Chrom&Spec

Chromatography Control Center

Manual

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Part I

Introduction

1 Introduction

1.1 General information

1.1.1 About the program

Chrom&Spec, version 3.4 is the name of the data acquisition and control software for PC-controlled chromatographic systems consisting of instruments from **Ampersand, Ltd.** and a number of other instrument manufactures. It was designed to operate under Windows XP, Windows Vista, Windows 7, Windows 8 and Windows 10. **FDA 21 CFR Part 11** 54 functions are available only if NTFS file system is used.

The operating software meets all the requirements you could place today on a modern integration and control software.

The Chrom&Spec is able to operate with several independent chromatographic instruments simultaneously. Great advantage of the software is the capability to acquire and process **Multichannel chromatograms** 146 (i.e. data from multi-detector system or multi-channel Diode Array Detector).

Characteristic features of the software are simple and intuitive user interface, top scientific level of solution of all data processing tasks and attractive price. Chrom&Spec was designed to bring the users the maximal level of automation of all routine works in chromatography analysis.

See also:

Hardware requirements 19

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Registration 20

1.1.2 Software basics

The "Chrom&Spec" program consists of data processing and system control software that provides a complete set of data processing tasks. These tasks include:

analog-to-digital conversion 19,

equipment control 77,

noise smoothing 133,

integration 159,

peak identification 166,

quantification 201,

reporting 318

The software is designed with **Good Laboratory Practice** 43 and **Good Automated Laboratory Practice** standards in mind.

It provides work with **sample queues** 237, **batch reprocessing** 271, **password protection** 45, and performs operations with **multichannel chromatograms** 146 and **spectral operations**.

1.1.3 Analog-to-digital conversion

During the analysis, the detector outputs an analog signal. Analog-to-Digital Converter (ADC) is used to convert analog signal of the detector into digital form that can be handled by the computer.

A24 and **E24** ADC devices can measure data from up to four detectors or channels.

Modern detectors usually contain a build-in ADC, are equipped with digital (e.g. RS-232, RS-422/485, USB or Ethernet) interface, and can be connected to the computer directly. In this case detector uses digital interface both to send chromatographic data, auxiliary information and current parameters to the computer, and to receive commands from the computer.

See also:

Equipment control 77
Software basics 18
Interfaces 107

1.1.4 Hardware and software requirements

For comfort work with Chrom&Spec software the following minimal hardware configuration is recommended:

Computer	x86-compatible with 1 GHz or higher
Operating system	Windows™ XP, Windows™ Vista, Windows™ 7, Windows 8, Windows 10 (in all cases both 32 and 64 bit versions) NTFS file system is required to activate **21 CFR Part 11** 54 capabilities (electronic signature and data protection features)
Free space on hard disk	50 Mb for program files 100 Mb minimum for data files (depends on user's requirements for chromatogram database)
Working memory RAM	512 Mb for Windows XP, and 1 Gb for Windows Vista, Windows 7, Windows 8 and Windows 10
Graphics resolution	1024x768 at 16-bit color depth, or better
Printer	any printer supported by the operating system
Mouse	mouse or any Windows-compatible pointing device
CD-ROM	CD or DVD drive of any type to install software

1.1.5 Demo version

If the “Chrom&Spec” is installed on a PC without security dongle, this software can be used as a demo version which is restricted to the display and recalculation of already recorded chromatograms.

Security dongle activates only Basic features of the ***Chrom&Spec*** software. Such enhanced features as factor analysis 451 or spectral analysis are optional and can be activated by entering a special activation key 20 in the "User info" window 20 .

1.1.5.1 Activation key

Optional software features can be activated for the current security dongle specifing the special activation code (*activation key*) in the "User Information" window 20.

The following options are avalable in the current version:

Spectral operations

Factor analysis 451

Calculated channels 152

User-defined formulas 288

Advanced reports 341

TimeBase (number of simultaneously running chromatograms)

See also:

Security dongle

1.1.5.2 User Information window

If the program is started for the first time, the "***User information***" window appears where **Company**, **Division** and **Name of responsible person** can be entered.

"Company" field should be filled in to skip this window for the next time.

Note: "***User Information***" window can be opened by [Ctrl]+[F9] keyboard combination or by **Help/ About/*<Registration>*** menu item.

Activation key 20 a sequence of bytes that is used to activate optional features of the software

<Update from file> load a new activation key from file

1.1.6 Registration

Please return us your Ampersand, Ltd. Registration card as soon as possible. Only registered users will get updated program versions at a special price, and free technical support by phone or E-mail.

Phone/Fax: +7 (499) 322-99-61
Mail: 123098, Moscow, Academik Kurchatov sq. 2, Ampersand
E-mail: support@ampersand.ru
Contact person: Yuri Kalambet, General Director
Internet site: http://www.chromandspec.com

1.2 Installation

This section of the documentation helps you install and uninstall the Chrom&Spec software.

In this section:

1.2.1 Installation of the software

"Chrom&Spec" software is supplied on CD-ROM

To install the software follow these steps:

1. Switch on PC and start operating system.
2. Insert installation CD into CD drive.
3. Select **<Start>** and Run. Find the file setup.exe on the CD and click on **<OK>**.
4. Follow the setup program instructions.
5. Follow the instructions given in the setup program.
6. During installation the user is prompted to specify two folders:
   Folder for software
   - the folder which stores the software executable files and other binary files which must not change. In most cases there are no need to change the folder which is proposed be default. This folder is referred to as **installation folder** further in this documentation.
   Folder for storing your data
   - the folder which stores all user settings and chromatographic data (chromatograms systems, methods, reports, etc). User can change the proposed default folder to another location which is more convenient for user. This folder is referred to as **installation data folder** further in this documentation.

Software shortcuts are created in the **Windows *start menu*** and on the desktop.

The following folders are created in the **installation data folder**:

Data	Folder for storage of chromatogram files (***.chw**) and batch reprocessing files (***.bar**) with several examples.
Methods	Folder for storage of data processing method files (***.mtw**) with several examples.
Systems	Folder for storage of system files (***.smt**) and sample queue files (***.que**)
Reports	Default folder for storage of report files and graphic files
Devices	Special folder for service usage
Accounts	Folder for storage of user accounts data. This folder is locked in **FDA 21 CFR part 11 mode** 54.
Log	Folder for storage of exception files.(***.exc**), history files (***.hst**), and log files (***.log**).
FLog	Folder for storage of audit trails files. This folder is locked in **FDA 21 CFR part 11 mode** 54.

See also:

File types 38

1.2.2 Removing the software

To uninstall the software follow these steps:

1. Open **Control panel** from **Windows *start menu.***
2. Locate and open **Add or remove program** (Windows XP) or **Uninstall program** (Windows Vista, 7, 8, 10).
3. Locate and select Chrom&Spec in the list of installed programs and click on **<Uninstall>**. This operation removes program files from **installation folder** and shortcuts from **Windows *start menu*** and on the desktop. This operation does not remove chromatography data and configuration files from **installation data folder**. If user do not need these files he should remove files and **installation data folder** manually.

1.3 Starting/closing the program...

1.3.1 Start the program

Start the program

Double-click the ***Chrom&Spec*** icon or the **Chrom&Spec.exe** file to start the "Chrom&Spec" program. The "Chrom&Spec**"** login window appears.

Enter **User name** and **Password**, and click the ***<LogIn>*** button.

Note: when the Chrom&Spec software is started for the first time, "***Add user***" window is opened. Enter *Short* and *Full name* of the user, and define then confirm a *password*, and then click ***<Add>*** button. New user with **Administrator** access level will be created in the List of users. Please, remember the password and short user name that are needed to log in the program.

See also:

Close the program 23

Security options 50

1.3.2 Close the program

(Chrom&Spec **/ File / Exit)**

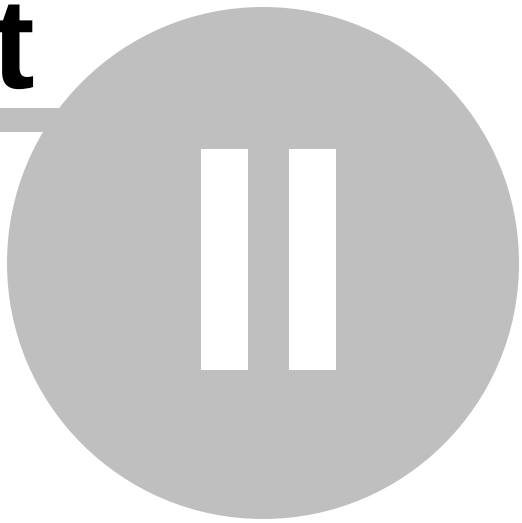
Exit the "Chrom&Spec" program.

The program is also quit by clicking on  in the upper right part of the main window or [Alt]+[F4] key combination.

See also:

Start the 22 Chrom&Spec

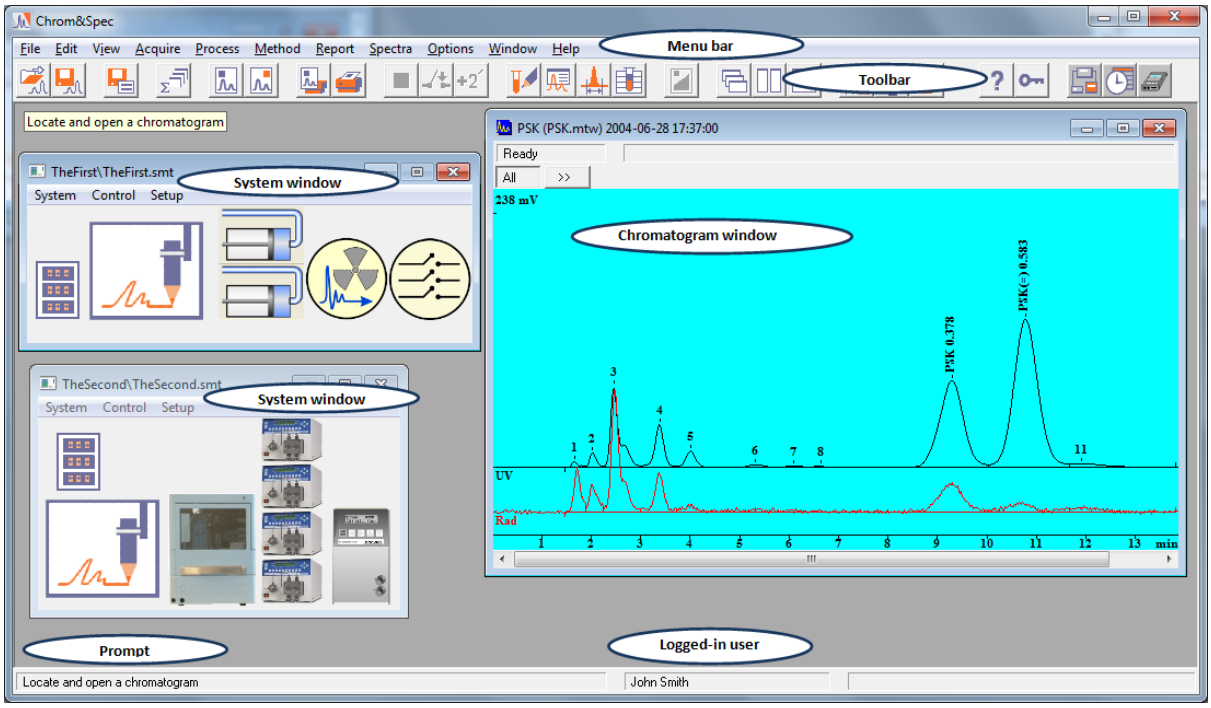
Part



2 Overview

2.1 Main window elements

The main window is the center of the “Chrom&Spec” software. Its elements are the menu bar, the toolbar and the status bar indicating prompts and logged-in user.



See also:

Main window menus 25

Toolbar 36

2.1.1 Menus

2.1.1.1 Main window menus

File 26	Handling of files, data import/export, printing.
Edit 29	Copy to clipboard.
Table 30	Functions for components table (replaces **Edit** menu if **Components table** is opened)
View 30	Functions for chromatogram display.
Acquire 30	General function of data acquisition manual control.
Process 31	Reprocessing functions.
Method 32	Data acquisition and evaluation parameters.

Report 32	Report parameters
Spectra 34	Spectral operations (available for multi-channel chromatograms only)
Options 34	General settings, security options.
Window 35	Tiling, opening and closing of windows.
Help 35	Program-specific online help.

2.1.1.1.1 File menu

New

Method... 123	Create a new method based on an existing method file (*.mtw).
System... 93	Create a new system file (*.smt) using the system wizard.

Open

Chromatogram... 207	Open an existing chromatogram file (*.chw).
Method... 123	Open an existing method file (*.mtw).
Batch reprocessing... 273	Open an existing batch reprocessing file (*.bar).
Last batch... 273	Open the last opened batch reprocessing file (*.bar).
Sample queue... 237	Open an existing or create a new sample queue file (*.que).
System... 79	Open an existing system file (*.smt).

Save

Chromatogram 210	Save the selected chromatogram.
Method 123	Save the modified method or extract and save the method from the chromatogram.
Save Method As... 123	Save the method in the file under the different name. Method can be extracted from the chromatogram.

Import from

AIA file... 27	Import chromatograms stored in the AIA (Analytical Instrument Association) format.
AIA file (raw data only)... 27	Import raw data stored in the AIA (Analytical Instrument Association) format and process them by the current method.
XML file... 28	Import chromatograms and methods stored in the XML (eXtended HTML) format.
Text file (raw data only)... 28	Import chromatographic raw data from a text file (ASCII format).
Other chromatogram types... 211	Import chromatograms recorded with other software versions.

Export to

AIA file... 212	Export chromatograms in the AIA (Analytical Instrument Association) format.
XML file... 29	Export chromatographic raw data to the XML file (extended HTML format)
Text file (raw data only)... 29	Export chromatographic raw data to the text file (ASCII format).

Close 211	Close selected chromatogram window.
Delete 211	Delete selected chromatogram.
Print... 233	Print report of selected chromatogram.

Preview 234	Display report print preview.
Printer setup 234	Change printer setup.
Exit 29	Terminate program.

See also:

Main window menus 25

2.1.1.1.1.1 Import

(*Main menu* File / Import from / AIA file...)

Import data from **AIA** (Analytical Instrument Association) format.

AIA is a universal format specially designed for data exchange between analytical programs. It may include processing options (such as calibration data) and processing results. So it can be imported to Chrom&Spec directly without specifying processing **method** (unlike XML and Raw data).

This import option reads as much as possible of the data and processing results supplied by another software.

See Import from AIA file (raw data only) 27 for alternative way for importing **AIA** format.

AIA files have ***.cdf** extention

See also:

Chromatogram import 211

(*Main menu* File / Import from / AIA file (raw data only)...)

Import data from **AIA** (Analytical Instrument Association) format and process them by the current method.

AIA is a universal format specially designed for data exchange between analytical programs. It may include processing options (such as calibration data) and processing results.

Still in most cases it is more convenient to specify the data processing options withing "Chrom&Spec" software, not the external software. This is done by configuring appropriate processing method 122.

This import option reads only raw data and sample description data from **AIA** file. After reading the "Chrom&Spec" software processes the data with preliminary configured **method** 122. To use this option user needs first to open an appropriate empty processing method 122.

See Import from AIA file 27 for alternative way for importing **AIA** format.

AIA files have ***.cdf** extention

See also:
Chromatogram import 211

(*Main menu* File / Import from / XML file...)

Import data from XML format

XML is a hypertext language (eXtended HTML). XML files also contain analytical channels only. Although it includes peak integration results and some processing results, it still requires empty processing Method 122 or Chromatogram 207 to be opened. In the later case existing data are replaced with data from XML file.

XML files have ***.xml** extention and are used for data export to text editors like MS Word or other applications.

See also:
Chromatogram import 211

(*Main menu* File / Import from / Text file (raw data only)...)

Import data from plain text files, containing raw data.

Raw data is an ASCII text format that contain analytical channels only. It does not include data processing settings, so it can be imported to Chrom&Spec only if empty processing Method 122 has been opened.

This command allows importing text data which were previously exported with export raw data to text file 29 operation.

See also:
Chromatogram import 211
Export raw data to text file 29

2.1.1.1.1.2 Export

(File / Export to / AIA file...)

Export the current chromatogram to AIA format.
AIA files contain both raw data and processing data, so they can be used for data exchange between various analytical programs without any losses.

(Main menu* File / Export to / XML file... *)

Export data from chromatogram to XML format

XML is a hypertext language (eXtended HTML). XML files contain analytical channels and include peak integration results and some processing results. However, it still requires empty processing Method 122 or Chromatogram 207 to be opened when importing.

XML files have ***.xml** extention and are used for data export to text editors like MS Word or other applications.

See also:

Chromatogram export 212

(File / Export to / Text file (raw data only)...)

Export raw data from chromatogram to plain text file, in raw data format.

Raw data is an ASCII text format that contain analytical channels only. It does not include processing results or processing Method 122. Format of exported data is defined in the "Export raw data" window

Raw data files have ***.txt** extention and are used for data export to electronic data sheets like Excel.

See also:

Chromatogram export 212

"Export raw data" window

2.1.1.1.1.3 Exit

This option terminates the program. If some chromatograms have not been saved yet, the software reminds about and offers to save them.
The standard combination [Alt]+[F4] does the same.

2.1.1.1.2 Edit menu

Copy to clipboard This option allows to copy a chromatogram plot from the active window to the clipboard so that it is available for other Windows applications, such as Word, Excel, etc.

See also:

Main window menus 25

2.1.1.1.3 Table menu

The **Table menu** replaces the **Edit menu** when the **Components table** 171 is active.

Add component	Add a new component (new row) to the **Components table** 171.
Delete component	Delete the current component from the **Components table** 171.
Clear table	Clear entire **Components table** 171.

See also:

Main window menus 25

2.1.1.1.4 View menu

Appearance 216	Change chromatogram appearance.
X full scale 223	Set X axis to full scale.
Y full scale 223	Set Y axis to full scale.
View all 223	Set X and Y axis to full scale.
Recorder autoscale 224	Chromatogram autoscaling.

See also:

Main window menus 25

2.1.1.1.5 Acquire menu

Start chromatogram 30	Generate manual **Inject signal** for the running **chromatogram** 207.
Finish! 31	Force **finish** for the running **chromatogram** 207.

See also:

Main window menus 25

2.1.1.1.5.1 Start chromatogram

(*Main menu* Acquire / Start chromatogram)

This command supplies manual **Inject signal** for the current **run**.

The command refers to the running **chromatogram** 207 which must be displayed in the active **chromatogram window**.

Typically instruments supply **Inject signal** and running **system** 79 automatically handles this signal. In

this case operator do not need to use this command.

Operator have to make manual **Inject** command if there are no instrumental support for the **Inject signal**.

The same action can be performed be pressing the **[SPACE]** keyboard key if **Global preferences** 41 has an appropriate configuration.

See also:

System definition 79

Start run 83

2.1.1.1.5.2 Finish!

(*Main menu* Acquire / Finish!)

This command forces finish for the running **chromatogram** 207.

The action of the command is analogous to **stop data acquisition** 84 command of the **system window** 80.

The command refers to the running **chromatogram** 207 which must be displayed in the active **chromatogram window**.

See also:

System definition 79

Start run 83

Stop run 83

Stop data acquisition 84

2.1.1.1.6 Process menu

Reintegrate... 231 start reintegration procedure

Peak editor 224 switch on peak editor mode.

Calibrate... 176 start recalibration procedure

Electronic signature 61 perform operations with electronic signatures for the current chromatogram

More... Opens a menu with additional options:

Subtract... 232 Subtract one chromatogram from the other.

Compare... 231 Compare two **chromatograms** 207 or **processing methods** 122

Data smoothing/Compress... 132 Settings for chromatogram noise smoothing and data compression (in the case of over-sampling).

Invert! 232 Invert chromatogram.

Peaks deconvolution by form 231 Master to perform chromatogram peaks de-convolution using Gauss, EMG or other peak approximation.

Cut Raw Data 232 Cuts chromatogram data

See also:

Main window menus 25

2.1.1.1.7 Method menu

Allows to edit a **method** 122 settings, either a "pure" one (free of data) or one attached to the chromatogram.

Method setup... 124	Parameter settings of method such as run time and acquisition rate.
Sample... 126	Edit sample description of the chromatographic run.
Channels setup... 147	Edit Channels table 112 of the Method.
Integration... 159	Describes how peaks are detected.
Calibration... 171	Parameter settings for calibration.
Extract stored system... 234	Extract system from chromatogram and save it in a file.

See also:

Main window menus 25

2.1.1.1.8 Report menu

Report menu consists of the following items:

Make quick report... 33	Make **advanced report** 341 from **report templates** 145 previously defined in the method. Opens "***Quick reports*** 33" window to perform an immediate report. If there are no reports defined in the method opens **"Edit report template"** 343 window for configuring and generating report.
Report setup... 145	Calls a **Method setup / "Reports" page** 145 for configuring **individual analysis reports** 320 for the current chromatogram or method.
Review stored report...	Navigate throw report files which were created earlier.
Sign stored report... 62	Run a wizard which helps user apply **electronic signature** 62 to previously created ***.PDF** report file. This option is valid if **21 CFR Part 11** 54 option is installed.
Setup and make plain report... 322	Setup simple plain-text report. Opens "**Report options** 322" window to setup a **plain report** 320 for the current chromatogram or method.

See also:

Main window menus 25

2.1.1.1.8.1 Quick reports

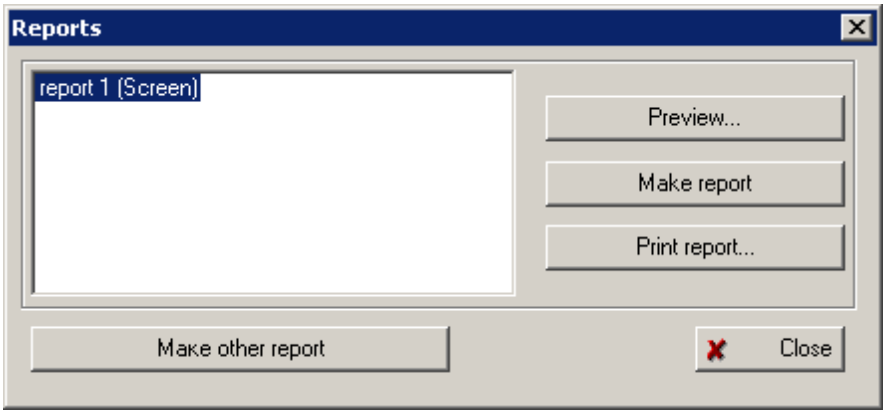
(*Main menu* Report / Make quick report...)

Opens **Reports** window for generating reports.

Reports window allows to immediately generate report for the **advanced report** 341 templates which were configured for the method or chromatogram. See **Method setup / "Reports" page** 145 for details.

This window appears if one ore more report templates are already configured and stored in the chromatogram.

If there are no report templates defined in the **Method setup / "Reports" page** 145 then **Edit report template** 343 window is opened instead of **Reports** window. In this case user can configure and generate report without storing report template in the method or chromatogram.



<Preview>	Preview report for the selected **advanced report** 341 template. Report is previewed on screen as WYSIWYG, according to settings defined in the **Edit report template** 343 window for the template selected.
<Make report>	Perform report output to printer, file or other destination according to settings defined in the **Edit report template** 343 window for the template selected.
<Print report>	Perform report output to printer. This is analogous to ***<Make report>*** action with the difference that output is performed to printer no matter what destination is chosen in the **Edit report template** 343 window for template. User can specify printer to use in the following ***Print Setup*** dialog.
<Make other report>	Generate an alternative report. Opens **"Edit report template"** 343 window to configure an alternative report options.

See also:

Report menu 32

Method setup / "Reports" page 145

Advanced reports 341

2.1.1.1.9 Spectra menu

Items of this menu become active if

- multichannel chromatogram 146 is loaded in the current chromatogram window
- appropriate activation key 20 is entered

The following menu items are available:

Spectral report 442
Spectral window 431
Recognition wizard 434
Factor analysis 451
Spectral analysis options 446

See also:

Main window menus 25

2.1.1.1.10 Options menu

Global preferences 41	General settings.
Choose UI Language... 44	Select software user interface language. Opens "***Choose language***" window.
Fonts... 43	Font settings for dialogs, reports, tables and plots.
Security settings... 47	Edit list of users with passwords and access levels (for users with **Administrator** access level) or change the current password (for users with **Master** and **Operator** access levels). See Security system 45 for details.
User logoff 53	Lock the system. Another valid user can login and proceed. Opens **LOGIN** window for locking the system or changing the user.
Lock access 54	Lock the system. Only current user or Administrator can unlock the software. Opens **LOGIN** window for locking the system.
Audit trail 67	Open "***History audit trail***" or "***Chromatogram audit trail***" window
Devices setup 77	Setup external devices. Display of workplace 77. Clicking this menu item opens the **WORKPLACE** window or brings it in front of all other windows.

Besides the **Options menu** includes a list of external devices 107 and systems 79 connected to workplace 89, in the following format:

"Folder \ System file"	Display of the **connected** System 79. Clicking this menu item opens the **SYSTEM WINDOW** or brings it in front of all other windows.
"Interface name"	Display of the connected **External devices (interface)** 107. Clicking this menu item opens the interface configuration window or brings it in front of all other windows.

See also:

Main window menus 25

2.1.1.1.11 Window menu

Cascade 75	Cascade all open windows.
Tile vertical 75	Tile all open windows vertically.
Tile horizontal 75	Tile all open windows horizontally.
Close all 75	Close all open windows.
1 ... N	Select a chromatogram window to be set active. It is possible to list chromatogram windows using [Ctrl]+[F6] key combination.

See also:

Main window menus 25

2.1.1.1.12 Help menu

On-line help	Calls up software on-line help.
About	Calls up "**ABOUT** Chrom&Spec" copyright information window.
Go to software web page	Navigate your default web browser to software support web site.
Manage my license	Allows you to review and upgrade your licence on-line.
Request for support	Navigate your default web browser to the support page where you could send your support request.
Collect data for support...	Launches wizard which allows user quickly and simply collect data required for support service. The collected data are stored in archive file which can be sent to specialists of support service by e-mail or transferred by another means. Just follow the instructions in the wizard.

See also:

Main window menus 25

2.1.1.2 Component window menus

2.1.1.2.1 Copy to clipboard

Copy to clipboard This option allows to copy the calibration graph of the selected component to the clipboard so that it is available for other Windows applications, such as MS Word, MS Excel, etc. The calibration graph is copied as a black-white picture.

2.1.1.2.2 Print/preview menu

Preview this	Display calibration graph print preview of the selected component.
Print this	Print selected calibration graph of the selected component.
Preview all	Display calibration graph print preview of all components.
Print all	Print selected calibration graph of all components.

2.1.2 Toolbar

The following icons are displayed in the toolbar of the Chrom&Spec main window:

Chrom&Spec icon

Open chromatogram 207

Save chromatogram 210

Save method or extract method from chromatogram 123

Open last **batch reprocessing** 271 file

Create plain report 322 for the selected chromatogram

Make quick report 33 for selected chromatogram by preconfigured templates

Preview plain report 234

Print plain report 233

Finish the current chromatogram and perform post-run data processing. It is equivalent to ***System / Control / Stop data acquisition*** operation

Generates **Inject event** . All events configured as **Start with inject** 91 are started (the run should be started first)

Prolongs the duration of the current chromatogram (data acquisition only) for 2 minutes

Edit sample description 126 of the current chromatogram or default **sample description** for the method

Method setup 124

Integration parameters 159

Components table 171

Make automated **spectral identification report** 442

Cascade 75 all opened chromatogram windows

Vertical tiling 75 of open chromatogram windows

Horizontal tiling 75 of open chromatogram windows

Chromatogram appearance 216

Manual peak editor 224 mode for chromatogram.

View all 223 **-** automatically scale chromatogram in the window

Help 35

Lock system 54

Workplace 77 configuration

Global time scheduler 78

ADC interface or other external device. Variety of devices are possible

Connected system 89 for instrument control

2.1.3 Program windows

" Chrom&Spec" consists of different windows whose functionality is linked together. The different windows are:

Chrom&Spec	Main program window with **menus** 25 for file administration, printing, method modification, options, login and user rights, window handling.
SYSTEM	**System window** 80 for control of interfaces and devices.
CHROMATOGRAM	**Chromatogram window** 212 for graphic plot of running or recorded chromatograms.
SYSTEM STATE	**System state** 98 window for status messages.
WATCH WINDOW	**Watch window** 103 for live display of instrument values.
SAMPLE QUEUE	**Sample queue control** 238 window for edition of sample queue tables and batch reprocessing tables.

2.2 File types

The following file types are produced by the "Chrom&Spec" software:

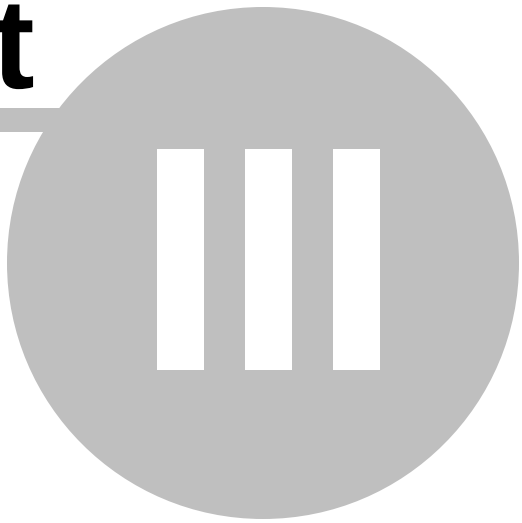
*.chw	**Chromatogram file** 207 (binary file) Contains raw chromatogram data, method configurations, and a copy of the system used for data acquisition. The ***.chw** files are stored automatically in the **Data** folder by default.
*.smt	**System** 79 **file** (binary file) Contains the instruments settings. The ***.smt** files are stored automatically in the sub folders of **Systems** folder.
*.mtw	**Method file** 122 (binary file) Contains the data processing settings, which can be linked to a system. The ***.mtw** files are stored in the in the **Systems** folder or in **Methods** folder by default.
*.que	**Sample queue file** 237 (binary file) Contains a sample data table. The ***.que** file is stored automatically in the **Systems** folder.
*.bar	**Batch reprocessing file** 271 (binary file) Contains batch reprocessing data. The *.bar file is stored automatically in the Data folder.
*.cal	**Calibration file** 198 (binary file) Contains calibration data, which can be exported and imported through chromatograms and methods. The ***.cal** file is stored automatically in the **Methods** folder
*.rtt	**Plain report template file** (ASCII file) Contains a report template for plain reports. The ***.rtt** files are stored in the program data folder.
*.ftt	**Advanced report template file** (binary file)

	Contains a report template for advanced reports. The ***.ftt** files are stored in the ***TEMPLATES*** folder by default.
*.dev	**Device** 105 **file** (ASCII file) Contains default settings for particular instrument. The ***.dev** files are stored in the **Devices** folder.
*.exc	**Exception file** (ASCII file) Contains exceptions from normal running and error messages. The ***.exc** files are stored automatically in one of the day sub-folders of the **Log** folder.
*.hst	**History file** (ASCII file) Contains history of commands and program actions. The ***.hst** files are stored automatically in one of the day sub-folders of the **Log** folder.
*.log	**Log file** (ASCII file) Contains log file of data communication between PC and instruments. The ***.log** files are stored automatically in one of the day sub-folders of the **Log** folder.

2.3 Context sensitive menus

Context sensitive menus are available in some Chrom&Spec windows and can be accessed by clicking the right mouse button somewhere in the window area. The pop up menu appears with different contents and functions that depend on the window or situation.

Part

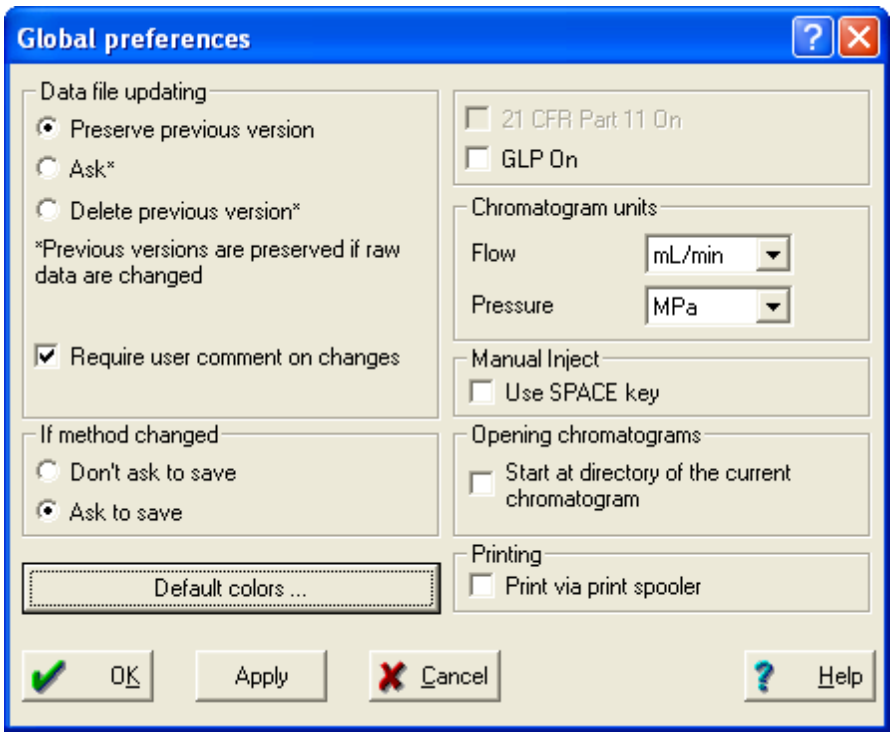


3 General settings and options

3.1 Global preferences

(*Main menu* Options / Global preferences)

This window is used for **global program settings**. It can be opened only by the user with Administrator 45 access level.



Note: if ☑ **GLP On** or ☑ **21 CFR Part 11 on** flags are set, some of settings in the form are fixed according to appropriate rules.

Data file updating

This section controls how software handles the procedure of updating chromatogram 207 data files.

⊙ **Preserve previous version**

Software keeps all previous versions of **chromatogram** files. A modified **chromatogram** is saved in the new file with file version number raised by 1.

⊙ **Ask***

The user is asked whether to keep the previous version of **chromatogram** file. A modified **chromatogram** is saved in the new file with file version number raised by 1.

⊙ **Delete previous version***

Previous version of **chromatogram** files is deleted. A modified **chromatogram** is saved in the new file with file version number raised by 1.

*Software always keeps previous version of **chromatogram** file if raw data changed (using **cut raw data** 232 function).

Software always keeps versions of **calibration chromatogram** files which where used to build **calibration** 165.

☑ **Require user comments on changes**

Operator is prompted to apply comments related to the update each time when updated chromatogram is saved to file. All comments can be reviewed in the **chromatogram audit trail** 68.

If method changed

Each **chromatogram** 207 stores its own copy of all **method** 122 settings. Operator can modify **method** 122 settings in the **chromatogram** 207 to get an optimal results.

This section controls how software handles modifications in the **chromatogram** 207 which refer to **method** 122 settings.

⊙ **Don't ask to save** — No prompts are shown to the operator and **method** 122 files is not updated an.

⊙ **Ask to save** — During saving **chromatogram** 207 the operator is asked to save **method** 122 modifications done in the **chromatogram** 207 to the **method** 122 file. Answer **"Yes"** overwrites the **method** 122 file from the **chromatogram** 207 settings.

"Good Laboratory Practice" (GLP) and "21 CFR Part 11" compliance

☑ **21 CFR Part 11 on** This flag indicates the operation of the software in the environment which requires **FDA 21 CFR Part 11** 54 compliance.

The flag is for indication only, it cannot be changed here. The **FDA 21 CFR Part 11** 54 compliance option must be configured during **software installation** 21.

☑ **GLP On** This flag sets the operation of the software in the environment which requires **"Good Laboratory Practice"** 43 compliance.

Chromatogram units

Indicates the preferred units for some physical measures:

Flow — Unit for flow rate: **µL/min**, **mL/min**

Pressure — Unit for pressure: **MPa**, **psi**, **bar**, **atm**

Manual inject

☑ **Use SPACE key** Pressing **[Space]** keyboard key supplies manual **Inject signal** for the running **chromatogram** 207 and **system** 79. See description for the **Start chromatogram** 30 command.

Opening chromatograms

☑ **Start with directory of the current chromatogram**

This options changes the default directory which is first displayed in the **Open chromatogram** 207 window form.
If this option is enabled, the directory is opened where the current active chromatogram is opened from.
If this option is disabled, the directory is opened where the last chromatogram was opened from.

☑ **Print via print spooler** Switch on/off printing via print spooler. Switch off this option if problems with printing occur.

<Default colors> Opens ***"Default colors"*** window to set default colors for elements of the **chromatogram window** 212.
"Default colors" window is similar to **"Colors" window** 222.

3.1.1 Good Laboratory Practice (GLP)

The "Chrom&Spec" software is designed to be compliant with a Good Laboratory Practice (**GLP**) and Good Automated Laboratory Practice (**GALP**) standards.

The most important embedded GLP features are:

- The complete equipment and data processing specifications as well as the raw data are stored in the same file and allow the complete reconstruction of the reported data or analysis later.
  See also: **Method** 122
- The security system on the basis of passwords enables to restrict **Access level** 45 of the user in accordance with his/her skill.
- Each run gets its unique serial number that is reported and cannot be changed by the user.
- Column test quantification method that provide a means to check the system for stability and reproducibility.
- **Audit trail** 67 options.
- Electronic signature features

Some useful GLP features can be switched on or off in the "**GLOBAL PREFERENCES**" window.

See also:
"Global preferences" window 41

3.2 Fonts

(*Main menu* Options / Fonts...)

This option allows to select fonts used by the system.

Font for dialogs This font is used in all dialogs boxes.

Font for reports This font is used for report output to the screen or printer.

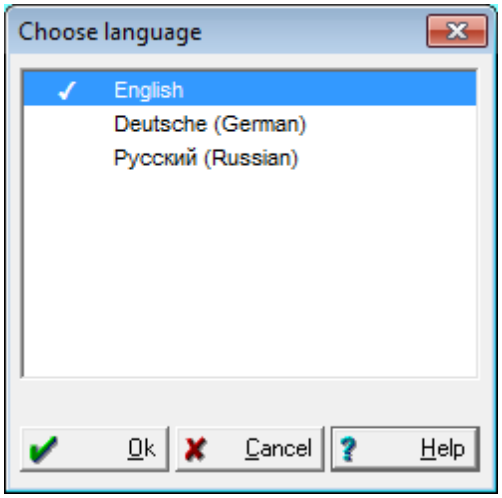
Font for tables This font is used for data presentation in tables on the screen (such as components table 171). It is not used for presentation of tables in the report.

Font for plots Choice of the font for labels on graphs (chromatogram plot, calibration curve, etc.).

3.3 Choose UI language

(*Main menu* Options / Choose UI Language...)

This command displays ***Choose language*** windows where language for software ***user interface*** can be selected:



Chrom&Spec provides **M**ultilanguage **U**ser **I**nterface (**MUI**).

So, it is possible to select the desired language from the list.

All menu, dialogs and messages inside the **Chrom&Spec** will be changed according to the selected language.

Note: In order to use new MUI settings, it is necessary to quit and restart Chrom&Spec application

Note: For reports 318 it is possible to use different languages with appropriate *report templates* no matter what language is selected for *user interface*. *Report templates* can be configured for languages which are not present in the list of *Choose language*

window.

3.4 Security system

In accordance with **GLP** 43 and **FDA 21 CFR Part 11** 54 requirements the "Chrom&Spec" software supports a security system with **password protection**.

Chrom&Spec implements reliable authentication system, based on recognized crypt algorithms (MD5 hashing with salt values and strong AES encryption). All sensitive user data (passwords, **certificates** 57, etc) are stored in encrypted form with encryption key based on user **password**.

Chrom&Spec does not use authentication and encryption supplied by **Windows™** operating system. Still Chrom&Spec software uses **Windows™** services for protected storage 74 to avoid occasional corruption or deletion of sensitive user data.

Several **access levels** 45 are available for users to control access to different software functions.

At first run of the "Chrom&Spec" software after installation the **"Add user" window** 51 is displayed which prompts to specify the account with **Administrator access level** 45.

Then **Administrator** can use **Options / Security settings...** 47 ***menu item*** to edit the **list of users** 50 and **security policies** 52.

Each time the Chrom&Spec starts the **Log in** 47 window prompts user for user name and password.

During the work it is possible to change the current user through the **User logoff** 53 **menu** command.

The user's name stamps methods, chromatograms and reports, created during the working sessin.

See also:

Log in window 47

Security settings 47

FDA 21 CFR Part 11 54

Certificates 57

How to modify a user 462

3.4.1 Access level

The access level is a part of the **Security system** 45. It is installed indirectly (together with the user name) when the user enters the password in the **Log in** 47 window.

There are three access levels that the user may have:

Administrator — Users with the highest **access level**. The administrator user is authorized to perform any tasks in the software, including ***administrative tasks***: configure **list of users** 50, set **access level** for users, configure **security policies** 52, configure **global preferences** 41.

Master — This **access level** is intended for experienced users. **Master** is allowed to perform any tasks in the software except ***administrative tasks***. **Master** can create, configure and update **systems** 79, **methods** 122 and data files, perform analyses and generate reports, apply **electronic signatures** 60.

Operator — This is a restricted **access level** intended for novice users. **Operator is** allowed to start and stop runs using existing preconfigured **systems** 79 and **methods** 122, run **sample queues** 237 and generate reports. Modifications of **systems** 79, **methods** 122 and data files are not allowed. Applying **electronic signatures** 63 is not not allowed.

Access level of the user can be modified by authorized users with **Administrator access level** throw " 50 ***User list*** 50 " page 50.

See also:

Status of the user 46

List of users 50

How to modify a user 462

3.4.2 Status of the user

Each user account can be in three states:

Active — Account of the user can be used for system log-in.

Inactive — Account of the user can not be used for system log-in. This status indicates that account is temporary inactivated in the system. System can automatically inactivate account after exceeding the ***Maximum number of login attempts*** 52.

Removed — Account of the user can not be used for system log-in. This status indicates that account is removed from the system (for example, when account owner leave the organization). Still **GLP** 43 and **FDA 21 CFR Part 11** 54 rules require that account data must be stored in the system.

Note: Status can be changed either by *Administrator* **access level** 45 throw " 50 ***User list*** 50 " page 50 or by the system automatically after exceeding the ***Maximum number of login attempts*** 52.

See also:

Log in window 47 .

Security system 45

List of users 50

3.4.3 "Log in" window

Log in window prompts the user to specify **User name** and **Password**.

Initial **user password** is defined by the **Administrator** when he creates a new user account in the **list of users** 50.

During first login user must modify password. So even **Administrator** does not know the password of the user.

There are no way to restore or reset the password for the user. If user forgets his password **Administrator** has to create a new account with a new password and inactivate the previous account.

System can automatically **inactivate** 46 account after exceeding the ***Maximum number of login attempts*** 52. Inactivated account can be activated again by **Administrator** only by changing **account status** 46.

If last active Administrator was **inactivated** 46, then there no way to restore **Administrator** account. If software operates with **21 CFR Part 11 on** 41 option then the software must be uninstalled and installed again. Organization must ensure that only individuals with appropriate credentials can install and uninstall software.

If software operates without **21 CFR Part 11 on** 41 option then it is possible to delete ***accounts.cfg*** file located in the ***Accounts*** directory. This action deletes all accounts from the **list of users** 50. Next time when Chrom&Spec starts it will prompt the user to specify new account for **Administrator**.

Software shows ***Log in*** window and locks other functions in the following cases:

- every time the software is started;

- after explicit logout using **User logoff** 53 **menu** command.

- after locking using **Lock access** 54 **menu** command.

- after automatic logout (by default system makes automatic logout after 30 min of user's inactivity);

- when user activated **Options / Security settings** menu item.

See also:

Security system 45

Status of the user 46

Security settings 47

3.4.4 Security settings

(*Main menu* Options / Security settings...)

When this item is chosen, the **Log in** 47 window is called up first to confirm user credentials.

If the specified account has an **Administrator** **access level** 45 then **Security options** 50 window is opened where **list of users** 50 and **security policies** 52 can be edited.

If the specified account has an **Operator** or **Master** **access level** 45 then **My Account** 48 window is opened.

See also:

Security system 45

FDA 21 CFR Part 11 54

3.4.4.1 "Security options" window

Security options window allows users with **Administrator** **access level** 45 to perform administrative tasks.

Log in 47 window is always called up first before displaying ***Security options*** window.

Security options window consists of 3 pages:

My account 48	Allows **Administrator** to perform operations with his own account.
User list 50	Add new users and modify existing users.
Password options 52	Set up security policies.

See also:

Security system 45

Security settings 47

Access levels 45

Log in window 47

3.4.4.1.1 My account

My account page is a part of the **Security options** 48 window. It allows the current user to perform operations with his password and **certificate** 57:

For users with **Operator** or **Master** **access level** 45 ***My account*** is shown as a separate window and other pages of **Security options** 48 window are not available.

<Change password> Alter password for the current user. **New password** 49 window is displayed.

My certificate Operations with **certificate** 57 for the current user.

- ***<View>*** 58 — View certificate information for the current user.
- ***<Export wizard>*** 59 — Execute special ***wizard*** which helps user to export his certificate to external file.
- ***<Import wizard>*** 60 — Execute special ***wizard*** which helps user to import his certificate from external file.

Note: Chrom&Spec software automatically generates the self-signed certificate for each new user when new account is created. Still this certificate cannot fully verify the identity of the individual who uses the certificate. To be fully compatible with **21 CFR Part 11** 54 requirements an organization must establish an appropriate **Certification Authority** 55 and issue ***"genuine"*** certificates for the employers who will work with the software. Certified users must import their certificates to the software using **Import wizard** 60.

See also:

Security system 45
Security options 50
Certificates and electronic signature: general information 55
Using certificates 57

3.4.4.1.1.1 "New password" window

New password window can be opened from the **My account** 48 page and is used to change a password for the current user.

New password is to be entered twice.

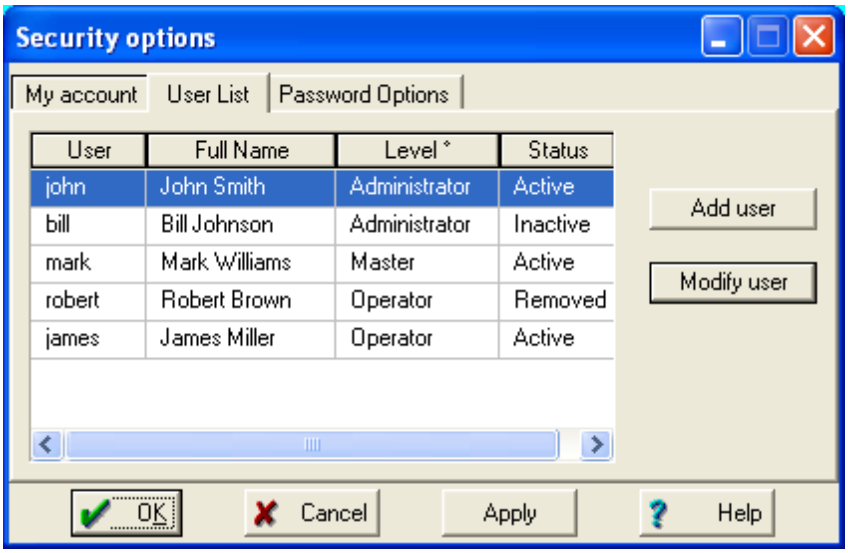
See also:

Security system 45
My Account 48

3.4.4.1.2 User List

User list page is a part of the **Security options** 48 window. It is available for **Administrator** **access levels** 45 only.

It allows **Administrator** to add new users to the list and to modify **names**, **access levels** 45 and **status** 46 of other users.



List of users contains the following columns:

User — Short user name (nickname). It is used in the **Log-in** 47 procedure.

Full name — User full name. This should be a real user name. **Full name** is used to mark chromatograms which user runs. Also **Full name** is displayed in the reports and in **audit trail** 67.

Level	**Access level** 45 of the current user
Status	**Status of the user** 46
<Add user>	Add a new user to the list. Opens **Add user** 51 window.
<Modify user>	Edit settings for the user selected in the list (**Full name**, **access levels** 45 and **status** 46). Opens **User** 52 window.

Note that there are no possibility to remove user from the list because **GLP** and **FDA 21 CFR Part 11** rules require that account data must be stored for audit purposes. Administrator should use **Removed status of the user** 46 to block account.

See also:

Security system 45

Security options 50

How to add a user 461

How to modify a user 462

3.4.4.1.2.1 "Add user" window

This window allows to add a new user to the **list of users** 50.

User, **Full name**, **Level** and **Password** items for the new user should be specified. Password should be repeated twice.

See descriptions in " 50 ***User list*** 50 " page 50.

Password for the user must meet requirements of security policies specified in the " 52 ***Password options*** 52 " page 52.

Administrator only can access the **Add user** window.

When a new user is created, the **Administrator** specifies a temporary password. When the user login

the program for the first time, he is forced to change password. So even **Administrator** does not know the actual password of the user.

There are no way to restore or reset the password for the user. If user forgets his password **Administrator** has to create a new account with a new password and inactivate the previous account.

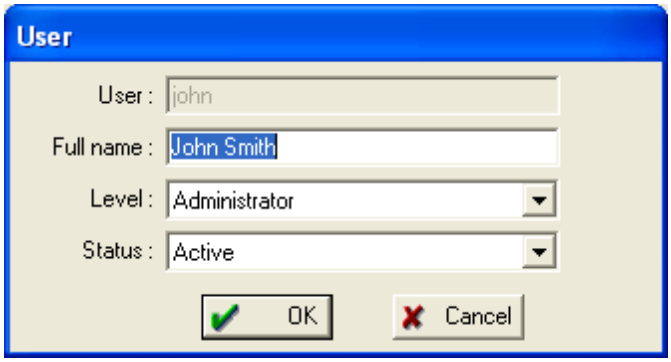
User is able to change his own password later through **My account** 48 page.

See also:

" 50 ***User list*** 50 " page 50

3.4.4.1.2.2 "User" window

User window enables to modify options for the selected user.



Full name, **Level** and **Status** items for the users can be modified here.

User item is for review only. It cannot be modified.

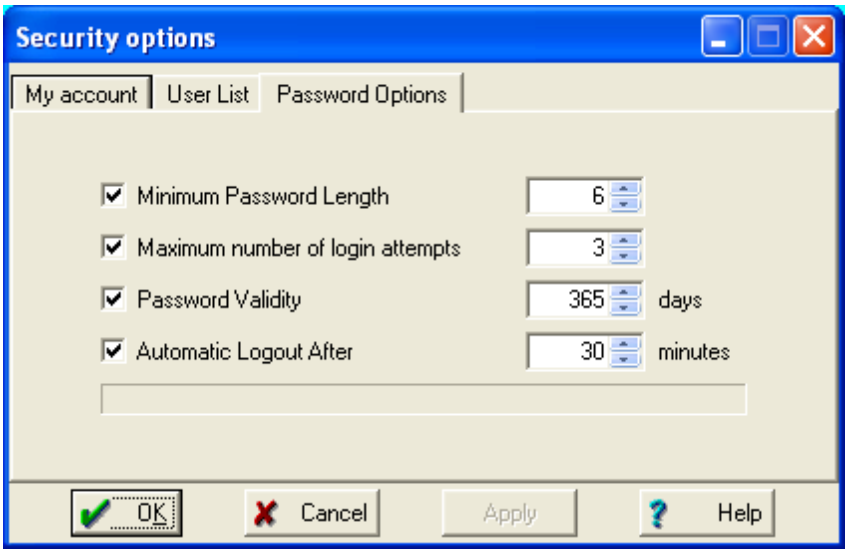
See also:

User list 50

3.4.4.1.3 Password options

Password options page is a part of the **Security options** 48 window. It is available for **Administrator access levels** 45 only.

It allows **Administrator** to set up security policies and password options.



☑ **Minimum password length**

a minimum allowable length of the password (a security precaution).
Default value: 6

☑ **Maximum number of login attempts**

A maximum number of log-in attempts in **Log in** 47 window. If this number is exceeded, the current user account is **inactivated** 46. See description of **Log in** 47 window for more details.
Default value: 3.

☑ **Password validity**

Duration of the password validity. When the time is over, the software prompts to change password.
Default value: 365 [days].

☑ **Automatic Logout after**

User's inactivity time (via keyboard or mouse) after which automatic log-out is performed.
Default value: 30 [min]

Each policy can by switched off by cleaning appropriate check-box ☑.

When software operates in **FDA 21 CFR Part 11** 54 mode the policies can not be switched off. **Administrator** is allowed to change values only.

See also:

" 48 ***My account*** 48 " page 48

" 50 ***User list*** 50 " page 50

3.4.5 User logoff

(*Main menu* Options / User logoff)

User Logoff function allows to lock system from unauthorized access.

Log in 47 is displayed and all other functions of the software are blocked.

Any authorized user can log in by entering his ***name*** and ***password***.
This operation can be used to change the current user.

Note: When system is locked automatically by specified time-out, this function is identical to *User logoff*.

See also:
Lock access 54
How to lock the system 463

3.4.6 Lock access

(*Main menu* Options / Lock access)

This option allows to lock the system while the user is on leave so that nobody could modify the data.
Log in 47 is displayed and all other functions of the software are blocked.
The system can be unlocked only by the user who locked it.

See also:

User logoff 53

How to lock the system 463

3.5 FDA 21 CFR part 11 compliance

3.5.1 21 CFR Part 11 definition

The "Chrom&Spec" software was designed to be compliant with Electronic Records and Signatures Rule, known as **21 CFR Part 11**, established by the U.S. Food and Drug Administration (FDA).

For this purpose, the program implements password protection and user administration 50, Electronic Signature 60, Audit Trail 67 and protected storage 74.

To be compliant with **21 CFR Part 11** requirements the software must be installed with appropriate option.

To use 21 CFR Part 11 it is necessary:

1) Install Windows operating system as specified in the **hardware and software requirements** 19 with **NTFS file system** on your computer.

2) Install " Chrom&Spec" software (the option ☑ 21 CFR Part 11 support in the corresponding dialog of the setup program must be activated).

3) Ensure that ☑ 21 CFR Part 11 On option in the "Global preferences" window 41 indicates the operation in compliant mode.

Note: **21 CFR Part 11** support can be activated if **NTFS file system** is used. If file systems other than NTFS are used, then convert disk partition where Chrom&Spec is to be installed to NTFS. Refer to Windows help or Microsoft support service.

If 21 CFR Part 11 support is installed, some additional restrictions appear:
- system folders as "Accounts", "Flog", and "Services" become protected and can not be accessed by other programs outside Chrom&Spec software.
- number of attempts to enter correct user name and password is restricted (default is 3) and then user name is deactivated. If Administrator is deactivated, the only way is to uninstall and then reinstall the Chrom&Spec software.

See also:

Electronic signature 60

"Global preferences" window 41

How to sign a chromatogram 463

3.5.2 Certificates

3.5.2.1 Certificates and electronic signature: general information

Certificates and Public Keys are regulated by 21 CFR part 11 54 requirements.

Certificate Services is one foundation for the Public Key Infrastructure (**PKI**) that provides the means for safeguarding and authenticating information. The relationship between a certificate holder, the certificate holder's identity, and the certificate holder's *public key* is a critical portion of PKI. This infrastructure is made up of the following parts:

- The Public/Private Key Pair
- The Certificate Request
- The Certification Authority
- The Certificate
- Your Public Key Used for Signature Verification

Public/Private Key Pair

PKI requires the use of *public/private key pairs*. The mathematics of public/private key pairs is beyond the scope of this documentation, but it is important to note the functional relationship between a public and a private key. PKI *cryptographic algorithms* use the public key of the receiver of an encrypted message to encrypt data, and the related *private key* and only the related private key to decrypt the encrypted message.

Similarly, a *digital signature* of the content, described in greater detail below, is created with the signer's private key. The corresponding public key, which is available to everyone, is used to verify this signature. The secrecy of the private key must be maintained because the framework falls apart after the private key is compromised.

Given enough time and resources, a public/private key pair can be compromised, that is, the private key can be discovered. The longer the key, the more difficult it is to use brute force to discover the private key. In practice, sufficiently strong keys can be used to make it unfeasible to determine the private key in a timely manner, making the Public Key Infrastructure a viable security mechanism.

A private key can be stored, in protected format, on a disk, in which case it can only be used with that specific computer unless it is physically moved to another computer. An alternative is to have a key on a

smart card that can be used on a different computer provided it has a smart card reader and supporting software.

The public key, but not the private key, of the subject of a digital certificate is included as part of the *certificate request*. (Hence, a public/private key pair must exist before making the certificate request.) That public key becomes part of the issued certificate.

The Certificate Request

Before a certificate is issued, a certificate request must be generated. This request applies to one entity, for example, an end-user, a computer, or an application. For discussion, assume that the entity is yourself. Details of your identity are included in the certificate request. After the request is generated, it is submitted to a *certification authority* (**CA**). The CA then uses your identity information to determine whether the request meets the CA's criteria for issuing a certificate. If the CA approves the request, it issues a certificate to you, as the entity named in the request.

The Certification Authority

Before issuing your certificate, the CA verifies your identity. When the certificate is issued, your identity is bound to the certificate, which contains your public key. Your certificate also contains the CA's digital signature (which can be verified by anyone who receives your certificate).

Because your certificate contains the identity of the issuing CA, an interested party that trusts this CA can extend that trust to your certificate. The issuance of a certificate does not establish trust, but transfers trust. If the certificate consumer does not trust the issuing CA, it will not (or at least should not) trust your certificate.

A chain of signed certificates allows trust to be transferred to other CAs as well. This allows parties who use different CAs to still be able to trust certificates (provided there is a common CA in the chain, that is, a CA that is trusted by both parties).

The Certificate

In addition to your public key and the identity of the issuing CA, the issued certificate contains information about the purposes of your key and certificate. Furthermore, it includes the path to the CA's list of revoked certificates, and it specifies the certificate validity period (beginning and ending dates).

Assuming the certificate consumer trusts the issuing CA for your certificate, the certificate consumer must determine if the certificate is still valid by comparing the certificate's beginning and ending dates with the current time and by checking that your certificate in not on the CA's list of revoked certificates.

Your Public Key Used for Signature Verification

A digital signature is used as confirmation that a message has not been altered and as confirmation of the message sender's identity. This digital signature is dependent on your private key and the message contents. Using the message as input and your private key, cryptographic algorithms create the digital signature. The contents of the message are not changed by the signing process. A recipient can use your public key (after checking your certificate's validity, issuing CA, and revocation status) to determine whether the signature corresponds to the message contents and to determine whether the message was sent by you.

If a third party intercepts the intended message, alters it (even slightly), and forwards it and the original signature to the recipient, the recipient, upon examination of the message and signature, will be able to determine that the message is suspect. Similarly, if a third party creates a message and sends it with a bogus digital signature under the guise that it originated from you, the recipient will be able to use your public key to determine that the message and signature do not correspond to each other.

Non repudiation is also supported by digital signatures. If the sender of a signed message denies

sending the message, the recipient can use the signature to refute that claim.

Note that the bulk of the activities listed here are also handled by software, not directly by the user.

See also:

Using certificates 57

3.5.2.2 Using certificates

Certificates are used to create and validate **electronic signatures** 60.

Chrom&Spec software supports ***X.509 certificates.***

X.509 is an internationally recognized standard for certificates that defines their required parts. ***X.509 digital certificates*** include not only a user's name and public key, but also other information about the user.

These certificates are more than stepping stones in a digital hierarchy of trust. They enable the **Certification Authority** 56 to give a certificate's receiver a means of trusting not only the public key of the certificate's subject, but also that other information about the certificate's subject. That other information can include, among other things, an e-mail address, an authorization to sign documents of a given value, or the authorization to become a **Certification Authority** 56 and sign other certificates.

Note: To use certificate issued for you and signed by **Certification Authority** 56, it is necessary to import it.

The following certificate services are supported by **Chrom&Spec** software.

- Software automatically generates "Self Signed" certificates with public/private key pair for new users. User is able to import them. Still these certificates cannot fully verify the identity of the individual who uses the certificate. To be fully compatible with 21 CFR part 11 54 requirements an organization must establishes an appropriate **Certification Authority** 56 and issue certificates for the employers who will work with the software. Certified users must import their certificates to the software using Import wizard.

- Software supports export and import of certificates. Private and public keys as well as whole certificates are transferred through "Personal Information Exchange -PKCS #12 (.PFX)" files. To maintain security, only user himself could export and import his certificate. See **Operations with certificates** 58 for details.

- Certificates and private keys are stored in the protected storage 74 and could not be accessed by regular means.

- Private keys are encrypted. That ensure that only user himself could use his private key.

- When user makes sign operation, software copies the public part of the user's certificate and stores it with the signature. Software enables to view corresponding certificate for each signature.

See also:

Certificates and electronic signature: general information 55

Security system 45
"My account" page 48

3.5.2.3 Operations with certificates

Operations with certificates are available from **My account** 48 page.

Use ***main menu*** **Options / Security settings...** to get access to this page.

<View> 58 View certificate information for the current user
<Export wizard> 59 Execute special wizard which helps user to export his certificate to external file.
<Import wizard> 60 Execute special wizard which helps user to import his certificate from external file.

See also:
Certificates and electronic signature: general information 55
Using certificates 57

3.5.2.3.1 View

<View> button at **My account** 48 page.

This command shows a certificate assigned to the current user. Subject and issuer names, certificate expiration date and other information can be viewed here.

Note: Chrom&Spec software automatically generates the self-signed certificate for each new user when new account is created. Still this certificate cannot fully verify the identity of the individual who uses the certificate. To be fully compatible with **21 CFR Part 11** 54 requirements an organization must establish an appropriate **Certification Authority** 55 and issue ***"genuine"*** certificates for the employers who will work with the software. Certified users must import their certificates to the software using **Import wizard** 60.

The window is divided into three pages:

General General information on the current certificate such as trust status, Certification authority, period of validity, etc
Details Provides a more detailed information including version, serial number, public key, subject, etc.
Certification path Hierarchy of the current certificate up to root certificate

See also:
"My account" page 48
Operations with certificates 58

3.5.2.3.2 Export

<Export> button at **My account** 48 page.

This command executes ***Certificate Export Wizard*** allowing to export the certificate to the external file.
The certificate can be exported with or without **private key** 55.

The certificate without **private key** 55 is not encrypted and is used for reviewing certificate owner data (name, e-mail etc).
The certificate without **private key** 55 is exported as ***Encoded Certificate X.509 (*.cer)***

The certificate with **private key** 55 is encrypted. Use it if you wish to transfer your certificate to another workstation.
The certificate with **private key** 55 is exported as **Personal Information Exchange (*.pfx)** file protected by user-defined password (compliant with ***PKCS #12*** specification).

Exported certificate with **private key** 55 can be imported to another PC with different **Chrom&Spec** installation. In this case it is possible to create identical electronic signatures for different software installations.

Certificate Export Wizard consists of the following steps:

- **Select "Export Private key" option**
  This step of the Certificate Export Wizard offers to choose if **private key** 55 should be included to exported certificate.
  Private keys 55 are password protected.
  If "⊙Yes, export the private key" option was selected, ***Wizard*** asks for password on the next step.

- **Type and confirm password**
  This step of the Certificate Export Wizard offers to enter and confirm password needed for private key protection.
  This page is displayed only if the export of the **private key** 55 is requested.

- **Specify file name to export certificate to**
  This step of the Certificate Export Wizard offers to enter file name for certificate storage.
  Personal Information Exchange (*.pfx) file is used for certificate files with **private key** 55
  or
  Encoded Certificate X.509 (*.cer) file if public part of the certificate is stored only

See also:
"My account" page 48
Operations with certificates 58
Import certificate 60

3.5.2.3.3 Import

<Import> button at **My account** 48 page.

This command executes ***Certificate Import Wizard*** allowing to import the certificate from the external file.

Personal Information Exchange (*.pfx) file compliant with ***PKCS #12*** specification must be used for importing certificates.
Certificates can be imported with **private key** 55 only.

The wizard allows to import certificate, supplied by **Certification Authority** 56, exported from **Chrom&Spec** software or produced by other means.

Warning: import procedure will destroy your current certificate! Use export procedure 59 to preserve the current certificate.

Follow ***wizard*** steps to import saved certificate .

Certificate Import Wizard consists of the following steps:

- **Specify the file name you want import *certificate* from**
  Click **<Browse>** button to select the desired file.
- **Specify the password**
  Password is used for protecting **private key** 55 in the **Personal Information Exchange (*.pfx)** file.

See also:
"My account" page 48
Operations with certificates 58
Export certificate 59

3.5.3 Electronic signature

In **Chrom&Spec** software ***electronic signature*** can be applied to chromatogram 207 data files and to ***report files*** stored in ***Portable document format (*.pdf)***.

Advanced reports 341 and **Advanced summary reports** 366 can be configured to produce output to ***Portable document format (*.pdf)*** files.

For applying ***electronic signature*** a **certificate** 57 of the user is used to ensure the identity of the signer.

By applying ***electronic signature*** to **chromatogram** 207 data files or to ***report files*** the user claims the validity of data processing settings and chromatographic results.

User can specify a meaning (such as ***review***, ***approval***, ***responsibility***, or ***authorship***) associated with the signature which clarifies the responsibility of the user.

Electronic signature is embedded to the **chromatogram** 207 data file. After applying ***electronic signature*** to **chromatogram** 207 data file the **Chrom&Spec** software prohibits any modifications of the signed file. Authorized user can ***revoke*** the ***electronic signature*** from the **chromatogram** 207 data file. After ***revoking*** the modification of any data processing settings is available again.

Signed **chromatogram** 207 data files can be copied and transferred to another workstation with another installation of **Chrom&Spec** software. The ***electronic signature*** can be reviewed and validated there. ***Electronic signature*** validation ensures the identity of the signer and the fact that no changes were applied to the **chromatogram** 207 data file since the time when it was signed. The **chromatogram** 207 validated with ***electronic signature*** can be used to generate reports and display validated results in a regular way.

Signed ***report files*** stored in ***Portable document format (*.pdf)*** format can be transferred to another workstation, for example, by ***Email***. The **Chrom&Spec** software is not required to be installed on the target workstation to validate embedded ***electronic signature*** in the ***PDF documents***. Most ***PDF*** viewers including ***Adobe®*** ***Reader®*** have a build-in tools for ***electronic signature*** validation.

User must have appropriate credentials (**Master** or **Administrator** **access level** 45) for applying or revoking ***electronic signatures***.

See also:

Electronic signature for chromatograms 61

Electronic signature for PDF reports 62

3.5.3.1 Electronic signature for chromatograms

(*Main menu* Process / Electronic signature)

Use this command to apply **electronic signature** 60 to **chromatogram** 207 data file.

Before signing the **chromatogram** 207 must be opened and displayed in the active **chromatogram window** 212.

The command displays the **electronic signature** 63 window where user must specify **user name**, **password** and **meaning** of the operation. Then user can perform signing or signature revoking operation.

See **electronic signature** 60 for details.

Once a **chromatogram** 207 is ***signed*** the **Chrom&Spec** software protects it from further modifications. To alter a signed chromatogram the signature has to be ***revoked***.

Several subsequent signatures can be applied to the signed **chromatograms** 207.

See also:

Electronic signature 60

"Electronic signature" window 63

Electronic signature for PDF reports 62

3.5.3.2 Electronic signature for PDF reports

(*Main menu* Report / Sign stored report...)

This menu command displays ***Sign PDF document*** window form.

User can apply electronic signature 60 to reports stored in ***Portable document format (*.pdf)*** files. Advanced 366 reports 341 and Advanced summary reports 366 can be configured to produce such reports.

To apply an electronic signature 60 first select the desired ***PDF*** report file. Click ***<Browse>*** button to browse for file.

Before signing user can review the document by pressing ***<Review...>*** button. This will open and display the ***PDF*** document with a default ***PDF*** viewer installed on user's workstation.

Note that user must install some ***PDF*** viewer (free ***Adobe®*** ***Reader®***, for example). Otherwise this

function will not work.

Then user should select a type of the signature: **visible signature** or **hidden signature**.

Visible signature will be displayed in the top of the first page of the signed of PDF document as a special mark with signer name, signature meaning and date of signature applying.
Visible signature will be present at report printout.

Hidden signature does not change the document view. **Hidden signatures** can be reviewed only in the special window or special section provided by your ***PDF*** viewer.

Both **Visible** and **Hidden** signatures are validated in the same way.

After selecting a type of the signature user should press ***<Sign or revoke signatures...>*** button.
This displays **Electronic signature** 63 window where user must specify **user name**, **password** and **meaning** of the operation. Then user can perform signing or signature revoking operation.

After successfully signing Document was successfully signed! message is displayed. User can review signed document by pressing ***<Review...>*** button.

Several subsequent signatures can be applied to the signed ***PDF*** document.

See also:

Electronic signature 60

"Electronic signature" window 63

Electronic signature for chromatograms 61

Advanced reports 341

Advanced summary reports 366

3.5.3.3 "Electronic signature" window

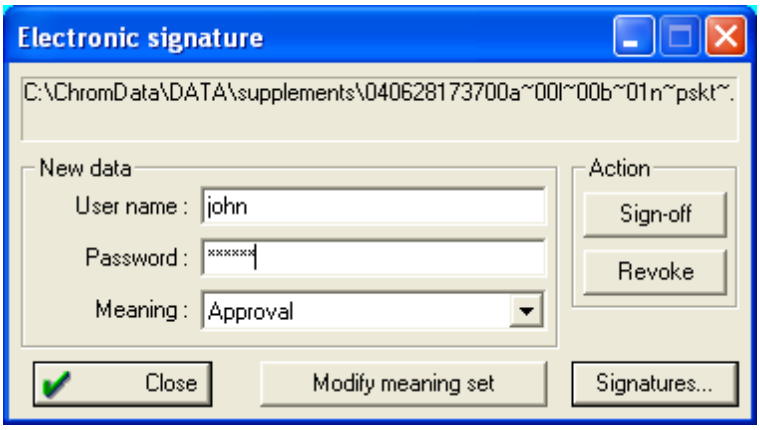
The **Electronic signature** window is used to ***sign*** the **chromatograms** 207 or reports stored in ***Portable document format (*.pdf)*** files.
This window is also used to ***revoke the signature*** if needed.

The **electronic signature** is a part of the 21 CFR Part 11 54 requirements. See **electronic signature** 60 article about details what is **electronic signature** and what it means.

Electronic signatures are embedded to the signed file. Several subsequent signatures can be applied to the **chromatograms** 207 and ***PDF*** documents.

To perform a signature operation user must specify his **user name**, **password** (see **security system** 45) and a **signature meaning** 65.

The **password** of the user is used do temporary decrypt a **private key** of the **user certificate** 55 so it is available for creating signature.



The full path and file name of the chromatogram or report is display in the top of the window.

User name Name of the user. User must have **Administrator** or **Master** **access level** 45.

Password A valid password of the user.

Meaning **Meaning of the signature** 65. It can be selected from a drop-down list. The set of possible meanings can be modified by pressing ***<Modify meaning set>*** button.

<Sign-off> Sign the chromatogram using the entered **user name**, **password** and the selected signature **meaning**.

<Revoke> Revoke signatures. All signatures are cleared from the object and corresponded notification is placed to the chromatogram audit trail 68.

<Modify meaning set> Displays **"Meaning set" window** 65 where user can review and modify the set of meanings available for **electronic signatures.** Only users with **Administrator** **access level** 45 can modify the list of meanings.

<Signatures...> Displays a list of signatures and signature validation status for the **chromatogram** 207 in the **signatures window** 66. This button is not available when operation is performed with ***PDF*** reports. Use signature tools of your ***PDF*** viewer (free ***Adobe®*** ***Reader®***, for example) to view and validate signatures of the ***PDF*** document.

Note: Once a chromatogram is signed it cannot be altered. To alter a signed chromatogram the signature has to be revoked.

See also:

Electronic signature 60

Electronic signature for chromatograms 61

Electronic signature for PDF reports 62

3.5.3.3.1 Signature meaning

Signature meaning is a short text description that clarifies what user means by applying **electronic signature** 60 to the object.

There is a predefined list of signature meanings in the **Chrom&Spec** software. This list can be modified or extended if necessary.

Only users with **Administrator** **access level** 45 can modify the list of meanings.

Meaning set 65 window is used for reviewing and modifying the list of signature meanings.

See also:

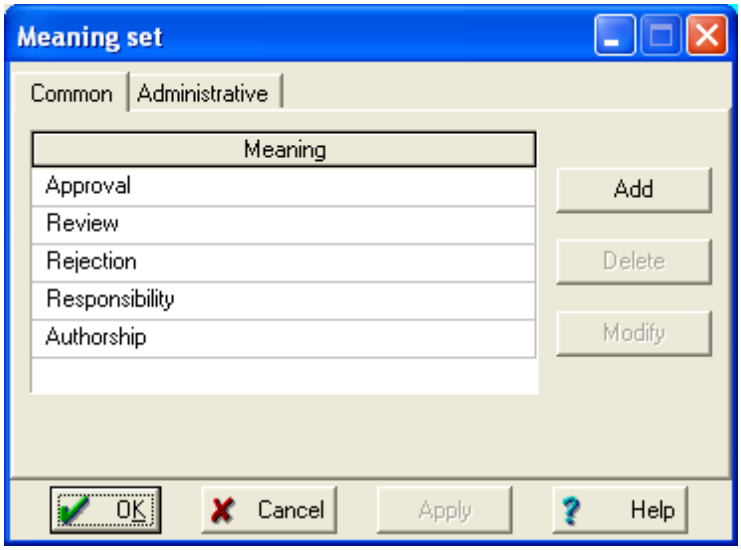
"Electronic signature" window 63

"Meaning set" window 65

3.5.3.3.1.1 "Meaning set" w indow

Meaning set window contains an editable list of meanings for the **electronic signature** 60.
<Modify meaning set> button in the **"Electronic signature" window** 63 is used to display this window. Only users with **Administrator** **access level** 45 can modify the list of meanings.

The list of signature meanings is used in the **"Electronic signature" window** 63 when user applies signature to the object or revokes signatures from the object.



Two types of signature meanings are available in the **Chrom&Spec** software.

Meanings listed in the **Common** list are available for users with **Administrator** or **Master** **access levels** 45.

Meanings listed in the **Administrative** list are available for users with **Administrator** **access level** 45 only.

The following predefined list of signature meanings is available in **Chrom&Spec** software: {Approval, Review, Rejection, Responsibility, Authorship}

<Add>	Add a new meaning of the signature to the list
<Delete>	Deletes the selected signature meaning from the list
<Modify>	Modify the selected signature meaning in the list

See also:

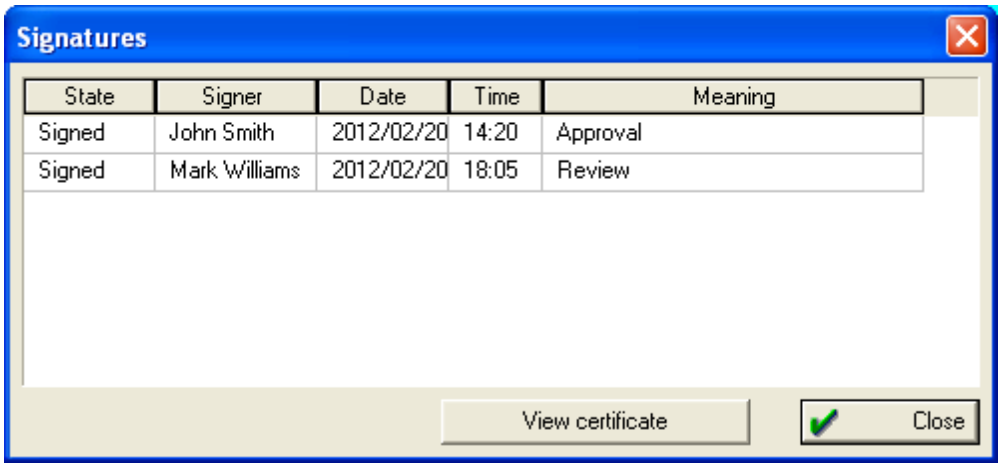
Electronic signature 60

"Electronic signature" window 63

3.5.3.3.2 Signatures window

Signatures window displays a list of signatures and signature validation status for the **chromatogram** 207.

<Signatures...> button in the **"Electronic signature" window** 63 is used to display this window.



State — Signature validation status Possible values are {***Signed***, ***Failed*** }

Signer — Signer full name, as it was specified in the **Chrom&Spec** software. It is defined in **"Add user" window** 51, **Full name** item. Note that this name can differ from the name specified in the user **certificate** 55. To review certificate use ***<View certificate>*** button.

Date — Date when the signature was created.

Time	Time when the signature was creating
Meaning	**Meaning of the signature** 65 which was specified by the signer.
<View certificate>	View the **certificate** 55 of the signer for the selected signature.

See also:

Electronic signature 60

"Electronic signature" window 63

3.5.4 Audit trail

3.5.4.1 Audit trail

(*Main menu* Options / Audit trail)

Audit trails keep history of actions performed by user while he makes configurations in the software and executes analyses.

Two types of **audit trails** are available in the software:

Chromatogram audit trail 68 available through ***main menu*** **Options / Audit trail / Chromatogram**

History audit trail 67 available through ***main menu*** **Options / Audit trail / History**

See also:

FDA 21 CFR Part 11 54 compliance

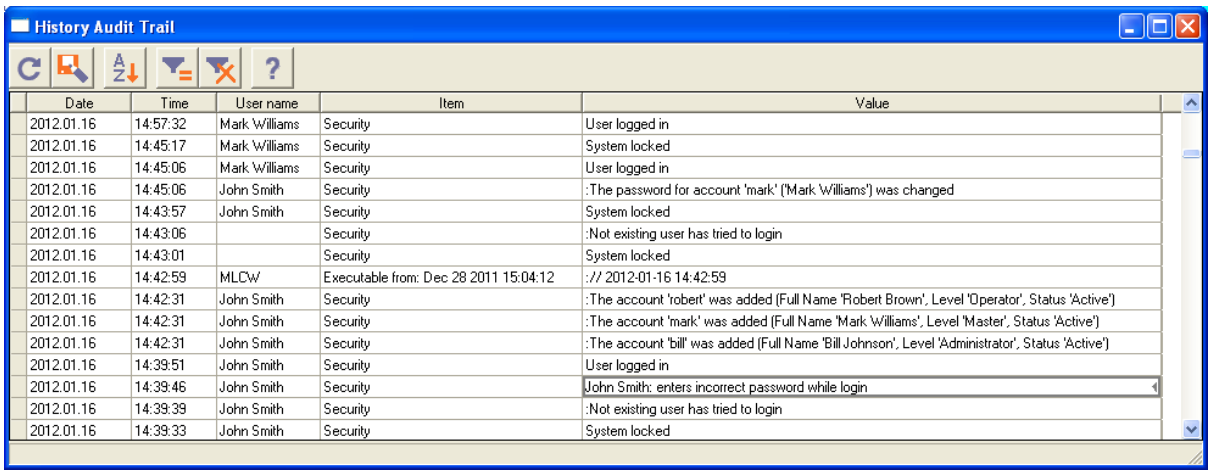
Good Laboratory Practice 43

Audit trail user interface 70

3.5.4.2 Audit trail: History

(*Main menu* Options / Audit trail / History)

History Audit trail window automatically traces all common user activity such as user login, password changing, analysis execution, opening of a windows, pushing a button etc..



Date	Time	User name	Item	Value
2012.01.16	14:57:32	Mark Williams	Security	User logged in
2012.01.16	14:45:17	Mark Williams	Security	System locked
2012.01.16	14:45:06	Mark Williams	Security	User logged in
2012.01.16	14:45:06	John Smith	Security	:The password for account 'mark' ('Mark Williams') was changed
2012.01.16	14:43:57	John Smith	Security	System locked
2012.01.16	14:43:06		Security	:Not existing user has tried to login
2012.01.16	14:43:01		Security	System locked
2012.01.16	14:42:59	MLCW	Executable from: Dec 28 2011 15:04:12	:// 2012-01-16 14:42:59
2012.01.16	14:42:31	John Smith	Security	:The account 'robert' was added (Full Name 'Robert Brown', Level 'Operator', Status 'Active')
2012.01.16	14:42:31	John Smith	Security	:The account 'mark' was added (Full Name 'Mark Williams', Level 'Master', Status 'Active')
2012.01.16	14:42:31	John Smith	Security	:The account 'bill' was added (Full Name 'Bill Johnson', Level 'Administrator', Status 'Active')
2012.01.16	14:39:51	John Smith	Security	User logged in
2012.01.16	14:39:46	John Smith	Security	John Smith: enters incorrect password while login
2012.01.16	14:39:39	John Smith	Security	:Not existing user has tried to login
2012.01.16	14:39:33	John Smith	Security	System locked

History audit trail table

It consists of the following columns:

Date Date of the entry.

Time Time of the entry.

User name Full name of the user who performed action or modification. See **security system** 45 and **Add user** 51 window.

Item Action identifier or source of the event.

Value Description of the event

See also:

Audit trail 67

Audit trail user interface 70

Chromatogram audit trail 68

FDA 21 CFR Part 11 54

Global preferences 41

3.5.4.3 Audit trail: Chromatogram

(*Main menu* Options / Audit trail / Chromatogram)

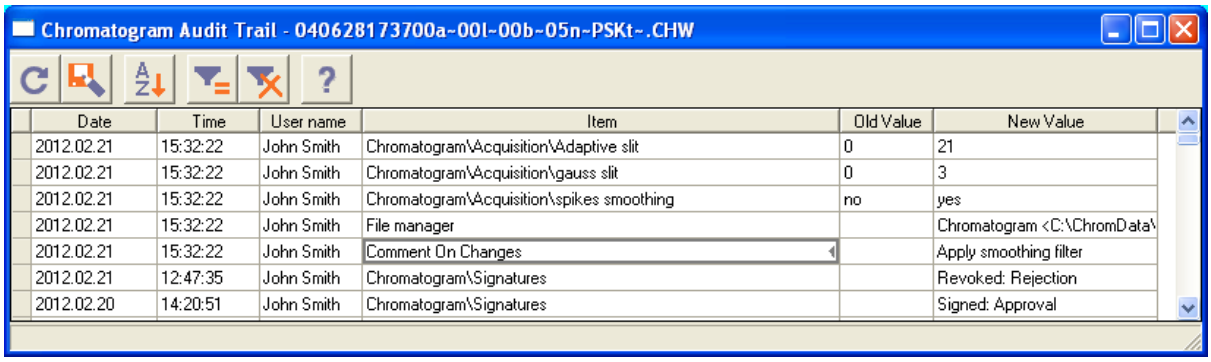
The **Chromatogram audit trail** window traces user activity concerned to the **chromatogram** 207.

Each **chromatogram** 207 keeps its own **audit trail** since the time when chromatogram file is created.

Chromatogram audit trail keeps history of all changes of the data processing settings which were introduced by users to the **chromatogram**. Also it keeps history of actions (such as applying or revoking **electronic signatures** 61) performed by users with **chromatogram**.

The **chromatogram audit trail** is updated automatically each time when updated **chromatogram** is saved to file. The ongoing changes which were not saved to file are not reflected in the **chromatogram audit trail**.

All entries in the **audit trail** are stamped automatically with user name, date, and time of the entry and cannot be cleared or edited.



Chromatogram audit trail table

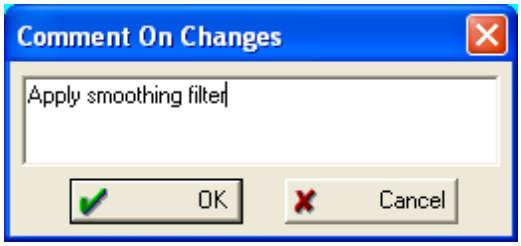
It consists of the following columns:

Date	Date of the entry.
Time	Time of the entry.
User name	Full name of the user who performed action or modification. See **security system** 45 and **Add user** 51 window.
Item	The name of modified parameter, action identifier or source of the event.
Old value	Old value of the parameter (before the modification). This item is empty when action was performed or event is logged.
New value	New value of the parameter (after the modification) or action description or event description.

In addition to automatic logging, user can specify free-text **user comments on changes** which describe the changes made. User specifies **comments on changes** at the time when the updated chromatogram is written to the file. **Comments on changes** can be reviewed in the **audit trail** along with other automatically generated entries.

☑ **Require user comment on changes** option of the **Global preferences** 41 window should be set to activate this function.

User comments are entered in the **Comments On Changes** window that appears before the chromatogram saving:



The chromatogram saving is not performed until user comments has been entered.

See also:

Audit trail 67

Audit trail user interface 70

History audit trail 67

FDA 21 CFR Part 11 54

Global preferences 41

3.5.4.4 Audit trail user interface

Chromatogram audit trail 68 and History audit trail 67 have similar user interface.

User interface offers filters 71 and sorting 73 capabilities to navigate through entries in audit trail 67.

Appropriate functions are supplied by toolbar 70 and item menu 71.

See also:

Audit trail 67

Chromatogram audit trail 68

History audit trail 67

3.5.4.4.1 Audit trail: toolbar

An ***audit trail toolbar*** contains button that perform the following operations:

Refresh information in the audit trail 67 window. By default the information is refreshed at the window opening. Press this button to view entries which appear after the time when audit trail 67 window was opened.

Save audit trail 67 entries to the disk file in text format. Name of the file is specified by the user.

Specify sorting rules for audit trail 67 entries. This command opens Sort 73 window.

Make a content of the selected cell as a **filter specifier**. Similar records are found and displayed while other are discarded. See audit trail: Filters 71.

Reset the filter. All entries of the table audit trail 67 are shown. See audit

trail: Filters 71.

Call the help topic for audit trails 67.

See also:

Audit trail user interface 70

3.5.4.4.2 Audit trail: filters

Audit trail user interface 70 supplies **filters** to help users to navigate through entries in the audit trail 67.

Filters are based on one or several **filter specifiers**.

Each **filter specifier** is a text mark which represent the partial or full content of the cell in some column of the audit trail 67.

Filter specifier can be ***inclusive*** (only entries which match the text mark are displayed) and ***exclusive*** (only entries which do not match the text mark are displayed).

For example, adding ***"John Smith"*** as ***inclusive* filter specifier** for **"User"** column displays all entries which refer to actions performed by user ***John Smith*** and hides all other entries.

Adding ***"Chromatogram\Calibration"*** as partial ***exclusive* filter specifier** for **"Item"** column hides all entries which refer to the updates in the calibration 165 settings (in chromatogram audit trail 68).

To create an inclusive **filter specifier** from the entire content of the selected sell user can use  button available at the toolbar 70.

To create inclusive or exclusive **filter specifier** from the entire or partial content of the selected sell the pop-up item menu 71 should be used.

Use  button available at the toolbar 70 to reset all **filter specifiers** and display all entries of the audit trail 67.

See also:

Audit trail: item menu 71

Audit trail user interface 70

3.5.4.4.3 Audit trail: item menu

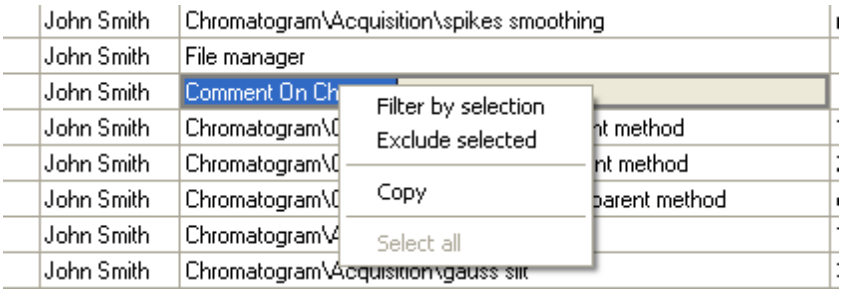
***Pop-up* item menu** for audit trail 67 supplies additional functions which help user to navigate through entries in audit trail 67.

Most functions in this menu are designed for specifying **audit trail filters** 71.

To use these functions first perform [Mouse Left Button Double Click] to select and highlight the required cell in the **audit trail** 67.
Then use ***mouse*** or ***keyboard*** to make a text selection in the highlighted cell.
The text selection can include any part of the cell content: beginning, end, middle, or entire content can be selected.

The selection in the cell can be used as a text mark for for ***inclusive*** or ***exclusive*** **filter specifier**. See **audit trail: filters** 71.

When selection is done perform [Mouse Right Button Click] at selected cell.
This displays ***Pop-up*** **item menu**:



The following commands are available:

Filter by selection	Creates ***inclusive*** **filter specifier**. Selected text is used as text mark for filter. See **audit trail: filters** 71.
Exclude selection	Creates ***exclusive*** **filter specifier**. Selected text is used as text mark for filter. See **audit trail: filters** 71.
Copy	Copy the selected text to clipboard
Select all	Select the entire text content of the cell.

Note, that for **filter specifier** it does matter what part of the text is selected in the cell.
The selection at the beginning of the text means that target text mark must appear at the beginning of the text of the cells at specified column.
The selection at the end of the text means that target text mark must appear at the end of the text of the cells at specified column.
The selection in the middle of the text means that target text mark can appear at any place of the text of the cells at specified column.
The selection of entire text means that target text mark must be equivalent to entire text of the cells at specified column.

For, examples let us consider ***inclusive*** filter created with **Filter by selection** command for **"Item"** column:
Selection for word *"Chromatogram"* at the begging of the text of the cell would display all entries where text at **"Item"** column starts with "*Chromatogram*" word.
Selection for word *"Chromatogram"* in the middle of the text of the cell would display all entries where text at **"Item"** column contains "*Chromatogram*" word at any place.

See also:

Audit trail: filters 71
Audit trail user interface 70

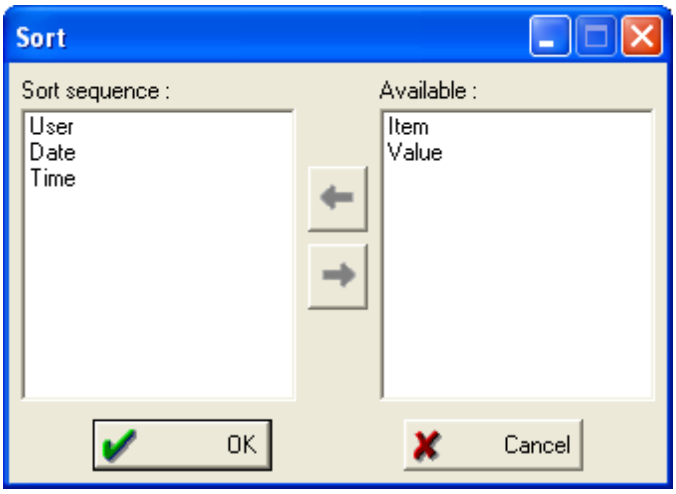
3.5.4.4.4 Audit trail:sorting

Sort window is opened by clicking on the  button located at the toolbar 70 of audit trail 67 window.

It is used to define sorting rules. Sorting is performed using content of the columns in accenting order.

It is possible to select several columns to sort. In this case sort operations are applied consecutively, according to sorting keys listed in the **Sort sequence** area.

Any available keys from **Available** area can be selected. Use arrow buttons ← and → to move keys between lists.



Sort sequence — List of chosen sorting keys which specifies sorting rule. Sorting operations are applied consecutively, in the order the keys are listed here.

Available — List of available sorting keys. They are equivalent to titles of the columns in the audit trail 67 window. See Chromatogram audit trail 68 and History audit trail 67 for details

See also:

Audit trail user interface 70

3.5.5 Protected storage

To ensure compatibility with **FDA 21 CFR Part 11** 54 Chrom&Spec" software implements ***protected storage***.

Protected storage option is installed only if ***21 CFR Part 11 support*** option is specified during software installation. See **FDA 21 CFR Part 11** 54 for details.

Protected storage uses services provided by **Windows™** operating system to restrict access to directories which are used as storage for sensitive information.

Protected storage ensures that sensitive information cannot be occasionally deleted or corrupted by users of the ***workstation***.

Data in the protected storage cannot be accessed by regular means.

The following directories establish the ***protected storage***:

Data	Used as a default storage for chromatogram data files. Regular means has a read-only access to this directory.
Flog	Used as a storage for audit trail 67 files. Regular means has a read-only access to this directory.
Accounts	Used as a storage for user account data. Regular means has no access to this directory. Additionally the sensitive user data (passwords, **certificates** 57, etc) are stored in encrypted form with encryption key based on user **password**. It is not possible to steal this information by breaking ***protected storage***.
SERVICES	Used as a placeholder for ***protected storage*** server binaries.

See also:

Security system 45

21 CFR Part 11 definition 54

3.6 Windows handling

3.6.1 Control menu

The **Control menu** is a standard Windows option. It is called up by [Alt]+[Space] short key combination or right-button click the upper part of the window.

It consists of the following commands:

Restore	Restore the window to its previous size after it has been maximized or minimized.
Move	Enable you to use the keyboard to move the window to another position.
Size	Enable you to use the keyboard to change the size of the window.
Minimize	Reduce the window to an icon.
Maximize	Enlarge the window to its maximum size.

Close Quit Windows, or close the window.

3.6.2 Cascade windows

(*Main menu* Window / Cascade)

Cascades all opened chromatogram windows.

3.6.3 Tile windows

(*Main menu* Window / Tile vertical)

Allows vertical tiling of open chromatogram windows.

(*Main menu* Window / Tile horizontal)

Allows horizontal tiling of open chromatogram windows.

3.6.4 Close all windows

(*Main menu* Window / Close all)

Close all opened chromatogram windows.

Part

4 Equipment control

Chrom&Spec implements native digital equipment control of hundreds devices from different manufactures: detectors, pumps, autosamplers, thermostats, valves, ADCs and so on. The list of supported instruments is continuously extended.

Most commonly chromatographic equipment is controlled automatically with parameters and time programs stored in a **System** 79. Manual control can also be used when required.

See also:

System 79

Software basics 18

4.1 Workplace

4.1.1 Workplace definition

The **workplace** contains all **external devices (interfaces)** 107. Also a **workplace** is place-holder of all **systems** 79 when they are in **connected** state (see **Connect to workplace** 89). The **workplace** can also contain some other auxiliary modules.

Workplace manages all available instrument resources. It ensures that resource used by some **system** in the analysis can not be accessed or affected some-how by another **system**.

The icons of all active interfaces, devices and systems are shown on the main **toolbar**.

They can also be displayed in the **Workplace window** 77 opened by selecting the **Options / Devices setup** menu item.

See also:

Workplace window 77

How to add an interface to the workplace 463

4.1.2 Workplace window

(*Main menu* Options / Devices setup)

Open the "**WORKPLACE**" window which shows all **interfaces** 107 and **devices** 105 installed. This window can be opened only by the user with **Administrator** access level.

<Setup>	Opens a configuration user interface of the selected device or module.
<Install device>	Installs a new interface. Opens **Add devices to WORKPLACE** 94 dialog form. This form is analogous to corresponding page of the **New system wizard** 93.
<Delete device>	Delete selected device from the workplace.

See also:

Workplace definition 77

Connect to workplace 89

How to add an interface to the workplace 463

4.1.3 Workplace common items

4.1.3.1 Timer

4.1.3.1.1 Global timer

The timer is used for programming system tasks which are started automatically daily or once at the desired time. The "**Global timer**" icon is available on the toolbar if the **Timer** has been installed with the **"New system" wizard** 93 or by using the **<Install device>** command of the **Workplace window** 77. By clicking this icon the **Timer window** 78 for parameter settings opens.

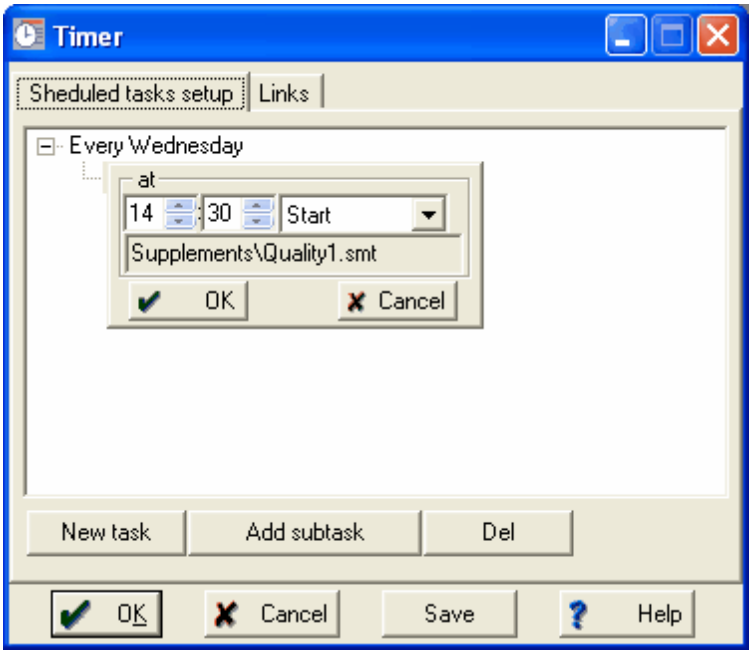
See also:

Timer program 78

How to install the global timer 465

4.1.3.1.2 Timer settings

Timer settings window provides user interface for configuring scheduled tasks.



The timer is used for programming system tasks which are started automatically daily or once at the desired time.

See also:

Global timer 78

How to install the global timer 465

4.2 Systems

4.2.1 System definition

System is a key definition of Chrom&Spec software. Chrom&Spec implements digital equipment control of hundreds devices from different manufactures: detectors, pumps, autosamplers, thermostats, valves, ADCs and so on.

To perform chromatographic analysis typically several devices must run synchronously.

System is an aggregated chromatographic complex consisting of several instruments operating together. **System** stores all instrument-specific settings and controls how instruments operate during chromatographic run. **System** may define control programs and alliances between devices.

System does not contain information on data processing algorithms, still it includes a reference to **Method** 122 that is used for data processing. This reference is handled by **Data recorder** 99 module.

Systems are stored as system files (***.smt**) in a sub-folder of **ChromData\Systems** folder. They can be opened using the corresponding **Open system** 79 menu.

Each opened **System** displays its user interface on the desktop in a separate **System window** 80. **System window** allows making configuration of the **System**, to set up hardware control parameters, and to start a new **chromatogram** 207. Several sequential runs of the **system** could be arranged to the **sample queue** 237.

Chrom&Spec software can run two or more **systems** at the same time. Generally this is possible if systems use different set of instruments. Sometimes several systems can share resources of some device. See **device definition** 105 topic for more details.

To create a new **system** use **Creating new system** 93 wizard.

See also:

Creating new system 93 wizard.

How to create a new system 466

How to open a system 467

How to select processing method and data source 467

4.2.1.1 Open system

(*Main menu* File / Open / System...)

Load an existing system file (***.smt**) from the **Systems** directory and open the corresponding **SYSTEM WINDOW** .

The name of the folder and of the system file are displayed in the title bar of the **SYSTEM** window.

The opened system is in off-line state. Still user can start it immediately. In this case the software will connect the system (see **Connect to workplace** 89) and will initiate device detection procedure.

See also:

Close system 82

How to open a system 467

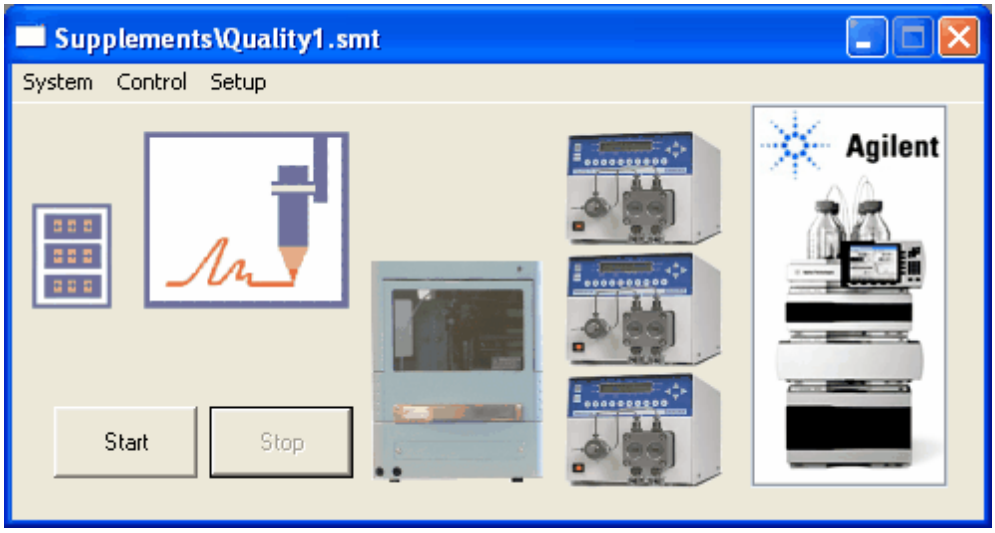
How to create a new system 466

4.2.2 System window

In "Chrom&Spec" software system stores information on the hardware configuration, and parameters that are needed for hardware control and data acquisition. Each system defines a set of instruments which must run synchronously to perform chromatographic measurement.

System window supplies user interface for configuring instruments. Each device or other module used by the system is shown as **icon**

in the systems window.



Double click icon. Shows instrument configuration user interface, which is specific for each instrument.

Right-button click icon. Displays instrument-specific menu. Typically it has the following items:

Open Shows instrument configuration user interface like **double clicking** the icon.

Unlink Removes instrument or other module from the system.

Besides additional instrument-specific items could be available, such as access to service functions, operating procedures and so on.

Note: Some instrument configurations are not available when system is in off-line mode. To make system on-line connect it using Control / Connect to workplace 89 menu.

System window menu

System 81	Handling of system files, sample queue.
Control 82	Start and stop functions, connect/disconnect system.
Setup 90	Setup of system functions.

4.2.2.1 System window menus

4.2.2.1.1 System menu

Save as... 81	Save the selected system in the file under the different name.
Change... 81	Change current system with a system from a different file.
Open other... 81	Open another system.
Sample queue... 237	Open an existing or create a new sample queue file (***.que**).
Close 82	Close selected **SYSTEM WINDOW** .

4.2.2.1.1.1 Save system as...

(*System menu* System / Save as...)

Make a copy of the system. Save the current system to file with a different name (***.smt**) in the desired folder in the **Systems** folder. The current file of the system remains unchanged.

4.2.2.1.1.2 Change system

(*System menu* System / Change...)

Open the selected new system in the desired system folder. The current system is disconnected and closed, and the new system is connected.

See also:

Open other system 81

How to open a system 467

4.2.2.1.1.3 Open other system

(*System menu* System / Open other...)

Load an existing system file (***.smt**) from the desired system folder in the **Systems** directory and open a new **SYSTEM WINDOW** for parameter settings. The old system remains connected.

See also:

Change system 81

How to open a system 467

4.2.2.1.1.4 Sample Queue...

(*System menu* System / Sample Queue...)

Load an existing or create new **sample queue** 237 **file** (***.que**).

When user specifies the existing file name (typically by clicking the **file name** shown in the form) the **sample queue** 237 is opened from the file specified.

User can specified a new non-existing file name. In this case a new **sample queue** 237 is created and opened.

It is assumed that **sample queue** 237 refer to the current **system**. The file of the current **system** (***.smt**) and file of the **sample queue** 237 (***.que**) must be located at the same directory.

See also:

Sample queue definition 237

4.2.2.1.1.5 Close system

(*System menu* System / Close)

Disconnect the system from the **workplace** (see **Disconnect from workplace** 90) and close the system.

The  icon corresponded to the system is removed from the **toolbar** 25.

Note that closing system using "cross button"  in the right top of the **SYSTEM window** 80 performs a rather different action. It just hides the **SYSTEM window** 80 still the **system** 79 remains active. The hidden system can run analyses and perform other instrument control actions.

The  icon is always present at the **toolbar** 25 for each active systems. Clicking this icon displays the corresponded **SYSTEM window** 80 again and brings it to the top of all other windows.

See also:

Open system 79

4.2.2.1.2 Control menu

Start run 83	Start run of the connected system.
Stop run 83	Stop current run.
Stop data acquisition 84	Stop data acquisition, but continue time program.
Startup hardware (Measure baseline) 84	Start pumps, thermostats, detectors, etc. User can observe the baseline stabilization process.
Shutdown hardware 85	Stop current run, switch off pumps, thermostats, lamps, etc.

Auto restart 85	Automatic start of a new run after preceding run has been finished.
Verify sample 85	Open sample passport window at each start of a run. User can specify sample-related information.
Connect to workplace 89	Connect system to the PC COM port.
Disconnect from workplace 90	Disconnect system from the PC COM port.

4.2.2.1.2.1 Start run

(*System menu* Control / Start run)

Start run command starts the instruments and performs initialization for the analysis.

It sends the **System startup values** to the devices.

Typically base-line monitoring is started (if supported by instruments). All instruments begin initialization (heating columns up to required temperature, switching on lamps of the detectors, calibrating detectors and so on).

When initialization finished devices with **immediate start** start their **time programs** (see **Start mode** 91 settings).

Other devices wait for **Inject** event.

When **Inject** is done chromatogram resets baseline monitoring and start measurement. Devices which **start with inject** start their **time programs** (see **Start mode** 91 settings).

Generally the run is stopped automatically when all devices finish their **time programs** and a chromatogram is finished (the duration of the chromatogram is defined in its **Method** 122)

A current run can be aborted by **Stop run** 83 command.

If you want just stop the data acquisition and let the **time programs** of the devices execute normally, select **Stop data acquisition** 84 command.

See also:

Stop run 83

Stop data acquisition 84

How to start a run 474

4.2.2.1.2.2 Stop run

(*System menu* Control / Stop run)

This command aborts the current run.

Data acquisition and time programs are terminated immediately. The recorded chromatogram is saved automatically only if the **Inject** was already done.
Alternatively the run can be stopped with **Finish!** 31 menu command from **main window menu** 25 or by  button from **main window toolbar** 36.

See also:

Start run 83

Stop data acquisition 84

How to stop a run 475

4.2.2.1.2.3 Stop data acquisition

(*System menu* Control / Stop data acquisition)

Stop data acquisition of the current run immediately.

Recorded chromatogram is saved automatically if the **Inject** was already done.

The **time programs** of the running devices continue normal execution.

See also:

Start run 83

Stop run 83

4.2.2.1.2.4 Startup hardware (Measure baseline)

(*System menu* Control / Startup hardware (Measure Baseline))

This command performs necessary instrument initialization without starting actual measurement.

Topically initialization involves the following actions:

- Send **System startup values** to the devices.
- Start **detectors**.
- Start monitoring of the baseline signal using the Method attached to the System.
- Start **solvent delivery system (pumps)**.
- Performs column heating.

Time programs of the devices are not started.

When to use

Some detectors may need time to enter the operating mode. In this case user can just startup hardware and evaluate the state of the detector by monitoring baseline signal.

Also this command useful for column washing and evaluating column state.

When all preparations are done proceed with actual analysis using **Start run** 83 command.

A run can be aborted using **Stop run** 83 command.

See also:

Shutdown hardware 85

4.2.2.1.2.5 Shutdown hardware

(*System menu* Control / Shutdown hardware)

This command shuts down the devices. Generally shutting down stops any activities of the devices.

Typically shutting down involves the following actions:

- Stopping **solvent delivery system (pumps)** to avoid eluent spending.
- Switching off lamps and other elements of the detectors to save their resources.
- Minimizing electric power consumption of the device (when supported).

Besides shutting down aborts running analysis of the system, if any.

See also:

Startup hardware 84

4.2.2.1.2.6 Auto restart

(*System menu* Control / Auto restart)

If this option is enabled, a new run is started automatically using the current system after the preceding run has been finished normally.

This option allows making an infinite **batch cycle** with the current system.

This option is ignored if a run is initiated from **sample queue** 237.

4.2.2.1.2.7 Verify sample

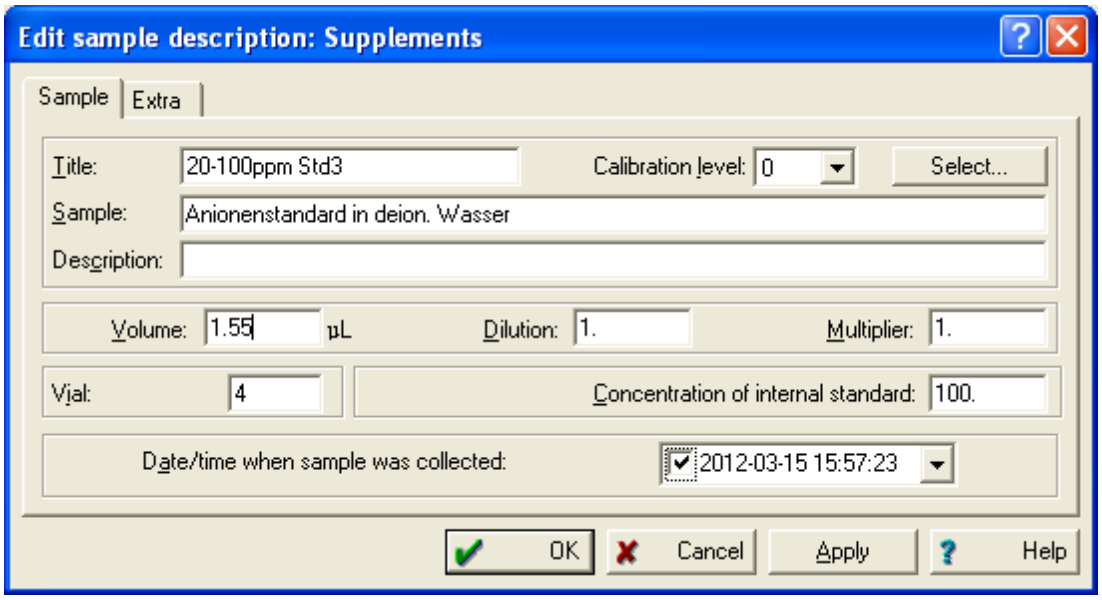
***(System menu* Control / Verify sample)**

If this option is **enabled**, the **Edit sample description** 85 window is opened automatically at the start of each run for entry of sample information.

This option is not used if a run is initiated from **sample queue** 237.

The **Edit sample description** window is opened automatically at each start of a run if the **Verify sample** 85 option of the **system control menu** 82 is enabled.

Sample page contains a set of items which describe sample used in this analysis. Items can be edited before performing the **injection**.



Title 126 — User defined identifier (title) for the chromatogram. **Title** 126 item at the **General** 124 page of the **Method setup** 124 for **Method** contains the default value for this item, which can be modified here. When chromatogram is finished **Title** 126 item at the **General** 124 page contains actual value for run.

Calibration level 199 — If the current run is used for calibration, specify the identifier of calibration level from a drop-down list. If the run is non-calibration measure, set this item to **0**.

Select... 87 — Opens **Select and edit calibration level** 87 helper dialog form. User can select a calibration level for run and modify concentrations if necessary. A selected calibration level is entered to **calibration level** item when finished.

The remaining items are analogous to that of the **Sample** 126 page of the **Method setup** 124. **Method** defines the default values which can be modified here.When chromatogram is finished **Sample** 126 page contains actual values for run.

Sample — User-defined sample name or basic sample description (max. 256 characters).

Description — Additional sample description (max. 256 characters).

Volume — Injected volume in micro liters.

Dilution — Dilution of the sample.

Multiplier — Sample multiplier. This is a sample concentrating factor.

Note. **Volume, Dilution and Multiplier ,** are interrelated items. They are used to calculate **component *quantity*** (e.g. **component *weight***) for both calibration run and analyte. See

adjusted volume 199 and **quantity** 200 for details.

Note. The detector response (peak area or height) is related directly to **component *quantity*** value**,** not **component** concentration**.** So **component *quantity*** is actually used to build **calibration curve** 182. For analyte a **component *quantity*** is calculated from calibration curve. See **quantification** 201 for details.

Note. Set **Dilution and Multiplier** values to 1.0 if these parameters are not used in your analysis.

Vial — Auto-sampler vial position identifier to take sample from. Typically this is a numeric value. Still some auto-samplers may require a vial position in a special string form. Refer to documentation of the auto-sampler which you use.

Concentration of internal standard — Concentration of the **standard component** for quantification using **relative concentration** 202 method.

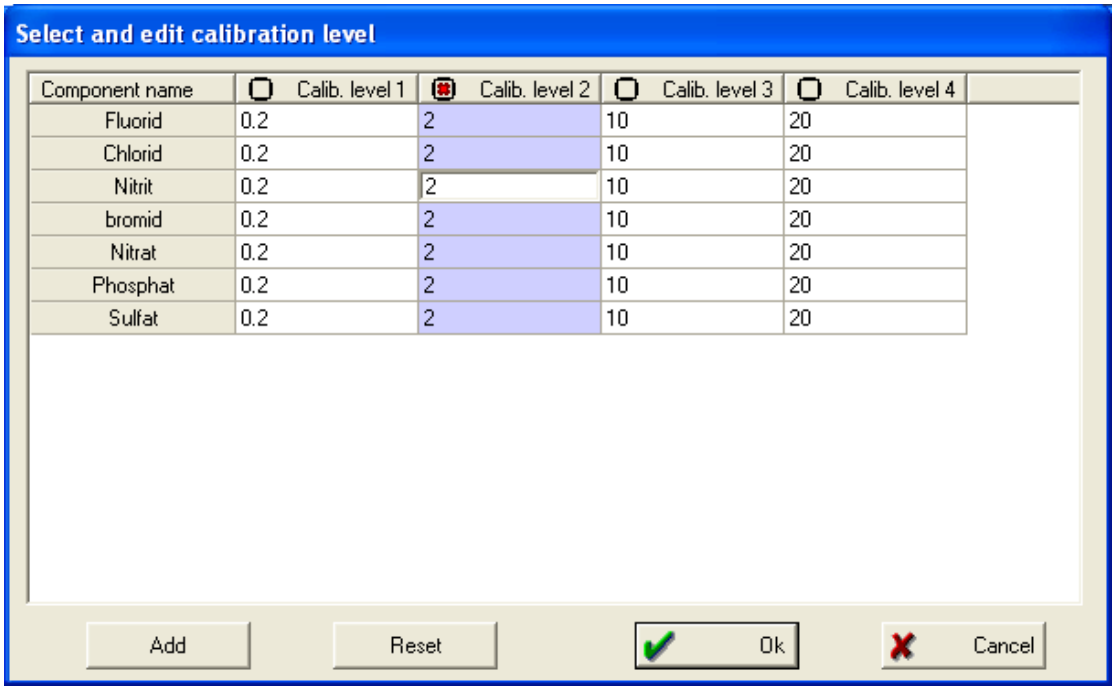
Date/time when sample was collected — This date/time stamp can be changed by the user, if date and time of the sample collection are essential. The default values are equal to the date and time when the chromatogram starts.

Note. **System** may contain autosamplers and other injected devices. Depending on capabilities of the devices user may configure them to use values defined in **Vial number, Volume, Dilution, Multiplier** in the injecting procedure. Alternatively some devices may ignore values defined here and overwrite them by actually used values which were defined some-how else in the device configuration. Refer to documentation of the auto-sampler which you use.

See also:

Select calibration level 87 dialog form
Edit sample extra parameters 89 page
Verify sample 85

This dialog form lets user to review components and concentrations of standards. The form is designed to help user to select an appropriate calibration level for the calibration run.



This form is similar to **Concentrations table** 174 for the **Method**.

To use this dialog form a **Components table** 171 must be already defined in the processing **Method**.

To select a calibration level click a header item of appropriate calibration level. The header item is marked as selected.

When calibration level is selected its concentrations can be edited if necessary.

Note. Typically concentrations of standards are defined in the **Method** in the **Concentrations table** 174. If concentrations are correct no modifications are required. When user decides to change the concentration of the standard this form allows inserting modifications "on the fly", without going to method modification. When run is finished all modifications are applied to **Method**.

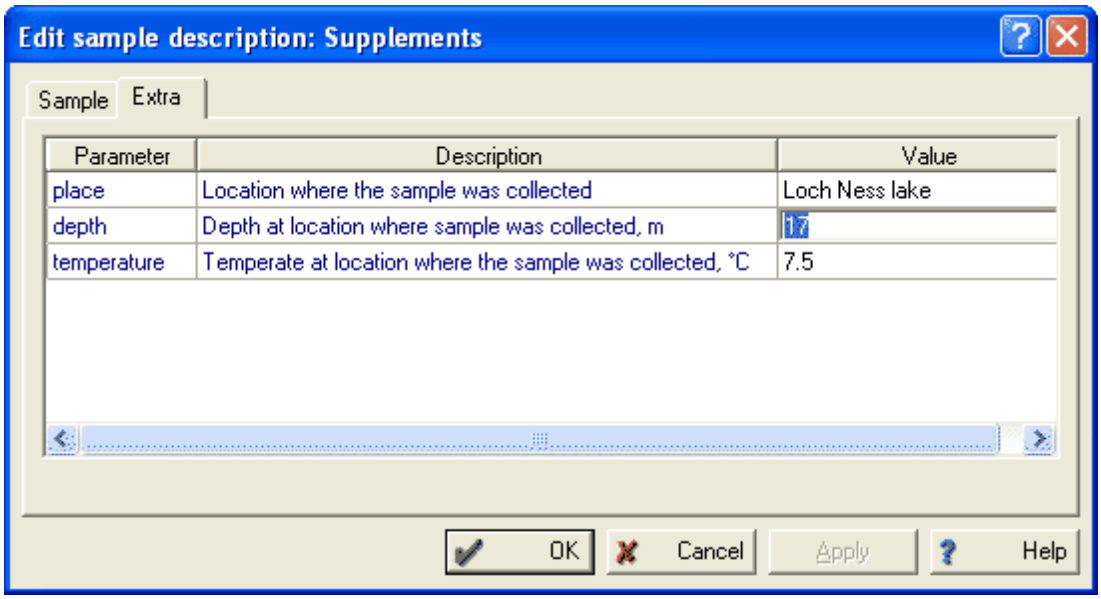
Note. User can modify concentrations of the selected calibration level only.

Add	Add a new calibration level. User is allowed to add only one calibration level at this form. Added calibration level is selected and no other calibration level can be selected any more. Added calibration level is used for current calibration run.
Reset	Resets all modifications made in this form and restores original values which were read from **Method**
Ok	Applies all modifications. The selected calibration level appears at **Calibration level** item of the **Sample** 85 page of **Edit sample description** 85 dialog form.
Cancel	Resets all modifications made in this form and closes the dialog form.

See also:

Edit sample description 85 dialog form.

Extra page allows user to edit values of **Method**-defined custom parameters for current sample run.



All items at this page are identical to items at the **Extra** 128 page of the **Method setup** 124 for **Method.**

The **Parameter** and **Description** items in the list are taken from the method. For consistency user is not allowed to modify them as well as delete items from the list or insert new items to the list. (These operations must be done at **Method** configuration, see **Extra** 128 page).

The default **Value** item are also taken from the **Method.** Still user is allowed to modify any **Value** items and set them to actual values for the processed sample.

See also:

Edit sample description 85 dialog form.

Extra page of the Method setup 128

4.2.2.1.2.8 Connect to w orkplace

(*System menu* Control / Connect to workplace)

This commands connects a selected system to the **workplace** 77 and puts it to **on-line** state.

When **system** is connected its device drivers are allowed to communicate with instruments and device drivers enable manual control functions if supported.

When **system** is connected it captures for exclusive use all the devices and other resources used by the system. Connection is not possible if some device or other resource is already captured by another connected system.

Some instrument configurations are available only if the system is connected (in **on-line** state).

For each connected **System** an  icon appears on the main **toolbar** 25. If this icon is clicked, the **SYSTEM** window is displayed over all other windows.

Note: "Start run" and "Startup hardware" commands automatically connect the System to workplace

See also:

Disconnect from workplace 90

How to connect a system to the workplace 467

4.2.2.1.2.9 Disconnect from w orkplace

(*System menu* Control / Disconnect from workplace)

This command disconnects selected system from the **workplace** 77.

When **system** is discounted it frees all devices and other resources which were used by it. Devices and other resources became available for another systems.

When **system** is connected its device drivers can not communicate with instruments. Manual control functions and some other instrument configurations are disabled.

Device drivers may support configurations which are available in **off-line** mode.

See also:

Connect to workplace 89

4.2.2.1.3 Setup menu

Drag icons 91	Drag and drop or resize icons in the **SYSTEM WINDOW** .
Zoom in	Scales icon in the **SYSTEM WINDOW** increasing size.
Zoom out	Scales icon in the **SYSTEM WINDOW** decreasing size.
Watch window 91	Contains a menu group related to the **watch window** 103.
Start mode... 91	Open the **Start mode** 91 window.

New devices

Install new device 92	Install **internal** devices to the system.
Link to existing device 92	Connect system to control module (sub-device) of **external** devices.

Parameters

Print 92	Prints system parameters and instruments settings in text report.

4.2.2.1.3.1 Drag icons

(*System menu* Setup / Drag icons)

If this option is enabled, the device icons can be resized and moved in the **SYSTEM WINDOW** and the **SYSTEM WINDOW** itself can be resized.

To resize an icon or the window, move the cursor to the desired object corner or border until arrow ⤡ appears. Press the left mouse button and resize the object to the desired size.

To move an icon, move the cursor to the desired object until ✛ appears. Press the left mouse button and move the object to the desired place.

When the editing is finished, check out the “Drag icons” item.

4.2.2.1.3.2 Watch window

(*System menu* Setup / Watch window)

This menu group of the **system window** 80 contains the following items:

Automatically open watch window	If this option is enabled, the **watch window** 103 is automatically opened when a run or measure baseline action is started.
Manual configuration	Manual configuration of the **watch window**. See **watch window** 103 for details.
Auto configuration	Auto configuration of the **watch window**. See **watch window** 103 for details.

See also:

Watch window 103

4.2.2.1.3.3 Start mode

(*System menu* Setup / Start mode)

This menu item opens the **START MODE** window with the following two fields:

Immediate start The time programs for the listed device drivers (or the data acquisition for Recorder driver) are started at the moment the run is started.

Start with inject The time programs for the listed device drivers (or the data acquisition for Recorder driver) are started at the moment the sample is injected.

The objects can be moved from one field to the other using the  or  button.

See also:

How to set the start mode 468

4.2.2.1.3.4 Install new devices

(*System menu* Setup / New devices / Install new device)

This command is used to install the new **internal device** 105 into the **system** 79.

Install new device command opens **Add devices to the system** window. This window is equivalent to **Add devices to the system** 95 page of the **New system wizard** 93.

See also:

Device definition 105

How to add devices to an existing system 466

4.2.2.1.3.5 Link to existing devices

(*System menu* Setup / New devices/ Link to existing device...)

This command is used to link the system to **sub-device** 109 of some **external device** 107.

The command opens **Control the external devices** window. This window is equivalent to **Control the external devices** 96 page of the **New system wizard** 93.

See also:

External devices 107

Sub-devices 109

How to add interface to System window 464

4.2.2.1.3.6 Print system parameters

(*System menu* Setup / Parameters / Print)

A report of the system parameters including the time program is created and opened using the "Wordpad" program. The ***.txt** file opened can be printed, saved and exported to other programs.

The system report includes the following elements:

STARTUP HARDWARE Name of the method linked to the system
Main measurement channel
Configuration settings for the devices
System startup values

IMMEDIATE START Objects defined in the **Start mode** 91 window. The time programs are printed if the programs are enabled.

START WITH INJECT Objects defined in the **START MODE** window. The time programs are printed if the programs are enabled.

See also:

4.2.3 System installation

4.2.3.1 Creating new system

(*Main menu* File / New / System...)

New system wizard is a main user interface designed for creating new systems.

When you start the wizard a **NEW SYSTEM WIZARD** window and a corresponded **SYSTEM** windows are opened.

The **New system wizard** guides you trough the installation routine step-by-step to build a new system. The next step of the system installation is reached with **<Next>**, the previous step with **<Back>** and the installation is completed with **<Finish>**.

Step 1 **Welcome to the New System Creation Wizard** 93

Step 2 **Add devices to WORKPLACE** 94

Step 3 **Add devices to the system** 95

Step 4 **Control the external devices** 96

Step 5 **Data recorder setup** 97

See also:

Open system 79

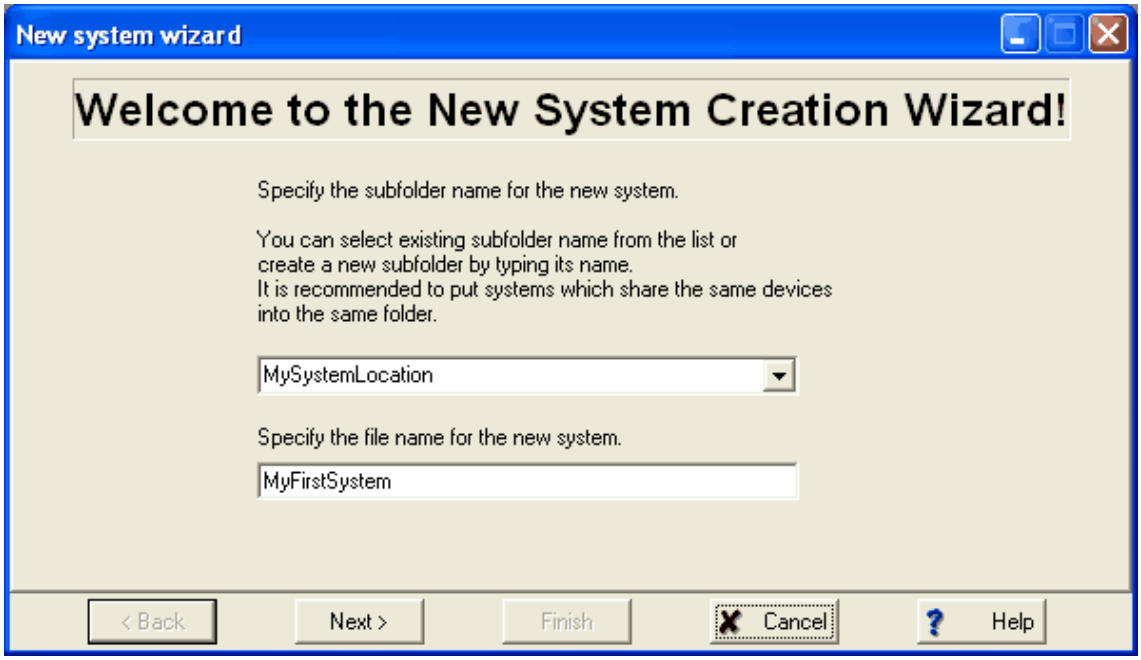
Close system 82

How to create a new system 466

4.2.3.1.1 New system wizard. Step 1

"Welcome to the New System Creation Wizard!" page.

The first step of the system installation is to enter a name for a system folder and a file name of the new system. System folder is created within the ChromData program path **...**\ChromData **\Systems**.



Usually you are creating a separate system for any analysis type you need. System and related method fully define the settings for analyses and data processing options.

It is recommended to put systems sharing the same instruments into the same folder, for example, when the same instruments are used in different kinds of analyses. This would allow software to effectively avoid instrument conflicts during sample queue execution.

See also:

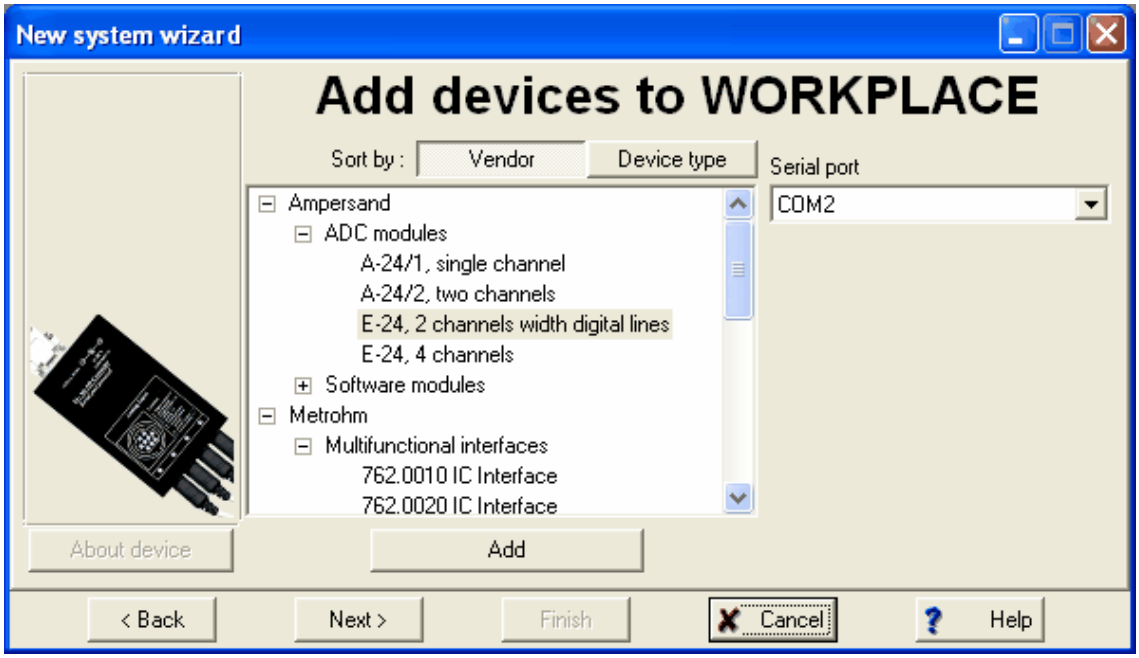
New system wizard 93

How to create a new system 466

4.2.3.1.2 New system wizard. Step 2.

"Add devices to WORKPLACE" page.

At the second step you can add **external devices** 107 to **Workplace** 77. **External device** is not owned by current system and could be shared by several systems simultaneously. A typical example of external devices is an **ADC** module. Two or more systems could link to different channels of multi-channel **ADC** module and perform different kinds of analyses at the same time.



Supported interfaces and other **external devices** 107 could by arranged by vendor or by type. Most devices need serial port to be specified. An icon of added module appears on the software toolbar.

Skip the second step if the desired module has been already added previously (during setup of another system) and its icon already shown on toolbar. You must not install the same external module twice!

See also:

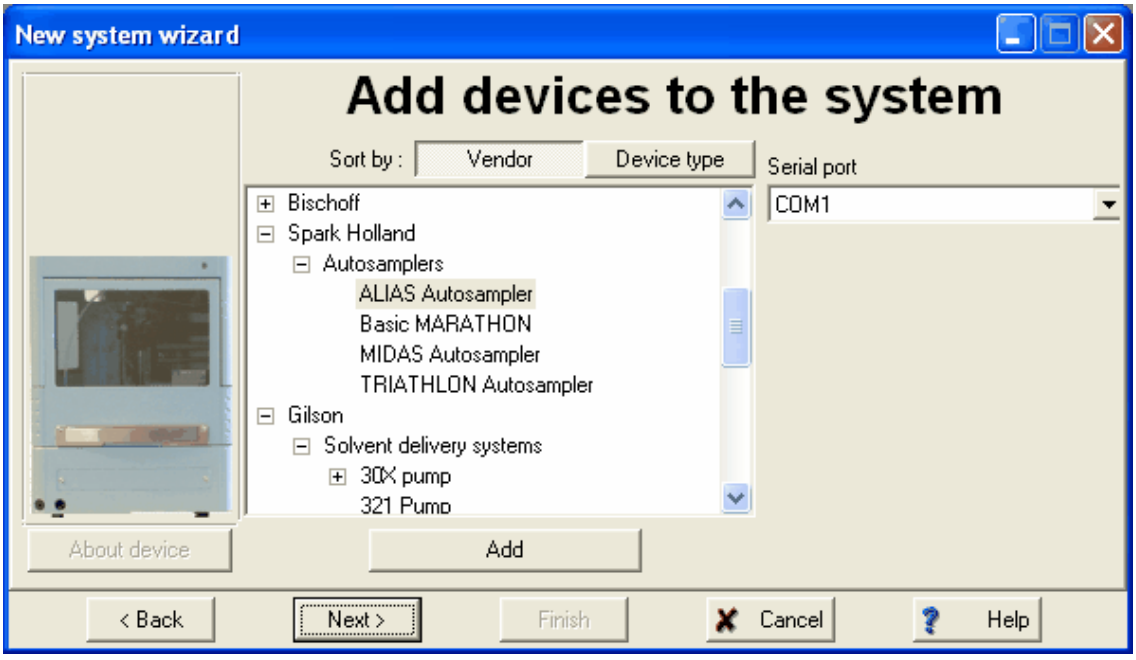
New system wizard 93

How to create a new system 466

4.2.3.1.3 New system wizard. Step 3.

"Add devices to the system" page.

At the third step you can add **internal devices** 105 to **System** 79. **Internal devices** are controlled by the system exclusively. Connected system locks all its internal devices so that no other systems could get access to them.



Supported devices could be arranged by vendor or by type. Typically a device needs a serial port to be specified. Some devices may need alternative communication settings: for example, when device operates through USB interface or through network.

To add a device, open the group which contains this device, select the device, specify the serial port where the device is connected to (or other communication option, if needed). After clicking on **<Add>**, the device is added to the system and its icon appears at the **SYSTEM WINDOW**.

If desired, an additional **data recorder** 99 can be added to the system.

See also:

New system wizard 93

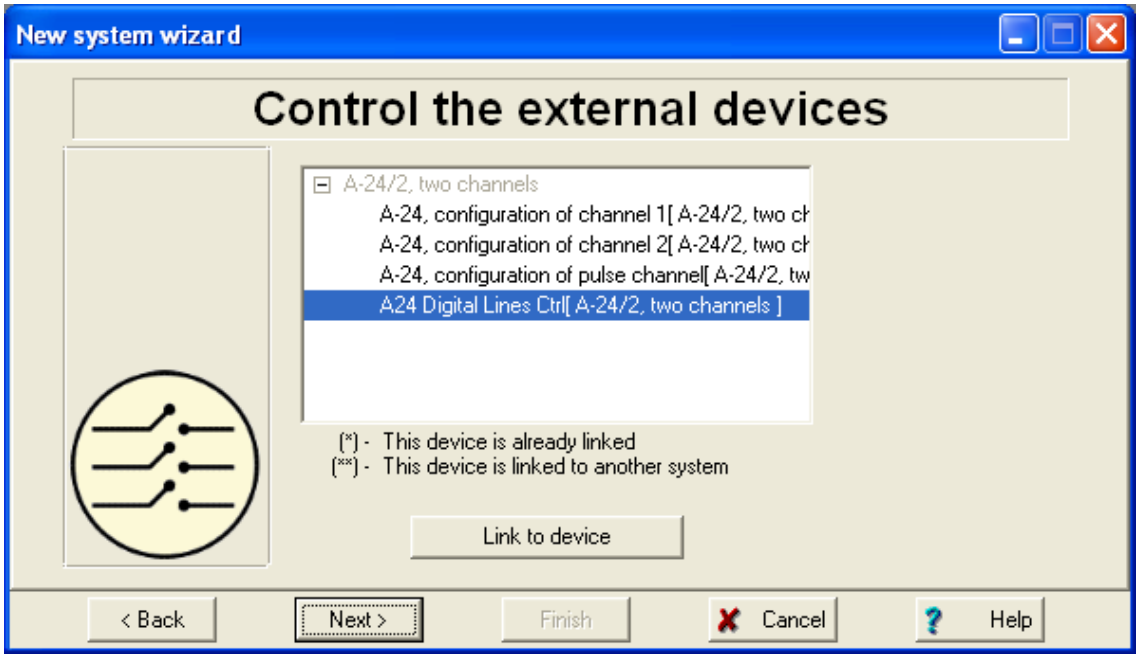
How to create a new system 466

4.2.3.1.4 New system wizard. Step 4.

"Control the external devices" page.

External devices 107 are not owned by current system and could be shared by several systems simultaneously.

Still external device can have so-called **sub-device** items. **Sub-device** item is a functional block or logical module which can be configured and controlled by current system.



Linked sub-device item is used by current system exclusively. When you link the sub-device item to the system, no other connected system is allowed to use it.

For example, consider 2-channel external ADC module A-24 which equipped with several switches which could be controlled by the software. You can setup **System 1** to use **channel 1** of **A-24** and link system to **A24 Digital Lines Ctrl** sub-device to control autosampler, valve or other devices.

Additionally, you can setup **System 2** for another type of analysis which needs no any digital lines control. **System 2** would use **channel 2** of **A-24 ADC** module and can run simultaneously with **System 1**.

In this configuration **System 2** could not be configured for controlling **A24 Digital Lines** because they are controlled exclusively by **System 1.** So **System 2** could not affect normal operation of **System 1.**

See also:

New system wizard 93

How to create a new system 466

4.2.3.1.5 New system wizard. Step 5.

"Data recorder setup" page.

The settings at this step are equivalent to **Data recorder setup** 100.

You are selecting **data processing method** 122 and configuring **data sources** 102 for chromatogram.

Press **<Finish>** button when done.

The new system is now ready for **starting run** 83.

See also:

New system wizard 93

How to create a new system 466

4.2.3.2 Install new devices

(*System menu* Setup / New devices / Install new device)

This command is used to install the new **internal device** 105 into the **system** 79.

Install new device command opens **Add devices to the system** window. This window is equivalent to **Add devices to the system** 95 page of the **New system wizard** 93.

See also:

Device definition 105

How to add devices to an existing system 466

4.2.3.3 Link to existing devices

(*System menu* Setup / New devices/ Link to existing device...)

This command is used to link the system to **sub-device** 109 of some **external device** 107.

The command opens **Control the external devices** window. This window is equivalent to **Control the external devices** 96 page of the **New system wizard** 93.

See also:

External devices 107

Sub-devices 109

How to add interface to System window 464

4.2.3.4 Delete systems

To delete an existing system, delete the ***.smt** file in the **Systems** folder.

Invoke a list of existing ***.smt** files (for example, use ***System menu*** **System / Change** option), select the desired System file, click the right mouse button to open a context menu, and execute "Delete" command.

4.2.4 System state window

The **SYSTEM STATE** window is automatically opened if a system is connected to workplace. It shows status and error messages for this system. Messages concerning a device are followed by **["device name"]**, messages concerning the loaded system are followed by **["folder name"]** (name of the folder that contains the system file). The following messages can appear:

Status messages

Checking on-line	Checking connection between PC and device.
On-line	Connection between PC and device is OK.

UploadStartupValues	Hardware or system startup values have been loaded to the device.
Initialization	Hardware or system initialization.
Ready	Device is ready.
Starting	Starting program or chromatogram data acquisition.
Running	Running program or chromatogram data acquisition.
Running program (xxx min left)	Running time program with time display.
Waiting for INJECT	Waiting for "INJECT" to start program and/or chromatogram data acquisition as defined in the **start mode** 91.
INJECT done	Injection valve has been switched to the "INJECT" position. Program and/or chromatogram data acquisition have been started.
Stopping	The run has been stopped.
Finished	Program or chromatogram data acquisition has been finished.
SHUTDOWN	System is **shutdown** 85.

General error messages

Detection of hardware failed	Bad connection between PC and device or device switched off (check connecting cable or switch on device).

4.2.5 System common items

4.2.5.1 Data recorder

The **Data recorder** is a component which present in a new **SYSTEM WINDOW** by default. If the system is connected and this icon is clicked with the right mouse button, the following menu appears:

Open 100	Open Data recorder setup window for selection of processing method and data source.
Open method 103	Load the processing method linked to the system and show an empty chromatogram window.
Unlink	Delete the **Data recorder** from the system (not recommended).

To record several single-channel chromatograms at the same time, additional data recorder must be installed for each detector. To record multi-channel chromatograms, only one data recorder icon must be installed, but several data source channels have to be linked to this data recorder. Some detectors (DAD and some other) can supply **spectral**channel. Single spectral channel as data source would expand to

multiple channels for each wavelength in the chromatogram.

See also:

Open processing method 103

Data recorder setup 100

Data source 102

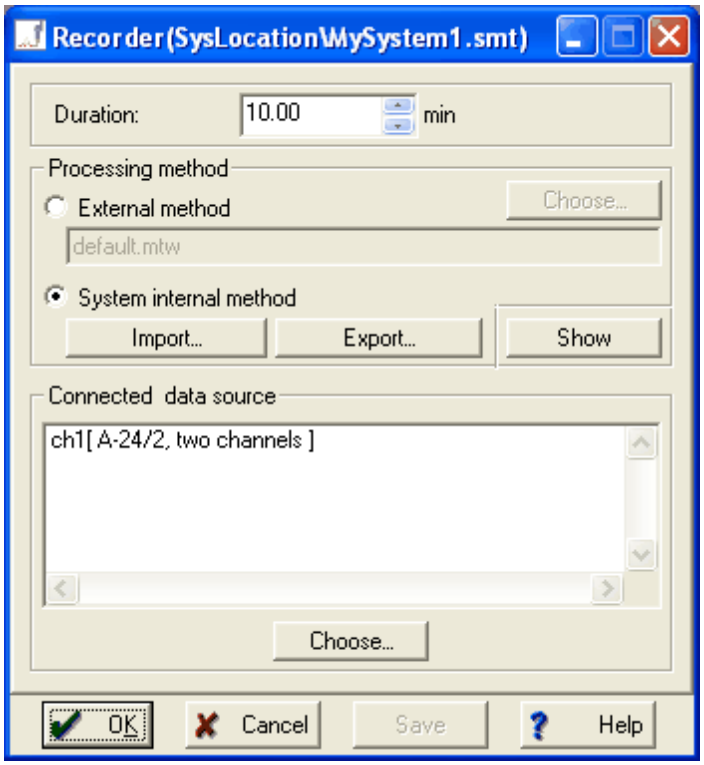
How to select processing method and data source 467

4.2.5.1.1 Data recorder setup

(Right click Data recorder icon, Open menu item of pop-up menu)

The same operation is performed by double-clicking the **Data recorder icon**.

Opens **"Recorder"** window for selection of data processing method and data source.
The title of the window contains also a name of the System (in brackets).



Duration — Duration of the chromatogram in **minutes**. It specifies the elution time after the inject. It is allowed to modify this value during the running of the chromatogram. This value is copied to **method** 122 when analysis starts. See **Duration** item in the **Method setup: "General" page** 124.

Processing method

Two options are available for the **processing method**.

External method

The method file is stored separately from the system, usually in ***ChromData\Methods*** folder. User can specify any valid file name for the external method. Several systems may use the same external method simultaneously. Changes in the method affect all systems which use it.

<Choose...> Select the external **method** 122 file (***.mtw**) to be linked to the system..

System internal method

Internal method is owned by its system. No other system can use it. Using internal method ensures integrity of **system + method** settings. The method file is stored in the same folder where system (***.smt**) file is stored in. System automatically assigns the file name for the internal method and user is not allowed to change it. Usually the file name of the internal method is the same as of the system file with (***.mtw**) extension.

<Import...> Import internal method for the current system from another method. If you have a method which is adequate for your needs click on **<Import...>** and select the desired **method** 122 file ***.mtw**. Imported method could be a basis for further configurations for your analysis

<Export...> Export internal method to another file. After exporting a newly created exported method file could by imported to another system or could be used by another system as external method. Usually exporting is done to ***ChromData\Methods*** folder.

<Show> For both **external** and **internal** methods. **Open processing method** 103 for review and configuration.

Note: In most practical cases using **System internal method** is preferable and is recommended. Take caution when using **External method** to avoid mistakes. Method files could be updated during performing the analysis (calibration and other settings). If you occasionally share the method through two or more systems which actually perform different types of analyses this would lead to incorrect analyses results.

Note: When you are configuring a new method at first step just specify analysis duration at the **General** 124 page of the **Method setup** 124. Then save the method and perform the first calibration run. When chromatogram finished, use it for final method setup: define integration parameters, components table, calibration, reports and other settings. Then save the method from the chromatogram using **Save method** 123 command.

Data source

Connected data source

Data source connected to the main measurement channel.

<Choose...> Select the **data source** 102 to be connected to the system.

Buttons

<OK> Apply or save changed settings and close window.

<Save> Save changed settings in the system file.

<Cancel> Cancel changes made and close window.

See also:

Open processing method 103

Data source 102

How to select processing method and data source 467

4.2.5.1.1.1 Data source

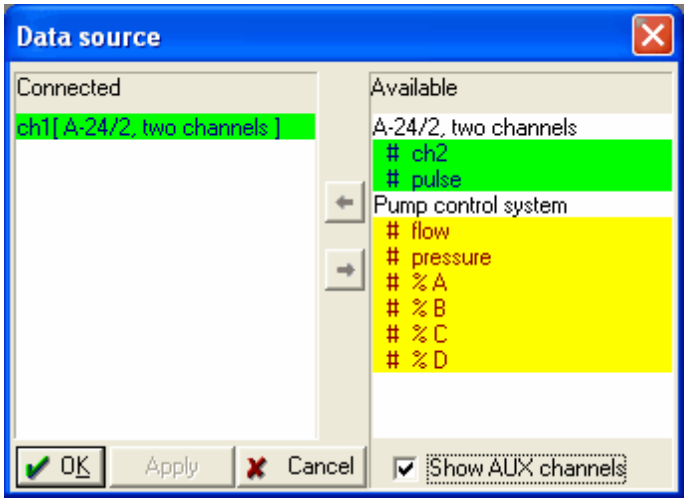
The "**DATA SOURCE**" window is used for selection of the data sources to be connected to the **data recorder** 99. Any data source from internal devices (that are installed in the current **System**) or any spare data source from external devices (that are installed at the **Workplace**) can be selected. Typically devices provide detector signals (called as data channels) which are used in chromatogram for analytical processing. Additionally devices can provide auxiliary channels, i.e. channels which monitor pressure, temperature, flow, or other parameters of devices.

It is possible to combine both auxiliary and data channels into a single multi-channel chromatogram.

Note: It is also possible to add extra **recorder** to the **system.** If you have detector or detectors which supply two or more **data signals** you can either combine all signals into the single multi-channel chromatogram or add one or more extra recorders to the **system** and get several single-channel chromatograms for single system run. Each single-channels chromatogram is processed independently by its own method. Both approaches are practical. You should select which is more appropriate for your needs.

The "**DATA SOURCE**" window is divided in two fields. The connected channels are placed on the left, and list of available data sources is on the right.

The data sources can be moved from one field to the other using the → or ← button.



Connected Connected data sources.

Available List of available data sources. Shared and analytical channels 113 are shown always.

☑ **Show AUX** if this box is checked, auxiliary channels are added to the list.

Buttons

<OK> Apply or save changed settings and close window.

<Apply> Apply changed settings.

<Cancel> Cancel changes made and close window.

See also:

Data recorder setup 100

How to select processing method and data source 467

4.2.5.1.2 Open processing method

(Right click Data recorder icon / Open method menu item of pop-up menu)

Load the **processing Method** 122 linked to the system and open an empty chromatogram window.

This operation allows to review and modify the processing method before starting a run. If the run is started, the chromatogram window is used for recording the measurement signal.

See also:

How to select processing method and data source 467

4.2.5.2 Watch window

(Watch window icon / Open)

The **watch window** displays the live parameters of the interfaces and devices included in the **connected** 89 **system** 79. Typically the **watch window** displays the actual signal level of the

detectors as well as auxiliary parameters such as current temperatures controlled by thermostats, flow rates of the pumps etc.

The **watch window** can be set for automatic open when a run or measure baseline is started. Use **Setup / Watch window / Automatically open watch window** 91 menu item for this configuration.

In most cases the **watch window** is configured automatically.

Manual configuration of the **watch window** is also possible. In this case user can specify what and how must be seen in the **watch window**.

The configuration of the **watch window** is done through **Setup / Watch window** 91 menu group of the **system window** 80.

Manual configuration 91 Possibility to select parameters which should be shown or to rearrange the sequence of the displayed parameters. This option opens the **Data source** 102 window for selection of the parameters to be displayed in the watch window. The ***Connected*** area shows the parameters to be displayed, the ***Available*** area shows the parameters not to be displayed. The parameters can be moved from one field to the other using the → or ← button.

Auto configuration 91 Automatic arrangement of all important parameters.

The **colors** 105 **of the watch window fields** can be changed by clicking the fields with the right mouse button. The colors set for this fields are also applied to the measurement display item in the control tabs of some interfaces and devices.

See also:

Watch window icon 104

Automatic watch window display 91

4.2.5.2.1 Watch window icon

The "**Watch window**" icon is one of the components always present in a new **SYSTEM WINDOW** . If the system is connected and this icon is clicked with the right mouse button, the following menu item appears:

Open Open the **watch window** 103 for live display of instrument values (this window can also be opened by double-clicking the watch window icon).

Unlink Delete the **watch window** 103 from the **SYSTEM WINDOW** (not recommended).

See also:

Watch window 103

Automatic watch window display 91

4.2.5.2.2 Color settings

The color settings for all display fields in the device settings windows, the "[103] and the "**SYSTEM STATE**" window can be changed. Click the right mouse button and select a field:

Choose color / Foreground / Out of range Set display color for field numbers if the measurement value is out of range (overflow or out of limits).

Choose color / Foreground / In range Set display color for field numbers if the measurement value is inside the normal range.

Choose color / Foreground / Active Set display color for field characters in the "**SYSTEM STATE**" window for running tasks.

Choose color / Foreground / Passive Set display color for field characters in the "**SYSTEM STATE**" window for finished tasks.

Choose color / Background / Out of range Set display color for field background if the measurement value is out of range (overflow or out of limits).

Choose color / Background / In range Set display color for field background if the measurement value is inside the normal range.

Choose color / Background / Active Set display color for field background in the "**SYSTEM STATE**" window for running tasks.

Choose color / Background / Passive Set display color for field background in the "**SYSTEM STATE**" window for finished tasks.

4.2.5.2.3 Watch window (menu group)

(*System menu* Setup / Watch window)

This menu group of the **system window** [80] contains the following items:

Automatically open watch window If this option is enabled, the **watch window** [103] is automatically opened when a run or measure baseline action is started.

Manual configuration Manual configuration of the **watch window**. See **watch window** [103] for details.

Auto configuration Auto configuration of the **watch window**. See **watch window** [103] for details.

See also:

Watch window [103]

4.3 Devices

4.3.1 Definition of device

Equipment control is based on the concept of **device drivers** (called also as **device** or **driver**). Normally each driver corresponds to some physical device (such as pump, detector, AD converter, etc.).

Driver provides control functions for the device and user interface for configuring device-specific settings.

Before using any instrument a corresponding **device driver** must be installed either inside the the

System 79 or to **Workplace** 77.

Typically device driver is installed inside the **system** 79. This is so-called **internal device**. **Internal device** stores instrument settings within **system** 79 file. **System** 79 owns its **internal devices** exclusively so that no other system could use it until owner system is in on-line state.

See **internal device installation** 106 article for details of device installation procedure.

Some drivers are installed **extra-system**. Such devices or modules are called **external devices** 107.

Some drivers can represent **virtual devices**. **Virtual device** is a helper modules which provide specific functionality for the system. The configuration of **virtual devices** is analogous to that of **internal devices**. The most common **virtual devices** are **Recorder** 99 and **Watch window** 104.

In most cases it is possible to build a chromatographic system using devices from different manufactures.

Chrom&Spec supports a digital control of variety of devices from different manufactures, including:

Detectors

Multi-wavelength detectors

Solvent delivery systems (Pumps)

Autosamplers

Thermostats

Valves and Fraction collectors

Compact chromatographic systems

Analog-to-Digital Converters

See also:
Internal device installation 106
External devices 107
How to create a new system 466
How to add devices to an existing SYSTEM window 466

4.3.2 Internal device installation

Installing:

Internal devices 105 can be installed in two ways:

1. Using the **Step 3: Add devices to the system** 95 of the **creating new system** 93 wizard.
2. Using **Install new device** 92 menu command of the **SYSTEM window** 80.

The icon of the **internal device** 105 appears in the **SYSTEM window** 80 after installation. **Clicking** this icon displays a user interface for device configuring for use in **system** 79. Clicking by **right-mouse-button** at icon displays a pop-up menu where additional configurations may be available.

The **internal device** 105 and its resources (such as **channels** 110) are available for components (such as **Recorder** 99) of the **system** 79 after installation.

Uninstalling:

To uninstall **internal devices** 105 from the **system** 79 locate icon of the device at the **SYSTEM window** 80. Click by **right-mouse-button** at icon to display a pop-up menu. Select an **Unlink** item in the menu.

The icon of the **internal device** 105 is removed from the **SYSTEM window** 80 after unlinking. The resources of the **internal device** 105 are not available for the **system** 79 any more. Some components of the the **system** 79 (such as **Recorder** 99) may need to be reconfigured if they used some resources of uninstalled devices.

See also:

Internal devices 105

External devices 107

4.4 External devices

4.4.1 Definition of external devices

External device or **Interface** means a **device driver** 105 that is installed **extra-system** to the **workplace** 77.

External device is not owned by any **system** 79 and could be shared by several **systems** 79 simultaneously.

A typical example of external devices is an **ADC** module. Two or more systems could link to different **channels** 110 of multi-channel ADC module and perform different analyses at the same time.

Besides **AD converters** 19 there are other **interfaces** which provide *COM ports sharing* or provide resources for connecting other devices.

See **external devices installation** 108 article about installation of **external devices**.

The icons of installed **external devices** are displayed at the main **toolbar** 36. Clicking this icon displays a user interface for device configuring. Clicking by **right-mouse-button** at icon displays a pop-up menu where additional configurations may be available.

In some cases the **external device** can supply so-called **sub-devices** 109. **Sub-device** 109 is a module of the **external device** which can be configured individually. The module can be logical or represent a real part of the **external device.**

See also:

External devices installation 108

Sub-devices 109

Internal devices 105

How to add an interface to the workplace 463

How to delete an interface 464

Analog-to-Digital Converters:

A-24: 2-channel 24-bit Analog-to-Digital Converter
E-24: 2 or 4-channel 24-bit Analog-to-Digital Converter

4.4.2 External devices installation

Installing:

External devices 107 can be installed in two ways:

1. Using the **step 2: "Add devices to WORKPLACE"** 94 of the **creating new system** 93 wizard.
2. Using **<Install device>** button at the **Workplace** 77 window.

The icon of the **external device** 107 appear at the main **toolbar** 36 after the installation. **Clicking** this icon displays a user interface for device configuring. Clicking by **right-mouse-button** at icon displays a pop-up menu where additional configurations may be available.

The **external devices** 107 and their resources (such as **channels** 110 or **line controls**) are available for all **systems** 79 after the installation.

Note that each **external device** 107 must be installed only once (this is unlike the **internal devices** 105 which must be installed into each system which uses them). For example, operator creates a new system with **creating new system** 93 wizard and installs multichannel **ADC** module (**step 2: "Add devices to WORKPLACE"** 94). The **data recorder** 99 of the system links to the ***channel 1*** of multichannel **ADC** module. Then operator creates another system and wishes to link it to the ***channel 2*** of multichannel **ADC** module. In this case operator must not install multichannel **ADC** module again because this module is already installed. Operator should just link the **data recorder** 99 of the second system to the ***channel 2*** of the previously installed multichannel **ADC** module.

Uninstalling:

To uninstall **external devices** 107 do one of the following:

1. Open the **Workplace** 77 window, locate the **external device** 107 which you need to uninstall and use **<Delete device>** button.
2. Locate the icon of the **external device** 107 at the main **toolbar** 36, click by **right-mouse-button** on it to display the pop-up menu and select **Unlink** item in the menu.

Once **external device** 107 is uninstalled no systems can use it any more. Systems which were configured for **external device** 107 must be redesigned or **external device** 107 must be installed again.

See also:
External devices 107
Internal devices 105

4.4.3 Sub-devices

External devices 107 are not owned by any system 79. Still external device 107 may need some configurations to be done for performing analysis.

In most typical cases user configures external devices 107 globally (on the workplace 77; user interface for configuration is displayed by clicking the icon of the device at the toolbar 36). Those configurations are applied to all systems 79 which use external device 107 and systems 79 cannot change them.

In some cases systems 79 may need to specify individual settings for external device 107 to perform a particular analysis. To fulfill this task the external device 107 can supply a set of so-called **sub-devices**.

Sub-device is an isolated module of the external device 107 which can be configured individually. The module can be logical or represent a real part of the external device 107.

The system 79 can be linked to 109 the **sub-device**. The system 79 owns the linked **sub-device** exclusively so that no other systems 79 can link to and configure the **sub-device** until the owner system is disconnected 90 or closed 82.

The linked **sub-device** appears as an icon in the SYSTEM window 80 and can be configured in the same way as internal device 105. Double clicking the icon displays the user interface for configuring the **sub-device**. Clicking by **right-mouse-button** at icon displays a pop-up menu where additional configurations may be available.

See also:
Linking to sub-devices 109
External devices 107
External devices installation 108

4.4.3.1 Sub-devices installation

As soon as external device 107 is installed all its sub-devices 109 are also available (if any). So sub-devices 109 do need to be installed separately. Still the system 79 must be linked to external device 107 to be able to apply configurations to it and to use its resources.

Linking to external device:

System 79 can be linked to sub-devices 109 in a two ways:

1. Using the step 4: "Control the external devices" 96 of the creating new system 93 wizard.
2. Using Link to existing devices 92 menu command of the SYSTEM window 80.

The icon of the sub-device 109 appear in the SYSTEM window 80 after linking. **Double clicking** the icon displays the user interface for configuring the sub-device 109. Clicking by **right-mouse-button** at icon displays a pop-up menu where additional configurations may be available.

Unlinking from external device:

To unlink the system 79 from the sub-device 109 locate the icon of the sub-device 109 in the SYSTEM window 80. Click by **right-mouse-button** at icon to display a pop-up menu. Select an **Unlink** item in the menu.

The icon of the sub-device 109 is removed from the SYSTEM window 80 after unlinking. The system 79 does not own the sub-device 109 any more so that another system can link to that sub-device 109.

See also:

Sub-devices 109

External devices 107

4.5 Channels

Detectors and other devices can supply a stream data of continuous measurement.

To deliver these data different devices implement **Channels**.

System 79 uses **channels** to deliver data from devices to other system components such as Data recorder 99 and Watch window 103.

Data recorder 99 then uses **channels** to deliver stream data to data processing method 122 to create a chromatogram 207.

DATA SOURCE 102 window is used for selection of **data sources** to be connected to the data recorder 99 (i.e. channels to be used for chromatogram plotting).

There are three types of channels which could be supplied by various detectors:

Analytical channels 113

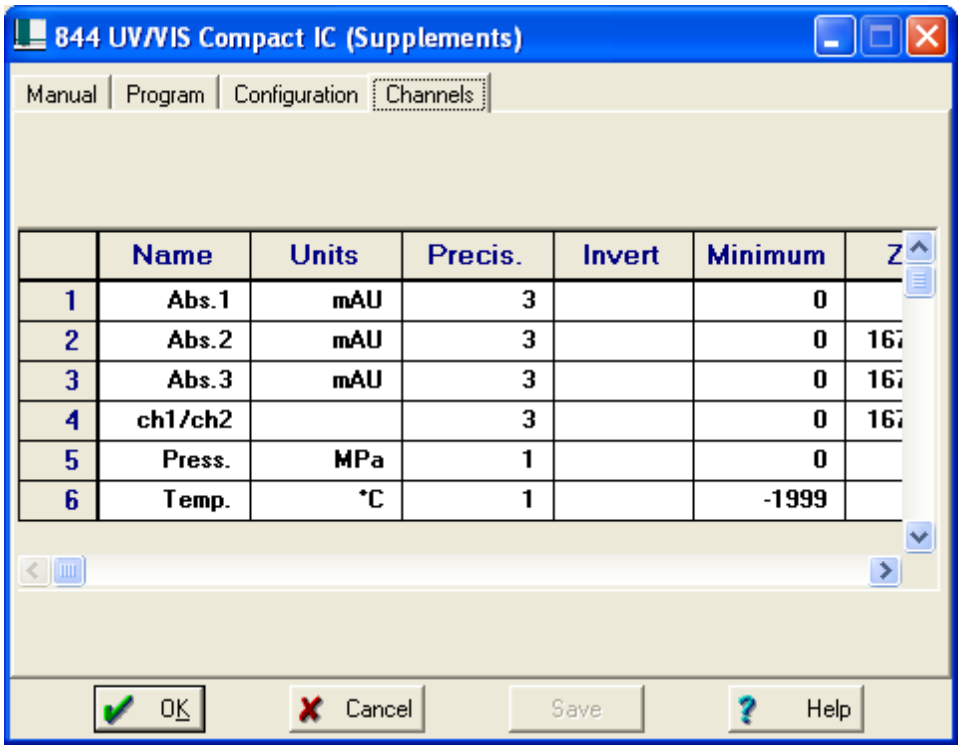
Spectral channels 113

Auxiliary channels 113

Several channels of any type can be implement by a single device.

4.5.1 Channels page

This page lists all **channels** 110 implemented by the particular **device driver**.



The parameters of each channel are presented as a **channels table** 112.

Note: Typically devices are supplied with already configured settings for **channels** in the **channels table** 112. It is not recommended to change these parameters unless you have a strong reason to do this. Modifying **channels table** 112 assumes an advanced knowledge of the instrument and software.

Note: Some devices can dynamically update some or all parameters in the **channels table** 112 depending upon operation mode of the instrument and/or other instrument settings. In this case modifying these parameters in the **channels table** 112 would have no effect. The instrument-specific values will be restored when analysis starts. Refer to documentation for individual devices for details.

See also:

Channels 110

4.5.1.1 Channel table

The **channel table** contains a set of parameters which describes the output of the **Analog-to-digital converter** 19 or any other **device** 105.

These parameters are used for recording a chromatogram and other purposes.

Name	Channel's name. This text appears as channel label in the chromatogram.
Units	Units of detector response.
Precis.	Number of decimal places to display in the **Watch window** 103 (and in other similar cells) for channel output.
Invert	Flag that inverts polarity of the detector signal: $R\ ?\ \ -R$. It is designed to convert negative peak to normal peaks. Typically **device drivers** 105 makes all necessary conversions internally. So there are no need to use this flag for them. The **Invert** flag can be useful for universal **Analog-to-digital converters** 19.
Minimum	Minimum value of the linear range of the AD converter (in ADC counts). This is an integer value in the range **[-2147483648...2147483647]**. This parameter is used to detect an underflow condition.
Zero	A signal level that is assumed to be on a baseline (in ADC counts). This is an integer value in the range **[-2147483648...2147483647]**. The value is used in the **Watch window** 103. Note, that chromatogram data processing does not uses this value. Data processing algorithm analyses actual data to determine baseline signal level as well as a drift of the base line.
Maximum	Maximum value of the linear range of the AD interface (in ADC counts). This is an integer value in the range **[-2147483648...2147483647]**. This parameter is used to detect overflow condition.
Range	A range of the values of input signal, in **Units**. **Range** = (**Maximum** - **Zero**) · **Coef** Setting this item recalculates **Coef**. parameter accordingly.
Coef	Conversion coefficient from ADC counts to physical measure units. $Vphysical$ [**Units**] = $Vadc$ · **Coef** Setting this item recalculates **Range** parameter accordingly.

See also:

Channels 110

Channels page 111

4.5.2 Analytical channels

Analytical (or data) channel provides a detector signal. Analytical channels are supplied by interfaces (such as ADC 191) and by **devices** 105 implementing various detectors.

Analytical channels can be shown in the **Watch window** 103 and can be added to the chromatogram.

Analytical channels are used for **data processing** by corresponded **data processing method** 122.

See also:
Spectral channels 113
Auxiliary channels 113
Data source window 102
Calculated channels 151

4.5.3 Spectral channels

Diode array detectors and some other multi-wavelength detectors can supply **spectral channels**.

Spectral channels are mostly analogous to the **analytical channels** 113.

Data recorder 99 expands each **spectral channel** of the device to several **analytical channels** 113 in the **chromatogram** 207. Each **channel** in the chromatogram refers to particular wavelength of the **spectral channel**.
Watch window 103 displays an averaged value for all wavelengths of the **spectral channel**.

See also:
Analytical channels 113
Auxiliary channels 113
Data source window 102
Calculated channels 151

4.5.4 Auxiliary channels

Auxiliary channels are used to control pressure, temperature, flow, or other current parameters of devices. They can be shown in the Watch window 103, in a special display of the particular device driver window or can be added as an additional channel to chromatogram.

Auxiliary channels can not be used for data processing!

See also:
Analytical channels 113
Spectral channels 113
Data source window 102

4.6 Documentation for individual devices and interfaces

4.6.2 Devices

4.6.2 Devices

4.6.2.1 SDU with 1...4 pumps

4.6.2.1.1 SDU features

SDU (Solvent Delivery Unit) is a virtual device driver that provides user interface to control high-pressure or low-pressure gradient mixture of one to four eluents. In High-pressure SDU a separate pump is used for each eluent while low-pressure SDU uses one pump with a special valve mixing device.

Various pump types supported by Chrom&Spec software can be used in SDU, appearance of SDU windows is independent on pump models

Each pump must be connected to the PC using a special data cable. Type of the data cable depends on pump type. RS232 protocol is usually used for data exchange of pump and PC.

The **SDU icon** 114 in the **SYSTEM window** is used to open the **SDU window** 115 for manual control and parameter settings.

See also:
SDU icon 114
SDU window 115
How to install SDU 119

4.6.2.1.2 SDU icons

The **SDU icon is available** in the **SYSTEM window** if a **SDU** (Solvent Delivery Unit) has been installed with the **New system wizard** 93 or by using the **Setup/New devices/Install new device** option of the **SYSTEM window** . The **SDU** icon consists of one to four Pump icons one above the other depending on the SDU type installed.

If the system is connected and the **SDU icon** is clicked with the right mouse button, the following menu appears:

Open 115 Open the **SDU** window for parameter settings.

Unlink Delete the **SDU icon** from the system.

See also:
SDU features 114
SDU window 115
How to install the SDU 119

4.6.2.1.3 SDU window

(SDU icon / Open)

Open the "**SDU**" window for parameter settings and manual control. The same operation is performed by double-clicking the **SDU icon** in **SYSTEM window** .

The title bar of this window displays Pump control system, and (in brackets) the name of the system folder and the system file. A star (*) at the end of the name indicates that the parameter settings have been modified since the last saving.

The "**SDU**" window can consist of the following tabs:

Manual 115	Parameter settings and display of pressure and flow.
Program 117	Gradient program for pumps.
Interfaces 118	Parameter settings and display of pressure and flow of the individual pumps.
Links 118	Window for COM port selection and settings (available for connected 89 system only).

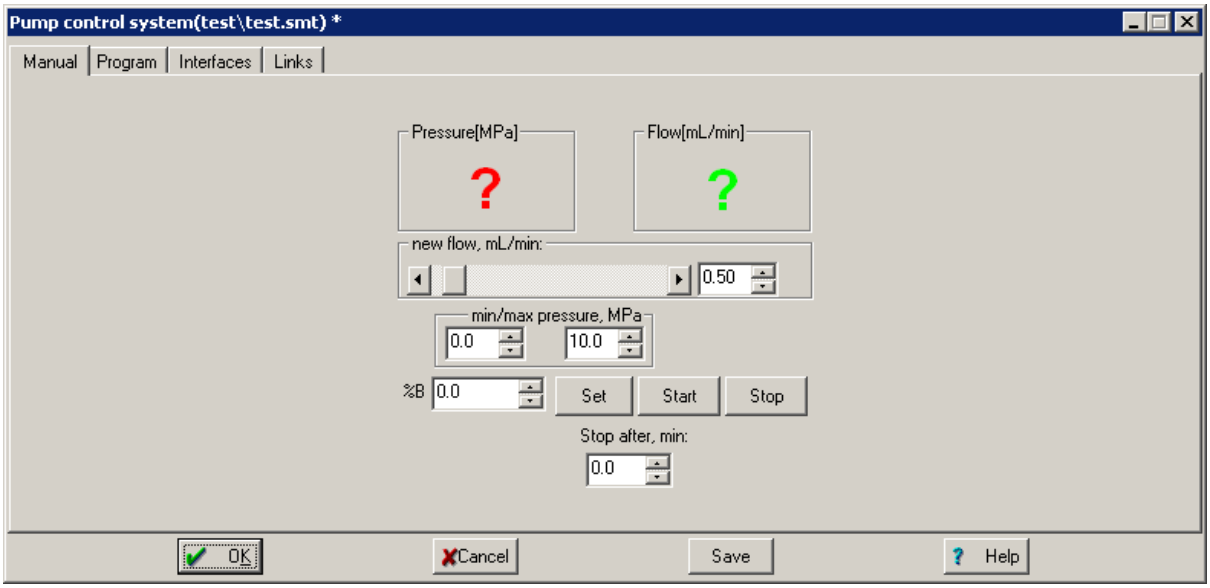
Buttons

<OK>	Apply or save changed settings and close window.
<Save>	Save changed settings in the system file.
<Cancel>	Cancel changes made and close window.

See also:
SDU features 114
SDU icon 114
How to install SDU 119

4.6.2.1.4 SDU "Manual"

The "**Manual**" page of the "**SDU**" window is available for a **connected system** only.



It contains the following display values and parameter settings for the pump control system:

Pressure — Live display of the current pressure in MPa. This value is also available for the **watch window** 103.

Flow — Live display of the current flow in mL/min. This value is also available for the **watch window**.

New flow — A new flow can be set by moving the scroll bar, by entering a value or by changing the value using the up and down arrows.
Entry range: 0.01 ... 20.00 [mL/min] (the range depends on number of pumps and type of pumps and pumpheads installed)

Min/Max pressure — The minimum and maximum pressure limits for the individual pump units can be set in steps of 0.1 MPa.
Entry range: 0.0 ... 50.0 [MPa]. (depends on type of pumps and pumpheads used)
The set maximum limit value that lie between 5 to 10 [MPa] above the particular operating pressure or the maximum admissible operating pressure of the column used. If the pump exceeds the preset limit value during operation, it is switched off immediately. At the same time, the **Pressure** field color in this window and in the **watch window** is changed to the value set for **Out of range**.
The set minimum limit value should lie far enough below the particular operating pressure. If the pump pressure falls below this preset lower limit during operation and this pressure drop persist for several revolutions of the pump cam due to leaks or interrupted inflow of the eluent, the pump is automatically switched off. At the same time, the "**Pressure**" field color in this window and in the **watch window** is changed to the value set for **Out of range**.

%B — Individual flow rate for pump B in percent of total flow. Appears if SDU includes two or more pumps
Entry range: 0 ... 100 [%]

%C — Individual flow rate for pump C in percent of total flow. Appears if SDU includes three or more pumps
Entry range: 0 ... 100 [%]

%D Individual flow rate for pump D in percent of total flow. Appears if SDU includes four pumps
Entry range: 0 ... 100 [%]

Stop after Stop time for all pump drives. This setting is active if gradient program 117 is enabled. It can be used in manual mode or when isocratic separation is running.
Entry range: 0.0 ... 99999.9 [min]

Buttons

<Set> Send current parameters immediately to the pump control system. Parameters are not stored in the system file (***.smt**) as long as the file is not saved.

<Start> Start all pump drives (preset eluent composition, flow, Max/Min pressure values are set, and timer for pump run is started).

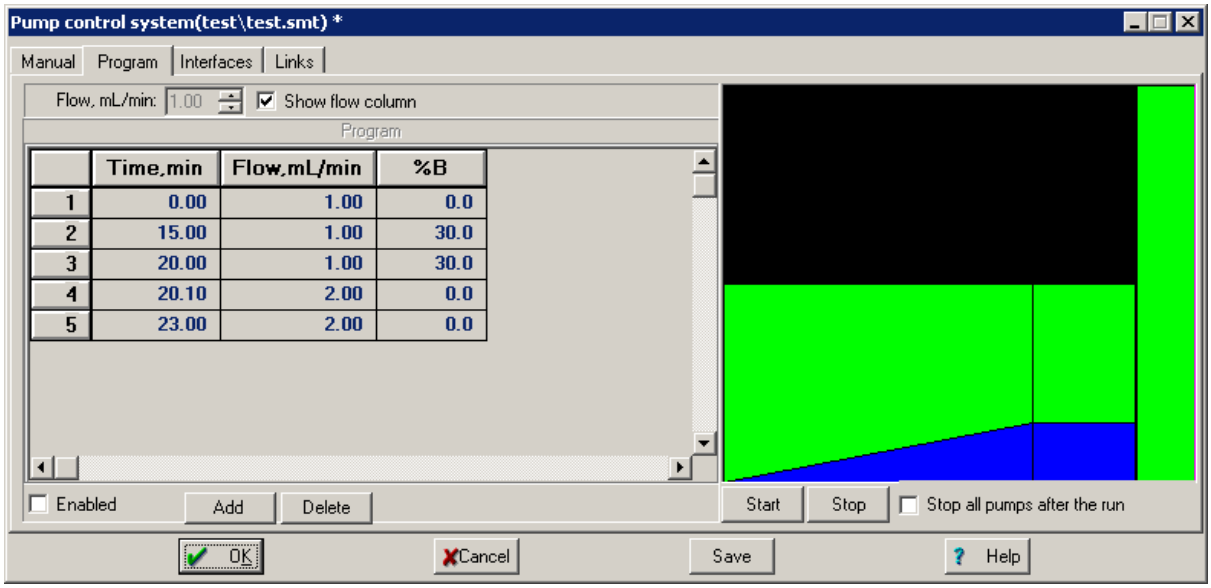
<Stop> Stop all pump drives immediately.

See also:
SDU interfaces 118
SDU icon 114
How to control SDU 120

4.6.2.1.5 SDU "Program"

The "**Program**" page of the "**SDU**" window contains a time program to define eluent gradients and shows a resulting Gradient graph

SDU allows to program both solvent composition and eluent flow.



Flow Overall flow of pump control system in mL/min. This value is also available for the **watch window** 103.
This field is available only if the **Show flow column** option is disabled. In this case **Flow** is constant during the gradient program.

Entry range: **0.01 ... 20.00** [mL/min] (flow range depends on pump type, type of pumpheads and number of pumps in SDU)

☑ **Show flow column** Show "**Flow**" column in the program table. In this case flow become a programmable value.

Program table

Number Row number in the program table (read-only).

Time **Time** at which the flow and/or gradient is changed.
Entry range: **0.00 ... 999999.99** [min]

Flow Overall flow of pump control system in mL/min.
Entry range: **0.01 ... 20.00** [mL/min] (depends on number of pumps and type of pumpheads)

%B (%C, %D) Individual flow rate for pump B (C, D) in percent of total flow.
Entry range: **0 ... 100** [%]

☑ **Enabled** Enable time program start (a disabled program is not started).

<Add> Add a new line to the gradient program.

<Delete> Delete the selected line from the gradient program.

<Start> Start gradient program in the manual mode.

<Stop> Stop gradient program in the manual mode

☑ **Stop pumps after the run** Stop pumps at the end of each run.

See also:

How to program SDU 120

4.6.2.1.6 SDU "Interfaces"

The "**Interfaces**" page of the "**SDU**" window is available for a **connected system** only.

Number of eluents Number of eluents used for gradient mixing.

Pumps List of used pumps for gradient mixing. Clicking on **<A>**, **<B>**, **<C>**, or **<D>** opens the window (for example **709 IC Pump**) for parameter settings and manual control of the selected pump.

Pressure checking Selection of the pump whose pressure is checked using the **Min/Max pressure** limits.

See also:

SDU manual settings 115

4.6.2.1.7 SDU "Links"

"**Links**" window contains information on all devices which function is linked with the current device. The most important function of the window is COM port changing and setting.

Alias Name of the interface or device. User is allowed to change this name. linked with the selected COM port.
USE: This area lists all devices that are used by the current device driver.

If the device driver controls a separate physical block, the COM # port used for connection is listed here.

Click the right mouse button on the COM port name to invoke the context menu:

Put on desktop	Open the **COM port** window. The same operation is performed by double-clicking the entry.
Change	Open the **COM port selection** window. To change the COM port used for the device connection, select the new unused COM port in the list, and accept the choice.

If the driver controls several devices (like SDU), all controlled devices are listed here. Double-click the desired item to open the device window.

USED BY:	This area contains a list of device drivers and systems that use the current device.
CHILDS:	This area lists sub-devices, data channels, and processes that are born by the current driver.

See also:

COM port settings

COM port log

COM port selection

4.6.2.1.8 How to install SDU

1. Switch off PC and all instruments connected to it.
2. For each pump used for the high-pressure gradient mixer system, connect the **RS232** socket on the pump and one of the RS232 sockets of PC using a appropriate cable.
3. Connect the outlet capillaries of Pumps as described in the installation manual.
4. Switch on PC and all instruments connected to it and start "Chrom&Spec" program.
5. For every Pump used, switch on the external control using the **<Ext.>** key on the Pump front panel (some pumps does not require this operation and switch to external mode automatically).
6. **Open the system** 467 in which the SDU is to be installed and click on **Setup / New devices / Install new device** 92 in the **SYSTEM window** to open the device selection window.
7. Select **SDU with one...four pumps** of the **solvent delivery systems** group and the **Serial port** of where the Pumps are connected to and click on **<Add to system>**. The **SDU icon** 114 will appear in the **SYSTEM window** .
8. Click on **<Close>** in the **Adding devices to your SYSTEM window** .
9. Click on **System / Save** in the **SYSTEM window** . Enter the name of the system file ***.smt** to be saved and click on **<Save>**.

Note: SDU can also be installed during the installation of a **new system** 93 using the system wizard.

See also:

SDU 114

4.6.2.1.9 How to control SDU

1. **Open the system** 467 with the SDU icon.
2. **Connect** 467 the system.
3. Double-click on the **SDU icon** 114 or click the icon using the right mouse button and select **Open**. The **Pump control system** 115 window is opened.
4. Select the **Manual** 115 page for manual control of the pump control system and modify the parameters to the desired values. Click on **<SET>** to send the new settings immediately to the Pumps.
5. Click on **<Start>** to start the pump control system or on **<Stop>** to stop the pump control system.
6. Click on **<Save>** to save the changed parameters in the system file.
7. Click on **<OK>** to close the **Pump control SYSTEM window** .

See also:

SDU Icon 114

SDU Control 115

4.6.2.1.10 How to program the SDU

1. **Open the system** 467 with the SDU icon.
2. Double-click the **SDU icon** 114 or click the icon using the right mouse button and select **Open** to open the **Pump control SYSTEM window** . Select the "**Program**" page for entry of a user-defined time **program** 117 suitable for the selected system.
3. Click on **<Add>** to add a new program line. Enter the time in min into the **Time** column (the time of the first line must be **0**). Enter the flow in mL/min into the **Flow** column. Enter the individual flow rates in percent for pump B, C and D in the **%B**, **%C** and **%D** column.
4. Click on **<Add>** to add new program lines or click on **<Delete>** to delete program lines.
5. Switch on the **Enabled** option.
6. If desired, start the program manually with **<Start>**.
7. Click on **<Save>** to save the program in the system file.
8. Click on **<OK>** to close the **Pump control SYSTEM window** .

See also:

SDU Program 117

Part V

Method

5 Method

5.1 Method definition

Method contains information necessary for data processing and producing report of analysis results.

Method stores peak integration parameters, calibration data, data processing options, report templates and other settings which define how data are proceeded. Also **Method** stores administrative information which describes the type of analysis.

To produce a chromatographic run **Method** operates in conjunction with related **System** 79. It is linked to system via **Data recorder setup** 99 settings. **Method** can be **internal** 100 or **external** 100 for the system. In most cases using **internal** method is recommended.

Method and related **System** 79 fully define the configuration of chromatographic analysis.

Methods are stored as ***.mtw** files.

Typically **method** is accessed by using **Open processing method** 103 command of **Data recorder** 99 module (see also **Data recorder setup** 100 user interface). Also **method** can be opened and saved using the corresponding **File menu** 26 commands.

The main settings of the **method** are configured from the **Method menu** 32 of the main **Chrom&Spec** menu.

Other configurations are available from **Main menu** 25, most settings are also accessible from **toolbar** 36.

Note: It is quite unusual making configuration of the empty method (without chromatogram data). Instead run the first calibration chromatogram for the newly created method. At this step you need just specify the chromatogram duration at the **General** 124 page of the **Method setup** 124. When chromatogram finished, make all necessary **method** configurations in this chromatogram: set integration parameters, define components table, setup calibration, reports and make other settings. When done save the method from the chromatogram using **Save method** 123 command.

During chromatogram run a complete copy of the **method**, as well as copy of the **system** used for data acquisition are attached to the chromatographic raw data and are written to chromatogram file. So all information used for data collection is always available to the user. It allows reviewing instruments configurations and processing parameters. Also it is possible to reproduce exactly the analysis later.

Several examples of the **methods** can be located in the **Method** folder.

5.2 Method file handling

5.2.1 New method

(*Main menu* File / New / Method..)

To create a new **external** 100 method just load an existing **method** 122 (***.mtw**) from the **Methods** directory and save it under a new name.

A new **internal** 100 method is created automatically during **System** 79 setup.

See also:

Open method 123

How to open a method 469

5.2.2 Open method

(*Main menu* File / Open / Method...)

Load an existing **external** 100 **method** 122 (***.mtw**) from the **Methods** directory and open an empty chromatogram window.

To load an **internal** 100 method of the **System** 79 use **Open processing method** 103 command of **Data recorder** 99 module. This command also opens **external** 100 **method** 122 which is linked to the **System** 79. See also **Data recorder setup** 100 user interface.

The title bar of the chromatogram window displays **Title** 126, **method file name**, and current run number. A star (*) at the end of the window title indicates that the method has been changed since the last saving.

See also:

How to open a method 469

5.2.3 Save method

(*Main menu* File / Save / Method)

Save the current **method** 122. This command is applied to methods and to chromatograms. For chromatogram the command updates the method which chromatogram refers to with settings from chromatogram.

5.2.4 Save method as

(*Main menu* File / Save Method As...)

Save the current **method** 122 to the file under the different name.

or

Extract the method from the current chromatogram and save it under the different name.

5.3 Method setup

(*Main menu* Method / Method setup...)

This section of the **Method menu** 32 allows to set or view the most common parameters of the Method.

General 124	the most common part of the chromatogram's ***Method setup.***
Sample 126	sample information.
Extra 128	custom (extra) sample parameters.
Comment 129	user comments on chromatogram.
Column 130	column information.
Eluent 131	eluent information.
Smoothing 132	selecting and tuning of **noise smoothing** methods.
Processing 135	set actions that are performed when the **chromatogram finishes**.
Export 136	setup automatic exports that are performed when the **chromatogram finishes**.
Math 138	parameters that are used for various types of calculations.
Noise 142	setup option for calculating signal ***noise***.
Quantification 144	open ***Quantification*** window to set up common parameters for quantification procedure.
Reports 145	open ***Reports*** window to set up advanced reports 341.

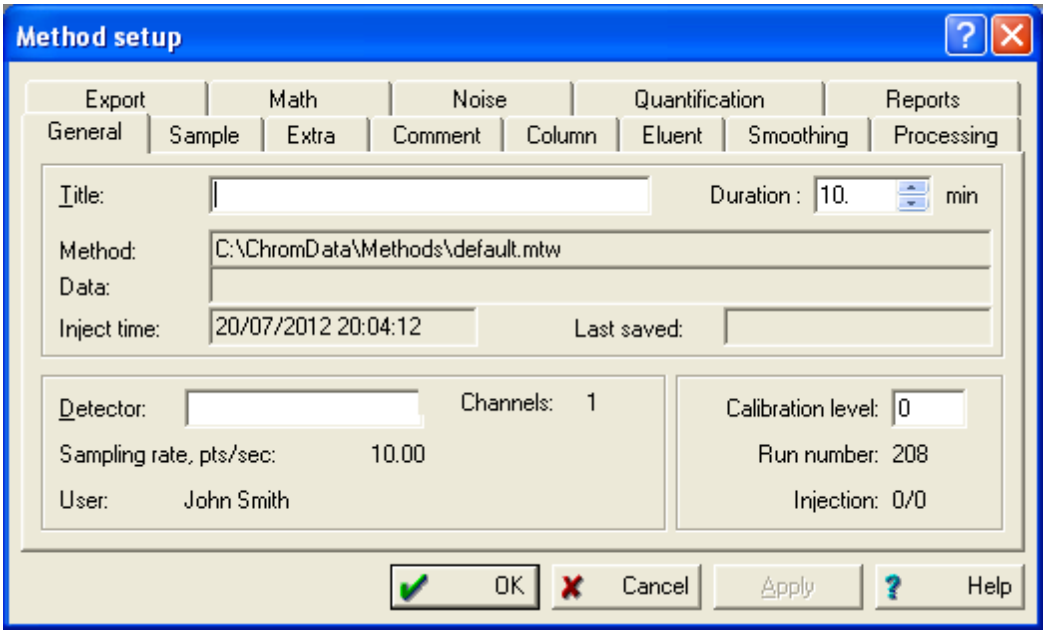
Buttons

<OK>	Accept parameters.
<Cancel>	Cancel changes.
<Apply>	Accept modified parameters.

5.3.1 General

General description of the method is a part of the chromatogram's **Method setup** 124.

General description can be included into the report by checking the ☑ **General** checkbox in the **Report options** 322 window.



Title 126 — User defined **identifier** (title) for the chromatogram. Usually this item refer to individual sample run, not to method. Still you could set this item and store it in the method. In this case stored value would be a default value for each later sample run of this method.
Sample queue: The **Title** field from the sample queue table replaces this value if **Sample queue** 237 is active.

Duration — Duration of the chromatogram in **retention units** 218. This value cannot be edited here, it is for review only. Use **data recorder setup** 100 to specify duration of the analysis.

Method — Path and file name of the **method** used for data acquisition (read-only).

Data — Path and file name of the current **chromatogram** (read-only).

Inject time — Date and time of the chromatogram start. This value can not be modified by anybody (read-only).

Last saved — Date and time of the last chromatogram modification and saving (read-only).

Detector — User-defined name of the **detector**. This item is a brief description of the instrument used.

Channels — Number of the **measure channels** for this analysis. This item set automatically when analysis run. For general-purpose LC/GC this is usually ***1***. This value is set to a different value for DAD detection.

Sampling rate, pts/sec — Value of the chromatogram data sampling rate.

User — Name of the **user** who produced this analysis. This item is set to the full name of currently logged-in user when analysis start. This item is empty for method.

Calibration level 199 — If the current run is used for calibration, the calibration level is a positive integer, otherwise it equals 0. You can modify this value when the chromatogram run is starting (in single-run scenario).
Sample queue: The **Calibration level** field from the sample queue table replaces this value if when **Sample queue** 237 is running.

Run number — Sequence number of the **current run** starting from the very first one. All runs are automatically numbered by the system (read-only).

Note: User can reset the **Run number** by pressing **[Ctrl]+[F8]** key combination. The "**ANALYSIS NUMBER**" window is opened where the run number for the next analysis can be modified to the desired value.

Injection — Specifies the injection number for the **current run** and total number of the injections for the **vial** 126. This item is filled when **sample queue** 237 is executed. See **Injections** and **Done** items in the **sample table** 244. If analysis was run without **sample queue** 237 this item is set to **1/1** value. For **methods** 122 this item is set to **0/0** value.

5.3.1.1 Title

Title is a header for the chromatogram that appears as title of the chromatogram window.

Title is displayed and can be modified in the **Method setup: "General" page** 124.

It is also displayed in the **Chromatogram open** 207 window as additional short information.

There are several ways to specify the title for the chromatogram:

Single analysis runs: The **Title** item from the **Edit sample description** 85 replaces this value when analysis is **executed** 83.

Sample queue 237**:** The **Title** item from the **sample queue table** 255 replaces this value when **sample queue** 237 is executed.

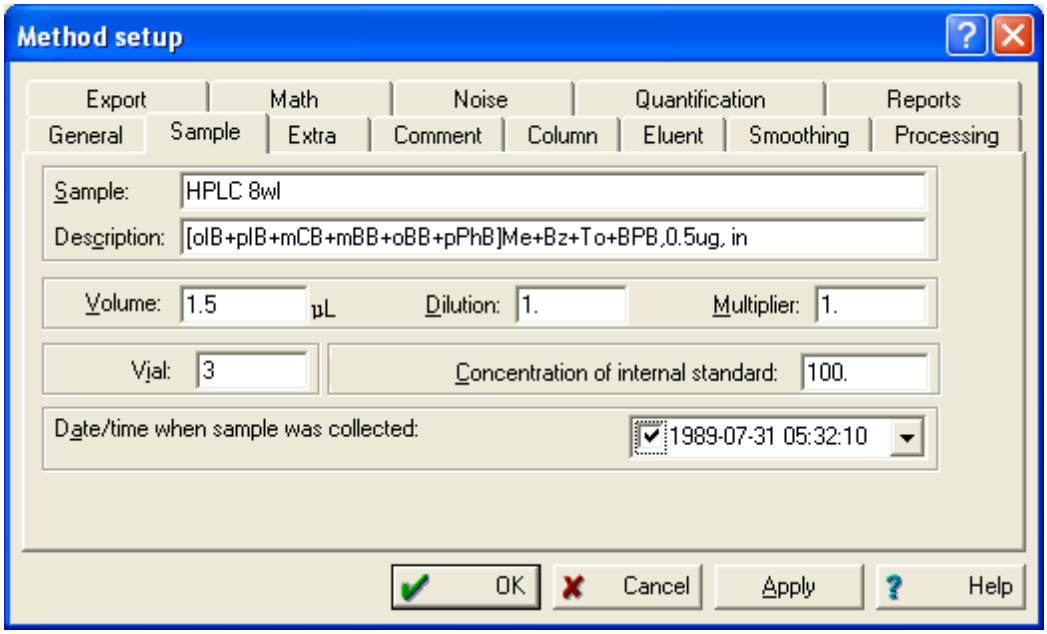
Batch reprocessing 271**:** The **Title** item from the **batch reprocessing table** 284 replaces this value when **batch reprocessing** 271 is performed.

5.3.2 Sample

(*Main menu* Method / Sample...)

Sample description is a part of the chromatogram's **Method setup** 124 It can be included into the report by checking the ☑ **Sample** checkbox in the **Report options** 322 window.

The information at this page refer to individual sample run. Still you could set any items here and store them in the method. In this case stored values would be default values for each later sample run of this method.



Sample — User-defined sample name or basic sample description(max. 256 characters).
Sample queue: The **Sample** field from the sample queue table replaces this value if **Sample queue** 237 is active.

Description — Additional sample description (max. 256 characters).
Sample queue: The **Sample description** field from the sample queue table replaces this value if **Sample queue** 237 is active.

Volume — Injected volume in micro liters.
Sample queue: The **Volume** field from the sample queue table replaces this value if **Sample queue** 237 is active.

Dilution — Dilution of the sample.
Sample queue: The **Dilution** field from the sample queue table replaces this value if **Sample queue** 237 is active.

Multiplier — Sample multiplier. This is a sample concentrating factor.
Sample queue: The **Multiplier** field from the sample queue table replaces this value if **Sample queue** 237 is active.

Note. **Volume, Dilution and Multiplier ,** are interrelated items. They are used to calculate **component *quantity*** (e.g. **component *weight***) for both calibration run and analyte. See **adjusted volume** 199 and **quantity** 200 for details.

Note. The detector response (peak area or height) is related directly to **component *quantity*** value**,** not **component** concentration**.** So **component *quantity*** is actually used to build **calibration curve** 182. For analyte a **component *quantity*** is calculated from calibration curve. See **quantification** 201 for details.

Note. Set **Dilution and Multiplier** values to 1.0 if these parameters are not used in your analysis.

Vial	Autosampler vial position to take sample from. **Sample queue:** The **Vial** field from the sample queue table replaces this value if **Sample queue** 237 is active.
Concentration of internal standard	Concentration of the **standard component** for quantification using **relative concentration** 202 method. See **Quantification page** 144. **Sample queue:** The **Concentration of internal standard** field from the **sample queue table** 255 replaces this value when **Sample queue** 237 is running.
Date/time when sample was collected	This date/time stamp can be changed by the user, if date and time of the sample collection are essential.

See also:
Extra sample parameters 128

5.3.2.1 Multiplier

Multiplier	**Sample queue:** The *Multiplier* value from the sample queue table replaces this value in the chromatogram Sample description 126 when Sample queue 237 is running.

Multiplier is a dimensionless coefficient

5.3.2.2 Dilution

Dilution	Dilution of the sample. **Sample queue:** The *Dilution* field from the sample queue table replaces this value in the Sample description 126 if Sample queue 237 is running.

Dilution is a dimensionless coefficient

5.3.3 Extra

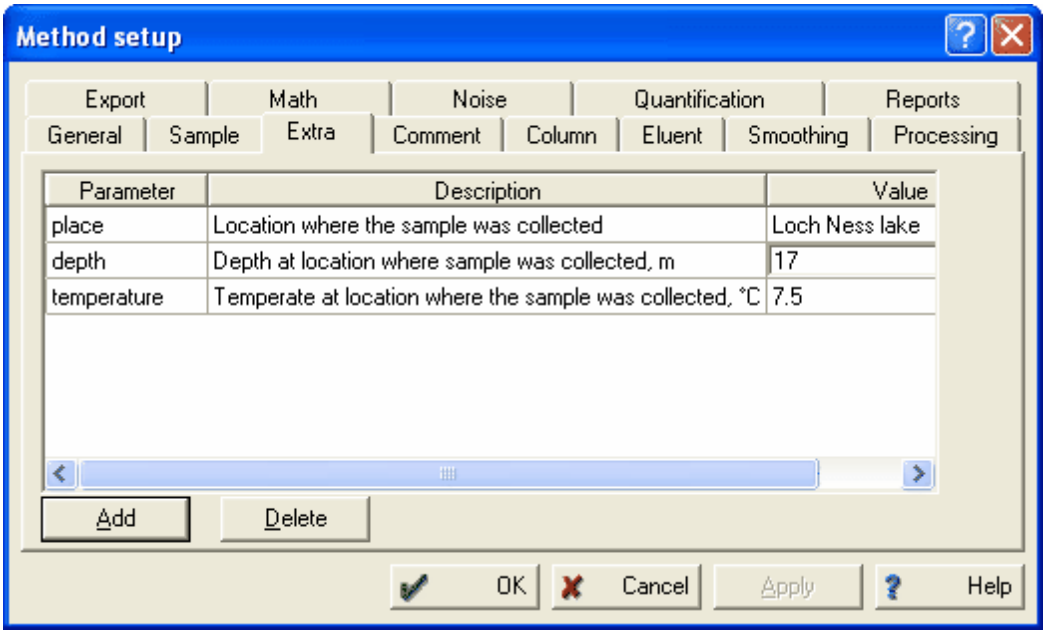
Sample **Extra** page is a part of the chromatogram's **Method setup** 124.

This page allows defining custom parameters. Usually these parameters refer to individual sample and expand **Sample** 126 page.

Extra parameters can be numerical or text strings.

In reports extra parameters are listed in **Sample** section (by default).

Custom parameters can be used in **custom formulas** 288 as well as in logical and arithmetical expressions in **advanced reports** 341.



Parameter — Literal parameter label. This label is required to identify parameter in **custom formulas** 288 and in **Sample queue** 237.

Description — Additional user-readable description of the parameter. Usually this is just description of what parameter means.

Value — Value of the parameter. When defined in the method this is a default value for every run. User can modify this value when analysis starts (in a single run scenario). Alternatively parameters can be defined in the **Sample queue** 237 for each run.

Add — Button to add another parameter in the list.

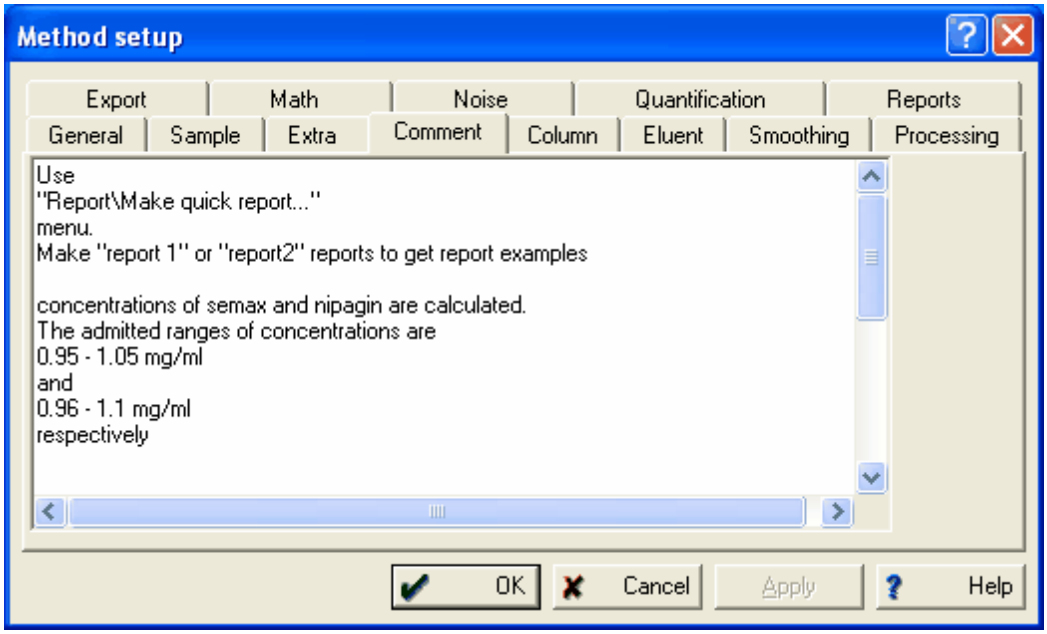
Delete — Button to permanently delete selected custom parameter from the list.

The list of parameters (**Parameter** and **Description** items) should be defined in the method while **Value** item refers to the particular sample run.

5.3.4 Comment

The **Comment** page is used to enter free-text **user comments** into the **method** or **chromatogram** description. Use this feature to enter any additional information about the chromatogram not included in other sections of the **Method setup** 124. Checking the ☑ Comment checkbox in the **Report options** 322 window will switch comment printing on.

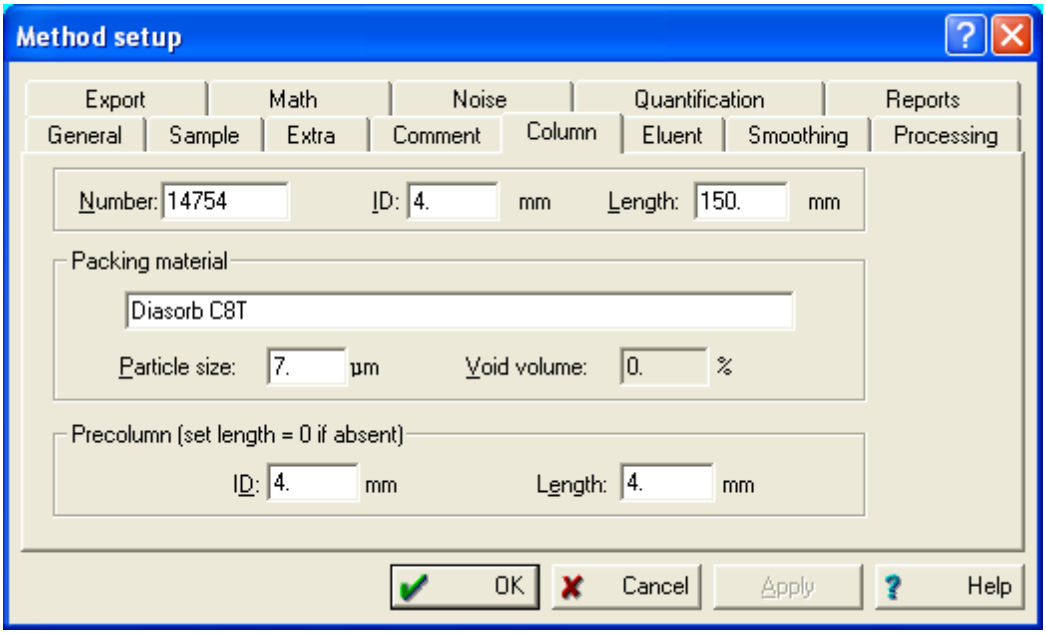
Comment is accessed via **Method setup** 124 window.



When comments are defined in the **method** subsequent runs of the **method** apply these comments to all chromatograms obtained by the method.

5.3.5 Column

Column description is a part of chromatogram's **Method setup** 124. Its settings can be included into the report by checking the ☑ Column checkbox in the **Report options** 322 window.



Number Column's **serial number**, text item.

ID **Internal diameter** of the column in mm.

Length **Length** of the column in mm. This value is used to calculate **linear flow rate** 198.

Packing material

Column **description**, text item.

Particle size **Particle size** of parking material in µm. This value is used for the calculation of reduced theoretical plate height (**reduced TP height** 335).

Void volume **Void volume** for the column in %. Used to compute **logarithmic index** 141, **capacity factor** 335 and **linear flow rate** 198. It is calculated by the system in accordance with **Math** 138 window settings.

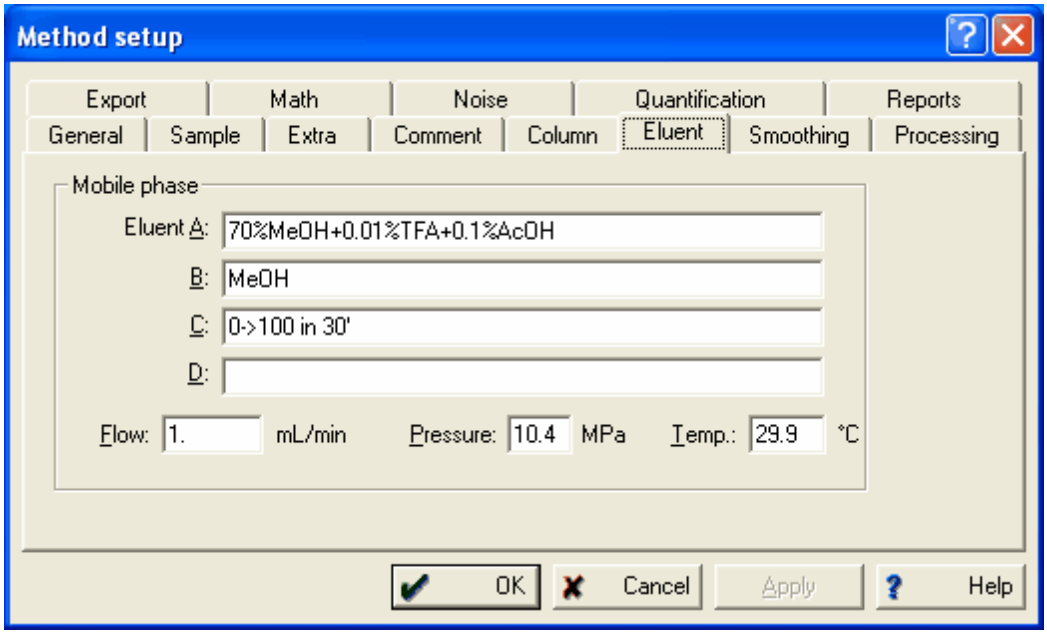
Precolumn

ID **Internal diameter** of the precolumn in mm.

Length **Length** of the precolumn in mm (set length to 0 if no precolumn is used).

5.3.6 Eluent

Eluent description is a part of chromatogram's **Method setup** 124. It can be included into the report by checking the ☑ Eluent in the **Report options** 322 window.



Eluent A **Description** of eluent composition.

Eluent B **Description** of eluent composition.

Eluent C **Description** of eluent composition.

Eluent D **Description** of eluent composition.

Flow	**Flow rate** in mL/min or µL/min. Flow rate is used to recalculate the retention time into volumetric units. The system startup value of the pump for the flow rate is entered automatically into this field at **inject**.
Pressure	**System pressure** in MPa, psi, bar, or atm. The measured value of the pump for the pressure is entered automatically into this field at the **inject**.
Temp.	Field where you can enter the **temperature** of the column's thermostat or the ambient temperature. The measured value of the thermostat (if available) for the temperature is entered automatically into this field at the **inject.**

5.3.7 Smoothing

(*Main menu* Process / More... / Data smoothing/Compress...)

Smoothing page is a part of chromatogram's **Method setup** 124.

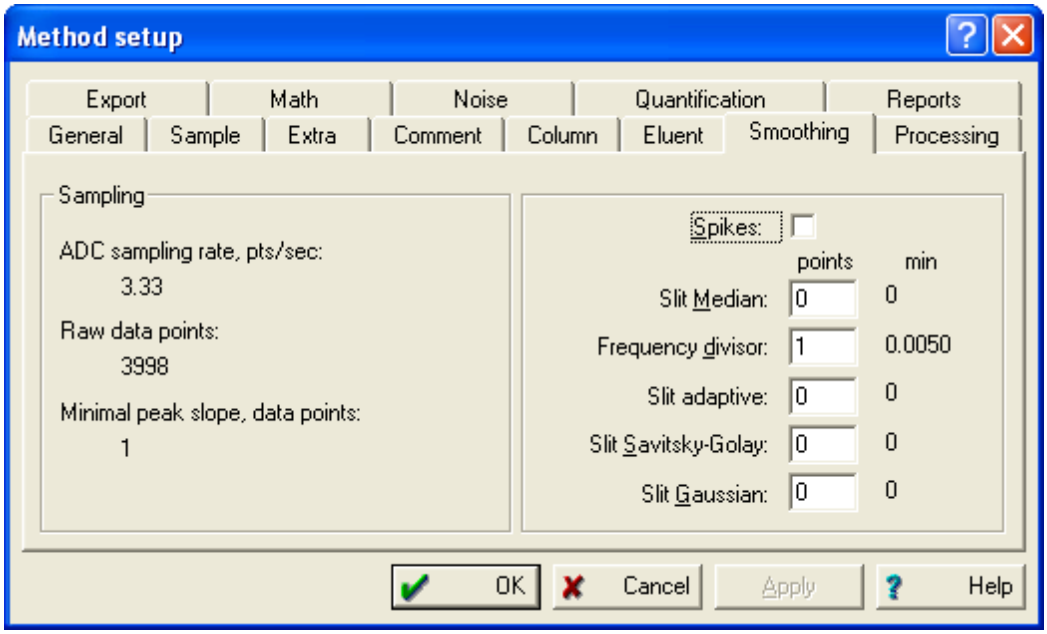
This user interface allows defining parameters for **noise smoothing** 133.

Noise smoothing is applied to raw data before they are processed.

For GLP compliance noise smoothing does not change the raw data. Chromatogram always stores internally the original raw data and never change them.

User can change the smoothing settings several times to get the best results. New noise smoothing settings are applied to original raw data.

Noise smoothing can significantly enhance the precision of peaks detection and identification, as well as improve visual representation of chromatogram.



Some smoothing require **slit** value to be entered. **Slit** is defined in data points and must be natural odd number or zero. Zero value means that corresponded smoothing filter is disabled.

Methods of noise smoothing

Spikes 133
Clear spikes only. The value of the spike is replaced with the half of the sum of two neighboring signal values.

Slit Median 133
Slit for **Median smoothing method**. Non-zero value activates this smoothing. This smoothing is applied before **Frequency divisor**. So the slit is defined in original raw data points.

points
Number of data points per smallest peak on the chromatogram (read-only). This information is a hint to apply **Frequency divisor** and/or select correct ***slit*** value for smoothing.

Frequency divisor 135
Divisor to reduce the sampling rate. **Entry range**: **1 ... 9999**.

Slit adaptive 133
Slit for **adaptive confidence smoothing filter** 135. Non-zero value activates this smoothing. This smoothing is applied after **Frequency divisor**. So the slit is defined in data points with reduced sampling rate.

Slit Savitsky-Golay 133
Slit for **Savitsky-Golay smoothing filter**. Non-zero value activates this smoothing. This smoothing is applied after **Frequency divisor**. So the slit is defined in data points with reduced sampling rate.

Slit Gaussian 133
Slit for **Gauss smoothing filter**. Non-zero value activates this smoothing. This smoothing is applied after **Frequency divisor**. So the slit is defined in data points with reduced sampling rate.

ADC sampling rate, pts/sec
Value of the chromatogram data sampling rate (read-only, actual only for running or recorded chromatograms).

Raw data points
Number of data points per chromatogram channel after applying **Frequency divisor** (read-only).

Minimal peak slope, data points
Number of data points per smallest peak on the chromatogram (read-only). This information is a hint to apply **Frequency divisor** and/or select corrects ***slit*** value for smoothing.

See also:

Noise smoothing 133
Calculated channels: Smoothing 157
System basics 18

5.3.7.1 Noise smoothing

Acquired data are stored in the computer memory as raw data points. After acquisition noise smoothing

may be used in some cases. There are several smoothing algorithms in the software: Spikes filter, Median smoothing filter, adaptive Confidence smoothing filter, Savitsky-Golay smoothing filter and Gauss smoothing filter. They can be applied to raw data in the order in which they are mentioned.

Some smoothings require **slit** value to be entered. **Slit** is defined in data points and must be a natural number.
When slit is required, the **gap** of the filter is calculated as
gap = slit * 2 + 1

The Spikes filter smoothes the first and last points of the chromatogram and the points identified as spikes. The spike is exchanged with half of the sum of two neighboring signal values.

Savitsky-Golay smoothing filter is well described in the literature. In this implementation it performs a local polynomial regression of third degree within **gap** range to determine the smoothed value for each point. Central value of polynomial regression is used. This smoothing filter does not does the area of the peaks.

In the Median smoothing filter the values within the **gap** are sorted by increasing response level and the response corresponding to the middle of the **gap** is replaced with the value in the middle of a sorted array. This method affects chromatographic peaks in minimal extent, improves baseline and very effectively eliminates single-point spikes. In this case spike will be replaced with one of the neighboring points.

Gauss smoothing filter calculates the weighted sum of all points within a **gap** with Gauss weights distribution. Calculated value replaces the original raw value. Peaks after smoothing become a bit smaller and wider, but their area does not change. The weight function of Gauss smoothing filter is defined as:

$$W_{gauss}(i) = \exp\left(\frac{-(i - i_0)^2}{slit^2}\right)$$

here i is an index of the point and $i0$ is an index of the central point in the **gap** (which is approximated)

Adaptive Confidence smoothing filter is based on conventional Savitsky-Golay smoothing filter. It performs a local polynomial regression of third degree within gap range analogous to conventional Savitsky-Golay smoothing filter. Still it varies **gap** and performs non-central approximation to get the best fit of raw data. Actual approximation can be performed using

$$2 \cdot gap,\ \sqrt{2} \cdot gap,\ gap,\ gap/\sqrt{2},\ gap/2,\ gap/(2 \cdot \sqrt{2})$$

depending upon the noise of the raw data and how fast the detector signal is changing. For details see the original article 135.

See also:

Method setup: "Smoothing" page 132
Calculated channels: Smoothing 157
System basics 18

5.3.7.2 Confidence smoothing filter

Enter topic text here.

5.3.7.3 Divisor

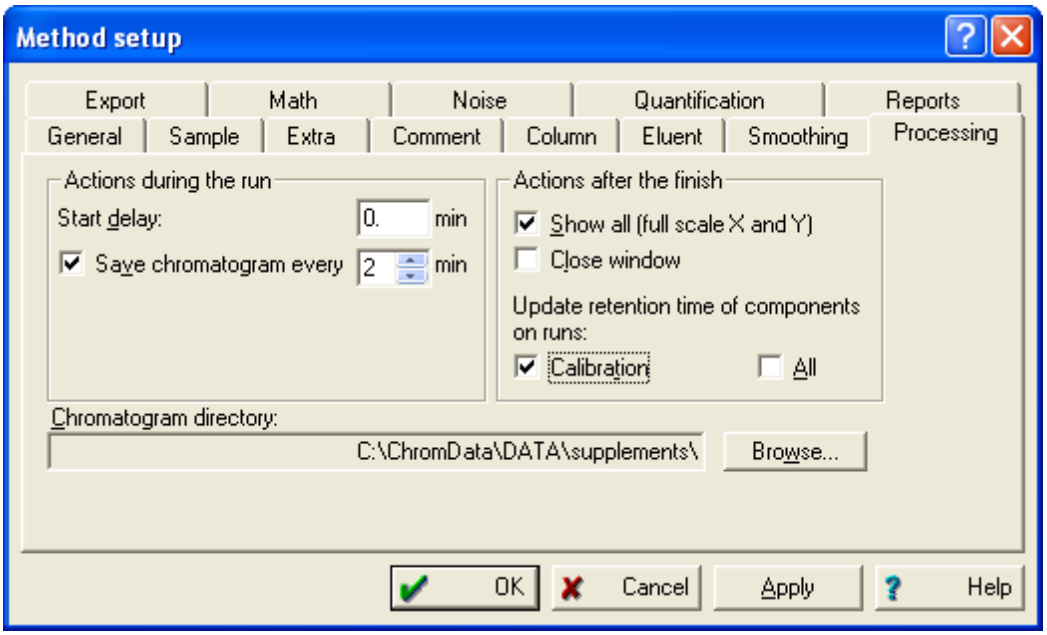
Frequency divisor allows to reduce the data sampling rate. A reduced rate eliminates over-sampling effects in the chromatogram data.

If the value of this parameter is different from 1 (default value), consecutive 'divisor' data points are summarized and the sum value is stored instead of the raw data points. The divisor value may be within the range of **1 - 9999**.

5.3.8 Processing

Processing page is a part of the chromatogram's **Method setup** 124.

This box contains a list of actions that are performed during the run or when the chromatogram finishes.



Actions during the run:

Start delay Time delay after **Inject** before starting actual data acquisition, in min. Use this option if there are useless data at the beginning of the chromatogram.

☑ **Save chromatogram every ... min**

If checked, autosaving of the chromatogram will be performed during acquisition run.

If some value is entered, chromatogram saving during the run will be performed in a regular intervals. If **0** is set, the chromatogram is not saved during the run

Actions after the finish:

☑ **Show all** — If checked, auto scaling on X and Y axes will be done so that the chromatogram fits the window.

☑ **Close window** — Close the window after the run is finished. It is recommended to set this option for analyses which run from the **sample queue**. Otherwise multiple windows of chromatograms could consume most system resources.

Update retention time on runs:

☑ **Calibration** — Calibration runs will update retention time for all components when chromatogram is finished.

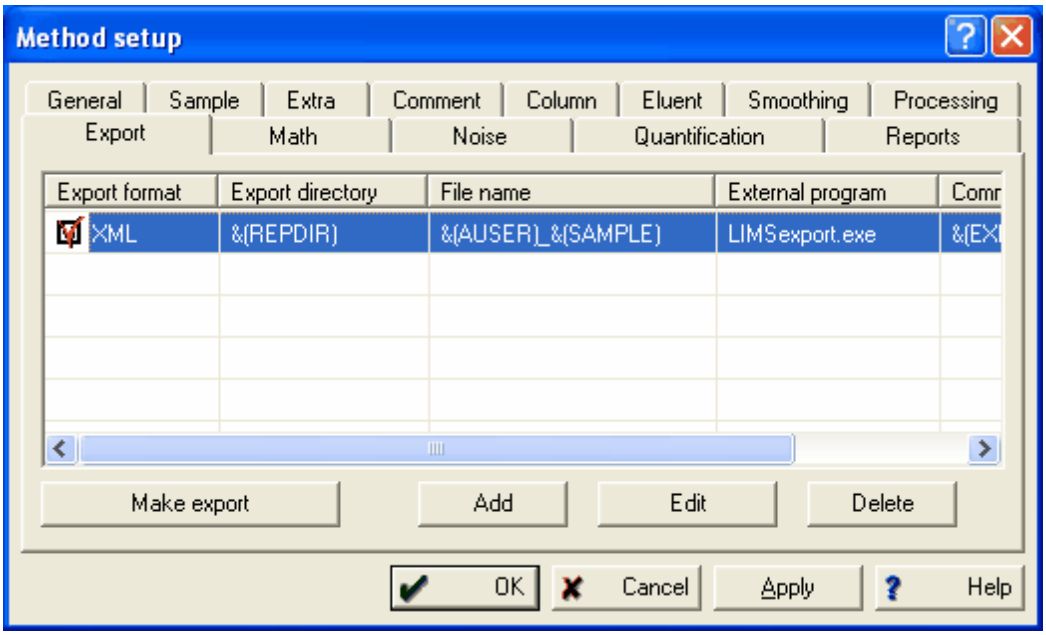
☑ **All** — Any run will update retention time for all recognized components when chromatogram is finished. Use this option with caution.

Chromatogram directory — directory where the chromatogram files are saved. Set it in the ***Method*** to define individual chromatogram storage for this method. Use the **<Browse>** button to select a new directory.

5.3.9 Export

Export page is a part of the chromatogram's **Method setup** 124.

You can set up an automated exports of the chromatogram data, method settings and analysis results. This may be convenient when integration with third-party software (such as **LIMS**) is required.



Software currently supports export in the the following data formats:

AIA file 212 — Export chromatograms in the AIA (Analytical Instrument Association) format.

Raw data into txt 212	Export chromatographic raw data to the text file (ASCII format).
XML file 29	Export method settings, chromatographic raw data and analysis results to the XML file.

Put this check mark to make export automatically when analysis finish.

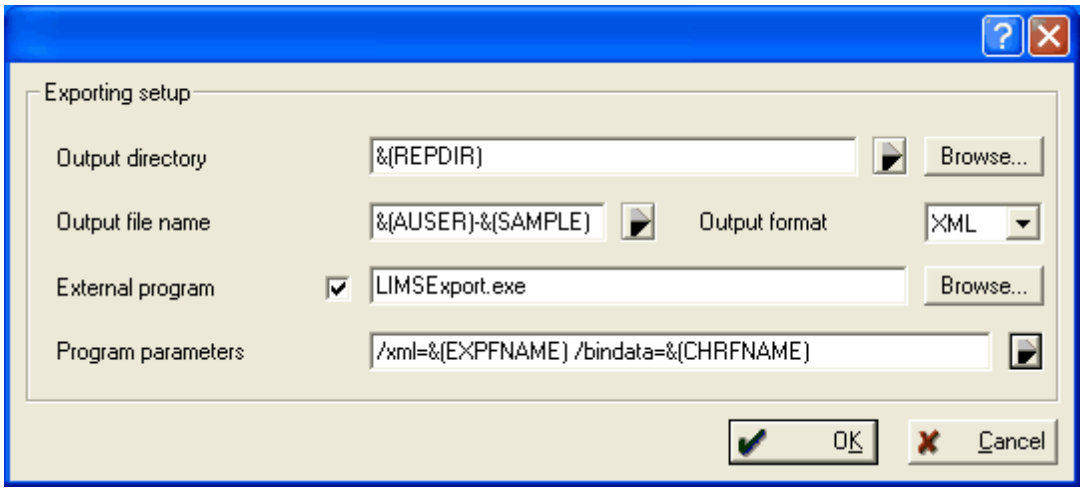
Make export	You can immediately make export for currently selected item in the export list by pressing this button.
Add	Add another export to the list. Exporting setup 137 dialog form is opened.
Edit	Edit currently selected item in the export list. Exporting setup 137 dialog form is opened.
Delete	Delete currently selected item from the export list.

See also:

Exporting setup 137 dialog form

5.3.9.1 Exporting setup

Use this dialog form to setup your exporting.



Some items in this dialog form can use file and directory macro language 486.

Use helper button to select available macro from the list.

Output directory	Directory name where software writes exported file.
Output file name	Name of the exported file. Do not specify file extension here! It is

appended automatically.

Output format — The export file format. The file extension is appended based on this selection.

External program — External program may be specified to be called immediately when export is done. The external program may perform it's own data processing, present user special reports, export data to LIMS or other databases and so on.

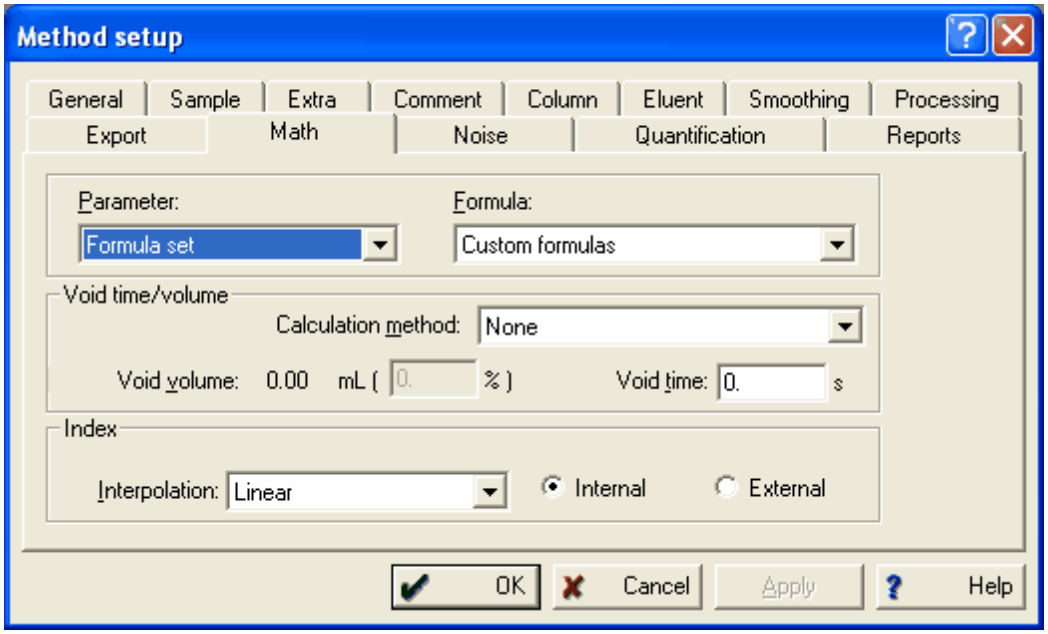
Program parameters — Additional parameters which may be required for external program. In most cases this is just full name of exported file which is specified through **&(EXPFNAME)** macro.

See also:

Method setup: "Export" page 136
File and directory macro language 486

5.3.10 Math

The **Math** page contains parameters that are used for various types of calculations.



Parameter 139 — Selection of calculation parameter.

Formula 139 — Selection of formula for the calculation parameter.

Void time/volume

Calculation method — Selection of the method for **void time** 141 calculation.

Void volume 141 — **Void volume** in mL and % of column volume. The % value can be entered manually if "From void volume %" calculation method is set.

Void time 141	**Void time** in sec. This value can be entered manually if "None" void time calculation method is set.

Index

Interpolation 141	Use of linear or logarithmic interpolation scale for retention index calculation.
Internal	The index scale is constructed on the basis of the current chromatogram. All components used for index scale calibration should be present in the current sample.
External	The index scale is constructed on the basis of another standard chromatogram.

5.3.10.1 Calculation parameter

Parameter and **Formula** fields on the **Math page** 138 define formulas for the calculation of the three parameters:

Efficiency, TP 139

Resolution 140

Asymmetry 140

Settings for Parameter:

Formula set	The following settings are available: Custom formulas: User can individually setup the calculation formulas for parameters. European Pharmacopoeia or US Pharmacopoeia: formulas are defined according to the corresponding Pharmacopoeia.
Efficiency, TP 139	Selection of calculation formula for **Efficiency, TP** (if "**Formula set**" = "Custom formulas").
Resolution 140	Selection of calculation formula for **Resolution** (if "**Formula set**" = "Custom formulas").
Asymmetry 140	Selection of calculation formula for **Asymmetry** (if "**Formula set**" = "Custom formulas").

5.3.10.1.1 Efficiency, TP

This item defines formula for **efficiency** per column.

The number of theoretical plates $N(i)$ per column for a chromatographic peak i is calculated by one of the formulas:

$N(i) = 2\ PI\ \cdot [\ T(i) \cdot H(i) / A(i)\ ]^2$	
$N(i) = 5.54\ \cdot [\ T(i) / W(i)\ ]^2$	this formula is default for European Pharmacopoeia
$N(i) = 16\ \cdot [\ T(i) / Wb(i)\ ]^2$	this formula is default for US Pharmacopoeia

where ***i*** is an index of the peak, ***PI*** is 3.1415926..., ***T(i)*** is a retention time, ***H(i)*** is a height, ***A(i)*** is an area, ***W(i)*** is a width on the half-height of the peak and ***Wb(i)*** is a width of the peak at the base line.

To calculate ***Wb(i)*** a tangential at inflection points is used to find intercept with base line on both sides of the peak.

5.3.10.1.2 Resolution

This item defines formula for **resolution**.

The **resolution** for a chromatographic peak ***i*** is calculated by one of the formulas:

R = (T(i+1) - T(i)) / (W(i+1) + W(i)) | 60.7%	The width ***W(i)*** of the peak ***i*** is calculated at 60.7% of the peak height.
R = 1.18 * (T(i+1) - T(i)) / (W(i+1) + W(i)) |50%	The width ***W(i)*** of the peak ***i*** is calculated at 50% of the peak height This formula is default for European Pharmacopoeia
R = 2 * (T(i+1) - T(i)) / (Wb(i+1) + Wb(i))	***Wb(i)*** is a width of the peak at the base line This formula is default for US Pharmacopoeia

Here ***(i)*** and ***(i+1)*** indices refer to the neighboring peaks.

To calculate ***Wb(i)*** a tangential at inflection points is used to find intercept with base line on both sides of the peak.

5.3.10.1.3 Peak asymmetry

This item defines formula for **asymmetry** of the peak.

The **asymmetry** for a chromatographic peak ***i*** is calculated by one of the formulas:

(Width after) / (Width before) | 10%	*Width after* - peak semi-width after the top at 10% of the peak height *Width before* - peak semi-width before the top at 10% of the peak height
(Full Width) / (2 * Width before) | 5%	*Full Width* - peak width at 5% of the peak height *Width before* - peak semi-width before the top at 5% of the peak height This formula is default for European Pharmacopoeia and for US Pharmacopoeia

As >1 for tailing peaks.

5.3.10.2 Void time

Void time is the net time needed by eluent to pass through the chromatographic system from injector to detector. This time is used in capacity factor, linear velocity and logarithmic index calculations.

Void volume is the volume corresponding to the void time. **Void time** and **Void volume** are related as

Void volume = **Void time** x **Flow rate**.

Usually unretained components are eluted as void time peak. Retention time of this peak may be used as void time estimate for the run.

The system allows to set up a way of recognizing a void time peak by the **Calculation method** parameter:

None	Void time, manually entered into respective field, is used for all calculations.
1st component	The peak corresponding to the first component is selected as a void time marker and its retention time replaces the previous value of the void time. If the first component is not identified, the **expected retention time** 168 of the component is used.
1st peak	The first detected peak is used as a void time marker for the run and its retention time is stored in the void time field.
From void volume %	For the calculation of the void time, the % value entered in the "**Void volume**" field is multiplied by the ratio of empty column volume and eluent flow rate.

If **Calculation method** is not set to **None**, every time when the chromatogram makes the **peak identification** 166, the void time value will be recalculated.

5.3.10.3 Retention index

The chromatogram has a primary retention scale, measured as time or volume of retention and a secondary scale, that appears after peak identification. This scale is called Index. A typical case is Kovatch' or linear indexes in gas chromatography.

Although this secondary scale is called Index, it may have quite different meanings and may be helpful in many cases. So, index can stand for boiling temperature, providing a mean for imitated distillation calculations in GC or for molecular mass for GPC (SEC) calculations.

The secondary scale can also be used as more accurate relative time indicator, if retention time is entered into "Index" fields of identified components in the calibration run and linear index interpolation is used.

For index calculation the user must define index values for at least two peaks and enter these values in the "Index" column of the **components table** 171. All other values will be calculated by the software using retention times of the preceding peak with known index value and the following one. If there is no peak with known index value either before or after the peak of interest, the software will extrapolate the index using the nearest two peaks with known index. Peaks with known index are those that match components with a non-zero value in the "Index" field of the **components table** 171.

The interpolation method (Linear or Logarithmic) for the index calculation can be selected in the **Math** 138 window:

Linear index is calculated by the formula:

$$I(i) = I(n) + [\, I(n+1) - I(n) \,] \bullet [\, T(i) - T(n) \,] / [\, T(n+1) - T(n) \,],$$

where:

I(i)	Index of the peak of interest (target peak).
I(n), I(n+1)	Indexes of the previous and the following components with known index value, respectively.
T(i)	Retention time for target peak.`
T(n), T(n+1)	Retention times of the peaks, corresponding to previous and following components with known index.

Logarithmic (or Kovatch') index is calculated by the formula:

$$I(i) = I(n) + [\, I(n+1) - I(n) \,] \bullet [\, \log T'(i) - \log T'(n) \,] / [\, \log T'(n+1) - \log T'(n) \,].$$

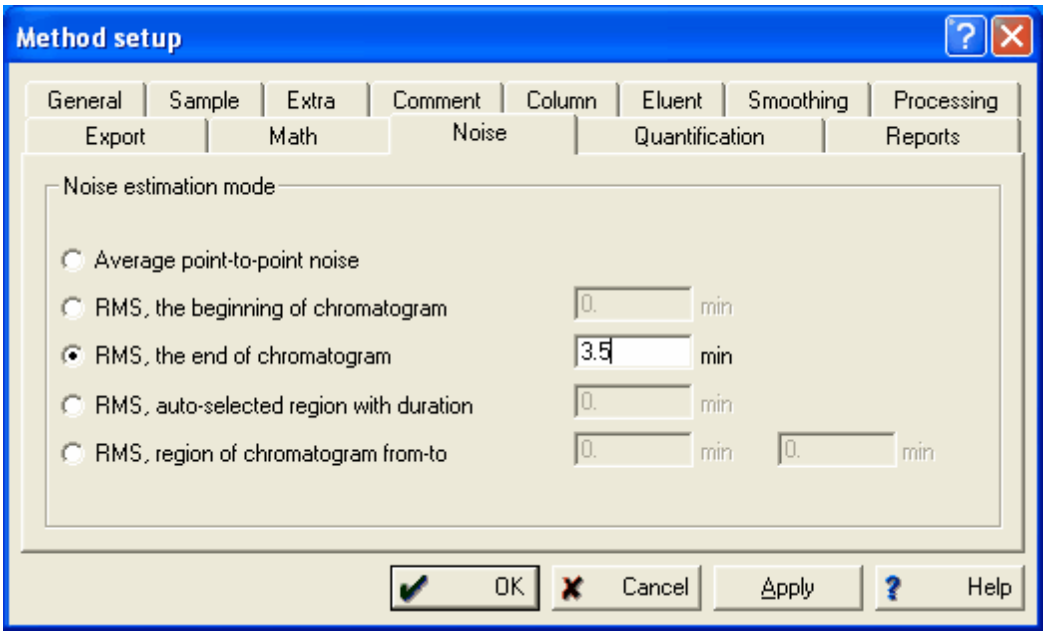
Two types of Indexes scales can be used: Internal index scale and External index scale. They are also selected in the **Math** 138 window.

Internal index scale intends that components used for the index scale calibration are present in all analyzed samples and their real retention times obtained in the current chromatogram are used for calculations.

In the case of External index scale the expected retention times 168 of the components, obtained in the previous calibration chromatogram, are used. Although this approach is less precise as compared with Internal index scale, it is often used and gives satisfactory results in most cases.

5.3.11 Noise

The **Noise** page contains settings how signal noise is calculated.



If there are more then one measure channels in the chromatogram the noise is calculated individually for each channel.

Settings of this page are applied to each channel.

***Noise estimation mode*:**

Average point-to-point noise	Noise estimation based on point-to-point approach. This mode was used in software versions **3.2** and earlier.
RMS, the beginning of chromatogram	Noise estimation based on RMS approach. A region for RMS calculation is taken at the beginning of the chromatogram.
RMS, the end of chromatogram	Noise estimation based on RMS approach. A region for RMS calculation is taken at the end of the chromatogram.
RMS, auto-selected region with duration	Noise estimation based on RMS approach. An algorithm looks for region of specified duration in chromatogram with minimal noise level. A noise is estimated at this region.
RMS, region of chromatogram from-to	Noise estimation based on RMS approach. A region for RMS calculation is defines in the middle of the chromatogram by **from** time and **to** time values.

Remarks

Software evaluates the dispersion (σ) of the noise using the specified ***noise estimation mode***. The dispersion of the noise is printed at the reports as **Noise** report item.

When RMS approach is used the software also calculates signal ***drift*** at specified chromatogram

region. The ***drift*** is subtracted from the original signal. So the drift of the signal has no effect on noise estimation.

Besides dispersion (σ - **noise**) software also calculates **peak-to-peak noise** at specified region.

Noise, **drift** and **peak-to-peak noise** are calculated after applying **smoothing** 132.

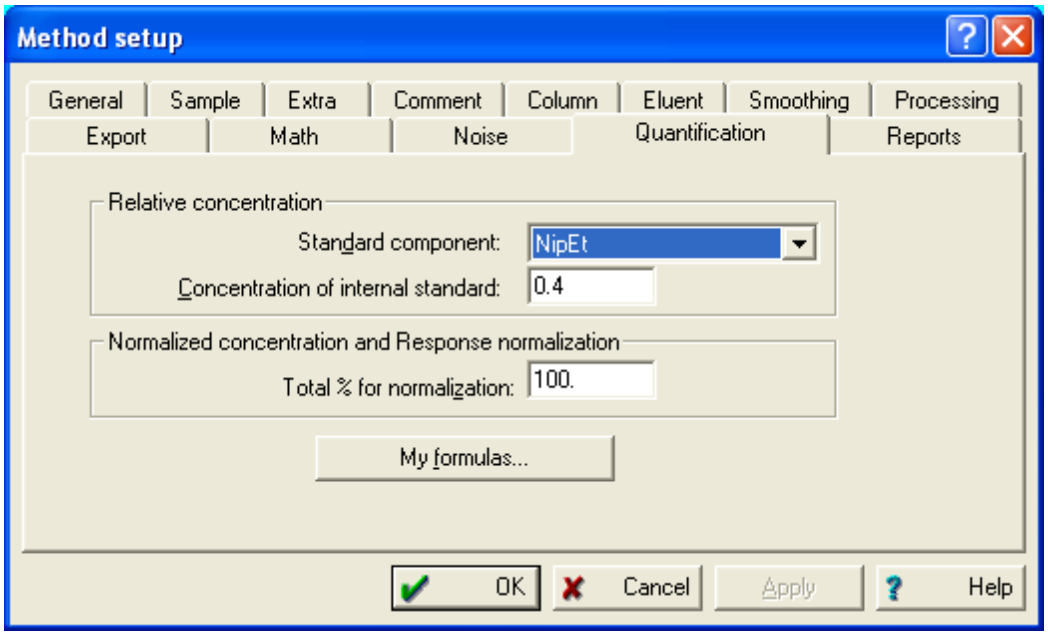
If **Average point-to-point noise** mode is specified in the method, then **drift** and **peak-to-peak** values are calculated using entire chromatogram.

For original raw data (before **smoothing** 132) the software also calculates **raw noise** using **average point-to-point noise** mode.

Default report templates for plain reports print **raw noise, noise**, **drift** and **peak-to-peak** values when user selects ***channel table*** 325 chapter in the **Report options** 322 dialog form.

5.3.12 Quantification

Quantification page is a part of the **Method setup** 124 window and allows to define common parameters of the quantification procedure for the current chromatogram 207 or Method 122.



Relative concentration

These parameters are used for **relative concentration** 202 quantification procedure.

Standard component Select the desired **standard component** 204 from the list

Concentration of internal standard: Enter a concentration of the standard component. The same

item is located at the **Sample** 126 page.

Normalized concentration and Response normalization

Parameters in this area are used to calculate normalized values.

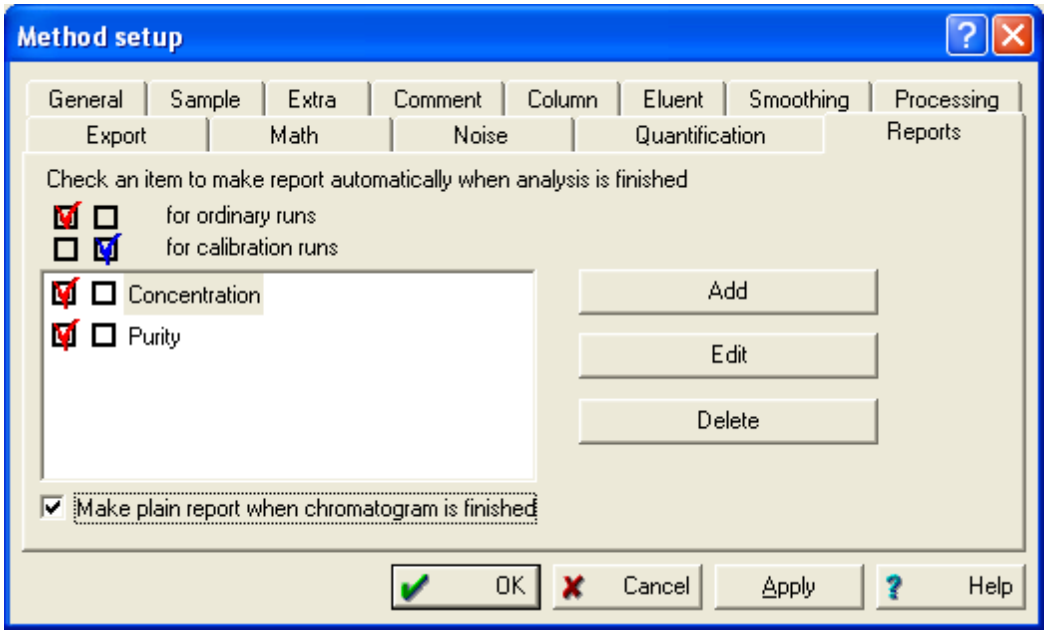
Total % for normalization value used for calculation of Normalized concentration 330 and Response normalization 329

<My formulas> this button opens "***Custom formulas*** 289" window to review and edit user-288 **defined formulas** 288. User formulas are saved in the method and are applied to all chromatograms collected with this method.

5.3.13 Reports

(*Main menu* Report / Report setup...)

Reports page is a part of the **Method setup** 124 window. It allows to define templates for **advanced reports** 341 for chromatograms running this method.



One or more **advanced reports** 341 could be defined. Each report could have it's own layout and could be directed to its own output(file of specified format, printer, screen).

User could put a check mark for the report item to generate report automatically when analysis finished: for ordinary runs, for calibration runs or both.

<Add> add a new report template to the list.
"***Add report***" window is opened prompting to enter a name of a new ***report***.

Then "***Edit report template*** 343" form is opened. User can define report items and configure report layout.

<Edit> Opens "***Edit report template*** 343" form for the selected item for editing report template.

<Delete> Delete the selected report item.

☑ **Make plain report when chromatogram is finished**

check this box to produce a **plain report** 320 (in addition to the advanced reports) when a chromatogram is finished.

See also:

Quick reports 33

5.4 Channels

Detectors and other devices can supply a stream data of continuous measurement. See **Channels** 110 description of instrument control.

The chromatogram obtains these data and stores data for **channels** in the chromatogram file.

Typically there is the only **analytical channel** 113 in the chromatogram. The chromatogram is a **multi-channel chromatogram** 146 when it contains more then one **analytical channels** 113.

Method 122 can define **noise smoothing** 133 options for channel data preprocessing.

Also operators can configure additional **calculated channels** 152 in the **Method** 122 and use them for data processing instead of usual **analytical channels** 113.

Chromatogram window can display **auxiliary channels** 113 produced by instruments for additional visual control by operators.

See also:

Instrument channels 110

Multi-channel chromatogram 146

Method: "Channels setup" 147

Noise smoothing 133

Calculated channels 152

5.4.1 Multi-channel chromatogram

Multi-channel chromatograms contain measurements produced by several data **channels** 146 simultaneously and provide a powerful tool for analysis of complex mixtures.

Two types of **multi-channel chromatograms** can be distinguished on the basis of signal source nature.

Some chromatographic detectors can provide not one, but several response values for each measurement. A typical example is a diode-array detector or a rapid scanning detector in LC. In this case all data channels are of the same physical nature (i.e. UV absorbance). Thus, DAD detector can provide measurements at up to several hundreds channels simultaneously. See **spectral channels** 113.

In other cases, several chromatographic detectors may be used to monitor the same chromatographic mixture. Typical examples are simultaneous use of thermo-conductivity and flame ionization detectors in GC, UV + refractive index or UV + radioactivity detectors in LC. As a rule, Physical nature of detectors is different in this case.

Both cases are handled by Chrom&Spec software in a similar way as **multi-channel chromatograms**.

The software provides a toolkit for handling of such data in peak detection, identification, calibration and quantification.

Additional features such as **factor analysis** 451 are specific for multi-channel chromatograms.

5.4.2 Cycle time

The **cycle time** of **analytical channels** 113 is a duration between the subsequent ADC measures. Typically **cycle time** is about ***0.1sec*** in chromatography.

The less **cycle time** the more measures are recorded per chromatogram peak.

To get a best accuracy the instruments should be configured for **cycle time** which provides not less then 15-20 measures per peak in **chromatogram** 207.

If **cycle time** is too low then it may cause ***oversampling effects*** (too much measure points per peak): typically the noise of ADC grows when **cycle time** is decreased.

To avoid ***oversampling effects*** user should configure his instrument to bigger **cycle time**. If not possible then **frequency divisor** 135 or **noise smoothing** 133 can be configured in the **processing method** 122 (see **Method setup: "Smoothing" page** 132).

For **multi-channel chromatograms** 146 it is possible that different channels has different **cycle time**. In this case the raw data are preprocessed and re-sampled to the same **cycle time** when chromatogram finished.

5.4.3 Channels setup window

(*Main menu* Method / Channels setup...)

Each Method 122 includes a Channels table 149 which is used as a basis for other configurations and allows to define additional Calculated channels 152.

"**CHANNELS SETUP**" window includes two pages:

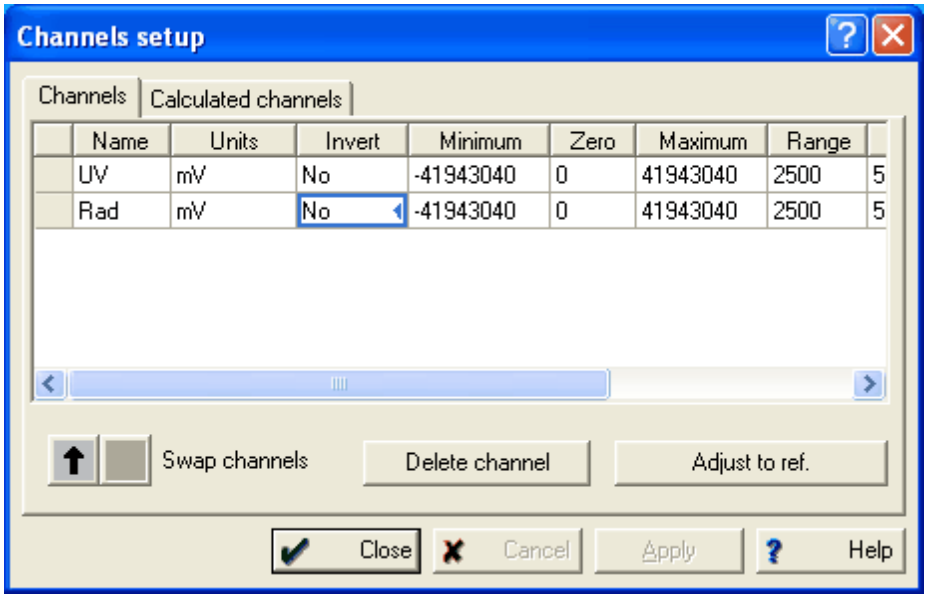
Channels 148 local Channels table that contains all data channels

Such operations as delete channel, swap channels, adjust channel's time shift are available

Calculated channels 151 this page allows to select and tune Calculated channels.

5.4.3.1 Channels setup window: Channels page

This page contains a **local channels table** containing parameters of all data channels in the current **Method** 122 or **chromatogram** 207.



For methods:

Invert and **Shift** parameters of the **channels table** 149 can be defined here. These parameters are preserved in the method and are used for data pre-processing when method runs next analysis.

To edit **Shift** parameter use ***Adjust to ref.*** button - see **adjust time shift** 150 for details.

Do not edit other settings of the channels here! **System** 79 overwrites a **local channels table** in the **method** 122 each time when analysis starts, so this table is a copy of the channels settings as specified by Data recorder setup 100 and Channels page 111 of the instruments.

Use Data recorder setup 100 of your system 79 to define a set of channels for chromatograms.

Use Channels page 111 of your instruments for changing channels configuration, if needed.

Local channels table is available in the **method** 122 after the first run of the system 79.

Local channels table is available for reviewing because it is used as a basis for other configurations of the **method** 122: **calculated channels** 152, **reference channel** 197, **channel for peak detection** 160 and other.

For chromatograms:

You should avoid editing **local channels table** for routine analysis. Instead use **Data recorder setup** 100 and **Channels page** 111 of the instruments for channels configurations.

Experienced users and method developers can edit **local channels table** to find a best

configuration for the method (based on the current chromatogram).

Note:	Modifying **local channels table** in the chromatogram can invalidate some other settings: peak detection configurations, calibration and so on.

Channels table 149 contains settings for all channels in the chromatogram.

The following functions are available:

Swap channels — This function enables to swap position of each selected channel in the table.
Move the selected channel up or down using arrow buttons.

<Delete channel> — delete the selected channel from chromatogram data.

<Adjust to Ref.> — adjust time shift 150 of the selected channel relative to reference one. Reference channel is selected in the Calibration Graphs window 178.

5.4.3.1.1 Channels table

All analytical data channels used in the current **method** 122, are combined in **local channels table** that has the following structure:

Name — Channel's name. This text appears as channel label in the chromatogram. This field can be changed by the user

Units — Units of detector response.

Invert — This flag allows to invert polarity of the channel's data.

Minimum — Minimum value of the linear range of the AD converter (in ADC counts). This parameter is used to detect an underflow condition.

Zero — A signal level that is assumed to be on a baseline. Note, that chromatogram data processing typically does not uses this value. Data processing algorithm analyses actual data to determine baseline signal level as well as a drift of the base line.

Maximum — Maximum value of the linear range of the AD interface (in ADC counts). This parameter is used to detect overflow condition.

Range — A range of the values of input signal, in **Units**.
Range = (**Maximum** - **Zero**) · **Coef**

Coef — Conversion coefficient from ADC counts to physical measure units. $Vphysical$ [**Units**] = $Vadc$ · **Coef**

Noise — Estimated baseline noise value of the channel in ADC conversion units (in ADC output units).

Shift — Shift of the current channel in time. See **adjust time shift** 150 function.

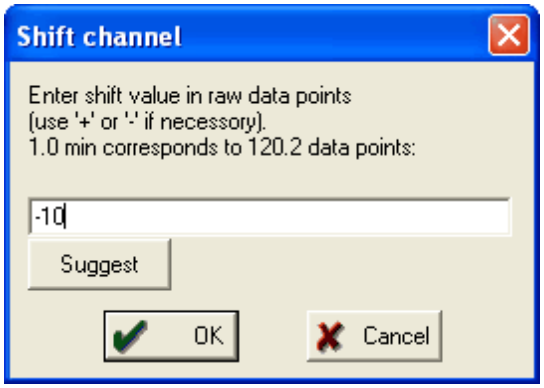
See also:

Channels setup window: Channels page 148

5.4.3.1.2 Adjust time shift

Shift channel dialog form can be called from the **Channels setup window: Channels page** 148 by pressing ***Adjust to ref.*** button.

This feature adjusts a retention time of all measures of the selected channel relative to the **reference channel** 197.



The **shift** value is specified in the ADC measures (sample data points - see **cycle time** 147).

Suggest - the software calculates the shift value which is a best match of the selected channel to **reference channel** 197. This function is used with a sample chromatogram during method configuration. The chromatogram should contain several peaks to get the best results.

Adjusting time shift is necessary when channel data are acquired from two different detectors with spatial distance between them. To get quasi-simultaneous detection it is necessary to shift one channel with respect to the other to compensate for time spent by a mobile phase to traveling from one detector to the other. This problem is common in multi-detector chromatography with void volumes between detectors (connecting lines, volumes of flow cells, etc.). A typical example is the in-line coupling of a catarometer and a flame ionization detector in gas chromatography. Two peaks of the same component will have a time shift.

In the case of Diode Array Detector time shift between data channels 0, so no time shift is required.

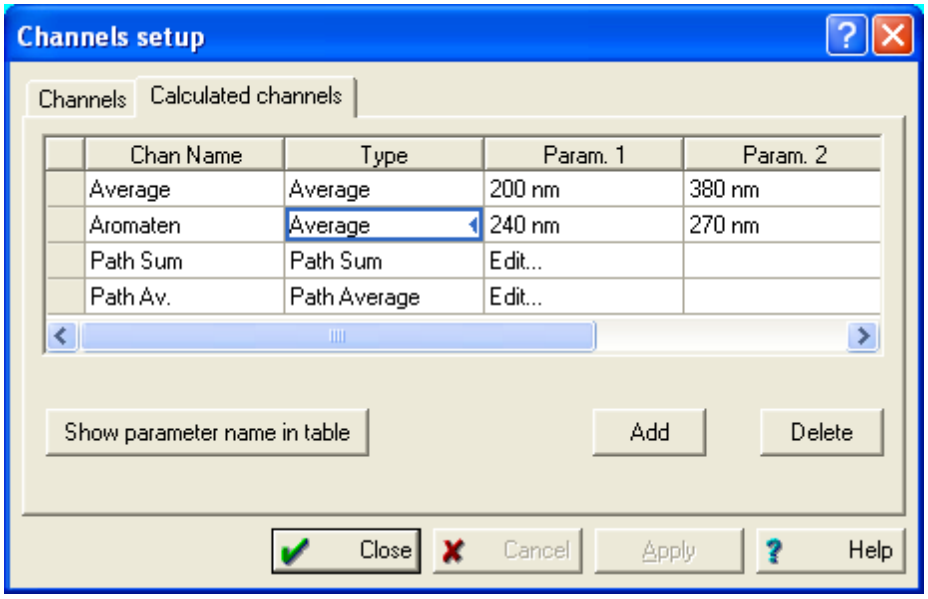
Channel shift is measured relative to the **reference channel** 197 in . Reference channel can be selected in the **Calibration graph** 178.

See also:

Multi-channel chromatogram 146
Channels setup window: Channels page 148

5.4.3.2 Channels setup window: Calc.Channels page

Calculated channels page allows to define and configure **calculated channels** 152 for your method.



The page consist of the following parts:

Calculated channels table 152	lists **calculated channels** 152 and includes additional parameters, needed for their computing. Double-click the left mouse button or press [Enter] in a desired item to edit parameter. It is possible either to enter text or numeric value, or to select a value from the list.
<Show parameter name in table>	this button toggles parameters values and parameters names (meaning) in the table.
<Add>	Add a new channel
<Delete>	Delete a selected channel

Note: Configure ***calculated channels*** in some sample chromatogram, created by preliminary configured **method** 122. The sample chromatogram is used to immediately evaluate the results of your configuration.When done save the method from the chromatogram using **Save method** 123 command. This applies configuration of ***calculated channels*** to your **method** 122.

See also:

Calculated channels 152
How to add calculated channel

5.4.3.2.1 Calculated channels table

Calculated channels table lists calculated channels and includes some additional parameters, needed for their computing.

Chan. name	User-defined name of the channel (up to 8 symbols)
Type 152	calculation algorithm used for the current channel
Param.1	first parameter needed for the channel calculation
Param. 2	second parameter needed for the channel calculation
Param. 3	third parameter needed for the channel calculation
Removable	removable channel is a temporary channel that is used for computing of other calculated channels only. Removable channel is deleted when computing of all channels is finished.

Note: Calculated channel can be used as an input for computing other calculated channels.

See also:

Channels setup: "Calculated Channels" 151

Calculated channels 152

How to add calculated channel

5.4.3.2.2 Calculated channels

Chrom&Spec software offers an ***Calculated channels*** technique which serves to optimize different aspects of data processing and to enhance accuracy of analysis results.

Calculated channels technique means creating an additional channels in the chromatogram by applying different computational algorithms to original **analytical channels** 113.

It is possible to use ***Calculated channels*** for data processing instead of original **analytical channels** 113, including integration and quantification. This provides a flexible tool for **method** developing and optimizing.

Calculated channels are listed in the **Calculated channels** 151 page that includes also some additional parameters, needed for channel computing.

It is possible to create as many calculated channels as necessary, each with different parameters.

The following calculated channels are available:

Total	**Total** channel is calculated as a sum of response-to-noise ratios for all channels of the selected channel range. Two additional parameters can be set: the first and the last channel of the range. By default all available data channels

are used. **Total** channel can not be used for quantification purpose, but it is usually the best choice for peak detection (integration).

Average — **Average** channel is calculated as a sum of responses for the selected channel range. Two additional parameters can be set: the first and the last channel of the range. By default all available data channels are used. It is possible to create as many **average** channels as necessary, each for the different wavelength range. **Average** channel can be used for both quantification and peak detection (integration) purposes.

Difference — **Difference** channel is calculated as a difference between two other channels. Three additional parameters should be set: the first channel (Reducible), the second channel channel (Deducted), and scale factor. Scale factor is used to multiply the second channel before subtraction. Default value for scale factor is **1**.

Integral — **Integral** channel allows to calculate integral value of the selected channel. Two additional parameters should be set: channel and Base parameters.

Channel channel to be integrated
Base parameter showing if baseline should be or should not be subtracted from channel value before integration {Use baseline; Ignore baseline}

Derivative — **Derivative** channel allows to calculate a derivative for a selected channel. Two additional parameters should be set: channel and Order parameters.

Channel calculates a derivative for channel.
Order order of the derivative to be calculated **{1, 2, 3}**

Angle 154 — Angle channel shows angle of spectral vector, created in multidimensional spectral space.

Resp./Time 155 — Each point of the channel is calculated as a ratio of response of base channel and retention time. The only additional parameter specifies a base channel for calculations.

Spec.Ratio — Ratio of channels response for two other channels. If some peak is homogeneous by spectra, all its spectral ratios are constant within boundaries of the peak. Two additional parameters should be set: Dividend and Divisor parameters.

Dividend The response value for the channel is used as dividend. The baseline value is subtracted from the response.
Divisor The response value for the channel is used as divisor. The baseline value is subtracted from the response.

Shift-Fit — This function calculates and applies an optimal shift between two channels. One channel is selected as *base* channel and the other –as *shifted*. Shift optimization is performed by maximizing correlation of specified channels. Additional ***Limit*** parameter specifies maximal shift [***-Limit***, ***+Limit***] of the *shifted* channel, in ADC cycles. Setting ***Limit=0***, assumes no restrictions for possible shift of the *shifted* channel.

Normalize — A selected channel can be normalized.
Channel parameter defines a base channel for normalization.
How parameter defines the way of normalization:
Max. response maximum response of the **Channel** is normalized

to **1.**

Max. peak area	**Channel** is normalized so that the maximal area of the peak equals to **1.**
Full area	**Channel** is normalized so that the total area of all peaks equals to **1.**

Note: **Calculated channels of the *Path-* type work similar to *Total* or *Average* channels, but allow to define an adjustable (over retention time) range of analytical channels for calculations. *Path-* type channels are intended for diode-array spectral detectors. See *Path editor*[155] for details.**

Path S/N	***Path S/N*** channel is calculated as a sum of response-to-noise ratios for the selected channel range. Channel range is configured in the ***Path editor***[155]. Double click on the ***Edit...*** cell to open ***Path editor***[155]. ***Path S/N*** channel can not be used for quantification purpose, but it is usually the best choice for peak detection (integration).
Path Sum	***Path Sum*** channel is calculated as a sum of responses for the selected channel range.Channel range is configured in the ***Path editor***[155]. Double click on the ***Edit...*** cell to open ***Path editor***[155]. ***Path Sum*** channel can be used for both quantification and integration purposes.
Path Average	***Path Average*** channel is calculated as an average response for the selected range of channels. Channel range is configured in the ***Path editor***[155]. Double click on the ***Edit...*** cell to open ***Path editor***[155]. ***Path Average*** channel can be used for both quantification and integration purposes.
From calib. level	The channel is imported from specified calibration chromatogram. Importing channel allows operator to compare visually the current analysis with calibration one. If calibration chromatogram contains more then one channel the **reference channel**[197] is imported. The only additional parameter ***Level*** specifies a **calibration level**[199]. **Calibration level**[199] defines a name of calibration chromatogram file where the channel is imported from.
Smoothing[157]	This channel allows configuring an individual smoothing filter for selected channel. See **Calculated channels: Smoothing**[157]. See also **noise smoothing**[133], **method setup: "Smoothing" page**[132]

Note: The computed data of ***Calculated channels*** are not stored in the chromatograms file but reevaluated each time the chromatogram is loaded.

See also:

Channels setup: “Calculated Channels”[151]

5.4.3.2.2.1 Angle channel

Angle calculated channel represents angle between spectra of two adjacent chromatogram points (in multi-dimensional spectral space).

See **spectral angle**[454] description.

Minimum on the angle curve corresponds to the best angle spectrum of the homogeneous peak.

Angle calculated channel has no parameters. All **analytical channels** 113 of **multi-channel chromatogram** 146 are used.

See also:

Channels setup: "Calculated Channels" 151

Calculated channels 152

5.4.3.2.2.2 Resp./Time

Each point of the channel is calculated as a ratio of response of base channel and retention time. The only additional parameter specifies a base channel for calculations.

This channel allows compensate flow variations from analysis-to-analysis.

Flow variations (up to 5-10%) can be caused by various reasons related to instrument maintenance.

For concentration-responsive detectors this would lead to similar variations of peak areas which in turn results in quantification errors.

Using **Resp./Time** calculated channel as a reference channel 197 can compensate most negative effects produced by flow variations (as well as some other similar effects).

Another well known approach for such compensation is using **[Area/Time]** value instead of **[Area]** for quantifications. Using **Resp./Time** calculated channel is more accurate.

The calculated channel is especially useful for capillary electrophoresis data processing. Still it also may be used in LC.

See also:

Channels setup: "Calculated Channels" 151

Calculated channels 152

5.4.3.2.2.3 Calculated channels: Path editor

Path editor is designed for configuring ***Path*** calculated channels: ***Path S/N*** 152, ***Path Sum*** 152, ***Path Average*** 152

Path calculated channels are intended for **Multi-channel chromatograms** 146, created with diode-array detectors.

Path calculated channels are used to eliminate overflow and non-liner responses at particulate

wavelengths for the analysis. Also they can eliminate "**blank**" areas of **multi-channel** 146 detection (minimizing noise of the resultant calculated channel).

This can significantly improve the usability and precision of the analysis.

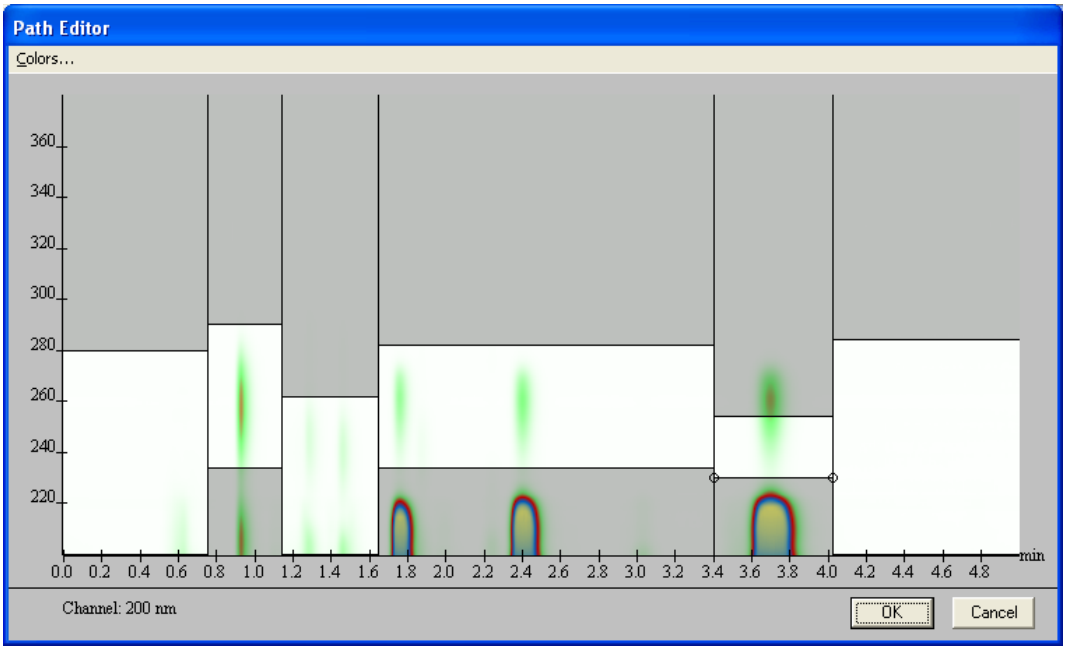
Use **Path editor** to define an adjustable (over retention time) range of analytical channels to calculate a resultant channel.

You would need a sample chromatogram (created by preliminary version of the **method** 122) to make a configuration.

Path editor shows the "top view" of the chromatogram. The horizontal line is a retention time and vertical line is a wavelength.

The detector response is displayed by colors.

Use **Colors...** 439 menu to setup a color palette.



All configurations within **Path editor** are done using ***mouse*** pointing device.

Use ***right mouse button*** to put a vertical ***split line***.

Vertical and horizontal ***split lines*** can be dragged using the ***left mouse button.***

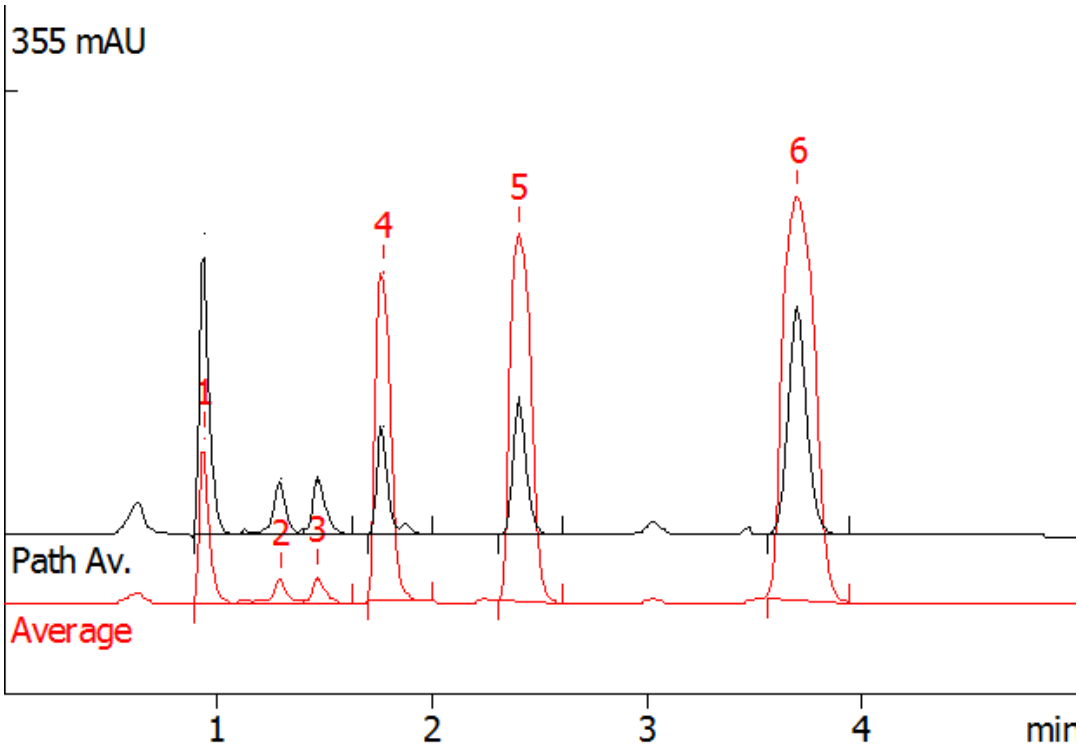
To remove a vertical ***split line*** just drag another vertical ***split line*** over it.

Note: As usual, configure ***calculated channels*** in some sample chromatogram, created by preliminary configured **method** 122. The sample chromatogram is used to immediately evaluate the results of your configuration.When done save the method from the chromatogram using **Save method** 123 command. This applies configuration of ***calculated channels*** to your **method** 122.

An example below shows the results produced by ***Path Average*** 152 compared to simple ***Average*** 152 calculated channels.

Average 152 (red line) includes overflow responses at some wavelengths. This appears as flatten tops of some peaks. Calculating concentration using this channel would produce significant error.

Path Average 152 (black line) has normal peaks and all responses are within range of linearity. So calculation of the concentrations using conventional **calibration procedure** 165 produces adequate results.



See also:

Channels setup: "Calculated Channels" 151

Calculated channels 152

5.4.3.2.2.4 Smoothing

Smoothing calculated channel allows configuring an individual smoothing filter for other channel. Other channel can be **analytical channel** 113 or **calculated channel** 152.

Smoothing calculated channel needs three additional parameters:

Channel	channel that is used as input for smoothing filter
Type	type of the smoothing filter, see below
Slit	slit for the smoothing filter, see description at **Method setup: "Smoothing" page** 132

The ***Type*** parameter specifies a type of the mathematical algorithm of the smoothing filter. The following types are available:

Median
Gaussian
Savitsky-Golay
Adaptive FS
Adaptive FS: CI
Adaptive FS: shift
Adaptive
Adaptive: CI
Adaptive: shift
Adaptive: slit

Median, **Gaussian**, **Savitsky-Golay** are equivalent to that defined at the **Method setup: "Smoothing" page** 132.

Adaptive FS defines an ***Adaptive Savitsky-Golay (confidence)*** smoothing filter ***without slit variation (Fixed Slit)***. See **confidence smoothing filter** 135 for details.

Adaptive defines an ***Adaptive Savitsky-Golay (confidence)*** smoothing filter ***with slit variation***. This filter is equivalent to **Adaptive** smoothing filter defined at **Method setup: "Smoothing" page** 132. See **confidence smoothing filter** 135 for details.

Other types **{ Adaptive FS: CI**, **Adaptive FS: shift**, **Adaptive: CI**, **Adaptive: shift**, **Adaptive: slit** } actually **do not** produce smoothing. The output channel contains specific values which demonstrate how **confidence smoothing filter** 135 works. For details see **confidence smoothing filter** 135.

Adaptive FS: CI	Shows a **C**onfidence **I**nterval for output of **Adaptive FS** smoothing filter at **0.95** confidence level.
Adaptive FS: shift	Shows a **shift** from the central point of the best polynomial smoothing probe. This is calculated for **Adaptive FS** smoothing filter.
Adaptive: CI	Shows a **C**onfidence **I**nterval for output of **Adaptive** smoothing filter at **0.95** confidence level.
Adaptive: shift	Shows a **shift** from the central point of the best polynomial smoothing probe. This is calculated for **Adaptive** smoothing filter.
Adaptive: slit	Shows an actually used **slit** value of the best polynomial smoothing probe obtained by **slit variation**. This is calculated for **Adaptive** smoothing filter.

See also:

Channels setup: "Calculated Channels" 151

Calculated channels 152

Noise smoothing 133

Method setup: "Smoothing" page 132

5.5 Peaks integration

(*Main menu* Method / Integration...)

This item allows to setup parameters for automated peak detector for **method**.

See also:

About peaks integration 159

Integration parameters 159

Integration setup 160

Integration events 162

5.5.1 About peaks integration

Integration procedure is used to detect **peaks** on the chromatographic curve and to draw a **baseline**.

The “Chrom&Spec” software includes a built-in integration algorithm for automated peaks detection. User configures the peaks detection for his analysis using **integration setup** 160 and **integration events** 163 which are parts of **integration parameters** 159 user interface.

Typically you should use an appropriate **chromatogram** 207 to configure parameters for **integration procedure** for your analysis. When you get an adequate results use **Save method** 123 command to save method from the chromatogram. This action applies settings to all subsequent runs of the method.

Manual **peak editor** 224 allows quickly correct results of automatic detection for chromatograms if required.

See also:

Integration setup 160

Integration events 162

Manual peak editor 224

Peak identification form 166

Quantification 201

Software basics 18

5.5.2 Integration parameters

(*Main menu* Method / Integration...)

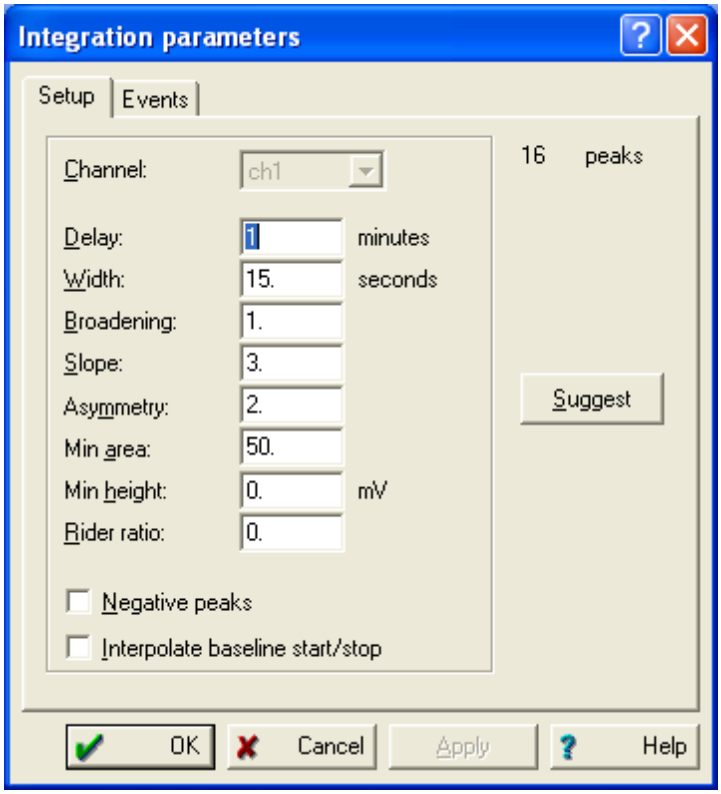
This window contains parameters used for the **integration** 159 procedure.

Integration parameters window consists of two pages:

Setup 160	Parameters for the integration procedure.
Events 162	Integration events.

5.5.2.1 Setup

This page of **Integration parameters** 159 contains the parameters that are used for the integration procedure.



Number of peaks	Number of peaks detected in the chromatogram (read-only).
Channel	Channel for peak detection for multi-channel analysis. This item is disabled for single-channel analysis. This channel can be different from **reference channel** 197.
Delay	Time delay before starting peak detection in minutes. Skips peak detection at the beginning of the chromatogram.
Width	Approximate expected width of the peak (at the baseline, in seconds). This parameter is used for setting baseline start and end points. It is recommended to enter the width of the narrowest peak, typically at the begging of the chromatogram.
Broadening	Broadening for width of the peaks at the end of the chromatogram compared to peaks at the beginning. This parameter is used for automatic adjustment of "**Width**".

Slope	Sensitivity threshold for peak detection. This is a key parameter for peaks integration. The built-in integrator algorithm is based on the use of the first derivative.The value of the first derivative (slope) of the curve is divided by the baseline noise (which is estimated using a special algorithm) and the result is compared with the "**Slope**" threshold value. Reasonable range of "**Slope**" parameter is 0.5...5. The threshold values for the upslope and downslope may differ. See **Asymmetry**.
Asymmetry	Ratio of slope at the start of the peak to slope at the end of the peak.
Min area	Minimum area of peaks to be detected. Skips peaks with areas less then specified.
Min height	Minimum height of peaks to be detected. Skips peaks with heights less then specified.
Rider ratio	Ratio of peak heights for two adjacent peaks. If this threshold value is exceeded, the smaller peak is separated from the higher one by tangent skimming. This function is switched off always if 0 is entered.
Negative peaks	Checking this checkbox allows to detect negative peaks.
Interpolate baseline start/stop	Checking this checkbox enables the interpolation of baseline start and stop points. This setting is recommended for very sensitive analyses with high noise level.

Buttons:

<Suggest> 161	Use automatic heuristic analysis of the current chromatogram to suggest a reasonable integration parameters.
<OK>	Accept integration parameters.
<Cancel>	Cancel changes.
<Apply>	Accept integration parameters and perform reintegration. This is used to estimate integration results after parameter changing.

Note: Always press **<Apply>** to estimate integration results after changing parameters! For chromatogram updated parameters produce immediate peaks re-integration.

See also:

About peaks integration 159

Integration events 162

5.5.2.1.1 Suggest

The Suggest mode sets up reasonable **integration** 159 parameters in the following way:

- "**Width**" and "**Broadening**" are calculated by fitting a straight line through the measured Peak halfwidth values vs. Retention time. "**Width**" is determined as the **y** value of this line at the "**Delay**" time, "**Broadening**" is calculated as the **y** value at the end of the chromatogram divided by the **y**

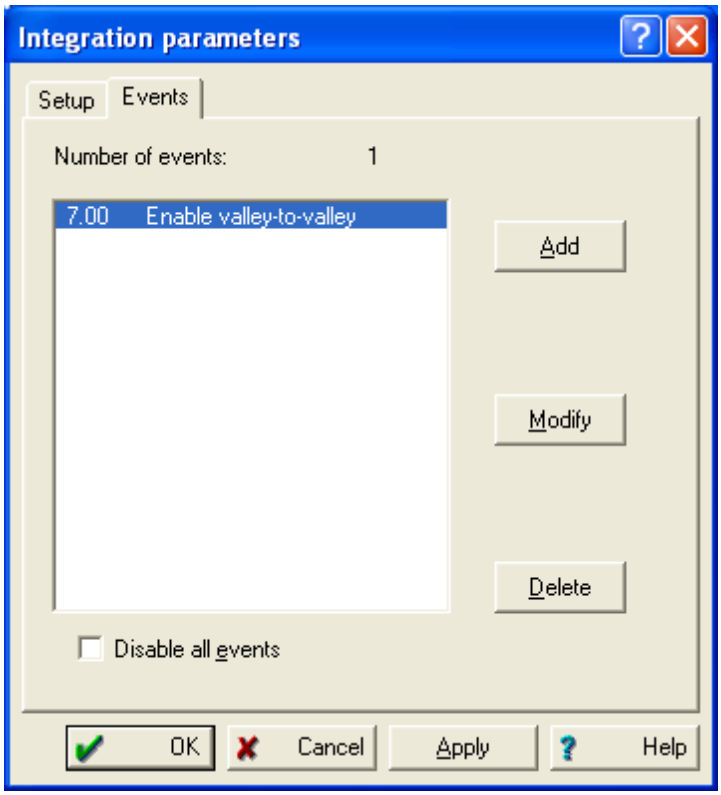
value at the "**Delay**" time. If this procedure does not provide adequate result,

- "**Width**" is set equal to the average value of peak width for the chromatogram.
- "**Broadening**" is set to **1**.

In many cases repeated (3 - 4 times) use of **<Suggest>** and **<Apply>** actions in combination leads to reasonable peak detection parameters even if the initial peak pattern is strongly inadequate.

5.5.2.2 Events

This page of **Integration parameters** 159 contains a list for defining special **integration events** 163.



Integration events are an advanced settings for fine tuning of integration procedure for particular analysis. Use it only if configuring general parameters at **Integration setup** 159 could not produce adequate results.

Integration events have higher priority than integration parameters defined at **integration setup** 160 page!

Note: Always press **<Apply>** to estimate integration results after changing parameters!

Number of events	Number of integration events (read-only).
<Add>	Add **event** 163 to the list.

<Modify> Edit the selected event.

<Delete> Delete the selected event.

<OK> Accept integration parameters.

<Cancel> Cancel changes.

<Apply> Accept integration parameters and perform reintegration. This is used to estimate integration results after parameter changing.

☑ **Disable all events** Checking this checkbox allows to ignore all determined events at the chromatogram integration.

See also:

About peaks integration 159

Integration setup 160

5.5.2.2.1 Integration events

Integration events are used for fine tuning of the **integration** 159 process. They should be used only in the case when problems cannot be solved by tuning a set of parameters from the **integration parameters** 159 window. They are especially useful for series of similar analyses.

If an integration event is added or modified, the "**EDIT INTEGRATION EVENT**" window is opened where the following parameters can be set:

Time Start time for event in min.

Event List box with items to be selected (see below).

Value Parameter value for selected integration event. This field appears for events that demand input of additional parameter.

Integration events for peak detection

Disable detection Set this mode to stop detection of new peaks. If a peak is available at the moment of the event it is either finished (downslope peaks) or rejected (upslope peaks).

Enable detection Clear **Disable detection** mode.

Enable negative peaks Enable detection of negative peaks. In some cases this mode may result in instability of detection algorithm.

Disable negative peaks Disable detection of negative peaks. This event does not influence negative peaks which already started.

Disable peak reject Set this mode, if a peak cannot be rejected because of its flat apex.

Enable peak reject Clear **Disable peak reject** mode.

Integration events for peak start/end

Set peak start Force the beginning of a new peak. If a peak is available at the moment of the event it is either rejected (upslope) or terminated (downslope).

Set peak end Force peak end at the time of the event. Upslope peaks are rejected (except those born by **Set peak start** event), downslope peaks are terminated.

Stop single peak mode Disable peak end detection. All peaks of any group after this event will

be treated as one peak. The group end will be treated as peak end.

Start single peak mode Set normal detection mode, when valley causes perpendicular drop or skim line separation.

Split peak Terminates the current peak and starts a new one.

Integration events for baseline

Enable valley-to-valley Disable perpendicular drop peak separation. All peaks are considered to be baseline-separated. The bottom of the valley becomes the baseline point.

Disable valley-to-valley Enable perpendicular drop peak separation.

Set horizontal baseline Set horizontal baseline for all peaks except the last one of adjacent peaks that are not separated. The baseline is drawn **forwards** from the peak start point.

Set back horizontal base Set horizontal baseline for all peaks except the first one of adjacent peaks that are not separated. The baseline is drawn **backwards** from the peak end point.

Set normal baseline Set default baseline detection mode.

Set baseline point Set defined baseline points for better evaluation of peaks on descending or ascending baselines. The baseline between two successive baseline points is set to zero for optimum integration.

Force horizontal baseline Set horizontal baseline for a single peak. The baseline is drawn **forwards** from the peak start point. The intersection of the baseline with the signal is defined as peak end point.

Cancel horizontal baseline Clear **Force horizontal baseline** mode.

Force horizontal base back Set horizontal baseline for a single peak. The baseline is drawn **backwards** from the peak end point. The intersection of the baseline with the signal is defined as peak start point.

Cancel horizontal base back Clear **Force horizontal base back** mode.

Enable baseline penetration Allow crossing of the signal by the baseline.

Disable baseline penetration Clear **Enable baseline penetration** mode.

Integration events for integration parameters

Set width Sets new "**Width**" parameter that supersedes default linear growth of expected peak width.

Set slope Sets new "**Slope**" value.

Set min height Sets a new "**Minimum peak height**" value.

Set rider ratio Sets a new value of the "**Rider ratio**" parameter.

5.6 Calibration

This section contains topics describing process of calibration in the Chrom&Spec software.

In this section:

5.6.1 About calibration

Calibration is a procedure which enables the response of an instrument to be related to the concentration of an analyte in a sample by first measuring the response from a sample of known composition, i.e. a standard. A series of standards is used to prepare a calibration curve in which instrument response is plotted as a function of quantity of the analyte over a given range.

The goal of the calibration is to provide information for the **quantification** 201 procedure.

The result of this procedure is a **calibration curve** 182 showing the dependence of **sample quantity** 200 versus **detector response** 200.

There are several ways to perform calibration. Basic experimental procedures are called **External standard calibration** 190 (or absolute calibration) and **Internal standard calibration** 190 (or relative calibration). In addition a modified external standard method called **Tabulated calibration** 193 (relative response factor) can be used. Methods differ in the way in which the calibration plot is constructed.

Calibration may be **single-point** 200 and **multi-point** 201.

See also:

5.6.2 Using calibration

This article describes typical scenarios of building and updating **calibration** 165.

The calibration procedure fulfills the following tasks:

1. Measures **retention times** 168 of peaks corresponded to **components**. This information is used in **peaks identification procedure** 166 recognize components in the analyte.
2. Build **calibration curve** 182 which relates detector response (peak **height** or **area**) and concentration of each component. This information is used in **quantification** 201 procedure for calculating concentrations of components in analyte.

Typically both tasks are executed simultaneously by running and processing the special **calibration samples** with known components and known concentrations.

See also:

About calibration 165

5.6.3 Peaks identification procedure

Peak identification is a process of cross-linking detected **peaks** and components listed at components table 171.

Columns from components table 171, responsible for peak identification, are listed below:

Name	Component name.
Time	Retention time 168 in calibration run.
Window%	Identification window 173 of the component.
Ref.	Reference component indicator.

Typically identification is done by matching retention time 168 of the chromatographic peak and expected retention time 168 of the component.

When needed an advanced two-step procedure is used for peak identification. This procedure recognizes reference components 174 on the first step. The second step uses relative retention times to identify ordinary components 174 (expected retention time 168 is corrected in accordance with actual retention times of reference components in the current run).

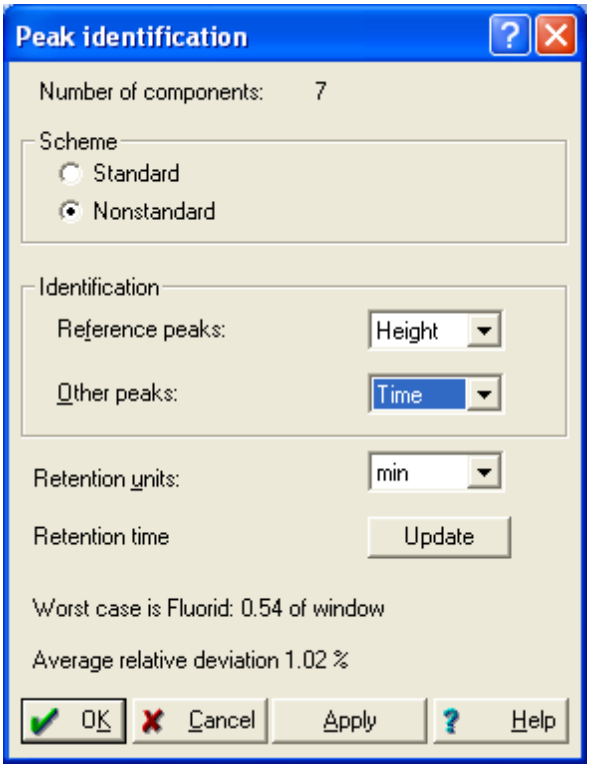
See also:

Peak identification window form 166

5.6.3.1 Peak identification

(*Main menu* Method / Calibration / Identification)

The "***Peak identification***" window contains parameters for configuring peak identification procedure 166.



Number of components Number of components in the **components table** 171 (read-only).

Scheme Quick choice of **identification parameters** 169 scheme.

Standard — Sets default (recommended) configuration for identification parameters:

Height for reference components

Time for all other components (ordinary components)

Use this scheme also if your **method** has no **reference components** 174

Nonstandard — Set custom configuration of identification parameters

Identification **Identification parameters** 169.

Reference peaks — Set **identification parameters** 169 for **reference components** 174. Default is **Height**.

Other peaks — Set **identification parameters** 169 for **ordinary components** 174. Default is **Time**.

Retention units 169 Choice of retention units. Default is "**min**".

Retention time 168

<Update> Updates the retention times stored for components in **components table** 171 according to retention times of the recognized peaks in the current chromatogram. This update changes **expected retention times** 168 for components.

Worst case... Information about current chromatogram: the component with the largest deviation of actual and expected retention time. Deviation is given as a part of component's **identification window** 173.

Average relative deviation — Relative deviation of retention times (as percent of **expected retention times** 168) averaged for all components.

Note: It is recommended to update the retention time of components if the deviation of some component or the Average relative deviation exceeds half of the identification window 173. Don't wait until the identification algorithm fails! Besides, if you use manual calibration, the software will identify such cases and will offer to update retention times before calibration is performed.

See also:

Peaks identification procedure 166

5.6.3.2 Retention time

Retention time of the peak is a time of the peak top elapsed since chromatogram start.

Algorithm uses polynomial approximation of the peak top to calculate an exact peak top position. This makes possible to calculate the position of the peak top with a precision better then ADC cycle time (ADC cycle time is a value reverse to ADC sampling rate 124 : ***ADC cycle time = 1 / ADC sampling rate***).

Polynomial approximation uses cubic polynomial with a gap depending on peak width at the half of peak height. For very narrow peaks a quadratic polynomial may be used instead of cubic one.

5.6.3.3 Expected retention time

Expected retention time of the component is used for **peak identification** 166.

Typically expected retention time of the component is a retention time of a component obtained in the calibration run.

In some cases an advanced technique should be used which assumes two-pass identification. Two types of components must be defined in **components table** 171: **reference components** 174 and **ordinary components** 174.

Expected retention time of the **reference components** 174 is a retention time of a component obtained in the calibration run. Thus, reference components use an absolute retention scale. Algorithm identifies **reference components** 174 at the first path of two-pass identification.

An expected retention time is corrected for **ordinary components** 174. Algorithm calculates a correction of expected retention time by matching expected retention time of the reference components and actual retention time of the corresponding peaks using piecewise-linear function. Thus, ordinary components use a relative retention scale. Analyte must contain at least some reference components.

For example, if a retention time of reference component (we will assume for simplicity, that only one component has been defined as reference) in the chromatogram was increased by 10% compared to its

expected retention time, the expected retention times for all other components will be also increased by 10%.

5.6.3.4 Identification parameter

This parameter configures **peak identification procedure** 166. It defines the way how peak in the chromatogram is identified as component from **components table** 171.

In all cases only those peaks are considered that fall within the **identification window** 173 for the component.

The possible selections are:

Time — The peak with the time closest to the **expected retention time** 168 is selected. Peaks that fall within the **identification window** 173 are only considered for the component.

This setting is default for ordinary components.

Remember, that if at least one **reference component** 174 is used the **expected retention time** 168 for **ordinary components** 174 differs from the retention time measured in the calibration run (stored in **components table** 171).

Area — The greatest peak by area is selected. Peaks that fall within the **identification window** 173 are only considered for the component.

Height — The greatest peak by height is selected. Peaks that fall within the **identification window** 173 are only considered for the component.

This setting is default for **reference components** 174.

Number — This setting is a simple identification method used when no other identifications could be used by some reason. **Identification procedure** 166 matches sequence number of the component from **components table** 171 to the sequence number of the peak in the chromatogram.

Take care when using this setting.The chromatogram must not contain peaks which has no related component from **components table** 171. Identification fails otherwise. All peaks of impurities and noise must by removed either by configuring **peaks integration** 159 procedure or **manually** 224.

This setting cancels **reference components** 174 and two-pass identification. Selecting this item for **Reference peaks** or for **Other peaks** in **peak identification form** 166 forces identification by **Number** for all peaks.

See also:

Peak identification 166

5.6.3.5 Retention units

The retention units for calibration (unit for retention time) is set in the **Peak identification** 166 form. The possible choices are:

sec	Seconds
min	Minutes
µL	Microliters
mL	Milliliters
Nmeas	Number of raw data points (Number of ADC measure cycles)

Volume units (**µL, mL**) use **flow** 131 rate parameter for calculating **retention volume**.

This parameter affects the way how the **peak areas** are calculated. See **peak area units** 170 for details.

This parameter also used in **reports** 318. Various report items are printed out in these units.

See also:

Retention units (appearance) 218

5.6.3.6 Peak area units

The **area of the peak** is most commonly used as **detector response** 200 for **calibration** 165 and **quantification** 201. See **calibration curve** 182 and **computed quantity** 201.

The **retention units** 169 parameter of **peak identification** 166 affects the way how **area of the peak** is calculated.

Measurement units for **area of the peak** are defined by the following rule:

If retention units are time (**sec** or **min**) then:

[Area] = [Measure units]*sec

If retention units are volume (**µL** or **mL**) then:

[Area] = [Measure units]*µl

If retention units are **Nmeas**:

[Area] = [Measure units]

the ***Area*** is calculated as a sum of ADC outputs through the peak range.

Here ***[Measure units]*** are physical measure units of the **channel** 146 at which area is calculated. In most cases this is a **reference channel** 197. See **channels table** 149 for details.

Using volume units makes it possible to use different **flow** 131 rates for calibration runs and for analyte because changing **flow** 131 rate preserves the same areas of the peaks.

See also:

Retention units (calibration) 169

Peak identification 166

5.6.4 Calibration user interface

Calibration user interface is a set of window forms and menu 171 which allow user to create, update and transfer calibration. The most important configurations are done using Components table 171, Concentrations table 174 and Calibration graphs 178 window forms.

See also:

Calibration menu 171
About calibration 165
Using calibration 165

5.6.4.1 Calibration menu

(*Main menu* Method / Calibration...)

This is a submenu of the **Method** menu that gives access to the following calibration actions:

Components 171	Edit Components table.
Identification 166	Set parameters for peak identification 166.
Concentrations 174	Edit Concentrations table.
Graphs 178	View and edit Calibration graphs.
Load from method 197	**Load** calibration from method in working memory to current chromatogram.
Save to method 198	**Save** calibration from current chromatogram to method in working memory.
Import calibration 198	**Import** calibration from file to current method / chromatogram.
Export calibration 198	**Export** calibration to file. Useful to transfer calibration from chromatogram-to-chromatogram.

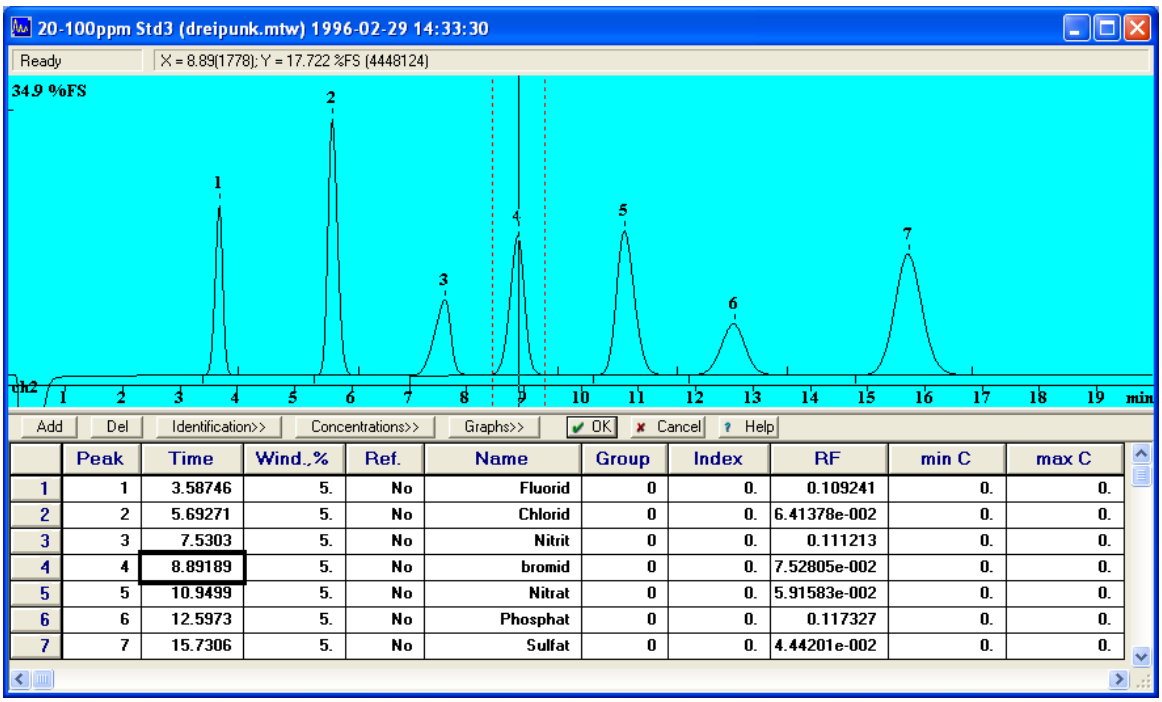
See also:

About calibration 165
Using calibration 165

5.6.4.2 Components table

(*Main menu* Method / Calibration / Components)

The **components table** stores information on the components to be analyzed. It contains components names and parameters necessary for peak identification 166 and quantification 201.



	Peak	Time	Wind.,%	Ref.	Name	Group	Index	RF	min C	max C
1	1	3.58746	5.	No	Fluorid	0	0.	0.109241	0.	0.
2	2	5.69271	5.	No	Chlorid	0	0.	6.41378e-002	0.	0.
3	3	7.5303	5.	No	Nitrit	0	0.	0.111213	0.	0.
4	4	8.89189	5.	No	bromid	0	0.	7.52805e-002	0.	0.
5	5	10.9499	5.	No	Nitrat	0	0.	5.91583e-002	0.	0.
6	6	12.5973	5.	No	Phosphat	0	0.	0.117327	0.	0.
7	7	15.7306	5.	No	Sulfat	0	0.	4.44201e-002	0.	0.

User creates **components table** on the basis of the **calibration chromatogram** (that is the chromatogram containing components with known concentrations).

When the **components table** is opened, the **chromatogram window is split into two parts**. The upper one shows the chromatogram, the **components table** appears in the bottom part of the screen. When moving into the **components table**, a special cursor in the upper part of the window jumps to the peak corresponding to the current component.

Columns of Components table

Number — Row (sequence) number in the **components table** (read-only).

Peak — Number of the peak in the chromatogram that corresponds to the given component. Setting this parameter automatically updates **Time** parameter.

Time — Retention time of the component measured by **retention time** 168 of the peak in the calibration run. See **expected retention time** 168.

Wind.% — **Identification window** 173 of the component.

Ref. — **Reference component** 174's trigger. **Yes** stands for reference component, **No** for ordinary component. See **peak identification** 166.

Name — Component's name (15 character limited).

Group — A **group** 173 number for the component. Any positive integer may be specified. A zero value has no effect (default).

Index — **Retention index** 141 for components with known index. In the case of an unknown index this value should be equal to 0. For index calculation the user must define index values for at least one peak (still two or more peaks are recommended), and all other values will be calculated by the software using linear or logarithmic approximation. See **Index** section at **Math page** 138.

RF — **Response factor** 201 (***K1*** coefficient in calibration formula). See also quantification without calibration 165.

min C (max C) Minimum (Maximum) concentration value for the component. These parameters are used for reports only.
Components whose concentrations are outside the range [**min C**, **max C**] are marked in the **Peak table** 327 by the sign "**!**"

Command buttons (above the components table)

<Add> Add a new component (an empty row) to the **Components table**.

<Del> Delete the current component from the **Components table**.

<Identification> 166 Edit peak identification parameters.

<Concentrations> 174 Edit the **Concentrations table**.

<Graphs> 178 Show calibration graphs and edit settings of calibration method.

<OK> Accept all changes and close **Components table** window.

<Cancel> Reject all changes and close **Components table** window.

See also:

How to modify the components table 471
About calibration 165
Using calibration 165

5.6.4.2.1 Identification window

Identification window is a user-defined maximum allowed difference of the actual retention time of the component and its **expected retention time** 168, measured as % of expected retention time. The component will be identified within its identification window only.

The identification window value is entered in the "Wind. %" column of the **components table** 171.

See also:

Peaks identification 166

5.6.4.2.2 Group number

Each component can have a **group number** that is defined in the "**Group**" column of the **components table** 171.

A **group number** is used in **reports** 318. Components in the same **group** may be grouped together in a separate table and group subtotals can be calculated and printed.

5.6.4.2.3 Reference component

Reference components are the characteristic components that can be easily found in the chromatogram. Usually peaks of those components are stand-alone or are the highest in their **identification window** 173. Moreover, at least some of them should be present in all samples analyzed by the method. Reference components are used to provide better **peak identification** 166 for **ordinary components** 174. Usually it is enough to choose 2 - 3 reference components.

To make a component a reference component, set the **Ref.** parameter in the **components table** 171 to **Yes**.

See also:

Expected retention time 168
Peaks identification 166

5.6.4.2.4 Ordinary component

Ordinary or other component is any component that is not a **reference component** 174. Ordinary components use a relative **expected retention time** 168 scale for **peak identification** 166.

To make a component an ordinary component, set the Ref. parameter in the **components table** 171 to **No**.

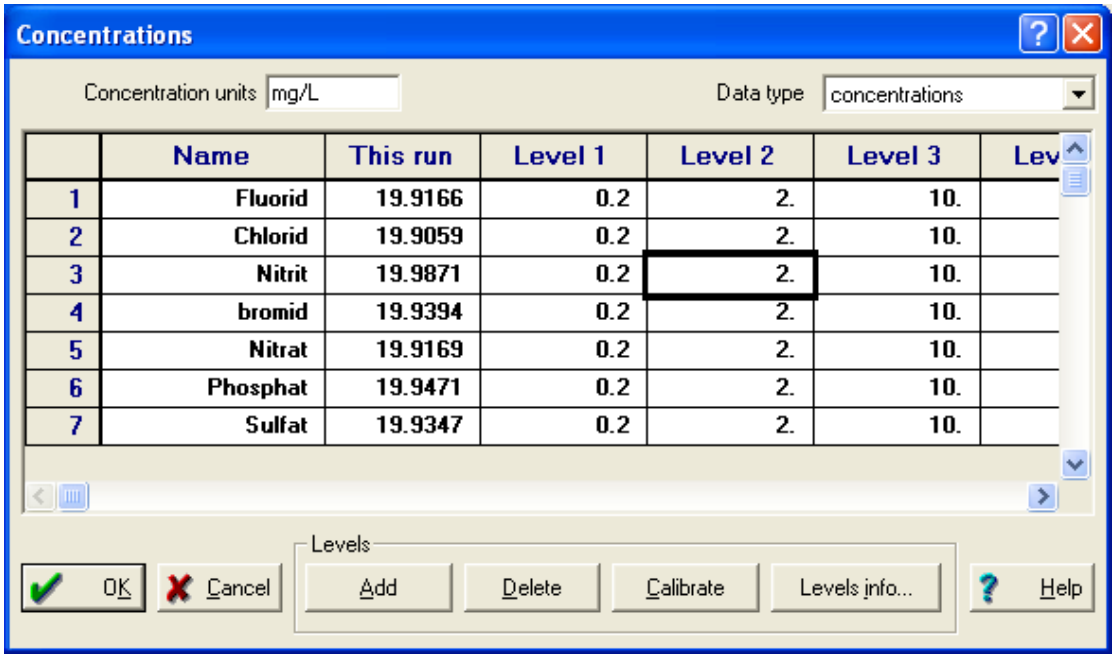
See also:

Peaks identification 166

5.6.4.3 Concentrations

(*Main menu* Method / Calibration / Concentrations)

Concentrations table contains concentrations of all components for all calibration samples (i.e. for all **calibration levels** 199).



Concentration units User-defined units of concentration. Units will appear in the report. Note, that changing concentration units does not cause recalculation of concentrations.

Data type Choice of the data type that will be shown in the concentrations table:

concentrations: shows user-defined concentrations for calibration levels. User can edit values here. See also **select and edit calibration level** 87 form used in single-run scenario (it is available when analysis starts).

heights: shows height of the peaks related to components measured in calibration runs.

areas: shows areas of the peaks related to components measured in calibration runs

Concentrations table consists of:

Number A sequence number of the component (read-only).

Name Name of the component taken from the **components table** 171 (read-only).

This run Contains concentrations (or other chosen values) obtained in the current run. The concentration is calculated using **calibration graph** 178 for both calibration samples and for analyte.

Level 1...Level N Contains user-defined concentrations (or other chosen concentrations) of components for corresponding **calibration level** 199.

Buttons

<Add> 176 Add a new calibration level to the **concentrations table**.

<Delete> Delete the current calibration level (where cursor is placed) from the **concentrations table**.

<Calibrate> 176 Calibrate the selected calibration level by measures from the current

chromatogram.

<Levels info...> 177 — Displays additional information about calibration levels.

<OK> — When editing of the **concentrations table** is finished, all calibration coefficients are recalculated.

<Cancel> — Reject all the latest changes and exit.

See also:

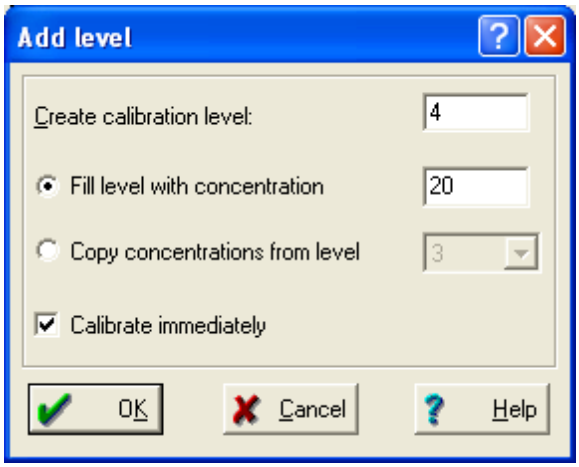
How to modify the concentrations table 472

About calibration 165

Using calibration 165

5.6.4.3.1 Add calibration level

Add a new **calibration level** 199 to the **concentrations table** 174.



Create calibration level — An index (sequence number) of calibration level to add.

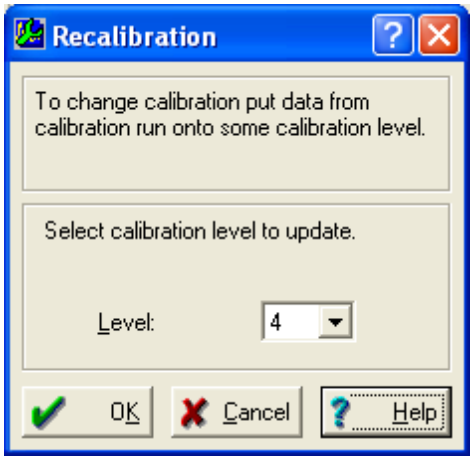
Fill level with concentration — Concentration to be filled in for all components.

Copy concentrations from level — Copy all concentrations from the specified calibration level.

Calibrate immediately — Calibrate the new calibration level by measures from the current chromatogram.

5.6.4.3.2 Recalibration

(*Main menu* Process / Calibrate...)



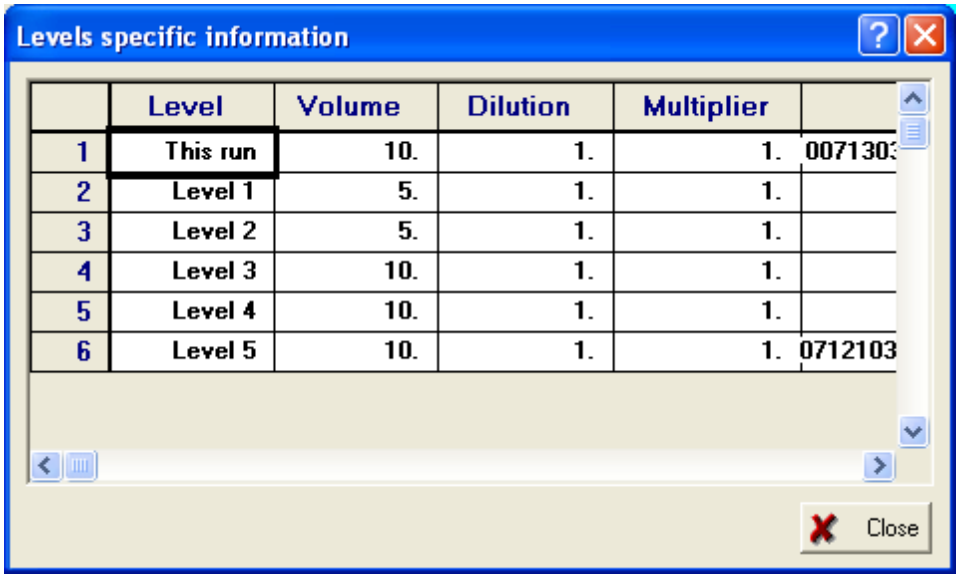
The ***Recalibration*** window allows to accept data from the current run, considering this run as a **calibration** 165. This option is usually used to recalibrate manually some calibration level.

Level Index (sequence number) of **Calibration level** 199. This item cannot be edited if current chromatogram was already used for some calibration level.

<OK> Fill in area and height information for the selected calibration level from the run and recalculate coefficients of all components

5.6.4.3.3 Levels Specific Info

Levels specific information form is a table that contains additional information on all Calibration levels 199 in the current chromatogram 207 or Method 122.



It includes the following data:

Level calibration level number. The current chromatogram is always presented as

"This run" level in the first row.

Volume	volume of the injected sample in calibration run. See **sample description** 126.
Dilution	dilution of the injected sample in calibration run. See **sample description** 126.
Multiplier	multiplier for the injected sample in calibration run. See **sample description** 126 .
File	filename of the chromatogram used for calibration level. The filename does not include path of the folder.

Volume, **Dilution** and **Multiplier** parameters are used to calculate **adjusted volume** 199 and components **quantity** 200 in calibration run to build **calibration curve** 182.

All information is for review only. It can not be edited here (because it refers to calibration run, not to current run or method).

See also:

Sample description 85

5.6.4.4 Calibration graphs

(*Main menu* Method / Calibration / Graphs)

There are two modes of calibration graphs available in the method settings: **simple** 180 and **advanced** 178 calibration.

Simple calibration 180 has settings for most commonly used types of analysis. It is a best choice for beginners to start with.

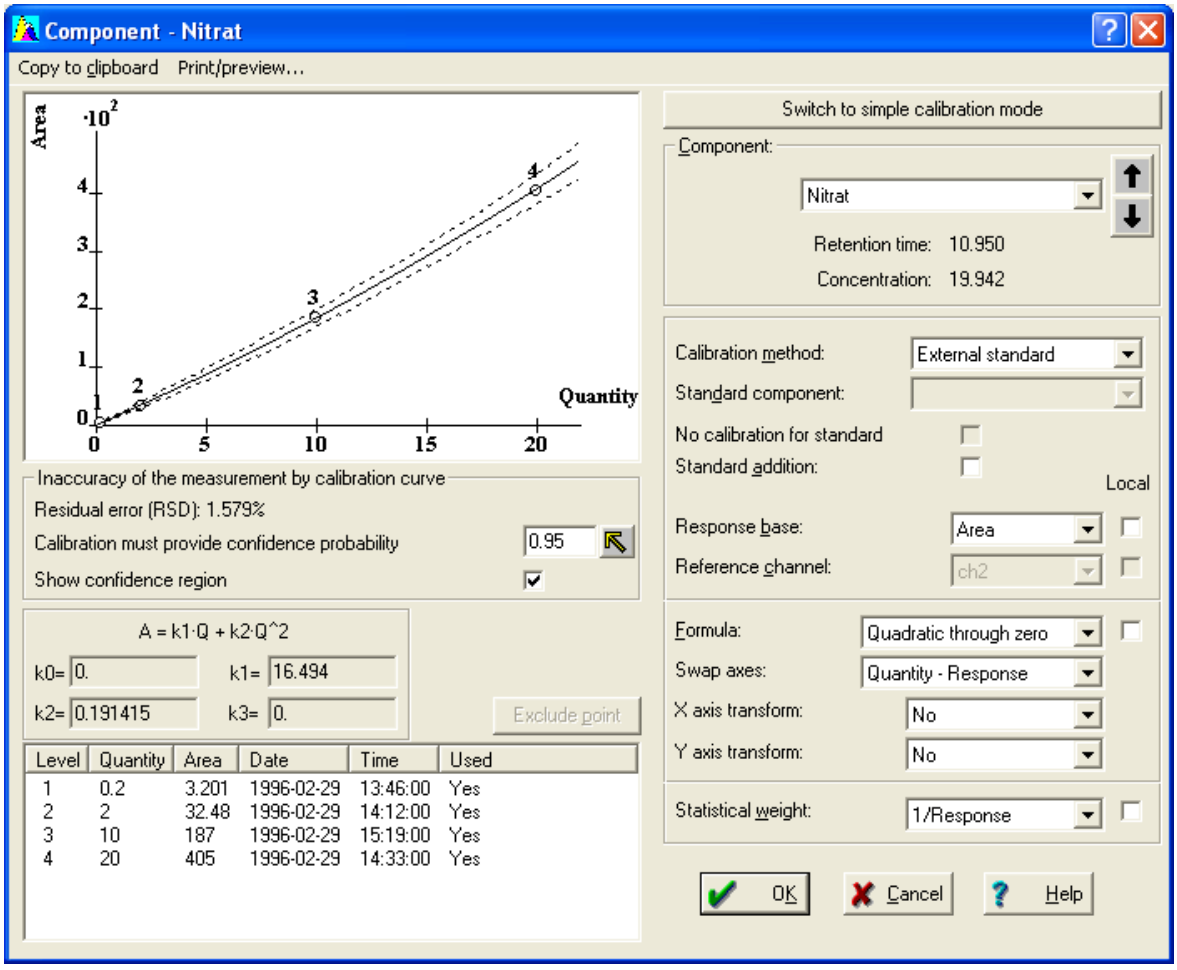
Advanced calibration 178 has a variety of additional settings to get best performance and best precision of the results.

See also:

About calibration 165
Using calibration 165

5.6.4.4.1 Calibration graphs (advanced)

(*Main menu* Method / Calibration / Graphs)



<Switch to simple calibration mode> Switches calibration to simple mode and displays **Calibration graphs (simple)** 180 form.

The calibration graphs window form for the **Component** includes the following areas:

Calibration curve 182

Calibration inaccuracy settings and results 183

Calibration results 185

Calibration points table 185

Component information 186

Calibration parameters 186

Additionally, local menu specifies the following commands:

Copy to clipboard	Copy the calibration curve of the selected component to the clipboard so that it is available for other Windows applications, such as MS Word, Excel etc.
Print/preview	Prints or previews calibration results including curve.
Preview this	Displays print preview for the selected component.
Print this	Prints the selected component.
Preview all	Displays print preview for all components.
Print all	Prints all components.

See also:

Calibration graphs 178
Calibration graphs (simple) 180
About calibration 165
Using calibration 165

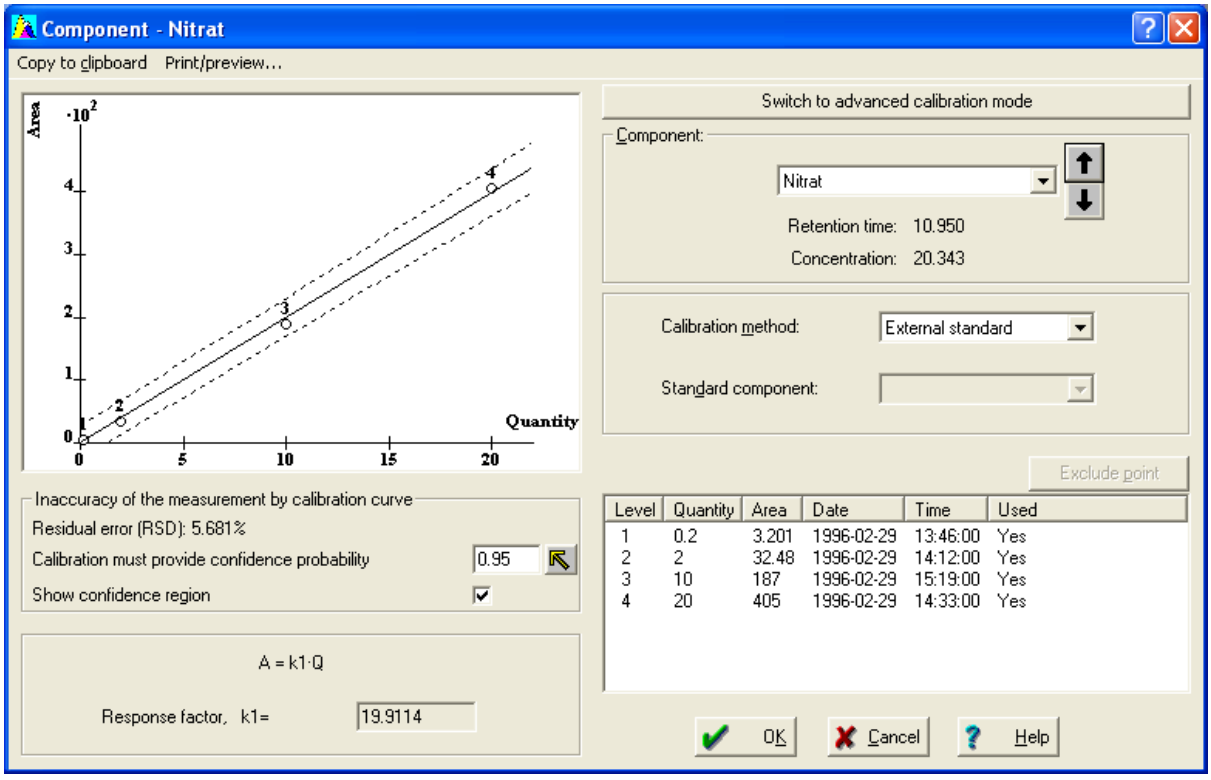
5.6.4.4.2 Calibration graphs (simple)

(*Main menu* Method / Calibration / Graphs)

This window form displays the simplified user interface for calibration configuration.

It is designed for novice users who may encounter difficulties with **Calibration graphs (advanced)** 178 configurations.

Simple calibration mode suitable for most commonly used types of analyses.



<Switch to advanced calibration mode> Switches calibration to advanced mode and displays **Calibration graphs (advanced)** 178 window form.

The calibration graphs window form for the **Component** includes the following areas:

Calibration curve 182

Calibration inaccuracy settings and results 183

Calibration results 185

Calibration points table 185

Component information 186

Those areas are analogous to that **Calibration graphs (advanced)** 178 window form

Calibration parameters 188 area is simplified compared to **Calibration graphs (advanced)** 178 window form.

It has minimal set of parameters for calibration configuration.

Additionally, local menu specifies the following commands:

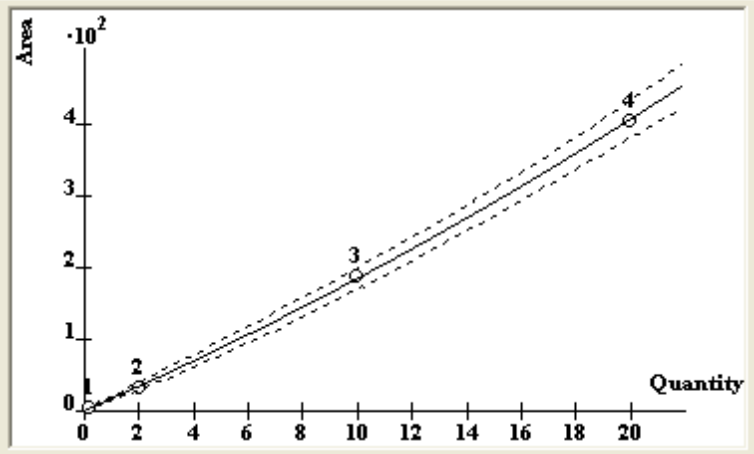
Copy to clipboard	Copy the calibration curve of the selected component to the clipboard so that it is available for other Windows applications, such as MS Word, Excel etc.
Print/preview	Prints or previews calibration results including curve.
Preview this	Displays print preview for the selected component.
Print this	Prints the selected component.
Preview all	Displays print preview for all components.
Print all	Prints all components.

See also:

Calibration graphs 178
Calibration graphs (advanced) 178
About calibration 165
Using calibration 165

5.6.4.4.3 Calibration curve

Chrom&Spec software calculates a calibration curve as a plot of component quantity 200 versus response 200. It is used to determine the computed quantity 201 value for an unknown concentration of the component.



Typically user builds calibration curve by varying component ***concentration*** in calibration runs.

Still sample ***volume*** 126, ***dilution*** 128 and ***multiplier*** 128 are also taken into account. It is also possible to vary these parameters for calibration construction.

The calibration curve is shown in **Quantity-Response** or **Response-Quantity** axes.

The **Response** could be **Area** or **Height**.

Recalculation of ***Quantity*** <-> ***Concentration*** is carried out using the formula:

Quantity = Concentration * Volume * Multiplier / Dilution

See **adjusted volume** 199 for details.

Calibration curve is constructed using weighted regression of the first, second or third order to get

coefficients of the polynomial that fits the calibration points in the best way.

The regression construction is controlled by **calibration parameters** 188 settings for **calibration advanced mode** 178 or **calibration parameters (simple mode)** 188 settings for **calibration simple mode** 180.

Optionally calibration graph can plot inaccuracy curves, that demonstrate a **confidence region** (or **confidence band**) of the **polynomial regression** for a specified **confidence probability**.

See also:

Calibration graphs (advanced) 178

Calibration graphs (simple) 180

Calibration inaccuracy 183

Confidence intervals for weighted polynomial calibrations 490

Notations 198

5.6.4.4.4 Calibration inaccuracy

Calibration inaccuracy settings are part of **Calibration graphs** 178 user interface (both **advanced** 178 and **simple** 180).

The **Inaccuracy of the measurement by calibration curve** section of the **Calibration graphs** 178 contains:

Relative error (RSD)	**Relative Standard Deviation** value to evaluate the error of calibration curve approximation.
Correlation coef.	**Correlation coefficient** value. It is available only for **linear** and **linear through zero** calibrations formulas without weighting.
Calibration must provide confidence probability	Setting for **confidence probability** for **polynomial regression.** A typical value is 0.95. This setting is used to calculate errors of concentrations for components in analyte. Also it is used to construct confidence region plot.
Show confidence region	Setting to show confidence region at Calibration curve 182 plot. Confidence region is calculated using specified **confidence probability**. **Confidence region** (or **confidence band**) specifies the possible variation of Y (ordinate) value (typically this is a detector response) for each X (abscissa) value (typically this is a component quantity 200) with a specified **confidence probability**. See **Confidence intervals for weighted polynomial calibrations** 490 article for more details.

Residual Standard Deviation is a measure of the quality of the polynomial regression.

The less Residual Standard Deviation the better calibration data are fitted by calibration curve 182.

The calibration data after applying **axis transform** 196 and **swap axes** 186 are represented by $\{x_i, y_i\}$ pair,

w_i is a **statistical weight** 186 of the point.

$$RSD = 100\,\% \cdot \sqrt{\frac{n}{n-k}} \cdot \frac{\sqrt{\frac{\sum w_i \cdot (\tilde{y}_i - y_i)^2}{\sum w_i}}}{\frac{\sum \sqrt{w_i} \cdot \tilde{y}_i}{\sum \sqrt{w_i}}}$$

where $\tilde{y}_i = \hat{F}(x_i)$ is a fitted value for point i obtained from constructed **calibration curve** 182,

n is a number of calibration points,

k is a number of independent coefficients in the **calibration formula** 195.

Correlation coefficient is a measure of linearity for dependence of two data sets $\vec{X}$ and $\vec{Y}$.

The closer correlation coefficient is to 1 the more linear is the dependence.

For two data sets (vectors) $\vec{X}$ and $\vec{Y}$ of the same dimension new vectors $\vec{X}'$ and $\vec{Y}'$ are constructed,

where $x_i' = x_i - \bar{x}$ and $y_i' = y_i - \bar{y}$ (indices are used for vector elements, $\bar{x}$ and $\bar{y}$ are average values for vectors $\vec{X}$ and $\vec{Y}$).

The correlation coefficient is calculated as:

$$Corr = \frac{\vec{X}' \cdot \vec{Y}'}{|\vec{X}'| \cdot |\vec{Y}'|}.$$

Vectors $\vec{X}$ and $\vec{Y}$ for each component are consisted of the responses (height or area) for calibration points and corresponding **quantities** 200 by applying **axis transform** 196 and **swap axes** 186.

Note: Correlation coefficient does not depend on the selected calibration formula and can be

calculated and included in the report for any formula (see Calibration results section of the Report options 322 window). However, it makes sense for liner dependences only. The Calibration graphs window 178 shows correlation coefficient for linear formulas with no weighting only.

See also:

Confidence intervals for weighted polynomial calibrations 490

Notations 198

5.6.4.4.5 Calibration results

This part of the **calibration graph** 178 window shows calibration coefficients and analytical expression for selected component.

Analytical expression A line looking like
Q = k3•A^3 + k2•A^2 + k1•A + k0.
This formula is used for approximation of the calibration curve.

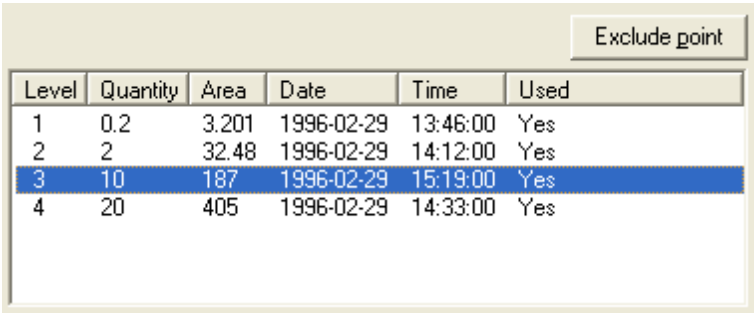
k0, k1, k2, k3 Calibration coefficients (coefficients of the calibration formula).

Weighted regression of the first, second or third order is used to get coefficients of the polynomial that fits the calibration points in the best way.

The regression construction is controlled by **calibration parameters** 188 settings for **calibration advanced mode** 178 or **calibration parameters (simple mode)** 188 settings for **calibration simple mode** 180.

5.6.4.4.6 Calibration points

This part of the **Calibration graphs** 178 window shows the calibration points table containing the basic information used to construct the **calibration curve** 182:



Level Sequence number of **calibration level** 199.

Quantity Quantity of the current component in the calibration sample. It is calculated using the concentration from **concentrations table** 174. See **Quantity** 200.

Area (or height) Peak height or area of the current component, depending on calibration **base** 186.

Used Information whether the calibration level is used for calculations or excluded from calibration.

<Exclude point> Exclude the chosen calibration point from the list and recalculate calibration coefficients for the current component. Repeated pressing includes the point again. You can exclude points that drop out of the calibration curve watching for **RSD** 183 values.

See also:

Calibration graphs (advanced) 178
Calibration graphs (simple) 180
Concentrations table 174
Levels Specific Info 177

5.6.4.4.7 Component

This part of the **calibration graph** 178 window shows information about currently selected component.

Component Allows to choose the current component from the list. It is possible also to scroll the list of components by mouse, using the special arrow buttons on the right.

Retention time Displays the retention time of the selected component (read-only).

Concentration Concentration of the selected component (read-only) in the current chromatogram.

5.6.4.4.8 Calibration parameters

This part of the **calibration graph** 178 window shows calibration parameters.

Calibration method 189 Selection of the method that is used for **calibration procedure**.

Standard component 194 Name of the standard component. It is used for **Internal standard** 190 or **Tabulated** 193 method.

☑ **Standard addition** 194 Calculate concentration of the selected component using **standard addition** method.

This option requires **external standard** 190 selection for **calibration method** 189.

☑ **No calibration for standard** Option used for **Internal standard** 190 selection for **calibration method** 189.

It directs using simplified approach for internal standard calibration method.

This approach assumes that the calibration curve for standard component is liner and goes through zero. No calibration for standard is needed.

☑ Local

If **Local** checkbox is marked then the corresponding parameter is applied for the currently selected component only. Otherwise this parameter is **Global** (i.e. applied for all components which do not set **Local** checkbox for the item).
See also: **Special component** 196

Response base

Base for calculations (**Area** or **Height**) in quantification and calibration procedures. Indicates, which parameter (**Area** or **Height**) is to be used as a peak response.

Reference channel 197

Channel which is used to calculate **Area** or **Height** values. These values are used in quantification and calibration procedures.

Formula 195

Calibration formula. The **Local** checkbox for this item affects on **Formula**, **Swap axes**, **X axis transform**, **Y axis transform** items.

Swap axes

Allows specifying which value (component **quantity** or detector **response**) is considered as independent measurement for the regression when building **calibration curve** 182.

Response - Quantity: An abscissa (X axis) is detector **response** (independent variable) and ordinate (Y axis) is component **quantity** (dependent variable).

Quantity - Response: An abscissa (X axis) is component **quantity** (independent variable) and ordinate (Y axis) is detector **response** (dependent variable).

Typically **Quantity - Response** dependence is used and is recommended. Still sometimes **Response - Quantity** is preferable. Use it, for example, when sample dosing error dominate in your analysis (compared to **area** or **height** measurement).

X axis transform 196

Axis transform setting for X axis (abscissa).

Y axis transform 196

Axis transform setting for Y axis (ordinate).

Statistical weight Specifies model of statistical weight for weighted regression. See **Calibration curve** 182.

Possible selection are:

No: No weighting. All calibration points are equivalent and their weights equal to identity.

1/Response: Use it when error of your detector can be approximated by $E_R \sim \frac{1}{\sqrt{\text{Response}}}$

1/(Response)^2: Use it when error of your detector can be approximated by $E_R \sim \frac{1}{\text{Response}}$

1/Quantity: Use it when error of your detector can be approximated by $E_R \sim \frac{1}{\sqrt{\text{Quantity}}}$

1/(Quantity)^2: Use it when error of your detector can be approximated by $E_R \sim \frac{1}{\text{Quantity}}$

In most cases No weighting is used. Still it may appear not quite correct because the error produced by the detector do depends upon the **response** value or substance concentration. To get best results use setting which is the most adequate to your instrument and your method.

5.6.4.4.8.1 Calibration parameters (simple mode)

This part of the **calibration graphs (simple)** 180 window shows calibration parameters.

It has minimal set of parameters for calibration configuration (compared to **advanced mode parameters** 186):

Calibration method 189 Selection of the method that is used for **calibration procedure**.

Standard component 194 Name of the standard component. It is used for **Internal standard** 190 or **Tabulated** 193 method.

There are no settings for:

☑ **Standard addition** 194	**Standard addition** method is not supported in **calibration simple mode** 180.
☑ **No calibration for standard**	**Calibration simple mode** 180 assumes that this flag is always **ON** for **Internal standard** 190.
☑ **Local**	All parameter are assumed to be **Global** (i.e. applied for all components) . There are no **Special components** 196.
Response base	**Area** is always assumed as a detector **response base**.
Reference channel	**Calibration simple mode** 180 is assumed to be used for single channel analyses only. This setting is not needed.
Formula 195	**Linear through zero** calibration formula is always assumed.
Swap axes	**Quantity - Response** (namely **Quantity - Area**: see **Response base**) dependence is always assumed.
X axis transform 196	No **Axis transform**
Y axis transform 196	No **Axis transform**
Statistical weight	**No** weighting is always assumed.

5.6.4.4.8.2 Calibration method

There are three basic methods of calibration in the "Chrom&Spec" software. Methods differ in the way how the calibration curve is constructed.

External standard calibration 190 (Absolute calibration). It is the basic calibration procedure.

Internal standard calibration 190 (Relative calibration).

Tabulated calibration 193 (Relative response factor calibration). It is a simplified method of external standard calibration.

See also:

About calibration 165

How to perform a single-point calibration 472

How to perform a multi-point calibration 473

This is the basic calibration method. It is called **absolute calibration** as well.

Calibration: One or more samples with known concentrations are used. The dependence of the **quantity** [200] of the injected component versus **response** (area or height) of the corresponding peak is constructed, using polynomial regression.

$Q(i) = C(i) \cdot V'$ - quantity of the component, where

V' is an **adjusted volume** [199] of the calibration sample

C is a concentration

i refers to component with sequence number i

The **calibration curve** [182] is constructed in $\{ R(i), Q(i) \}$ axes.

Quantification: The component's quantity in the unknown sample is calculated from the **calibration curve** [182] using the **response** (area or height) of the corresponding peak.

Typically **external standard** calibration is used together with **absolute concentration** [202] **quantification method**. The concentration of the component is calculated from its quantity using **adjusted volume** [199] of the unknown sample.

A concentration of the component is reported in **raw concentration** [337] item of the **peak table** [327].

External standard calibration can be used together with **relative concentration** [202] **quantification method**. See **relative concentration** [337] item of the **peak table** [327].

See also:

Notations [198]

Calibration method [189]

Calibration curve [182]

How to perform a single-point calibration [472]

How to perform a multi-point calibration [473]

Internal standard (ISTD) technique is made to increase the accuracy of calculation with the help of the component with known concentration, called **Internal standard**. A known concentration of the **Internal standard** is added to analyte.

The "classical" internal standard implementation builds calibration in $\{ R(i) / R(s), C(i) / C(s) \}$ axes where

R is a detector response (**area** or **height**)

C is a concentration

s refers to standard component

i refers to all other components

Chrom&Spec software uses rather different implementation of the **internal standard**, which has some advantages.

First of all, Chrom&Spec software treats differently **internal standard method** used for **calibration** 165 and **internal standard method** used for **quantification** 201.

In most cases when "classical" internal standard is used the **relative concentration** 202 **quantification method** based on **internal standard** technique is a better solution. It uses simple **external standard** 190 calibration and can handle non-liner detector responses fitted by quadratic or cubic polynomials. "Classical" internal standard implementation can handle liner detector responses only. See description for **relative concentration** 337 report item of the same name for more details.

Below is a description of the **Internal standard method** used for **calibration**.

Internal standard calibration method provides a mean to construct a more precise calibration curve by partly or fully eliminating dosing error for calibration samples.

Two modes of the **Internal standard calibration** are available: with and without calibration of the standard component. **No calibration for standard** 186 option of the **calibration graphs** 178 sets this mode.

No calibration for standard 186 is ***off***:

The calibration curve for standard component is constructed using **external standard** 190 calibration.

The calibration of the standard component is used to calculate a corrected volume of the calibration sample, eliminating (at least partly) dosing error:

$$V' = Q(s)\{R(s)\} / C(s)$$

The corrected quantity of other components in calibration sample is calculated using

$$Q(i) = C(i) \bullet V'$$

The calibration curve of other components is constructed in $\{ R(i), Q(i) \}$ axes.

The calibration obtained could be used for **quantification** 201 using both **Absolute concentration** 202 and **Relative concentration** 202 **quantification method**.

This configuration differs from "classical" **internal standard method** because calibrating standard component relies on absolute value of its **Quantity** 200, so needs a correct value of injected **volume** 126 to be specified.

An advantage is that unlike "classical" **internal standard** implementation this approach handles correctly non-liner detector responses fitted by quadratic or cubic polynomials.

No calibration for standard 186 is ***on***:

This configuration is generally equivalent to "classical" **internal standard method** still preserving some advantages.

The calibration relies on ratios of concentrations of standard component and other components.

The absolute value of **Quantities** 200 of components is of no interest in this approach (ratios only are used). So the injected **volume** 126 is fully eliminated from the calibration thus excluding any dosing errors.

Additional requirements for this configuration:

- A **Relative concentration** 202 **quantification method** 201 only must be used to calculate unknown concentrations of analyte.
- **Standard component for quantification** 204 and **standard component for calibration** 194 must be the same.
- The calibration curve for standard component is assumed to be linear and goes through zero.

Summary:

The calibration curves for all components besides standard are constructed in { ***R(i), W(i)*** } axes, where

$$W(i) = C(i) \cdot R(s) / C(s)$$

A concentration of component ***i*** in analyte is calculated by **relative concentration** 202 method as:

$$C(i) = W(i)\{R(i)\} \cdot (C(s) / R(s))$$

where ***C(s)*** is a known concentration of the standard component in the analyte

Details:

Using approach specified above:

$$Q(s)=k(s) \cdot R(s)$$

where ***k(s)*** is some constant value. It gives for calibration:

$$V' = Q(s)\{R(s)\} / C(s) = k(s) \cdot R(s) / C(s)$$ - volume of the calibration sample

$$Q(i) = C(i) \cdot V' = k(s) \cdot C(i) \cdot R(s) / C(s)$$ - corrected quantity of the component ***i***

We are defining a helper value

$$W(i) = Q(i) / k(s) = C(i) \cdot R(s) / C(s)$$

As soon as non-standard components also has linear through zero detector response

$$Q(i)=k(i) \cdot R(i)$$

we can write

$$W(i)=(k(i) / k(s)) \cdot R(i) = k'(i) \cdot R(i)$$

where $k'(i) = k(i) / k(s)$ is just some constant which can be defined from the calibration curve.

The calibration curves for all components besides standard are constructed in { ***R(i), W(i)*** } axes, that is { ***R(i), C(i) • R(s) / C(s)*** }

As specified for **relative concentration** 202 the unknown concentration of component ***i*** is calculated by:

$$C(i) = Q(i)\{R(i)\} / V' = Q(i)\{R(i)\} \cdot C(s) / Q(s)\{R(s)\} = Q(i)\{R(i)\} \cdot C(s) / (k(s) \cdot R(s)) = (Q(i)\{R(i)\} / k(s)) \cdot (C(s) / R(s)) = W(i)\{R(i)\} \cdot (C(s) / R(s))$$

The value of $W(i)\{R(i)\}$ is calculated from the calibration curve for the component i. The known concentration $C(s)$ of the standard component is specified by operator.

As seen from the above, the absolute value $k(s)$ is eliminated from the final result. So the calibration of the standard is not needed and not actually constructed by the software.

For simplicity we can always assume that

$k(s) = 1$ and $Q(s) = 1 \cdot R(s)$

Note: "Classical" internal standard method builds calibration in { $R(i) / R(s), C(i) / C(s)$ } axes. This is generally equivalent using implementation of **internal standard** without calibrating standard (that is **No calibration for standard** 186 is **on**) where calibration is done in { $R(i), C(i) \cdot R(s) / C(s)$ } axes.

See also:

Relative concentration 202 **quantification**

Relative concentration 337 report item

Calibration method 189

External standard 190 calibration method

Notations 198

The **Tabulated** calibration method is a simplified way of **External standard** 190 calibration.

A single **standard component** 194 is calibrated using the **external standard** 190 method.
The calibration curves of other components are obtained by multiplying the calibration curve of the standard component by the **relative response factor**.

$$Q(i)\{R(i)\} = K1(i) \cdot Q(s)\{R(s)\}$$

Operator specifies the **relative response factor** of the component in the **response factor** 201 item of the **components table** 171. Also it can be specified at $K1$ coefficient in the **calibration graph** 178 window.

This means that $K1$ coefficient (the synonym of **Response factor** 201) has a different meaning for **Tabulated calibration**, as specified in the above expression.

Relative response factors $K1(i)$ can be known from the literature or obtained from theoretical considerations or measured experimentally.

See also:

Notations 198

About calibration 189

How to perform a single-point calibration 472

How to perform a multi-point calibration 473

5.6.4.4.8.3 Standard component (calibration)

Standard component is selected in the **calibration graphs** 178 window.

This setting is used for **internal standard** 190 or **tabulated** 193 calibration methods.

The meaning of **standard component** is specific for each calibration method. See descriptions of calibration methods for details.

See also:

Internal standard 190

Tabulated 193

5.6.4.4.8.4 Standard addition

The method of **standard addition** is used in instrumental analysis to determine concentration of a substance (analyte) in an unknown sample by comparison to a set of samples of known concentration, similar to using a calibration curve for **external standard** 190. Standard addition is used instead of a calibration curve to solve the matrix effect problem.

The standard solution (solution of known concentration) is added to the unknown solution so any impurities in the unknown are accounted for in the calibration. The operator does not know how much was in the solution initially but knows how much standard solution was added, and knows how the detector response changed before and after adding the standard solution. Software can extrapolate and determine the concentration contained initially in the unknown solution.

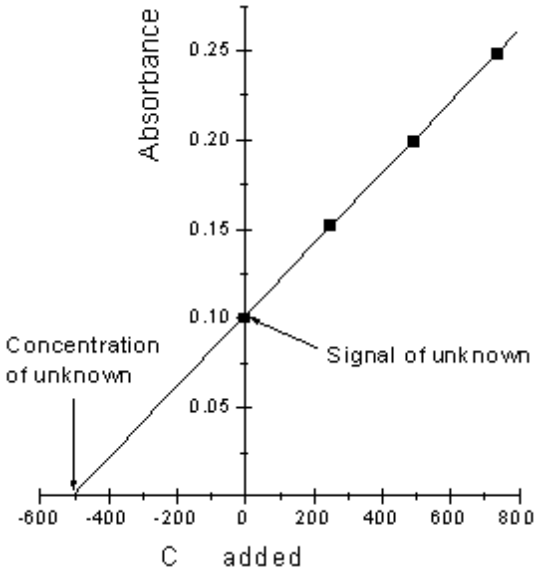
A typical procedure involves preparing several solutions containing the same amount of unknown, but different amounts of standard.

For example, five 25 mL volumetric flasks are each filled with 10 mL of the unknown. Then the standard is added in differing amounts, such as 0, 1, 2, 3, and 4 mL. The flasks are then diluted to the mark and mixed well.

The idea of this procedure is that the total concentration of the analyte is the combination of the unknown and the standard. Minimal number of flasks with different concentrations of standard is 2 in this case.

Operator must fill **concentrations table** 174 taking into account concentrations which comes from added standards only. One or several components in the solution can be processed using **standard addition method**.

If unknown solution contains some initial concentration of the component, the resultant calibration does not come through the origin. The "shift" of the calibration from the origin defines the initial concentration.



Note: By default initial concentration in the unknown solution is reported in the "**Calibration results**" section of the report, not in the "**Peak table**" section. Look for "**Concentration before standard addition**" item in the report. Initial concentration is a property of the calibration, it is not a property of the current run!

Note: Peak table in the report may contain **Concentration** item for any run! The value of the **Concentration** is calculated from the calibration curve taking into account initial concentration. So the value reported in this item is a sum of the initial concentration and concentration of the added standard. It is not an initial concentration.

5.6.4.4.8.5 Calibration formula

There are six possible **calibration** 165 dependencies which describe the shape of the **calibration curve** 182. The corresponding calibration formula is selected in the **Formula** field of the **calibration graph** 178 window.

Linear through zero:	$Y = K1 \cdot X$
Linear:	$Y = K1 \cdot X + K0$
Quadratic through zero:	$Y = K2 \cdot X^2 + K1 \cdot X$
Quadratic:	$Y = K2 \cdot X^2 + K1 \cdot X + K0$
Cubic through zero:	$Y = K3 \cdot X^3 + K2 \cdot X^2 + K1 \cdot X$
Cubic:	$Y = K3 \cdot X^3 + K2 \cdot X^2 + K1 \cdot X + K0$

In most cases the calibration dependence is linear so the coefficient ***K1*** is often called as **Response**

factor 201.

See also:

Special component 196

5.6.4.4.8.6 Axis transform

Axis transform allows transform values on horizontal X or vertical Y axis or both.

Possible transformations are:

No: No transformations.

Logarithmic: A value at specified axis is transformed using logarithmic function $Z \to \log(Z)$.

Transformed values are used for the regression when **calibration curve** 182 is constructed. Reverse transform is used when necessary for the **quantification** 201 procedure.

It is preferable to use linear functions in the regression procedure (which uses least-squares approach) when possible. Non-linear polynomials lead to complicated metrology and may produce instabilities related to error estimations. In many cases **axis transform** feature allows using linear formula in the regression instead of quadratic or cubic, still correctly handles non-linear detector responses.

For example, detector response of the form $R \sim Q^{\alpha}$ can be handled by logarithmic axis transform for R and Q values.

Another example is a raw absorption at photometric detectors. In this case $R \sim e^{-\lambda \cdot Q}$ and logarithmic transform at R value would give linear regression. Still note, that most photometric detectors perform logarithmic transformation internally.

5.6.4.4.8.7 Special component

Special components can use some calibration parameters (**base**, **reference channel**, **formula**, **weight**) which are different from the default values.

Default values are indicated in **Calibration graphs (advanced)** 178 form when no **Local** marks are set for component.

To set special calibration parameters for component set the **Local** mark near required parameter for component and set parameter to value needed.

Special components are marked by the 'p' sign in the **Type** 339 column of the **Custom** 332 report.

See also:

Component type 339

5.6.4.4.8.8 Reference channel

Reference channel is a channel in the multi-channel chromatogram that is used for calculation peaks **Areas** and **Heights**.

These values are used in **calibration** and **quantification** procedures.
Also these values may be reported in the **Peak table** section of the **Report** 322.

Some components can have individual settings for their **reference channel**. See **Special component** 196 and **Calibration parameters** 186 for details.

Note: **Reference channel** could differ from the channel that was used for peak detection (See peak integration setup 160). It is quite common in multi-channel chromatography when peaks are detected at some channel (for example, **Total** calculated channel, which is typically the best for peak detection) and **Areas** or **Heights** are calculated on a different channel (**Average** calculated channel or **Path** 155 special calculated channel).

See also:

Analytical channels 113
Calculated channels 151
Auxiliary channels 113
Current channel 221
Selected channels 221

5.6.4.5 Load from method

(Method / Calibration / Load from method)

Load the calibration from the method. This option is used to update the calibration in the chromatogram for the current run by the one taken from the method associated with chromatogram.

See also:

Calibration menu 171
About calibration 165
Using calibration 165

5.6.4.6 Save to method

(Method / Calibration / Save to method)

Save the current calibration to the method. This option is used to transfer the updated calibration from the run to the method (i.e. the method associated with the current chromatogram).

See also:

Calibration menu 171
About calibration 165
Using calibration 165

5.6.4.7 Import calibration

(Method / Calibration / Import calibration)

Use this option to **import a calibration** stored in a ***.cal** file to the current method or chromatogram. It is used to transfer the updated calibration from chromatogram-to-chromatogram or from method-to-method. Different methods can be processed in this case.

See also:

Load calibration from method 197
Save calibration to method 198

5.6.4.8 Export calibration

(Method / Calibration / Export calibration)

Use this option to **exports a calibration** and store it in a ***.cal** file. It is useful to transfer a calibration from chromatogram to another method or to another chromatogram which was obtained by different method.

See also:

Load calibration from method 197
Save calibration to method 198

5.6.5 Calibration references

5.6.5.1 Notations

R	Stands for **response** 200 value, either **area** or **height**, depending on setting, selected in the **Calibration graphs** 178 window.
V	**Sample volume** 126 injected.
D	**Dilution coefficient** 126, shows number of times to which the initial solution is dissolved before injection.
A	**Multiplier coefficient** 126, sample concentrating factor.
V' = V * A / D	**Adjusted volume** 199 of injected sample. A correction is made for the dilution

	coefficient.
C	Component concentration in the initial solution (before dilution).
Q = C • V'	**Quantity** 200 of component, used for calibration curve construction.
t	Retention time.
t0	**Void time** 141.
t' = t - t0	Corrected retention time.
L	Column length.
v = L / t0	Linear flow rate.
Q{R}	Calibration dependence (component **quantity** 200 vs. detector **response** 200). In the case of the most common linear calibration curve ***Q = Q{R} = k1R*** it comes through the origin. The concentration of the component in the analyzed mixture is calculated by the formula ***C = Q{R} / V'***.

Subscript values used

j	Stands for j-th calibration level run.
s	For standard component.
i	For component number ***i***.

5.6.5.2 Adjusted volume

Adjusted volume is the injected **volume** 126 of the sample corrected by the sample **dilution** 126 and the sample **Multiplier** 126 parameters.

It is equal to the volume of original sample which was actually used to perform ***injection***.

$$V' = V \cdot Multiplier / Dilution$$

The eluted quantity of the component is given by the formula

$$Q(c) = C(c) \cdot V' = C(c) \cdot Volume \cdot Multiplier / Dilution.$$

When component quantity is known, its concentration can be calculated by

$$C(c) = Q(c) / V' = Q(c) / (Volume \cdot Multiplier / Dilution).$$

See also:

Notations 198

5.6.5.3 Calibration level

Calibration level (calibration point) corresponds to one calibration run and collects all information from that run necessary for calculations. These are component quantity, peak area, peak height, and **adjusted injection volume** 199. Information on all calibration levels is summarized in the

concentrations table 174.

Prior to the calibration procedure it is necessary to fill in component concentrations for all calibration levels that are to be used.

If several injections of the same solution are to be made, it is necessary to make a separate calibration level for each injection.

If the calibration level has no information on the height and area of a corresponding peak, this level is considered to be empty and information from it is not included into calculations.

See also:

About calibration 165

5.6.5.4 Quantity

Quantity or amount of the component in the calibration mixture is the value calculated as a product of the component concentration C to **adjusted volume** 199 V'.

$Q = C \cdot V'$ For **External standard** 190 or **Tabulated** 193 calibration or

$Q = C \cdot Q(s)\{R(s)\} / C(s)$ For **Internal standard** 190 calibration.

where

$Q(s)\{R(s)\}$ **Computed quantity** 201 of internal standard component in the same calibration run.

$C(s)$ Concentration of internal **standard component** 194 in the calibration mixture.

See also:

About calibration 165

Computed quantity 201

5.6.5.4.1 Response

Detector response for the component is area or height of the corresponding **peak**, depending on the **Response base** for quantification defined in the **Calibration graphs** 178.

The Response units for the ADC channel is set in the **Channel table** 112 which can be included into a **report** 322.

5.6.5.5 Single-point calibration

Single-point calibration means that only one calibration sample is used for the **calibration** 165 of the component, only one point is available on the curve and the dependence is linear with the line going through the origin.

See also:

Calibration method 189

Multi-point calibration 201

How to perform a single-point calibration 472

How to perform a multi-point calibration Ht_multi_calibration>Proc

5.6.5.6 Multi-point calibration

Multi-point calibration means that multiple experiments were made to construct a **calibration curve** 182 and there are many points on the curve. In this case the dependence is approximated by the curve, the curve may be not only linear, but of other type. Using the RSD technique it is possible to calculate calibration coefficients, describing the curve that fits all experimental data in the best way.

See also:

Calibration level 199

Calibration method 189

Single-point calibration 200

How to perform a single-point calibration 472

How to perform a multi-point calibration 473

5.6.5.6.1 Computed quantity

Computed quantity is determined from the **calibration curve** 182 for ***i***-th component.

$$Q = Q(i)\{R(i)\}$$

The ***R*** parameter is a value of **response** 200 for the peak.

Computed quantity is used to compute the **raw concentration** 202 of the component and other values.

5.6.5.7 Response factor

In most cases calibration curves are linear and come through the origin. So the most informative coefficient in the **calibration formula** 195 is ***K1***. That is why the ***K1*** coefficient only is present in the **components table** 171, even if a non-linear **calibration formula** 195 is used. Nevertheless, all other calibration coefficients are included into the **components table** and are used for calculations. All calibration coefficients are available in the **calibration graphs** 178 window and can be included into the report by checking the ☑ **Calibration results** item in the **"Report options"** 322 window.

5.7 Quantification

Quantification is the procedure aimed to answer the question "What is the concentration of components in the test sample?".

The basic **quantification** options available are:

Absolute concentration 202

Relative concentration 202

Response normalization 204

Normalized concentration 204

Typically **quantification** uses preliminary constructed **calibration** 165 to calculate unknown concentrations. **Absolute concentration** 202 quantification method is most commonly used.

Relative concentration 202 quantification is recommended in the cases when "classical" **internal standard** is used. See also **internal standard** 190 calibration method.

Besides basic options from the above list a variety of derived quantification methods can be configured with using **custom formulas** 288.

5.7.1 Absolute concentration

Absolute concentration is also called a **raw concentration**.

This concentration is calculated from the **calibration curve** 182.

The **quantification** 201 procedure calculates the concentration $C(i)$ of the component i as

$$C(i) = Q(i)\{R(i)\} / V'.$$

where V' is an **adjusted volume** 199 of the sample,

and $Q(i)\{R(i)\}$ is a **computed quantity** 201 of the component in the sample.

Quantification 201 procedure needs **calibration** 165 to be preliminary constructed using the standard samples.

Absolute concentration quantification cannot be used if **No calibration for standard** 186 option is on for **internal standard** 190 calibration.

The calculated value is in **concentration units** that are defined by customer in the **method** 122 (see **concentrations table** 174).

Important: The unknown concentrations of the components are reported in the **Raw concentration** 337 item of the **Peak table** 327. Use **Absolute concentration** 330 quantification setting in the **Report options** 322 form to get the correct report output.

See also:

Quantification 201

Relative concentration 202

5.7.2 Relative concentration

This **quantification** 201 procedure uses the known concentration of the **standard component** 204 which

is present in the analyte to calculate the concentration of the other components.

Relative concentration is used when the volume of analysed sample is not known or could not be effectively controlled (for example, because of complicated sample preparation procedure which could include several stages of diluting or concentrating).

In this case the standard component is used to evaluate an effective volume of the sample which was injected.

A known concentration of the standard component must be present in (added to) the original sample before starting sample preparation.

Concentration of component is calculated by the formula:

$$C(i) = Q(i)\{R(i)\} / V' = Q(i)\{R(i)\} \bullet C(s) / Q(s)\{R(s)\}$$

where $V' = Q(s)\{R(s)\} / C(s)$ – effective volume of the injected sample calculated from known concentration of **internal standard**.

Quantification 201 procedure needs **calibration** 165 to be preliminary constructed using the standard samples. **Calibration** 165 can be constructed by any **external standard** 190 or **internal standard** 190 calibration method.

The calculated value is in **concentration units** that are defined by customer in the **method** 122 (see **concentrations table** 174).

In most cases **relative concentration** can be used instead of "classical" **internal standard** method of concentration calculation. Still the calibration may be done by the simple **external standard** 190 method. See **internal standard** 190 calibration method for details.

Important: The unknown concentrations of the components are reported in the **Relative concentration** 337 item of the **Peak table** 327, not in the **Raw concentration** 337 item! Use **relative concentration** 331 quantification setting in the **Report options** 322 form to get the correct report output.

The **Quantification page** 144 is used to select a **standard component** 204 and set the concentration of the **standard component** in the analyte. The concentration in the analyte can also be defined by operator in the **Edit sample description** 85 form at single analysis start or in **sample queue editor** 245 when multiple analyses are executed.

See also:

Quantification 201

Absolute concentration 202

Internal standard calibration method 190

5.7.2.1 Standard component (quantification)

Standard component for quantification is used for calculating concentrations using **relative concentration** 202 quantification method.

Standard component is selected in **Quantification** 144 page of the **Method setup** 124 window.

When **relative concentration** 202 quantification method is used with **internal standard** 190 calibration method it is strongly recommended to set the same component as **standard component for calibration** 194 and **standard component for quantification**.

Relative concentration 202 quantification method can also be used together with **external standard** 190 calibration method. In this case **standard component for calibration** 194 is not used and any component could be selected as **Standard component for quantification**.

See also:

Internal standard calibration method 190

Relative concentration 202

5.7.3 Response normalization

The method normalizes the responses for all peaks in the chromatogram to the ***NORM*** factor

The response is a **peak area** or **height**.

NORM factor is configured by operator in the **Total% for normalization** field of the **Quantification page** 144. It is also available at **Report options** 322 window.

$$R(i)\% = NORM \cdot R(i) \,/\, sum\,[R(i)]$$

(***R*** is **area** or **height**)

All peaks are processed no matter whether they have been recognized or not.

This **quantification** 201 needs no **calibration** 165.

Important: The calculated values are reported at **Area%** or **Height%** items of the **Peak table** 327. Use **Response normalization** 329 quantification setting in the **Report options** 322 form to get the correct report output.

See also:

Quantification 201

5.7.4 Normalized concentration

This quantification method calculates **normalized concentrations.**

NORM factor is configured by operator in the **Total% for normalization** field of the **Quantification**

page 144. It is also available at Report options 322 window.

The **normalized concentrations** are calculated as:

$$C(i)\% = NORM \cdot Q(i)\{R(i)\} / Sum[Q(i)\{R(i)\}]$$

where $Q(i)\{R(i)\}$ is a computed quantity 201 of the component in the sample.

The default value for $NORM$ factor is **100.0**.

Important:	The calculated values are reported at **Concentration%** item of the Peak table 327. Use Normalized concentration 330 quantification setting in the Report options 322 form to get the correct report output.

See also:

Quantification 201

Part

6 Chromatogram

6.1 Chromatogram definition

A chromatogram is presented to user as a graphic plot of the elution curve (signal vs. time) following a chromatographic separation and is displayed in the **chromatogram window** 212.

Chromatograms are stored as **chromatogram files** (***.chw**) in the **Data** directory.

These files contain the measurement raw data and a copy of the **method** 122 settings used to acquire and process these data. They can be opened, saved, closed, deleted, imported and exported using the corresponding **File menu** 26 items.

Some **chromatogram examples** 235 can be found in the **Data** folder.

See also:

Multichannel chromatogram 146

6.2 Chromatogram file handling

6.2.1 Open chromatogram

(*Main menu* File / Open / Chromatogram...)

This window is used to manipulate chromatogram files. It contains a list of chromatograms 209 for the selected directory and a description of the current (selected) chromatogram.

By default all chromatograms in the list are sorted by time: the last obtained file is on the top of the list. However, any other column can be selected for sorting by clicking mouse pointer on the title of the desired column. Repeated clicking changes the sorting order: descending or ascending. Only one-key sorting is supported in the current version.

To load a chromatogram select it first (use arrow keys to move through the list or use mouse) and then press the **<OK>** button or [Enter] key. Double-clicking the left mouse button does the same.

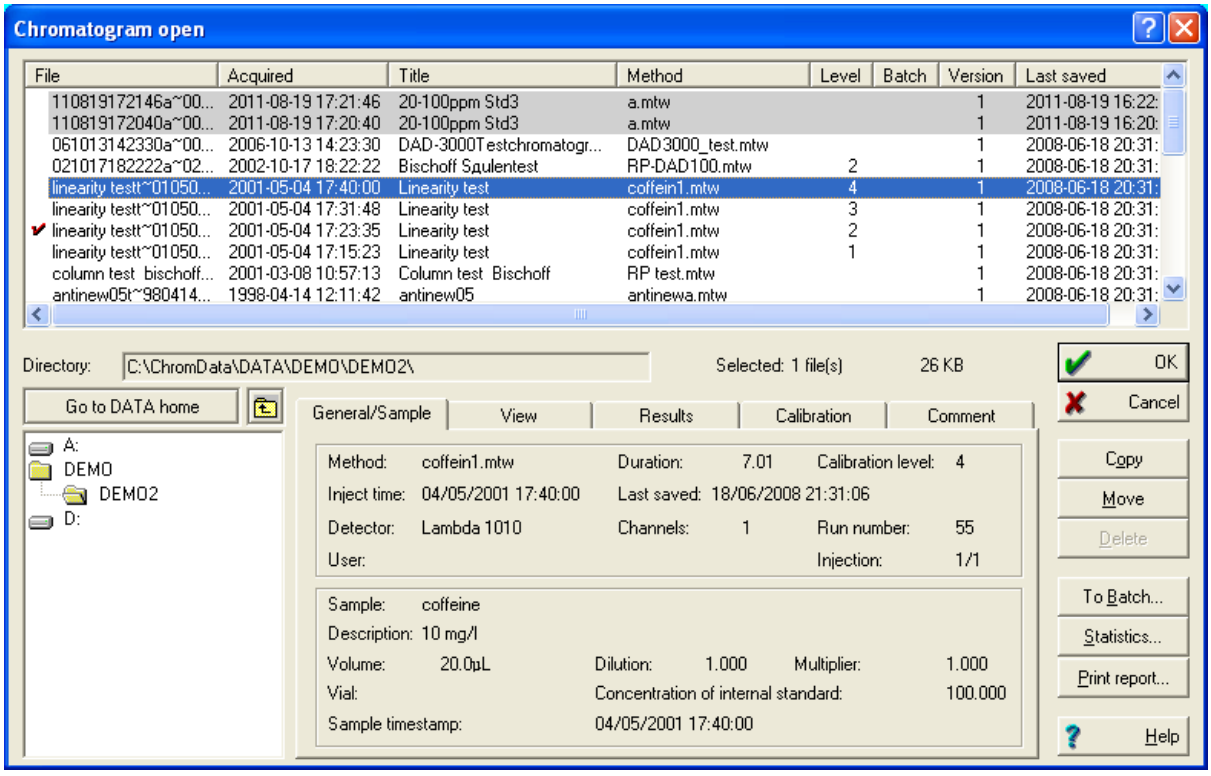
It is possible to get a more detailed information for the current chromatogram: "**Passport**", "**View**", "**Results**", "**Calibration**", or "**Comment**" page can be shown.

Several chromatograms can be selected at once. Press [Shift] and the left mouse button to select all chromatograms up to last item clicked, press [Ctrl] and the left mouse button to add a single chromatogram to the selection already made. All selected items are painted. Press the **<OK>** button, and all selected chromatograms will be opened, each in its own window. It is also possible to copy, move or delete chromatogram files from the selected directory.

When multiple chromatograms are selected then there is a single **current chromatogram** in the **File list** 209 window. **Current chromatogram** is a chromatogram which is last clicked by the user when he makes selection. **Current chromatogram** is marked by slight dotted frame around it in the **File list** 209 window. **Chromatogram description** 210 area displays information for **current chromatogram**.

Note: **Chromatograms that were acquired last and that have not been reported yet, are marked with gray background.**

Note: **Signed chromatograms are marked with green background.**



"Chromatogram open" window areas

File list 209 — list of chromatogram files in the selected directory. Default chromatogram directory is stored in the chromatogram (Method) . Depending on the flag Ignore last data directory set in the "Global preferences" window, either default or the last data directory will be used.

Selected — number of chromatograms, selected in the "Chromatogram open" window, and their total size.

Directory — a currently selected directory. It is possible to travel one level up by clicking icon. Working directory can be changed in the Directories area where directory tree is shown.

Directories — area where directory tree is shown. It is possible to move up and down the tree and change disk drive by mouse clicking. Use scroll-bar on the right or arrow keys to move along large lists.

Chromatogram description 210 — area where detailed information on the **current chromatogram** can be previewed.

Buttons

<Copy>	Copy selected chromatograms to another location.
<Move>	Move selected chromatograms to another location.
<Delete>	Delete selected chromatograms. It is not available when **21 CFR Part 11** 54 option is installed.
<To Batch...>	Create a new **batch reprocessing** 271 for all selected chromatograms. Information on selected chromatograms is stored in the user-editable batch reprocessing file. See **creating a new batch reprocessing** 271 for details.
<Statistics...>	Performs statistics or summary report for the selected chromatograms. Opens **Statistics** 375 window where report can be configured.
<Print report...>	Generate and print **plain report** 320 for selected chromatograms. Report is generated for each selected chromatogram according to it's settings in **Report options** 322 window.
<OK>	Load and open all selected chromatograms.
<Cancel>	Close this window without any action.

See also:

Save chromatogram 210

Delete chromatogram 211

Close chromatogram 211

How to open a chromatogram 475

6.2.1.1 Open chromatogram: file list

The most important information taken from the chromatogram is shown here.

The following columns are presented in the list of chromatograms:

File	filename of the chromatogram. The current version uses automatically generated file names.
Acquired	date and time of the chromatogram acquisition start.
Title 126	short title of the chromatogram. Title is especially useful for seeking in the chromatogram database. So, it is recommended to use informative titles.
Method 122	the name of the file of processing method used for the current chromatogram
Level 199	calibration chromatograms display the corresponded **calibration level** 199
Batch	batch counter showing history of batch processing; this item is not empty if the chromatogram was processed with **batch reprocessing** 271
Version 210	counter showing the chromatogram version.
Last saved	date and time of the last modification of the chromatogram file

6.2.1.1.1 Chromatogram version

GLP 43 and 21 CFR Part11 specification demands that primary data as well as all copies of chromatograms derived from it were stored and can not be changed. So, several copies of the same chromatogram shoud be stored. Version number allows to distinguish such copies of the same chromatogram.

Version number for primary chromatogram always equals 1. Each chromatogram derived from the parent one directly, will get version number 2. If this chromatogram will be changed in turn and saved, the copy will get version number 3, etc.

If default sorting ("File" column) is applied, chromatograms will be sorted by the second sort-key also, namely by version key.

Note: several versions with the same number can exist for chromatogram.

Note: up to two new chromatogram versions per single operation can be created in some cases. Thus, batch reprocessing with recalibration option will create two new versions for each chromatogram. This pecularity is because

Note: if 21CFR Part 11 option is installed, it is not allowed to delete any chromatogram.

6.2.1.2 Chromatogram description

Information on the selected chromatogram can be previewed.

The following pages are available:

General/Sample	Selected fields related to chromatogram run and **sample description** 126.
View	preview of the graph of the selected chromatogram.
Results	**peak table** 327 for the selected chromatogram is shown here. Peak table is shown according to the settings in the **Report options** 322 window.
Calibration	calibration parameters and main calibration results for all components of **components table** 171 are shown here.
Comment	user-defined comment for the selected chromatogram can be viewed here.

6.2.2 Save chromatogram

(*Main menu* File / Save / Chromatogram)

This command saves the modified **chromatogram**.

The chromatogram is always saved in the location where it was opened from. You can move the chromatogram to another location using **Move** command in **Open chromatogram** 207 form.

A new file name is automatically generated each time a modified **chromatogram** is saved (according to its **version number** 210).

A previous versions of the chromatogram can be stored or deleted according to **global preferences** 41 settings.

Each chromatogram contains a copy of all settings of the **data processing method** 122. When operator modifies any **method** 122 settings in the chromatogram a prompt window may appear asking for updating method file. **Global preferences** 41 are used to configure this behavior.

See also:

Open chromatogram 207

Delete chromatogram 211

Close chromatogram 211

Main window menu 25

6.2.3 Close chromatogram

This option closes the active chromatogram window. If the data were not saved or the **method** 122 was modified, the software reminds about.

Usually it is more convenient to close the window by clicking the  button at the top corner area.

See also:

Open chromatogram 207

Save chromatogram 210

Delete chromatogram 211

6.2.4 Delete chromatogram

Close current window and delete current chromatogram from the directory. A warning will be generated by the software.

See also:

Open chromatogram 207

Save chromatogram 210

Close chromatogram 211

6.2.5 Import chromatogram

(*Main menu* File / Import from)

Allows import of chromatograms recorded with other programs.

AIA file... 27 Import chromatograms in the AIA (Analytical Instrument Association)

format.

XML file... 29	Import chromatograms in the XML (eXtended HTML) format
Text file (raw data only).. 28	Import chromatographic raw data from a text file (ASCII format).
Other chromatogram types...	Import chromatograms of the following format:
Chrom&Spec for DOS (*.chm)	Chromatogram files of the **"Chrom&Spec"** program (DOS version).
Hyper/Metrodata (*._rd)	Chromatogram files of the **"714 IC Metrodata"** program (DOS version). After selection of the file to be imported you are asked to load a method.
EnviroChrom (*.chr)	Chromatogram files of the **"EnviroChrom"** program.
AtomChrom (*.dar)	Chromatogram files of the **"AtomChrom"** program.
LongInteger (*.*)	Chromatogram files in Long Integer format.

Note: Some imports need a method 122 for importing to. You need first open some method 122 file (using File / Open / Method menu). Otherwise import function is not available.

See also:

Export chromatogram 212

6.2.6 Export chromatogram

(*Main menu* File / Export to)

Allows export of the actual chromatogram into one of the following file formats:

AIA file... 28	Export chromatograms in the AIA (Analytical Instrument Association) format (***.cdf**).
XML file... 29	Export chromatograms in the XML (eXtended HTML) format (***.xml**).
Text file (raw data only)... 29	Export chromatographic raw data into an ASCII text file (***.txt**). Opens "Export raw data" window

See also:

Import chromatogram 211

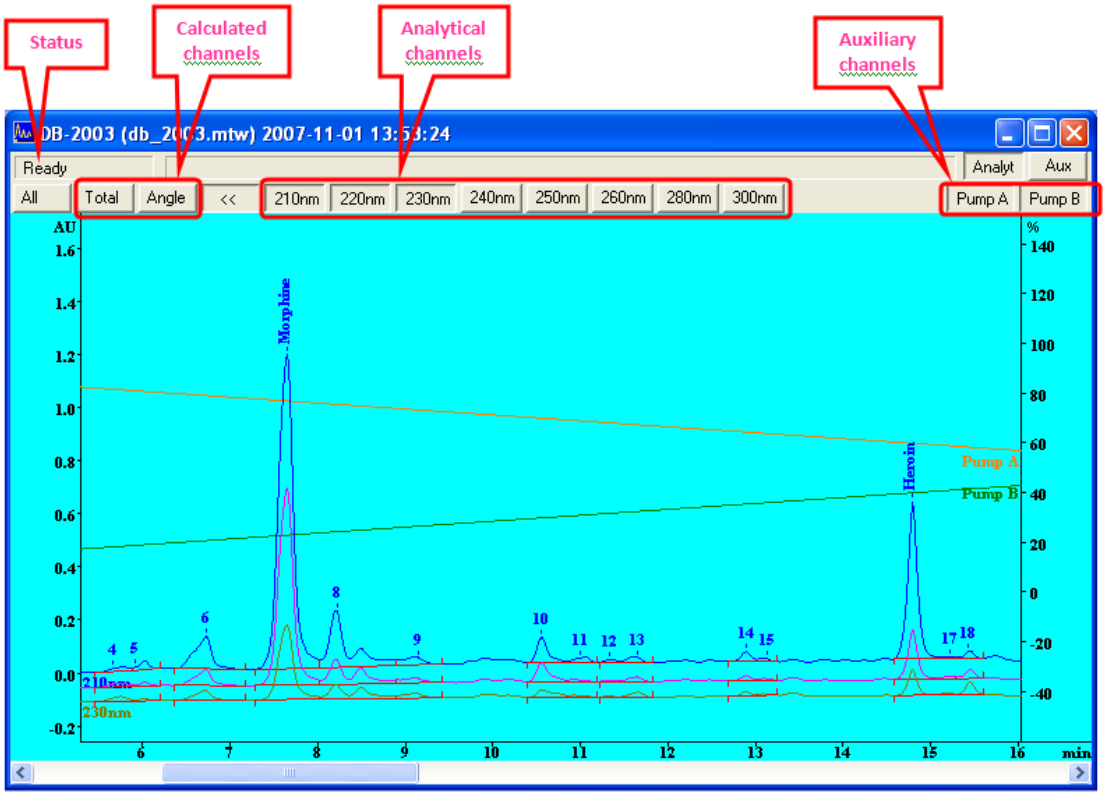
How to export a chromatogram 476

6.3 Chromatogram window

The **chromatogram window** is used to show a running or recorded **chromatogram** 207.

The **chromatogram window** contains a graph of the chromatogram and controls for changing

chromatogram appearance.



Depending on the content of the chromatogram the window may have or may have not some controls.

The chromatogram window includes:

- **Title bar** with window name and buttons for minimizing, maximizing and closing the window. The window name is generated according to:
  chromatogram title [126] **(method file name** [122]**) date and time of the chromatogram start** [124]
- **Status bar** with display of **measurement status** [215]. Running chromatograms also display the running time, analysis time and value of measuring signal. **Peak editor** [224] mode displays X and Y values of the cursor.
- **Channels display toolbar**.

  Buttons [***Analyt***] and [***Aux***] switch scaling mode for **analytical channels** [113] and **auxiliary channels** [113] respectively.

  Button [***All***] toggles view (**on** and **off**) for all **analytical channels** [113] available.

  Buttons [**>>**] [**<<**] show and hide individual buttons for **analytical channels** [113] at the toolbar.

  Buttons for **calculated channels** [152] toggles view (**on** and **off**) for individual **calculated**

channel. Last shown channel became a **current channel** 221.

Buttons for **analytical channels** 113 toggles view (**on** and **off**) for individual **analytical channel.** Last shown channel became a **current channel** 221.

Buttons for **auxiliary channels** 113 toggles view (**on** and **off**) for individual **auxiliary channel.**

- **Chromatogram area**.

  Left axis refers to **analytical channels** 113. **Current channel** 221 is used to draw axis ticks. Other channels are scaled.

  Right axis refers to **auxiliary channels** 113. Last toggled **auxiliary channel** is used to draw axis ticks.

  Horizontal axis refers to retention time displayed in **retention units** 218.

  To scale a chromatogram select an appropriate part of the chromatogram by [Left] mouse button.

  Double click [Left] mouse button on chromatogram area to perform automatic scaling.

  Other chromatogram scaling functions are available through **keyboard or mouse hot keys** 214.

  Scaling and other appearance settings can be configured using **Appearance** 216 window form.

  Appearance is also controlled via **view menu** 30 and analogous **context (pop-up) menu** called by clicking [Right] mouse button on **Chromatogram area**

  Some of the window handling functions are collected in the **Window menu** 35.

See also:

Keyboard or mouse functions 214

Appearance window form 216

View menu 30

6.3.1 Keyboard and mouse functions

The mouse helps in zooming a chromatogram.
To zoom a portion of the plot it is necessary to place the mouse cursor to the upper left corner of the square to zoom, press the left mouse button and drag the cursor to the lower right corner of the rectangle. After releasing of the left mouse button the selected region will be zoomed full-screen.

The keyboard can also be used to scale a chromatogram in the window, as described below.

KEYBOARD QUICK REFERENCE

Keyboard and mouse shortcuts for chromatogram window:

[Up] Increases sensitivity on the axis Y.

[Down]	Reduces sensitivity on the axis Y.
[Right]	Expands a chromatogram on the axis X.
[Left]	Shrinks a chromatogram on the axis X.
[Ctrl] + [Home]	Autoscale procedure on the axis X (shows all on X).
[Ctrl] + [End]	Autoscale procedure on the axis Y (shows all on Y).
[Alt] + [V]	Autoscale procedure on the axis X and Y (shows all on X and Y).
[Mouse Left Button Double Click],	Autoscale procedure on the axis X and Y (shows all on X and Y).
[Page Up],	Shifts a chromatogram on 1/10 part of a screen upwards.
[Mouse Wheel Down],	Shifts a chromatogram upwards.
[Page Down],	Shifts a chromatogram on 1/10 part of a screen downwards.
[Mouse Wheel Up],	Shifts a chromatogram downwards.
[Shift] + [Up]	Increases a distance between channels of a multi-channel chromatogram.
[Shift] + [Down]	Reduces a distance between channels of a multi-channel chromatogram.
[Ctrl] + [Right]	Scroll chromatogram right (without change of scale on X and Y axes).
[Ctrl] + [Left]	Scroll chromatogram left (without change of scale on X and Y axes).
[Home]	Shows the beginning of a chromatogram (without change of scale on X and Y).
[End]	Shows the end of a chromatogram (without change of scale on X and Y).
[0 (Zero)]	Adjusts a zero on the last point of a chromatogram (running chromatogram) or its lowest level (finished run).
[Z]	Adjusts a zero on the last point of a chromatogram (running chromatogram) or its lowest level (finished run).
[Space]	Manual **Inject (start)** signal for the running chromatogram. It is active only when related option is set in the **Global Preferences** 41.

See also:

Chromatogram window 212

6.3.2 Chromatogram measurement status

Text at the left top corner of the **chromatogram window** 212.

Indicates the current status of the chromatogram, one of listed below:

Ready	Chromatogram is ready to start.
Waiting	Chromatogram is waiting for the first measuring points.
Measure	Chromatogram is being measured.
Measure(Baseline)	Recording of baseline.
Finished	Measurement finished, but the chromatogram is not processed.
Processing	Chromatogram is being processed after finishing.

See also:

Chromatogram window 212

6.3.3 Appearance

(*Main menu* View / Appearance...)

Opens an **Appearance** window form.

This window form defines the appearance of the chromatogram and consists of four pages:

Chromatogram axes 216	Scaling of chromatogram axes.
Labels 218	Settings for peak labels and baseline drawing.
Select channel 220	Select channels to be displayed (only available for multi-channel chromatograms).
Colors 222	Color settings for chromatogram elements.

Buttons

<OK>	Accept modified parameters and close window.
<Cancel>	Cancel changes and close window.
<Apply>	Apply modified parameters to chromatogram window.

Note: By design, modifying appearance settings is not considered as modification of the chromatogram. So modified appearance settings do not produce a prompt asking for save changes on closing the chromatogram. Operator can save chromatogram explicitly after modification in order to have the same appearance after reopening the chromatogram.

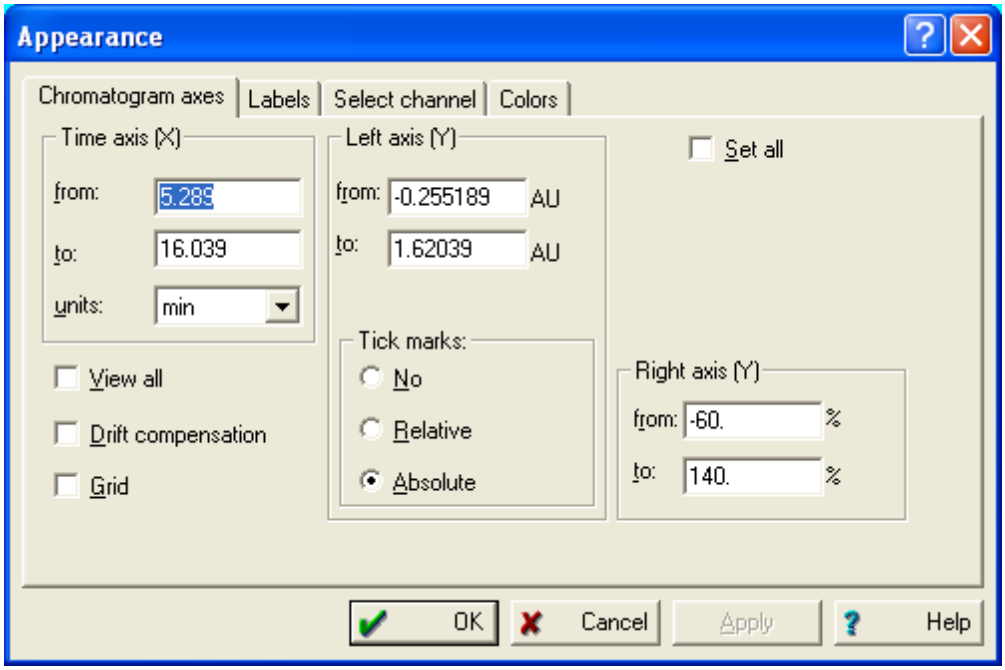
See also:

Chromatogram window 212

How to change the appearance 475

6.3.3.1 Chromatogram axes

This page of **Appearance** 216 form defines scaling parameters of the chromatogram graph 212.



Time axis (X) Specifies the scaling over the horizontal axis.

- **from** Beginning of the window on X axis.
- **to** End of the window on X axis.
- **units** Choice of the **retention units** 218 for X axis.

Left axis (Y) Specifies the scaling over the left vertical axis. **Current channel** 221 is used as a basis for scaling. Other channels are scaled automatically.

- **from** Beginning of the window on Y axis.
- **to** Set scale on Y axis.
- **Tick marks** Specifies the way how ticks are drawn on vertical axis:
  - **No** No vertical axis is drawn; scaling is analogous to **Relative**
  - **Relative** Zero value is always assumed at axis origin. **[PageUp]**, **[PageDown]** **hot keys** 214 move graph vertically relatively fixed ticks.
  - **Absolute** Ticks refer to actual detector response of the **current channel** 221. **[PageUp]**, **[PageDown]** **hot keys** 214 move graph and axis ticks vertically.

Right axis Specifies the scaling over the right vertical axis. Right axis refers to **Auxiliary channels** 113. Ticks always refer to the actual value of the **auxiliary channel.**

- **Y from** start point for Y axis.

Y to end point for Y axis.

Buttons

☑ **View all** Set scales on X and Y axes so that the whole chromatogram is visible.

☑ **Drift compensation** Software estimates the drift on each analytical 113 and calculated 152 channel. The drift is subtracted from the channel value when a graph is constructed. Drift compensation has no effect while a chromatogram is running.

☑ **Grid** Prints dotted grid lines in the chromatogram window.

☑ **Set all** Apply axis scaling settings to all opened chromatograms. This option allows to view several similar chromatograms in exactly the same scaling.

See also:

Appearance window form 216

Chromatogram window 212

6.3.3.1.1 Retention units

The retention units for appearance (unit for retention time) is set in the **chromatogram axes** 216 page of the **appearance** 216 form.

The possible choices are:

sec Seconds
min Minutes
µL Microliters
mL Milliliters
Nmeas Number of raw data points (Number of ADC measure cycles)

Volume units (**µL, mL**) use **flow** 131 rate parameter for calculating retention volume.

This parameter defines how retention is displayed in the chromatogram window 212 and in the reports.

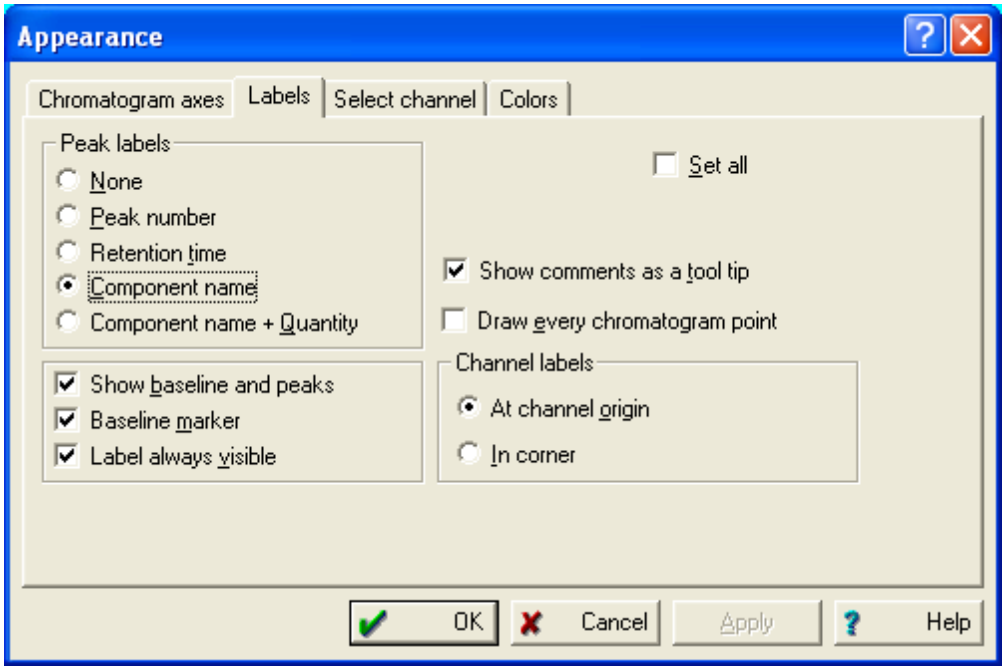
See also:

Chromatogram axes 216

Retention units (calibration) 169

6.3.3.2 Labels

This page of **Appearance** 216 configures the way how peaks and labels are drawn in the **chromatogram graph** 212.



Peak labels

Defines the label which appears at the peak top.

None — No peak labels.

Peak number — Peak number.

Retention time — Retention time.

Component name — Component's name.

Component name + Quantity — Name and quantity of component.

Channel labels

Defines where channel label is printed.

At channel origin — Channel label is shown near the left vertical axis where channel graph begin.

In corner — Channel label is shown in the upper left corner of the chromatogram.

Buttons

☑ **Show baseline and peaks** — Baselines are shown under the peak.

☑ **Baseline marker** — Start and end of baselines are marked.

☑ **Label always visible** — Peak label is shown always with zooming. If not set peak label is not printed if the peak top is outside the printed area.

☑ **Show comments as a tool tip** — Show the content of the "Comment" page 129 as a tool tip over chromatogram window 212.

☑ **Draw every chromatogram point** — Exact drawing of the chromatogram graph in **chromatogram window** 212. If not set the drawing works faster still visual uncertainties may appear. This option is designed to support low-performance workstations.

☑ **Set all** — Apply settings of this page to all opened chromatograms. This option allows to view several similar chromatograms in exactly the same manner.

See also:

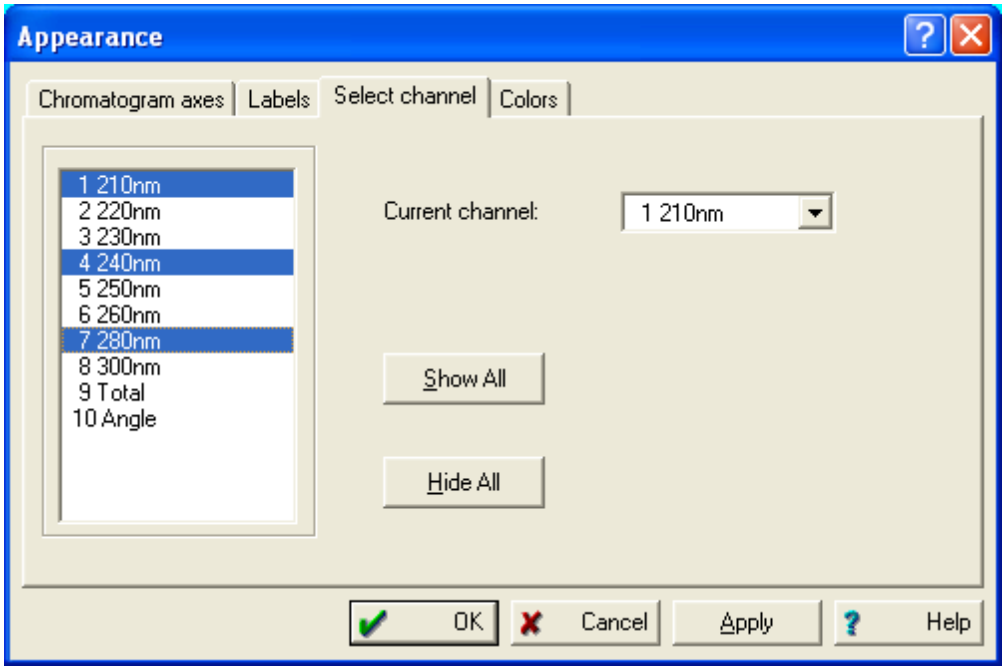
Appearance window form 216

Chromatogram window 212

6.3.3.3 Select channels

This page of **Appearance** 216 is available only for chromatograms with two or more channels.

Use this page to select channels which are visible in the **chromatogram window** 212 and in reports.



Selection list — The selection window shows **channels** 146 of the chromatograms which can be selected for display. The list includes **analytical channels** 113 and **calculated channels** 152. See **selected channels** 221.

<Show all>	Select all **analytical channels** 113 and hide all **calculated channels** 152.
<Hide all>	Hide all **channels** 146 of the chromatogram.
Current channel	Select a channel which is used as a **current channel** 221 in the chromatogram.

See also:

Appearance window form 216

Chromatogram window 212

6.3.3.3.1 Current channel

The **current channel** is used for the following functions:

- to plot peak labels on the chromatogram.
- to scale chromatogram using autoscale procedure 214.
- to calculate and draw ticks of the left vertical axis of the chromatogram.
- to edit peaks using manual peak editor 224.

Any analytical channel 113 or calculated channel 151 of the chromatogram can be chosen as **current channel**.

Use Appearance/Select channels 220 page to set a **current channel**.

Channels buttons in the chromatogram window 212 also set a **current channel**. The last shown channel is considered as current one.

See also:

Selected channel 221

Reference channel 197

Analytical channels 113

Calculated channels 151

Auxiliary channels 113

6.3.3.3.2 Selected channels

Selected channels are those to be shown on the chromatogram plot.

Channels can be selected:

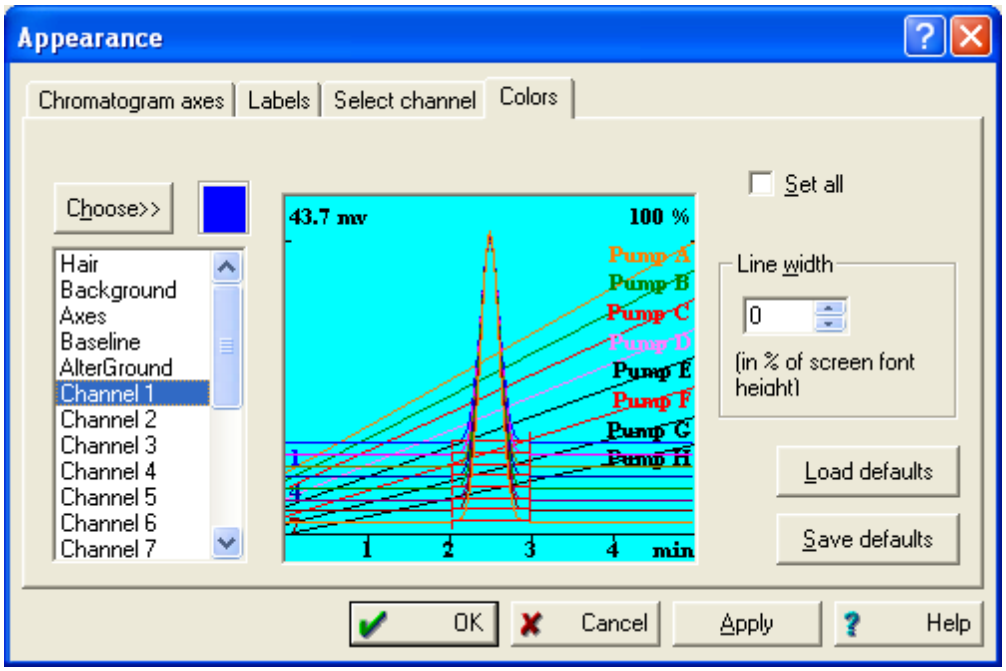
- in the Appearance/Select channels 220 page.
- using special channel buttons in the chromatogram window 212.

See also:

Current channel 221
Reference channel 197
Analytical channels 113
Calculated channels 151
Auxiliary channels 113

6.3.3.4 Colors

This page of **Appearance** 216 includes the following parameters for customizing the **colors** of a chromatographic window:



<Choose> — Choose a new color for the selected element. An example of the chosen color is shown beside the button.

Hair — Cursor's color.

Background — Background color.

Axes — Axes and axes labels color.

Baseline — Baseline color.

AlterGround — Background color prior to the moment of sample injection.

Channel 1...8 — Color of the selected analytical 113 or calculated 152 channel. Each channel

	can be of a unique color. If there are more then **8** **selected channels** 221 in the chromatogram the colors are applied cyclically.
Aux 1...8	Color of the selected auxiliary channel 113. Each channel can be of a unique color.
Line width	Line width for the selected item (**Axes** or **Channel 1...8** or **Aux 1...8**) in % of selected plot font height. Range: **0** ... **232**
<Load defaults>	Load default colors into the chromatogram.
<Save defaults>	Save color settings of this chromatogram as default.

Buttons

☑ **Set all**	Set colors of all opened chromatograms automatically to the settings in the selected chromatogram window.

See also:

Appearance window form 216

Chromatogram window 212

6.3.4 "View" menu commands

6.3.4.1 View all

(*Main menu* View / View all)

Show chromatogram that fits window both **horizontally and vertically**. Keyboard shortcut [**Alt - V**].

If ***<Analyt>*** button is pressed in the chromatogram window 212, this option is applied in vertical direction for analytical channels 113 only, otherwise auxiliary channels 113 only are to be scaled vertically. Horizontal full scaling is carried out for both auxiliary and analytical channels

6.3.4.2 X full scale

(*Main menu* View / X full scale)

Show chromatogram that fits window **horizontally**. Keyboard shortcut [Ctrl - Home].

6.3.4.3 Y full scale

(*Main menu* View / Y full scale)

Show chromatogram that fits window **vertically** within current retention limits. Keyboard shortcut is [Ctrl - End].

If ***<Analyt>*** button is pressed in the chromatogram window 212, this option is applied for analytical

channels 113 only, otherwise Auxiliary channels 113 are to be scaled.

6.3.4.4 Recorder autoscale

(*Main menu* View / Recorder autoscale)

This option allows to look at the chromatogram so that the last point is always visible on the screen while data are acquired.

If *Recorder autoscale* is switched on, the following autoscaling rules apply:

- If the last acquired point comes out of the window down, Autozero is performed.
- If the last point is too high, the recorder scale shrinks twice until the point comes to screen.
- If the last point comes outside of the plotting area to the right, the window is shifted half-screen right.

If *Recorder autoscale* is switched off, the window scale does not change automatically during data acquisition.

6.4 Peak editor

(*Main menu* Process / Peak editor)

The **peak editor** can also be activated by clicking the Peak editor icon  in the toolbar of the **main window** 25.

The **peak editor** is used for manual correction of the peaks when it is not possible to get adequate results using **automated peaks detection** 159.

Before using **peak editor**:

- verify that settings in the **setup of the** 160 **automated peaks detection** 159 are correct and optimal for your **method** 122. Optimal settings may avoid the need of manual corrections.
- consider using **events for the automated peaks detection** 162.

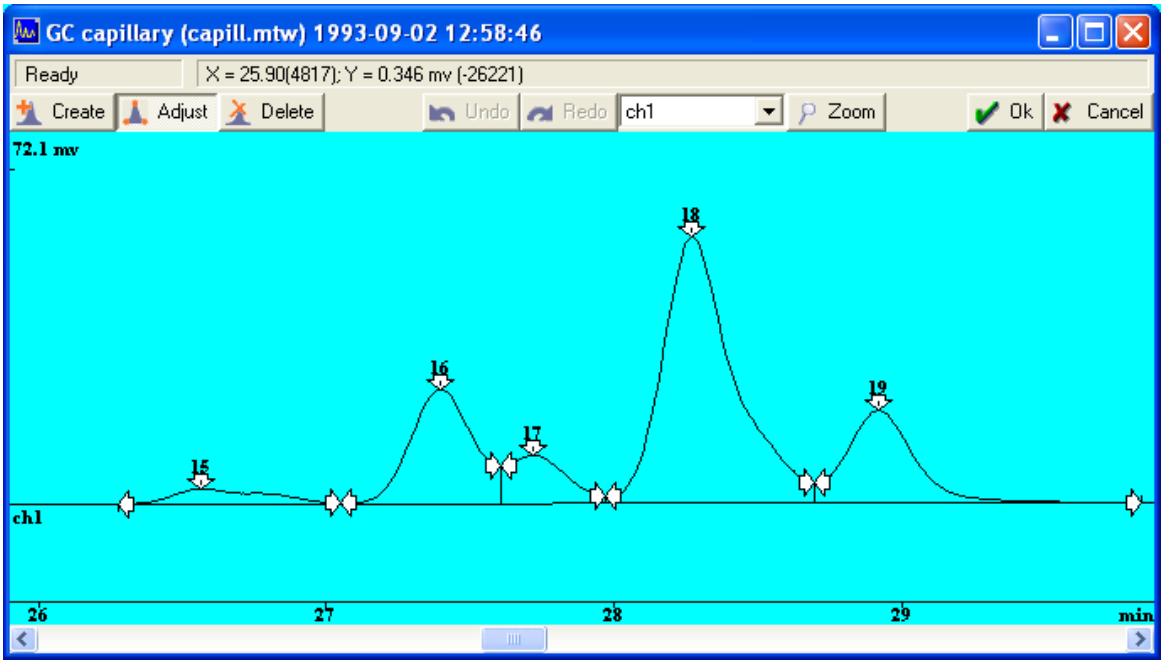
It is recommended to avoid using manual peak corrections when it is possible because this correction would introduce subjectivity of the operator.

When peaks are corrected manually using **peak editor** this fact is reflected in the reports (in the **General** section by default).

When the **Peak editor** is activated, the vertical **cursor** 226 bar appears in the chromatogram window and **Peak editor *toolbar*** appears at the top of **chromatogram window** 212.

A **current channel** 221 is displayed only; other channels are hidden.

All manipulations with peaks are done using ***computer mouse*** pointing device.



[*Create*] Switches peak create mode 226 for **peak editor**

[*Adjust*] Switches peak adjust mode 229 for **peak editor**

[*Delete*] Switches peak delete mode 230 for **peak editor**

[*Undo*] Undo the last peak operation. Operator can undo several or all operation by repeatedly pressing [*Undo*] button.

[*Redo*] Redo the last peak operation.

{*channel list*} A drop-down list containing the names of **analytical** 113 and **calculated** 152 channels. Operator can select any channel to set it as a **current channel** 221 and display it in the **chromatogram area**.

[*Zoom*] Zooming is done by [Right] mouse button. It acts in the same way as [Left] mouse button do in the normal **chromatogram window** 212.

To scale a chromatogram select an appropriate part of the chromatogram by [Right] mouse button.

Double click [Right] mouse button on chromatogram area to perform automatic scaling.

Operator can use keyboard and mouse functions 214 in the same way as in normal **chromatogram window** 212.

[*Ok*] Apply all peak operations and exit **peak editor**.

[*Cancel*] Cancel all peak operations and exit **peak editor**.

Note: Operator can edit the ***peak control points*** only: ***peak start, peak end*** and ***peak top.*** The baseline under the peak is always calculated automatically. Operator cannot modify the position of the baseline. **Interpolate baseline start/stop** option of the **peak integration setup** 160 controls the way how baseline is calculated.

See also:

About peaks integration 159
Integration setup 160
Integration events 162
Chromatogram window 212

6.4.1 Cursor

Cursor is a vertical bar in the chromatogram window that helps to change peak integration patterns manually with the help of the **peak editor** 224.

Just activate the peak editor to activate the cursor.

Moving cursor by mouse

The cursor can be dragged using ***computer mouse*** pointing device. The position of the cursor is displayed in the status bar of the **chromatogram window** 212.

Use [Left] mouse button to make actions by the cursor.

See also:

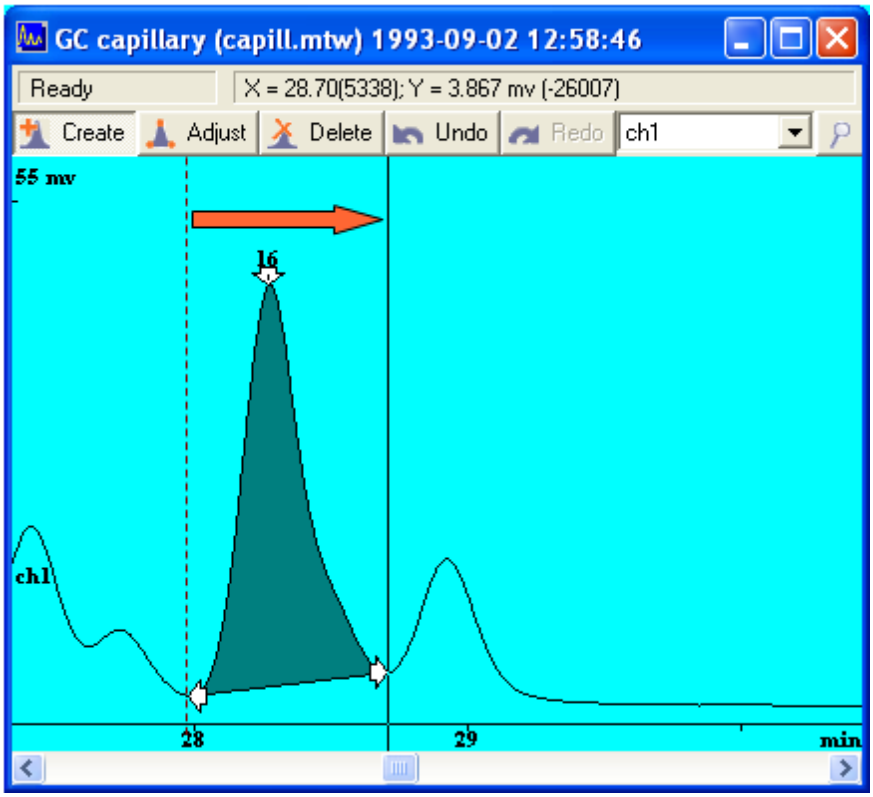
Peak editor 224

6.4.2 Peak editor: Create peak mode

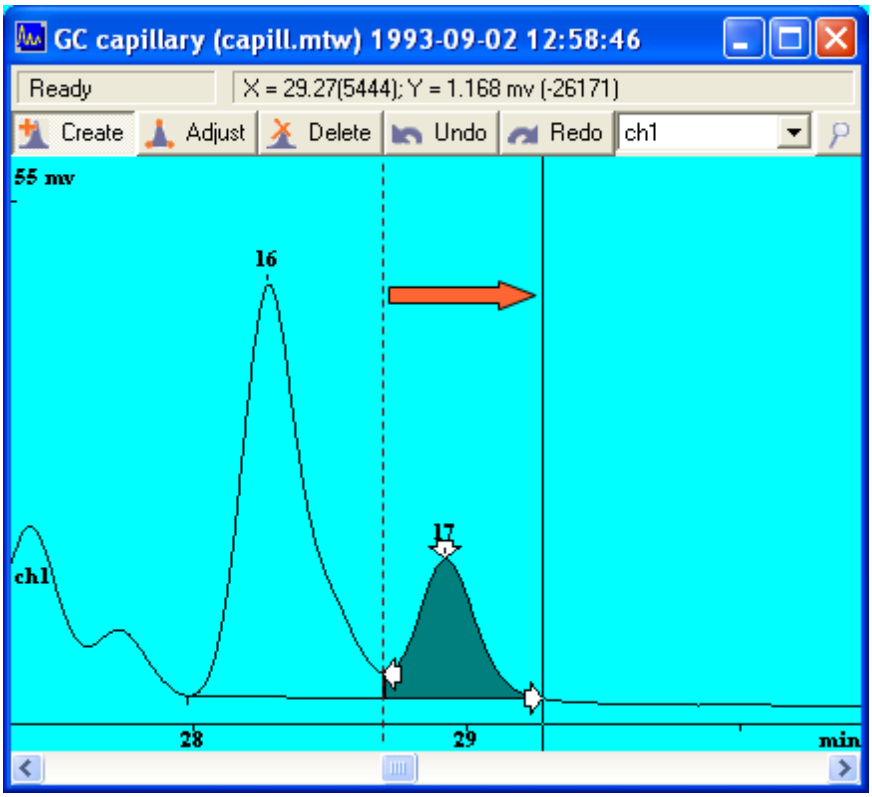
This mode is activated by pressing [***Create***] button at the **peak editor** 224 ***toolbar***.

Use this mode to create a new normal ***peaks*** or **rider *peaks***.

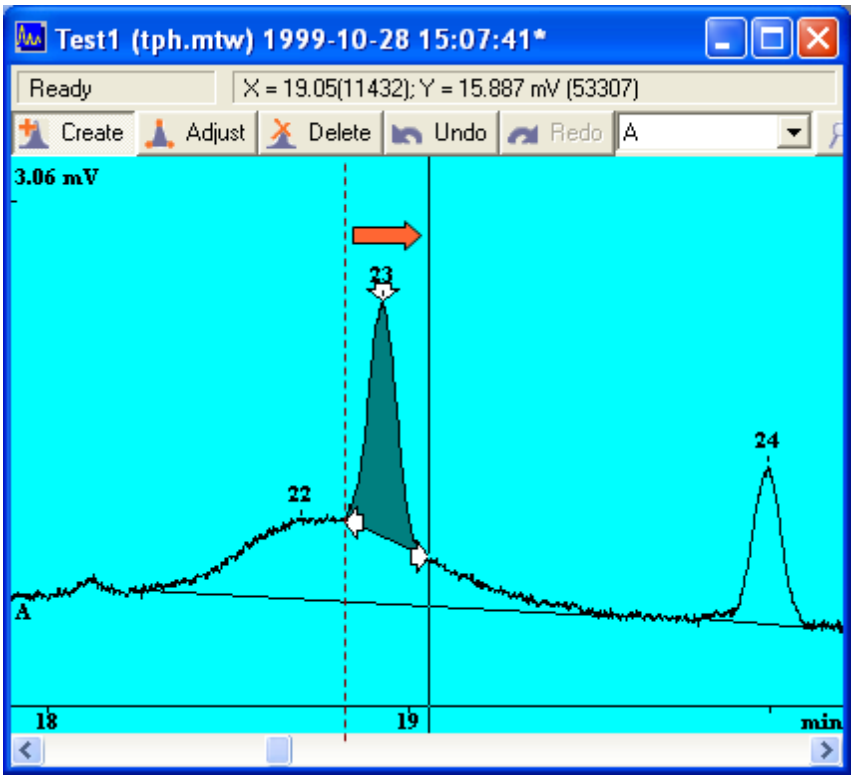
To create a stand-alone ***peak*** move cursor 226 to the ***peak start***, press and hold [Left] mouse button, move cursor 226 to the ***peak end*** not overlapping nearby peaks and release the [Left] mouse button.



To create a ***peak*** with common baseline with nearby peak make the same actions overlapping slightly nearby peak:



To create a **rider *peak*** perform analogous actions over the **rider host *peak*.** Note that it is not possible to create a **rider *peak*** covering the top of the **rider host *peak*.** Operator can move the top of the ***peak*** using **adjust peak mode** 229 if necessary.



See also:

Peak editor 224

6.4.3 Peak editor: Adjust peak mode

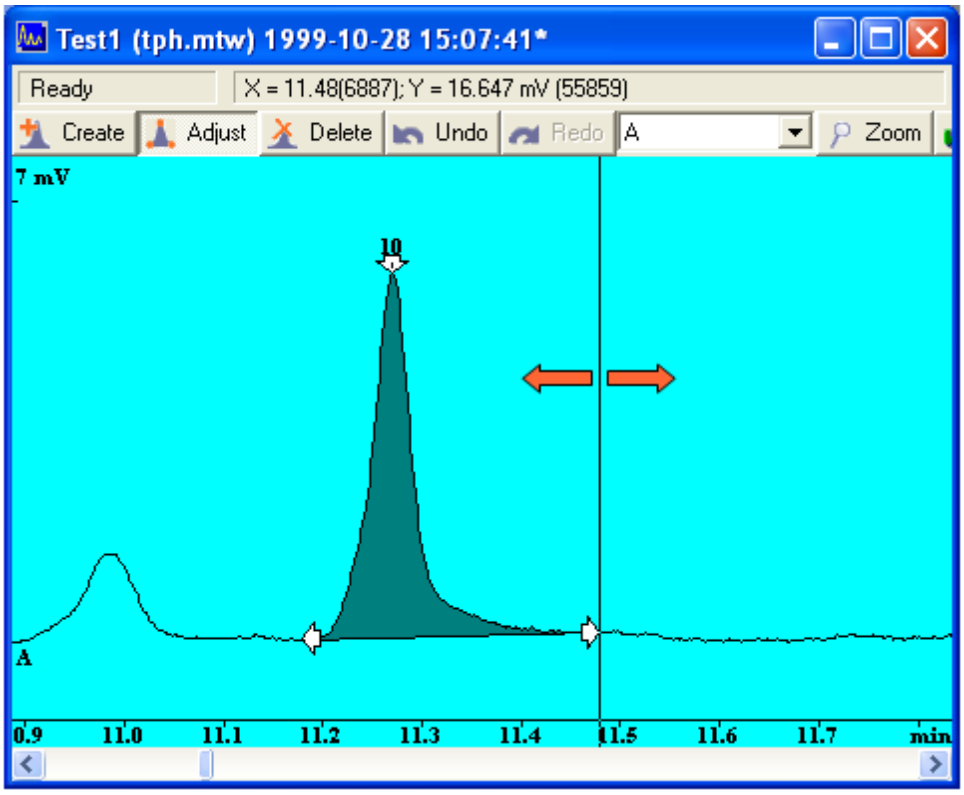
This mode is activated by pressing [***Adjust***] button at the **peak editor** 224 ***toolbar***.

Use this mode to adjust boundaries (***peak start*** and ***peak end***) of the peaks and the position of the ***peak top.***

To adjust ***peak*** move cursor 226 to the ***peak control point*** (the ***control points*** are marked by white arrows), press and hold [Left] mouse button, move cursor 226 to the new location and release the [Left] mouse button.

Software restricts an incorrect adjustments. For example, it is not possible to move ***peak top*** outside the ***peak*** boundaries.

The adjustment can also modify, delete or convert to **rider** the overlapped nearby ***peaks*** if necessary.



Tow or more ***peaks*** may have a common **baseline**. ***Peaks*** must have a common boundary to have a common baseline. That is the ***peak end*** point of the peak must be the ***peak start*** point of the other peak. Otherwise the ***peaks*** are considered as independent and the **baseline** is calculated separately for each ***peak***.

Note: The baseline under the peak is always calculated automatically. Operator cannot modify the position of the baseline. **Interpolate baseline start/stop** option of the **peak integration setup** 160 controls the way how baseline is calculated.

See also:

Peak editor 224

6.4.4 Peak editor: Delete peak mode

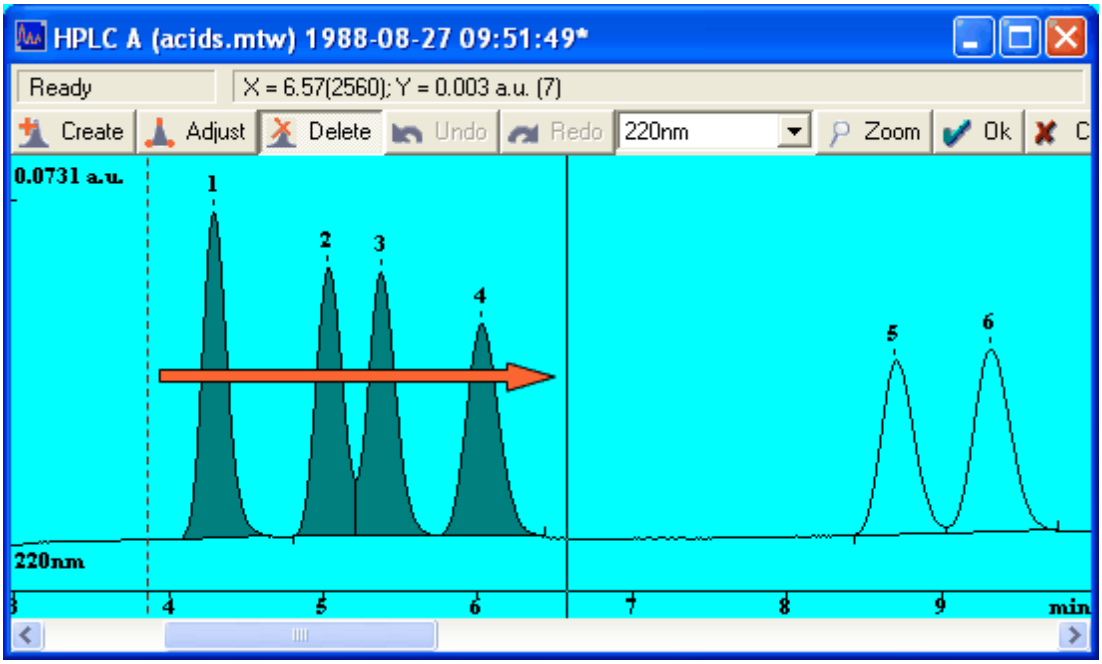
This mode is activated by pressing [***Delete***] button at the **peak editor** 224 ***toolbar***.

Use this mode to delete ***peaks*** from the chromatogram.

To delete ***peaks*** move cursor 226 to any point in the **chromatogram**, press and hold [Left] mouse button, move cursor 226 to the new location and release the [Left] mouse button. All **peaks** within the selected range will be deleted.

To delete a single ***peak*** the range must be within the ***peak*** boundaries. To delete a **rider** ***peak*** select a

range within this ***peak*** - the host peak will not be deleted in this case.



See also:

Peak editor 224

6.5 Peak deconvolution

6.5.1 Peak deconvolution

(*Main menu* Process / More... / Peaks deconvolution by form)

6.6 Chromatogram processing commands

6.6.1 Reintegrate

(*Main menu* Process / Reintegrate...)

This menu item opens the **Integration parameters** 159 window. Modify these parameters and press the **<Apply>** button for reintegration of the selected chromatogram.

6.6.2 Compare Chromatograms

(*Main menu* Process / More... / Compare...)

Use this command to compare the current **chromatogram** or **method** with another **chromatogram** or **method**.

The compared **chromatograms** or **methods** should be opened first.

Compare with chromatograms window is displayed containing a list of opened objects for comparison. Operator should select a desired object from the list.

Click **<Compare>** button to proceed . Differences window 232 will be opened where all founded differences will be displayed .

6.6.2.1 "Differences" window

Differences window presents all differences, founded between two selected **chromatograms** or **methods**. The left area displays a tree of chromatogram branches, and the right area contains a table of all items (in the selected branch) that are different for two chromatograms.

See also:

"Compare Chromatograms" command 231

6.6.3 Invert

(*Main menu* Process / More... / Invert!)

This menu item inverts the response curves for all channels of the chromatogram so that negative peaks become positive and vice versa (useful for chromatograms with wrong input polarity).

6.6.4 Subtract

(*Main menu* Process / More... / Subtract...)

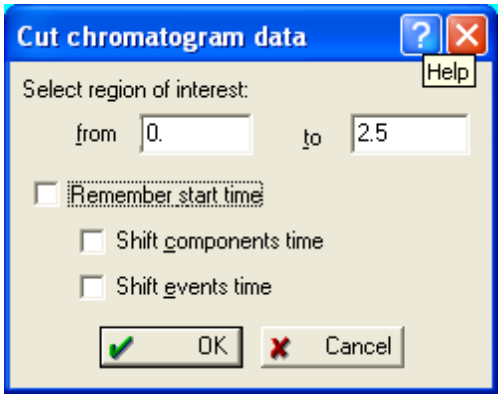
This menu item allows to subtract any opened chromatogram from the active (selected) chromatogram.

Select the chromatogram that should be subtracted in the "***Subtract chromatogram***" window, click on **<Subtract>** and then on Chrom&Spec **/ View / View all**. The result is shown in the active chromatogram window, which is considered as a new chromatogram and will be stored under a new name to avoid overwriting of old data.

6.6.5 Cut raw data

(*Main menu* Process / More... / Cut Raw Data)

This option enables to cut any desired part of the chromatogram and to reject all unneeded data.



Select region of interest from... to ...
select start and end points of the desired chromatogram region, in **retention units** 218.
Retention time units can be selected in the **Chromatogram axes** 216 page.

☑ **Remember start time**
set this box to count time scale for the selected part from the beginning of the initial chromatogram (time axis is unchanged)
If this box is **cleared**, time scale is measured from the begging of the selected region (time axis start is shifted to the first point of the region), and the following two items become available:

☑ **Shift components time** shifts components retention times in the Components table 171 to ensure correspondence with a new time scale

☑ **Shift events time** shifts integration events 163 time to ensure correspondence with a new time scale.

Note: "Cut raw data" operation modifies raw data! The chromatogram will be saved as a new file (it does not matter what settings are set in the Global preferences 41 dialog box).

6.7 Chromatogram printing

6.7.1 Print

(File / Print menu item)

Clicking the  button or selecting the **menu item File / Print** sends the **plain report** 320 to the printer. Before printing, the **Windows© system** standard **Print** window is opened where printer, printing range and number of copies can be defined.

All settings defined in the **Report options** 322 window will be used except the destination of the printout.

If you want to modify the report options for the printout, use the  button or the **menu item Report / Setup and make &plain report...**

See also:

Toolbar 36
Preview 234
Printer setup 234
Page layout 340
How to print a chromatogram 476

6.7.2 Preview

(File / Preview menu item)

By clicking the  button or selecting the **menu item File / Preview** the ***Preview*** window of **plain report** 320 is displayed. The report is generated using settings defined in the **report options** 322 window form and stored in the chromatogram. The report is formatted for the printer defined by **printer setup** 234.

See also:

Toolbar 36
Print 233
Printer setup 234
Page layout 340

6.7.3 Printer setup

(File / Printer setup menu item)

By selecting the **menu item File / Printer setup** the **Windows© system *Print*** window is opened where ***printer***, ***paper size*** and other settings can be defined.

The settings are used for printing **plain reports** 320 only.

Advanced reports 341 can define an individual settings for printing.

See also:

Print 233
Preview 234
Page layout 340

6.8 Other chromatogram operations

6.8.1 Extract stored system

(*Main menu* Method / Extract stored system...)

The instrument configurations for the chromatographic analysis are stored in the **system** 79 file (***.smt**).

When analysis is executed the entire content of the **system** 79 file is copied to the chromatogram and is stored in the **chromatogram files** (***.chw**).

Later the stored **system** 79 can be extracted from the chromatogram using **Extract stored system**.

This command can be used to review the instrument settings as they were defined when analysis was executed.

Extracted system can be saved to another **system file** and then it can be used to perform other analyses (still some reconfigurations may be needed).

6.9 Chromatogram examples

6.9.1 Chromatogram examples

The **Data** folder contains several example chromatogram files. They demonstrate different aspects of Chrom&Spec usage.

Part VII

7 Sample queue

7.1 Sample queue definition

A **sample queue** is an automated sequence of several analysis. It is used to facilitate the work with multiple routine analyses. Use of **sample queue** together with auto-samplers is most effective.

Operator can perform **method** 122 **(re)calibration** 165 and run a set of analyte samples in a single strictly defined sequence.

Sample queue can be configured to perform various actions during execution:

- Create **individual analysis reports** 341, including **calibration validation** 263 and other validation reports.
- Create **summary reports** 366 (**statistics**) for a specified set of analysis or for all analysis in the **sample queue**.
- Pause the **sample queue** during execution, promoting the operator to perform a specific actions.
- Create notification messages during **sample queue** execution, as needed by the working scenario.
- Shut down instruments when needed.

A **sample queue** defines a table containing sample description and sample-specific data. Once the queue has been started, the sample-specific data are transferred line-by-line to the running **system** 79 and are stored in the resulting **chromatograms** 207.

A **sample queue** are stored in a **sample queue file** (***.que**). Sample queue uses **systems** 79 to run analyses. Several different **systems** 79 can be used in the same **sample queue**, still all system files must be located in the directory where **sample queue file** (***.que**) is.

Most commonly **sample queue** uses only single **system** 79 to run all analysis. Operator can create or open the **sample queue** using **System / Sample Queue...** 82 **menu item** of the **system window** 80 .

The **sample queue** can also be opened using **File / Open / Sample queue** 237 **menu item** of the **main window** 25.

The execution of the **sample queue** is controlled with **sample queue control** 238 window form.

To edit and configure the **sample queue** **sample queue editor** 245 user interface is used.

7.2 Sample queue file handling

7.2.1 Open sample queue

(*Main menu* File / Open / Sample queue...)

This menu command displays **Windows© system** standard **File open** window for opening a **sample queue file**.

Select the desired directory and file to open an existing **sample queue** and display the **sample queue control** 238 window form.

To create a new **sample queue**, select the desired directory and enter a new name in the **File name** field. This creates and opens a new **sample queue control** 238 window form with a single row containing default values.

See also:

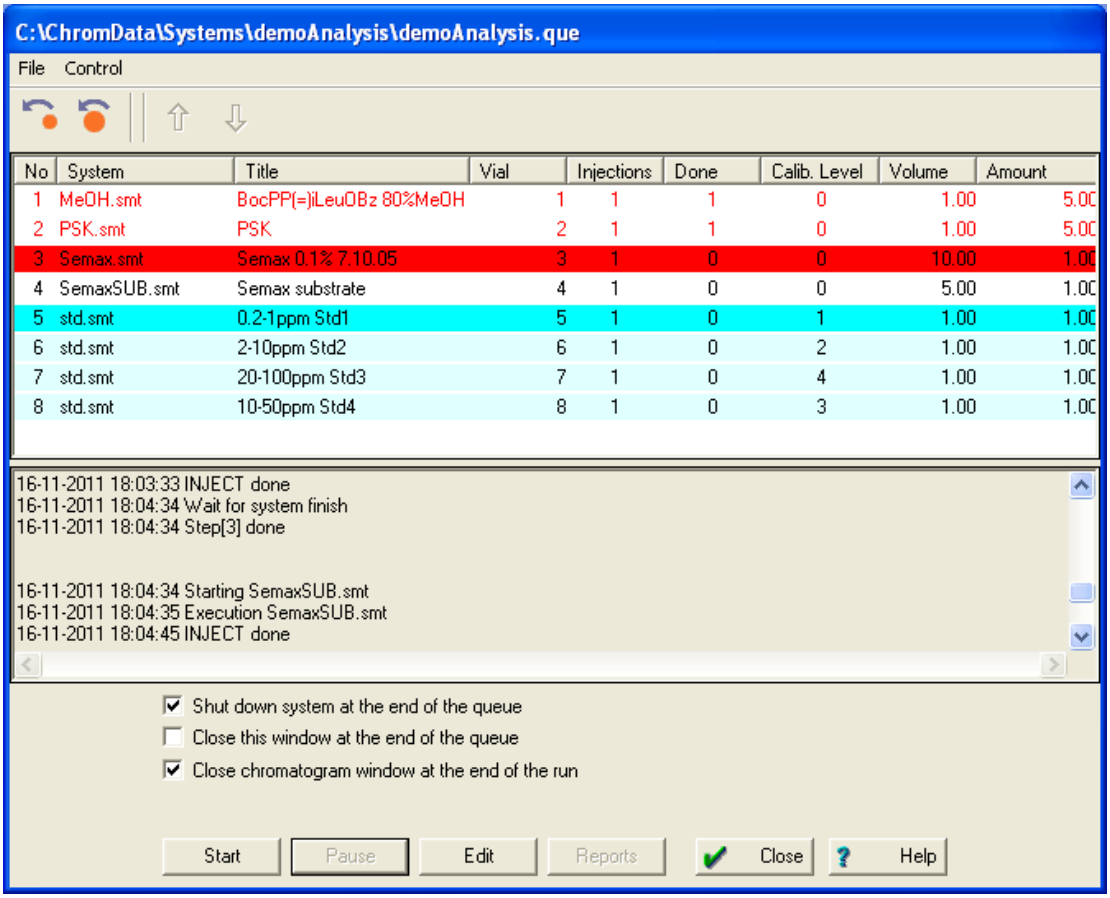
Delete sample queue 240

Save sample queue 247

How to open a sample queue 481

7.3 Sample queue control

The **sample queue control** window is used to control the execution of the **sample queue.**



The window contains the following items:

- **Queue control menu** 239
- **Queue control toolbar** 243
- **Sample table** 244
- **Sample queue execution log** 245

Options and buttons

Shut down system at the end of the queue

If this option is checked, the **sample queue** **shuts down the system** 85 used in the last analysis of the queue. The system remains connected to workplace 89.

Close this window at the end of the queue

When checked closes **sample queue control** window when sample queue is finished.

Close chromatogram window at the end of the run

If this option is checked, the **chromatogram window** 212 is forced closed when analysis finished. Otherwise the **chromatogram window** 212 is controlled by the **Close window** option at the **method setup: "Processing" page** 135.

<Start>	Start sample queue 240
<Pause>	Pause sample queue 241
<Edit>	Edit sample queue 240
<Reports>	Generate reports 242
<Close>	Close the **sample queue control** window.

See also:

Sample queue definition 237
Sample queue editor 245

7.3.1 Queue control menu

The menu of the **sample queue control** 238 window contains the following items:

File

Save as...	Save the sample queue to a file with a different name.
Edit...	Edit sample queue 240
Delete queue...	Delete sample queue 240

Control

Start...	Start sample queue 240
Pause...	Pause sample queue 241
Cancel last run...	Cancel last run 241
Reset...	**Reset sample queue** 242
Reports	**Generate reports** 242
Abort queue	Abort the execution of the **sample queue** and close **sample queue control** 238 window.
Move Up	**Reorder samples** 243 **in the sample table** 244
Move Down	**Reorder samples** 243 **in the sample table** 244

7.3.1.1 Edit sample queue

File / Edit... menu item

or

<Edit> button

Open the **sample queue editor** 255 program for editing the sample queue table.

See also:

Sample queue control 238
How to edit the sample queue table 481

7.3.1.2 Delete sample queue

File / Delete queue... menu item

Delete the file of the **sample queue** and close the **sample queue control** 238 window.

See also:

Sample queue control 238
Open sample queue 237
Save sample queue 247

7.3.1.3 Start sample queue

Control / Start menu item

or

<Start> button

Start execution of the sample queue from the first or from the row where execution was **paused** 241.

For each row, the sample-specific data are transferred to the appropriate **system** 79 (corresponded to the current run) and are stored in the resulting **chromatograms** 207.

The currently executing row is marked by **RED** color in the **sample table** 244.

A running sample queue can be interrupted by pressing the ***<Pause>*** 241 button or selecting **Control / Pause... menu item**.

An interrupted sample queue execution can be restarted by pressing the ***<Start>*** button or selecting **Control / Start menu item**.

See also:

Sample queue control 238
Pause sample queue 241
Cancel last run 241
Reset sample queue 242
How to start a sample queue 481

7.3.1.4 Pause sample queue

Control / Pause... menu item

or

<Pause> button

Interrupt execution of the sample queue.

The next run specified by **sample queue** will not start until operator restart the execution using **<Start>** button or **Control / Start menu item**.

Note, that current run will not be interrupted and will continue until finish. Use **Control / Stop run** menu command of the **system window** 80 to interrupt the current run if needed.

The **sample queue** is paused automatically when operator performs actions to force stop of the current run (using **Control / Stop run** menu command of the **system window** 80, for example)

See also:

Sample queue control 238
Start sample queue 240
Cancel last run 241
Reset sample queue 242
How to pause a sample queue 482

7.3.1.5 Cancel last run

Control / Cancel last run... menu item

Cancels the last started run in the **sample queue**. It is used when problems occur during the run, for example, because of incorrect **system** or **method** configuration or because of instrument issues.

The canceled run can be repeated afterwards after fixing the source of the problem.

The **Done** parameter of the last executed sample item from sample table 244 is decreased by 1.

This function is only available if the sample queue has been ***paused*** by pressing the **<Pause>** button or selecting **Control / Pause... menu item.**

When the queue is restarted, the canceled item from the sample table 244 is executed again.

See also:

Sample queue control 238
Start sample queue 240
Pause sample queue 241
Reset sample queue 242

7.3.1.6 Reset sample queue

Control / Reset... menu item

Resets entire **sample queue.** Sets **Done** parameter to zero for all sample items in the **sample table** 244.

This function is only available if the sample queue has been finished or interrupted (see **pause sample queue** 241).

After resetting the **sample queue** can be started again from the beginning.

See also:

Sample queue control 238
Start sample queue 240
Pause sample queue 241
Cancel last run 241

7.3.1.7 Generate reports

Control / Reports menu item

or

<Reports> button

Generates all reports specified in the **sample queue.** This function is available for the ***finished* sample queue** only.

Sample queue can be configured to generate **individual analysis reports** 341 and **summary reports** 366 (**statistics**). See **sample queue editor** 245 for details**.**

Typically reports are generated during **sample queue** execution as soon as related runs are finished.

Operator may wish to reproduce all reports of the finished **sample queue** afterwards using **Reports** command.

See also:

Sample queue control 238

7.3.1.8 Reorder samples

Control / Move Up **menu item**
Control / Move Down **menu item**

These commands give the operator a simple and quick way to change the order of execution of sample items in the sample table 244.

The commands can be used during **sample queue** execution and when the **queue** is in the ***paused*** state (see pause sample queue 241).

There are some restrictions applied to the sample reordering:

- the order of the already finished or started samples can not be changed
- samples item can not be moved to or moved from the **sample group** (see **sample queue editor** 245)

See also:

Sample queue control 238

7.3.2 Queue control toolbar

Buttons in the toolbar give a quick access to frequently used operations.

Cancel last run 241

Reset sample queue 242

Move Up, samples reordering 243

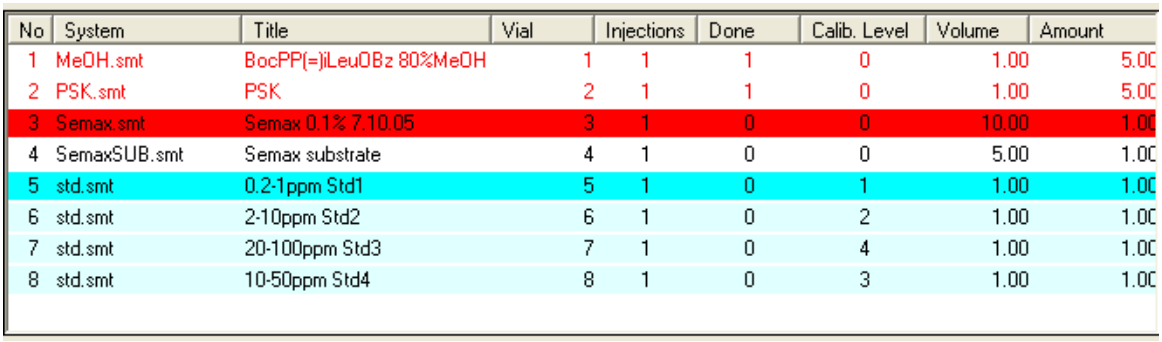
Move Down, samples reordering 243

These operations are also available through **queue control menu** 239

See also:

Sample queue control 238 window form.

7.3.3 Sample table



No	System	Title	Vial	Injections	Done	Calib. Level	Volume	Amount
1	MeOH.smt	BocPP(=)LeuOBz 80%MeOH	1	1	1	0	1.00	5.00
2	PSK.smt	PSK	2	1	1	0	1.00	5.00
3	Semax.smt	Semax 0.1% 7.10.05	3	1	0	0	10.00	1.00
4	SemaxSUB.smt	Semax substrate	4	1	0	0	5.00	1.00
5	std.smt	0.2-1ppm Std1	5	1	0	1	1.00	1.00
6	std.smt	2-10ppm Std2	6	1	0	2	1.00	1.00
7	std.smt	20-100ppm Std3	7	1	0	4	1.00	1.00
8	std.smt	10-50ppm Std4	8	1	0	3	1.00	1.00

Sample table contains the following items:

No	The sequence number of the row.
System	**System** 79 file to be used for the run.
Title 126	User defined **title** for chromatogram. The value will appear in the **general page** 124 when the chromatogram finish.
Vial	Autosampler **vial position** to take sample from. If the system uses autosampler this value can be handled by autosampler device. The value will appear in the **sample page** 126 when the chromatogram finish.
Injections	Number of the injections requested for the same vial position.
Done	Number of the injections which were already done; this value is automatically updated during **sample queue** execution.
Level	**Calibration level** 199 for a given sample. Level **0** stays for normal analysis (analyte run), levels **1** and greater for calibration runs. The **calibration** 165 of the **method** 122 used by the **system** 79 must be properly configured. The **concentrations table** 174 defines calibration levels and appropriate concentrations of the standard components. Specifying **Level** parameter produces automatic calibration of the **calibration level** 199 when analysis is finished.
Volume	Injected volume of sample, in micro liters. If the system uses autosampler this value can be handled by autosampler device. The value will appear in the **sample page** 126 when the chromatogram finish.
Multiplier	Sample multiplier parameter. See **adjusted volume** 199. The value will appear in the **sample page** 126 when the chromatogram finish.

Sample table contains a subset of sample description parameters which are most important for running **sample queue**.

All sample parameters can be reviewed and edited with **sample queue editor** 245.

Sample table highlights with **RED** color the line corresponding the currently executing sample.

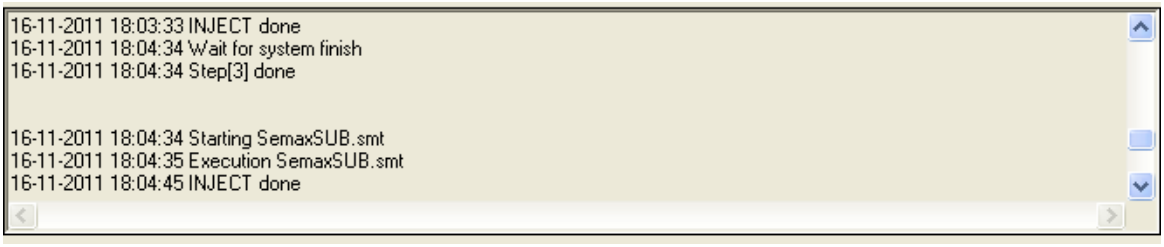
Sample table also highlights the **sample groups** 262.

The group **start** is marked with **CYAN** color and other samples in the group are marked with **LIGHT CYAN** color.

See also:

Sample queue definition 237
Sample queue control 238
Sample queue editor 245

7.3.4 Sample queue execution log



Sample queue execution log contains a list of time-stamped messages notifying operator about important events during **sample queue** execution.

This list also contains user-defined messages and prompts which are configured in sample queue editor 245 using options panel 257 (see User message before analysis 264, User message after analysis 265 for details).

See also:

Sample queue definition 237
Sample queue control 238

7.4 Sample queue editor

Sample queue editor is a tool provided to edit a list of samples for sample queue 237 and perform all other necessary configurations.

To launch a **sample queue editor** first open the sample queue 237 using File / Open / Sample queue 237 **menu item** of the main window 25 or System / Sample Queue... 82 **menu item** of the system window 80.
Use edit sample queue 240 command of the sample queue control 238 window to launch a **sample queue editor**.

Sample queue editor displays a window form which provides the following elements (see sample queue editor window elements 246):

- Menu 246
- Toolbar 254
- Sample table 255
- Options panel 257

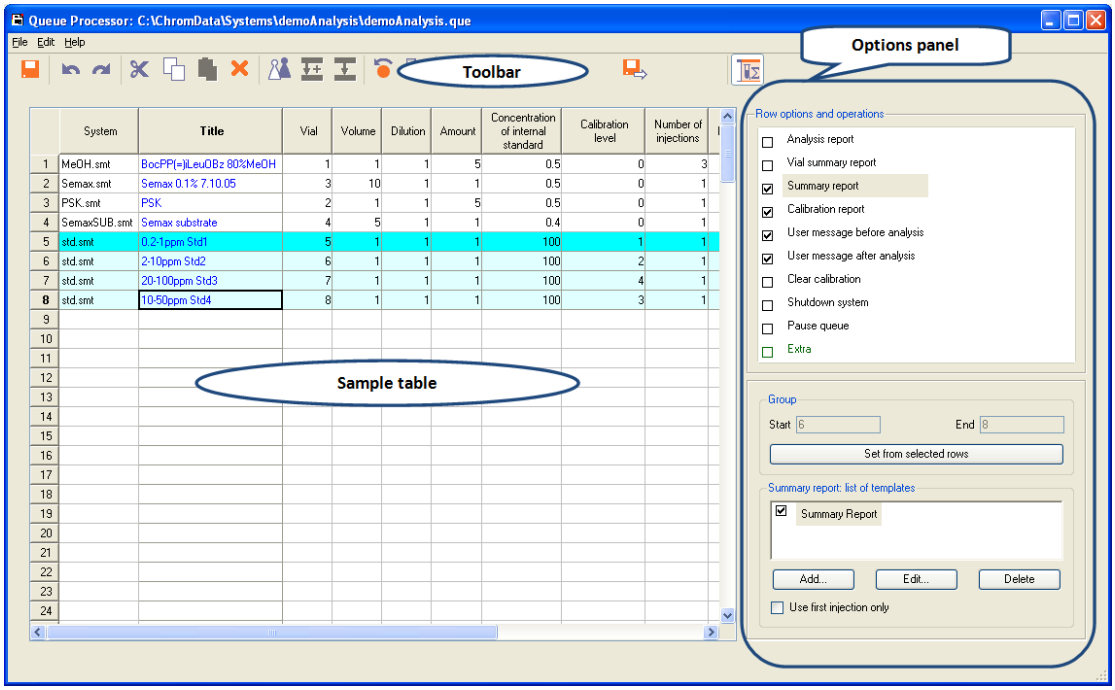
The main configurations of the sample queue are edited within sample table 255.

The optional (advanced) configurations are available at **options panel** 257.

See also:

Sample queue definition 237
Sample queue control 238

7.4.1 Sample queue editor window elements



	System	Title	Vial	Volume	Dilution	Amount	Concentration of internal standard	Calibration level	Number of injections
1	MeOH.smt	BocPP(=)iLeuOBz 80%MeOH	1	1	1	5	0.5	0	3
2	Semax.smt	Semax 0.1% 7.10.05	3	10	1	1	0.5	0	1
3	PSK.smt	PSK	2	1	1	5	0.5	0	1
4	SemaxSUB.smt	Semax substrate	4	5	1	1	0.4	0	1
5	std.smt	0.2-1ppm Std1	5	1	1	1	100	1	1
6	std.smt	2-10ppm Std2	6	1	1	1	100	2	1
7	std.smt	20-100ppm Std3	7	1	1	1	100	4	1
8	std.smt	10-50ppm Std4	8	1	1	1	100	3	1

See also:

Sample queue definition 237
Sample queue editor 245

7.4.2 Sample queue editor menu

File

Save 247
Save & exit 247
Exit... 247

Edit

Undo 248
Redo 248
Cut 249
Copy 249
Paste 249
Delete 250
Duplicate 250

7.4.2.1 Save

(File / Save menu item)

Save the changes made in **sample queue editor** to the file. Operator can continue editing.

See also:

Sample queue definition 237
Sample queue editor 245
Sample queue editor menu 246

7.4.2.2 Save & exit

(File / Save & exit menu item)

Save all changes to the file and close the **sample queue editor**.

All changes are applied to the sample queue control 238 window. The operator can run **sample queue**.

See also:

Sample queue definition 237
Sample queue editor 245
Sample queue editor menu 246
Sample queue control 238

7.4.2.3 Exit

(File / Exit menu item)

Close the **sample queue editor** without saving changes to file.

See also:

Sample queue definition 237
Sample queue editor 245
Sample queue editor menu 246

7.4.2.4 Undo

(Edit / Undo menu item)

Undo the last operation made in the sample queue editor.

Operator can use **Undo** repeatedly.

Undo affects all modifications done in the sample table 255, options panel 257 and all modifications done using editing commands of the **menu** 246 **and toolbar** 254.

Restriction of the **Undo** operation:

Operator can specify analysis reports 258, calibration reports 263, summary reports 260 and vial summary report 259 in the options panel 257.

These options needs **report templates** to be specified. **Report templates** can be modified using special external editor for **report templates**.

Modifications in the **report templates** cannot be undone using the **Undo** command of the **sample queue editor** 245.

See also:

Redo 248
Sample queue definition 237
Sample queue editor 245
Sample queue editor menu 246

7.4.2.5 Redo

(Edit / Redo menu item)

Redo the operation which was undone by the Undo 248 command.

Operator can use **Redo** repeatedly until all modifications are restored.

See also:

Undo 248
Sample queue definition 237
Sample queue editor 245
Sample queue editor menu 246

7.4.2.6 Cut

 **(Edit / Cut menu item)**

Cuts entire rows of the selected items 257 in the **sample table** 255.
The rows are placed into the internal buffer and removed from the **sample table** 255.

Paste 249 operation can put the rows from the internal buffer to another location in the **sample table** 255.

See also:

Sample queue definition 237
Sample queue editor 245
Sample queue editor menu 246

7.4.2.7 Copy

 **(Edit / Copy menu item)**

Copies entire rows of the selected items 257 in the **sample table** 255.
The copy of the rows is placed into the internal buffer.

Paste 249 operation can put the rows from the internal buffer to another location in the **sample table** 255.

See also:

Sample queue definition 237
Sample queue editor 245
Sample queue editor menu 246

7.4.2.8 Paste

 **(Edit / Paste menu item)**

Puts the rows from the internal buffer to the selected 257 location in the **sample table** 255.
The rows starting from selected 257 location and below are shifted down as needed to make space for inserted rows.

This command works in conjunction with Cut 249 and Copy 249 operations.

See also:

Sample queue definition 237

Sample queue editor 245
Sample queue editor menu 246

7.4.2.9 Delete

 **(Edit / Delete menu item)**

Deletes entire rows of the selected items 257 from the **sample table** 255.

See also:

Sample queue definition 237
Sample queue editor 245
Sample queue editor menu 246

7.4.2.10 Duplicate

 **(Edit / Duplicate menu item)**

Makes a copy of the entire rows of the selected items 257 in the **sample table** 255.

To use this function select 257 a range of sample items at one or more rows in the **sample table** 255.
Call the **Duplicate** command using **menu** 246 or **toolbar** 254.
The copy of the selected rows is placed below the selected range. The lower rows are shifted downward.

See also:

Sample queue definition 237
Sample queue editor 245
Sample queue editor menu 246

7.4.2.11 Increment

 **(Edit / Increment menu item)**

This function is designed to simplify creating sequential values for items in the **sample table** 255.
It can be applied to **Title**, **Vial**, **Level**, **Sample**, and **Description** items.

To use this function select 257 several items within one of the column from the above list. The top item must have a value which ends with one or more digits.
Call the **Increment** command using **menu** 246 or **toolbar** 254.
The value from the top item will be used to create sequential values for lower items.

For example, the first **Title** item has a name test01. Operator selects 257 6 items below starting from test01 and calls **Increment**. This produces sequential values:

Title
test01
test02
test03
test04
test05
test06

See also:

Sample queue definition 237
Sample queue editor 245
Sample queue editor menu 246

7.4.2.12 Propagate

 **(Edit / Propagate menu item)**

This function is designed to simplify copying values of items in the **sample table** 255.

To use this function select 257 a rectangular range of items within several rows and one or more columns.
Call the **Propagate** command using **menu** 246 or **toolbar** 254.
The value from the top selected row will be copied to all lower rows of the selection 257.

See also:

Sample queue definition 237
Sample queue editor 245
Sample queue editor menu 246

7.4.2.13 Reset

 **(Edit / Reset menu item)**

This command acts analogous to **reset sample queue** 242 command of the **sample queue control** 238 .

Sample queue editor 245 allows editing the sample queue which was partly executed.

The rows which refer to already executed samples are highlighted with **RED** color and cannot be changed.

Other rows can be edited and new rows can be inserted to the **sample queue** 237.

The command resets entire ***sample queue*** so that any rows could be edited. After resetting the execution of the **sample queue** 237 starts from the first

See also:

Sample queue definition 237
Sample queue editor 245
Sample queue editor menu 246

7.4.2.14 Change system

 **(Edit / Change system menu item)**

Changes the **System** item for all rows in the selection 257.

Displays the **Windows© system** standard **File open** window for selecting **system** 79 file to run an analysis.

Note, that it is possible to select a **system** 79 file from another directory. Still **system** 79 files used by **sample queue** must be located in the same directory where **sample queue file** (***.que**) is.

Operator must copy or move all **systems** 79 and **sample queue file** (***.que**) to the same directory to run a **sample queue**.

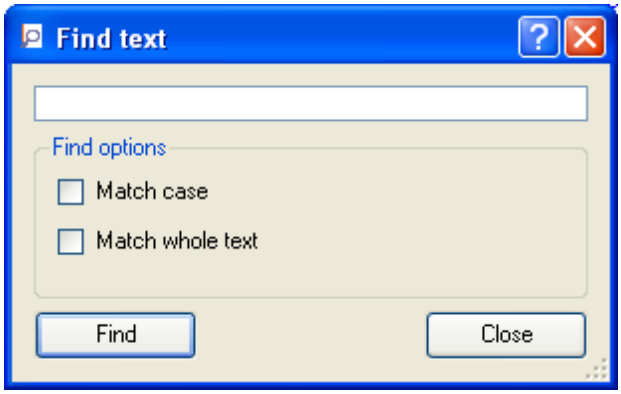
See also:

Sample queue definition 237
Sample queue editor 245
Sample queue editor menu 246

7.4.2.15 Find...

 **(Edit / Find... menu item)**

Displays ***Find Text*** window.



Find a row and item in the sample table 255 containing the specified text.
The search starts from the selected row till the last row in the sample table 255.

See also:

Sample queue definition 237
Sample queue editor 245
Sample queue editor menu 246

7.4.2.16 On-line help...

(Help / On-line help... menu item)

Displays sample queue editor 245 on-line help page.

See also:

Sample queue definition 237
Sample queue editor 245
Sample queue editor menu 246

7.4.2.17 About...

(Help / About... menu item)

Displays the short description of the sample queue editor 245 tool.

See also:

Sample queue definition 237
Sample queue editor 245
Sample queue editor menu 246

7.4.3 Sample queue editor: Toolbar

 **Save** 247

 **Save & exit** 247

 **Undo** 248

 **Redo** 248

 **Cut** 249

 **Copy** 249

 **Paste** 249

 **Delete** 250

 **Duplicate** 250

 **Increment** 250

 **Propagate** 251

 **Reset** 251

 **Change system** 252

 **Move up** 254

 **Move down** 254

 **Find...** 252

 Toggles **options panel** 257 on and off

7.4.3.1 Move up, Move down

 **Move up**

 **Move down**

Move the selected 257 row or rows up or down

These commands give the operator a simple and quick way to change the order of execution of sample items in the sample table 255.

There are some restrictions applied to the sample reordering:

- the order of the already finished or started samples can not be changed
- samples item can not be moved to or moved from the **sample group** 262 (see summary report option 260)

See also:

Sample queue definition 237
Sample queue editor 245
Sample queue editor menu 246

7.4.4 Sample table

Sample queue table defines **systems** 79 which must be used to run an analysis and parameters of the **samples**. This is a most important part of the **sample queue** configuration.

Each row of the **sample queue table** refers to individual analysis. Calibration and analyte runs can be configured.

The parameters for the analysis are arranged within the following columns:

No	Sequence number of the analysis in the **sample queue**.
System	**System** 79 file to be used to acquire and process data.
Title	User defined **title** 126 for chromatogram. This value will be placed into appropriate field in the **General page** 124 of the resulting chromatogram.
Vial	Autosampler **vial position** to take sample from. Typically this is a numeric value. Still some autosamplers may require a vial position in a special string form. Refer to documentation of the auto-sampler which you use. If your **system** 79 do not use set this item to any numeric value. This value will be placed into appropriate field in the **Sample page** 126 of the resulting chromatogram.
Volume	**Injected volume** of sample, in micro liters. This value will be placed into appropriate field in the **Sample page** 126 of the resulting chromatogram.
Dilution	**Dilution** of sample. This value will be placed into appropriate field in the **Sample page** 126 of the resulting chromatogram.
Multiplier	**Multiplier** of sample. This value will be placed into appropriate field in the **Sample page** 126 of the resulting chromatogram.

Note. **Volume, Dilution and Multiplier ,** are interrelated items. They are used to calculate **component *quantity*** (e.g. **component *weight***) for both calibration run and analyte. See **adjusted volume** 199 and **quantity** 200 for details.

Note. The detector response (peak area or height) is related directly to **component *quantity*** value**,** not **component** concentration**.** So **component *quantity*** is actually used to build **calibration curve** 182. For analyte a **component *quantity*** is calculated from calibration curve. See **quantification** 201 for details.

Note. Set **Dilution and Multiplier** values to 1.0 if these parameters are not used in your analysis.

Concentration of internal standard — Concentration of the **standard component** for quantification using **relative concentration** 202 method.

This value will be placed into appropriate field in the **Sample page** 126 of the resulting chromatogram. Set this value to **100.0** if you do not use **quantification** 201 with **relative concentration** 202 .

Level — **Calibration level** 199 for sample which is used for **calibration** 165. Level **0** defines analyte runs (no calibration), levels **1** and greater define **calibration runs**. When calibration run is finished software automatically updates the specified **calibration level** 199 and updates **calibration curve** 182 in the **method** 122. The updated **calibration** 165 will be used in the subsequent runs of appropriate **method** 122. **Components table** 171 and **concentrations table** 174 must be preliminary configured in the **method** 122 to enable calibration from **sample queue**.

Injections — Number of injections for the same vial position. Topically this value set to **1**. Operator can set another value to perform several injections of the same **sample**. Each injection can be processed separately as individual run with its own report. Also a **vial summary report** 259 can be configured.

Done — Indication of the fact that the sample run has been started:

0 sample run not yet started

1 … Injections Number of runs which were started

Sample — User-defined sample name or basic sample description.

This value will be placed into appropriate field in the **Sample page** 126 of the resulting chromatogram.

Description — Additional sample description.

This value will be placed into appropriate field in the **Sample page** 126 of the resulting chromatogram.

Items in the **sample table** are edited in-place. Also operator can use **editor functions** available through **menu** 246 and **toolbar** 254.

Additional options can be defined for each sample through **options panel** 257.

When sample is started the **Done** item is updated, related row in the **sample table** is marked with **RED** color and its items cannot be edited any more until **resetting** 251 the **sample queue**.

See also:

Sample queue editor 245

How to edit the sample queue table 481

7.4.4.1 Selecting sample queue items

Some operations need one or several sample queue items to be selected in the **sample table** 255.

To select a single item just click it with a **left mouse button.**

To select several items within rectangular range click and hold the **left mouse button** at the left-top item, drag the mouse cursor to the right-bottom item and release the **left mouse button.**

Alternatively click the **left mouse button** at the left-top item, press and hold **SHIFT** keyboard button and click the right-bottom item.

To select an entire column click the column header.

To select an entire row click the sequence number item of the string.

The following operations work with selections in the **sample table** 255:

- Cut 249
- Copy 249
- Paste 249
- Delete 250
- Duplicate 250
- Increment 250
- Propagate 251
- Change system 252
- Specifying summary reports 260

See also:

Sample table 255

Sample queue editor 245

7.4.5 Options panel

Besides general items available through sample table 255 additional options can be defined for each ***sample.***

Options are configured through **options panel.**

 button at the toolbar 254 toggles **options panel** on and off.

Options panel consists of two parts. The upper **"Sample options and operations"** is a list of available options. The lower contains configurations for each option.

The following options are available in the **"Sample options and operations"** list:

Analysis report 258
Vial summary report 259
Summary report 260
Calibration report 263
User message before analysis 264
User message after analysis 265
Clear calibration 266
Shutdown system 267
Pause queue 267
Extra 268 (user-defined sample parameters)

See description of the particular option from the list above to know how to configure it.

See also:

Sample queue editor 245
Sample table 255

7.4.5.1 Analysis report

Analysis report option is available in the **"Sample options and operations"** list of the **options panel** 257.

This option configures **advanced report** 341 for individual analysis.

Option configuration:

Select **Analysis report** option in the **"Sample options and operations"** list by clicking it's text, not the check mark ☑.

This displays a **"Analysis report: list of templates"** at the lower part of the **options panel** 257 where **report templates** can be configured.

Samples in the **sample table** 255 can be linked to one or several **report templates**. Each **report template** is available for any sample.

<Add...>	Add a new **advanced report** 341. **Report editor** 343 is used for configuring new report. **Report editor** 343 allows importing the desired **report template** from the previously created file.
<Edit...>	Edit selected **advanced report** 341 **template** with **report editor** 343.
<Delete>	Delete the selected **advanced report** 341 **template** from the list.

To configure **analysis report** for the sample do the following actions:

- Make a **selection** 257 which includes one or more samples (rows in the **sample table** 255). It doesn't matter what items are actually selected. The configuration is applied to all selected samples.

- Put a check mark ☑ near **Analysis report** item in the **"Sample options and operations"** list. "**Analysis report: list of templates"** appears in the lower part of the **options panel** 257
- If the required **report template** is already in the **"Analysis report: list of templates"** put a check mark ☑ near it. Operator can select several reports from the list. In this case all selected reports will be generated when analysis finished.
- If the required **report template** is not in the **"Analysis report: list of templates"** click ***<Add...>*** button to add a new **advanced report** 341 template. Use **report editor** 343 to configure **report template** (or import **report template** from previously created file). Exit **report editor** 343 when finished. Put a check mark ☑ near the newly created **report template** in the "**Analysis report: list of templates"**.
- Repeat previous action if you need more reports to be generated.

If multiple injections are defined in the **Injections** item of the **sample table** 255, the report is generated for each injection.

To remove this option for the sample do the following actions:

- Make a **selection** 257 which includes one ore more samples (rows in the **sample table** 255). It doesn't matter what items are actually selected. The configuration is applied to all selected samples.
- Clear a check mark ☑ near **Analysis report** item in the **"Sample options and operations"** list.

See also:

Options panel 257
Sample queue editor 245

7.4.5.2 Vial summary report

Vial summary report option is available in the **"Sample options and operations"** list of the **options panel** 257.

This option configures **advanced summary report** 366 for all injections produced by the sample. This option is used when **Injections** parameter for the sample in the **sample table** 255 is **2** or greater.

Vial summary report allows to get more precise measurements by averaging results from several independent runs of the same sample.

Option configuration:

Select **Vial summary report** option in the **"Sample options and operations"** list by clicking it's text, not the check mark ☑.

This displays a **"Vial summary report: list of templates"** at the lower part of the **options panel** 257 where **report templates** can be configured.

Samples in the **sample table** 255 can be linked to one or several **report templates**. Each **report template** is available for any sample.

<Add...>	Add a new **advanced summary report** 366. **Summary report editor** 367 is used for configuring new report. **Summary report editor** 367 allows importing the desired **report template** from the previously created file.
<Edit...>	Edit selected **advanced summary report** 366 **template** with **summary report editor** 367.
<Delete>	Delete the selected **advanced summary report** 366 **template** from the list.

To configure **vial summary report** for the sample do the following actions:

- Make a **selection** 257 which includes one or more samples (rows in the **sample table** 255). It doesn't matter what items are actually selected. The configuration is applied to all selected samples.
- Put a check mark ☑ near **Vial summary report** item in the **"Sample options and operations"** list. "**Vial summary report: list of templates"** appears in the lower part of the **options panel** 257.
- If the required **report template** is already in the **"Vial summary report: list of templates"** put a check mark ☑ near it. Operator can select several reports from the list. In this case all selected reports will be generated when analysis finished.
- If the required **report template** is not in the **"Vial summary report: list of templates"** click *<Add...>* button to add a new **advanced summary report** 366 template. Use **summary report editor** 367 to configure **report template** (or import **report template** from previously created file). Exit **summary report editor** 367 when finished. Put a check mark ☑ near the newly created **report template** in the "**Vial summary report: list of templates"**.
- Repeat previous action if you need more reports to be generated.

To remove this option for the sample do the following actions:

- Make a **selection** 257 which includes one ore more samples (rows in the **sample table** 255). It doesn't matter what items are actually selected. The configuration is applied to all selected samples.
- Clear a check mark ☑ near **Vial summary report** item in the **"Sample options and operations"** list.

See also:

Options panel 257
Sample queue editor 245

7.4.5.3 Summary report

Summary report option is available in the **"Sample options and operations"** list of the **options panel** 257.

This option configures **advanced summary report** 366 for a **group of samples** 262 in the **sample table** 255.

Summary reports allows combining results from multiple analysis in the single report and perform statistical computations.

Option configuration:

Select **Vial summary report** option in the **"Sample options and operations"** list by clicking it's text, not the check mark ☑.

The lower part of the **options panel** 257 will display **"Group"** and **"Summary report: list of templates"** configuration items.

"Group" item is used to configure a **group** of samples for the **summary report**.

Start	Indicates the **group** start sample, that is the sample from the **sample table** 255 which defines the start of the **group**.
End	Indicates the **group** end sample, that is the sample from the **sample table** 255 which defines the end of the **group**.
<Set from selected rows>	Sets or updates the **group** using the current **selection** 257 of the **sample table** 255.

See **group of samples** 262 for more details.

The **summary report** is generated when the last analysis of the **group** is finished.

"Summary report: list of templates" item is used to configure **report templates** for **summary reports**.

Samples in the **sample table** 255 can be linked to one or several **report templates** from the list. Each **report template** is available for any sample.

<Add...>	Add a new **advanced summary report** 366. **Summary report editor** 367 is used for configuring new report. **Summary report editor** 367 allows importing the desired **report template** from the previously created file.
<Edit...>	Edit selected **advanced summary report** 366 **template** with **summary report editor** 367.
<Delete>	Delete the selected **advanced summary report** 366 **template template** from the list.
☑ **Use first injection only**	Multiple injections can be defined using **Injections** item of the **sample table** 255. When checked the first injection only will be used to produce **advanced summary report** 366. Otherwise all injections will be used.

To configure **summary report** for the sample do the following actions:

- Make a **selection** 257 which includes one or more samples (rows in the **sample table** 255). It doesn't matter what items are actually selected. The configuration is applied to all selected samples.
- Put a check mark ☑ near **Summary report** item in the **"Sample options and operations"** list. Alternatively you can press ***<Set from selection>*** button from the **"Group"** item. This creates and highlights the **group of samples** 262 from the **selection** 257 of the **sample table** 255.
- If the required **report template** is already in the **"Summary report: list of templates"** put a check mark ☑ near it. Operator can select several reports from the list. In this case all selected reports will be generated when the last analysis of the **group** is finished.
- If the required **report template** is not in the **"Summary report: list of templates"** click ***<Add...>*** button to add a new **advanced summary report** 366 template. Use **summary report editor** 367 to configure **report template** (or import **report template** from previously created file). Exit **summary**

report editor 367 when finished. Put a check mark ☑ near the newly created **report template** in the **"Summary report: list of templates"**.

- Repeat previous action if you need more reports to be generated.

To remove this option for the samples do the following actions:

- Click any sample in the **group of samples** 262 in the **sample table** 255. It doesn't matter what items are actually selected.
- Clear a check mark ☑ near **Summary report** item in the **"Sample options and operations"** list.

This operation removes **group of samples** 262 from the **sample table** 255.

See also:

Options panel 257
Sample queue editor 245

7.4.5.3.1 Group of samples

Several subsequent samples in the **sample table** 255 can be combined into the **group**. One or more **groups** can be defined in the single **sample queue** 237.

The **group** is used for **summary report** 260 configuration.

To create and configure **group** select **Vial summary report** option in the **"Sample options and operations"** list by clicking it's text, not the check mark ☑.

"Group" item in the lower part of the **options panel** 257 is used to configure a **groups**.

	System	Title	Vial number	Volume	Dilution	Amount	Concentration of internal standard	Calibration level	Number of injections
1	MeOH.smt	BocPP(=)iLeuOBz 80%MeOH	1	1	1	5	0.5	0	1
2	PSK.smt	PSK	2	1	1	5	0.5	0	1
3	std.smt	0.2-1ppm Std1	3	1	1	1	100	1	1
4	std.smt	2-10ppm Std2					100	2	1
5	std.smt	20-100ppm Std3					100	4	1
6	std.smt	10-50ppm Std4	6	1	1	1	100	3	1
7	Semax.smt	Semax 0.1% 7.10.05	7	10	1	1	0.5	0	1
8	SemaxSUB.smt	Semax substrate	8	5	1	1	0.4	0	1
9									

Group of samples

To create a **group** for the sample do the following actions:

- Make a **selection** 257 which includes one or more samples (rows in the **sample table** 255). It doesn't

matter what items are actually selected.

- Press *<Set from selection>* button from the **"Group"** section. This creates and highlights the **group** from the **selection** 257 of the **sample table** 255. Putting a check mark ☑ near **Summary report** item in the **"Sample options and operations"** list performs the same action.

The **group** start (the first **sample** in the **group**) is marked with **CYAN** color and other samples in the **group** are marked with **LIGHT CYAN** color.

The created group can be modified.

To extend the group make a new **selection** 257 which includes samples you wish add to the **group**. The selection must overlap at least partly the group which you are modifying. Press *<Set from selection>* button from the **"Group"** section. This action places all selected samples into the **group**.

To shrink the group make a new **selection** 257 within the **group** including samples for new **group**. Press *<Set from selection>* button from the **"Group"** section. This action shrinks the **group** to the **selection** 257. Samples not in the **selection** 257 will be removed from the **group**.

To remove a **group** click any item of any **sample** within the **group**. Clear a check mark ☑ near **Summary report** item in the **"Sample options and operations"**. This operation removes **group of samples** 262 from the **sample table** 255.

See also:

Summary report 260

Options panel 257

Sample queue editor 245

7.4.5.4 Calibration report

Calibration report option is available in the **"Sample options and operations"** list of the **options panel** 257.

Calibration report is used when **calibration** 165 is performed or updated by the **sample queue** 237. See description of the **Level** item in the **sample table** 255.

Calibration report option is mostly equivalent to **analysis report** 258 option and is configured in the same way. **Advanced** 366 **report** 341 for this option is configured to report results of the calibration so that operator could easily control the correctness of the **calibration** 165. **Calibration report** should include **Calibration** 354 and **Calibration results** 357 chapters.

Typically **calibration report** is configured for the last **calibration sample** in the **sample table** 255. Still **calibration report** can be configured for any **sample**.

Option configuration:

Select **Calibration report** option in the **"Sample options and operations"** list by clicking it's text, not the check mark ☑.

This displays a **"Calibration report: list of templates"** at the lower part of the **options panel** 257 where **report templates** can be configured.

Samples in the **sample table** 255 can be linked to one or several **report templates**. Each **report template** is available for any **sample**.

<Add...>	Add a new **advanced report** 341. **Report editor** 343 is used for configuring new report. **Report editor** 343 allows importing the desired **report template** from the previously created file.
<Edit...>	Edit selected **advanced report** 341 **template** with **report editor** 343.
<Delete>	Delete the selected **advanced report** 341 **template** from the list.

To configure **calibration report** for the sample do the following actions:

- Make a **selection** 257 which includes one or more samples (rows in the **sample table** 255). It doesn't matter what items are actually selected. The configuration is applied to all selected samples.
- Put a check mark ☑ near **Calibration report** item in the **"Sample options and operations"** list. **"Calibration report: list of templates"** appears in the lower part of the **options panel** 257
- If the required **report template** is already in the **"Calibration report: list of templates"** put a check mark ☑ near it. Operator can select several reports from the list. In this case all selected reports will be generated when analysis finished.
- If the required **report template** is not in the **"Calibration report: list of templates"** click *<Add...>* button to add a new **advanced report** 341 template. Use **report editor** 343 to configure **report template** (or import **report template** from previously created file). Exit **report editor** 343 when finished. Put a check mark ☑ near the newly created **report template** in the **"Calibration report: list of templates"**.
- Repeat previous action if you need more reports to be generated.

To remove this option for the sample do the following actions:

- Make a **selection** 257 which includes one ore more samples (rows in the **sample table** 255). It doesn't matter what items are actually selected. The configuration is applied to all selected samples.
- Clear a check mark ☑ near **Analysis report** item in the **"Sample options and operations"** list.

See also:

Options panel 257
Sample queue editor 245

7.4.5.5 User message before analysis

User message before analysis option is available in the **"Sample options and operations"** list of the **options panel** 257.

This option configures a text message which is shown to the operator **before** starting the analysis. The message is configured individually for each sample.

The message is displayed in the **sample queue execution log** 245 of the **sample queue control** 238 during **sample queue** execution.

Option configuration:

To add a **user message before analysis** for the sample or samples do the following actions:

- Make a **selection** 257 which includes one or more samples (rows in the **sample table** 255). It doesn't matter what items are actually selected. The configuration is applied to all selected samples.
- Select **User message before analysis** option in the **"Sample options and operations"**. **"User message before analysis"** text box appears at the lower part of the **options panel** 257.
- Type a text message in the **"User message before analysis"** text box. A check mark ☑ appears near **User message before analysis** item in the **"Sample options and operations"** list when the text box is not empty.

To remove a **user message before analysis** for the sample or samples do the following actions:

- Make a **selection** 257 which includes one or more samples (rows in the **sample table** 255). It doesn't matter what items are actually selected. The configuration is applied to all selected samples.
- Clear a check mark ☑ near **User message before analysis** item in the **"Sample options and operations"** list. This clears a message text from the **"User message before analysis"** text box.

See also:

Options panel 257
Sample queue editor 245

7.4.5.6 User message after analysis

User message after analysis option is available in the **"Sample options and operations"** list of the **options panel** 257.

This option configures a text message which is shown to the operator **after** the finish of the analysis and before starting the next analysis. The message is configured individually for each sample.

The message is displayed in the **sample queue execution log** 245 of the **sample queue control** 238 during **sample queue** execution.

Option configuration:

To add a **user message after analysis** for the sample or samples do the following actions:

- Make a **selection** 257 which includes one or more samples (rows in the **sample table** 255). It doesn't matter what items are actually selected. The configuration is applied to all selected samples.
- Select **User message after analysis** option in the **"Sample options and operations"**. **"User message after analysis"** text box appears at the lower part of the **options panel** 257.

- Type a text message in the **"User message after analysis"** text box. A check mark ☑ appears near **User message after analysis** item in the **"Sample options and operations"** list when the text box is not empty.

To remove a **user message after analysis** for the sample or samples do the following actions:

- Make a **selection** 257 which includes one or more samples (rows in the **sample table** 255). It doesn't matter what items are actually selected. The configuration is applied to all selected samples.
- Clear a check mark ☑ near **User message after analysis** item in the **"Sample options and operations"** list. This clears a message text from the **"User message before analysis"** text box.

See also:

Options panel 257
Sample queue editor 245

7.4.5.7 Clear calibration

Clear calibration option is available in the **"Sample options and operations"** list of the **options panel** 257.

This option instructs the **sample queue** 237 to clear **calibration** 165 in the **method** 122 used for the **sample.** **Sample queue** 237 clears the calibration when analysis starts.

The option is designed for **calibration samples** when **method** 122 **(re)calibration** 165 is performed from the **sample queue** 237.
Calibration sample is a sample where **Level** item is set to value other then **0** in the **sample table** 255.

Typically **calibration samples** update calibration data for its **level** only. This may lead to situation when outdated calibration data are mixed with updated calibration data. To avoid this situation use **Clear calibration** option for the first calibration sample in the **sample queue** 237.

Option configuration:

To set a **clear calibration** option for the sample do the following actions:

- **Select** 257 a sample in the **sample table** 255.
- Put a check mark ☑ near **Clear calibration** item in the **"Sample options and operations"** list.

To remove a **clear calibration** option for the sample do the following actions:

- **Select** 257 a sample in the **sample table** 255.
- Clear a check mark ☑ near **Clear calibration** item in the **"Sample options and operations"** list.

See also:

Options panel 257

Sample queue editor 245

7.4.5.8 Shutdown system

Shutdown system option is available in the **"Sample options and operations"** list of the **options panel** 257.

This option instructs the **sample queue** 237 to perform **shutdown hardware** 85 operation for the **system** 79 after finishing the analysis for which this option is configured**.**

Most commonly the **sample queue** uses the same **system** 79 for all **samples**. In this case **Shut down system at the end of the queue** option of the **sample queue control** 238 can be used.

When more then one **systems** 79 are used in the **sample queue** 237 the operator can configure **shutdown hardware** 85 operation for each **system** 79 individually.

Option configuration:

To set a **shutdown system** option for the sample do the following actions:

- **Select** 257 a sample in the **sample table** 255.
- Put a check mark ☑ near **Shutdown system** item in the **"Sample options and operations"** list.

To remove a **shutdown system** option for the sample do the following actions:

- **Select** 257 a sample in the **sample table** 255.
- Clear a check mark ☑ near **Shutdown system** item in the **"Sample options and operations"** list.

See also:

Options panel 257
Sample queue editor 245

7.4.5.9 Pause queue

Pause queue option is available in the **"Sample options and operations"** list of the **options panel** 257.

This option instructs the **sample queue** 237 to perform the **pause** 241 action during execution after finishing the analysis for which this option is configured**.**

This option can be combined with **user message after analysis** 265 option. In this case a message may contain a prompt for the operator to perform a specific actions (for example, perform instrument reconfiguration or maintenance operations.)

Option configuration:

To set a **pause queue** option for the sample do the following actions:

- **Select** 257 a sample in the **sample table** 255.
- Put a check mark ☑ near **Pause queue** item in the **"Sample options and operations"** list.

To remove a **pause queue** option for the sample do the following actions:

- **Select** 257 a sample in the **sample table** 255.
- Clear a check mark ☑ near **Pause queue** item in the **"Sample options and operations"** list.

See also:

Options panel 257
Sample queue editor 245

7.4.5.10 Extra

Extra option is available in the **"Sample options and operations"** list of the **options panel** 257.

This option configures the custom sample parameters. See description of **Method setup: "Extra" page** 128.

Option configuration:

Select **Analysis report** option in the **"Sample options and operations"** list by clicking it's text.
This displays a **"Custom sample parameters"** table at the lower part of the **options panel** 257.
Parameter, Description and **Value** items of the **"Custom sample parameters"** table have the same meaning as for **Method setup: "Extra" page** 128.

<Add parameter>	Add a new parameter to the **"Custom sample parameters"** table**.**
<Delete parameter>	Delete the selected item from the **"Custom sample parameters"** table**.**

Items in the **"Custom sample parameters"** table can be edited in-place.
Parameter and **Description** are the same for all **samples** in the **sample table** 255. The **Value** item can be set individually for each **sample**.

Empty **Value** item means that the value is not set for the **sample** and this parameter is not applied to the chromatogram for the **sample**.

To set or update a **Value** item for the sample do the following actions:

- Make a **selection** 257 which includes one or more samples (rows in the **sample table** 255). It doesn't matter what items are actually selected. The configuration is applied to all selected samples.
- Edit the **Value** item in the **"Custom sample parameters"** table as needed.

To remove a **Value** item for the sample do the following actions:

- Make a **selection** 257 which includes one or more samples (rows in the **sample table** 255). It doesn't matter what items are actually selected. The configuration is applied to all selected samples.
- Clear a **Value** item in the **"Custom sample parameters"** table as needed.

Note, the **method** 122 used for **sample** processing can also define **custom sample parameters** (using **Method setup: "Extra" page** 128). When analysis is executed the **custom sample parameters** from the **sample queue** 237 are merged with one defined in the **method** 122 and applied to the resulting **chromatogram**. The merged list of the **custom sample parameters** can be reviewed in the resulting **chromatogram** in the **Method setup: "Extra" page** 128.

The following rules are used for merging:

- If the **Value** item of the **parameter** in the **sample queue** 237 is empty for the **sample** then this **parameter** is ignored (it is not applied to the chromatogram).
- If the **Value** item of the **parameter** in the **sample queue** 237 is not empty and the same **Parameter** item (parameter label) exists in the **Method setup: "Extra" page** 128 then the content of the **Value** item for the **parameter** is copied from the **sample queue** 237. If **sample queue** 237 defines non-empty content of the **Description** item for the **parameter** then **Description** is also updated in the **chromatogram**.
- If the **Value** item of the **parameter** in the **sample queue** 237 is not empty and the **Parameter** item (parameter label) not exists in the **Method setup: "Extra" page** 128 then **parameter** (including **Parameter, Description** and **Value** items) is added to parameter list in the resulting **chromatogram**.
- If **Method setup: "Extra" page** 128 of the **method** 122 contains **Parameter** item which is not present in the **sample queue** 237 then this **parameter** is applied unchanged to the resulting **chromatogram**.

See also:

Method setup: "Extra" page 128

Options panel 257

Sample queue editor 245

Part VII

8 Batch reprocessing

8.1 Batch reprocessing definition

Batch reprocessing is a recalculation of previously recorded chromatograms.

Typically processing of analysis data is performed immediately when analysis finished. If **processing method** 122 is configured correctly there is no need for **reprocessing**.

Still it is quite usual that operator makes a number of analysis before noticing that some method settings are incorrect or not optimal.

Batch reprocessing is tool which allows operator to apply corrected settings to multiple **chromatograms.** Operator can perform repeated calibration by including calibration chromatograms to the **batch**.

To run a **batch reprocessing** the operator should create a **batch reprocessing file** (***.bar**) which lists chromatograms for reprocessing.

All chromatograms for **batch reprocessing** and **batch reprocessing file** (***.bar**) must be located in the same directory.

The chromatograms for the **batch reprocessing** must be of the same analysis type (that is refer to the same **processing method** 122).

If operator combines chromatograms which were processed by different **methods** 122 then the method settings from the **example chromatogram** 273 are applied to all other chromatogram.

See **creating a new batch reprocessing** 271 article for details how to create a **batch reprocessing file**.

"Reprocess" window form 273 is used for configuring options for **batch reprocessing**.

See also:

Creating a new batch reprocessing 271

"Reprocess" window form 273

How to perform batch reprocessing 482

Sample queue 237

8.2 Creating a new batch reprocessing

Before creating a batch reprocessing operator should choose an **example chromatogram** 273 and use

it for configuring **processing method** 122.

Parameters of the **method** 122 are configured in a regular way, as for any other method or chromatogram. Operator should open a **chromatogram file** (***.chw**) of **example** 273 and apply all necessary **method** 122 configurations to it.

The most important parameters for **batch reprocessing** 271 are:

- **Method setup** 124 (**Column** 130, **Eluent** 131, **Smoothing** 132, **Math** 138, **Noise** 142 pages)
- **Calculated channels** 152 (see **calculated channels page** 151)
- **Peak integration parameters** 159.
- All settings related to **calibration** 165.

When **method** 122 configuration is finished do not forget to save changes in the **example chromatogram** 273 file using **File / Save / Chromatogram** 210 command of the **main menu** 25.

After configuring and saving the **example chromatogram** 273 the **batch reprocessing** file can be created.

- Invoke **File / Open / Chromatogram...** 207 menu item of the **main menu** 25 to display an **Chromatogram open** window form.
- Navigate to the location of your chromatograms using **Directories** control. All chromatograms for the **batch reprocessing** must be located in the same directory, including an **example chromatogram** 273.
- Make a selection in the **File list** 209 area of the **Chromatogram open** 207 window form. The selection must include an **example chromatogram** 273 and all other **chromatograms** which you intend to reprocess. Multiple chromatograms are selected by using [Shift] and the left mouse button or by [Ctrl] and the left mouse button.
- Press **<To Batch...>** button. Type a file name for new **batch reprocessing** when prompted. The **batch reprocessing file** (***.bar**) will be placed into the same directory where chromatograms are located.
- **"Reprocess" window form** 273 is opened.
- Ensure that **example chromatogram** 273 is selected in the **Use method from file for reprocessing** item of **"Reprocess" window form** 273.
- Proceed with configuring options for **batch reprocessing**.

See also:

Batch reprocessing definition 271
Example chromatogram 273
"Reprocess" window form 273
"Chromatogram open" window form 207

8.2.1 Example chromatogram

An **example chromatogram** for **batch reprocessing** 271 is a chromatogram which is used as reference for all settings of **processing method** 122.

The settings of **processing method** 122 from example chromatogram are applied to other chromatograms during executing **batch reprocessing** operation.

An **example chromatogram** must be properly configured and saved to **chromatogram file** (***.chw**) before creating **batch reprocessing**. See **creating a new batch reprocessing** 271 for details.

Operator must select an **example chromatogram** 273 in the **Use method from file for reprocessing** item of **"Reprocess" window form** 273.

See also:

Batch reprocessing definition 271
Creating a new batch reprocessing 271

8.3 Open batch reprocessing file

(*Main menu* File / Open / Batch reprocessing...)

Load an existing batch reprocessing file (***.bar**) from the **Data** directory and open the **"Reprocess" window** 273.

(*Main menu* File / Open / Last batch...)
Load the last opened batch reprocessing file (***.bar**) from the **Data** directory and open the **"Reprocess" window** 273.

See also:

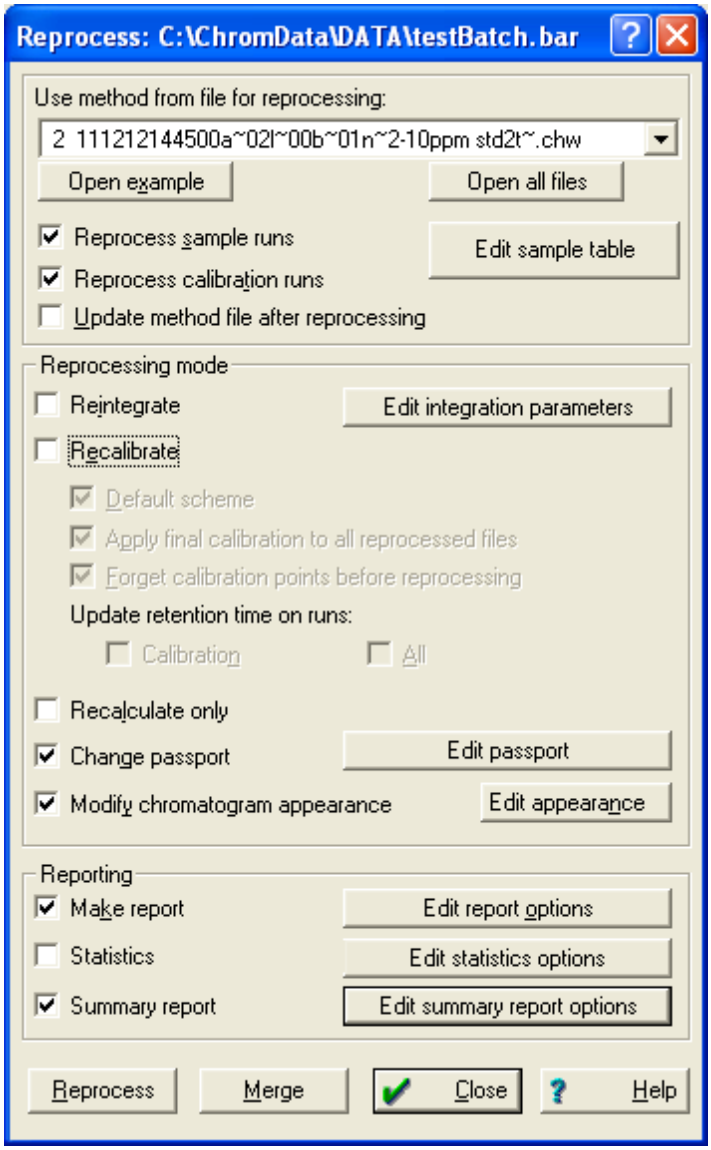
Creating a new batch reprocessing 271

Save batch reprocessing file 279

8.4 Reprocess options window

The **"Reprocess"** window form is used for setting the options for **batch reprocessing** and performing the **batch operations**.

The name of **batch reprocessing file** (***.bar**) is displayed in the window title.



All options are grouped in three areas:

General settings

Reprocessing mode

Reporting

General settings

Use method from file for reprocessing

Select the desired chromatogram file from the list which will be used as **example chromatogram** 273. Read **creating a new batch reprocessing** 271 article for details.

<Open example> Open the **example chromatogram** 273 selected above for reviewing.

<Open all files> Open all chromatograms of the **batch reprocessing** for reviewing.

<Edit sample table> Open the **batch reprocessing table editor** 278 program to edit a list of chromatograms and sample parameters.

☑ **Reprocess sample runs**
Reprocess all **analyte sample** chromatograms (**calibration level = 0**).

☑ **Reprocess calibration runs**
Reprocess all **calibration** chromatograms (**calibration level > 0**).

☑ **Update method file after reprocessing**
The method file (***.mtw**) of the **example chromatogram** 273 will be updated after reprocessing. Use this option to apply final **calibration** calculated in the **batch** for subsequent runs of the **method** 122.

Reprocessing mode

☑ **Reintegrate** Reintegrate chromatograms according to the settings of the **Integration setup** 160 and **Integration events** 162 parameters.

<Edit integration parameters> Open the **Integration parameters** 159 window for reviewing integration parameters. The settings are taken from **example chromatogram** 273. Operator can modify settings if necessary.

☑ **Recalibrate** Reprocess all calibration chromatograms, recalculate and update **calibration** 165. During **batch reprocessing** each calibration chromatogram updates its own **calibration level** 199 (defined in the **batch reprocessing table** 284). The new **calibration** 165 will be applied to all sample chromatograms. The **calibration** 165 settings are taken from **example chromatogram** 273. **Example chromatogram** 273 must contain a properly configured **components table** 171, define concentrations of standards in **concentrations table** 174 and define all calibration parameters in the **peak identification** 166 and **calibration graphs** 178.
This option also recalculates **calculated channels** 152 using settings from **example chromatogram** 273.

☑ **Default scheme** Default setting for recalibration reprocessing.
The two options ☑ **Apply final calibration to all reprocessed files** and ☑ **Forget calibration points before reprocessing** are switched on. A new calibration is performed with the calibration runs included into the **batch** and the resulting **calibration curve** 182 is applied to all runs.

☑ **Apply final calibration to all reprocessed files**
This option defines **two-pass batch reprocessing**. At first path calibration chromatograms are proceeded only to build **calibration curve** 182. At the second path a final calibration is applied to all chromatograms (analyte and calibration) and is used to calculate unknown concentrations. If this option is not set the calibration and analyte chromatograms are processed in the **single pass** in order defined by the **batch reprocessing table** 284.

☑ **Forget calibration points before reprocessing**

Clears calibration data for all **calibration levels** 199 before performing **batch reprocessing**. This option ensures that the calibration chromatograms from the current **batch** are only used to build **calibration curve** 182. Otherwise calibration levels from **example chromatogram** 273 not updated by the **batch** will be preserved and used for building **calibration curve** 182. This option has no effect if all calibration chromatograms are included into the **batch**.

Update retention time on runs

☑ **Calibration** — Calibration runs will update retention time for all components when reprocessed.

☑ All — Any runs (calibration and analyte) will update retention time for all recognized components when chromatogram is finished. Use this option with caution.

☑ **Recalculate only** — Performs **quantification** 201 of chromatograms with values for "**Volume**", "**Dilution**", "**Multiplier**" and "**Concentration of internal standard**" entered in the **batch reprocessing table** 284. This option also recalculates **calculated channels** 152 using settings from **example chromatogram** 273.

Note: The recalculation is done automatically if the **Reintegrate** and/or **Recalculate** options are enabled. If the **Recalculate only** option is enabled, the **Reintegrate** and **Recalculate** options are disabled automatically.

☑ **Change passport** — If this option is enabled, the settings of **Column** 130, **Eluent** 131, **Smoothing** 132, **Math** 138, **Noise** 142 pages of **Method setup** 124 from the **example chromatogram** 273 will be applied to all chromatograms in the **batch**.

<Edit passport> — Open the **Passport** window where settings of **Column** 130, **Eluent** 131, **Smoothing** 132, **Math** 138, **Noise** 142 pages of **Method setup** 124 can be reviewed and modified if necessary.

☑ **Modify chromatogram appearance** — If this option is enabled, the **appearance settings** 216 from the **example chromatogram** 273 will be applied to all chromatograms in the **batch**.

<Edit appearance> — Open the **Appearance** 216 window form where settings from the **example chromatogram** 273 can be reviewed and modified if necessary.

Reporting

☑ **Make report** — Generate **plain report** 320 for all chromatograms using settings as defined in the **example chromatogram** 273.

<Edit report options> — Open the **Report options** 322 window form where settings for **plain report** 320 can be reviewed and modified if necessary.

☑ **Statistics** — Generate **plain statistics report** 360 based on all reprocessed

chromatograms after **reprocessing**.

<Edit statistics options> Open the **Statistic options** 361 window form where settings for **plain statistics report** 360 can be defined.

☑ **Summary report** Generate **advanced summary report** 366 based on all reprocessed chromatograms after **reprocessing**.

<Edit summary report options> Open the **Summary report editor** 367 window form where settings for **advanced summary report** 366 can be defined.

<Reprocess> Press this button to start **reprocessing procedure** according to parameters set in the window.

<Merge> Perform **merge chromatograms** 277 operation. No reprocessing is performed. This function needs only a list of chromatograms defined in the **batch reprocessing file** (***.bar**). Other settings are ignored.

See also:

Batch reprocessing 271

Creating a new batch reprocessing 271

Batch reprocessing table editor 278

8.4.1 Merge chromatograms

Reprocess 273 **/ <Merge> button**

Merge chromatograms operation combines **channels** 113 from all chromatograms of the **batch reprocessing file** (***.bar**) into single **multi-channel chromatogram**.

This feature allows operator to visually compare measurements obtained by several analyses. Typically no further processing of the resulting **multi-channel chromatogram** is performed.

If **merge** operation is used to combine several **multi-channel chromatogram** then the **reference channel** 197 of each chromatogram is used for the resulting chromatogram.

The **channels** 113 from the source chromatograms are displayed in the same order as in the **batch reprocessing table** 284 slightly displaced one upon the other. The distance between the curves can be increased by pressing [Shift] + [Up] and decreased by pressing [Shift] + [Down]. See keyboard and mouse functions 214 for other capabilities.

The chromatogram axes, labels and colors can be set in the **Appearance** 216 window.

The multi-channel chromatogram can be saved with **File / Save chromatogram** 210.

See also:

How to merge chromatograms 477

8.5 Batch reprocessing table editor

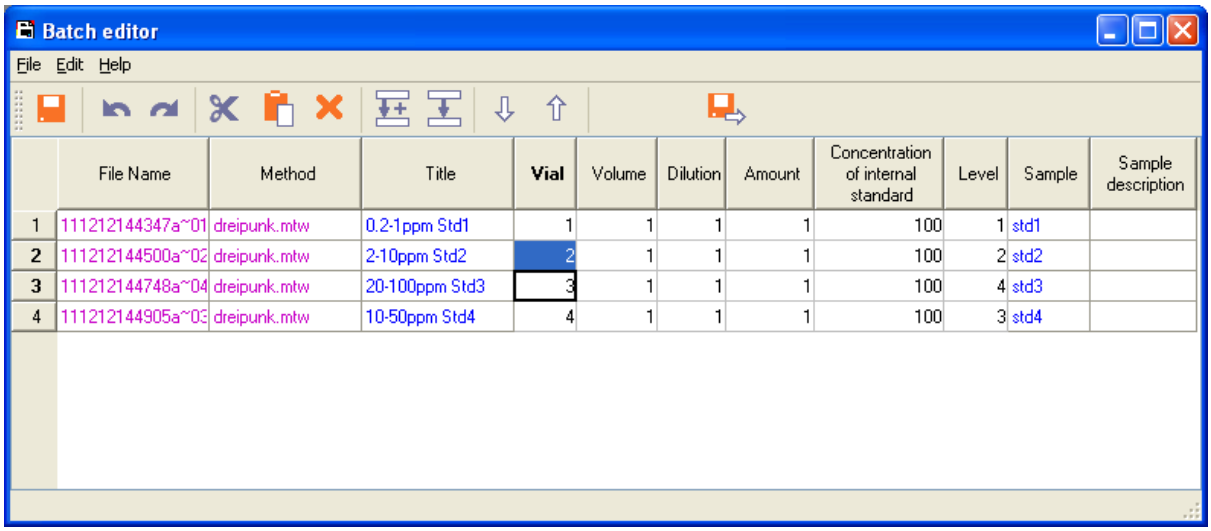
Batch editor is tool which allows operator to review a list of **chromatograms** for **batch reprocessing** 271 and edit **sample parameters** for each **chromatogram** if needed.

Sample parameters are applied to the corresponded chromatograms during execution of the **batch reprocessing** 271 and are used for **quantification** 201 and for report output.

Batch editor is opened from **"Batch reprocess" window** 273 by clicking ***<Edit sample table>*** button.

In the current implementation there are no possibility to add a chromatogram file to the existing **batch reprocessing table** 284. If you need to add a chromatogram file to the list just **create a new batch reprocessing file** 271. This is done from **chromatogram open** 207 window form by using **<To Batch...>** button.

Chromatograms can be excluded from the list using **delete** 281 function.



Batch reprocessing includes:

Batch editor menu 279

Batch editor toolbar 283

Batch reprocessing table 284

See also:

Creating a new batch reprocessing 271

Open batch reprocessing file 273

8.5.1 Batch editor menu

File

- Save 279
- Save as... 279
- Save & exit 280
- Exit... 280

Edit

- Undo 280
- Redo 280
- Cut 281
- Paste 281
- Delete 281
- Increment 282
- Propagate 282

Help

- On-line help... 283
- About... 283

8.5.1.1 Save

(File / Save menu item)

Save the changes made in **batch reprocessing editor** to the file. Operator can continue editing.

See also:

Batch reprocessing definition 271
Batch reprocessing table editor 278

8.5.1.2 Save as...

(File / Save as... menu item)

Save the changes made in **batch reprocessing editor** to the file with a different name. Operator can continue editing.

Note, that it is possible to save the **batch table** to the file in another directory. Still chromatogram 207 files listed in the batch table 284 must be located in the directory where **batch reprocessing file** (***.bar**) is.

See also:

Batch reprocessing definition 271
Batch reprocessing table editor 278

8.5.1.3 Save & exit

 **(File / Save & exit menu item)**

Save all changes to the file and close the **batch reprocessing editor** program.

See also:

Batch reprocessing definition 271
Batch reprocessing table editor 278

8.5.1.4 Exit...

(File / Exit... menu item)

Close the **batch reprocessing editor** program without saving changes to file.

See also:

Batch reprocessing definition 271
Batch reprocessing table editor 278

8.5.1.5 Undo

 **(Edit / Undo menu item)**

Undo the last operation made in the **batch reprocessing editor**.
Operator can use **Undo** repeatedly.

Undo affects all modifications done in the batch reprocessing table 284 and all modifications done using editing commands of the menu 279 and toolbar 283.

See also:

Redo 280
Batch reprocessing definition 271
Batch reprocessing table editor 278

8.5.1.6 Redo

 **(Edit / Redo menu item)**

Redo the operation which was undone by the Undo 280 command.
Operator can use **Redo** repeatedly until all modifications are restored.

See also:

Undo 280
Batch reprocessing definition 271

Batch reprocessing table editor 278

8.5.1.7 Cut

 **(Edit / Cut menu item)**

Cuts entire rows of the selected items 286 in the **batch reprocessing table** 284.
The rows are placed into the internal buffer and removed from the **batch reprocessing table** 284.

Paste 281 operation can put the rows from the internal buffer to another location in the **batch reprocessing table** 284.

See also:

Batch reprocessing definition 271
Batch reprocessing table editor 278

8.5.1.8 Paste

(Edit / Paste menu item)

Puts the rows from the internal buffer to **selected** 286 location in the **batch reprocessing table** 284.
The rows starting from **selected** 286 location and below are shifted down as needed to make space for inserted rows.

This command works in conjunction with **Cut** 281 operation.

See also:

Batch reprocessing definition 271
Batch reprocessing table editor 278

8.5.1.9 Delete

 **(Edit / Delete menu item)**

Deletes entire rows of the **selected items** 286 from the **batch reprocessing table** 284.

See also:

Batch reprocessing definition 271
Batch reprocessing table editor 278

8.5.1.10 Increment

 **(Edit / Increment menu item)**

This function is designed to simplify creating sequential values for items in the **batch reprocessing table** 284.

It can be applied to **Title**, **Vial**, **Level**, **Sample**, and **Description** items.

To use this function **select** 286 several items within one of the column from the above list. The top item must have a value which ends with one or more digits.

Call the **Increment** command using **menu** 279 or **toolbar** 283.

The value form the top item will be used to create sequential values for lower items.

For example, the first **Title** item has a name test01. Operator **selects** 286 6 items below starting from test01 and calls **Increment**. This produces sequential values:

Title
test01
test02
test03
test04
test05
test06

See also:

Batch reprocessing definition 271
Batch reprocessing table editor 278

8.5.1.11 Propagate

 **(Edit / Propagate menu item)**

This function is designed to simplify copying values of items in the **batch reprocessing table** 284.

To use this function **select** 286 a rectangular range of items within several rows and one or more columns.

Call the **Propagate** command using **menu** 279 or **toolbar** 283.

The value from the top selected row will be copied to all lower rows of the **selection** 286.

See also:

Batch reprocessing definition 271
Batch reprocessing table editor 278

8.5.1.12 On-line help...

(**Help / On-line help...** menu item)

Displays batch reprocessing table editor 278 on-line help page.

See also:

Batch reprocessing definition 271
Batch reprocessing table editor 278

8.5.1.13 About...

(**Help / About...** menu item)

Displays the short description of the batch reprocessing table editor 278 tool.

See also:

Batch reprocessing definition 271
Batch reprocessing table editor 278

8.5.2 Batch editor: Toolbar

 Save 279

 Save & exit... 280

 Undo 280

 Redo 280

 Cut 281

 Paste 281

 Delete 281

 Increment 282

 Propagate 282

 Move up 284

 Move down 284

8.5.2.1 Move up, Move down

Move up

Move down

Move the selected 286 row or rows up or down

Theses commands give the operator a simple and quick way to change the order of execution of sample items in the **batch reprocessing table** 284.

See also:

Batch reprocessing definition 271
Batch reprocessing table editor 278
Batch editor menu 279

8.5.3 Batch reprocessing table

Batch reprocessing table contains a list of **chromatograms** for **batch reprocessing** 271 and defines **sample parameters** for each **chromatogram**.

	File Name	Method	Title	Vial	Volume	Dilution	Amount	Concentration of internal standard	Level	Sample	Sample description
1	111212144347a~01	dreipunk.mtw	0.2-1ppm Std1	1	1	1	1	100	1	std1	
2	111212144500a~02	dreipunk.mtw	2-10ppm Std2	2	1	1	1	100	2	std2	
3	111212144748a~04	dreipunk.mtw	20-100ppm Std3	3	1	1	1	100	4	std3	
4	111212144905a~03	dreipunk.mtw	10-50ppm Std4	4	1	1	1	100	3	std4	

The **batch reprocessing table** contains the following columns:

No — Row number.

File name — Name of the **chromatogram file *.chw**.
This item cannot be modified, it is intended for review only.

Method — Name of the **method** 122 **file *.mtw** used for recording the chromatogram.
This item cannot be modified, it is intended for review only.
Note that the name of the **method** 122 from the **example chromatogram** 273 will replace this value in the resulting chromatograms after reprocessing.

Title — User defined **title** 126 for chromatogram.
This value will replace an appropriate field in the **General page** 124 of the resulting chromatogram.

Vial — Autosampler **vial position**.
This value will replace an appropriate field in the **Sample page** 126 of the resulting chromatogram.

Volume — **Injected volume** of sample, in micro liters.

This value will replace an appropriate field in the **Sample page** 126 of the resulting chromatogram.

Dilution — **Dilution** of sample.

This value will replace an appropriate field in the **Sample page** 126 of the resulting chromatogram.

Multiplier — **Multiplier** of sample.

This value will replace an appropriate field in the **Sample page** 126 of the resulting chromatogram.

Note. **Volume, Dilution and Multiplier ,** are interrelated items. They are used to calculate **component *quantity*** (e.g. **component *weight***) for both calibration run and analyte. See **adjusted volume** 199 and **quantity** 200 for details.

Note. The detector response (peak area or height) is related directly to **component *quantity*** value**,** not **component** concentration**.** So **component *quantity*** is actually used to build **calibration curve** 182. For analyte a **component *quantity*** is calculated from calibration curve. See **quantification** 201 for details.

Note. Set **Dilution and Multiplier** values to 1.0 if these parameters are not used in your analysis.

Concentration of internal standard — Concentration of the **standard component** for quantification using **relative concentration** 202 method.

This value will replace an appropriate field in the **Sample page** 126 of the resulting chromatogram. Set this value to **100.0** if you do not use **quantification** 201 with **relative concentration** 202 .

Calibration level — **Calibration level** 199 for sample which is used for **calibration** 165. Level **0** defines analyte runs (no calibration), levels **1** and greater define **calibration runs**. During **reprocessing** software automatically updates the specified **calibration level** 199 and updates **calibration curve** 182. The updated **calibration** 165 will be used in the subsequent analyses in the **batch. Components table** 171 and **concentrations table** 174 must be properly configured in the **example chromatogram** 273 to enable calibration from **batch reprocessing**.

Sample — User-defined sample name or basic sample description.

This value will replace an appropriate field in the **Sample page** 126 of the resulting chromatogram.

Sample description — Additional sample description.

This value will replace an appropriate field in the **Sample page** 126 of the resulting chromatogram.

When **batch reprocessing file** (***.bar**) is **created** 271 the **sample parameters** and other items in the **batch reprocessing table** are filled with values stored in the corresponded chromatograms.

Items can be edited in-place and by using editing function of **menu** 279 and **toolbar** 283.

Updated values are applied to the corresponded chromatograms during execution of the **batch**

reprocessing 271 and are used for **quantification** 201 and for report output.

See also:

How to edit the batch reprocessing table 482

8.5.3.1 Selecting batch table items

Some operations need one or several batch table items to be selected in the **batch reprocessing table** 284.

To select a single item just click it with a **left mouse button.**

To select several items within rectangular range click and hold the **left mouse button** at the left-top item, drag the mouse cursor to the right-bottom item and release the **left mouse button.**

Alternatively click the **left mouse button** at the left-top item, press and hold **SHIFT** keyboard button and click the right-bottom item.

To select an entire column click the column header.

To select an entire row click the sequence number item of the string.

The following operations work with selections in the **batch reprocessing table** 284:

- Cut 281
- Paste 281
- Delete 281
- Increment 282
- Propagate 282

See also:

Batch reprocessing table 284

Batch reprocessing table editor 278

Part IX

User-defined formulas

9 User-defined formulas

9.1 About user-defined formulas

The most important part of data processing results is calculation of different metrics of peaks in the **chromatogram** 207.

Concentration of component in the peak, peak ***area*** and peak ***height*** are the most typical metrics of the peak.

Chrom&Spec software offers a wide predefined set of peak metrics which can be calculated and included into **reports** 318. To view a list of predefined peak metrics see the **custom peak table** 332 article.

Besides predefined peak metrics it is possible to create **user-defined formulas**. This is a powerful tool which allows to process very specific user tasks. Calculations done with **user-defined formulas** can be included into the **peaks table** in the **reports** 318 along with standard metrics.

User creates formulas with a special **macro-language** 291. Each formula defines a specific metric of the peaks.

In formula it is possible to refer to standard metrics of the peak (such as concentration or area), to standard metrics of other peaks or even to metrics of peaks in other chromatograms. Also it is possible to call special functions and perform various mathematical computations.

User creates **user-defined formulas** individually for particular **method** 122.

Also it is possible to configure **user-defined formulas** for **advanced summary reports** 366.

For **method** 122 **user-defined formulas** are configured from **Method setup: "Quantification" page** 144 by pressing ***<My formulas>*** button. Alternatively **user-defined formulas** can be reviewed and configured from ***Report options*** 322 window by pressing ***<Formulas...>*** button (see **peak table configuration** 327 for details). Those formulas are saved in the **method** 122 file and are applied to all chromatograms processed by the method.

For **advanced summary reports** 366 **user-defined formulas** are configured in **summary report configuration** 367 window and are applied to results produced by this **summary report** 366 only.

In both cases **Custom formulas** 289 window is used to configure **user-defined formulas**.

See also:

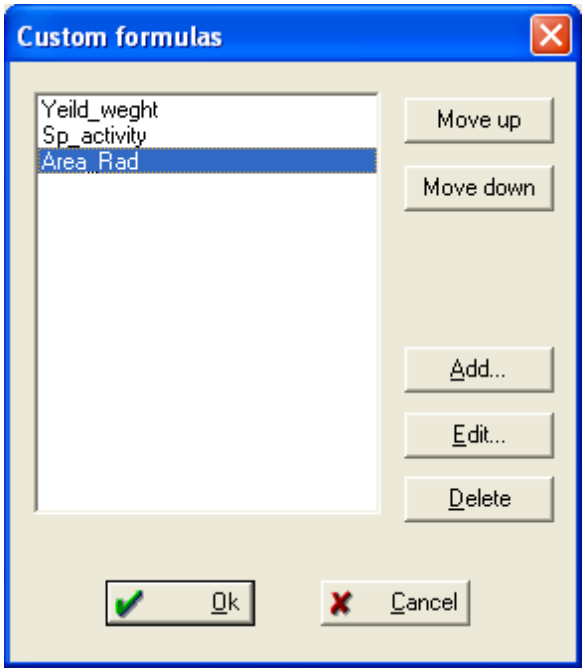
"Custom formulas" window 289

"Build new peak parameter" window 290

Macro language for user-defined formulas 291

9.2 "Custom formulas" window

Custom formulas window displays a list of user-defined formulas. User can add new formulas, edit, delete or sort item in the list.



<Move up>	Sorting: moves the formula up in the list.
<Move down>	Sorting: move the formula down in the list.
<Add>	Add new formula to the list. Opens **Build new peak parameter** 290 window to create a new formula.
<Edit>	Review and edit the selected formula. Opens **Build new peak parameter** 290 window to edit the selected formula.
<Delete>	Delete the selected formula from the list.

In the reports (see **peak table** 327 of **plain report** 320, for example) the formulas are calculated and printed in the order they appear in this list.

See also:

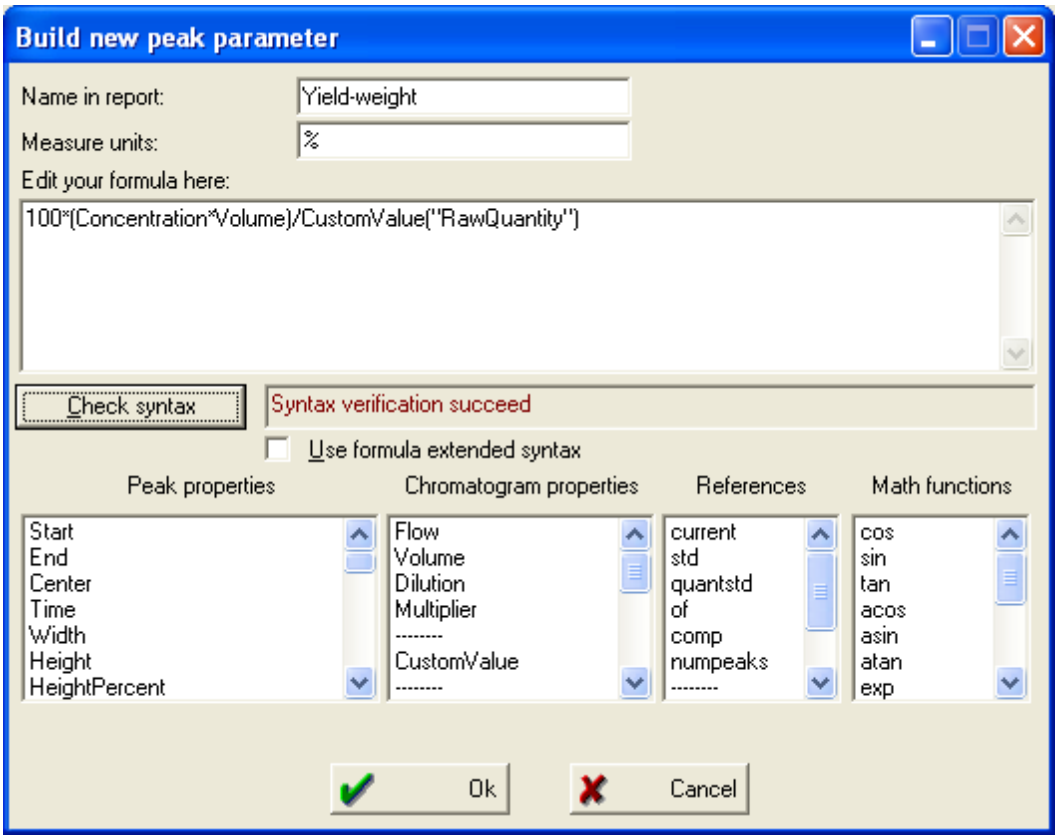
About user-defined formulas 288

"Build new peak parameter" window 290

Method setup: "Quantification" page 144

9.2.1 "Build new peak parameter" window

Custom formulas window allows to create and edit **user-defined formulas**.



Name in report: Name of the user-defined formula. Any ASCII symbols can be used including space, punctuation characters, numbers. etc. This name appears in the **Custom formulas** 289 window and can be printed in the **reports** 318.

Measure unit: User can specify optional **measure units** for return value of the formula. Units can be printed in the **reports** 318.

Edit your formula here: This text field is used to write expression of the formula. Formulas are described using a special **macro-language** 291.
Use ***<Check syntax>*** button to check syntax of the expression.

<Check syntax> This button verifies the correctness of the formula expression. "*Syntax verification succeeded*" or "*Syntax verification failed*" message is shown in the field on the right from the button.

Available **macro definitions** 294 are grouped in the lists:

- **Peak properties** 294
- **Chromatogram properties** 306
- **References** 310
- **Math functions** 314

These lists help user to edit formula.

Locate the required **macro definition** 294 in the lists and use **[Mouse Left Button Double Click]**. This inserts the **macro definition** 294 to the formula expression in the place where cursor is located. Any **macro definitions** 294 can also be typed from the keyboard.

☑ **Use formula extended syntax** — This option changes the way how **macro definition** 294 are inserted to the formula expression from the lists by **[Mouse Left Button Double Click]**. If checked **extended** syntax is used and **simple** syntax is used otherwise. For details see syntax description for each macro group.

See also:

About user-defined formulas 288

Custom formulas window 289

Macro language for user-defined formulas 291

Macro definitions 294

9.3 Macro language for user-defined formulas

The **macro-language** for **user-defined formulas** 288 defines **data types** 291 and **mathematical operators** 292 which allow to build ***mathematical expressions*** from a set of available **macro definitions** 294.

User-defined formulas 288 are evaluated for each peak in the chromatogram no matter whether the peak is recognized or not.

See also:

About user-defined formulas 288

"Build new peak parameter" window 290

9.3.1 Data types

The following data types are supported by ***Chrom&Spec*** software:

Data type	Description	Syntax	Examples
real	real numbers of double precision.	**<fractional-part><exponent-part>** **<fractional-part>:**	**14.25** **-40.53** **12.15e23**

		<sign><digit-sequence>.<digit-sequence> **<exponent-part>:** **e**<sign><digit-sequence> or **E**<sign><digit-sequence> <sign>: + or – If not specified, + assumed	**-0.123E-8** **123e5**
integer	integer numbers	<sign><digit-sequence> <sign>: + or – If not specified, + assumed	**123** **-14** **+150**
string	string expressions	"<letters-sequence>"	**"Component"** **"Chloride"**
boolean	boolean expressions	true or false	Typically *boolean* type is not used directly. Some expressions can be evaluated to *boolean* ***type*** in intermediate calculations.

The final result of each **user-defined formula** must be of *real* **data type**.

Other data types are used for intermediate computations or as input parameters for **macro definitions** 294.

See also:

Macro language for user-defined formulas 291

9.3.2 Mathematical operators

The macro-language supports the following mathematical operators, where ***M1***, ***M2*** and ***M3*** are any valid operands:

M1 - M2 subtraction
Example: End - Start

M1 + M2 addition
Example: (End + Start) / 2

M1 * M2 multiplication

Example: Concentration * Volume

M1 / M2 division
Example: Area / Time

M1 ? M2 : M3 conditional operator (similar to "C" conditional operator)
if ***M1*** evaluates to true then expression evaluates to ***M2***; if ***M1*** evaluates to false then expression evaluates to ***M3***
Example: (Area > Area[of("Fluoride")]) ***?*** Area / Area[of ("Fluoride")] ***:*** 0
If area of the current peak is higher than area of the peak, identified as "Fluoride", returns ratio of areas of current peak to "Fluoride", otherwise returns 0.

M1 > M2 logical greater than
Example: Area **>** Area[of("Fluoride")]

M1 >= M2 logical greater than or equal to
Example: Area **>=** Area[of("Fluoride")]

M1 < M2 logical less than
Example: Area **<** Area[of("Fluoride")]

M1 <= M2 logical less than or equal to
Example: Area **<=** Area[of("Fluoride")]

M1 == M2 logical equal to
Example: current **==** of("Fluoride")

M1 != M2 logical not equal to
Example: current ***!=*** of("Fluoride")

M1 || M2 logical OR
Example: (Area < Area[of("Fluoride")]) **||** (current == of ("Nitrit"))

M1 && M2 logical AND
Example: (Area > Area[of("Fluoride")]) ***&&*** (Area < 10*Area[of ("Fluoride"))

! M1 logical NOT
Example: ***!***((Area < Area[of("Fluoride")]) || (current == of("Nitrit")))

Precedence (order of evaluation) of operators.

!	logical NOT
** , /*	multiplicative
+, -	additive
<, >, <=, >=	relational
==, !=	equality

? :	conditional-expression

Operators in the table are listed in descending order of precedence
In complicated formulas braces should be used:
(End-Start) / Width.

See also:
Macro language for user-defined formulas 291

9.3.3 Macro definitions

Each **macro definition** can be treated as a function which returns value of type 291 *real* or *integer*.
Some **macro definitions** can have additional parameters.

All macro-definitions are grouped according to their functionality.

Peak properties 294	these macro-definitions return properties, corresponding to the chromatographic peak, described in the current peak table line (current peak).
Chromatogram properties 306	these macro-definitions return properties, corresponding to the whole chromatogram.
References 310	these macro-definitions allow access to an arbitrary peak or channel of the chromatogram.
Mathematical functions 314	these macro-definitions supply different mathematical functions and constants

Macro definitions can be used with **simple** or **extended** syntax. For details see description of the syntax for each macro group above.

See also:
Macro language for user-defined formulas 291

9.3.3.1 Peak properties

These macro-definitions return properties, corresponding to the chromatographic peak.
Macro-definitions of this type return ***real*** (floating-point, see data types 291) values.

See **syntax of peak properties** 295 article for syntax description.
See **list of peak properties** 296 for available **macro definitions** of **peak properties**.

See also:

References 310 (how to address **peak properties** of other peaks).
Macro definitions 294

9.3.3.1.1 Syntax of peak properties

The following syntax can be used for **peak properties** 294:

Simplified syntax:

PeakMacro

- for macro definitions without additional parameters

or

PeakMacro(param1, param2, ...)

- for macro definitions with additional parameters

-

When **simplified syntax** is used the returned value of macro-definition refers to the ***current peak***, that is the peak, for which **user-defined formula** 288 is evaluated.

Extended syntax:

It is possible to build a formula expression for a peak which refers to **peak property** 294 of another peak in the chromatogram. In this case the **extended syntax** must be used:

PeakMacro[npeak] or *PeakMacro[npeak](param1, param2, ...)*

- returns the value of **peak property** 294 which refers to peak with index *npeak* in the chromatogram.

or

PeakMacro[npeak1, npeak2] or *PeakMacro[peak1, peak2](param1, param2, ...)*

- returns the sum of values of **peak properties** 294 for several peaks in the chromatogram from *npeak1* to *npeak2*.

npeak, npeak1, npeak2 : *integer*

They must be a valid sequence numbers of peaks in the chromatogram. *1* defines the first peak and *numpeaks* (see **references** 310) defines the last peak in the chromatogram.

Peak references macro-definitions (see **references** 310) can be used as *npeak, npeak1, npeak2*. Also any valid mathematical expressions are allowed for peak references. For example:

Area[current+1]

returns area of the next peak

Summary extended syntax:

Summary extended syntax is used only in **peak table** 372 of **advanced summary reports** 366. It allows to build a formula expression for a peak which refers to **peak property** 294 of any peak in any chromatogram from summary list.

PeakMacro{"chromatogram title"}<Extended Section>

or

PeakMacro{"chromatogram title", nInjection}<Extended Section>

where

"chromatogram title" : *string*	is a text string specifying a **title of the chromatogram** 126.
nInjection : *integer*	is a sequence number of the injection for the current vial; Typically this value equals to *1*. Other values are possible when **Injections** item in **sample queue table** 255 specifies several injections for a vial.
<Extended Section>	is peak references and additional parameters as described for **extended syntax**. The *<Extended Section>* can be of the form: *[npeak]* *[npeak](param1, param2, ...)* *[npeak1, npeak2]* *[peak1, peak2](param1, param2, ...)* Note, that *current* is not allowed as **reference** 310 when *{.....}* section is specified. The *current* identifies the index of the currently reported peak in the current chromatogram. The *current* is undefined for any other chromatogram. Other references from **reference** 310 list are allowed.

The *{"chromatogram title", nInjection}* section can be omitted. In this case *PeakMacro* refers to the **peak property** 294 of the current chromatogram, that is the chromatogram of the peak for which the **user-defined formula** 288 is evaluated.

See also:

Peak properties 294

List of peak properties 296

9.3.3.1.2 List of peak properties

Here is a list of macro definitions related to **peak properties** 294.

All macro-definitions of this type return *real* (floating-point, see **data types** 291) values.

Macro definition	Description

Start	Returns formal **time of peak start**, in seconds. This is a time of ADC data point which was identified as ***start of the peak*** by **peak integration procedure** 159. **No parameters.**
End	Returns formal **time of peak end**, in seconds. This is a time of ADC data point which was identified as ***end of the peak*** by **peak integration procedure** 159. **No parameters.**
Center	Returns **approximate time of peak top** in seconds. This is a time of ADC data point which was identified as a ***top of the peak*** by **peak integration procedure** 159. See also *Time* macro. **No parameters.**
Time	Returns **retention time** 333 of the peak. See also *Center* and *TimeEx* macro. **No parameters.**
Width	Returns **width (h/2)** 334 metric of the peak. **No parameters.**
Height	Returns **height** 334 of the peak. **No parameters.**
HeightPercent	Returns **height %** 334 for the peak. **No parameters.**
Area	Returns **area** 334 of the peak. See also *AreaEx* macro. **No parameters.**
AreaPercent	Returns **area %** 334 for the peak. **No parameters.**
Capacity	Returns **capacity factor k** 335. **No parameters.**
Resolution(SecondPeak, Formula)	Returns *resolution for the peak pair*. This is similar to **resolution** 335 property in report output. **Parameters:** *SecondPeak* : *integer* The index of the second peak used to calculate the resolution with respect to the current peak. *current+1* is a default which indicates the next peak. See **references** 310 for other possibilities for peak references. *Formula* : *integer* **[-1, 0, 1, 2]** Number that defines formula for calculation of **resolution** 140

	-1: *Formula* is used as specified in the **method** 122 settings (see the **Math page** 138). This is a default value. **0**: ***(T(** SecondPeak **) - T(i)) / (W(** SecondPeak **) + W (i)) | 60.7%*** **1**: ***1.18 * (T(** SecondPeak **) - T(i)) / (W (SecondPeak) + W(i)) |50%*** **2**: ***2 * (T(** SecondPeak **) - T(i)) / (Wb(** SecondPeak **) + Wb(i))***
Efficiency(Formula)	Returns *efficiency (theoretical plates)* calculated for the peak. This is similar to **efficiency TP** 335 property in report output. See **efficiency** 139. **Parameters:** *Formula* : *integer* **[-1, 0, 1, 2]** Number that defines formula for calculation of **efficiency** 139 **-1**: *Formula* is used as specified in the **method** 122 settings (see the **Math page** 138). This is a default value. **0**: ***2 PI • [T(i) • H(i) / A(i)]^2*** **1**: ***5.54 • [T(i) / W(i)]^2*** **2**: ***16 • [T(i) / Wb(i)]^2***
Asymmetry(Formula)	Returns *asymmetry* of the peak. This is similar to **asymmetry** 336 property in report output. See **asymmetry** 140. **Parameters:** *Formula* : *integer* **[-1, 0, 1]** Number that defines formula for calculation of **asymmetry** 140. **-1**: *Formula* is used as specified in the **method** 122 settings (see the **Math page** 138). This is a default value. **0**: ***(Width after) / (Width before) | 10%*** **1**: ***(Full Width) / (2 * Width before) | 5%***
ResponseFactor	Returns **response factor** 336 of the ***component*** associated with the peak. Returns **0**, if peak has no component associated with it or when calculation is not possible. **No parameters.**
Concentration	Returns **concentration** 337 of the ***component*** associated with the peak. Returns **0**, if peak has no component associated with it or when calculation is not possible. **No parameters.**
ConcentrationPercent	Returns **concentration %** 337 of the ***component*** associated with the peak.

	Returns **0**, if peak has no component associated with it or when calculation is not possible. **No parameters.**
RelativeConcentration	Returns **relative concentration** 337 of the ***component*** associated with the peak. Returns **0**, if peak has no component associated with it or when calculation is not possible. **No parameters.**
RelativeConcentrationPercent	Returns **relative concentration %** 338 of the ***component*** associated with the peak. Returns **0**, if peak has no component associated with it or when calculation is not possible. **No parameters.**
Quantity	Returns **quantity** 338 of the ***component*** associated with the peak. Returns **0**, if peak has no component associated with it or when calculation is not possible. **No parameters.**
SignalToNoise	Returns **signal/noise** 336 ratio for the peak. **No parameters.**
Index(Type, Interpolation)	Returns *retention index* of the peak. This is similar to **index** 338 property in report output. See **retention index** 141. **Parameters:** *Type* : *integer* **[-1, 0, 1]** Number that defines the **index type** 141. **-1**: *Type* is used as specified in the **method** 122 settings (see the **Math page** 138). This is a default value. **0**: Internal index scale **1**: External index scale *Interpolation* : *integer* **[-1, 0, 1]** Number that defines the interpolation method 141. **-1** : *Interpolation* is used as specified in the **method** 122 settings (see the **Math page** 138). This is a default value. **0** : Linear index **1** : Logarithmic (or Kovatch') index
Section(HeightPercent)	Returns the duration from ***upslope*** to ***downslope*** of the peak, in ***seconds***. The duration is calculated at the height defined by *HeightPercent* parameter. **Parameters:**

	HeightPercent : *real* The percent of the ***peak height*** which defines the height from the ***baseline*** at which *Section* is calculated.
SectionLeft *(HeightPercent)*	Returns the duration from ***upslope*** of the peak to ***peak top***, in ***seconds***. The duration is calculated at the height defined by *HeightPercent* parameter. **Parameters:** *HeightPercent* : *real* The percent of the ***peak height*** which defines the height from the ***baseline*** at which *SectionLeft* is calculated.
SectionRight	Returns the duration from the ***peak top*** to ***downslope*** of the peak, in ***seconds***. The duration is calculated at the height defined by *HeightPercent* parameter. **Parameters:** *HeightPercent* : *real* The percent of the ***peak height*** which defines the height from the ***baseline*** at which *SectionRight* is calculated.
ConcErrorMinus *(Confidence)*	Returns *lower uncertainty of concentration* which is defined from **confidence region** of **calibration curve** 182 of the ***component*** associated with the peak. The *uncertainty* is calculated for specified **confidence probability**. The returned value is similar to **lower uncertainty of concentration** 351 property in report output. **Parameters:** *Confidence* : *real* **[0.0, 0.9999999]** The **confidence probability** for **polynomial regression** which defines the **confidence region.** See **calibration inaccuracy** 183 and **calibration curve** 182 for details. Use *default_probability* macro to specify the **confidence probability** from the **method** 122 settings (see the **Calibration graphs** 178). This is a default value. Remarks: Note that this uncertainty applies to **concentration** 337, not the **relative concentration** 337. For **relative concentration** 337 use *ConcErrorPercentMinus* macro.
ConcErrorPlus	Returns *upper uncertainty of concentration* which is defined from **confidence region** of **calibration curve** 182 of the ***component***

(Confidence)	associated with the peak. The *uncertainty* is calculated for specified **confidence probability**. The returned value is similar to **upper uncertainty of concentration** 351 property in report output. **Parameters:** *Confidence* : *real* **[0.0, 0.9999999]** The **confidence probability** for **polynomial regression** which defines the **confidence region.** See **calibration inaccuracy** 183 and **calibration curve** 182 for details. Use *default_probability* macro to specify the **confidence probability** from the **method** 122 settings (see the **Calibration graphs** 178). This is a default value. Remarks: Note that this uncertainty applies to **concentration** 337, not the **relative concentration** 337. For **relative concentration** 337 use *ConcErrorPercentPlus* macro.
ConcError(Confidence)	Returns maximal value from *ConcErrorMinus(Confidence)* and *ConcErrorPlus(Confidence)* **Parameters:** *Confidence* : *real* **[0.0, 0.9999999]** It has the same meaning as for *ConcErrorMinus* and *ConcErrorPlus*. Remarks: The returned value can be considered as a general uncertainty of concentration calculated from **calibration curve** 182. Note that this uncertainty applies to **concentration** 337, not the **relative concentration** 337. For **relative concentration** 337 use *ConcErrorPercent* macro.
ConcErrorPercentMinus(Confidence)	Returns *lower relative uncertainty*, in **%**, which is defined from **confidence region** of **calibration curve** 182 of the ***component*** associated with the peak. The *uncertainty* is calculated for specified **confidence probability**. The returned value is similar to **lower relative uncertainty, %** 352 property in report output. **Parameters:** *Confidence* : *real* **[0.0, 0.9999999]** The **confidence probability** for **polynomial regression** which defines the **confidence region.** See **calibration inaccuracy** 183 and **calibration curve** 182 for details. Use *default_probability* macro to specify the **confidence probability** from the **method** 122 settings (see the **Calibration graphs** 178). This is a default value. Remarks:

	The relative uncertainty can be applied to **concentration** 337, **relative concentration** 337 and **quantity** 338 of the component.
ConcErrorPercentPlus (Confidence)	Returns *upper relative uncertainty*, in **%**, which is defined from **confidence region** of **calibration curve** 182 of the ***component*** associated with the peak. The *uncertainty* is calculated for specified **confidence probability**. The returned value is similar to **upper relative uncertainty, %** 352 property in report output. **Parameters:** *Confidence* : *real* **[0.0, 0.9999999]** The **confidence probability** for **polynomial regression** which defines the **confidence region**. See calibration inaccuracy 183 and calibration curve 182 for details. Use *default_probability* macro to specify the **confidence probability** from the **method** 122 settings (see the **Calibration graphs** 178). This is a default value. Remarks: The relative uncertainty can be applied to **concentration** 337, **relative concentration** 337 and **quantity** 338 of the component.
ConcErrorPercent (Confidence)	Returns maximal value from *ConcErrorPercentMinus(Confidence)* and *ConcErrorPercentPlus(Confidence)* **Parameters:** *Confidence* : *real* **[0.0, 0.9999999]** It has the same meaning as for *ConcErrorPercentMinus* and *ConcErrorPercentPlus*. Remarks: The returned value can be considered as a general uncertainty of concentration calculated from **calibration curve** 182.
TimeEx(Channel, Formula)	Returns *retention time* of the peak calculated by alternative method at specified channel. The output value is in **retention units(calibration)** 169. **Parameters:** *Channel* : *integer* Reference to **channel** 146 which will be used to calculate the alternative *retention time*. See **references** 310 how to specify the reference to the channel. *Formula* : *integer* **[1, 2]** Number that defines the formula for calculation of alternative *retention time*. The possible values are: *T_MEDIAN* (or **1**) : The ***median*** *retention time*. This is a time which splits the area of the peak at two equal parts.

	T_CMASS (or **2**) : The ***center-of-mass*** *retention time*. It is calculated as $$\frac{\int t \cdot R(t) \cdot dt}{\int R(t) \cdot dt} = \frac{\int t \cdot R(t) \cdot dt}{Area}$$ where t is a retention time, $R(t)$ is a detector response after baseline subtraction; integration is performed within the limits of peak duration.
HeightEx(Channel)	Returns *peak height* calculated at the specified channel. The output value is in **physical measure units** 149 of the specified channel. **Parameters:** *Channel* : *integer* Reference to **channel** 146 which will be used to calculate the *peak height*. See **references** 310 how to specify the reference to the channel.
AreaEx(Channel)	Returns *peak area* calculated at the specified channel. The output value is in **peak area units** 170 where ***[Measure units]*** of specified channel are used. **Parameters:** *Channel* : *integer* Reference to **channel** 146 which will be used to calculate the *peak area*. See **references** 310 how to specify the reference to the channel.
SpRatio(Channel, Basechannel)	Returns *spectral ratio* for detector responses corresponded to the peak at specified **channels** 146. The returned value is similar to **spectral ratio** 339 property in report output. Adaptive formula calculates the detector response corresponded to the peak in the same way as for **spectral ratio** 339 property. **Parameters:** *Channel* : *integer* and *Basechannel* : *integer* References to **channels** 146 which will be used to calculate the *spectral ratio*. See **references** 310 how to specify the reference to the channel. Remarks: The returned spectral ratio is calculated as ***Response(Channel) / Response(Basechannel)***
Momentum(Channel, Order)	Returns the *momentum* of detector response for the peak. The calculation is performed at specified channel. The calculation algorithm depends upon *Order* parameter. **Parameters:**

	Channel : *integer* Reference to **channel** 146 which will be used to calculate the *momentum*. See **references** 310 how to specify the reference to the channel. *Order* : *integer* **[0, 1, 2, 3, 4]** The order of the momentum; There are different approaches for calculation of momentum for different orders. **0 :** $\int R(t) \cdot dt$ This moment is analogous to peak area. It is returned in **peak area units** 170. **1 :** $\frac{\int t \cdot R(t) \cdot dt}{\int R(t) \cdot dt} = \frac{\int t \cdot R(t) \cdot dt}{Area}$ This momentum is a retention time of peak's center of mass. It is returned in **retention units(calibration)** 169. **2, 3, 4 :** $\frac{\int (t - T_c)^n \cdot R(t) \cdot dt}{\int R(t) \cdot dt} = \frac{\int (t - T_c)^n \cdot R(t) \cdot dt}{Area}$ These are central moments. Here T_c is a time of peak's center of mass (*momentum* of order **1**) and n is a specified order of the *momentum*. The returned value is in the **[Time]** ^{n} units where **[Time]** is **retention units(calibration)** 169. Remarks: All integrations are performed over time of peak duration. $R(t)$ defines a detector response after baseline subtraction.
SignalSpecial(Channel, Metric)	Returns *special metrics* of detector response within the peak at specified channel. **Parameters:** *Channel* : *integer* Reference to **channel** 146 which will be used to calculate the *special metrics*. See **references** 310 how to specify the reference to the channel. *Metric* : *integer* **[0, 1, 2, 3, 4, 5, 6]** Number that defines the formula for calculation of alternative *retention time*. **[** `SP_RMS`, `SP_PKTOPK`, `SP_AVERAGE`, `SP_DRIFT`, `SP_SUM`, `SP_BLSUM`, `SP_SQSUM`] macro can be used instead of specifying numbers.

0 or SP_RMS **:** ***Root mean square*** deviation of the detector response in the range of the peak. The deviation is calculated after subtracting ***linear drift*** from detector response (see SP_DRIFT metric). The output value is in **physical measure units** 149 of the specified channel.

1 or SP_PKTOPK **:** Maximal (***peak-to-peak***) deviation of the detector response in the range of the peak. The deviation is calculated after subtracting ***linear drift*** from detector response (see SP_DRIFT metric). The output value is in **physical measure units** 149 of the specified channel.

2 or SP_AVERAGE **:** ***Average*** value of signal in the range of the peak. ***Average*** is calculated without subtracting baseline and without subtracting ***linear drift***. The output value is in **physical measure units** 149 of the specified channel.

3 or SP_DRIFT **:** Calculates the ***linear drift*** of the of the detector response in the range of the peak. Calculation is performed by fitting the the detector responses by linear function. The output value is is in **[R]/sec** units where **[R]** is **physical measure units** 149 of the specified channel.

4 or SP_SUM **:** Calculates the sum of the detector responses (integral) in the range of the peak. The calculation is performed without subtracting baseline and without subtracting ***linear drift***. The output value is is in **[R]*sec** units where **[R]** is **physical measure units** 149 of the specified channel.

5 or SP_BLSUM **:** Calculates the sum of the detector responses (integral) in the range of the peak. The calculation is performed with subtracting baseline. Riders (if any) are not subtracted from detector response. The output value is is in **[R]*sec** units where **[R]** is **physical measure units** 149 of the specified channel.

6 or SP_SQSUM **:**Calculates the sum of the squared detector responses (squared integral) in the range of the peak. The calculation is performed without subtracting baseline and without subtracting ***linear drift***. The output value is is in **[R]** ^{2}***sec** units where **[R]** is **physical measure units** 149 of the specified channel.

Remarks:

Typically *SignalSpecial* macro is not used with a "real" peak (which is detected by **peaks identification procedure** 166 or by other means). The most topical usage of *SignalSpecial* is an advanced technique for

	calculating noise in the chromatogram. In this case *SignalSpecial* macro is used to calculate metrics of detector response at some range of the **chromatogram**. Usually there are no peaks at all at this range. Operator can use **manual peak editor** 224 or **integration events** 163 to create an "artificial" peak which would cover the range required. Then *SignalSpecial* macro can be used to calculate metrics for this range.

See also:
Peak properties 294
Syntax of peak properties 295

9.3.3.2 Chromatogram properties

These macro-definitions return properties, corresponding to the entire chromatogram.
Macro-definitions of this type return ***real*** (floating-point, see **data types** 291) values.

See **syntax of chromatogram properties** 306 article for syntax description.
See **list of chromatogram properties** 307 for available **macro definitions** of **chromatogram properties**.

See also:
Macro definitions 294

9.3.3.2.1 Syntax of chromatogram properties

The following syntax can be used for **chromatogram properties** 306:

Simplified syntax:

ChromatogramMacro

- for macro definitions without additional parameters

or

ChromatogramMacro(param1, param2, ...)

- for macro definitions with additional parameters

-

When **simplified syntax** is used the returned value of macro-definition refers to the ***current chromatogram***, that is the chromatogram of the peak, for which **user-defined formula** 288 is evaluated. (Remember that **individual analysis reports** 320 use single chromatogram, so simplified syntax is only possible for these reports.)

Summary extended syntax:

Summary extended syntax is used only in **peak table** 372 of **advanced summary reports** 366. It allows to build a formula expressions which refers to **chromatogram properties** 306 of any chromatogram from summary list.

ChromatogramMacro{"chromatogram title"}

- for macro definitions without additional parameters

or

ChromatogramMacro{"chromatogram title", nInjection}(param1, param2, ...)

- for macro definitions with additional parameters; some or all parameters can be optional

where

"chromatogram title" : *string*	is a text string specifying a **title of the chromatogram** 126.
nInjection : *integer*	is a sequence number of the injection for the current vial; Typically this value equals to *1*. Other values are possible when **Injections** item in **sample queue table** 255 specifies several injections for a vial.

The *{"chromatogram title", nInjection}* section can be omitted. In this case *ChromatogramMacro* refers to the current chromatogram, that is the chromatogram of the peak for which the **user-defined formula** 288 is evaluated.

See also:

Chromatogram properties 306

List of chromatogram properties 307

9.3.3.2.2 List of chromatogram properties

Here is a list of macro definitions related to **chromatogram properties** 306.

All macro-definitions of this type return *real* (floating-point, see **data types** 291) values.

Macro definition	Description
Flow	Returns eluent *flow rate*. See **"Eluent" page** 131 for details. The output value is always in ***[µL / min]***. **No parameters.**
Volume	Returns *injected volume* of the sample. See **"Sample" page** 126 for

	details. The output value is in ***[µL]***. **No parameters.**
Dilution	Returns *dilution* of the sample. See **"Sample" page** 126 and **dilution** 128 for details. **No parameters.**
Multiplier	Returns *multiplier* for the sample. See **"Sample" page** 126 and **multiplier** 128 for details. **No parameters.**
CustomValue *(ParameterID)*	Returns a *real* number corresponded to *custom parameter* for the sample. See **"Extra" page** 128 for details. **Parameters:** *ParameterID* : *string* The string which identifies the *custom parameter*. It must match the **Parameter** item in the table of **"Extra" page** 128. The matching is case sensitive. *CustomValue* returns **0** if no matches are found. Remarks: The **Value** item in the **"Extra" page** 128 is a string. *CustomValue* converts this string to a *real* number. To be properly converted the string in the **Value** item must match syntax specified for *real*: see **data types** 291. The valid *real* number in the **Value** item can be followed by arbitrary sequence of characters. In this case the conversion is performed until the first character which cannot be converted. For example, string ***"7.55 miles"*** will be converted to ***7.55*** *real* number.
ColumnLength	Returns *length of the column*. See **"Column" page** 130 for details. The output value is in ***[mm]***. **No parameters.**
ColumnDiameter	Returns *internal diameter of the column*. See **"Column" page** 130 for details. The output value is in ***[mm]***. **No parameters.**
ColumnPorosity	Returns *porosity* for the column, that is the *void volume percent* of column volume. See **"Column" page** 130 for details.The output value is in ***[%]***. **No parameters.**
ColumnParticleSize	Returns *particle size* of the column ***packing material***. See **"Column" page** 130 for details.The output value is in ***[µm]*** - micrometers. **No parameters.**
VoidTime	Returns the *void time* as it is calculated by the software. See **"Column" page** 130, **"Math" page** 138 and **void time** 141 for details. The output value is in ***[s]*** .

	No parameters.
NoiseInChan(Channel)	Returns the *noise estimation* for the specified channel. The noise is calculated in the way specified at the **"Noise" page** 142. The output value is in **physical measure units** 149 of the specified channel. **Parameters:** *Channel* : *integer* Reference to **channel** 146 which will be used to calculate the *noise*. See **references** 310 how to specify the reference to the channel.
NoiseInChanRMS (Channel, Start, End)	Returns the alternative *noise estimation* for the specified channel. Noise estimation is based on **RMS** approach. It is calculated for the specified range of the chromatogram. The output value is in **physical measure units** 149 of the specified channel. **Parameters:** *Channel* : *integer* Reference to **channel** 146 which will be used to calculate the *noise*. See **references** 310 how to specify the reference to the channel. *Start*, *End* : *real* The ***start*** and the ***end*** time of the range of the chromatogram for which *noise* is calculated. The time must be specified in ***[s]***.
RawNoiseInChan (Channel)	Returns the alternative *noise estimation* for the specified channel. Noise estimation is based on **average point-to-point** approach. See **"Noise" page** 142. This macro calculates the noise using original raw data, that is raw data before applying any smoothing filters specified at **"Noise" page** 142. The output value is in **physical measure units** 149 of the specified channel. **Parameters:** *Channel* : *integer* Reference to **channel** 146 which will be used to calculate the *noise*. See **references** 310 how to specify the reference to the channel.
ResponseAt(Channel, Time)	Returns the *detector response* value for specified channel at specified time. The output value is in **physical measure units** 149 of the specified channel. **Parameters:** *Channel* : *integer* Reference to **channel** 146 for obtaining *detector response*. See **references** 310 how to specify the reference to the channel. *Time* : *real* The time of the chromatogram for obtaining *detector response* . The time must be specified in ***[s]***.

CycTime	Returns the *cycle time* for ADC measurements for **channels** 146 of the chromatogram. See **cycle time** 147 for details. The output value is in ***[s]***. **No parameters.**

See also:
Chromatogram properties 306
Syntax of chromatogram properties 306

9.3.3.3 References

References macro-definitions are used as input parameters for other macro-definitions such as **peak properties** 294 and **chromatogram properties** 306.

Two types of **references** are available.

Peak references allow access to the property of an arbitrary peak in the chromatogram.

The macro-definition of this type returns *integer* value (see data types 291) which indicates the index of the peak in the chromatogram.

The first peak in the chromatogram has index 1 and *numpeaks* macro indicates the index of the last peak.

Channels references allow addressing to a specific **channel** 146 of the chromatogram.

The macro-definition of this type returns *integer* value (see data types 291) which indicates the index of the **channel** 146 (sequence number in the **channels table** 148) in the chromatogram.

See **syntax of references** 311 article for syntax description.
See **list of references** 312 for available **macro definitions** of **references**.

See also:
Macro definitions 294
Peak properties 294
Chromatogram propertie 306

Adjust time shift 150

Peak Indexing rules

Indexing allows to address parameters of other peaks while making calculations for the current one. Indexing is allowed for all macro-definitions of *Peak parameters type*.

References (i.e. *serial number*) of the peak has to be written in brackets just after the macro-definition name. Peak numbering starts from 1.

Note: macro-definition of Peak parameters type 294 returns 0, if index of non-existing peak is found in brackets!

Note: index is omitted for the current peak

Example:

Area / Area[**1**]

calculates ratio of the *current peak* to the *first peak*.

If macro-definition needs additional parameters, index in brackets is placed before parameters:

Example:

Section[**1**](50.0)

returns width at 50% height for the first peak.

Note: Peak indices can use their own macro-definitions.

Note: There is a group of indices macrodefinitions that operate with any specified channel. These type of parameters are grouped together in the bottom part of the parameters list, after delimiter ----------.

Examples:

Area[*quantstd*]	returns area of quantification standard.
Section[*of*("Chloride")](50.0)	returns width at half-height of the peak, identified as "Chloride"
Area[**current+1**]	returns area of the next peak.

Macro-definitions of *Peak indices type* can be used as parameters for other macro-definitions:

Resolution(current+1, -1)	returns *resolution of the current peak with respect to the next* using resolution formula, specified in the chromatogram.
*Resolution***[current-1]**(current+1, -1)	returns *resolution of the previous peak with respect to the next* using resolution formula, specified in the chromatogram.

9.3.3.3.1 Syntax of references

The **simplified syntax** is only available for **references** 310.

Simplified syntax:

ReferenceMacro

- for macro definitions without additional parameters

or

ReferenceMacro(param1, param2, ...)

- for macro definitions with additional parameters.

Summary extended syntax is not used with **references** 310 macro-definitions directly.

Still **peak property** 294 or **chromatogram property** 306 can be used with **summary extended syntax** of the form

PropertyMacro{"chromatogram title", nInjection}<.....>

See **syntax of peak properties** 295 and **syntax of chromatogram properties** 306 for details.

In this case **summary extension section** *{"chromatogram title", nInjection}* is propagated on all *ReferenceMacro* items which are used as input parameters for **peak property** 294 or **chromatogram property** 306.

For example an expression

Area{"20-100ppm Std3", 2}[of("Chlorid"), of("Phosphat")]

will calculate the sum of areas of all peaks from peak which was recognized as *Chlorid* to peak which was recognized as *Phosphat* in the injection 2 of the sample with title *"20-100ppm Std3"*.

Any mathematical expressions are allowed with **references** 310.

For example, an expression

of("Chlorid") + 1

indicates the peak next to the peak which was recognized as *Chlorid*.

See also:

References 310

List of references 312

9.3.3.3.2 List of references

Here is a list of macro definitions related to **chromatogram properties** 306.

All macro-definitions of this type return *integer* (floating-point, see **data types** 291) values.

Macro definition	Description
Peak references	
current	This pseudo-reference returns the index of the *current peak*, that is the index of the peak, for which **user-defined formula** 288 is evaluated. **No parameters.** Remarks: The pseudo-reference term means that this macro cannot be used for **peak property** 294 or **chromatogram property** 306 with **summary extended syntax** (see **syntax of peak properties** 295 and **syntax of chromatogram properties** 306 for details). The *current* identifies the

	index of the currently reported peak in the current chromatogram. The *current* is undefined for any other chromatogram.
std	Returns the index of the peak which was identified as **standard component (calibration)** 194 It returns **0** (non-existing peak) if **external standard calibration** 190 is used or if the standard component was not identified. **No parameters.**
quantstd	Returns the index of the peak which was identified as **standard component (quantification)** 204. It returns **0** (non-existing peak) if **standard component (quantification)** 204 is not defined in the method or if the standard component was not identified. **No parameters.**
of(ComponentName)	Returns the index of the peak which was identified as component with name *ComponentName*. It returns **0** (non-existing peak) if the specified component was not identified. **Parameters:** *ComponentName* : *string* The name of the component as it was specified in the **components table** 171.
comp(ComponentIdx)	Returns the index of the peak which was identified as component with index *ComponentIdx*. It returns **0** (non-existing peak) if the specified component was not identified. **Parameters:** *ComponentIdx* : *integer* The index (sequence number) of the component as it displayed in the **components table** 171. Remarks: This reference is similar to *of(ComponentName)* macro. The difference is that component index is used instead of component name to specify the component required.
numpeaks	Returns the total number of the detected peaks in the chromatogram. This is also the index of the last peak in the chromatogram. **No parameters.**
Channel references	
refchan	Returns the index of **reference channel** 197 of the chromatogram. **No parameters.**

	Remarks: Some components can have individual settings for their **reference channel** (see **reference channel** 197 for details). *refchan* macro returns the index of the **reference channel** which is default for all components.
detchan	Returns the index of the channel which was specified as a channel for peak detection. See **Integration setup** 160 for details. **No parameters.**
chan(ChanName)	Returns the index of the channel with name *ChanName*. If channel with specified name was not found it returns *refchan* value. **Parameters:** *ChanName* : *string* Channel name as it appears in the **channels table** 148. It also can be a name of the **calculated channel** 152 as it was specified at **Calculated Channels** 151 page. Remarks: Normally there should be no channels with the same name in the chromatogram. If there are more then one channel with the name specified in the chromatogram then the index of the first occurrence is returned.

See also:
References 310
Syntax of references 311

9.3.3.4 Mathematical functions

Different mathematical functions allow user to build a complicated mathematical expressions.
Macro-definitions of mathematical function return ***real*** (floating-point, see data types 291) values.

See **syntax of mathematical functions** 314 article for syntax description.
See **list of mathematical functions** 315 for available **macro definitions** for **mathematical functions**.

See also:
Macro definitions 294
Mathematical operators 292

9.3.3.4.1 Syntax of mathematical functions

The following syntax is used for **mathematical functions** 314:

MathMacro

- for macro definitions without additional parameters (these are just mathematical constants such as *e* or *pi*)

or

MathMacro(param1, param2, ...)

- for macro definitions with additional parameters.

Any valid mathematical expressions can be used as parameters for **mathematical functions** 314. In turn **mathematical functions** 314 can be combined at mathematical expressions and can be used as parameters for another **mathematical functions** 314.

Example:

log(Height / Height[of("Chloride")])

Returns natural logarithm of the ratio of heights of the current peak and the peak identified as "Chloride"

See also:

Mathematical functions 314

List of mathematical functions 315

9.3.3.4.2 List of mathematical functions

Here is a list of macro definitions related to **mathematical functions** 314.

All macro-definitions of this type return *real* (floating-point, see **data types** 291) values.

All parameters if any are also of *real* **data type** 291.

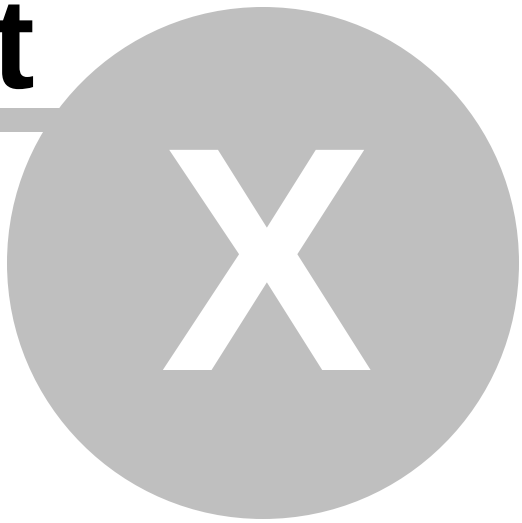
Macro definition	Description
cos(param)	Returns cosine of the *param* value
sin(param)	Returns sine of the *param* value
tan(param)	Returns tangent of the *param* value
acos(param)	Returns arccosine of the *param* value
asin(param)	Returns arcsine of the *param* value
atan(param)	Returns arctangent of the *param* value
exp(param)	Returns the exponential value of the *param*
log(param)	Returns natural logarithm of the *param* value
log10(param)	Returns base-10 logarithm of the *param* value
pow(base, exponent)	Returns *base* raised to the power of *exponent*.
sqrt(param)	Returns square root of the *param* value
abs(param)	Returns absolute value of the *param* value
e	Defines constant – base of natural exponent, *e = 2.71828182845904523536*

pi	Defines constant, *pi = 3.14159265358979323846*

See also:

Mathematical functions 314
Syntax of mathematical functions 314

Part



Reports

10 Reports

Reports present user the results of the analyses or results of series of analyses.

The report can be a hardcopy printout, a display on the screen or can be stored in the file.

Reports for individual analysis 320 are the most commonly used. As stated these reports present user the results of data processing and associated information which refer to single **chromatogram** 207.

In more complicated cases the results produced by several chromatograms can be combined into the single report. See **summary reports** 359 for more details and cases of use.

Chrom&Spec software supplies several options for configuring and producing reports.

Reports for individual analysis	
Plain reports 320	These are ease-to-use reports for most common tasks. Reports allow to review the results of analysis with minimal configurations. The output is based on the plain text. Reports can be displayed on the screen, printed, stored as ***.TXT** files and exported to external programs for further processing.
Advanced reports 341	This is a powerful tool for building reports that conform to specific needs of the users. Users have control over font, text formatting, and colors. It is possible to insert pictures, graphs, logos, and other graphics into the reports. Build-in script engine and **user-defined formulas** 288 allow to perform additional computations as necessary. User can strictly specify what information must be in the report and how this information must look. Reports can be stored as ***.PDF, *.RTF, *.HTML** or text files. Software supplies tools for previewing, displaying and printing reports. **Electronic signature** 62 can be applied to reports stored in ***.PDF.** Software supplies a set of predefined report templates for most common tasks so that user can start using **advanced reports** 341 with minimal configurations.

Generally **reports for individual analysis** should be configured for the **method** 122. See **method setup: "Reports" page** 145 for details.

Typically reports are produced automatically when analysis finish.

Configured reports can be generated manually for chromatogram using **Report / Make quick report...** 33 menu command.

Plain reports 320 are configured and executed using **setup and make plain report...** 322 menu command.

There are several alternatives in **Chrom&Spec** software for configuring and getting **reports for individual analysis**:

1. User can use ***<Make other report>*** option of **Report / Make quick report...** 33 menu command for producing advanced report without configuring **method** 122.

2. **Analysis report** 258 and **calibration report** 263 options can be configured in the **sample queue** 237.
3. User can configure **Make report** option in **"Reprocess" window form** 273 for **batch reprocessing** 271.
4. User can use **<Print report...>** button in **Open chromatogram** 207 window form to print the **plain report** 320 which was previously configured for selected **chromatograms** 207.

Summary reports	
Plain statistics reports 360	These are simple and easy-to-use reports which allow calculate the statistical metrics of **peak parameters** 332 over the set of chromatograms. The output is based on the plain text. Reports can be displayed on the screen, printed or stored as ***.TXT** files and exported to external programs for further processing.
Advanced summary reports 366	This is a powerful tool which allows combining results from the several analyses into the single report. Reports can be easily configured for computation of statistical metrics of **peak parameters** 332 over the set of chromatograms. The statistics can also be performed for special peak parameters specified with **user-defined formulas** 288. Build-in script engine and **user-defined formulas** 288 allow to perform additional computations producing specific values derived from the results of several independent analyses. The advanced capabilities of the these reports are analogous to **advanced reports** 341 for individual analysis. Reports can be stored as ***.PDF, *.RTF, *.HTML** or text files. Software supplies tools for previewing, displaying and printing reports. **Electronic signature** 62 can be applied to reports stored in ***.PDF.** Software supplies a set of predefined report templates for most common tasks so that user can start using **advanced summary reports** 366 with minimal configurations.

There are several ways how **summary reports** can be configured and produced in **Chrom&Spec** software.

1. From **Open chromatogram** 207 window form by pressing **<Statistics...>** button.
2. In the **sample queue** 237 by configuring **summary report** 260 or **vial summary report** 259 options in the **options panel** 257.
3. In the **batch reprocessing** 271 by configuring **Statistics** or **Summary report** options in the **"Reprocess" window form** 273.

See also:

Individual analysis reports 320

Summary reports 359

Plain reports 320

Advanced reports 341

Plain statistics reports 360

Advanced summary reports 366
Method setup: "Reports" page 145
Report / Make quick report... 33
Analysis report in the sample queue 258
Calibration report in the sample queue 263
Summary report in the sample queue 260
Vial summary report in the sample queue 259
“Reprocess” window form 273
Electronic signature for PDF reports 62

10.1 Individual analysis reports

Individual analysis reports reports present user the results of data processing and associated information which refer to single **chromatogram** 207.

Two types of **individual analysis reports** are available in **Chrom&Spec** software:

Plain reports 320 - ease-to-use tool with simple configuration for most common tasks.

Advanced reports 341 - an advanced tool which allows user to fully customize the view of the report and produce reports in various document formats.

To overview **individual analysis reports** see also a general **Reports** 318 article.

See also:

Reports 318
Summary reports 359
Method setup: "Reports" page 145
Report / Make quick report... 33
Analysis report in the sample queue 258
Calibration report in the sample queue 263
“Reprocess” window form 273
Electronic signature for PDF reports 62

10.1.1 Plain reports

Plain reports is an ease-to-use tool for most common tasks with simple configuration.

Plain reports allow to quickly review the results of analysis with minimal configurations.

The output is based on the plain text.

Reports can be displayed on the screen, printed, stored as ***.TXT** files and exported to external programs for further processing.

The printout and print preview of **plain reports** can contain graphics such as plot of **chromatogram** 207

and plots of **calibration curves** 182.

Configuring plain reports 321 article explains how user can configure and generate **plain reports** in **Chrom&Spec** software.

See also:
Configuring plain reports 321
Report options 322
Advanced reports 341
Individual analysis reports 320
Reports 318

10.1.1.1 Configuring plain reports

Plain reports 320 are a particular case of **individual analysis reports** 320.

Generally reports of this type should be configured for the **method** 122. Report configuration is performed at **Report options** 322 window which is called by **Report / Setup and make plain report...** menu command of **Report** 32 menu.

Method 122 can be configured to generate **plain report** 320 automatically when analysis finished. **Make plain report when chromatogram is finished** option at **method setup: "Reports" page** 145 is used for this task.

Still it is quite unusual making configuration of **plain report** 320 in the empty method (without chromatogram data). User would find much more convenient using an appropriate sample chromatogram for report configuration. A calibration chromatogram can be used as a sample.

To configure **plain report** 320 call **Report options** 322 window for sample chromatogram (sample chromatogram must be obtained using the **method** 122 to be configured). Make all necessary configurations. Review results using **<Preview>** button in the **Report options** 322 window. When finished use **<Accept>** button to apply changes to **chromatogram** 207. Then save **method** 122 from **chromatogram** 207 using **Save method** 123 menu command or appropriate button from the **toolbar** 36. This action applies configuration of the report to all subsequent runs of the **method** 122.

Additional configuration of the report is possible by editing **report templates** stored in ***.RTT** files. **RTT**-files are plain text files with a simple syntax which provide report layout. They are located in the root of ***software data folder*** which was specified during software installation. See **software installation** 21 for details.

Report templates (RTT) can be edited with any test editor, for example **Notepad** supplied with **Windows™** .

Chrom&Spec software supplies a set of default **report templates** for several languages. User can use them as a bases for creating their own **report templates**. Still editing report templates requires appropriate experience from the user.

There are several alternatives in **Chrom&Spec** software for configuring and getting **plain reports** 320:

1. User can configure **Make report** option in **"Reprocess" window form** 273 for **batch reprocessing** 271.
2. User can use **<Print report...>** button in **Open chromatogram** 207 window form to print the **plain report** 320 which was previously configured for selected **chromatograms** 207.

See also:

Plain reports 320

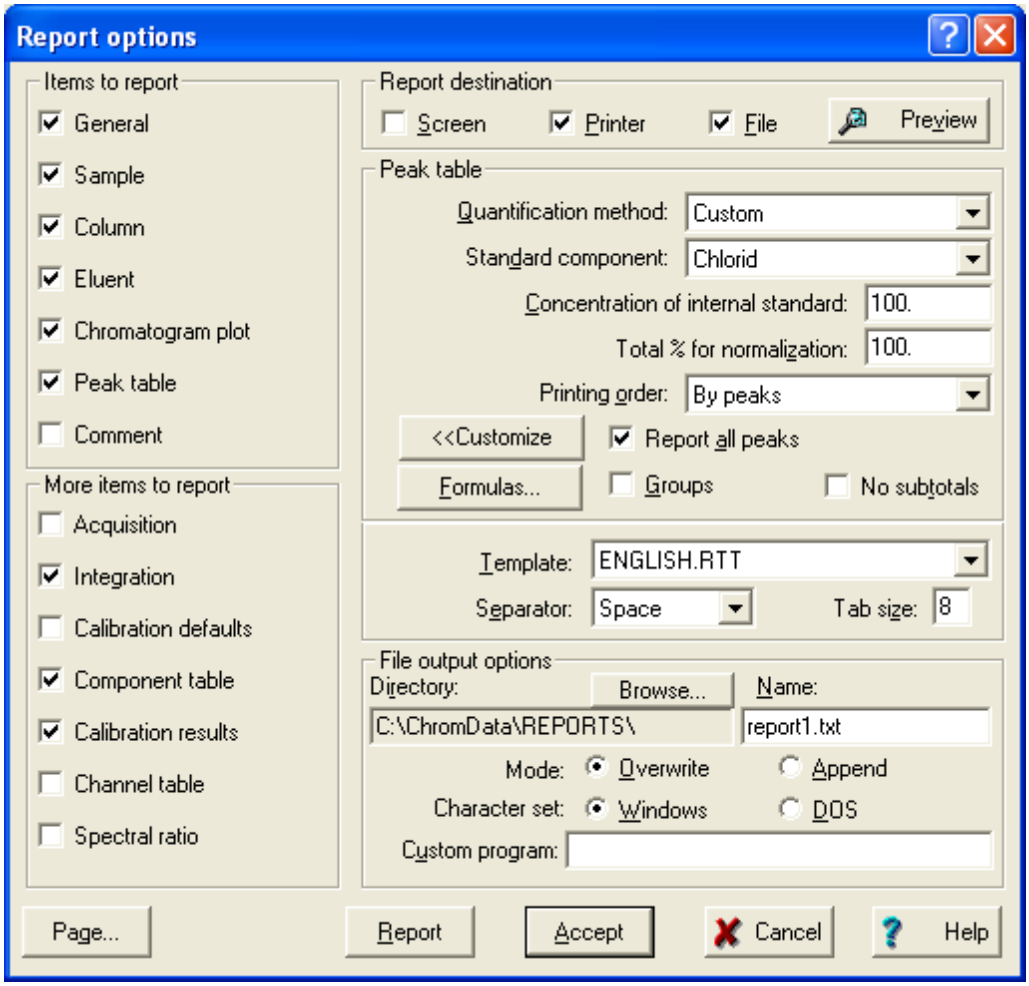
Report options window 322

10.1.1.2 "Report options" window

(*Main menu* Report / Setup and make plain report...)

This window form is used for configuring **plain report** 320 for **method** 122 or **chromatogram** 207 as well as producing report output.

See **configuring plain reports** 321 article for general overview of **plain report** 320 configuration.



The **Report options** window is divided into several areas that group parameters on their functionality.

Items to report 324 Main items to be included into a report.

More items to report 325 Additional items to be included into a report.

Note: The **plain report** 320 is organized as a set of chapters which are printed one after another. Each item in the **Items to report** 324 or **More items to report** 325 areas specifies a particular chapter in the report. The content of each chapter is defined by the **report template** stored in the ***.RTT** file (see **Template options**). It is possible to change the content of each chapter by editing existing **RTT** file or creating your own **RTT** file. See **configuring plain reports** 321 for more details.

Report destination 326 Specifies destination for the report. Several destinations can be specified.

Peak table 327 Settings for **peak table** – the main chapter producing the results of the analysis.

Template options Selection of **report template**, separator and tab size.

File output options 340 Specifies directory, file name and other options for report output to file.

Buttons:

<Page...> 340 Review and modify page layout for printing to the printer. This option is only available if the **Printer** report destination is set.

<Report>	Apply changes and generate a report according to **Report destination** 326.
<Accept>	Apply changes made to chromatogram or method and close the window. The settings of the report can be stored in the chromatogram or method so that report can be reproduced in the same form next time when needed. Do not forget save changes to file to make the them persistent.
<Preview>	Preview the report on screen.
<Cancel>	Cancel changes and close the window.

See also:

Plain reports 320
Configuring plain reports 321
Individual analysis reports 320
Advanced reports 341
How to modify report options 478
How to print a report 479
How to display a report 479
How to export a report 480

10.1.1.2.1 Items to report

The **plain report** 320 is organized as a set of chapters which are printed one after another.

This part of the **Report options** 322 window contains a list of important report chapters that can be included into the **plain report** 320 on the user's choice.

Check items required by the mouse click.

General	Chapter containing general description of the analysis. Typically this chapter presents information from **General** 124 page.
Sample	Chapter containing description of the sample. Typically this chapter presents information from **Sample** 126 page and lists custom sample parameters specified at the **Extra** 128 page.
Column	Chapter containing description of the column. Typically this chapter presents information from **Column** 130 page.
Eluent	Chapter containing description of eluting conditions (flow, pressure, temperature) and descriptions of eluents. Typically this chapter presents information from the **Eluent** 131 page.

Chromatogram plot Plot of the chromatogram.
The plot is displayed when **Report destination** 326 is set to **Printer** and for **<Preview>** action.
If **Report destination** 326 is set to **File** software produces a plot file in ***widows metafile*** format. A plot file has the same name as a report file with ***.WMF** extension and is stored in the directory which is specified in the **File output options** 340.
The plot **is not** displayed if **Report destination** 326 is set to **Screen**.
As alternative user can use **Edit \ Copy to clipboard** 29 menu command to get a plot of the chromatogram.
Advanced reports 341 provide user much more flexible tools for displaying plots and other graphics.

Peak table **Peak table** is a main chapter of the report producing the results of the analysis. The content of this chapter is defined by **Peak table** 327 settings in the **Report options** 322 window.

Comment Chapter containing user comments. Normally the content of this chapter is taken from the **Comment** 129 page.

See also:
Plain reports 320
Report options window 322

10.1.1.2.2 More items to report

The **plain report** 320 is organized as a set of chapters which are printed one after another.

This part of the **Report options** 322 window contains a list of additional report chapters that can be included into the **plain report** 320 on the user's choice.

Check items required by the mouse click.

Acquisition Chapter contains various parameters of data acquisition environment, data preprocessing options etc. Typically this chapter presents settings of your instrument (as they were defined at the time when analysis was run; note that not all instruments support reporting of their parameters). Also this chapter displays sampling rate, analysis duration and **noise smoothing** options defined at **Smoothing** 132 page.

Note: **Chromatogram** 207 stores an exact copy of the **system** 79 as it was configured at the time when analysis was run. This copy of the system can be extracted from the chromatogram using **Method / Extract stored system...** 234 menu command.

Integration Chapter containing parameters of **peaks integration procedure** 159. Typically this chapter presents information of **Integration setup** 160 and lists **Integration events** 162.

Calibration defaults Chapter containing calibration parameters common for all components. Typically this chapter presents parameters specified at **Calibration graphs** 178 and **Peak identification** 166 windows.

Note: User can specify individual calibration settings for some components. This is done at **Calibration graphs (advanced)** 178 window by setting **Local** options (see **calibration parameters** 186). **Local** component settings **are not** displayed at this chapter. Use **Calibration results** chapter to view **Local** component settings in the report.

Components table — Chapter containing list of components and their parameters as specified at **Components table** 171 window.

Calibration results — Chapter containing results of calibration for each component. This chapter is processed in a special way.
This chapter consists of several pages. Report engine forms a separate page for each component defined in **Components table** 171.
Typically each page contains calibration settings for component (specified in **Calibration graphs** 178 window taking into account **Local** flags defined for component), the equation and plot of **calibration curve** 182 for component, list of calibration points used to build a **calibration curve** 182 and a set of metrics which indicate the accuracy of the calibration.
The plot of **calibration curve** 182 is displayed when **Report destination** 326 is set to **Printer** and for **<Preview>** action. The plot of **calibration curve** 182 **is not** produced if **Report destination** 326 is set to **Screen** or **File**.
As alternative user can use **Copy to clipboard** and **Print/preview...** menu command of **Calibration graphs** 178 window to get plots of the **calibration curves** 182.
Advanced reports 341 provide user much more flexible tools for displaying plots and other graphics.

Channel table — Chapter containing parameters of the measure channels of the chromatogram. Typically this chapter presents information of **Channels page** 148 and results of noise calculations for each channel (see **Method setup: "Noise" page** 142 and ***Remarks*** at this article).

Spectral ratio — Chapter presents the results of calculations of **spectral ratio** 339 for all peaks and for all channels. **Spectral ratios** 339 are calculated relative to **reference channel** 197. This option should be used for **multi-channel chromatograms** 146 only.
The *SpRatio* 296 macro available at **user-defined formulas** 288 provides additional capabilities for calculating **spectral ratios**.

See also:

Plain reports 320

Report options window 322

10.1.1.2.3 Report destination

This part of the **Report options** 322 window specifies output destination for the report. Several output destinations can be selected simultaneously in any combination.

☑ **Screen** — Report output to screen (text only). All graphics are skipped when output is performed to screen.

☑ **Printer**	Report output to printer. If this item is checked, the **<Page...>** 340 button is enabled. Click **<Page...>** 340 button to modify page layout.
☑ **File**	Report output to file. The output is performed according to specified **File output options** 340.
<Preview>	Previews complete report on screen in WYSIWYG mode. Report is formatted exactly in the same way as it will be on printer's hard copy. Click **<Page...>** 340 button to modify page layout.

See also:

Plain reports 320

Report options window 322

10.1.1.2.4 Peak table

The **peak table** is a main chapter of the report producing the results of the analysis (see **items to report** 324). Typically this chapter contains a list of identified components and their concentrations along with additional peak metrics.

The **Report options** 322 window has an appropriate configurations grouped in **Peak table** area. This area contains an essential parameters for **quantification procedure** 201. Here user can control the content of the **peak table** chapter in the report.

Quantification method	Specifies **quantification procedure** 201 for data processing. Actually this option just defines a set of peak parameters which will be displayed in the **peak table** chapter. See description of **Quantification method** 329 option for more details.
Standard component	**Internal standard component** 204 for **relative concentration** 202 quantification procedure. It is used when **Quantification method** 329 option is set to **Relative concentration** 331 or analogous **Custom** 332 quantification. Typically **internal standard component** 204 is specified for method at **Method setup: "Quantification" page** 144. For convenience **Report options** 322 window duplicates the same item so that user can review and modify it if necessary.
Concentration of internal standard	Concentration of the **internal standard component** 204 for **relative concentration** 202 calculations. Typically **Concentration of internal standard** should be specified before analyses run: at **Edit sample description** 85 window for single analysis runs or in **sample table** 255 for runs from **sample queue** 237. For convenience **Report options** 322 window also supplies **Concentration of internal standard** item so that user can review and modify it if necessary. **Concentration of internal standard** can also be reviewed and modified at the **Sample** 126 page of the chromatogram.
Total % for normalization	A value to which the sum of concentrations is normalized. It is used for **Response normalization** 329 and **Normalized**

	concentrations 330 quantification methods. The default value is 100. Typically this item is configured for method 122 at the Method setup: "Quantification" page 144. For convenience Report options 322 window duplicates this item so that user can review and modify it if necessary.
Printing order	Determines the order of the components in the peak table.
By peaks	Lists run results by peaks. Missing components are not listed.
By components	Lists run results by components. Missing components are included into the report and their concentrations are reported as zero.
☑ **Report all peaks**	When checked all detected peaks are included into the report. When not checked recognized peaks only are included into the report. The concentration of the unrecognized peaks are reported as zero (because those peaks are not calibrated). Still other peak metrics, such as **peak area** and **peak height** are calculated and reported. This option is available only if Quantification method 329 option is set to ***Index*** or ***Column test*** or ***Custom***. This option requires **Printing order** to be set to ***By peaks*** value. This option has no effect if **Printing order** is set to ***By components*** value.
☑ **Groups**	If this checkbox is checked, a separate **peak table** report is generated for each group 173 specified in the components table 171. All components belonging to the same group are grouped together. For each group a separated subtotals can be calculated. The **group tables** follow the main **peak table** in the report.
☑ **No subtotals**	If checked, no subtotals are reported for **peak table** and for group's **peak tables**.
<<Customize	This option allows user to customize the list of peak parameters in the **peak table**. The option is available if Quantification method 329 is set to ***Custom*** value. See Quantification method 329 and Custom method 332 for details.
Formulas...	This option allows user to specify, review and edit the user-defined formulas 288. Each user-defined formula 288 specifies additional peak parameter which will be reported in the **peak table**. Custom formulas 289 and Build new peak parameter 290 window forms are used to review and edit the user-defined formulas 288. The option is available if **Quantification method** option is set to ***Custom*** value. Typically user-defined formulas 288 are configured for method 122 (at the Method setup: "Quantification" page 144, ***<My***

formulas> button). For convenience **Report options** 322 window also allows reviewing and editing **user-defined formulas** 288.

See also:

Plain reports 320

Report options window 322

10.1.1.2.4.1 Quantification method

The **Quantification method** option of the **Report options** 322 window defines a set of peak parameters reported in the **peak table** chapter of the report (see **Peak table** 327).

"Chrom&Spec" software supplies several predefined sets corresponding to most common **quantification procedures** 201.

Note that in "Chrom&Spec" software the **quantification** is rather flexible. In most cases parameters which refer to different **quantification procedures** 201 can be calculated simultaneously and reported in the single report. For example, in some cases it is possible to calculate **absolute concentration** 202 and **relative concentration** 202 simultaneously and have both values in the report (the values may be rather different). Also it is not a problem to calculate **response normalization** 204 and **normalized concentration** 204 together with **absolute concentration** 202.

Experienced user can specify **Custom** 332 **Quantification method** to freely manipulate the set of peak parameters reported in the **peak table**. Additionally **user-defined formulas** 288 can be used. **User-defined formulas** 288 is a powerful tool for defining specific peak parameters and creating specific procedures for calculating concentrations. **User-defined formulas** 288 are configured in the **Peak table** 327 of the **Report options** 322 window (*<Formulas...>* button).

Below is a list of **Quantification method** option available for the **Peak table** 327. View description of each option for a list of corresponded peak parameters. To view a list of all peak parameters available read **Custom** 332 article.

Quantification methods available:

Response normalization 329

Normalized concentration 330

Absolute concentration 330

Relative concentration 331

Index 338

Column test 331

Custom 332

See also:

Quantification procedure 201

Report options window 322

Peak table 327

This selection for the **Quantification method** 329 option specifies a predefined set of peak parameters

designed for **response normalization** 204 **quantification procedure** 201.

All peaks are calculated and reported no matter whether they have been recognized or not.

Peak table chapter of the report includes the following parameters:

Peak number - the sequence number of the peak in the chromatogram
Retention time 333
Area 334 or **Height** 334 - the choice is controlled by the **Response base** setting; see **Calibration parameters** 186.
Area% 334 or **Height%** 334 - the choice is controlled by the **Response base** setting; see **Calibration parameters** 186.
Component name - as specified in the **Components table** 171

See also:

Quantification method 329

Quantification procedure 201

This selection for the **Quantification method** 329 option specifies a predefined set of peak parameters designed for **normalized concentration** 204.

Recognized peaks are reported only.

Peak table chapter of the report includes the following parameters:

Peak number - the sequence number of the peak in the chromatogram
Retention time 333
Height 334
Area 334
Response factor 336
Concentration% 337
Component name - as specified in the **Components table** 171

See also:

Quantification method 329

Quantification procedure 201

This selection for the **Quantification method** 329 option specifies a predefined set of peak parameters designed for **absolute concentration** 202 **quantification procedure** 201.

This is a most common **quantification procedure**.

Recognized peaks are reported only.

Peak table chapter of the report includes the following parameters:

Peak number - the sequence number of the peak in the chromatogram
Retention time 333
Height 334
Area 334
Response factor 336
Concentration 337

Concentration% 337
Component name - as specified in the **Components table** 171

See also:

Quantification method 329

Quantification procedure 201

This selection for the **Quantification method** 329 option specifies a predefined set of peak parameters designed for **relative concentration** 202 **quantification procedure** 201.

This option requires **standard component** 204 and **concentration of internal standard** to be specified in the corresponded items of the **Report options** 322 window. (The same items can be specified at **Method setup: "Quantification"** 144 page).

Recognized peaks are reported only.

Peak table chapter of the report includes the following parameters:

Peak number - the sequence number of the peak in the chromatogram
Retention time 333
Height 334
Area 334
Response factor 336
Relative Concentration 337
Relative Concentration% 338
Component name - as specified in the **Components table** 171

See also:

Quantification method 329

Quantification procedure 201

This selection for the **Quantification method** 329 option is used for calculating **retention indexes** 141 of the peaks.

Peak table chapter of the report includes the following parameters:

Peak number - the sequence number of the peak in the chromatogram
Retention time 333
Width (h/2) 334
Height 334
Index 338
Component name - as specified in the **Components table** 171

See also:

Quantification method 329

This selection for the **Quantification method** 329 option is not related to any **quantification procedure**. Instead this option specifies a predefined set of peak parameters which are useful for auxiliary tasks, such as evaluating the performance of column and method developing.

Peak table chapter of the report includes the following parameters:

Peak number - the sequence number of the peak in the chromatogram
Retention time 333
Capacity factor 335 *k* 335
Number of theoretical plates per column 335
Number of theoretical plates per meter 335
Reduced height equivalent to theoretical plate 335
Peak asymmetry 336
Component name - as specified in the **Components table** 171

See also:

Quantification method 329

User can specify an arbitrary combination of peak parameters for **peak table** chapter by setting **Quantification method** 329 option to ***Custom***.

Note however that experienced users only should use this configuration. Although all peak parameters are always available for selection, some of them can produce meaningless values in the report. The particular parameters produce valid results only if **method** 122 is configured properly.

After selecting ***Custom*** **Quantification method** 329 in the **Report options** 322 window user should click **<<Customize>>** button. This displays a list of peak parameters available for selection.

The list contains the following items:

peak number The sequence number of the peak in the **chromatogram**.
retention time 333
width (h/2) 334
height 334
height% 334
area 334
area% 334
capacity factor 335 *k* 335
resolution 335
efficiency TP 335
efficiency, TP/m 335
reduced TP height 335
signal/noise 336
asymmetry 336
response factor 336

concentration 337

concentration% 337

rel. concentration 337

rel. concentration% 338

quantity 338

index 338

type 339

group 173 Number of the group for the component.

spectral ratio 339

component Name of the recognized component as specified in the **components table** 171..

file name File name of the chromatogram. This is an auxiliary item which may be useful when text report is processed by external program (for the purpose of data export etc).

title **Title** 126 of the chromatogram. This is an auxiliary item which may be useful when text report is processed by external program (for the purpose of data export etc).

Note: Values listed here are pre-defined in the Chrom&Spec software. Additionally user-defined formulas 288 can be used. User-defined formulas 288 is a powerful tool for defining specific peak parameters and creating specific procedures for calculating concentrations.

See also:

Quantification method 329

Peak table 327

This chapter represents the information from the **Comment** 129 page.

No tables and **sort fields** 401 are assumed for this chapter.

See also:

Chapters 346

Retention time of the component.

The **exact time** of the top of the peak is calculated by polynomial approximation of data points near the peak top.

The output value is in **retention units (calibration)** 169.

If **subtotals** are requested (see **Peak table** 327) then the **subtotal value** for this item is equal to the duration of the chromatogram.

The **width** of the peak calculated **at half maximum** of the peak.

The output value is in **retention units (calibration)** 169.

If **subtotals** are requested (see **Peak table** 327) then the **subtotal value** for this item is equal to the average **width** of the reported peaks of the chromatogram.

The **height** of the peak.

The **exact height** of the top of the peak is calculated by polynomial approximation of data points near the peak top.

The **height** is calculated from the peak top to base line under the peak.

The output value is in **physical measure units** 149 of **reference channel** 197.

If **subtotals** are requested (see **Peak table** 327) then the **subtotal value** for this item is equal to the sum of **heights** of the reported peaks of the chromatogram.

The **normalized height** of the peak.

See **response normalization** 204.

Typically the ***NORM*** is configured to 100 value. This is a default value for **method** 122.

In this case the reported value is just a percent of the **peak height** which is calculated relatively to the sum of heights of all peaks in the chromatogram.

If **subtotals** are requested (see **Peak table** 327) then the **subtotal value** for this item is equal to the sum of **normalized heights** of the reported peaks of the chromatogram.

The **area** of the peak.

The **area** is calculated with subtracting the base line under the peak from the detector response.

The output value is in **peak area units** 170.

If **subtotals** are requested (see **Peak table** 327) then the **subtotal value** for this item is equal to the sum of **areas** of the reported peaks of the chromatogram.

The **normalized area** of the peak.

See **response normalization** 204.

Typically the ***NORM*** coefficient is configured to 100 value. This is a default value for **method** 122.

In this case the reported value is just a percent of the **peak area** which is calculated relatively to the

sum of areas of all peaks in the chromatogram.

If **subtotals** are requested (see **Peak table** 327) then the **subtotal value** for this item is equal to the sum of **normalized areas** of the reported peaks of the chromatogram.

Capacity factor $k(i)$ of the component is equal to the ratio of its corrected retention time $(t - t_0)$ to the **void time** 141 (t_0) of the system:

$$k(i) = [t(i) - t_0] / t_0$$

If **subtotals** are requested (see **Peak table** 327) then the **subtotal value** for this item is equal to the **capacity factor of the last peak** of the chromatogram.

Resolution for two neighboring peaks $R(i,i+1)$.

The **resolution** is calculated according to **resolution** 140 configuration of the **method** 122: see **Method setup: "Math" page** 138.

The **subtotal value** (see **Peak table** 327) is always blank for this item.

Efficiency for the peak in number of theoretical plates.

The **efficiency** is calculated according to **efficiency, TP** 139 configuration of the **method** 122: see **Method setup: "Math" page** 138.

If **subtotals** are requested (see **Peak table** 327) then the **subtotal value** for this item is equal to the average **efficiency TP** of the reported peaks of the chromatogram.

Efficiency for the peak in number of theoretical plates per meter.

The number of theoretical plates per meter N' for the given peak is calculated as

$$N'(i) = N(i) \cdot 1000 / (L_{col} + L_{precol})$$

where L_{col} and L_{precol} are length of the column and precolumn respectively, in mm (see **Method setup: "Column" page** 130) and $N(i)$ is **efficiency, TP** 139 for the i-th peak.

If **subtotals** are requested (see **Peak table** 327) then the **subtotal value** for this item is equal to the average **efficiency TP/m** of the reported peaks of the chromatogram.

Reduced height, equivalent to theoretical plate $H(i)$ is calculated by formula:

$$H(i) = 1000 \cdot (L_{col} + L_{precol}) / (N(i) \cdot dp)$$

where L_{col} and L_{precol} are length of the column and precolumn respectively, in mm; dp is particle size in μm (see Method setup: "Column" page 130) and $N(i)$ is efficiency, TP 139 for the i-th peak.

If **subtotals** are requested (see Peak table 327) then the **subtotal value** for this item is equal to the average **reduced TP height** of the reported peaks of the chromatogram.

Signal-to-noise ratio for the peak.

The signal-to-noise ratio (S/N) influences the precision of quantification 201 and is calculated from the equation

$$S/N = 2H/h$$

H - height of the peak 334 in the chromatogram 207, measured from the maximum of the peak to the extrapolated baseline of the signal observed.

h - range of the background noise in a chromatogram. The noise is obtained at reference channel 197 for recognized component or at calibration default reference channel 197 for unrecognized peaks.

Software evaluates h as

$$h = 6\sigma$$

σ - standard deviation of the noise at reference channel 197, obtained using settings of the Method setup: "Noise" page 142.

The equation for signal-to-noise ratio can be rewritten in the form

$$S/N = H/(3\sigma)$$

If **subtotals** are requested (see Peak table 327) then the **subtotal value** for this item is equal to the average **signal-to-noise ratio** of the reported peaks of the chromatogram.

Asymmetry of the peak.

The **asymmetry** is calculated according to peak asymmetry 140 configuration of the method 122: see Method setup: "Math" page 138.

If **subtotals** are requested (see Peak table 327) then the **subtotal value** for this item is equal to the average **asymmetry** of the reported peaks of the chromatogram.

Response factor for the peak.

This is a coefficient $K1$ of the calibration curve 182. See response factor 201

description for details.

If the reported peak is not recognized as any component from components table 171 then zero value is

printed.

Typically the **response factor** 201 should be included into the report only if the **calibration curve** 182 for components is linear (see **calibration formula** 195).

The **subtotal value** (see **Peak table** 327) is always blank for this item.

Absolute (or **raw**) **concentration**.

This is a **concentration** calculated with **absolute concentration** 202 quantification procedure.

The output value is in **concentration units** which are defined by customer in the **concentrations table** 174 (this is an item of **method** 122 configuration).

If the reported peak is not recognized as any component from **components table** 171 then zero value is printed.

If **subtotals** are requested (see **Peak table** 327) then the **subtotal value** for this item is equal to the sum of **absolute concentrations** of the reported peaks of the chromatogram.

Normalized absolute concentration

This value is calculated as described in **normalized concentration** 204 quantification procedure.

Typically the ***NORM*** coefficient is configured to 100 value. This is a default value for **method** 122.
In this case the reported value is just a percent of the **absolute concentration** 337 which is calculated relatively to the sum of **absolute concentrations** of all peaks in the chromatogram.

If **subtotals** are requested (see **Peak table** 327) then the **subtotal value** for this item is equal to the sum of **normalized absolute concentrations** of the reported peaks of the chromatogram.

Relative concentration.

This is a **concentration** calculated with **relative concentration** 202 quantification procedure.

This item requires **standard component** 204 and **concentration of internal standard** to be specified in the corresponded items of the **Report options** 322 window. (The same items can be specified at **Method setup: "Quantification"** 144 page).

The output value is in **concentration units** which are defined by customer in the **concentrations table** 174 (this is an item of **method** 122 configuration).

If the reported peak is not recognized as any component from **components table** 171 then zero value is printed.

If **subtotals** are requested (see **Peak table** 327) then the **subtotal value** for this item is equal to the sum of **relative concentration** of the reported peaks of the chromatogram. Still the value related to the **standard component** 204 is excluded from the sum.

Normalized relative concentration

This value is analogous to **concentration %** 337. The equation for this value is rather similar to equation for **normalized concentration** 204. The only difference is that quantity of the **standard component** 204 is excluded from the summation:

$$C(i)\% = NORM \cdot Q(i)\{R(i)\} / (Sum[Q(i)\{R(i)\}] - Q(s)\{R(s)\})$$

Typically the ***NORM*** coefficient is configured to 100 value. This is a default value for **method** 122.

In this case the reported value is just a percent of the **relative concentration** 337 which is calculated relatively to the sum of **relative concentrations** of all peaks in the chromatogram excluding **standard component** 204.

If **subtotals** are requested (see **Peak table** 327) then the **subtotal value** for this item is equal to the sum of **normalized relative concentrations** of the reported peaks of the chromatogram. Still the value related to **standard component** 204 is excluded from the sum.

The **quantity** of the component in the injected sample.

This is a **computed quantity** 201 value determined from the **calibration curve** 182.

If the reported peak is not recognized as any component from **components table** 171 then zero value is printed.

There is an equation which relates the **quantity, raw concentration** 202 and **adjusted volume** 199 for ***i***-th component:

$$Q(i) = C(i) \cdot V'$$

The output value is in units:

[Quantity] = [**Concentration**]*µL

where [**Concentration**] units are defined by customer in the **concentrations table** 174 (this is an item of **method** 122 configuration).

If **subtotals** are requested (see **Peak table** 327) then the **subtotal value** for this item is equal to the sum of **quantities** of the reported peaks of the chromatogram.

Retention index for the peak.

See **retention indexes** 141 article for details.

The **retention index** is calculated according to **Index** settings in the **Method setup: "Math" page** 138 window.

If **subtotals** are requested (see **Peak table** 327) then the **subtotal value** for this item is a special value calculated by formula:

$$I = sum\ [\ I(i)\ C(i)\ ]\ /\ sum\ [C(i)]$$

where summation is performed by all reported peaks.

The **type** code for the peak and related component.

The **type** code may contain several letters. Each letter indicates the particular property of the peak or related component.

First two letters indicate how peak is separated from another peaks:

BB Indicates the stand-along peak that starts and ends at **baseline** (**B**).

BD Peak starts on the **baseline** (**B**) and ends on the **drop line** (**D**) (that separates it from another adjacent peak).

DB Peak starts on the **drop line** (**D**) and ends on the **baseline** (**B**) .

DD Peak starts and ends on the **drop line** (**D**).

Other letters have the following meaning:

R The peak is a rider.

S **Standard component (quantification)** 204 for **relative concentration** 202 quantification procedure.

C **Standard component (calibration)** 194 for calibration **internal standard** 190 method.

? The overloaded peak. Some points of the peak are out of ADC or detector range - the quantification results may be incorrect .

! Component concentration is outside of **minimum** or **maximum** limits defined in the **components table** 171 (**min C** and **max C** parameters).

p Component has one or more **special** 196 options defined in **Calibration graphs** 178 window.

N The **response** of the peak (**area** 334 or **height** 334) is outside of calibrated region.

The final **type** code may look like **BBR: ! N**.

The **subtotal value** (see **Peak table** 327) is always blank for this item.

Spectral ratio for multi-chan 146 **n** 146 el chromatograms 146.

The spectral ratio is calculated by formula for each *Channel* of **multi-channel chromatogram** 146

$$Response(\ Channel\ )\ /\ Response(\ Refchannel\ )$$

where *Refchannel* is a **reference channel** 197.

The adaptive formula calculates the ***Response*** based on **resolution** 335 for the peak (relatively to nearby peaks).

If the **resolution** 335 is enough then **area** 334 is used as ***Response***. Otherwise the **height** 334 of the peak is used as ***Response***.

The **subtotal value** (see **Peak table** 327) is always blank for this item.

10.1.1.2.5 File output options

The set of file parameters are activated when ☑ **File** option is specified as **report destination** 326 in the **Report options** 322 window:

Directory — Specifies the output directory where file report will be generated to. User can use **<Browse>** button to navigate to the desired directory.

Name — Name of the file for the report with file extension. The report is saved in text form in the ANSI or ASCII format. Typically ****.txt*** file extension is used. If the **Chromatogram plot** item is set in the **Items to report** 324 then the software also produces a plot file in ***windows metafile*** format. The plot is saved in a separate file with the same name and ****.wmf*** file extention.

Mode — Report mode: ***Overwrite*** or ***Append*** existing file. ***Overwrite*** option removes the previous report file with the same name (if any) and generates a new file. ***Append*** option writes the text of new report at the end of the existing report file.

Character set — **Windows (ANSI)** or **DOS (ASCII)**. This setting specifies the code page for text output. This setting is essential for printing of non-English symbols only.

Custom program — Full path and file name of the external program to be started after report output. This option enables post-processing of text reports by external programs so that analysis results can be transferred to database, electronic table or other actions can be performed.

See also:

Plain reports 320

Report options window 322

10.1.1.2.6 Page layout

The ***Page layout*** window is displayed when user presses ***<Page...>*** button in **Report options** 322 window.

The ***Page layout*** window defines the following parameters:

Length units — Selection of ***inches*** or ***centimeters***: the length units for other items in

	this window.
Page margins	***Left***, **right**, ***top*** and **bottom** margins for printed report.
Chromatogram plot size	***Width*** and ***height*** of the chromatogram plot. Specifies the size of the plot for **Chromatogram plot** option of **Items to report** 324.
Calibration graph size	***Width*** and ***height*** of the calibration curve plot. Specifies the size of the plot for **Calibration results** option of **More items to report** 325.
<Load default>	Loads the default values for page layout parameters.
<Save as default>	Saves the set of page layout parameters as default set.

See also:

Plain reports 320

Report options window 322

Print 233

Preview 234

10.1.2 Advanced reports

Advanced reports are a particular case of **individual analysis report** 320.

Introduction

Being able to produce clear, visual representations of analytical results is key to productivity. In most cases, plain text reports are not sufficient; the principal results can be lost among data of secondary importance.

Chrom&Spec provides powerful tools for building reports that conform to specific needs of the customer. **Advanced reports** allows user to fully customize the view and contents of his report.

Advanced reports are easy to read because users have control over font, text formatting, and colors. Users can insert pictures, graphs, logos, and other graphics into the reports.

For quality control, continuous monitoring of particular parameters is usually required (usually the controlled parameter is a concentration of a specific substance).

Chrom&Spec software allows you to highlight the errant condition using special colors in the reports when a concentration runs out of the admissible range.

Chrom&Spec generates reports at the end of every run, marking critical data by color immediately attracting the operator's attention.

Advanced reports supply a vast number of special functions to define the content of the report. These include data sorting and filtering, calculating minimal, maximal, average and other statistical values, defining your own functions and conditional statements. Any meaningful parameters related to analysis can be individually added or removed from the report.

Chrom&Spec allows you to define conditional report fields (comments, warnings, etc) and conditional report sections which appear in the report only if analysis results meet specific conditions.

Regardless of the wide variety of functions and configuration options, **advanced reports** are easy to use. **Chrom&Spec** comes with a set of predefined **report templates** suitable for most commonly used chromatography methods. As a matter of initial convenience, the report is divided by sections with strict meaning (such as ***Sample***, ***Column***, ***Calibration***, ***Peaks*** and so on). To begin, a user can simply check the necessary sections with a click of the mouse – no complicated.

See also:

Features and capabilities of advanced reports 342
Configuring advanced reports 342

10.1.2.1 Features and capabilities of advanced reports

Here is a summary list of features available in **advanced reports** 341.

Features related to advanced representation of the reports

- Configurable text fonts, text colors ant text backgrounds for any item of the report.
- The possibility to insert pictures, plots, logos and other graphics into the report.
- Reports can be stored as ***.PDF, *.RTF, *.HTML** or text files. No doubts the report can be viewed on the screen and printed.
- **Electronic signature** 62 can be applied to reports stored in ***.PDF** files.

Features related to the content of the reports

- User can specify mathematical and logical expressions and include them to the report.
- User can specify conditional sections of the report: the section appears in the report only if analysis results conform to (or not conform to) the specific conditions.
- User can specify conditional fonts and text colors: the report items are printed differently depending upon the results of analysis. For example, user can specify the "red" text color to highlight the specific rows in the peak table where the concentration of the component is out of the permissible range.
- Data filtering and data sorting capabilities.
- Summary and statistical computations.

For details see the **configuring advanced reports** 342 article.

10.1.2.2 Configuring advanced reports

Advanced reports 341 are a particular case of **individual analysis report** 320.

Generally reports of this type should be configured for the **method** 122. Report configuration is started from a **Method setup: "Reports" page** 145. This page can be called from the **main menu** 25 with **Report / Report setup...** menu command.

Configured settings of **advanced report** 341 are stored in the **report templates**. For configuring **report templates** the **Advanced report configuration** 343 window is used. **Method** 122 can store several different **report templates** where each report is configured for its own tasks. Software can generate all

these reports automatically when analysis finishes.

Typically **advanced reports** 341 are not configured in the empty **method** 122 (without chromatogram data). User would find much more convenient using an appropriate sample chromatogram for report configuration. A calibration chromatogram can be used as a sample.

To configure a **advanced report** 341 user should call the **Advanced report configuration** 343 window for sample chromatogram (sample chromatogram must be obtained using the **method** 122 to be configured) and make all necessary configurations. User can immediately review the results using **<Preview>** button in the **Advanced report configuration** 343 window. When finished user saves **method** 122 from **chromatogram** 207 using **Save method** 123 menu command or appropriate button from the **toolbar** 36. This action applies configuration of the **report templates** to all subsequent runs of the **method** 122.

It is quite easy to start using the **advanced reports** 341. At first approach user can just select a set of required **chapters** 346 in the **Advanced report configuration** 343 window. This produces a report with preconfigured chapters. **Chrom&Spec** software supplies a preconfigured chapters for several languages. By default the **advanced report** 341 is produced at the language of software user interface: see **choose UI language** 44.

Advanced users can use **advanced report designer** 378 which allows to fully customize the view and content of each **chapter** 346 of **advanced report** 341.

Typically reports are produced automatically when analysis finish.

Configured reports can be generated manually for chromatogram using **Report / Make quick report...** 33 menu command.

There are several alternatives in **Chrom&Spec** software for configuring and getting **advanced reports** 341 for individual analysis:

1. User can use ***<Make other report>*** option of **Report / Make quick report...** 33 menu command for producing advanced report without configuring **method** 122.
2. **Analysis report** 258 and **calibration report** 263 options can be configured in the **sample queue** 237.

See also:

Advanced reports 341

Features and capabilities of advanced reports 342

"Advanced report configuration" window 343

10.1.2.2.1 "Advanced report configuration" window

This window is intended for configuring the **report template** for **advanced report** 341.

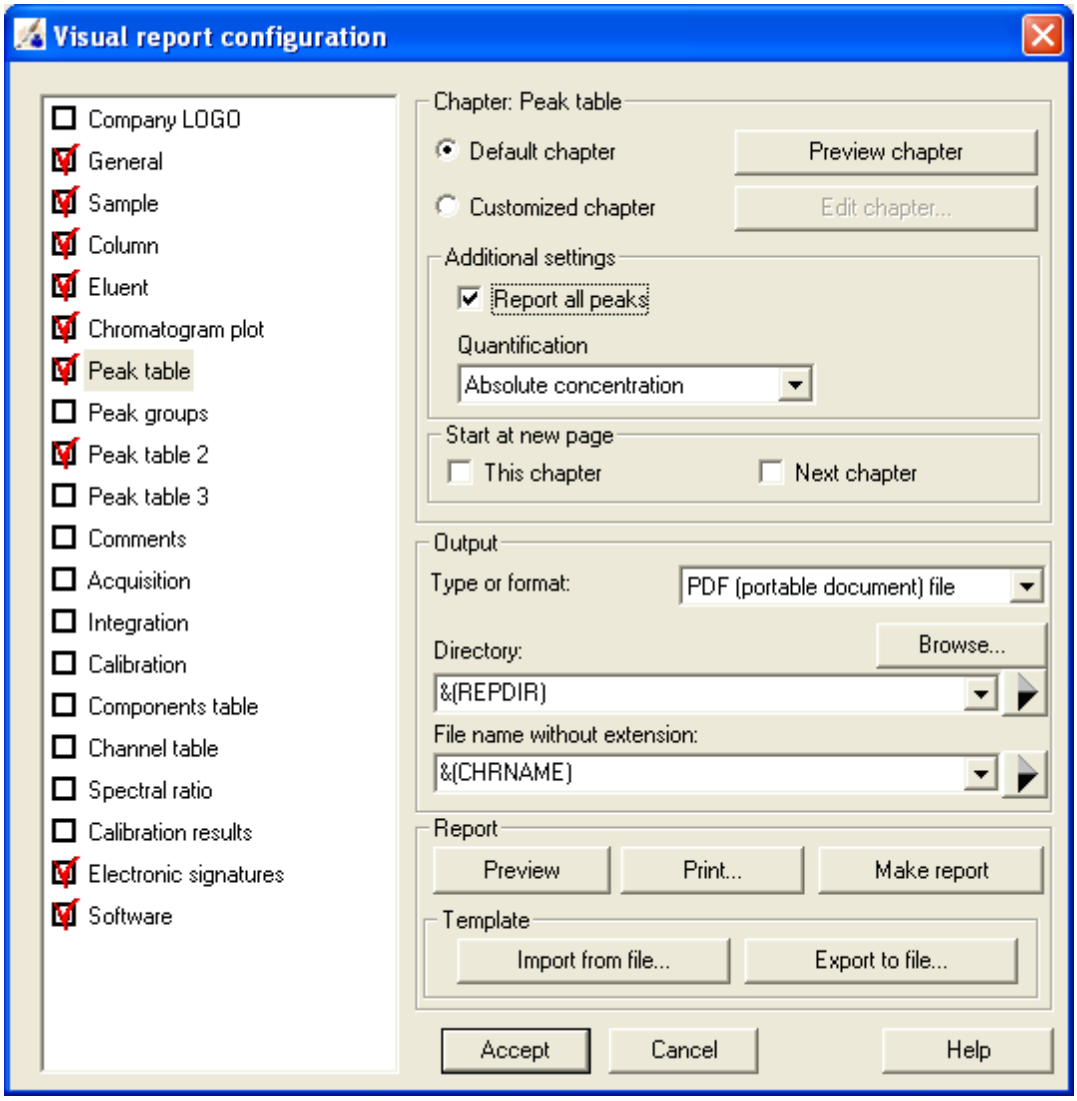
Typically the window is called from **Method setup: "Reports" page** 145 (by ***<Add>*** or ***<Edit>*** buttons).

This window is also used in:

- **Quick reports** 33 option (***<Make other report>*** button) for producing **advanced report** 341 without configuring **method** 122.
- **Analysis report** 258 and **calibration report** 263 options of the **sample queue** 237 for configuring the

report template.

See **configuring advanced reports** 342 article for general description of configuring **advanced report** 341.



Chapters

The **advanced report** 341 is organized as a set of **chapters** 346 which are printed in the report one after another. The left panel of the **Advanced report configuration** window displays the list of available chapters. User includes the chapter into report by putting a check mark ☑ near it.

Chapter: (Chapter title)

Each **chapter** 346 can be individually configured. To configure a chapter click the text label in the list of available chapters to select it. The currently selected item is drawn in dark background.

Note: User should differentiate two different actions with items in the list: checking item with a check mark  to include the chapter into the report and selecting item by clicking text label for configuring chapter.

An area at the top-right of the window (it is titled **Chapter: [chapter label]**) displays configurable options for the **chapter** 346.

Typically these options contain:

⊙ **Default chapter**	The default configuration for the **chapter** is used. Setting this option resets the configuration of the chapter to the default state. The language for the default configuration is the same as specified at **choose UI language** 44 window.
⊙ **Customized chapter**	Activates ***<Edit chapter...>*** button for editing chapter with **Report designer** 378.
<Preview chapter>	Displays a **preview window** for the selected **chapter** only.
<Edit chapter...>	Press this button to launch a **Report Designer window** 381 for configuring the contents of the chapter. Note that using **report designer** 378 may require some experience from the user.

Start at new page

☑ **This chapter**	Forces page break in the report output before the selected chapter.
☑ **Next chapter**	Forces page break in the report output after the selected chapter.

Other chapter-specific configuration options may be displayed (for example **peak table** 349 has additional options). See individual description for the **chapter** in the **chapters** 346 list.

Output

The **Output** area of the window contains settings related to specifying the output destination for the report.

Type or format Specifies the output destination for the report. Other options appear below depending upon what is selected here.

Here is a list of available options:

Screen	The report will be generated to the screen. No additional options.
Printer	The report will be printed. Additional options are displayed allowing user to select a printer for the report and to define printing preferences for it.

RTF (rich text) file

PDF (portable document) file

HTML (web page) file

Text (comma delimited) file

Text (tab delimited) file

All these items define a set of file output options (**RTF**, **PDF**, **HTML** and several text formats)
Additional options are displayed allowing user to specify a directory and file name for the report. Note that special file and directory macro language 486 can be used for specifying file names.

Report

The **Report** area allows user to perform various actions with configured report template.

<Preview> Displays a **preview window** for the entire report. All checked **chapters** 346 are included to the report as it would be in the final output (compare this action with action of ***<Preview chapter>*** button).

<Print...> Prints the report. The **printer configuration** window is displayed allowing user to select a printer and to define printing preferences. The settings specified in the **Output** area are ignored.

<Make report> Generates report using the settings specified in the **Output** area.

Note: The functions producing report (such as ***<Preview>***, ***<Print...>*** and ***<Make report>***) use the **saved copy of the chromatogram**, which is stored in the chromatogram file. User may open chromatogram and modify it. Still all modifications **will not** be reflected in the report until user finish his modifications and save chromatogram to file. This behavior differs from the **plain reports** 320 which immediately reflect all modifications done by the user.

<Import from file...> Import the entire **report template** 379 from the external file ***.ftt**.

<Export to file...> Export this **report template** 379 to the external file ***.ftt**.

Using exporting and importing functions allows user to exchange**report templates** 379 between different **methods** 122 (that is to reuse **report templates**). Also **report template** can be configured for sample chromatogram, exported and then imported into the **sample queue** 237 (see **analysis report** 258 and **calibration report** 263).

<Accept> Applies all changes to the **report template** 379 and close this window

<Cancel> Cancels all modifications of the **report template** 379 and close this window

See also:

Advanced reports 341

Configuring advanced reports 342

Features and capabilities of advanced reports 342

10.1.2.2.1.1 Chapters

The **advanced report** 341 for individual analysis is organized as a set of **chapters** which are printed in the report one after another.

The list of all available **chapters** is displayed in the left panel of the **Advanced report configuration** 343 window. User includes the **chapter** into report by putting a check mark near it.

Review the general **chapters of advanced reports** 380 article for details about **chapters**.

The following chapters are available for the **advanced reports** 341 for individual analysis:

Company LOGO 347
General 347
Sample 348
Column 348
Eluent 348
Chromatogram plot 348
Peak table 349
Peak groups 353
Comments 333
Acquisition 354
Integration 354
Calibration 354
Components table 355
Channel table 356
Spectral ratio 356
Calibration results 357
Electronic signatures 357
Software 358

See also:
Advanced reports 341
"Advanced report configuration" window 343

This chapter is designed to represent a general header of the report.
User can modify the chapter to include the company name, company logo and other appropriate information.

No tables and **sort fields** 401 are assumed for this chapter.

See also:
Chapters 346

This chapter represents the general description and settings for the analysis.
Typically this chapter refers to the **General** 124 page. Still it can also contain other data on user's choice.

No tables and **sort fields** 401 are assumed for this chapter.

See also:
Chapters 346

This chapter represents the description of the sample.
Typically this chapter refers to information from **Sample** 126 page and lists custom sample parameters specified at the **Extra** 128 page.

The chapter can produce the only table displaying custom sample parameters from the **Extra** 128 page. This table needs no **sort fields** 401.

See also:
Chapters 346

This chapter represents the description of the column.
Typically this chapter refers to information from **Column** 130 page.

No tables and **sort fields** 401 are assumed for this chapter.

See also:
Chapters 346

This chapter represents the description of eluting conditions (flow, pressure, temperature) and descriptions of eluents.
Typically this chapter refers to information from the **Eluent** 131 page.

No tables and **sort fields** 401 are assumed for this chapter.

See also:
Chapters 346

This chapter is designed to display a plot of the chromatogram.

The chapter can also contain another data related to the analysis on user's choice. The default **report template** displays the analysis sequence number, analysis date and time, operator name. If some preprocessing options are defined in the **Method setup: "Smoothing" page** 132 then these options are

also displayed in this section by default.

No tables and **sort fields** 401 are assumed for this chapter.

See also:
Chapters 346

Peak table is a main chapter of the ***advanced report*** 341 producing the results of the analysis.

This chapter contains a table which lists identified components, their concentrations and/or other peak metrics which are needed. It can also contain other data on user's choice.

The chapter has individual settings which are displayed in the **Additional settings** area of the **Advanced report configuration** 343 window when **peak table** item is selected. (See **Advanced report configuration** 343 about selecting chapter item.)

☑ **Report all peaks**	When checked all detected peaks are processed in the report. When not checked recognized peaks only are processed in the report. The concentration of the unrecognized peaks are reported as zero (because those peaks are not calibrated). Still other peak metrics, such as **peak area** and **peak height** are calculated and reported.
Quantification template	Software supplies several predefined configurations corresponding to most common **quantification procedures** 201. User can select one of the predefined templates from this list. It is also possible to create a customized configuration of the **peak table** based on the predefined templates. To do that select the most appropriate template from **Quantification template** list, select ⊙ **Customized chapter** in the **Advanced report configuration** 343 window and press ***<Edit chapter...>*** button to launch a **report designer** 378. Note that **Quantification template** option is similar to **Quantification method** 329 option for **peak table of plain report** 327. Below is a list of the predefined configurations (compare it with a **Quantification method** 329 option) ***Response normalization*** ***Normalized concentration*** ***Absolute concentration*** ***Relative concentration*** ***Index***

All peak parameters listed in the **custom method** 332 (for plain reports) are available for customization of **peak table** chapter.

Additionally several advanced metrics are supplied for **peak table** of ***advanced reports***:

uncertainty of concentration 350

lower uncertainty of concentration 351

upper uncertainty of concentration 351

relative uncertainty, % 352

lower relative uncertainty, % 352

upper relative uncertainty, % 352

gaussian factor 353

User-defined formulas 288 can be used along with predefined peak parameters. **User-defined formulas** 288 is a powerful tool for defining specific peak parameters and creating specific procedures for calculating concentrations. **User-defined formulas** 288 are configured for **method** at the **Method setup: "Quantification" page** 144 (***<My formulas>*** button).

Peak table chapter supplies several **sort fields** 401 for customizing peak table:

peak number (PEAK_NUMBER) - The sequence number of the peak in the **chromatogram**.

group (PEAK_GROUP) - The **group** 173 of the peak.

formula number (MF_INDEX) - The sequence number of the **user-defined formula** 288 specified in the processing **method**.

If no **sorting sections** 387 are specified then the implicit sorting is assumed:

1. ***peak number (PEAK_NUMBER)***
2. ***formula number (MF_INDEX)***.

The sorting of the predefined report templates for **peak table** is:

1. ***peak number (PEAK_NUMBER)*** (explicit - defined by **sorting section** 387)
2. ***formula number (MF_INDEX)***. (implicit)

User can specify up to 3 different **peak table** chapters in the report ("***Peak table***", "***Peak table 2***", "***Peak table 3***"). Additionally **peak groups** 353 chapter is available.

Peak groups 353 chapter is a chapter which is processed in the same way as **peak table** chapter. Still **peak groups** 353 chapter supplies an alternative predefined templates with a different sorting. The sorting of the predefined **peak groups** 353 templates is:

1. ***group (PEAK_GROUP)*** (explicit - defined by **sorting section** 387)
2. ***peak number (PEAK_NUMBER)*** (implicit)
3. ***formula number (MF_INDEX)*** (implicit)

See also:

Chapters 346

"Advanced report configuration" window 343

User-defined formulas 288

Peak table of plain report 327

The maximal value from **lower uncertainty of concentration** 351 and **upper uncertainty of concentration** 351

The lower (negative) limit of **confidence region** in concentration units, which is defined from **confidence region** of **calibration curve** [182] of the ***component*** associated with the peak.

The **confidence region** (or **confidence band**) is calculated for the **confidence probability** specified in the **Calibration graphs** [178] window (see **calibration curve** [182] and **calibration inaccuracy** [183]).

For a measured detector **response** [200] the **confidence region** for **computed quantity** [201] is calculated as described in the **confidence intervals for weighted polynomial calibrations** [490] article.

The returned value is calculated as

$$\Delta_C^{lower} = \frac{\Delta_Q^{lower}}{V'}$$

where

Δ_C^{lower} - returned **lower uncertainty of concentration**

Δ_Q^{lower} - lower uncertainty of **quantity** [201], calculated from **confidence region** of **calibration curve** [182]

V' - adjusted volume [199] of the analyte.

The upper (positive) limit of **confidence region** in concentration units, which is defined from **confidence region** of **calibration curve** [182] of the ***component*** associated with the peak.

The **confidence region** (or **confidence band**) is calculated for the **confidence probability** specified in the **Calibration graphs** [178] window (see **calibration curve** [182] and **calibration inaccuracy** [183]).

For a measured detector **response** [200] the **confidence region** for **computed quantity** [201] is calculated as described in the **confidence intervals for weighted polynomial calibrations** [490] article.

The returned value is calculated as

$$\Delta_C^{upper} = \frac{\Delta_Q^{upper}}{V'}$$

where

Δ_C^{upper} - returned **upper uncertainty of concentration**

Δ_Q^{upper} - upper uncertainty of **quantity** 201, calculated from **confidence region** of **calibration curve** 182

V' - adjusted volume 199 of the analyte.

The maximal value from **lower relative uncertainty, %** 352 and **upper relative uncertainty, %** 352

Returns **lower relative uncertainty**, in **%**, which is defined from **confidence region** of **calibration curve** 182 of the ***component*** associated with the peak.

The **confidence region** (or **confidence band**) is calculated for the **confidence probability** specified in the **Calibration graphs** 178 window (see **calibration curve** 182 and **calibration inaccuracy** 183).

For a measured detector **response** 200 the **confidence region** for **computed quantity** 201 is calculated as described in the **confidence intervals for weighted polynomial calibrations** 490 article.

The returned value is calculated as

$$\Delta_R^{lower} = \frac{\Delta_Q^{lower}}{Q} \cdot 100\%$$

where

Δ_R^{lower} - returned **lower relative uncertainty**

Δ_Q^{lower} - lower uncertainty of **quantity** 201, calculated from **confidence region** of **calibration curve** 182

Q - **computed quantity** 201 of the component associated with the peak.

Returns **upper relative uncertainty**, in **%**, which is defined from **confidence region** of **calibration curve** 182 of the ***component*** associated with the peak.

The **confidence region** (or **confidence band**) is calculated for the **confidence probability** specified in the **Calibration graphs** 178 window (see **calibration curve** 182 and **calibration inaccuracy** 183).

For a measured detector **response** [200] the **confidence region** for **computed quantity** [201] is calculated as described in the **confidence intervals for weighted polynomial calibrations** [490] article.

The returned value is calculated as

$$\Delta_R^{upper} = \frac{\Delta_Q^{upper}}{Q} \cdot 100\%$$

where

Δ_R^{upper} - returned **upper relative uncertainty**

Δ_Q^{upper} - upper uncertainty of **quantity** [201], calculated from **confidence region** of **calibration curve** [182]

Q - **computed quantity** [201] of the component associated with the peak.

This special value is calculated as

$$Gs = 1.83 \cdot \frac{W_{50\%}}{W_{10\%}}$$

where

$W_{N\%}$ is a width of the peak calculated at specified percent of the peak **height** [334]. See also *Section* [296] macro in **user-defined formulas** [288].

Peak groups chapter is similar to **Peak table** [349] chapter.

This chapter is processed by software exactly in the same way as **Peak table** [349] chapter.

Peak groups and **Peak table** [349] chapters differ only in predefined report templates.

The predefined report templates for **peak groups** chapter are designed with the following sorting:

1. ***group (PEAK_GROUP)*** (explicit - defined by **sorting section** [387])
2. ***peak number (PEAK_NUMBER)*** (implicit)
3. ***formula number (MF_INDEX)*** (implicit)

See **peak table** 349 chapter for more details.

Note that report templates designed for **peak groups** chapter can be used in the **peak table** 349 chapter and vice-versa.

See also:
Chapters 346
"Advanced report configuration" window 343
Peak table of plain report 327

This chapter represents instrument parameters defined in the data acquisition **system** 79.

Typically the content of this chapter is similar to the report produced with **print system parameters** 92 menu command.
The data for this chapter are taken from the acquisition **system** 79 at the moment when analysis starts. The **chromatogram** 207 stores these data in its file so that they cannot be modified any more.
So **acquisition** chapter displays instrument parameters as they were specified during **chromatogram** 207 acquisition.

No tables and **sort fields** 401 are assumed for this chapter.

See also:
Chapters 346

This chapter contains parameters of **peaks integration procedure** 159.
Typically this chapter presents information of **Integration setup** 160 and lists **Integration events** 162.

If **Integration events** 162 are present the chapter produces the corresponded table.
No **sort fields** 401 are assumed for this chapter.

See also:
Chapters 346

This chapter contains parameters of the **calibration** 165.

Calibration chapter supplies several **sort fields** 401 for customizing corresponded tables:

component ID (COMP_ID) - The sequence number of the component as it is viewed in the

Components table 171

level ID (LEVEL_ID) - The identification number of the **calibration level** 199 as it is viewed in the **Concentrations table** 174

If no **sorting sections** 387 are specified then the implicit sorting is assumed:

1. ***component ID (COMP_ID)***.
2. ***level ID (LEVEL_ID)***.

Calibration, **Component table** 355 and **Calibration results** 357 chapters are processed by software exactly in the same way.

These chapters are differed only in default report templates. Still report template designed for one of the above chapters can be used for another chapter without restrictions.

The default report template of the **Calibration** chapter displays calibration parameters common for all components. These parameters are taken from **Calibration graphs** 178 and **Peak identification** 166 windows.

Also the default report template displays a table of calibration chromatograms similar to that displayed in the **Levels Specific Info** 177 window. To produce this table the template defines the following sorting:

1. ***level ID (LEVEL_ID)*** (explicit - defined by **sorting section** 387).
2. ***component ID (COMP_ID)*** (implicit).

Note: User can specify individual calibration settings for some components. This is done at **Calibration graphs (advanced)** 178 window by setting **Local** options (see **calibration parameters** 186). **Local** component settings **are not** displayed at this chapter. Use **calibration results** 357 chapter to view **Local** component settings in the report.

See also:

Chapters 346

Component table 355

Calibration results 357

This chapter is processed in the same way as **calibration** 354 chapter.

The default report template of the chapter produces a ***components table*** similar to that displayed in the **Components table** 171 window.

To produce this table the template defines the following sorting:

1. ***component ID (COMP_ID)*** (implicit).
2. ***level ID (LEVEL_ID)*** (implicit).

For more details about processing **Components table** chapter review **calibration** 354 chapter.

See also:
Chapters 346
Calibration 354
Calibration results 357

This chapter contains parameters of the analytical 113 and calculated 152 channels of the chromatogram.

Typically this chapter produces **local channels table** similar to that displayed at the Channels 148 page (the calculated 152 channels are generated based on settings at Calculated channels 151 page). The table also presents results of noise calculations for each channel (see Method setup: "Noise" page 142 and ***Remarks*** at this article).

No sort fields 401 are assumed for this chapter.

See also:
Chapters 346

The most common task of this chapter is to produce the table of spectral ratio 339 for all peaks and for all channels for the multi-channel chromatograms 146.
The default report template is functionally mostly equivalent to spectral ratio 325 chapter of the plain reports 320.

Still by redesigning the report template this chapter can be configured for performing other more complicated tasks.
All peak parameters available for peak table 349 chapter are also available for this chapter (excluding user-defined formula 288).
Spectral ratio 339 is calculated relative to reference channel 197.

Spectral ratio chapter supplies several sort fields 401 for customizing corresponded tables:

peak number (PEAK_NUMBER)	- The sequence number of the peak in the **chromatogram**.
group (PEAK_GROUP)	- The group 173 of the peak.
channel index (PEAK_ISPECCHAN)	- The sequence number of the channel Channels 148 page; analytical 113 channels are followed by average and other statistical calculated 152 channels.

If no sorting sections 387 are specified then the implicit sorting is assumed:

1. ***peak number (PEAK_NUMBER)***.
2. ***channel index (PEAK_ISPECCHAN)***.

Default report template for **Spectral ratio** chapter uses the following sorting:

1. ***peak number (PEAK_NUMBER)*** (explicit - defined by **sorting section** 387).
2. ***channel index (PEAK_ISPECCHAN)*** (implicit).

See also:

Chapters 346

Peak table 349

Channel table 356

This chapter is processed in the same way as **calibration** 354 chapter.

The default report template of the chapter produces results of calibration for each component. Functionally the chapter is mostly equivalent to the **calibration results** 325 chapter of the **plain reports** 320.

For each component from the **Components table** 171 window a separated page is generated (it is possible to create more compact reports without splitting to pages by redesigning the default report template).

Typically each page contains calibration settings for component (specified in **Calibration graphs** 178 window taking into account **Local** flags defined for component), the equation and plot of **calibration curve** 182 for component and a set of metrics which indicate the accuracy of the calibration. Report also produces a table of calibration points used to build a **calibration curve** 182 for component. The table is similar to that displayed in the **Calibration graphs** 178 window.

Default report template for **Calibration results** chapter uses the following sorting:

1. ***component ID (COMP_ID)*** (explicit - defined by **sorting section** 387).
2. ***level ID (LEVEL_ID)*** (implicit).

For more details about processing **Components table** chapter review **calibration** 354 chapter.

See also:

Chapters 346

Calibration 354

Component table 355

This chapter produces a table which lists all **electronic signatures** 61 applied to the chromatogram.

The default report template prints data from the **Signatures window** 66. Besides it prints details related to **user certificate** 55 corresponded to each **electronic signature** 61.

Remember that ***21 CFR part 11*** compliant reports must be stored as ***.PDF** documents and must be independently signed (see **Electronic signature for PDF reports** 62).

Review the **FDA 21 CFR part 11 compliance** 54 article for more details.

No **sort fields** 401 are assumed for this chapter.

See also:
Chapters 346
FDA 21 CFR part 11 compliance 54

This chapter is designed to represent a general footer of the report.
The default report template prints software name and version information.

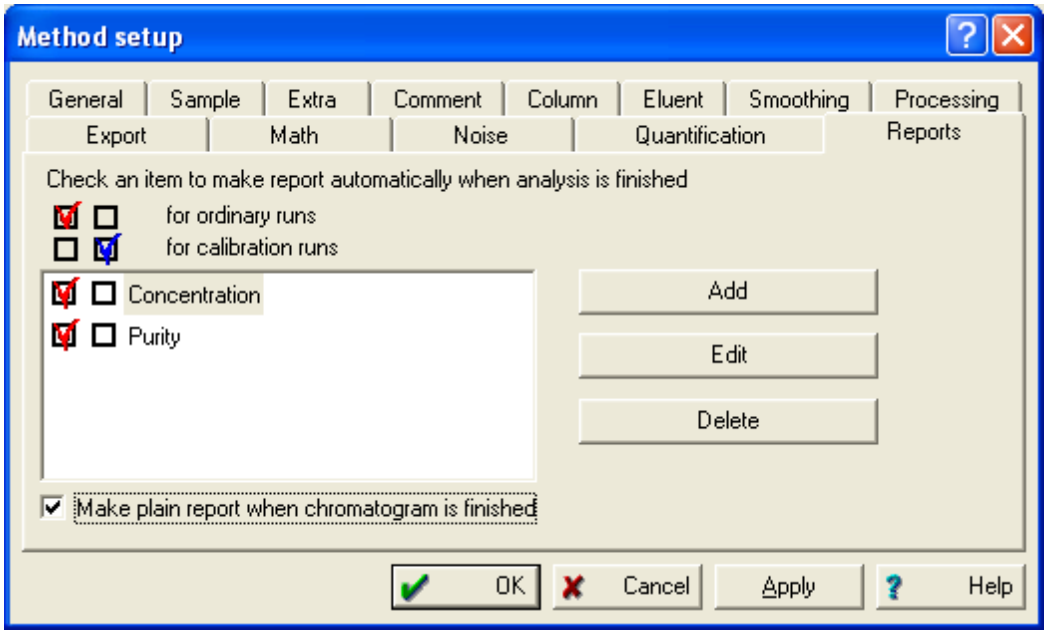
No tables and **sort fields** 401 are assumed for this chapter.

See also:
Chapters 346

10.1.2.2.2 "Reports" page

(*Main menu* Report / Report setup...)

Reports page is a part of the **Method setup** 124 window. It allows to define templates for **advanced reports** 341 for chromatograms running this method.



One or more **advanced reports** 341 could be defined. Each report could have it's own layout and could be directed to its own output(file of specified format, printer, screen).

User could put a check mark for the report item to generate report automatically when analysis finished: for ordinary runs, for calibration runs or both.

<Add>	add a new report template to the list. "***Add report***" window is opened prompting to enter a name of a new ***report***. Then "***Edit report template***[343]" form is opened. User can define report items and configure report layout.
<Edit>	Opens "***Edit report template***[343]" form for the selected item for editing report template.
<Delete>	Delete the selected report item.

☑ **Make plain report when chromatogram is finished**

check this box to produce a **plain report**[320] (in addition to the advanced reports) when a chromatogram is finished.

See also:
Quick reports[33]

10.2 Summary reports

Summary reports combine results produced by several **chromatograms**[207] into the single report.

An important function of the **summary reports** is a possibility to calculate various statistical metrics of user-specified chromatographic parameters. This allows analyzing how the parameters vary from run to run.

Two types of **individual analysis reports** are available in **Chrom&Spec** software:

Plain statistics reports[360] - ease-to-use tool with simple configuration which produces text output.

Advanced summary reports[366] - an advanced tool which allows user to fully customize the view of the report, perform complicated statistical computations and produce reports in various document formats.

To overview **summary reports** see also a general **Reports**[318] article.

See also:
Reports[318]
Individual analysis reports[320]
Statistics window[375]
Summary report (sample queue)[260]
Vial summary report (sample queue)[259]

10.2.1 Plain statistics reports

Plain statics report is an ease-to-use tool with simple configuration which produces text output.

Plain statics report allows user to combine chromatographic results from a set of chromatograms and calculate statistical metrics for **peak parameters** of the recognized **components** 171.

The list of **peak parameters** which can be handled by **plain statics report** is similar to that defined for **peak table** 327 (see **custom peak parameters** 332):

- **retention time** 333
- **width (h/2)** 334
- **height** 334
- **height%** 334
- **area** 334
- **area%** 334
- **capacity factor** 335 *k* 335
- **resolution** 335
- **efficiency TP** 335
- **efficiency, TP/m** 335
- **reduced TP height** 335
- **signal/noise** 336
- **asymmetry** 336
- **response factor** 336
- **concentration** 337
- **concentration%** 337
- **rel. concentration** 337
- **rel. concentration%** 338
- **quantity** 338

For each selected **component** 171 and each selected **peak parameter** the following statistical metrics can be calculated:

Max - maximal value of **peak parameter** (for the set of chromatograms)

Min - minimal value of **peak parameter** (for the set of chromatograms)

Mean - mean (average) value of **peak parameter** (for the set of chromatograms)

StdDev - corrected standard deviation of the **peak parameter**. It is calculate as:

$$StdDev = \sqrt{\frac{\sum (p_i - \bar{p})^2}{N-1}}$$

where summation is performed for all chromatograms in the set

%RSD - relative standard deviation, in percent; it is calculated as

$$\%RSD = 100\% \cdot \frac{StdDev}{Mean}$$

NegDev/RSD - negative deviation factor; it is calculated as *(Min - Mean) / StdDev*

PosDev/RSD - positive deviation factor; it is calculated as *(Max - Mean) / StdDev*

Statistic options 361 window form is used for most configurations for **plain statics report**. Here user can specify a list of **peak parameters** of interest, define a list of components or **groups** 173 of components, specify output format of the report (**report type**).

Generated **plain statics report** can be viewed with any plain text viewer. By default the **Notepad** program is used (it is supplied with any version of ***Windows***).
User can change report viewer using **Statistics: Advanced...** 365 configurations.

The **plain statics report** can be produced in **Chrom&Spec** software using:

1. **Open chromatogram** 207 window form. Press **<Statistics...>** button and use **Plain report** page of the **Statistics window** 375 to make settings for report.
2. The **batch reprocessing** 271. Open **"Reprocess" window form** 273, check ☑ **Statistics** option and press ***<Edit statistics options>*** button to make settings for report.

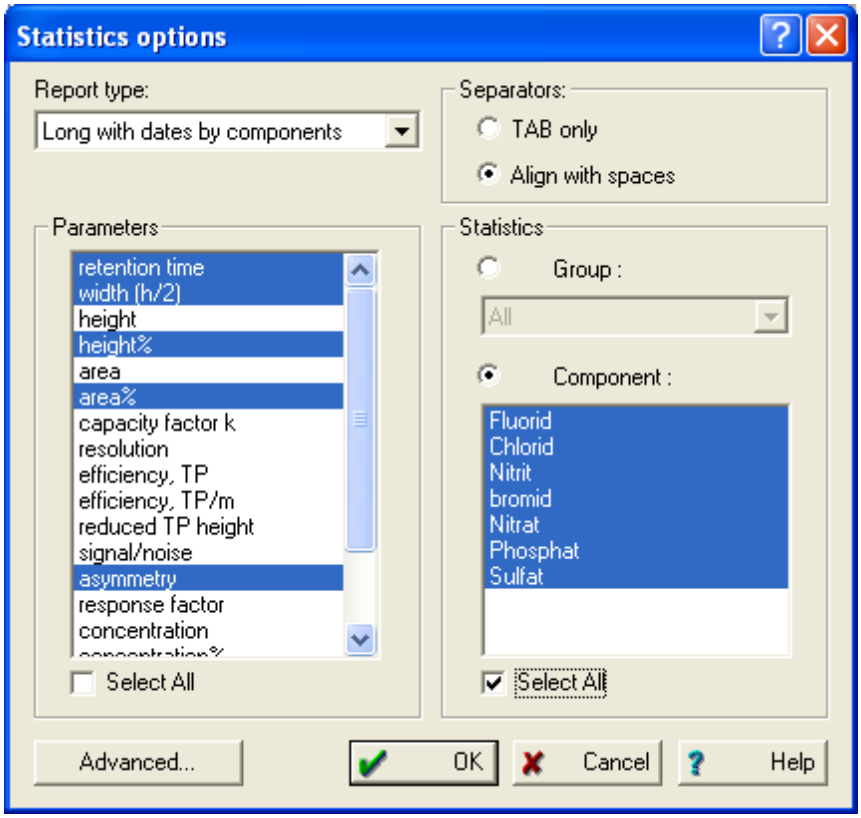
See also:

Statistics options window 361
Statistics window 375
Advanced summary reports 366
Summary reports 359
Reports 318

10.2.1.1 Statistics options

Statistics options window is used for configuring **plain statistics reports** 360.

Statistics options window is opened form the **Reprocess** 273 window by pressing ***<Edit statistics options>*** button.
The similar page is displayed in the **Statistics** 375 window (as **Plain report** 375 page); **Statistics** 375 window is opened form **Open chromatogram** 207 window by pressing the **<Statistics...>** button.



Report type

Specifies the output form of the report

Several predefined report forms are available

Short by components	short format
Long by components	the most complete format but without date/time column
Long with dates by components	the most complete format with date/time column
Short by parameters	short format
Long by parameters	the most complete format but without date/time column
Long with dates by parameters	the most complete format with date/time column

Reports ***"... by components"*** generate outputs ordered by *components* first: for each selected *component* all selected *parameters* are reported.

Reports ***"... by parameters"*** generate outputs ordered by *parameters* first: for each selected *parameter* all selected *components* are reported.

Reports ***"Short ..."*** generate short report output including statistical metrics only (see **plain statistics reports** 360) of the selected parameters.

Reports ***"Long ..."*** generate report output including values from each processed chromatogram and resulting statistical metrics of the selected parameters.

Reports ***"Long with dates ..."*** are similar to ***"Long ..."*** but include **sample date and time** 126 for each processed chromatogram.

Separators

Select the separator between columns in the tables of the report

⊙ ***TAB only*** use tabs between columns in the report. It is useful when the report output is further processed by ***Microsoft Excel*** or another table-oriented viewer.

⊙ ***Align with spaces*** columns of tables are aligned with spaces. Use this option to view the results in the simple text viewers, ***Notepad*** for example.

Parameters

Specifies a list of parameters that will be used for calculations and report output.

The list of **peak parameters** which can be handled by **plain statics report** is similar to that defined for **peak table** 327 (see **custom peak parameters** 332):

- **retention time** 333
- **width (h/2)** 334
- **height** 334
- **height%** 334
- **area** 334
- **area%** 334
- **capacity factor** 335 *k* 335
- **resolution** 335
- **efficiency TP** 335
- **efficiency, TP/m** 335
- **reduced TP height** 335
- **signal/noise** 336
- **asymmetry** 336
- **response factor** 336
- **concentration** 337
- **concentration%** 337
- **rel. concentration** 337
- **rel. concentration%** 338
- **quantity** 338

☑ **Select all** check this flag to select all available parameters in the list

⊙ Group

Select a **group** 173 for statistical calculations.

It is possible to select any **group** 173 defined in the **Components table** 171 or ***"All"*** item.

An **example chromatogram** 364 is used for reading components and **groups** from.

All components belonging to the selected **group** are processed and reported.

If ***"All"*** item is selected the statistics is done for all components (components of all available **groups** 173 including components with ***zero*** **group**).

⊙ Component

Select **component** or several **components** from the list for statistical calculations.

All selected components are processed and reported.

An **example chromatogram** 364 is used for reading list of components from.

All components defined in the **components table** 171 are available.

☑ Select all check this flag to select all available components

<Advanced...> Opens **Statistics: Advanced...** 365 window for additional configurations of the report output.

See also:

Plain statistics reports 360

Example chromatogram 364

Batch reprocessing window 273

Statistics window 375

10.2.1.1.1 Example chromatogram (plain statics report)

Configuration of **plain statistics reports** 360 requires some information from the **method** 122.
Specifically, the list of components and **groups** 173 settings from **components table** 171 are needed.

Each **chromatogram** 207 stores a copy of the its **method** 122. So the required information is taken form the **example chromatogram** rather then from the **method** 122 file. This is done to avoid inconsistencies between copy of the **method** 122 stored in the chromatograms and **method** 122 file: statistic may be performed at old chromatograms which were acquired some time ago and **method** 122 file may be modified since that time.

When **plain statistics reports** 360 is done from **batch reprocessing** 271 then its **example chromatogram** 273 is also an **example chromatogram** for statistics.

When **plain statistics reports** 360 is configured from **Open chromatogram** 207 window then **current chromatogram** (see **Open chromatogram** 207) is an **example chromatogram** for statistics.

Note: Statistic calculations assume that all proceeded chromatograms were acquired with the same processing method 122 and contain the same components table 171. If it is not so then the results of the statistical report may be incorrect.

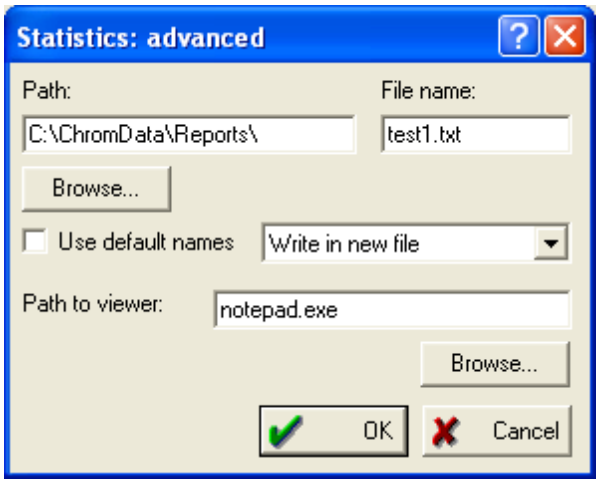
See also:

Plain statistics reports 360
"Statistic options" window 361

10.2.1.1.2 Statistics: advanced

Statistics: advanced dialog box is opened by clicking ***<Advanced...>*** button in the **Statistic options** 361 window.

It allows to set additional options related to the statistical report output.



Path User-defined output directory for the **plain statistics report** 360

<Browse> Press this button to navigate and select another output directory.

File name User-defined name of the output file for the **plain statistics report** 360;

☑ **Use default names**

The **Path** is set to the ***default report directory*** (see installation of the software 21).
The **File name** is set to automatically generated unique name.
The ***file overwriting*** is set to ***Overwrite old report***.
All these options are disabled so that user cannot modify them any more.
When statistics report is created and displayed user can change the name of the file and its location using **Save as...** function of the report viewer.

File overwrite settings

Overwrite old report If the file with the specified name already exists then the file will be destroyed; new file with the same name will be created containing the generated statistics report.

Write in new file If the file with the specified name already exists then new file name is generated appending several digital symbols to the user specified **File name**. This is done each time when statistic report is produced.

Path to viewer

Path and file name of the external program which will be used as viewer for statistics report.
The output of the **plain statistics report** 360 is a plain text file so any program which reads plain text can be used.
By default the ***Notepad*** program is used. It is supplied with any version of ***Microsoft Windows***.

User may wish to use ***Microsoft Excel*** program for additional calculations. In this case the full path to the ***Microsoft Excel*** should be specified. It is also recommended to set the ***TAB only*** **Separator** in the **Statistic options** 361 window.

<Browse> Press this button to navigate to and select the external program for report viewing.

See also:

Statistics options window 361

10.2.2 Advanced summary reports

Advanced summary reports is a powerful tool which allows combining results from the several analyses into the single report.

Reports can be configured for computation of statistical metrics of **peak parameters** 332 over the set of chromatograms (analogous to that of the **plain statistics reports** 360). The statistics can also be performed for special peak parameters specified with **user-defined formulas** 288. Additionally the build-in script engine and **user-defined formulas** 288 allow to perform various computations producing derived values from the results of several independent analyses.

The advanced capabilities of these reports are analogous to **advanced reports** 341 for individual analysis. Review also **Features and capabilities of advanced reports** 342 article.

Advanced summary reports can be stored as ***.PDF, *.RTF, *.HTML** or text files. Software supplies tools for previewing, displaying and printing reports. **Electronic signature** 62 can be applied to reports stored in ***.PDF** files.

The configuration of the **advanced summary reports** is based on the **report templates** 379 which are edited with **Summary report configuration** 367 window.

Software supplies a set of predefined report templates for most common tasks so that user can start using **advanced summary reports** with minimal configurations.

The **advanced summary reports** can be produced in **Chrom&Spec** software using:

1. **Open chromatogram** 207 window form. Press **<Statistics...>** button and use **Summary report** 376 page of the **Statistics window** 375 to configure and produce report.
2. The **sample queue** 237. **Summary reports** 260 and **Vial summary reports** 259 can be configured for a set of runs using **Options panel** 257 of **Sample queue editor** 245.
3. The **batch reprocessing** 271. Open **"Reprocess" window form** 273, check ☑ **Summary report** option and press ***<Edit summary report options>*** button to make settings for report.

See also:

"Summary report configuration" window 367

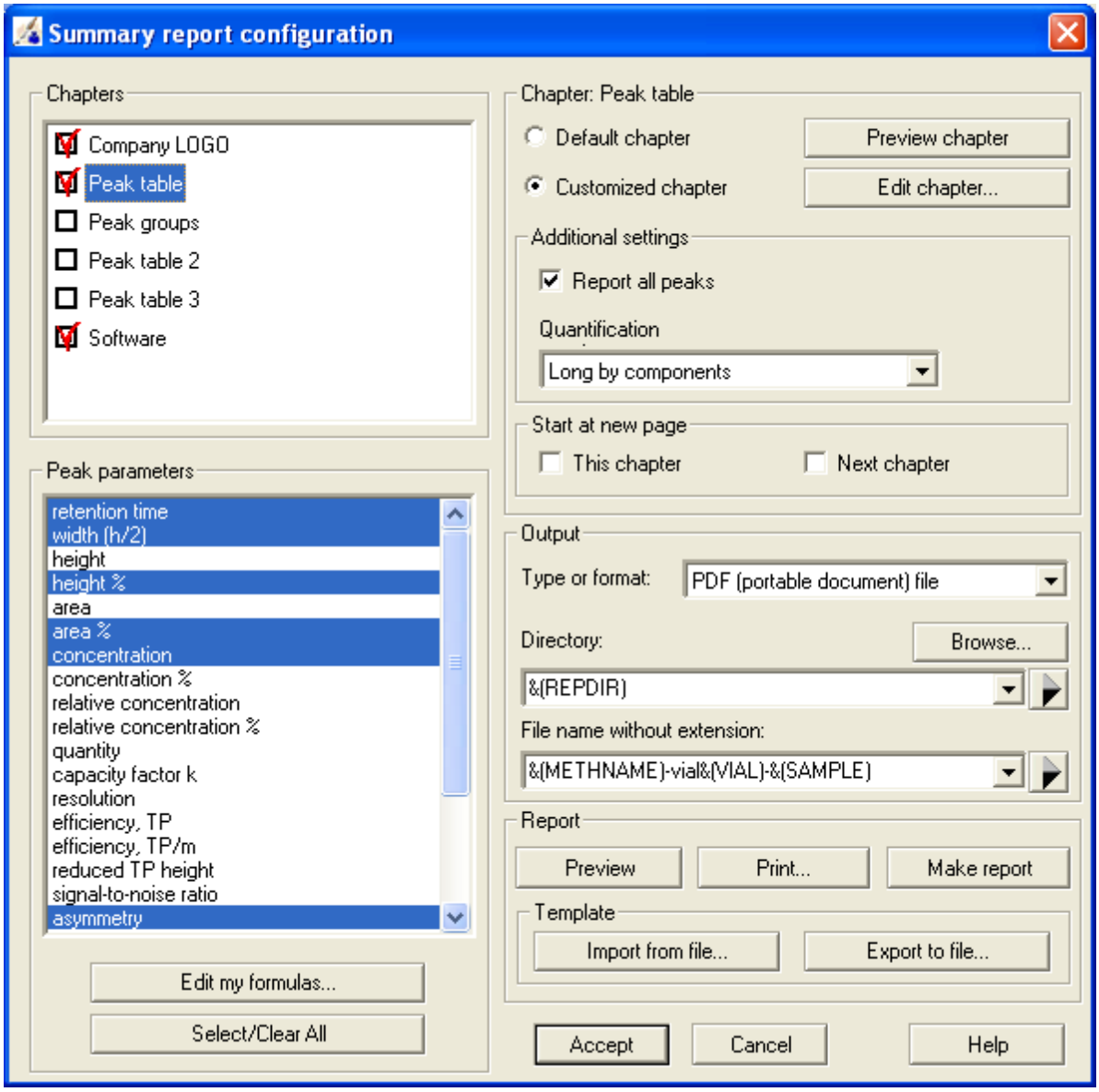
Summary reports 359

Plain statistics reports 360
Reports 318

10.2.2.1 Summary report configuration

Summary report configuration window.
This window is intended for configuring the report template 379 for advanced summary reports 366.

This window can be called from the Summary report 376 page, from Summary reports 260 and Vial summary reports 259 panels of Sample queue editor 245, and from "Reprocess" window form 273.



Chapters

The **Advanced summary report** 366 is organized as a set of **chapters** 372 which are printed in the report one after another. The left-top panel of the ***Summary report configuration*** window displays the list of available chapters. User includes the chapter into report by putting a check mark ☑ near it.

Chapter: (Chapter title)

Each **chapter** 372 can be individually configured. To configure a chapter click the text label in the list of available chapters to select it. The currently selected item is drawn in dark background.

Note: User should differentiate two different actions with items in the list: checking item with a check mark ☑ to include the chapter into the report and selecting item by clicking text label for configuring chapter.

An area at the top-right of the window displays configurable options for the **chapter** 372.
Typically these options contain:

⊙ **Default chapter**	The default configuration for the **chapter** is used. Setting this option resets the configuration of the chapter to the default state. The language for the default configuration is the same as specified at **choose UI language** 44 window.
⊙ **Customized chapter**	Activates ***<Edit chapter...>*** button for editing chapter with **Report designer** 378.
<Preview chapter>	Displays a **preview window** for the selected **chapter** only.
<Edit chapter...>	Press this button to launch a **Report Designer window** 381 for configuring the contents of the chapter. Note that using **report designer** 378 may require some experience from the user.

Start at new page

☑ **This chapter**	Forces page break in the report output before the selected chapter.
☑ **Next chapter**	Forces page break in the report output after the selected chapter.

Other chapter-specific configuration options may be displayed (for example **peak table** 372 has additional options). See individual description for the **chapter** in the **chapters** 372 list.

Peak parameter

This list displays an available **peak parameters**. User can select one, several or all parameters for building statistics in the summary report. See **peak parameters for summary reports** 370 for more details.

<Edit my formulas...>	Opens **Custom formulas** 289 window where user can specify **custom peak parameters**. See **peak parameters for summary reports** 370 for details.
<Select/Clear All>	Selects or clears all parameter.

Note that selection of **peak parameters** is optional. This selection may be required or may be not used depending upon the configuration of the **peak table** 372 **chapters**. The predefined configurations { ***Response normalization***, ***Normalized concentration***, ***Absolute concentration***, ***Relative concentration***, ***Index*** } do not use selection from ***Peak parameter*** list. The predefined configurations {***Short by components***, ***Long by components***, ***Long with dates by components***, ***Short by parameters***, ***Long by parameters***, ***Long with dates by parameters***} require no-empty selection from ***Peak parameter*** list.

Output

The area of the window contains settings related to specifying the output destination for the report.

Type or format	Specifies the output destination for the report. Other options appear below depending upon what is selected here.

Here is a list of available options:

Screen The report will be generated to the screen.
No additional options.

Printer The report will be printed. Additional options are displayed allowing user to select a printer for the report and to define printing preferences for it.

RTF (rich text) file
PDF (portable document) file
HTML (web page) file
Text (comma delimited) file
Text (tab delimited) file

All these items define a set of file output options (**RTF**, **PDF**, **HTML** and several text formats)
Additional options are displayed allowing user to specify a directory and file name for the report. Note that special **file and directory macro language** 486 can be used for specifying file names.

Report

The ***Report*** area allows user to perform various actions with configured report template.

<Preview> Displays a **preview window** for the entire report. All checked **chapters** 346 are included to the report as it would be in the final output (compare this action with action of ***<Preview chapter>*** button).

<Print...> Prints the report. The **printer configuration** window is displayed allowing user to select a printer and to define printing preferences. The settings specified in the **Output** area are ignored.

<Make report> Generates report using the settings specified in the ***Output*** area.

<Import from file...> Import the entire **report template** 379 from the external file ***.ftt**.

<Export to file...> Export this **report template** 379 to the external file ***.ftt**.

Using exporting and importing functions allows user to exchange **report templates** 379 between different **method** 122 (that is to reuse **report templates**). Also **report template** can be configured for sample chromatogram, exported and then imported into the **sample queue** 237 (see **analysis report** 258 and **calibration report** 263).

<Accept> Applies all changes to the **report template** 379 and close this window.
<Cancel> Cancels all modifications of the **report template** 379 and close this window.

10.2.2.1.1 Peak parameters for summary reports

The list of **peak parameters** which can be handled by **advanced summary report** 366 is similar to that defined for **peak table** 327 (see **custom peak parameters** 332):

retention time 333

Additionally user can define **custom peak parameters** using **user-defined formulas** 288 and process them as usual **peak parameters**.

Use ***<Edit my formulas...>*** button in the **Summary report configuration** 367 window to create or modify a list of **custom peak parameters**.

Pressing ***<Edit my formulas...>*** button opens **Custom formulas** 289 window where user can specify **custom peak parameters** using a special **macro-language** 291.

The specified **custom peak parameters** appear in the bottom of the ***Peak parameter*** list of the **Summary report configuration** 367 window. User can select them and process with the **summary report** in a regular way.

See also:
"Summary report configuration" window 367

10.2.2.1.2 Chapters

The **advanced summary report** 366 is organized as a set of **chapters** which are printed in the report one after another.

The list of all available **chapters** is displayed in the top-left panel of the **Summary report configuration** 367 window. User includes the **chapter** into report by putting a check mark near it.

Review the general **chapters of advanced reports** 380 article for details about **chapters**.

The following chapters are available for the **advanced summary report** 366:

Company LOGO 372
Peak table 372
Peak groups 374
Software 374

See also:
"Summary report configuration" window 367

10.2.2.1.2.1 Company LOGO

This chapter is designed to represent a general header of the report.

User can modify the chapter to include the company name, company logo and other appropriate information.

No tables and **sort fields** 401 are assumed for this chapter.

See also:
Chapters 372

10.2.2.1.2.2 Peak table

Peak table is a main chapter of the **advanced summary report** 366.

Generally the chapter is similar to the **peak table** 349 chapter of the **advanced reports** 341 for single analysis.

This chapter contains a table which displays identified components and corresponded **peak parameters** 370. Various statistical metrics can be calculated for each component and each **peak parameter** 370 over the set of chromatograms using build-in **report script engine** (see **calculated fields** 399).

Note that it is possible to combine build-in **report script engine** with **user-defined formulas** 288 which provide a wide capabilities in customizing your summary report.

The chapter has individual settings which are displayed in the **Additional settings** area of the **advanced summary report** 366 window when **peak table** item is selected. (See **advanced summary**

report 366 about selecting chapter item.)

☑ **Report all peaks** — When checked all detected peaks are processed in the report. When not checked recognized peaks only are processed in the report.
The concentration of the unrecognized peaks are reported as zero (because those peaks are not calibrated). Still other peak metrics, such as **peak area** and **peak height** are calculated and reported.

Quantification — Software supplies several predefined configurations corresponding to most common quantification procedures 201. User can select one of the predefined templates from this list.
It is also possible to create a customized configuration of the **peak table** based on the predefined templates. To do that select the most appropriate template from **Quantification template** list, select ⦿ **Customized chapter** in the advanced summary report 366 window and press ***<Edit chapter...>*** button to launch a report designer 378.

Below is a list of the predefined configurations (compare it with a Quantification method 329 option)

- ***Response normalization***
- ***Normalized concentration***
- ***Absolute concentration***
- ***Relative concentration***
- ***Index***
- ***Short by components***
- ***Long by components***
- ***Long with dates by components***
- ***Short by parameters***
- ***Long by parameters***
- ***Long with dates by parameters***

All peak parameters listed in the custom method 332 (for plain reports) are available for customization of **peak table** chapter. They are used for building simple summary reports based on predefined templates { **Response normalization**, ***Normalized concentration***, ***Absolute concentration***, ***Relative concentration***, ***Index*** }.

Statistical reports use another approach. User should select appropriate peak parameters in ***Peak parameter*** list of the Summary report configuration 367 ***window***. User-defined formulas 288 can be used to add custom peak parameters to the list. Predefined templates { ***Short by components***, ***Long by components***, ***Long with dates by components***, ***Short by parameters***, ***Long by parameters***, ***Long with dates by parameters*** } demonstrate basic approaches for building statistical reports.

Peak table chapter supplies several sort fields 401 for customizing peak table:

chromatogram data file name (CHR_FILE) - The name of the **chromatogram** data file form the summary set.

peak number (PEAK_NUMBER) - The sequence number of the peak in the **chromatogram**.

group (PEAK_GROUP) - The group 173 of the peak.

formula number (MF_INDEX) - The sequence number of the user-defined formula 288 specified in the processing **method**.

User can specify up to 3 different **peak table** chapters in the report ("***Peak table***", "***Peak table 2***", "***Peak table 3***"). Additionally **peak groups** 374 chapter is available.

Peak groups 374 chapter is a chapter which is processed in the same way as **peak table** chapter. Still **peak groups** 374 chapter supplies an alternative predefined templates with a different sorting.

See also:
Chapters 372
"Summary report configuration" window 367
User-defined formulas 288

10.2.2.1.2.3 Peak groups

Peak groups chapter is similar to **peak table** 372 chapter.

This chapter is processed by software exactly in the same way as **peak table** 372 chapter.

Peak groups and **peak table** 372 chapters differ only in predefined report templates.

Review the content of the predefined report templates to see what is a difference.

See **peak table** 372 chapter for more details.

Note that report templates designed for **peak groups** chapter can be used in the **peak table** 372 chapter and vice-versa.

See also:
Chapters 372
"Summary report configuration" window 367

10.2.2.1.2.4 Software

This chapter is designed to represent a general footer of the report.

The default report template prints software name and version information.

No tables and **sort fields** 401 are assumed for this chapter.

See also:
Chapters 372

10.2.3 Statistics (from Open chromatogram)

Statistics window is opened from **Open chromatogram** 207 form by pressing the **<Statistics...>** button. It allows to configure and immediately produce **plain statistics report** 360 or **advanced summary report** 366 for a selected set of **chromatograms** 207.

Before performing **statics** reports a required set of chromatograms must be selected in the **file list** 209 of the **Open chromatogram** 207.

Statistics window contains two pages:

Statistics: Plain report 375: for configuring and producing **plain statistics report** 360

Statistics: Summary report 376 for configuring and producing **advanced summary report** 366

<Make report> Press this button to generate the configured report. The type of the generated report relates to the page which is currently active: if **Plain report** 375 page is currently active then the **plain statistics report** 360 is created; if **Summary report** 376 page is currently active then the **advanced summary report** 366 is produced.

For details about configuring **statistics** reports see descriptions for each page of the ***Statistics*** window.

See also:

Summary reports 359
Open chromatogram window 207

10.2.3.1 Statistics: Plain report

Plain report page of the **Statistics** 375 window is used for configuring **plain statistics report** 360.

Functionally this page is equivalent to the **Statistics options** 361 window: review its documentation to know how to configure your report.

This page uses information from **example chromatogram** 364 - which is a **current chromatogram** from the **Open chromatogram** 207 window.

To get a **plain statistics report** 360 follow these steps**:**

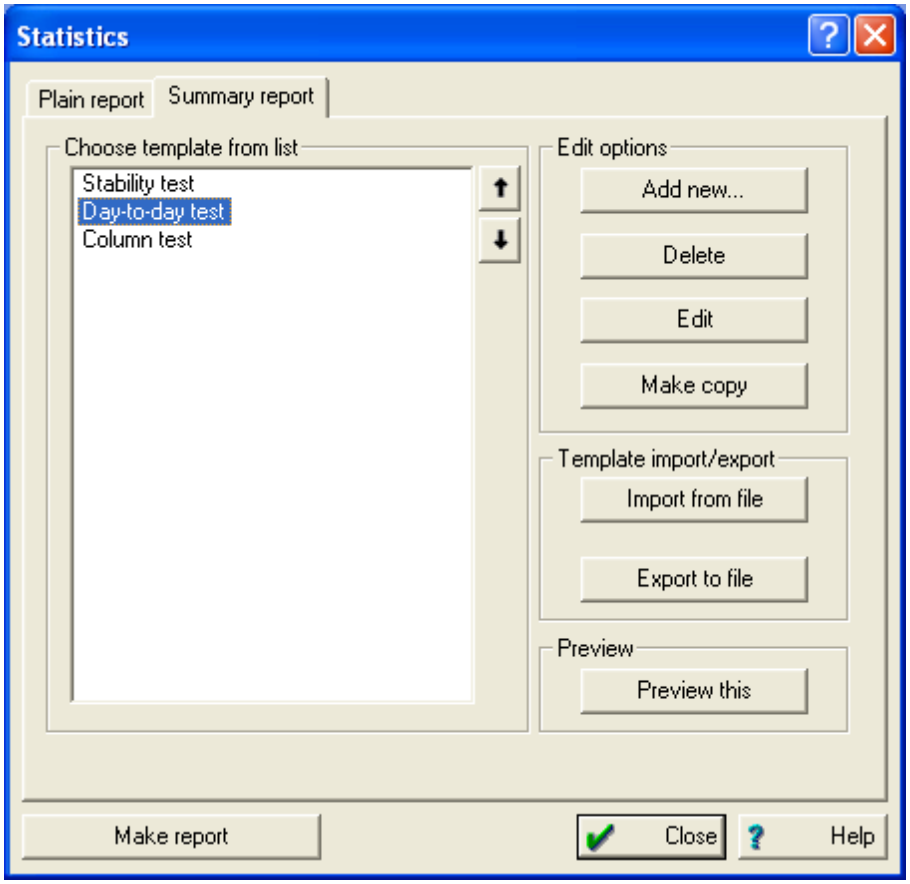
1. Select required chromatograms in the **Open chromatogram** 207 window.
2. Press **<Statistics...>** button in the **Open chromatogram** 207 window. **Statistics** 375 window is opened.
3. Make ***Plain report*** page active.
4. Make all necessary configurations.
5. Press ***<Make report>*** button.

See also:

Statistics window 375
Summary reports 359

10.2.3.2 Statistics: Summary report

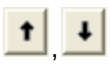
Summary report page of the Statistics 375 window is used for configuring report templates 379 for advanced summary reports 366, navigating through previously configured report templates 379 and producing advanced summary report 366 for a set of chromatograms selected in the Open chromatogram 207 window.



Choose template from list

This panel at the left part of the page contains a list of configured report templates 379 for advanced summary reports 366. Software stores this list so that configured report templates 379 can be reused later for another set of chromatograms.

One item in the list can be made selected by ***left-mouse-button*** click.


buttons can be used to order items by moving selected item upward or downward.

User can rename the selected item. To do it make a ***left-mouse-button*** click on the selected item again. Note that the second ***left-mouse-button*** click must not be too fast (otherwise the system would interpret it as ***double-click***)

The panels at the right part of the page are intended for **report templates** 379 editing and manipulation.

Edit options

<Add new...> - Create a new **report template** 379 for **advanced summary report** 366. User is prompted to enter name for **report template**. When done the **Summary report configuration** 367 window is opened where user can make configuration. When configuration is finished the name of the new **report template** is appears in the list of the left panel.

<Delete> - Delete the selected **report template** 379 from the list.

<Edit> - Edit the **report template** 379 selected in the list. The **Summary report configuration** 367 window is opened where user can make configuration.

<Make copy> - Create a copy of the **report template** 379 selected in the list. A new **report template** appears immediately in the list with a new name. User then can edit **report template** in a usual way. This feature allows user to create a new **report template**s based on previously created.

Template import/export

<Import from file> - Import the **report template** 379 from the external ****.fst*** file. Imported **report template** appears as a new item in the list of the left panel.

<Export to file> - Export the **report template** 379 selected in the list to the external ****.fst*** file. Exported file can be transferred to another workstation. Also they can be used to transfer **report template** into the **sample queue** 237 (see **summary report in sample queue** 260).

Note: **.fst* files can also be exported and imported using *<Import from file...>* and *<Export to file>* functions of the Summary report configuration 367 window.

Preview

<Preview this> - Generates and displays a preview report for the **report template** 379 selected in the list.

<Make report> - Press this button to generate **advanced summary report** 366 for the **report template** 379 selected in the list of left panel. The report output will be as specified at the **Output** settings of **Summary report configuration** 367 window for the **report template**.

To get a **advanced summary report** 366 follow these steps:

1. Select required chromatograms in the **Open chromatogram** 207 window.

2. Press **<Statistics...>** button in the **Open chromatogram** 207 window. **Statistics** 375 window is opened.
3. Make ***Summary report*** page active.
4. Select a desired **report template** 379 in list from **Choose template from list** panel. You can create a new **report template** if necessary.
5. Press ***<Make report>*** button.

See also:

Statistics window 375

Summary reports 359

10.3 Advanced report designer

Report designer is an application dedicated to develop report layouts for **report chapters** 380.

The **advanced report** is organized as a set of **chapters** 380 which are printed in the report one after another (see for example **advanced report configuration** 343 and **chapters** 346 of **advanced reports** 341).

Report designer is a powerful tool which allows user to configure the data layout individually for each **chapter** of the report.

Chrom&Spec software provides default report templates with typical layouts for every **chapter**. If user wishes to customize the **chapter** it is a good approach to start with the default layout and modify it as needed. The intuitive graphical interface in conjunction with predefined templates makes it easy to create or edit complicated report layouts for users without a special experience.

Remember that different **chapters** 380 of the report are processed in a different ways. This means that layout designed for one **chapter** generally cannot be used for another **chapter**.

Review the documentation related to the particular **chapter** for details about its layout and compatibility with another chapters.

Report Designer window 381 is a main part of the **report designer** where user makes an actual design.

Basic features of the Report designer

- Various text formatting capabilities: configurable text fonts, text colors ant text backgrounds for any item of the report.
- The possibility to insert pictures, plots, logos and other graphics into the report.
- Data filtering capabilities based on the rules specified by the user. This feature allows to print only the desired subset of the chromatographic data.
- User can specify conditional fonts and text colors based on logical expressions. The report items can be printed differently depending upon the results of analysis. For example, user can specify the "red" text color to highlight the specific rows in the peak table where the concentration of the component is

out of the permissible range.

- User can specify conditional **sections** 387 based on logical expressions. The entire **section** 387 appears in the report only if analysis results conform to (or not conform to) the specific conditions.
- User can specify mathematical and logical expressions and include calculated items into the report.

See also:

Report template 379

Report Designer window 381

Report chapter 380

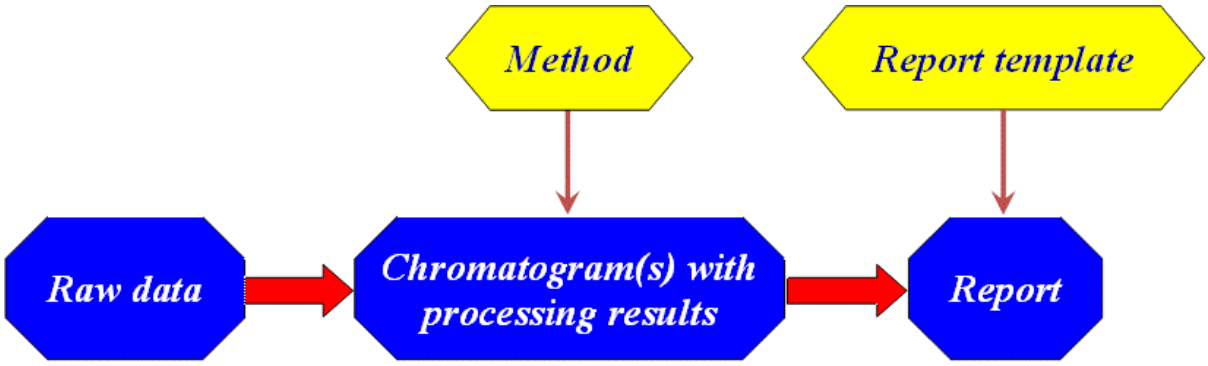
Advanced report configuration 343

Summary report configuration 367

10.3.1 Report template

There are two types of the **advanced reports** implemented in **Chrom&Spec** software: **advanced reports for individual analysis** 341 and **advanced summary reports** 366. The reports of both types are configured and generated in a similar way.

The advanced reports are generated according to the following schema:



Chromatograms supply the data for the report while **report templates** define the layout of the report.

Report templates can also supply the special data post-processing rules (custom formulas, data sorting, filters, etc). This post-processing is additional to the processing performed by **processing method** 122.

Each **report template** is organized as a set of **chapters** 381 which are printed in the report one after another. User specifies the set of chapters for the report at **Advanced report configuration** 343 window (individual analysis) or at **Summary report configuration** 367 window (summary reports).

Individual **chapters** 381 of the report can be designed with **Report Designer window** 381.

See also:

Advanced report designer 378
Report Designer window 381
Advanced report configuration 343
Summary report configuration 367

10.3.2 Report chapter

The advanced reports 341 and advanced summary reports 366 are organized as a set of **chapters** which are printed in the report one after another.

Each **chapter** represents a specific portion of the data and processing results related to the chromatographic analysis. The information required for the report is taken from chromatogram 207 files.

The list of all available **chapters** is displayed in the left panel of the Advanced 343 report configuration 343 window or Summary report configuration 367 window. User includes the **chapter** into report by putting a check mark near it.

Typically each **chapter** can produce a specific table of chromatographic data. For example a Peak table 349 **chapter** produces a table containing the main results of chromatographic analysis (calculated concentrations, peak areas, heights, etc).

The layout of the data in the report is configured individually for each chapter using Advanced report designer 378.
Report chapter contents 381 article describes what each **chapter** consists of and how it is processed to produce the final report.

Different **chapters** of the report are processed in a different ways. This means that layout designed for one **chapter** generally cannot be used for another **chapter**.
There are some sets of **chapters** where **chapters** do compatible with each other. Typically these chapters represent the same type of information but in a different layout.
Review the documentation related to the particular **chapter** for details about its layout and compatibility with another chapters.

Chrom&Spec software provides default report templates with default layouts for every **chapter** available. If user wishes to customize the **chapter** it is a good approach to start with the default chapter layout and modify it as needed.

For details which data and which tables are represented by the chapters see description of the appropriate chapters for individual reports 346 or chapters for summary report 372.

See also:
Report chapter contents 381

Advanced report designer 378
Advanced report template 379
Advanced report configuration 343
Summary report configuration 367

10.3.2.1 Report chapter contents

Each report chapter 380 consists of one or several report sections 387.

Generally report section 387 can be considered as a placeholder for all report fields 390 such as data fields, string labels, graphs etc.

Several types of report sections 387 are available for report designing. Each type supplies a specific processing logic and report functionality. So it does matter where a data field is placed to. The same data field would produce different results depending upon where it is located. See sections concept 387 for more details.

The most typical **chapter** consists of the following **sections**:

Chapter header - used as general description of the chapter
Detail section - used for displaying table data
Chapter footer - used for displaying table summaries

User can add new sections into the report using **Sections / *New*** menu command 383.
To delete the section from the **chapter** use **Sections / *Delete*** menu command 383.

User adds a report fields 390 into the section with a menu commands located in the **Insert** menu group 383.

See also:
Report chapter 380

10.3.3 Report Designer window

The ***Report Designer window*** is an essential part of the Advanced report designer 378.
This tool is used for creating the layout of each report chapter 380 including visual representation and logical scheme of data constructions.

Chrom&Spec software provides default report templates with default layouts for every chapter 380. Typically the minor changes for default templates are only desirable when configuring **chapters** for particular analysis. Sure an advanced users can create a rather different **chapter** layouts from the scratch.

To open ***Report Designer window***:

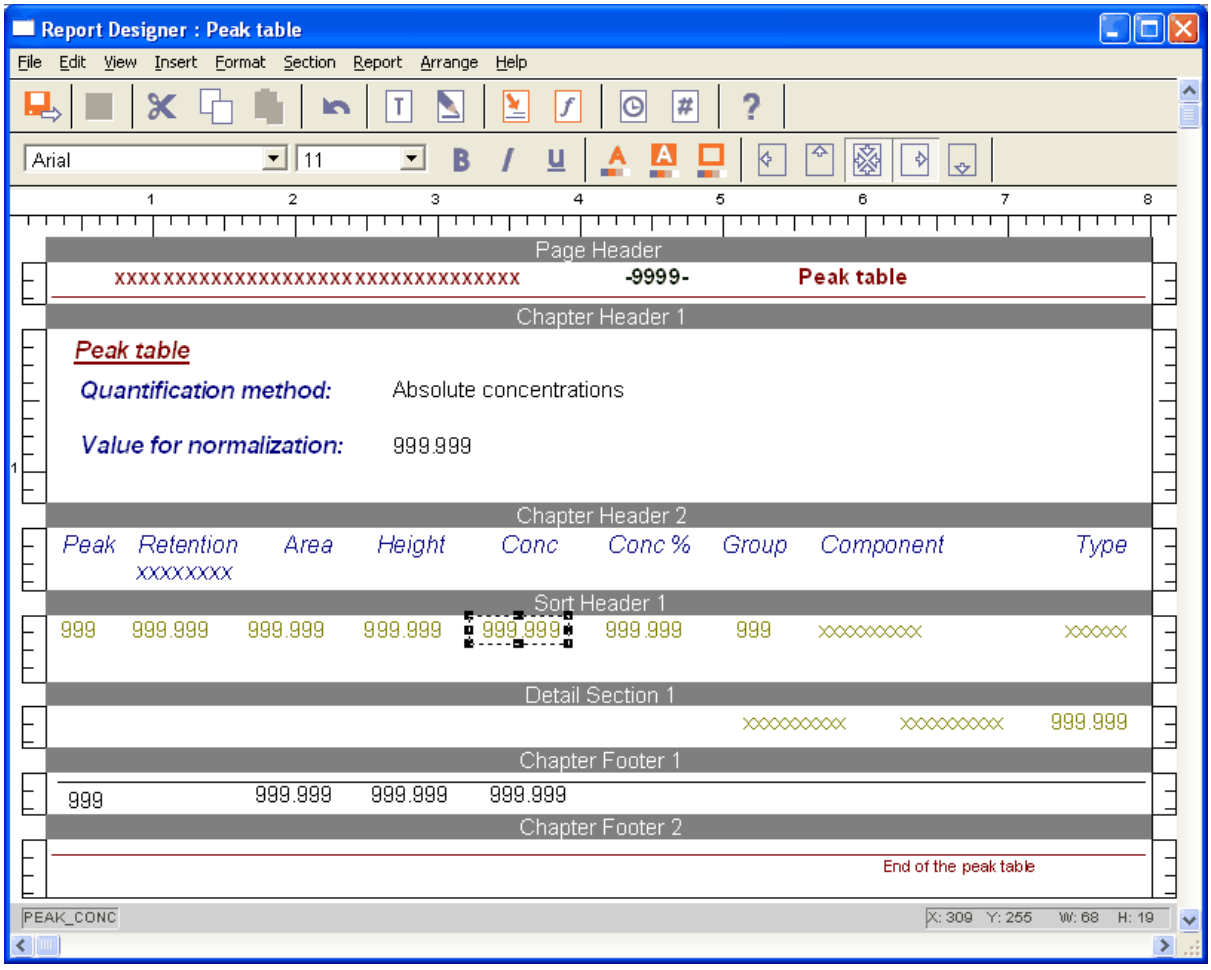
- Select the desired **chapter** 380 from the list of chapters (left panel of **Advanced report configuration** 343 or **Summary report configuration** 367 window)
- Check the ⊙ **Customized chapter** option
- Click ***<Edit chapter...>*** button.

Most editing is performed with mouse by dragging various items in the window. The items can be sized by simply pulling the sizing tabs.

Multiple items can also be selected and manipulated. Item arrangement tools can be used to align the items horizontally or vertically.

Other editing and configuration operations are done using ***Menu*** 383 and ***Toolbar*** 385.

Some configurations can be done with a context menu which is called by right-mouse-button click on the selected item (such as **report field** 390 or **report section** 387).



See also:

Menu (Report Designer window) 383

Toolbar (Report Designer window) 385

Sections concept 387

Fields concept 390

How to create report template 420

10.3.3.1 Menu

The **menu** of the **Report Designer window** 381 contains the following options:

File

New	clear the current template contents. It is useful to start a new template design from the scratch.
Save (F2)	save template for the current **chapter** 380 and stay ***Report Designer*** opened. **[F2]** is a shortcut for the operation.
Import	import template for the **chapter** 380 from ***.FPC** file. ***.FPC** files can be created using the **Export** operation. User must not import templates which were designed for a different **chapter** 380, see **report chapter** 380 for details.
Export	export the current **chapter** 380 template to the ***.FPC** file. User specifies the name and location of the file.
Page setup (Shift+F4)	select page size and orientation. **[Shift]+[F4** is a shortcut for the operation.
Save and exit	save template for the current **chapter** 380 and close ***Report Designer*** window.
Exit (Ctrl+F10)	exit the ***Report Designer*** and discard all changes. **[Ctrl]+[F10]** are short keys for the operation.

Edit

Undo	undo the last operation.
Cut (Ctrl+X)	cut the selected item(s) and place them to the clipboard. **[Ctrl]+[X]** is a shortcut for the operation.
Copy (Ctrl+C)	copy the selected item(s) to the clipboard **[Ctrl]+[C]** is a shortcut for the operation.
Paste (Ctrl+V)	paste the item(s) from the clipboard **[Ctrl]+[V]** is a shortcut for the operation.
Delete	delete the selected item(s) **[Del]** is a shortcut for the operation.
Label	if label 397 is selected, "***Edit label"*** window is opened. The same operation is performed by double clicking on the desired label.
Formula field	if calculated field 399 is selected, "***Edit calculate field"*** window is opened for editing of the field. The same operation is performed by double clicking on the desired calculated field.
Rename formula field	if calculated field 399 is selected, this operation enables to change its name
✓ **Snap to grid**	when this option is checked, position of elements is snapped to grid when moving moving can be done either by dragging items with mouse or using **[Up]**, **[Down]**, **[Left]**, **[Right]**, buttons of the keyboard.

View

✓ **Show field names**	when this option is checked, field names are shown instead of their

values

✓ **Lowcase field names** when this option is checked, field names are printed in lowcase

✓ **Show field boundaries** when this option is checked, boundaries of fields are shown

Insert

Data field insert data field 398 to the desired position

System field insert system field 399 to the desired position

Formula field insert formula field 399 to the desired position

Dialog field insert dialog field 400 to the desired position

Label insert label 397 to the desired position

Line insert line 396 to the desired position

Picture insert picture 395 to the desired position

Format

Font open "***Fonts"*** window to set font attributes for the selected item(s)

✓ **Conditional font** allows to assign a conditional font for selected field(s). This menu item is checked for all fields that are tied with a conditional font.

Apply default item formatting apply default formatting for the selected template item. Default formatting for each type of item is defined from ***Report/Set item formatting as default*** menu item.

Apply default field properties apply default properties for the selected field. Default properties for each type of field is defined from ***Report/Set field properties as default*** menu item.

Alignment open "**Alignment**" window to align item position in its frame box

Borders opens **"Borders"** window to define border around the selected item(s)

Background color opens **"Background color"** window to define type of the background for the selected item

Center in report aligns position of the selected item to the center of the page

Field edit format of the selected field.

Label edit format of the selected label.

Line edit format of the selected line.

Section edit format of the selected section.

Sections

New create a new section 387. Type of the section can be selected from the list offered by the software.

Delete delete the current section
[Del] is a shortcut for the operation.

Sort field modify a **sort field** associated with a **sort header** 387 section.

Break field modify a **break field** associated with a **sort header** 387 section. Typically the break **break field** should be the same as **sort field**.

Selection formula open "388 **Section selection criteria** 388" window 388 to define selection expression.

Report

Filter open "388 **Record selection criteria"** 388 window 388 to define expression for selection of the report item 378.

Named fonts... 419 a group of operations with **named fonts**

Conditional fonts... 419	a group of operations with **conditional fonts**
Dialog fields...	a group of operations with **dialog fields**
Set item formatting as default	save formatting of the current item as default. Default formatting will be applied to all new items of the current type
Set field properties as default	save properties of the current field as default. Default properties will be applied to all new fields of the current type
Size...	open submenu to format size of the selected area
Options	
Arrange	
Align...	open submenu to align several selected elements with different ways
Spacing...	open submenu to set uniform spacing for a group of several elements
Sizing...	open submenu to set uniform size for a group of several elements
Help	calls help topic for the "***Report designer***" window

10.3.3.2 Toolbar

Most frequently used commands in the **Report Designer window** 381 are grouped in **toolbar**.

Save and exit	save all changes for the **report chapter** 380 and close **Report Designer window.** 381
Save (F2)	save all changes for the **report chapter** 380. **Report Designer window** 381 stays opened and user can continue editing.
Cut (Ctrl+X)	cut the selected item(s) and place to the clipboard. **[Ctrl]+[X]** is a shortcut for the operation.
Copy (Ctrl+C)	copy the selected item(s) to the clipboard **[Ctrl]+[C]** is a shortcut for the operation..
Paste (Ctrl+V)	paste the selected item(s) from the clipboard **[Ctrl]+[V]** is a shortcut for the operation..
Undo	undo the last operation
Label	insert label 397 field to the desired position
Line	insert line 396 to the desired position
Data field	insert data field 398 to the desired position

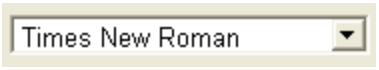
Formula field insert formula field 399 to the desired position

Insert time insert **time field** that will be filled with the current time at the moment of the report output

Page number insert **page number field**

Help call online help topics

Text formatting options:



Text font change ***text font*** for the current item or selected item(s)

Text font size change the ***size of the text font*** for the current item or selected item(s)

Bold font set the style of the text font to ***bold*** for the current item or selected item(s)

Italic font set the style of the text font to ***italic*** for the current item or selected item(s)

Underline font set the style of the text font to ***underline*** for the current item or selected item(s)

Color options:

Text color change text color for the current item or selected item(s)

Fill color change background color for the current item or selected item(s)

Border color change border or line color for the current item or selected item(s)

Align options:

Align left align contents of the selected box(es) to left

Align top align contents of the selected box(es) to top

Center reset alignment of the selected box(es) to center both horizontally and vertically

Align right align contents of the selected box(es) to right

Align bottom align contents of the selected box(es) to bottom

10.3.4 Sections concept

Report Designer organizes a report template by sections. A report should have one section at least.

Each section can include a **section filter** i.e.condition when the section is to be used in the report.

The following sections can be used:

Chapter *header* is printed only once in the beginning of the report (that can include several pages).
Among other things, this section can be used to print a detail description for the report.

Chapter *footer* is printed at the end of the report. This section can be used to print the report summary.

Page Header this section is automatically printed after the top margin on every page. It can be used to print the report name, current date, page number, column headers, etc.

Page Footer is automatically printed before the bottom margin on every page.
It can be used to print the page totals or other pertinent text and data.

Sort Header up to 9 section headers are allowed that are numbered from 1 to 9. The section number 1 is the highest level section, where as the section number 9 is the lowest level section. A lower level section header can be created only if all higher level section headers are already exist.
A section header is always associated with a **sort field**. When a new section is created, the user is provided with a list of sort fields to choose from.

Sort Footer up to 9 section footers are allowed that are numbered from 1 to 9. Similarly, a section footer is allowed only if the corresponding section header is already created.
The footer sections are used to print **summarized values** 400 for all records within the section . A summarized field is like an ordinary field but with the summarization attribute turned on.

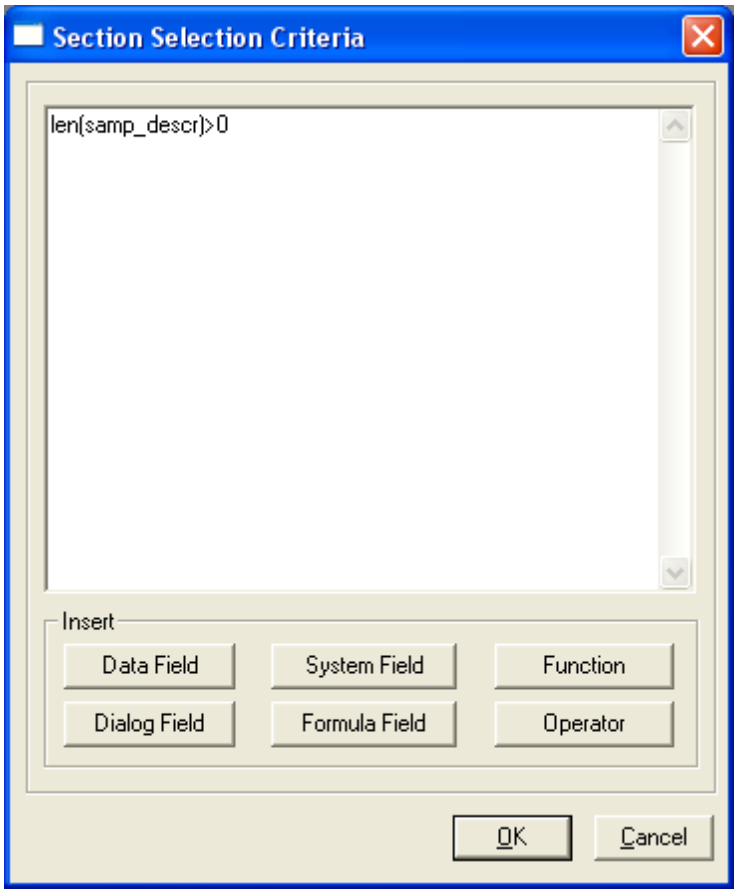
Detail section A report can have up to 9 detail sections. Typically, a report has only one detail section.
Every detail section is printed for each record. The lower numbered detail sections are printed before the higher numbered detail sections.
Detail section has additional parameters that can be tuned by double-clicking on the section's header.

10.3.4.1 Section filter

(Section / Selection formula)

Once a section is created, by default it will be printed in its proper execution sequence. However, you can define an expression to print the section selectively. If a selection expression is provided, the section will print only if the expression evaluates to a **TRUE** value.

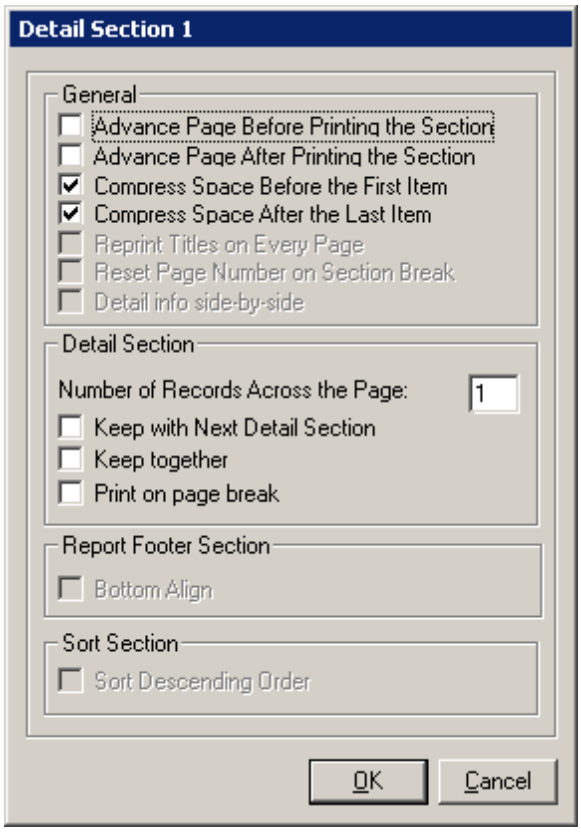
A selection expression can use data fields 398, system fields 399, dialog fields 400, operators and functions 401. This feature is useful when designing complex reports.



Similar dialog window is used to define criteria for each report item 378 (**Report/Filter**).

10.3.4.2 Section parameters

Double-click on the section's header calls a dialog for tuning properties of the section.



These parameters can be selected for any section:

- Advance to the next page before printing the section.
- Advance to the next page after printing the section.
- Compress space between the beginning of the section and the topmost item in the section.
- Discard space after the bottom most item in the section. This attribute can be used to allow large memo (word-wrapped) fields. This attribute will automatically suppress the space after the smaller word-wrapped text data.
- Print sort header and detail records side-by-side. This flag is valid for only the innermost sort header section. The detail section field must be placed toward the right so that they don't overlap the sort header fields on the left side.

Other parameters are section-dependent.

Detail Section

Number of records across the page f

☑ ***Keep with next Detail Section*** set this flag to keep the current and next Detail Sections together (on the same page)

☑ ***Keep together***

☑ ***Print on page break***

Report Footer Section

☑ ***Bottom align*** — set this flag to keep the current Footer Section together on the bottom of the page.
All Footer Sections with higher numbers will be printed below the Footer section

Sort Section

☑ ***Sort descending order*** — use descending order for the current Sort Section.
Normally ascending order is used

10.3.5 Fields concept

A **field** represents a value to be printed in the report.

The **Report Designer** supports the following types of objects (report fields 391): **text**, **numeric**, **float**, **logical, date, line,** and **picture**

Data for report fields can come from one of the following sources 398:

Data Field	a field that is associated with a data record in the file.
Calculation Field	specified using constants, operators, functions and other fields to perform numerical calculations.
System Field	page number, current date, record number, and other system parameters
Dialog Field	Used to prompt the user for data during the report execution. It can also be printed in the report for information purposes.
Picture	picture in BMP or JPG format. Filename or name of the graph variable should be specified by the user directly.

In addition there are two special objects as Line and Label:

Line	graphic lines that can be used as delimiters. You can control the color, thickness, style and slope of the line objects. Line parameters and position are defined by the user directly and are constant for the report layout.
Label	user-defined text labels that are constants for report layout.

Note: ***Labels*** **and** ***Lines*** **are constants. Their value and position are strictly defined in the report template and can not be changed by the software when the report is generated.**

See also:

Report fields 391

Source of field data 398

Summary fields 400

10.3.5.1 Field placement and width

When a field is inserted using a menu option or the field button, the **Report Designer** displays a cursor rectangle. Use the mouse to position the cursor rectangle and click any mouse button. The new field is created where the cursor rectangle is positioned.

The field rectangle contains a text that represents the data type and the current format specification for the field.

For a **'text' type field**, the field rectangle contains a string of 'x' symbols. The 'x' symbols are capitalized if the capitalization is turned on for the field. The number of 'x' symbols is equal to the data width of the field or the maximum number of symbols that can be accommodated within the current rectangle.

For a **numeric field**, the field format can consist of the symbol '9', a decimal symbol and a set of comma symbols. The currency symbol is also shown when the field rectangle is large enough.

For a **date field**, the field text describes the format of the date (example: mm/dd/yy, dd/mm/yy, mmm dd, yyyy etc).

A **logical field** is denoted by a single 'Y' character.

Operations with fields:

When a field is selected, the name of the field appears on the status line. The field width is initially set to the default value. Once a field is inserted in the report template, you are free to adjust its **location** by selecting the item and dragging the mouse. The field **width** can be changed by simply pulling the sizing tabs. A field can be **deleted** by simply selecting the field and then pressing the **[Del]** key.

Double click the left mouse button on the desired field to **edit** its properties.

10.3.5.2 Report Fields

Report fields are used to print values in the report. Properties and position of each field in the layout are determined individually.

Report Designer supports **6** types of field values :

Text 392

Numeric 393

Float 393

Date 394

Picture 395

Logical 396

In other words, **Report fields** are variables that can contain data of definite type and are distinguished by their names (identificators).

Dimensions and position of **Report fields** in the report layout can be changed with mouse by drag-and-drop procedure.

In addition there are two special objects as Line and Label:

Line 396	graphic lines that can be used as delimiters. You can control the color, thickness, style and slope of the line objects. Line parameters and position are defined by the user directly and are constant for the report layout.
Label 397	user-defined text labels that are constants for report layout.

Note: ***Labels*** **and** ***Lines*** **are constants. Their value and position are strictly defined in the report template and can not be changed by the software when the report is generated.**

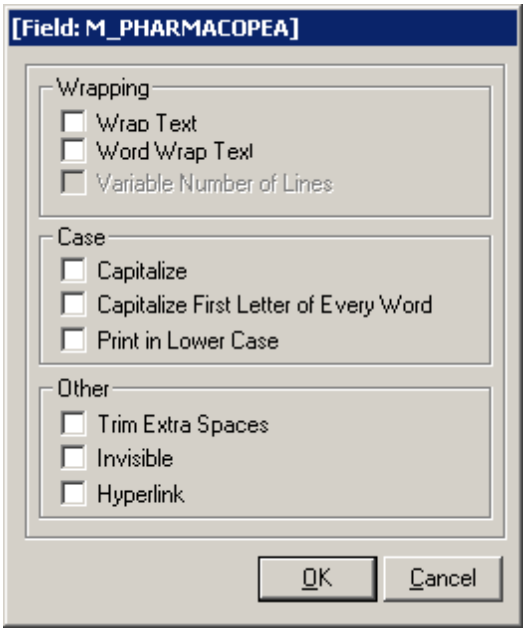
10.3.5.2.1 Text

Text field holds data that consists of characters and digits. The examples of the text fields would be a name, description or comments.

The formatting options that are available for a text field include:

- printing in capital letters
- printing in small letters
- capitalizing the first letter of each word in the field
- word wrapping. The word wrapping option allows a long text field to be printed in multiple lines.

Properties of a text Field are set in the following window that is opened by double mouse clicking on the desired text field:



Window header contains identifier of the field variable

Wrapping

☑ ***Wrap text*** this option wraps the text that is larger than the field width

☑ ***Word Wrap text*** this option breaks the text at the word boundary

☑ ***Variable number of lines*** this option will compress the space after the last text line

Case

☑ ***Capitalize*** this option capitalize all characters in the field

☑ ***Capitalize First Letter*** this option the first letter of every word in the field

☑ ***Capitalize*** this option capitalize all characters in the field

Other

☑ ***Trim extra spaces*** trim extra spaces between words

☑ ***Invisible*** make the item visible only during the design session.
This option can be useful for creating intermediate calculation fields that should not be displayed in the report

☑ ***Hyperlink***

See also:

Report fields 391

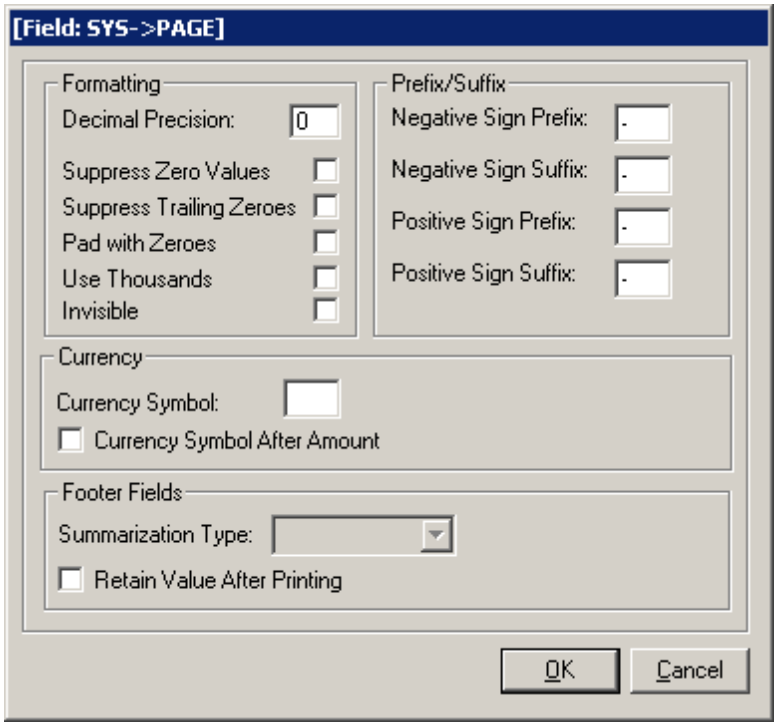
10.3.5.2.2 Number and Float

These fields hold numeric values. The numeric fields hold whole numbers, whereas the Float fields hold floating point numbers.

The formatting options that are available with these fields include:

- number of decimal places
- currency symbol
- prefix and suffix for positive and negative numbers
- zero padding or suppression
- comma formatting.

Properties of a **Numeric** and **Float** field are set in the following window that is opened by double mouse clicking on the desired number field:



Window header contains identifier of the field variable

Formatting

XXX ***Decimal Precision***	the number of digits to the right of the decimal point
☑ ***Suppress Zero Values***	suppress the printing of a field if it contains a zero value
☑ ***Suppress Trailing Zeroes***	suppress the trailing zeroes for a decimal field. For example, values 1.30 and 1.00 would be printed as 1.3 and 1 respectively
☑ ***Pad with Zeroes***	insert zeros before the number if the field value occupies less spaces than specified by the field width
☑ ***Use Thousands***	use an additional space between thousands
☑ ***Invisible***	the item is visible only during the design session. This option is useful for intermediate calculation fields that should not be displayed in the report.

Prefix/Suffix

These settings define appearance of negative and positive values (add an additional symbol before or after the number)

Footer Fields

These options are available for the fields located in a footer section only.

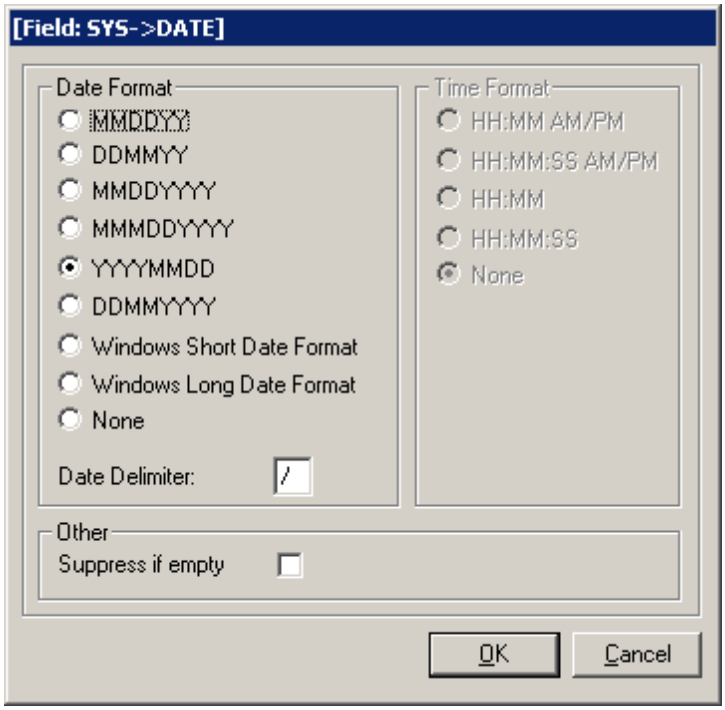
Summarization type	select instruction to print **totals**, **average**, **maximum**, **minimum** or **count** of a field. Specify **Value** to print value for the last record before the footer section
☑ ***Retain Value after Printing***	normally, when a total (or average, maximum, minimum, count) is printed, the internal accumulator is cleared to start the next iteration of the section from zero. However, if you wish to print the running totals, check this option

See also:

Report fields 391

10.3.5.2.3 Date

Properties of a **Date** field are set in the following window that is opened by double mouse clicking on the desired Date field:



Date Format

Number of different date formats are available.

Data Delimiter	delimiter to separate month, day and year. Default value is "***/***"
☑ ***Suppress if empty***	suppress Date field printing if its value is empty

Time format

These settings become available if ⊙ **Windows Short Date Format** or ⊙ **Windows Long Date Format** is selected.

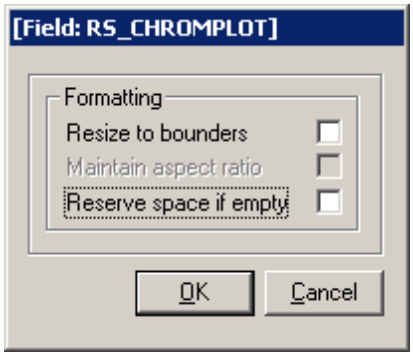
See also:

Report fields 391

10.3.5.2.4 Picture

Picture field denotes a picture id that can be replaced with data from disk file or clipboard. The picture file must be in ***BMP*** or ***JPEG*** format

Properties of a **Picture field** are set in the following window that is opened by double mouse clicking on the desired **Picture field**:



Formatting

☑ ***Resize to boundaries*** shrink or stretch size of he picture to fit it to the field boundaries

☑ ***Maintain aspect ratio*** preserve picture's aspect ratio when resizing.
This option become available when Resize to boundaries flag is set.

☑ ***Reserve space if empty*** leave empty space in the report if the picture is absent.

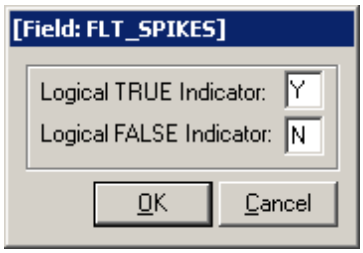
See also:

Report fields 391

10.3.5.2.5 Logical

Logical field contains a **boolean value** that can have only one of two values, such as **yes/no**, **true/false**, **black/white**.

The formatting options available with this type allows you to specify the text to be printed for a true and false value:



Single-letter indicators can be used only.

See also:

Report fields 391

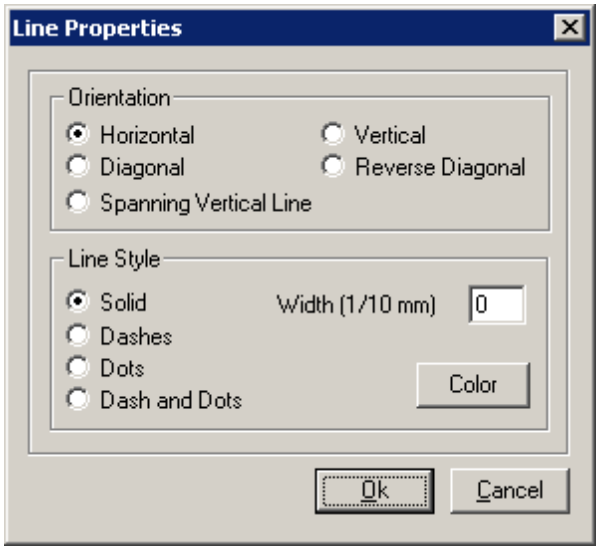
10.3.5.2.6 Line

Line is a graphic object that can be placed in any place of the report layout and is used as delimiter.

It is possible to control color, thickness, style and slope of the line objects. Line parameters and position are defined by the user directly and are constant for the report layout.

Note: ***Lines*** **are constants. Their value and position are strictly defined in the report template and can not be changed by the software when the report is generated.**

Properties of the **Line field** are set in the following window that is opened by double mouse clicking on the desired **Line field**:



See also:

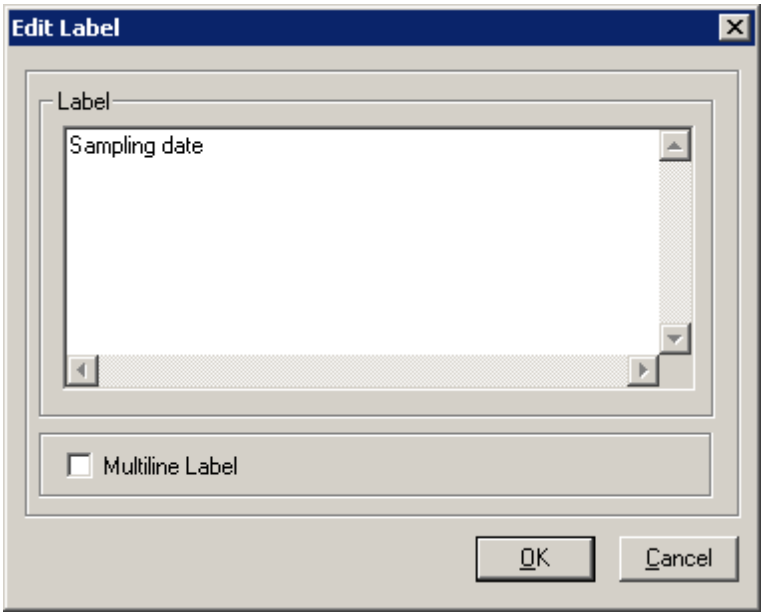
Report fields 391

10.3.5.2.7 Label

Label is a string object that can be placed in any place of the report layout and is used as description of other report fields.

Note: ***Labels*** **are constants. Their value and position are strictly defined in the report template and can not be changed by the software when the report is generated.**

Text of the **Label field** is entered in the following window that is opened by double mouse clicking on the desired **Label field**:



☑ ***Multiline label*** check it if the label is too long and can not fit a single line

It is possible to control **font**, **size**, **color**, **style** and **alignment** of the label text using icons from the tool panel or items in the **Format** menu. It is possible also to click the right mouse button on the desired label field and select the required option from the context menu.

See also:

Report fields 391

10.3.5.3 Source of field data

Each **Report field** 391 may represent the following data:

data value 398

calculated value 399

system value 399

user entered value (dialog) 400

10.3.5.3.1 Data field

Data field is associated with the application data file. Your application provides a list of fields to choose from. The application can organize data fields by files and use some prefixes to distinguish them.

Note: When the user inserts a data field into a report template, the Report Designer calls a field selection routine provided by the Chrom&Spec. This routine allows the user to select a data field from the available list. Then Chrom&Spec passes the field name along with other required information in a field structure .

See also:

Source of field data 398

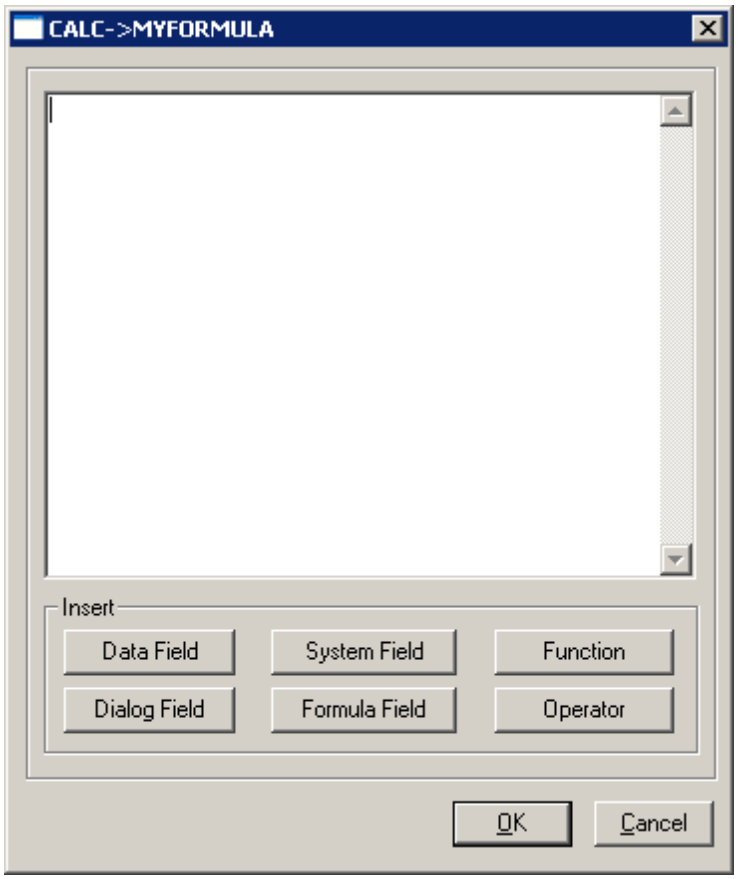
10.3.5.3.2 Calculated field

The calculated fields allow you to print a value which is derived using other fields, operators and functions.

A calculated field is specified using a calculation expression.

Each calculated field is assigned a name that can be used in the current template in other calculations.

Calculation expression is created in the "***Calc***" window:



See also:

Source of field data 398

10.3.5.3.3 System field

System fields are used to print information such as:

- calendar date
- time
- page
- record number.
- SECTION_ITEM_COUNT field that can be used within the innermost section footer to print the number of detail records inside this section.

See also:

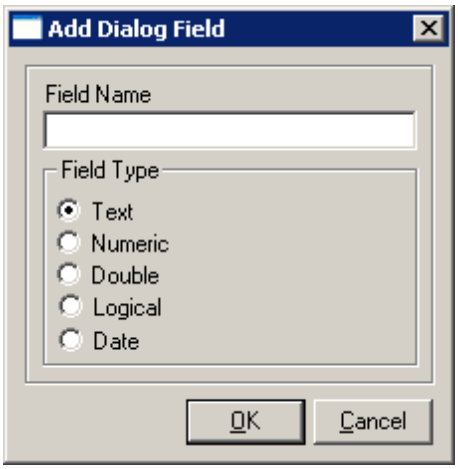
Source of field data 398

10.3.5.3.4 Dialog field

Dialog fields allow to ask the user for additional data before the report is executed.

Report Designer allows you to create a list of dialog fields. Dialog fields can be placed anywhere in the report (as other fields can). Typically, a dialog field for the report date appears in the report header. It is also possible to use dialog fields in the report selection criteria that are applied to filter out some records.

Before using a dialog field, it is necessary to define it in the "***Add Dialog Field***" window (**Report/Dialog Fields/New**).



Enter **Field name** (name of the dialog) and select field type. The value returned by the dialog can be placed in any position of the template similar to other Data fields 398.

See also:

Source of field data 398

10.3.5.4 Summary fields

Report Designer allows you to summarize a numeric or float field. The summarized value of a field can be printed in any footer section.

The following types of **Summary Fields** are available:

Totals	accumulates all records of this type within the current section.
Average	average value for all records of this type within the current section is calculated.
Minimum	computes the minimum value of all records of this type within the current section.
Maximum	computes the maximum value of all records of this type within the current section.
Count	calculates the number of records of this type within the current section.

10.3.5.5 Sort fields

Enter topic text here.

10.3.6 Calculated expressions

The calculation expressions can be used to:

- Define the **calculated fields**.
- Define the **report selection criteria**. The expression must evaluate to a TRUE or FALSE value.
- Define the **section selection criteria**. The expression must evaluate to a TRUE of FALSE value.

A calculation expression consists of **operands** and operators 401.

The operands can be:

- fields 398
- functions 409
- result of an if/then/else statement 419

Operator Precedence:

In an expression with multiple operators, the execution priority of an operator is determined by its precedence. The operator with the highest precedence gets executed first. The lower precedence operators use the result of the higher precedence operators as operands. You can override the default precedence by using parentheses.

10.3.6.1 Operators

The following operations can be used in Report Designer's expressions:

Logical "OR" 402
Logical "AND" 402
Logical "NOT" 403
Logical EQUAL 402
Logical "NOT EQUAL" 403
Logical "GREATER THAN" 403
Logical "LESS THAN" 404
Logical "GREATER THAN OR EQUAL" 404
Logical "LESS THAN OR EQUAL" 404
Logical "Part of" 405

Addition 405
Subtraction 406
Multiplication 406
Division 407

TOTAL OF 407
AVERAGE OF 407
MAXIMUM OF 408

MINIMUM OF 408
COUNT OF 409

10.3.6.1.1 Or

Operator Symbol	**.OR.**
First Operand Type	logical
Second Operand Type	logical
Result Type	logical
Precedence Rank	100
Description	The logical OR operator returns a TRUE value if either the first operand or the second operand is TRUE. Otherwise, it returns a FALSE value.

Examples:

10=(20-2).OR.10=(20-10) -> TRUE

10=(20-2).OR.10=(20-8) -> FALSE

10.3.6.1.2 And

Operator Symbol	**.AND.**
First Operand Type	logical
Second Operand Type	logical
Result Type	logical
Precedence Rank	200
Description	The logical AND operator returns a TRUE value if both the first operand and the second operand are TRUE. Otherwise, it returns a FALSE value.

Examples:

10=(30-20).AND.10=(20-10) -> TRUE

10=(30-20).AND.10=(20-8) -> FALSE

10.3.6.1.3 Equal

Comparison

Operator Symbol	**=**
First Operand Type	Numeric, float, text, date, logical
Second Operand Type	Same as the first operand type
Result Type	logical
Precedence Rank	300
Description	This operator returns a TRUE value if the first operand is equal to the second operand. Otherwise, it returns a FALSE value.

Examples:

10=(30-20) -> TRUE

10=(30-10) -> FALSE

10.3.6.1.4 Not

Operator Symbol	**.NOT.**
First Operand Type	logical
Second Operand Type	N/A
Result Type	logical
Precedence Rank	800
Description	This operator negates the logical value of the first operator. Being a unary operator, it accepts only one operand.

Examples:

.NOT.(10=(20-10))	-> FALSE
.NOT.(10=(20-8))	-> TRUE
.NOT.("KEEP"$"KEEPING")	-> FALSE

10.3.6.1.5 Notequal

Comparison

Operator Symbol	**<>**
First Operand Type	Numeric, float, text, date, logical
Second Operand Type	Same as the first operand type
Result Type	logical
Precedence Rank	300
Description	This operator returns a TRUE value if the first operand is not equal to the second operand. Otherwise, it returns a FALSE value.

Examples:

10<>(40-20) -> TRUE

10<>(20-10) -> FALSE

10.3.6.1.6 Greater

Comparison

Operator Symbol	**>**
First Operand Type	Numeric, float, text, date, logical
Second Operand Type	Same as the first operand type
Result Type	logical

Precedence Rank	400
Description	This operator returns a TRUE value if the first operand is greater than the second operand. Otherwise, it returns a FALSE value.

Examples:

10>(30-22) -> TRUE

10>(30-10) -> FALSE

"ABC">"ACC" -> FALSE

10.3.6.1.7 Less

Comparison

Operator Symbol	**<**
First Operand Type	Numeric, float, text, date, logical
Second Operand Type	Same as the first operand type
Result Type	logical
Precedence Rank	400
Description	This operator returns a TRUE value if the first operand is less than the second operand. Otherwise, it returns a FALSE value.

Examples:

10<(30-22) -> FALSE

10<(30-10) -> TRUE

"ABC"<"ACC" -> TRUE

10.3.6.1.8 Greater or Equal

Comparison

Operator Symbol	**>=**
First Operand Type	Numeric, float, text, date, logical
Second Operand Type	Same as the first operand type
Result Type	logical
Precedence Rank	400
Description	This operator returns a TRUE value if the first operand is either greater or equal to the second operand. Otherwise, it returns a FALSE value.

Examples:

10>=(30-22) -> TRUE

10>=(30-10) -> FALSE

"ABC">="AB" -> TRUE

10.3.6.1.9 Less or Equal

Comparison

Operator Symbol	**<=**

First Operand Type	Numeric, float, text, date, logical
Second Operand Type	Same as the first operand type
Result Type	logical
Precedence Rank	400
Description	This operator returns a TRUE value if the first operand is either smaller or equal to the second operand. Otherwise, it returns a FALSE value.

Example:

10<=(30-22) -> FALSE

10<=(30-10) -> TRUE

"ABC"<="ABCD" -> TRUE

10.3.6.1.10 Part of

String operation

Operator Symbol	**$**
First Operand Type	text
Second Operand Type	text
Result Type	logical
Precedence Rank	500
Description	This operator returns a TRUE value if the first operand is contained within the second operand. Otherwise, it returns a FALSE value.

Examples:

"KEEP"$"HOUSE KEEPER" ->TRUE

"KEEPING"$"HOUSE KEEPER" ->FALSE.

10.3.6.1.11 Addition

Arithmetic, string, date operation

Operator Symbol	**+**
First Operand Type	numeric, float, text, date
Second Operand Type	same as the first operand type when the first operand type is numeric, float or text. When one of the operands is a 'date', the other operand must be numeric. Two dates can not be added.
Result Type	same as the first operand type when both operands are numeric, float, or text. When one of the operand is a 'date', the result is also a 'date.
Precedence Rank	600
Description	This operator adds the second operand to the first operand. If one of the operands is numeric and the other is float, the result will be of the float type. If the operand type is text, the second string is appended to the first string.

Examples:

10 + 20 -> 30

10 + 20.5	-> 30.5
"Good " + "Day"	-> "Good Day"
"5/9/99" + 1	-> "5/10/99"

10.3.6.1.12 Subtraction

Arithmetic, string, date operation

Operator Symbol	-
First Operand Type	numeric, float ,text, date
Second Operand Type	same as the first operand type when the first operand is numeric, float or text. When the first operand is a 'date', the second operand can be a 'date' or numeric. Similarly, when the second operand is a 'date', the first operand can be a 'date' or numeric.
Result Type	same as the first operand type when both operands are numeric, float, or text. When both operands are 'date', the result is a number of days calculated by subtracting the second date from the first date. When the first operand is a date and the second operand is numeric, then the result is a date calculated by subtracting the number of days (second argument) from the date (first argument).
Precedence Rank	600
Description	This operator subtracts the second operand from the first operand. If one of the operands is numeric and the other float, the result will be of float type. If the operand type is text, the second string is appended to the first string. However, any spaces after the first string are truncated and transferred at the end of the output string.

Examples:

10 - 20	-> -10
10 - 20.5	-> -10.5
"Good " - "Day"	-> "GoodDay "
"5/9/99" - "5/8/99"	-> 1
"5/9/99" – 1	-> "5/8/99"

10.3.6.1.13 Multiply

Arithmetic operation

Operator Symbol	*
First Operand Type	numeric, float
Second Operand Type	numeric, float
Result Type	numeric, float
Precedence Rank	700
Description	This operator multiplies both operands. If one of the operands is numeric and the other float, the result will be of float type.

Examples:

10 * 20 -> 200

10 * 20.5 -> 205.

10.3.6.1.14 Divide

Arithmetic operation

Operator Symbol	**/**
First Operand Type	numeric, float
Second Operand Type	numeric, float
Result Type	numeric, float
Precedence Rank	700
Description	This operator divides the first operand by the second operand. If one of the operand is numeric and the other float, the result type will be float.

Examples:

10 / 2	-> 5
10 * 20	-> 0
10 * 20.0	-> .5

10.3.6.1.15 Total of

Footer section summary operation

Operator Symbol	**.TOTAL-OF.**
First Operand Type	numeric or float type field
Second Operand Type	N/A
Result Type	Same as the first operand type
Precedence Rank	900
Description	The operand for this operator must be a field. Being a unary operator, it accepts only one operand. This operator is allowed only in the calculation fields that are placed in a footer section. The operator will calculate the subtotal for the field indicated by the first operand.

Example:

.TOTAL-OF.sales	->amount calculates the total sales amount for the footer section field.

10.3.6.1.16 Average

Footer section summary operation

Operator Symbol	**.AVE-OF.**

First Operand Type	numeric or float type field
Second Operand Type	N/A
Result Type	Same as the first operand type
Precedence Rank	900
Description	The operand for this operator must be a field. Being a unary operator, it accepts only one operand. This operator is allowed only in the calculation fields that are placed in a footer section. The operator will calculate the average value for the field indicated by the first operand.

Example:

.AVE-OF.sales	->amount calculates the average sales amount for the footer section field.

10.3.6.1.17 Maximum

Footer Section summary operation

Operator Symbol	**.MAX-OF.**
First Operand Type	numeric,float type field
Second Operand Type	N/A
Result Type	Same as the first operand type
Precedence Rank	900
Description	The operand for this operator must be a field. Being a unary operator, it accepts only one operand. This operator is allowed only in the calculation fields that are placed in a footer section. The operator provides the largest value of the field indicated by the first operand.

Example:

.MAX-OF.sales	->amount returns the largest sales amount for the **footer section field**.

10.3.6.1.18 Minimum

Footer Section summary operation

Operator Symbol	**.MIN-OF.**
First Operand Type	numeric,float type field
Second Operand Type	N/A
Result Type	Same as the first operand type
Precedence Rank	900
Description	The operand for this operator must be a field. Being a unary operator, it accepts only one operand. This operator is allowed only in the calculation fields that are placed in a footer section. The operator provides the smallest value of the field indicated by the first operand.

Example:

.MIN-OF.sales	->amount returns the smallest sales amount for the **footer section**

field.

10.3.6.1.19 Count of

Footer Section summary operation

Operator Symbol	**.COUNT-OF.**
First Operand Type	numeric,float type field
Second Operand Type	N/A
Result Type	Same as the first operand type
Precedence Rank	900
Description	The operand for this operator must be a field. Being a unary operator, it accepts only one operand. This operator is allowed only in the calculation fields that are placed in a footer section. The operator provides the record count for a section.

Example:

.COUNT-OF.sales	->amount returns the number of records processed within the current section.

10.3.6.2 Functions

The Report Designer can use functions in the calculation expressions.

A function accepts a predefined number of arguments and returns a value of a predefined type.

In addition to predefined standard functions user-defined functions 288 can be used in report. Custom functions have access to a more detailed chromatogram parameters than Report Designer has.

The following functions can be used:

10.3.6.2.1 AddtLine

Function Name:	**AddLine**
First Argument Type:	text
Second Operand Type:	N/A
Result Type:	text
Description:	This function is used to add text to the next line. A new blank line is not created if the text is blank. This function can be used to print address using a calculation field.

Example:

Name+AddLine(company)+AddLine(address1)+AddLine(address2)

10.3.6.2.2 Length

Function Name:	**LEN**
First Argument Type:	text
Second Operand Type:	N/A
Result Type:	numeric
Description:	This function returns the length of a text string.

Examples:

```
LEN("ABCD") -> 4
LEN("GOOD DAY") -> 8
```

10.3.6.2.3 InStr

Function Name:	**InStr**
First Argument Type:	text

Second Operand Type: text

Result Type: numeric

Description: This function returns the position of the second string within the first string. It returns 0 if the second string is not found within the first string. The string search is case-sensitive.

Examples:

```
InStr("catdog","cat") -> 1
InStr("catdog","dog") -> 4
InStr("catdog","mouse") -> 0
```

10.3.6.2.4 ToDate

Function Name: **ToDate**

First Argument Type: text

Second Operand Type: N/A

Result Type: Date

Description: This function converts a text type argument to date type.

Examples:

```
ToDate("12/31/2002") -> 12/31/2002
```

10.3.6.2.5 Upper

Function Name: **UPPER**

First Argument Type: ***text***

Second Operand Type: N/A

Result Type: text

Description: This function converts the given string to the upper case.

Examples:

UPPER("abcd") -> "ABCD"

UPPER("Good Day") -> "GOOD DAY"

10.3.6.2.6 LOWER

Function Name: **LOWER**

First Argument Type: text

Second Operand Type: N/A

Result Type: text

Description: This function converts the given string to the lower case.

Examples:
LOWER("ABCD") -> "abcd"
LOWER("Good Day") -> "good day"

10.3.6.2.7 TRIM

Function Name:	**TRIM**
First Argument Type:	text
Second Operand Type:	N/A
Result Type:	text
Description:	This function returns a string by removing spaces from the beginning and ending of given string.

Examples:
TRIM(" ABCD ") -> "ABCD"
TRIM("Good Day ") -> "Good Day"

10.3.6.2.8 WORD

Function Name:	**WORD**
First Argument Type:	text
Second Operand Type:	numeric
Result Type:	text
Description:	This function extracts a word from the input string. The second argument specifies the word position to be extracted.

Examples:
WORD("It is a Good Day",1) -> "It"
WORD("It is a Good Day",2) -> "is"

10.3.6.2.9 CHAR

Function Name:	**CHAR**
First Argument Type:	text
Second Operand Type:	numeric
Result Type:	text
Description:	This function extracts a character from the input string. The second argument specifies the character position to be extracted.

Examples:

CHAR("It is a Good Day",1) -> "I"

CHAR("It is a Good Day",2) -> "t"

10.3.6.2.10 FIRST

Function Name:	**FIRST**
First Argument Type:	text
Second Operand Type:	numeric
Result Type:	text
Description:	This function extracts the specified number of characters (argument #2) from the beginning of the specified (argument #1) text string.

Examples:

FIRST("It is a Good Day",5) -> "It is"

FIRST("It is a Good Day",2) -> "It"

10.3.6.2.11 LAST

Function Name:	**LAST**
First Argument Type:	text
Second Operand Type:	numeric
Result Type:	text
Description:	This function extracts the specified number of characters (argument #2) from the end of the specified (argument #1) text string.

Examples:

LAST("It is a Good Day",8) -> "Good Day"

LAST("It is a Good Day",3) -> "Day"

10.3.6.2.12 TEXT

Function Name:	**TEXT**
First Argument Type:	numeric, float, date, logical
Second Operand Type:	N/A
Result Type:	text
Description:	This function converts any other type argument to the text type data using the default format specifications.

Examples:

TEXT("3/4/92") -> "3/4/92" (text)

TEXT(123) -> "123"

10.3.6.2.13 MIN

Function Name:	**MIN**
First Argument Type:	numeric, float
Second Operand Type:	numeric, float
Result Type:	numeric, float
Description:	This function returns the smaller of the first and second arguments. If one of the arguments is numeric and the other is float, then the return type will be float.

Examples:

MIN(10,20) -> 10

MIN(10,20.0) -> 10.0

10.3.6.2.14 MAX

Function Name:	**MAX**
First Argument Type:	***numeric, float***
Second Operand Type:	numeric, float
Result Type:	numeric, float
Description:	This function returns the larger of the first and second arguments. If one of the arguments is numeric and the other is float, then the return type will be float.

Examples:

MAX(10,20) -> 20

MAX(10,20.0) -> 20.0

10.3.6.2.15 ROUND

Function Name:	**ROUND**
First Argument Type:	float
Second Operand Type:	numeric
Result Type:	float
Description:	This function rounds the first argument to the number of decimal places specified by the second Argument.

Examples:

ROUND(10.153,2) -> 10.15

ROUND(10.153,1) -> 10.2

10.3.6.2.16 INT

Function Name:	**INT**
First Argument Type:	float, text, date, logical
Second Operand Type:	N/A
Result Type:	numeric
Description:	This function converts any other type argument to the numeric type. For a 'float' type of argument, this operation discards any decimal digits from the first argument. The date type argument is converted to YYYYMMDD formatted numeric value. The logical type is converted either 1 or 0.

Examples:

INT(10.153) -> 10

INT("123") -> 123

INT("3/4/92") -> 19920304

INT(1<>2) -> 1

10.3.6.2.17 ToNumber

Function Name:	**ToNumber**
First Argument Type:	text
Second Operand Type:	N/A
Result Type:	float
Description:	This function converts a text type argument to float type.

Examples:

ToNumber("10.153") -> 10.153

ToNumber("123") -> 123

ToNumber("-123.456") -> -123.456

10.3.6.2.18 ABS

Function Name:	**ABS**
First Argument Type:	numeric,float
Second Operand Type:	N/A
Result Type:	Same as the Argument
Description:	This function returns the absolute value of the given argument.

Examples:

ABS(-10.153) -> 10.153

ABS(10.153) -> 10.153

ABS(-12) -> 12

10.3.6.2.19 WEEKDAY

Function Name:	**WEEKDAY**
First Argument Type:	date
Second Operand Type:	N/A
Result Type:	text
Description:	This function returns the weekday for given date.

Examples:

WEEKDAY("4/13/92") -> "Monday"
WEEKDAY("4/14/92") -> "Tuesday"

10.3.6.2.20 DAY

Function Name:	**DAY**
First Argument Type:	date
Second Operand Type:	N/A
Result Type:	numeric
Description:	This function extracts the day (1 to 31) from the given date.

Examples:

DAY("4/13/92") -> 13
DAY("4/14/92") -> 14

10.3.6.2.21 MONTH

Function Name:	MONTH
First Argument Type:	date
Second Operand Type:	N/A
Result Type:	numeric
Description:	This function extracts the month (1 to 12) from the given date.

Examples:

MONTH("4/13/92") -> 4
MONTH("5/14/92") -> 5

10.3.6.2.22 YEAR

Function Name: YEAR
First Argument Type: date
Second Operand Type: N/A
Result Type: numeric
Description: This function extracts the year from the given date. The year is returned using 4 digits.

Examples:

YEAR("4/13/92") -> 1992
YEAR("5/14/08") -> 2008
YEAR("5/14/2008") -> 2008

10.3.6.2.23 BREAKS

Function Name: BREAKS
First Argument Type: numeric
Second Operand Type: N/A
Result Type: numeric
Description:

When the argument value is a value from 1 to 9, this function returns the number of sort breaks encountered thus far for the given sort level. Consider a report which lists invoice items for each invoice for each customers.

If you wish to print the number of invoices for a customer, create the following calculation expression in the footer section of the customer:
BREAKS(2)

If you wish to print the number of customers in the entire report, create following expression in the report footer:
BREAKS(1)

You can also set the first argument to 0 to retrieve the number of detail records in the last sort section. For example, if you wish to report the number of items for an invoice, create the following calculation expression in the footer section of the invoice:
BREAKS(0)

In the above examples the summarization type should be reset to 'value', since by default the calculation expressions entered in a footer section is assigned the summarization type of 'Total'.

10.3.6.2.24 TotalBreaks

Function Name: TotalBreaks
First Argument Type: numeric
Second Operand Type: N/A
Result Type: numeric

Description:

When the argument value is a value from 1 to 9, this function returns the number of sort breaks encountered thus far for the given sort level. The difference between this function and the 'Breaks' functions is that this function allows you to access the sort-break count (or detail record count) of any level from any footer.

Consider a report which lists invoice items for each invoice for each customers for each department:
Department (sort level 1)
Customer (sort level 2)
Invoice (sort level 3)
Invoice items (detail records)

If you wish to print the number of invoices for a department, create the following calculation expression in the footer section for the department:
TotalBreaks(3) (The argument value 3 indicates the sort level of the 'invoice' sort)

If you wish to print the number of departments in the entire report, create following expression in the report footer:
TotalBreaks(1) (The argument value 1 indicates the sort level of the 'department' sort)

You can also set the first argument to 0 to retrieve the number of detail records encountered thus far at the current sort footer. For example, if you wish to report the number of invoice-items for a customer, create the following calculation expression in the footer section of for customer:
TotalBreaks(0)

In the above examples the summarization type should be reset to 'value', since by default the calculation expressions entered in a footer section is assigned the summarization type of 'Total'.

10.3.7 Additional features

Report designer allows additional features that can be used for sophisticated reports.

Named fonts 419	it is possible to define names to some useful font settings. For example, it is possible to use blue color for values that are less then the lower limit, red color for values that exceed some upper level and green color for values that fit the range. Named fonts are used in **conditional font expessions**. For example, "blue", "green" and "red" are names of the correspondent fonts
Conditional fonts 419	it is possible to define font formating for data fields that fit some condition. Conditions are created using the same rules as conditional statements 419 are, however named fonts are used as substatements.

Example:

.IF.(peak_name="sodium".AND.peak_conc<6.0.AND.peak_conc>1.0).THEN."green".ELSE.
(.IF.(peak_name="sodium".AND.peak_conc>7.0).THEN."red" .ELSE."blue")

Conditional font expression can be applied for each field or selected region of fields (for example, row in the table). Select the desired field(s) and use **Format / Conditional font** menu item to apply.

Note: a set of named fonts and conditional font expressions is individual for each report section

10.3.7.1 Named fonts

(Report/Named fonts...)

It is possible to define a so called "**named fonts**", i.e. user-defined names for the most frequently used font attributes. Named fonts are used in **conditional font expressions** 419

The following operations with named fonts are available in this menu:

- Use **Report/Named fonts/New** menu item to create a new Named font
- Use **Report/Named fonts/Edit** menu item to view defined font list in the Select named font window, and then edit the selected named font.
- Use **Report/Named fonts/Delete** menu item to view defined font list in the Select named font window, and then delete the selected named font.

10.3.7.2 Conditional fonts

(Report / Conditional fonts...)

This submenu operates with **conditional fonts**.

It is possible to define font formatting for data fields that fit some condition. Conditions are created using the same rules as conditional statements 419 are, however **named fonts** are used as substatements.

The following operation are available in this menu:

- Use **New** menu item to create a new conditional font expression
- Use **Edit** menu item to view a list of conditional font expressions in the Select font expression window, and then edit the selected conditional font expression.
- Use **Delete** menu item to view a list of conditional font expressions in the Select named font window, and then delete the selected item.
- Use **Rename** menu item to view a list of conditional font expressions in the Select named font window, and then rename the selected item.

See also:

Named fonts 419

10.3.7.3 Conditional statements

The **Report Designer** allows to use an **.IF.condition.THEN.substatement1.ELSE.substatement2** construction. This statement evaluates if the condition is a TRUE or FALSE value. If the value is TRUE, then the entire expression evaluates to the subexpression1 following the **THEN** statement. Otherwise the entire expression evaluates to the subexpression2 following the **ELSE** statement.

Examples:

.IF.comp_irbase="0".THEN."Area%".ELSE."Height%"

This example compares the **comp_irbase** parameter and returns a text string. The resulting text string is equal to "**Area%**" when comp_irbase=0. Otherwise it is equal to "**Height%**".

Note: It is important that the subexpression following the then and the else statement must

return the same type result.

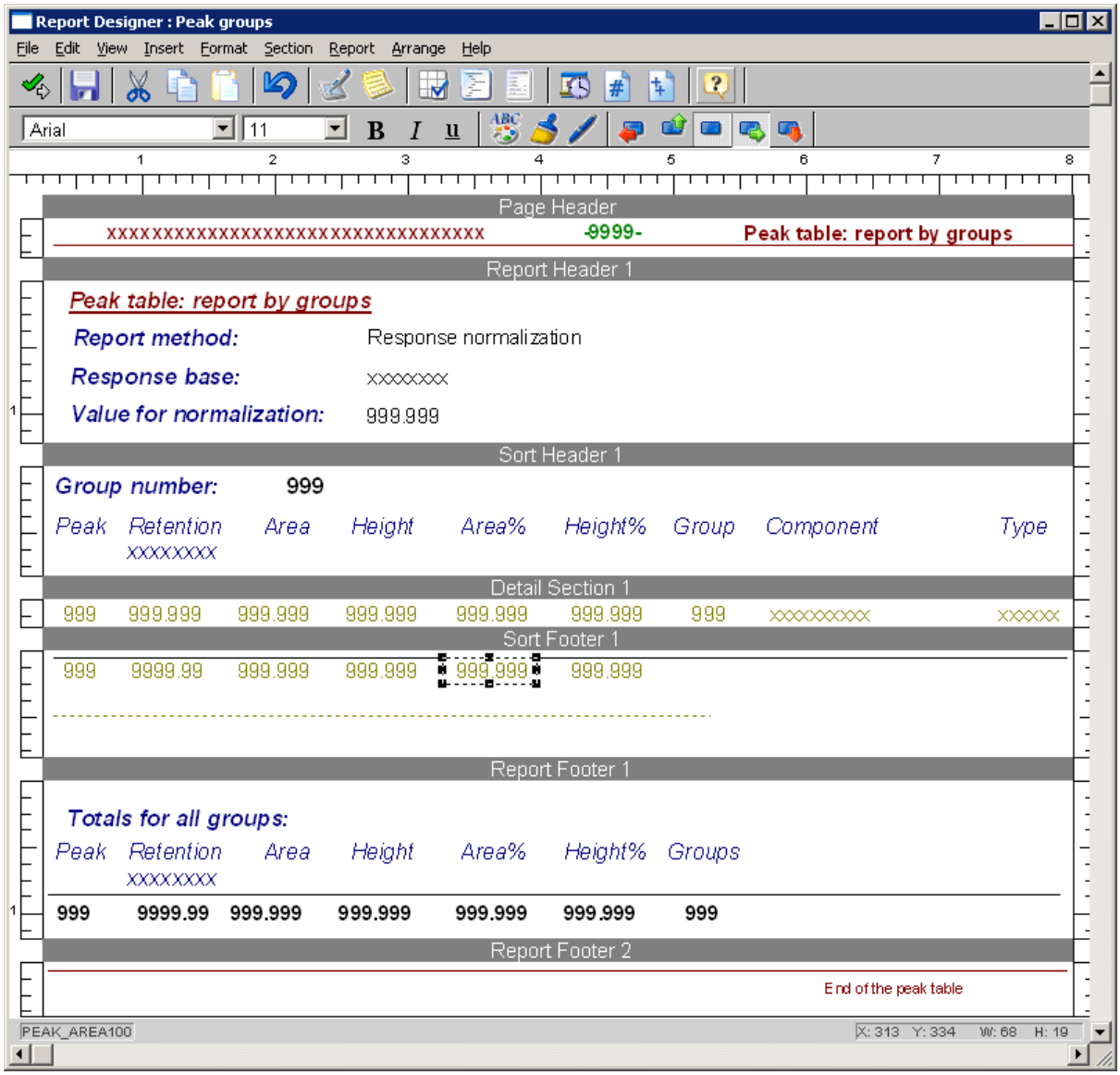
Examples of invalid statements:

.IF.comp_irbase=0.THEN."Area%".ELSE."Height%"	comp_irbase parameter is a string value
.IF.comp_irbase="0".THEN."Area%".ELSE.(100)	THEN and ELSE statements are to be of the same type.

10.3.8 How to create a report template

The following procedure can be used.

- Open "***Reports***145" page (**Method/Method setup/Reports**).
- Click ***<Add>*** button and enter the desired name of the **report layer** to be created. Default name **Report #** is offered.
  If the desired layer already exists, select it and click ***<Edit>*** button.
- "***Select report items***343" window will be opened. Select the desired template item for editing, choose ⊙ **Customized report** option, and click ***<Edit report>*** button.
  Report designer will be opened, and a default template for the current item will be loaded from the **default.dtt** file



The example of Peak table report template for **Response normalisation** method and **reporting by groups** is given here.

It is possible to add or remove fields, change their formatting and properties, move their position. Desired Sections also can be added and removed, their properties can be edited and different filters can be applied.

- Add information that is to be printed on each page header.
- Add as many Report headers as necessary (up to 9 Report Header Sections are allowed). Those sections will be printed consequtively. If it is necessary to apply some filter to the section (i.e. skip or include it to the report on some condition), click the right mouse button on the header of the desired section, select the **Section filter** option and create condition criteria using instuments from "Section selection criteria" window.
- Add **Sort Header** if records are to be sorted by some parameter (by groups in the current example). Click the right mouse button, select **Edit sort field** item, and choose the desired sort parameter from the list. In the current example **Peak_Group** sorting parameter is chosen. Place a header of the group's peak table in the section.

- Add **Detail section** to the Sort Header to organize body of the group's peak table.
- Add **Sort Footer** that calculates summary for each group. Use the same set of fields that were used in the **Detail Section**, but set the desired summarization type for each value in its "***Properties***" window (envoked by clicking the right mouse button)
- Add **Report footer** with the same values to calculate summary values for all peaks in all groups.

The following operations are often used:

- Add a ***Label*** (arbitrary user-defined text field) .

  Click on **Insert/Label** menu item (or  icon), place the appeared positioning rectangle to the desired position with a mouse, and click any mouse button to accept position of the label. Double-click the label and enter the desired text. It is possible to change font size, style, color and some other attributes of the text. Dimentions of the label rectangle can be changed with mouse.
- Add a ***Data field***.

  Click on **Insert/Data field** menu item (or  icon). "***Select report item*** 343" window will be opened. Select the desired variable and place the appeared positioning rectangle to the desired position with a mouse, and click any mouse button to accept the position.
  Double click the left mouse button to edit parameters of the data field.
- Add a ***Formula field***.

  Click on **Insert/Data field** menu item (or  icon).
  Enter name for the formula. This name is local and can be used in the current template only.Click ***<OK>*** to accept.
  In the "***Calc***" window create the desired formula using available **Data Fields** 398, **System Fields** 399, **Dialod Fields** 400, **Formula fields** 399, and embedded functions 409 and operations 401
- Graphical objects. It is possible to use lines 396 and pictures 395 in reports

Part XI

Spectral operations

11 Spectral operations

11.1 Spectrum definition

Spectrum is a set of responses for all channels in the multi-channel chromatogram. Several types of spectra can be distinguished in the **Chrom&Spec** software:

- spectrum at the peak apex.
- spectrum averaged for all points of the selected chromatogram peak.
- best angle spectrum for the peak.

Spectra are shown in a special Spectrum window 431 where several spectral operations can be performed.

Note: Spectra in **Chrom&Spec** software are calculated relative to baseline (i.e. after baseline subtraction).

11.2 Multi-channel chromatogram definition

Multi-channel chromatograms contain several data channels at the same time and provide a power tool for analysis of complex mixtures.

Two types of multi-channel chromatograms can be distinguished on the basis of signal source nature.

In some cases, the chromatographic detector provides not one, but several response values for each measurement. A typical example is a diode-array detector or a rapid scanning detector in LC. In this case all data channels are of the same physical nature (i.e. UV absorbance). Thus, DAD100 detector can provide measurements at up to 100 channels simultaneously.

In other cases, several chromatographic detectors may be used to monitor the same chromatographic separation. Typical examples are simultaneous use of thermo conductivity and flame ionization detectors in GC, UV + refractive index or UV + radioactivity detectors in LC. As a rule, physical nature of detectors is different in this case.

Both cases are handled by Chrom&Spec software in a similar way as multi-channel chromatograms 146.

The software provides a complete toolkit for correct handling of such data in peak detection, identification, calibration and quantification.

Additional instruments such as factor analysis 451 and spectral operations 424 are specific for multi-channel chromatograms.

11.3 Spectral module overview

Chrom&Spec software includes a special **Spectral module** dedicated for spectral operations in the case of multi-channel chromatograms 146.

All spectral operations are available in the Spectrum window 431 activated by **Process / Spectrum** menu item.

The following basic operations are available using the Spectral module

2D-spectra presentation 438

3D-spectra presentation 438

Calculating spectra for a peak 434
Creation of spectra database on disk
Recognition of the current spectrum 455
Factor analysis of the selected peak 435
Peak recognition by spectrum 455
Performing quantification by spectrum 458

The following procedures are to be available in the nearest future versions:

A new peak identification scheme using spectra database

Note: spectral module is available in any multi-channel chromatogram. However, it should have 3 analytical channels at least.

See also:

Factor analysis basics 450
Factor analysis of the chromatogram site 451
How to perform factor analysis of the peak 454
How to perform factor analysis of the chromatogram site 453

11.4 Spectral analysis definitions

The spectral analysis of the chromatogram site (or peak) is based on comparison of all its points (instant spectra) using tools of **vector algebra** (i.e. **factor analysis**). Spectral analysis procedure allows to analyze chromatogram site (or peak) and to make conclusion on a degree of its spectral homogeneity, and in the case of overlapped chromatographic peaks it is possible to receive spectra of individual components and their real elution profiles. Often spectral analysis is called as factor analysis.

The first step of the factor analysis is to calculate **a table of spectral components**. This table is resulted from the **covariance matrix** composed of a specially normalized spectral raw data poitns. The total number of table elements equals to number of own vectors of the **covariance matrix** (coincides with number of wavelengths on the chromatogram), and each element equals to a square root from the corresponding **own number** of the covariance matrix. For convenience these table elements are normalized to 100%.

Each element of the table meets an **abstract spectral component** (that is a vector), and expresses its **length**. Real spectrum can be expressed as a **superposition** of these abstract spectral components. The larger element value, the more contribution of the component to the resultant spectrum. Strictly speaking, the initial signal can be exactly restored if all abstract components are used. However, due to limited signal-to-noise values and limited number of real spectral components on the chromatogram site, most of abstract spectral components are insignificant and can be rejected. **Significant components** are proposed automatically on the basis of internal threshold values, or can be selected manually (by default table elements under 1% are considered as insignificant). If the only significant component can be selected, the peak can be considered as homogeneous by spectra.

See also:

Theory of spectral operations 426
Factor analysis basics 450

11.5 Theory of spectral operations

- What is a spectrum?

Analytical chemistry usually deals with spectra as a set of electromagnetic waves emitted or absorbed by the sample. A classical example of the spectrum is an absorption UV-spectrum of some substance solution. This is a contiguous spectrum by physical nature, nevertheless due to digital processing methods UV-spectra are usually stored and handled as a set of measurements made with some permanent wavelength step. Wavelength step depends obviously on the spectrometer resolution and precision. It is no much sense to store a more detailed spectrum than optical resolution of the device or even thin structure of the spectrum itself.

Bischoff DAD100 diode array detector is able to measure an instant UV-spectrum of eluate in the range 190-390 nm, with a frequency about 10 Hz, with wavelength step of 2 nm, without eluent flow stop. Each instant spectrum corresponds to a single point on the multi-channel chromatogram, and chromatogram itself consists of large number of such points-spectra. In this case each channel of chromatogram corresponds to one wavelength. Thus, in the case of DAD100 detector an instant spectrum consists of 101 data points.

In common case, spectrum can be composed of measurements made with a variable wavelength step (but wavelengths should be sorted in ascending order). Furthermore, it is possible to define a spectrum for any multi-channel chromatogram, even if various physical values from different detectors are recorded in different channels.

It is also possible to calculate an average spectrum for peak (**Peak spectrum**) or even for chromatogram site (**Site spectrum**).

The absolute values of the detector signal are stored in the chromatogram. A more useful in chromatographic practice is to measure a magnitude of the detector signal relatively to a baseline level (we shall name this value as the **detector response**).

Note: all spectra in Chrom&Spec software are considered to be spectra od detector responses.

Apart from the three-dimensional view of a chromatogram offered by many photodiode-array detection software systems, Chrom&Spec uses a different approach for multi-channel chromatograms processing. A chromatogram is considered as a curve in multi-dimensional space, where each coordinate represents a detector response on each wavelength. One point in the **detector response (DR) space** represents one spectrum.

If we subtract the baseline in such a chromatogram, the curve will become tightly grouped around zero with peaks looking like curve fragments starting from zero and returning back to zero. However, the analysis of curves in DR-space is not very convenient, and the main reason is that spectral analysis techniques is based on root-mean-square (RMS) approach. The RMS approach can be successfully used only if the expected errors are comparable for all axes, otherwise the result will not be adequate.

There is a natural way to construct the unified space coordinates that are suitable for all kinds of spectral analyses - measurement units equal to the noise (or the expected measurement error) should be used for each axis. In this instance each coordinate axis will represent the signal-to-noise ratio (S/N) for one channel. This reduced coordinate system is called as a **noise-normalized detector response (NNDR) space**. One point in the NNDR space represents the normalized spectrum.

NNDR and DR spaces may be transformed into one another by linear transformation:

$$D = R*W \qquad (1)$$

where ***D*** = normalized spectrum from NNDR space (detection vector);
W = weight matrix with $w_{ij} = (i \times j)$ and $w_{ii} = 1/Ei$, where Ei is an expected error for the channel i;
R = *(R1,…,RN)* = detector response vector, and
N = number of channels (wavelengths)

Note: NNDR space can be used to analyze physically different signals, e.g., absorption, conductivity and radioactivity, in a unified way, within the same multi-channel chromatogram.

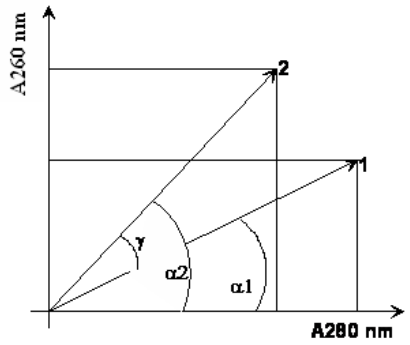
. Comparison of spectra

The most important part of the additional information obtained from the multi-channel chromatogram is founded on comparison of spectra. So, to estimate homogeneity of chromatographic peak all instant spectra within the peak should be compared, spectral identification is based on the comparison of the peak spectrum with library spectra, etc. Therefore, the correct choice of criterion for spectra comparison is of great importance.

There are a lot of methods to compare spectra. The most widespread of them are:

- comparison of **spectral ratios**;
- comparison based on a **correlation coefficients**;
- comparison based on **angle between spectra**.

An example of two elementary spectra (1 and 2) obtained on two wavelengths is given below. It is possible to illustrate basic ways of spectra comparison, using two elementary spectra obtained with two wavelengths only.



The figure represents a frame of two axes, each standing for absorption at a definite wavelength, say 260 and 280 nm. Then each two-wavelength spectrum is plotted as a point on a plane. It is obvious that each point on the plane sets a vector. Generally speaking, each spectrum is represented by a vector in many-dimensional space of wavelengths, therefore a concept of a vector is equivalent to a spectrum.

Note: each spectrum can be presented by a vector in NNDR space.

Spectral ratio is attitude of the detector response on one wavelength to the response on other (basic) wavelength. It is clear, that if both responses are inside the linear range of the detector, such ratio should not depend on a component concentration, and is individual for each substance. For calculating the spectral ratio it is necessary to know detector responses on each wavelength of the spectrum. However with number of wavelengths increasing the amount of the possible spectral ratio precipitately grows, and, for example, for a spectrum on 8 wavelengths 8!/(8-2)!/2!=28 of the spectral ratio exist. And

for 100 wavelengths number of spectral ratio would be 4950!

Correlation coefficient of two vectors (i.e. of two spectra) equals to a cosine of an angle between them, and therefore, angle and correlation coefficient are one-to-one connected, therefore we shall not consider a correlation coefficient as a measure of spectra comparison any more.

Angle between two vectors of spectra (γ) also can be used as a measure of their difference. And in most cases its using is more preferential. So the angle, as opposed from a correlation coefficient, is a metric value (or distance) in strictly mathematical sense, since the disparity of a triangle is fulfilled (for any three points A, B, and C the distance |AC| no more than sum of distances |AB| + |BC|). Unlike the spectral ratio, the angle is an integrated measure of spectra difference: for any pair of spectra there is only one angle between them, irrespective of the number of wavelengths. However, it is not very simple to receive a significant value of the angle difference.

Normalization of spectral axes

For more obvious discussion of the problem, let us to consider another simple model. Let's assume, that the analyzed component contains an isotope of some radioactive element, and the eluent measuring is carried out by two detectors: 1) UV-detector with a wavelength of 280 nm and 2) detector on radioactivity with giving output value in counts per second. A frame with the indicated axes is shown in Fig. 3. It is also possible to name points on the plane as spectra, however units on different axes are different. In such space it is impossible to apply concepts of an angle between vectors or vector length: the angle depends on an axis scale used, and vector length will be received by addition of square optical units with square counts per second and subsequent square root extraction from this chimera.

In the case of spectrum with uniform coordinates (for example, UV-spectra) the same problem remains, as the measuring errors on different wavelengths can be essentially different, and spectra comparison considering an error of gauging will give more reliable results.

So, a procedure of axes normalization is performed. Axes are transformed so that instead of the detector response, ratio of the response to some averaged measuring error is used. The units for coordinate axes become identical in this case, and the angle between spectra again can be used for their comparison. Thus, spectra are translated in some normalized spectral space, where detector response on each channel is normalized on an error of gauging (**E**rror-**N**ormalized **D**etector **R**esponse (***ENDR***) space is used).

Spectral homogeneity of a peak

Spectral information contained in the multi-channel chromatogram can be used to check homogeneity of the chromatographic peak.

Nevertheless, two additional conditions are necessary to distinguish components inside the peak:
1) all components should have different spectra
2) all components should have at least a small difference in retention time.

When homogeneity of chromatographic peak is being checked, a comparison of great number of spectra is performed: all spectra (i.e. points of the multichannel chromatogram) which are inside the chromatographic peak. The supposition being checked: all spectra relate to one substance. If it actually so, all spectra vectors of the tested chromatographic peak, submitting the **Lambert-Beer's law**, should lay along one straight line within error of measuring.

Such supposition is checked within the framework of multi-dimensional regression analysis, by carrying out the best straight line on experimental points. The method of principal components allows to calculate:

- a direction of the vector of a spectrum;
- average magnitudes of deflections;
- amount of individual spectral components in peak (their spectra and lengths, at which the deflections are minimum).

Lambert-Beer's law shows a linear relationship between the flow cell path length and absorbance.

$$Abs = -\log T = \log \frac{I_0}{I} = \varepsilon \cdot c \cdot d$$

where

T is the transmission, defined as the quotient of the intensity of the transmitted light I divided by the intensity of the incident light, I0

ε is the extinction coefficient, which is a characteristic of a given substance under a precisely-defined set of conditions of wavelength, solvent, temperature and other parameters

c is the concentration of the absorbing species (usually in g/l or mg/l)

d is the path length of the cell used for the measurement.

Analysis of a peak homogeneity

Spectral homogeneity of a peak is a criterion for its purity: if some admixture presents, spectral homogeneity is disturbed.

If a homogeneous peak is analyzed, all its instant spectra should be obtained by multiplication of a component spectrum on instant component concentration. In this case 100 % of a signal should be composed of a single own vector and this vector should be a spectrum of the component. In practice the matter is not absolutely so.

The error of gauging results in that some part of a signal is distributed on other components. The allowable part of a signal coming on non-significant components, signal-to-noise ratio of the chromatogram. For a diode-array detector baseline noise should not exceed 1% if the detector response is about 1 AU. This magnitude was accepted as a threshold of a spectral component significance.

D = c * Q + e

where **D** is a detector response vector,
c is a concentration of the component,
Q is a component spectrum reduced to NNDR space,
e – error vector.

The significance limit of 1% can be adequate only at preliminary analysis of the peak. The real value should be determined experimentally, performing a chromatographic analysis of the pure individual component using the same chromatographic conditions and approximately the same concentration as in working analysis. The real significance threshold will be given by spectral analysis of this obviously homogeneous peak, and will equal to the value of the second-largest own vector.

Non-homogenous chromatographic peak results in several significant own vectors in the table of spectral components:

$$D = \sum C_i \cdot Q_i + e$$

The number of significant own vectors is called as "rank".

In the case when pure spectra for all substances within an overlapped peak are known in advance, one can use the RMS approach to decompose every measured spectrum of the peak into spectra of this pre-defined basis of spectra. In the case of known spectra, eqn. 3 represents a set of N equations with K unknowns, where K is the number of individual components and N, as before, is the number of channels (wavelengths). In the case when K J N we can apply the RMS approach which gives a solution of the above eqn. in the form:

$$C = D \cdot Q^T \cdot (Q \cdot Q^T)^{-1}$$

where **C** = (c1, c2, ..., ck) is a concentration vector,
D = detection vector, and
Q = (N*K) matrix composed of K detection vectors made from pure component spectra

Of course, the spectra of pure components should be linearly independent (not too similar), otherwise matrix inversion in eqn. 4 cannot be applied. If these conditions are fulfilled, decomposition is allowed and gives a unique concentration vector C.

Spectral separation of overlapped peaks can not be performed if:
- their spectra are identical;
- their retention times are the same.

By making spectrum decomposition for every peak point, we can obtain a concentration profile for each component.

It is also possible to analyze a multi-channel chromatogram without any a priori knowledge of component spectra. A multi-dimensional space mathematics, i.e., principal component and factor analysis should be applied in this case. The theory and a detailed description of the algorithms for this type of analysis will not be discussed here. An overview of the calculations allowed by Chrom&Spec software are presented here.

Factor analysis procedure is applied as following.

(a) A subspace with a minimum number of dimensions that contain the entire peak curve within admissible error is constructed using the principal component approach. The number of subspace dimensions represent the number of components in the peak, and peak spectra should be a linear combination of subspace basis vectors.

(b) Noise is filtered by placing the whole curve for the peak into subspace.

(c) The best candidates for the role of "pure spectrum" for each component is selected among all peak points. The assumption is made that some point exists within the peak where the first component is "pure" and assume the spectrum at this point to be a true pure first-component spectrum, and so on.

(d) Elution profiles of each component within the peak is constructed and their amounts are calculated.

To apply this type of curve analysis, one should note the propositions made: (a) eluted substances have linearly independent (i.e. different) spectra; and (b) the elution profiles are shifted with respect to each other so that for each component there is a point within an analyzed chromatogram region where only this component is present.

Reasons of apparent peak non-homogeneity

In some cases a faulty conclusion on peak or site non-homogeneity can be done. The following cases can be suggested.

- **Errors of the baseline subtraction** are most typical in the case of peak overlapping and improper tuning of integration parameters. These errors can be revealed at close visual analysis of the chromatogram. The baseline can be corrected by the user, as it is described in McDAD manual. It is recommended to perform automatic integration (or manual correction) using the "total"channel.
- **Errors of interpolation**. The interpolation of measurements to the same moment is applied for rapid-scanning detectors or several detectors connected consecutively. The higher is sampling rate the lower interpolation error is. The same recommendation as for quantification or integration procedure can be applied: the narrowest peak should be described by 30 data points at least. In the case of several detectors additional peak broadening can be derived from extra-detector lines.
  For diode-array detectors this type of error can be ignored.
- **Detector signal is out of linear dynamic range**. Signal overscaling can occur for large peaks. Both

ADC and detector have a guaranteed linear dynamic range where measuring error does not exceed some threshold value. Channels with the signal coming out of this range will be discarded during the spectral analysis procedure. Of cause, accuracy of the factor analysis will be lowered compared with non-overscaled chromatogram.
Note that detector's linear range on some channels can be considerably lower than in the device specification due to eluent absorption.

- **A gradient of concentration in the cell** can be observed for narrow peaks. This effect can be minimized by optimization of dynamic properties of the detector cell (in the ideal case dynamic volume of the cell is equal to its geometrical volume)
- **Refractometric effect** in the cell can be observed for high concentration of component in the eluate. This effect also can be minimized by proper geometry of the cell. In addition high component concentrations in the cell can cause a violation of Bouguer's law.
- **Fluorescence** of the component. Fluorescence of the component in the cell and series of other causes also can result in non-linearity of the detector response (violation of Bouguer's law).

The indicated effects lead to apparent separation of homogeneous chromatographic peak on two or more peaks with very similar spectra, and the shape that considerably differs from the gaussian, characteristic for chromatographic peaks.

11.6 Spectrum window

(*Main menu* Spectra / Spectral window...)

"**Spectrum**" window shows all calculated or loaded from disk spectra and provides all available operations with them. Each spectrum is drawn by different color and has a legend (ID number and name) . Spectrum name coincides with a correspondent peak name from the components table.

"**Spectrum**" window is invoked by **Process / Spectrum** menu item.

Note: "**Spectrum**" window can be opened for multi-channel chromatograms 146 only.

All operations are performed via "**Spectrum**" window menu

File 432

Edit 433

View 437

Note: All spectra are calculated after baseline subtraction. Spectra without baseline subtraction are available in the "**2D-spectrum**" window.

Spectrum can be calculated for a chosen peak only.

See also:

Scaling of spectra 432

11.6.1 Spectrum window menu

11.6.1.1 Scaling of spectra

Spectra in the "***Spectrum***" window can be scaled using arrow key:

<Up>	stretch scale on Y axis
<Down>	shrink scale on Y axis
<Right>	stretch scale on X axis
<Left>	shrink scale on X axis

The same keys being pressed together with **[Shift]**, move spectra along X or Y axes without scaling.

Double clicking on the left mouse button performs autoscale operation for both axes.

Contents of spectral window will be printed exactly as is on the screen (WYSIWYG function).

11.6.1.2 File

(Spectrum / File)

File menu provides disk operations with spectra in the current "**Spectrum**" window.

Save spectra 432	save the contents of the "**Spectrum**" window to disk as ***.spe** file
Add to 432	add the contents of the "**Spectrum**" window to an existing ***.spe** file
Load spectra 432	add new spectra from a selected ***.spe** file to the existing "**spectrum**" window
Clear spectra 433	delete entire contents of the current "**spectrum**" window
Import from text 433	import spectra from other file formats
Export from text 433	import spectra from other file formats

11.6.1.2.1 Save spectra

(***Spectrum* / File / Save spectra**)

This operation enables to save spectra from the current "**Spectrum**" window. If several spectra are present in the window, all them are saved.

Any directory and filename according to Windows rules can be specified for spectra storage. To create a new directory click **Create new folder button** in the "**Save to spectrum file**" window

11.6.1.2.2 Add spectra to

(Spectrum / File / Save to)

This option enables to add spectra from the current "**Spectrum**" window to an existing ***.spe** file. If several spectra are present in the window, all them are added.

"**Save to spectrum file**" window is opened, and any directory and filename can be specified for spectra storage according to Windows rules.

11.6.1.2.3 Load spectra

(Spectrum / File / Load spectra)

This option enables to load spectra to the current "**Spectrum**" window.

If the "**Spectrum**" window is not empty, loaded spectra is added to the existing one.

"**Open spectrum file**" window is opened where any directory and filename can be selected.

11.6.1.2.4 Clear spectra

(Spectrum / File / Clear spectra)

This operation deletes all spectra in the current "**Spectrum**" window.

Note: no precaution is generated even if spectra in the current "**Spectrum**" window have not been saved.

11.6.1.2.5 Import spectra

(***Spectrum* / File / Import)**

This option enables to import spectra from other file formats to the current "**Spectrum**" window.

The following formats are supported:

EasyChrom spectrum (***.spm**) spectrum files generated by the *EasyChrom* chromatography package.

11.6.1.2.6 Spectrum_Export

(***Spectrum* / File / Export to text**)

This option enables to export spectra to file in text format. This option is useful for user's spectral database creation and editing

11.6.1.3 Edit

(Spectrum / Edit)

Edit menu provides the following operations with spectra in the current "**Spectrum**" window and (or) current chromatogram window.

Calculate 434
Recognize 434
Apply all 436
Apply manually 436
Options 436

11.6.1.3.1 Calculate spectrum

(Spectrum / Edit / Calculate)

This option opens Spectrum calculating window 434 allowing to calculate spectra for a selected peak.

11.6.1.3.2 "Spectrum calculating" window

(Spectrum / Edit / Calculate)

"**Spectrum calculating**" window allows to calculate spectrum for any selected peak of multi-channel chromatogram, and put it to the current Spectrum window 431.

Calculate spectra of the peak # selection of the peak to calculate spectrum for.

Calculation method

Average peak spectrum 435 — resultant spectrum is calculated as average spectrum for all points of the peak

Best angle spectrum 435 — spectrum is taken in the site of the peak where spectral angle between neighbouring points is minimal

Center of the peak spectrum 435 — resultant spectrum is taken as spectrum at the peak apex point

Factor analysis

Factor analysis of the peak 435 — calls a factor analysis procedure for the selected peak

See also:

How to calculate peak spectrum 454

11.6.1.3.3 Recognize spectrum

(*Main menu* Spectra / Recognition wizard...)

Recognize item opens Spectrum recognition window to performs spectra comparison in the "**Spectrum**" window with a etalon spectra stored on disk.

See also:

Spectrum recognition 455

11.6.1.3.3.1 "Spectrum calculating" window

(Spectrum / Edit / Calculate)

"**Spectrum calculating**" window allows to calculate spectrum for any selected peak of multi-channel chromatogram, and put it to the current Spectrum window 431.

Calculate spectra of the peak # selection of the peak to calculate spectrum for.

Calculation method

Average peak spectrum 435 — resultant spectrum is calculated as average spectrum for all points of the peak

Best angle spectrum 435	spectrum is taken in the site of the peak where spectral angle between neighbouring points is minimal
Center of the peak spectrum 435	resultant spectrum is taken as spectrum at the peak apex point

Factor analysis

Factor analysis of the peak 435	calls a factor analysis procedure for the selected peak

See also:

How to calculate peak spectrum 454

11.6.1.3.3.2 Average peak spectrum

Average peak spectrum is calculated using a formula

11.6.1.3.3.3 Best angle spectrum

Best angle spectrum is calculated using a formula.

This type of spectrum has the best signal-to-noise ratio and can be recommended for etalon spectra calculating.

11.6.1.3.3.4 Center of the peak spectrum

Center of the peak spectrum is taken at the apex point of the selected peak

11.6.1.3.3.5 Factor analysis of the peak

(Spectrum / Edit / Calculate)

This option activates a factor analysis procedure for the selected peak.

Note: this procedure looks like the factor analysis of the chromatogram site 451 procedure, but deals with a single peak on the chromatogram, and has not influence on integration results.

Factor analysis of the peak procedure allows to control peak homogeneity and to divide overlapping chromatographic peaks into individual components using a special processing algorithm.

Factor analysis of the peak procedure enables to determine a number of significant components within the selected peak and to calculate individual spectra of the components. Resulting spectra of components are presented in the Spectrum window 431 and can be saved to disk or compared with etalon spectra on disk.

See also:

Factor analysis basics 450

Spectrum calculating window 434

How to perform factor analysis of the peak 454
How to perform factor analysis of the chromatogram site 453

11.6.1.3.4 Apply all

(Spectrum / Edit / Apply all)

11.6.1.3.5 Apply manually

(Spectrum / Edit / Apply manually)

This procedure applies a recognized spectrum from the disk database to the current chromatogram.

Note: the spectrum should be added to the **Spectrum window** first, by using ***<Set>*** procedure in the Spectrum recognition window

The result depends on settings of the How to apply recognized component 436 window. For example, the component that has the closest spectrum to etalon can be added to the components table

11.6.1.3.6 Options

(Spectrum / Edit / Options)

"**How to apply recognized components?**" window defines rules of how to apply recognized peaks information in the case of existing components table.

Previous component assigned to peak action

(if recognized by spectrum peak has already been assigned to some item from components table, and names of spectrum and item are different)

Leave unchanged — ignore spectrum recognition and use recognition using current components table (default value)

Leave in components table, but make unrecognized — use spectrum recognition, ignore recognition using components table, and make former component unrecognized (its retention time is set to Zero).

Delete from components table — use spectrum recognition, ignore recognition using components table, and delete former component information and substitute it by spectrum recognition data.

Existing component with the same name action

(if component identified by spectrum already exist in components table)

Reassign to recognized peak — use spectrum recognition, delete former component information and substitute it by spectrum recognition data.

Leave unchanged, ignore spectrum recognition — ignore spectrum recognition and use recognition using components table info

11.6.1.4 Veiw

(Spectrum / View)

View menu provides the following operations with spectra in the current "**Spectrum**" window.

Representation 437	select a way of spectra normalization in the current Spectrum window 431
Info 437	show information on spectra in the current "**Spectrum**" window
Chrom 3D 438	draw a 3D-presentation of the current chromatogram
Chrom 2D 438	draw a 2D- presentation of the current chromatogram

See also:

11.6.1.4.1 Spectra view window

(Spectrum / View / Representation)

"**Spectra view**" window is used to select a method of spectra normalization. Normalization is applied for spectra comparison.

All spectra in the "**Spectrum**" window can be normalized using the following methods

Don't normalize	don't use any normalization. All spectra are shown "as are", i.e. as a set of detector responses for all chromatogram channels
For sum of squares	after normalization sum of squares are equal for all spectra
For integral	after normalization spectra integrals (areas) are equal.
For maximum value	maximum value in each spectrum is taken per unit.
For value at wavelength	value at the selected wavelength is taken per unit for each spectrum. All normalized spectra cross at the selected wavelength.
☑ **Draw with shift**	take into account systematic shift of spectra

Note: this procedure changes spectra appearance only and does not alter spectral data themselves.

11.6.1.4.2 Info window

(Spectrum / View / Info)

"**Info**" window shows properties for all spectra in the "**Spectrum**" window and allows to edit them. Spectra properties are listed as the following table

ID	ordinal number of a spectrum
Peak	peak number in the current chromatogram corresponding to the spectrum. If spectrum was loaded from disk (i.e. it does not refer to chromatogram), this column contains "**0**".
Component	name of the component. When spectrum is calculated for a selected peak, its name from the components table is inserted automatically. "*Component*" field can be edited directly in the "**Info**" window.
Etalon	this flag shows if the spectrum should be considered as etalon.
Quantification	this flag shows if quantification by spectrum is to be performed for the current component. When the flag is cleared, quantification is not performed, and "**Quantity calculation**" window is unavailable.

Quant	component quantity calculated by using spectrum and additional parameters from the "**Quantity calculation**" window.
Quant units	user-defined units for calculated quantity (set in the "**Quantity calculation**" window)

Note: Double-click the left mouse button on the desired cell, or place cursor to the desired position and press [Enter]

Buttons:

<Delete>	delete the selected spectrum form the table and the current "**Spectrum**" window.
<Merge> 440	open "**merge**" window allowing to select a spectrum from "**Spectrum**" window to be merged with the current spectrum.
<Shift>	open "**Select**" window allowing to select an etalon spectrum that will be compared with the current spectrum for shift value calculating.
<More...> 441	opens "**More info**" window to edit parameters of the selected spectrum
<Quant...> 442	opens "**Quantity calculating**" window to set parameters needed for the current component quantification by spectra

11.6.1.4.3 "Chrom 3D" window

(Spectrum / View / Chrom 3D)

"**Chrom 3D**" window allows to view 3D-image of the current multi-channel chromatogram. 3D-image is calculated on the basis of detector responses for each channel, i.e. after baseline subtraction. That is why in the absence of peaks 3D-image looks like a plane.

The following operations with 3D-image are available:

-rotation (by the mouse moving while the left mouse button is pressed)

-scaling (by moving mouse up or down while [Shift] key is pressed)

11.6.1.4.4 "Chrom 2D" window

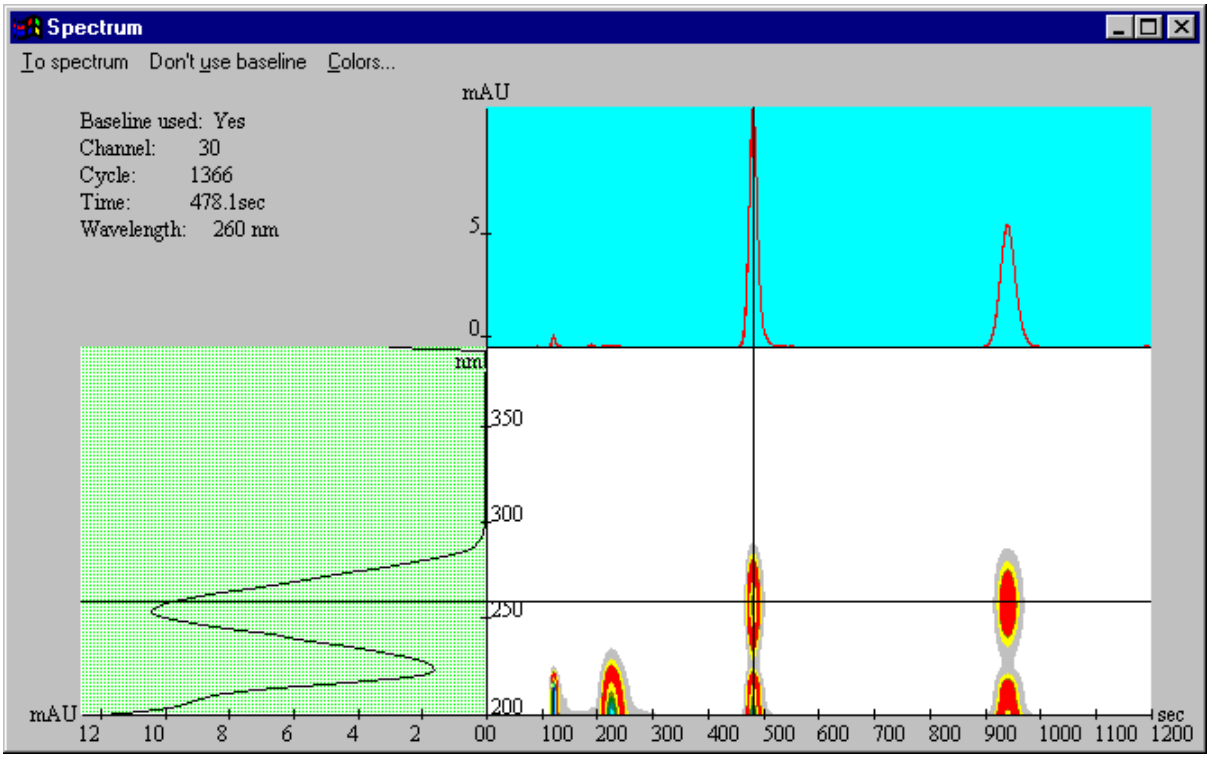
(Spectrum / View / Chrom 2D)

"**Chrom 2D**" window allows to view 2D-image of the current multi-channel chromatogram. 2D-image is shown on the basis of detector responses for each channel (i.e. after baseline subtraction). Different colors can be defined to map signal value on plane.

It is possible to select point (press the left mouse button and move mouse to the desired point on 2D-image) that defines two sections of the spectra:

- the first section is eluent spectra at the defined time moment. It is plotted on the left hand side from the 2D-image. It is possible to switch if baseline should be subtracted or not, by clicking **<Don't use baseline>** menu item.

– the second section presents a chromatogram at the selected wavelength



The following menu is available:

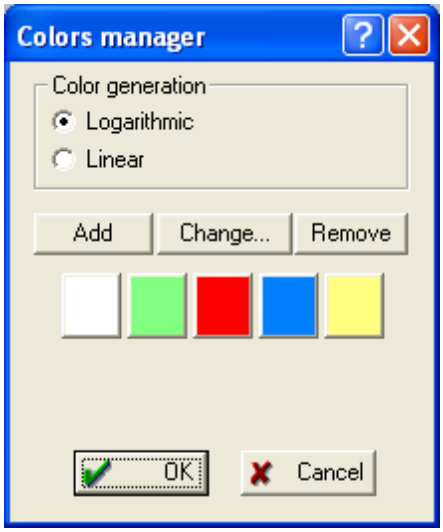
To spectrum copy the spectrum section of 2D-image to Spectrum window 431 for further processing.

Don't use baseline toggle a baseline subtraction option. Spectrum section can be calculated on the basis of absolute detector signal (i.e. without chromatogram baseline subtraction, the first point of the chromatogram is taken as zero), or on the basis of the detector response (i.e. baseline subtraction is performed)

Colors open Colors manager 439 window to define or tune colors of 2D-image.

11.6.1.4.4.1 Colors manager

Colors manager window allows to define color palette and color scheme



Color generation

Two color schemes can be applied:

⊙ **Logarithmic**	logarithmic scale for signal value is used. It gives a more distinct picture for lower response level
⊙ **Linear**	linear scale for signal value is used (default value)

<Add>	Add a new color to the palette
<Change...>	Change a selected color in the palette
<Remove>	Remove the selected color from the palette

See also:

Path editor 155
Spectral: Chrom 2D window 438

11.6.1.4.5 "Merge spectrum" w indow

Merge operation can be used, for example, to improve signal-to-noise ratio by merging several identical spectra, or to obtain a more detailed spectrum (in the case of some rapid-scanning detectors).

"**merge**" window allows to select a spectrum from "**Spectrum**" window to be merged with the spectrum previously selected in the "**Info**" window. The resultant spectrum replaces the second one.

Available spectra (all except for the current one) are given as the following table:

ID	spectrum ID (the same as in "**Info**" window and "**Spectrum**" window)
Component	spectrum name (is taken from "**Info**" window and can be edited there)
Discrepancy	discrepancy between the spectrum selected in the "**Info**" window and spectrum chosen in the "Merge" window
Angle	angle between above two spectra.
☑ **Don't remove original spectrum**	use this flag to prevent replacement of the original spectrum by the resultant one.
☑ **Ignore exceeding maximum allowed discrepancy**	when the flag is set, software will not control if spectra to be merge are similar

or not. Only similar spectra can be merged otherwise.

See also:

Operations with spectra

11.6.1.4.6 Spectrum: “More” window

"**More**" window shows additional parameters that present or can be entered for component related to the current spectrum. Some parameters taken from the source chromatogram are also present here.

The following parameters are available:

Component component name that appears as legend in the "**Spectrum**" window. Component name is taken from the components table 171 if it existed at the moment of the spectrum calculating, or can be entered manually here.

Eluent Eluent composition. Is automatically taken from the passport or can be entered by the user

Channels number of channels in the spectrum (corresponds to channels number of the parent chromatogram)

Volume volume of the parent peak that was used for the spectrum calculating. This parameter is used in the quantification by spectrum procedure.

Flow Eluent flow value, taken from the parent chromatogram. Flow units can be selected in the Global preferences window 41.

Start time time of the component's peak start

End time time of the component's peak end

Molec.weight molecular weight of the component. This parameter is used in the quantification by spectrum procedure.

Spectrum units units on the spectral axis ([nm] is used by default)

Response units units for the spectrum response axis. Is taken from the channels table 149 of the parent chromatogram

Date date of the parent chromatogram start

Time time of the parent chromatogram start

Operator Name of the current user at the moment of the spectrum calculation. It is taken from the List of users, in accordance with the password entered at the program starting.

Peak peak number in the current chromatogram corresponding to the spectrum. If spectrum was loaded from disk (i.e. it does not refer to chromatogram), this column contains "**0**".

Source file file of the parent chromatogram

Shift value the current spectrum should be shifted to compensate detector optical error or solvent shift.

See also:

Operations with spectra

11.6.1.4.7 Spectrum: “Quantity calculating” window

"**Quantity calculating**" window allows to perform quantity calculation for the current component using spectral information. The window is available for spectra with "*Quantification*" flag set to **Yes** in the "**Info**" window.

All data for quantification are taken from the spectrum description (i.e. from the corresponding chromatogram) or can be entered by the user. In the later case "**Quantity calculating**" window can be used to recalculate any parameter (it is necessary to click a corresponding **<Get>** button to reculculate the desired parameter).

Component — component name that appears as legend in the "**Spectrum**" window. Component name is taken from the **components table** 171 if it existed at the moment of the spectrum calculating, or can be entered manually in the **Info window** 437.

Molecular weight — molecular weight of the component. This parameter is used in the quantification by spectrum procedure. Default value is 1.

Volume — volume of the parent peak that was used for the spectrum calculating. This parameter is used in the *quantification by spectrum* procedure. It is calculated automatically as a difference between retention volumes of peak start and end, or can be entered manually.

Absorbance [o.u.] — average absorbance of the peak (**Aav**)

$$Aav = \frac{\int_{v1}^{v2} A \cdot dv}{(v2 - v1)}$$

where **v1** and **v2** are retention volume of the peak start and peak end, **A** – current absorbance.

Wavelength [nm] — user-selectable wavelength that is to be used for calculations.

Extinction [AU*l/mol] — value of the extinction factor. It can be calculated automatically for components on the basis of calibration chromatogram or entered by the user.

Quant — quantity of the component in the peak.

User-selectable units for *quantity* of the current component:

Volume units: [l, ml]

Mass units: [mole, mmole, μmole, nmole]
[g, mg, μg, ng]

<Get> — recalculates the desired parameter on the basis of user-entered value(s). All other parameters are considered unchanged. Several values can be changed by the user at the same time.

11.7 Spectral report

(*Main menu* Spectra / Spectral report...)

This option performs an automatic identification of components in the current chromatogram on the basis of existing spectral database, and generates a report/ Report is exported to the text editor for preview (MS Word, MS WordPad or some other can be used). Further printing can be done from the text editor after report viewing.

All peaks on the chromatogram are processed according to rules set in the "***Spectral autorecognition setup***" window. All recognized peaks will be reported.

11.8 Spectrum recognize wizard

McDAD2ES / Spectra / Recognize wizard

Spectrum recognize wizard enables to obtain spectrum of the desired peak and to perform its recognition using a spectra database on disk. In other words, it facilitates one of the most often used spectral operations that otherwise could be performed manually via Recognize option.

After *Spectrum recognize wizard* activation "**Spectrum**" and "**Recognize wizard**" windows are opened at the same time.

Fill all necessary fields in the "**Recognize wizard**" window and click **<Continue>** button to go to the next wizard step.

Spectrum recognize wizard includes the following steps:

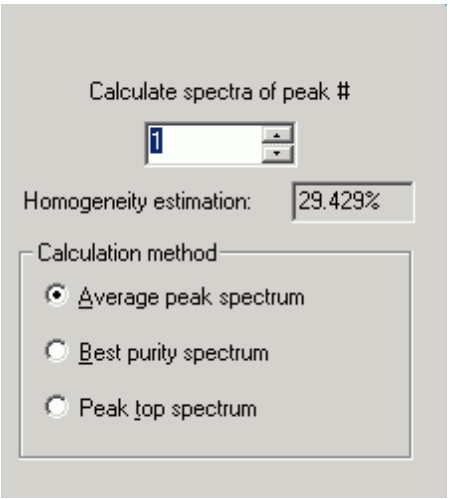
Spectrum calculating for the desired peak

Seaching in the spectral database

Show results

11.8.1 Spectrum recognize wizard: step 1

The first step of the *Spectrum recognize wizard* consists in spectra calculating for the desired peak:



Both "**Spectrum**" and "**Recognize wizard**" windows are opened.

Just select a desired peak number and choose a preferred type of spectra calculation.

Homogeneity estimation parameter shows a degree of peak homogeneity estimated on the basis of spectral analysis of the peak. The closer this parameter is to 100% the more uniform is the peak. Value of the parameter shows how completely the entire peak spectra can be described by the first **significant spectral component** (calculated as a result of the factor analysis).

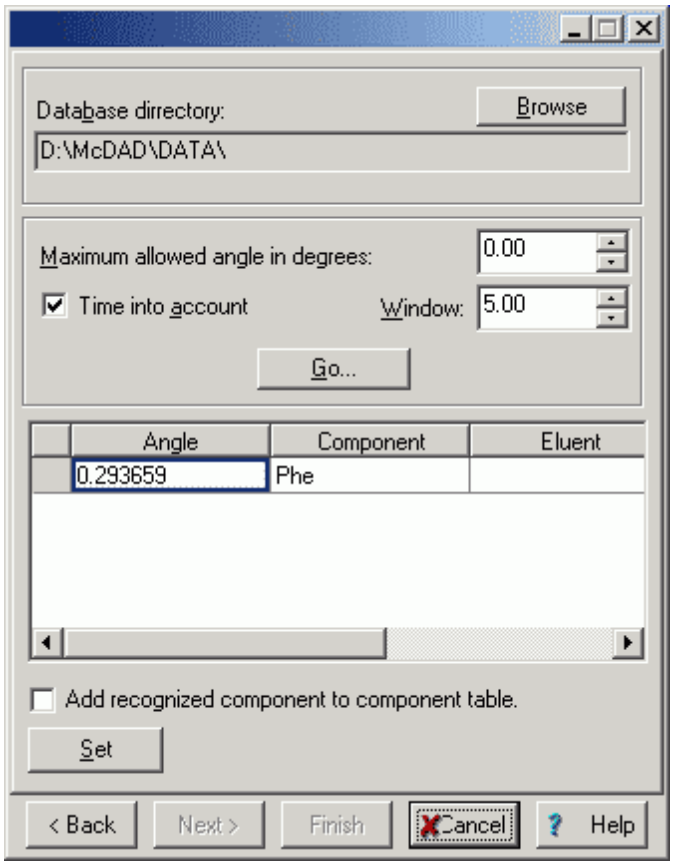
Click **<Next>** button to perform spectrum calculation and go to the next Wizard step.

See also:

Factor analysis basics 450
Theory of spectral operations 426

11.8.2 Spectrum recognize wizard: step 2

The second step of the *Spectrum recognize wizard* consists in spectra calculating for the desired peak:



Spectrum of the selected peak will be calculated and plotted in the "**Spectrum**" window that is opened alongside.
Although this window does not contain a menu, spectra scaling 432 buttons are fully functional.

A table that shows all spectra in database that are similar to the current peak spectrum. Angle between spectra is used as criteria.

Database directory shows the directory where etalon spectra are stored.
<Browse> change an etalon directory.

Maximum allowed angle Enter a maximum allowable angle between the current spectrum and etalon spectrum. All etalon spectra from disk that has a lower angle difference (in multidimensional spectral space) with the current spectra,

will be listed in the Spectra recognition table after **<Go>** procedure executing.

☑ ***Time into account*** set this flag to take into account retention of the etalon component as an additional search parameter. Only etalon spectra within the preset retention window will be taken.

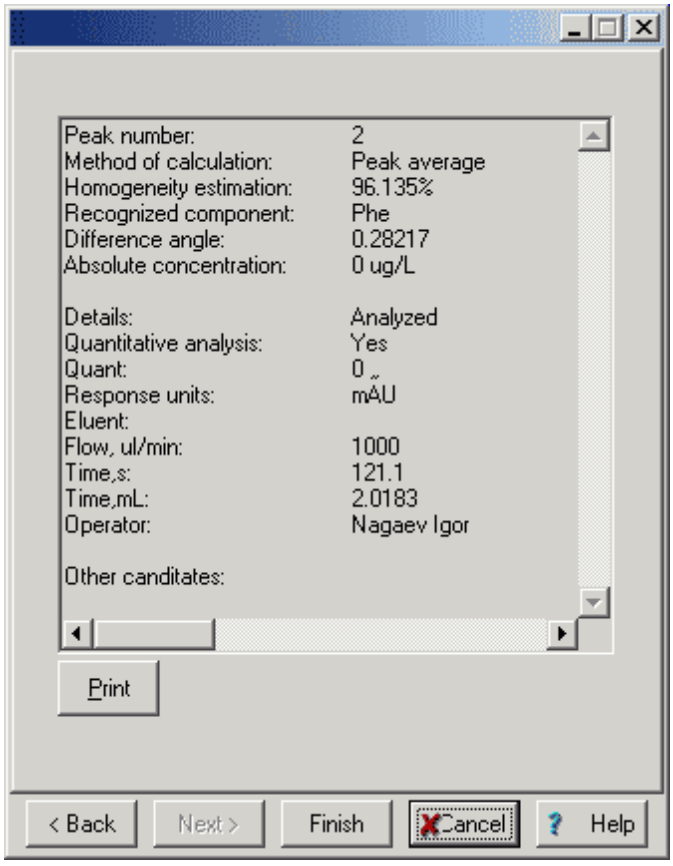
<Go> Execute recognition procedure

☑ ***Add recognized component*** Set this flag to add recognized component to Components table.

<Set> Accept and execute settings.
Spectrum that was found in the database is added in the left window.

11.8.3 Spectrum recognize wizard: step 3

The fourth step of the *Spectrum recognize wizard* shows results of the recognition.



Results can be printed by clicking **<Print>** button.

Parameters and results of the recognition procedure

Peak number peak that was processed by the *Recognize Wizard*

Method of calculation method of spectrum calculation

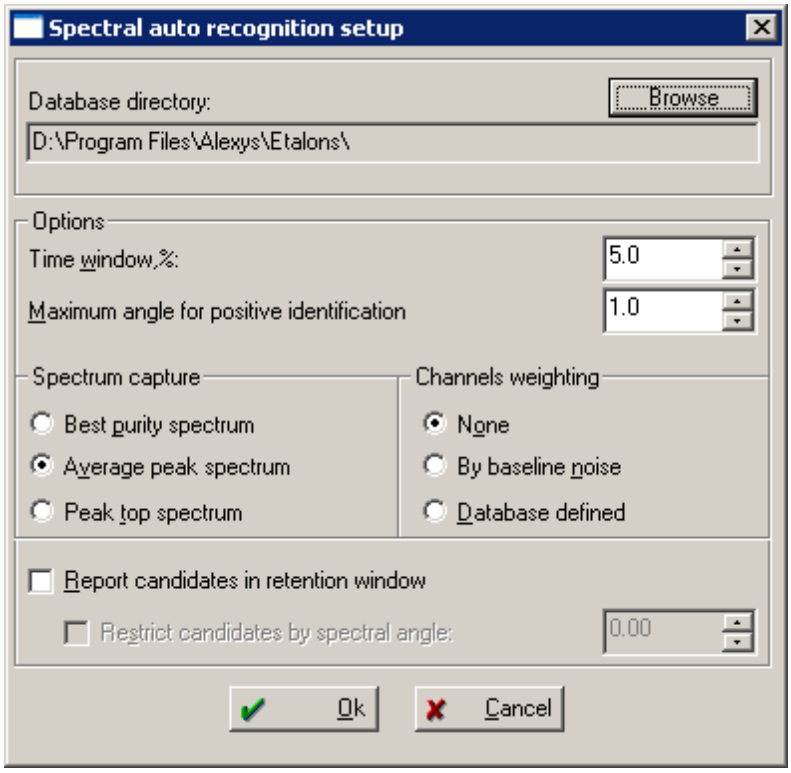
Homogeneity estimation the closer this value to 100% the more homogeneous the peak is.

Recognized component	component name is present if peak spectrum is identified in the existing database, and standard spectrum has a complete description.
Difference angle	angle between current and standard spectra. The lower the difference is the more identical these spectra are. Usually value of "1" means a very good spectra coincidence.
Absolute concentration	average concentration of the component in the eluate. The value is calculated if the standard spectrum has a complete description.
Details	
Quantitative analysis	(Yes/No) This flag shows if quantitative analysis is allowed
Quantity	calculated quantity of the component in the peak
Response units	units for Y axes on chromatogram
Eluent	eluent description from the passport of the chromatogram
Time, s	retention time of the peak **[s]**
Time, ml	elution volume of the peak **[ml]**
Operator	current operator
Other candidates	a list of other components with similar spectra that were found in the database. It is a good idea to use retention time as an additional parameter for recognizing procedure. However, spectra database should be obtained in the same conditions as the analyzed chromatogram.
<Finish>	this button completes the recognition procedure

11.8.4 Spectral Autorecognition Setup

(*Main menu* Spectra / Spectral analysis options...)

"***Spectral Auto recognition setup***" window allows to tune default spectral analysis options used by Recognition Wizard 443.



Database directory shows the directory where etalon spectra are stored.

<Browse> change an etalon directory.

Options

Time window Only etalon spectra within the preset retention window will be taken into account (if retention of the etalon component is selected as additional search parameter).

Maxixum angle a maximum allowable angle between the current spectrum and etalon spectrum. All etalon spectra from disk that has a lower angle difference (in multidimensional spectral space) with the current spectra, will be listed in the Spectra recognition table. The lower is this value the stricter is seach condition.

Spectrum capture

Average peak spectrum 435 resultant spectrum is calculated as average spectrum for all points of the peak

Best angle spectrum 435 spectrum is taken in the site of the peak where spectral angle between neighbouring points is minimal

Peak top spectrum 435 resultant spectrum is taken as spectrum at the peak apex point

Channels weighting

None No channels weighting is performed during spectra calculation. This way is often used in other spectral software. However, it doen not take into account a difference in the data accurity for various channels due to noise value.

By baseline noise	baseline noise for each channel is considered to calculate spectra. This is the recommended way of operation if spectra are used in qualitative analysis only leading to higher reliability of spectral recognition in this case.
Database defined	channebs are weigted as defined in spectral database file selected in this window

☑ *Report candidates in retention window*

check this box if other candidates within *time window%* are to be shown (othewise only one best fit component is shown).
Check ☑ *Restrict candidates by spectral angle* box to use additional filter for possible candidated

11.8.5 Peak homogeneity

Spectral information contained in the multi-channel chromatogram can be used to check homogeneity of the chromatographic peak.

Nevertheless, two additional conditions are necessary to distinguish components inside the peak:
1) all components should have different spectra
2) all components should have at least a small difference in retention time.

When homogeneity of chromatographic peak is being checked, a comparison of great number of spectra is performed: their number equal to number of chromatogram points in the peak. The supposition being checked: all spectra relate to one substance. If it is actually so, all spectra vectors of the tested chromatographic peak, submitting the **Lambert-Beer's law**, should lay along one straight line within error of measuring.

Such supposition is checked within the framework of multi-dimensional regression analysis, by carrying out the best straight line on experimental points. The method of principal components allows to calculate:

- a direction of the vector of a spectrum;
- average magnitudes of deflections;
- amount of individual spectral components in peak (their spectra and lengths, at which the deflections are minimum).

Lambert-Beer's law shows a linear relationship between the flow cell path length, concentration and absorbance (***Abs***).

$$Abs = -\log T = \log \frac{I_0}{I} = \varepsilon \cdot c \cdot d$$

where

T	is the transmission, defined as the quotient of the intensity of the transmitted light ***I*** divided by the intensity of the incident light, I_0
ε	is the extinction coefficient, which is a characteristic of a given substance under a precisely-defined set of conditions of wavelength, solvent, temperature and other parameters
c	is the concentration of the absorbing species (usually in mole/l)
d	is the path length of the cell used for the measurement.

The peak homogeneity is calculated as

Note: the current Chrom&Spec version does not take into account peak shape. Only spectral analysis is performed.

See also:

Reasons of peak non-homogeneity 449

11.8.6 Peak non-homogeneity reasons

In addition of real non-homogeneity of peaks due to presence of admixture conponents, a faulty conclusion on peak or site non-homogeneity can be done in some cases. The following cases can be suggested.

- **Errors of the baseline subtraction** are most typical in the case of peak overlapping and improper tuning of integration parameters. These errors can be revealed at close visual analysis of the chromatogram. The baseline can be corrected by the user, as it is described in McDAD manual. It is recommended to perform automatic integration (or manual correction) using the "total"channel.
- **Errors of interpolation**. The interpolation of measurements to the same moment is applied for rapid-scanning detectors or several detectors connected consecutively. The higher is sampling rate the lower interpolation error is. The same recommendation as for quantification or integration procedure can be applied: the narrowest peak should be described by 30 data points at least. In the case of several detectors additional peak broadening can be derived from extra-detector lines.
  For diode-array detectors this type of error can be ignored.
- **Detector signal is out of linear dynamic range**. Signal overscaling can occur for large peaks. Both ADC and detector have a guaranteed linear dynamic range where measuring error does not exceed some threshold value. Channels with the signal coming out of this range will be discarded during the spectral analysis procedure. Of cause, accuracy of the factor analysis will be lowered compared with non-overscaled chromatogram.
  Note that detector's linear range on some channels can be considerably lower than in the device specification due to eluent absorption.
- **A gradient of concentration in the cell** can be observed for narrow peaks. This effect can be minimized by optimization of dynamic properties of the detector cell (in the ideal case dynamic volume of the cell is equal to its geometrical volume)
- **Refractometric effect in the cell** can be observed for high concentration of component in the eluate. This effect also can be minimized by proper geometry of the cell. In addition high component concentrations in the cell can cause a violation of Bouguer's law.
- **Fluorescence of the component**. Fluorescence of the component in the cell and series of other causes also can result in non-linearity of the detector response (violation of Bouguer's law).

The indicated effects lead to apparent separation of homogeneous chromatographic peak on two or more peaks with similar spectra, and the shape that considerably differs from the gaussian, characteristic for chromatographic peaks.

See also:

Peak homogeneity 448

11.9 Factor analysis

In the modern liquid chromatography various spectral detectors, such as rapid-scanning and diode array, are often used. These detectors are able to monitor eluent absorbence at several wavelengths giving a multi-channel chromatogram 146. Several individual detectors, connected consecutively or in parallel, also can produce a multi-channel chromatogram (but number of channels is much less in this case and physical nature of detectors may be different).

A set of responses of all these channels, taken at a definite moment, or averaged for any chromatogram part or component peak, can be considered as a discrete spectrum 424, similar to the conventional UV absorption spectra. The main difference is that in chromatography not absolute eluate absorbance, but absorbance corrected to the pure eluent background (baseline), is measured.

Exploring and comparing normalized spectra at different points of the same peak allow to decide if the peak is homogeneous (i.e. consists of the single component only) or not. If the peak contains a single component only, its spectrum along the peak will be unchanged. In the opposite case the peak can be presented as a superposition of several components with different spectra.

To perform analysis of spectra, it is convenient to express them as a vectors. In the case of 2-channel chromatogram this vector exists in the plane and its projection to X and Y axes equals to response of the first and second channel, respectively. Measure of the difference between spectra is the angle between their vectors.

The spectrum for multi-channel chromatogram is a vector in the abstract multidimensional space. **Angle** between two vectors in this case also measures a difference between two spectra.

For homogeneous chromatographic peak the angle between spectra is close to zero for any points. If the peak is non-homogeneous, this angle appreciably increases, reaching maximum in the field of a maximum overlap of peaks and minimum, where one of components essentially prevails only.

The angle between spectra allows to define, whether this or that peak is homogeneous, and to estimate number of significant components in the chromatogram region. To decide, which components are significant on the analyzed site of a chromatogram, the strict factor analysis algorithm is applied. The maximum number of components (factors) to be defined equals to number of channels in the chromatogram.

It is possible to analyze a multi-channel chromatogram without any a priori knowledge of component spectra. A multi-dimensional space mathematics, i.e., principal component and factor analysis should be applied in this case. The theory and a more detailed description of algorithms for spectral analysis is presented in the Theory of spectral operations 426 topic.

See also:

Theory of spectral operations 426

Spectral analysis definitions 425

11.9.1 Factor analysis of the peak

(Spectrum / Edit / Calculate)

This option activates a factor analysis procedure for the selected peak.

Note: this procedure looks like the factor analysis of the chromatogram site 451 procedure, but deals with a single peak on the chromatogram, and has not influence on integration results.

Factor analysis of the peak procedure allows to control peak homogeneity and to divide overlapping

chromatographic peaks into individual components using a special processing algorithm.

Factor analysis of the peak procedure enables to determine a number of significant components within the selected peak and to calculate individual spectra of the components. Resulting spectra of components are presented in the Spectrum window 431 and can be saved to disk or compared with etalon spectra on disk.

See also:

Factor analysis basics 450

Spectrum calculating window 434

How to perform factor analysis of the peak 454

How to perform factor analysis of the chromatogram site 453

11.9.2 Factor analysis of the chromatogram site

(*Main menu* Spectra / Factor analysis...)

This function performs a factor spectral analysis procedure for the selected site of multi-channel chromatograms 146.

Factor analysis is a procedure allowing to control peak homogeneity and to divide overlapping chromatographic peaks into individual components using a special processing algorithm.

Note: The chromatogram part that is presented in the current chromatogram window, is analyzed.

Factor analysis procedure enables to determine a *number of significant components* on the selected chromatogram site and to perform reintegration of the site according to the obtained results.

The integration of the chromatogram site can be changed according to the factor analysis results.

See also:

Factor analysis basics 450
How to perform factor analysis procedure 453
Factor analysis: Page 1 451
Factor analysis: Page 2 452
Factor analysis: Page 3 452

11.9.3 Factor analysis: Page 1

This page presents results on the first step of the factor analysis. The total spectrum of the chromatogram region is presented as a superposition of elementary spectra of components (factors). The software founds number of significant components, i.e. rank of the total spectrum.

The field contains a list of calculated factors and their contribution to the total signal (absolute and in %). The total number of factors is equal to number of channels in the chromatogram. The software automatically determines a number of significant factors (i.e. factors with contribution greater than error of their measurement).

Factors are listed in accordance with their contribution to the total signal. The last of significant parameters is selected. The user is able to change the rank according to his(her) desire.

☑ Overlapping 2 peaks only	this flag restricts number of overlapping peaks for each point of the chromatogram region. Each point of chromatogram can be considered as a superposition of 2 elementary spectra only.
☑ No negative concentrations	excludes results that correspond to negative concentration
☑ Manual choice	allows to set position of the pure component manually. In this case automatically calculated positions are offered.

11.9.4 Factor analysis: Page 2

This page shows a contribution of each significant factor for chosen chromatogram channel. User is able to choose a channel that will be used for quantification (i.e. channel, that was used for calibration). Overlapping area on the chosen channel will be divided according to this contribution.

The left field contains a list of all chromatogram channels, and the right - a contribution (absolute and in %) of significant components to the signal of the selected channel.

<Back>	click this button to return to the previous step of the procedure.
<Next>	click this button to go to the next step of the factor analysis procedure.
<Cancel>	click this button to cancel the factor analysis procedure and close the window.

11.9.5 Factor analysis: Page 3

This page presents results of spectral deconvolution of the selected chromatogram channel to separate components.

☑ Channel	set the flag to show initial channel signal (in dotted line)
☑ Angle	set the flag to show the angle diagram (angle is measured between two adjacent points). The diagram will be represented by a continuous red line.
☑ Base	
☑ Shift	plot channels shifted on Y axis for better visualization.

Scaling the spectra

It is possible to change scale of the spectra plot by using standard mouse and keyboard scaling functions that are used for ordinary chromatograms. It is possible to zoom the spectra window to full screen using the "Zoom" icon in the upper right corner. Click somewhere in the spectra window to perform scaling.

<Save>	puts the resulting graph to a separate window as a new chromatogram. The graph can be saved to disk as an ordinary multi-channel chromatogram using the  icon.
<Close>	closes the window with the factor analysis result. The button "Close" in the right corner does the same. The closed window can be opened again by clicking on the graph place.
<Back>	use this button to return to the previous step (in order to try another chromatogram channel)

<Finish> button to complete the factor analysis procedure. The "**FACTOR ANALYSIS**" window is closed and integration results are modified.

11.9.6 How to perform factor analysis procedure

How to perform factor analysis of the site

1. Use mouse or keyboard to select the desired chromatogram region, where inhomogeneous peaks probably exist. It is not recommended to fall outside the merged peaks group.
2. Execute the command ***Process/More.../Factor analysis***. The "**FACTOR ANALYSIS**" window will be opened.
3. Look through the list of calculated factors. If necessary, change the rank 453 of the spectra (if possible, it is necessary to decrease number of significant parameters. Their number should be equal to the number of real components in the region of interest).
   In most cases it can be recommended to set Overlapping 2 peaks only 453 and No negative concentrations 454 checkboxes.
4. Click **<Next>** button to continue. The next dialog page will appear.
5. Select the channel that will be used for quantification. As a rule, the reference channel that was used for calibration and quantification of overlapped components, is selected.

Note: If real number of components in the analyzed region or their calibration (relative response factors at least) is unknown, it is impossible to perform correct quantification!

6. Click **<Next>** button. The window that presents resultant spectral data for the selected channel, will appear.
7. If necessary to save calculated components spectra on disk, click **<Save>** button. The spectra will appear in a separate chromatogram window and can be saved as an ordinary multi-channel chromatogram.
8. Click **<Finish>** to complete the factor analysis operation. The "**FACTOR ANALYSIS**" window is closed and integration results are modified.

11.9.7 Rank of the spectrum

Rank of the spectrum

Spectrum rank is a number of significant components (factors) in the spectrum, determined as a result of factor analysis procedure. It corresponds to a minimum number of components with different spectra, which superposition is able to describe the initial spectrum with a desired precision.

Rank is determined automatically, but it can be modified manually by the user.

11.9.8 FA1_Overlapping

☑ Overlapping 2 peaks only this flag restricts number of overlapping peaks for each point of the chromatogram region. Each point of chromatogram can be considered as a superposition of 2 elementary spectra of components only.

11.9.9 FA1_NoNagative

☑ No negative concentrations excludes results that correspond to negative concentration

11.10 Spectral references

11.10.1 Spectral angle

Angle is a quantitative measure of similarity of two spectra.

When detection is performed at N wavelengths

11.11 Spectral operations: how to ...

11.11.1 How to calculate spectrum of peak

1. Open the desired multi-channel chromatogram
2. From the current chromatogram window select ***Process / Spectrum*** item to open Spectrum window 431
   Note: only one spectrum window for each chromatogram can be opened.
3. Check that peak integration procedure 159 was carried out properly. If necessary, use peak editor 224 for manual correction.
4. Choose **Spectrum** ***/ Edit / Calculate*** item to open Spectrum calculation 434 window
5. Select peak number (according to chromatogram) to calculate spectrum for.
6. Select the desired spectrum calculation method.
7. Click **<OK>** to execute. Spectrum of the desired peak will appear in the "**Spectrum**" window. By default the spectrum gets a name (is taken from Components table 171).
   It is possible to edit parameters and description for each spectrum in the Info 437 window and perform other operations available for spectra
8. If necessary, repeat the above operations to add spectra for other components

See also:

Operations with spectra

Spectrum window: context menu

11.11.2 How to perform factor analysis of the peak

Factor analysis of the peak procedure enables to check if the selected peak is homogeneous or contains impurities of other compounds.

Two conditions should be fulfilled for successful operation:

- spectra of overlapped components should be different

– overlapped components should differ in retention time

1. Open the desired chromatogram
2. Open the "**Spectrum**" window (**Chrom&Spec** ***/ Process / Spectrum***)
3. Open "**Spectrum calculation**" window (**Spectrum** ***/ Edit / Calculate***)
4. Select peak number (it corresponds to the peak number on the current chromatogram)
6. Select ⊙ **Factor analysis of the peak** item and click **<OK>** to start the procedure
7. In the first "**Factor analysis**" window select rank 453 of the peak spectrum (select the desired

position in the list using mouse). Estimated contribution of several spectra to the resultant peak spectrum are given here.
As a rule ☑ **No negative concentration** restriction is used

8. Select wavelength (channel) that will be used for plotting results. If results are satisfactory, complete the procedure using **<Finish>** button or repeat previous step(s) clicking **<Back>**.
9. When finished, several new spectra (according to selected spectrum rank) appear in the spectrum window

See also:

Factor analysis basics 450

Spectrum calculating window 434

Factor analysis of the peak 435

How to perform factor analysis of the chromatogram site 453

Operations with spectra

11.11.3 How to perform spectrum recognition

Spectrum recognition procedure seeks spectra in the etalon database that are similar to the selected spectrum in the "**Spectrum**" window. All spectra from database with angle difference with the current spectrum less than some threshold value, will be listed.

1. Open the desired chromatogram
2. Open the "**Spectrum**" window (**Chrom&Spec / *Process* / *Spectrum***)
3. Calculate spectra 454 of desired peaks or load them from disk 456
3. Select **Spectrum / *Edit* / *Recognize*** menu item to open Spectrum recognition window
4. Select catalog where etalon spectra are stored (use **<Browse>** button)
5. Select current spectrum number (if several spectra presents in the "**Spectrum**" window)
6. Enter a maximum allowed angle (threshold value). All etalon spectra that fit this condition, will be listed.
   Look through listed components and select lower threshold angle if too many items were found. Increase it in the opposite case, and try once more (Note that your etalon database may not include the desired spectra).
7. It is possible to add one of the founded etalon spectra to current "**Spectrum**" window by checking the ☑ Add etalon spectrum to Spectrum window flag.

Note that this spectrum will be added to the local database. In this case recognition results can be further applied 455 to the chromatogram.

See also:

Operations with spectra

11.11.4 How to perform peak recognition by spectrum

This procedure applies result of peak recognition to the current chromatogram

Note: this procedure can be performed after spectrum recognition only.

1. Calculate spectrum 454 of the desired peak
2. Execute recognition 455 of the spectrum.

Check ☑ Add etalon spectrum to Spectrum window flag.
Click **<Set>** button.
Close "**Spectrum recognition**" window.
A new etalon spectrum from the database will be added to the "**Spectrum**" window.

3. Repeat the above procedure for all components of interest.
4. Execute **Spectrum / Edit / Apply all** operation. All recognized components will be added to the components table according to the How to apply recognized components 436 window settings.

It is possible to perform this procedure separately to any of the recognized component by using **Spectrum / Edit / Apply manually** option.

5. Two cases can be distinguished:

- No components table exists or it does not include components with retention times close to the founded by spectrum peak. In this case a new line in components table will appear.
- Components table exists. In this case settings of Spectrum options 436 window will be used.

See also:

Operations with spectra

11.11.5 How to save spectrum to disk

Note: if several spectra are present in the "Spectrum" window, all them are stored as a single file.

1. Obtain as many spectra as you need 454
2. Enter spectra description 457 if necessary
3. Select **Spectrum / *File / Save spectrum*** menu item.
4. Enter the desired spectrum name (by default name of the first calculated spectra is offered)
5. Select the desired catalog for storage
6. Click **<Save>** button.

See also:

Operations with spectra

11.11.6 How to load spectrum from disk

Note: it is possible to add several spectra to the current "Spectrum" window

1. In the Spectrum window 431 select ***File / Load spectra*** item
2. Select the desired catalog
3. Select the desired spectrum name from the list
4. Click **<Open>** button.

See also:

Operations with spectra

11.11.7 How to edit spectrum description

Each spectrum includes a relevant information that is either taken automatically from the chromatogram or can be entered by the user. This additional information can be descriptive or used in the quantification or recognition procedures. It is possible to look it and edit in the Info 437 window (short form that lists all spectra in the "**Spectrum**" window) or in the More Info 441 window (a more detailed data on the single selected spectrum).

1. Open the "**Spectrum**" window (**Chrom&Spec / *Process* / *Spectrum***)
2. Calculate spectra 454 of desired peaks or load them from disk 456
3. Open the "**Info**" window (**Spectrum / *View* / *Info***)
4. The following parameters can be edited:
   Component name of the component
   Quantification toggle this flag to **Yes** if the spectrum will be used for quantification
   All other parameters can not be edited here.
5. Select the desired spectrum and click **<More>** button to open "**More Info**" window
6. The following parameters are usually edited:
   Component name of the component
   Eluent eluent description (spectra can change with eluent composition or pH)
   Molec.weight molecular weight of the component (is used for quantification)
   All other parameters taken from chromatogram automatically or are of no significance.

See also:

Operations with spectra

11.11.8 How to merge spectra

Spectrum merge procedure enables to merge two selected spectra. As a rule, only similar spectra are allowed to merge. Nevertheless, it possible to merge a completely different spectra if the flag ☑ **Ignore exceeding maximum allowable difference** is set.

1. Open the "**Spectrum**" window (**Chrom&Spec / *Process* / *Spectrum***)
2. Calculate spectra 454 of desired peaks or load them from disk 456
3. Open the "**Info**" window (**Spectrum / *View* / *Info***)
4. Select the current spectrum (it will be modified by adding another spectrum)
5. Click **<Merge>** button. Merge spectrum 440 window will open.
6. Select a spectrum to be merged (it will be deleted after this procedure).
   If different spectra are to be merged, set ☑ **Ignore exceeding maximum allowable difference** flag.
7. Click **<OK>** to finish the operation.

See also:

Operations with spectra

11.11.9 How to calculate spectrum shift

Spectrum shift procedure enables to calculate shift between the selected spectrum and etalon spectrum. Shift calculating procedure can be applied to similar spectra only. The resultant shift value is placed to the "More info" window 441

1. Open the "**Spectrum**" window (**Chrom&Spec / *Process* / *Spectrum***)

2. Calculate spectra 454 of desired peak or load it from disk 456.
   Note that desired etalon spectrum also should be loaded.
3. Open the "**Info**" window (**Spectrum / *View / Info***)
4. Select the current spectrum.
5. Click **<Shift>** button. Select window will open.
6. Select etalon spectrum to be compared with the current spectrum.
7. "**More info**" window for current spectrum will be opened, containing the calculated shift value.
8. Save the modified spectrum to disk (all unneeded spectra can be removed from "**Spectrum**" window using **<Delete>** option in the "**Info**" window).

See also:

Operations with spectra

11.11.1(How to perform quantification by spectrum

Quantification by spectrum procedure is performed in the Quantity calculation 442 window.

The following operations can be carried out:

- Calculate component quantity in the selected peak on the basis of etalon spectrum (etalon spectra are obtained on the basis of calibration chromatogram)
- Calculate component quantity in the selected peak on the basis of entered extinction factor at the selected wavelength
- Calculate extinction factor at the selected wavelength on the basis of entered component quantity
- Calculate absorbance of the sample on the basis of component extinction factor, solution volume, and component quantity.

  All lacking data are replaced by default values to avoid "division to zero" situation.

1. Open the "**Spectrum**" window (**Chrom&Spec / *Process / Spectrum***)
2. Calculate spectra 454 of desired peaks or load them from disk 456
3. Open the "**Info**" window (**Spectrum / *View / Info***)
4. Select the current spectrum
5. Set *Quantification* flag for the spectrum to **Yes**.
6. Click **<Quant>** button to open "**Quantity calculation**" window
7. Enter the desired value(s)
   For example, to calculate component quantity in the peak, enter molecular mass, select wavelength and corresponding extinction factor, and choose the desired units. Volume of the peak will be taken from the chromatogram.
8. Click **<Get>** button to calculate a desired parameter.

See also:

Operations with spectra

Part XII

How to ...?

12 How to ...?

12.1 Installation and configuration

12.1.1 How to install the software

"Chrom&Spec" software is supplied on CD-ROM

To install the software follow these steps:

1. Switch on PC and start operating system.
2. Insert installation CD into CD drive.
3. Select **<Start>** and Run. Find the file setup.exe on the CD and click on **<OK>**.
4. Follow the setup program instructions.
5. Follow the instructions given in the setup program.
6. During installation the user is prompted to specify two folders:
   Folder for software
   - the folder which stores the software executable files and other binary files which must not change. In most cases there are no need to change the folder which is proposed be default. This folder is referred to as **installation folder** further in this documentation.
   Folder for storing your data
   - the folder which stores all user settings and chromatographic data (chromatograms systems, methods, reports, etc). User can change the proposed default folder to another location which is more convenient for user. This folder is referred to as **installation data folder** further in this documentation.

Software shortcuts are created in the **Windows *start menu*** and on the desktop.

The following folders are created in the **installation data folder**:

Data	Folder for storage of chromatogram files (***.chw**) and batch reprocessing files (***.bar**) with several examples.
Methods	Folder for storage of data processing method files (***.mtw**) with several examples.
Systems	Folder for storage of system files (***.smt**) and sample queue files (***.que**)
Reports	Default folder for storage of report files and graphic files
Devices	Special folder for service usage
Accounts	Folder for storage of user accounts data. This folder is locked in **FDA 21 CFR part 11 mode** 54.
Log	Folder for storage of exception files.(***.exc**), history files (***.hst**), and log files (***.log**).
FLog	Folder for storage of audit trails files. This folder is locked in **FDA 21 CFR**

part 11 mode 54.

See also:

File types 38

12.1.2 How to deinstall the software

To uninstall the software follow these steps:

1. Open **Control panel** from **Windows *start menu.***
2. Locate and open **Add or remove program** (Windows XP) or **Uninstall program** (Windows Vista, 7, 8, 10).
3. Locate and select Chrom&Spec in the list of installed programs and click on **<Uninstall>**. This operation removes program files from **installation folder** and shortcuts from **Windows *start menu*** and on the desktop. This operation does not remove chromatography data and configuration files from **installation data folder**. If user do not need these files he should remove files and **installation data folder** manually.

12.1.3 How to switch on instruments and start program

1. Switch on PC.
2. Switch on AC100 Interface.
3. Switch on Decade Detector(s).
4. Switch on LC100 Pump(s).
5. Switch on peripheral units like OR100 organizer.
6. Switch on AS100 Autosampler
7. **Start the program** 22 by double-clicking the Chrom&Spec **icon** or the Chrom&Spec.exe file.
8. Enter the Nickname and Password and click the **<LogIn>** 47 button.

See also:

Start the program 22

12.2 Security system

12.2.1 How to add a user

1. Click on Chrom&Spec **/ Options / Security** to open the **LogIn** 47 window.
2. Enter Short User name and Password and click on **<LogIn>** to open the **Security options** 50 window.

Note: "**SECURITY OPTIONS**" window can be opened only by users with **Administrator access level** 45.

3. Click on **<Add user>** button. "**ADD USER**" window will be opened.
4. Enter **Short name** and **Full name** for a new user.
5. Select access **level** 45 (**Novice**, **Master**, or **Administrator**) for a new user.
6. Enter and confirm a password for the user.
6. Click **<Add>** button to close the "**ADD USER**" window and to accept the information.

7 Click **<OK>** button to close the "**SECURITY OPTIONS**" window.

Note: Administrator adds a new user, sets his access level and defines initial password, but is not able to change a password. This is prerogative of the user himself.

See also:

Security options 50

How to modify a user 462

How to delete a user 462

12.2.2 How to modify a user

1. Click on Chrom&Spec **/ Options / Security** to open the **LogIn** 47 window.
2. Enter Short user name and Password and click on **<LogIn>** to open the **Security options** 50 window.

Note: The "**SECURITY OPTIONS**" window can be opened only by users with **Administrator access level** 45.
Users with **Master** or **Novice** level will be able to use this menu option for password changing only.

3. Select the user to be modified in the **List of users**.
4. Click on **<Modify user>** to open "**USER**" window.
5. Modify **Full name**, access **level** 45, and Status 46 for the selected user.
6. Click **<OK>** to accept changes and close the "**USER**" window
7. If necessary, set additional parameters in the "Password options" page 52
8. Click **<OK>** to close the "**SECURITY OPTIONS**" window.

See also:

Security options 50

How to add a user 461

How to delete a user 462

12.2.3 How to delete a user

Note: According to 21 CFR Part 11 regulations, it is not allowed to remove any user from the list of users completely. However, Administrator is able to change a Status 46 of each existing user.

1. Click on Chrom&Spec **/ Options / Security** to open the **LogIn** 47 window.
2. Enter the Password and click on **<LogIn>** to open the **Security options** 50 window.

Note: The "**SECURITY OPTIONS**" window can be opened only by users with **Administrator access level** 45.

3. Select the user to be removed or deactivated.
4. Click on **<Modify user>** to invoke the "**USER**" window.
5. Select the desired status.
6. Click on **<OK>** to accept changes and close the "**USER**" window.

See also:

Security options 50
How to add a user 461
How to modify a user 462

12.2.4 How to lock the system

1. Click on Chrom&Spec **/ Options /** Lock system 54.
2. The **LogIn** 47 window is opened and the program is locked until valid **short user name** and **Password** are entered.

See also:

Security options 50

12.2.5 How to sign a chromatogram

1). Open the desired chromatogram.
If several chromatograms are opened, select the desired one by clicking on its window. The chromatogram in the active window will be signed.

1) Select **Process / Electronic signature** menu item, the **Electronic signature** 63 window opens.

2) Enter User name and Password.

3) Select an existing meaning for the signature
(Approval, Authorship, Review, Rejection, Responsibility)
or click **<Modify meaning set>** button to modify or create your own signature meaning.

4) Click on **<OK>** to close the "***Electronic signature***" window.

12.3 Interfaces

12.3.1 How to add an interface to the workplace

1. Click on Chrom&Spec **/ Options /** Devices setup 77 to open the **WORKPLACE** window.
2. Click on **<Install device>** to open the "**ADDING INTERFACES TO YOUR WORKPLACE**" window.

3. Select the desired interface from the available groups.
4. Select the **Serial port** on the PC where the interface is connected to.
5. Click on **<Add to workplace>**. The interface icon will appear on the toolbar.
6. Click on **<Close>** in the "**ADDING INTERFACES TO YOUR WORKPLACE**" window.
7. Close the **WORKPLACE** window by clicking on  in the upper right part of the window.

Note: Interfaces can also be installed during the installation of a **new system** 93 using the system wizard.

See also:

Devices setup 77

How to add an interface to the SYSTEM window 464

How to delete an interface 464

12.3.2 How to add an interface to a system window

1. Click on **SYSTEM WINDOW / Setup / New devices / Link to existing device** 92.
2. Select the desired interface and click on **<OK>** to add the interface icon to the **SYSTEM**.

See also:

Link to existing device 92

How to add an interface to the workplace 463

How to delete an interface 464

12.3.3 How to delete an interface

1. Click on Chrom&Spec **/ Options / Devices setup** 77 to open the "**WORKPLACE**" window.
2. Select the desired interface and click on **<Delete device>**.
3. Close the "**WORKPLACE**" window by clicking on  in the upper right part of the window.
4. Confirm the question "**Equipment configuration is modified. Save changes?**" by clicking on **<Yes>**.

See also:

Devices setup 77

How to add an interface to the workplace 463

How to add an interface to the SYSTEM window 464

12.3.4 Global timer

12.3.4.1 How to install the global timer

1. Click on Chrom&Spec **/ Options /** **Devices setup** 77 to open the "**WORKPLACE**" window.
2. Click on **<Install device>** to open the "**ADDING INTERFACES TO YOUR WORKPLACE**" window.
3. Select the **Timer** option from the **More modules** group.
4. Click on **<Add to workplace>**.
5. Click on **<Close>** in the "**ADDING INTERFACES TO YOUR WORKPLACE**" window.
6. Close the "**WORKPLACE**" window by clicking on  in the upper right part of the window.
7. Confirm the question **Equipment configuration is modified. Save changes?** by clicking on **<Yes>**.

Note: The global timer can also be installed during the installation of a **new system** 93 using the system wizard.

See also:

Global timer 78

12.3.4.2 How to program the global timer

1. Click the **Timer icon** 78 on the toolbar using the left mouse button or click the icon using the right mouse button and select **Open** to open the "**TIMER**" window.
2. Click on **<New task>** to add a new program task. Click on **<Daily>** to define a daily task or on **<Once>** to define a single task.
3. **Daily task**: Select the days at which the task should be started and click on **<OK>**. Click on **<Add subtask>** to a add a new subtask for the daily task. Enter the time at which the subtask should be started. Select the desired **program instruction** and select the system file to which this instruction should be applied.
4. **Single task**: Enter time and date at which the task should be started. Select the desired **program instruction** and select the system file to which this instruction should be applied.
5. Click on **<Save>** to save the timer program.
6. Click on **<OK>** to close the **Timer** window.

See also:

Timer program 78

Timer program instructions

12.4 Systems and devices

12.4.1 Systems

12.4.1.1 How to create a new system

1. Click on Chrom&Spec **/ File /** **New System** 93 to open the "**NEW SYSTEM WIZARD**" window.
2. Enter a name for the new system folder where the new system file is stored and click on **<Next>**.
3. If the interface to which the devices of the new system are connected has not been already installed to the toolbar, select the desired **interface** 107 from the **Interfaces** groups, select the **Serial port** and click on **<Add to workplace>**.
4. Click on **<Next>** to open the window for selection of the devices for the new system. For every device of the system, open the group which contains this device, select the device and the serial port of the interface where the device is connected to, and click on **<Add to system>**.
5. Click on **<Next>** to open the window for selection of **processing method** 122 and **data source** 102.
6. Click on **<Choose>** for the **Processing method** and select the desired **method** 122 file ***.mtw**.
7. Click on **<Choose>** for the **Connected data source** and select the desired **data source channel** 102. Check the **Shared** option in the **Data source** window and select the desired data source channel **# ch#** (for AC100 pump), **# Cell**(for Decade detector) or **# Press** (pressure of LC100) to be connected in the **Available** field and move it into the **Connected** field using the  button.
8. Click on **<OK>** to close the **Data source** window.
9. Click on **<Finish>** to close the "**NEW SYSTEM WIZARD**" window.
10. Enter a name for the new system file (***.smt**) to be saved and click on **<Save>**.

See also:

New system 93

12.4.1.2 How to add devices to an existing system

1. **Open the system** 467.
2. Click on **SYSTEM WINDOW / Setup / New devices / Install new device** 92 to open the **Adding devices to your SYSTEM WINDOW** .
3. For every device to be added, open the group which contains this device, select the device and the serial port of the interface where the device is connected to, and click on **<Add to system>**.
4. Click on **<Close>** to close the **Adding devices to your SYSTEM WINDOW** .
5. Click on **System / Save** in the **SYSTEM WINDOW** . Enter the name of the system file ***.smt** to be saved and click on **<Save>**.

See also:

Install new device 92

12.4.1.3 How to open a system

Open a system if no system is open

1. Click on **File / Open / System** in the main window.
2. Open the desired folder and select the desired **system** 79 **file *.smt**.
3. Click on **<Open>** to open the **SYSTEM WINDOW** for the selected system.

Open a system if a system is already open

1. Click on **System / Open other** in the **SYSTEM WINDOW** .
2. Select the desired **system** 79 **file *.smt**.
3. Click on **<Open>** to open a new **SYSTEM WINDOW** for the selected system.

Change a system

1. Click on **System / Change** in the **SYSTEM WINDOW** . If the current system has been changed, the user is asked to save the system.
2. Select the desired **system** 79 **file *.smt**.
3. Click on **<Open>**. The old system is closed and the selected system is automatically opened and connected.

See also:

Open system 79

Open other system 81

Change system 81

How to connect a system 467

12.4.1.4 How to connect a system

1. **Open the system** 467.
2. Click on **Control / Connect to workplace** in the **SYSTEM WINDOW** .

See also:

Connect a system 89

Disconnect a system 90

12.4.1.5 How to select processing method and data source

1. **Open the system** 467.
2. Verify that a system is in connected state. Use system menu "**Control\Connect to workplace**" to connect the system.
3. Click the **Data recorder icon** 99 using the right mouse button and select **Open**. The **RECORDER** 100 window is opened.
4. Using internal method is recommended in most cases. Select **"System internal method"** option.

5. If you already have method which is adequate for your needs click on **<Import...>** and select the desired **method** 122 file ***.mtw**. Skip this step to configure new method.

6. Click on **<Choose>** for the **Connected data source** and select the desired **data source channel (s)** 102. **Data source channels** are supplied by instruments. Instruments must be already installed to the **system** (internal modules) or to **Workplace** (external modules). Available data sources are located in the **Available** field. Drag and drop desired data sources into the **Connected** field or use the  button.

7. Click on **<OK>** to close the **Data source** window.

See also:

Data recorder setup 100

Data source 102

12.4.1.6 How to set the start mode

1. **Open the system** 467.

2. Click on **Setup / Start mode** in the **SYSTEM WINDOW** to open the **Start mode** 91 window.

3. Move the objects **RECORDER** (**data acquisition**) and **"Device name"** (**time program** for the selected device) to the **Immediate start** area or to **Start with inject** area as desired using the  or  button.

4. Click on **<Close>** to close the **Start mode** window.

5. Click on **System / Save** in the **SYSTEM WINDOW** . Enter the name of the system file ***.smt** to be saved and click on **<Save>**.

See also:

Start mode 91

12.4.2 System timer

12.4.2.1 How to install the system timer

1. **Open the system** 467 in which the system timer is to be installed and click on **Setup / New devices / Install new device** 92 in the **SYSTEM WINDOW** to open the device selection window.

2. Select **Timer** of the **More modules** group and click on **<Add to system>**. The **Timer icon** will appear in the **SYSTEM WINDOW** .

3. Click on **<Close>** in the **Adding devices to your SYSTEM WINDOW** .

4. Click on **System / Save** in the **SYSTEM WINDOW** . Enter the name of the system file ***.smt** to be saved and click on **<Save>**.

Note: The system timer can also be installed during the installation of a **new system** 93 using the system wizard.

See also:

Global timer 78

How to install the global timer 465

12.4.2.1.1 How to program the system timer

1. **Open the system** 467 with the system timer icon.
2. Double-click the **Timer icon** or click the icon using the right mouse button and select **Open** to open the **Timer** window.
3. Click on **<New task>** to add a new program task. Click on **<Daily>** to define a daily task or on **<Once>** to define a single task.
4. **Daily task**: Select the days at which the task should be started and click on **<OK>**. Click on **<Add subtask>** to a add a new subtask for the daily task. Enter the time at which the subtask should be started. Select the desired **program instruction** which will be applied to the system.
5. **Single task**: Enter time and date at which the task should be started. Select the desired **program instruction** which will be applied to the system.
6. Click on **<Save>** to save the timer program.
7. Click on **<OK>** to close the **Timer** window.

See also:

Timer program 78

Timer program instructions

12.5 Methods

12.5.1 How to open a method

Open the method belonging to a system

1. **Open the system** 467 desired.
2. **Connect** 467 the system.
3. Click **Data recorder icon** 99 using the right mouse button and select **Open method** to open the method. An empty **chromatogram window** 212 is opened.

Open a method from the METHODS directory

1. Click on **File / Open / Method** in the main window.
2. Select the desired **method** 122 **file *.mtw**.
3. Click on **<Open>** to open the method. An empty **chromatogram window** 212 is opened.

Open and edit the method belonging to a chromatogram

Typically user needs some sample chromatogram to setup a **Method**. The best way is using a first calibration run.

Each chromatogram holds its own copy of all method settings. You can use chromatogram to make any settings for its method. Then settings can be saved to the method file for use in subsequent **Method** run.

1. Click on  or **File / Open / Chromatogram** in the main window.
2. Select the desired **chromatogram** 207 **file *.chw** in the **Chromatogram open** 207 window.
3. Click on **<Open>** to open the chromatogram and also open the **method** 122.
4. Make changes for **Method** settings.
5. Save the **Method** using **File / Save / Method** or **File / Save method as...** commands.

See also:

Open method 123

How to modify a method 470

12.5.2 How to modify a method

1. **Open the method** 469 desired.
2. Click on  or **Method / Method setup** in the main window. Modify the parameters on the different tabs of the **Method setup** 124 window as desired.
3. Click on  or **Method / Integration** in the main window. Modify the parameters on the **Setup** 160 page and enter integration events on the **Events** 162 page of the **Integration parameters** 159 window as desired.
4. Click on  or **Method / Calibration / Components** in the main window. Modify the existing or create a new **components table** 471.
5. Click on **<Identification>** in the **CHROMATOGRAM** window or **Method / Calibration / Identification** in the main window. Modify the parameters in the **Peak identification** 166 form as desired.
6. Click on **<Concentrations>** in the **CHROMATOGRAM** window or **Method / Calibration / Concentrations** in the main window. Modify the existing or create a new **concentrations table** 472 as desired.
7. Click on **<Graphs>** in the **CHROMATOGRAM** window or **Method / Calibration / Graphs** in the main window. Modify the parameters in the **Component** 178 window for each component as desired.
8. Click on  or **Method / Report options** in the main window. Modify the parameters for report creation in the **Report options** 322 window as desired.
9. Click on **File / Save / Method** in the main window to save the modified method.

Note: If you want to modify the appearance parameters for a method, open a chromatogram with this method and click on  or **View / Appearance** in the main window. Modify the parameters for chromatogram axes, labels and colors in the **Appearance** 216 window as desired. Then, click on **File / Save / Method** in the main window to save the modified method.

See also:

How to open a method 469

12.6 Calibration

12.6.1 How to modify the component table

1. **Open the method** 469 desired.

2. Click on  or **Method / Calibration / Components** in the main window. As a result, the **Components table** 171 appears below the chromatogram. It is possible to erase the entire old table by selecting the Chrom&Spec **/ Table / Clear table** option.

3. Press the **<Add>** button in the ribbon over the components table (or select the Chrom&Spec **/ Table / Add component** item). A new row will be added to the table.

- Enter the number of the peak you are going to include into the components table and press the right arrow key. The cursor will jump to the chosen peak apex and it's retention time value will appear in the **Time** column.

- Enter the **Wind. %** value (identification window) for peak recognition (typically 5...10%).

- Enter the **Name** of the component.

- Fill other columns if necessary:

  Ref (Yes/No) Indicator of the **Reference component** 174.

  Group **Group** 173 number for given component. Is used when Group identification is performed.

  Index Retention **Index** 338 of the component.

  RF **Response factor** 201. Default value is 1.

4. Repeat the procedure for each component of the chromatogram.

5. Close the components table by pressing the **<OK>** button.

6. Save the method (Chrom&Spec **/ File / Save Method**) or the chromatogram (Chrom&Spec **/ File / Save Chromatogram**).

See also:

Components table 171

How to modify the concentrations table 472

How to perform a single-point calibration 472

How to perform a multi-point calibration 473

12.6.2 How to modify the concentration table

1. **Open the method** 469 desired.
2. Click on  or **Method / Calibration / Components** in the main window. As a result, the **Components table** 171 appears below the chromatogram.
3. **Modify the components table** 471.
4. Click on the **<Concentrations>** button to open the Concentrations table. "**Name**" and "**This run**" columns will be filled by data from the **Components table** and the current **calibration chromatogram**.
5. Press the **<Add>** button to add a new **calibration level** 176. Fill in the "**Level 1**" column by concentrations of components in the first **calibration sample**.
6. In a similar way create all other calibration levels. For each calibration point (sample) a separate calibration level should be created. If the same sample should be injected for several times, several calibration levels with the same concentrations are needed.

Hint: To obtain a more accurate calibration graph using only one calibration mixture just **use sample dilution**. In this case all calibration levels should contain the same concentrations of the components. Don't forget to enter appropriate values to "**Volume**" and "**Dilution**" fields of the **Sample description** 126!

See also:

Components table 171

How to modify the components table 471

How to perform a single-point calibration 472

How to perform a multi-point calibration 473

12.6.3 How to perform a single-point calibration

1. **Open the system** 467 desired.
2. **Connect the system** 467.
3. **Start a run** 474 and inject a standard solution containing all components to be determined to obtain the **calibration chromatogram**.
4. Modify the **integration parameters** 159 if necessary.
5. **Modify the components table** 471 if necessary.
6. **Modify the concentrations table** 472 if necessary.
7. Click on **<Calibrate>** 176 in the **Concentrations** window or select Chrom&Spec**/ Process / Calibrate** 176. Enter the Level number "**1**" and click on **<OK>**. The **calibration level** 199 1 will be filled by peak areas (or heights) and the calibration coefficients will be (re)calculated for all identified components.
8. Click on **<Graphs>** 178 in the "**CONCENTRATIONS**" window or select Chrom&Spec**/ Method /**

Calibration / Graphs 178. Modify the parameters for the calibration curve for each component as desired.

9. Close the chromatogram and answer **<Yes>** for all questions concerning the saving and overwriting of the method and the chromatogram.

See also:

How to perform a multi-point calibration 473

12.6.4 How to perform a multi-point calibration

1. **Open the system** 467 desired.
2. **Connect the system** 467.
3. **Start a run** 474 and inject the first standard solution containing all components to be determined to obtain the first **calibration chromatogram**.
4. Open the finished chromatogram and modify the **integration parameters** 159 if necessary.
5. **Modify the components table** 471 if necessary.
6. **Modify the concentrations table** 472 by adding a **calibration level** 199 for the first standard and all other standards to be injected and entering the concentrations for each level.
7. Save the chromatogram and also the method.
8. Click on  or **File / Open / Chromatogram** in the main window and select all the recorded standard **chromatogram** 207 **files *.chw** in the **Chromatogram open** 207 window.
9. Click on **<To Batch>** to open the chromatograms into a batch reprocessing file ***.bar**. Enter a name for the new batch reprocessing file and click on **<OK>**.
10. Click on **<Edit sample table>** in the **Reprocess** 273 window. The sample table for all standard chromatograms loaded is opened.
11. For each standard, enter the corresponding **calibration level** 199 number into the **Calibration level** column.
12. Click on  or **File / Save & Exit** in the **Queue editor** 284 window to save the sample table settings and return to the Reprocess window.
13 Make sure that the following options are enabled in the **Reprocess** 273 window: **Reprocess calibration runs**, **Update method file in <METHODS> directory after reprocessing**, **Recalibrate**, **Default scheme**.
14. Click the **<Reprocess>** button to start the recalibration and evaluation of the multi-point calibration curve.
15. **Open the method** 469 used to record the standard chromatograms.
16. Select Chrom&Spec**/ Method / Calibration / Graphs** to open the **calibration graphs** 178 window. Modify the parameters for the calibration curve for each component as desired. Select another function in the **Formula** field if the displayed calibration curve does not fit optimally the calibration

points. Close the “**COMPONENT**” window by clicking on **<OK>**.

17. Close the chromatogram window and confirm the question **Method *.mtw was modified. Save changes?** with **<Yes>**.

See also:

How to perform a single-point calibration 472

12.7 Determination and measurement

12.7.1 How to measure the baseline

1. **Open the system** 467 desired.
2. **Connect the system** 467.
3. If desired, open the individual system devices and modify the startup values.
4. Click on **Control / Startup hardware (Measure baseline)** 84 in the **SYSTEM WINDOW** .

The **Startup values** are automatically set at all devices of the system and a chromatogram window is opened where the measurement signal is recorded until the data acquisition is stopped with **Stop data acquisition** 84 or a new run is started with **Start run** 83. Alternatively the baseline recording can be stopped by clicking the  icon of the **chromatogram window**. In this case the user is asked if the recorded baseline should be saved or not.

See also:

Measure baseline 84

12.7.2 How to start a determination

1. **Open the system** 467 desired.
2. **Connect the system** 467.
3. If desired, open the individual system devices and modify the startup values.
4. Click on **Control / Start run** 83 in the **SYSTEM WINDOW** . At this start command, the **Startup values** are set at all devices of the system. The device programs and the data recording are started either immediately (**immediate start** mode) or after switching the injection valve to the "Inject" position (**start with inject** mode) as set in the **Start mode** 91 window.
5. If you want to stop a current run before the set time duration has been reached, select the **Control / Stop run** 83 menu item.
6. If you want to stop only the data acquisition but not the running time program, select the **Control / Stop data acquisition** 84 menu item.

See also:

Start run 83

How to stop a run 475

12.7.3 How to stop a determination

1. **Start the run** 474.
2. If you want to stop a current run before the set time duration has been reached, select the **Control / Stop run** 83 menu item. Data acquisition and time program are terminated immediately. The recorded chromatogram is saved automatically only if the **Inject** was done during the run.
3. Alternatively the run can be stopped by clicking the  icon of the **chromatogram window**.
4. If you want to stop only the data acquisition but not the running time program, select the **Control / Stop data acquisition** 84 menu item.

See also:

Stop run 83

How to start a run 474

12.8 Chromatogram

12.8.1 How to open a chromatogram

1. Click on  or **File / Open / Chromatogram** in the main window.
2. Select the desired chromatogram file and click ***<OK>***.

See also:

Open chromatogram 207

12.8.2 How to change the appearance

1. **Open the chromatogram** 475.
2. Click on  or **View / Appearance** 216 in the main window.
3. On the **Chromatogram axes** 216 page, modify the parameters for **Time axis** and **Response axis** as desired. Check the **View all**, **Drift compensation** and **Grid** option if desired. Set the scaling of the chromatogram axes by checking the desired **Tic marks** options. Check the **Set all** option, if these settings should be applied to all opened chromatograms.
4. On the **Labels** 218 page, select the desired options for peak labeling and baseline display. Check the **Set all** option, if these settings should be applied to all opened chromatograms.
5. On the **Colors** 222 page, select the desired colors for axes, channels, baseline, background and cursor. Check the **Set all** option, if these settings should be applied to all opened chromatograms.
6. If you want to save the appearance settings permanently in the chromatogram, select the **File / Save / Chromatogram** option to save the chromatogram.
7. If you want to save the appearance settings permanently in the method, select the **File / Save / Method** option to save the method.

See also:

Appearance 216

12.8.3 How to print a chromatogram

1. **Open the chromatogram** 475.
2. Select the chromatogram view to be printed by **zooming** 214 the desired region.
3. If desired, **change the appearance** 475 of the chromatogram.

Note: If you change the settings on the **Colors** 222 page of the "**APPEARANCE**" window, the new settings are not applied immediately for printing and print preview. In this case, save the chromatogram with **File / Save / Chromatogram**, close the chromatogram and open it again.

4. If desired, **modify the report options** 478. Make sure that the **Chromatogram plot** item is checked.
5. If desired, select the **File / Printer setup** option to change the parameters for printer selection, paper size and format in the **Printer setup** 234 window.
6. If desired, select the **File / Page layout** option to change the parameters in the **Page layout** 340 window.
7. If desired, click on  or **File / Preview** to open the **Preview** 234 window where the report is shown in the appearance formatted for the selected printer.
8. Click on  or **File / Print** 233 to send the report to the printer. Before printing, the "**PRINTING**" window is opened where printer, printing range and number of copies can be defined.

Note: If you print the chromatogram on a printer with a high resolution, the lines may be too thin. In this case, reduce the printer resolution if possible or increase the **Line width** on the "**COLORS**" page of the "**APPEARANCE**" window for **Axes** and **Channel #**.

See also:

Print 233

Printer setup 234

Preview 234

12.8.4 How to export a chromatogram

Export via clipboard

1. **Open the chromatogram** 475.
2. Select the chromatogram view to be exported by **zooming** 214 the desired region.
3. If desired, **change the appearance** 475 of the chromatogram.
4. Click on **Edit / Copy to clipboard** 36 to copy the selected chromatogram view to the clipboard so that it is available for other Windows applications, such as Word, Excel, etc.

Export via file report

1. **Open the chromatogram** 475.

2. Select the chromatogram view to be exported by **zooming** 214 the desired region.
3. If desired, **change the appearance** 475 of the chromatogram.

Note: If you change the settings on the **Colors** 222 page of the "**APPEARANCE**" window, the new settings are not applied immediately for printing and print preview. In this case, save the chromatogram with **File / Save / Chromatogram**, close the chromatogram and open it again.

4. Click on  or **Method / Report options** in the main window. Switch on the **File** option under **Report destination** in the **Report options** 322 window.
5. Enter a name for the file to be saved in the **Name** field under **File output options**. If desired, change the **Directory** for saving reports and chromatograms (default directory is **.../Reports**) and set the other parameters under **File output options** as desired.
6. Make sure that the **Chromatogram plot** item is checked and select the other report items as desired.
7. Click on **<Report>** to save the chromatogram as ***.wmf** file (graphic file) and the text report as ***** file (text file) in the selected report directory from where they can be inserted into other Windows applications, such as Word, Excel, etc.

Export to AIA file

1. **Open the chromatogram** 475.
2. Click on **File / Export / AIA file**.
3. Enter name and directory for the ***.cdf** file to be exported and click on **<Save>**.

Export as measurement point table

1. **Open the chromatogram** 475.
2. Click on **File / Export to / Text file (raw data only)...**
3. Select the parameters desired in the **Report raw data** window.
3. Enter name and directory for the ***.txt** file to be exported and click on **<Save>**.

See also:

Print 233

12.8.5 How to merge chromatograms

1. Click on  or **File / Open / Chromatogram** in the main window.
2. Select the desired chromatograms to be merged and click on **<To Batch>**.
3. Enter the name of the new batch reprocessing file ***.bar** and click on **<OK>**.
4. Click on **<Merge>** 277 to open a new chromatogram window with all chromatograms combined in a single multi-channel chromatogram. The chromatograms are displayed in the same order as in the batch reprocessing table slightly displaced one upon the other.

5. If desired, press [Shift] + [up] to increase the distance between the chromatograms and press [Shift] + [down] to decrease the distance.
6. If desired, **change the appearance** 475 of the multi-channel chromatogram.
7. If desired, save the multi-channel chromatogram with **File / Save chromatogram** 210.

See also:

Merge chromatograms 277

12.8.6 How to sign a chromatogram

1). Open the desired chromatogram.
If several chromatograms are opened, select the desired one by clicking on its window. The chromatogram in the active window will be signed.

1) Select **Process / Electronic signature** menu item, the **Electronic signature** 63 window opens.

2) Enter User name and Password.

3) Select an existing meaning for the signature
(Approval, Authorship, Review, Rejection, Responsibility)
or click **<Modify meaning set>** button to modify or create your own signature meaning.

4) Click on **<OK>** to close the "***Electronic signature***" window.

12.9 Report

12.9.1 How to modify report options

1. **Open the chromatogram** 475.
2. Click on  or **Method / Report options** in the main window to open the **Report options** 322 window.
3. Select the desired report elements in the **Items to report** and **More items to report** column.
4. Select the desired **Report destination(s)** for manual or automatic report output.
5. Select the desired **Quantification method** 329 and other parameters for the **Peak table** section.
6. If you want to customize the peak table, select Custom for **Quantification method** 329 and click on **<Customize>** 332. Select all desired elements for output in the peak table report and click on **Customize>** 332 again.
7. Select the desired **report template** (**english.rtt** for English report, **deutsch.rtt** for German report).

8. If the **File** option is enabled for **Report destination**, modify the **File output options** 340 parameters as desired.

9. Click on **<Accept>** to save the report options and close the window with **<OK>**.

See also:

Report options 322

12.9.2 How to print a report

1. **Open the chromatogram** 475.

2. If the chromatogram plot is included in the report, select the chromatogram view to be printed by **zooming** 214 the desired region. If desired, **change the appearance** 475 of the chromatogram.

3. **Modify the report options** 478 as desired.

4. If desired, select the **File / Printer setup** option to change the parameters for printer selection, paper size and format in the **Printer setup** 234 window.

5. If desired, select the **File / Page layout** option to change the parameters in the **Page layout** 340 window.

6. If desired, click on  or **File / Preview** to open the **Preview** 234 window where the report is shown in the appearance formatted for the selected printer.

7. Click on  or **File / Print** 233 to send the report to the printer. Before printing, the **Printing** window is opened where printer, printing range and number of copies can be defined.

See also:

Print 233

Printer setup 234

Preview 234

12.9.3 How to display a report

1. **Open the chromatogram** 475.

2. Click on  or **Method / Report options** in the main window to open the **Report options** 322 window.

3. **Modify the report options** 478 as desired. Make sure that the **Screen** option is enabled for **Report destination**.

4. Click on **<Report>** to open the report window displaying the selected report items without chromatogram.

See also:

Report options 322

12.9.4 How to export a report

Export via clipboard

1. Open the chromatogram 475.
2. Click on  or **Report / Report options** in the main window to open the **Report options** 322 window.
3. **Modify the report options** 478 as desired. Make sure that the **Screen** option is enabled for **Report destination**.
4. Click on **<Report>** to open the report window displaying the selected report items without chromatogram.
5. Click on **Edit / Copy to clipboard** 36 to copy the report to the clipboard so that it is available for other Windows applications, such as Word, Excel, etc.

Export via file report

1. Open the chromatogram 475.
2. Click on  or **Method / Report options** in the main window. Switch on the **File** option under **Report destination** in the **Report options** 322 window.
3. Enter a name for the file to be saved in the **Name** field under **File output options**. If desired, change the **Directory** for saving reports and chromatograms (default directory is **.../Reports**) and set the other parameters under **File output options** as desired.
4. Click on **<Report>** to save the text report as ***** file (text file) in the selected report directory from where they can be inserted into other Windows applications, such as Word, Excel, etc.

Export "Peak table" to Excel

1. Open the chromatogram 475.
2. Click on  or **Method / Report options** in the main window.
3. Switch on the **Peak table** item in the "**Items to report**" window and switch off all other items.
4. Switch on the **File** option in the "**Report destination**" field and switch off all other options.
5. Select **Custom** in the "**Quantification method**" field.
6. Click on **<Customize>** and select all data elements to be exported.
7. Select the **excele.rtt** (for English report) or **exceld.rtt** (for German report) in the **Template** field.
8. Select **Semicolon** in the "**Separator**" field.
9. Enter a name and the extension **.csv** for the exported file in the "**Name**" field. If desired, change the **Directory** (default directory is **.../Reports**).

10. Select the **Windows** option for **Character set**.
11. Click on **<Report>** to save the report as ***.csv** file.
12. Open the exported file *.csv in Microsoft Excel.

See also:

Report options 322

12.10 Sample queues

12.10.1 How to open a sample queue

1. Click on **File / Open / Sample queue** in the main window or **System / Sample queue** in the **SYSTEM WINDOW** .
2. Select the desired directory and ***.que** file to open an existing sample queue file or enter a new name ***.que** to create a new sample queue file.
3. Click on **<Open>** to open the **sample queue overview** 238 window.

See also:

Open sample queue 237

12.10.2 How to edit the sample queue table

1. **Open the sample queue** 481.
2. Click on **<Edit>** 240 in the **sample queue overview** 238 window.

Note: A running sample queue can not be edited. If you want modify sample queue entries, **pause** 482 the queue, edit the sample queue table and **restart** 481 the sample queue.

3. Use **sample queue editor** 245 to modify **sample queue**.
4. Click on  or **File / Save & Exit** to save the modified sample queue table and close the sample queue editor window.

See also:

Sample queue control 238

Sample queue table 255

12.10.3 How to start a sample queue

1. **Open the sample queue** 481.
2. **Edit the sample queue table** 481.
3. Switch on the **Shut down system after the queue finishes** option if desired.
4. Click on **<Start>**Start_sq>Main in the **sample queue overview** 238 window. The sample queue is started using the first row with **Started = 0**. The current row is highlighted.

See also:

Start sample queue 240

How to pause a sample queue 482

12.10.4 How to pause a sample queue

1. **Start the sample queue** 481.
2. Click on **<Pause>** 241 in the **sample queue overview** 238 window. The sample queue is stopped after the current run has been finished.

See also:

Pause sample queue 241

How to start a sample queue 481

12.11 Batch reprocessing

12.11.1 How to create a batch reprocessing file

Read **creating a new batch reprocessing** 271 article.

12.11.2 How to edit the batch reprocessing table

1. **Create a new batch reprocessing file** 271 or click on  or **File / Open last batch** to open the last opened batch reprocessing file.
2. Click on 

in the **Reprocess options** 273 window.
3. Modify the **batch reprocessing table** 284 using the **editor function** 278 program as desired.
4. Click on  or **File / Save & Exit** to save the modified batch reprocessing table and close the batch reprocessing editor window.

See also:

Reprocess options window 273

Batch reprocessing table 284

12.11.3 How to perform batch reprocessing

1. **Create a new batch reprocessing file** 271 or click on  or **File / Open last batch** to open the last opened batch reprocessing file.
2. **Edit the batch reprocessing table** 481 if desired.
3. Select the desired method for reprocessing in the **Use method from file for reprocessing** field of the **Reprocess options window** 273.
4. Check the **Reprocess sample runs** option, if the sample runs (**calibration level = 0**) should be reprocessed.
5. Check the **Reprocess calibration runs** option, if the calibration runs (**calibration level > 0**)

should be reprocessed.

6. Check the **Update method file...** option if the modified method should be saved automatically after reprocessing.

7. Check the **Reintegrate** option if the chromatograms should be reintegrated. If desired, **the <Edit integration parameters>** button can be used to modify the **integration parameters** 159.

8. Check the **Recalibrate** option if the chromatograms should be recalibrated and select the according options **Default scheme**, **Apply final calibration...** or **Forget calibration points...** .

9. Check the **Recalculate only** option if the chromatograms should be recalculated without reintegration or recalibration.

Note: The recalculation is done automatically if the **Reintegrate** and/or **Recalculate** options are enabled. If the **Recalculate only** option is enabled, the **Reintegrate** and **Recalculate** options are disabled automatically.

10. Check the **Change passport** option if the method parameters of all chromatograms should be overwritten by the parameters entered after clicking the **<Edit passport>** button.

Note: Only some of the passport parameters can be modified. The passport parameters **Ident**, **Sample Info 1** and **Sample Info 2** entered in the batch reprocessing table are overwritten if these values are modified in the passport window.

11. Check the **Modify chromatogram appearance** option if the **appearance** 216 parameters entered after clicking the **<Edit appearance>** button should be applied to all chromatograms.

12. Check the **Make report** option if a report should be printed for all chromatograms using the current report settings of the selected chromatogram in the "Use method..." field. If desired, **the <Edit report options>** button can be used to modify the parameters of the **Report options** 322 window.

14. Click on **<Reprocess>** to start the reprocessing.

See also:

Reprocess options window 273

12.11.4 How to merge chromatograms

1. Click on  or **File / Open / Chromatogram** in the main window.

2. Select the desired chromatograms to be merged and click on **<To Batch>**.

3. Enter the name of the new batch reprocessing file ***.bar** and click on **<OK>**.

4. Click on **<Merge>** 277 to open a new chromatogram window with all chromatograms combined in a single multi-channel chromatogram. The chromatograms are displayed in the same order as in the batch reprocessing table slightly displaced one upon the other.

5. If desired, press [Shift] + [up] to increase the distance between the chromatograms and press [Shift] + [down] to decrease the distance.

6. If desired, **change the appearance** 475 of the multi-channel chromatogram.

7. If desired, save the multi-channel chromatogram with **File / Save chromatogram** 210.

See also:

Merge chromatograms 277

Part XIII

Appendix

13 Appendix

13.1 File and directory macro language

A full path name to your file written in a regular way could be something like
"C:\Documents and Settings\All Users\Application Data\ChromData\Reports\MyReport.pdf"

Some settings in the method, reports and other software entities require file names and paths to be specified.
When user specify path and file name in a regular way this may result in the following problems:

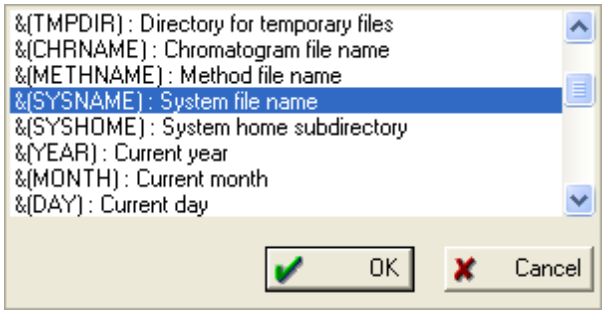
- Method (or other entities) appears to be not transferable. It is not possible to re-use method on a different machine because different machine may have different disks a directory structure. Also software may be installed into the different directory.
- In routine analysis several files may be produced (reports, exports, etc). For example, If the report file name is specified somewhere in the method in a regular way then the file will be overwritten in subsequent runs.
- Uniqueness of the file name can be done by upending some number to the file name. Still this makes it hard to identify what analysis a particular report file refers to.

To avoid those problems a simple macro language was introduced.

In many places where directory or file name is required a macro items can be used instead of regular literal names.

A special button  near the file or directory name or other text item notifies that macro definitions are possible for the item.

Pressing the button opens a list of available macro:



Macro are processed when the item is actually used by the software (typically when related file is created).

Currently software supports the following macro definitions:

&(WORKINGDIR)	Expands to **software working directory**, the root directory which holds all the software data. This directory is specified during software installation.
&(DATADIR)	Expands to software **chromatogram data** directory. It is equivalent to &(WORKINGDIR)\DATA
&(METHDIR)	Expands to the directory where external **methods** are stored by default. It is equivalent to &(WORKINGDIR)\Methods
&(SYSDIR)	Expands to the directory where **systems** are stored by default. It is equivalent to &(WORKINGDIR)\Systems
&(REPDIR)	Expands to the directory where **reports** are stored by default. It is equivalent to &(WORKINGDIR)\Reports
&(RTDIR)	Expands to the directory where **report templates** are stored by default. It is equivalent to &(WORKINGDIR)\Templates
&(TMPDIR)	Expands to the directory for **temporary** files. It is equivalent to &(WORKINGDIR)\TMP
&(CHRNAME)	Expands to **chromatogram file name**, with no path, no extension
&(METHNAME)	Expands to **method file name**, with no path, no extension
&(SYSNAME)	Expands to **system file name**, with no path, no extension
&(SYSHOME)	Expands to name of **system home directory**, with no path
&(YEAR)	Expands to current date, **year**
&(MONTH)	Expands to current date, **month**
&(DAY)	Expands to current date, **day**
&(HOUR)	Expands to current time, **hour**
&(MINUTES)	Expands to current time, **minutes**
&(SECONDS)	Expands to current time, **seconds**
&(AYEAR)	Expands to date when analysis was started, **year**
&(AMONTH)	Expands to date when analysis was started, **month**
&(ADAY)	Expands to date when analysis was started, **day**
&(AHOUR)	Expands to time when analysis was started, **hour**
&(AMINUTES)	Expands to time when analysis was started, **minutes**
&(ASECONDS)	Expands to time when analysis was started, **seconds**
&(USER)	Expands to currently logged-in **user**

&(AUSER)	Expands to **user** who started the analysis
&(TITLE)	Expands to chromatogram **title** 124
&(VIAL)	Expands to sample **vial** 126
&(SAMPLE)	Expands to **sample** 126
&(SAMPLE2)	Expands to sample **description** 126
&(LEVEL)	Expands to chromatogram **calibration level** 124
&(NRUN)	Expands to chromatogram **run number** 124
&(EXPFNAME)	Expands to **export file full name**, including path
&(CHRFNAME)	Expands to **chromatogram file full name**, including path
&(METHFNAME)	Expands to **method file full name**, including path
&(SYSFNAME)	Expands to **system file full name**, including path

Part XIV

Articles

14 Articles

14.1 Confidence intervals for weighted polynomial calibrations

Confidence intervals for weighted polynomial calibrations

Summary

In many chromatographic software products, weighted polynomial regression is used for the calibration curves. Weighting is a useful mean to account for the measurement error that may depend on the detector response value. Confidence intervals show how accurate a measurement is with the help of a calibration curve.
We have extended the confidence interval theory to the frequent case of weights, expressed as a function of Y value, in particular 1/Y and $1/Y^2$. This extension allows accurate calculation of concentrations with confidence intervals for calibration curves, constructed using point weighting. Examples are shown that demonstrate applications of weighted calibration curves with confidence intervals in chromatography.

Introduction

General theory of linear regression analysis is usually used for calculating confidence intervals. However, in analytical chemistry, we may face a practical problem where the regression analysis cannot be applied directly and needs some adaptation.

A very common situation in analysis is that the error is not the same for different signal levels. The error can be proportional to the signal itself, that is $\Delta_R \sim R$. For radioactivity measurements we would have $\Delta_R \sim \sqrt{R}$. Here, R is the detector response and Δ_R is a related measurement error. Correct handling of such errors and calculating true errors in the resulting concentration requires special consideration.

Another example of weighted regression is curve fitting by polynomial of second or third power. Conventional linear regression analysis gives tools for calculating confidence intervals for this case. Exact formulas are typically not present in specialized literature for analytical chemistry.

The most important practical cases related to the confidence intervals are the following:

1. We build the regression of value y_i which is measured with error at the precisely known set x_i (calibration). Then, we make a set of measurements of the detector response Y_* at known x_*. What is the variation of Y_* value and how does it differ from the expected value $\hat{Y}_*$, calculated from calibration at x_*?
2. We build the regression of value y_i which is measured with error over the precisely known set x_i (calibration). Then, we measure the detector response Y_* at some unknown x_*. A value $\hat{x}_*$ from calibration curve at Y_* is used as the estimate of x_*. What is a variation of $\hat{x}_*$ value and how it differs from "true" x_*?

I. Regression Without Weighting

Regression without weighting assumes that the error of measurement depends on neither the detector response nor the concentration. Regression can be linear through origin or not through origin. Also, it can be a polynomial of second or third order.
This case is considered in details in the literature.

A regression is defined by the expression:

$$\mathbf{Y} = \mathbf{X} \cdot \boldsymbol{\beta} + \boldsymbol{\varepsilon} \qquad \text{(I.1), (Seber 3.2)}$$

where $\mathbf{X}$ is a regression matrix. For example, quadratic regression not going through origin it is

$$\mathbf{X} = \begin{Bmatrix} 1 & x_1 & x_1^2 \\ 1 & x_2 & x_2^2 \\ \dots & \dots & \dots \\ 1 & x_n & x_n^2 \end{Bmatrix}$$

The lower index refers to the number of calibration point.
$\mathbf{Y} = \{y_1 . y_2 ... y_n\}$ is vector of detector response values
$\boldsymbol{\varepsilon} = \{\varepsilon_1, \varepsilon_2, ..., \varepsilon_n\}$ - a related vector of errors of measurements.
$\boldsymbol{\beta} = \{\beta_0, \beta_1, \beta_2\}$ - a regression coefficients which must be calculated.

It is assumed that errors of measurements follow the rule:
$\text{cov}[\varepsilon_i, \varepsilon_j] = \delta_{ij} \cdot \sigma^2$
$\mathbf{D}[\varepsilon] = \sigma^2 \cdot \mathbf{I_n}$
That is, errors ε_i are not correlated and have the same dispersion.
The solution of the dispersion is

$$\hat{\boldsymbol{\beta}} = (\mathbf{X}' \cdot \mathbf{X})^{-1} \mathbf{X}' \cdot \mathbf{Y} \qquad \text{(I.2), (Seber 3.5)}$$

Confidence interval at $100 \cdot (1 - \alpha)$ level for response value at a given X_*

We are building the regression of response values y_i measured with errors over the precisely known set x_i (calibration). After building the calibration curve, we make another measurement Y_* at some known x_*.
Then, the confidence interval of the single measurement is given by the expression:

$$\mathbf{Y}_* = \hat{\mathbf{Y}}_* \pm t_{n-p}^{(1/2)\alpha} \cdot S \cdot (1 + u_*)^{1/2} \qquad \text{(I.3), (Seber 5.22)}$$

where

$$S^2 = \frac{(\mathbf{Y} - \mathbf{X}\hat{\boldsymbol{\beta}})' \cdot (\mathbf{Y} - \mathbf{X}\hat{\boldsymbol{\beta}})}{n - p} \qquad \text{(Seber § 3.3)}$$

$$u_* = \mathbf{x}_*' (\mathbf{X}' \cdot \mathbf{X})^{-1} \mathbf{x}_* \qquad \text{(Seber 5.17)}$$

$\mathbf{x}_*' = \{1, x_*, ..., x_*^p\}$ – if polynomial curve does not go through

$\hat{\mathbf{Y}}_* = \mathbf{x}_*'\hat{\boldsymbol{\beta}}$ (Seber § 5.2)

n – number of calibration points

p – power of the polynomial

t_m^{δ} – Student's coefficient at confidence probability $(1-\delta)$ with m degrees of freedom.

Confidence interval for prediction in solving the inverse problem (discrimination)

We build the regression of response values y_i measured with errors at the precisely known set x_i (calibration). After building a calibration curve, we make another measurement Y_*. Using the calibration curve, we find $\hat{x}_*$ - an estimate of the true value x_*:

$$\mathbf{Y}_* = \hat{\mathbf{x}}_*'\hat{\boldsymbol{\beta}}$$

We have to follow the reasoning of (Seber § 7.2.6)

Let $\mathbf{x} = \mathbf{x}_*$ – true value of $\mathbf{x}$ in our measurement.

We define $\hat{\mathbf{Y}}_*$ so that

$$\hat{\mathbf{Y}}_* = \mathbf{x}_*\hat{\boldsymbol{\beta}}$$

Then, from (I.3) we have:

$\mathbf{Y}_* - \hat{\mathbf{Y}}_* \sim N(0, \sigma^2(1+u_*))$

and

$$T = \frac{\mathbf{Y}_* - \hat{\mathbf{Y}}_*}{S\sqrt{1+u_*}} \sim t_{n-p}$$

Thus a set of $\mathbf{x}$ which satisfy the condition

$$(\mathbf{Y}_* - \hat{\mathbf{Y}}_x)^2 \le (t_{n-p}^{(1/2)\alpha})^2 \cdot S^2 \cdot (1+u_x) \qquad \text{(I.4)}$$

form a confidence region at $100\cdot(1-\alpha)$ level for $\mathbf{x}_*$

Here we use:

$$\hat{\mathbf{Y}}_x = \mathbf{x}\cdot\hat{\boldsymbol{\beta}} \qquad \text{(I.5)}$$

$$u_x = \mathbf{x}'(\mathbf{X}'\cdot\mathbf{X})^{-1}\mathbf{x} \qquad \text{(I.6)}$$

In the particular case of linear regression, formula (I.4) is equivalent to (Seber § 7.11).

For linear regression going through origin, formula (I.4) gives result equivalent to (Seber § 7.18).

II. Weighted Regressions

Assumptions, which were used in the previous chapter for constructing the regression

$$\mathbf{Y} = \mathbf{X} \cdot \boldsymbol{\beta} + \boldsymbol{\varepsilon} \qquad \text{(II.1)}$$

are

$\operatorname{cov}[\varepsilon_i, \varepsilon_j] = \delta_{ij} \cdot \sigma^2$

$\mathbf{D}[\varepsilon] = \sigma^2 \cdot \mathbf{I_n}$

Still, following to (Seber § 3.6), we can build a generalized method of least squares.
Let $\mathbf{D}[\varepsilon] = \sigma^2 \cdot \mathbf{V}$, where $\mathbf{V}$ is a known positively-defined matrix of size $(n \times n)$.
In this case, non-singular matrix $\mathbf{K}$ exists so that

$\mathbf{V} = \mathbf{K} \cdot \mathbf{K}'$

We define

$\mathbf{Z} = \mathbf{K}^{-1} \cdot \mathbf{Y}$,

$\mathbf{B} = \mathbf{K}^{-1} \cdot \mathbf{X}$

$\boldsymbol{\eta} = \mathbf{K}^{-1} \cdot \boldsymbol{\varepsilon}$

and build another regression

$$\mathbf{Z} = \mathbf{B} \cdot \boldsymbol{\beta} + \boldsymbol{\eta} \qquad \text{(II.2)}$$

In this regression $E[\boldsymbol{\eta}] = 0$ и $\mathbf{D}[\boldsymbol{\eta}] = \sigma^2 \cdot \mathbf{I_n}$
This means that model (II.2) is equivalent to model (I.1), where all ε_i are not correlated and have the same dispersion.

Least-squires estimate $\hat{\boldsymbol{\beta}}$ for vector $\boldsymbol{\beta}$ is calculated by minimizing of value $\boldsymbol{\eta}' \cdot \boldsymbol{\eta}$ and is given by expression

$$\hat{\boldsymbol{\beta}} = (\mathbf{B}' \cdot \mathbf{B})^{-1} \mathbf{B}' \cdot \mathbf{Z} = (\mathbf{X}' \cdot \mathbf{V}^{-1} \cdot \mathbf{X})^{-1} \mathbf{X}' \cdot \mathbf{V}^{-1} \cdot \mathbf{Y} \qquad \text{(II.3)}$$

Just in the same way the expected value $\hat{Y}_*$ at a given known x_* is given by

$\hat{\mathbf{Y}}_* = \mathbf{x}_*' \hat{\boldsymbol{\beta}}$

and true unknown x_* for measured Y_* is estimated by $\hat{x}_*$:

$\mathbf{Y}_* = \hat{\mathbf{x}}_*' \hat{\boldsymbol{\beta}}$

Methods of evaluating confidence intervals are not directly applicable, although (II.2) and (I.1) seems to be equivalent.
We can expect that the statistical behavior of vector $\hat{\boldsymbol{\beta}}$ from (II.3) is analogous to the conventional regression model because (II.3) is the usual estimate made by the least squares method. In the experiment, we are measuring or setting values x_* and Y_*. In general, we cannot match them related values b_* and Z_* in inverted regression.

Fortunately, in some practically significant cases such a match is possible.

Let us assume that errors ε_i are not correlated as previously, that is $\mathrm{cov}[\varepsilon_i, \varepsilon_j] = 0$ when $i \neq j$.
Now the dispersions are not the same.
Let us assume that we are making multiple measurements of the detector response at a given strictly known $\tilde{x}$ and by averaging responses we obtain a true response $\tilde{Y}$.
Also, assume that the dispersion of the error depends on $\tilde{x}$ and $\tilde{Y}$ only, that is

$$\tilde{\varepsilon}^2 = \frac{\sigma^2}{w(\tilde{x}, \tilde{Y})} \qquad \text{(II.4)}$$

Also, we have to assume that errors are the same for calibration and for analyte and they follow (II.4).
In practice a particular form of (II.4) is known approximately and is defined by the type of physical experiment.

The most important models are listed below:

$w(x,Y) = 1$ (II.5.1) – conventional regression, no weighting

$w(x,Y) = \frac{1}{|Y|}$ (II.5.2) – error of measurement is proportional to $\sqrt{|Y|}$. For example, this is a case of radioactivity detector.

$w(x,Y) = \frac{1}{Y^2}$ (II.5.3) – Constant relative error? That is $\delta Y \sim |Y|$ and $\frac{\delta Y}{|Y|} = const$

$w(x,Y) = \frac{1}{|x|}$ (II.5.4) – error of measurement is proportional to $\sqrt{|x|}$. Analogous to (II.5.2), if we replace Y with x.

$w(x,Y) = \frac{1}{x^2}$ (II.5.5) – error of measurement is proportional to $|x|$. Analogous to (II.5.3), if we replace Y with x.

We define matrix $\mathbf{V}$ as:

$$\mathbf{V} = diag\{\frac{1}{w(x_i, Y_i)}\} \approx diag\{\frac{1}{w(\tilde{x}_i, \tilde{Y}_i)}\} = \tilde{\mathbf{V}} \qquad \text{(II.6)}$$

where i – is a number of the calibration point.

When we are building the calibration, a precise value $\tilde{Y}_i$ for calibration point is unknown. Therefore, we have to use approximation by replacing $\tilde{Y}_i \to Y_i$. This means that a true error matrix $\tilde{\mathbf{V}}$ is replaced by an approximate $\mathbf{V}$.

An inverse matrix for $\mathbf{V}$ is:

$$\tilde{\mathbf{V}}^{-1} \approx \mathbf{V}^{-1} = diag\{w(\tilde{x}_i, \tilde{Y}_i)\}$$

Confidence interval at $100\cdot(1-\alpha)$**level for the response value at a given** x_***.**

Using (II.3) we can estimate the true detector response Y_* at a given known x_*. A natural estimate is:

$\hat{\mathbf{Y}}_* = \mathbf{x}_*'\hat{\boldsymbol{\beta}}$

We define

$w_* = w(x_*, \hat{Y}_*) \approx w(x_*, Y_*) = \tilde{w}_*$

so

$$\varepsilon_*^2 = \frac{\sigma^2}{w(x_*, \hat{Y}_*)} \approx \frac{\sigma^2}{w(x_*, Y_*)} = \tilde{\varepsilon}_*^2$$

is an estimate of dispersion of measured response Y_*, according to (II.4).

Now we define

$$\frac{1}{k_*} = \sqrt{w_*}, \quad Z_* = \frac{Y_*}{k_*}, \quad b_* = \frac{x_*}{k_*},$$

so that

$$\hat{Z}_* = \mathbf{b}_*' \cdot \hat{\boldsymbol{\beta}} = \frac{\mathbf{x}_*'}{k_*} \cdot \hat{\boldsymbol{\beta}} = \frac{\hat{\mathbf{Y}}_*}{k_*}$$

is an estimate for Z_* in inverted regression (II.2).

This means that the method for calculating confidence intervals from chapter for (I) is applicable for Z_* and $\hat{Z}_*$.

Then, a confidence interval for response value of single measurement is given by:

$$Z_* = \hat{Z}_* \pm t_{n-p}^{(1/2)\alpha} \cdot S \cdot (1 + u_*)^{1/2} \qquad \text{(II.7)}$$

Where

$$S^2 = \frac{(\mathbf{Z} - \mathbf{B}\hat{\boldsymbol{\beta}})' \cdot (\mathbf{Z} - \mathbf{B}\hat{\boldsymbol{\beta}})}{n - p}$$

$u_* = \mathbf{b}_*'(\mathbf{B}' \cdot \mathbf{B})^{-1}\mathbf{b}_*$

Now, we need to convert from (b, Z) back to (x, Y). We get:

$$Y_* = \hat{Y}_* \pm t_{n-p}^{(1/2)\alpha} \cdot S \cdot \left(\frac{1}{w_*} + U_*\right)^{1/2} \qquad \text{(II.8)}$$

where

$$S^2 = \frac{(\mathbf{Y} - \mathbf{X}\hat{\boldsymbol{\beta}})' \cdot \mathbf{V}^{-1} \cdot (\mathbf{Y} - \mathbf{X}\hat{\boldsymbol{\beta}})}{n - p}$$

$U_* = \mathbf{x}_*'(\mathbf{X}' \cdot \mathbf{V}^{-1} \cdot \mathbf{X})^{-1}\mathbf{x}_*$

Confidence interval for prediction in solving an inverse problem (discrimination).

We are making an estimate $\hat{x}_*$ of a true value x_* using the regression (II.3) at a measured detector response Y_*:

$$\mathbf{Y}_* = \hat{\mathbf{x}}'_*\hat{\boldsymbol{\beta}}$$

We need to repeat the reasoning, analogous to the one we made for confidence interval for response value.
In the same way we get:

$$w_* = w(\hat{x}_*, Y_*) \approx w(x_*, Y_*) = \tilde{w}_*$$

$$\frac{1}{k_*} = \sqrt{w_*}\,, \quad Z_* = \frac{Y_*}{k_*}$$

$$\mathbf{Z}_* = \frac{\mathbf{Y}_*}{k_*} = \frac{\hat{\mathbf{x}}'_*}{k_*}\hat{\boldsymbol{\beta}} = \hat{\mathbf{b}}_*\hat{\boldsymbol{\beta}}$$

We define $b_* = \frac{x_*}{k_*}$. An estimate of confidence intervals from chapter (I) is applicable for b_* and $\hat{b}_*$. Namely, a set of all $\mathbf{b}$ which follow the condition

$$(\mathbf{Z}_* - \hat{\mathbf{Z}}_b)^2 \le (t_{n-p}^{(1/2)\alpha} \cdot S)^2 \cdot (1 + u_b) \qquad \text{(II.9)}$$

form a confidence region for $\mathbf{b}_*$ at $100 \cdot (1-\alpha)$ level.
Here we define:

$$\hat{\mathbf{Z}}_b = \mathbf{b} \cdot \hat{\boldsymbol{\beta}}$$

$$u_b = \mathbf{b}'(\mathbf{B}' \cdot \mathbf{B})^{-1}\mathbf{b}$$

Now we need to convert back from (b, Z) to (x, Y). Assuming $\mathbf{b} = \frac{\mathbf{x}}{k_*}$ we get a confidence region for $\mathbf{x}_*$ at $100 \cdot (1-\alpha)$ level. This is a set of all $\mathbf{x}$, which follow the condition:

$$(\mathbf{Y}_* - \hat{\mathbf{Y}}_x)^2 \le (t_{n-p}^{(1/2)\alpha})^2 \cdot S^2 \cdot (\frac{1}{w_*} + U_x) \qquad \text{(II.10)}$$

where

$$S^2 = \frac{(\mathbf{Y} - \mathbf{X}\hat{\boldsymbol{\beta}})' \cdot \mathbf{V}^{-1} \cdot (\mathbf{Y} - \mathbf{X}\hat{\boldsymbol{\beta}})}{n - p}$$

$$U_x = \mathbf{x}' \cdot (\mathbf{X}' \cdot \mathbf{V}^{-1} \cdot \mathbf{X})^{-1} \cdot \mathbf{x}$$

$$\hat{\mathbf{Y}}_\mathbf{x} = \mathbf{x} \cdot \hat{\boldsymbol{\beta}}$$

III. Examples

The examples below represent typical regressions of different polynomial powers and different weighting models. For demonstration purposes, the simulated data are generated with significant error. Confidence intervals for response values at 0.95 confidence probability are drawn.

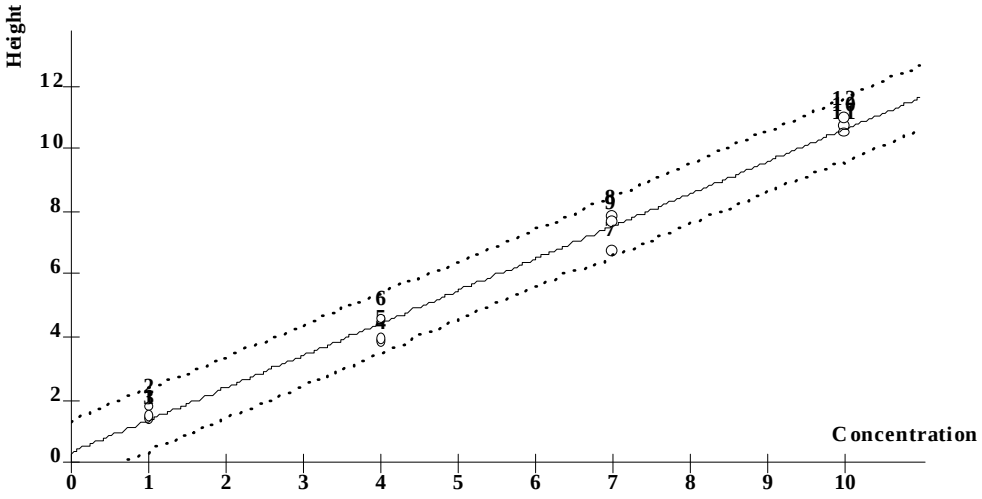


Figure 1. Linear polynomial not going through the origin. The dispersion of error is the same for all measurements, no weighting.

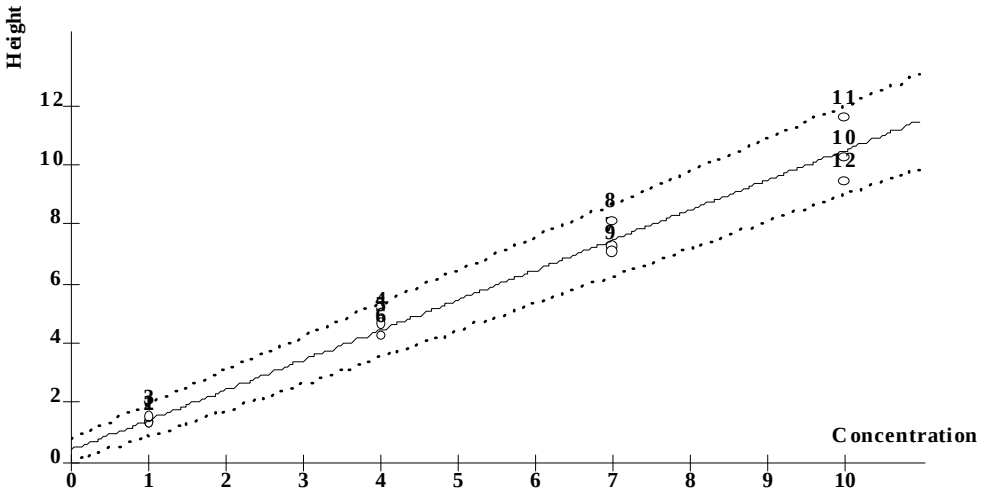


Figure 2. Linear polynomial not going through the origin. The dispersion of error is proportional to $\sqrt{Height}$. Weighting 1/*Height*.

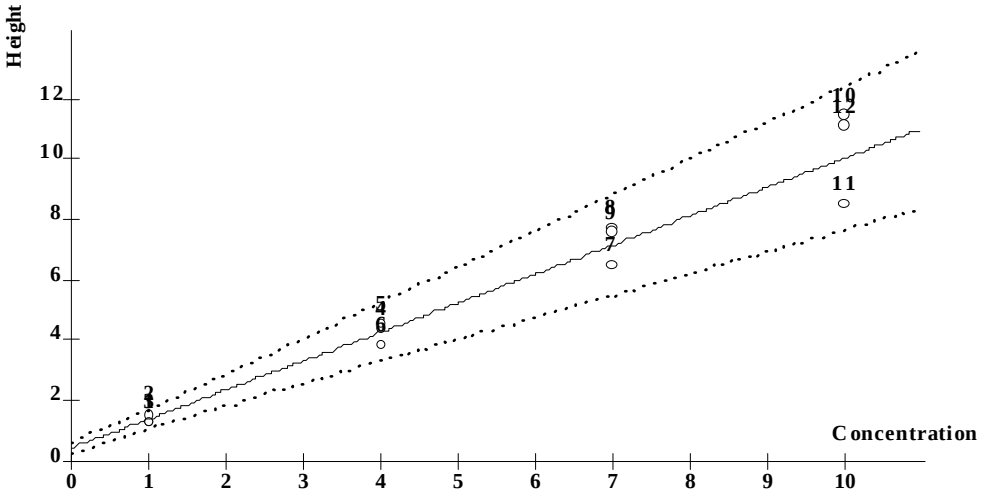


Figure 3. Linear polynomial not going through the origin. The dispersion of error is proportional to *Height* (constant relative error). Weighting $1/Height^2$.

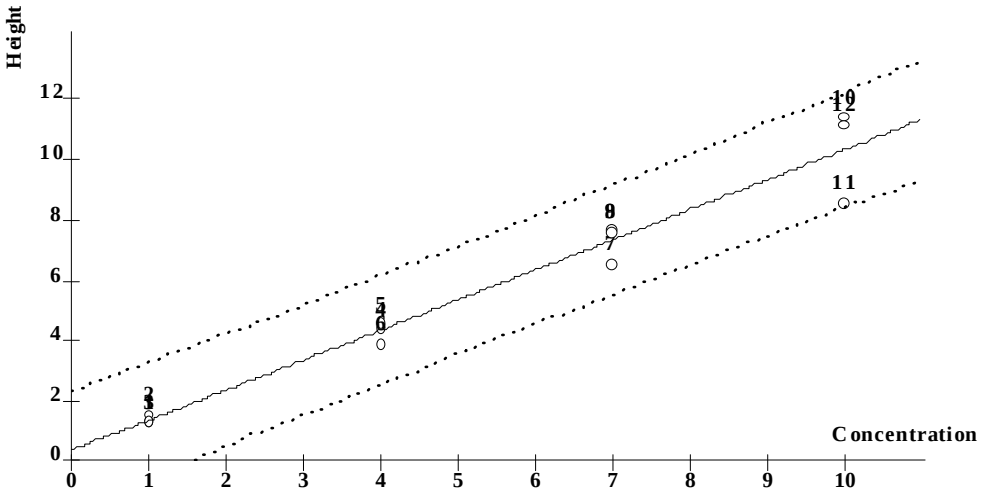


Figure 4. Linear polynomial not going through the origin, the same data as on Fig.3. The dispersion of error is proportional to *Height* (constant relative error). Regression is constructed without weighting (just as if absolute error is constant). This regression gives an approximation formula that is not quite correct and has incorrect confidence intervals.

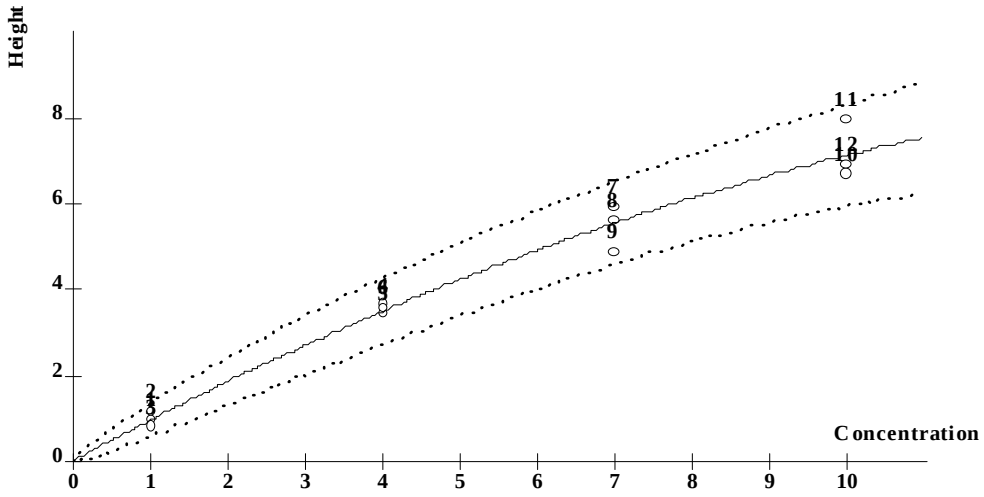


Figure 5. Quadratic polynomial through the origin. The dispersion of error is proportional to $\sqrt{Height}$. Weighting $1/Height$.

A correct test plan for calibration is especially important when building regression with a non-linear polynomial. Let us consider a regression of the simulated data which should be approximated by quadratic polynomial. If we select 3 concentrations and make measurements twice at each concentration, the calibration curve could look quite nice. Still, when we calculate and draw related confidence intervals we would notice that adequate results are possible near the initial concentrations only. Therefore, this test plan is incorrect.

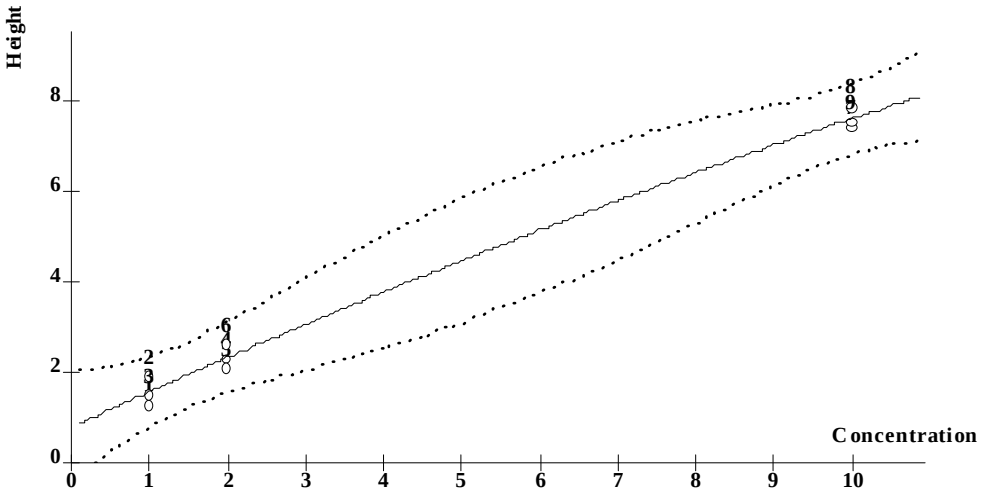


Figure 6. Quadratic polynomial not going through origin. The dispersion of error is the same for all measurements, no weighting. The simulated detector response is measured three times at three concentrations. This test plan produces a poor prediction.

A prediction becomes much better if we select uniformly distributed concentrations for the calibration. This calibration curve would supply good predictions over an entire range of calibration.

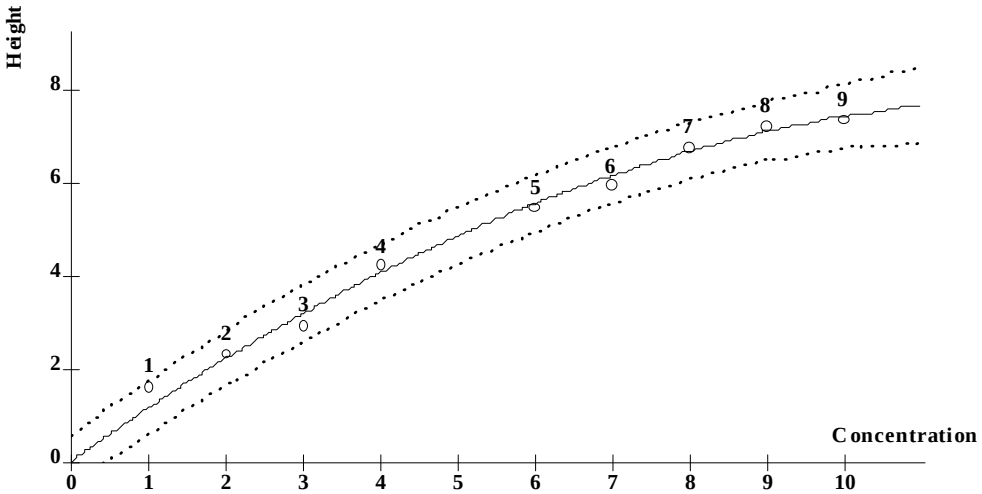


Figure 7. Quadratic polynomial not going through origin. The errors are the same for all measurements, no weighting. The concentrations for calibration are uniformly distributed. This test plan produces an adequate prediction.

IV.Conclusion

We have strict mathematical expressions for confidence intervals for detector response and for the prediction in an inverse problem in the case of generalized regression with weighting. An expressions (II.8) and (II.10) are generalizations of (I.3) and (I.4) respectively. They are applicable either for linear regressions or for regressions with polynomial of other powers (quadratic, cubic etc.).

Literature:

1. G. Seber Linear Regression Analysis

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