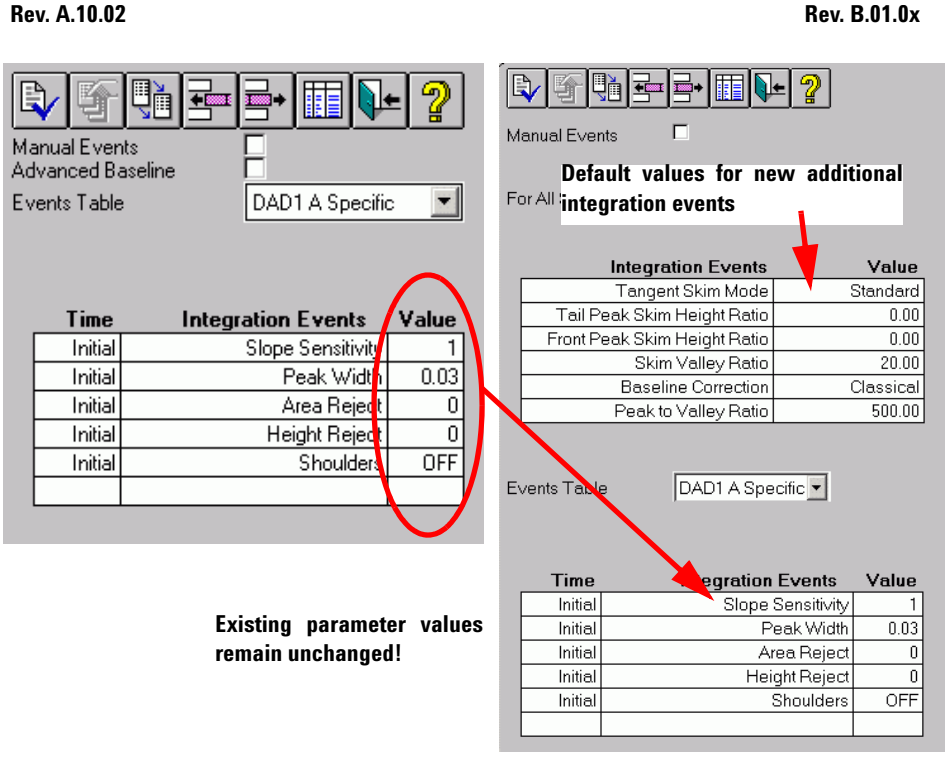


Figure 23 Parameter values in Rev. A.10.02 and in Rev. B.0x.0x

NOTE

When methods are loaded for the first time into a Rev. B.0x.0x ChemStation system, the new integration events are automatically set to default values. The method modified flag is not set when the default values are assigned.

Improvements in the accuracy of peak start and stop times may result in small changes to the integration results, e.g. area, height, peak width. Changed integration results will result in changes to values calculated using these integration results, e.g. S/N, peak symmetry. The greatest variation is to be expected for small-area peaks, sharp and narrow peaks, and non-symmetric (non Gaussian-shaped) peaks. Small and sharp peak forms tend to contain a

low number of data points, where single data point changes have a greater effect. These peak forms can be expected to provide the greatest changes in results, especially if combined with a noisy baseline.

The following section demonstrates potential result differences based on example demo data. The impact on integration results may differ depending upon the integration complexity (e.g. use of timed events) and the individual characteristics of the chromatogram e.g. baseline noise, peak shape, peak resolution etc.

The example data used in this document to highlight potential integration impacts will not necessarily reflect your specific data. It is not possible to represent all potential scenarios within the scope of this document.

Examples for Improved Peak Start and Stop Time Position Determination

To illustrate the different integration results after upgrading ChemStation A.xx.xx methods to Rev. B.0x.0x ChemStation a set of chromatograms was integrated using identical integration events for both ChemStation Rev. A.10.02 and B.0x.0x. The results of this comparison are listed in tables according to the chromatogram set. Report print outs are also attached. The comparison is based on peak area, peak height, peak width, peak start time, peak end time and amount results.

Example Chromatogram No. 1

Data/Settings used for System Comparison.

To compare integration results an area% calculation was done, based on the following data file in Rev. A.10.02 and Rev. B.01.01 ChemStation.

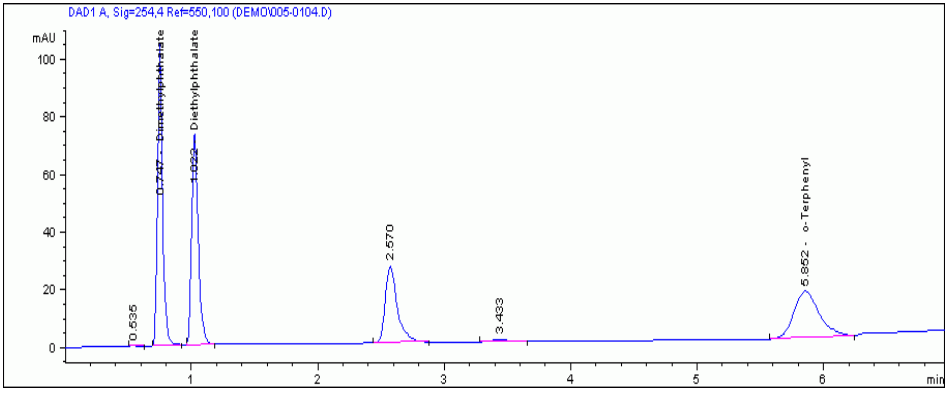


Figure 24 ChemStation A.10.02 Example Chromatogram No 1

Table 18 Data Files used for Example No. 1

Report used	Data File	Signal Description
Area % Calculation	005-0104.D	Signal A, 254,4 Ref. 550,100

Integration settings:
The Method has been set up using the 'Enhanced Integrator' with the following integration event values:

Slope Sensitivity	3
Peak Width	0.04
Area Reject	0
Height Reject	0
Shoulders	Off

Steps performed: Rev. A.10.02:

1 The sample file was processed to obtain integration results and an Area% report has been generated. (for the Area% report refer to Figure 36, "Area% Report for Sample 005-0104.d - generated on ChemStation A.10.02," on page 153 in the Appendix).

Rev. B.01.01:

2 The method uploaded in Rev. B.01.01 ChemStation was used to reprocess the same sample file and an Area% report has been generated.
(for the Area% report refer to, Figure 37, "Area % Report for Sample 005-0104.d - generated on ChemStation B. 01.01," on page 154 in the Appendix).

Result Comparison: Comparison of reported integration results peaks shows differences for nearly all peaks. The area calculation for these peaks differs due to the improved peak start and stop position determination. In this case the start and end time differences on the x-scale are not present for the shown number of digits. The y-position of the start and stop determination are not printed in the reports, they are available as register entries. Changes in the determination of start and stop time position affects the baseline construction. Therefore all integrator results may be effected

Table 19 Integration Results for Comparison of data file 005-0104.D Example No. 1

	A.10.02	B.01.01	Differences Absolute	Differences Relative /%	Name
Retention time	0.5347561240	0.5347561240	0.0000000000	0.000	<unknown>
	0.7465666533	0.7465666533	0.0000000000	0.000	Dimethylphthalate
	1.0216099024	1.0216099024	0.0000000000	0.000	Diethylphthalate
	2.5699408054	2.5699408054	0.0000000000	0.000	<unknown>
	3.4325516224	3.4325516224	0.0000000000	0.000	<unknown>
	5.8524289131	5.8524289131	0.0000000000	0.000	o-Terphenyl
Area	0.2853316367	0.2853193283	0.0000123084	0.004	<unknown>
	294.8515014648	294.8515014648	0.0000000000	0.000	Dimethylphthalate
	261.4009399414	261.4132385254	0.0122985840	0.005	Diethylphthalate
	175.7781066895	175.8833465576	0.1052398681	0.060	<unknown>
	5.4511561394	5.4511113167	0.0000448227	0.001	<unknown>
	229.3132476807	229.3127593994	0.0004882813	0.000	o-Terphenyl
Height	0.3549563885	0.3549563885	0.0000000000	0.000	<unknown>
	104.6963195801	104.6963195801	0.0000000000	0.000	Dimethylphthalate
	75.4323272705	75.4323272705	0.0000000000	0.000	Diethylphthalate
	26.6097583771	26.6126747131	0.0029163360	0.011	<unknown>
	0.6711332798	0.6711332798	0.0000000000	0.000	<unknown>
	16.2621154785	16.2621154785	0.0000000000	0.000	o-Terphenyl
Peak Width	0.0213782471	0.0213778429	0.0000004042	0.002	<unknown>
	0.0448563062	0.0448563062	0.0000000000	0.000	Dimethylphthalate
	0.0524293184	0.0524312221	0.0000019037	0.004	Diethylphthalate
	0.1010673866	0.1011050791	0.0000376925	0.037	<unknown>
	0.1227603480	0.1227595583	0.0000007897	0.001	<unknown>
	0.2125124931	0.2125121504	0.0000003427	0.000	o-Terphenyl
Start Time	0.5080894828	0.5080894828	0.0000000000	0.000	<unknown>
	0.6945833564	0.6945833564	0.0000000000	0.000	Dimethylphthalate
	0.9605301023	0.9605301023	0.0000000000	0.000	Diethylphthalate
	2.4412500858	2.4412500858	0.0000000000	0.000	<unknown>
	3.2827787399	3.2827787399	0.0000000000	0.000	<unknown>
	5.5745835304	5.5745835304	0.0000000000	0.000	o-Terphenyl

Table 19 Integration Results for Comparison of data file 005-0104.D Example No. 1

	A.10.02	B.01.01	Differences Absolute	Differences Relative /%	Name
End Time	0.6279166937	0.6279166937	0.0000000000	0.000	<unknown>
	0.9212499857	0.9212499857	0.0000000000	0.000	Dimethylphthalate
	1.1879166365	1.1879166365	0.0000000000	0.000	Diethylphthalate
	2.8812499046	2.8812499046	0.0000000000	0.000	<unknown>
	3.6545832157	3.6545832157	0.0000000000	0.000	<unknown>
	6.2448053360	6.2448053360	0.0000000000	0.000	o-Terphenyl
Area%	0.0295044415	0.0294996001	0.0000048414	0.016	<unknown>
	30.4888339137	30.4851459574	0.0036879563	0.012	Dimethylphthalate
	27.0299109999	27.0279130072	0.0019979927	0.007	Diethylphthalate
	18.1761648623	18.1848471676	0.0086823053	0.048	<unknown>
	0.5636715206	0.5635987041	0.0000728165	0.013	<unknown>
	23.7119142620	23.7089955637	0.0029186983	0.012	o-Terphenyl
Total	967.08028	967.19728			

Example Chromatogram No. 2

Data/Settings used for System Comparison.

To compare integration results and calculated values (amounts) a multi – level calibration was used based on the following three data files in Rev. A.10.02 ChemStation.

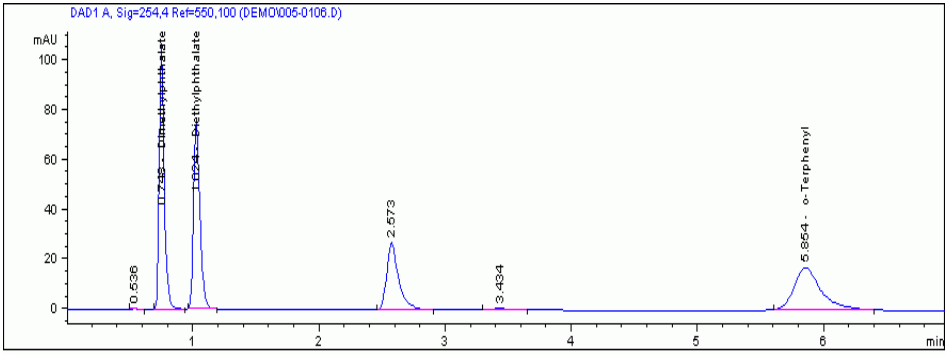


Figure 25 ChemStation A.10.02 Example Chromatogram No 2: Sample File

Table 20 Data Files used for Example No. 2

Used for	Data File	Signal Description	Amount
Calibration Data, Level 1	005-0101.D	Signal A, 254,4 Ref. 550,100	3
Calibration Data, Level 2	006-0201.D	Signal A, 254,4 Ref. 550,100	5
Calibration Data, Level 3	007-0301.D	Signal A, 254,4 Ref. 550,100	7
Sample Data	005-0106.D	Signal A, 254,4 Ref. 550,100	to be calc.

Integration settings:
The Method has been set up using the ‘Enhanced Integrator‘ with the following integration event values:

Slope Sensitivity	3
Peak Width	0.04
Area Reject	0
Height Reject	0
Shoulders	Off

Steps performed:

Rev. A.10.02

1 A three level calibration table was created. The sample file was processed to obtain results and an ESTD report has been generated.
(see Figure 38, “ESTD Report for Sample 005-0106.d - generated on ChemStation A.10.02,” on page 155 in the Appendix).

Rev. B.01.01

2 The method uploaded in Rev. B.01.01 ChemStation was recalibrated using the ‘Replace‘ option for each calibration level. The same sample file was used to reprocess the results and an ESTD report has been generated.
(see Figure 39, “ESTD Report for Sample 005-0106.d - generated on ChemStation B.01.01,” on page 156 in the Appendix).

Result Comparison:

Comparison of reported amounts based on calibrated peaks shows some differences in the amount results (see Table 22, “Integration Results for Comparison of data file 005-0106.D after recalibration,” on page 127.).

After recalibrating the method in Rev. B.01.01 the resulting calibration table showed update areas when compared with the original calibration from Rev. A.10.02, see Table 21, “Area Comparison of calibration table data A.10.02 system / recalibrated B.01.01 system,” on page 127. The calibration level areas changed and should to be updated with the reprocessed calibration data.

In this particular case an data file was used as an example, where the area for the three calibrated peaks are the same in A.10.02 and B.01.01. This example demonstrate the impact of the updated calibration areas used for the calibration curve.

Table 21 Area Comparison of calibration table data A.10.02 system / recalibrated B.01.01 system

Level	Compound	Area A.10.02	Area B.01.01	Differences Absolute	Differences Relative /%
Level 1	Dimethylphthalate	294.8071899414	294.9114379883	0.1042480469	0.0354
	Diethylphthalate	260.7143249512	260.9624023438	0.2480773926	0.0952
005-0101.d	o-Terphenyl	251.7360076904	251.7360076904	0.0000000000	0.0000
Level 2	Dimethylphthalate	458.7709655762	458.7012634277	0.0697021484	0.0152
	Diethylphthalate	409.6070556641	409.3640441895	0.2430114746	0.0593
006-0201.d	o-Terphenyl	394.7962341309	394.5599365234	0.2362976074	0.0599
Level 3	Dimethylphthalate	645.0082397461	644.9074096680	0.1008300781	0.0156
	Diethylphthalate	577.7369995117	577.3869018555	0.3500976563	0.0606
007-0301.d	o-Terphenyl	557.1237182617	557.1237182617	0.0000000000	0.0000

Table 22 Integration Results for Comparison of data file 005-0106.D after recalibration

	A.10.02	B.01.01	Differences Absolute	Differences Relative /%	Compound
Retention time	0.748061	0.7480610609	0.000000	0.000000	Dimethylphthalate
	1.023835	1.0238345861	0.000000	0.000000	Diethylphthalate
	5.853765	5.8537645340	0.000000	0.000000	o-Terphenyl
Area	300.7270507813	300.7270508	0.000000	0.000000	Dimethylphthalate
	266.6829528809	266.6829529	0.000000	0.000000	Diethylphthalate
	256.1013793945	256.1013794	0.000000	0.000000	o-Terphenyl
Height	106.9831390381	106.9831390381	0.000000	0.000000	Dimethylphthalate
	77.3352508545	77.3352508545	0.000000	0.000000	Diethylphthalate
	17.0476074219	17.0476074219	0.000000	0.000000	o-Terphenyl
Amount	3.2155806766	3.215654120	0.0000734	0.0023	Dimethylphthalate
	3.1973308873	3.197973012	0.0006421	0.0201	Diethylphthalate
	3.1833136562	3.183981658	0.0006680	0.0210	o-Terphenyl
Total	9.59623	9.59761	0.00138	0.0144	

Example Chromatogram No. 3

This example shows the improved accuracy of detection of peak start and stop times for small-area peaks that include a valley. In the example chromatogram No.2 the valley location between the peak at 0.372 and 0.516 min. is determined differently in Rev. A.10.02 and Rev. B.01.01. The Chem32 integrator improves the determination of the exact valley, as seen in Figure 26 and Figure 27 on page 129. The system reports different areas for peak on either side of the valley Figure 23 on page 129. For peak 0.372 min. the absolute area difference is calculated as 0.052122 area counts and for the peak of 0.5016 min. the absolute area difference is calculated as 0.051955 area counts.

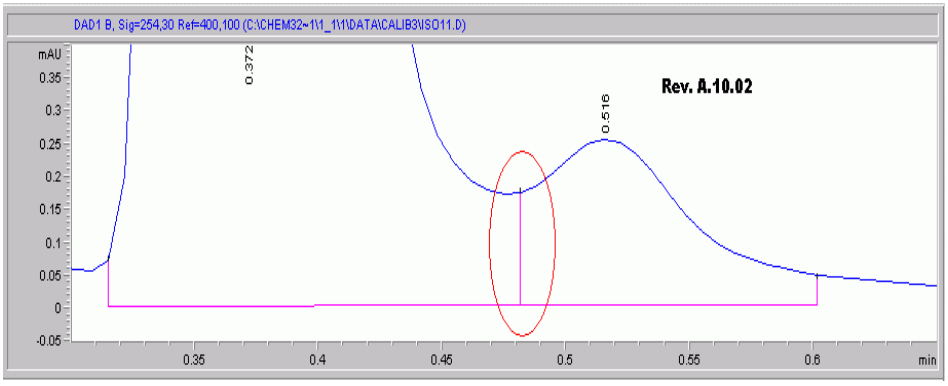


Figure 26 ChemStation A.10.02 Example Chromatogram No 3

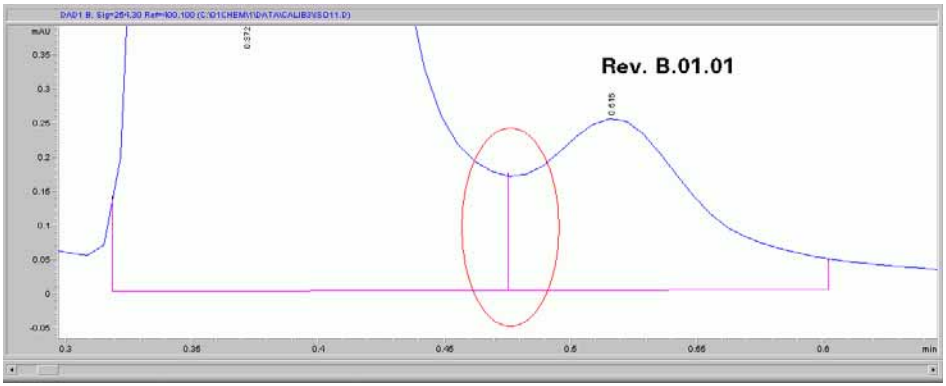


Figure 27 ChemStation B.01.01 Example Chromatogram No 3

Table 23 Integration Results for Example Data No.3

	Peak at	A.10.02	B.01.01	Differences Absolute	Differences Relative /%
Area	0.372	54.9091682434	54.8570480347	0.0521202087	0.095
	0.516	1.0940805674	1.1460355520	0.0519549847	4.749
Height	0.372	18.7451038361	18.7451038361	0.000000000	0.000
	0.516	0.2533660233	0.2533660233	0.000000000	0.000
Peak Width	0.372	0.0461746305	0.0461421907	0.0000324398	0.070
	0.516	0.0623787865	0.0647711381	0.0023923516	3.835
Start Time	0.372	0.3151666522	0.3151666522	0.000000000	0.000
	0.516	0.4818333387	0.4767456055	0.0050877333	1.056
End Time	0.372	0.4818333387	0.4767456055	0.0050877333	1.056
	0.516	0.6018333435	0.6018333435	0.000000000	0.000

Example Chromatogram No. 4

The following example shows the impact of peak start and stop times differences between neighboring peaks. This example can be seen as extreme, because it purposefully includes multiple factors that highlight potential result differences.

The factors used in this example include

- a small peak area of 2.06 area counts
- a peak with baseline penetration: The total area is calculated as the difference between the positive and the negative peak sections. Changes to the baseline construction have twice the impact of a plain positive peak
- the integration events used in this example do not result in a satisfying baseline construction for this peak, due to the baseline penetration. In general this results in a low precision.

In example chromatogram No. 4 the peak at 1.29 min. reports a minor absolute area difference of 0.00584 area counts. However, due to the small area, the relative difference is calculated as 0.284%, see Table 24 on page 132.

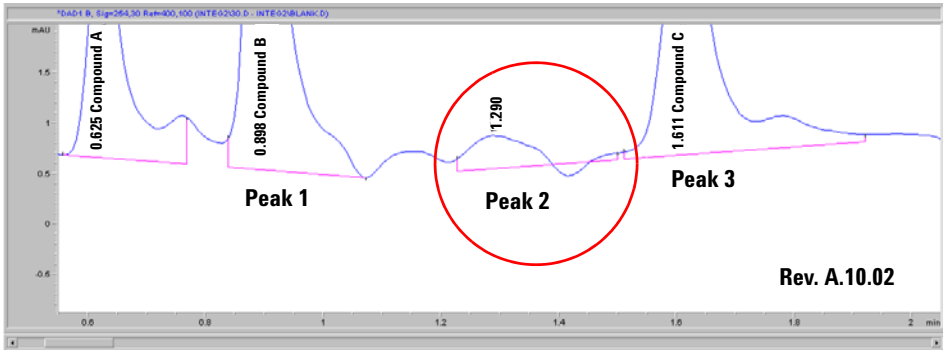


Figure 28 ChemStation A.10.02: Example Chromatogram 4

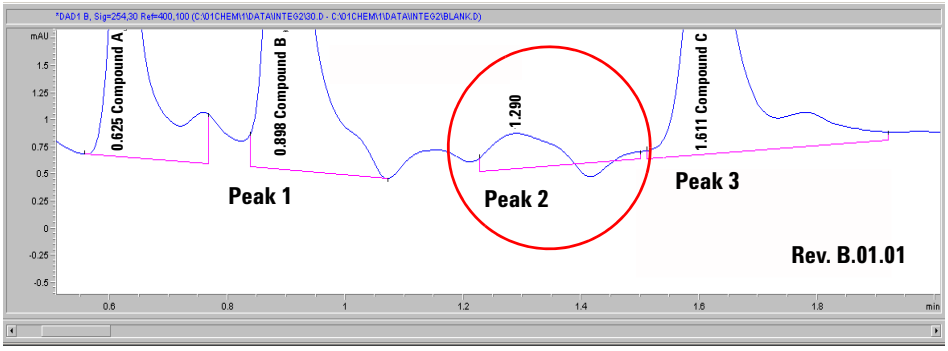


Figure 29 ChemStation B.01.01: Example Chromatogram 4

Looking at peak start and stop times of the peak of interest, neither value shows a difference between the ChemStation Revisions, also no visual differences is observed (see Figure 28 and Figure 29). The peak start and stop times of the current peak as well as previous and following peaks need to be taken into consideration, because of a potentially different baseline construction. By looking closely at the values in Table 24, Table 25 and

Table 26 on page 132, you can see that the peak stop time of the previous peak differs. This results in a different baseline construction and an area difference of 0.00058 area counts.

Table 24 Integration results for example No 4: Areas

Peak No.	RT A.10.02	Area A.10.02	Area B.01.01	Differences Absolute	Differences Relative /%
Peak 1	0.898035347	24.03518105	24.04627800	0.011096954	0.046
Peak 2	1.289547563	2.057008743	2.062850475	0.005841732	0.284
Peak 3	1.610636592	17.13418198	17.13872719	0.004545212	0.027

Table 25 Integration results for example No 3 Peak Starts

Peak No.	RT A.10.02	Peak Start A.10.02	Peak Start B.01.01	Differences Absolute	Differences Relative /%
Peak 1	0.898035347	0.838035345	0.8380353450	0.000000000	0.000
Peak 2	1.289547563	1.227166653	1.227166653	0.000000000	0.000
Peak 3	1.610636592	1.510636568	1.510636568	0.000000000	0.000

Table 26 Integration results for example No 3: Peak Ends

Peak No.	RT A.10.02	Peak End A.10.02	Peak End B.01.01	Differences Absolute	Differences Relative /%
Peak 1	0.898035347	1.071937919	1.0721049310	0.000167012	0.016
Peak 2	1.289547563	1.500499964	1.500499964	0.000000000	0.000
Peak 3	1.610636592	1.92050004	1.920500040	0.000000000	0.000

Impact on Validated Systems - based on 'Enhanced Integrator'

The improved integration algorithm in Chem32 integrator provides more accurate and reproducible integration results: area, height, peak width, etc. You may see changes within your reported integration results. Amounts are affected less, and typically are within the accuracy of analytical request.

Depending upon the specific application, you generally see the greatest changes in the integration results for small and non-symmetrically shaped peaks. These peaks reflect the improved start and stop peak position determination in the Chem32 integrator to the greatest extent. When the number of data points over a peak envelope is small, the impact of a different point e.g. start point, has more influence and is expressed in the improved integration result.

Based on these results, be aware that the new Chem32 integrator improvements may affect the following areas:

Results:	Amounts, Calibration areas, Response factors, etc.
User Requirement Specifications:	E.g Acceptance Criteria
Functional Specifications:	E.g Signal to Noise, Peak Symmetry, etc.

The improvement in the Chem32 Integrator may affect your work, if

- you continue working with the existing uploaded methods,
- you compare defined specification in various documents,
- you have to upload 'old' data for reprocess or to compare results exchanged e.g. between different laboratories.

Continue to work with existing Methods from A.xx.xx based on 'Enhanced Integrator'

The integration events from the 'Enhanced Integrator' remain for the 32–bit structured ChemStation. The values in the signal specific integration events are the defined values from the 'Enhanced Integrator' method in A.xx.xx ChemStation. Due to the outlined affects of the improvements in the integrator, integration results may differ. You should make an example recalibration for each of your methods using data previously calibrated in Rev. A.xx.xx to assess the need for recalibration for each of your methods. You have

to assess whether a partial method revalidation is necessary. Since data acquisition parameters stay unchanged, the re-validation can be based on existing data sets.

You use defined Product Specifications relating to integration values

The improved integration events in Rev. B.0x.0x have an impact on the following results: area, height, peak width, peak symmetry, start and end time peak, etc. Amounts are less affected and typically are within the accuracy of analytical request. If your product specifications are based on one of these results, the integration events need to be changed accordingly. You need to assess if parts of the method might need revalidation. Since data acquisition parameters remain unchanged, a re-validation can be based on existing data sets.

You need to upload ChemStation Rev. A.xx.xx data for reprocessing, exchanging data

You need to upload ChemStation Rev. A.xx.xx data for reprocessing or exchanging data between system using different ChemStation Revisions, audit purposes or other reasons:

Exchanging results between ChemStation systems on different revisions

In order to compare results from a lab using Rev. A.xx.xx and a lab using Rev. B.0x.0x ChemStation, you need to document all of the conditions used for the experiment. For the comparison or interpretation of results, the integration type and events must be documented (e.g. for ruggedness test during method validation process), so that the variation between integrators can be taken into account and appropriately documented.

Restoring Rev. A.xx.xx ChemStation data for Audit reasons, Inspections etc.

In the case of an audit situation, where you need to restore or replay your results for old Rev. A.xx.xx data files, it might be necessary to reprocess the old data files. The Chem32 integrator in Rev. B.0x.0x may yiel different integration results.

However, the integrator allows you to define integration events generating an equivalent baseline construction. If the new baseline construction visually matches the original baseline construction, the remaining result deviation is significantly lower than the analytical accuracy. A manual baseline construction should be considered if the baseline construction does not match and cannot be achieved using the integration events. ChemStation Plus users can retrieve peak start and stop times for manual baseline reconstruction from the ChemStore database.

NOTE

This “Upgrade guide” is important for regulatory audit purposes and should be made available for inspections in case of an auditor request to reprocess data generated on ChemStation Rev. A.xx.xx. using a method with ‘Enhanced Integrator’ settings.

Upgrade from Enhanced Integrator with Advanced Baseline

When a method that contains the ‘Advanced Baseline Option’ within the Enhanced Integrator of the Rev. A.xx.xx ChemStation is loaded into a Rev. B.0x.0x system, the system displays a dialog. The dialog indicates that a method containing non-updated integration settings has been loaded and advises that the method will be automatically updated to allow it to be used in a Rev. B.0x.0x system. You must select ‘OK’ (see Figure 30) to continue. The method is updated automatically.

Figure 30 System dialog

NOTE

The new integration events are saved only if you save the method. If you wish to save a copy of the original 16-bit method, save the method with a new name.

The original method remains and is backwards-compatible with ChemStation Rev. A.xx.xx. You are always prompted to change the name when saving a 16-bit method in a Rev. B.0x.0x system.

The ChemStation 32 integrator in Rev. B.0x.0x is an improved version of the familiar ‘Enhanced Integrator’ used in Rev. A.xx.xx. The Chem32 integrator is the standard integrator for Rev. B.0x.0x ChemStations. The ‘Advanced Baseline Option’ has been replaced by a more powerful feature, called ‘Baseline Correction’ (see Figure 31 on page 137).

NOTE

The new Chem32 ‘Baseline Correction’ parameter is much more powerful than the ‘Advanced Baseline’ option. They are different events and behave differently.

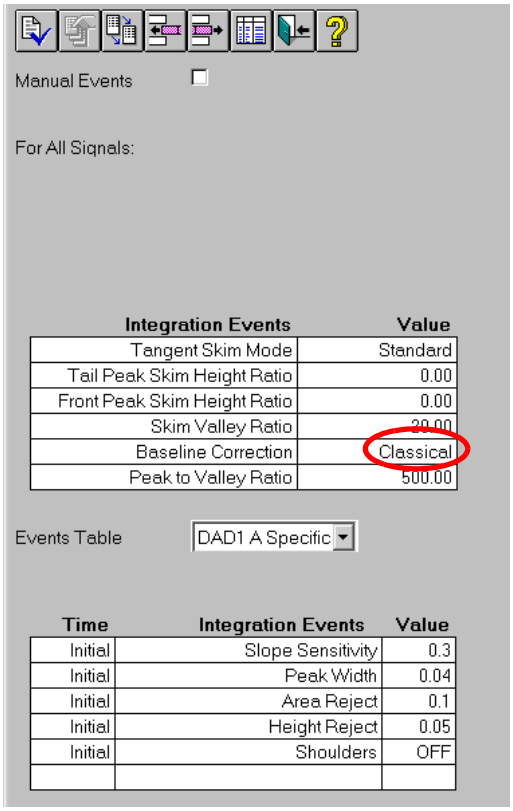


Figure 31 Example screen shot Chem32 Integrator

The system can work in the following modes:

1 'Classical' mode (default), with no additional baseline treatment

2 The option 'No Penetration' performs a baseline reconstruction. In an additional review pass, the system removes any baseline penetration. The start and the end of the peak are shifted along the signal towards the peak top until there is no penetration left.

3 The option 'Advanced' combines the penetration removal with an additional start/stop peak position determination. The baseline construction is reallocated.

The parameter set for Baseline Correction is described in detail in the integration section of 'Understanding your ChemStation' manual.

Impact on Validated Systems - based on ‘Enhanced Integrator with Advanced Baseline’

With the removal of the ‘Advanced Baseline’ option, the additional review to reallocate unassigned areas and redefine baseline allocation has been removed. Therefore, the integration results from Rev. A.xx.xx are not comparable with the integration results given by the Chem32 integrator within Rev. B.0x.0x. The integration settings need to be adjusted according to the Chem32 integrator. We suggest that you use the new integration features in Rev. B.0x.0x to improve your integration. The newly implemented integration events allow improved accuracy of baseline treatment.

Be aware that the integrator change may affects your:

Results:	E.g. Amounts, Calibration areas, Response factors, etc.
User Requirement Specifications:	E.g Acceptance Criteria
Functional Specifications:	E.g Signal to Noise, Peak Symmetry, etc.

These changes may have an impact on you, if

- you continue working with the existing uploaded methods
- you compare defined specification in various documents
- you have to upload ‘old’ data for reprocess or to compare results exchanged e.g. between different laboratories.

Continue to work with existing Methods from A.xx.xx based on ‘Enhanced Integrator with Advanced Baseline’

After uploading methods in Rev. B.0x.0x and editing the integration settings, the Advanced Baseline option has been removed. The integration parameter values reflect your specific settings from integration events of the ‘Enhanced Integrator’ in A.xx.xx ChemStation. All new additional integration events are set to default values. The Chem32 integrator default values are shown on Figure 31 on page 137. Integration events need to be redefined accordingly. Agilent recommends that you use the new integration events available in the Chem32 integrator to take advantage of the integration improvements.

After optimizing the integrator settings, existing calibration tables need to be updated by the recalibration/replace function to obtain an updated calibration curve in Rev. B.0x.0x. The updated calibration table contains the newly calculated areas corresponding to your updated integration settings. The difference between the original calibration curve in Rev. A.xx.xx and the updated calibration curve in Rev. B.0x.0x needs to be evaluated for each of your methods.

You need to assess whether a partial method or system revalidation is necessary. Since data acquisition parameters remain unchanged, a re-validation can be based on existing data sets.

You use defined Product Specifications relating to integration values

The updated integration events have an impact on the following results: area, height, peak width, peak symmetry, peak start and end time peak, etc. If your product specifications are based on one of those mentioned results, the integration events needs to be changed accordingly.

You need to assess whether a partial method or system revalidation is necessary. Since data acquisition parameters remain unchanged, a re-validation can be based on existing data sets.

You need to upload ChemStation Rev. A.xx.xx data for reprocessing, exchanging data

You need to upload ChemStation Rev. A.xx.xx data for reprocessing or exchanging data between system using different ChemStation Revisions, audit purposes or other reasons:

Exchanging results between ChemStation systems on different revisions

In order to compare results from a lab using Rev. A.xx.xx and a lab using Rev. B.0x.0x ChemStation, you need to document all of the conditions used for the experiment. For the comparison or interpretation of results, the integration

type and events must be documented (e.g. for roughness test during method validation process), so that the variation between integrators can be taken into account and appropriately documented.

Restoring Rev. A.xx.xx ChemStation data for Audit reasons, Inspections etc.

In the case of an audit situation, where you need to restore or replay your results for old Rev. A.xx.xx data files, it might be necessary to reprocess the old data files. The Chem32 integrator in Rev. B.0x.0x yields different integration results. However, the integrator allows you to specify integration events generating an equivalent baseline construction. The differences are significantly lower compared to the analytical accuracy in cases where the baseline construction visually matches the original baseline construction. A manual baseline construction should be considered if the baseline construction does not match and cannot be achieved using the integration events. ChemStation Plus users can retrieve peak start and stop times for manual baseline reconstruction from the ChemStore data base.

NOTE

This “Upgrade guide” is important for regulatory audit purposes and should be made available for inspections if an auditor requests the reprocess of data generated on ChemStation Rev. A.xx.xx. using a method with ‘Enhanced Integrator with Advanced Baseline’ settings.

8 Spectra/Purity Options using ChemStation Rev. B.03.0x. (relevant for Rev. A Upgrades only)

(LC, CE and LC/MS Systems only)

Introduction of the Spectra/Purity Tools Sets

NOTE This chapter applies only for upgraded methods using the“old” spectra/purity tool sets available in ChemStation Rev. A.xx.xx. All ChemStation methods since Rev. A.04.02 using the “new” spectra/purity tool set continue to use this. The “new” spectra/purity tool of ChemStation Rev. A.xx.xx is the standard tool set within ChemStation Rev. B.

Since Agilent ChemStation Rev. A.04.02, up to and including Rev. A.10.02, two different spectra/peak purity options have been available:

- the “old” spectra/purity settings (since Rev. A.04.01)

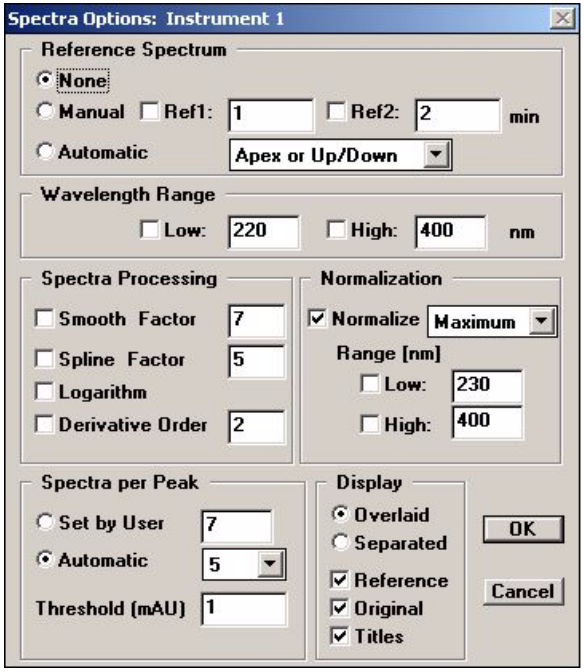


Figure 32 “old” spectra/purity settings (since Rev. A.04.01)

- the “new” spectra/purity settings (since Rev. A.04.02).

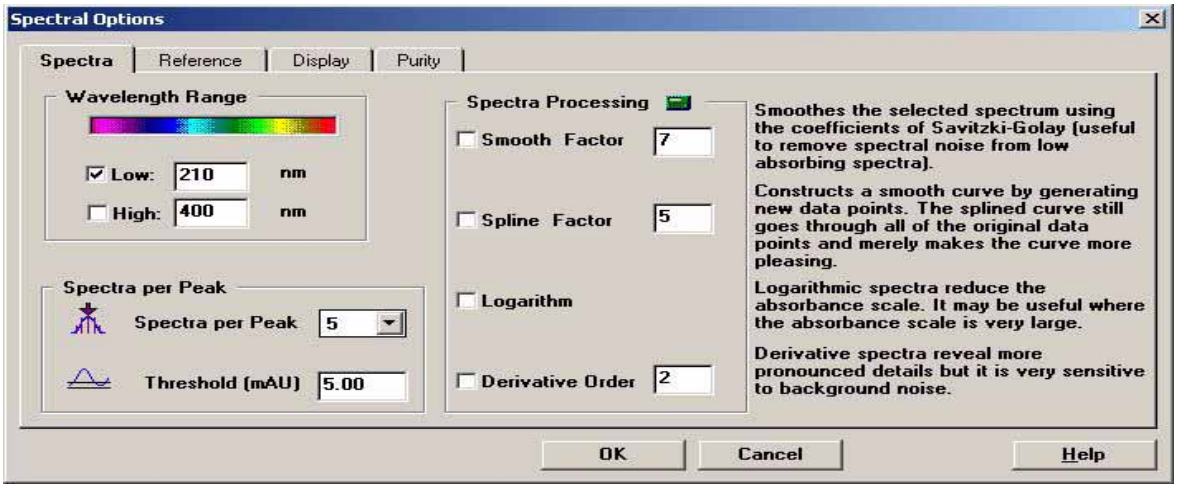


Figure 33 "new" spectra/purity settings (since Rev. A.04.02)

New methods starting from ChemStation Rev. A.04.02 contain two spectra/purity tools. Entering the spectra/peak purity settings for the first time triggers the decision for one of the tool sets. Once the spectra/purity settings have been selected, they are stored with the method.

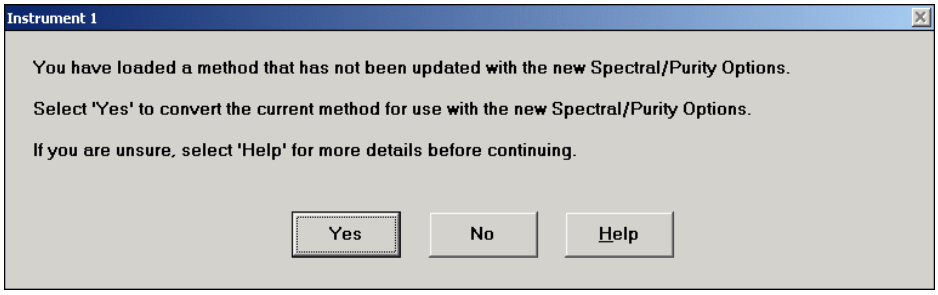


Figure 34 Rev. A.04.02 and higher: choosing spectra/peak purity settings

With the introduction of ChemStation Rev. B. ChemStation, the "new" spectra/purity settings are the standard; the "old" spectra/purity tool set is no longer available.

Upgrading to the “New” Spectra/Purity Tool Set

When you load a method Rev. A.xx.xx containing the “old” spectra/purity tool set into ChemStation Rev. B. you are alerted about the change to the “new” spectra/purity tool set.

Figure 35 Upgrade alert for methods containing an “old” spectra/purity tool set

The spectra/purity values defined in A.xx.xx are transferred to the “new” spectra tool set, and the method gets a ‘method modified flag’ to visualize the change. If the method is saved using the original name, it is no longer backwards compatible, and contains the “new” spectra/purify tool set. In order to prevent the method from being overwritten, save the updated method under a new name.

The “old” and the “new” spectra/purity parameters work slightly differently: the “newer” spectra/purity tool set is more automated. Therefore, the results of the both tools sets are not directly comparable and need expert comparison.

To allow comparison of both spectra/purity tool sets, the following tables should be give an overview of the parameters used and their differences. The tables are split into sections: spectra and purify. In the “older” tool set this was two different menu items within the Data Analysis item ‘spectra’, whereas in the “newer” tool set both items are addressed as two tabs of the ‘spectra options’ menu item within the Data Analysis item ‘spectra’.

Table 27 Comparison Spectra Tool Set "old" versus "new"

Parameter	"old" SPECTRA SET A.04.01 till B.0x.0x	"new" SPECTRA SET A.04.02 till B.0x.0x	Comment
Reference Spectra	Parameter to determine the Reference Spectra used for display and calculation. Parameter is defined separately for both spectra and purity display/calculations. - None - Manual - Automatic (Apex, Up/Down Nearest Baseline **Peak Baseline**)	Parameter to determine the Reference Spectra used for display and calculation. Same Parameters used for both, spectra and purity display/calculations - None - Manual - Automatic (Depending on the Data Acquisition parameter the reference is determined, see help) **Note:** The Automatic mode corresponds to "old" Automatic mode: Peak BaseLine	To improve usability and comparison, the specified values for the reference spectra are now the same within Spectra and Purity definition. This avoids misleading information when different values are chosen in the spectra and purity sets. The automatic mode for the reference spectra has been improved: the selected reference spectra/spectrum depends on the spectrum mode, spectrum type and availability of baseline spectra. **Note**: For comparison reasons standard values are used, therefore the user selection for the automation mode has been removed. **Impact: on UV Library**: depending on the reference used, different spectra are stored within the UV library. It is recommended to update the spectra library when upgrading the spectra/purity options.
Wave-length Range	Parameter to define the Wavelength Range for Signal Display. Parameters are defined separately for both spectra and purity display	Parameter to define the Wavelength Range for Signal Display. Same Parameters used for both spectra and purity display	

Table 27 Comparison Spectra Tool Set "old" versus "new" (continued)

Parameter	"old" SPECTRA SET A.04.01 till B.0x.0x	"new" SPECTRA SET A.04.02 till B.0x.0x	Comment
Spectra processing	Allow processing a spectrum from a data file before display. - Smooth Factor - Spline Factor - Logarithm - Derivative Order Parameters are defined separately for both spectra and purity display	Allow processing a spectrum from a data file before display. - Smooth Factor - Spline Factor - Logarithm - Derivative Order Same Parameters used for both spectra and purity display	
Spectra per peak	Parameter specifies how many spectra are extracted from a datafile. Parameters are defined separately for both, spectra and purity display. - User-defined spectra per peak - Automatic defined spectra per peak - Threshold	Parameter specifies how many spectra are extracted from a Data file. The parameter is used only for the spectra extraction in the spectra display. - Automatic defined spectra per peak - Threshold	The User-defined spectra per peak set takes x defined spectra at about equidistant points over the peak. Using Automatic and choosing a value of five, for example, the ChemStation extracts five spectra across the peak according to the peak width and symmetry. **Note:** For comparison reasons, standard values should be used therefore the user-defined option has been removed.
Normalization	Display options for Normalization modes can be separately defined for both spectra and purity windows	Same Display options is used for both spectra and purity calculations	
Display	Parameter to define display settings for spectra windows	Parameter to define display settings for spectra windows	

Table 28 Comparison Purify Tool Set "old" versus "new"

Parameter	"old" PURITY SET A.04.01 till B.0x.0x	"new" PURITY SET A.04.02 till B.0x.0x	Comment
Reference Spectra	Parameter to determine the Reference Spectra used for display and calculation. For purity calculations, a reference MUST be defined; when you use the option NONE, a pop up message forces you to specify a reference. - None - Manual - Automatic (Apex, Up/Down Nearest Baseline **Peak Baseline**)	Parameter to determine the Reference Spectra used for display and calculation. Same Parameters used for both spectra and purity display/calculations. Option options can be used for purity calculations. - None - Manual - Automatic (Depending on the Data Acquisition parameter the reference is determined, see help) **Note:** The Automatic mode corresponds to "old" Automatic mode: Peak BaseLine	To improve usability and comparison, the specified values for the reference spectra are now the same within Spectra and Purity definition. This avoids misleading information when different values are chosen in the spectra and purity sets. The automatic mode for the reference spectra has been improved, The selected reference spectra/spectrum depends on the spectrum mode, spectrum type and availability of baseline spectra. **Note:** For comparison reasons, standard values are used; therefore the user selection for the automation mode has been removed. **Impact on UV Library:** depending on the used reference, different spectra are stored within the UV library. It is recommended to update the spectra library when upgrading the spectra/purity options.
Spectra per peak	Parameter specifies how many spectra are used to calculate the average spectra for comparison. - User-defined spectra per peak - Automatic defined spectra per peak - Threshold	Five spectra per peak are used to assess purity: two spectra on each of the up and down slopes and one at the top (top or apex spectrum). The five spectra are averaged and compared with all spectra recorded in the spectra.	The User-defined spectra per peak set takes x defined spectra at about equidistant points over the peak. Using Automatic and choosing a value of five, for example, the ChemStation extracts five spectra from across the peak according to the peak width and symmetry. **Note:** For comparison reasons, standard values are used; therefore the user-defined option has been removed. **Impact on match results:** match result depends on the used average spectra for comparison

Table 28 Comparison Purify Tool Set "old" versus "new" (continued)

Parameter	"old" PURITY SET A.04.01 till B.0x.0x	"new" PURITY SET A.04.02 till B.0x.0x	Comment
Spectra per peak	Parameter to define display options	All purity-related graphical options are displayed in the purity windows	
Purity level calculation	Specifies which spectra are used to calculate the purity level of the peak, or to construct the similarity and threshold curve(s). The default value is the average spectrum, which decreases the contribution of noise in the spectrum	Specifies which spectra are used to calculate the purity level of the peak, or to construct the similarity and threshold curve(s). The default value is the average spectrum, which decreases the contribution of noise in the spectrum	Exactly the same parameters, but the calculation differs when average spectra are used for calculation. **Impact on purity factor:** purity factor result might depend on the used average spectra for comparison
Noise calculation	Defines how to calculate the threshold curve from the background noise	Defines how to calculate the threshold curve from the background noise	The noise calculation remains the same for both spectra/purity sets

UV-Libraries and Their Results

The UV libraries are built upon the selected spectra, and have been stored using the settings defined in the spectra/purify tool set. Depending on these parameters, libraries were created based on either pure spectra or spectra corrected by a reference. The comparison of a library spectrum against the spectrum of an unknown sample still needs expert interpretation, because there are many influences that need to be taken into account.

In ChemStation Rev. B.0x.0x, the “new” spectra/purify tool set of the Rev. A.xx.xx ChemStation is now the standard tool set. This tool set is more automated and enhanced and allows easier comparison of spectra.

UV libraries built upon the “old” spectra/purify tool set included the option to specify the mode used for ‘reference spectra’, and to define the ‘spectra per peak’ used for the purity calculations. Both options are automated using the “new” spectra/purify tool set and they now use either automatically calculated settings or fixed values (e.g. the ‘spectra per peak’ is now fixed to 5 spectra for purity calculations).

Because of these changes, match factors and purity results may differ between the A.xx.xx ChemStation and the B.0x.0x ChemStation, even when using the same methods, datafiles and UV-Libraries. In order to compare results from systems using different spectra/purify tool sets, you need to document the details of the spectra/purity settings used, so that the variation can be taken into account and appropriately documented.

NOTE This “upgrade preparation guide” is important for regulatory audit purposes and should be made available for inspections if an auditor requests the reprocess of data generated on ChemStation Rev. A.xx.xx. using a method with “old” spectra/purity tool sets.

It may be necessary to recreate the spectra entry of interest using the “new” spectra/purify tool. After you have upgraded the method in Rev. B.0x.0x, the UV-Library entries should be checked, to ascertain if any entries or whole libraries created using the “old” spectra/purify tool require rework. The best options is to establish a new UV-Library set up by using the standard spectra/purify tool set in Rev. B.0x.0.x.

9 Appendix

ChemStation Reports

Overview

Within the appendix the various ChemStation reports are listed, used to demonstrate the upgrade from ChemStation A.10.02 to ChemStation Rev. B.01.01. All ChemStation reports found in the appendix are related to the example chromatogram No. 1 and No. 2 used in Chapter 7, “Upgrade from Enhanced Integrator,” starting on page 118.

Example chromatogram No. 1

Rev. A.10.02:

1 The sample file was processed to obtain integration results and an Area% report was generated (see Figure 36, “Area% Report for Sample 005-0104.d - generated on ChemStation A.10.02,” on page 153).

Rev. B.01.01:

2 The method uploaded in Rev. B.01.01 ChemStation was used to reprocess the same sample file. An Area% report was generated (see Figure 37, “Area % Report for Sample 005-0104.d - generated on ChemStation B. 01.01,” on page 154).

Example chromatogram No. 2

Rev. A.10.02

1 A three level calibration table was created. The sample file was processed to obtain results and an ESTD report was generated (see Figure 38, “ESTD Report for Sample 005-0106.d - generated on ChemStation A.10.02,” on page 155).

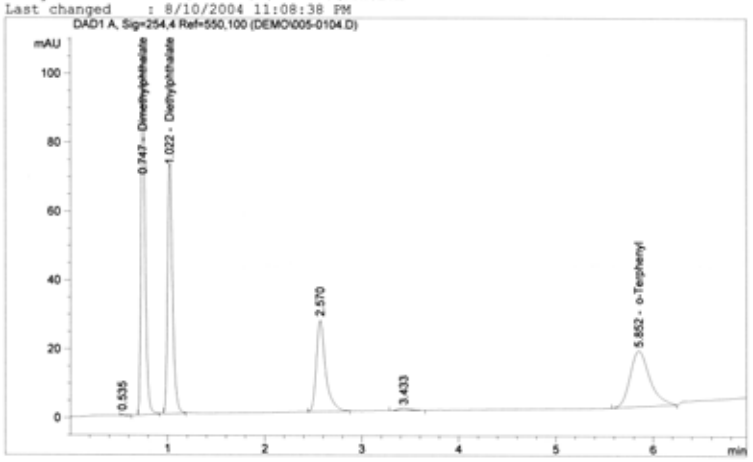
Rev. B.01.01

2 The method uploaded in Rev. B.01.01 ChemStation was recalibrated using the ‘Replace‘ option for each calibration level. The same sample file was used to reprocess the results and an ESTD report was generated (see Figure 39, “ESTD Report for Sample 005-0106.d - generated on ChemStation B.01.01,” on page 156).

Example Chromatogram 1 A.10.02

Data File C:\HPCHEM\1\DATA\DEMO\005-0104.D Sample Name: Isocratic Std. 1

```
Injection Date  : 4/19/94 8:08:45 AM          Seq. Line :   1
Sample Name     : Isocratic Std. 1            Location : Vial 5
Acq. Operator   : a.g.h.                         Inj :   4
Acq. Instrument : HP LC 1050                 Inj Volume : 2 µl
Acq. Method     : DEMO.M
Analysis Method : C:\HPCHEM\1\METHODS\DEMO1.M
Last changed    : 8/10/2004 11:08:38 PM
```



Area Percent Report

```
Sorted By             :      Signal
Calib. Data Modified  :      Tuesday, August 10, 2004 11:08:36 PM
Multiplier            :      1.0000
Dilution              :      1.0000
Use Multiplier & Dilution Factor with ISTDs

Signal 1: DAD1 A, Sig=254,4 Ref=550,100

Peak RetTime  Type   Width     Area      Area     Name
  #   [min]          [min]   [mAU*s]      %
----|-------|------|-------|----------|--------|--------------------
   1   0.535 PP      0.0214 2.85332e-1   0.0295 ?
   2   0.747 BB      0.0449  294.85150  30.4888 Dimethylphthalate
   3   1.022 BB      0.0524  261.40094  27.0299 Diethylphthalate
   4   2.570 BB      0.1011  175.77811  18.1762 ?
   5   3.433 PP      0.1228    5.45116   0.5637 ?
   6   5.852 PP      0.2125  229.31325  23.7119 o-Terphenyl

Totals :                    967.08028

 Results obtained with enhanced integrator!
```

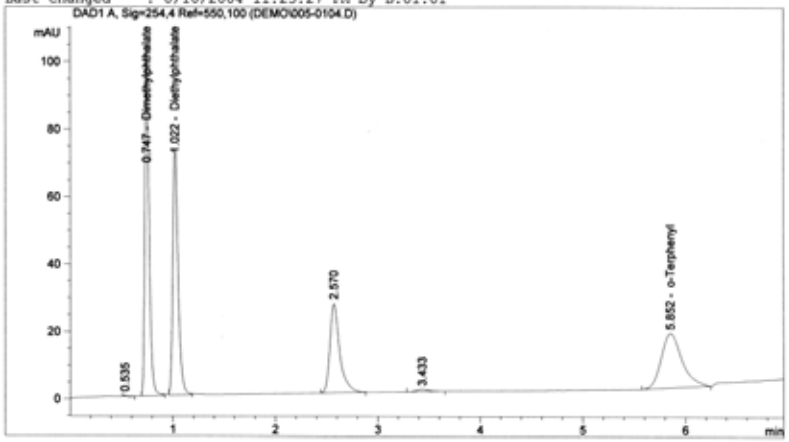
*** End of Report ***

Instrument 1 8/10/2004 11:09:00 PM Page 1 of 1

Figure 36 Area% Report for Sample 005-0104.d - generated on ChemStation A.10.02

Example Chromatogram 1 B.01.01:

```
Data File C:\CHEM32\1\DATA\DEMO\005-0104.D
Sample Name: Isocratic Std. 1

================================================================================
Injection Date  : 4/19/94 8:08:45 AM              Seq. Line :   1
Sample Name     : Isocratic Std. 1                 Location : Vial 5
Acq. Operator   : a.g.h.                             Inj :   4
Acq. Instrument : HP LC 1050                     Inj Volume : 2 µl
Acq. Method     : DEMO.M
Analysis Method : C:\CHEM32\1\METHODS\DEMO1_32A.M
Last changed    : 8/10/2004 11:23:27 PM by B.01.01
```



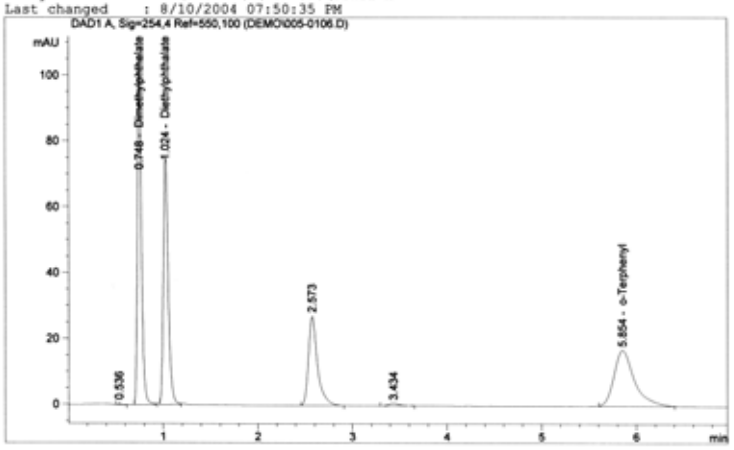

```
================================================================================
                              Area Percent Report
================================================================================

Sorted By             :      Signal
Calib. Data Modified  :      Tuesday, August 10, 2004 11:23:24 PM
Multiplier            :      1.0000
Dilution              :      1.0000
Use Multiplier & Dilution Factor with ISTDs

Signal 1: DAD1 A, Sig=254,4 Ref=550,100

Peak RetTime  Type   Width     Area      Area    Name
  #   [min]          [min]    [mAU*s]      %
----|-------|------|-------|----------|--------|--------------------
   1   0.535 BB      0.0214 2.85319e-1   0.0295 ?
   2   0.747 BB      0.0449  294.85150  30.4851 Dimethylphthalate
   3   1.022 BB      0.0524  261.41324  27.0279 Diethylphthalate
   4   2.570 BB      0.1011  175.88335  18.1848 ?
   5   3.433 BB      0.1228    5.45111   0.5636 ?
   6   5.852 BV      0.2125  229.31276  23.7090 o-Terphenyl

Totals :                     967.19728

================================================================================
                            *** End of Report ***


Instrument 1 8/10/2004 11:26:27 PM B.01.01                    Page   1 of 1
```

Figure 37 Area % Report for Sample 005-0104.d - generated on ChemStation B. 01.01

Example Chromatogram2 A.10.02

Data File C:\HPCHEM\1\DATA\DEMO\005-0106.D Sample Name: Isocratic Std. 1

```
Injection Date  : 4/19/94 8:25:02 AM          Seq. Line :   1
Sample Name     : Isocratic Std. 1            Location : Vial 5
Acq. Operator   : a.g.h.                        Inj :   6
Acq. Instrument : HP LC 1050                Inj Volume : 2 µl
Acq. Method     : DEMO.M
Analysis Method : C:\HPCHEM\1\METHODS\DEMO1.M
Last changed    : 8/10/2004 07:50:35 PM
```



External Standard Report

```
Sorted By             :      Signal
Calib. Data Modified  :      Tuesday, August 10, 2004 07:50:31 PM
Multiplier            :      1.0000
Dilution              :      1.0000
Use Multiplier & Dilution Factor with ISTDs

Signal 1: DAD1 A, Sig=254,4 Ref=550,100

RetTime  Type     Area      Amt/Area    Amount   Grp   Name
 [min]          [mAU*s]                 [mg/l]
-------|------|----------|----------|----------|--|-----------------
  0.748 BB      300.72705 1.06927e-2    3.21558    Dimethylphthalate
  1.024 BB      266.68295 1.19893e-2    3.19733    Diethylphthalate
  5.854 BB      256.10138 1.24299e-2    3.18331    o-Terphenyl

Totals :                                9.59623

 Results obtained with enhanced integrator!
```

*** End of Report ***

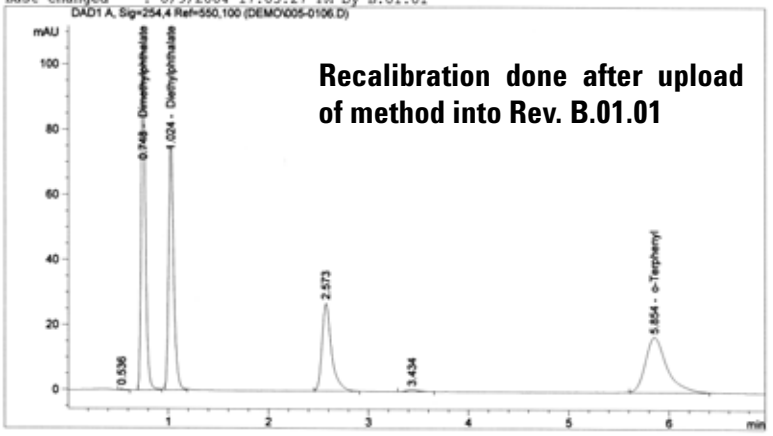
Instrument 1 8/10/2004 11:08:17 PM Page 1 of 1

Figure 38 ESTD Report for Sample 005-0106.d - generated on ChemStation A.10.02

Example Chromatogram2 B.01.01

Data File C:\CHEM32\1\DATA\DEMO\005-0106.D
Sample Name: Isocratic Std. 1

```
Injection Date  : 4/19/94 8:25:02 AM            Seq. Line :   1
Sample Name     : Isocratic Std. 1              Location : Vial 5
Acq. Operator   : a.g.h.                           Inj :   6
Acq. Instrument : HP LC 1050                  Inj Volume : 2 µl
Acq. Method     : DEMO.M
Analysis Method : C:\CHEM32\1\METHODS\DEMO1_32_RECAL.M
Last changed    : 8/9/2004 17:05:27 PM by B.01.01
```




```
                        External Standard Report

Sorted By             :      Signal
Calib. Data Modified  :      Monday, August 09, 2004 17:05:24 PM
Multiplier            :      1.0000
Dilution              :      1.0000
Use Multiplier & Dilution Factor with ISTDs

Signal 1: DAD1 A, Sig=254,4 Ref=550,100

RetTime  Type     Area      Amt/Area    Amount   Grp   Name
 [min]          [mAU*s]                 [mg/l]
-------|------|----------|----------|----------|--|------------------
  0.748 BB      300.72705 1.06929e-2    3.21565    Dimethylphthalate
  1.024 BB      266.68295 1.19917e-2    3.19797    Diethylphthalate
  5.854 BB      256.10138 1.24325e-2    3.18398    o-Terphenyl

Totals :                                9.59761

                        *** End of Report ***

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```

Figure 39 ESTD Report for Sample 005-0106.d - generated on ChemStation B.01.01

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In This Book

Use this handbook when you upgrade the Agilent ChemStation from an Revision A/B.xx.xx to Revision B.03.01.

This handbook describes the necessary steps to perform an upgrade to Rev. B.03.01 of Agilent ChemStation. It gives details about modifications compared to previous ChemStation revisions and explains how to operate with update ChemStation files (e.g. methods, sequences, etc.).

This handbook lists the PC hardware and software requirements that need to be met in order to upgrade and operate the Agilent ChemStation successfully.

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