

PrepCon

Abgelaufene Zeit: 00:00:00

Lösemittel A: 100.0 %

Lösemittel B: 0.0 %

Lösemittel C: 0.0 %

Lösemittel D: 0.0 %

Pumpen Status: EIN

Flussrate: 200.00 ml

Volumen: 58.42 ml

Druck: 40.1 Bar

Fraktion Nr.: 1

Channel 1: 0.096 mV

Channel 2: 0.059 mV

Channel 3: 0.028 mV

Channel 4: 0.047 mV

Fraktionslimit: EIN

Ventilsteuerung: Ventil 1 - Positiv

Probe Nr.:

# PrepCon5

Chromatogramm

Peakkerl

Kein Peakfenster

Maximum

Peak

Schulter

Tal

Start

Ende

Lösemittelvorrat

A B C D Waste

Schließen Mehr Details >>

PrepCon Zeitablen-Editor (TimeControlExample.tcf)

Zeit (Min)	Funktion	Parameter
0.00	Komposition Hauptpumpe(n)	90.0 , 10.0 , 0.0 , 0.0
0.00	Flussrate Hauptpumpe(n)	100.00 ml/min Konstantfluss
0.00	Fraktionslimit	Limit = 140.00 ml
0.00	Temperatur	Column Oven = 25 °C
0.00	Temperatur	Sample Heater = 25 °C
0.00	Ventilposition	Waste / Fraction Valve = 'Waste Injection'
0.10	Beschreibung	
0.10	Injektion Probengeber	
0.18	Event Box Ausgang	Ausgang 1 = PULS
0.20	Start Chromatogramm	Kanal 1,2,P (500 ms)
0.75	Komposition Hauptpumpe(n)	90.0 , 10.0 , 0.0 , 0.0
1.99	Schwellwert	1.03 Min / 59.06 mV

TimeControlExample.tcf

Resultat

Zeit (Min)	Funktion	Parameter
0.00	Komposition Hauptpumpe(n)	10.0 , 90.0 , 0.0 , 0.0
0.00	Flussrate Hauptpumpe(n)	1.03 Min / 59.06 mV
0.00	Fraktionslimit	0.58 Min / 55.84 mV
0.00	Temperatur	0.32 Min / 173.08 mV
0.00	Temperatur	0.60 Min / 44.64 mV
0.00	Ventilposition	
0.10	Beschreibung	
0.10	Injektion Probengeber	
0.18	Event Box Ausgang	
0.20	Start Chromatogramm	Kanal 1,2,P (500 ms)
0.75	Komposition Hauptpumpe(n)	90.0 , 10.0 , 0.0 , 0.0
1.99	Schwellwert	1.03 Min / 59.06 mV
3.33	Schwellwert	0.58 Min / 55.84 mV
3.43	Peaküberwachung	0.32 Min / 173.08 mV
5.55	Schwellwert	0.60 Min / 44.64 mV
6.50	Komposition Hauptpumpe(n)	10.0 , 90.0 , 0.0 , 0.0

Fraktionsrack (Vario4000-Prep.rck)

1	20	21	40	41	60
2	19	22	39	42	59
3	18	23	38	43	58
4	17	24	37	44	57
5	16	25	36	45	56
6	15	26	35	46	55
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# Manual



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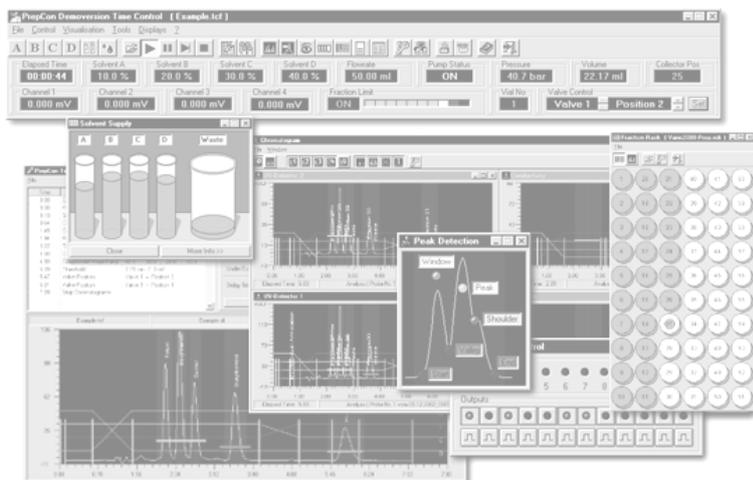
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## 2. Introduction

As a preparative data and control system, PrepCon meets all the requirements of an up-to-date program for use in preparative chromatography. Its superior flexibility and modular construction mean that the program can be adapted to suit any user's system. As a further development of the previous versions of the program, PrepCon 5 has the added advantages of a simpler user interface and improved method construction. All the advantages of networks can be exploited without restrictions. National and international regulations, such as 21 CFR Part 11, are fully supported.



The program allows isocratic elution of up to four solvents, gradient programming and gradient support. Switching valves and fraction collectors can be controlled by time, threshold values or automatic peak sampling. Eluent programming can be carried out in units of time, units of volume of the solvent supported or in units of column volume.

The screen displays the pump condition, flow rate, pressure, the solvent being pumped, solvent supply, detector signals and valve positions. The entire run is displayed in a visualisation diagram of the system, which can be individually formatted, and in a time control file which indicates the stage in progress at all times.

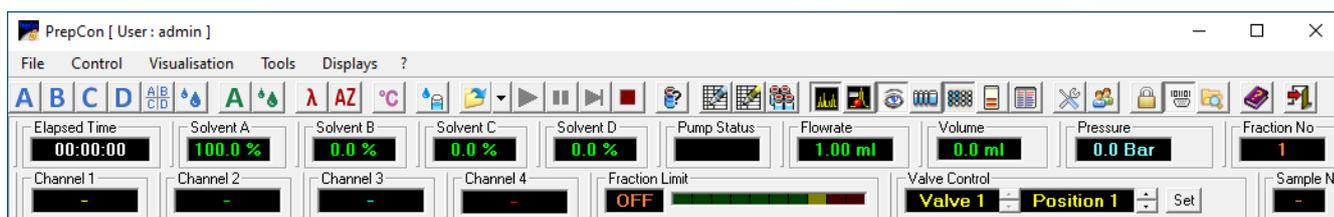
The display settings and function buttons in the main window can be personalized by the user.

The screen keys and visualisation diagram of the system allow manual control of the pumps and valves.

During the flow of a preparative eluent, the functions of the time control file can be adjusted using a graphic time control editor. This allows compensation for retention time shifts.

The results data from a run includes all the chromatograms recorded, with integration results, the time control tables, the autosampling table, a protocol of the entire run and a fraction table with links to the fraction rack and the appropriate chromatograms. Thus PrepCon 5 allows the user to re-establish all the relevant information needed to reproduce the run from the results data alone.

### 3. The Main Window



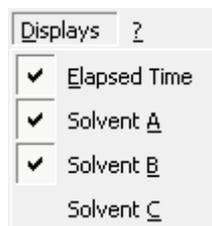
#### 3.1 General

The main window is made up of a toolbar with function buttons, plus a display bar in which the current system data is displayed. The arrangement of the function buttons and displays can be personalized by the user. The size and position of the window can also be changed, and will be saved when the program is closed.

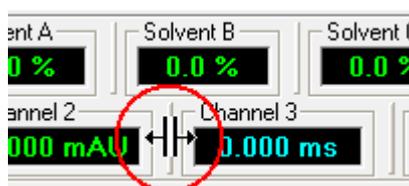


To make changes to the toolbar, double-click on an empty space on the toolbar. The “Customize Toolbar” will open, where you can add

and remove buttons. To hide a button, deselect the checkbox under it. The settings will be saved when you exit the program.



To add or remove displays, select the relevant display from the “Displays” menu. The selected displays will be ticked in the menu. To change the display colour, right-click on a display and select the menu option “Edit display colour”. The colour dialogue that appears will allow you to choose a new colour.



To move displays, click on the vertical line in front of the display and drag it to its new position. If you drag a display down and out of the window, a new display bar will appear. The arrangement of the toolbar and display bar is saved when you exit the program and will reappear this way the next time you open it.

### 3.2 Function buttons in the main window

-  100% Solvent A Major Pump starts the Major Pump System with 100% eluent A and the currently set flow rate.
-  100% Solvent B Major Pump starts the Major Pump System with 100% eluent B and the currently set flow rate.
-  100% Solvent C Major Pump starts the Major Pump System with 100% eluent C and the currently set flow rate.
-  100% Solvent D Major Pump starts the Major Pump System with 100% eluent D and the currently set flow rate.
-  Solvent Composition Major Pump starts the Major Pump System with the solvent composition shown in the "Solvent Composition" window and the currently set flow rate.
-  Flow rate Major Pump opens a window to show the flow rate. A change to the flow rate does not start the pumps, but it will take immediate effect if the pumps are running.
-  100% Solvent A Minor Pump starts the Minor\_Pump System with 100% eluent A and the currently set flow rate.
-  100% Solvent B Minor Pump starts the Minor Pump System with 100% eluent B and the currently set flow rate.
-  100% Solvent C Minor Pump starts the Minor\_Pump System with 100% eluent C and the currently set flow rate.
-  100% Solvent D Minor Pump starts the Minor Pump System with 100% eluent D and the currently set flow rate.
-  Solvent Composition Minor Pump starts the Minor Pump System with the solvent composition shown in the "Solvent Composition" window and the currently set flow rate.
-  Flow rate Minor Pump opens a window to show the flow rate. A change to the flow rate does not start the pumps, but it will take immediate effect if the pumps are running.
-  Wavelength opens a window where you can enter the wavelength of a controlled detector.
-  Autozero will return a serial controlled detector to zero.
-  Set Reference Spectrum sets the current DAD spectrum as reference spectrum.
-  Temperature Control opens a window where you can set the temperature for the temperature control.
-  Limiter Value opens a window where you can enter the maximum value for the fraction limiter.

-  Load Control File opens a data file selection window where you can load a time control or autosampler control file. In the file type box of this window, you can select either \*.tcf (Time Control File) or \*.acf (Autosampler Control File). If the option “Start Pumps after loading Time Control File” is selected in the time control file, the pumps will begin once loading is complete, with the solvent composition and flow rate programmed for time point 0.00 minutes.
-  Start Control File starts the time control file or autosampler control file that has been loaded. If the function “Hold Time Control File or Autosampler Control File” was executed first, the run will resume.
-  Hold Control File pauses the time flow of a time control file or autosampler table. If the option “Stop Pumps at Time Control Hold” is selected in the time control file, the pumps will have a flow rate of 0 ml. While the Hold function is activated, the flow rate of the pumps can be adjusted manually using the “Flow rate” function. “Start Time Control File or Autosampler Control File” resumes the run at the time point where it was paused.
-  Jump to next Line jumps forward in time to the next line programmed in the time control table. The first time you use this function, you must confirm it in a dialogue box, but it is possible here to select the option “Don’t ask again” to avoid seeing this box in future.
-  Stop all stops the pumps and the time control file from running. It is not possible to resume the run at the point where it was stopped.
-  Manual Sample ID enables you to enter a sample identifier when starting a time control file. This option is not possible when running an autosampler control file, because the sample identifiers are derived from the accompanying sample identifier file.
-  Create / Edit Time Control File opens the time control file editor to create or edit a time control file.
-  Create / Edit Sequence Table opens the sequence table editor to create or edit a sequence.
-  Create / Edit Autosampler Control File opens the autosampler control file editor to create or edit an autosampler control file.
-  Chromatogram opens the chromatogram window to show the analysis, reconstruction and reprocess areas.
-  Peak Detection opens the window with the automatic peak sampling displays.
-  System Visualisation opens the system visualisation window.
-  Mass spectrometer opens the window for visualisation, setup and manual control of the mass spectrometer.
-  Solvent Supply opens the window with the solvent supply display.
-  Waste Management opens the window with the waste management display.
-  Fraction Rack opens the window with the fraction rack visualisation.

-  Event Box Control opens the window with the visualisation and manual control of the event box.
-  Time Control Visualisation opens the window with the visualisations of the time control file and autosampler control file in table form.
-  Setup opens the setup window, in which communication settings, device parameters and device descriptions etc. can be set.
-  User Administration opens the user administration window.
-  Key lock makes it possible for you to lock the program. After activation, a “Key lock deactivation” window appears on the task bar, which will unlock the program when you enter the user password. The initial password following installation is “SCPA” (see Chapter 5.2).
-  Communication Log opens a terminal window showing the communication, in which you can make entries in linked interfaces.
-  Open current working folder opens a Windows Explorer Window showing the content of the current working folder.
-  Online Help opens the program’s online help.
-  Exit ends the program.

### 3.3 The main window displays

 Elapsed Time shows the time that has elapsed in a time control file. If the time control file is on “Hold,” then the display will flash between the elapsed time and “Hold”. During the injection phase, the display flashes between the elapsed time and “Injection”. Following the time control file command “Wait for input,” the display will flash between the elapsed time and “Waiting”.

 Solvent A shows the current percentage of eluent A being pumped by the main pump.

 Solvent B shows the current percentage of eluent B being pumped by the main pump.

 Solvent C shows the current percentage of eluent C being pumped by the main pump.

 Solvent D shows the current percentage of eluent D being pumped by the main pump.

Pump Status  
**ON**

Pump Status shows the current main pump status. ON = pump is running, OFF = pump has been stopped, OVER = pump has stopped because the pressure was too high, UNDER = pump has stopped because the pressure was too low.

Flowrate  
**10.00 ml**

Flow rate shows the main pump's current flow rate.

Volume  
**3.80 ml**

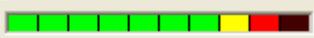
Volume indicates the volume pumped through with the main pump since pumping began. When the pumps are stopped, the volume display returns to 0. Depending on the volume pumped, the display unit changes automatically from µl through ml to l.

Pressure  
**42.7 bar**

Pressure indicated the current pump pressure. You can change the display value in Setup, under "Presets," using an offset and a factor.

Fraction No  
**1**

Fraction No shows the current fraction number.

Fraction Limit  
**ON** 

Fraction Limit indicates the fraction limiter status. OFF = limiter is inactive, ON = Limiter is active. The LED band display indicates the volume pumped of the current fraction in steps of 10%. When the last red LED has lit up (100%), the limiter triggers a step in the fraction collector.

Valve Control  
**Valve 1** 

Valve Control shows the current position of the selected valve and is also a way of switching the valve manually. To do this, select the desired valve and the required position, and use the "Set" button to change the position.

Vial No  
**1**

Vial No indicates the current vial number of the current autosampler injection.

Run No  
**1 of 6**

Run No. shows the number of the current run in association with the function "Restart".

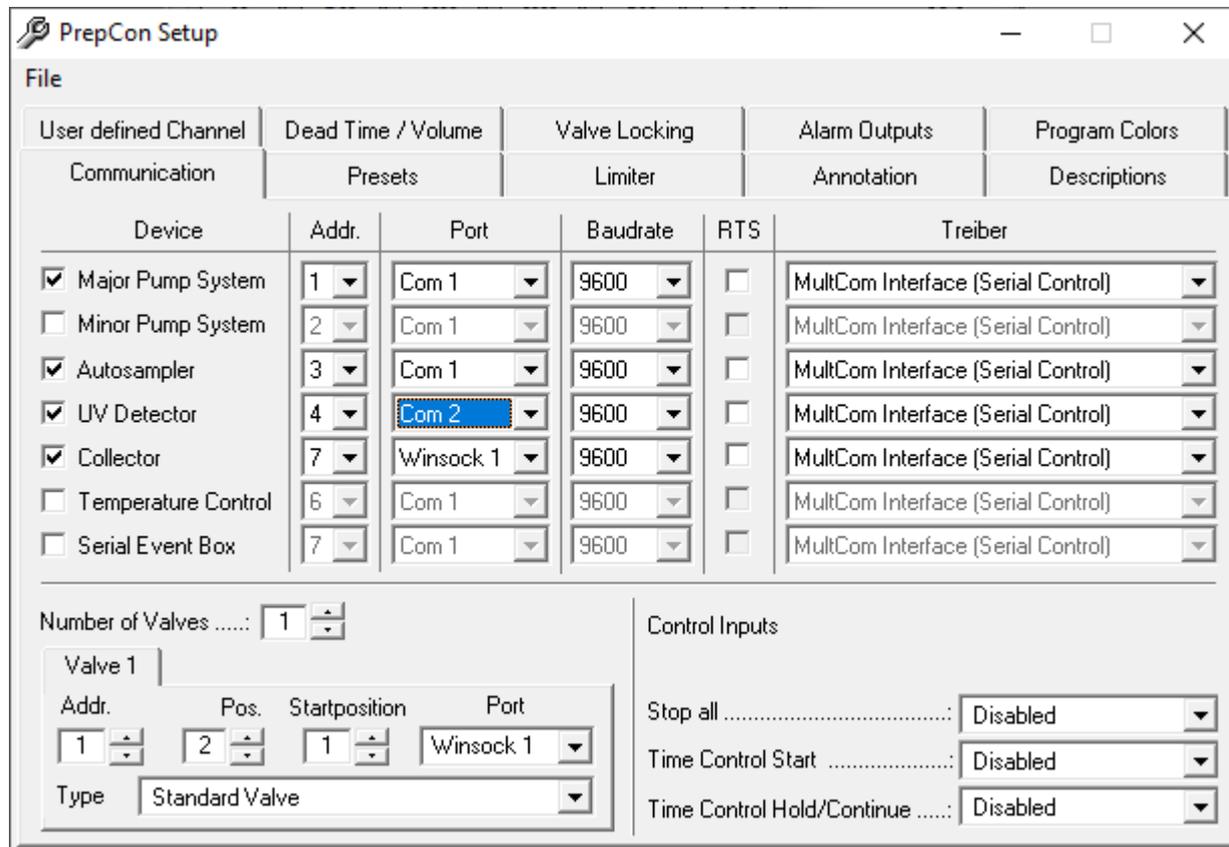
Channel 1  
**0.043 mV**

Channel 1 – Channel ... show the values of the device connected to each analogue entry. In the Analysis window, under "Channel setup," you can change the displays for each device using an offset, a factor and a dimension.

## 4. Program setting (Setup)

The function key or the menu option “Setup” in the main window opens the program settings window. This window contains 10 tabs, whose content is described below.

### 4.1 Communication



In the Communication setup you can configure your systems control interfaces and valves. “Device” lists all the controllable interfaces, which can be activated or deactivated. “Addr.” defines the device address. This corresponds to the address of MultCom interfaces, which is set with the help of the round encoding switch (see illustration). Under “Port”, you can select the serial or winsock port to which the interface is connected. With “Baudrate” and “RTS”, you can configure the serial port settings if used. Under “Driver”, you can select whether your device is controlled by a MultCom interface or a specific software driver.

You can configure your systems controlled valves in the bottom left corner. With “Number of Valves” you enter the number of valves. For each valve the address, number of positions and port then is configured in the corresponding tab.

Under “Control Inputs” you can define event box inputs or game port inputs that trigger one of the following events: stop a run (“Stop all”), start a run (“Time Control Start”) or temporarily pause and then resume a run (“Time Control Hold/Continue”).

## 4.2 Presets

Device	Addr.	Port	Baudrate	RTS	Treiber
<input checked="" type="checkbox"/> Major Pump System	1	Com 1	9600	<input type="checkbox"/>	MultCom Interface (Serial Control)
<input type="checkbox"/> Minor Pump System	2	Com 1	9600	<input type="checkbox"/>	MultCom Interface (Serial Control)
<input checked="" type="checkbox"/> Autosampler	3	Com 1	9600	<input type="checkbox"/>	MultCom Interface (Serial Control)
<input checked="" type="checkbox"/> UV Detector	4	Com 2	9600	<input type="checkbox"/>	MultCom Interface (Serial Control)
<input checked="" type="checkbox"/> Collector	7	Winsock 1	9600	<input type="checkbox"/>	MultCom Interface (Serial Control)
<input type="checkbox"/> Temperature Control	6	Com 1	9600	<input type="checkbox"/>	MultCom Interface (Serial Control)
<input type="checkbox"/> Serial Event Box	7	Com 1	9600	<input type="checkbox"/>	MultCom Interface (Serial Control)

Number of Valves .....: 1

Valve 1	Addr.	Pos.	Startposition	Port	Type
1	1	2	1	Winsock 1	Standard Valve

Control Inputs

Stop all .....: Disabled

Time Control Start .....: Disabled

Time Control Hold/Continue .....: Disabled

You can set standard and maximum values for the devices being controlled in the Presets setup. You can enter the following values in “Major Pump System” and “Minor Pump System”:

- Flow rate (the standard flow rate transmitted to the pumps when the program starts.)
- Max. Pressure (maximum pressure, the point at which the pumps will stop.)
- Serial Cycle (time interval at which the status of serial controlled pumps is requested.)
- Valve Cycle (time for a mix cycle of a low pressure gradient system at a flow rate of 10 ml/min.)
- Valve Min. Cycle (minimum permissible switching time for the gradient mix valves in use.)
- Max. Flow rate (maximum flow rate of the pumps.)
- Max. Voltage (maximum controlling voltage for voltage controlled pumps.)
- Gradient Valves (must be activated when a low pressure gradient system is used.)
- Different Pumps (can be activated with voltage controlled pumps with different maximum flow rates. In the tabs, which appear underneath, the controlling voltage and the maximum flow rate for each pump can be set separately.)

“Collector Start Position” indicates the starting position of the fraction collector when the program starts.

“Collector Stop Position” indicates the last possible position of the fraction collector. The usage of not equipped rack positions can be prohibited by this function.

“Temperature Control” indicates two system temperatures that are set when the program starts (e.g. column oven and sample heater).

“UV-Detector” show the wavelengths of the UV detector when the program starts.

You can use “Pressure Display” to change the program’s pressure display to match that of the pumps with the help of an offset and a factor.

### 4.3 Limiter

The screenshot shows the 'PrepCon Setup' dialog box with the 'Limiter' tab selected. The 'Limiter activation' section has four rows, each with a checkbox, a label, a dropdown menu, and another dropdown menu. The first row is checked and set to 'Valve 1 - ( 2 Positions )' and 'Not Position 1'. The other three rows are unchecked and set to 'Off'. The 'Limiter Output' section has three radio buttons, with the first one selected and set to 'Controlled Collector ( Next Vial )'. The other two are set to 'Valve 1 - ( 2 Positions )' and 'Event Box Output 1'. The 'Limiter Value' section has two radio buttons, with the first one selected and set to '10.0 ml' and the second one set to '5 sec'.

The fraction limiter is configured in the limiter setup.

Enter when the fraction limiter becomes active in “Limiter activation.” As a rule, this is the point of switching between waste and the fraction.

- “Controlled Valve” should be activated if you are using a serial controlled valve for this. The following position must be the position “fraction.”
- “Event Box Output” should be activated if you are using an event box output for this. The following output state must be the state “fraction”.
- “Event Box Input” should be activated if you are recording the fraction position with an event box input. The following input state must be the one for the state “fraction”.
- “Auxiliary Output” should be activated if you are using the auxiliary output of the pump interface for this. The following output state must be the one for the state “fraction”.

Enter in “Limiter Output” what the limiter should act on when the fraction limit is reached.

The device you are fractionating with should be activated here.

- “Controlled Collector” should be activated if you are using a serial controlled fraction collector. When the fraction limit is reached, a “step” is carried out.

- "Controlled Valve" should be activated if you are using a serial controlled motor switching valve. When the fraction limit is reached, it switches to the next position.
- "Event Box Output" should be activated if you are using a fraction collector controlled by the event box. When the fraction limit is reached, there is a "pulse" at the indicated output.

Enter the volume or time limit for the fractions in "Limit Value".

#### 4.4 Annotation

The screenshot shows the 'PrepCon Setup' window with the 'Annotation' tab active. The 'File' menu is visible at the top. The 'Annotation' tab contains the following settings:

Text Type	Text	+ (Elapsed Time)
<input checked="" type="checkbox"/> Waste Text	Waste	<input type="checkbox"/>
<input checked="" type="checkbox"/> Fraction Text	Fraction	<input type="checkbox"/>
<input checked="" type="checkbox"/> Step Text	Step to Position	<input type="checkbox"/>

Device Type	Device	Position
<input checked="" type="radio"/> Waste Annotation Device	Valve 1 - ( 2 Positions )	Position 1
<input type="radio"/> Fraction Annotation Device	Event Box Output 1	Off
<input type="radio"/> Step Annotation Device	Event Box Input No 1	Off
<input type="radio"/>	Game Port Input 1	Off
<input type="radio"/>	Auxiliary Output	Off

The automatic annotations in the chromatograms are configured in the annotation tab

"Waste Text" allows you to activate or deactivate an annotation when switching to waste. You are free to choose the text of the waste annotation. The option "+(Elapsed Time)" adds the elapsed time to the text.

"Fraction Text" allows you to activate or deactivate an annotation when switching to the "fraction" position. You are also free to choose the text of the fraction annotation.

The fraction number is automatically appended to the text. If you select the "+(Elapsed Time)" option, the elapsed time is also added.

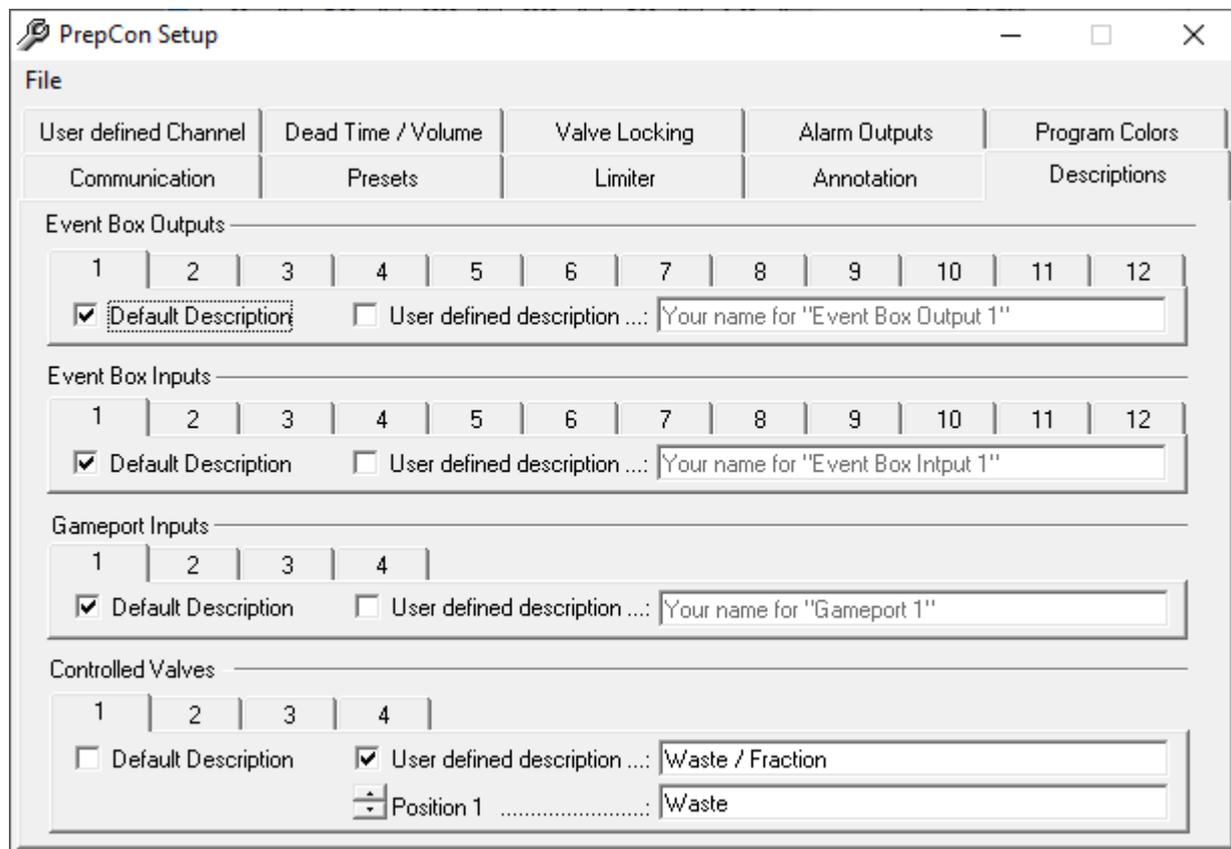
"Step Text" allows you to activate or deactivate an annotation when changing a position. You are also free to choose the text of the step annotation. The fraction number is automatically appended to the text. If you select the "+(Elapsed Time)" option, the elapsed time is also added.

In "Waste Annotation Device" you can enter the device with its position or state that corresponds to the "waste" position.

In “Fraction Annotation Device” you can enter the device with its position or state that corresponds to the “fraction” position.

In “Step Annotation Device” you can enter the device with which you are fractionating or controlling the fractionating.

### 4.5 Descriptions

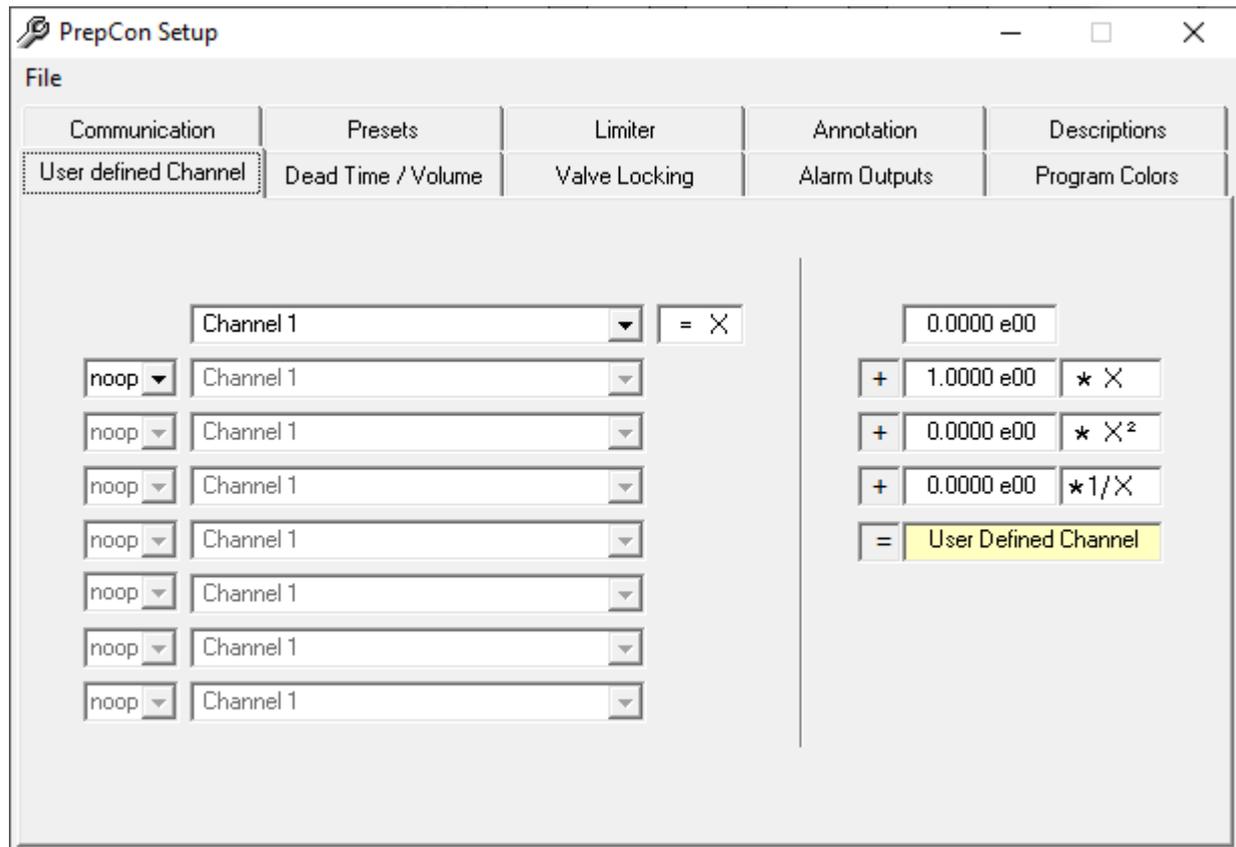


You can give your own names to the event box inputs and outputs, controlled valves in the descriptions tab. This makes it easier to program time control files. It also makes the visualisations clearer, since the inputs, outputs and valves are can be listed by function.

The “Default Description” option gives these inputs, outputs and valves their standard description (“Event Box Output ...”, “Event Box Input ...”, “Valve No ...”)

The “User defined Description” gives you the possibility of entering your own descriptions in the adjacent text boxes.

## 4.6 User Defined Channel



You can set up a user-defined data channel in the user defined channel setup. This data channel is used in the same way as one of your analogue channels, and carries the description "U".

On the left hand side, you can activate one or more of your analogue signals as a data source. You have a choice of possible operations between these channels:

- "NOOP" (No operation)
- "+" (Addition of the following channel)
- "-" (Subtraction of the following channel)
- "\*" (Multiplication by the following channel)
- "/" (Division by the following channel)

The result of these operations is on the right side available as value "X" to calculate the "User defined Channel". You can enter an offset in the first box. In the second box you can enter a factor to "X". In the third box you can enter a factor to the square of "X" and in the fourth box, you can enter a factor to the reciprocal of "X". The addition of the four lines gives the value of your "User defined Channel."

## 4.7 Dead Time / Dead Volume

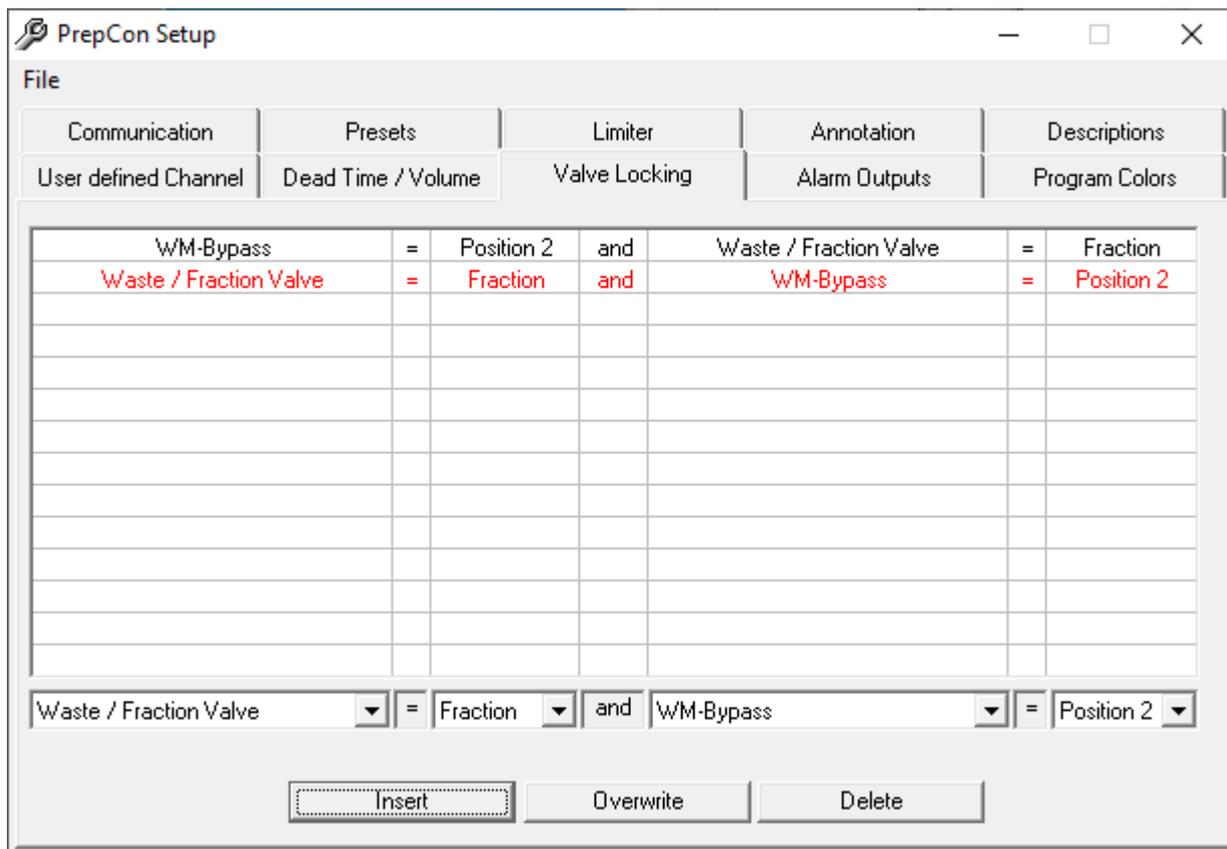
The screenshot shows the 'PrepCon Setup' window with the 'Dead Time / Volume' tab selected. The interface is organized into several sections:

- File:** A menu bar with options: Communication, Presets, Limiter, Annotation, Descriptions.
- User defined Channel:** A sub-menu bar with options: Dead Time / Volume (selected), Valve Locking, Alarm Outputs, Program Colors.
- Controlled Collector:** A section with two radio buttons: 'Volume' (selected) with a text box containing '2.50' [ml], and 'Time' with a text box containing '0' [sec].
- Controlled Valves:** A section with a dropdown menu showing '1' and two radio buttons: 'Volume' (selected) with a text box containing '2.50' [ml], and 'Time' with a text box containing '0' [sec].
- Event Box Outputs:** A section with a grid of 12 numbered tabs (1-12) and two radio buttons: 'Volume' (selected) with a text box containing '0.00' [ml], and 'Time' with a text box containing '0' [sec].
- Auxilliary Output:** A section with two radio buttons: 'Volume' (selected) with a text box containing '0.00' [ml], and 'Time' with a text box containing '0' [sec].

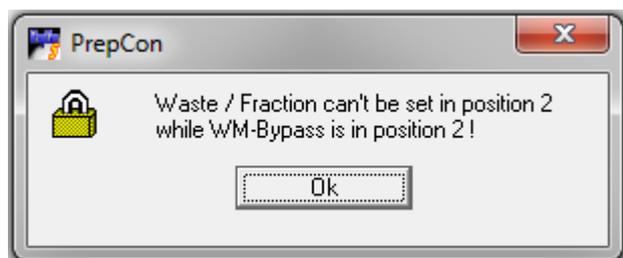
A considerable dead volume can occur in the tubing and valves between the detector cell and the waste/fraction switching valve, which results in a time delay when fractionating, especially at low flow rates. In the Dead Time / Dead Volume setup, you can define the dead volume or dead time of your system.

When you enter a dead volume, the program calculates the necessary dead time for each device according to the current flow rate. Functions triggered by threshold values or automatic peak detection are also carried out with this delay. When you enter a dead time, this is carried out on a 1:1 basis. Annotations are recorded in the chromatogram without the time delay.

### 4.8 Valve Locking



When using several valves, it is possible to switch to non-permitted valve positions or even close off the flow through the system without intending to do so. In order to prevent this, you have the possibility to enter all the non-permitted valve positions in a list in the valve-locking setup.

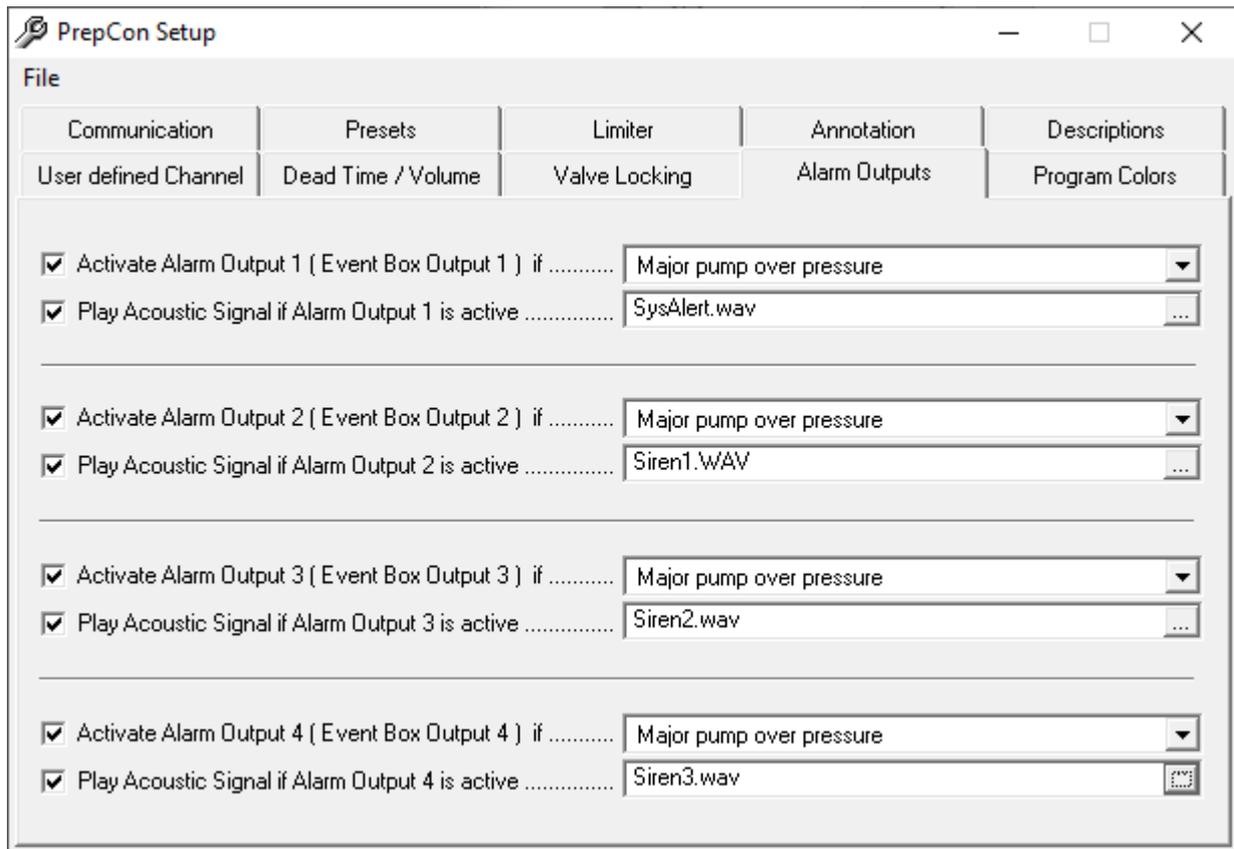


The program will constantly check for these combinations and prevent them from being carried out. If these non-permitted valve positions occur, a message will appear on screen (see illustration). To fill in the table, select the non-permitted valve positions in the editing bar underneath the table, and use the *Insert* button to add it.

*Overwrite* allows you to write over the row marked in red, or you can delete it with the *Delete* button. The possible choice of valves in the editing bar only includes the valves configured in "Communication".

Valve Lock Conditions are formatted as "if.. then" combinations. I.e. if the valve position on the left hand site is already selected the valve position on the right hand site can not be switched to. If a combination of two valve positions must never occur regardless of which valve is switched first this combination must be entered a second time with reversed order of positions.

### 4.9 Alarm Outputs

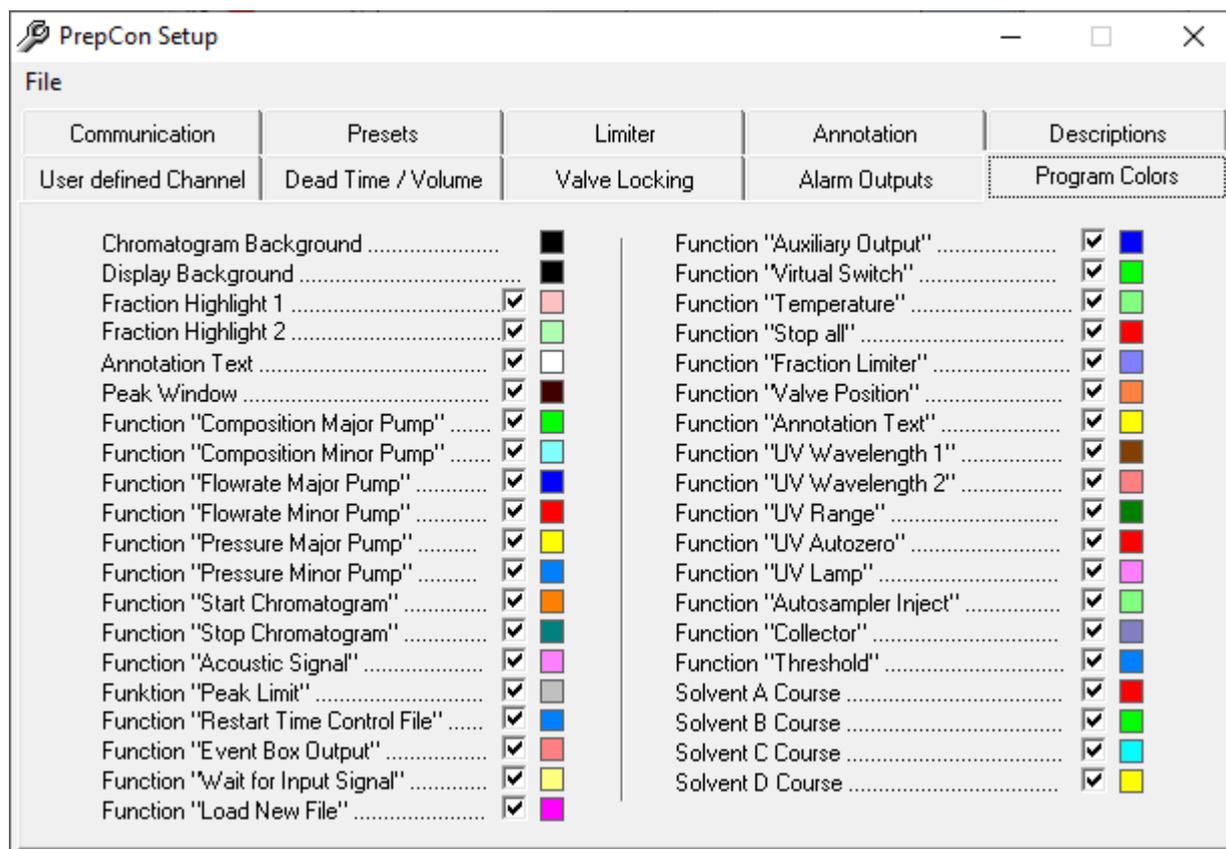


Up to 4 alarm outputs can be activated in the alarm outputs set-up. The alarm outputs 1 to 4 are set using event box outputs.

Using the corresponding dropdown-lists, you can configure the respective situations leading to an alarm by choosing from several predefined situations.

The option "Play Acoustic Signal if Alarm Output n is active" activates an acoustic signal, which will be played while the alarm output is active. The signal file can be selected in the adjacent field.

### 4.10 Program Colors



The Program Colors set-up allows the configuration of colors for chromatogram background, annotation texts, peak windows and the graphic time table functions.

For each graphic element or function, an adjacent checkbox determines whether the element or function will be displayed. Clicking on the colored boxes opens a color dialog window in which the corresponding display colors can be selected.

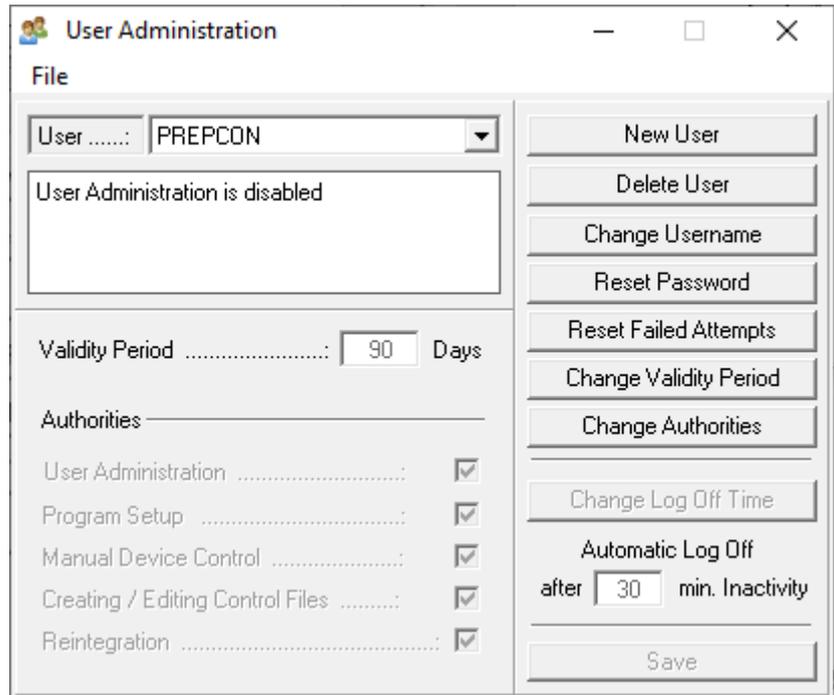
## 5. User Administration

### 5.1 General

The user administration allows you to set up administrators and users who can be allocated user authorities.

### 5.2 Working without user administration

At initial installation, the user administration is deactivated. This setting can be re-establish any time. To work without user administration name the administrator "PREPCON" and allocate the password "SCPA". This combination of name and password deactivates the user administration.

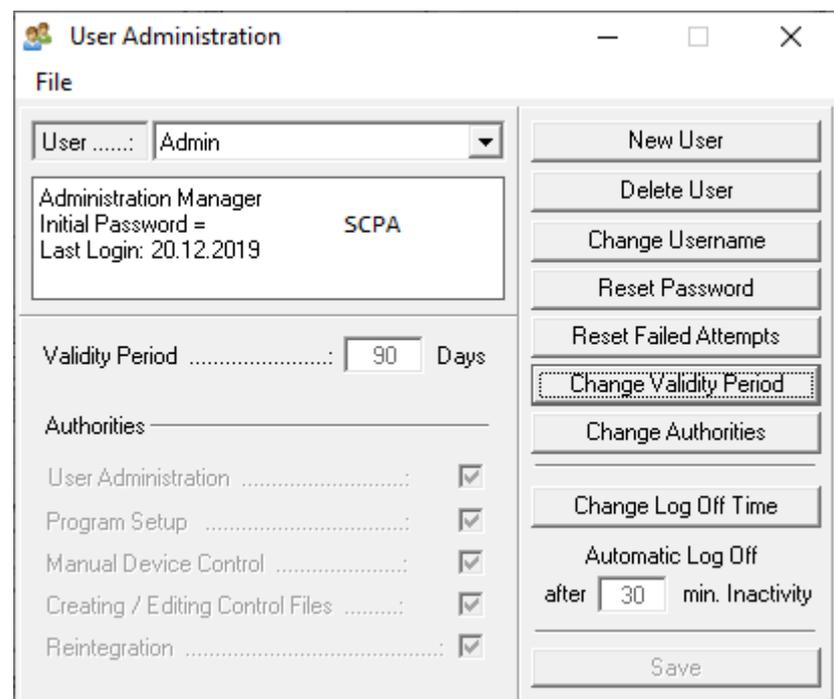


### 5.3 How to activate the user administration

The user administration will be activated when the password or the user name of the administrator is changed. To change the name of the administrator press the button "Change Username". When entering a new name you need to respect following restrictions:

1. Case sensitivity
2. No blanks
3. At least 3 characters

To confirm the input of the new user name press the "Save" button. In the status



window you will get an “Initial Password” which you need to use at your first login. The first user in the list cannot be deleted and always has administrative rights, which cannot be deactivated.

### 5.4 Adding Users

To create a new user profile click on the button “New User”. Into the new user interface, you can enter the user name, the validity period of the password and assign user authorities. To confirm the input press the “Save” button.

- User name: Need to have at least 3 characters, no blanks and attend to case sensitivity.
- Validity period: Defines the duration when the password is valid. After the entered period of time the user need to enter a new password. The validity period can be between 7 and 180 days long.
- User Administration: Allows access to the user administration
- Program Setup: Allows access to the program setup
- Manual Device Control: Allows manual operation of the system using the manual control functions in the main window or the visualisation
- Creating / Editing Control Files: Allows the creating and editing of time control and autosampler control files
- Reintegration: Allows the belated integration of the result files

- Automatic Log Off: Determines the time of inactivity after the user is logged out. To deactivate Automatic Log Off enter 0 Minutes.

By pressing the button of the combination-field behind the user name, you can switch between the different user interfaces. The initial password for the first login you will find in the status window of the user interface of the new registered operator.

It also shows the administrator some additional information (last login, expiry date of the password).

### **5.5 Resetting a password**

The administrator can reset a forgotten or unsafe password for the affected user. When pressing the "Reset Password" button a new initial password will be generated. The operator needs to use this password for the next login.

### **5.6 Resetting failed attempts**

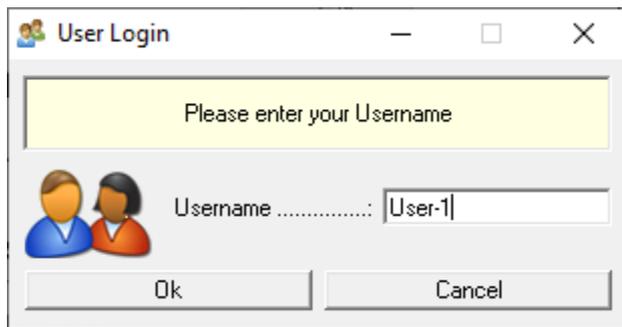
After three failed attempts to login, the account of the operator will be locked. The administrator has the possibility to reset these attempts to give the operator another try to login.

The administrator will get the information, if a user is locked due to failed attempts, in the status window of the user interface.

### **5.7 Deleting Users**

In order to delete a user, select the user and press the „Delete User“ button. Deletion of a user must be confirmed with "Ok" in the following dialog window.

## 5.8 User Login

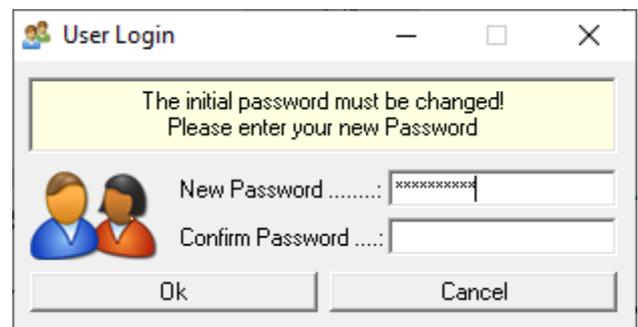


When the user administration is activated, the operator will get a request window for the login when starting PrepCon. The operator needs to identify by entering user name and password.

At the first login after activation or resetting of the password the operator need to use the assigned initial password that was generated when creating the user profile or resetting the password. After the successful input of the initial password, the operator is requested to define and enter a new password.

The new password has to be at least 8 characters long and must contain characters from three of the following four categories:

- lower case letters (a – z)
- upper case letters (A - Z)
- base 10 digits (0 – 9)
- non-alphanumeric special characters:  
! " # \$ % & ' ( ) \* + ' -  
. / : ; < = > ? @ [ \ ] ^ \_ ` { | } ~



For safety reasons the operator needs to confirm the password with a second entry.

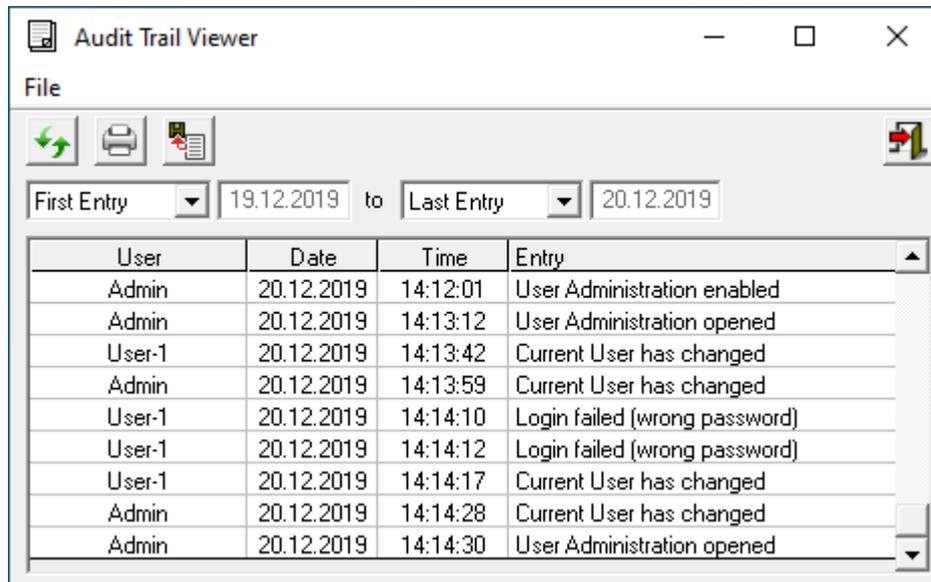
At the end of the validity period of the password, the operator is also asked to enter a new password. The previously used password will not be accepted.

## 5.9 Printing the User Administration

In order to print a list of all users and their rights select „Print User Administration“ in the „File“ menu. The passwords are not part of the list.

## 5.10 View Audit Trail

In order to view the audit trail select „View Audit Trail“ in the „File“ menu. The displayed list shows all events related to the user administration since installation of PrepCon.



In order to only display a part of this time period select „Date“ instead of „First Entry“ or „Last Entry“. Then the desired dates between which the audit trail should be displayed can be entered. Pressing enter or clicking the „Refresh“ button updates the content of the list.

## 5.11 Function Buttons in the Audit Trail Window



„Refresh display“ refreshes the list according to the selected time period.



„Print Audit Trail“ opens the printer dialog in order to print the audit trail for the selected time period.



„Export Audit Trail“ opens a file selection window in order to export the audit trail to CSV.

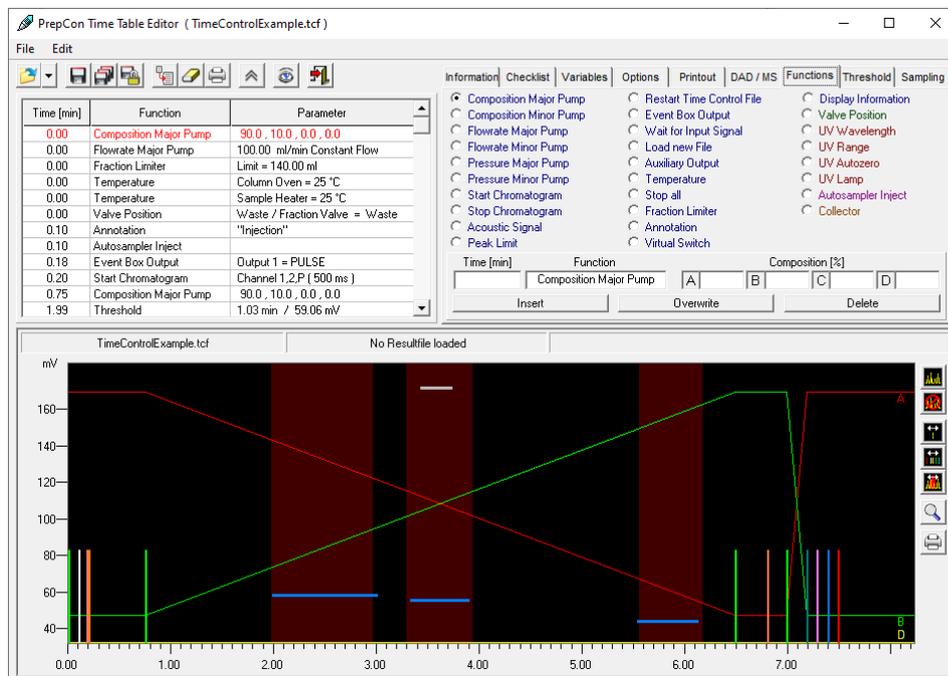


„Exit“ closes the audit trail window.

## 6. Creating Time Control Files

### 6.1 General

You can open the time control file editor with the function button or the menu option "Create / Edit Time Control File" in the main window. The editor shows the time control file



in both table and graphic form. The graphic display also allows you to load a chromatogram as a background image, with the help of which the functions of the time control file can be adjusted and checked along the time and intensity axes. The graphic presentation of the functions, particularly the display of the gradient, ensures increased clarity when programming and

thus helps you to avoid making mistakes.

The functions of the time table need not be programmed in chronological order. They are sorted automatically in the right order on inserting into the time table.

Time [min]	Function	Parameter
0.30	Auxiliary Output	Auxiliary = ON
0.60	Annotation	"My individual Annotation"
0.75	Composition Major Pump	10.0 , 20.0 , 30.0 , 40.0
1.00	Start Chromatogram	Channel 2 ( 200 ms )
1.62	Composition Major Pump	40.0 , 20.0 , 30.0 , 10.0
2.06	Threshold	1.00 min / 14.00 mV
2.06	Peak Limit	
3.01	Event Box Output	Your name for "Event Box Output 1"
3.14	Wait for Input Signal	Your name for "Event Box Input 1" :
3.20	Start Chromatogram	Channel 3 ( 200 ms )
3.38	Threshold	0.58 min / 14.00 mV
4.18	Composition Major Pump	40.0 , 20.0 , 30.0 , 10.0

If you want to move more than one function of the time table to another time, click with the right mouse key into the first line of the functions to be moved. On clicking into "cut/insert time" an entry box

1.00	Start Chromatogram
1.62	
2.06	<input type="text" value="2.00"/> <input type="button" value="Min"/> <input type="button" value="Ok"/>
2.06	Peak Limit

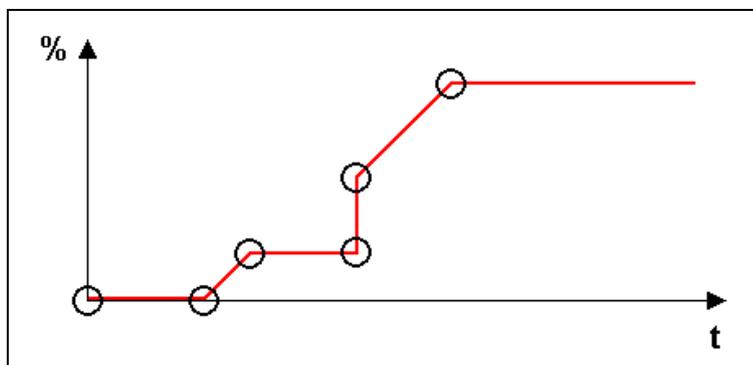
appears, where a positive or a negative time can be

entered. A positive time moves all following functions to a later time, a negative time moves all functions to an earlier time.

There are certain things you should bear in mind when creating or editing a time control file.

It is a basic principle that every time control file must begin at a time point of 0.00 minutes with an eluent composition and a flow rate, so that the initial conditions of the pumps are set.

All the functions programmed for time point 0.00 minutes are carried out when the time control file is loaded. For this reason, it is sensible use this point in the program to set all the controlled valves to a basic position and to set the event box exits used, so that the system is not left in an undefined state because of previous use or manual operation.



eluent composition programmed will run isocratic until the time control file is ended (by the program or manually).

If you want to program a gradient, you should take care that you include all the angles of this gradient as eluent compositions in the time control file. A linear gradient will be calculated between two different eluent compositions at two different times. If you want to program a stepped gradient, add start and end points with a time difference of 0.01 minutes. The last

## 6.2 Creating a time control file

On the right hand side of the window is the toolbar for the time control file editor. The functions are listed here in the order that corresponds to the display:



“Open Time Control File” loads an available time control file into the editor. The types of file you can select to load are: “Time Control File“ (\*.tcf), “Result File“ (\*.rfp) or “PrepCon4 File“ (\*.lgr). The “Result File“ option allows you to load a time control file from results data. “PrepCon4 File“ allows you to import time control files created with PrepCon Version 4.



“Save Time Control File” saves the time control file under its existing name.



“Save Time Control File as ...” saves the time control file under a new name.



“Save Time Control File as validated” saves the time control file as a validated file. This file cannot be modified any more.



“Import Time Control Part” is used to import an element of a time control file. The content of the selected tab can be imported from an existing time control file.



“Clear all” deletes the content of a time control file. In order to prevent the file from being deleted by mistake, this function requires a further confirmation from you before being carried out.



“Print Time Control File” opens a printer dialogue to print out the time control file.



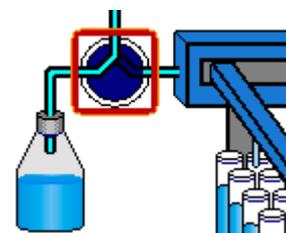
“Hide Graphic / Show Graphic” hides or shows the graphic time table editor. The window of the time table editor will be reduced or enlarged.



“Simulation mode” activates a simulation mode for the loaded time table in the time table editor. By clicking a line in the editor the correspondent situation is displayed in the system visualisation. The selected line is marked in the table with two arrows. With the

5.60	Threshold	0.60 min / 12.00 mV
▶ 6.81	Valve Position	Valve 1 = Position 1    aste ◀
7.20	Stop Chromatogram	All started Channels

arrow keys on the keyboard the next or the previous line can be selected. Using this simulation, basic functions of time tables can be tested. In the system visualisation a red blinking frame marks the appropriate graphic object. In addition value labels are showing the parameters of the selected line (solvent compositions, flow rates, UV wavelengths, etc.)



“Exit” closes the time control file editor.

### 6.2.1 Storing of general information

In the “***Information***” tab, you can enter information about the author of the file, the eluents

Information

Author.....:	Axel Wilharm	Date .....	Tuesday, 08.02.2011
Comment ...:	Time table for PrepCon 5		
Solvents .....	A	Methanol + Water	
	B	Saline Solution	
	C	Buffer pH 4	
	D	Buffer pH7	
Column .....	Glass Column, Maximaldruck 10 Bar		
Sample .....	Sample No. 123		

used, the column use, a sample identifier and a general comment. The date is automatically generated when you save the file. The sample identifier is not included when using an autosampler or when the “Manual Sample ID” option

is activated. The information entered is saved in the results file generated and can be reopened later.

### 6.2.2 Creation of a checklist

The „**Checklist**“ tab allows you to create an instruction list or a checklist. The editor bar is at the bottom of the tab, where you can choose between “*Checkbox*” or “*User Input*”:

Type	Requirement
Check Box	Solvent restock ?
<b>Check Box</b>	<b>Waste container empty ?</b>
Check Box	Fraction vials restock ?

Check Box | Waste container empty ?

Insert    Overwrite    Delete

- „*Checkbox*“ is an instruction or a control statement. Enter the text of the statement in the input field on the right. This item has to be ticked off by the user before he can start this time control file.
- „*User Input*“ is an input prompt. Enter the text of the prompt in the input field on the right. The user has to enter the demand before he can start this time control file.

The “*Insert*” button adds the content of the current editor bar to the checklist. The “*Overwrite*” button overwrites the content of the line you have selected with the contents of the editor bar. The “*Delete*” button deletes the line you have selected. To change the order of the lines, left-click on a line and while keeping it pressed move it to the desired place.

If the checklist of a time control file contents rows, the checklist window will open before starting this file. The user has to ticked off all checkboxes and enter all demands before

Solvent restock ?	<input checked="" type="checkbox"/> OK
Waste container empty ?	<input type="checkbox"/> OK
Fraction vials restock ?	<input checked="" type="checkbox"/> OK

Start    Cancel

the run begins. A forgotten line will be highlight red and prevents the start. The checklist will be logged in the result file.



## 6.2.4 Optional settings

The “**Options**” tab allows you to set the dimensions of the x-axis in “*Programming Mode*”. You have a choice between units of time, volume or column volume. You can also select

the size of the units beside each programming mode. To help you determine the column volume when programming in units of column volume, you can use the mini-calculator on the right. To do this, enter the length and internal diameter of the column and click on the “**Calculate**” button. The column volume will then appear in the “Column Volume” box.

In “*Extended Pump Options*”, you can use the “*Start Pumps after loading Time Control File*” option to determine whether the pumps should start after loading the time control file, with the parameters programmed for time point 0.00 minutes. The “*Stop Pumps at Time Control Hold*” lets you determine whether the pumps should stop when the “*Hold Time Control File*” occurs at a flow rate of 0 ml.

“*Sampling Control*” allows you to deactivate the peak sampling programmed by selecting the “*Disable Peak Sampling*” option. “*Disable Thresholds*” deactivates the thresholds programmed for this time control file. These options allow you to deactivate the collective functions without needing to delete the threshold values or peak samples from a valuable program you may need later.

“*Result file*” allows you to enter the names of the result files to be generated by this time control file. You can set the file names using the following 9 name segments:

1. “*User-Defined Name*” adds a user-defined text to the file name. (It should be short enough to fit into the text box.)
2. “*Username*” (adds the name of the current user to the file name.)
3. “*Author*” (adds the name of the author of the time control file to the file name.)
4. “*Time Control File*” (adds the name of the time control file to the file name.)
5. “*Sample Identifier*” (adds the sample identifier to the file name.)
6. “*Vial + Injection*” (adds the number of the current sample vial and the current injection to the file name.)
7. “*Actual Date*” (adds the current date to the file name.)
8. “*Actual Time*” (adds the current time to the file name.)
9. “*Auto Increment*” (Adds a four-digit consecutive number to the end of the file name, in order to stop result files with the same name from being overwritten. If you do not want to lose your last file, you should always select this name segment.)

## 6.2.5 Printout options

The **„Printout“** tab allows you to setup the content and design of your report file for automatic printing.

The screenshot shows the 'Printout' dialog box with the following settings:

- Content:**
  - Chromatogram
  - Peak Results
  - Column Coefficients
  - Fraction Table
  - Checklist
  - Run Protocol
  - Time Control File
- Options:**
  - Automatic Printout
  - Monochrome Printout
  - Chromatograms in separate Windows
- Orientation:**
  - Portrait
  - Landscape
- Parameter:**
  - Headline Text: PrepCon Report
  - Text Font: Arial
  - Chromatogram Linewidth: 1.5
- Company Logo:**
  - Company Logo: SCPA.bmp
  - Preview: SCPA logo

In the section **“Content”** you can define which data you want to include in your printout. Besides the chromatogram you can choose different data, tables and protocols.

In the section **“Options”** you can checkmark, if the printout should be executed automatically after each run. It is also possible to choose the option to have each data channel in a separate window and the option for a monochrome printout.

The layout can be varied between portrait and landscape in the section **“Orientation”**.

In the section **“Parameter”** and **“Company Logo”** you can adapt your individual design with an individual headline, text font, line width of the data traces and a company logo.

The size of the logo should be 154 to 42 pixels and the type Bitmap.

## 6.2.6 Settings for Diode Array Detectors and Mass spectrometer

The parameters of the diode array detector and/or mass spectrometer are defined in the **„DAD / MS“** tab. Select the source of the data channel under **„Data selection“**. You can choose either the A/D converter board by **„A/D Converter“** or the data of the DAD by **„DAD“** or the data of the MS by **„MS“**. Choose the wavelength range of the DAD channels or the mass range of the MS channels in the adjacent entry boxes. The selection of data channels is automatically adopted when loading the time table.

		DAD / MS				
Data Selection						
	ADC	DAD	MID			
Channel 1	<input type="radio"/>	<input checked="" type="radio"/>	<input type="radio"/>	254	-	254 nm
Channel 2	<input type="radio"/>	<input checked="" type="radio"/>	<input type="radio"/>	310	-	310 nm
Channel 3	<input type="radio"/>	<input checked="" type="radio"/>	<input type="radio"/>	280	-	280 nm
Channel 4	<input checked="" type="radio"/>	<input type="radio"/>	<input type="radio"/>			
Channel 5	<input checked="" type="radio"/>	<input type="radio"/>	<input type="radio"/>			
Channel 6	<input checked="" type="radio"/>	<input type="radio"/>	<input type="radio"/>			
Channel 7	<input checked="" type="radio"/>	<input type="radio"/>	<input type="radio"/>			
Channel 8	<input checked="" type="radio"/>	<input type="radio"/>	<input type="radio"/>			

Slicewidth	500	ms
<b>DAD</b>		
Bandwidth	2	nm
<input checked="" type="checkbox"/> Save 2D-Data		
<b>MID</b>		
Mode .....	XIC	
Range :	25	
Makeup Flow :	1000	µl
Attenuat	50.0 - 800.0	
<input type="checkbox"/> Save 2D-Data		

Enter the slice width of the DAD and MS channels in the **„Slicewidth“** entry box.

The **„Bandwidth“** parameter is used for averaging the measured values in order to reduce signal noise. For a bandwidth of e.g. 5 nm the signal of each wavelength is averaged over a range of  $\pm 2$  nm. No average value is calculated when a bandwidth of 1 nm is entered.

By choosing the **„Save 2D-Data“** option the spectra data set of the DAD is saved in the ChromStar DAD data format.

The parameters for the MS channels will be described in chapter 19. Control of mass spectrometers.

## 6.2.7 Time control file commands

You will find a list of all the programmable functions of the time control file in the “**Functions**” tab. The editor bar is at the bottom of the tab, where all the functions are to be entered with their time and parameters. The parameter boxes in the editor bar change depending on the function selected. The “**Insert**” button adds the content of the current editor bar to the time control file. The order in which you make your entries is irrelevant, since all the lines of program are ordered chronologically. The “**Overwrite**” button overwrites the content of the line you have selected with the contents of the editor bar. The “**Delete**” button deletes the line you have selected.

“**Composition Major Pump**” determines the eluent composition for the primary pumps in the system. Entries are made in percent, and while you are making the entries, the entry in the following box always makes up the difference to 100%.

“**Composition Minor Pump**” determines the eluent composition for the secondary pumps in the system (e.g. column conditioning, sample application etc.) Entries are also made in percent.

“**Flow rate Major Pump**” determines the flow rate of the primary pumps in the system. Changes are made in steps, i.e. a flow rate gradient cannot be generated. Entries are made in ml/min.

“**Flow rate Minor Pump**” determines the flow rate for the secondary pumps in the system. Entries are also made in ml/min.

„**Pressure Major Pump**“ determines the behaviour of the pump at the inscribed value.

- Minimum Pressure: Pausing of the method and stopping of the pump when the pressure was constantly below the appointed value for 20 seconds.
- Maximum Pressure: Pausing of the method and stopping of the pump when the pressure when the appointed value is exceeded.
- Pressure Limit (has to be supported from the pump): automatic flow rate control starts working when the appointed value is achieved.

„Pressure Minor Pump“ determines the behaviour of the pump at the inscribed value.

- Minimum Pressure: Pausing of the method and stopping of the pump when the pressure was constantly below the appointed value for 20 seconds.
- Maximum Pressure: Pausing of the method and stopping of the pump when the pressure when the appointed value is exceeded.
- Pressure Limit (has to be supported from the pump): automatic flow rate control starts working when the appointed value is achieved.

„Start Chromatogram“ starts plotting the chromatogram for the analogue channels selected, with the data point density entered under „Slice Width“.

„Stop Chromatogram“ stops plotting the chromatogram for the analogue channels selected or, if „all active“ is selected, stops plotting the chromatogram for all the analogue channels started.

„Acoustic Signal“ initiates a sound reproduction of the wave file selected with an interval of 4 seconds. The test button  allows you to hear the file. The sound will end when the time control file is stopped.

„Peak Limit“ is used to monitor peak heights and peak times. It works in conjunction with the „Restart“ command and takes effect when the time control file is restarted during cyclic effluents. The end time in minutes („End“) and the limit value in mV („Value“) must be entered as parameters. A peak limit only allows the time control file to restart when one or more peaks exceeds the limit value and then falls back below this value during the time duration of the time control file. If one or more peak limits fail, the „Restart“ command will be ignored and you will receive an error message on screen.

„Restart Time Control File“ is used to restart the time control file. You can select the parameter „Loop“ for an endless loop, or „Repeats“ in order to enter a certain number of repeats. Once all the repeats have been carried out, this command will be ignored.

„Event Box Output“ is used to switch one of the 12 event box outputs. The required event box output and the state to be switched to (Off, On, Pulse) must be selected as parameters.

„Wait for Input“ interrupts the continuation of the time control file through time („Hold Function“) until the selected event box input or the game port has the state programmed „Off“, „On“ or „Pulse“. This function can be used when injecting by means of a manual injection valve, for example.

„Load new File“ is used to load and start the time control file selected. This allows you to link several time control files together.

„Auxiliary Output“ is used to switch the pump interface's auxiliary output. You can select „On“ or „Off“ as parameters.

„Temperature“ is used to program up to two system temperatures. The parameters are the temperatures in °C.

„Stop all“ is used to end a run and stop the pumps.

„Fraction Limiter“ is used to program fraction limits. You can enter a maximum volume in ml or a maximum time in seconds. The value programmed will not change the limiter setup, but will be adopted as a current value.

„Annotation“ is used to add manual text annotations to the chromatograms.

„Virtual Switch“ is used to program up to 10 virtual switches. These virtual switches can have the state “on” or “off”.

„Display Information“ is used to display user defined information which are shown in the “Information label” of the system visualisation.

„Valve Position“ is used to switch valves. Select the desired valve and position as parameters.

„UV-Wavelength“ is used to program the wavelength of an UV detector. Enter the desired wavelength in nm and channel as the parameter.

„UV-Range“ is used to program the range value of a UV detector.

„UV-Autozero“ makes the UV detector automatically return to zero.

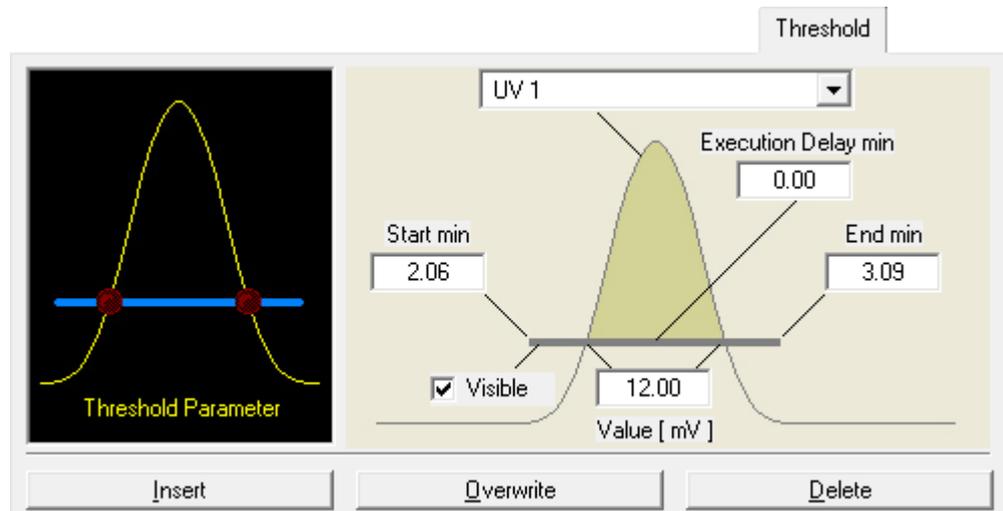
„UV-Lamp“ is used to switch on or off the lamp from the UV-detector. (Only when supported)

„Autosampler Inject“ is used to carry out an injection from an autosampler. This function can only be used in conjunction with an autosampler control file. The course of the time control file is paused during the injection phase and the “Elapsed Time” display in the main window shows the time passed and “Injection” alternately.

„Collector“ is used to program a fraction collector position. The parameters can be a return to the home position (“Home”), a move to a further position (“Step”) or a position number (“Position”).

### 6.2.8 Programming thresholds

The “**Threshold**” tab allows you to program thresholds, meaning that a series of device control functions can be executed if a value exceeds or drops below the threshold. The threshold values allow individual fractionating or system monitoring possibilities, thanks to their selectable data source, programmable time frames for activities and programmable threshold levels. Up to 50 threshold values can be active at any one time.



The graph on the left of the tab is used to select the threshold parameters. Click on the graph next to the LEDs and the boxes for the general threshold parameters will appear. You can select the data source of a threshold value in the upper box. You can choose between all the analogue channels, the system pressure, the event box inputs and the game port inputs.

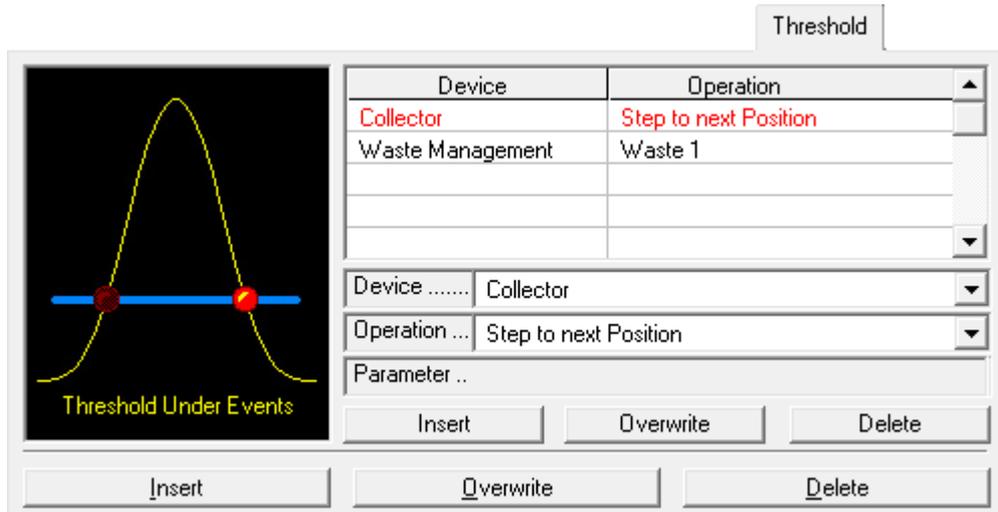
The boxes “Start Time” and “End Time” set the time frame for the activity of the threshold

The “Value” box is for the threshold value. When using event box or game port inputs, this parameter is not available, since the data source only has two possible states (Low = Threshold Under Event, High = Threshold Over Event).

The “Execution Delay” parameter delays the execution of all programmed “Over Event Functions” in this Threshold.

By choosing the “Visible” option the graphic line of this Threshold will be displayed in the analysis windows. Otherwise, it will be invisible.

Click on the left-hand LED in the graph and the function table of the “Over Event Functions” will appear, in other words, the functions that are carried out if the threshold



value is exceeded. The selection boxes “Device“ and “Operation“ allow you to set the desired function, and the “Insert” button adds these functions to the time control file.

You can use the “Overwrite” button to overwrite a selected line, and “Delete” to delete it. If you click on the right-hand LED, the function table of the “Under Event Functions“ appears, i.e. the functions that are carried out when the value is less than the threshold. Functions can be set in exactly the same way here as for “Over Events“.

### 6.2.9 Using logic gates

As Over and Under Events functions the inputs of logic gates can be set. Logic gates can be used to monitor several channels simultaneously and to use the combination of these channels as input for the fractionation. PrepCon5 handles 10 individual logical gates. For each gate several inputs of four internal gates can be set to 0 or 1. The four internal gates are or-gates (OR), and-gates (AND), not-and-gates (NAND) and exclusive-or-gates (XOR). These internal gates are evaluated in the order: OR-AND-NAND-XOR. If an internal gate gives a result of 0 the evaluation is stopped and the logic gate is set to 0 in total. E.g. if inputs of the OR-gate are evaluated and the result is 0 the other logical gates are not processed.

The several inputs and one output of a logic gate can have the binary values 0 or 1. The

A	B	Y
0	0	0
0	1	1
1	0	1
1	1	1

OR-Gate

A	B	Y
0	0	0
0	1	0
1	0	0
1	1	1

AND-Gate

A	B	Y
0	0	1
0	1	1
1	0	1
1	1	0

NAND-Gate

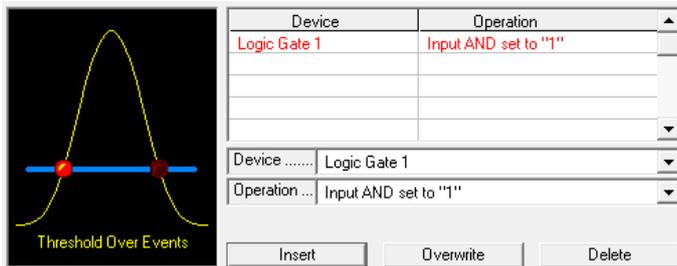
A	B	Y
0	0	0
0	1	1
1	0	1
1	1	0

XOR-Gate

output of the OR-gate has the value 1 if at least 1 input value is 1. The output of the AND-gate is 1 if all inputs are 1. The output of the NAND-gate is 1 if at least one input is 1 and the output of the XOR-gate is 1 if exactly 1 input is 1. The logical operations leading to the outputs are illustrated in the truth tables for the four logic gates used.

Example:

Logic gates can be used to collect fractions in case a defined DAD-channel (channel 1) and a defined MS-channel (channel 2) are above threshold while another MS-channel (channel 3) is not above threshold.

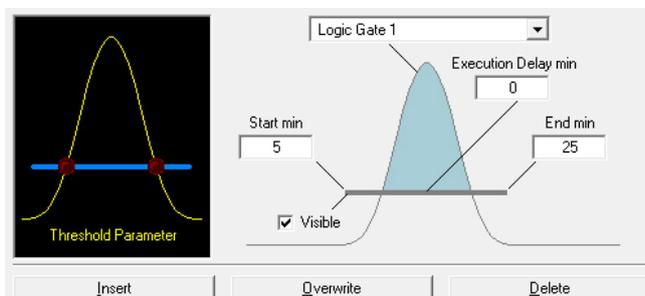


Threshold 1 is programmed for channel 1: if the threshold is exceeded an AND-input of logic gate 1 is set to 1, if the channel value falls below the threshold the input is set back to 0. This is done by setting an AND-input of logic gate 1 to 1 and 0 in case of an „Over Event“ or „Under Event“.

In the same way another threshold monitoring channel 2 is programmed, setting another AND-input of logic gate 1 to 1 and to 0, respectively. A third threshold monitors channel 3 and sets the NAND-input of logic gate 1 to 1 and 0 in case of an „Over Event“ or „Under Event“.

A	B	C	Y
0	0	0	0
0	1	0	0
1	0	0	0
1	1	0	1
0	0	1	0
0	1	1	0
1	0	1	0
1	1	1	0

The output of logic gate 1 now is 1 in case both signals of channel 1 and 2 are above threshold while channel 3 is below threshold. This behaviour can also be demonstrated by the corresponding truth table combining the AND-inputs A and B with the NAND-input C to output Y of the logical gate. If the AND of channels 1 and 2 is 0 the NAND is not evaluated (hashed fields in the truth table).

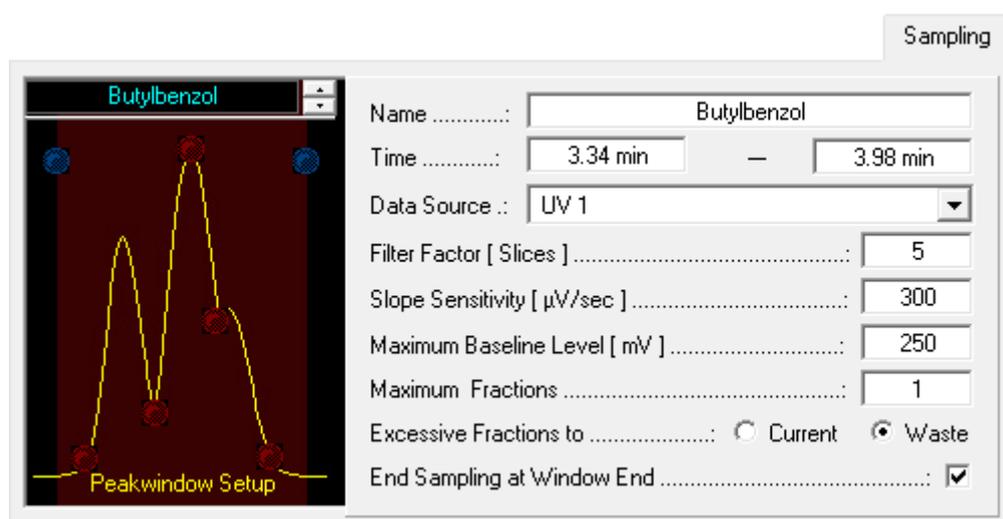


Another threshold using logic gate 1 as input can be used for the fractionation.

### 6.2.10 Programming peak sampling

The “**Sampling**” tab allows you to program peak sampling. Peak sampling is a way of carrying out a series of device control functions based on automatically recognised peak situations. Peak sampling takes place in peak windows, the start and end times of which can be set by the user. You can select the data source, sensitivity of peak recognition and the functions to be carried out separately for each peak window. This allows you to react to single peaks on an individual basis. When fractionating in combination with threshold values, the thresholds and peak samples always combine to form one fraction event. This means that as long as the threshold is still exceeded or the peak sampling has not yet recognised the end of a peak, fractionating continues.

The graph of peak situations is used to select the peak sampling parameters and peak situations. Click on the graph next to the LEDs and the boxes where you can enter the peak sampling parameters will appear. You can choose the peak window you require from the graph.



The name of the peak window can be entered in the “**Name**” box.

The “**Time**” boxes are for the time point where the window starts and ends.

In “**Data Source**” you can select the data sources for these time windows.

The “**Filter Factor**” parameter indicates the number of data points used for the first derivation when calculating the gradient.

The “**Slope Sensitivity**” indicates the size of the gradient above which the start of a peak is recognised.

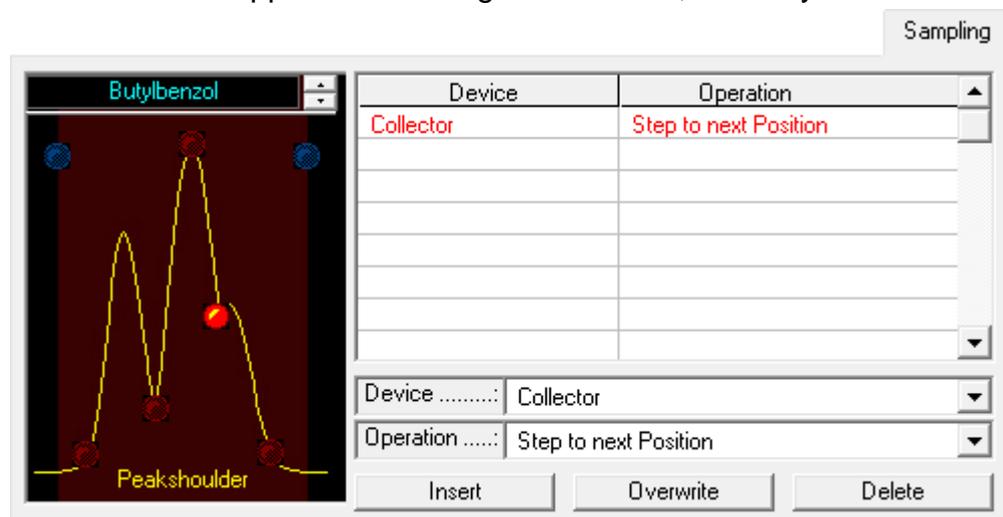
“**Maximum Baseline Level**” is used as a threshold value for peak sampling. No peak end is recognised above the value entered.

The “**Maximum Fractions**” parameter is only relevant to the “**Defined by Peak Window**” setting, which is a possible position setting for motorised switching valves. It indicates the maximum number of fractions that can arise in this peak window.

The “**Excessive Fractions to**” option determines where the fractions that exceed the maximum number of fractions should be pumped. “**Current**” pumps them in the current position, and “**Waste**” pumps them into the waste.

The “End Sampling at Window End” option indicates whether fractionating should continue after the end of the time period of a peak window, or whether the system should switch to waste.

To program peak sampling functions, click on the LED at the desired location. A function table will then appear on the right-hand side, which you can fill in with functions. The



selection boxes “Device” and “Operation” allow you to select the required function and add it to the time control file with the “Insert” button. The “Overwrite” button allows you to overwrite a selected line, and the “Delete” button deletes it.

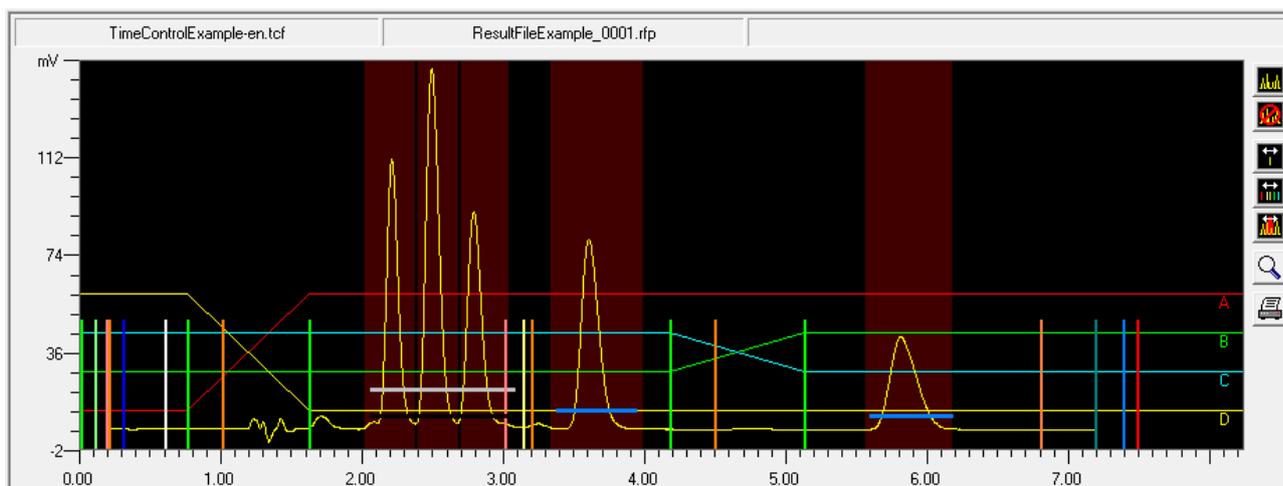
The possible peak sampling situations are:

- “Peak Window Start” (Blue LED on the left) is the time when a peak window begins.
- “Peak Window End” (Blue LED on the right) is the time when a peak window ends.
- “Peak Start” is the start of a peak as recognised by the peak sampling.
- “Peak Valley” is a dip in a peak recognised by the peak sampling.
- “Peak Shoulder” is the shoulder of a peak recognised by the peak sampling.
- “Peak End” is the end of a peak as recognised by the peak sampling.

The following rules apply to the sensitivity of peak sampling:

- The smaller the data point density (slice width), the faster and more sensitive the peak sampling. (However, bear in mind that very small slice widths lead to large results files)
- The smaller the “Filter Factor”, the faster and more sensitive the peak sampling. (Bear in mind that the factor range is from 5 to 15, and the value entered must be an odd number)
- The smaller the “Slope Sensitivity” value, the more sensitive the peak sampling

### 6.3 The graphic time control file editor



The graphic time control file editor is used to create a graphic presentation of a time control file and allow visual editing. All the functions of the time control file are shown as coloured lines which can be moved horizontally (movement in time) and vertically (changing the threshold value or peak limit) with the mouse. A highlighted function in the table representation of the time control file will flash on the graph. Clicking on a function on the graph will likewise highlight the corresponding line of the table. Peak windows are also represented graphically and can be created and edited with the mouse.

A programmed gradient development is also represented by coloured lines, whereby 0% is the y-axis minimum and 100% is the y-axis maximum.

You can load a chromatogram as a background image, which you can then use to adjust the functions of your time control file. The display colours of all the functions can be selected at will in the graphic time control file editor setup, and any functions you do not want to show can be deactivated.



The status bar in the graphic time control file editor shows the name of the time control file loaded, the name of the chromatogram loaded and an information box indicating the following:

- The time control file function over which your mouse cursor is positioned, or which you are moving by means of the "Single Function Moving" function.
- The time by which you are shifting the functions when using the "Multi Function Moving" function.
- The name and times of the peak window over which your mouse cursor is positioned when using the "Create / Edit Peak Window" function.

The graphic time editor tool bar is on the right-hand side of the window. Its functions are listed here in the order they appear on screen:



“Load Chromatogram” opens a chromatogram being used as a background image.



“Clear Chromatogram” removes the loaded chromatogram from the graph.



“Single Function Moving” allows single functions to be moved.



“Multi Function Moving” allows multiple functions to be used. To do this, begin by drawing a time window with the left mouse button held down. All the functions within this window can then be moved with the mouse at the same time. Holding down the right mouse button will adopt the time shift.



“Create / Edit Peak Window” allows peak windows to be created and edited. To create a peak window, simply hold down the left mouse button and draw a new window on screen. When you release the mouse button, you will be asked for the name of the new window. You can edit an existing peak window by moving the mouse cursor over the window. The cursor will change, depending on its position in the window, from an arrow pointing left (on the left-hand side of the window) to an arrow pointing right (on the right-hand side of the window) or an arrow pointing both ways (in the centre of the window). By holding down the left mouse button, you can now extend or move the window to the left and right. If you right-click over a peak window, menu options to rename or delete the window will appear.



“Zoom Graphic” is used to enlarge part of a graph. To do this, drag out a window with the left mouse button held down to include the area you wish to enlarge. In order to return to the original graph size, right-click with the mouse.



“Print Graphic” prints the graph shown.

## 7. Creating Sequence Tables

### 7.1 General

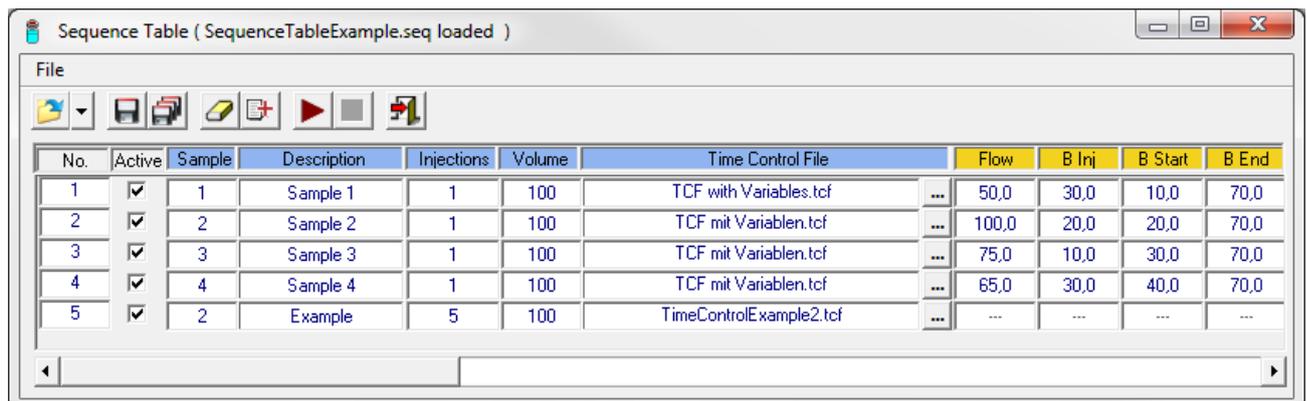
You can open the sequence table editor with the function button or the menu option „Create / Edit Sequence Table“ in the main window.

A sequence table processes a sequence of time control files. These time control files may or may not use autosampler injection via the command „Autosampler Inject“. For time control files with autosampler injection the sample position, number of injections and injection volume of the autosampler can be programmed in the sequence table.

If time control files, which use variables, are inserted into the sequence table, columns for each variable will be added to the sequence table. For each sequence table line different values can be assigned to the time control file variables.

Time control files incorporating the functions „Restart Time Control File“ and „Load New File“ can not be used in the sequence table. If you want to connect different time control files this can only be done using the sequence table lines.

### 7.2 Creating a sequence table



No.	Active	Sample	Description	Injections	Volume	Time Control File	Flow	B Inj	B Start	B End
1	<input checked="" type="checkbox"/>	1	Sample 1	1	100	TCF with Variables.tcf	50,0	30,0	10,0	70,0
2	<input checked="" type="checkbox"/>	2	Sample 2	1	100	TCF mit Variablen.tcf	100,0	20,0	20,0	70,0
3	<input checked="" type="checkbox"/>	3	Sample 3	1	100	TCF mit Variablen.tcf	75,0	10,0	30,0	70,0
4	<input checked="" type="checkbox"/>	4	Sample 4	1	100	TCF mit Variablen.tcf	65,0	30,0	40,0	70,0
5	<input checked="" type="checkbox"/>	2	Example	5	100	TimeControlExample2.tcf	...	...	...	...

On the left hand side of the window is the toolbar for the sequence table editor. The functions are listed here in the order that corresponds to the display:



„Load sequence table“ loads an available sequence table into the editor.



„Save sequence table“ saves the sequence table under its existing file name as .seq file.



„Save sequence table as ...“ saves the sequence table under a new name



„Clear sequence table“ deletes all entries in all lines of the sequence table.



„Add row“ enters a new empty line into the sequence table.

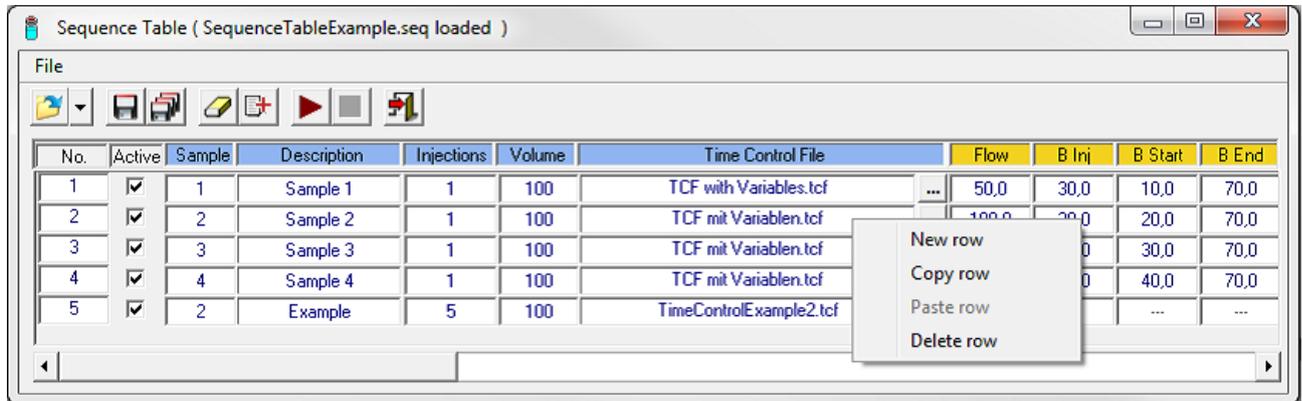


„Exit“ closes the sequence table editor.

After selection of a time control file (.tcf file) in a sequence table line, the columns on the right hand side will be adjusted automatically displaying one column for each variable used in any sequence table line. For each line the variables used in the selected time control file

can be entered in the sequence table line. This allows for modification of the time table within the sequence table.

The right mouse click opens a menu with items for copying, inserting and deleting rows into the time table.



The Menu item „File – Import Autosampler Control File“ opens a dialog window for the selection of an autosampler control file (.acf). The lines of the autosampler control file will be imported into the sequence table.

### 7.3 Execution of a sequence table

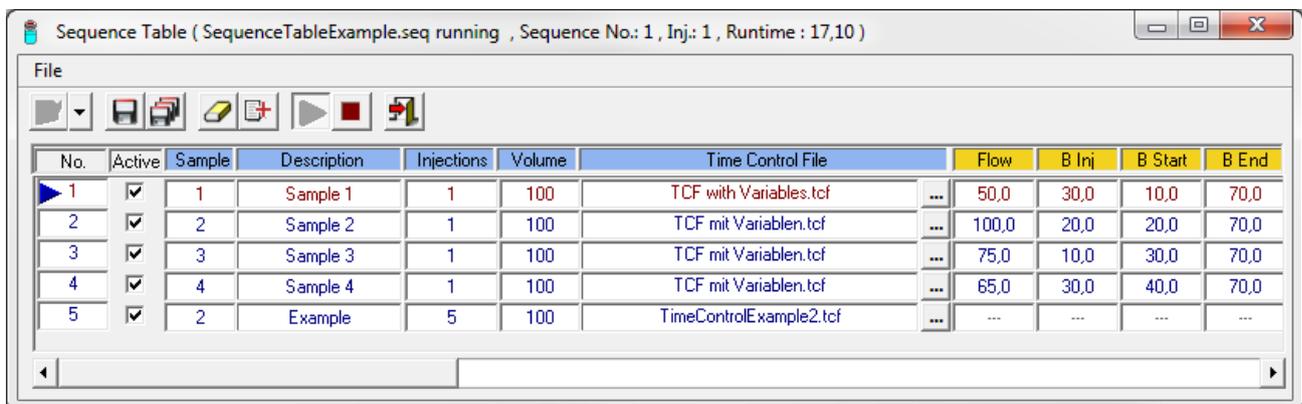


„Start sequence table“ starts the execution of a sequence table.

All sequence table lines with the check box in column *Active* activated will be executed successively. During the execution the current row will be highlighted with a blue arrow and the caption of the sequence table editor window displays the current sequence, injection and runtime. Future lines can be edited during execution.



„Stop sequence table“ or the button „Stop All“ in the main window stops the execution of the sequence table.



## 8. Creating autosampler control files

### 8.1 General

The function key and the menu option “Create / Edit Autosampler Control File” in the main window open the autosampler control file editor.

An autosampler control file works on the principle of a series of time control files, each of which is allocated an automatic sample injection. The command for the sample injection is programmed into the corresponding time control file with the command “Inject”.

During injection, the time progression is paused (Time Control Hold). The parameters for the injections are programmed into the autosampler control file. These parameters include the vial numbers, the number of injections per vial, the injection volume and the column oven temperature. However, certain values for the time control file can also be pre-set. To do this, the parameter “AS” must be entered in the time control file. Then the parameter “AS” will act as a variable and obtain its values from the current line of the autosampler control file.

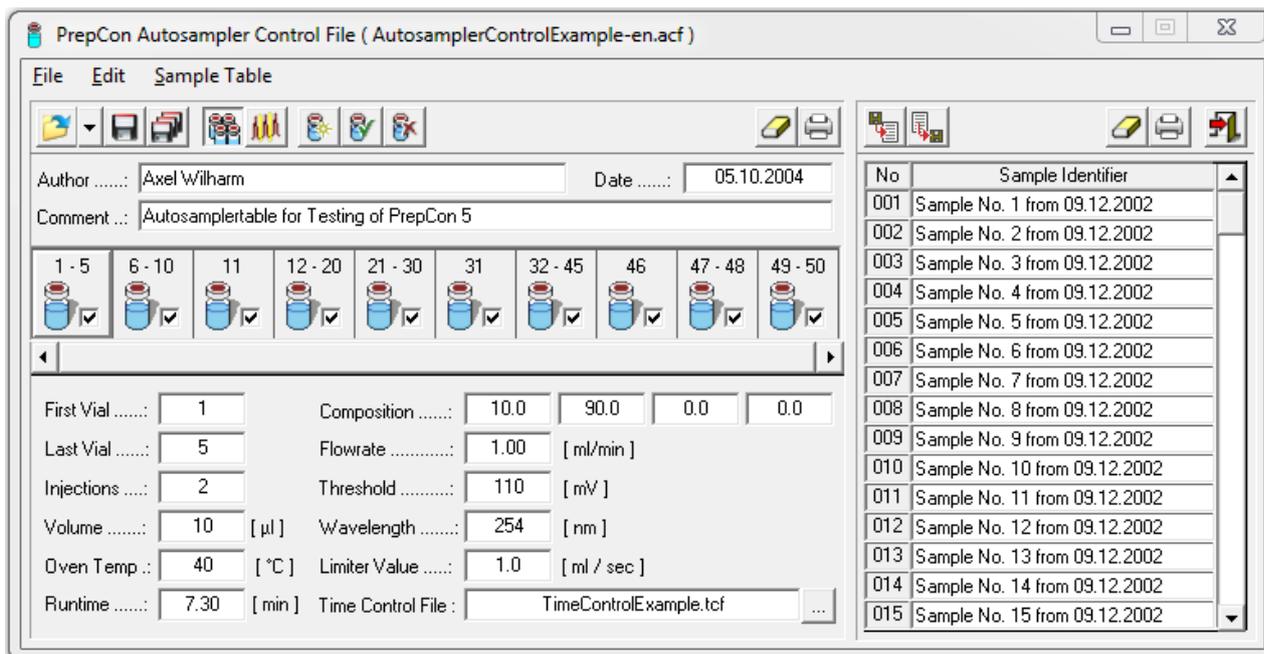
Possible commands include:

Solvent	(eluent composition for the pump)
Flow rate	(flow rate for the pumps)
Threshold	(level of a programmed threshold value)
Wavelength	(UV detector wavelength)
Limiter Value	(maximum size of the fractions obtained)

The running time programmed into the autosampler control table determines the time after which the current or a new time control file is started for the next injection. In other words, the time progression of an autosampler control file determines which time control file is started and how long it runs for. Restarting a time control file will only occur for as long as further injections take place. After the last injection, the corresponding time control file will therefore continue running until the system stops. This function can be useful if you program a “Stop all” in the time control file after the programmed running time of the autosampler control file. For as long as there are further injections waiting, this command will not be carried out, because the time control file will always restart first. It is only after the last injection that the time control file will reach this line of the program, and the system will stop automatically.

Autosampler injections can be programmed either singly or as a sequence. The sample identifiers of the individual vials can be entered in a sample table. For each injection, the identifier corresponding to the sample number will be read from this table.

## 8.2 Creating an autosampler control file



The editor toolbar is in the upper part of the window. The functions are listed in the order they appear on screen:



„Open Autosampler Control File“ loads an existing autosampler control file into the editor. The possible file types to be loaded are “Autosampler Control File” (\*.acf) or “Result file” (\*.rfp). “Result file” allows you to load an autosampler control file from a result file.



„Save Autosampler Control File“ saves the autosampler control file under its existing name.



„Save Autosampler Control File as ...“ saves the autosampler control file under a new name.



„Injection Parameter“ opens the panel with the input fields of the injection Parameter.



„Stacked Injection Parameter“ opens the panel with the input fields of the stacked injection Parameter.



„Stacked Injection enable / disable“ activates or deactivates the stacked injection-function of the autosampler control file.



„Insert Autosampler Sequence“ adds the autosampler sequence in the editor box to the autosampler control file.



„Overwrite Autosampler Sequence“ overwrites the highlighted autosampler sequence with the one in the editor box.



„Delete Autosampler Sequence“ deletes the highlighted autosampler sequence.



„Clear all“ deletes the contents of the autosampler control file. In order to prevent accidental deletion, this function is only carried out after you have confirmed it.



„Print Autosampler Control File“ opens a printer dialogue box to print out the

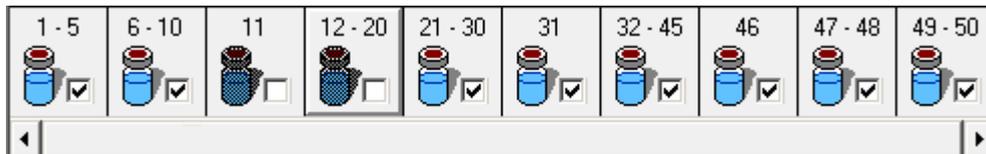
autosampler control file.



„Exit“ closes the editor.

You can enter your name and a comment on the autosampler control file in the “Author” and “Comment“. The date is generated automatically when you save the file.

The sequence bar shows all the autosampler sequences. The highlighted line is shown as raised. If there are more than 10 sequences, you can scroll along the sequence bar using



the scroll bar underneath. Each sequence is shown with the vial numbers

programmed. You can tick the sequence icons to activate or deactivate them for processing. When you resume an interrupted run, you can use this function to deactivate the sequences that have already been processed.

Beneath the sequence bar is the editor box with entry boxes for a sample sequence. The parameters to be entered are the following:

„First Vial“ is the number of the first vial in a sample sequence.

„Last Vial“ is the number of the last vial in a sample sequence. If you are only injecting from one vial, enter the same number in “First Vial” and “Last Vial“.

„Injections“ indicates the number of injections per vial.

„Volume“ indicates the injection volume in  $\mu\text{l}$ .

„Oven Temp“ indicates the temperature of the column oven.

„Runtime“ indicates the running time after which the current or a new time control file will begin with the next injection. The running time should always be shorter than the last line in the corresponding time control file that still has to be carried out.

„Solvent“ indicates an eluent composition entered in the solvent lines of a time control file with the eluent composition “AS” as a parameter.

„Flow Rate“ indicates a flow rate entered in the flow rate lines of the time control file with the flow rate parameter “AS”.

„Threshold“ indicates a threshold level entered in the threshold lines of the time control file with the threshold value “AS” as a parameter.

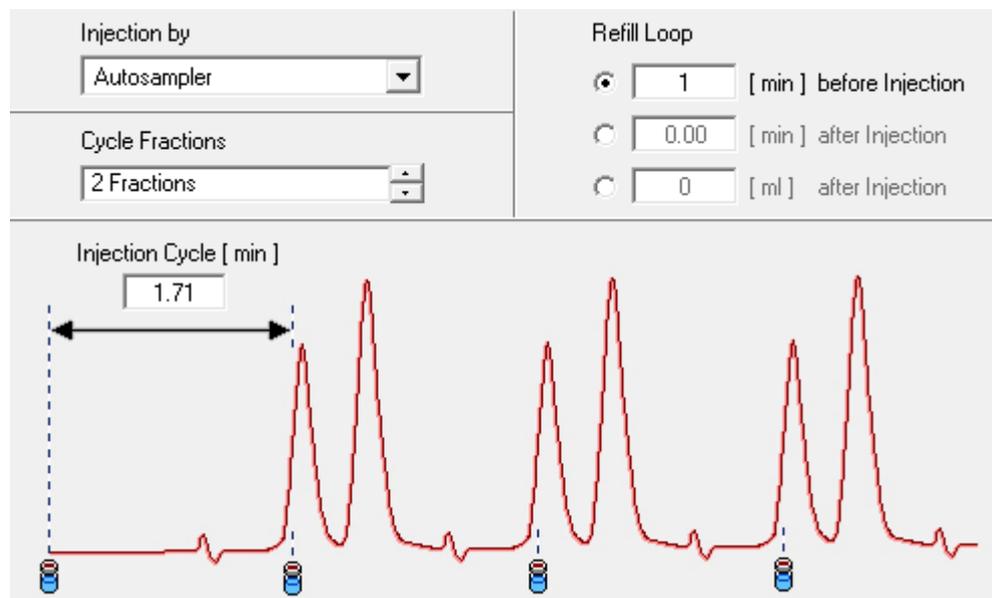
„Wavelength“ indicates a wavelength entered in the wavelength lines of the time control file with the wavelength parameter “AS”.

„Limiter Value“ indicates a maximum volume entered in the limiter lines of the time control file with the maximum volume parameter “AS”.

„Time Control File“ indicates the time control file which is started for every injection in this sequence.

### 8.3 Stacked Injection

The function „stacked injection“ allows for multiple nested injections of identical probes in order to save solvents and time. During the elution, time of one sample the following



sample is already charged onto the column. If the function „stacked injection“ is activated, all entries of the sample table will be executed within one run. In the select list under the item „Injection by...“ one can choose whether samples are automatically injected by an

autosampler or by a valve. In case of injection by valve the main pump aspirates sample and switches the injection valve into position 2 until the required amount of sample is pumped into the system.

The Parameter „fractions per cycle“ defines the number of fractions collected within one cycle. After this number is reached, the cycle is repeated and the following fraction is again collected into the start position.

In case of injections using an autosampler the parameter „sample loop fill“ defines at what time the sample loop is refilled. Possible options are „time before injection“, „time after injection“ and „volume after injection“.

The time table for a run using stacked injections corresponds to that of a single injection but will be automatically extended for each additional injection (see example tables below). The parameter „injection cycle“ defines the time between two consecutive injections. The injection times are indicated by sample vials in the chromatogram as can be seen in the upper figure.

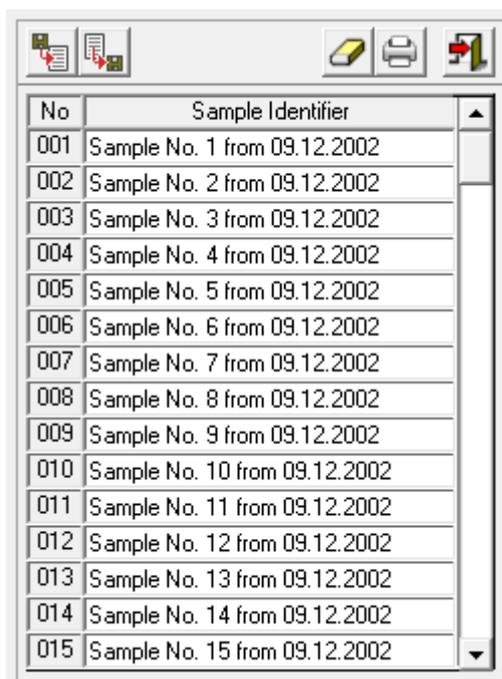
Initial time table

Time [min]	Function	Parameter
0.00	Composition Major Pump	100.0 , 0.0 , 0.0 , 0.0
0.00	Flowrate Major Pump	100.00 ml/min Constant Flow
0.15	Autosampler Inject	
0.20	Start Chromatogram	Channel 1 ( 200 ms )
1.00	Threshold	4.90 min / 25.00 mV
6.00	Stop Chromatogram	All started Channels
6.10	Stop all	

Time table after 10 „Stacked Injections“

Time [min]	Function	Parameter
0.00	Composition Major Pump	100.0 , 0.0 , 0.0 , 0.0
0.00	Flowrate Major Pump	100.00 ml/min Constant Flow
0.15	Autosampler Inject	
0.20	Start Chromatogram	Channel 1 ( 200 ms )
1.00	Threshold	20.29 min / 25.00 mV
1.86	Autosampler Inject	
3.57	Autosampler Inject	
5.28	Autosampler Inject	
6.99	Autosampler Inject	
8.70	Autosampler Inject	
10.41	Autosampler Inject	
12.12	Autosampler Inject	
13.83	Autosampler Inject	
15.54	Autosampler Inject	
21.39	Stop Chromatogram	All started Channels
21.49	Stop all	

## 8.4 Creating a sample identifier table



No	Sample Identifier
001	Sample No. 1 from 09.12.2002
002	Sample No. 2 from 09.12.2002
003	Sample No. 3 from 09.12.2002
004	Sample No. 4 from 09.12.2002
005	Sample No. 5 from 09.12.2002
006	Sample No. 6 from 09.12.2002
007	Sample No. 7 from 09.12.2002
008	Sample No. 8 from 09.12.2002
009	Sample No. 9 from 09.12.2002
010	Sample No. 10 from 09.12.2002
011	Sample No. 11 from 09.12.2002
012	Sample No. 12 from 09.12.2002
013	Sample No. 13 from 09.12.2002
014	Sample No. 14 from 09.12.2002
015	Sample No. 15 from 09.12.2002

The sample identifier table is located on the right hand side of the editor. The sample numbers are displayed in the first column of the table, and the sample identifiers in the second column. The sample identifiers can be written directly into the table.

Before each injection, the identifier corresponding to the sample number is read from this table and used as the "Sample Identifier". The number of rows in the table can be set in the file "PrepCon5.ini" with the command "[MaximumSamples]". 100 sample identifiers are possible as standard.

Above the table is the sample identifier table toolbar. Its buttons have the following functions:



„Import Sample Table“ imports a sample identifier table from a text file.



„Export Sample Table“ exports the sample identifier table as a text file.



„Clear Sample Table“ deletes the content of the sample identifier table. In order to avoid accidental deletion, this function will only be carried out after confirmation from the user.

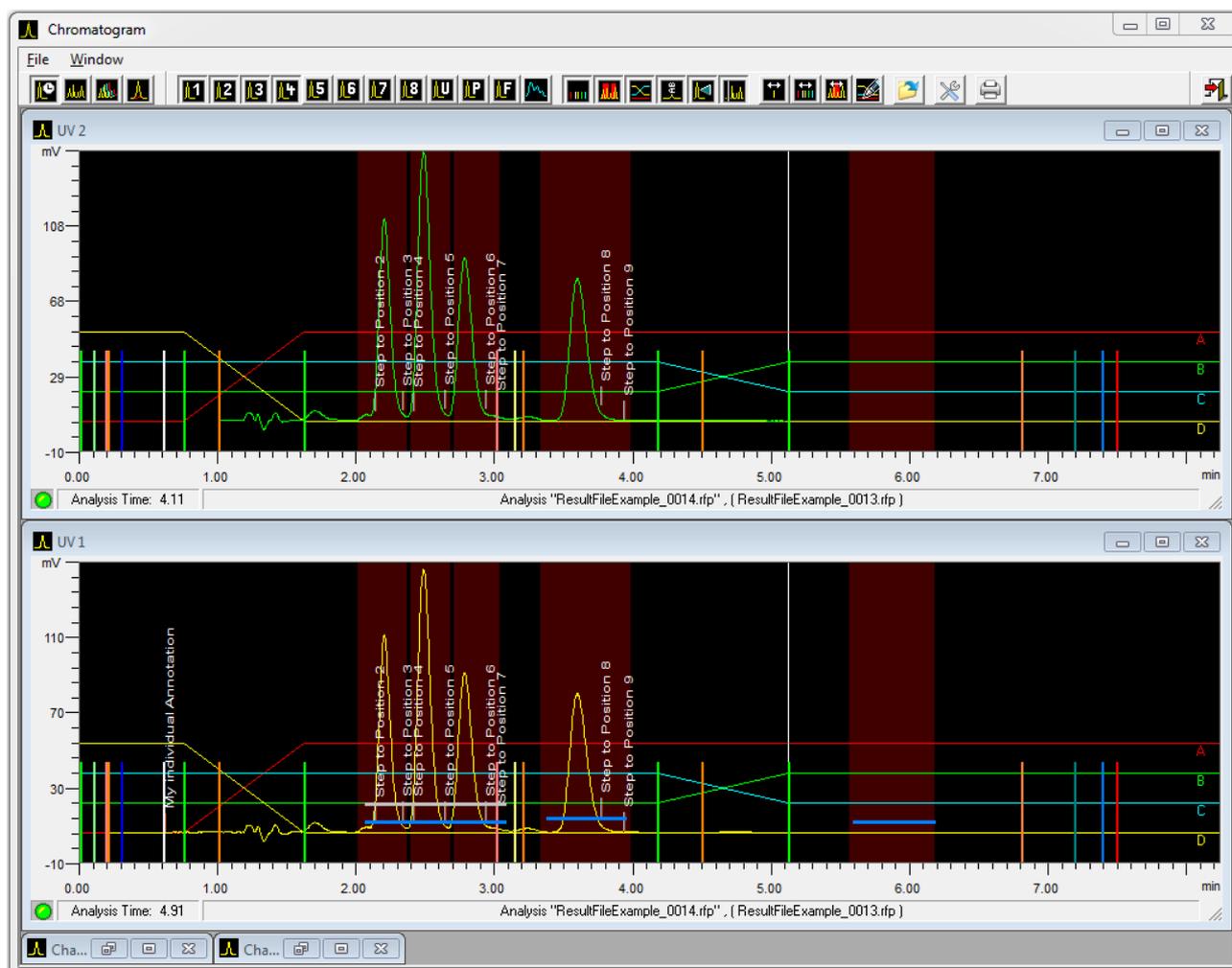


„Print Sample Table“ opens a printer dialogue box to print out the sample identifier table.

## 9. Data recording (Analysis)

### 9.1 General

The function key and the menu option “*Chromatogram*” in the main window open the chromatogram window. The first area is data recording (Analysis).



The data-recording window is used to display and record analogue signals. The requirement for this is an analogue/digital converter card in your PC. Up to 8 analogue signals can be recorded at once. The automatic peak sampling can only work with these analogue signals.

Data recording is started in the time control file with the command “*Start Chromatogram*” and stopped with “*Stop Chromatogram*”. Chromatograms can be started simultaneously or with a delay.

While a time control file is running, the graphic display of the time control file, the current chromatogram trace, the programmed peak windows, the gradient and the current chromatogram labels are displayed in the data recording windows. Just like in the graphic time control file editor, you have the possibility to edit time control file functions and peak windows in the data recording windows. These changes take effect on the current run and can also be saved in the time control file loaded. This means you have the possibility of intervening in a process “online”. However if you move a gradient, this will not take effect until the next time the time control file starts.

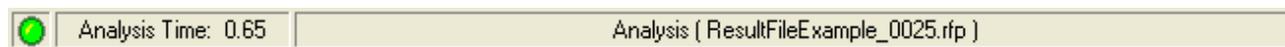
## 9.2 Function buttons in the data recording window

-  Channel... is used to open or close a data channel window. Only the buttons for the channels that can be selected are shown. The “U” button belongs to a user-defined channel (see chapter 4.6). Data channels which are programmed into a time control file are automatically opened upon loading. If no data recording is active, the data track selected runs in base line mode, i.e. from the left to the right edge in about 8 minutes as an endless loop. Data recording is started with the time control file command “Start Chromatogram” and stopped with the command “Stop Chromatogram”.
-  Pressure Channel shows the pressure data of the pump. This channel can be used like the data channels described above.
-  Flow Rate Channel shows the actual value of the flow rate performed by the major pump system. It can be used like the data channels described above. It is especially useful when using the option „pressure limit“ in a time control file programming. Then it will show when and in which intensity the automatic flow rate control was active.
-  Spectrum Channel is used to show or hide the spectrum window of the DAD.
-  Show Functions is used to show or hide the time control file functions. When the functions are hidden, the contents of the window are scaled to fit the area of the data recording.
-  Show Peak Windows is used to show or hide the peak windows.
-  Show Gradient is used to show or hide the programmed gradients.
-  Show Annotations is used to show or hide the current annotations.
-  Show Last Chromatogram automatically loads the last chromatogram as a background image in the data channel window.
-  Show Elapsed Time Line is used to show or hide the vertical line indicating the elapsed time.
-  Single Function Moving enables you to move single functions (see chapter 6.3). Changes take immediate effect in the current run, and after deselecting these functions you will be asked if they should be saved in the time control file as well.
-  Multi Function Moving enables you to move multiple functions (see chapter 6.3). Changes take immediate effect in the current run, and after deselecting these functions you will be asked if they should be saved in the time control file as well.
-  Create / Edit Peak Window allows you to create and edit peak windows (see chapter 5.6). Changes take immediate effect in the current run, and after deselecting these functions you will be asked if they should be saved in the time control file as well.
-  Edit Gradient opens a window where you can edit the running Gradient. Changes take immediate effect in the current run, and after closing the window you will be asked if they should be saved in the time control file as well.
-  Load last Chromatogram is used to load the last chromatogram manually, as a background image for the data channel window.

 Channel Setup opens the window with the settings for the individual data channels. The different parameters have already been described in chapter 9.4.

 Automatic Print activates or inactivates the automatic printing of the report after the recent run.

### 9.3 The status bar in the data recording window



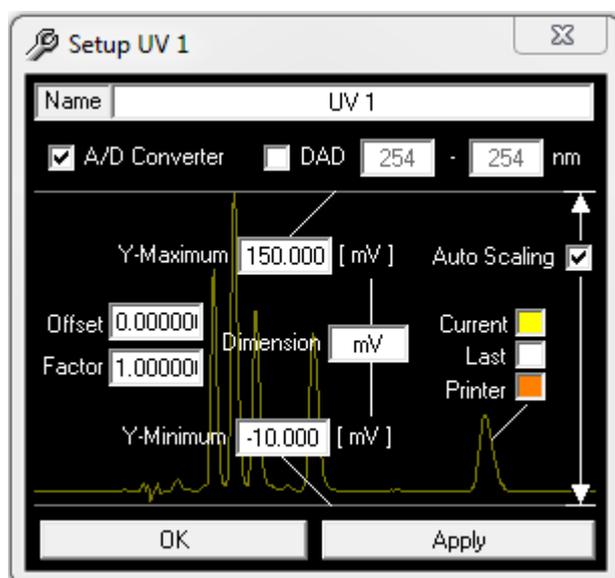
The data recording status is displayed with a graphic in the left-hand box of the status bar. The meaning of the symbols is as follows:

	<u>Baseline</u>	(Baseline is displayed)
	<u>Ready</u>	(data channel is in use, but has not yet started)
	<u>Chromatogram running</u>	(data recording is active)
	<u>Chromatogram finished</u>	(data recording has finished)

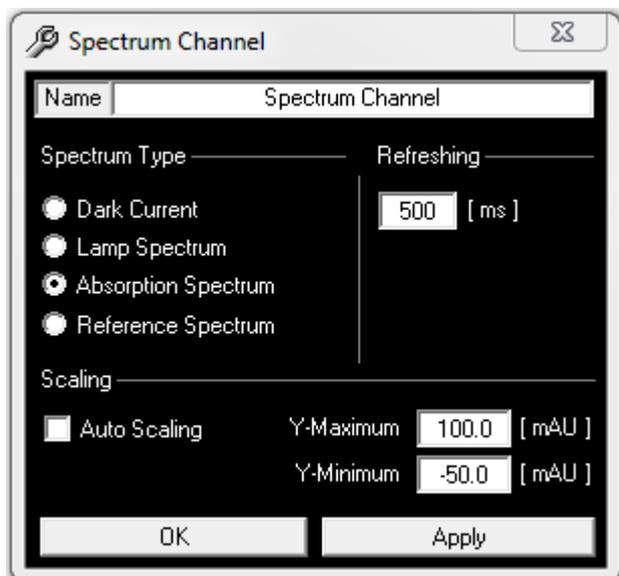
The central box shows the chromatogram running time, and the right-hand box shows the current status, with the name of the results file.

### 9.4 Data Channel settings

The window always shows the data of the selected channel, i.e. the analysis window in focus. You can change the name of the channel in the "Name" window. You can use the options "A/D Converter" or "DAD" to determine the data source of the channel. Select "A/D Converter" for the the data of the A/D conversion cards and "DAD" for the data of the DAD. You can set the the DAD wavelength range in the adjacent text boxes. The "Offset" parameter is used to compensate for a detector offset. The value entered will be added to the analogue signal, and can be positive or negative. The "Factor" parameter is used to correct the size of the analogue signal indicated. A factor of 1 shows the analogue signal at its original size. The "Y-Maximum" and "Y-Minimum" values set the scale of the y-axis. The "Auto Scaling" option automatically corrects the scaling when these values exceed or drop below the corresponding maximum or minimum signal. You can set the measurement unit of each channel in the "Dimension" box. Clicking on the "Current", "Last" or "Printer" box opens a colour selection dialogue, which you can use to set the colour of each chromatogram trace. Current is the colour of the current chromatogram and Last is the colour of the last chromatogram, which is displayed if you use the "Show last Chromatogram" function and "Printer" is the colour of the printed chromatogram. The "Apply" button applies the settings, and the "OK" button closes the window at the same time.



Choose the type of the displayed spectrum in the setup window for the DAD spectrum under „Spectrum type“. „Dark Current“ is the remaining current without exposing the diode array. The „Lamp Spectrum“ is the measured spectrum of the diode array minus the dark current. The „Reference Spectrum“ is a saved lamp spectrum. A reference spectrum can be set manually by the „Set Reference Spectrum“ function key.



The „Absorption Spectrum“ of the DAD is the logarithm of the reference spectrum minus the logarithm of the actually measured lamp spectrum.

The „Refreshing“ parameter defines after which time the spectrum display is actualized.

The „Y-Maximum“ and „Y-Minimum“ values define the scaling of the y-axis. The „Auto Scaling“ option automatically fits the scaling according to the signal maximum and minimum.

## 10. Control file visualisation

The function key and the menu option “Control File Visualisation” in the main window open the window where you can visualise the time and autosampler control files. When you are running a time control file, it will be displayed in the form of a table. All the lines that have

The screenshot shows a window titled "Control File Visualisation" with two tables. The top table, "AutosamplerControlExample-en.acf", has columns for Vial, Inj, Volume, Time, and Sample. The bottom table, "TimeControlExample.tcf", has columns for Time [min], Function, and Parameter. In both tables, rows that have already been executed are highlighted in red, and rows that are still to be executed are highlighted in blue.

Vial	Inj	Volume	Time	Sample
1	1	10	7.30	Sample No. 1 from 09.12.2002
1	2	10	7.30	Sample No. 1 from 09.12.2002
2	1	10	7.30	Sample No. 2 from 09.12.2002
2	2	10	7.30	Sample No. 2 from 09.12.2002
3	1	10	7.30	Sample No. 3 from 09.12.2002
3	2	10	7.30	Sample No. 3 from 09.12.2002
4	1	10	7.30	Sample No. 4 from 09.12.2002
4	2	10	7.30	Sample No. 4 from 09.12.2002
5	1	10	7.30	Sample No. 5 from 09.12.2002
5	2	10	7.30	Sample No. 5 from 09.12.2002
6	1	20	7.30	Sample No. 6 from 09.12.2002
7	1	20	7.30	Sample No. 7 from 09.12.2002

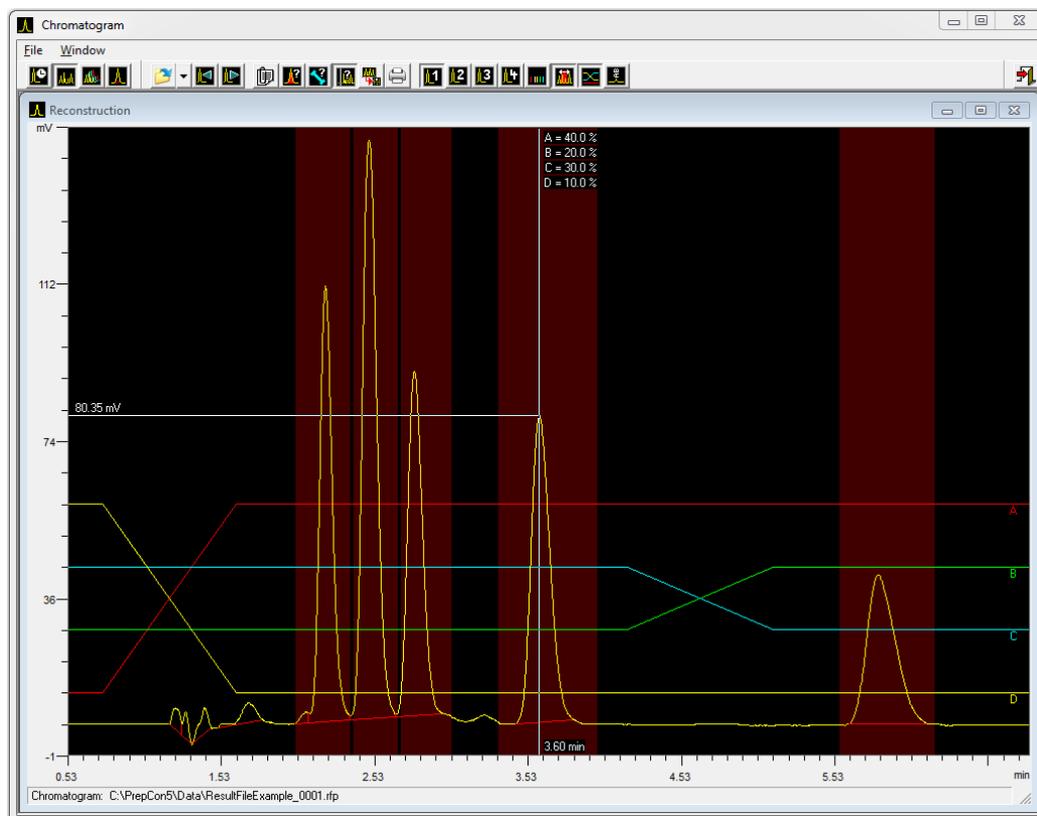
  

Time [min]	Function	Parameter
0.00	Composition Major Pump	10.0 , 20.0 , 30.0 , 40.0
0.00	Flowrate Major Pump	5.50 ml/min Constant Flow
0.00	Fraction Limiter	Limit = 18.00 ml
0.00	Temperature	Column Oven = 25 °C
0.00	Temperature	Sample Heater = 25 °C
0.10	Autosampler Inject	Vial 1 , Injection 1
0.18	Event Box Output	Output 12 = PULSE
0.20	Start Chromatogram	Channel 1 ( 200 ms )
0.30	Auxiliary Output	Auxiliary = ON
0.60	Annotation	"My individual Annotation"
0.75	Composition Major Pump	10.0 , 20.0 , 30.0 , 40.0
1.00	Start Chromatogram	Channel 2 ( 200 ms )

already been worked through will be displayed in red, and those still to come will be in blue. The blue line above the table shows the name of the time control file loaded. When you are running an autosampler control file, another table shows all the injections in the sequences programmed. Here, too, the injections that have already been made are in red and those still to come are in blue. The columns of the table show you the number of each vial, the injection number, the sample volume injected, the running time of the time control file and the sample identifier. The yellow field above this table shows the name of the autosampler control file. The tables automatically scroll down in such a way that the current line is always visible.

## 11. Displaying chromatograms (Reconstruction)

### 11.1 General

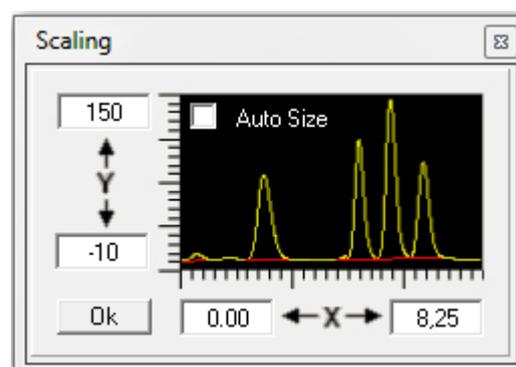


The function key and the menu option "Chromatogram" in the main window open the chromatogram window. The second area displays the chromatograms (reconstruction).

You can load and display result files in the reconstruction window. Chromatograms, time control file functions, peak windows, gradients, chromatogram labels and the protocol of the run can all be displayed. The chromatograms can be displayed singly or, in the case of multiple channel data recording, superimposed. To enlarge the display of certain areas, you can drag out a zoom window by holding down the left mouse button. When you release the mouse button, the display will automatically zoom in on this area. You can repeat this process up to the maximum zoom level. To return to the original size, click on the chart with the right mouse button.

Double clicking on the chromatogram scaling opens a window, in which you can fix the scaling by values. After this, the scaling will be displayed highlight. The option "Auto-Size" automatically fits the chromatogram in the reconstruction window.

The status bar at the bottom of the window shows the path and name of the result file loaded. If you move the mouse cursor over a time control file function, the time and parameter values of this function will be displayed in the status bar.



## 11.2 Function buttons in the reconstruction window



Open Result File opens a results file (\*.rfp). Temporary results files (\*(H).tmp) can also be opened. The temporary results files are created at the end of a method run and usually are deleted after they have been summarized to the results file. On an unexpected end of a run such as power failure or system crash the temporary files still exist. On opening a temporary results file a normal results file is automatically created. The maximum loss of data will be 100 data points. This corresponds to a loss of 50 seconds of chromatographic time when using a slice width of 500ms.



Previous Result File loads the result file that comes before the loaded file in the order of their names.



Next Result File loads the result file that comes after the loaded file in the order of their names.



View Protocol opens a window that displays the run protocol ordered by time.



View Peak Results opens the window with the display of the integration results in table form.



View Column Coefficients opens the window with the display of the column coefficients in table form. To calculate the capacity enter the column dead Time in the field „Column Dead Time“.



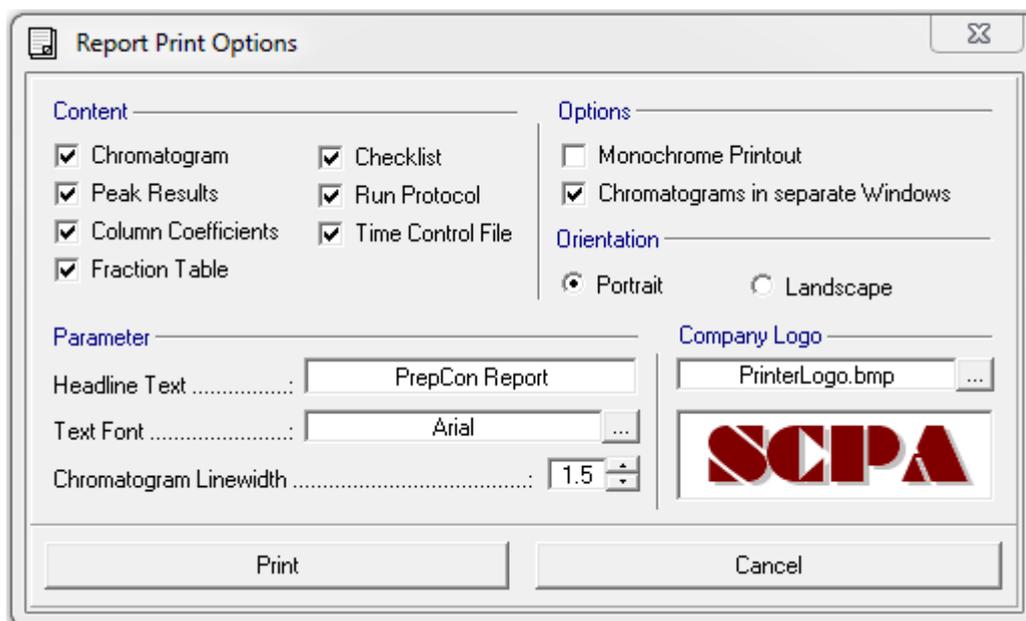
View Peak Value is used to register the peak values. After selecting this function, cross hairs will appear on the graph, which you can move along the chromatogram trace. The time and intensity will be displayed on the cross hair lines. In a multiple channel result file, only one chromatogram can be selected to register peak values. At any time in the chromatogram the appropriate spectrum can be shown when the chromatogram is recorded by a DAD detector and a DAD result file exists. Click with the right mouse key in the chromatogram and choose "Show Spectrum". A new window appears showing the spectrum belonging to the chosen time. This operation can be repeated by clicking again with the right mouse key or by moving the mouse with pressed right key.



Export Chromatogram is used to export one or more chromatograms. The export formats can be selected in the file selection window as file types. Possible export formats are "Comma Separated Value File" for export to Excel, "AIA/Andi File" for export in Andi file format or "Slicefile" for export to ChromStar.



Print Result File is used to print the result file loaded. After selecting this function, a



window opens in which you activate or deactivate elements of the results data to appear on the printout. (see chapter 6.2.5 for the print out settings)



Show Channel ... shows or hides each chromatogram. Hidden chromatograms are not displayed on screen, and they do not appear on the printout either.



Show Functions shows or hides the time control file functions. When the functions are hidden, the window contents are scaled to fit the area of the data recording.



Show Peak Windows shows or hides the peak windows.



Show Gradient shows or hides the gradient.

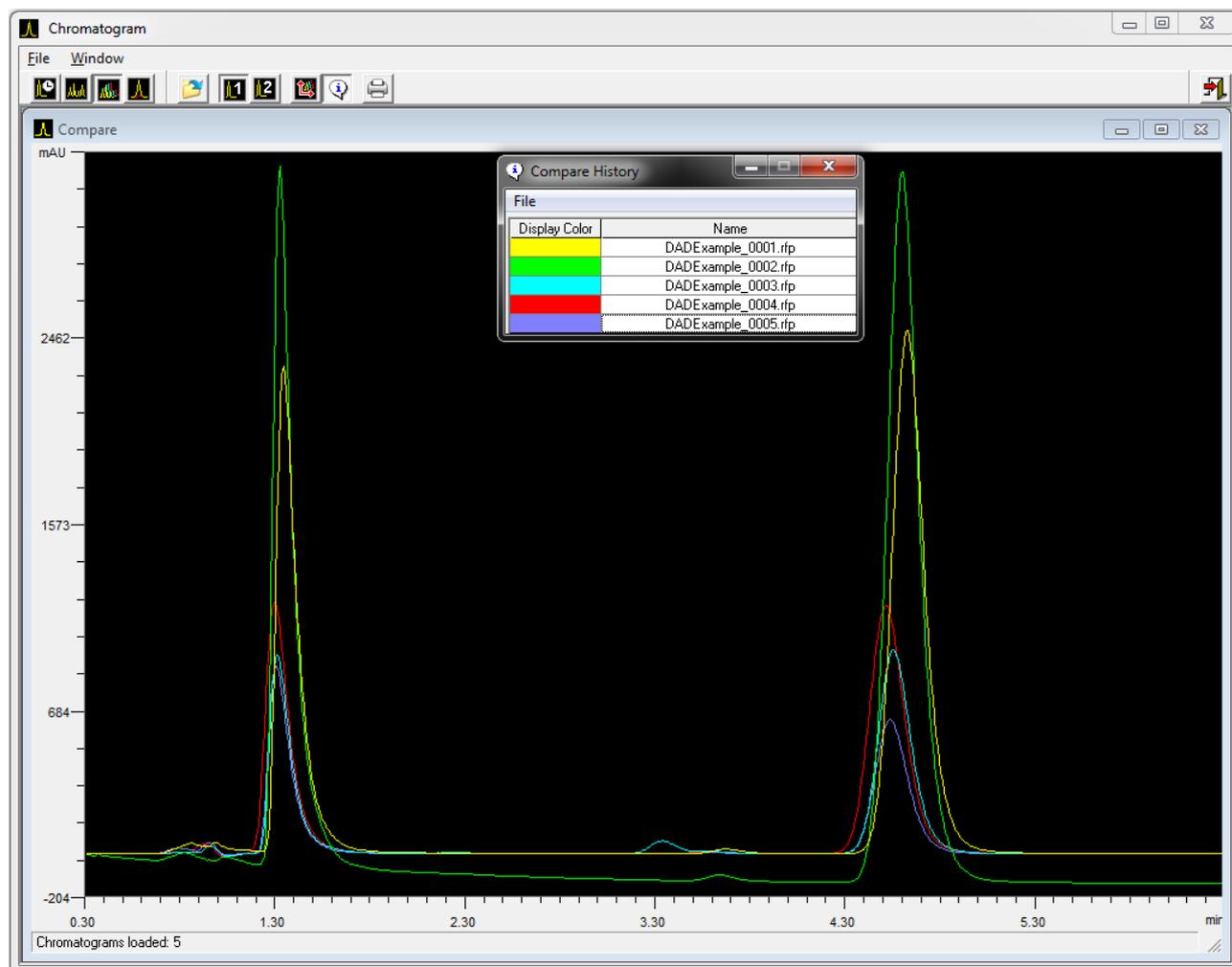


Show Annotations shows or hides the annotations.

## 12. Comparing Chromatograms (Compare)

### 12.1 General

The chromatogram window is opened in the main window via function key or menu procedure „Chromatogram“. The third function key opens the compare chromatograms window (Compare).

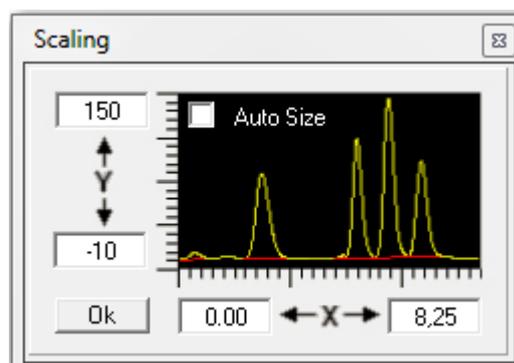


Several result files (.rfp) can be loaded. Only the chromatogram is displayed.

A zoom window can be opened by pressing the left mouse button and dragging the mouse. On depressing the mouse button the zoomed window is shown. This procedure can be repeated until a maximum of magnification is reached. By clicking the right mouse button the original size is restored.

Double-clicking on the chromatogram scaling opens a window, in which you can fix the scaling by values. After this, the scaling will be displayed highlight. The option "Auto-Size" automatically fits the chromatogram in the reconstruction window.

The status bar in the bottom shows the number of loaded result files.



## 12.2 Function keys in the Compare window



Open Resultfiles opens one or more result files. Multiple selection of several result files can either be done by using the Ctrl key or the Shift key and the result files simultaneously.



Channel ... chooses the channel the chromatograms of which are to be shown in the Compare window.



Chromatogram Offset is used to offset the loaded Chromatograms. By using the cursor keys the chromatograms will be moved on x axis and y-axis. The status bar shows the offset in pixel.



Compare History opens a window that shows the list of the result files and the corresponding colors. The column „Display Color“ shows the color and the column „Name“ shows the name of the result file.

Using the menu procedure „File“ and „Display Color“ the colors in the display can be chosen. By using „Printer Color“ the colors in the print-out can be chosen. A double click in one of the colors opens a dialog box in which the color can be changed.

Display Color	Name
Yellow	ResultFileExample_0001.rfp
Green	ResultFileExample_0002.rfp
Cyan	ResultFileExample_0003.rfp
Red	ResultFileExample_0004.rfp
Blue	ResultFileExample_0005.rfp
Magenta	ResultFileExample_0006.rfp
Orange	ResultFileExample_0007.rfp
Light Green	ResultFileExample_0008.rfp
White	ResultFileExample_0009.rfp
Yellow	ResultFileExample_0010.rfp

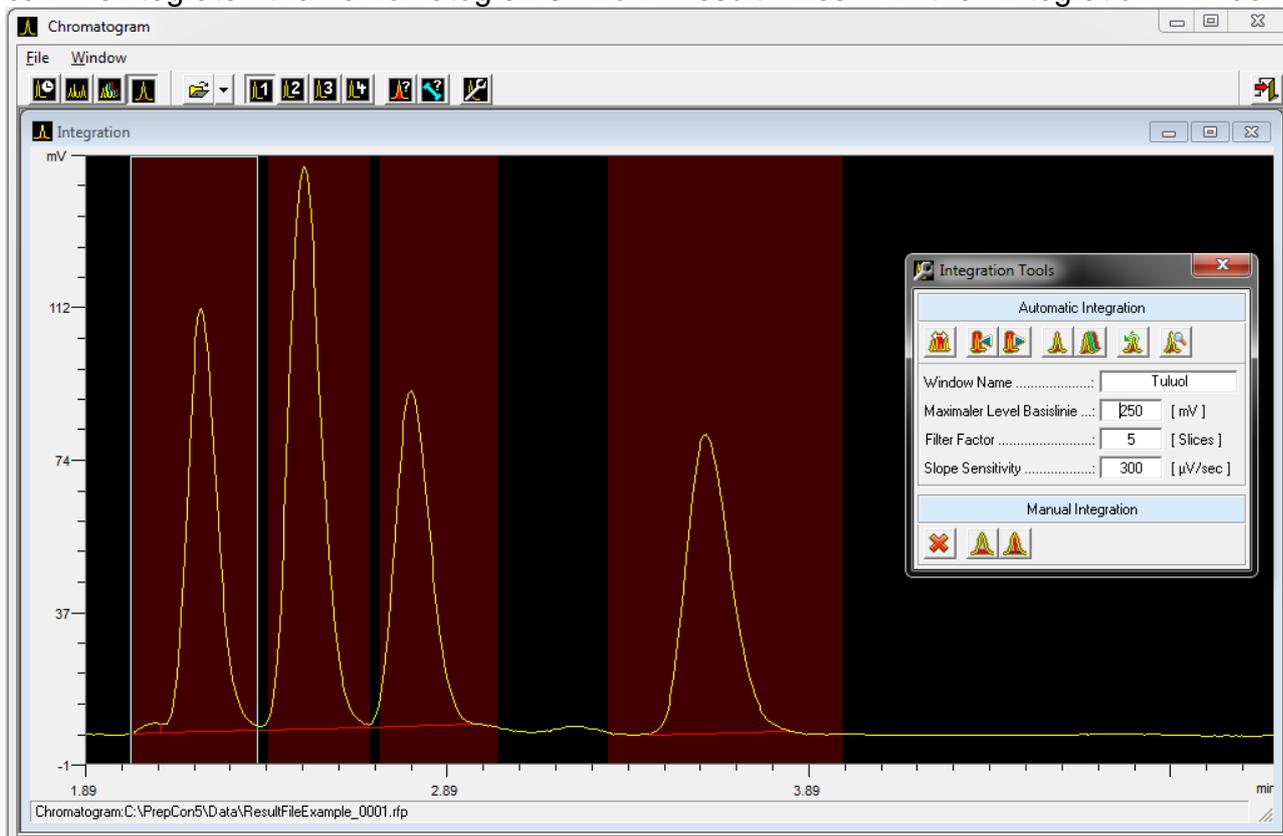


Print Resultfiles prints out the graphic representation of the loaded result files and the color references.

## 13. Reintegrating Chromatograms

### 13.1 General

The function key and the menu option Chromatogram in the main window open the chromatogram window. The fourth area displays the reintegration of chromatograms. You can reintegrate the chromatograms from result files in the integration window.



The chromatograms can be reintegrated singly or collectively in the case of multiple channel data recording. Once reintegration has been carried out, it is saved automatically. The original integration remains in the result file, so that you always have the possibility of reverting to the original.

Reintegration allows you to optimise the integration of your chromatograms later on. If you load the time control file from a reintegrated results file into the time control file editor, the program will recognise the reintegration and ask you if you want to load the reintegration parameters. This time control file will be identical to the run completed, but will contain the integration parameters of the reintegration. You can then save this time control file under a new name, or overwrite the old file.

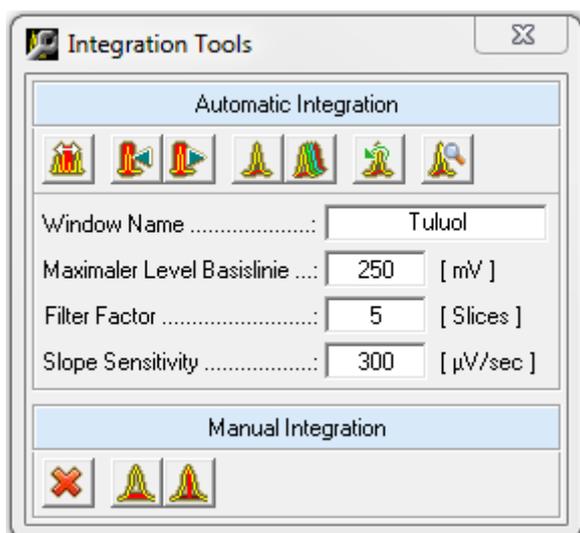
To enlarge the display of certain areas, you can drag out a zoom window by holding down the left mouse button. When you release the mouse button, the display will automatically zoom in on this area. You can repeat this process up to the maximum zoom level. To return to the original size, click on the chart with the right mouse button.

The status bar at the bottom of the window shows the path and name of the result file loaded.

## 13.2 Function buttons in the reintegration window

-  Open Result File opens a result file.
-  Channel ... is used to select the chromatogram shown in the reintegration window.
-  View Peak Results opens the window with the display of the integration results in table form.
-  View Column Coefficients opens the windows with the display of the column coefficients
-  Integration Tools opens the window with the function buttons and parameter boxes for reintegration.

The Integration Tools window contains the tools needed for reintegration. As described in chapter 6.2, the integration parameters are saved with the peak windows. Carrying out a reintegration always concerns the part of the chromatogram within the peak window selected. Outside of the peak windows the default parameters are applied as defined in „PrepCon5.ini“ (see chapter 20.2). The buttons in the tools window have the following functions:



 Create / Edit Peak Window enables you to create and edit peak windows (see chapter 6.2.10).

  Previous Peakwindow and Next Peakwindow are used to select the peak window. The peak window selected is framed in the graph in the reintegration window. The name of the window is displayed in the box below the toolbar.

 Integrate Selected Channel reintegrates the selected chromatogram.

 Integrate All Channels reintegrates all the chromatograms of the result file loaded.

 Original Integration reverts to the original integration.

The reintegration parameters have the following meanings:

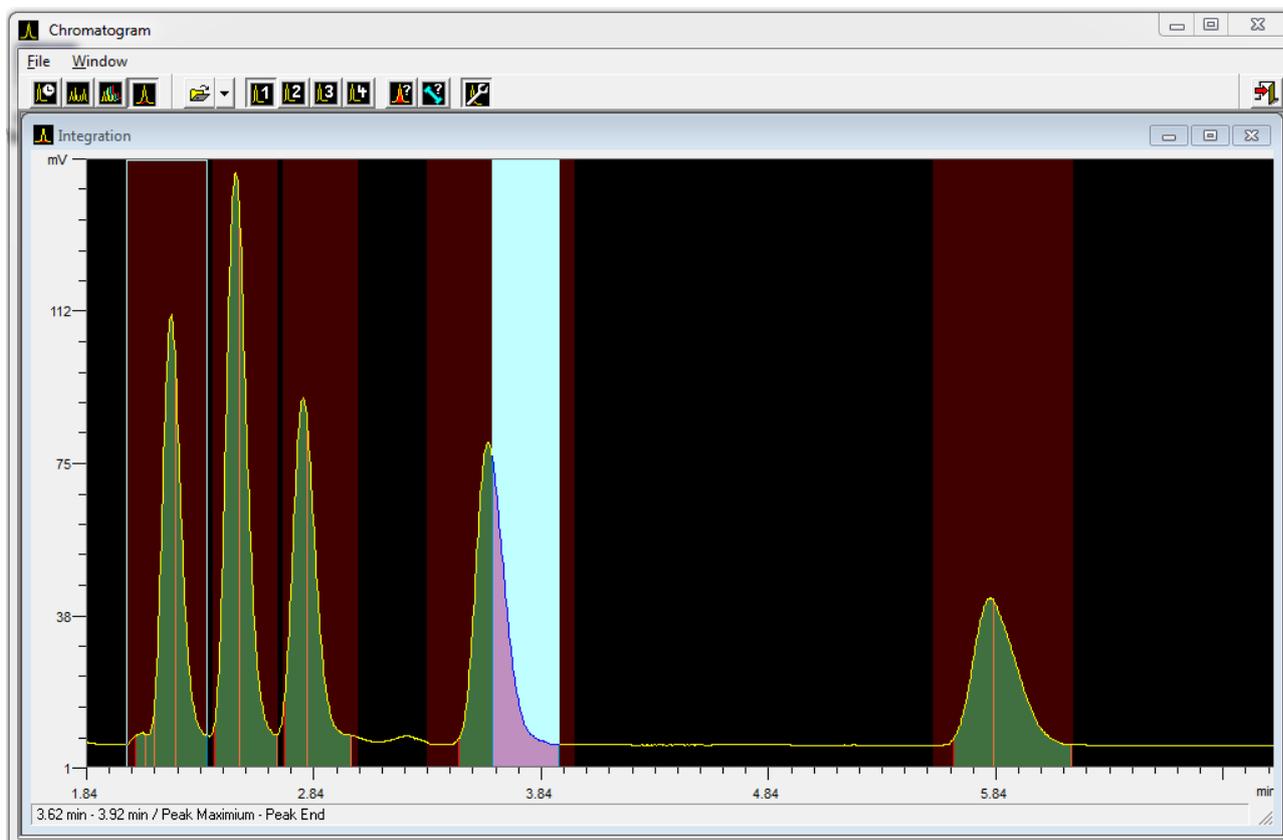
Maximum Baseline Level functions as a threshold for peak sampling. No more peak ends are recognised above the value entered in mV.

The parameter Filter Factor shows the number of slices used to form the first derivative of the gradient calculation.

The parameter Slope Sensitivity indicates the size of the gradient where a peak beginning is recognised in µV/sec.



Peaksampling Preview displays the result of the online peak sampling. The peaks that will be recognised by the online peak sampling correspond to the filled green areas under the chromatogram. Orange vertical lines indicate different peak situations. When moving the mouse over the recognised peak situations the area between two successive peak situations is highlighted. The corresponding start and end time as well as the respective situation names are displayed in the status bar.



Clear Integration deletes all integration results of the displayed channel.



Set manual Baseline allows inserting a baseline manually. Starting point and end point can be fixed by left mouse button. Placed points can still be shifted by left mouse button. After releasing the key the baseline will be used automatically.

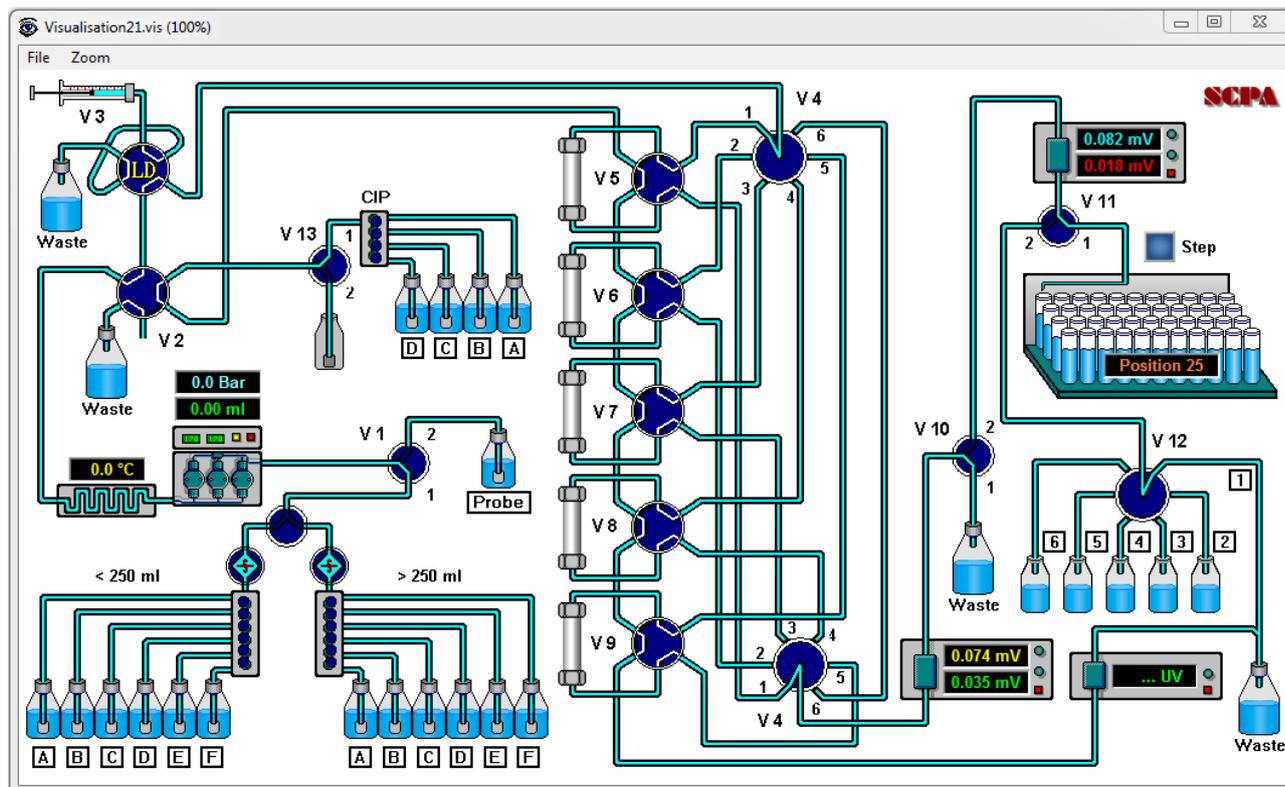


Set manual Drop allows inserting a drop line manually. The time of the drop can be fixed by left mouse button. The placed drop line can still be shifted by left mouse button. After releasing the key the drop line will be used automatically.

## 14. System Visualisation

### 14.1 General

The function key or the menu option "System Visualisation" in the main window opens the system visualisation window.



The system visualisation is used to display the flow process graphically, as well as to operate manually all the devices that can be controlled by means of the visualisation. What is more, the display boxes can show data relating to the current pressure, eluent composition, flow rate, detector signals, autosampler vial numbers, fraction collector position and temperature.

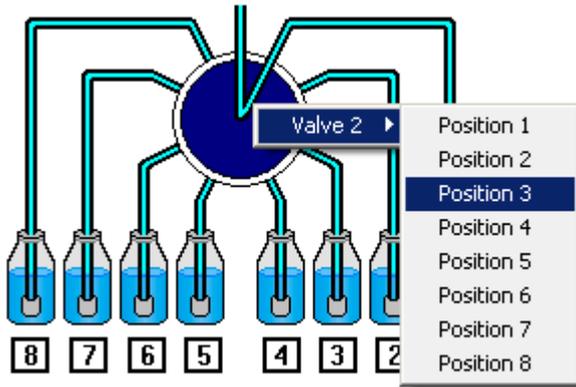
A library of graphic objects and the use of background images in Windows Bitmap Format (\*.bmp) allow the user to create an individually configured system visualisation.

Each of the devices that can be visualised displays its current position or state at all times.

The visualisation window can be scaled freely using the menu option *Zoom* or by dragging the borders of the window.

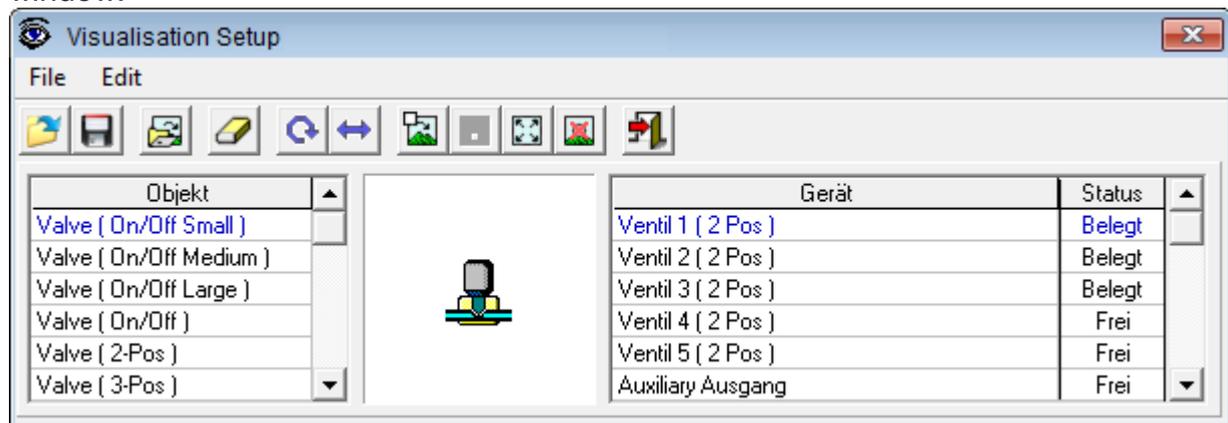
## 14.2 System Visualisation functions

All the devices that can be visualised can be controlled from within the visualisation by means of a popup menu. To see these menus, right-click the mouse on the device required. The first menu option in the popup menu that appears is the device name, followed by the positions or states to which the device in question can be switched. By left clicking on the menu options, the device is switched to the corresponding position or state. The "Button" object can be used like a function button by left clicking with the mouse. Right clicking on a box (value label) shows the value label's data source.



## 14.3 Creating a system visualisation

The menu option "Setup" in the visualisation window opens the system visualisation setup window.



The function buttons in the toolbar have the following functions:

-  **Load Visualisation** opens a previously created visualisation. All the visualisations are to be found in the "Visualisation Files" folder. This folder can be found in the program directory in the subfolder "Visualisation".
-  **Save Visualisation** saves a newly created visualisation.
-  **Load Background Picture** opens a background image in Windows Bitmap Format. All the background images are stored in the "Visualisation Backgrounds" folder. This folder can be found in the program directory in the subfolder "Visualisation".
-  **Clear Visualisation** deletes the loaded visualisation and all its objects. To avoid accidental deletion, this function is only carried out after confirmation from the user.
-  **Rotate Object 90** rotates the selected object 90° clockwise
-  **Flip Object** flips the selected object horizontally.
-  **Insert Object** adds the selected object to the chosen arrangement in the visualisation window. All objects are inserted in their basic position (e.g. valves in position 1).



Place Object places the inserted object at the chosen position in the visualisation.



Move Object moves an already placed object.



Delete Object deletes an already placed object.



Exit Setup closes the visualisation setup window

To create a new visualisation, first draw a background image that corresponds to the devices and tubing in your system. You can use the windows program “*Paint*” for this. You will find a number of models for the single elements in the system in the “*Bitmap Library*” folder. You must then save the background image in the “*Visualisation Backgrounds*” folder, and load it as a background image using the Load Background Picture function.

Now you have to position the appropriate graphic objects for each of the devices to be visualised. The left-hand table in the setup window contains all the graphic objects and the right-hand table contains all the devices in your system that can be visualised. If you choose a value label as an object, all the values that can be visualised will be the only thing shown in the device table.

The graphic objects are displayed in the preview box in the centre of the setup window. Check here that the object is the same way up as the corresponding element in your background image.

Use the Rotate Object 90° and Flip Object functions to adjust the alignment. Once you have chosen an appropriate device for your system in the right-hand table, you can add the object to the visualisation window with the Insert Object function. It will appear in the top right corner, and can be put in the right place with the mouse or the cursor keys. When you have done this, use the Place Object function to add it to the visualisation.

When all the objects have been added, you must save the visualisation using the Save Visualisation function. All the visualisations must be saved in the “*Visualisation Files*” folder.

## 15. Displaying the Solvent Supply

### 15.1 General

The function button or the menu option "Solvent Supply" in the main window opens the solvent supply display window.

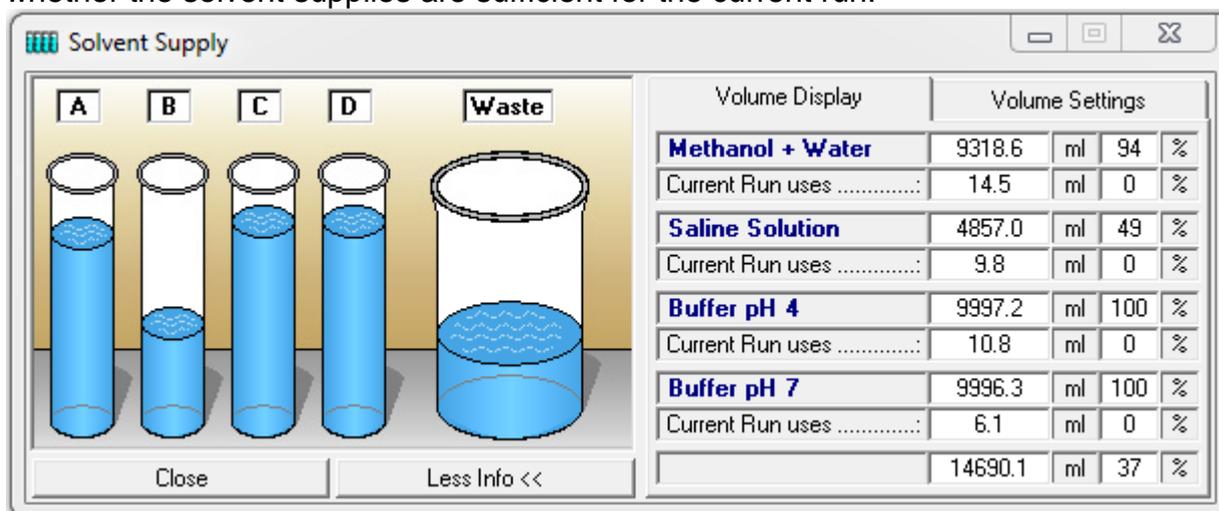
The solvent supply display is used to control the supply of solvents. To prevent a column from running dry, you have the possibility of setting two volume limits in percent. When the volume drops below the first limit, an alarm will sound, and when it drops below the second limit, the pumps will stop.

The values displayed are based on the calculated used volume of solvent at the current flow rate and time passed. This means that there is no provision for pump tolerance in this calculation. For this reason, the volume limits for the warning and turning off the pumps should allow a certain leeway. Regular control of the supply containers also helps to prevent a column from running dry.

### 15.2 Solvent visualisation

The supply of solvents A to D and the level of the waste container are shown as a graphic on the left-hand side of the window. They are intended to allow the user to make instant checks.

You can open the right-hand side of the window with the "More Info" button. You can then use the "Less Info" button to close it again. The right-hand side of the window displays the solvent names and the numerical solvent quantities. It also shows the solvent consumption for the current run. The values are shown as absolute volumes and as percentages of the total volume. The values next to "Actual Run Uses" show the solvent consumption of the time control file loaded as a volume and percentage. This display is intended as a check of whether the solvent supplies are sufficient for the current run.



A solvent that has dropped below the minimum percent level set, or a waste volume that has exceeded the maximum percent level, will be marked with a red exclamation mark.

### 15.3 Solvent Supply display settings

Volume Settings		
Name	Total [ml]	Current [ml]
Methanol + Water	10000.0	9318.6
Saline Solution	10000.0	4857.0
Buffer pH 4	10000.0	9997.2
Buffer pH 7	10000.0	9996.3
Waste	40000.0	14690.1
<input checked="" type="checkbox"/> Acoustic Warning at .....		10 %
<input checked="" type="checkbox"/> Hold with Pump stop		5 %
Save		Refill all
		[ ml ]

In the "Volume Settings" part, you can enter your own names for the solvents A to D under "Name". Enter the total volume of the individual solvent containers in the boxes under "Total" and enter the current solvent volume in the containers under "Actual". The pumps should be stopped when you enter the current solvent volume, since the values in the boxes are constantly updated when the pumps are running, meaning that your entries will be overwritten. Use the "[I]" to switch the unit of volume between [ml] and [l]. The "Refill All" button returns all the

current solvent volumes to the total volume of the corresponding containers and the waste container to zero. The "Save" button applies and saves the settings. The option "Acoustic warning at" sets a percentage threshold at which the alarm will sound. The second threshold with the option "Stop all" or "Hold with Pump stop" is used to stop the pumps, in order to prevent the column from running dry. "Stop all" stops the time control file and the pumps, and "Hold with Pump stop" pauses the running of the time control file and sets the pumps to a flow rate of 0 ml. When the solvent containers have been refilled, you can resume the time control file using "Continue".

## 16. Waste Management

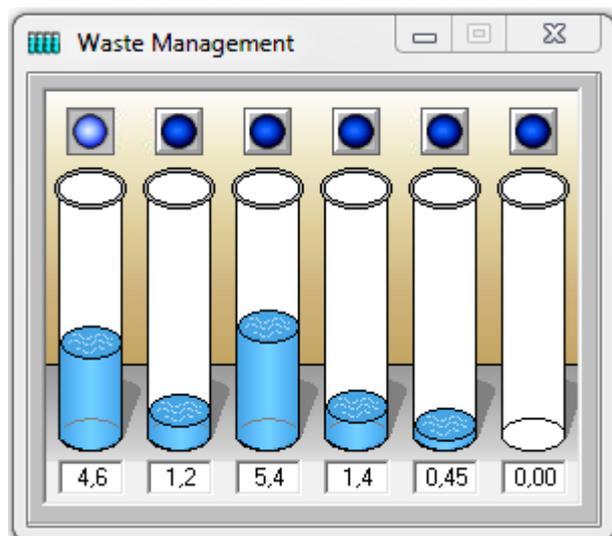
### 16.1 General

The function key and menu option “Waste Management” in the main window opens the window where you can visualise the waste management display.

In the PrepCon5.ini-file [WasteManagement] (see appendix) you can define the valve that should function as the waste management valve. The number of the possible containers comply with the number of valve positions.

### 16.2 Display of the waste management

The window will show the number of containers in order of the configured valve positions.



The LED above the containers shows if the position on the valve is chosen. At the same time it is also a button for setting the valve position. Below the containers a value display will show the calculated volume inside the container. With a right-button click with the mouse, you can “empty” the container

### 16.3 How to use the waste management

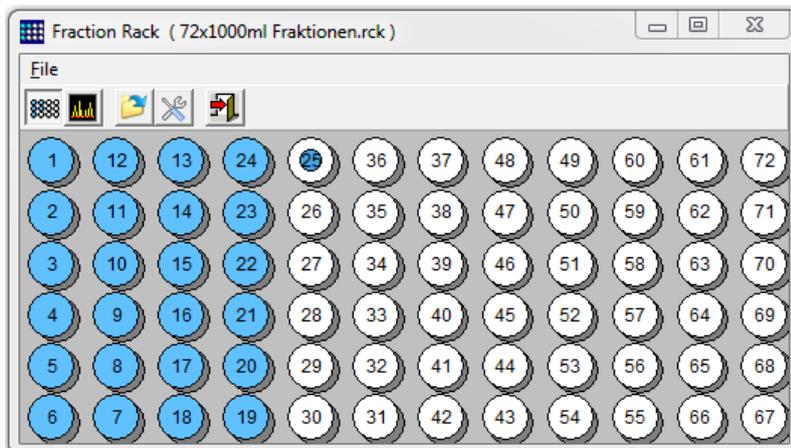
A typical usage of the waste management is the automatic sample. In such an application, you can collect the non-valuable fractions of each injection separately in case a sample did not bind to the column or the elution went

wrong. In a cyclic time control file programming the position will switch to the next position after each run or when the set volume for the container is reached. A new run will only start when the container of the designated position is marked as “empty”. Otherwise the method will switch to “hold”. In that case, you will get an error message on the screen.

## 17. The rack display of the fraction collector (fraction rack)

### 17.1 General

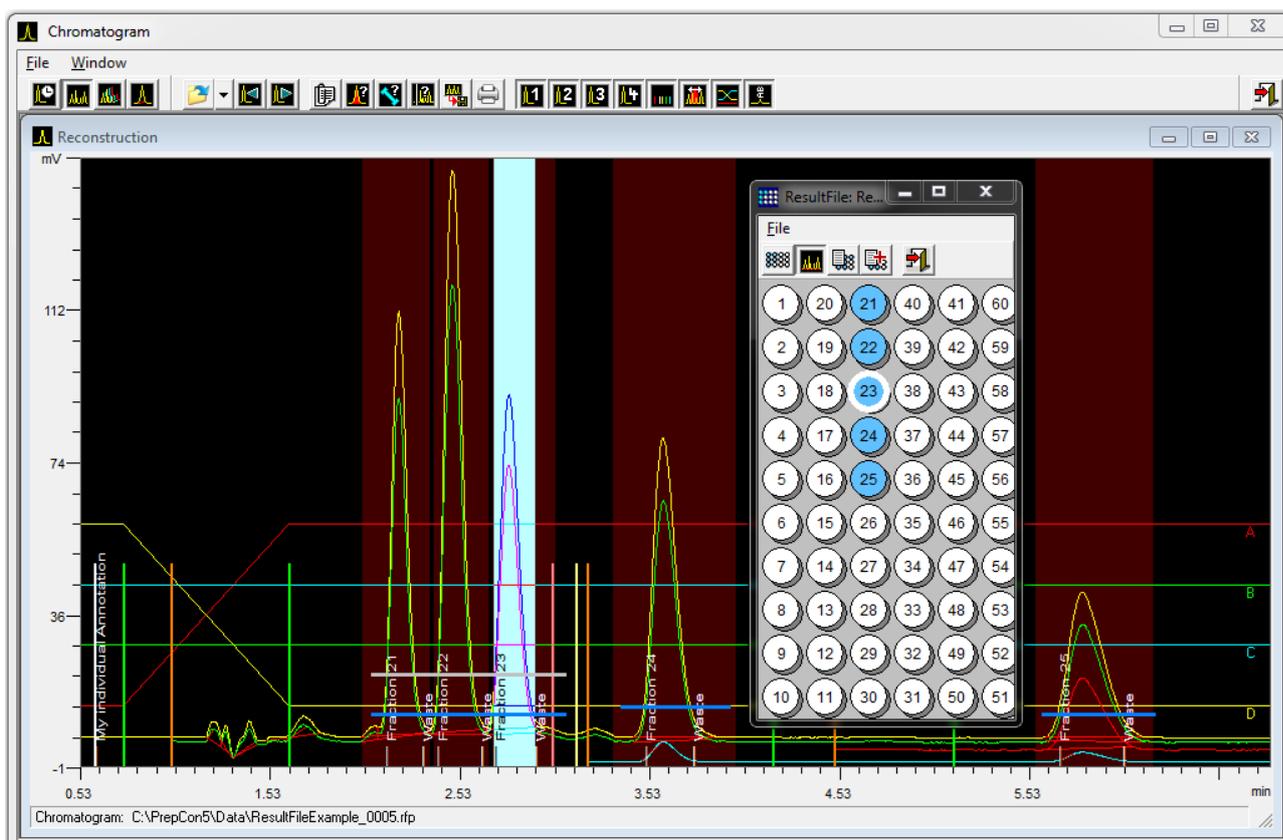
The function key or the menu option "Fraction Rack" in the main window opens the window with the rack display of the fraction collector.



The fraction rack can be displayed in two ways:

The current view shows the fraction collector rack with all the positions. The filled fractions are displayed in blue and the empty ones in white. The current position is indicated by the blue dot.

The reconstructed view shows the fractions produced by the result file loaded into the reconstruction window.



If you left-click on one of the filled fractions, this part of the chromatogram will be displayed inverted. If you left-click on a peak, you will see the position of this fraction in the rack. This will give you a direct graphic relation between the chromatogram and the fraction produced in the fraction collector rack. If you move the mouse over one of the filled fractions, the fraction number and the volume fractionated will be displayed.

## 17.2 Fraction collector rack functions



Show Rack changes to the current view of the fraction collector rack.



Show Reconstruction changes to the reconstruction view of the fraction collector rack, displaying the result file loaded into the reconstruction window.



Load Rack File opens a rack file to display a fraction collector rack. You can also open a rack file out of a result file. The rack file is the same that was used in this run.



Rack Setup opens the window to create a rack file to display a fraction collector rack



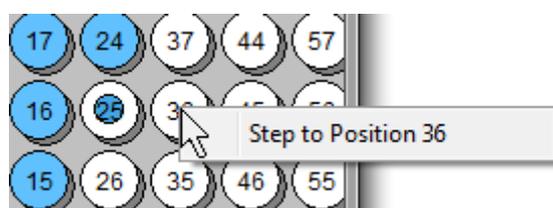
Open Fraction Table opens a window where a fraction table can be created.



Add Fractions to Fraction Table adds all fractions of the loaded results file into the fraction table



Exit closes the rack display of the fraction collector.



The rack display allows you to enter the fraction collector positions directly. To do this, click with the right mouse button on a fraction and then select the menu option “Step to Position...” with the left mouse button.

## 17.3 Fraction Table

No	Sample	Injection	Result File
1	Sample No. 1 from 09.12.2002	1	C:\LaboChrom5\Data\ResultFileExample_0001.rfp
2	Sample No. 1 from 09.12.2002	1	C:\LaboChrom5\Data\ResultFileExample_0001.rfp
3	Sample No. 1 from 09.12.2002	1	C:\LaboChrom5\Data\ResultFileExample_0001.rfp
4	Sample No. 1 from 09.12.2002	1	C:\LaboChrom5\Data\ResultFileExample_0001.rfp
5	Sample No. 1 from 09.12.2002	1	C:\LaboChrom5\Data\ResultFileExample_0001.rfp
6	Sample No. 1 from 09.12.2002	2	C:\LaboChrom5\Data\ResultFileExample_0002.rfp
7	Sample No. 1 from 09.12.2002	2	C:\LaboChrom5\Data\ResultFileExample_0002.rfp
8	Sample No. 1 from 09.12.2002	2	C:\LaboChrom5\Data\ResultFileExample_0002.rfp
9	Sample No. 1 from 09.12.2002	2	C:\LaboChrom5\Data\ResultFileExample_0002.rfp
10	Sample No. 1 from 09.12.2002	2	C:\LaboChrom5\Data\ResultFileExample_0002.rfp

The fraction table contains a list of fractions, which the user has selected manually in the fractions rack window. Fractions can be inserted into the fraction table by clicking into a fraction of the rack display with the right mouse key and choosing the menu point „Add to Fraction Table“. All fractions of a fractionation run can be added into the fraction table by clicking the button „Add Fractions to Fraction Table“ (chapter 13.2) in the fractions rack window. The table contains the following columns: the fraction number, a sample description, the injection number, the name and the path of the corresponding result file.

The toolbar of the fraction table contains the following function buttons:



Import Fraction Table imports an already existing fraction table.



Export Fraction Table converts the fraction table into the CSV format (Comma separated Value).



Print Fraction Table opens a dialog window for the printout of the fraction table.



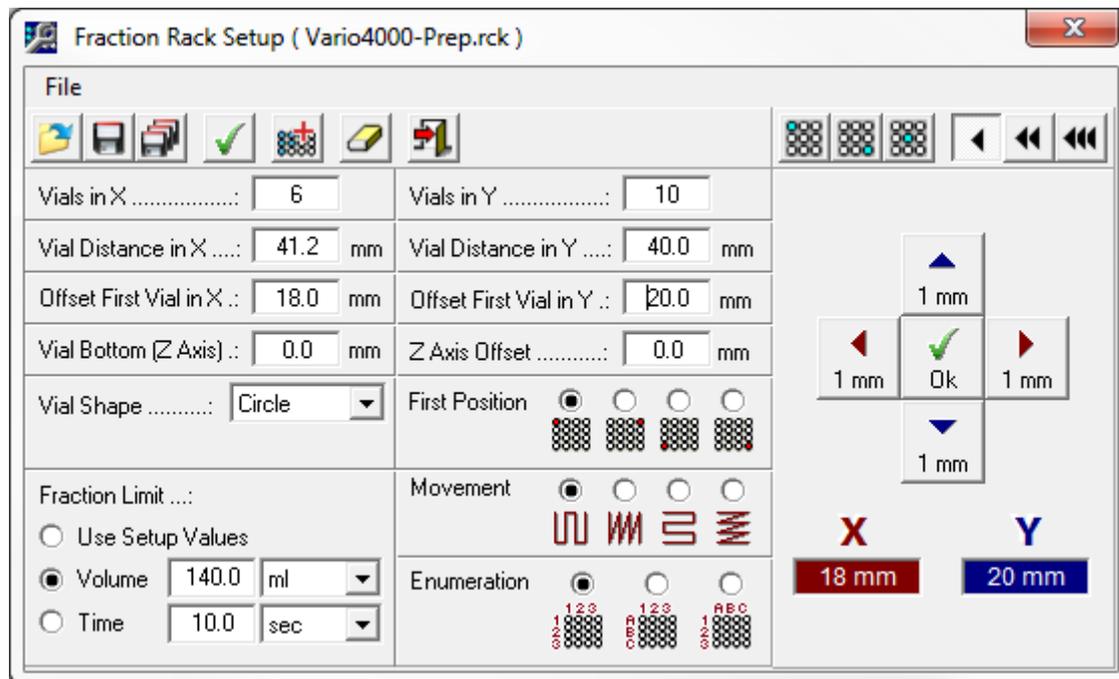
Clear Fraction Table deletes the content of the fraction table.



Exit closes the fraction table.

## 17.4 Fraction Rack Setup

The function button Rack Setup opens the window to create or edit a rack file. Rack files contain information about the geometry of the rack and the relation between the number and the corresponding absolute co-ordinates of a fraction.



„Vials in X“ and „Vials in Y“ indicate the number of fractions in the x and y axes. You can enter the distances between the midpoints of the fraction vials in the x and y axes in the boxes „Vial Distance in X“ and „Vial Distance in Y“.

You can use „Offset First Vial in X“ and „Offset First Vial in Y“ to define the x and y distance of the midpoint of the first fraction from the home position.

„Vial Bottom“ determines the depth of the fraction vials when a Z Axis is used and „Z Axis Offset“ sets the offset of the Z Axis during a fraction step.

„Vial Shape“ determines the shape of a fraction. Options are „Circle“, „Rectangle“ or „Square“. For „Rectangle“ the parameter „Aspect Ratio“ defines the ratio of height and width of the fractions displayed as rectangles.

“*First Position*” determines the angle for the first position “*Movement*” sets the procedure for fractionating.

You can add a maximum fraction volume or fraction time for the fraction limiter in “*Fraction Limit*”. The values from the limiter setup will be replaced by the rack file values when loading this rack file. If the option “*Use Setup Values*” is selected, the values in the limiter setup will be retained.

The tool bar on the left side of the window contains the following function buttons:



Load Rack File to load a previously created rack file.



Save Rack File to save a new or changed rack file



Save Rack File as... to save a rack file under a new name.



Create Symmetrical Rack creates with the help of given data a symmetrical Rack.



Append Rack File appends an already created Rack file to the current loaded one.



Clear Rack file to clear the content of the boxes.



Exit to close the rack file setup window.

The teaching module of the setup is on the right hand side of the window. This module, allows the positions of the individual fractions to be determined and corrected step by step when using fraction collectors that are controlled by co-ordinates.

The tool bar in the teaching module contains the following function buttons:



Teaching top left Position selects the mode to move to the top left-hand fraction. The co-ordinates are automatically entered in the boxes “*Offset First Vial in X*” and “*Offset First Vial in Y*”.



Teaching bottom right Position selects the mode to move to the bottom right-hand fraction. The co-ordinates express the X and Y distances of the fractions one above the other. They are automatically entered in the boxes “*Vial Distance in X*” and “*Vial Distance in Y*”.



Teaching single Position selects the mode for the corrector of the fraction that is indicated in the rack display as the current fraction.



Teach width 1mm sets the step distance when moving to a fraction at 1 mm.



Teach width 10mm sets the step distance when moving to a fraction at 10 mm.



Teach width 50mm sets the step distance when moving to a fraction at 50 mm.



A click on one of the *Teaching Buttons* moves the arm of the fraction collector by the distance set in the corresponding direction.



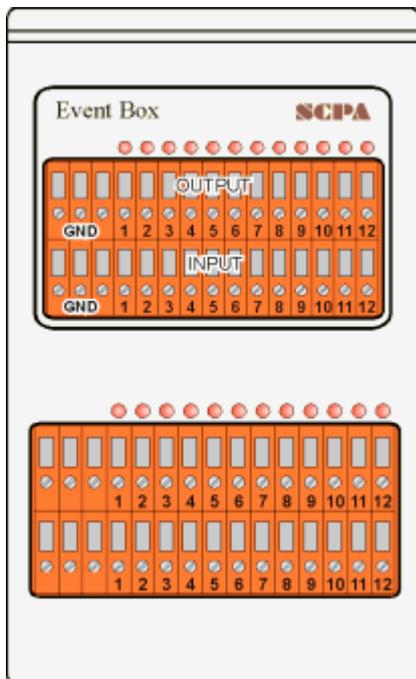
When it has reached the position required, the co-ordinates can be recorded by clicking on the *Set* button.



The current position of the fraction collector is shown in the X and Y co-ordinate displays.

## 18. The Event Box

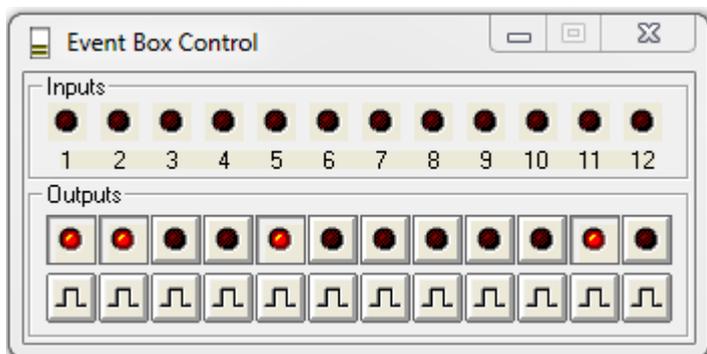
### 18.1 General



The event box consists of 12 outputs, which are used to control system components, and 12 inputs used to capture statistical system signals. It is driven with the help of an interface card in the computer. The outputs are open collector outputs and switch the signals to ground (GND). The inputs are low active, i.e. they are considered active when they are connected to ground or when the input voltage is around 0 volts. The three connections on the left of the inputs and outputs are the mass connections. To switch devices such as magnetic valves, an external source of voltage is required. The maximum alternating voltage is 30 volts and the maximum current is 500 mA. Examples of applications that require an event box include: switching smaller magnetic valves, autozero on detectors, reporting back from an injection valve, controlling devices with TTL inputs etc.

### 18.2 Manual control of the event box

The function button or the menu option “*Event Box*” in the main window opens the event box window. The upper row of LEDs represent the inputs. An active input is shown by a lit up LED. The buttons in the lower part of the window are used to switch the outputs manually. The upper row of buttons switch the outputs on or off statically. The LEDs in the buttons show the status of each output. The lower row of buttons switch the outputs with a pulse lasting one second.



The function button or the menu option “*Event Box*” in the main window opens the event box window. The upper row of LEDs represent the inputs. An active input is shown by a lit up LED. The buttons in the lower part of the window are used to switch the outputs manually. The upper row of buttons switch the outputs on or off statically. The LEDs in the buttons show the status of each output. The lower row of buttons switch the outputs with a pulse lasting one second.

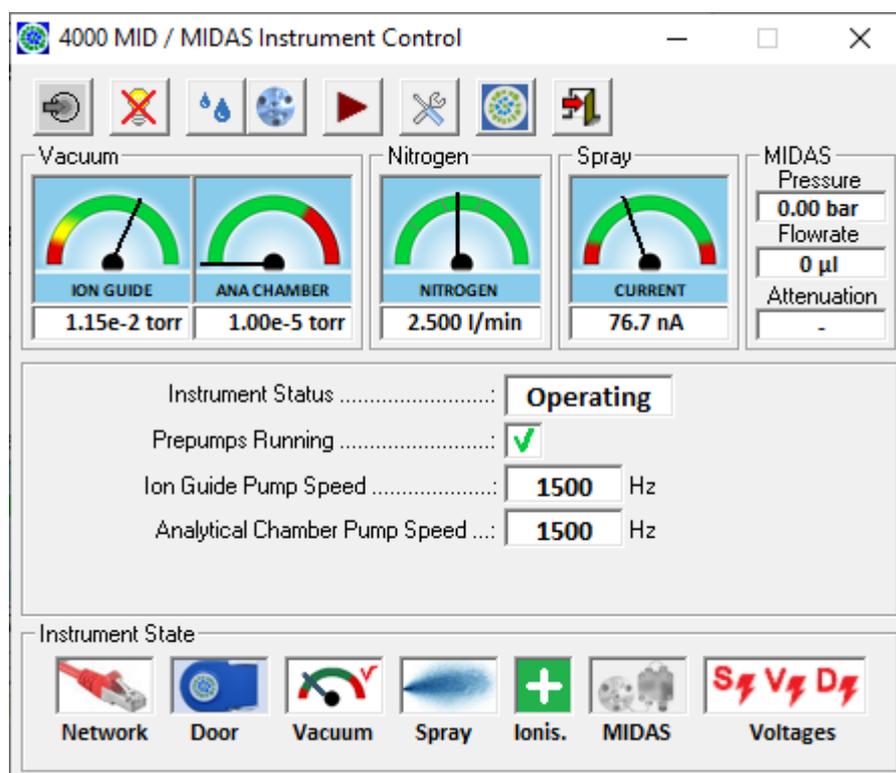
## 19. Control of mass spectrometers

### 19.1 General

Mass spectrometers can be implemented in PrepCon either via MS-LC coupling or via direct control with the PrepCon software. So far the mass spectrometer 4000 MID by Microsaic is implemented.

The control of the 4000 MID follows the logic of the control within the Masscape® software by Microsaic. Complex and not often used functions like calibration of the spectrometers are not available in PrepCon5. In order to perform these tasks there is a possibility to switch from PrepCon to the Masscape® software using TightVNC for the remote connection.

### 19.2 Control of the 4000 MID / MIDAS Spectrometer



**Function buttons of the 4000 MID/ MIDAS Spectrometer control window:**

 Pump down, Vent, Vent disabled:

If the mass spectrometer is vented pressing Pump down starts the vacuum pumps. If the spectrometer is evacuated but not in operation the system can be vented.

On the measurement is started using ,Operate' the spectrometer cannot be vented and this function button is disabled.



start measurement (Operate), stop measurement: The operate function button is available as soon as the vacuum has sufficient quality. During operation the measurement can be stopped using this function button. In case makeup pump and/or attenuator are active, they will be switched off as well.



start and stop makeup pump: This function is only available while the MIDAS is switched on and activated with the Masscape Software and the measurement is in operation.



start and stop attenuator: This function is only available while the MIDAS is switched on and activated with the Masscape Software and the measurement is in operation.



start and stop scan: This function is available once the measurement is in operation. Starting a time control file will start scan automatically. Scan cannot be stopped during execution of a time control file.



Setup: opens setup window. This function is only available while scan is not started. See below for details.



Masscape: Stops control of the 4000 MID Spectrometer by PrepCon and allows for a remote desktop connection via TightVNC to the internal Linux PC of the MID running the Masscape® software. This function is not available while the measurement is in operation.

### 19.3 Displays in 4000 MID/ MIDAS Spectrometer Control Window

Display for vacuum, N usage, spray current as well as makeup pump pressure and flowrate and the attenuation are available while scan is not started.

In addition displays are available for:

- spectrometer status
- prepump status (on/off)
- speed of the ion chamber turbo pump
- speed of the separation chamber turbo pump
- warning messages

While scan is active the numerical measurement values (e.g. number of detected ions, gate time) for the selected mass acquisition channels (defined in the setup, see below) as well as the total ion current (TIC) will be displayed.

### 19.4 Status Displays



Network: indicates whether a connection to the mass spectrometer could be established.



Door: Shows the status of the cover of the spray source – open or closed. If the door is opened, the spray voltage is switched off and the measurement cannot be started.



Vacuum: indicates if pressures are sufficient for measurement.



Spray: Status of the spray source.



Ionisation: Shows which ionisation is selected in the setup.



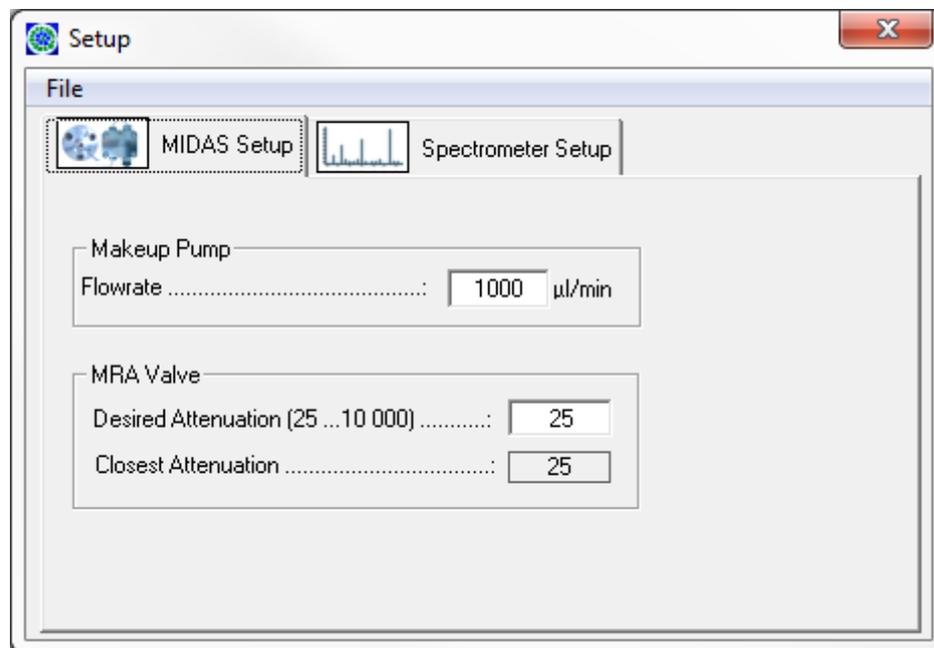
MIDAS: shows if makeup pump an attenuator are started.



Voltages: indicates whether spray voltage, voltage of ion optics and high voltage of the detector are designed values during operation all three voltages must be switched on.

### 19.5 4000 MID / MIDAS Setup

The parameters entered in the setup window may be partly overwritten by parameters in the time control file.

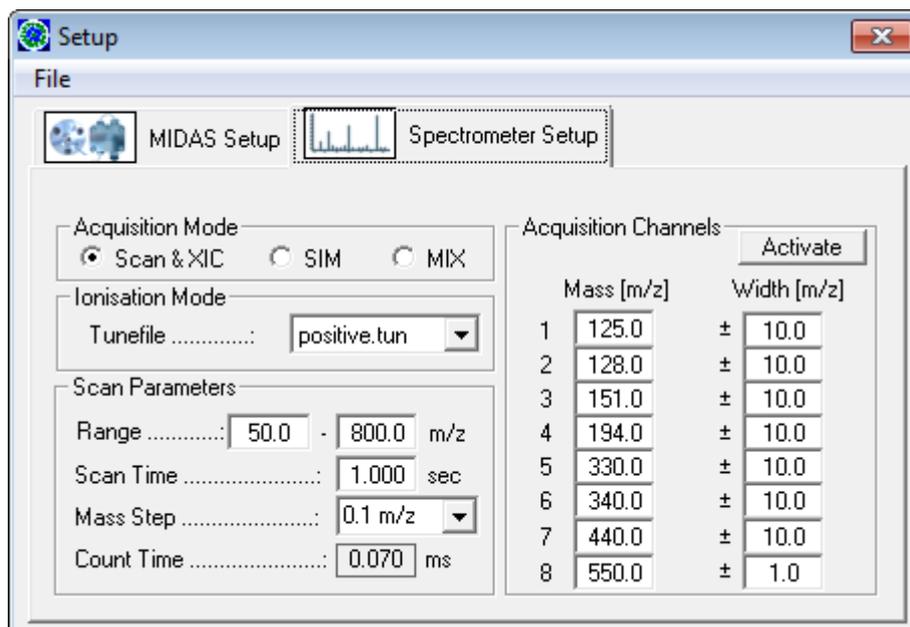


On the tab MIDAS Setup the flowrate of the makeup pump and the attenuation can be entered

## Spectrometer Setup:

There are three modes of acquiring data: Scan & XIC, SIM or MIX. The default acquisition mode is Scan & XIC. In the Scan & XIC mode PrepCon acquires complete mass spectra and single mass data tracks are extracted as chromatograms.

PrepCon can save the complete spectrum into the result file. In the SIM acquisition mode only selected ion masses are measured, no spectra can be saved. In the MIX mode selected ion masses are measured as in SIM mode, but the full spectrum is recorded as well. The sensitivity in MIX mode for the selected masses is slightly lower than in SIM mode.



**Ionisation mode:** Depending on the chemical properties of the samples the positive or negative ionisation mode can be used. The ion mode is selected via parameter files (tune files) e.g. positive.tun and negaitve.tun. The tune files can only be adjusted using the Microsaic Massscape software.

**Mass range:** Ranges between 50 and 800 m/z can be selected. Masses below 50 cannot be measure.

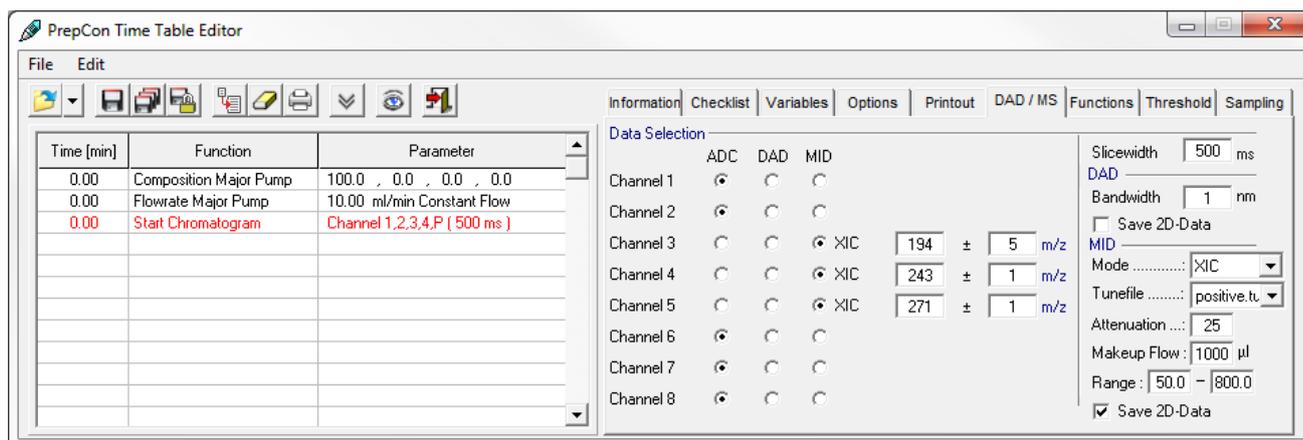
**Scan time:** overall scan time for a full spectrum

**Mass step:** can be set to 0.1 or 0.2 m/z

**Count Time:** Count time for one single point. The count time is calculated using mass range, scan time and mass step.

**Acquisition channels:** Up to eight masses can be define for the chromatogram channels. These parameters will be overwritten by the entries for MS channels (see below) in the time control file when loading the file.

### 19.6 Mass spectrometer parameters in the time control file



The following parameters for the control of the mass spectrometer are available on the DAD/MS tab of the time control file editor:

**Data selection:** for up to 8 channels you can chose whether an AD-Converter is used as data source (also choose this option for the channels of a UV detector), which wavelength range is used for channels of diode array detector or which mass tracks are acquired from the mass spectrometer.

**Slicewidth:** the data point density, slicewidth in milliseconds. Same value for the slice width in the DAD/MS tab and in the start chromatogram command have to be applied.

**Mode:** The acquisition mode of the mass spectrometer: XIC SIM or MIX (see MS setup, above)

**Attenuation:** Setup for the MIDAS-Attenuator

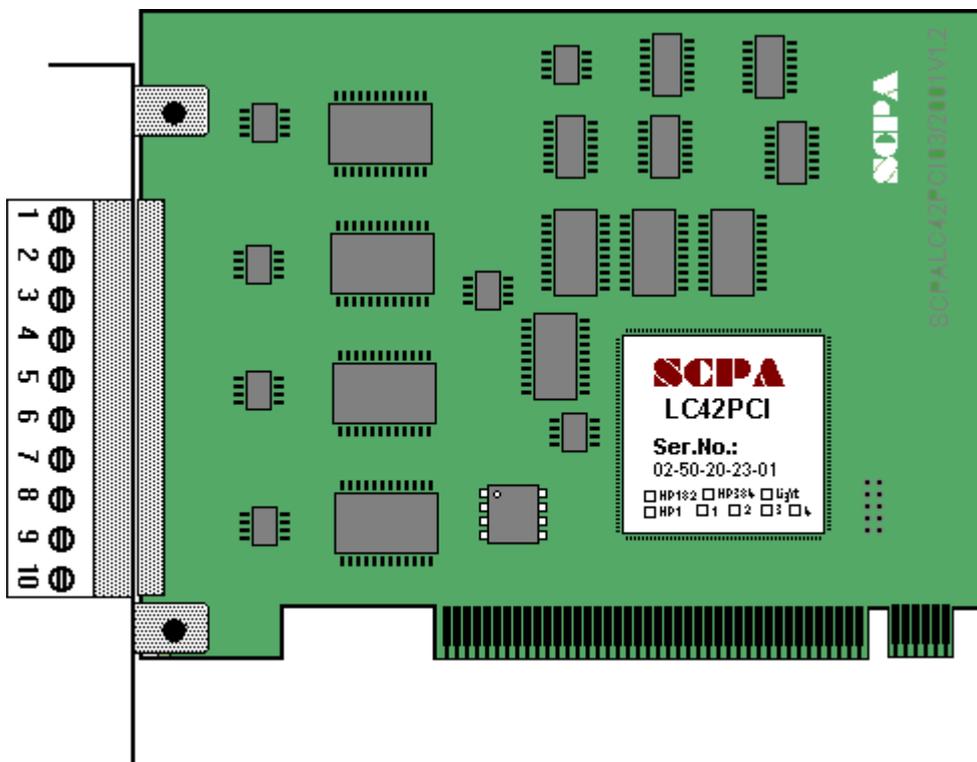
**Makeup Flow:** flow rate of the MIDAS makeup pump.

**Range:** mass range for the scan (see MS setup, above)

**Save 2D-Data:** If this option is selected, all mass spectra acquired during the data acquisition will be saved to the result file. Saved spectra can be viewed in the reconstruction window.

## 20. Appendix

### 20.1 Location of the connections on A/D conversion cards



Pin	1 Channel Standard Performance	2 Channel Standard Performance	2 Channel High Performance	4 Channel Standard Performance
1	- Channel 1	- Channel 1	- Channel 1	- Channel 1
2	+ Channel 1	+ Channel 1	+ Channel 1	+ Channel 1
3	n.c.	- Channel 2	Shielding	- Channel 2
4	n.c.	+ Channel 2	- Channel 2	+ Channel 2
5	n.c.	n.c.	+ Channel 2	- Channel 3
6	n.c.	n.c.	Shielding	+ Channel 3
7	n.c.	Start Channel 2	Start Channel 1	- Channel 4
8	n.c.	GND	GND	+ Channel 4
9	Start Channel 1	Start Channel 1	Start Channel 2	Start Channel 1
10	GND	GND	GND	GND

## 20.2 The entries in the file PrepCon5.ini

### [MainWindow]

AlwaysOnTop=0	[ 0 or 1 ]	The main window is always in the foreground.
SolventConfirm=0	[ 0 or 1 ]	Starting the pump with the eluent buttons must always be confirmed by the user
DataPathSelection=0	[ 0 or 1 ]	After loading a time control file the user can select a folder for the resultfiles
MultiLingual=0	[ 0 or 1 ]	The program is corresponding to the operating-system multilingual ( german / English)
DateFormat=YYYY.MM.DD		The programs date format
WavelengthRequest=0	[ 0 or 1 ]	Before starting a time control file, the user will be asked for a uv wavelegth.

### [Boards]

Order=PCIFIRST	[PCIFIRST or ISAFIRST ]	Order of the analog channels if ISA and PCI cards are used combined.
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### [WinsockPorts]

Port1=	[ IP,Port ]	IP-Address and portnumber of the used Winsock-Ports. The portnumber will be appended with a comma after the IP-address. Winsock-Ports who are not used should do not have parameters.
Port2=		
Port3=		
Port4=		
...		
Port16=		

### [EthernetBox]

URL1=192.168.0.215	[ IP,Port ]	IP-Address and portnumber of the used Winsock-Ports of the Ethernet-A/D-Converter
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### [AutomaticDataFiles]

CSVFile=0	[ 0 or 1 ]	A chromatogram file in *.csv format will be saved automatically at the end of a run
FrationTable=0	[ 0 or 1 ]	A fraction table in ascii format will be saved automatically at the end of a run.
SaveResultWithSequence=0	[ 0 or 1 ]	While executing a sequence table save resultfiles (.rfp) in the same folder (1) as the sequence files (.seq) or (0) as the time control file (.tcf)

### [User Company]

Name=SCPA	[Text]	User defined company name for all prints.
FontName=Braggadocio	[Text ]	Name of the font for the company name.
FontSize=18	[Value]	Fontsize for the company name
FontBold=0	[0 or 1]	Bold font for the company name
FontItalic=0	[0 or 1]	Italic font for the company name
FontColor=128	[Value]	Font color for the company name

### [Pumps]

ConstantModeMajor=0	[0 or 1]	The pump system supports a constant pressure mode, i.e. a flow rate control for working at a constant pressure
ConstantModeMinor=0		

OnlineMoving=1	[0 or 1]	The pump system supports the online gradient shift
Autozero=0	[0 or 1]	The pump interface supports a potential free switch for a uv-autozero function
MaxPressFactor=1	[0 or 1]	The maximum pressure value will be scaled appropriate to the pressure range
PressureChannel=0	[0 or 1 - 8]	The pump pressure signal will be acquired by the specified A/D-conversion channel
FlowrateChannel=0	[0 or 1 - 8]	The pump flow rate signal will be acquired by the specified A/D-conversion channel
ParameterChange=0	[0 or 1]	The buttons 100% Solvent A-D and flowrate are enabled during a time control run
FlowDimension=ml	[ $\mu$ l , ml , l]	Dimension of the pump flowrate
FlowGradient=-1	[0,1,-1]	The pump supports flowrate gradients. A value of -1 supresses sending the command.
FlowGradientMinor=-1		
IOControl=0	[0 or 1]	Pump interface supports an emulation of an eventbox
IOControlMinor=0		
LimiterVolumeMinor=0	[0 or 1]	Limiter volume calculate using the minor pump flow
PumpStopRequestFlag=0	[0 or 1]	Don't stop the pump without additional confirmation
SoftwareHPG=0	[0 or 1]	The software driver for the main pump system controls a high pressure gradient
SoftwareHPGPort2=0	[IP]	IP address of pump B for the software high pressure gradient
SoftwareHPGPort3=0	[IP]	IP address of pump C for the software high pressure gradient
SoftwareHPGPort4=0	[IP]	IP address of pump D for the software high pressure gradient
<b>[PressureSensor]</b>		
Enabled=0	[0 or 1]	Activates external pressure sensor via ethernet
IP=192.168.0.140	[IP]	IP address of the external pressure sensor
Port=100	[Value]	Portnumber of the external pressure sensor
Channels=0	[Value]	Amount of channels of external pressure sensor
<b>[Autosampler]</b>		
MaximumSamples=100	[1 - ...]	Maximum sample capacity of the autosampler.
LoopVolume=10000	[1 - ...]	Input limitation for programming injection volumes
ArmenInjection=0	[0 or 1]	Sample injection using an Armen pump
VolumeDimension	[ $\mu$ l or ml]	Dimension of the injection volume
AS3000=0	[0 or 1]	The autosampler is a SCPA AS3000
VarioPrep=0	[0 or 1]	The autosampler is an SCPA VarioPrep
Wash=0	[Value]	Washvolume of the dispenser
SampleCentering=0	[0 or 1]	Place sample in the middle of the loop using wash liquid

**[SequenceTable]**

MinSamplePosition=0	[0 - ...]	Input limit in sequence table
MaxSamplePosition=100	[0 - ...]	Input limit in sequence table
MinInjections=0	[0 - ...]	Input limit in sequence table
MaxInjections=1	[0 - ...]	Input limit in sequence table
MinVolume=0	[0 - ...]	Input limit in sequence table
MaxVolume=10000	[0 - ...]	Input limit in sequence table
DefaultVolume=100	[0 - ...]	Preset in sequence table.
OLBImport=0	[0 or 1]	Import sequence from MassLynx-.olb file possible
EnableInit=0	[0 or 1]	activates dialog window on start of a sequence allowing for initialisation
ColectorOnlyLine1=0	[0 or 1]	Fraction collector executes position commands only in the first row of the sequence file
TimeShiftThreshold=1	[0 or 1]	Variable time shift acts on start and end time of thresholds
AdditionalFields=0	[0 or 1]	Additional text fields in the sequence table and the report printout
MaxPeaklimitFailed=1	[0 or 1]	Maximum allowed number of runs with failed peak limit condition before stopping sequence

**[Collector]**

Cetac=0	[0 or 1]	Activates the direct control of Cetac fraction collector
StepAtWaste=0	[0 or 1]	Automatic fraction collector step when switching to waste
HomeOutput=0	[1 - 12]	Event box output for a home fraction collector
StepOutput=0	[1 - 12]	Event box output for a fraction collector step
CollectorArray=0	[0 or 1]	Serial switching of several fraction collectors
Collectors=2	[2 - ...]	Number of fraction collectors in the series
CollectorValve=2	[1 - ...]	Number of the waste/fraction valve when several collectors are switched in series
Autozero=0	[0 or 1]	The collector supports a potential free switch for a uv-autozero function
DiverterPort=0	[0 or 1]	Diverting using an external waste/fraction valve
AutomaticRestart=0	[0 or 1]	At the last position of the rack restart automatically at the first position

**[FrationCleaning]**

Enabled=0	[0 or 1]	Automatic fraction cleaning enabled / disabled.
WashTime=2	[Value]	Wash time in the washing station
XOffset=71	[Value]	X-offset to reach the fraction coordinate
YOffset=-20	[Value]	Y-offset to reach the fraction coordinate
ZOffset=0	[Value]	Z-offset to reach the fraction coordinate

**[Aliqoutation]**

Enabled=0	[0 o 1]	Automatic aliquotation enabled / disabled
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**[Detector]**

AutozeroAnnotation=1	[0 or 1]	On each autozero an annotation will be written into the chromatogram
WavelengthAnnotation=1	[0 or 1]	On each wavelength change an annotation will be written into the chromatogram

**[ProStar]**

Enabled=0	[0 or 1]	Activates Varian ProStar UV detector
IP=192.168.0.2	[Ip]	IP address of the UV detector
Port=2346	[Value]	Portnumber of the UV detector
Attenuation1=1.0	[Value]	Attenuation for wavelength 1
Attenuation2=1.0	[Value]	Attenuation for wavelength 2
WaveLenth1=254	[Value]	Wavelength for channel 1 in nm
WaveLenth2=280	[Value]	Wavelength for channel 2 in nm
DualMode=2	[Value]	Dualmode for Varian ProStar
Bunching=1	[Value]	Bunching for Varian ProStar
AnalogSource1=0	[Value]	Analogsource for channel 1
AnalogSource2=0	[Value]	Analogsource for channel 2
CellType=4	[Value]	Index of the cell type
CellRatio=32.22	[Value]	Size ratio of the cell
ConnectionTimeout=5	[Value]	Timeout for establishing connection
AnswerTimeout=5	[Value]	Timeout for sending commands

**[S3245]**

Port=0	[0 or 1]	Activates Sykam S3245 US detector
Channels=1	[1 or 2]	Number of channels
Wavelength1=254	[Value]	Wavelength channel 1 in nm
Wavelength2=254	[Value]	Wavelength channel 1 in nm

**[LaboCord5000]**

Enabled=0	[0 or 1]	Activates LaboCord-5000 UV detector
IP=192.168.0.101	[IP]	IP address of the UV detector
Port=10001	[Value]	Port number of the UV detector
Wavelength1=254	[Value]	Wavelength channel 1 in nm
Wavelength2=254	[Value]	Wavelength channel 1 in nm
DataRate=2	[Value]	Data rate per second
ConnectionTimeout=2	[Value]	Timeout for establishing connection

**[KnauerUVD]**

Enabled=0	[0 or 1]	Activates Knauer UV detector
IP=192.168.0.101	[IP]	IP address of the UV detector
Port=10001	[Value]	Port number of the UV detector
BaudRate=9600	[Value]	Baudrate in case of serial control
Wavelength1=254	[Value]	Wavelength channel 1 in nm
DataRate=2	[Value]	Datarate per second
Channels=1	[Value]	Number of channels
Type=UVD2.1S	[Text]	Type of detector

**[TOYODADMWD]**

Enabled=0	[0 or 1]	Activates ECOM DAD as MWD
IP=192.168.0.101	[IP]	IP address of the detector
Port=10001	[Value]	Port number of the detector

Channels=4	[Value]	Number of channels
LampOff=0	[0 or 1]	switch lamp off at shutdown of PrepCon
<b>[KnauerIFU21]</b>		
Port=0	[0 or 1]	Activates Knauer IFU A/D converter
Datarate=1	[Value]	Datarate per second
Channels=4	[Value]	Number of channels
<b>[KnauerCM21S]</b>		
Enabled=0	[0 or 1]	Activates Knauer CM21S LF detector
IP=192.168.0.101	[IP]	IP address of the detector
Port=10001	[Value]	Port number of the detector
DataRate=9600	[Value]	Datarate per second
Channels=3	[Value]	Number of channels
<b>[ThermoControl]</b>		
Enabled=0	[0 or 1]	Activates temperature control
IP=192.168.0.101	[IP]	IP address of the temperature control interface
Port=10001	[Value]	Port number of the temperature control interface
Channels=3	[Value]	Number of channels
<b>[DAD]</b>		
Enabled=0	[0 or 1]	Activates DAD
Diodes=254	[Value]	Number of diodes in the DAD array
ScanStart=100	[Value]	Start of the spectrum of an ECOM-DAD
ScanEnd=600	[Value]	End of the spectrum of an ECOM-DAD
SliceWidth=500	[Value]	Standard value for the DAD slice width
IntegrationTime=500	[Value]	Integration time of the DAD
IntegrationBandwidth=1	[Value]	Standard value for DAD bandwidth.
AutomaticReference=1	[0 or 1]	At the start of each method a reference spectrum is recorded automatically
SpecType=ABS		detector delivers absorption spectra
<b>[MMS]</b>		
Port=COM2	[COM1 - ...]	Com port number of ECOM –DAD
<b>[Smartline2600]</b>		
Integration=20	[Value]	Integration time of Knauer Smartline DAD
<b>[Calibration]</b>		
p0=1.900000000E+002	[Value]	Calibration factor 0 of the DAD
p1=2.000000000E+000	[Value]	Calibration factor 1 of the DAD.
p2=0.000000000E+000	[Value]	Calibration factor 2 of the DAD.
p3=0.000000000E+000	[Value]	Calibration factor 3 of the DAD.
p4=0.000000000E+000	[Value]	Calibration factor 4 of the DAD.
<b>[Microsaic]</b>		
Enabled=0	[0 or 1]	Activates Microsaic MS
IP=192.168.0.111	[IP]	IP address of the Microsaic MS

Factor=1	[Value]	Factor applied to all MS counts
StopScan=0	[0 or 1]	Stopping MS scan after stopping run
MixMode=1	[0 or 1]	Microsaic Interleave Mode available
<b>[Eventbox]</b>		
Pulselength=0.5	[Value]	Pulse length of the event box outputs in seconds
<b>[Signal Inverting]</b>		
Eventbox=0	[1 – 12]	Listed EventBox or Game port inputs will be inverted
GamePort=0	[1 – 4]	
<b>[Temperature]</b>		
FunctionName1=	[Text]	User defined name of the function „Temperature 1“.
FunctionName2=	[Text]	User defined name of the function „Temperature 2“.
StirrerSpeed=150	[Value]	Heater stirrer speed
<b>[MultiSystem]</b>		
Enabled=0	[0 or 1]	PrepCon5 is running several times on one computer.
DataChannel1=1	[ 0 or 1 ]	Number of the data channel that is allocated to the first system in a multiple system
DataChannel1=2	[ 0 or 1 ]	Number of the data channel that is allocated to the second system in a multiple system
DataChannel3=3	[ 0 or 1 ]	Number of the data channel that is allocated to the third system in a multiple system
DataChannel4=4	[ 0 or 1 ]	Number of the data channel that is allocated to the fourth system in a multiple system
<b>[IntegrationPresets]</b>		
IntegrationInhibit=0	[o or ...]	Data channels that are not to be automatically integrated, are to be entered separated by commas.
MaxBaselineLevel=250	[ ... ]	Preset values for integration outside peak windows (explanation in Chapter 6.2.10).
FilterFactor=5	[-5 – 15]	
SlopeSensitivity=500	[ ... ]	Enables an input field in the threshold programming where a delay time for crossing execution can be entered
AreaDelay=0	[0 or 1]	
TailingFactor=0	[0 or 1]	display tailing factor instead of asymmetry
<b>[SolventSupply]</b>		
AnalogA=0	[1 - 8]	Number of the channel that records the level signal of solvent A.
AnalogB=0	[1 - 8]	Number of the channel that records the level signal of solvent B.
AnalogC=0	[1 - 8]	Number of the channel that records the level signal of solvent C.
AnalogD=0	[1 - 8]	Number of the channel that records the level signal of solvent D.

AnalogWaste=0	[1 - 8]	Number of the channel that records the level signal of waste.
SoundfileWaste=*.wav	[*.wav]	Sound wave file that plays automatically when the waste level is upper maximum
SoundfileSolvents=*.wav	[*.wav]	Sound wave file that plays automatically when a solvent level is under minimum.
<b>[WasteMannagement]</b>		
ValveNo=1	[1 - ...]	Number of the waste/fraction valve when using waste management
BypassValve=0	[1 - ...]	Number of the bypass valve when using waste management.
Volume=10000	[Value]	Volumes of waste containers when using waste management
ErrorInput=0	[1 - 12]	Number of the EventBox-Input for an error signal
Soundfile=Fehler.wav	[*.wav]	Sound wave file that plays automatically when an error occurs.
<b>[LeakageInput]</b>		
LeakageInput1=0	[1 - 12]	Event box input for leakage sensor 1
LeakageInput2=0	[1 - 12]	Event box input for leakage sensor 2
...		
LeakageInput6=0	[1 - 12]	Event box input for leakage sensor 6
Message1=Leakage	[Text]	Display text for leakage sensor 1
Message2=Leakage	[Text]	Display text for leakage sensor 2
...		
Message6=Leakage	[Text]	Display text for leakage sensor 6
LeakageCountdown=120	[0 - ...]	Countdown in seconds until the system is stopped following the detection of a leak
WindowsShutdown=1	[0 or 1]	At the end of countdown shutdown windows
Soundfile=Fehler.wav	[*.wav]	Sound wave file that plays automatically when a leak has been detected
EluentValveA=2	[1 - ...]	Valve number for sealing off eluent Solvent A
EluentValveB=2	[1 - ...]	Valve number for sealing off eluent Solvent B
EluentValveC=2	[1 - ...]	Valve number for sealing off eluent Solvent C
EluentValveD=2	[1 - ...]	Valve number for sealing off eluent Solvent D
<b>[DemoMode]</b>		
Chromatogram=*.rfp	[*.rfp]	Resultfile which is used for chromatograms in demo mode
<b>[Visualisation]</b>		
ValvePartitioning=0	[1 - ...]	Index of the fractionation valve divided in horizontal position segments. Double clicking this valve in the system visualisation switches into the corresponding position instead of the next position.
<b>[TandemValve]</b>		
Index=0	[1 - ...]	Index of the tandem valve
SecondPort=1	[1 - ...]	COM port number of the second tandem valve
PositionRequest=0	[0 or 1]	At the start of every run the user is asked which valve position to use for the tandem

valve

**[Recycling]**

Sovent=A

[A,B,C,D]

Solvent to be recycled

ValveIndex=0

[1 - ...]

Index of recycling valve

ValvePosition=2

[1 - ...]

valve position for solvent recycling; an error message is displayed in case the recycling valve is in this position and recycled solvent is not set to 100 %

**[SedexLC]**

Enabled=0

[0 or 1]

Activates Sedex ELSD detector

Port=2

[Value]

COM port number of the detector

TempZone=1

[Value]

Temperature control of ELSD using

Temperature Zone [1-8]

### 20.3 PrepCon5 file types

<b>*.tcf</b>	PrepCon5-Time Control File
<b>*.acf</b>	PrepCon5-Autosampler Control File
<b>*.rfp</b>	PrepCon5-Result File. Includes the result data of a run
<b>*.dad</b>	PrepCon5-DAD-File. Includes the spectra of a DAD run
<b>*.rck</b>	PrepCon5-Fraction Collector Rack File. Includes the geometric data of a fraction collector rack.
<b>*.vis</b>	PrepCon5-Visualisation File. Includes the data of a system visualization.
<b>*.cfg</b>	PrepCon5-Configuration File. Includes the data of the program configuration