Agilent ChemStation

Upgrade Preparation Guide

Agilent Technologies

Notices

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Software Revision

This guide is valid for revision B.04.02 SP1 or higher of the Agilent ChemStation software.

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CAUTION

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For Research Use Only

In This Guide...

This guide describes the upgrade to Agilent ChemStation B.04.02 SP1 software and the steps to configure your analytical system. The documentation should be used as resource prior to a ChemStation upgrade.

1 Introduction to Agilent ChemStation Rev B.04.02 SP1

This chapter provides an overview about the changes in Agilent ChemStation Rev. B.04.02 SP1 with respect to the previous revision and information regarding the content of this guide.

2 Prerequisites to Upgrade to Agilent ChemStation Rev. B.04.02 SP1

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.04.02 SP1

This chapter describes how to upgrade to Agilent ChemStation Rev. B.04.02 SP1. This includes the treatment of Add-On Solutions during the upgrade.

4 The First Time You Start Up Your ChemStation Rev. B.04.02 SP1

This chapter covers most of the recognizable changes compared to previous revisions, e.g. graphical and design changes. 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. In addition for updates from Rev. A systems, the upload process and modifications for 16-bit files into the 32-bit ChemStation are described.

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 such as Macros and the necessary actions to adapt the Unicode format.

7 Upgrade Impact on time stamps of reprocessed data and methods on reports

This chapter is relevant for upgrades from Rev. A.xx.xx. only.

8 Upgrade Impact on Quantification Methods (Relevant for Upgrades from Rev. A.xx.xx 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.

9 Upgrade Impact on LC Methods

This chapter outlines the differences between storage of acquisition parameters for LC ChemStation when using classic drivers or RC.NET drivers, respectively.

10 Spectra/Purity Options using ChemStation Rev. B.04.0x (Relevant for Upgrades from Rev. A.xx.xx 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 no longer available.

11 Appendix

The appendix offers Example Chromatograms produced with different versions.

Contents

1 Introduction to Agilent ChemStation Rev B.04.02 SP1

This chapter provides an overview about the changes in Agilent ChemStation Rev. B.04.02 SP1 with respect to the previous revision and information regarding the content of this guide.

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 since Rev. B.01.01

Changes and new functionality introduced with ChemStation revision B.04.02 and B.04.02 SP1:

- **Easy Sequence**: a new easy-to-use user interface for sequence planning, generation and queuing.
- Improved functionality of the **Easy Sequence** Queue (B.04.02 SP1)

- LC specific:
  - Support for the Agilent 1120 Compact LC (B.04.02 DSP1), the new SFC Fusion A5 (B.04.02 SP1), and the new Agilent 1290 Infinity LC System.

    The Agilent 1290 Infinity LC System consists of the following hardware modules:
    - Agilent G4220A 1290 Binary Pump
    - Agilent G4226A 1290 High Performance Autosampler
    - Agilent G1316C 1290 Thermostatted Column Compartment
    - Agilent G4212A 1290 DAD
    - Agilent G4227A Infinity Flexible Cube (B.04.02 SP1)
  - A new user interface for LC instrument control in the **Method and Run Control** view with:
    - Flexible sizing of the instrument control panel to make best use of the available desktop space.
    - Show/hide functionality to reduce the display to the most essential information
    - Graphical representation of multiple devices of the same kind (e.g. two pumps)
    - Graphical representation of all valves
    - Direct access to the method parameters and all import functions for each module
    - Status display for the individual modules and resulting overall instrument status

  - Tooltips reveal most important information on specific functions
  - Tabular display of the sample information for the current run or sequence line
  - Direct access to data analysis parameters and settings for OpenLAB ECM (only with G2189BA ChemStation OpenLAB option)

- GC specific
  - 7693A Automatic Liquid Sampler support with the Agilent 6890 and 6850 GCs
  - Agilent 7820A GC (B.04.02 DSP2)
  - G7300AA Easy SamplePrep (B.04.02 SP1)
  - Improved Method Resolution with the new 78xx (Version 3.01) and the new 68xx (Version 6.01) Software Drivers (B.04.02 SP1)
  - Ability to make column, valve, gas type, and syringe size changes from Method Edit with the new 78xx (Version 3.01) and the new 68xx (Version 6.01) Software Drivers (B.04.02 SP1)
  - Barcode support with the new 68xx (Version 6.01) Software Driver (B.04.02 SP1)

- LC/MSD specific
  - Support for the new Agilent 6100B Series Single Quad LC/MS Systems, including the G6120B, G6130B and G6150B
  - Support for the Agilent Jet Stream (compatible with G6150B only)

- CE specific
  - Support for the new Agilent 7100 CE System (B.04.02 DSP1)

- ChemStation OpenLAB Option
  - Support for OpenLAB Intelligence Reporter A.02.01 with the following new features:
    - Report Template Editor
    - Chromatogram and spectra display in the OpenLAB Intelligence reports

Changes and new functionality introduced with ChemStation revision B.04.01 SP1:

- 7693A Automatic Liquid Sampler system G4513A (ALS), G4514A (Tray), and G4515A (BCR) support with the Agilent 7890A GC.
- Support for Method Development System and Method Scouting Wizard for LC and LC/MSD ChemStation.

Changes and new functionality introduced with ChemStation revision B.04.01:

- Custom Fields for samples and compounds to store additional information
- Enhanced overlay capabilities in **Data Analysis** view
- Data acquisition into an existing sequence container (**Unique Folder Creation** switched on)
- Storage of manual integration events with the data file
- Usability enhancements for sequence and method handling in Data Analysis
- GC Specific:
  - eMethods
- Agilent 7890A GC specific:
  - Sampling diagram
  - **Method Resolution** dialog box displays a report detailing method and hardware differences
  - Column Compensation
  - Digital auto zero
  - Graphics plot shown in edit parameters screen
  - Editing GC Parameters during a run via software for single runs
  - Edit GC Parameters includes a new method editing page to specify how the GC determines its readiness
  - Runtime event editing enhancements
  - Out of limit values are highlighted

- LC Specific:
  - Support for Agilent 1200 G1314D VWD and G1314E VWD SL Plus
  - Support for Agilent 1200 G1367D High Performance Autosampler SL Plus
- For users of the ChemStation OpenLAB Option:
  - Direct access to ECM information such as object properties and location
  - Configurable automatic storage of data in ECM
  - Automatic update of local methods and sequences with ECM data
  - Automatic deletion of local data
- Furthermore, the ChemStation OpenLAB Option provides a set of new features that allow the enforcement of tighter security where needed and enable users to comply with 21 CFR Part 11 and similar regulations for electronic records and electronic signatures:
  - Mandatory login/connection to ECM
  - Configurable session locking (interactive as well as time-based)
  - Configurable ChemStation user roles and privileges
  - Full data traceability through audit trails for methods and results
  - Full versioning of data including master methods and sequence templates

Changes and new functionality introduced with 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 Advisor* 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 Software in Chinese and Japanese

Changes and new functionality introduced with 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

Changes and new functionality 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

Changes and new functionality 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 x 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* is applicable only for customers upgrading an existing ChemStation. The document refers to *changes* in comparison to previous ChemStation Revisions only.

NOTE ChemStation B.04.02 SP1 is supported on Windows XP and Windows Vista (32 bit). Windows XP is supported with SP3 only. Windows Vista is supported with SP2 only. In order to upgrade to ChemStation B.04.02 SP1 the operating system needs to be updated PRIOR to the ChemStation upgrade, if necessary. Please also check the PC minimum requirements, see "PC Requirements" on page 18.

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

A.03.0x or higher to Agilent ChemStation Rev. B.04.02 SP1

B.0x.0x to Agilent ChemStation Rev. B.04.02 SP1

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 DVD-ROM, 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.04.02 SP1

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.

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.04.02 SP1 and greater is supported on personal computers with an Intel Pentium IV 1.5 GHz or higher (Windows XP) or 3.4 GHz (Windows Vista). Using a GPIB interface, one PCI slot is required. Alternatively, the Agilent USB-GPIB interface device 82357A or 82357B can be used. For details about GPIB and the USB-GPIB interface requirements, refer to the LC/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.

PC Requirements

Minimum hardware requirements for your Agilent Technologies ChemStation software (version B.04.02 SP1) are:

- A personal computer with an Intel Pentium IV processor (1.5 GHz for Windows XP, 3.4 Ghz single core for Windows Vista)
- 1280 x 1024 Super VGA resolution, 17 inch display, 16k colors or better (recommended: 19 inch, resolution 1440 x 900)
- 40 GB hard disk (with 600 MB free disk space) for Windows XP, 160 GB hard disk for Windows Vista
- DVD-ROM drive
- Windows XP: 512 MB RAM (recommended: 1 GB); Windows Vista: 1 GB RAM (recommended: 2 GB)
- MS Windows compatible pointing device

- LAN = Ethernet IEEE 802.3 Industry Standard 10/100 Base T
- LAN Cabling between the hub and LAN boards, category 4 or greater UTP with RJ-45 connections
- Maximum supported cable distance = 100 meters
- Operating system compatible printer:
  - For the English system a printer using PCL 5c, 5e, 5e, 5.02 or 6
  - For Japanese system use Canon LBP-430, 450, 470, 1310, or 3410
  - for the Chinese System a printer using PCL 6
- Either a Microsoft Windows XP Professional (Service Pack 3) or Microsoft Windows Vista Business (Service Pack 2) operating environment
- TCP/IP protocol support installed, if you are using LAN communications
- If you are using GPIB communication: The 82350 (A or B model) GBIB Board or 82357 (A or B model) USB-GPIB interface, depend on suitable personal computer, and Agilent IO Libraries Suite 15.0. Refer to the Manuals\Installation folder of the ChemStation DVD for IO Libraries Suite installation instructions.

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.

Non-HP Computers

The Agilent ChemStation is designed to successfully run on a wide range of compatible personal computers equipped with accessories and peripherals that adhere to the programming standards for the Intel PC platform and Microsoft Windows operating systems.

However, Agilent has tested the Agilent ChemStation software mainly on Hewlett-Packard/Compaq equipment. All configuration information listed in this manual applies to Hewlett-Packard/Compaq Kayak, Vectra and EVO computers and may not be optimized for other vendor's PCs. The standard configuration of the GPIB interface, for instance, may conflict with the

memory configuration of a non Hewlett-Packard 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 check the documentation supplied with it and the accessories to eliminate resource conflicts in your PC's setup, especially regarding the configuration of the GPIB interface.

Printers for the Agilent ChemStation

The Agilent ChemStation is designed to work with printers that are compatible with the operating system. Printers may be attached to a local (preferably parallel) or networked port on the PC. Serial port printers are supported by the operating system but may exhibit speed performance limitations. Networked printers must be shared by a network server running a network protocol supported by the Microsoft operating system. We recommend printers that are capable of interpreting an escape code language (such as PCL) or page description language (such as PostScript®). Host-based printers (such as GDI or PPA printers) impose more printer processing tasks on the CPU and are not recommended for use with Agilent ChemStation online sessions.

For best printing results with your Agilent ChemStation, use HP LaserJet printers. High performance HP DeskJet printers may also be used if the amount of printing required is low. Check the readme.txt files for information on recommended printer driver versions.

Agilent Technologies has not tested all printer and printer driver combinations that are supported in the Windows environment. Print performance and results may vary on other manufacturer's printers and appropriate drivers.

The printers listed in Table 1 on page 21 have been successfully tested at the time this handbook was printed.

Table 1 Successfully tested Printers

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 (C9707A)	PCL 6 Driver
OfficeJet Pro K550DTWN	PCL 3 Driver
OfficeJet Pro K5400	PCL 3 Driver
HP LaserJet 2200D	HP PS 5.02 or PCL 6 Driver
HP LaserJet 2300dn	HP PS 5.02 or PCL 6 Driver
HP LaserJet 2300D (Q2474A)	HP PCL 5e Driver or PCL 6 Driver
HP LaserJet 2420D	HP PCL 6 Driver
HP LaserJet P3005D	PCL 6 Driver
Adobe Acrobat	version 7.0, 8.0
Amyuni PDF Converter	version 2.50
PDF-XChange	version 4.0 installed during ChemStation installation

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 it will not work with the Agilent ChemStation, but it has simply not been tested.

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 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.04.02 SP1 is available in English, as well as in localized versions for Japanese and Chinese. Depending of your choice of ChemStation, you will need the corresponding Microsoft Windows XP Professional *(Service Pack 3)* or Microsoft Windows Vista Business *(Service Pack 2)* operating system:

- English Microsoft Windows XP Professional *(Service Pack 3)*
- Japanese Microsoft Windows XP Professional *(Service Pack 3)*
- Chinese Microsoft Windows XP Professional *(Service Pack 3)*
- English Microsoft Windows Vista Business *(Service Pack 2)*
- Japanese Microsoft Windows Vista Business *(Service Pack 2)*
- Chinese Microsoft Windows Vista Business *(Service Pack 2)*

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

Windows XP Professional and Windows Vista Business (32 bit) are the only supported operating systems 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.

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 devices shown in Table 2 on page 24, and Table on page 31.

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.

1100/1200 LC Instrument firmware requirements

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 DVD.

Table 2 LC 1100/1200 Series Instrument Firmware Requirements

LC Instrument	Product Number	Firmware Revision
Samplers		
Agilent 1100/1200 Automation Interface	G2254A	A.06.10 or newer
Agilent 1100 Autosampler	G1313A	A.06.10 or newer
Agilent 1100/1200 Thermo. Autosampler	G1329A	A.06.10 or newer
Agilent 1200 Thermo. Autosampler SL	G1329B	A.06.10 or newer
Agilent 1100 Micro Sampler	G1389A	A.06.10 or newer
Agilent 1100/1200 Preparative Autosampler	G2260A	A.06.10 or newer
Agilent 1100 Well Plate Autosampler	G1367A	A.06.16 or newer
Agilent 1200 High Performance Autosampler	G1367B	A.06.16 or newer

Table 2 LC 1100/1200 Series Instrument Firmware Requirements

LC Instrument	Product Number	Firmware Revision
Agilent 1200 High Performance Autosampler SL	G1367C	A.06.16 or newer
Agilent 1200 High Performance Autosampler SL Plus	G1367D	A.06.16 or newer
Agilent 1100 Thermost. Well Plate Autosampler	G1368A	A.06.10 or newer
Agilent 1100/1200 Micro Well Plate Autosampler	G1377A	A.06.16 or newer
Agilent 1100/1200 Thermost. Micro Well Plate Autosampler	G1378A	A.06.10 or newer
Agilent 1100/1200 Dual Loop Autosampler PS	G2258A	A.06.16 or newer
Agilent 1290 Infinity High Performance Autosampler	G4226A	A.06.30 or newer
Column Compartments		
Agilent 1100/1200 Thermostatted Column Compartment	G1316A	A.06.10 or newer
Agilent 1200 Thermostatted Column Compartment SL	G1316B	A.06.10 or newer
Agilent 1290 Infinity Thermostatted Column Compartment	G1316C	A.06.30 or newer
Agilent 1100/1200 Chip Cube Interface	G2240A	A.06.11 or newer
Pumps		
Agilent 1100/1200 Isocratic Pump	G1310A	A.06.10 or newer
Agilent 1100/1200 Quaternary Pump	G1311A	A.06.10 or newer
Agilent 1100/1200 Binary Pump	G1312A	A.06.10 or newer
Agilent 1200 Binary Pump SL	G1312B	A.06.11 or newer
Agilent 1290 Infinity Binary Pump	G4220A	B.06.30 or newer
Agilent 1100/1200 Capillary Pump	G1376A	A.06.11 or newer
Agilent 1100/1200 Preparative Pump	G1361A	A.06.11 or newer
Agilent 1100/1200 Nano Pump	G2226A	A.06.11 or newer

Table 2 LC 1100/1200 Series Instrument Firmware Requirements

LC Instrument	Product Number	Firmware Revision
Detectors		
Agilent 1100 DAD	G1315A	A.06.10 or newer
Agilent 1100/1200 DAD	G1315B	A.06.10 or newer
Agilent 1100/1200 DAD SL	G1315C	B.06.30 or newer[1]
Agilent 1200 DAD	G1315D	B.06.30 or newer[2]
Agilent 1290 Infinity DAD	G4211A	A.06.10 or newer
Agilent 1100 MWD	G1365A	A.06.10 or newer
Agilent 1100/1200 MWD	G1365B	A.06.10 or newer
Agilent 1100/1200 MWD SL	G1365C	B.06.30 or newer[1]
Agilent 1200 MWD	G1365D	B.06.10 or newer[2]
Agilent 1100/1200 FLD	G1321A	A.06.11 or newer
Agilent 1100 VWD	G1314A	A.06.13 or newer
Agilent 1200 VWD	G1314B	A.06.13 or newer
Agilent 1200 VWD SL	G1314C	A.06.13 or newer
Agilent 1200 VWD	G1314D	B.06.25 or newer[3]
Agilent 1200 VWD SL Plus	G1314E	B.06.25 or newer[3]
Agilent 1100/1200 RID	G1362A	A.06.10 or newer
Agilent 1100/1200 UIB	G1390A	A.06.10 or newer
Fraction Collectors		
Agilent 1100 Fraction Collector	G1364A	A.06.10 or newer
Agilent 1100/1200 Fraction Collector PS	G1364B	A.06.10 or newer
Agilent 1100/1200 Fraction Collector AS	G1364C	A.06.10 or newer
Agilent 1100/1200 Micro Fraction Collector	G1364D	A.06.10 or newer

Table 2 LC 1100/1200 Series Instrument Firmware Requirements

LC Instrument	Product Number	Firmware Revision
Valves		
2Pos/10Port Valve	G1157A	A.06.10 or newer
2Pos/6 Port Valve	G1158A	A.06.10 or newer
2Pos/6 Port Valve SL	G1158B	A.06.10 or newer
6Position Selection Valve	G1159A	A.06.10 or newer
12Pos/13 Port Selection Valve	G1160A	A.06.10 or newer
2Pos/6 Port Micro Valve	G1162A	A.06.10 or newer
2Pos/10 Port Micro Valve	G1163A	A.06.10 or newer
Agilent 1290 Infinity Flexible Cube	G4227A	C.06.30 or newer
Others		
Agilent 1100/1200 Degasser	G1322A	All Revisions
Agilent 1100 Micro Degasser	G1379A	All Revisions
Agilent 1200 Micro Degasser	G1379B	All Revisions
Agilent 1100/1200 Manual Injector	G1328B	All Revisions
Agilent 1100/1200 Thermostat f. Sampler/ Fraction Collectors	G1330B	All Revisions
Agilent 1100 Local User Interface (A.02.03)	G1323A	A.05.xx[4]
Agilent 1100/1200 Local User Interface (B.03.22 and below)	G1323B	A.05.xx
Agilent 1100/1200 Local User Interface (B.04.02 and above)	G1323B	A.06.01/02/05/1x; B.01.02/06/1x; B.06.2x
Agilent 1100/1200 Control Module Instant Pilot	G4208A	B.02.09 or newer
Agilent 1200 SFC Fusion A5	G4301A	use firmware included on CD shipping with the hardware

[1] 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.

[2] 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.

[3] The Agilent G1314D and G1413E VWD modules require minimum firmware B.06.20. This firmware is only compatible with firmware A.06.1x or higher. As soon as a G1314D/E is used in an 1100/1200 stack, the whole stack needs to be compatible using firmware A.06.1x or higher.

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

1120 Compact LC firmware requirements

The LC ChemStation software requires firmware B.06.2x for the 1120 compact LC.

GC Instrument Firmware Requirements

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

Table 3 GC Instrument Firmware Requirements

GC Instrument	Product Number	Firmware Revision	Part Number
GC System			
Agilent 7890A GC System	G3440A	A.01.10.3	n.a.[1]
Agilent 7820A GC System	G4350A	7820A.01.10.013.1.bin - for English, Chinese and Japanese languages. 7820A.01.10.013.Ru.bin - for Russian language.	n.a.
Agilent 6890N	G1530N, G1540N	N.06.07 for 7693A support, And N.05.06 LAN assembly 04.7B3	n.a.[1]
Agilent 6890Plus, 6890A	G1530A, G1540A	A.03.08	G1530-61706
Agilent 6850N Series GC serial# >= US10243001	G2630A	N.06.07 for 7693A support And N.05.06 LAN assembly 04.7B3	n.a.[1]
Agilent 6850 Series GC serial# <= US00003200	G2630A	A.03.07 for 7693A support and A.03.03	n.a.[1]
Agilent 6850 Handheld Controller	G2629A	A.05.06 (not supported with 7693A)	n.a.[1]
GC Autosampler			
7693A Injector	G4513A	A.10.02	n.a.[1]
7683B Autoinjector	G2913A	A.11.03	n.a.[1]
7673C Autoinjector	G1513A	A.09.15	n.a.[1]
7683A/6890Plus ALS interface board	G2612A	A.02.01	n.a.[1]
7683A Autoinjector Module	G2613A	A.10.07	n.a.[1]
6850 Automatic Liquid Sampler	G2880A	A.10.05	n.a.[1]

Table 3 GC Instrument Firmware Requirements

GC Instrument	Product Number	Firmware Revision	Part Number
GC Tray			
7693A Tray	G4514A	A.10.11	n.a.[1]
7673C Tray	18596C	No Revision	
7683 ALS Tray for 5890	G2916A	A.02.01	n.a.[1]
7683A Tray module	G2614A	A.02.01	n.a.[1]
Bar Code			
BCR/Mixer	G4515A	A.10.03	n.a.[1]
BCR/Mixer	G2615A	No Revision	
BCR/Mixer	G1926A	No Revision	
GC Controller			
7693A ALS card upgrade for 6890Plus	G4517A	A.01.01	n.a.[1]
7693A Touchstone 2 Accessory for 6890A	G4516A	A.01.01	n.a.[1]
7673C ALS Controller	G1512A	A.01.12	n.a.[1]
A/D Converter			
35900E	35900E	E.01.02	n.a.[1]

[1] The 7890A, 7820A, 6890N, and 6850 GC Systems, Autosampler (ALS) and 35900E instruments have flash ROM memory. Either Agilent Instrument Utilities or Agilent Lab Advisor can be used to update firmware. 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 *Installing your GC ChemStation* manual.

35900E A/D converter firmware requirements

Agilent 35900E A/D converter have flash ROM memory. The GC Firmware Update Utility is provided on the ChemStation DVD under the Support directory. 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

A/D Converter	Product Number	Firmware Revision
35900E		E.01.02

LC/MS Instrument Firmware Requirements

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

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)

Table 4 LC/MS Instrument Firmware Requirements

LC/MS Instrument	Product Number	Firmware Revision
Agilent 6100 Series LC/MS	G6110A, G6120A/B, G6130A/B, G6140A, G6150B	3.02.36 or higher
Agilent 1100/1200 Series LC/MSD	G1946C/D G1956A/B	3.03.36 or higher

CE Instrument Firmware Requirements

The CE ChemStation software requires the following minimum firmware revisions in order to work with the devices shown in Table 5 on page 33.

Table 5 CE Instrument Firmware Requirements

CE Instrument	Firmware Revision
G1601A	
Built-in DAD	Rev. 1.2 or higher
Mainframe Agilent CE G1601A	Rev. 2.3 or higher
G7100	Rev. B.06.25 or higher

Communication Components

Using LAN Communication

If you connect your instrument using a standard TCP/IP protocol, it 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 to LAN connection, you must install the required LAN communication components and reconfigure your instrument.

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.04.02 SP1. 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 DVD.

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.04.0x. In addition, a USB-GPIB Interface can be used. For details, please refer to Table 6 on page 35.

NOTE Agilent LC 1100 and 35900E using GPIB communication are no longer supported. These systems need an upgrade to LAN connection PRIOR to the upgrade to ChemStation Rev. B.04.0x.

Table 6 GPIB and Analytical Hardware Compatibility Matrix

Instrument Type	Agilent 82350 A	Agilent 82350 B	Agilent USB-GPIB Interface 82357A	Agilent USB-GPIB Interface 82357B
Agilent 1100/1200 LC	No	No	No	No
Agilent 1120 Compact LC	No	No	No	No
HP 5890 GC, 4890D GC	No	Yes	No	Yes
Agilent 7890A GC System	No	No	No	No
Agilent 7820A GC System	No	No	No	No
Agilent 6890N GC	No	No	No	No
Agilent 6890A and 6890 Plus GCs	No	Yes	No	Yes
Agilent 6850 GC	No	No	No	No
G1600A Capillary Electrophoresis	Yes	Yes	Yes	Yes
7100 Capillary Electrophoresis	No	No	No	No
35900E	No	No	No	No

CAUTION

Electronic boards and components are sensitive to electrostatic discharge (ESD).

ESD can damage electronic boards and components.

➔ Be sure to hold the board by the edges and do not touch the electrical components. Always use an ESD protection (for example, an ESD wrist strap) when handling electronic boards and components.

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 DVD-ROM in the Manual/Installation folder.

3 How to Upgrade to Agilent ChemStation Rev. B.04.02 SP1

This chapter describes how to upgrade to Agilent ChemStation Rev. B.04.02 SP1. This includes the treatment of Add-On Solutions during the upgrade.

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 "Upgrade Procedure for ChemStation Systems with Add-On Solutions" on page 46, prior to starting the upgrade procedure. Verify that your Add-On Solution is supported on ChemStation B.04.02 SP1. If you have used GPIB communication, read the section "Communication Components" on page 34 prior to starting the upgrade procedure.

Licenses in ChemStation Rev. B.04.0x

ChemStation Rev. A.xx.xx License numbers in general allow the upgrade to ChemStation Rev. B.04.0x. 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.04.0x. 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 to ChemStation Rev. B.04.02 SP1 from any revision between B.01.01 and B.04.02

The upgrade of an existing ChemStation revision between B.01.01 and B.04.02 to revision B.04.02 SP1 can be performed using the installation routine on your ChemStation DVD.

The Installation Wizard uninstalls the current ChemStation, and a backup copy is saved under a new backup directory. The original installation directory name is used to create this directory, by default CHEM32_001. All files from the previous installation directory are filed in this directory.

After the upgrade installation, the instruments that had been configured previously will be available. There is no need to reconfigure them. Additional instruments can be added using the **Add Instrument** tool. For more information please see the respective *Install Your ChemStation* manual.

NOTE ChemStation B.04.02 SP1 is supported on Windows XP and Windows Vista only. Older ChemStation B.0x.0x versions had been supported Windows 2000, so in order to upgrade to ChemStation B.04.02 SP1 the operating system needs to be updated PRIOR the ChemStation upgrade. Please check as well the PC minimum requirements, see "PC Requirements" on page 18.

NOTE When upgrading from ChemStation B.01.01, the instrument configuration is not automatically available with the new B.04.02 SP1 installation. At the end of the upgrade process, the instruments have to be configured again in the **Add Instrument** dialog. Please make sure that you have your ChemStation licenses for the instruments available.

NOTE When upgrading a ChemStation revision B.0x.0x with a service release or patch installed, you may either remove the service release or patch via Windows' **Add or Remove Program** tool, or install the upgrade without removing them. If the patches and service releases are not removed before the upgrade, the corresponding entries in **Add or Remove Program** may still be available after the upgrade, although the previous ChemStation version including patches has been upgraded correctly. Do not try to remove these entries later.

NOTE Before starting the upgrade, close all programs and reboot your system.

1 Insert the ChemStation DVD-ROM into the DVD drive.

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

3 At the command line, type:
`x:\Install\Setup.exe` (where x represents the letter of your DVD drive), then click on **OK**.

NOTE

Agilent ChemStation B.04.02 SP1 requires Microsoft .NET Framework 3.5 SP1 and PDF-XChange 4.0 installed. Microsoft. NET Framework improves security and speed of the used applications and generates a basis for programs of various programming languages. PDF-XChange 4.0 is required by the ChemStation to provide the file type .PDF in the **Specify Report** and **Sequence Output** dialogs. If these two prerequisite applications are not already installed on your computer, you will be asked to install them. In the corresponding dialogs, press the **Install** button. For Microsoft .Net Framework 3.5 SP1 also accept the License agreement.

4 The Setup Wizard for Rev. B.04.0x starts and guides you through the upgrade process. On the Welcome screen, wait until the setup wizard has computed the disk space requirements, then press **Next**.

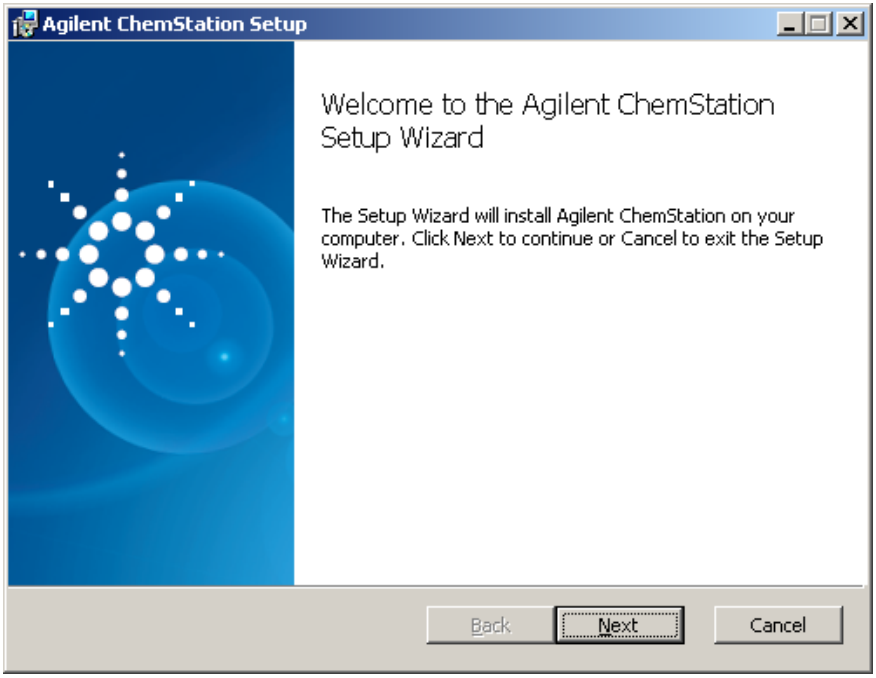


Figure 1 Agilent ChemStation **Setup** dialog

5 On the End-User License Agreement Screen, read the license agreement and then select **I accept the terms in the License Agreement**. Press **Next** to continue.

6 On the Upgrade Installation screen, the user is informed that the setup wizard has detected a previous B.0x.0x version of ChemStation. The user is informed that a backup of the current installation directory will be created and the new revision B.04.0x will be installed. Press **Next** to continue.

7 On the next screen the user is informed that the setup wizard is ready to start the upgrade installation. Press **Install** to start the installation process. During the installation process, the setup wizard moves the files of the previous ChemStation installation directory into a backup folder CHEM32_001 and removes all ChemStation related entries from the registry, the Windows Path variable and the ChemStation.ini file.

   Afterwards the new ChemStation B.04.02 SP1 files are installed. The setup wizard will restore the licenses used in the previous revision, the instrument configuration and files from the previous installation.

8 At the end of the upgrade process, press **Finish** to complete the upgrade installation.

9 Your software upgrade is now complete. Remove and store your DVD in a safe place.

10 Run IQT Report to check out the upgrade installation. Details about IQT Report are documented in your appropriate *Installing your ChemStation* manual.

Additional Upgrade Instructions

During an upgrade installation, the Setup Wizard moves user created files from backup folder Chem32_001 into the new installation. This covers all files created by the ChemStation user. If the user stores the files in the default directories, these are:

- Chem32\x\data*.d files: user-created data files
- Chem32\x\methods*.m files: user-created methods
- Chem32\x\sequences*.s files: user-created sequences
- Chem32\x\hypersequences*.hyp files: user-created hypersequences
- Chem32\x\verify*.val files: user-created system verification tests

In addition, also user-created spectral library files are moved when stored in the default location:

- Chem\speclibs*.uvl files: user-created UV library files

Data files, methods, sequences, and spectral libraries are also copied to the new installation, if the default path for these file types has been changed in the Configuration Editor.

Starting with ChemStation B.02.01, it is possible to set up additional paths for data files, methods, and sequences. Files in these additional locations are not copied if they are not located below the instrument directory chem32/x, where x is the is instrument number.

The following files, if they exist, need to be moved manually to the corresponding path in ChemStation Rev. B.04.0x:

- Chem32\repstyles*.frp files: user-created report styles
- Chem32\core*.mac, mcx files: specially user-created macro files, including user.mac
- Chem32\core*.xml: user-created xml files
- 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 "Impact on Customized Solutions" on page 105.

Manual Upgrade from ChemStation Rev. A.xx.xx to Rev. B.04.02 SP1

NOTE ChemStation B.04.02 SP1 is supported on Windows XP or Windows Vista only. In order to upgrade from ChemStation A.xx.xx to ChemStation B.04.02 SP1 the operating system needs to be updated PRIOR to the ChemStation upgrade. Please check as well the PC minimum requirements, "PC Requirements" on page 18.

ChemStation revisions A.xx.xx cannot be upgraded automatically to ChemStation B.04.02 SP1. In order to upgrade, the PC hardware and software requirements, as well as the firmware requirements, need to be checked. If the prerequisites are met, you can backup your data, uninstall the current ChemStation revision and then run the Setup Wizard of Rev. B.04.0x. The other upgrade possibility is to install ChemStation Rev. B.04.0x on a supported, clean system.

After installation, move the required user-created files manually to the appropriate directories. Be sure to backup all your necessary data. If you load methods, sequences, etc. within Rev. B.04.0x, they are saved using the new file format. Files saved in ChemStation Rev. B.04.0x are not backwards-compatible with any ChemStation Rev. A.xx.xx.

Instrument Specific Upgrade Instructions

LC-Specific Upgrade Instructions

LC 1100 modules communication

The following HPLC 1100/1200-specific file is moved to the upgraded ChemStation:

- chem32\x\clusterx.mth: system-created configuration file for LC 1100/1200 modules when using classic LC drivers

  or

- RapidControl.InstrumentConfig.xml: system-created configuration file for LC 1100/1200 modules when using RC.NET drivers for LC

Wellplate Configuration

The following Wellplate Sampler-specific file is moved to the upgraded ChemStation if it is stored in a directory below the instrument subdirectory, by default:

- chem32\x*.wpt files: user-created Wellplate definition file

GC-Specific Upgrade Instructions

Add-on products such as HeadSpace, CTC PAL Autosampler, and SimDis and LTM software must be uninstalled before the ChemStation software upgrade.

Companion is included in the GC ChemStation beginning with B.01.01 and is no longer a separate add-on product.

If Retention Time Locking Software is installed as an add-on with B.01.0x and B.02.0x. For these revisions RTL must be removed from the add/remove programs in control panel before the upgrade. RTL is no longer an add-on beginning with revision B.03.01 and no longer needs to be removed.

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.04.0x, 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.04.0x 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

There are no CE or CE/MS-specific upgrade instructions.

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.04.02 SP1. Refer to Table 7 on page 47, 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. B.01.01 or higher to ChemStation Revision B.04.0x. 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 the ChemStation.ini file (located in the WINDOWS directory of your system) in order to maintain the Add-On solution program.

During the upgrade process, the upgrade program reads all 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 chemstation.ini file that are not removed during the uninstallation; these entries may need to be MANUALLY removed from the chemstation.ini file AFTER the uninstallation of the Add-On solution, but PRIOR to the upgrade installation.

Supported Add-On Solution Products with ChemStation B.04.02 SP1

NOTE Verify PRIOR to the upgrade, that your installed Add-On Solution is supported on ChemStation B.04.0x. Not every Add-On Solution software is initially supported. The supported Add-On Solutions are documented in Table 7 on page 47.

Please find below the supported Rev. of Add-On Solutions to be installed on ChemStation Rev. B.04.02 SP1:

Table 7 Supported Add-On Solution Products with ChemStation Rev. B.04.02 SP1

Add-On Solution for ChemStation Rev. B.04.02 SP1	Required Revision for ChemStation Rev. B.04.02 SP1	Uninstall from ChemStation Rev. B.04.02 SP1
G2181BA ChemStore Client/Server	B.04.02	Uninstalls completely from the **Add/Remove Programs** in Control Panel, including entries in the chemstation.ini.
G2183BA Security Pack	B.04.02	Uninstalled during ChemStore uninstall.
G226xAA 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.
G3382AA Control for CTC PAL Autosampler for GC Systems	A.01.06	Uninstalls completely from the **Add/Remove Programs** in Control Panel, including entries in the chemstation.ini.
G3383AA Control for CTC PAL Autosampler for LC and LC/MS Systems	A.01.06	Uninstalls completely from the **Add/Remove Programs** in Control Panel, including entries in the chemstation.ini.
G2924AA Integrated HeadSpace software for GC	A.02.01 (supported on Windows XP SP3 only)	Uninstalls completely from the **Add/Remove Programs** in Control Panel, including entries in the chemstation.ini.
G2887BA SimDis software for GC	A.02.02	Uninstalls completely from the **Add/Remove Programs** in Control Panel, including entries in the chemstation.ini.

Table 7 Supported Add-On Solution Products with ChemStation Rev. B.04.02 SP1

Add-On Solution for ChemStation Rev. B.04.02 SP1	Required Revision for ChemStation Rev. B.04.02 SP1	Uninstall from ChemStation Rev. B.04.02 SP1
G6586AA Low Thermal Mass (LTM) software for GC	A.01.01 SP1	Uninstalls completely from the **Add/Remove Programs** in Control Panel, including entries in the chemstation.ini.
G7300AA Easy Sample Prep software for GC	A.02.01	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.
G2725AA Easy -Access	A.05.01	Uninstalls completely from the **Add/Remove Programs** in Control Panel, including entries in the chemstation.ini.
G3785AA Mass Hunter LC SQ Integrat software	B.01.00	Uninstalls completely from the **Add/Remove Programs** in Control Panel, including entries in the chemstation.ini.
G3772AA Masshunter Analytical Studio Reviewer	B.02.00	Uninstalls completely from the **Add/Remove Programs** in Control Panel, including entries in the chemstation.ini.
G2201BA CE/MS	B.04.02	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.0x.0x with installed Add-On solution. e.g. Purify:

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 **Add/Remove Programs**.

Table 8 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
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.
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

Table 8 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
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	B.01.02 B.01.03	[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	
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
G2887BA SimDis software for GC	starting A.02.01	[PCS, Instrument number] ADDONS=x (whereas x is the number of installed Add-Ons) ADDONx=C:\CHEM32\Core\SDSetup.MAC	Yes, removes completely all related entries in chemstation.ini
G6586AA Low Thermal Mass (LTM) software for GC	starting A.01.01	[PCS, Instrument number] ADDONS=x (whereas x is the number of installed Add-Ons) ADDONx=C:\CHEM32\LTM\LTMAddon.MAC	Yes, removes completely all related entries in chemstation.ini

Table 8 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
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.01.01	[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.

NOTE The win.ini entries related to the installed Add-On solutions are listed in Table 9 on page 52.

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 uninstalled 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.

8 Backup your ChemStation data.

9 Uninstall ChemStation, following the instructions in the *Installing Your ChemStation* manual of the currently installed ChemStation revision A.xx.xx.

10 Install ChemStation B.04.02 SP1.

Table 9 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.

Table 9 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
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
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.

Table 9 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
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 HeadSpace software for GCStandalone	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
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.

Table 9 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
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.xx.xx 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. B.0x.0x or higher ChemStation to ChemStation Revision B.04.0x. 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

The G2181BA ChemStore software on top of ChemStation Rev. B cannot be updated. 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 G2170BA/G2180BA ChemStation to revision B.04.02 SP1. The Add-on software must be upgraded after the ChemStation upgrade.

Purify Software

The following Purification Add-On Solution Software cannot be automatically upgraded to next higher revision B.04.0x. To upgrade, the software needs to be uninstalled manually.

Refer to the uninstallation section of the appropriate manual:

- G2262AA Purification/HighThroughput SW module
- G2263AA Mass based fraction collection add-on SW (LC/MS specific)
- G2265AA Standalone Purification/HighThroughput DA SW

The uninstallation shield of the Purification software removes all Purification related entries from the ChemStation.ini file. For details refer to Table 9 on page 52.

GC-Specific Add-On Solutions

All Add-On software products need to be uninstalled before any upgrade of G2070BA ChemStation to ChemStation B.04.02 SP1. The Add-On software must be upgraded after the ChemStation upgrade.

Retention Time Locking

Retention Time Locking G2080BA software is no longer an add-on beginning with B.03.01 and no longer needs to be uninstalled.

If RTL is installed as an add-on with B.01.0x – B.02.0x, it must be removed using the add/remove programs in control panel before upgrading.

Companion

Companion is no longer an add on product and is not uninstalled before an upgrade. 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.04.02 SP1. 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.04.0x. The Add-on software version must be reinstalled after the ChemStation upgrade. Please ensure that you install a compatible version.

Purify Software

The following Purification Add-On Solution Software cannot be automatically upgraded to next higher revision B.04.0x. To upgrade, the software needs to be uninstalled manually.

Refer to the uninstallation section of the appropriate manual:

- G2262AA Purification/HighThroughput SW module
- G2263AA Mass based fraction collection add-on SW (LC/MS specific)
- G2265AA Standalone Purification/HighThroughput DA SW

The uninstallation shield of the Purification software removes all Purification related entries from the ChemStation.ini file. For details refer to Table 9 on page 52.

Active Splitter Software

The Active Splitter Add-On software must be removed using **Add/Remove Programs** in the Control Panel before ChemStation for LC/MSD Rev. B.04.0x software is installed.

G1979A Multi-Signal Output Accessory Software

The G1979A Multi-Signal Output Accessory Add-On software must be removed using **Add/Remove Programs** in the Control Panel before the ChemStation for LC/MSD Rev. B.04.0x 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 ChemStation for LC/MSD Rev. B.04.0x is installed. The Analyst Rev. 1.4 Add-on software should not be removed before ChemStation for LC/MSD Rev. B.04.0x software is installed. ChemStation for LC/MSD Rev. B.04.0x should be installed while the Analyst Rev. 1.4 is still installed.

Easy-Access Software

The Easy Access Add-on software must be removed using **Add/Remove Programs** in the Control Panel before the ChemStation for LC/MSD Rev. B.04.0x software is installed.

CTC Cycle Composer Software

The CTC Cycle Composer Add-on software must be removed using **Add/Remove Programs** in the Control Panel. In addition, the CTC Cycle Composer add-on entries in win.ini must be manually deleted before the ChemStation for LC/MSD Rev. B.04.0x is installed.

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.04.02 SP1. 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 DVD-ROM.

NOTE The Agilent 82350 A/B cards are supported on Windows XP Professional or Windows Vista Business using ChemStation Rev. B.04.0x, for all analytical hardware as described in Table 6 on page 35.

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.04.0x.

Agilent LC 1100 and 35900E using GPIB communication are no longer supported with ChemStation Rev. B.04.0x.

4
The First Time You Start Up Your ChemStation Rev. B.04.02 SP1

This chapter covers most of the recognizable changes compared to previous revisions, e.g. graphical and design changes. 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. In addition for updates from Rev. A systems, the upload process and modifications for 16-bit files into the 32-bit ChemStation are described.

Startup Changes Introduced with B.04.02 SP1

Easy Sequence

Easy Sequence is a new user interface for quick and easy setup of sequences from templates. The template specifies parameters that should be viewed or edited by the user. Calibration setup provides an easy to use drag and drop interface to specify calibration types and sample positions, and displays an overview of the sequence. With **Easy Sequence**, multiple sequences can be submitted to the sequence queue to be run on the data system.

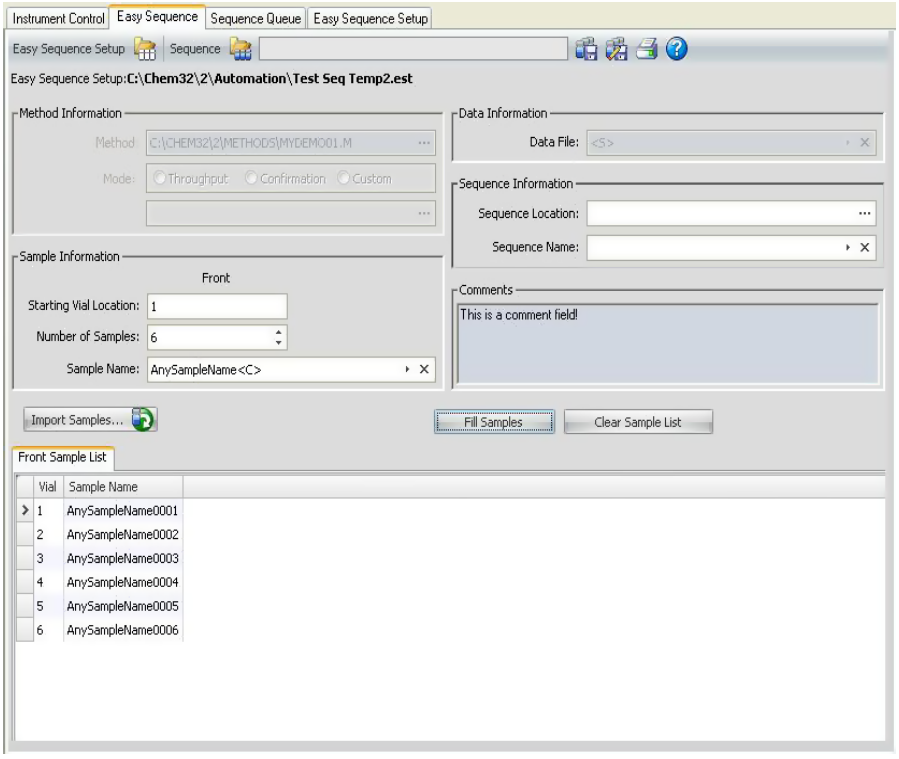


Figure 2 **Easy Sequence** tab

Using Easy Sequence Setup Tab (Template)

Easy Sequence Setup is used to create templates which are the starting point for creating sequences. There are two panels: Samples and Calibration. The **Samples** panel specifies the method, sample, data, and sequence information. The template is also used to specify what parameters are hidden or read-only. The **Calibration** panel provides a graphical interface to configure and view calibration runs. It provides an easy-to-use drag and drop interface to specify calibration types, cyclic and bracketed, and sample positions.

Creating an Easy Sequence template:

1 From the **Easy Sequence Setup** tab, select the **Samples** panel. Open an existing template or create a new template.

2 Select the **Method**. Dual injection options will be shown if the method's injection source is Dual. A back analysis method can be specified for the back signal. The method is the only parameter required for a template.

3 Specify the **Starting Vial Location**, **Number of Samples**, and the **Sample Name**.

4 Select the **Data Location**

5 Select the **Sequence Location** and specify the **Sequence Name**.

6 Enter any comments for the template.

7 Specify which parameters are hidden or read-only. Enter a default value for **injections/vial**, **sample amount**, **ISTD amount**, **injection volume**, etc. This helps to minimize the chance for errors when creating a sequence in the **Easy Sequence** Tab.

8 Save the template.

To define Calibrations:

The method used in the template should have been calibrated to the necessary levels.

1 From the **Easy Sequence Setup** tab, select the **Calibration** panel

2 Select **Cyclic** or **Bracketing** from the **Calibration Mode** drop down list.

3 The **Sequence Diagram** has the following sections:

- **Sequence Start**
- **Cyclic/Bracketing**

- **Samples**
- **Sequence End**

4 In the **Samples** area for the Sequence, set the **Calibration Interval** based on number of samples or number of injections.

5 Setup the **Sample type**, **Blank**, **Calibrant**, or **QC Sample** by dragging the icon from the **Sample Type** area to the **Sequence Diagram** section.

6 Setup the parameters for each Sample type and set to **Hide** or **Read-Only**.

7 Verify the cyclic/bracketing calibration in the **Easy Sequence** Overview.

8 Save the template.

Using Easy Sequence Tab (Sequence)

Easy Sequence tab is used to create a sequence from the template created in the **Easy Sequence** Setup. Samples saved as a CSV format can also be imported.

To define a Sequence

1 From the **Easy Sequence** tab, open a template by clicking on the Open Easy Sequence Setup icon.

2 Make updates if required. This may include sample vial locations, calibrant vial locations, data, or sequence location. Parameters available for editing depend on the template configuration.

3 If the pre-filled samples do not match new sample locations, click **Fill Samples** to refill the table.

4 Click **Preview/Print Sequence...** to preview the Sequence

5 Save the sequence.

HINT The sequence can be edited as long as its status is **Pending** in the queue.

6 Click **Save and Add to Queue** to submit the Sequence to the Sequence Queue.

To import Sample Data

Sample data set can be imported into **Easy Sequence**. Before importing samples, the CSV file must be set up and formatted properly. Refer to online help for more information on how to create a CSV sample data file.

1 From the **Easy Sequence** tab, open a template by clicking on the **Open Easy Sequence Setup** button
2 Click **Import Samples...**
3 Select the CSV file you want to import.

   All valid fields are imported.

NOTE To import sample data to the **Back Sample List**, make sure that the **Back Sample List** is selected and displaying before pressing the **Import Samples** button.

4 Verify the fields by reviewing the Sample List.

Using the Sequence Queue Tab (Queue)

Multiple and different sequences can be added to the queue. The first sequence added to the queue starts when the data system is ready. Additional sequences are added to the end of queue and the order in which the sequence is run can be changed. The **Easy Sequence** can be edited while in the queue as long as its status is pending.

For more information, see the online help system. **Easy Sequence Setup** tutorials are available in online help.

New User Interface in LC ChemStation

ChemStation B.04.02 introduces a new user interface for LC ChemStation.

The new user interface offers:

- Flexible sizing of the instrument control panel to make best use of the available desktop space
- Show/hide functionality to reduce the display to the most essential information
- Graphical representation of multiple devices of the same kind (for example, two pumps)
- Graphical representation of all valves
- Direct access to method parameters and all important functions for each module

- Status display for the individual modules and resulting overall instrument status
- Tool-tips reveal most important information on specific functions
- Tabular display of the sample information for the current run or sequence line
- Direct access to data analysis parameters

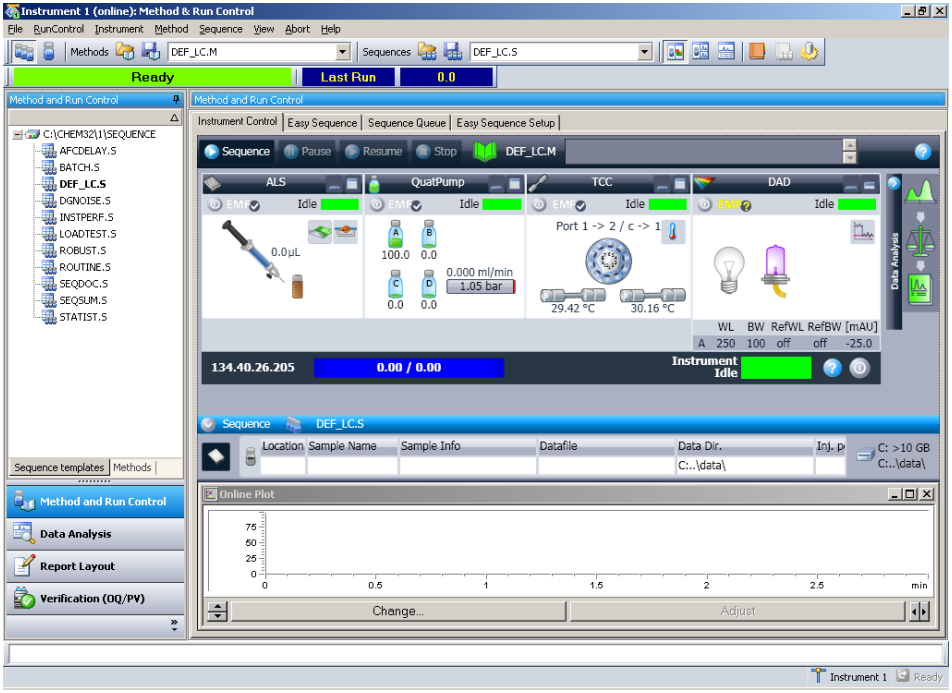


Figure 3 **Method and Run Control** view with RC.NET drivers

Availability of the new user interface (UI) for LC depends on the instrument drivers used for the 1100/1200 modules. ChemStation B.04.02 introduces support for a new set of drivers, the Rapid Control.NET drivers. Only if these drivers are used, the new UI will be available. With classic drivers, the UI will remain unchanged. Please refer to tables Table 10 on page 68to Table 14 on page 71 for availability of RC.NET drivers.

For most of the 1100/1200 modules both classic and RC.NET drivers are available. However, a few modules only support one of these driver types. Within one ChemStation instrument it is only possible to use either classic or RC.NET drivers.

Table 10 Available Drivers for Agilent Detectors

Module/ Device	Product Number	Classic Driver	RC.net Driver
Agilent 1100 VWD	G1314A	Yes	Yes
Agilent 1200 VWD	G1314B/D	Yes	Yes
Agilent 1200 VWD SL	G1314C	Yes	Yes
Agilent 1200 VWD SL Plus	G1314E	Yes	Yes
Agilent 1100/1200 DAD	G1315A/B	Yes	Yes
Agilent 1100/1200 DAD SL	G1315C	Yes	Yes
Agilent 1200 DAD	G1315D	Yes	Yes
Agilent 1290 Infinity DAD	G4211A	No	Yes
Agilent 1100/1200 FLD	G1321A	Yes	Yes
Agilent 1100/1200 RID	G1362A	Yes	Yes
Agilent 1100 MWD	G1365A	Yes	Yes
Agilent 1100/1200 MWD	G1365B	Yes	Yes
Agilent 1100/1200 MWD SL	G1365C	Yes	Yes
Agilent 1200 MWD	G1365D	Yes	Yes
Agilent 1100/1200 UIB	G1390A	Yes	Yes
Agilent ELSD	G4218A	Yes	No

Table 11 Available Drivers for Agilent Sampling Systems

Module/ Device	Product Number	Classic Driver	RC.net Driver
Agilent 1100 Autosampler	G1313A	Yes	Yes
Agilent 1100/1200 Autosampler (Thermostatted)	G1327A and G1329A/B	Yes	Yes
Agilent 1100/1200 Well Plate Autosampler (Thermostatted)	G1367A and G1368A	Yes	Yes
Agilent 1200 High Performance Autosampler (SL)	G1367B/C	Yes	Yes
Agilent 1200 High Performance Autosampler SL Plus	G1367D	Yes	Yes
Agilent 1100/1200 Microwell Plate Autosampler (Thermostatted)	G1377A and G1378A	Yes	No
Agilent 1100 Micro Autosampler	G1389A	Yes	No
Agilent 1200 Well Plate Handler	G2257A	Yes	No
Agilent 1200 Dual Loop Autosampler	G2258A	Yes	No
Agilent 1100/1200 Preparative Autosampler (Thermostatted)	G2260A and G2261A	Yes	No
Agilent 1290 High Performance Autosampler	G4226A	No	Yes
CTC HTC PAL Autosampler	G4270	Yes	No
CTC HTS PAL Autosampler	G4271	Yes	No

Table 12 Available Drivers for Agilent Pumps

Module/ Device	Product Number	Classic Driver	RC.net Driver
Agilent 1100/1200 Isocratic Pump	G1310A	Yes	Yes
Agilent 1100/1200 Quaternary Pump	G1311A	Yes	Yes
Agilent 1100/1200 Binary Pump	G1312A	Yes	Yes
Agilent 1200 Binary Pump SL	G1312B	Yes	Yes
Agilent 1200 Preparative Pump	G1361A	Yes	No

Table 12 Available Drivers for Agilent Pumps

Module/ Device	Product Number	Classic Driver	RC.net Driver
Agilent 1100/1200 Capillary Pump	G1376A	Yes	No
Agilent 1100/1200 Nano Pump	G2225A and G2226A	Yes	No
Agilent 1290 Infinity High Performance Binary Pump	G4220A	No	Yes

Table 13 Available Drivers for other Agilent Modules

Module/ Device	Product Number	Classic Driver	RC.net Driver
Agilent 1100 Fraction Collector	G1364A	Yes	No
Agilent 1100/1200 Preparative Fraction Collector	G1364B	Yes	No
Agilent 1100/1200 Analytical Fraction Collector	G1364C	Yes	No
Agilent 1100/1200 Micro Fraction Collector	G1364D	Yes	No
Agilent 1100/1200 Thermostatted Column Compartment	G1316A	Yes	Yes
Agilent 1200 Thermostatted Column Compartment SL	G1316B	Yes	Yes
Agilent 1290 Infinity Thermostatted Column Compartment	G1316C	Yes[1]	Yes
1100 Chip Cube Interface	G1390A	Yes	No
Agilent 1200 SFC Fusion S5	G4301A	No	Yes[1]

[1] no support for new 2/10 and 2/6 valves and Method Development solution

Table 14 Available Drivers for Agilent Valves

Module/ Device	Product Number	Classic Driver	RC.net Driver
9Pos/7Port Valve	G1156A	Yes	Yes
2Pos/10Port Valve	G1157A	Yes	Yes
2Pos/6 Port Valve (SL)	G1158A/B	Yes	Yes
6Position Selection Valve	G1159A	Yes	Yes
12Pos/13 Port Selection Valve	G1160A	Yes	Yes
2Pos/6 Port Micro Valve	G1362A	Yes	Yes
2Pos/10 Port Micro Valve	G1363A	Yes	Yes
Valve Kits	G4230A/B	No	Yes
Agilent 1290 Infinity Flexible Cube	G4227A	No	Yes

ChemStation B.04.02 provides a **Configuration Assistant** that helps in selecting the driver set for your current LC instrument configuration. The **Configuration Assistant** starts automatically if the option **Use configuration assistant to configure LC system** is selected when finishing the Setup Wizard. For details about the **Configuration Assistant** please refer to the *ChemStation Installation Manual for LC and CE systems*.

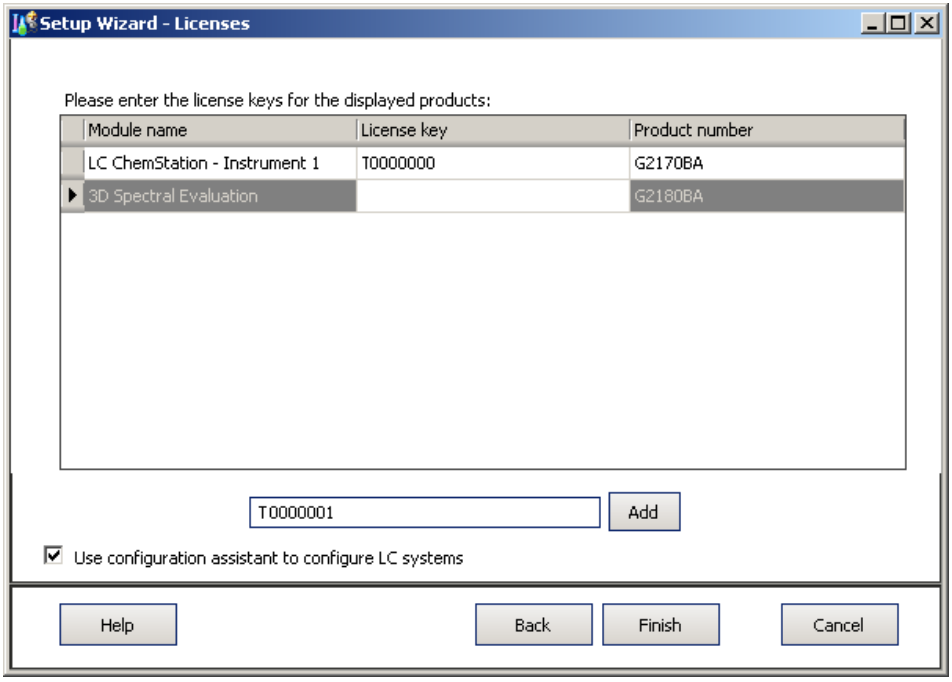


Figure 4 Setup Wizard with option **Use configuration assistant** selected

Using RC.NET drivers for LC ChemStation also changes the internal structure of the ChemStation methods. Please refer to "Upgrade Impact on LC Methods" on page 147 for more details how this impacts existing methods. "Impact on Customized Solutions" on page 105 describes how macro customized solutions are impacted.

Startup Changes Introduced with B.04.01

The data organization scheme introduced in revision B.02.01 was enhanced by the following new features:

- Enhanced overlay capabilities in Data Analysis view
- Data acquisition into an existing sequence container (Unique Folder Creation switched on)
- Storage of manual integration events with the data file
- Usability enhancements for sequence and method handling in Data Analysis For more details, refer to the manual Getting Started with New ChemStation Workflow.

For more details, refer to the manual *Getting Started with New ChemStation Workflow*.

Custom Fields

ChemStation provides numerous fields where you can enter information on a sequence, on specific samples, or on the expected compounds. These fields suffice for many standard analysis tasks. However, for some specific tasks you may need to save additional information on the samples or compounds. In this case, you can define the so-called custom fields.

Custom fields are available for sample information and for compound information. The custom fields definition is saved as part of the method definition. When you define custom fields, you can define, according to your needs, a suitable field name and data type for the additional information.

Once you defined the custom fields, you can enter the actual values in the sequence table of the current sequence. These values will be shown on ChemStation reports.

Setting up Custom Fields

The custom fields definition is part of the method. You can define up to ten custom fields related to the samples, and up to ten custom fields related to the compounds. Also, you can import the custom fields definitions from an other, existing method.

To define new custom fields:

1 Select the **Method and Run Control** view.

2 Load the required method.

3 Select **Method > Custom Fields Setup**.

The **Set up Custom Fields definitions** dialog opens. It contains two sections, one for sample custom fields, and one for compound custom fields.

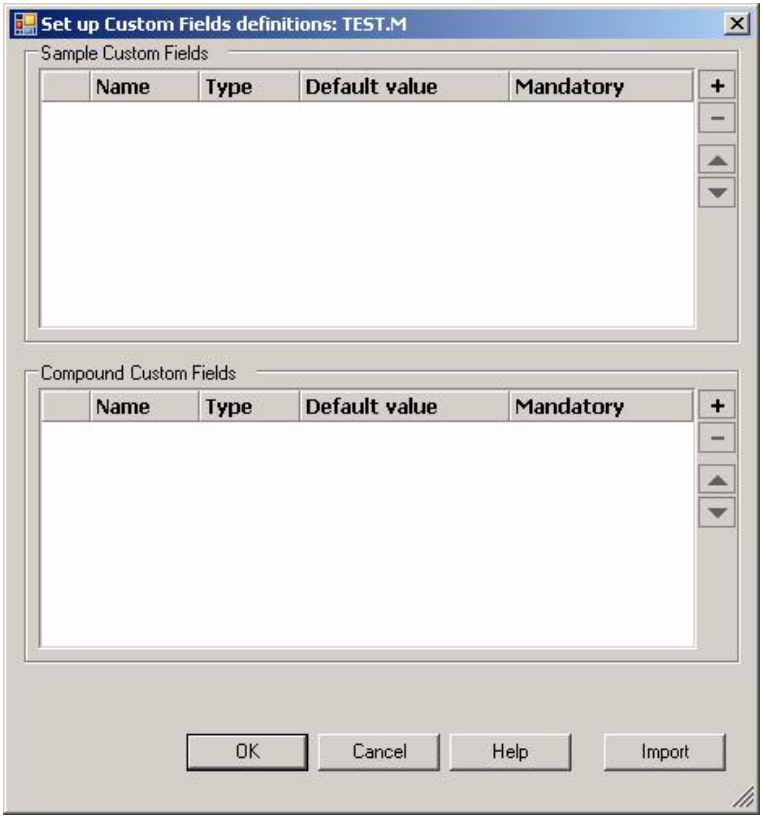


Figure 5 **Set up Custom Fields definitions** dialog

4 Click + to add a new custom field in the according section.

5 Enter a suitable name for the new custom field (for example, Color).

6 Select a suitable data type (for example, TEXT).

7 If appropriate, enter a default value (for example, Blue).

8 If appropriate, select the **Mandatory** check box to ensure that the custom field is always filled.

NOTE For mandatory fields, it may be useful to also provide a default value.

9 If required, click - to delete a selected custom field.

10 If required, adjust the order of the custom fields with the Up and Down buttons.

To import custom fields from an existing method:

1 Make sure the method with the custom fields is available in your local file system.

2 Load the target method (the one where you want to import the custom fields definition).

3 Select **Method > Custom Fields Setup**.

4 Click **Import**. A dialog opens where you can select the source method from the local file system.

5 Click **OK**.

Specifying Custom Field Values

The specific values of the predefined custom fields depend on the actual sequence. Therefore, the values are specified in the sequence table.

To provide sample custom field values:

1 In the **Method and Run Control** view, load the required sequence.

2 Select **Sequence > Sequence Table** to open the sequence table.

3 Click **Custom Fields**.

The **Set up Custom Fields values** dialog opens. The **Sample Custom Fields** tab is active. Each predefined custom field is shown in a separate column. Mandatory custom fields are marked with (*) in front of the field name.

The lines correspond to the lines in the sequence table.

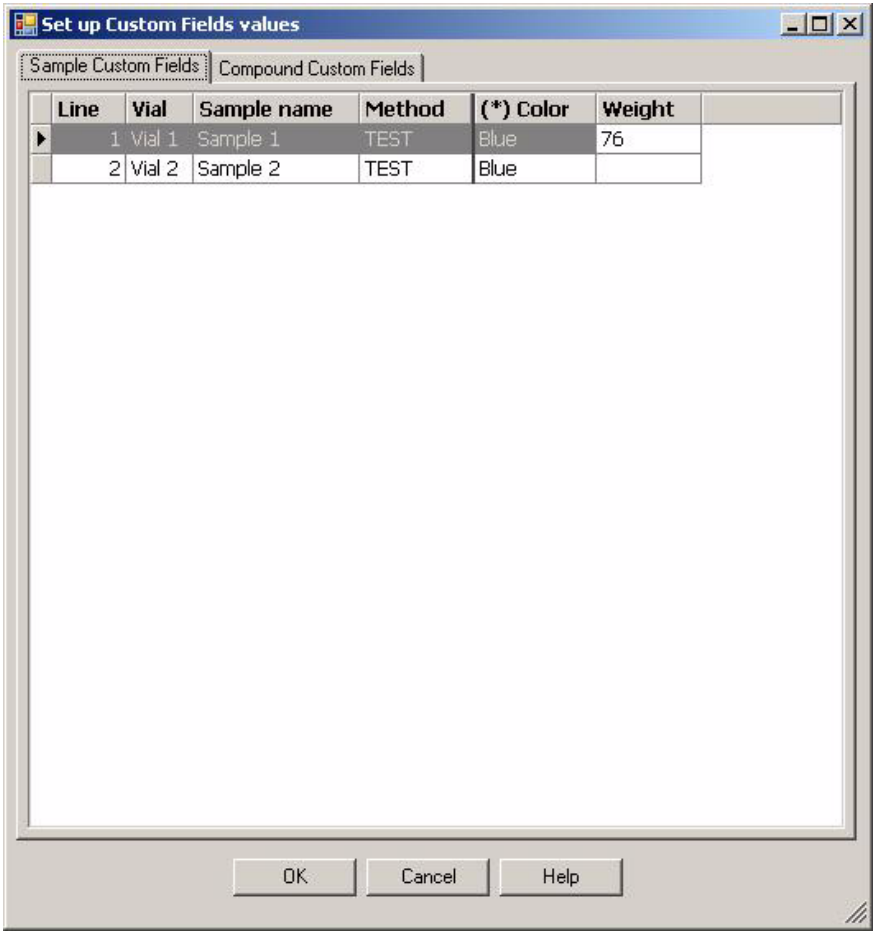


Figure 6 Set up Custom Fields values - Sample Custom Fields

4 Enter the required values for each sample and custom field.

NOTE You can not start a sequence as long as the mandatory fields are not completed.

To provide compound custom field values:

1 Select the **Compound Custom Fields** tab.

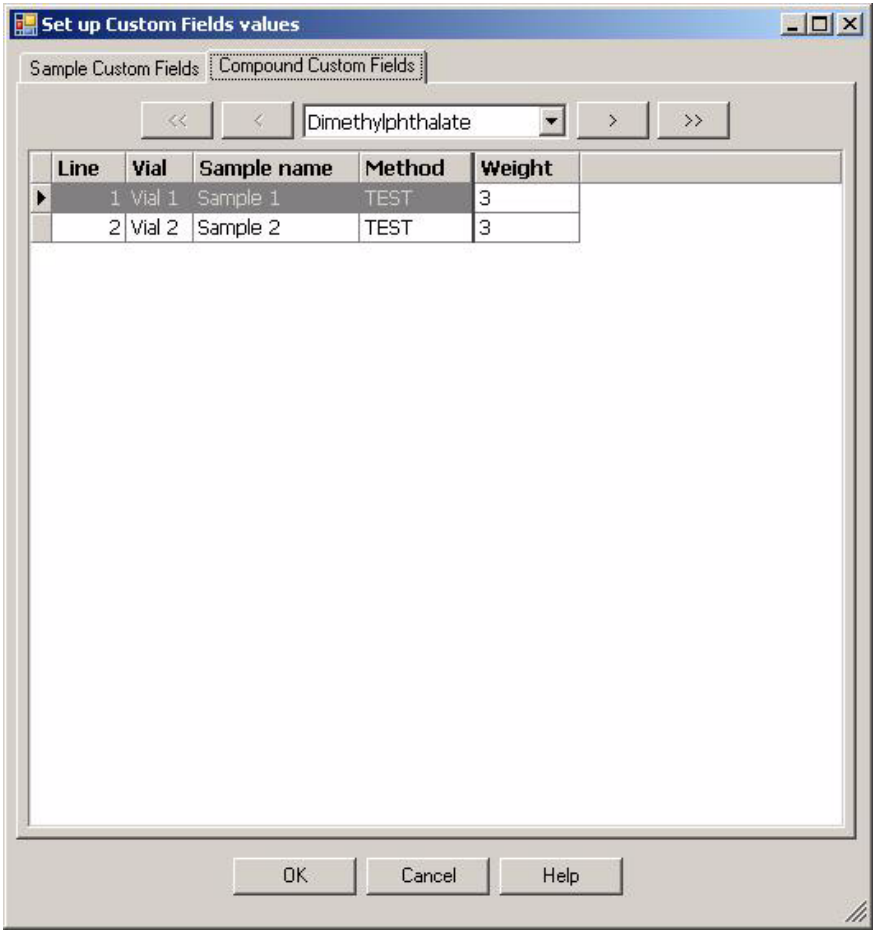


Figure 7 Set up Custom Fields values - Compound Custom Fields

2 Select the required compound from the drop-down list at the top, or click <<, <, >, or >> to navigate to the required compound.

3 Enter the required values for each sample and custom field.

4 Select the other compounds and provide the values accordingly.

5 Click **OK**.

Reporting of Custom Fields

Custom field values are not automatically shown in ChemStation reports. If you want to display the custom fields in your ChemStation reports, you must first adjust the report options.

To display custom fields in ChemStation reports:

1 Select the **Data Analysis** view.

2 Select **Report** > **Specify Report**.

3 Select the check boxes **Add Sample Custom fields to Sample info** and **Add Compound Custom fields.**

4 Click **OK**.

The custom fields and the according values will now be displayed on ChemStation reports.

Reprocessing

It is possible to modify the values of the custom fields during reprocessing. The custom field values are available when editing the Sequence Table in Data Analysis view in preparation for reprocessing in the same way as described in section "Specifying Custom Field Values" on page 75.

After acquisition, only the values the custom fields of a sample can be changed. It is not possible to attach new custom fields to the sample, even if the method used for reprocessing contains other custom fields than the ones employed for acquisition.

Only if **Unique Folder Creation** is switched off, it is possible to change the custom fields attached to a sample. The Sequence Parameters **According to Runtime Checklist** or **Acquisition Only** need to be selected as parts of the method to be run. After adding a method with different custom fields, switch to **Reprocessing Only**, to attach the new fields to the reprocessed samples.

Startup Changes Introduced with B.03.0x, 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. The ChemStation Explorer allows you to navigate to the different ChemStation elements such as **Method and Run Control**, **Data Analysis** and **Report Layout**. 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 15 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.

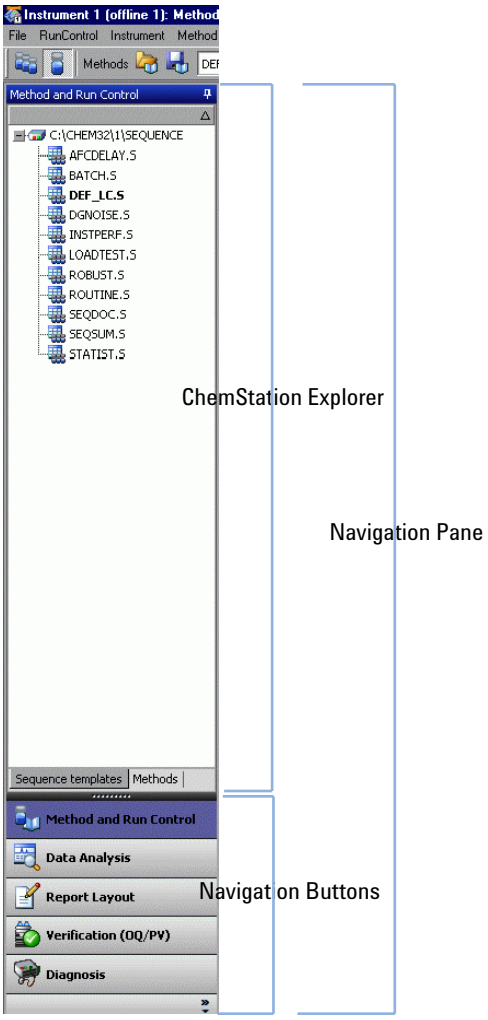


Figure 8 Navigation Pane showing ChemStation Explorer and Navigation Buttons

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.

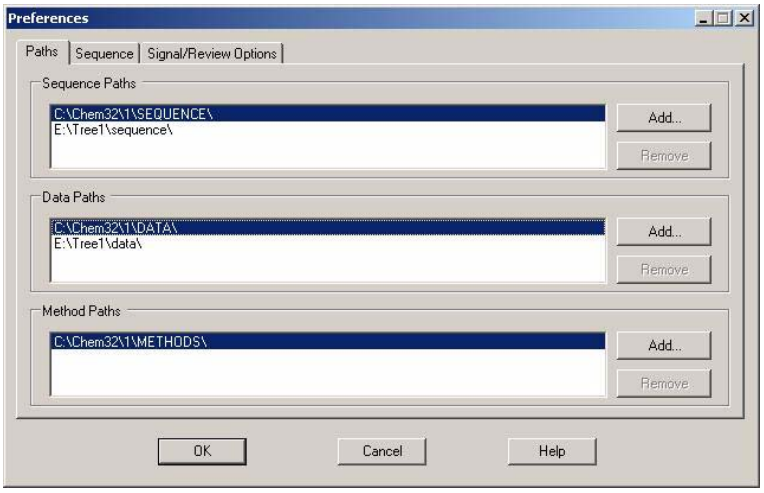


Figure 9 Paths preferences for the ChemStation Explorer

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 **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.

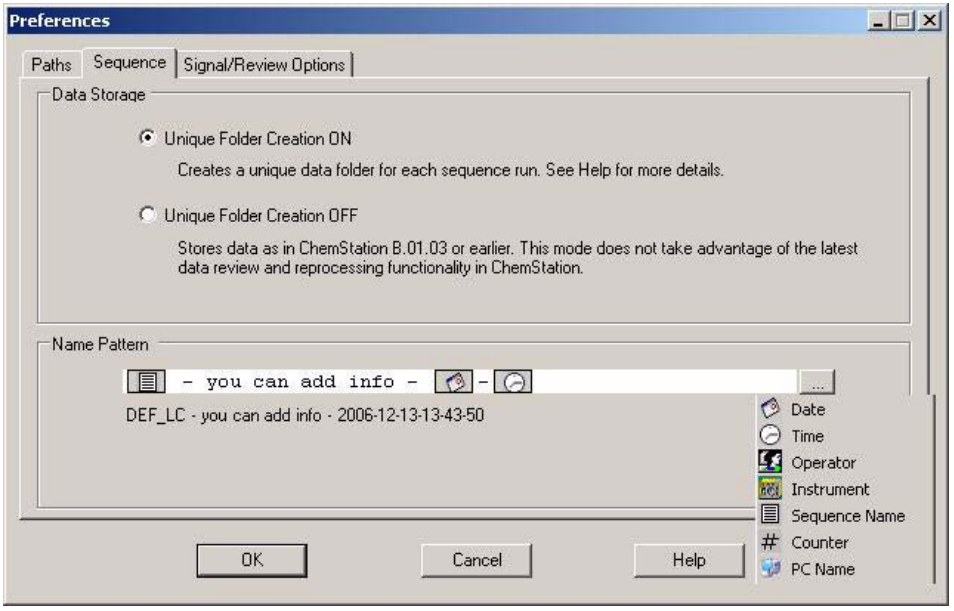


Figure 10 Preferences for sequence naming

The sequence name pattern can contain various sections; 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

Since 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 snapshot.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

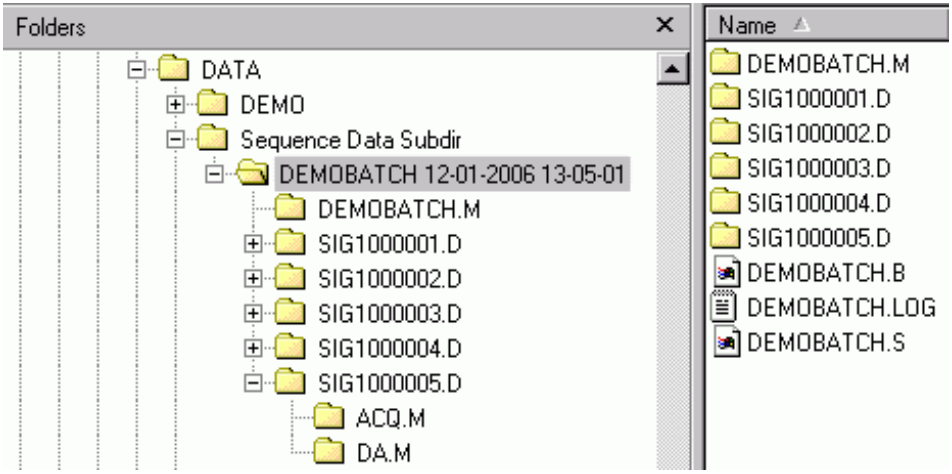


Figure 11 Sequence Data Container Content

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.

With B.04.01 this scheme was enhanced by the following new features:

- Enhanced overlay capabilities in **Data Analysis** view
- Data acquisition into an existing sequence container (**Unique Folder Creation** switched on)
- Storage of manual integration events with the data file
- Usability enhancements for sequence and method handling in Data Analysis

For more details, refer to the manual *Getting Started with New ChemStation Workflow*.

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 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.

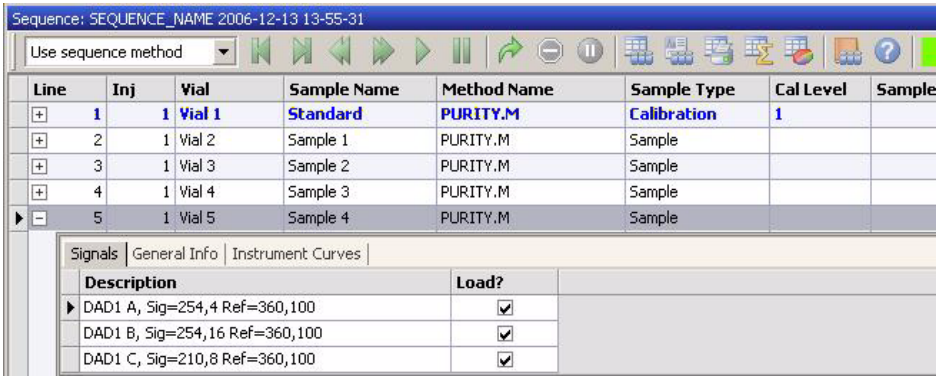


Figure 12 Navigation Table in Data Analysis

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, 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.

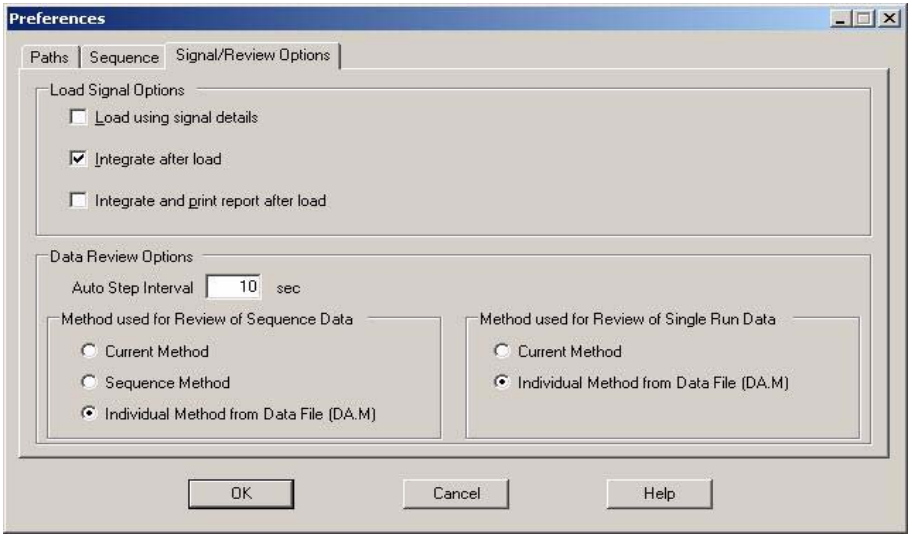


Figure 13 Preferences for Signal options

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 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.

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.

Switching Unique Folder Creation off

The new data organization scheme 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 acquired 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 offers a **Data Storage** section. Here you can choose between **Unique Folder Creation ON** and **Unique Folder Creation OFF** (Figure 14 on page 92). Per default, **Unique Folder Creation ON** is selected. **Unique Folder Creation ON** enables the data storage

concept as outlined above. **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 14 **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 OpenLAB Integration or ChemStore/Security Pack installed.

The enhanced ChemStation user interface as introduced with ChemStation B.02.01 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**.

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 15 **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 file names to fit all information onto the report template.

```
Method and Injection Info Part:

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

Figure 16 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.

File Naming Conventions

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 a file or directory name:

< > : " / \ | @ % * ? ' & blanks (spaces) etc.

Using these characters in file or directory names may cause problems when loading files in ChemStation. In addition, if these characters are used in the installation folder, the reprocessing copy does not start, if the character % is used in the installation folder, some 'Agilent Chemstation B.04.02 SP1' shortcuts do not work properly.

The following rules apply in addition:

Table 16 Restricted characters

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

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

- CON, PRN, AUX, NUL
- COMx (where x is a number from 1 to 9)
- LPT1x (where 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 17 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

Table 17 Maximum Length of ChemStation file names and subdirectories

DataFile/Subdirectory/Path	Max. Input Length	Auto append	Example
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

All ChemStation logbooks report system messages in an extended format and information strings are printed over multiple lines. Certain reports, e.g. Sequence report, may truncate filenames to fit all information onto the report template.

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 18 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 data file can be integrated and used within B.0x.0x, and remains backwards-compatible. Data files acquired with Rev. B.0x.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 17 on page 98). These method parameters are automatically converted to the new B.0x.0x functionality. The method receives a **method modified** flag to reflect the changes. Details regarding this conversion are documented in “Upgrade Impact on Quantification Methods (Relevant for Upgrades from Rev. A.xx.xx only)” on page 115.

Figure 17 Integrator alert

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 152”.

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

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

General Compliance Information for Upgrade Rev. B.04.0x

Overview

After installing 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.

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.04.0x. 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 **IQT Report** 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 as a so-called *reference file*. A modified or corrupted reference file has a different checksum and is thus detected by the **IQT Report** 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.

In addition, the **IQT Report** 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.04.0x of the Agilent ChemStation features the same **Verification View** as 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.04.0x. In order to do so, you must backup them before uninstalling ChemStation A.xx.xx. After uninstalling ChemStation

A.xx.xx, the new revision B.04.0x can be installed. After the installation of B.04.0x has been completed, you can copy the files from your backup directory onto the new ChemStation directory (assuming the default directory was used for installation):

The OQ/PV methods should be copied to:

- C:\CHEM32\X\METHODS\OQPV, were x is the instrument number

The OQ/PV sequences should be copied to:

- C:\CHEM32\X\SEQUENCE\OQPV, were x is the instrument number

NOTE Running the OQ/PV tests is only possible with ChemStation B.04.02 SP1 if using classic LC drivers.

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

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

Impact of new data structure on 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 Microsoft.NET Framework.

Customizing 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.04.02 SP1 unmodified. Please check the online help for more information.

Customizing 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.04.02 SP1 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.04.02 SP1 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.03.0x, B.02.0x, and B.01.0x” on

page 79. **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 paths items.

The following path variables apply when using **Unique Folder Creation** ON in ChemStation revision B.02.01 SR1 and higher:

Table 19 Sequence paths

	Method & RunControl		**Data Analysis**	
	Sequence run	**No sequence run**	**Reprocessing**	**No reprocessing**
_DataPath$	Path to sequence data container [1]	Default data path (_ConfigDataPath$)	Path to sequence data container being reprocessed	Default data path (_ConfigDataPath$)
_DataSeqSubDir$	Empty	Subdirectory of current sequence template	Empty	Empty
_SeqPath$	Path to sequence data container	Path to the current sequence template	Path to the current sequence data container	Path to the currently loaded sequence data container
DaDataPath$	Undefined	Undefined	Path to sequence data container being reprocessed	Path to the currently loaded sequence data container

[1] at sequence startup (before the Pre-Sequence hook is executed) the _DATAPATH$ variable is set as follows: _DATAPATH$ = _DATAPATH$ + _DATASEQSUBDIR$ + <Name of Sequence container> (if path in the Sequence Parameter Dialog is set to the Default Data Path) _DATAPATH$ = TabHdrText$(_Sequence, "SeqParm", "DataDir") + _DATASEQSUBDIR$ + <Name Sequence container> (if path in the Sequence Parameter Dialog is not equal the default data path)

Table 20 Single Run paths

	Method & RunControl	
	Single run	**No run**
_DataPath$	Data directory a current run (=ConfigDataPath$)	Default data directory
_ConfigDataPath$	Data directory a current run	Contains the data directory set in the **Sample Info** dialog; set to _DataPath$ at ChemStation startup
_DataSubDir$	Subdirectory of current run	Subdirectory set in **Sample Info** dialog

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.

The following path variables apply when using **Unique Folder Creation** Off in ChemStation revision B.02.01 SR1 and higher:

Table 21 Path variables when **Unique Folder Creation** OFF

	Method & RunControl		**Data Analysis**	
	Sequence run	**No sequence run**	**Reprocessing**	**No reprocessing**
_DataPath$	Default data path (_ConfigDataPath$)	Default data path (_ConfigDataPath$)	Default data path (_ConfigDataPath$)	Default data path (_ConfigDataPath$)
_DataSeqSubDir$	Subdirectory of current sequence template	Subdirectory of current sequence template	Empty	Empty
_SeqPath$	Path to the current sequence template	Path to the current sequence template	N.A.	Path to the last sequence data container loaded
DaDataPath$	Undefined	Undefined	N.A.	Path to the currently loaded sequence data container

Impact of upgrade from ChemStation A.xx.xx on Macro Solutions

Overview

With the upgrade to ChemStation Rev. B.04.0x, 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 DVD-ROM. 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, per default c:\chem32\Core.

In the user.mac you place commands to load and execute your own macros within the ChemStation. During an upgrade from ChemStation Rev. B.0x.0x to ChemStation Rev. B.04.0x, your own macros are moved to the Chem32_001 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.

If your custom application is not able to open Unicode-based files, a conversion to ANSI is required. Please see “Converting Unicode to ANSI” on page 111.

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:

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

Note: 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 not supported with Chemstation B.04.02. Agilent delivers the option to use XML as data interchange format, as well as ChemStore as Data Management system.

Impact of using RC.NET drivers in LC ChemStat on Macro Solutions.

ChemStation B.04.02 provides a new set of drivers (RC.NET drivers) for most of the 1100/1200 LC instrument modules (see Table 10 on page 68 up to Table 14 on page 71). When these drivers are used a more modern user interface is available (see "New User Interface in LC ChemStation" on page 66). The new architecture of these instrument drivers requires a new way of storing instrument parameters with the method. When using classic drivers as in revisions of ChemStation prior to B.04.02, the instrument parameters are stored in .reg files, e.g. LPMP1.reg for the pump parameters.

When using RC.NET drivers for the 1100/1200 modules, the acquisition parameters are stored in files of type .xml. This change implies changes in macro commands that write and read instrument parameters of a method.

Summary of changes

The new RC.NET drivers still provide a register interface to access e.g. method parameters or status information. The major differences are:

- The register names are different from the ones used by the classic drivers.
- The content of the former module status register has been split into two registers, a status register and a configuration register.
- Most of the header item and table names inside a register are different.
- Some header items have been split into two parts. *Example*: the **StopTime** is now split into a **StopTime_Time** and a **StopTime_Mode**, where **StopTime_Mode** is either **SET** or **NOLIMIT**.
- The injector program of a sampler is no longer part of the method register but resides now in a new **Pretreatment** register.

For compatibility reasons, some of the commonly used commands like `SendModule$` are also available for RC.NET drivers, additionally new RC.NET specific commands can be used.

7 Upgrade Impact on time stamps of reprocessed data and methods on reports

This chapter is relevant for upgrades from Rev. A.xx.xx. only.

When data files or methods from 16-bit ChemStation A.xx.xx are reviewed or reprocessed in 32-bit ChemStation B.0x.0x, time stamps may differ from those displayed in reports from 16-bit ChemStation. It is common industry standard for software applications to store any time stamps in a universal time (UTC). This allows to exchange data between different time zones and still show the correct date and time information in local time.

For the conversion between local time and universal time Microsoft Windows provides specific functions in their API (Application Programming Interface). These Windows functions use the time zone information configured on the indivual PC. All 16-bit programs (e.g. in our case the 16-bit ChemStation rev. A.xx.xx) use the 16-bit Windows API. In the 16-bit environment Windows uses a specific environment variable called TZ to determine the time zone of a PC. If this variable is not set, Windows uses Pacific Standard Time (PST) as the default time zone.

Unfortunately the knowledge about the existence of this variable is not widely spread, so most Windows PCs do not have this variable configured (i.e. the 16-bit Windows API is considering this PC is in the PST time zone). This applies also to 16-bit programs running on a 32-bit Windows operating system. All 32-bit programs (e.g. 32-bit ChemStation rev. B.0x.0x) use the 32-bit Windows API functions. In this environment Windows uses the time zone information configured in the **Control Panel** for any time conversion.

In contrast to the TZ variable, in most cases the time zone for the 32-bit environment is correctly configured, because Windows asks the user for these settings at first startup. Therefore a typical PC (outside of the PST time zone) has a different time zone configured for 16-bit Windows environment than for

the 32-bit environment.As a consequence 32-bit Windows programs interpret any UTC time stamp with a different time zone than what was used for their creation. This leads to a difference in the display that matches the delta between the correct local time zone and PST (which was used by 16-bit Windows environment as the default). As an example, time stamps in CET (Central European Time) time zone would be 9 hours off.

In ChemStation, the following time stamps are of interest: **Injection Time** for a data file, **Last changed** time, and **Last modified** time for a method. When methods and data files that were created with a 16-bit ChemStation are imported to a 32-bit ChemStation, the following issue is observed with these time stamps if the TZ variable had not been specified on the Windows system when using 16-bit ChemStation: The time stamps as shown in 16-bit ChemStation and as shown in 32-bit ChemStation differ by the time difference of the actual time zone and PST.

Examples:

- France (GMT + 1h):
  - Injection time ChemStation A.xx.xx : 11.00
  - Injection time ChemStation B.0x.0x : shift to 20.00 (= 11.00h + 9h)
- China (Peking) (GMT + 8h):
  - Injection time ChemStation A.xx.xx : 11.00
  - Injection time ChemStation B.0x.0x : shift to next day, 03.00 (= 11.00h +16h)

NOTE The ChemStation PLUS applications uses a TZ variable to calculate local time and this is placed on the report. Therefore ChemStation PLUS systems will NOT see the variation in the time stamps.

8 Upgrade Impact on Quantification Methods (Relevant for Upgrades from Rev. A.xx.xx 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.

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 18 on page 118) 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 18 on page 118.

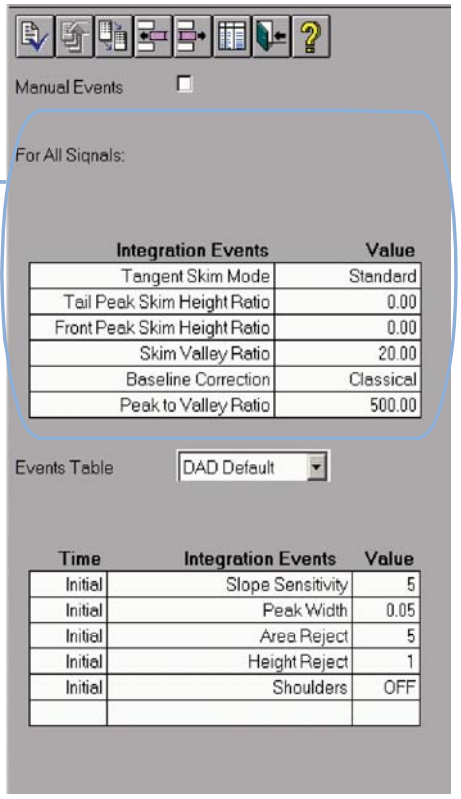


Figure 18 The default values for the new integration events

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 18 on page 118.

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 as 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 22 on page 120 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 ChemStation Rev. B.0x.0x .

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

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

Table 22 Agilent ChemStation Rev. A.xx.xx Integrators

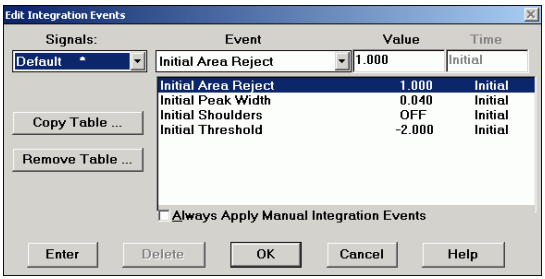
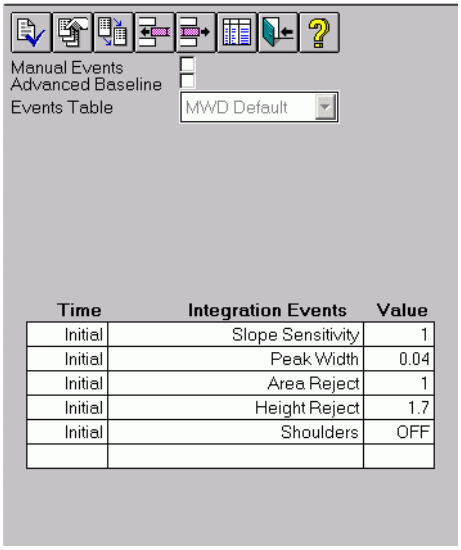
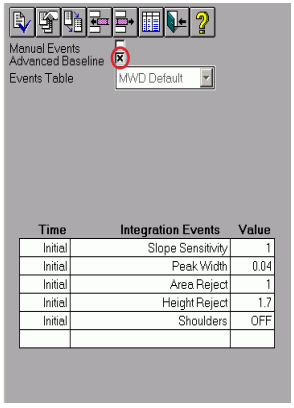
Description	Available since	Example Screen shots
Standard Integrator Please refer to "Upgrade from Standard Integrator" on page 122	Rev. A.02.xx (1993)	

Table 22 Agilent ChemStation Rev. A.xx.xx Integrators

Description	Available since	Example Screen shots
Enhanced Integrator Default integrator Please refer to "Upgrade from Enhanced Integrator" on page 126	Rev. A.04.01 (1996) A.05.01 (1997)	
Enhanced Integratorwith **Advanced Baseline** option Please refer to "Upgrade from Enhanced Integrator with Advanced Baseline" on page 141	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 19 on page 122 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 19 Automatic update of the method

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 23 on page 123).

Uploaded methods using the **Standard Integrator** of Rev. A.xx.xx need to readjust their integration parameters accordingly.

Table 23 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 18 on page 118. 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 20 on page 126).

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.

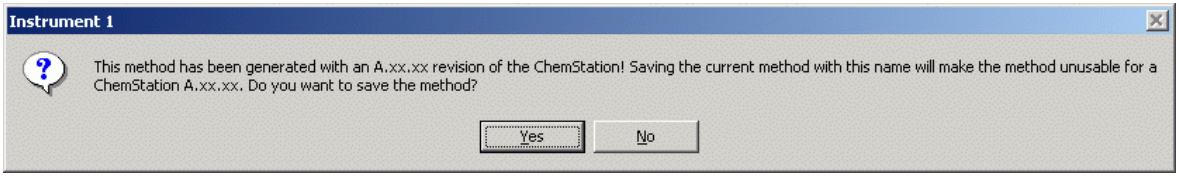


Figure 20 Prompt for changing the name

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 21 on page 127.

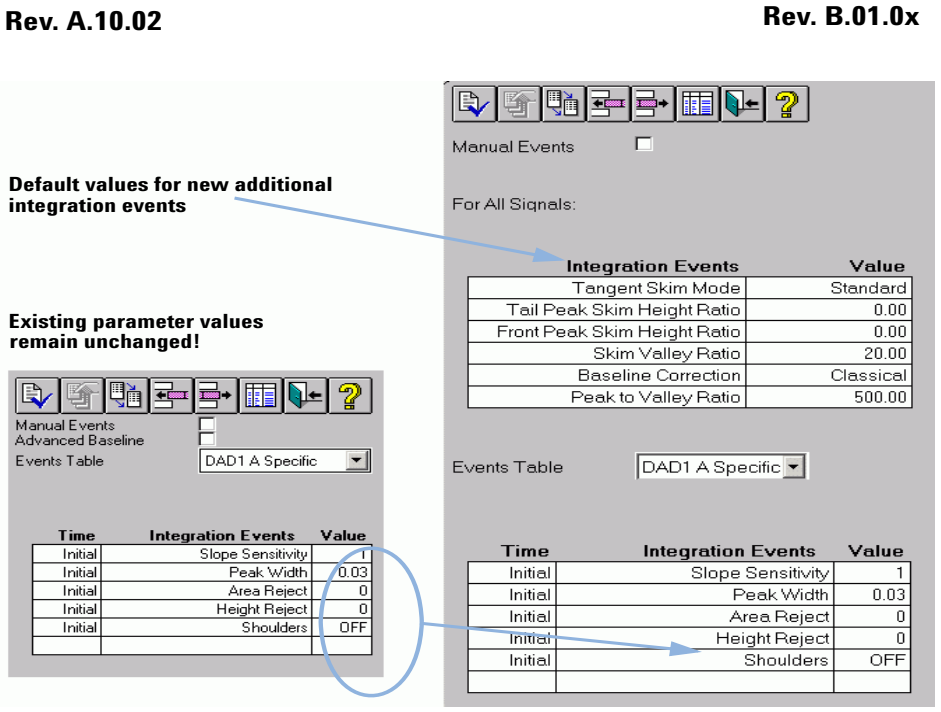


Figure 21 Parameter values in Rev. A.10.02 and in Rev. B.0x.0x

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.

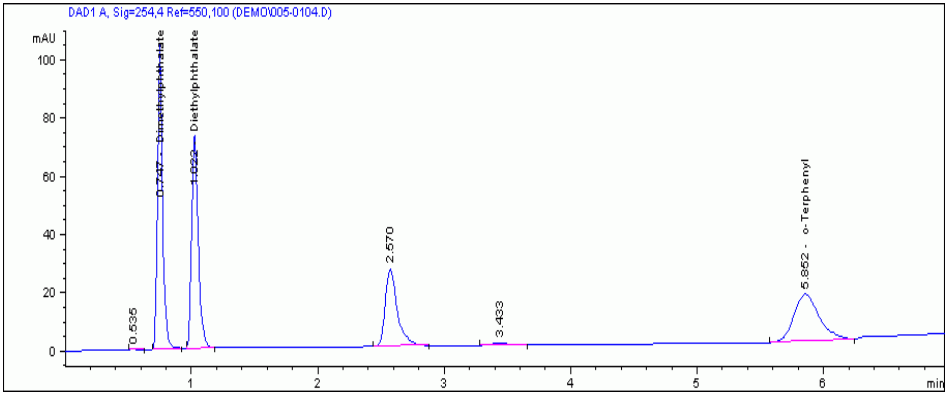


Figure 22 ChemStation A.10.02 Example Chromatogram No 1

Table 24 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:

1 Rev. A.10.02:

The sample file was processed to obtain integration results and an Area% report has been generated. (for the Area% report refer to Figure 34 on page 161 in the Appendix).

2 Rev. B.01.01:

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 35 on page 162 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 affected.

Table 25 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 25 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.

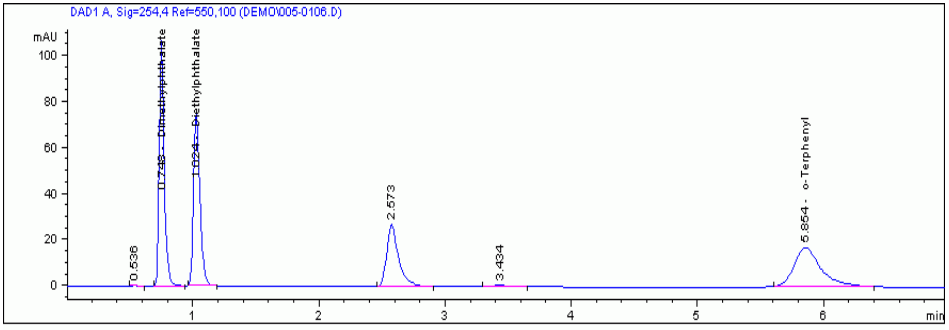


Figure 23 ChemStation A.10.02 Example Chromatogram No 2: Sample File

Table 26 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:

1 Rev. A.10.02

A three level calibration table was created. The sample file was processed to obtain results and an ESTD report has been generated. (see Figure 36 on page 163 in the Appendix).

2 Rev. B.01.01

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 37 on page 164 in the Appendix).

Result Comparison:

Comparison of reported amounts based on calibrated peaks shows some differences in the amount results (see Table 28 on page 133.).

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 27 on page 133. 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 27 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 28 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	3.21565412 0	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 24 on page 134 and Figure 25 on page 134. The system reports different areas for peak on either side of the valley Table 29 on page 135. 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.

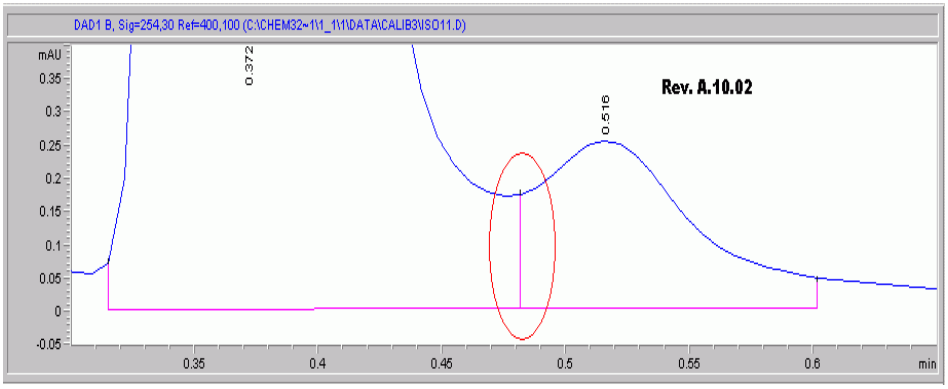


Figure 24 ChemStation A.10.02 Example Chromatogram No 3

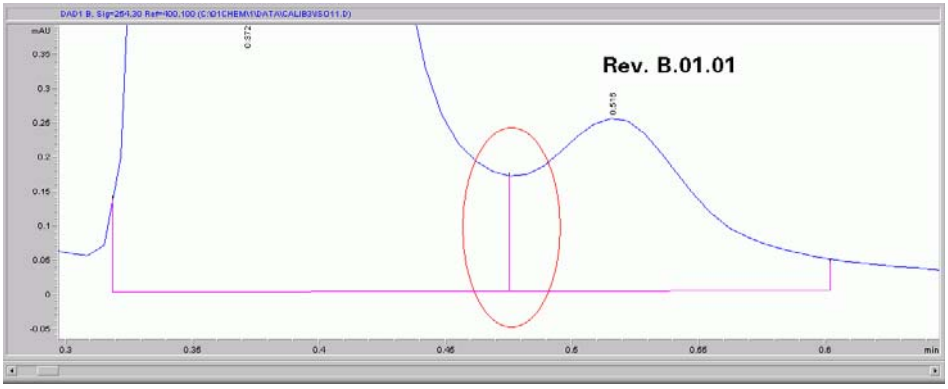


Figure 25 ChemStation B.01.01 Example Chromatogram No 3

Table 29 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 30 on page 137.

Figure 26 ChemStation A.10.02: Example Chromatogram 4

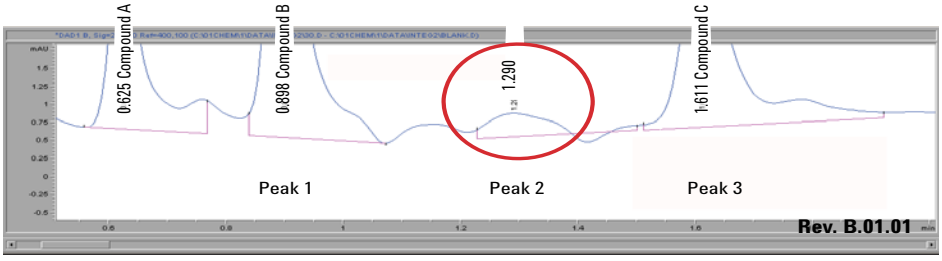


Figure 27 ChemStation B.01.01: Example Chromatogram 4

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 26 on page 136 and Figure 27 on page 136). 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 30 on page 137, Table 31 on page 137 and Table 32 on page 137, 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 30 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	24.046278 00	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 31 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	0.838035345 0	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 32 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	1.072104931 0	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 yield 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 28 on page 141) to continue. The method is updated automatically.

Figure 28 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 29 on page 142).

NOTE

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

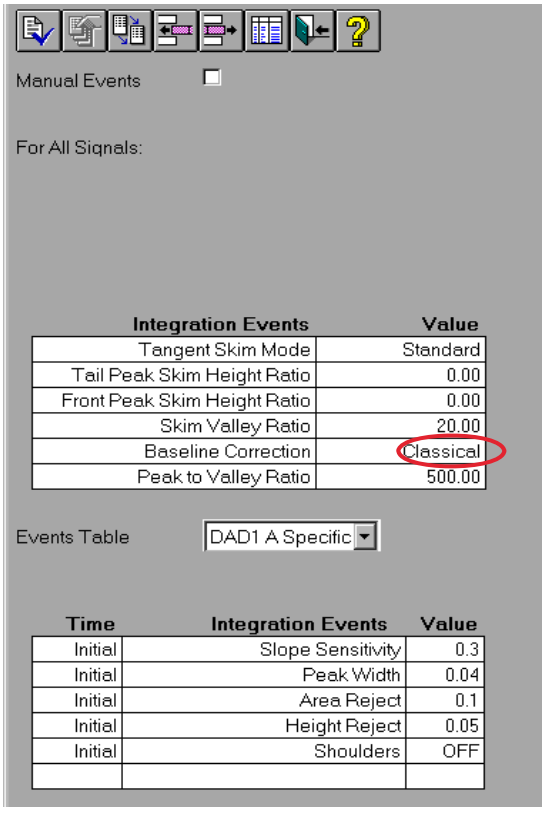


Figure 29 Example screen shot Chem32 Integrator

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 29 on page 142. 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

You need to upload ChemStation Rev. A.xx.xx data for reprocessing or exchanging data between systems 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.

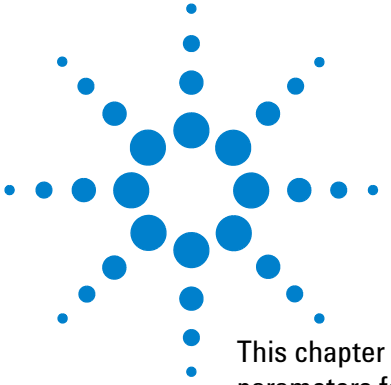
In the case of an audit situation, where you need to restore or replay your results for old Rev. A.xx.xx data files, it might be necessary to reprocess the old data files. The Chem32 integrator in Rev. B.0x.0x yields different integration results. However, the integrator allows you to specify integration 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 Upgrade Impact on Quantification Methods (Relevant for Upgrades from Rev. A.xx.xx only)

Upgrade from Enhanced Integrator with Advanced Baseline



9
Upgrade Impact on LC Methods

This chapter outlines the differences between storage of acquisition parameters for LC ChemStation when using classic drivers or RC.NET drivers, respectively.

Technical Background

ChemStation B.04.02 provides a new set of drivers (RC.NET drivers) for most of the 1100/1200 LC instrument modules (see Table 10 on page 68 up to Table 14 on page 71). When these drivers are used a more modern user interface is available (see "New User Interface in LC ChemStation" on page 66.).

The new architecture of these instrument drivers requires a new way of storing instrument parameters with the method. When using classic drivers as in ChemStation revision B.04.01 and prior, the instrument parameters are stored in .reg files, e.g. LPMP1.reg for the pump parameters. When using RC.NET drivers for the 1100/1200 modules, the acquisition parameters are stored in files of type .xml. This change in the storage of instrument parameters requires a migration of existing methods.

Method Migration

Method migration will be run automatically by the ChemStation when loading a method based on classic drivers into an LC ChemStation using RC.NET drivers.

The acquisition parameters stored in the .reg files are written into corresponding .xml files for the currently configured modules. The .reg files are not deleted, but renamed to files called .reg.bak.

NOTE There is no migration available for methods that were created when using RC.NET drivers. Such methods cannot be used in an instrument controlled by classic drivers. Also after migration, the method can no longer be loaded in the classic instrument.

10 Spectra/Purity Options using ChemStation Rev. B.04.0x (Relevant for Upgrades from Rev. A.xx.xx 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 no longer available.

Introduction to 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)

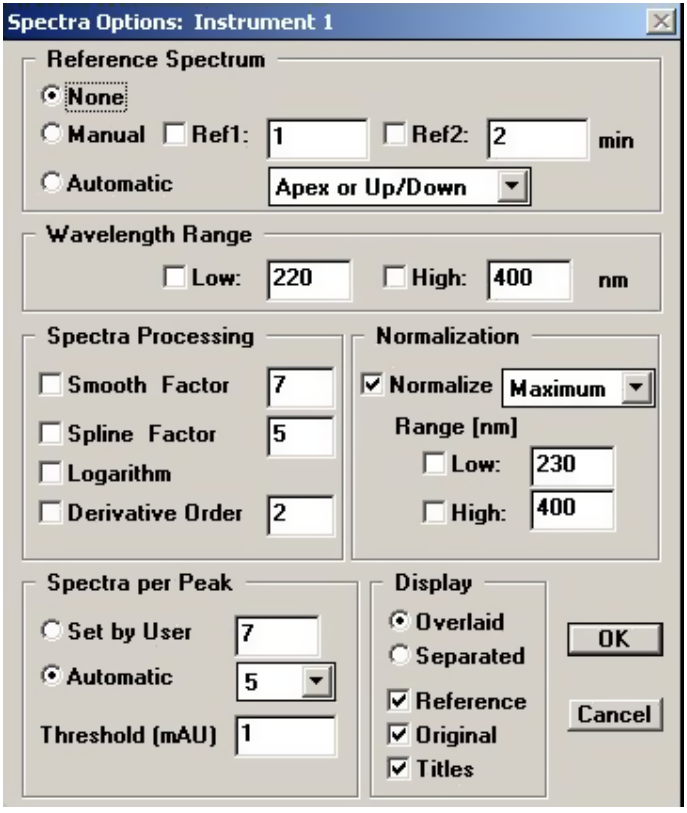


Figure 30 "old" spectra/purity settings (since Rev. A.04.01)

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

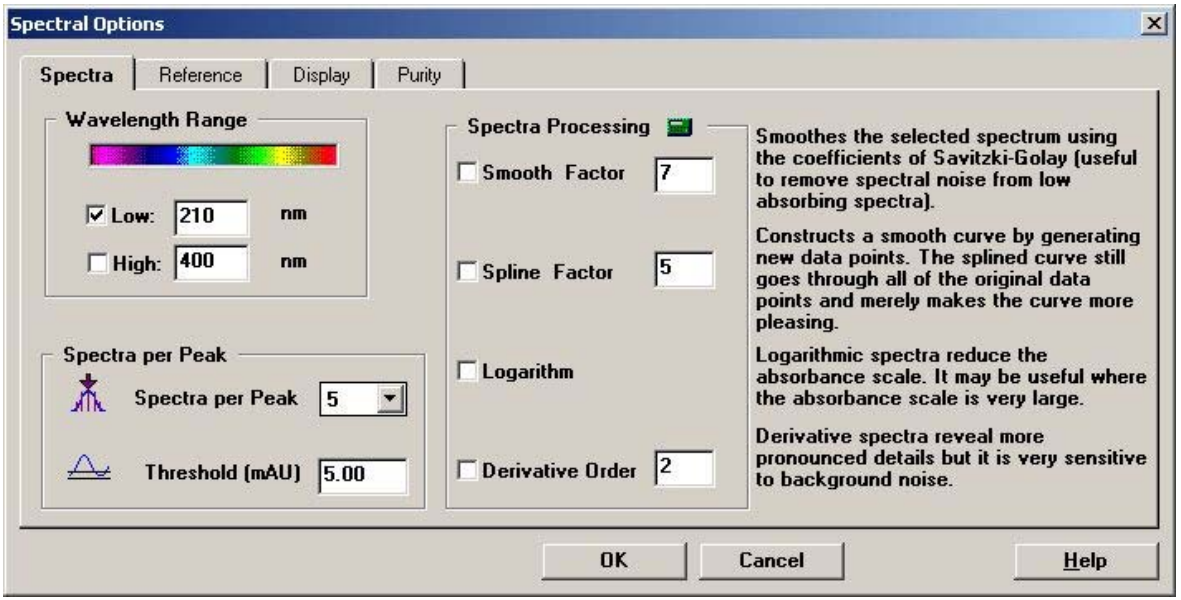


Figure 31 “new” spectra/purity settings (since Rev. A.04.02)

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.

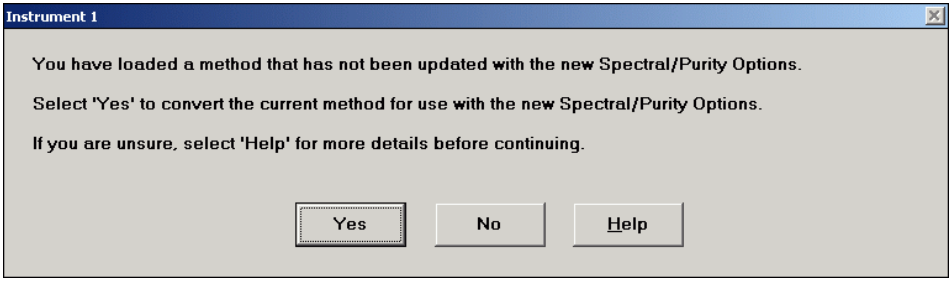


Figure 32 Rev. A.04.02 and higher: choosing spectra/peak purity settings

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 33 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 different: 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 tabs of the **Spectral Options** menu item within the Data Analysis item **Spectra**.

Table 33 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.
Wavelength Range	Parameter to define the Wavelength Range for Signal Display. Parameters are defined separately for either spectra or purity display	Parameter to define the Wavelength Range for Signal Display. Same parameters used for both spectra and purity display	

Table 33 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
Spectra processing	Allow processing a spectrum from a data file before display. • Smooth Factor • Spline Factor • Logarithm • Derivative Order Parameters are defined separately for either spectra or 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 either spectra or 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 defined separately for both spectra and purity windows	Same display options are 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 34 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 asks 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
Spectra per peak	Parameter to define display options	All purity-related graphical options are displayed in the purity windows	

Table 34 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
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.

11
Appendix

The appendix offers Example Chromatograms produced with different versions.

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 "Upgrade from Enhanced Integrator" on page 126.

Example chromatogram No. 1

1 Rev. A.10.02:

The sample file was processed to obtain integration results and an Area% report was generated (see Figure 34 on page 161).

2 Rev. B.01.01:

The method uploaded in Rev. B.01.01 ChemStation was used to reprocess the same sample file. An Area% report was generated (see Figure 35 on page 162).

Example chromatogram No. 2

1 Rev. A.10.02

A three level calibration table was created. The sample file was processed to obtain results and an ESTD report was generated (see Figure 36 on page 163).

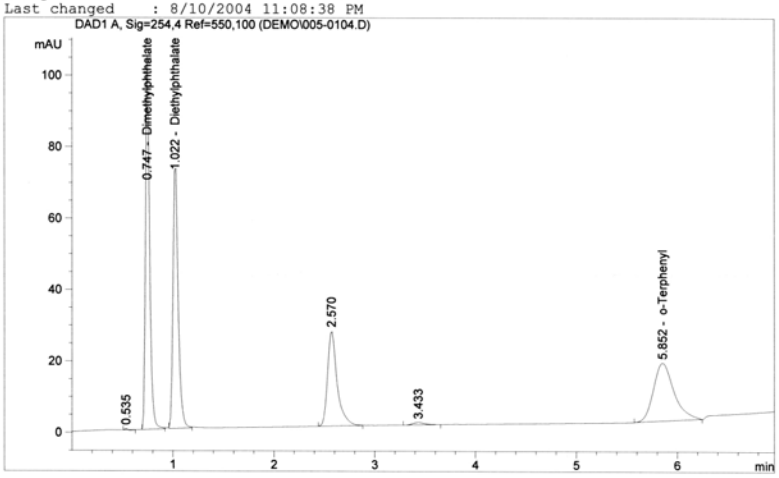
2 Rev. B.01.01

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 37 on page 164).

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
```



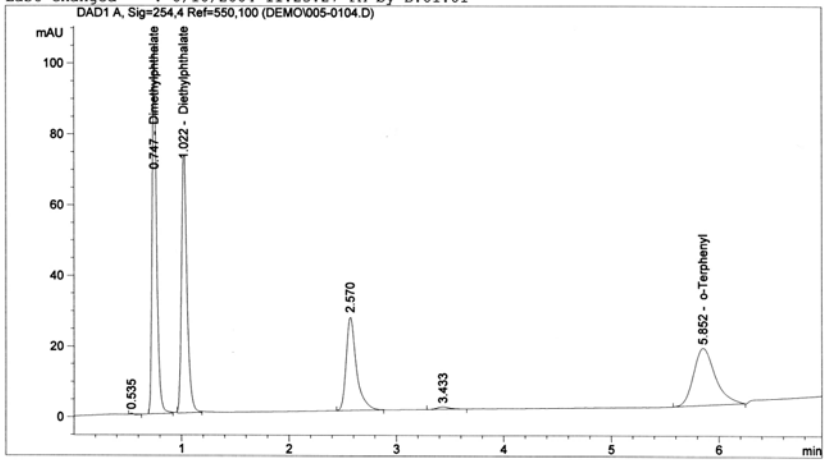

```
                          Area Percent Report

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 34 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
```



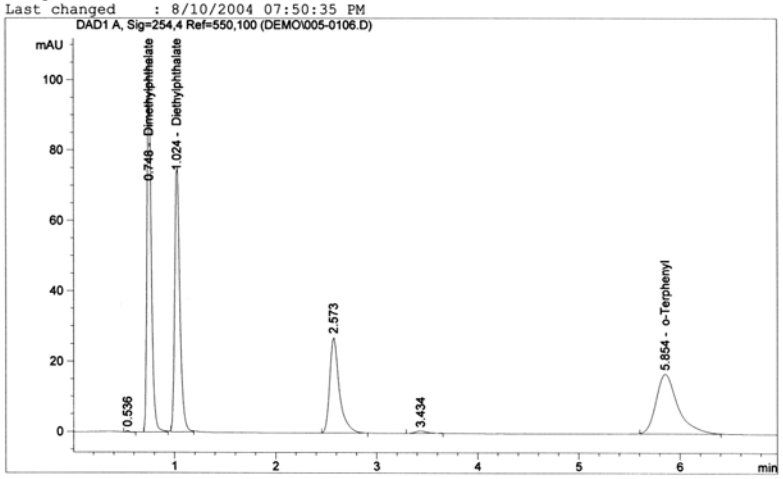

```
================================================================================
                              Area Percent Report
================================================================================

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 35 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 [min]	Type	Area [mAU*s]	Amt/Area	Amount [mg/l]	Grp	Name
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 ***

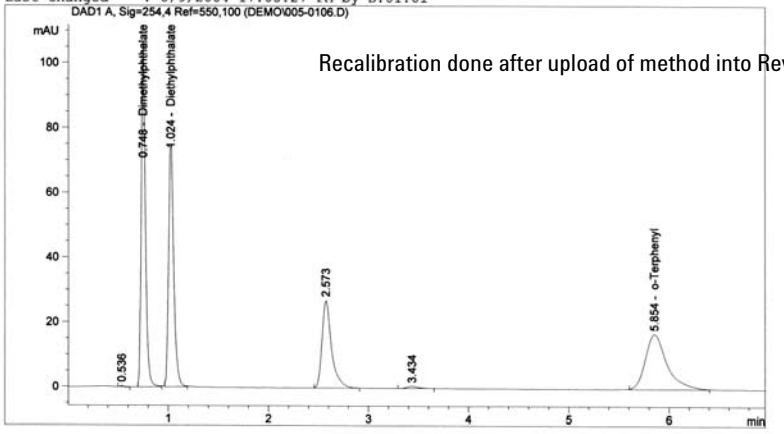
Instrument 1 8/10/2004 11:08:17 PM Page 1 of 1

Figure 36 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		



Recalibration done after upload of method into Rev. 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 [min]	Type	Area [mAU*s]	Amt/Area	Amount [mg/l]	Grp	Name
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 ***

Instrument 1 8/10/2004 11:26:52 PM B.01.01 Page 1 of 1

Figure 37 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.04.02 SP1.

This handbook describes the necessary steps to perform an upgrade to Rev. B.04.02 SP1 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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