

Getting Started With UNICORN 5.0



Getting Started with UNICORN 5.0
03-0014-92 Edition AB
2004-02

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Table of Contents

1 Introducing UNICORN

- About this chapter** This chapter contains:
- An overview of the UNICORN™ system and general information that you need before you can start.
 - Information about the user documentation for UNICORN and how to use it.
 - A Quick Start Guide that can be used as a shortcut for experienced users that want to start right away.
-

In this chapter This chapter contains these sections.

Topic	See
About UNICORN	1.1
About this manual	1.2
About the UNICORN user documentation	1.3
Quick Start Guide	1.4

1.1 About UNICORN

Introduction

This section is a general overview of the UNICORN system.

What is UNICORN?

UNICORN is a complete package for control and supervision of chromatography systems. It consists of control software and a controller card for interfacing the controlling PC to the chromatography liquid handling module.

Liquid chromatography is used in separation processes, for analytical purposes or in the biochemical process industry.

Operating environment

UNICORN 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 UNICORN, including:

- cut and paste
- right-click short-cut menus

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

Compatible chromatography systems

UNICORN can be used with a number of systems including

- ÄKTA™ design systems
- BioProcess™ systems

Note: All examples in this guide are based on an ÄKTAexplorer™ 100 system that operates with the E100F400 strategy. If you use another system you may find that the descriptions and instructions do not match your system on every point. In that case you also need to refer to the user documentation for your specific chromatography system.

System networks UNICORN can be installed on a stand-alone computer to control only a single, locally attached system. However, a stand-alone computer can control up to a maximum of four separate systems. In a network installation each computer workstation can operate many systems regardless if they are locally connected or not. Each system can only be operated by one workstation at a time, but several may view the output data.



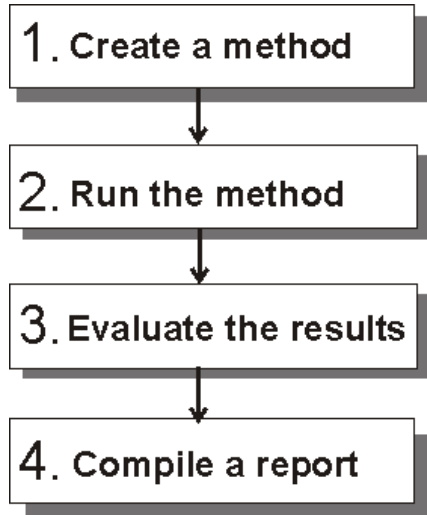
Software modules The UNICORN control software consists of four integrated modules:

Module	Function
UNICORN Manager	File handling and administration, e.g. definition of systems and user profiles etc.
Method Editor	To create and edit methods for pre-programmed control of chromatography systems.
System Control	To control and monitor the separation processes online, through method-based or manual control.
Evaluation	To evaluate and present stored results from separation processes.

Note: All modules are active when the program is operating, and are not closed when they are minimized. A minimized **System Control** unit may control a process.

Work flow

The work flow in UNICORN can be divided into four distinct stages. Each stage is described in separate chapters in this manual. The flow chart below shows the work flow stages.



Help functions

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

If you want to access...	Then...
the general help utility.	open the Help menu in any of the software modules.
context-specific help topics.	<ul style="list-style-type: none"> • click the Help button in the dialog box. <i>or</i> • press the F1 key on your keyboard.

Security

The table below describes the main security functions in UNICORN:

Feature	Function
Access Security	Only authorized users can access UNICORN. Each user is assigned an access level, which defines the functions that the user is permitted to use.
Connection Security	A running system can only be controlled from one connection. Systems may be locked with a password to prevent other, un-authorized users from changing parameters.

Feature	Function
Data Security	Result files from an ongoing separation run can be saved automatically at preset intervals to minimize data loss if the system fails. The results are saved locally if the network communication fails.
Electronic Signatures	Method and result files can be signed electronically for enhanced security and accountability.

1.2 About this manual

Introduction This section provides a general description of the manual, the contents and the pre-requisites for the examples and instructions that are presented in the Getting Started guide.

The purpose of Getting Started The purpose of Getting Started is to present a quick and easy guide to the system for a user with limited or no experience of UNICORN. The work flow is presented in the form of practical instructions for how to operate a model system. These instructions form a basic framework that the reader can expand on by reading selected parts in the other manuals.

The model system UNICORN software can be used in numerous possible system variations. For practical reasons the user documentation is based on a model system that consists of:

- **ÄKTAexplorer 100**
- Strategy **E100F400**
- **Frac-950**

Note: If you use another system you may find that the descriptions and instructions do not match your system on every point. In that case you also need to refer to the user documentation for your specific chromatography system.

Refer to other manuals The examples and instructions that are presented in this manual are deliberately limited to a minimum to reduce the number of pages that you will need to read. In almost all cases you will find additional information about each topic in the User Reference Manual.

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. The section begins with an introduction that summarizes the content.

A section is divided into blocks of information with separating lines. The blocks are identified by labels in the margins. This makes it easier for you to quickly scan a page to find the exact topic you are looking for.

The manual contents Getting Started contains ten chapters that can be sorted logically into 4 major topics:

Topic	Chapter
Background information.	1. Introducing UNICORN 2. UNICORN concepts

Topic	Chapter
How to prepare the system.	3. How to start your system 4. How to create a method
How to run the system.	5. How to perform method runs 6. Scouting
How to use the results.	7. How to view results 8. How to print chromatograms 9. How to evaluate and save the results 10. How to create and print reports

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:Windows:Customise** (i.e. the menu command **Customise** in the sub-menu **Windows** from the **View**-menu).

Text entries that UNICORN generates or that the user must type are represented by a monotype typeface:

- *Example:* `Connection change`

Pre-requisites

The following pre-requisites must be fulfilled before you can use this manual the way it was intended:

- You need to have a general understanding of how your PC and Windows works. In most cases universal computer functions will not be explained.
- UNICORN must be installed and configured correctly on your computer.
- You need to understand the concepts of liquid chromatography. Terminology and functionalities will be explained only when they differ from normal practise.
- Before you try to operate a chromatography system based on the instructions in this manual you need to study and understand the safety information that is part of the system documentation.

1.3 About the UNICORN user documentation

Introduction

The user documentation for UNICORN is divided into three separate manuals. This section is an overview of the contents and the relationship between the manuals.

The manuals

The three manuals are:

- Getting Started with UNICORN(See section 1.2 About this manual on page 8)
 - UNICORN User Reference Manual
 - UNICORN Administration and Technical Manual
-

User info about Getting Started

The questions and answers in the table below describe the features of the Getting Started manual.

Question	Answer
Who should read Getting Started?	Users that are new to the UNICORN system and with limited experience from other chromatography systems.
What do I need before I start?	A basic knowledge of PC and Windows functions and an understanding of the concepts and terminology of liquid chromatography.
What are the contents of Getting Started?	Basic descriptions of UNICORN and its use, based on a model system.
How should I use Getting Started?	Read in front of your computer and test the instructions at the same time.
When do I need to refer to the User Reference Manual?	When you need: <ul style="list-style-type: none">• more in-depth information,• alternative ways to perform a task.
When do I need to refer to the Administration and Technical Manual?	When you need: <ul style="list-style-type: none">• general information about the network functions of UNICORN,• to set up and configure a UNICORN workstation in a network,• to trouble-shoot a workstation with network problems.

**User info about
the User Reference
Manual**

The questions and answers in the table below describes the features of the User Reference Manual.

Question	Answer
Who should read the User Reference Manual?	<ul style="list-style-type: none"> • Users that are experienced with previous UNICORN system versions. • Users with vast experience from other chromatography systems.
What do I need before I start?	<ul style="list-style-type: none"> • Knowledge of PC and Windows functions. • An understanding of the concepts and terminology of liquid chromatography. • Preferably some previous experience with UNICORN.
What are the contents of the User Reference Manual?	<ul style="list-style-type: none"> • Detailed descriptions of UNICORN. • Instructions on how to use the system, with suggested alternatives. <p><i>Note:</i> Most instructions are based on a model system.</p>
How should I use the User Reference Manual?	<p>Depending on your previous experience you can either read</p> <ul style="list-style-type: none"> • whole chapters from the beginning to the end • only selected sections for reference.
When do I need to refer to Getting Started?	When you need brief, step-by-step instructions for a selected task.
When do I need to refer to the Administration and Technical Manual?	<p>When you need</p> <ul style="list-style-type: none"> • general information about the network functions of UNICORN. • to set up and configure a UNICORN workstation in a network. • to trouble-shoot a workstation with network problems.

**User info about
 The Administration and Technical
 Manual**

The questions and answers in the table below describes the features of the Administration and Technical Manual.

Question	Answer
Who should read the Administration and Technical Manual?	System administrators.
What do I need before I start?	<ul style="list-style-type: none"> • General knowledge of UNICORN. • Knowledge of PC, Windows and general network administration functions. • An understanding of the concepts and terminology of liquid chromatography.
What are the contents of the Administration and Technical Manual?	<p>Detailed instructions of</p> <ul style="list-style-type: none"> • how to install and maintain UNICORN in a network environment. • how to create and administrate user profiles. <p><i>Note:</i> Most instructions are based on a model system.</p>
How should I use the Administration and Technical Manual?	<ul style="list-style-type: none"> • If you are an experienced administrator of previous UNICORN versions you can read selected sections for reference. • If this is your first experience of UNICORN administration we recommend that you study the manual in detail.
When do I need to refer to Getting Started?	When you need brief, step-by-step instructions for a selected task.
When do I need to refer to the User Reference Manual?	When you need more information about the basic functions of UNICORN.


1.4 Quick Start Guide

Introduction

This guide is intended for users who are fully familiar with the safety precautions and operating instructions that are described in all manuals, i.e. experienced users of previous versions of UNICORN. The instructions assume that all installations were made according to the instructions, that the model system is used and is connected.

Quick Start instructions

The table below describes the easiest way to create a method, run the system and generate a printed chromatogram. The procedure is based on an **Instant run**.

Step	Action
1	<p>Click the Instant run icon in the UNICORN Manager.</p>  <p><i>Result:</i> The Instant run dialog box opens.</p>
2	<ul style="list-style-type: none"> • Select Wizard. • Select a system (if necessary). • Click the Run button. <p><i>Result:</i> The Method Wizard opens in the System Control module.</p>
3	<p>Go through all selections on the Method Wizard pages. Click the Next button to proceed from page to page.</p>
4	<p>Click the Run button on the last page.</p> <p><i>Result:</i> The start protocol opens.</p>
5	<p>Verify the method on the Variables page and change values as required. Click the Next button to proceed through several pages.</p>
6	<p>Select Print_Chromatogram in the Evaluation procedures page.</p> <p><i>Result:</i> A printout will automatically be generated after the run.</p>
7	<p>Click the Start button on the last page.</p> <p><i>Result:</i> The run starts.</p>

2 UNICORN concepts

Introduction This chapter contains definitions and descriptions of some of the specific concepts that are presented in this manual and in the other UNICORN manuals. General concepts and common chromatography terminology are not explained here.

In this chapter This chapter contains this section.

Topic	See
Concept definitions	2.1

2.1 Concept definitions

- Introduction**
- This section contains explanations and definitions of a number of UNICORN concepts that are used in this manual.
 - The concepts are sorted in alphabetical order.

Note: The section also lists some concepts that are described only in the User Reference Manual. These concepts are included for reference since they may be found in menus and dialogs that you will use while working with this manual.

- Alarms**
- Systems settings or method instructions specify acceptable limits for monitor signals during a separation run. An **Alarm** dialog box will be displayed on the screen and an optional alarm can sound if a specified limit is exceeded. The system will be paused.

Note: Refer to the User Reference Manual for information about **Alarms**. The topic is not covered in this manual.

- Batch run**
- You can perform a **Batch run** of a number of result files in the **Evaluation** module. The files do not have to be open and the run operates in the background. The procedure is useful if you want to print a number of results with the same settings, or if you want to perform integration with the same parameter settings on many results.

Note: Refer to the User Reference Manual for information about **Batch runs**. The topic is not covered in this manual.

- BufferPrep**
- BufferPrep** is a function to prepare a buffer of different pH and salt concentrations online from four stock solutions. This eliminates the need to manually prepare new buffers every time the pH needs to be changed.

Note: **BufferPrep** is only available for some ÄKTAdesign systems. Refer to the User Reference Manual for information about **BufferPrep**. The topic is not covered in this manual.

- 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 chromatography run are defined in a **Method**. A **Method** is normally divided into blocks that represent steps in the separation process. Each block consists of a series of instructions that request specific operations in the system.

MethodQueue **MethodQueues** are used to link several methods together, on the same or on different systems.

Example: A **MethodQueue** can be set up to conduct a CIP study of a number of columns, through a controlled series of scouting runs.

Note: A method can be placed in a **MethodQueue** if the system is busy when the operator wants to run the method. Refer to the User Reference Manual for information about **MethodQueues**. The topic is not covered in this manual.

Method Wizard The **Method Wizard** is a user-friendly tool to create new methods. The **Wizard** takes the user step-by-step through the creation process.

Method Wizards are supplied with UNICORN installations for ÄKTAdesign systems.

Result files UNICORN 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, calibration settings, scouting parameters, text method etc.

- Saved results from evaluations of the run data

Example: Peak integrations, simulated peak fractionations etc.

Scouting **Scouting** is used to repeat a series of **Method runs** automatically with predetermined changes in the values for one or more **Variables**. A **Scouting Scheme** is defined as part of the method.

Scouting is used for optimizing chromatographic processes.

Strategy

Part of the UNICORN software is specific for the system that it is set up to operate. The system specific part is usually referred to as the **Strategy**. The **Strategy** defines available method and manual instructions, system settings, run data, curves and method templates.

UNICORN

Note: The examples in this guide are generally based on the **E100F400** strategy.

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.

Variable

Values at breakpoints in the **Method** and instruction parameters may be defined as **Variables**. **Variables** makes it easy to adapt a method to a particular chromatography run.

- A framework **Method** with default parameters can be changed to create variants.
 - A **Method** can be used in automatic **Method Scouting**, where one or more parameter **Variables** are changed systematically.
-

Warnings

Systems settings or method instructions specify acceptable limits for monitor signals during a separation run. A **Warning** dialog box may be displayed on the screen if a specified limit is exceeded. The system will still continue to run after a **Warning**.

Note: Refer to the User Reference Manual for information about **Warnings**. The topic is not covered in this manual.

3 How to start your system

Introduction The first step when you begin your work with UNICORN is to start the system. This chapter describes how to start the program and log on as a user.

In this chapter This chapter contains the section below.

Topic	See
How to start UNICORN and log on	3.1


3.1 How to start UNICORN and log on

Introduction This section describes how to start the UNICORN program and how to log on as a user.

Username and password The system administrator creates and defines users and may also create your initial password. (You may change the initial password to another later). The program can also be set up so you can logon without a password.

How to start the program *Note:* If UNICORN is already started by a previous user, proceed to "How to log on".

There are two ways to start the program:

If you start with...	then...
a UNICORN icon on your desktop,	double-click the icon. 
the Windows Start menu,	locate the program under Programs:Unicorn and click UNICORN .


The Logon dialog box This is an illustration of the **UNICORN Logon** dialog box:



Note: The **Logon** dialog has a **Password** text box only if a password is required.

How to log on

The table below describes how to log on to UNICORN.

Step	Action
1	<ul style="list-style-type: none">• Select Tools:Logon. <p><i>or</i></p> <ul style="list-style-type: none">• Click the Logon/Logoff icon in the UNICORN Manager. 
2	Select your username in the list.
3	Type your password (optional).
4	Click OK .

The four program windows

The program has four windows or modules. When you start the program and log on you work in the **UNICORN Manager**. UNICORN also automatically opens the **Method Editor**, the **System Control** and the **Evaluation** modules. These modules are minimized until you activate them.

Log off after you are finished

Always log off when you leave the computer to prevent others from accidentally changing or deleting your files, or disturbing your method runs. There are two ways to log off:

- Select **Tools:Logoff**.

or

- Click the **Logon/Logoff** icon.



4 How to create a method

Introduction Chromatography runs are programmed as **Methods** in UNICORN. Before you can proceed with a chromatography run you need either to use an existing method or create a new method. This chapter describes two different ways to create new methods.

In this chapter This chapter contains the sections below.

Topic	See
How to use the Method Wizard	4.1
How to use text instructions	4.2

4.1 How to use the Method Wizard

Introduction

This section describes how to use the **Method Wizard** to create a new method. For most purposes, customized methods can be created simply by setting appropriate values for the method variables.

Are wizards always available?


Wizards are available for **AKTAdesign** systems delivered with standard strategies. If your system is a process systems please refer to the system documentation.

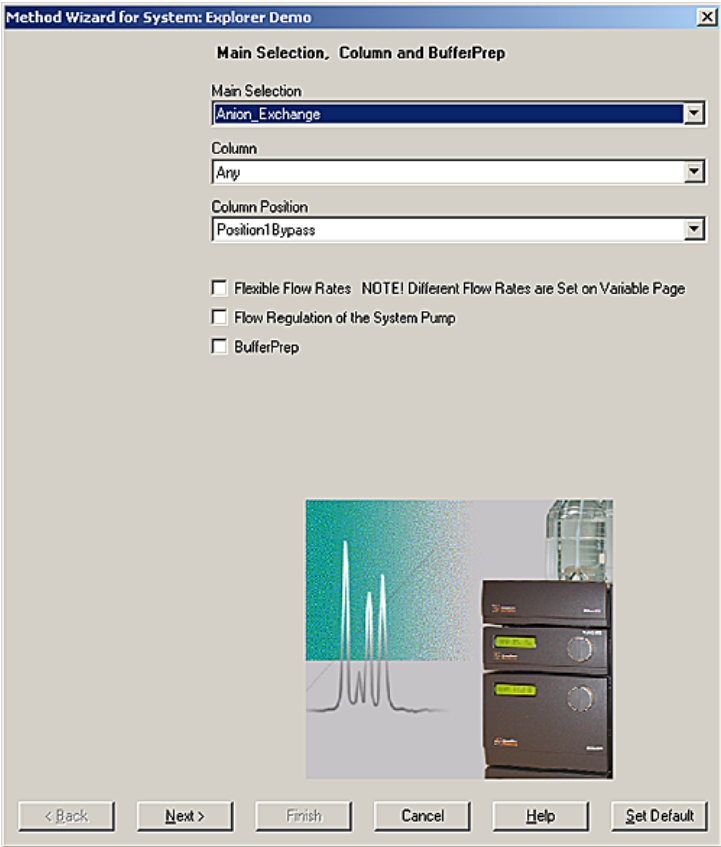
How does the wizard work?

The **Method Wizard** consists of a number of dialog boxes in which you answer questions and receive instructions on how to create your method. The options in subsequent boxes depend on the choices you have made in the initial dialog box.

How to create a new method

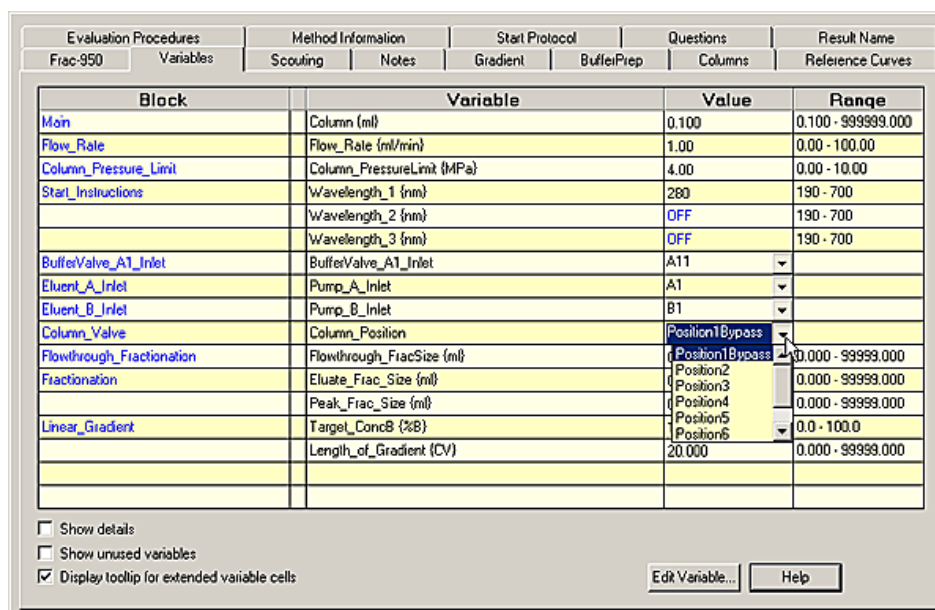
The table below describes an example of how to create a method with the **Method Wizard**.

Step	Action
1	<p>Click the Method Wizard icon in the Method Editor module.</p>  <p><i>Result:</i> The Method Wizard dialog box appears.</p> <p><i>Note:</i> If several systems are available you must first select which system you want to use.</p>

Step	Action
2	<p>Select the appropriate parameter values and click Next.</p>  <p><i>Note:</i> Click Set Default to restore all settings to the default values.</p>
3	<p>On each new dialog page, select the appropriate parameter values and click Next to continue.</p>
4	<p>Click Finish in the last window.</p> <p><i>Result:</i> Run Setup opens.</p>

The Run Setup

The **Run Setup** consists of a number of tab pages. Click the tabs at the top of the dialog box to select a tab page.



Run Setup Variables

The method is represented by a number of blocks on the **Variables** tab. The blocks are typical steps in a chromatographic run.

Each block contains a number of **Variables**, with suitable default values that can be changed to suit your application. Some values are normally hidden. Click the checkbox **Show Details** to display hidden variables.

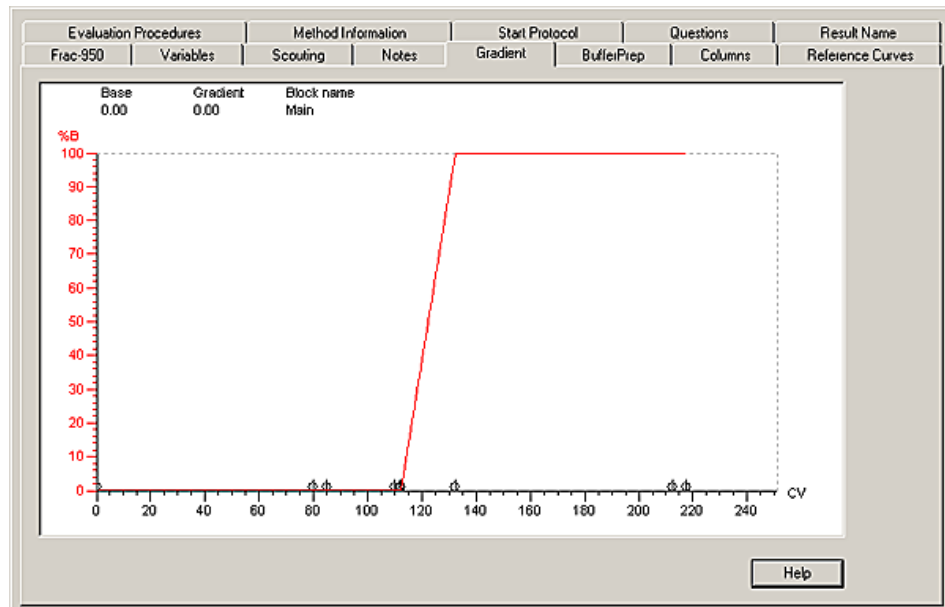
Default values

When you select a column, default values will be set for:

- The correct column volume.
- The recommended flow rate.
- The correct pressure limit.

Note: If you exceed the recommended values for the selected column you will receive a warning when you save your method.

The Gradient page The **Gradient** tab shows the method graphically:



The length of each block is marked at the bottom of the graph.

- Click the x-axis to view the method in time, volume or column volumes (CV).

The Start Protocol The **Start Protocol** tab shows the items that will be displayed as dialog boxes in the **Run Setup** sequence.

- Click the checkboxes for the items that you want to select.

How to save your method

Before you can run your method you must save it.

- Select **File:Save**.

or

- Click the **Save** icon.



4.2 How to use text instructions

Introduction Sometimes you need more advanced editing facilities, which are available when you work directly in the **Text Instructions Editor** in the **Method Editor**. This section is a brief description of this process.


The Text Instructions Editor You can use the **Text Instructions** in the **Method Editor** to build your method step by step. You can also use the editor to modify instructions in methods created by wizards or based on templates.

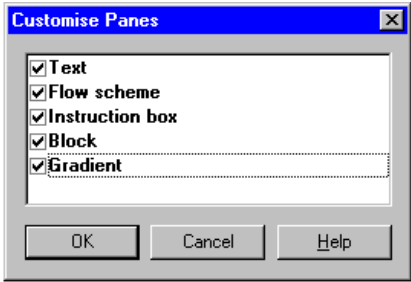
When do I use Text Instructions? Use text instructions when you want to:

- change selected instructions in the method, e.g. the outlet valve position,
- add blocks or instructions, e.g. **Watch** instructions,
- change method instructions to adapt to non-standard system configurations,
- create new methods for applications not covered by the supplied templates or wizards.

Valid instructions The system strategy determines the available instructions. A method that is developed for one system may not be valid for another.

How to open the Editor The table below describes how to open the **Text Instructions Editor**.

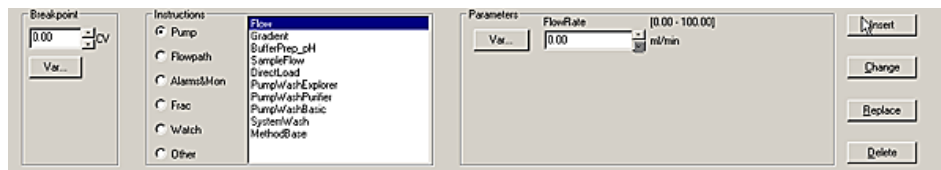
Step	Action
1	Select the Method Editor module.
2	Select File:New . <i>Result:</i> The New Method dialog opens.
3	<ul style="list-style-type: none"> • Select a system (if more than one is available) • Select Method Editor and click OK. <i>Result:</i> The Method Editor module opens in text edit mode.
4	Proceed with step 5 and 6 if the screen is blank.
5	Click the Customise Panes icon. 

Step	Action
6	Select Text and Instruction Box and click OK . 

How to enter Text Instructions

The text instructions are selected in the **Instruction box** in the lower part of the **Method Editor**. Applicable parameters can be edited for each selection. Use the buttons to **Insert**, **Change**, **Replace** or **Delete** the selected instructions. All text entries are shown in the **Text** pane.

The illustration below shows the **Instruction box**:



5 How to perform method runs

Introduction

Once you have a defined method in place you can perform a method run. You can monitor its progress in the **System Control** module. This chapter describes how to perform the method run, the data display, how you can focus on the information you are interested in and make adjustments while the method run is in progress.

In this chapter

This chapter contains the sections below.

Topic	See
How to run your method	5.1
The System Control module	5.2
How to change the way your run is displayed	5.3
Manual control	5.4

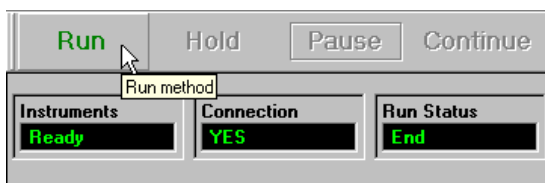
5.1 How to run your method

Introduction

Follow the instructions in this section if you want to start a separation run based on the method you created and saved in the previous chapter. Also use this procedure if you want to run other methods.

Connect to the system

Before you can start a run, you must connect to the system. Open the **System Control** window and look at the **Connection** panel in the **Run Data** section. If you are not connected the panel will show the text **NO**. Once you are connected the text changes to **YES**. Refer to the User Reference Manual if your system is not connected.




Prepare the system

After the system is connected it must be prepared. Verify that this already has been done or refer to your system documentation for the correct procedure.

How to start a method run

You initiate the method run in a series of dialog boxes in the **Run Setup** in the **System Control** module. The **Start Protocol** for the method decides which pages you need to fill in. The steps in the table below is an example of a **Run Setup** sequence. When you are finished in one dialog box you click **Next** to proceed.

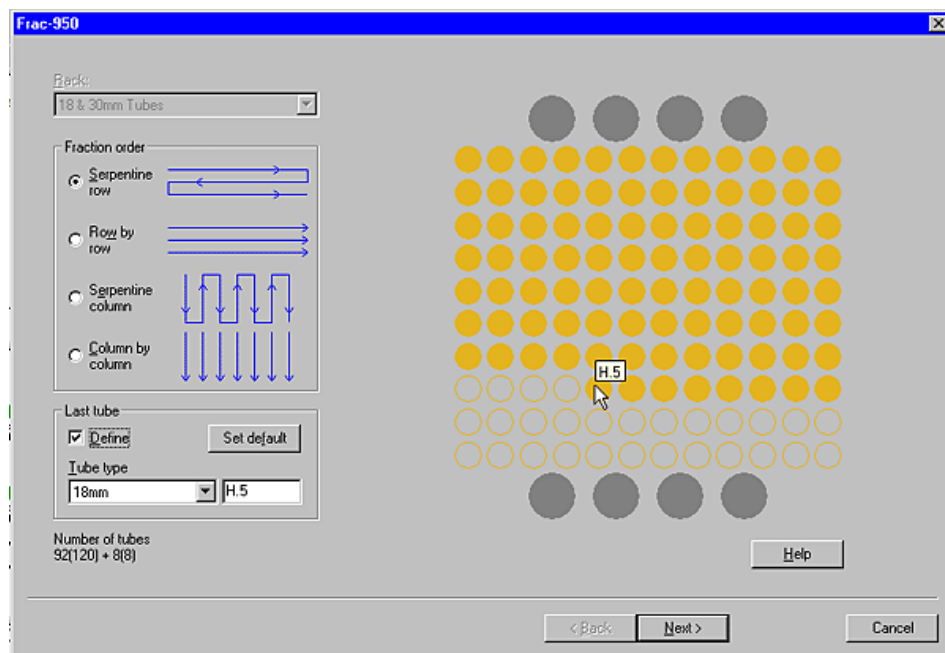
Step	Action
1	<ul style="list-style-type: none"> Select the File:Run menu command <p><i>or</i></p> <ul style="list-style-type: none"> click the Run toolbar icon. 
2	The Run Setup opens. Select a method and click OK .
3	If your method run involves a fraction collector, i.e. Frac-950, the first step is usually the setup dialog box. See "How to set up Frac-950" below.
4	The Variables dialog box opens next. Verify and fine tune your method before you proceed.
5	In the Notes dialog box some information can already be present. Click the Start Notes tab and add your own comments.

Step	Action
6	In the Questions dialog box some questions may be mandatory and must be answered before you can start.
7	In Evaluation Procedures you select the automated operations you want the system to perform after the UNICORN run. Select Print_Chromatogram for an automatic print-out after the run.
8	The Method Information page is a summary of information about the run. Click Next to proceed to name your result file and define where it should be stored.

How to set up Frac-950

In the **Frac-950** setup dialog box you can define the order of fractionation and set up the last tube. The system will be paused when the last tube is reached and the fractionation will stop.

The illustration below shows the **Frac-950** setup dialog box:



How to name the result file

The final step before starting is to name your result file and define where it should be stored. The default file name is defined in the **Result Name** page of the **Run Setup**. By default the result file name will either be the same name as the method, the date of the run or a pre-defined name. The name is followed by a three-digit sequence number starting with 001. You can change this name and select a new directory by clicking **Browse**.

You can also select to have the software add a unique identifier to the file name.

How to start the method run

Click the **START** button in the **Result Name** dialog box. This will initiate the method run and you can follow its progress in the **System Control** module.


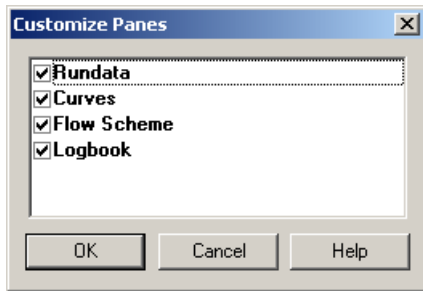
5.2 The System Control module

Introduction

All data on your separation run are displayed in the **System Control** module. You have a choice of four different panes that can be open one at a time or all at once in separate parts of the window.

How to select displays

The table below describes how to select the panes that are displayed in the **System Control** module.

Step	Action
1	<ul style="list-style-type: none"> Select the View:Panes menu command. <p><i>or</i></p> <ul style="list-style-type: none"> Click the Customise Panes icon. 
2	Click the check boxes for the panes that you want to display. 
3	Click OK .

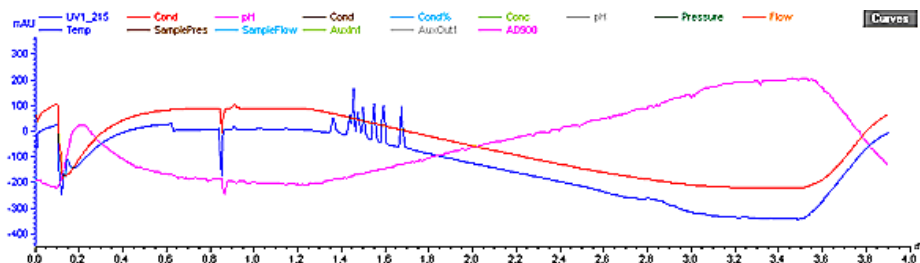
The Run Data pane

The **Run Data** pane shows the current values for the running parameters. When the system is running, the text **Run** is displayed in the **Run Status** panel. If the system is operated manually the text **Manual** is displayed. The illustration below shows only part of the **Run Data** pane.



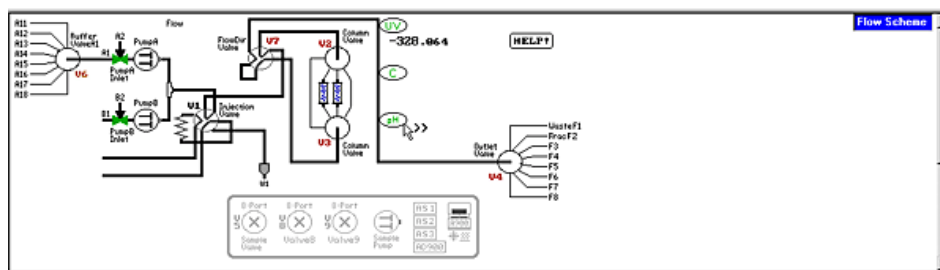
The Curve Data pane

The **Curve Data** pane shows selected monitor signals as curves during your method run. All curves are stored in the result file. Normally the curves are scaled with auto scaling, i.e. the scale is adjusted continually to the highest and lowest values for each curve.



The Flow Scheme pane

The **Flow Scheme** pane shows a schematic view of your system configuration.



The Logbook pane

The **Logbook** pane is shown at the bottom. The **Logbook** shows exactly when the instructions in the method were executed during the run. It also shows all manual instructions that were performed and all alarms and warnings that were registered.

```

0.00 min Method Run 3/26/2002 8:47:16 AM, Method: idtest, Result: v:\Niklas\idtest001.res
0.00 min Batch ID: 4E9820F4-380A-11D6-AC46-00D0B72BBCC0
0.00 min Base CV: 0.10 (ml)
0.05 min Block Flow_Rate
0.05 min Base SameAsMain
0.05 min Flow 1.00 ml/min
0.05 min End Block
0.05 min Block Column_Pressure_Limit
0.05 min Base SameAsMain
0.05 min Alarm_Pressure Enabled, 400 MPa, 0.00 MPa
0.05 min End Block
0.05 min Block Start_Instructions
0.05 min Base SameAsMain
0.05 min Wavelength 280 nm, OFF, OFF
0.05 min AveragingTimeUV 2.56 sec
0.05 min End Block
0.05 min Block BufferValve_A1_Inlet
    
```

How to view a single pane

If you want....	then....
to enlarge a pane	right-click and select Maximize .
to return to the original size	right-click and select Restore .

5.3 How to change the way your run is displayed

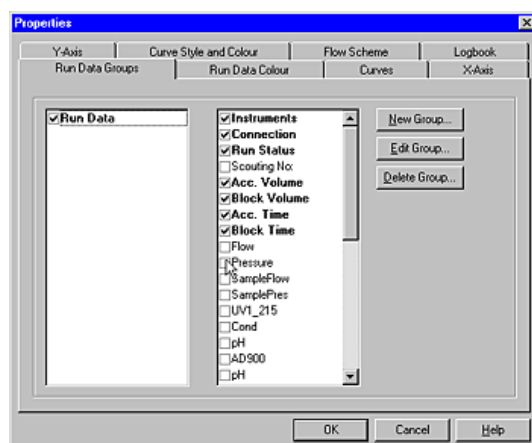
Introduction

There are a number of ways to change the way your method run data is displayed in the **System Control** module. This section describes a few of the options.

How to edit the pane displays

The table below describes how to open the **Properties** dialog box to edit the way the panes are displayed.

Step	Action
1	Right-click in the pane you want to edit.
2	Select Properties from the menu.
3	Click the tab for the pane you want to edit. <i>Result:</i> The page shows all the options that you can select in this particular pane. You also have a choice of different styles, colors and axis layouts for your curves.



How to change the Y-axis scale display

You can select which curve the Y-axis scale refers to in two different ways:

- Click the curve name at the top of the **Curve Data** pane.

or

- Click the Y-axis scale to toggle between the curve scales.

How to set fixed values for the Y-axis

The table below describes how to set a fixed value range for the Y-axis for a selected curve in the **Properties** dialog box.

Step	Action
1	Click the Y-axis tab.

Step	Action
2	Click the curve you want to edit.
3	Click the Fixed radio button.
4	Type a minimum and a maximum value. The maximum range values allowed are shown above the entry boxes.
5	Repeat steps 2 to 4 for all other curves you want to edit.
6	Click OK .

5.4 Manual control

Introduction

In some applications you may want to change some parameters manually during a run. This section exemplifies how you can change the pump flow manually.

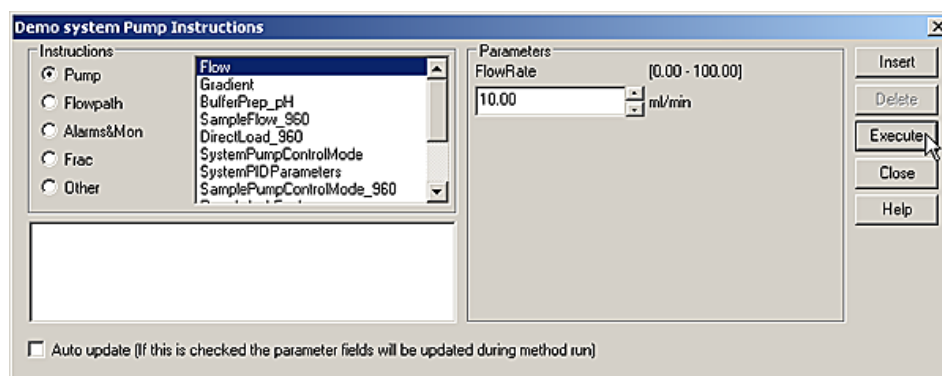
How to change the pump flow

The table below describes how to change the pump flow.

Step	Action
1	Select Manual:Pump . <i>Result:</i> the System Pump Instructions dialog box opens The Pump radio button is selected.
2	Click the function you want to change, i.e. Flow .
3	Enter a new value (FlowRate) under Parameters . You can use the arrows to step the value up or down.
4	<ul style="list-style-type: none"> Click Execute to execute the instruction immediately. <p>or</p> <ul style="list-style-type: none"> Click Insert to add the instruction to the list below the instructions menu. <p><i>Note:</i> If there are instructions on the list, the Execute button will execute all instructions on the list at the same time.</p>
5	Click Close to close the dialog box.

The System Pump Instructions box

The illustration below shows the **System Pump Instructions** dialog box:



Note: The parameter values will be updated continually during the run if the **Auto update** checkbox is selected.

How to end your run manually

Click the **End** button to end the method run before it is finished. You can save the partial result the same way that you save a completed run.



6 Scouting

Introduction You can use **Scouting** to automatically repeat a series of method runs with a systematic variation of one or more parameters. This chapter gives an example of how to use **Scouting**.

In this chapter This chapter contains the section below.

Topic	See
How to set up a Scouting Scheme	6.1

6.1 How to set up a Scouting Scheme

Introduction

When you prepare your method you can define a number of variables in the method for **Scouting**. The definition of how the series of method runs will be performed is called a **Scouting Scheme**.

When to use Scouting

You can use **Scouting** for example:

- to screen for the best column,
- to find the optimal pH,
- to test column capacity (sample volume),
- to find the optimal flow rate for binding and elution,
- to optimize gradient length and slope.

Before you start

Scouting Schemes are defined in the **Run Setup** in the **Method Editor**. Before you can start you need to create a new method, for example by using a method wizard. You can also add a **Scouting Scheme** to an existing method.

Note: Variables must be defined for **Scouting**.

Example: Flow-Rate Scouting

The table below describes how to set up a **Scouting Scheme**.

Step	Action
1	Click the Scouting tab in the Run Setup . <i>Result:</i> A Scouting Variables dialog box opens.
2	<ul style="list-style-type: none">• Click the checkbox for the variable Flow_Rate and any other variable you wish to scout, e.g. BufferPrep_pH.• Click OK. <i>Result:</i> The selected scouting variables will appear in a column.
3	Click Add to create a second column for the next run. This column will have the same values as the previous column.
4	Change variable values in the same manner as on the Variables page. See 4.1 How to use the Method Wizard on page 24
6	Repeat steps 3 and 4 until you have defined all the runs you require.
7	Select the File:Save menu command.

7 How to view results

Introduction This chapter describes how to view the results from your method run in the **Evaluation** module.

In this chapter This chapter contains the sections below.

Topic	See
How to view and edit a result layout	7.1
How to view the run documentation	7.2
How to compare curves	7.3

7.1 How to view and edit your result layout

Introduction

This section describes the basics of how to view and edit the layout of your results in the **Evaluation** module.

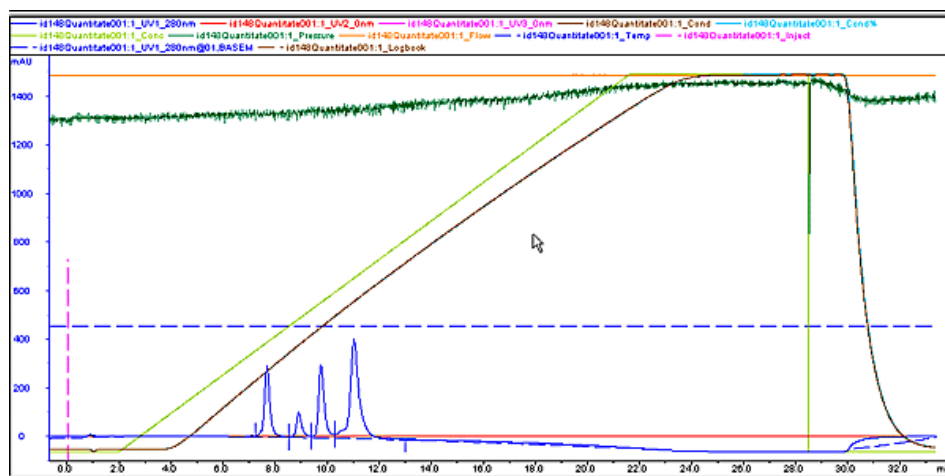
How to open the result file

The table below describes how to view the results.

Step	Action
1	Complete the method run.
2	Locate the result file in the Results pane in the UNICORN Manager module.
3	Double-click the file. <i>Result:</i> The file opens in the Evaluation module.

The Raw Chromatogram Data

The result file is opened in a **Chromatogram** window. The default view shows all the curves as in the illustration below.



How to change the chromatogram layout

The table below describes how to change the layout of the **Chromatogram** display.

Step	Action
1	Right-click in the Chromatogram window and select Properties . <i>Result:</i> The Chromatogram Layout dialog box opens.
2	Click the Curve tab.
3	Click the check-boxes to de-select the curves that you do not want to display.

Step	Action
4	Click OK .

Raw data curves are saved

Your selections determine the curves that are displayed in the **Chromatogram** window and shown on printouts.

Note: The original raw data curves can never be modified, renamed or deleted from the result file.

How to change the Y-axis scale

Normally the curves are auto scaled, i.e. the highest and lowest values for each curve set the scale. The table below describes how to change auto scaled Y-axis scales to fixed values in the **Chromatogram Layout** dialog box.

Step	Action
1	Click the Y-axis tab.
2	Click the curve you want to edit.
3	Click the Fixed radio button.
4	Enter new minimum and maximum values.
5	Repeat steps 2 to 4 for all other curves you want to edit.
6	Click OK to execute the changes and close the window.

How to change the Y-axis scale display

You can select which curve the Y-axis scale refers to in two different ways:

- Click the curve name at the top of the **Curve Data** window.

or

- Click the Y-axis scale to toggle between the curve scales.

How to view curve details

The table below describes how you can zoom in on a curve to view more details.

Step	Action
1	Place your cursor in a corner of the area you want to enlarge.
2	Press and hold the left mouse button and drag diagonally over the area. <i>Result:</i> A rectangle appears.
3	Release the mouse button. <i>Result:</i> The area within the rectangle is enlarged.

Step	Action
4	Repeat steps 1 - 3 to enlarge the selected area further.
5	Right-click and select Undo Zoom to zoom out one step.
6	Right-click and select Reset Zoom to return to the full window view.

How to save a layout

You can save your edited layout. It can be applied later to any result file. Follow the steps in the table below.

Step	Action
1	Right-click and select Properties to open the Chromatogram layout dialog box.
2	Select the Layout library tab.
3	Click the Save current layout as... button.
4	Enter a name for the layout and click OK .

How to apply a saved layout

Select a layout from the **Saved layouts** list in the **Layout library**. Click the **Apply selected layout** button.

7.2 How to view the run documentation

Introduction

The full documentation of a method run is stored in the result file. You can view this information in the **Documentation** dialog box in the **Evaluation** module. This section gives an example of how to view the **Logbook**.

How to open the run documentation

Maximize the **Evaluation** module and either:

- Select the **View:Documentation** menu command

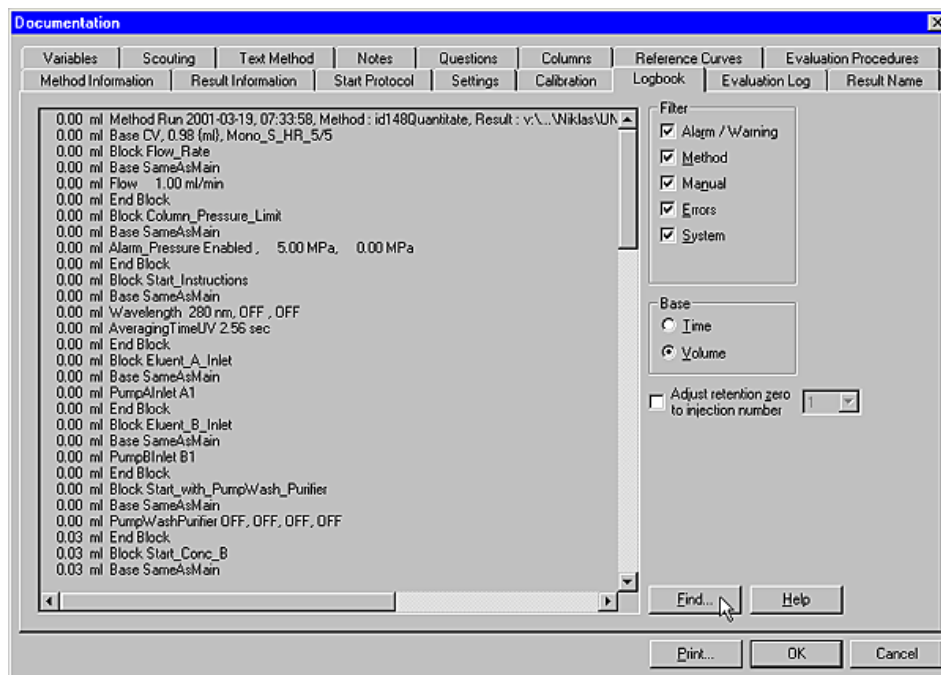
or

- Click the **View Documentation** icon.



The documentation window

This is an illustration of the **Documentation** dialog box with the **Logbook** tab selected. Click the tabs to view other information.



7.3 How to compare curves

Introduction

You can import or copy curves from different method runs into one chromatogram for comparison. This section is an example of how you can use the function **Open to compare** to import curves.

Open the dialog box

First open the dialog box **Open Curves to Compare**. You can either:

- Select **File:Open to compare:Curves**.

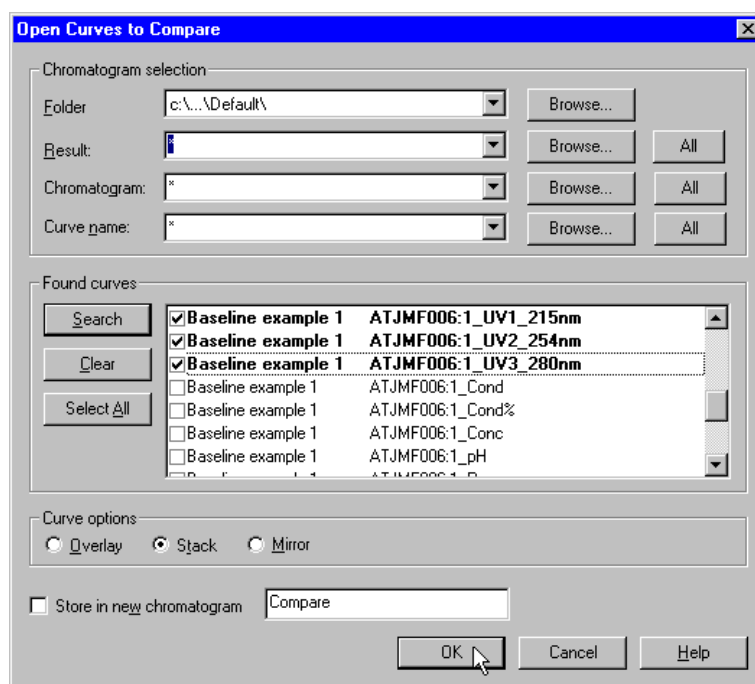
or

- Click the **Open curves to compare** icon.



The Open curves to compare dialog box

The illustration below shows the dialog box **Open Curves to Compare**.



How to import the curves

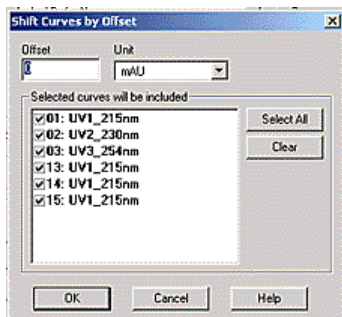
The table below describes how to import curves and store them in a new chromatogram.

Step	Action
1	Define search criteria for the folder, result, chromatogram and/or curve name. Use the Browse command buttons.

Step	Action
2	Click Search . <i>Result:</i> A list of found curves is displayed.
3	Repeat step 1 - 2 to add more curves to the list.
4	<ul style="list-style-type: none"> Select the individual curves that you want to import. <p>or</p> <ul style="list-style-type: none"> Click Select all to import all curves.
5	Click the checkbox Store in new chromatogram and enter a name in the text box (Compare is default). <i>Note:</i> You can also save the curves in the active chromatogram.
6	Select one of the Curve options: Overlay, Stack or Mirror . <i>Result:</i> This will decide how the curves are displayed.
7	Click OK .

How to set the stack offset

If you selected the **Stack** option the **Shift Curves by Offset** dialog box is opened automatically. Adjust the offset distance between the curves to a suitable value.



8 How to print your chromatograms

Introduction This chapter describes how to print open chromatograms. Proceed to **10 How to create and print reports** on page 57 if you want to add text information to your prints or create a complete report.

In this chapter This chapter contains the section below.


Topic	See
How to print active chromatograms	8.1

8.1 How to print active chromatograms

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

Before you print Open all chromatograms that you want to print in the **Evaluation** module before you proceed.

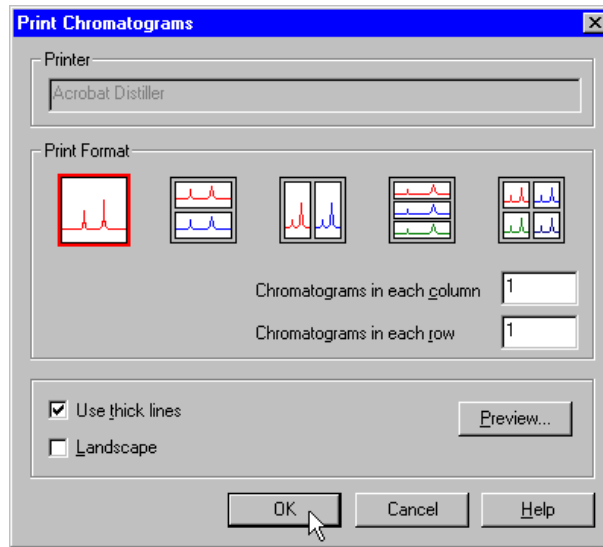
How to print The table below describes how to print active chromatograms.

Step	Action
1	<ul style="list-style-type: none">• Select the File:Print menu command. <p><i>or</i></p> <ul style="list-style-type: none">• Click the Print icon.  <p><i>Result:</i> The Print Chromatograms dialog box opens.</p>
2	Select print formats and layout options.
3	Click Preview . Result: The Customise Report window opens.
4	<ul style="list-style-type: none">• Verify that the layout is correct.• Click Edit Mode to make changes, e.g. change the order of the chromatograms. Click Preview to return to preview mode.• Click Exit to return to the Print Chromatograms dialog box.
5	Click OK .

The Print Chromatograms dialog box

This is an illustration of the **Print Chromatograms** dialog box.

Note: The selected print format is outlined in red.



9 How to evaluate and save the results

Introduction This chapter describes how to perform basic evaluation procedures and how to save the results of the evaluations.

In this chapter This chapter contains the sections below.

Topic	See
How to perform a basic peak integration	9.1
How to save the results	9.2

9.1 How to perform a basic peak integration

Introduction Peak integration is used to identify and measure curve characteristics, including peak areas, retention times and peak widths.


Baseline calculations A correct baseline must be calculated before the peak areas can be calculated. There are several alternative ways to perform this calculation:

- use automatic calculation,
- subtract a blank run curve from the source curve,
- use a **Zero baseline**, i.e. no baseline subtraction at all,
- re-use an existing baseline,
- edit a baseline manually from any curve in the chromatogram.

The default options are used for the example in this section, i.e. automatic calculation (**Calculate baseline**) with a **Morphological** algorithm.

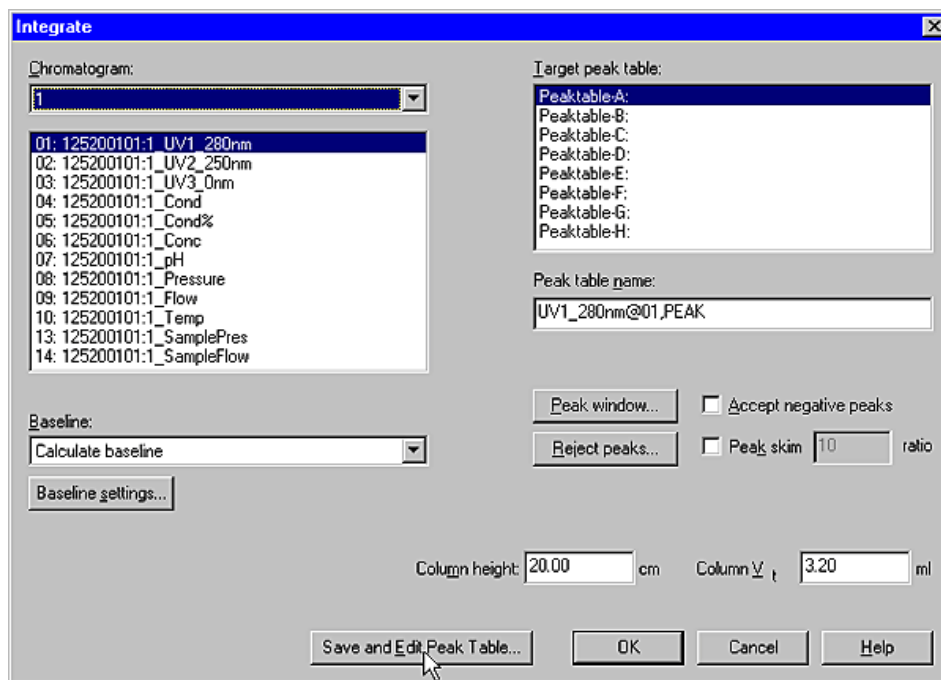
How to perform the peak integration

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

Step	Action
1	<ul style="list-style-type: none"> • Select the Integrate:Peak Integrate menu command. <p><i>or</i></p> <ul style="list-style-type: none"> • Click the Peak Integrate icon.  <p><i>Result:</i> The Integrate dialog box opens.</p>
2	Select a source curve.
3	Select a peak table destination from the Target peak table list.
4	Select Calculate baseline in the Baseline list.
5	Click OK .

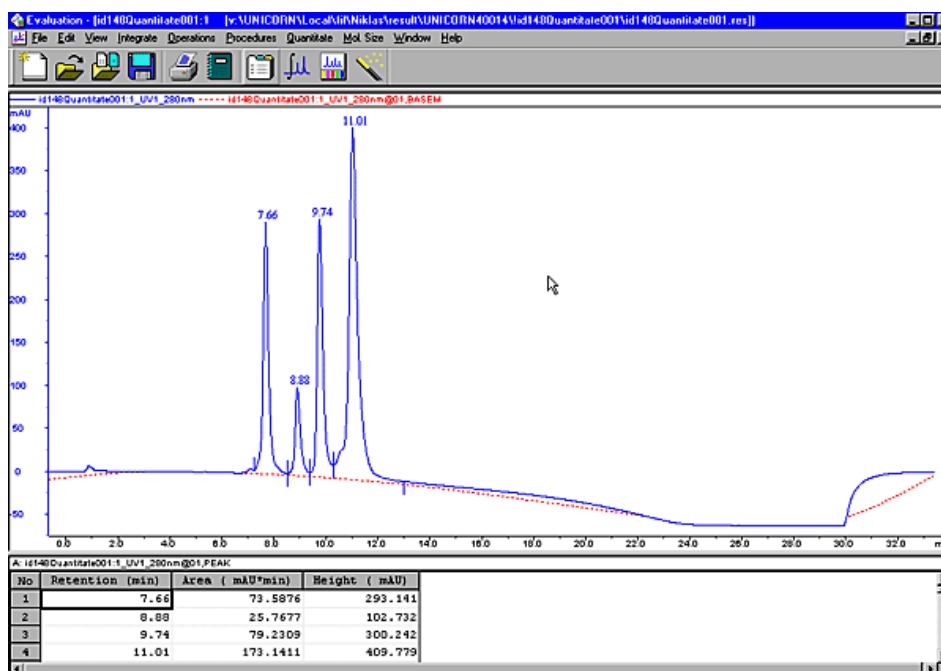
The Integrate dialog box

This is an illustration of the **Integrate** dialog box.



Peak integration results

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



Note: 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**.

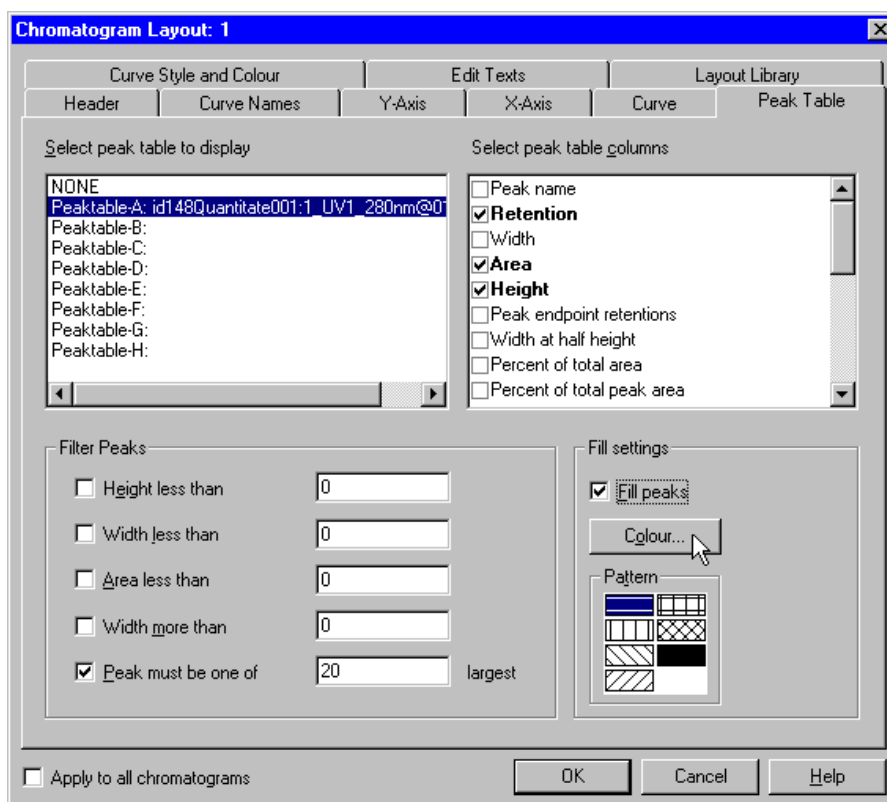
How to display peak characteristics

The peaks in the integrated chromatogram are automatically labelled with their retention times. Several other peak characteristics are also calculated automatically. The table below describes how to display other characteristics.

Step	Action
1	Right-click in the active chromatogram.
2	Select Properties . <i>Result:</i> The Chromatogram Layout dialog box opens.
3	Click the Peak Table tab.
4	Select the options that you want to display from the Select peak table columns list. <i>Result:</i> The selected items will be displayed in the peak table.
5	Click OK .

The Peak Table dialog box

This is an illustration of the **Peak Table** dialog box.



9.2 How to save the results

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. Some of these curves may not be needed anymore.

- Select **Edit:Delete:Curves** to remove all unwanted 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 results in the original file or in a new result file.

If you want to save...	then...
in the original result file	<ul style="list-style-type: none">• choose File:Save <p><i>or</i></p> <ul style="list-style-type: none">• click the Save icon. 
in a new result file	<ul style="list-style-type: none">• choose File:Save as.

10 How to create and print reports

Introduction The **Evaluation** module provides extensive tools to create detailed reports. This chapter describes how to create reports.

In this chapter This chapter contains the sections below.

Topic	See
How to print an existing report format	10.1
How to edit an existing report format	10.2
How to create and print a customized report format	10.3


10.1 How to print an existing report format

Introduction

This section describes how to use an existing report format to print a basic report with a chromatogram and text.

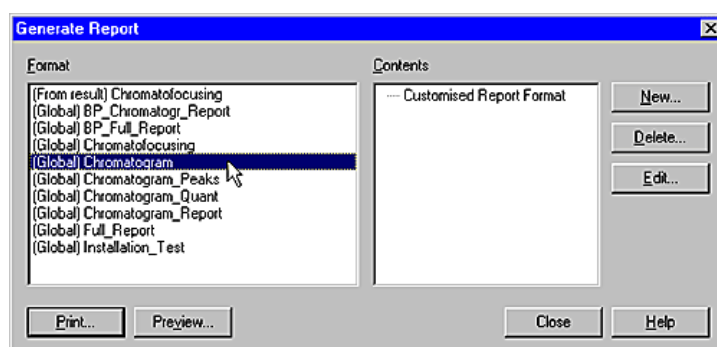
How to print a report

The table below describes how to print a report.

Step	Action
1	<ul style="list-style-type: none">Choose File:Report. <p>or</p> <ul style="list-style-type: none">Click the Report icon.  <p><i>Result:</i> The Generate Report dialog box opens.</p>
2	Select format (Global) Chromatogram . <i>Result:</i> This creates a report containing the chromatogram and the answers to the questions from the Run Setup Questions page.
3	Click Print . <i>Result:</i> The Print dialog box opens.
4	Click OK .

The Generate Report dialog box

This is an illustration of the **Generate Report** dialog box.




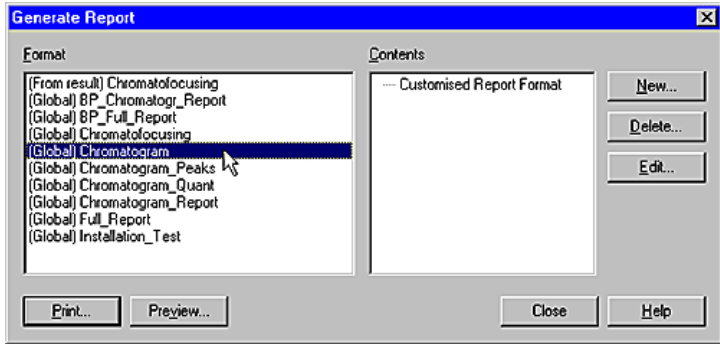
10.2 How to edit an existing report format

Introduction

This section describes how to open an existing report format to edit the items that are included in the report.


How to open and edit a report format

The table below describes how to open and edit a report format.

Step	Action
1	<ul style="list-style-type: none"> Choose File:Report <p>or</p> <ul style="list-style-type: none"> Click the Report icon.  <p><i>Result:</i> The Generate Report dialog box opens.</p> 
2	Select a report format.
3	<ul style="list-style-type: none"> Click Edit. <p><i>Result:</i> The Customize Report window opens in edit mode.</p>
4	<ul style="list-style-type: none"> Double-click an item that you want to edit in the report. <p><i>Result:</i> A Setup dialog box specific for the item opens.</p>
5	<ul style="list-style-type: none"> Edit the item. Repeat step 4 for all other items you want to edit.

How to apply the report format

Once you have finished editing the report items you can apply the format.

If you want to...	then...
to print the report	<ul style="list-style-type: none">click the Print icon. 
to preview the changed report layout	<ul style="list-style-type: none">click the Preview button.
to save the format	<ul style="list-style-type: none">choose File:Save As and enter a name for the report format.


10.3 How to create and print a customized report format

Introduction

You can select a number of different objects (including chromatograms, methods, images, free text etc.) and create a customized report format. The objects can be aligned, re-sized and positioned to fit your specific layout. This section describes only some of the formatting options.

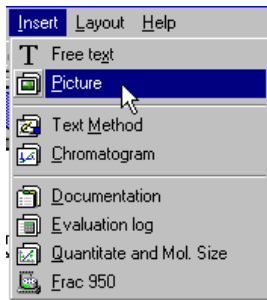
How to create a new report format

The table below describes how to create a new customized report format.

Step	Action
1	<ul style="list-style-type: none"> Choose File:Report. <p>or</p> <ul style="list-style-type: none"> Click the Report icon.  <p><i>Result:</i> The Generate Report dialog box opens.</p>
2	<p>Click the New button.</p> <p><i>Result:</i> The Create New Report Format dialog box opens.</p>
3	<p>Choose Customised Format and click OK.</p> <p><i>Result:</i> The Customise Report window opens.</p>
4	<p>Proceed to "How to add items to the empty report".</p>

How to add items to the report

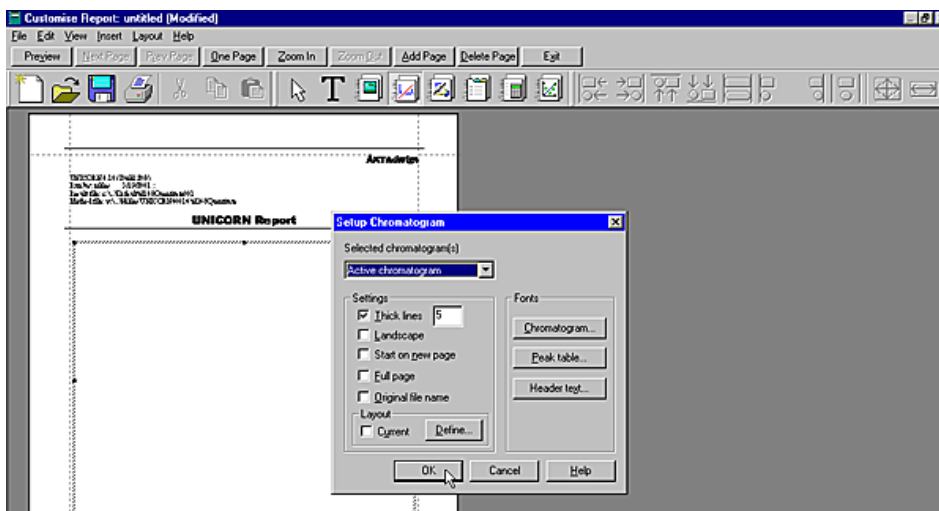
The table below describes how to add items to your empty report format.

Step	Action
1	<p>Select an information item.</p> <ul style="list-style-type: none"> Click one of the item icons in the toolbar. <p>or</p> <ul style="list-style-type: none"> Select an item from the Insert menu. 

Step	Action
2	Press and hold down the left mouse button, and drag out a box to the size of the item you want to insert. <i>Note:</i> The mouse pointer shows a symbol for the type of item you have selected.
3	Release the mouse button. <i>Result:</i> A Setup dialog box opens. The dialog box is specific to the type of item that you want to insert.
4	Select the options you want.
5	Click OK .
6	Repeat steps 1 to 5 for each new item you want to insert.
7	Click Preview to view the final results.

The Setup Chromatogram dialog box

The illustration below shows the **Setup Chromatogram** dialog box in the **Customise Report** window.



How to set up the page format

The table below describes how to set up the page formatting.

Step	Action
1	Double-click anywhere in the Customise Report window. <i>Result:</i> The Page Setup dialog box opens.
2	Click the Page Setup tab and enter values for all Margins .
3	Click the First Header tab and select the items that you want to include in the first page header.

Step	Action
4	Click the Footer tab and select the items that you want to include in the footer.
5	Click the Header tab and select the items that you want to include in the header. <i>Note:</i> This tab is not available if you selected Same header on all pages in the Page Setup tab.

The Page Setup dialog box

The illustration below shows the **First Header** tab in the **Page Setup** dialog box.

