# Table of Contents

1. Introducing PrimeView........................................................................................................3  
   1.1. About PrimeView...............................................................................................4  
   1.2. About this manual.............................................................................................5  

2. PrimeView concepts............................................................................................................6  
   2.1. Concept definitions...........................................................................................7  
   2.2. The PrimeView user interfaces......................................................................................8  
      2.2.1. The PrimeView module.................................................................................9  
      2.2.2. The PrimeView Evaluation module...............................................................11  
      2.2.3. Search functions.......................................................................................13  
      2.2.4. Help functions..........................................................................................15  
      2.2.5. Snapshots.................................................................................................16  

3. Software Installation.........................................................................................................18  
   3.1. How to install PrimeView for the first time.........................................................19  

4. Files and folders in PrimeView...........................................................................................24  
   4.1. How to create folders.......................................................................................25  
   4.2. How to open and preview files..........................................................................26  
   4.3. How to arrange and locate your files..................................................................28  
   4.4. How to copy, delete, rename and backup files and folders...................................29  

5. How to perform method runs..............................................................................................32  
   5.1. How to start a method run................................................................................33  
   5.2. How to monitor a method run.......................................................................................37  
      5.2.1. How to customize PrimeView panes.............................................................38  
      5.2.2. The Curves pane........................................................................................40  
      5.2.3. The Logbook pane.....................................................................................45  

6. How to view results...........................................................................................................47  
   6.1. How to open a result file..................................................................................48  
   6.2. Basic presentation of chromatograms...........................................................................49  
      6.2.1. Introduction and temporary chromatograms..................................................50  
      6.2.2. The chromatogram window.........................................................................52  
   6.3. How to optimize the presentation of a chromatogram.............................................56  
      6.3.1. How to make changes in the Chromatogram Layout dialog box.......................57  
      6.3.2. The Curve tab and Curve Names tab..............................................................58  
      6.3.3. The Curve Style and Color tab.....................................................................59  
      6.3.4. How to change and fix the axes...................................................................61  
      6.3.5. How to save and apply a layout...................................................................63
1 Introducing PrimeView

Introduction

This chapter contains:

- A general overview of the PrimeView™ system.
- Information about the user documentation for PrimeView and how to use it.

In this chapter

This chapter contains the following sections

<table>
<thead>
<tr>
<th>Topic</th>
<th>See</th>
</tr>
</thead>
<tbody>
<tr>
<td>About PrimeView</td>
<td>1.1</td>
</tr>
<tr>
<td>About this manual</td>
<td>1.2</td>
</tr>
</tbody>
</table>
1.1 About PrimeView

Introduction
This section is a general overview of the PrimeView system.

What is PrimeView?
PrimeView is a complete control software package for supervision of ÄKTAprime™ automated liquid chromatography systems.

Operating environment
PrimeView runs on a PC under Microsoft® Windows® 2000 or Microsoft Windows XP. It is designed to run under English keyboard settings.

Note: Microsoft and Windows are registered trademarks of the Microsoft Corporation in the United States and/or other countries.

Windows functions
Most Windows functions are also available in PrimeView, including
• cut and paste
• right-click short-cut menus

Note: Drag and drop is not available. File and folder handling in PrimeView also differs from the general Windows file manager standard.

Help functions
An online help utility is included in the PrimeView software. The table below describes how to access the help utility.

<table>
<thead>
<tr>
<th>If you want to access...</th>
<th>Then...</th>
</tr>
</thead>
<tbody>
<tr>
<td>the general help utility.</td>
<td>open the Help menu in any of the software modules.</td>
</tr>
<tr>
<td>context-specific help topics.</td>
<td>• click the Help button in the dialog box or • press the F1 key on your keyboard.</td>
</tr>
</tbody>
</table>

Note: An online version of the PrimeView User Manual is available on the installation CD.
1.2 About this manual

Introduction
This section is a general description of the manual, the contents and the
pre-requisites for the examples and instructions that are presented in the PrimeView

Document structure
The manual is divided into chapters. Each chapter starts with a brief overview that
presents the contents and the headings for the sections that the chapter contains.
Most sections begin with an introduction that summarizes the content. Some
sections are divided into sub-sections.
A section is divided into blocks of information with separating lines. The blocks
are identified by a label in the margin. This makes it easier for you to quickly scan
a page to find the exact topic you are looking for.

Typographical representations
Menu commands, field names and other text items from the software are quoted
exactly as they appear on the screen, in a bold typeface:
Example: Run Setup
Search paths are shown in a bold typeface with a separating colon between each
level:
Example: View:Panels:Customize (i.e. the menu command Customize in the sub-menu
Panels from the View-menu).
Text entries that PrimeView generates or that the user must type is represented by
a monotype typeface:
Example: Connection change
2 PrimeView concepts

Introduction

This chapter contains:

• Definitions and descriptions of some of the specific concepts that are presented in this manual.

• An overview of the PrimeView user interface.

Note: General concepts and common chromatography terminology are not explained here.

In this chapter

This chapter contains the following sections

<table>
<thead>
<tr>
<th>Topic</th>
<th>See</th>
</tr>
</thead>
<tbody>
<tr>
<td>Concept definitions</td>
<td>2.1</td>
</tr>
<tr>
<td>The PrimeView user interfaces</td>
<td>2.2</td>
</tr>
</tbody>
</table>
2.1 Concept definitions

Introduction
This chapter contains explanations and definitions of a number of PrimeView concepts that are used in this manual.
The concepts are organized in alphabetical order.

Chromatogram
A chromatogram is a collection of data represented by a number of curves that have been created during a separation run, including UV, conductivity, pH, fraction marks etc. The original raw data curves cannot be deleted or modified. They can be used as a basis for evaluation procedures and subsequent creation of new curves.
A chromatogram can also contain curves that have been created and saved during an evaluation session.

Curves
The monitor signals from the chromatography run are displayed graphically as curves.

Method
The program instructions for a run are defined in a Method. The Method is programmed in the ÄKTAprime system.

Result files
The ÄKTAprime system creates Result files when a method is run. The Result files contain:
- Run data from the monitors in the chromatography system.  
  Example: UV absorbance, flow rate, conductivity etc.
- Documentation from the run.  
  Example: Logbook entries, settings, text method etc.
- Saved results from evaluations of the run data.  
  Example: Peak integrations, etc.

Template
Templates are basic methods that can be used as a starting point for developing customized methods. The method variables in a suitable Template is adjusted to create a method for another application.
Method Templates are supplied with the ÄKTAprime system.
2.2 The PrimeView user interfaces

Introduction

This section is an overview of the two PrimeView modules with descriptions of some of the elements of the user interfaces. The section also contains a description of the search functions in PrimeView.

In this section

This section contains the following sub-sections

<table>
<thead>
<tr>
<th>Topic</th>
<th>See</th>
</tr>
</thead>
<tbody>
<tr>
<td>The PrimeView module</td>
<td>2.2.1</td>
</tr>
<tr>
<td>The PrimeView Evaluation module</td>
<td>2.2.2</td>
</tr>
<tr>
<td>Search functions</td>
<td>2.2.3</td>
</tr>
<tr>
<td>Help functions</td>
<td>2.2.4</td>
</tr>
<tr>
<td>Snapshots</td>
<td>2.2.5</td>
</tr>
</tbody>
</table>
2.2.1 The PrimeView module

Introduction

The PrimeView module is used to monitor separation runs.

The PrimeView panes

The PrimeView module contains two different display panes that can be opened both at once or one at a time:

- The Curves pane.
- The Logbook pane.

The Curves pane

The Curves pane displays monitor signal values graphically. See the illustration below:

![Curves pane illustration](image1)

The Logbook pane

The Logbook pane displays all actions during a separation run, e.g. method start and end, base instruction, method instructions and manual instructions such as Pause or Hold. See the illustration below:

![Logbook pane illustration](image2)

The Status bar

The Status bar in the bottom of the PrimeView module displays the current status of the separation run. See the illustration below:

![Status bar illustration](image3)

The current system status is represented by the colored dot:

- A green dot represents a running system.
- A red dot represents a system in Pause state.
- A yellow dot represents a system in a Hold state.
- A white dot represents a system in an End state.
The table below describes the toolbar icons in the module:

<table>
<thead>
<tr>
<th>Icon</th>
<th>Function</th>
</tr>
</thead>
<tbody>
<tr>
<td><img src="CustomisePanes.png" alt="Customise Panes" /></td>
<td>The Customise Panes icon opens the Customise Panes dialog box, which is used to select the display panes that are open.</td>
</tr>
<tr>
<td><img src="ViewDocumentation.png" alt="View Documentation" /></td>
<td>The View Documentation icon opens the documentation pages. Run notes can be entered in the Notes page and settings can be changed.</td>
</tr>
<tr>
<td><img src="ViewProperties.png" alt="View Properties" /></td>
<td>The View Properties icon opens the Properties dialog box, which is used to control the data display in the PrimeView panes.</td>
</tr>
</tbody>
</table>
2.2.2 The PrimeView Evaluation module

Introduction

The PrimeView Evaluation module provides extensive facilities to present and to evaluate curve data.

The module window

Opened result files are displayed in the Evaluation module window. See the illustration below:

<table>
<thead>
<tr>
<th>Icon</th>
<th>Function</th>
</tr>
</thead>
<tbody>
<tr>
<td><img src="image" alt="Open Icon" /></td>
<td>The Open icon displays all available result files and result folders in the Open Result dialog box.</td>
</tr>
<tr>
<td><img src="image" alt="Save Icon" /></td>
<td>The Save icon saves the edited result file.</td>
</tr>
<tr>
<td><img src="image" alt="Print Icon" /></td>
<td>The Print icon opens the Print Chromatograms dialog box.</td>
</tr>
<tr>
<td><img src="image" alt="Report Icon" /></td>
<td>The Report icon opens the Generate Report dialog box, which is used to select a report format.</td>
</tr>
<tr>
<td><img src="image" alt="View Documentation Icon" /></td>
<td>The View Documentation icon opens the Documentation dialog box, which is used to view and edit the result documentation.</td>
</tr>
</tbody>
</table>
### 2.2.2 The PrimeView Evaluation module

<table>
<thead>
<tr>
<th>Icon</th>
<th>Function</th>
</tr>
</thead>
<tbody>
<tr>
<td><img src="image" alt="Peak Integrate Icon" /></td>
<td>The <strong>Peak Integrate</strong> icon opens the <strong>Integrate</strong> dialog box, which is used to select peaks to integrate in a modified peak table.</td>
</tr>
<tr>
<td><img src="image" alt="Chromatogram Layout Icon" /></td>
<td>The <strong>Chromatogram Layout</strong> icon opens the <strong>Chromatogram Layout</strong> dialog box, which is used to select and format curves and display items in the chromatogram.</td>
</tr>
</tbody>
</table>
2.2.3 Search functions

Introduction
This section describes the general search functions that can be used to locate for example chromatograms, curves and text strings in PrimeView. These functions can be used in several program modules, dialog boxes and wizards.

Search the Folder list
The search will take place in the displayed folder only. To select another folder, click the Browse button and open the desired folder.

Search the Result list
- The search will take place in all result files within the selected folder as denoted by the asterisk (*). To select specific result file(s), click the Browse button and select the result file(s).
- You can use wildcard characters to search for chromatograms within result files with a specific name profile.
  - * represents any number of characters
  - ? represents any single character

Wildcard character examples:
- iex will search files named “iex”
- iex* will search all files with names that begin with “iex”
- *iex will search all files with names that end with “iex”
- ?iex will search only 4-character names that end with iex

Search the Chromatogram list
The asterisk (*) indicates that all chromatograms within a result file will be selected. Click Browse to select one or several specific chromatograms.

Search the Curve name list
The UV curves are identified by number. To search for all UV curves, select *UV* in the Curve name text field.

Find a text string
The Find command is used to search for text strings:

<table>
<thead>
<tr>
<th>Field</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Find what</td>
<td>Type the text string you want to find.</td>
</tr>
<tr>
<td>Field</td>
<td>Description</td>
</tr>
<tr>
<td>------------------------------</td>
<td>-----------------------------------------------------------------------------</td>
</tr>
<tr>
<td>Match whole word only</td>
<td>Select the check-box if you only want complete string matches, not partial matches.</td>
</tr>
<tr>
<td>Match case</td>
<td>Select the check-box if you only want matches which correspond according to upper-case and lower-case letters.</td>
</tr>
<tr>
<td>Search from top of document</td>
<td>Select the check-box to start the search from the top of the document, otherwise the search will start from the cursor position.</td>
</tr>
<tr>
<td>Direction</td>
<td>Choose whether to search upwards or downwards in the document.</td>
</tr>
</tbody>
</table>

Commands
Use the commands below to find more occurrences of a text string after you have found the first one:

- Press **F3** to search for the next occurrence of the string or right-click and choose **Find next**.
- Right-click and choose **Find previous** to search for a previous occurrence.

General information about searches
- The default setting is to search in all result files or chromatograms.
- User-entered search filters (to a maximum of 10) will be saved in the drop-down menus for both Result and Chromatogram selections. More than one string can be used as a search delimiter (insert “;” between strings), and search filters are automatically saved and stored within user profiles.
- Click **All** to return to the default setting to search in all result files or chromatograms.
2.2.4 Help functions

Introduction
There are different ways to get help and instructions in PrimeView:
- From the Help menu in each module
- From the context-sensitive help in each dialog box
- By pressing the <F1> key

The Help menu
- From the Help menu in each module you can access the Help file.

The illustration below shows the Help menu of the Evaluation module:

The Help file
The table below describes how to open and use the Help file:

<table>
<thead>
<tr>
<th>Step</th>
<th>Action</th>
</tr>
</thead>
</table>
| 1    | Choose Help:Index.  
*Result:* The Help file is displayed |
| 2    | Type a word you want help on in the text box in the left pane.  
*Result:* The closest matches are displayed in the list.  
Select a match and click the Display button.  
*Result:* The associated help text is displayed in the right pane. |
| 3    | You can also click the Contents tab to view the contents of the Help file divided into sections.  
Click the plus signs to expand the tree structure.  
Click a topic to read the associated help text. |

Context-sensitive help
In each dialog box there is a Help button. If you press that button, either of the following will be displayed:
- A message box with relevant information, for example the dialog box options.
- The Help file, with relevant information displayed in the right pane.
Snapshots

Introduction

A Snapshot provides information about a method run at a certain point in time. It contains monitor values at the selected point. Snapshot functionality is available in

- the Evaluation module, where you can take Snapshots from a result file using the Marker.
- the PrimeView module, where you can take Snapshots during a run using the Marker.

How to take Snapshots in the Evaluation module

The table below describes how to take Snapshots in the Evaluation module:

<table>
<thead>
<tr>
<th>Step</th>
<th>Action</th>
</tr>
</thead>
</table>
| 1    | • Open a result file in the Evaluation module.  
      • Right-click and select Marker in the menu.  
      
      Result: A vertical line indicating a certain point is displayed. |
| 2    | Click the marker line and drag it to the desired point where you want to take a Snapshot. |
| 3    | Right-click and select Snapshot in the menu.  
      
      Result: The Snapshot is displayed in the Snap Shot dialog box. |
| 4    | • Click the Save to File button if you want to save the information as an Excel file (.xls) or a tabbed text file (.txt).  
      • You can also copy the information to the clipboard:  
        - Click and drag the mouse in the table to select the information you want to copy.  
        - Press CTRL+C.  
        
        The information can now be pasted in a text editor.  
      • Click the Print button if you want to print the information.  
      • Click the Close button. |
| 5    | Repeat steps 2 to 4 if you want to view more Snapshots. |
The table below describes how to view Snapshots in the **PrimeView** module during a method run:

<table>
<thead>
<tr>
<th>Step</th>
<th>Action</th>
</tr>
</thead>
</table>
| 1    | A method is running and the **PrimeView** module is running:  
  • Right-click in the **Curves** pane and select **Marker** in the menu.  
  **Result:** A vertical line is displayed. |
| 2    | Click the marker line and drag it to the desired point where you want to take a Snapshot. |
| 3    | Right-click in the **Curves** pane and select **Snapshot** in the menu.  
  **Result:** The Snapshot is displayed in the **Snap Shot** dialog box. |
| 4    |  
  • Click the **Save to File** button if you want to save the information as an Excel file (.xls) or a tabbed text file (.txt).  
  • You can also copy the information to the clipboard:  
    - Click and drag the mouse in the table to select the information you want to copy.  
    - Press **CTRL+C**.  
    The information can now be pasted in a text editor.  
  • Click the **Print** button if you want to print the information.  
  • Click the **Close** button. |
| 5    | Repeat steps 2 to 4 if you want to view more Snapshots. |
3 Software Installation

Introduction

The PrimeView software is normally pre-installed by a Amersham Biosciences representative. Follow the instructions in this chapter to install the program yourself if your system is not pre-installed.

In this chapter

This chapter contains the following section

<table>
<thead>
<tr>
<th>Topic</th>
<th>See</th>
</tr>
</thead>
<tbody>
<tr>
<td>How to install PrimeView for the first time</td>
<td>3.1</td>
</tr>
</tbody>
</table>
3.1 How to install PrimeView for the first time

**Installation prerequisites**
Before you start the installation procedure the following prerequisites have to be met:
- The operating system, Windows 2000/XP, must be correctly installed on your computer. See the operating system documentation for details.

**Installation notes**
Also notice the following:
- You can exit the installation at any point by clicking on either the **Cancel** button or the **Exit** button. If you do this, however, the installation will be incomplete and the software cannot be used.

**Upgrading a PrimeView installation**
Installing a new version of the PrimeView software over an existing PrimeView installation is no problem. You do not have to uninstall the previous version before installing the new version.

**Do not copy the CD-ROM or decompress the files**
PrimeView is supplied on a CD-ROM. Files on the CD-ROM are compressed and cannot simply be copied onto the hard disk. During the installation procedure, the required folder structure is created on the hard disk and the files are decompressed. Do not attempt to decompress the files using any other file decompression utility.

**Step 1 - Insert the Setup CD**
Follow the instructions in the table below to begin the installation:

<table>
<thead>
<tr>
<th>Step</th>
<th>Action</th>
</tr>
</thead>
</table>
| 1    | • Insert the CD-ROM disk into the CD-ROM drive.  
The PrimeView Setup Program should start automatically. If not,  
• click the Windows **Start** button and select **Run**  
• type the command `d: setup`, where `d:` is the unit for your CD-ROM drive.  
• click **OK**. |
| 2    | The PrimeView Setup Program is launched. Continue the setup below. |
This table describes how to complete step 2 of the PrimeView Setup Program:

<table>
<thead>
<tr>
<th>Step</th>
<th>Action</th>
</tr>
</thead>
</table>
| 1    | • The Welcome dialog box is displayed.  
      • Click the **Next** button to continue. |
| 2    | • The **PrimeView Software License Agreement** dialog box is displayed.  
      You must accept the license agreement to install PrimeView.  
      • Click the **Yes button** to continue. |
| 3    | • The **User Information** dialog box is displayed. Type your name,  
      company and the product serial number of the software. The serial number can be found on the License Agreement that is shipped with the CD.  
      • Click the **Next button** to continue. |

### Step 3 - Select the COM port

You must define the **COM** port which the AKTAprime system is connected to.
- Select the appropriate **COM** port.
- Click the **Next** button to proceed.
In the Select Drive dialog box you choose the installation folder for the PrimeView software.

Follow the instructions in the table to select a disk drive:

<table>
<thead>
<tr>
<th>Step</th>
<th>Action</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>Select the disk drive where the program is to be installed. This should be a physical disk drive (usually C:) on the computer where you install PrimeView, not a network disk drive.</td>
</tr>
</tbody>
</table>
| 2    | - Click the Next button to continue.  
- Click the Yes button if asked whether Setup should create the UNICORN™ program folder.  
Note: The UNICORN folder will contain all PrimeView files and folders. |
In the Select Program Folder dialog box you choose where to store the program icon.

The table below describes how to select a program folder for the PrimeView icon:

<table>
<thead>
<tr>
<th>Step</th>
<th>Action</th>
</tr>
</thead>
</table>
| 1    | In the Select Program Folder dialog box, you select the Start menu folder where you want the PrimeView icon to be placed. You can either  
* accept the suggested folder named UNICORN (recommended)  
or  
* create a new folder. Type the name of the new folder in the text field Program Folders.  
or  
* select a folder that already exists by clicking its name on the list. |
| 2    | Click the Next button to continue. |
The Start Copying Files dialog box displays the installation choices made.

The table describes how to start copying the program files from the CD:

<table>
<thead>
<tr>
<th>Step</th>
<th>Action</th>
</tr>
</thead>
</table>
| 1    | The setup program is ready to copy the files. The Start Copying Files dialog box displays all the selections that have been made and the components to be installed.  
*Note:* If you want to make any changes you can click the Back button one or more times. |
| 2    | If the settings are correct, click the Next button to copy the files. |

The installation is complete and the computer must be restarted:  
- Click the Finish button to exit the setup program and automatically restart the computer.
Files and folders in PrimeView

Introduction
All PrimeView data is organized in files and folders. Files and folders are handled like in any other Windows application, with some exceptions. This chapter describes how to work with PrimeView files and folders, with the focus on the topics that are specific for PrimeView.

In this chapter

This chapter contains the following sections

<table>
<thead>
<tr>
<th>Topic</th>
<th>See</th>
</tr>
</thead>
<tbody>
<tr>
<td>How to create folders</td>
<td>4.1</td>
</tr>
<tr>
<td>How to open and preview files</td>
<td>4.2</td>
</tr>
<tr>
<td>How to arrange and locate your files</td>
<td>4.3</td>
</tr>
<tr>
<td>How to copy, delete, rename and backup files and folders</td>
<td>4.4</td>
</tr>
</tbody>
</table>
## 4.1 How to create folders

### Introduction

This section describes how folders are organized in PrimeView and how to create a new user-specific folder for the user’s methods and results.

### How to create a new folder

The table below describes how to create a new folder in the **Evaluation** module.

<table>
<thead>
<tr>
<th>Step</th>
<th>Action</th>
</tr>
</thead>
</table>
| 1    | • Select **File:Open**.  
|      |   or   |
|      | • Click the **Open** icon.  
|      | **Result**: The **Open Result** dialog box opens. |
| 2    | • Right-click on an empty area of the dialog box.  
|      | • Select **New Folder** from the shortcut menu.  
|      | **Result**: The **Create New Folder** dialog box opens. |
| 3    | • Type a name for the new folder.  
|      | • Click **OK**.  
|      | **Result**: The new folder is displayed in the **Open Result** dialog box. |
4.2 How to open and preview files

Introduction

This section describes how to open your saved result files. You can also preview your result files to identify the correct file before you open it.

How to open a result file

The table below describes how to open result files in the **Evaluation** module.

<table>
<thead>
<tr>
<th>Step</th>
<th>Action</th>
</tr>
</thead>
</table>
| 1    | • Choose **File:Open:Result**  
      |   or  
      | • Click the **Open** icon.  
      |  
      | Result: The **Open Result** dialog box opens. |
| 2    | • Double-click the result file  
      |   or  
      | • Select the result file and click the **OK** button  
      |  
      | Result: The file is opened in the **Evaluation** module. |

Quick View

Quick View is a preview function for result files to make it easier to select the correct result file. You can preview the first curve in the first chromatogram.
The table below describes how to preview result files in Quick View.

<table>
<thead>
<tr>
<th>Step</th>
<th>Action</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>Select a result file in the <strong>Open Result</strong> dialog box.</td>
</tr>
</tbody>
</table>
| 2    | • Right-click and choose **Quick View** from the short-cut menu.  
**Result:** The **Quick View** dialog box opens. |
| 3    | • Click the **Open** button.  
**Result:** The result file that is displayed in the dialog box opens in the **Evaluation** module. |
4.3 How to arrange and locate your files

Introduction
This section describes how to arrange the way the files are displayed in the Open Results dialog box and how to locate files through a search.

Different view modes
You can choose how the files and folders are displayed in the Open Results dialog box. The options are the standard Windows alternatives:

- Details
- List
- Large icons
- Small icons.

How to change the view mode
If you want to change the view you:

- Right-click and select View and the option that you want from the shortcut menu.

Sort order
The files can be sorted in different orders. The table below shows the options.

<table>
<thead>
<tr>
<th>Sorted by:</th>
<th>Order</th>
</tr>
</thead>
<tbody>
<tr>
<td>Name</td>
<td>Alphabetical order or reverse alphabetical order.</td>
</tr>
<tr>
<td>Size</td>
<td>Smallest or largest files first.</td>
</tr>
<tr>
<td>Type</td>
<td>Alphabetical order of file extension type.</td>
</tr>
<tr>
<td>Modified</td>
<td>Most recently modified files first.</td>
</tr>
<tr>
<td>Created</td>
<td>Most recent creation dates first.</td>
</tr>
</tbody>
</table>

How to change the sorting order
Select one of the methods below to change the sorting order:

- Right-click and select Sort and the option that you want from the short-cut menu.

or

- Click the column header for the option that you want to sort by (a second click on the same header will reverse the order).
## 4.4 How to copy, delete, rename and backup files and folders

### Introduction

PrimeView has some file and folder handling functions that are slightly different from the general Windows functions. This section focuses on the differences.

### How to copy or move files and folders

If you copy a folder you will also at the same time copy all files and folders that it contains. The table below describes how to copy files and folders.

*Note:* Follow the same steps but select **Move** to move files and folders.

<table>
<thead>
<tr>
<th>Step</th>
<th>Action</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>Select a file or folder in the <strong>Open Results</strong> dialog box.</td>
</tr>
</tbody>
</table>
| 2    | Right-click and select **Copy** from the short-cut menu.  
*Result:* The **Copy** dialog box is opened. |
| 3    | Select a target folder or floppy disk drive. |
| 4    | Click **OK**. |

### The function Copy to External

Use the function **Copy to External** when you need to copy files and folders outside of your own user folders. **Copy to External** should be used specifically when you need:

- to copy to a floppy disk drive. (The files are automatically compressed into a zip-file. The file will also automatically be spanned across several disks if necessary.)

### How to Copy to External

The table below describes how to use the function **Copy to External**.

<table>
<thead>
<tr>
<th>Step</th>
<th>Action</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>Select the file you want to copy.</td>
</tr>
</tbody>
</table>
| 2    | Right-click and select **Copy to External** from the shortcut menu.  
*Result:* the **Copy to External** dialog box opens. |
| 3    | Select the destination drive and folder. |
| 4    | Click the **Save** button. |
The function **Copy from External** can be used to import files and folders:

- If the files were saved using the function **Copy to External** they will automatically be decompressed.

### How to use Copy from External

The table below describes how to use the function **Copy from External**.

<table>
<thead>
<tr>
<th>Step</th>
<th>Action</th>
</tr>
</thead>
</table>
| 1    | Right-click in the **Open Results** dialog box and select **Copy from External**.  
*Result:* The **Copy from External** dialog box opens. |
| 2    | Select the files you want to copy. |
| 3    | Click **Save**.  
*Result:* The result files are copied into the open folder in the **Open Results** dialog box. |

### How to rename files and folders

The table below describes how to rename files and folders in the **Open Results** dialog box.

<table>
<thead>
<tr>
<th>Step</th>
<th>Action</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>Select the item that you want to rename.</td>
</tr>
</tbody>
</table>
| 2    | Right-click and select **Rename** from the shortcut menu.  
*Result:* The **Rename** dialog box opens. |
| 3    | Type a new name. |
| 4    | Click **OK**. |

### How to delete files and folders

The table below describes how to delete files and folders in the **Open Results** dialog box.  

*Note:* Home folders cannot be deleted this way.

<table>
<thead>
<tr>
<th>Step</th>
<th>Action</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>Select the item that you want to delete.</td>
</tr>
</tbody>
</table>
| 2    | Right-click and select **Delete** from the shortcut menu.  
*or*  
Press the **Delete** key. |
## Backup security

Backup copies should be taken regularly to avoid data loss in the event of hard disk failure or accidental deletion. You can use the function **Copy to External** to save your files on the network server.

*Note:* Amersham Biosciences cannot accept responsibility for the replacement of results that were lost as a result of computer failure or other incidents.

<table>
<thead>
<tr>
<th>Step</th>
<th>Action</th>
</tr>
</thead>
<tbody>
<tr>
<td>3</td>
<td>Confirm the delete action in the confirmation dialog box</td>
</tr>
</tbody>
</table>
How to perform method runs

Introduction
This chapter describes how to perform and monitor different kinds of runs from the PrimeView module. It also describes how to control the system with manual commands and instructions.

In this chapter
This chapter contains the following sections

<table>
<thead>
<tr>
<th>Topic</th>
<th>See</th>
</tr>
</thead>
<tbody>
<tr>
<td>How to start a method run</td>
<td>5.1</td>
</tr>
<tr>
<td>How to monitor a method run</td>
<td>5.2</td>
</tr>
</tbody>
</table>
5.1 How to start a method run

Before you start a method, make sure that

- the ÄKTAprime system is prepared according to the instructions in the ÄKTAprime system documentation

Four ways to start an ÄKTAprime run

The method runs are all operated from the ÄKTAprime unit. There are four different types of ÄKTAprime runs:

- **Application template** runs
- **Method template** runs
- Operator created method runs
- Manual runs

How to start an application template run

Application templates are available for the most frequent purifications. All process parameters except the sample volume are preset. The table below describes how to start an **Application template** run on the ÄKTAprime unit. All parameters are selected with the arrow buttons on the unit. The selections are confirmed with the **OK** button.

<table>
<thead>
<tr>
<th>Step</th>
<th>Action</th>
</tr>
</thead>
</table>
| 1    | • Choose the **Templates** menu.  
   • Press the **OK** button.  
   *Result*: The **Templates** menu is displayed. |
| 2    | • Choose the **Application template** menu.  
   • Press the **OK** button.  
   *Result*: The first application template is displayed. |
| 3    | • Step through the list of application templates with the up or down buttons until the desired template is displayed.  
   • Press the **OK** button.  
   *Result*: The **Sample appl. volume** menu is displayed. |
| 4    | • Set the sample volume with the up or down buttons.  
   • Press the **OK** button.  
   *Result*: The **Press OK to start run** prompt is displayed.  
   • Press the **OK** button.  
   *Result*: The purification run starts. |
Note: If needed, the sample volume should include the sample wash out volume.

The four most common purification techniques are available as method templates. Some parameters must be set by the operator when a run is prepared from a method template. The settings can be saved for later use before the run is started.

ÄKTAprome

method templates

The table below describes how to start a method template run on the ÄKTAprome unit. All parameters are selected with the arrow buttons on the unit. The selections are confirmed with the OK button.

<table>
<thead>
<tr>
<th>Step</th>
<th>Action</th>
</tr>
</thead>
</table>
| 1    | • Choose the Templates menu.  
      • Press the OK button.  
      
      Result: The Templates menu is displayed. |
| 2    | • Choose the Method template menu.  
      • Press the OK button.  
      
      Result: The first method template is displayed. |
| 3    | • Step through the list of method templates with the up or down buttons until the desired template is displayed.  
      • Press the OK button.  
      
      Result: The Sample inject by menu is displayed. |
| 4    | • Select sample injection through the injection valve or through the system pump.  
      • Press the OK button.  
      • Continue to set method parameters with the up and down buttons in the subsequent menus and press the OK button to proceed.  
      • After all parameters are set, navigate to the Method ready? menu with the arrow button.  
      • Press the OK button.  
      
      Result: The Save Method menu is displayed. If you want to save the method, continue with step 5 below. If not, select no in the next menu and proceed to step 6. |

5.1 How to start a method run
5. Choose **yes** and press the **OK** button.
   - Use the up and down keys to select a free method number and press the **OK** button.

   **Note:** Up to 40 methods can be stored. If the method number already is used you can press **OK** and then clear the number in the **Clear Method** menu.

6. Press the **OK** button at the **Press OK to start run** prompt.

   **Result:** The method runs starts.

---

**How to run a saved method**

The table below describes how to run a saved method on the ÄKTAprime unit. All parameters are selected with the arrow buttons on the unit. The selections are confirmed with the **OK** button.

<table>
<thead>
<tr>
<th>Step</th>
<th>Action</th>
</tr>
</thead>
</table>
| 1    | • Choose the **Run Stored Method** menu.  
      • Press the **OK** button.  
      **Result:** The **Run Stored Method** menu is displayed. |
| 2    | • Select **System** or **PC**.  
      • Press the **OK** button.  
      • Choose the method number.  
      • Press the **OK** button.  
      **Result:** The **Press OK to start run** menu is displayed. |
| 3    | • Press the **OK** button.  
      **Result:** The method runs starts. |

**Note:** Important parameter values are displayed on the ÄKTAprime unit during the run. Refer to the ÄKTAprime User Manual for instructions on how to change some of these parameters if needed.
The table below describes how to run the ÄKTAprime unit manually. All parameters are selected with the arrow buttons on the unit. The selections are confirmed with the OK button.

<table>
<thead>
<tr>
<th>Step</th>
<th>Action</th>
</tr>
</thead>
</table>
| 1    | • Choose the **Manual Run** menu.  
      | • Press the OK button.  
      | **Result**: The **Set Method Base** menu is displayed. |
| 2    | • To edit the method base, press OK and select the base with the arrow buttons.  
      | • Proceed to select parameters with the arrow buttons in the subsequent menus and press OK to continue. |
| 3    | • After the last parameter selection, navigate to the **Start run** menu.  
      | • Press the OK button.  
      | **Result**: The method runs starts. |

**Note**: Refer to the ÄKTAprime User Manual for instructions on how to select the parameters if needed.

How to finish the run

Press the OK button to finish the run at the **Method Complete** prompt. This will cause all valves to return to the default position 1. The run can be aborted before it is complete at any time by pressing the **End** button.
5.2 How to monitor a method run

Introduction

This section describes how to monitor a method run by using the PrimeView module and how to customize the different panes.

In this section

This section contains the following sub-sections

<table>
<thead>
<tr>
<th>Topic</th>
<th>See</th>
</tr>
</thead>
<tbody>
<tr>
<td>How to customize PrimeView panes</td>
<td>5.2.1</td>
</tr>
<tr>
<td>The Curves pane</td>
<td>5.2.2</td>
</tr>
<tr>
<td>The Logbook pane</td>
<td>5.2.3</td>
</tr>
</tbody>
</table>
How to customize PrimeView panes

The PrimeView module displays the status of the ÄKTAprime system run. The PrimeView module can be open on the Windows desktop before a run is started, in which case it will either display a blank Curves pane or show the curves from the previous run. The PrimeView module can also be opened after the run has been started, in which case it will display the whole progress of the run from the beginning. The list below describes how to open the PrimeView module.

- Click the PrimeView icon.

Result: The PrimeView module opens.

Illustration

The illustration shows the PrimeView module with the Curves and Logbook panes displayed.

How to select what panes to display

The PrimeView module displays one or two panes for monitoring different aspects of the run. To select what panes to display, either

- click the Customize Panes icon,
How to customize PrimeView panes

Change the size
Select a split-bar and drag up and down to change the size of a specific pane.

Maximize, restore or hide
Right-click a pane and select the appropriate option to:

- maximize,
- restore
  or
- hide the pane.
5.2.2 The Curves pane

**Introduction**

The Curves pane of the PrimeView module displays monitor signal values graphically. The figure below shows an example of the Curves pane:

![Curves pane example](image)

The table describes how to select the curves to be displayed on the screen.

<table>
<thead>
<tr>
<th>Step</th>
<th>Action</th>
</tr>
</thead>
</table>
| 1    | In the PrimeView module, select View:Properties.  
*Result:* The Properties dialog box is displayed. |
| 2    | Select the Curves tab. |
| 3    | In the Display curves list, select the curves you want to display.  
If you want all curves to be displayed, click the Select All button. If you do not want any curves to be displayed, click the Clear All button.  
Click OK. |

**How to display a vertical marker line**

The table below describes how to display a vertical marker line:

<table>
<thead>
<tr>
<th>Step</th>
<th>Action</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>Right-click the Curves pane and select Marker.</td>
</tr>
</tbody>
</table>
| 2    | Drag the marker line with the mouse.  
*Result:* Where the line bisects the curve, the X-axis and Y-axis values are displayed at the top right corner of the pane. |

*Note:* Right-click and select Snapshot to record the marker position values. See 2.2.5 Snapshots on page 16 for more information about the Snapshot function.

**How to set a reference point**

When the vertical marker is displayed, you can set a reference point to display curve data. The table describes how to set a reference point:
### How to change the curve colors and styles

The **Curves** pane displays graphs for the selected curves in different colors. The table below describes how to change the curve colors and styles:

<table>
<thead>
<tr>
<th>Step</th>
<th>Action</th>
</tr>
</thead>
</table>
| 1    | Select **View:Properties**.  
*Result:* The **Properties** dialog box is displayed. |
| 2    | Select the **Curve Style and Color** tab. |
| 3    | • Select a curve from the **Curve** list.  
• Select an appropriate color and style. |

### How to change the scale of the Y-axis

In most cases, the Y-axis is automatically scaled for each of the curves. Values on the Y-axis apply to the curve with the same color as the axis markings. To get the correct Y-axis, click the legend. The table below describes how to fix the scale of individual curves.

<table>
<thead>
<tr>
<th>Step</th>
<th>Action</th>
</tr>
</thead>
</table>
| 1    | • Select **View:Properties**.  
*Result:* The **Properties** dialog box is displayed.  
• Select the **Y-axis** tab. |
| 2    | • Select the appropriate curve.  
• Select **Fixed** and type a minimum and maximum range in the fields within the specified limits. |
| 3    | Repeat step 2 for other curves if needed. |
| 4    | Click **OK**. |
How to change the scale of the X-axis

The table below describes how to change the scale of the X-axis:

<table>
<thead>
<tr>
<th>Step</th>
<th>Action</th>
</tr>
</thead>
</table>
| 1    | Select View:Properties.  
      Result: The Properties dialog box is displayed.  
      - Select the X-axis tab. |
| 2    | Select the appropriate base, Time or Volume.  
      Note: Curves are collected in time and recalculated for display in volume. Thus, the resolution of the two bases may appear slightly different. |
| 3    | Select the appropriate Axis scale:  
      - Total will show the curves as far as they have come in the run.  
      - Window allows you to set the portion of the total pane to be displayed, either in minutes or ml depending on the selected base.  
      - Click OK. |

How to switch between time and volume units

- Click the legend of the X-axis
- or
- right-click and select Base Type

to switch the display between time and volume units. The run is controlled according to the time/volume base defined in the current block, regardless of the base in the curves display.

How to zoom in the Curves pane

The table below describes how to zoom in on a selected region of the curve pane:

<table>
<thead>
<tr>
<th>Step</th>
<th>Action</th>
</tr>
</thead>
</table>
| 1    | Press and hold the left mouse button and drag a rectangle out on the screen to encompass the area to be viewed.  
      - Release the mouse button.  
      Result: The display is now zoomed in on the selected area. |
| 2    | Repeat the process for further magnification of selected areas. |

How to zoom out

To reduce the scale of the zoom, right-click in the Curves pane, and select one of the following options:
- **Undo Zoom**: reverses each zoom-in action a step at a time.
- **Reset Zoom**: reverses all zoom-in actions to the default scale.

If the **Pressure** curve is displayed in the **Curves** pane, you can set the displayed units. The table below describes how to do this:

<table>
<thead>
<tr>
<th>Step</th>
<th>Action</th>
</tr>
</thead>
</table>
| 1    | Right-click in the **Curves** pane, and select **Properties** in the displayed menu.  
*Result*: The **Properties** dialog box is displayed. |
| 2    | Select the **Y-Axis** tab. |
| 3    | Select the **Pressure** curve and select the appropriate **Pressure unit** button.  
Click **OK**. |

You can select the way that text is aligned for the **Logbook** and **Fraction** curves. You can also select to show only part of the **Logbook** information. The table below describes how to do this:

<table>
<thead>
<tr>
<th>Step</th>
<th>Action</th>
</tr>
</thead>
</table>
| 1    | Right-click in the **Curves** pane, and select **Properties** in the displayed menu.  
*Result*: The **Properties** dialog box is displayed. |
| 2    | Select the **Curve Style and Color** tab. |
| 3    | Select the following:  
- **Logbook** or **Fraction** curve in the **Curve** list as appropriate.  
- Select the appropriate **Logbook text alignment** or **Fraction text alignment** option:  
  - Horizontal  
  - Vertical  
  - Fly over (displays the text if you place the mouse pointer over the generated mark).  
Click **OK**. |
At some breakpoints there can be more logbook information than what is possible to conveniently display in the **Curves** pane. The additional information that is not displayed is indicated by an arrow point symbol by the break point.

- Hold the mouse cursor over the break point to display the complete information in a flyover text box, as shown in the illustration below.
5.2.3 The Logbook pane

Introduction

All actions (including method start and end, base instruction, method instructions and manual interventions such as Pause or Hold) and unexpected conditions such as warnings and alarms are logged for every run, with date, time and current user name where appropriate. The logbook thus provides a complete history of any given run. The log is saved in the result file.

Illustration

The illustration below shows an example of the Logbook pane:

Note: The second logbook line is the BatchID that is automatically generated.

Autoscroll

The Logbook pane can autoscroll to display the latest entries. Right-click in the pane, and select Autoscroll. You can also select the Autoscroll option in the Properties dialog box (View: Properties and select the Logbook tab).

How to filter the logbook contents

You can choose to display only selected items in the logbook. The table below describes how to activate the filter.

<table>
<thead>
<tr>
<th>Step</th>
<th>Action</th>
</tr>
</thead>
</table>
| 1    | • Right-click in the Logbook pane and choose Properties.  
Result: The Properties dialog box opens. |
| 2    | • Choose the Logbook tab.  
• Select the items you want to display in the logbook (all items are selected by default).  
• Click the OK button.  
Result: Only the selected items will be displayed in the logbook. The Logbook title in the upper right corner will show the text (Filter on) to indicate that not all items are visible. All items will still be logged in the result file. |
### How to find logbook text entries

The logbook can be searched for specific text entries. The table below describes the function:

<table>
<thead>
<tr>
<th>Step</th>
<th>Action</th>
</tr>
</thead>
</table>
| 1    | Right-click in the **Logbook** pane and choose **Find**.  
*Result*: The **Find** dialog box opens. |
| 2    | • Type the text you want to locate.  
• Select search criteria if necessary.  
• Click **OK**.  
*Result*: The located logbook entry is highlighted. |
How to view results

Introduction

A result file is automatically generated at the end of a method run and contains a complete record of the method run, including method, system settings, curve data and method run log. The Evaluation module offers extensive facilities for presentation and evaluation of curve data.

This chapter describes how to present the chromatograms and curves of your result file and how to create and print reports.

In this chapter

This chapter contains the following sections

<table>
<thead>
<tr>
<th>Topic</th>
<th>See</th>
</tr>
</thead>
<tbody>
<tr>
<td>How to open a result file</td>
<td>6.1</td>
</tr>
<tr>
<td>Basic presentation of chromatograms</td>
<td>6.2</td>
</tr>
<tr>
<td>How to optimize the presentation of a chromatogram</td>
<td>6.3</td>
</tr>
<tr>
<td>How to print active chromatograms</td>
<td>6.4</td>
</tr>
<tr>
<td>How to create and print a customized report</td>
<td>6.5</td>
</tr>
<tr>
<td>Run documentation</td>
<td>6.6</td>
</tr>
</tbody>
</table>
How to open a result file

The **PrimeView Evaluation** module provides facilities for the presentation and evaluation of separation results. The module is independent from the **PrimeView** module and can be started even if the **PrimeView** module is not operating.

- Click the **PrimeView Evaluation** icon on the Windows desktop.

Result: The **PrimeView Evaluation** module opens.

The table below describes how to open a result file in the PrimeView Evaluation module.

<table>
<thead>
<tr>
<th>Step</th>
<th>Action</th>
</tr>
</thead>
</table>
| 1    | • Select **File:Open**  
   or  
   • Click the **Open** icon |

Result: The **Open Result** dialog box opens.

<table>
<thead>
<tr>
<th>Step</th>
<th>Action</th>
</tr>
</thead>
<tbody>
<tr>
<td>2</td>
<td>• Select the result file and click <strong>OK</strong>.</td>
</tr>
</tbody>
</table>

Result: All contents of the opened result file are transferred to the **Evaluation** module.

**Note:** By default, the chromatograms in a run are shown as opened windows. The chromatogram window on top is the active window. There is also a minimized **Temporary** chromatogram window. See 6.2 Basic presentation of chromatograms on page 49 for further information about chromatograms.
6.2 Basic presentation of chromatograms

Introduction

This section describes how to access result files and optimize the presentation of a chromatogram and its curves via the Chromatogram Layout dialog box.

In this section

This section contains the following sub-sections

<table>
<thead>
<tr>
<th>Topic</th>
<th>See</th>
</tr>
</thead>
<tbody>
<tr>
<td>Introduction and temporary chromatograms</td>
<td>6.2.1</td>
</tr>
<tr>
<td>The chromatogram window</td>
<td>6.2.2</td>
</tr>
</tbody>
</table>
6.2.1 Introduction and temporary chromatograms

Contents of a chromatogram

Chromatograms can be viewed in the Evaluation module.

A chromatogram includes a number of curves that have been created during a method run, such as UV, conductivity, pH, fraction marks, etc. A chromatogram also contains the curves created and saved during an evaluation session. The original raw data curves cannot be deleted or modified.

Temporary chromatograms

A Temporary chromatogram is essentially an empty chromatogram that is specific to the Evaluation module.

Information contained within a Temporary chromatogram is automatically saved from one evaluation session to the next, but is not saved within the result files.

How to copy curves into Temporary

Curves can be copied into Temporary and comparisons or evaluations can be performed. This is particularly useful if you do not want to clutter up your original chromatograms with a large number of curves. It can also be used to keep blank run curves or curves to compare when you open different result files.

The table below describes how to copy curves into Temporary:

<table>
<thead>
<tr>
<th>Step</th>
<th>Action</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>Open a result file.</td>
</tr>
</tbody>
</table>
| 2    | Select Edit:Copy:Curves.  
*Result:* The Copy Curve dialog box is displayed. |
| 3    | Select a source chromatogram and a curve to be copied in the Source Chromatogram fields. |
| 4    | Select Temporary as the target chromatogram and a position for the new curve in the Target Chromatogram fields. |
| 5    | Click the Copy button.  
*Result:* The curve is copied into the Temporary chromatogram.  
Click the Close button. |

How to clear a temporary chromatogram

The table below describes how to clear the contents of a temporary chromatogram:

<table>
<thead>
<tr>
<th>Step</th>
<th>Action</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>Open the relevant result file.</td>
</tr>
<tr>
<td>Step</td>
<td>Action</td>
</tr>
<tr>
<td>------</td>
<td>--------</td>
</tr>
</tbody>
</table>
| 2    | • Select **Edit:Clear Temporary Chromatogram**.  
      • Click the **Yes** button to confirm. |
6.2.2 The chromatogram window

Main views

The chromatogram window is divided into two main views:
- curves
- peak tables

The displayed areas for the views can be adjusted by dragging the borders with the mouse cursor between the views.

How to view peak table information

The table below describes how to display peak table information if the result has been integrated:

<table>
<thead>
<tr>
<th>Step</th>
<th>Action</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>Open a result file.</td>
</tr>
</tbody>
</table>
| 2    | Choose **Edit: Chromatogram Layout**.  
*Result:* The **Chromatogram Layout** dialog box opens. |
| 3    | Click the **Peak Table** tab.  
- Select a peak table in the **Select peak table to display** list.  
- Select what peak table columns to display.  
- Check if global peak table data should be displayed or not.  
- Click **OK**. |
The first time a result file is opened and viewed, a default layout is applied to display all the original curves. The default layout can be changed by the user (see 6.3.5 How to save and apply a layout on page 63).

Information for each curve
Each curve is automatically assigned a default color and style, with default information about each curve displayed in the key above the curves. This information includes
- result file name
- chromatogram name
- curve name.

Choose the Y-axis scale
Each curve has a correspondingly colored Y-axis. To choose the appropriate Y-axis scale
- click on the Y-axis until the desired scale is displayed
- click on the name of the curve.

Run curves, shortcut menu
When viewing curves in the Evaluation module, you can access a menu that provides a quick alternative to menu commands. Right-click the run curves view to display the menu shown in the picture below:
The chromatogram window can be minimized and maximized using ordinary Windows commands. The table below describes extra features to optimize the workspace:

<table>
<thead>
<tr>
<th>Use the command</th>
<th>if you want...</th>
</tr>
</thead>
<tbody>
<tr>
<td>Window:Arrange icons</td>
<td>to arrange icons of minimized windows.</td>
</tr>
<tr>
<td>Window:Tile</td>
<td>to view several chromatogram windows side by side.</td>
</tr>
<tr>
<td>Window:Cascade</td>
<td>to stack the open windows like a deck of cards.</td>
</tr>
</tbody>
</table>

The table below describes how to display a vertical marker line:

<table>
<thead>
<tr>
<th>Step</th>
<th>Action</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>Right-click the Curves pane and select Marker.</td>
</tr>
<tr>
<td>2</td>
<td>Drag the marker line with the mouse.</td>
</tr>
</tbody>
</table>

**Result:** Where the line bisects the curve, the X-axis and Y-axis values are displayed at the top right corner of the pane.

**Note:** Right-click and select Snapshot to record the marker position values. See 2.2.5 Snapshots on page 16 for more information about the Snapshot function.

The table describes how to set a reference point:

<table>
<thead>
<tr>
<th>Step</th>
<th>Action</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>• Display a Marker in the Curves pane.</td>
</tr>
<tr>
<td></td>
<td>• Right-click and select Set Marker Ref. Point to define a reference point for the marker position.</td>
</tr>
<tr>
<td>2</td>
<td>When the marker is moved from the reference point, the X-axis and Y-axis values for the new position are displayed together with:</td>
</tr>
<tr>
<td></td>
<td>• the new position in relation to the reference point,</td>
</tr>
<tr>
<td></td>
<td>• the minimum, maximum and average values for the curve interval between the reference point and the new position.</td>
</tr>
</tbody>
</table>
The table below describes how to display the logbook entries as an overlay in the chromatogram.

<table>
<thead>
<tr>
<th>Step</th>
<th>Action</th>
</tr>
</thead>
</table>
| 1    | • Right-click in the chromatogram window and choose **Properties** on the shortcut menu.  
**Result:** The **Chromatogram Layout** dialog box opens. |
| 2    | • Choose the **Curve** tab.  
• Select the **Logbook** curve. |

**How to view the complete logbook information**

At some breakpoints there can be more logbook information than what is possible to conveniently display in the chromatogram window. The additional information that is not displayed is indicated by an arrow point symbol by the break point.

• Hold the mouse cursor over the break point to display the complete information in a flyover text box, as shown in the illustration below:
6.3 How to optimize the presentation of a chromatogram

Introduction

This section describes some of the ways you can optimize the presentation of a chromatogram.

In this section

This section contains the following sub-sections

<table>
<thead>
<tr>
<th>Topic</th>
<th>See</th>
</tr>
</thead>
<tbody>
<tr>
<td>How to make changes in the Chromatogram Layout dialog box</td>
<td>6.3.1</td>
</tr>
<tr>
<td>The Curve tab and Curve Names tab</td>
<td>6.3.2</td>
</tr>
<tr>
<td>The Curve Style and Color tab</td>
<td>6.3.3</td>
</tr>
<tr>
<td>How to change and fix the axes</td>
<td>6.3.4</td>
</tr>
<tr>
<td>How to save and apply a layout</td>
<td>6.3.5</td>
</tr>
<tr>
<td>How to show part of a curve</td>
<td>6.3.6</td>
</tr>
</tbody>
</table>
6.3.1 How to make changes in the Chromatogram Layout dialog box

The Chromatogram Layout dialog box is used to make changes regarding chromatogram presentation. The main features of the Chromatogram Layout dialog box regarding chromatograms are described in the subsequent sections in this chapter. Features regarding peak tables are described in 8.2 How to perform a peak integration on page 89.

The table below describes how to make changes in the Chromatogram Layout dialog box:

<table>
<thead>
<tr>
<th>Step</th>
<th>Action</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>Open a result file.</td>
</tr>
</tbody>
</table>
| 2    | • Right-click the chromatogram window and select Properties or  
|      | • Choose Edit:Chromatogram Layout.  
|      | Result: The Chromatogram Layout dialog box is displayed. The view from which you activate the Properties command determines the tab that is displayed in the Chromatogram Layout dialog box. |
| 3    | Carry out the changes on the different tabs to get the desired layout for header, curves and peak table.  
|      | Select Apply to all chromatograms if you want to apply changes made in the Chromatogram Layout dialog box to all open chromatograms.  
|      | Click OK. |
6.3.2 The Curve tab and Curve Names tab

The Curve tab of the Chromatogram Layout dialog box contains a list of all the curves included in the chromatogram. Select the curves you want to display in the chromatogram, and click OK.

You select options for the curve name appearance on the Curve Names tab. This is an example of a default curve name:

**Result:11_UV**

The table below describes the three components that make up the default curve name:

<table>
<thead>
<tr>
<th>Component</th>
<th>Description</th>
<th>Example</th>
</tr>
</thead>
<tbody>
<tr>
<td>Result name</td>
<td>Name of the result.</td>
<td>Result</td>
</tr>
<tr>
<td>Chromatogram name</td>
<td>Number given automatically during a run or a name defined by the New Chromatogram instruction.</td>
<td>11</td>
</tr>
<tr>
<td>Curve name</td>
<td>Curve type, for example detection of an eluted component.</td>
<td>UV</td>
</tr>
</tbody>
</table>

You can choose to view only part of the curve name. The table below describes how to do this:

<table>
<thead>
<tr>
<th>Step</th>
<th>Action</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>Open a result file.</td>
</tr>
</tbody>
</table>
| 2    | Choose *Edit:Chromatogram Layout*.  
*Result:* The Chromatogram Layout dialog box is displayed. |
| 3    | Click the Curve Names tab. |
| 4    | • Select the appropriate boxes for Curve name appearance.  
• Select the appropriate Curve legend position.  
• Click OK. |

**Note:** It is usually sufficient to select the Curve Name option if only one chromatogram is being evaluated. However, confusion can arise when more than one chromatogram is shown, so more complete names might be necessary.
6.3.3 The Curve Style and Color tab

Introduction

All curves within a chromatogram are represented by a default color and line style. Curves imported into the chromatogram or newly created curves are automatically assigned a color and line style.

Peak label settings

Peaks can be labeled on the Curve Style and Color tab of the Chromatogram Layout dialog box. Use a combination of the following labels:

- **Retention** (the default label)
- sequential **Number**
- user-defined **Peak name**.

Fraction text and Logbook text alignment settings

Both Fraction text and Logbook text can be set to the following alignment options:

- **Vertical**
- **Horizontal**
- **Fly Over**, which sets text labels as hidden text that appears only when the cursor is carefully positioned over a fraction mark.

How to change the color and style of a curve

The table below describes how to change the color and style of a curve:

<table>
<thead>
<tr>
<th>Step</th>
<th>Action</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>Open a result file.</td>
</tr>
</tbody>
</table>
| 2    | Choose **Edit:Chromatogram Layout**.  
**Result:** The Chromatogram Layout dialog box is displayed. |
| 3    | Click the Curve Style and Color tab. |
| 4    | • Select the curve you want to change from the list.  
• Select the desired color and style.  
• Click **OK**. |

How to display a hatched background

The table below describes how to display a hatched background in the chromatogram window:

<table>
<thead>
<tr>
<th>Step</th>
<th>Action</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>Open a result file.</td>
</tr>
</tbody>
</table>
### 6.3.3 The Curve Style and Color tab

<table>
<thead>
<tr>
<th>Step</th>
<th>Action</th>
</tr>
</thead>
</table>
| 2    | • Choose **Edit:Chromatogram Layout**.  
      | *Result:* The **Chromatogram Layout** dialog box is displayed. |
| 3    | • Click the **Curve Style and Color** tab.  
      | • Select the **Hatch** box.  
      | • If desired, select the **Apply to all chromatograms** box and click **OK**.  
      | *Result:* Hatch marks are displayed as a background. |

**Note:** You can also right-click in the **Chromatogram** window and select **Hatch**.
## 6.3.4 How to change and fix the axes

The table below describes how to change and fix the Y-axis:

<table>
<thead>
<tr>
<th>Step</th>
<th>Action</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>Open a result file.</td>
</tr>
</tbody>
</table>
| 2    | Choose **Edit:Chromatogram Layout.**  
*Result:* The **Chromatogram Layout** dialog box is displayed. |
| 3    | Click the **Y-Axis** tab. |
| 4    | • Select the appropriate curve from the list.  
• Click the **Fixed** option. |
| 5    | • Type the desired minimum and maximum values.  
• Click the **All with this unit** button if you want other curves with the same Y-axis units as the current scaled curve to be similarly scaled.  
  
*Note:* The values will only be applied to existing curves. They will not be applied to new curves created after this function was last used.  
• Click the appropriate **Pressure unit (MPa, psi, bar)** option to change Y-axis units for pressure curves.  
• Click **OK**. |

The table below describes how to add a second Y-axis to the chromatogram:

<table>
<thead>
<tr>
<th>Step</th>
<th>Action</th>
</tr>
</thead>
</table>
| 1    | Choose **Edit:Chromatogram Layout.**  
*Result:* The **Chromatogram Layout** dialog box is displayed. |
| 2    | Click the **Y-Axis** tab. |
| 3    | • Select the appropriate curve from the **Right Axis** droplist.  
• Click the **OK** button. |
The table below describes how to change and fix the X-axis:

<table>
<thead>
<tr>
<th>Step</th>
<th>Action</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>Open a result file.</td>
</tr>
</tbody>
</table>
| 2    | Choose **Edit:Chromatogram Layout**.  
Result: The **Chromatogram Layout** dialog box is displayed. |
| 3    | Click the **X-Axis** tab. |
| 4    | Select the appropriate option in the **Base** field:  
- **Time** of retention  
- **Volume**  
Note: Some calculated curves, for example baselines, exist in only one base and might seem to disappear when the base is changed. Curves are collected in time and recalculated for display in volume. Thus, switching the base between **Time** and **Volume** can slightly alter the resolution. |
| 5    | • Click the **Fixed** option in the **Axis scale** field to set the axis limits manually.  
• Type the desired minimum and maximum values.  
• Click **OK**. |
6.3.5 How to save and apply a layout

Introduction

All configurations that you make in the Chromatogram Layout dialog box can be saved as a layout. It is possible to apply saved layouts to other chromatograms. All saved layouts are user-specific.

How to save a layout

The table below describes how to save a layout:

<table>
<thead>
<tr>
<th>Step</th>
<th>Action</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>Open a result file.</td>
</tr>
</tbody>
</table>
| 2    | Choose Edit:Chromatogram Layout.  
Result: The Chromatogram Layout dialog box is displayed. |
| 3    | Make the appropriate layout configuration within the various tabs.  
View your changes  
Click OK if you want to return to the chromatogram window to see the applied affects of a given configuration. Return to the Chromatogram Layout dialog box to perform further changes. |
| 4    | • Select the Layout Library tab.  
• Click the Save current layout as button.  
Result: The Save Layout dialog box is displayed. |
| 5    | • Type a name for the layout.  
• If you want the current layout to be the new default layout, select the Save as default option.  
• Click OK.  
Result: The new name is added to the Saved layouts list.  
• Click OK. |

How to apply a layout

The table below describes how to apply a layout:

<table>
<thead>
<tr>
<th>Step</th>
<th>Action</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>Select the Layout Library tab on the Chromatogram Layout dialog box.</td>
</tr>
</tbody>
</table>
### How to save and apply a layout

<table>
<thead>
<tr>
<th>Step</th>
<th>Action</th>
</tr>
</thead>
</table>
| 2    | • Select a layout from the *Saved layouts* list.  
      • Click the *Apply selected layout* button.  
      *Result:* The layout is automatically applied to the active chromatogram window.  
      • If the same layout is to be applied to all chromatograms on the *Evaluation* workspace, select the *Apply to all chromatograms* checkbox.  
      • Click *OK*. |
6.3.6 How to show part of a curve

Introduction

You can select a part of a curve in order to examine details more closely. It is also possible fix the axes, see 6.3.4 How to change and fix the axes on page 61.

How to use the zoom function

In the active chromatogram window, you can zoom in on a designated area of the chromatogram. This is the easiest and quickest way to enlarge different parts of a curve. The table below describes how to do this:

<table>
<thead>
<tr>
<th>Step</th>
<th>Action</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>Open a result file.</td>
</tr>
</tbody>
</table>
| 2    | • Place the mouse pointer in any corner of the area you want to magnify.  
• Press and hold the left mouse button. A magnifying glass icon will be added to the mouse pointer arrow on the screen.  
• Drag a box to cover the area to be magnified, and release the mouse button.  
Result: The selected region is now displayed in the entire chromatogram window, together with appropriate scales for the Y and X axes. |
| 3    | Use the arrow keys on the keyboard to move around in the chromatogram at the current zoom scale. |
| 4    | **Undo zoom**  
Right-click in the window and select **Undo zoom** to undo the last zoom step.  
**Reset zoom**  
Right-click in the window and select **Reset zoom** to reset all zoom steps at once. |
6.4   How to print active chromatograms

Introduction

This section describes how to print the chromatograms that are open in the Evaluation module.

The Print Chromatograms dialog box

This is an illustration of the Print Chromatograms dialog box.

*Note:* The selected print format is outlined in red.

Instruction

The table below describes how to print active chromatograms on the default Windows printer.

<table>
<thead>
<tr>
<th>Step</th>
<th>Action</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>Open all chromatograms that you want to print in the Evaluation module.</td>
</tr>
</tbody>
</table>
| 2    | • Select **File:**Print.  
  
  *or*  
  • Click the **Print** toolbar icon.  
  
  *Result:* The Print Chromatograms dialog box opens.  
| 3    | Select print format and layout options. |
| 4    | • Click **OK** to print.  
  
  *or*  
  • Proceed with step 5 to preview and edit the layout. |
<table>
<thead>
<tr>
<th>Step</th>
<th>Action</th>
</tr>
</thead>
</table>
| 5    | Click the **Preview** button.  
Result: The **Customise Report** window opens. |
| 6    | • Click the **Edit Mode** button to make changes, e.g. change the order of the chromatograms (see 6.5 **How to create and print a customised report** on page 68 for more information about how to edit).  
• Click the **Preview** button to return to preview mode. |
| 7    | • Select **File:Print**.  
*or*  
• Click the **Print** toolbar icon.  
*Result: The **Print** dialog box opens.* |
| 8    | • Select the print range and number of copies.  
• Click **OK**. |
6.5 How to create and print a customized report

You can choose from a variety of objects to include in a report, including chromatograms, methods, documentation, free text and more in the customized report interface. You can also place, align and size the objects as you please. This section describes how to create a customized report format.

Should you need to store your reports in an electronic format you can save them as PDF files. Select an Adobe™ Acrobat™ printer as default Windows printer and print the reports.

The table below describes how to open the Report Editor in Edit mode to create a customized report format.

<table>
<thead>
<tr>
<th>Step</th>
<th>Action</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>Open a result file in the Evaluation module.</td>
</tr>
</tbody>
</table>
| 2    | • Select **File:Report**.  
or  
• Click the **Report** icon.  
**Result**: The Generate Report dialog box opens. |
| 3    | • Click the **New** button.  
**Result**: The Report Editor opens in Edit mode. |

The illustration below shows the Report Editor window in Edit mode with a blank report open:

The table below describes the different functions of the Edit mode toolbar buttons in the Report Editor:

<table>
<thead>
<tr>
<th>Toolbar button</th>
<th>Function</th>
</tr>
</thead>
<tbody>
<tr>
<td>Preview/Edit</td>
<td>This button toggles between a print preview of the report and the Edit mode.</td>
</tr>
<tr>
<td>Next Page</td>
<td>This button displays the next page or pair of pages (where there are more than one page).</td>
</tr>
<tr>
<td>Toolbar button</td>
<td>Function</td>
</tr>
<tr>
<td>--------------------</td>
<td>--------------------------------------------------------------------------</td>
</tr>
<tr>
<td>Prev Page</td>
<td>This button displays the previous page or pair of pages (where there are more than one page).</td>
</tr>
<tr>
<td>One Page/Two Pages</td>
<td>This button toggles between single page view and pairs of pages view, when there is more than one page.</td>
</tr>
<tr>
<td>Zoom In</td>
<td>This button increases the magnification of the view.</td>
</tr>
<tr>
<td>Zoom Out</td>
<td>This button decreases the magnification of the view.</td>
</tr>
<tr>
<td>Add Page</td>
<td>This button adds a blank page to the report.</td>
</tr>
<tr>
<td>Delete Page</td>
<td>This button deletes the current page from the report.</td>
</tr>
<tr>
<td>Exit</td>
<td>This button closes the Customize Report window.</td>
</tr>
</tbody>
</table>

**How to add and delete report pages**

The table below describes how to add or delete report pages in the Report Editor:

<table>
<thead>
<tr>
<th>If you want...</th>
<th>then...</th>
</tr>
</thead>
<tbody>
<tr>
<td>to add new pages,</td>
<td>• click the Add Page toolbar button.</td>
</tr>
<tr>
<td></td>
<td>Result: A new page is added after the last page.</td>
</tr>
<tr>
<td>to delete a page while in One Page mode,</td>
<td>• select the page with Next Page or Prev Page,</td>
</tr>
<tr>
<td></td>
<td>• click the Delete Page toolbar button and confirm the deletion.</td>
</tr>
<tr>
<td>to delete a page in Two Page mode,</td>
<td>• select the page with Next Page or Prev Page,</td>
</tr>
<tr>
<td></td>
<td>• click an object on the page,</td>
</tr>
<tr>
<td></td>
<td>• click the Delete Page toolbar button and confirm the deletion.</td>
</tr>
</tbody>
</table>

**How to change the page layout**

The page layout is changed in the Page Setup dialog box. The table below describes how to set up the page layout:

<table>
<thead>
<tr>
<th>Step</th>
<th>Action</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>Double-click anywhere on the report page in the Report Editor (not on an object).</td>
</tr>
<tr>
<td></td>
<td>Result: The Page Setup dialog box opens.</td>
</tr>
<tr>
<td>Step</td>
<td>Action</td>
</tr>
<tr>
<td>------</td>
<td>--------</td>
</tr>
</tbody>
</table>
| 2    | • Type new values for the **Margins** if necessary.  
       • Select the appropriate **Settings** and **Unit**.  
*Note:* An extra **Header** tab will appear if you de-select the option to have the same header on all pages. The **First Header** tab is used for the first page header only, and the **Header** tab is used for all subsequent pages.  
       • Click the **First Header** tab. |
| 3    | • Select all the items you want to include in the header from the **Select Items** list.  
       • Click the **Font** button to change the font for all items if necessary. |
| 4    | • Type header text in the **Free text** box and click the **Font** button to alter the default font if necessary.  
       • Type the report title in the **Report title** box and click the **Font** button to alter the default font if necessary. |
| 5    | • Select the **Logo** check box and click the **Browse** button if you want to locate and select a logo image file.  
       • Select the **Alignment** for the logo, if necessary.  
*Note:* The logo file must be in bitmap format (.bmp) and smaller than 64 kB. Larger logo files or files in other formats must be inserted as **Picture** objects. |
| 6    | If you want to have a line under or over the header, select the appropriate option in the **Layout** field. |
| 7    | • Repeat steps 3 to 6 on the **Footer** tab and the subsequent pages **Header** tab.  
*Note:* All **Header** and **Footer** tabs contain the same options. You can have all information in either the header or footer or split information between the header and footer as required.  
       • Click **OK**. |
The table below describes how to add objects to the report. The various objects are described below this table.

<table>
<thead>
<tr>
<th>Step</th>
<th>Action</th>
</tr>
</thead>
</table>
| 1    | • Click the appropriate icon in the **Report items** toolbar.  
      | or     
      | • Choose an object from the **Insert** menu. |
| 2    | • Press and hold the left mouse button on the report page, and drag out a box to the size of the item you want to insert.  
      | **Note:** The mouse pointer shows a symbol for the type of item you have selected.  
      | • Release the mouse button.  
      | **Result:** A **Setup** dialog box opens. The dialog is specific to the type of item that you want to insert. |
| 3    | • Select the desired options and click **OK**.  
      | **Result:** The object is inserted onto the page. |

**Note:** If you want to edit an object later, double-click the object box.

The table below describes how to add free text to the report:

<table>
<thead>
<tr>
<th>Step</th>
<th>Action</th>
</tr>
</thead>
</table>
| 1    | • Click the **Free Text** icon.  
      | • Press and hold the left mouse button on the report page and drag out a box to the size of the text. Release the button.  
      | **Result:** The **Setup Free Text** dialog box opens. |
| 2    | • Type text in the edit field.  
      | • Select if the text is to start on a new page.  
      | • Select if the text box should be automatically sized.  
      | • Select if the text should appear in the same position on all pages, for example as header and footer text. |
Click the **Font** button to change the default font.

*Result*: The *Font* dialog box opens.

- Make the necessary changes and click **OK** to return.
- Click **OK**.

*Result*: The text object is inserted onto the page.

---

**How to add a picture**

The *Picture* dialog box is useful to insert logos, pictures or other figures in the report. The table below describes how to add a picture object to the report:

<table>
<thead>
<tr>
<th>Step</th>
<th>Action</th>
</tr>
</thead>
</table>
| 1    | • Press and hold the left mouse button on the report page and drag out a box to the size of the picture item. Release the mouse button.  
• Click the **Picture** icon.  

*Result*: The *Picture* dialog box opens. |
| 2    | • Click the **Browse** button to locate the desired picture file.  
• Select the picture file and click the **Open** button.  

*Note*: The file formats .bmp, .emf, .jpg and .tif can be used.  

*Result*: A preview of the selected picture is displayed. |
| 3    | • Select the desired **Settings** and click **OK**.  

*Result*: The picture is inserted onto the page. |
The table below describes how to add a chromatogram to the report. The layout can also be defined to include a peak table if desired.

<table>
<thead>
<tr>
<th>Step</th>
<th>Action</th>
</tr>
</thead>
</table>
| 1    | • Click the **Chromatogram** icon.  
  • Press and hold the left mouse button on the report page and drag out a box to the size of the chromatogram. Release the mouse button.  
  
  **Result:** The **Setup Chromatogram** dialog box opens. |
| 2    | Select which chromatogram(s) to insert from the **Selected chromatogram(s)** drop list.  
  • **Active chromatogram** inserts the chromatogram that currently is active in the **Evaluation** module.  
  • **All chromatograms** inserts all chromatograms that are open in the **Evaluation** module.  
  • **1, 2...etc.** inserts the corresponding chromatogram. |
| 3    | • Select the desired **Settings**.  
  • If desired, change the **Fonts**.  
  
  **Note:** Separate fonts can be selected for the **Chromatogram**, the **Peak table** and the **Header text**. |
Action
Step 4  
- Click the Define button in the Layout field if you want to re-define the layout of the chromatogram.

- Make the appropriate changes and click OK to return to the Setup Chromatogram dialog box.

Note: The changes that you make will only affect the report and not the view of the chromatograms in the Evaluation module.

Step 5
- Click OK.

Result: The chromatogram is inserted onto the page.

Note: All curves can be de-selected in the Report Chromatogram Layout dialog box leaving only the selected peak table(s) in the report.

<table>
<thead>
<tr>
<th>Step</th>
<th>Action</th>
</tr>
</thead>
</table>
| 4    | - Click the **Define** button in the **Layout** field if you want to re-define the layout of the chromatogram.  
  **Result:** The **Report Chromatogram Layout** dialog box opens.  
  - Make the appropriate changes and click **OK** to return to the **Setup Chromatogram** dialog box.  
  **Note:** The changes that you make will only affect the report and not the view of the chromatograms in the **Evaluation** module. |
| 5    | - Click **OK**.  
  **Result:** The chromatogram is inserted onto the page. |

How to add documentation

The table below describes how to add documentation to the report:

<table>
<thead>
<tr>
<th>Step</th>
<th>Action</th>
</tr>
</thead>
</table>
| 1    | - Click the **Documentation** icon.  
  - Press and hold the left mouse button on the report page and drag out a box to the size of the item. Release the button.  
  **Result:** The **Setup Documentation** dialog box opens. |
| 2    | - Select the items to be included in the report:  
  - **Select All** includes all items in the report.  
  - **Clear All** removes all selections. |
| 3    | - If desired, change the **Fonts**.  
  - Select if the documentation should start on a new page.  
  - If was selected, make the necessary changes to the **Base** and **Logbook filter** settings.  
  - Click **OK**.  
  **Result:** The selected documentation items are inserted into the report. |
The table below describes how to add the Evaluation Log to the report:

<table>
<thead>
<tr>
<th>Step</th>
<th>Action</th>
</tr>
</thead>
</table>
| 1    | • Click the Evaluation Log icon.  
      • Press and hold the left mouse button on the report page and drag out a box to the size of the item. Release the mouse button.  
      *Result*: The Setup Evaluation Log dialog box opens. |
| 2    | • If desired, change the Fonts.  
      • Select if the Evaluation Log should start on a new page.  
      • Click OK.  
      *Result*: The Evaluation Log is inserted into the report. |

The table below describes how to select, move and resize objects freely:

<table>
<thead>
<tr>
<th>If you want...</th>
<th>then...</th>
</tr>
</thead>
</table>
| to select a single object, | • click the Select icon,  
      • click the object of interest. |
| to select several objects, | • click the Select icon,  
      • press and hold the <Ctrl> key while you click the objects. |
| to move the selected object(s), | click on the objects, hold down the left mouse button and drag the object(s) to the new position. |
| to resize the selected object(s), | click one of the object border anchors, either in the corners or in the middle of a border, and drag the box to the new size.  
  *Note*: Some Text objects cannot be resized. |
Objects can be placed in exact positions and sized in relation to other objects. The table below describes the function of the **Alignment** toolbar icons in the **Report Editor**:

<table>
<thead>
<tr>
<th>Tool-bar icon</th>
<th>Function</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Align left</strong></td>
<td>Matches the left alignment of all selected objects to that of the highlighted object.</td>
</tr>
<tr>
<td><strong>Align right</strong></td>
<td>Matches the right alignment of all selected objects to that of the highlighted object.</td>
</tr>
<tr>
<td><strong>Align top</strong></td>
<td>Matches the top alignment of all selected objects to that of the highlighted object.</td>
</tr>
<tr>
<td><strong>Align bottom</strong></td>
<td>Matches the bottom alignment of all selected objects to that of the highlighted object.</td>
</tr>
<tr>
<td><strong>Adjust to margins</strong></td>
<td>Stretches the selected object(s) to the left and right margins.</td>
</tr>
<tr>
<td><strong>Adjust to left margin</strong></td>
<td>Adjusts the selected object(s) to the left margin.</td>
</tr>
<tr>
<td><strong>Adjust to right margin</strong></td>
<td>Adjusts the selected object(s) to the right margin.</td>
</tr>
<tr>
<td><strong>Adjust to centre</strong></td>
<td>Adjusts the selected object(s) to the center of the page.</td>
</tr>
<tr>
<td><strong>Make same size</strong></td>
<td>Adjusts the selected objects to the same size as the highlighted reference object.</td>
</tr>
<tr>
<td><strong>Make same width</strong></td>
<td>Adjusts the selected objects to the same width as the highlighted reference object.</td>
</tr>
<tr>
<td><strong>Make same height</strong></td>
<td>Adjusts the selected objects to the same height as the highlighted reference object.</td>
</tr>
</tbody>
</table>
**Note:** The **Make same size** and **Make same width** functions can only be used to resize the width of chromatograms, free text and picture objects.

The table below describes how to print the report:

<table>
<thead>
<tr>
<th>Step</th>
<th>Action</th>
</tr>
</thead>
</table>
| 1    | • Choose **File:Print**.  
       | *or*  
       | • Click the **Print** icon. |

**Result:** The **Print** dialog box opens.  
**Note:** The report will be printed on the default Windows printer.

<table>
<thead>
<tr>
<th>Step</th>
<th>Action</th>
</tr>
</thead>
</table>
| 2    | • Select the printing range.  
       | • Select the number of copies.  
       | • Click **OK**. |

**Note:** You can also print the report from the **Generate Report** dialog box.

The table below describes how to save the finished report format:

<table>
<thead>
<tr>
<th>Step</th>
<th>Action</th>
</tr>
</thead>
</table>
| 1    | • Choose **File:Save**.  
       | *or*  
       | • Click the **Save** icon. |

**Result:** The **Save Report Format** dialog box opens.

<table>
<thead>
<tr>
<th>Step</th>
<th>Action</th>
</tr>
</thead>
</table>
| 2    | • Type a name for the format.  
       | **Note:** The name for the default format will automatically be changed to **DEFAULT**.  
       | • Click **OK**. |
6.6 Run documentation

The full documentation for a method run is stored in the result file. This section describes:

- how to view and print the run documentation,

The table below describes how to view and print the run documentation.

<table>
<thead>
<tr>
<th>Step</th>
<th>Action</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>Open a result file.</td>
</tr>
</tbody>
</table>
| 2    | Choose **View: Documentation** in the **Evaluation** module.  
     | *or*  
     | • Click the view **Documentation** icon. |
|      | **Result:** The **Documentation** dialog box opens. |
| 3    | • Click the **Print** button.  
     | **Result:** The **Print** dialog box opens.  
     | • Select the documentation items you want to print and click **OK**.  
     | **Result:** The documentation is printed on the default Windows printer. |
How to edit results

Introduction

This chapter describes

- how to edit the results that are presented in the Evaluation module
- how to export results.

For more information about how to view results, see chapter 6 How to view results on page 47.

In this chapter

This chapter contains the following sections

<table>
<thead>
<tr>
<th>Topic</th>
<th>See</th>
</tr>
</thead>
<tbody>
<tr>
<td>How to enter and edit text in the chromatogram</td>
<td>7.1</td>
</tr>
<tr>
<td>How to rename chromatograms, curves and peak tables</td>
<td>7.2</td>
</tr>
<tr>
<td>How to export results</td>
<td>7.3</td>
</tr>
<tr>
<td>How to save results and exit the Evaluation module</td>
<td>7.4</td>
</tr>
</tbody>
</table>
7.1 How to enter and edit text in the chromatogram

How to enter text

Text can be added to the chromatogram. The table below describes how to do this:

<table>
<thead>
<tr>
<th>Step</th>
<th>Action</th>
</tr>
</thead>
</table>
| 1    | • Right-click the curves view of the chromatogram window and select Add text from the menu.  
      or  
      • Choose Edit:Text:Add. |
| 2    | • Click where you want to insert text in the chromatogram.  
      Result: A text box opens.  
      • Type the text.  
      • Click outside the text box to set the text. |

How to edit the text

The table below describes how to edit inserted text:

<table>
<thead>
<tr>
<th>Step</th>
<th>Action</th>
</tr>
</thead>
</table>
| 1    | Choose Edit:Text:Edit.  
      Result: The Edit Texts tab of the Chromatogram Layout dialog box is displayed. |
| 2    | • Select the text that you want to edit and make the appropriate changes in the Selected text field.  
      • Click the Change text button or the Delete text button.  
      • Use the Font and Set Orientation buttons if needed, and make the desired changes in the resulting dialog boxes.  
      • Click OK to apply the changes. |

Shortcut option

You can also right-click outside the text box and select Edit Text Mode from the shortcut menu. This activates all the text boxes in the chromatogram. The list below describes how to edit the text:

• Click the text and type the new text.
• Click outside the text box to set the text.
### 7.2 How to rename chromatograms, curves and peak tables

The table below describes how to rename chromatograms, curves or peak tables in the *Evaluation* module:

<table>
<thead>
<tr>
<th>Step</th>
<th>Action</th>
</tr>
</thead>
</table>
| 1    | Choose *Edit:Rename* and the relevant option *Chromatogram, Curve* or *Peak Table*.  
*Result:* The *Rename* dialog box opens. |
| 2    | • Select the appropriate object.  
• Type a new name in the *Name* field.  
• Click *OK*. |

*Note:* The original raw data curves cannot be renamed. They will not be listed as options in the dialog box.
7.3 How to export results

Introduction
This section describes how to export curves in different formats and how to copy data and curves to the clipboard.

Data formats
You can export data in the following formats:
- AIA (.cdf)
- ASCII (.asc)
- Lotus 1-2-3 (.wks)
- Excel (.xls)
- XML (.xml)

Export options
Select File:Export in the Evaluation module to export data from an open result file. The following export options are available:
- Curves
- Export curve to AIA
- Peak table
- Documentation
- Evaluation log

How to export curves
The table below describes how to export curves in the Evaluation module.

<table>
<thead>
<tr>
<th>Step</th>
<th>Action</th>
</tr>
</thead>
</table>
Action

Step 2
- Select the curve(s) you want to export.
- Enter parameters to limit the curve(s) if necessary.
- Click the Select button.
- Repeat Step 2 to select more curves.

Step 3
- Click the Export button.
  
  Result: The Export Curves to File dialog box opens.

Step 4
- Select the export file format from the Save as type drop list.
  - ASCII files (*.asc)
  - Lotus 1-2-3 files (*.wks)
  - Excel files (*.xls)
  - AIA files (*.cdf)

Step 5
- Select a destination folder.
- Type a file name and click OK.

Note: Curves are exported as series of numerical coordinates that refers to the time/volume and signal respectively.

---

How to edit results

You can optimize the exported curves to only the parts that you want to focus on, in the Export Curves dialog box. The table below describes how to use these editing options.

<table>
<thead>
<tr>
<th>Dialog box option</th>
<th>Instruction</th>
</tr>
</thead>
<tbody>
<tr>
<td>Cut curves</td>
<td>Enter retention values in the text boxes to limit the curve to only a portion of the original curve.</td>
</tr>
<tr>
<td>Cut graphically</td>
<td>This button opens the Export Cut dialog box. Move the vertical markers to the correct cutoff points.</td>
</tr>
<tr>
<td>Reduce number of samples</td>
<td>Adjust the factor value or the maximum number of samples. To reduce the number of samples by a factor of five means that only every fifth point will be sampled for export.</td>
</tr>
<tr>
<td>Normalise retention</td>
<td>Select the Normalise retention checkbox to have all exported curves normalized to a common X-axis.</td>
</tr>
</tbody>
</table>
### How to export curves in AIA format

The table below describes how to export curves in AIA format.

<table>
<thead>
<tr>
<th>Step</th>
<th>Action</th>
</tr>
</thead>
</table>
| 1    | Select **File:Export:Export curve to AIA**.  
*Result:* The **Export curve in AIA format** dialog box opens. |
| 2    | • Select the source chromatogram and the curve you want to export.  
• Click the **Export** button.  
*Result:* The **Export Curves to File** dialog box opens. |
| 3    | • Select a destination folder.  
• Type a file name.  
• Click **OK**. |

### How to export peak tables

The table below describes how to export peak tables.

<table>
<thead>
<tr>
<th>Step</th>
<th>Action</th>
</tr>
</thead>
</table>
| 1    | Choose **File:Export:Peak Table**.  
*Result:* The **Export Peak Table** dialog box opens. |
| 2    | • Select the source chromatogram and the peak table you want to export.  
• Click the **Export** button.  
*Result:* The **Export Peak Table to File** dialog box opens. |
| 3    | Select the export file format from the **Save as type** drop-list.  
• **ASCII files** (*.asc)  
• **Lotus 1-2-3 files** (*.wks)  
• **Excel files** (*.xls)  
• **XML files** (*.xml) |
| 4    | • Select a destination folder.  
• Type a file name.  
• Click **OK**. |

*Note:* Peak tables are exported as text strings in ASCII format and numerical values in the Lotus 1-2-3 formats. All possible columns in the peak table are exported.
The table below shows how to export documentation and evaluation logs:

<table>
<thead>
<tr>
<th>Step</th>
<th>Action</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>Select the data you want to export.</td>
</tr>
</tbody>
</table>
| 2    | • Select options in the dialog box.  
      | • Click the **Export** button. |
| 3    | • Select a destination folder and type a file name.  
      | • Click **OK**. |

You can also use the **Windows** clipboard to copy the contents of the active window and paste it into other programs, e.g. **Microsoft Word**. Curves and documentation are copied as Windows enhanced metafiles (.emf) and peak tables are copied as text. Only the peak table columns that are selected in the spreadsheet will be copied.
7.4 How to save results and exit the Evaluation module

Introduction

After you have finished the evaluation process, you can save all the changes you have made to the chromatograms, including newly created curves and chromatograms that you have imported and created.

How to delete unwanted curves

All the curves that you created during your manipulations will be saved in the chromatogram. If some of these curves are not be needed anymore, select Edit:Delete:Curves in the Evaluation module to remove the curves.

Note: The original curves that were created during the run can never be deleted.

How to save the results

You can either save your edited results in the original file or in a new result file. The table below describes how to save the results in the Evaluation module.

<table>
<thead>
<tr>
<th>If you want to save the edited results...</th>
<th>then...</th>
</tr>
</thead>
<tbody>
<tr>
<td>in the original result file</td>
<td>• select File:Save.</td>
</tr>
<tr>
<td></td>
<td>or</td>
</tr>
<tr>
<td></td>
<td>• click the Save toolbar icon.</td>
</tr>
<tr>
<td>in a new result file</td>
<td>• select File:Save as.</td>
</tr>
</tbody>
</table>

Note: The previous version of the result file will be overwritten if you save the changes. This cannot be reversed. However, the raw data curves remain unchanged.

How to exit the Evaluation module

The table below describes how to exit the Evaluation module:

<table>
<thead>
<tr>
<th>Step</th>
<th>Action</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>Choose File:Exit.</td>
</tr>
<tr>
<td></td>
<td><em>Result:</em> If there are unsaved changes, a dialog box opens with an option to save the changes before exit.</td>
</tr>
<tr>
<td>2</td>
<td>Select Yes if you want to save the changes.</td>
</tr>
<tr>
<td></td>
<td><em>Result:</em> The result file is closed.</td>
</tr>
</tbody>
</table>
Peak integration is used to identify and measure a number of curve characteristics including peak areas, retention time and peak widths. This chapter describes:

- How to perform peak integrations.
- How to optimize peak integrations.

This chapter contains the following sections:

<table>
<thead>
<tr>
<th>Topic</th>
<th>See</th>
</tr>
</thead>
<tbody>
<tr>
<td>Baseline calculation</td>
<td>8.1</td>
</tr>
<tr>
<td>How to perform a peak integration</td>
<td>8.2</td>
</tr>
<tr>
<td>How to optimize the baseline with a morphological algorithm</td>
<td>8.3</td>
</tr>
<tr>
<td>How to optimize the baseline with a classic algorithm</td>
<td>8.4</td>
</tr>
<tr>
<td>How to edit the baseline manually</td>
<td>8.5</td>
</tr>
<tr>
<td>How to edit the peaks</td>
<td>8.6</td>
</tr>
<tr>
<td>How to integrate part of a curve and how to exclude or skim peaks</td>
<td>8.7</td>
</tr>
<tr>
<td>Measurements</td>
<td>8.8</td>
</tr>
</tbody>
</table>
8.1 Baseline calculation

Introduction
The first step when you integrate peaks is to calculate a baseline. A correct baseline is crucial for accurate calculation of the peak areas. This section describes the options for how to calculate baselines in the Integrate dialog box.

Baseline options
The Evaluation module offers several options for how to create an accurate baseline:
- To use the automatic Calculate baseline function.
- To create a baseline based on a blank curve.
- To use a Zero baseline.
- To reuse an existing baseline.

The Calculate baseline function
The Calculate baseline instruction provides automatic calculation of the baseline. In most cases the measurement is very accurate. The calculation can be performed using the Morphological algorithm or the Classical algorithm.

Baselines based on a blank curve
A blank curve can be used as the baseline for peak integration.
- You can use a blank curve with the same chromatographic conditions as the corresponding sample.

or
- You can subtract the blank run from the source curve and then perform peak integration on the resulting curve with the Calculate baseline instruction.

Note: In addition to blank run curves, it is also possible to select any curve from the current chromatogram as the baseline, e.g. an edited baseline.

Zero baseline
To use a Zero baseline means that there is no baseline subtraction at all.

Reuse an existing baseline
To reuse an existing baseline for the selected curve is the default alternative whenever there is an existing baseline available. The option Correlated baseline is selected if this is the case.
## 8.2 How to perform a peak integration

The table below describes how to perform a basic peak integration.

<table>
<thead>
<tr>
<th>Step</th>
<th>Action</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>Open a result file in the <strong>Evaluation</strong> module.</td>
</tr>
</tbody>
</table>
| 2    | • Choose **Integrate:Peak Integrate**.  
      or  
      • Click the **Peak Integrate** toolbar icon.  
      
      **Result:** The **Integrate** dialog box opens.  
| 3    | • Select a source curve.  
      • Select a baseline or a calculation method from the **Baseline** list.  
      • Click **OK** to integrate with the default selections.  
      or  
      • Proceed with steps 4 to 6 to change the default selections.  
      **Note:** See also 8.3 How to optimize the baseline with a morphological algorithm on page 94 and 8.4 How to optimize the baseline with a classic algorithm on page 98. |
| 4    | • Click the **Baseline settings** button to change the calculation algorithm in the **Settings** dialog box. The default algorithm is **Morphological**.  
      • Change the selections or values.  
      • Click **OK** |
| 5    | • Click the **Peak window** button to edit the peak window limits if necessary.  
      • Click the **Reject peaks** button to set the parameters for peak rejection if necessary.  
      • Edit the **Column height** or **Column V** values if necessary. |
<table>
<thead>
<tr>
<th>Step</th>
<th>Action</th>
</tr>
</thead>
</table>
| 6    | • Click **OK** to integrate and close the dialog box.  

*or*

• Click **Save and Edit Peak Table** to save the integration and open the integrated curve for editing.  
  - See **8.5 How to edit the baseline manually** on page 106  
  - See **8.6 How to edit the peaks** on page 109  
  - See **8.7 How to integrate part of a curve and how to exclude or skim peaks** on page 116 |

---

**Peak integration results**

The peak table is displayed underneath the active chromatogram. The start point and end point of each peak are marked by vertical marks, **drop-lines**, in the chromatogram. The peaks are automatically labelled according to what is selected in the **Curve Style and Color** tab of the **Chromatogram Layout** dialog box.

This is an illustration of the results after a peak integration:

![Peak integration results](image)

*Note:* Peak tables can be copied from one chromatogram to another with the **Edit:Copy** command. However, to display the table you must right-click in the chromatogram, choose **Properties** and then select the new peak table on the **Peak Table** tab of the **Chromatogram Layout** dialog box.
The peak retention times and several other peak characteristics are calculated automatically. The table below describes how to display other peak characteristics.

<table>
<thead>
<tr>
<th>Step</th>
<th>Action</th>
</tr>
</thead>
</table>
| 1    | • Right-click in the active chromatogram.  
      | • Select Properties from the shortcut menu.  
      | *Result:* The **Chromatogram Layout** dialog box opens. |
| 2    | Click the **Peak Table** tab. |
| 3    | • Select options from the **Select peak table columns** list.  
      | • Click **OK**.  
      | *Result:* The selected items will be displayed in the peak table. |

Peaks can be removed from display in a peak table. The table below describes how to filter the peaks:

<table>
<thead>
<tr>
<th>Step</th>
<th>Action</th>
</tr>
</thead>
</table>
| 1    | • Right-click in the active chromatogram or peak table.  
      | • Select Properties from the shortcut menu.  
      | *Result:* The **Chromatogram Layout** dialog box opens. |
| 2    | Click the **Peak Table** tab. |
| 3    | • Click the check boxes in the **Filter Peaks** field to select the filter criteria.  
      | • Specify filter values.  
      | • Click **OK**. |

The table below describes the major differences in the effect of filtering peaks compared to excluding the peaks by rejection:

<table>
<thead>
<tr>
<th>Filter peaks...</th>
<th>Reject peaks...</th>
</tr>
</thead>
<tbody>
<tr>
<td>excludes the peaks from display,</td>
<td>permanently excludes peaks from the integration,</td>
</tr>
<tr>
<td>does not exclude the peaks from the calculation of the total peak area,</td>
<td>excludes the peaks from the calculation of the total peak area,</td>
</tr>
<tr>
<td>can be reversed.</td>
<td>cannot be reversed.</td>
</tr>
</tbody>
</table>
Peaks can be labelled with their retention, sequentially numbered, or be marked with specific identification names. See table below for an instruction on how to display peak labels.

The label type can be selected on the **Curve Style and Colour** tab in the **Chromatogram Layout** dialog box. De-select all label options to hide the labels, e.g. for presentations.

The illustration below shows the **Chromatogram Layout** dialog box with the **Curve Style and Colour** tab opened:

<table>
<thead>
<tr>
<th>Step</th>
<th>Action</th>
</tr>
</thead>
</table>
| 1    | • Choose **Edit: Chromatogram Layout**.  
  **or**  
  • Click the **Chromatogram Layout** icon.  
  **Result:** The **Chromatogram Layout** dialog box opens. |
<p>| 2    | Click the <strong>Curve Style and Colour</strong> tab. |</p>
<table>
<thead>
<tr>
<th>Step</th>
<th>Action</th>
</tr>
</thead>
</table>
| 3    | Select one or more of the following labelling options in the Peak label field:  
  - **Number**  
  *Result:* The peaks will be numbered sequentially.  
  - **Peak Name**  
  *Result:* Peak names will be displayed. See 8.6 How to edit the peaks on page 109 for information about how to name the peaks.  
  - **Retention**  
  *Result:* The retention volume or time will be displayed.  
  - Click **OK**.  

---

* p 93
8.3 How to optimize the baseline with a morphological algorithm

Introduction

The first choice when you want to optimize the peak integration is to change the baseline parameters. This section describes how to optimize the baseline with a morphological algorithm.

The Morphological algorithm

The Morphological algorithm can be described as a line that follows the chromatogram parallel to the X-axis. Data points for the baseline are created whenever the line touches the curve, and the points are joined at the end to create a baseline.

The Morphological algorithm gives the best result in curves with drifting baseline and peak clusters. The morphological baseline follows the curve faithfully, and a curve with a baseline at a more even level can be created by subtracting the morphological baseline.

The Morphological algorithm does not work well if there are negative peaks or if quantitative data from negative peaks are important in the run.

Note: The Morphological algorithm is the default baseline setting.

How to set a Morphological baseline

The table below describes how to choose a Morphological algorithm and define baseline settings.

<table>
<thead>
<tr>
<th>Step</th>
<th>Action</th>
</tr>
</thead>
</table>
| 1    | Select Integrate:Peak Integrate.  
Result: The Integrate dialog box opens. |
| 2    | Click the Baseline settings button in the Integrate dialog box.  
Result: The Settings dialog box opens. |
| 3    | • Select the Morphological algorithm.  
• Change the Baseline parameters if necessary.  
See more information about the parameters below this table.  
• Click OK. |

Note: The same settings can be edited in the Calculate Baseline dialog box when a new baseline is created. Choose Integrate:Calculate Baseline to open the dialog box.
The parameters for the Morphological algorithm are:
- **Structure width**
- **Noise window**
- **Minimum distance between points**

**Structure width** determines the length of the straight line that follows the chromatogram. The default value is set at the widest peak in the chromatogram multiplied by 1.5.

The illustration below is an example of how a morphological baseline follows the peaks at the different levels in the curve:
Too low settings
Too low Structure width settings can result in a baseline that reaches too high up in the peaks of the curve. Sometime a wider peak is not recognized because it contains a cluster of smaller peaks. The Structure width is then set to a value according to the largest width of the identified narrower peaks, and must be increased.

Too high settings
Too high Structure width settings mean that narrower peaks, especially in fluctuating curves, are not properly followed. This happens when an artifact in a curve is identified as the widest peak by the morphological algorithm, and then is used to set the default Structure width value.

The illustration below is an example of baselines using the default morphological algorithm settings (A) and a morphological algorithm with an increased Structure width value (B).

Noise window
Sometimes you get too many peaks after the peak integration, usually because noise on the baseline is erroneously detected as peaks.

The solution to this is to increase the Noise window parameter. However, this can result in peak limits too high up on the peak slopes.

Note: You can also use the Reject peaks function in the Integrate dialog box to reduce the number of peaks based on the total number of accepted peaks or the minimum peak height.
The **Minimum distance between points** is a measure of the distance between the data points used to generate a baseline. The largest number of data points is produced at the slopes of the curves. If you increase the **Minimum distance between points** value, fewer points will be collected on the slopes.

The illustration below is an example of a baseline (A) that is created with the **Minimum distance between points** parameter set at a low value. The number of data points is reduced when the **Minimum distance between points** parameter is set to a higher value (B).
8.4 How to optimize the baseline with a classic algorithm

Introduction

The first choice when you want to optimize the peak integration is to change the baseline parameters. This section describes how to optimize the baseline with a classical algorithm.

What is the Classic algorithm?

The **Classic algorithm** searches for all parts of the source curve that are longer than a defined minimum baseline segment and fall within limiting parameters. Together, the parameter values define the limits for a rectangular box. A part of the source curve must fit entirely inside this rectangular box to be identified as a baseline segment.

The **Classic algorithm** is particularly useful when you need to integrate curves with negative peaks and when quantitative data from negative peaks are important.

Classic algorithm parameters

The parameters for the **Classic algorithm** are:

- **Shortest baseline segment**
- **Noise window**
- **Max baseline level**
- **Slope limit**

See more information about the parameters below this table.

How to set a Classic baseline

The table below describes how to set a **Classic algorithm** and define a baseline.

<table>
<thead>
<tr>
<th>Step</th>
<th>Action</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>Click the <strong>Baseline settings</strong> button in the <strong>Integrate</strong> dialog box. <em>Result:</em> The <strong>Settings</strong> dialog box opens.</td>
</tr>
</tbody>
</table>
| 2    | • Select the **Classic** algorithm.  
      • Change the **Baseline** parameters.  
      See more information about the parameters below this table.  
      • Click **OK**. |

**Note:** The same settings can be edited in the **Calculate Baseline** dialog box when a new baseline is created. Choose **Integrate:** **Calculate Baseline** to open the dialog box.
The best way to optimize the baseline is to change the baseline parameters step by step and then check the resulting baseline after each change. When the desired effect is accomplished it is best to go back and try a parameter value in between the two last settings to avoid an unnecessarily low or high value.

How much the values should be changed depends on the cause of the peak integration problem. The table below is a general guideline.

<table>
<thead>
<tr>
<th>Baseline parameter</th>
<th>Recommended initial change</th>
</tr>
</thead>
<tbody>
<tr>
<td>Shortest baseline segment</td>
<td>20-50%</td>
</tr>
<tr>
<td>Noise window</td>
<td>10-30%</td>
</tr>
<tr>
<td>Max baseline level</td>
<td>Usually not necessary to adjust</td>
</tr>
<tr>
<td>Slope limit</td>
<td>25-50%</td>
</tr>
</tbody>
</table>

**Note:** If necessary, click the Default button to restore the default values.

If a too high Shortest baseline segment value is set, short curve segments between peaks in the middle of the chromatogram are not identified as baseline segments. The calculated baseline does not follow the source curve, see below:
The **Shortest baseline segment** value is decreased by 50% in this example:

---

**Slope limit**

A changed **Slope limit** will often improve the baseline calculation. The **Slope limit** sets the maximum slope of the curve to define when a peak is recognized. A too high **Slope limit** will cause the up-slopes of the peaks to be recognized as baseline segments.

The example above was improved by the shorter baseline segments but the high slope of the short segments in the region between the second and the fourth peak still makes the baseline unacceptable. In the example below the **Slope limit** is increased by a factor of 2.5, which produces a correct baseline:
A too high **Slope limit** value can cause peak limits too high up on the peaks. This can be the case when the chromatogram includes a very large flow-through or solvent peak. The large peak affects the calculation of the default parameters and leads to too high values for the **Slope limit**.

*Note:* A too high value for the **Noise window** can have the same effect and be caused by the same situation, often also in combination with a high **Slope limit**.

Peak limits are defined on peaks in the example below due to the high **Slope limit**:

The example below has a much lower **Slope limit**, and a lower **Noise window**:
Sometimes you get too many peaks after the peak integration, usually because noise on the baseline is erroneously detected as peaks.

The solution to this is to increase the **Noise window** parameter. However, this can result in peak limits too high up on the peak slopes.

The illustration below is an example of noise detected as peaks (A) and the result of a second peak integration with an increased **Noise window** (B).

---

**Note:** You can also use the **Reject peaks** function in the **Integrate** dialog box to reduce the number of peaks based on the total number of accepted peaks or the minimum peak height.
Sometimes obvious peaks are not detected in the peak integration. The probable cause is that the **Noise window** is set too high. See the illustration below:

All peaks are detected if the **Noise window** is decreased, see example below:

*Note*: Missing peaks can also be caused by improper settings for **Reject peaks** in the **Integrate** dialog box, or **Filter peaks** in the **Chromatogram layout** dialog box.
In rare cases the top of a broad, flat peak can be incorporated as a baseline segment. This is one of the very few situations where it is useful to change the Max baseline level. The illustration below is an example:

---

### How to set the Max baseline level

The table below describes how to set the Max baseline level.

<table>
<thead>
<tr>
<th>Step</th>
<th>Action</th>
</tr>
</thead>
</table>
| 1    | Right-click in the chromatogram and select Marker.  
**Result:** A vertical line is set in the chromatogram. A text box in the top left corner of the chromatogram displays the X-axis and Y-axis values of the curve at the point where the vertical Marker line crosses the curve. |
| 2    | • Move the Marker with your mouse.  
• Measure the height of the peak you want to exclude from the baseline. |
| 3    | Choose Integrate:Calculate baseline. |
| 4    | • Select the Classic checkbox as the Chosen algorithm.  
• Type a new value for Max baseline level. Set the level slightly lower than the value that you measured in step 2.  
• Click OK. |
The illustration below is an example of a correct baseline after the **Max baseline level** has been changed:
8.5 How to edit the baseline manually

You can edit the baseline manually in the Edit Baseline dialog box in the Evaluation module:

- Select Integrate:Edit Baseline to display the dialog box.

The Edit Baseline dialog box displays the baseline and the curve it was calculated from. The baseline points are marked with green squares. Hold the cursor above the baseline point to display its coordinates. See the illustration below:

<table>
<thead>
<tr>
<th>Step</th>
<th>Action</th>
</tr>
</thead>
</table>
| 1    | • Click the Zoom icon.  
   | Result: The cursor is changed into a magnifying glass. |
| 2    | • Press and hold the left mouse button.  
   • Drag the cursor over the area you want to zoom in on.  
   • Release the mouse button.  
   | Result: The area is enlarged. Right-click and select Reset zoom to restore the full view. |
The table below describes how to edit and insert baseline data points:

<table>
<thead>
<tr>
<th>Step</th>
<th>Action</th>
</tr>
</thead>
</table>
| 1    | Select **Integrate:Edit Baseline**.  
*Result:* If there are more than one baseline available, the **Select Baseline to Edit** dialog box opens. If not, proceed to step 2.  
- Select the baseline you want to edit from the list.  
- Click **OK**.  
*Result:* The **Edit Baseline** dialog box opens |
| 2    | - Click the **Set Curve Points** icon.  
*Result:* The cursor is changed into a cross. |
| 3    | **Add a data point**  
- Click the left mouse button to place a new baseline point in the chromatogram.  
*Result:* A new point is created, marked by a green square. The baseline curve is redrawn as a spline function based on the old and the new points. The baseline is guided by the points, but does not necessarily pass through them.  
- **Delete a data point**  
  - Double-click the data point.  
  *or*  
  - Click the data point to select it and click the **Delete** button.  
  *or*  
  - Right-click the data point and select **Delete Point** from the shortcut menu.  
*Result:* The data point is deleted and the curve is redrawn. |
| 5    | **Move a data point**  
- Select the data point and drag it to a new position.  
*Result:* The baseline curve is redrawn. |
| 6    | Click **OK**.  
*Result:* The **Save Edited Baseline** dialog box opens. |
8.5 How to edit the baseline manually

<table>
<thead>
<tr>
<th>Step</th>
<th>Action</th>
</tr>
</thead>
</table>
| 7    | • Confirm the location and type a new name if necessary.  
      | • Click **OK**.  
      | *Result:* The new baseline is saved. |

**Edited baseline**

The illustration below is an example of a baseline before and after editing:

![Baseline Illustration]

**How to draw a straight line**

The table below describes how to force a straight baseline between two points.

<table>
<thead>
<tr>
<th>Step</th>
<th>Action</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>Select the first of the two points in the point list.</td>
</tr>
</tbody>
</table>
| 2    | Click the **Draw straight to next point** button.  
      | *Result:* The baseline is drawn through the points as a straight line. |
8.6 How to edit the peaks

Introduction
Once a peak table has been generated based on an appropriate baseline, it is possible to split or join peaks and to manually adjust the peak start and end points. The peaks will then be renumbered and the peak values will all be recalculated.

How to open the peak table for editing
The table below describes how open the peak table for editing. The editing options are described below this table:

<table>
<thead>
<tr>
<th>Step</th>
<th>Action</th>
</tr>
</thead>
</table>
| 1    | Select **Integrate:Edit Peak Table**.  
*Result*: If there are more than one peak table available, the **Select Peak Table to Edit** dialog box opens. The name of the baseline on which the peak table was based is displayed at the bottom of the panel. |
| 2    | • Select the peak table from the list and click **OK**.  
• Select one or more **Help Curves** to be displayed for reference if necessary.  
*Result*: The **Edit Peak Table** dialog box opens.  
*Note*: The **Edit Peak Table** dialog box will be opened immediately if you select **Save and Edit Peak Table** as the last step of the peak integration. |
| 3    | Perform the changes (described in the instructions below). |
| 4    | Click **OK**.  
*Result*: The **Save Edited Peak Table** dialog box opens. The dialog box displays a suggested name and location for the peak table. |
| 5    | Confirm the name and location and click **OK**. |

How to adjust the baseline
The baseline can be adjusted graphically (see also 8.5 **How to edit the baseline manually** on page 106) in the **Edit Peak Table** dialog box. The table below describes this:

<table>
<thead>
<tr>
<th>Step</th>
<th>Action</th>
</tr>
</thead>
</table>
| 1    | • Click the **Set Curve Points** icon.  
*Result*: The cursor is changed into a cross. |
Perform the operations below as desired:

- Click to insert a new data point.
- Double-click on a data point or right-click the point and select **Delete Point** from the short-cut menu to delete the point.
- Click a data point and drag the point to a new position to move the baseline.

*Note: Accept negative peaks* must be selected before the peak integration if you want to be able to drag a data point to move the baseline above the curve.

### How to calculate a new baseline

The baseline can be recalculated in the **Edit Peak Table** dialog box. The table below describes how to do this:

<table>
<thead>
<tr>
<th>Step</th>
<th>Action</th>
</tr>
</thead>
</table>
| 1    | Select **Baseline:New:Calculate**.  
      | or  
      | Right-click and select **New Calculate** from the shortcut menu.  
      | **Result:** The **Settings** dialog box opens. |
| 2    | Select an algorithm (**Morphological** is default). |
| 3    | Adjust the **Baseline** parameters as desired.  
      | or  
      | Click the **Default Values** button for the default values. |
| 4    | Click **OK**.  
      | **Result:** The baseline is recalculated. |

*Note: Select **Baseline:New:Zero Baseline** to replace the calculated baseline with a zero baseline.*
The illustration below shows the **Edit Peak Table** dialog box.

The table below describes how to delete a peak in the **Edit Peak Table** dialog box:

<table>
<thead>
<tr>
<th>Step</th>
<th>Action</th>
</tr>
</thead>
</table>
| 1    | • Click the **Edit peaks** icon.  
      |       | • Click the peak in the curve or in the peak table to select the peak.  
|      | 2      | • Right-click and select **Delete Peaks** from the shortcut menu.  
      |       | *or*  
      |       | • Select **Edit:Delete Peaks**.  
      |       | **Result:** The peak is deleted and the remaining peaks are renumbered. |
How to add color to a peak

The table below describes how to add a fill color and a pattern to a peak in the Edit Peak Table dialog box:

<table>
<thead>
<tr>
<th>Step</th>
<th>Action</th>
</tr>
</thead>
</table>
| 1    | • Click the Edit peaks icon.  
• Move the cursor over the peak you want to edit.  
*Result*: The cursor is changed into a larger arrow.  
• Click to select the peak. |
| 2    | • Right-click and select Fill Peak from the shortcut menu.  
*or*  
• Select Edit:Fill Peak.  
*Result*: The Color and Pattern dialog box opens.  
• Select a color and a pattern.  
• Click OK.  
*Result*: The peak is filled according to the selections. |

*Note*: The color and pattern selections will override the general Fill settings that can be selected for all peaks on the Peak Table tab in the Chromatogram Layout dialog box.
The beginning of each peak is marked with a drop-line above the curve, and the end of each peak is marked with a drop-line below the curve. The illustration below shows an example of start and end point drop-lines:

Where there are two peaks beside one another, the end of the first peak will be at the same point as the beginning of the next peak. Thus, there will be a drop-line below and above the curve at the same point. See the illustration below:

How to split a peak

It is possible to split the peak into two new peaks by inserting a drop-line. The table below describes how to split a peak in the Edit Peak Table dialog box:

<table>
<thead>
<tr>
<th>Step</th>
<th>Action</th>
</tr>
</thead>
</table>
| 1    | • Click the Edit peaks icon.  

• Click the peak in the curve or in the peak table to select the peak. |
| 2    | • Right-click and select Split Peak from the shortcut menu.  

or  

• Select Edit:Split Peaks.  

Result: A new drop-line is inserted at the middle point between the two existing drop-lines and the peak is split. |

Note: The area under each new peak will not be the same if the symmetry of the original peak was not perfect.
### How to join peaks

It is possible to join the areas of adjacent peaks if they are separated by a drop-line. The table below describes how to join adjacent peaks in the *Edit Peak Table* dialog box:

<table>
<thead>
<tr>
<th>Step</th>
<th>Action</th>
</tr>
</thead>
</table>
| 1    | • Click the *Edit peaks* icon.  
      | • Click the peak in the curve or in the peak table to select the peak. |
| 2    | • Right-click and select *Join Left* or *Join Right* from the shortcut menu.  
      | *or*  
      | • Select *Edit:Join Left* or *Edit:Join Right*.  
      | **Result:** The original intervening drop-line is removed and all peaks are renumbered. |

### How to add peak names

The table below describes how to add names in the *Edit Peak Table* dialog box to identify the peaks:

<table>
<thead>
<tr>
<th>Step</th>
<th>Action</th>
</tr>
</thead>
</table>
| 1    | • Click the *Edit peaks* icon.  
      | • Click the peak in the curve or in the peak table to select the peak. |
| 2    | • Right-click and select *Peak Name* from the shortcut menu.  
      | *or*  
      | • Choose *Edit:Peak name*.  
      | *or*  
      | • Double-click the peak in the peak table or the curve.  
      | **Result:** The *Edit Peak Name* dialog box opens. The number and retention of the selected peak is displayed. |
| 3    | Type a name in the *Peak name* textbox and click *OK*. |
How to adjust peak areas with drop-lines

The table below describes how to move the drop-lines to adjust the peak area in the *Edit Peak Table* dialog box.

<table>
<thead>
<tr>
<th>Step</th>
<th>Action</th>
</tr>
</thead>
</table>
| 1 | • Click the **Edit peaks** icon.  
  • Click the peak in the curve or in the peak table to select the peak.  
  **Result:** Two vertical bars become superimposed over the drop-lines that delimit the selected peak. The area between the bars is filled with a yellow fill pattern. |
| 2 | Drag the bars to define the new limits for the selected peak.  
  **Result:** The drop-lines are moved and the peak areas are automatically recalculated. |

**Note:** A drop-line can never be moved beyond another drop-line or beyond a point where the peak meets the baseline.

How to use the zoom function

The table below describes how to use the zoom function in the *Edit Peak Table* dialog box.

<table>
<thead>
<tr>
<th>Step</th>
<th>Action</th>
</tr>
</thead>
</table>
| 1 | • Click the **Zoom** icon.  
  **Result:** The cursor is changed into a magnifying glass. |
| 2 | • Press and hold the left mouse button.  
  • Drag the cursor over the area you want to zoom in on.  
  • Release the mouse button.  
  **Result:** The area is enlarged. Right-click and select **Reset zoom** to restore the full view. |

The Integrate menu

If needed you can use the selections on the **Integrate** menu to perform a peak integration in the *Edit Peak Table* dialog box. This is useful for example if you want to re-integrate the curve using different settings or integrate only part of a curve with different settings.

See 8.7 *How to integrate part of a curve and how to exclude or skim peaks* on page 116 for more information.
8.7 How to integrate part of a curve and how to exclude or skim peaks

Introduction

There are several possibilities to improve the results if the peak integration is unsatisfactory. This section describes:

- How to select only part of a curve for integration.
- How to exclude peaks.
- How to skim peaks.

These operations can be performed both in the Integrate dialog box in preparation for the peak integration, or in the Edit Peak Table dialog box to adjust an unsatisfactory peak integration. This section describes both alternatives.

How to select part of a curve

The table below describes how to select only a part of a curve for peak integration in the Integrate dialog box:

<table>
<thead>
<tr>
<th>Step</th>
<th>Action</th>
</tr>
</thead>
</table>
| 1    | • Choose Integrate:Peak Integrate.  
      | Result: The Integrate dialog box opens.  
      | • Click the Peak Window button.  
      | Result: The Peak window dialog box opens. |
| 2    | • Type new X-axis values for the Left limit and the Right limit.  
      | or  
      | • Drag the vertical cursor lines to define the limits. |
How to exclude peaks

You can define criteria to exclude peaks from integration. The table below describes how to define peaks to be excluded in the Integrate dialog box.

<table>
<thead>
<tr>
<th>Step</th>
<th>Action</th>
</tr>
</thead>
</table>
| 1    | Click the Reject peaks button.  
*Result:* The Reject Peaks dialog box opens. |
| 2    | • Select the appropriate checkboxes and type values for height, width and area.  
• Define how many of the largest peaks you want to include.  
• Click OK. |

How to include negative peaks

Select the Accept negative peaks checkbox of the Integrate dialog box to include negative peaks in the integration.  
*Result:* The negative peaks will be reported as negative areas in the peak table. By default, negative peaks are not included in the integration.
The area under a peak can be calculated either using separating drop-lines or peak skimming:

- **Drop-lines** are vertical marks that split two peaks at the valley. Drop-lines are used mostly for peaks of relatively similar size. When a peak has a shoulder, splitting with drop-lines will cause the first peak to lose too much of its area to the peak that forms its shoulder.

- The **Peak skim** option can be used to skim off the smaller peak with a straight line that starts in the valley between the peaks and ends at the other side of the smaller peak, at the point where the skim line and the curve slope are equal.

The illustration below is an example of how a drop-line (A) and a skimmed peak (B) affects the area under the main peak and the peak shoulder. The peak shoulder area is marked in gray:

<table>
<thead>
<tr>
<th>Step</th>
<th>Action</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>Select the <strong>Peak skim</strong> checkbox.</td>
</tr>
<tr>
<td>2</td>
<td>Determine the ratio when peak skimming should be applied based on the relationship in the illustration below:</td>
</tr>
</tbody>
</table>

*Note: The default ratio value is 10.*
Part of a curve can be selected in the **Edit Peak Table** dialog box and integrated with settings that differ from the rest of the curve. The table below describes how to do this.

<table>
<thead>
<tr>
<th>Step</th>
<th>Action</th>
</tr>
</thead>
<tbody>
<tr>
<td>3</td>
<td>Type the ratio value in the text box.</td>
</tr>
</tbody>
</table>

**Note:** All operations described below will only affect the selected part of the curve.
<table>
<thead>
<tr>
<th>Step</th>
<th>Action</th>
</tr>
</thead>
</table>
| 3    | If desired, change the integration parameters:  
|      | **Reject peaks**  
|      | • Choose **Integrate:Settings**.  
|      | **Result**: The **Reject Peaks** dialog box opens.  
|      | • Change the settings as desired and click **OK**.  
|      | **Skim peaks**  
|      | • Choose **Integrate:Peak Skim**.  
|      | **Result**: The **Peak Skim** dialog box opens.  
|      | • Select the **Skim Peaks** checkbox and type a ratio.  
|      | • Click **OK**.  
| 4    | • Choose **Integrate:Peak Integrate**.  
|      | **Result**: The selected part of the curve is peak integrated based on the changed parameters. |
8.8 Measurements

Introduction

It is possible to determine the coordinates of any point on a curve and to obtain values for retention and peak height. This is a useful tool for many other functions, such as for measuring the parameters used in baseline calculations.

Measurement options

Coordinates can be obtained in two ways:

- Through direct measurement.
- From peak table data.

How to make direct measurements

The table below describes how to make direct measurements in a chromatogram:

<table>
<thead>
<tr>
<th>Step</th>
<th>Action</th>
</tr>
</thead>
</table>
| 1    | Right-click in the chromatogram and select Marker.  
*Result:* A vertical line is set in the chromatogram. A text box in the top left corner of the chromatogram displays the X-axis and Y-axis values of the curve at the point where the vertical Marker line crosses the curve. See the illustration below: |
| 2    | Move the Marker with your mouse to display the peak data. |
| 3    | Click the curve name legend above the chromatogram to change to another curve.  
*Result:* The Y-axis is changed to the one corresponding to the new curve. |
| 4    | Right-click and select Marker again to de-select the function. |

Note: The color of the Marker is the same as the selected curve.
How to set a reference point

The table describes how to set a reference point:

<table>
<thead>
<tr>
<th>Step</th>
<th>Action</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>Right-click in the chromatogram and select <strong>Set Marker Ref. Point</strong> to define a reference point for the marker position.</td>
</tr>
</tbody>
</table>
| 2    | When the marker is moved from the reference point, the X-axis and Y-axis values for the new position are displayed together with:  
    • the new position in relation to the position of the reference point,  
    • the minimum, maximum and average values for the curve interval between the reference point and the new position. |

How to record a Snapshot

The table below describes how to record a **Snapshot** of the current curve values:

<table>
<thead>
<tr>
<th>Step</th>
<th>Action</th>
</tr>
</thead>
</table>
| 1    | • Right-click in the chromatogram and select **Snapshot** from the shortcut menu.  
    **Result**: The **Snapshot** dialog box opens. |
| 2    | The dialog box displays all the curve data that was current at the moment the snapshot was taken.  
    • Click the **Save to file** button to save the snapshot as an Excel file.  
    • Click the **Print** button to print the snapshot. |

How to select peak table data

The retention time and amplitude of any peak can be viewed directly in a peak table after an integration. This data and more is selected in the **Chromatogram Layout** dialog box. The table below describes how to select peak table data.

<table>
<thead>
<tr>
<th>Step</th>
<th>Action</th>
</tr>
</thead>
</table>
| 1    | Click the **Chromatogram Layout** icon.  
    **Result**: The **Chromatogram Layout** dialog box opens. |
| 2    | Click the **Peak Table** tab. |
| 3    | • Select the checkboxes on the **Select peak table columns** list for all items that you want to display in the table.  
    • Click **OK**. |
A Evaluation functions and instructions

Introduction

This appendix describes the functions that are implemented in the Evaluation module.

In this chapter

This chapter contains the following sections

<table>
<thead>
<tr>
<th>Topic</th>
<th>See</th>
</tr>
</thead>
<tbody>
<tr>
<td>Baseline calculation theory</td>
<td>A.1</td>
</tr>
<tr>
<td>Peak table column components</td>
<td>A.2</td>
</tr>
</tbody>
</table>
A.1 Baseline calculation theory

Overall process

The table below describes the overall process of a baseline calculation.

<table>
<thead>
<tr>
<th>Stage</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>The baseline segments are defined.</td>
</tr>
<tr>
<td>2</td>
<td>The baseline points are selected.</td>
</tr>
<tr>
<td>3</td>
<td>The baseline is drawn.</td>
</tr>
</tbody>
</table>

Baseline segment definition

Baseline parameters are used to find the baseline segments. The default values for the parameters are determined from the source curve. The baseline segments are found by different parameters that are based on the type of algorithm that is selected.

Note: The parameters can be displayed in the Evaluation module if you choose Integrate:Calculate baseline function. You can also click the Baseline settings button in the Integrate:Peak integrate dialog box.

Morphological algorithm

The Morphological algorithm searches for all parts of the source curve where:

- The curve parts come into contact at both ends of a horizontal line of the length defined in the Structure width parameter. The default value of this parameter is based on the widest detected peak in the curve. The horizontal line is moved along the curve up the peak until it reaches the contact points. The curve parts below the horizontal line and the line will now form a "curve" with a plateau. The center point in the plateau formed by the horizontal line will be the data point for the baseline.
- The data points fulfil the Minimum distance between data points. This parameter reduces the total number of data points that are created from a curve.

Classic algorithm

The Classic algorithm searches for all parts of the source curve where:

- The curve parts are longer than the Shortest baseline segment. This parameter determines the minimum length for a part of the source curve to be considered a possible baseline segment.
- The curve has no point outside the Noise window. The noise window is defined as a rectangular corridor parallel to the slope of the curve and centered on the first and last points within the currently inspected segment.
- The slope is less than the Slope limit. This limits the maximum slope of the baseline to differentiate baseline segments from peaks.
- The curve parts are lower than the Max baseline level. This parameter determines the highest acceptable signal level for the baseline.
The baseline parameters can be illustrated as a rectangular box that the source curve has to fit into in order to be identified as a baseline segment, where:

- The length of the box corresponds to the **Shortest baseline segment**.
- The height of the box corresponds to the maximum level of noise on the baseline segments. This is referred to as the **Noise window**.
- The box is allowed to be tilted with a maximum slope corresponding to the **Slope limit**.
- The box is not allowed to move up above the **Max baseline level**.

The illustrations below shows the baseline parameters graphically.
The table below describes the baseline segment identification process:

<table>
<thead>
<tr>
<th>Stage</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>The box is virtually moved along the source curve in steps of one third of the <strong>Shortest baseline segment</strong> length to look for baseline segments.</td>
</tr>
<tr>
<td>2</td>
<td>A baseline segment is found whenever the currently examined part of the source curve fits completely within the box.</td>
</tr>
<tr>
<td>3</td>
<td>The found baseline segments are joined by connecting adjacent segments, provided that the slope of the joining lines does not exceed the <strong>Slope limit</strong>.</td>
</tr>
</tbody>
</table>

When the baseline segments have been defined and joined, they are replaced by baseline points at the start and end of each segment. The line between these is also filled with points.

**Note:** The baseline points are shown as green squares in the **Integrate:** Edit baseline function of the **Evaluation** module.

The baseline points are used to create the baseline curve using a spline interpolation. The spline function ensures that the baseline curve is guided by the baseline points. However, the curve does not necessarily pass through the baseline points. The baseline will be a smoothly curved function passing close to or through the points.

To reduce the effect of noise at the peak integration, the created baseline is forced equal to the source curve in every position where the difference between the baseline and the source curve is small enough. Choose **Integrate:** Calculate Baseline. If the **Accept negative peaks** option is off, the baseline will be forced down to the level of the source curve whenever the created baseline goes above the source curve.

You can try to measure the **Shortest baseline segment** length directly on your chromatogram. The table below describes how to do this:

<table>
<thead>
<tr>
<th>Step</th>
<th>Action</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>Locate the shortest segment of the curve that you consider a part of the baseline.</td>
</tr>
<tr>
<td>2</td>
<td>Use the marker box on the chromatogram to measure the length of the segment.</td>
</tr>
<tr>
<td>3</td>
<td>Choose <strong>Integrate:</strong> Calculate Baseline and insert this value as the <strong>Shortest baseline segment</strong> value.</td>
</tr>
</tbody>
</table>
Curve coordinates can also be used to measure noise levels on the source curve. The table below describes how to do this:

<table>
<thead>
<tr>
<th>Step</th>
<th>Action</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>Use the <strong>Zoom</strong> function to focus on a part of the curve that is representative for the baseline noise.</td>
</tr>
<tr>
<td>2</td>
<td>Select an appropriate Y-axis scale.</td>
</tr>
<tr>
<td>3</td>
<td>Measure the Y-axis coordinates.</td>
</tr>
</tbody>
</table>
| 4    | • Calculate the noise range as the difference between the max. and min. values.  
      • Add an extra 20%.  
      • Choose **Integrate:Calculate Baseline** and insert this value as the **Noise window** value. |
A.2  Peak table column components

Introduction

This section contains a list of peak parameters with explanations and calculation formulae when applicable.

Peak parameters - illustration

The diagram below illustrates the peak parameters. See the parameter list below for explanations.

Peak parameter descriptions

The list below contains descriptions of the peak parameters.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Area</td>
<td>Calculated as the area between the curve and baseline, between the peak start and peak end, time or volume base. (Gray area in the diagram above.)</td>
</tr>
<tr>
<td>Asymmetry</td>
<td>Peak asymmetry (indicator of column packing). See definition below this table.</td>
</tr>
<tr>
<td>Baseline height</td>
<td>Baseline amplitude at peak start, peak maximum and peak end. (A, F and G in the diagram above.)</td>
</tr>
<tr>
<td>Parameter</td>
<td>Description</td>
</tr>
<tr>
<td>---------------------------------</td>
<td>---------------------------------------------------------------------------------------------------------------------------------------------</td>
</tr>
<tr>
<td>Fraction tube id</td>
<td>Fraction number at peak start, peak maximum and peak end.</td>
</tr>
<tr>
<td>Height</td>
<td>Maximum amplitude above the baseline. (C-F in the diagram above)</td>
</tr>
<tr>
<td>Plate height (HETP)</td>
<td>Height equivalent to theoretical plate and plates/meter. The column height must be entered in the Integrate dialog box for this parameter to be calculated. See definition below this table.</td>
</tr>
<tr>
<td>Peak endpoint heights</td>
<td>Amplitude above the baseline at left (A in the diagram above) and right peak limits (E-G in the diagram above).</td>
</tr>
<tr>
<td>Peak endpoint retention</td>
<td>Retention value at peak start and peak end, time or volume base. (A and G in the diagram above.)</td>
</tr>
<tr>
<td>Peak name</td>
<td>Name of the peak.</td>
</tr>
<tr>
<td>Percent of total area</td>
<td>Peak area as a percent of the total area under the curve above the baseline. Time or volume base.</td>
</tr>
<tr>
<td></td>
<td><em>Note:</em> This value can differ in time and volume base if the flow rate is not constant throughout the method.</td>
</tr>
<tr>
<td>Percent of total peak area</td>
<td>Peak area as a percent of the sum of all integrated peaks.</td>
</tr>
<tr>
<td></td>
<td><em>Note:</em> This value can differ in time and volume base if the flow rate is not constant throughout the method.</td>
</tr>
<tr>
<td>Resolution</td>
<td>Peak resolution. See definition below this table.</td>
</tr>
<tr>
<td>Retention</td>
<td>Retention at the peak maximum, time or volume base. (C in the diagram above.)</td>
</tr>
<tr>
<td>Sigma</td>
<td>Standard deviation for a Gaussian-shaped peak. See definition below this table.</td>
</tr>
<tr>
<td>Parameter</td>
<td>Description</td>
</tr>
<tr>
<td>----------------------------</td>
<td>-----------------------------------------------------------------------------</td>
</tr>
<tr>
<td>Type of peak limits</td>
<td>Identifies the criteria for peak start and peak end as either the baseline intersection or dropline to the baseline or skim line.</td>
</tr>
<tr>
<td>Width</td>
<td>Difference in retention between the peak end and peak start, time or volume base. (G-A in the diagram above.)</td>
</tr>
<tr>
<td>Width at half height</td>
<td>Calculated by taking the maximum height of the peak above the baseline, then determining the peak width at half this value above the baseline. Time or volume base. (B-D in the diagram above, where BD bisects CF.)</td>
</tr>
</tbody>
</table>

### Sigma formula

The formula below is used to calculate **Sigma**.

\[
\text{Sigma} = \sqrt{\frac{\sum (x_i - \bar{x})^2}{n}}
\]

Where:
- \( n \) is the number of data points.
- \( x \) is the volume or time value.
- \( x_{\text{ymax}} \) is the volume or time value at the maximum amplitude value.
- \( A_{\text{peak}} \) is the area of the peak.

**Note**: The peak width for a Gaussian peak is \((4 \times \text{Sigma})\).

### Peak resolution algorithms

The peak resolution is calculated with one of the following three algorithms:

1. \((V_{R2} - V_{R1}) / ((W_{b2} + W_{b1}) / 2)\)
2. \((V_{R2} - V_{R1}) / ((\text{Sigma}_2 + \text{Sigma}_1) \times 2)\)
3. \(((V_{R2} - V_{R1}) / (2 \times (W_{h2} + W_{h1})) / 2.354)\)
Where:
- $V_{R1}$, $W_{h1}$, $\Sigma_{1}$ and $W_{h1}$ are the retention, width, $\Sigma$ and width at half height of the previous peak.
- $V_{R2}$, $W_{h2}$, $\Sigma_{2}$ and $W_{h2}$ are the retention, width, $\Sigma$ and width at half height of the current peak.

The formula below is used to calculate the **Capacity factor**.

Where:
- $V_R$ = retention volume.
- $V_t$ = total liquid volume.

The formula below is used to calculate the **Asymmetry**.

Asymmetry = $B / A$

Where:
- $A$ is a partial peak width, measured at a percentage of the peak height, for the leading part of the peak.
- $B$ is a partial peak width, measured at a percentage of the peak height, for the tailing part of the peak.
The formula below is used to calculate the HETP value.

\[
\text{HETP} = \frac{L}{N}
\]

\[
N = 5.54 \times (V_R/w_h)^2
\]
assuming a Gaussian peak.

Where:
- \(N\) = no. of theoretical plates.
- \(L\) = bed height in cm.
- \(V_R\) = peak retention (elution) volume or time.
- \(w_h\) = peak width at half height expressed in the same units as \(V_R\).
A

Application templates
   How to start a run, 33

B

Baseline
   Calculation options, 88
   The Calculate function, 88
   Reuse existing, 88
   How to edit manually, 107
   How to adjust the baseline graphically, 109
   Definition of a segment, 124
   Parameters, 125

BatchID
   Logbook illustration, 45

Blank curve
   Calculate baseline based on, 88

C

Chromatogram Layout
   Curve tab, 58
   Default curve names, 58
   How to choose curve name appearance, 58
   The Curve Style and Color tab, description, 59

Chromatogram window
   Shortcut menu, 53
   How to optimize the workspace, 54
   How to display a vertical marker, 54
   How to display the Logbook overlay, 55

Chromatograms
   Description, 50
   Temporary chromatogram, 50
   How to make layout changes, general, 57
   How to change and fix the Y-axis, 61
   How to add a second Y-axis, 61
   How to change and fix the X-axis, 62
   How to save a layout, 63
Index

How to apply a layout, 63
How to print active chromatograms, 66
How to add annotations, 80
How to edit annotation text, 80
How to rename, 81
How to set a reference point, 122

Classic algorithm
Definition, 98
Parameters, 98
How to set, 98
Shortest baseline segment, 99
Slope limits, 100
Noise window, 102
Missing peaks, 103
When to change the Max baseline level, 104
How to set Max baseline level, 104
Definition, 124
How to measure baseline segments, 126
How to measure noise level, 127

Curves
How to copy into the Temporary chromatogram, 50
Run curves default appearance, 53
How to choose the Y-axis scale, 53
Default curve names, 58
Peak labels, 59
Fraction text alignment options, 59
Logbook text alignment options, 59
How to change the color and style, 59
How to set a hatched background, 59
How to change and fix the Y-axis, 61
How to add a second Y-axis, 61
How to change and fix the X-axis, 62
How to save a layout, 63
How to apply a layout, 63
How to use the zoom function, 65
How to rename, 81
Export options, 82
How to export, 82
How to export in AIA format, 84
How to delete unwanted curves, 86

Curves pane in PrimeView
Description, 40
How to display a vertical marker, 40
How to set a reference point, 40
How to change curve colors and styles, 41
How to change scale of the Y-axis, 41
How to change scale of the X-axis, 42
How to zoom in regions of the pane, 42
Reduce scale of zoom, 42
How to select curve pressure units, 43
How to select text alignment, 43
How to display complete Logbook information, 44

D
Delete files and folders, 30
Documentation
  How to view, 78
  How to export, 85

E
Evaluation
  How to start the Evaluation module, 48
Chromatogram window views, 52
  How to display peak table information, 52
Chromatogram window shortcut menu, 53
  How to optimize the chromatogram workspace, 54
How to display a vertical marker, 54
How to set a reference point, 54
How to make chromatogram layout changes, general, 57
How to exit the module, 86
Evaluation logs
  How to export, 85

F
Files and folders
  Copy to external, 29
  How to copy from external, 30
Folders
  How to create, 25
I

Installation
  Software, 19
  Prerequisites, 19
  Software license agreement, 20

L

Logbook
  How to display an overlay in the Curves pane in PrimeView, 44
  How to display an overlay in the chromatogram window, 55
Logbook pane
  Description, 45
  Autoscroll function, 45
  How to filter the contents, 45
  Search function, 46

M

Manual runs
  How to run the system manually, 36
Measurements
  How to make direct, 121
Method runs
  Logbook pane, description, 45
Method templates
  How to start a run, 34
Methods
  How to run a saved method, 35
Morphological algorithm
  Description, 94
  How to set, 94
  Structure width, 95
  Incorrect structure width, 96
  Noise window, 96
  Minimum distance between points, 97
  Definition, 124
Peak integration
   How to perform, 89
   Differences between to filter peaks and to reject peaks, 91
   How to display peak labels, 92
   How to select part of a curve for peak integration, 116

Peak skim
   Compared to drop-lines, 118
   How to select a ratio, 118

Peak table
   How to display information, 52
   How to rename, 81
   How to export, 84
   How to select contents, 122

Peaks
   How to filter from view, 91
   Labels, 92
   How to display peak labels, 92
   How to open the peak table, 109
   How to delete a peak, 111
   How to add a fill color and pattern, 112
   Drop-lines, description, 113
   How to split a peak, 113
   How to join peaks, 114
   How to add peak names, 114
   How to exclude before integration, 117
   Include negative peaks in integration, 117
   How to select a skim ratio, 118
   Edit integration for part of a curve, 119
   Peak parameters, 128

PrimeView module
   How to open, 38
   How to select the displayed panes, 38
   How to customize the panes, 39

Quick View
   How to preview result files, 27
Index

R

Rename files and folders, 30
Reports
- How to create a blank customized report, 68
- Edit mode toolbar buttons, 68
- How to add or delete pages, 69
- How to change the page setup, 69
- How to add objects to a report, 71
- How to add free text, 71
- How to add picture objects, 72
- How to include chromatograms, 73
- How to include a peak table, 73
- How to add documentation, 74
- How to add the Evaluation log, 75
- Toolbar icons in Report Edit Mode, 76
- How to print, 77
- How to save the report format, 77

Result files
- How to open, 26
- How to save, 86

S

Searches
- General functions, 13

Security
- Backup, 31

Snapshots
- How to view, 16

System Control module
- Description, 9

T

Templates
- How to start a run from an application template, 33
- How to start a run from a method template, 34

Temporary chromatogram
- Description, 50
Index

Toolbar icons
   In the PrimeView module, 10

Y

Y-axis
   How to choose the Y-axis scale, 53

Z

Zero baseline
   Definition, 88
Zoom function
   How to enlarge parts of a curve, 65