MagIC Net

Metrohm
Ion analysis

Tutorial

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Metrohm AG
CH-9100 Herisau
Switzerland
Phone +41 71 353 85 85
Fax +41 71 353 89 01
info@metrohm.com
www.metrohm.com

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Technical Communication
Metrohm AG
CH-9100 Herisau
techcom@metrohm.com

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This documentation has been prepared with great care. However, errors can never be entirely ruled out. Please send comments regarding possible errors to the address above.

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1 Introduction

1.1 Structure of the tutorial

This tutorial describes the first steps with the ***MagIC Net*** software. You will be introduced to the most important controls by means of the recording of a chromatogram. The introduction follows the determination of the concentration of the anions F^-, Cl^-, NO_2^-, Br^-, NO_3^-, PO_4^{3-} and SO_4^{2-} in tap water. A 940 Professional IC Vario and a Metrosep A Supp 5 - 100/4.0 column with integrated chip are used for the determinations.

The tutorial is arranged in 4 parts:

- Configuring the hardware that is managed with the system and used in the method
- Creating a method for performing a determination
- Carrying out the determination
- Analyzing the determination, reprocessing and report output

It will be demonstrated how the determination is carried out with a simple system with manual injection. In addition, a determination with an automated system with sample changer is also described.

1.2 Program description

MagIC Net comprises the following program parts:

Workplace

- Opening/closing workplaces
- Entering sample data
- Starting single determinations and sample series
- Live representation of chromatograms and system parameters (Watch window)
- Report display

Database

- Opening/closing databases
- Managing determinations
- Reprocessing determinations
- Creating reports

Method

- Entering the device combination used and their parameters
- Defining the time program
- Entering integration parameters
- Entering the analytes
- Result definition
- Calibration parameters

Configuration

- Information on instruments, columns, eluents, accessories, solutions, amperometric cells, rotors, common variables and rack data
- User administration
- Security settings
- Program administration

Manual control

- Manual control of the instruments used in the method loaded in the workplace
- Manual control of all the connected instruments

1.3 Symbols and conventions

The following icons and formatting are used in this documentation:

1	**Instruction step** Carry out these steps in the sequence shown.
Method	**Dialog text, parameter** in the software
File ▶ New ▶	Menu or menu item
[Continue]	**Buttons** or **keys**
	Note This symbol highlights additional information and tips.

2 Configuration

Metrohm devices that are switched on and connected to the PC via a USB connector are automatically recognized when the program is started, as are devices connected to MSB connectors of USB devices (Dosinos, stirrers, pumps, Remote Box). Certain instruments need to be added to the device table manually. This includes devices that are connected to the PC via the RS-232 interface, the barcode reader and the 771 IC Compact Interface.

All the hardware components that are used in a method must be set up in the **Configuration** program part. This may include:

- Instruments (940 Professional IC Vario, 858 Professional Sample Processor etc.)
- Columns
- Eluents
- Accessories (pump tubing, pump tubing connectors etc.)
- Solutions
- Common variables
- Rack data
- Amperometric cells
- Rotors

2.1 Starting the software

NOTICE

Devices and intelligent columns are recognized automatically. All elements can be monitored by the system.

Starting MagIC Net

1 Click on the ***MagIC Net*** icon on the desktop.

2 Enter a user name and password, if requested, and click on **[OK]**.

3 Click on the **[Configuration]** icon.

The dialog for the **Configuration** program part opens.

A total of 9 subwindows can be displayed here:

Devices	Display of the automatically recognized and manually added devices.
Columns	Display of the automatically recognized and manually added columns.
Eluent	Display of the manually added eluents.
Accessories	Display of the manually added accessories.
Solutions	Display of the automatically recognized solutions in a dosing unit and of the solutions that have been added manually.
Rack data	Display of the automatically recognized and manually imported Metrohm sample racks.
Common variables	Display of all the common variables.
Amperometric cells	Display of the automatically recognized and manually added cells of the amperometric detector.
Rotors	Display of the manually added rotors with rotor type and serial number.

The subwindows to be displayed can be determined with the icon or via the **View ► Change layout...** menu item.

2.2 Configuring devices

Follow these steps to start up the **940 Professional IC Vario** for the first time:

Connecting the 940 Professional IC Vario

1 Connecting the device

Connect the device to the PC using a USB cable.

2 Switching on the device

The device parameters of the **940 Professional IC Vario** are automatically recognized.

3 Saving the device in the table

Confirm the message with **[Yes]**.

4 Checking the properties

Check the information in the **Properties** dialog and close by clicking on **[OK]**.

The **940 Professional IC Vario** is entered in the device list in the **Devices** subwindow.

5 Changing the device name (optional)

Follow these steps to give your device a different name:

- Double-click on the line with the entry **940 Professional IC Vario** in the device table.
- Select the **General** tab.
- Enter the new name in the **Device name** field.
- Close the dialog with **[OK]**.

If you carry out your determination with a sample changer, the instrument must be connected first.

Connecting the 858 Professional Sample Processor

1 Connecting the device

Connect the device to the PC using a USB cable.

2 Switching on the device

The device parameters of the **858 Professional Sample Processor** are automatically recognized.

3 Saving the device in the table

Confirm the message with **[Yes]**.

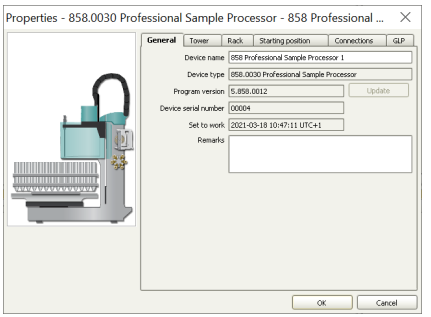
4 Checking the properties

Check the information in the **Properties** dialog and close by clicking on **[OK]**.

The **858 Professional Sample Processor** is entered in the device list in the **Devices** subwindow.

5 Defining rack parameters

- Double-click on the line with the entry **858 Professional Sample Processor** in the device table.



- Select the **Rack** tab.
  If a standard rack is used, the **Rack name** field contains the number 6.2041.440.
  If a different rack was placed on the sample changer, its respective number is entered. In this case, the correct positions may differ from the following description. Please make sure you use the correct selection.
- Click on the **[Rack data]** button.
- Select the **Lift positions** tab.
- Enter the value **125** in the **Work position** field.
- Select the **Special beakers** tab.
- Click on **[Edit]** to open the **Special beaker 1** dialog.
- Enter the value **149** in the **Rack position** field.
- Enter the value **125** in the **Work position Tower 1** field.

- Edit the two other special beakers in the same way.
- Close all dialogs with **[OK]**.

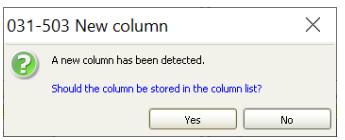
2.3 Configuring the column

Column with chip

An installed column with column chip is automatically recognized and entered in the **Columns** subwindow in the column table when the IC instrument is connected. The parameters of Metrohm columns with integrated chip are entered in the corresponding tab.

1 Inserting the column into the holder

The column is recognized by **MagIC Net**.



2 Saving the column in the table

Confirm the message with **[Yes]**.

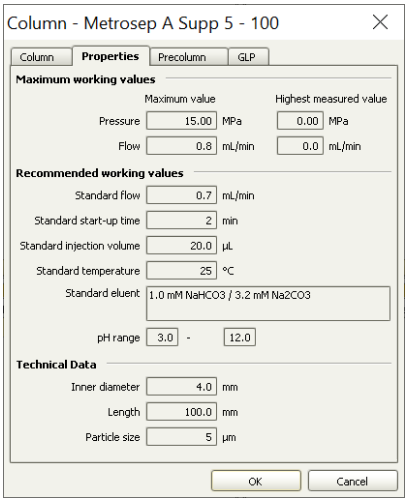
The column is entered in the column table in the **Columns** subwindow.

3 Editing the Column tab

Enter the name **Metrosep A Supp 5 - 100** in the **Column name** field in the **Column - Metrosep A Supp 5 - 100/4.0** dialog on the **Column** tab.

4 Editing the Properties tab

The parameters of the used column (max. pressure, max. flow etc.) are already entered.



5 Editing the Guard column tab

Activate the **Use guard column** check box.

Activating this feature simultaneously defines that the guard column is monitored with the column.

6 Monitoring tab

NOTICE

This tab is only available for automatically recognized columns with chip.

- Enter the value **500** (example) in the **Determinations** field and enable the **Monitoring** check box.

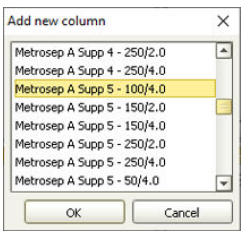
- Enter the value **72** (example) in the **Operating hours** field and enable the **Monitoring** check box.
- Enter the same limit values for the **Determinations** and the **Operating hours** of the **Guard column** as for the column and activate the check boxes for their monitoring.
  The guard column is monitored in the same way as the column.
- Activate the check box **Acoustic signal** in the **Message** area.

Column without chip

If a column without a chip is used, it must be configured first. Use the **[Edit]** menu in the **Columns** subwindow to do so. For known columns, some parameters are entered automatically and for unknown columns, these parameters can be found on the column leaflet and must be entered manually.

1 Adding a column

Open the **Add new column** dialog via the **Edit ► New...** menu.



2 Selecting the column

Mark the **Metrosep A Supp 5 - 100/4.0** column in the list and click on **[OK]**.

The **Column - Metrosep A Supp 5 - 100/4.0** dialog opens.

3 Editing the column

- Select the **Column** tab.
- Enter the name **Metrosep A Supp 5** in the **Column name** field.
- Click on the ... button in the **Set to work** field and select the date of the initial start-up.
  The **Column type** and **Order number** fields are automatically filled in for known columns.
  Entries in the **Serial number**, **Batch number** and **Comment** fields are optional. We recommend to enter information here for better traceability and for troubleshooting in the event of an error.

4 Editing the Properties tab

For known columns, the values for pressure, flow etc. are entered automatically. For unknown columns, these values can be found on the column leaflet and must be entered manually.

5 Editing the Guard column tab

For known columns, these fields are automatically filled in. For unknown columns, these values can be found on the column leaflet and must be entered manually.

Follow these steps to enter the date of the initial start-up:

- Select the **Guard column** tab.
- Activate the **Use guard column** check box.
- Click on the ... button of the **Set to work** field.
- Select the date and click on **[OK]**.

6 Editing the GLP tab (optional)

This tab only has to be edited if monitoring according to the GLP (Good Laboratory Practice) rules is necessary.

- Select the **GLP** tab.

- In the **GLP test date** field, click on the ... button and select the date of the last GLP test.
- Activate the **Monitoring of GLP validity** check box.
- Enter the value **100** (example) in the **GLP test interval** field.
  The date of the next GLP test is automatically entered in the **Next GLP test** field.
- Activate the check box **Acoustic signal** in the **Message** area.
- In the **Action** area, enable the **Display message** option.
- Close the dialog by clicking on **[OK]**.

2.4 Defining the eluent

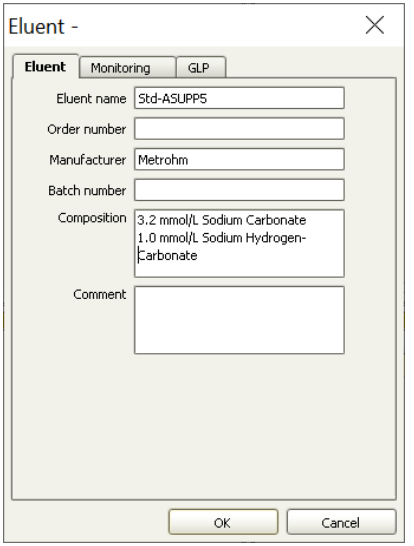
Eluents are defined in the **Eluent** subwindow.

1 Open the **Eluent** dialog via the **Edit ► New...** menu.

2 **Eluent properties**

- Select the **Eluent** tab.
- Make the following entries:

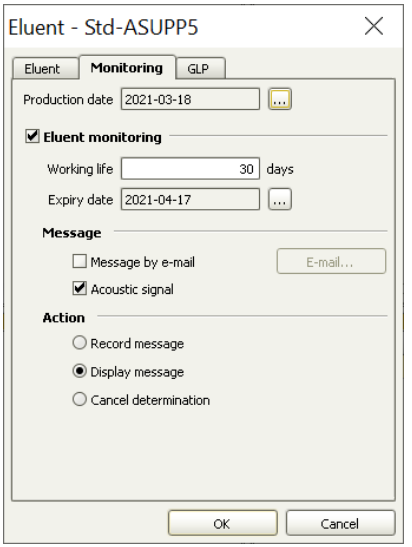
Field	Entry
Eluent name	Std-ASUPP5
Order number	optional
Manufacturer	optional
Batch number	optional
Composition	3.2 mmol/L sodium carbonate, 1.0 mmol/L sodium hydrogen carbonate
Comment	optional



3 Editing the Monitoring tab

- Select the **Monitoring** tab.
- The date of the initial start-up is entered automatically when the eluent is entered.
- Activate the **Monitor eluent** check box.
- Enter the value **30** in the **Working life** field (the working life depends on the type of eluent used).
  The date is automatically entered in the **Expiry date** field.
- Activate the check box **Acoustic signal** in the **Message** area.

- In the **Action** area, enable the **Display message** option.

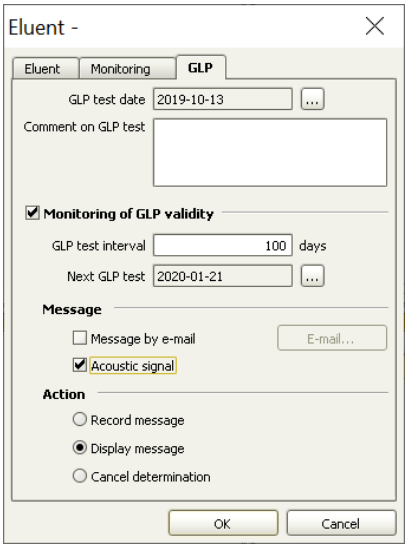


- Close the dialog by clicking on **[OK]**.

4 Editing the GLP tab (optional)

- Select the **GLP** tab.
- In the **GLP test date** field, click on the button and select the date of the last GLP test.
- Activate the **Monitoring of GLP validity** check box.
- Enter the value **100** (example) in the **GLP test interval** field.
  The date is automatically entered in the **Next GLP test** field.
- Activate the check box **Acoustic signal** in the **Message** area.

- In the **Action** area, enable the **Display message** option.



- Click on **[OK]** and close the **Eluent Std ASUPP5** dialog.

2.5 Setting up solutions

Solutions that are connected to a 800 Dosino with a 807 Dosing Unit are automatically recognized when they are connected. The parameters of the integrated chip are entered in the corresponding tabs in the **Solutions** subwindow. For unknown solutions, these parameters must be entered manually.

Solutions for the suppressor are defined in the **Solutions** subwindow.

1 Open the **Solution** dialog via the **Edit ► New...** menu.

2 Editing the **Solution** tab

- Enter the name **MSM regeneration solution H_2SO_4** in the **Solution name** field.
- Enter the concentration value **100** in the **Concentration** field and select the concentration unit **mmol/L** in the list box.
- Click on the ... button in the **Production date** field.
- Select the date and click on **[OK]**.
- Activate the **Monitor solution** check box.
- Enter the value **100** in the **Working life** field.
  The date is automatically entered in the **Expiry date** field.
- Activate the check box **Acoustic signal** in the **Message** area.
- In the **Action** area, enable the **Display message** option.
- Close the dialog by clicking on **[OK]**.

3 Editing the GLP tab (optional)

- Select the **GLP** tab.
- In the **GLP test date** field, click on the ... button and select the date of the last GLP test.
- Activate the **Monitoring of GLP validity** check box.
- Enter the value **100** in the **GLP test interval** field.
  The date is automatically entered in the **Expiry date** field.
- Activate the check box **Acoustic signal** in the **Message** area.

- In the **Action** area, enable the **Display message** option.

- Click on **[OK]** and close the **Solution** dialog.

2.6 Setting up accessories

Accessories always have to be set up and configured manually. The individual steps are carried out in the **Accessories** sub-window.

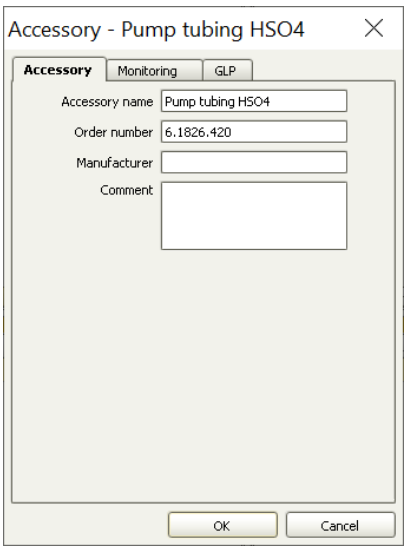
A pump tubing and a pump tubing connection with security lock and filter is added. The pump tubing connection with inline filter is used to protect the suppressor from a possible contamination from the regeneration solution.

Setting up new accessories

1 Open the **Accessories** dialog via the **Edit ▶ New...** menu.

2 Enter the name **Pump tubing H_2SO_4** on the **Accessories** tab in the **Accessory name** field.

3 Enter the number **6.1826.420** in the **Order number** field.



4 Select the **Monitoring** tab.

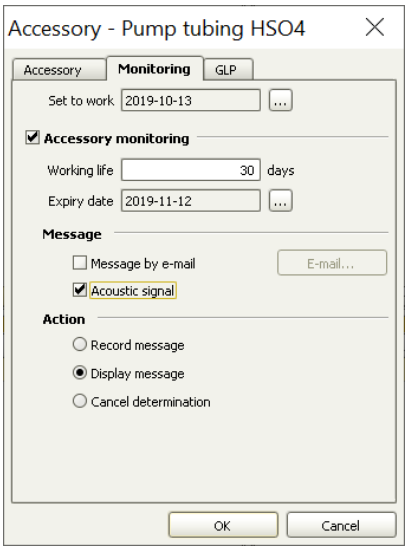
5 Activate the **Monitor accessories** check box.

6 Enter the value **30** in the **Working life** field.

The date is automatically entered in the **Expiry date** field.

7 Activate the check box **Acoustic signal** in the **Message** area.

8 In the **Action** area, select the **Display message** option.



The order number of the **Pump tubing connection with security lock and filter** is **6.2744.180**. The order number of the **Filter** is **6.2821.130**.

2.7 Setting up the rotor

The rotor is set up in the **Rotors** subwindow.

Setting up a new rotor

1 Adding a rotor

Open the **Add new rotor** dialog via the **Edit ► New...** menu.

2 Selecting the rotor

Select the rotor **MSM A**.

The **Rotor** dialog is opened.

3 Editing the rotor

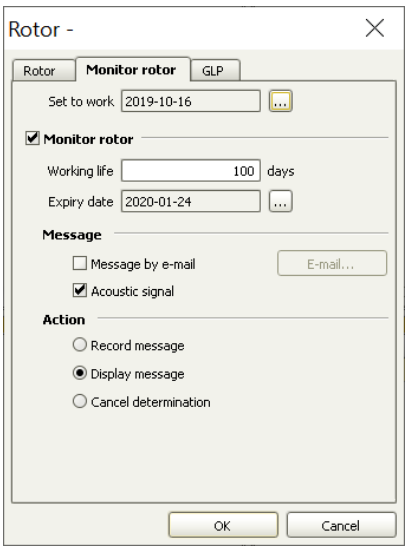
- Select the **Rotor** tab.
- Enter the name **MSM Rotor** in the **Rotor name** field.
- The **Order number** field is filled in automatically for known rotors.
  Entries in the **Serial number** and **Comment** fields are optional. We recommend to enter information here for better traceability and for troubleshooting in the event of an error.

4 Editing the Monitor rotor tab (optional)

This tab only has to be edited if monitoring of the rotor is necessary.

- Select the **Monitor rotor** tab.
- The date of the initial start-up is entered automatically when the rotor is entered.
- Activate the **Monitor rotor** check box.

- Enter the value **365** (example) in the **Working life** field.
  The date is automatically entered in the **Expiry date** field.
- Activate the check box **Acoustic signal** in the **Message** area.
- In the **Action** area, enable the **Display message** option.



5 Editing the GLP tab (optional)

This tab only has to be edited if monitoring according to the GLP principles is required.

- Select the **GLP** tab.
- In the **GLP test date** field, click on the ... button and select the date of the last GLP test.
- Activate the **Monitoring of GLP validity** check box.

- Enter the value **100** (example) in the **GLP test interval** field.
  The date of the next GLP test is automatically entered in the **Next GLP test** field.
- Activate the check box **Acoustic signal** in the **Message** area.
- In the **Action** area, enable the **Display message** option.
- Close the dialog by clicking on **[OK]**.

3 Creating a method

A method is a run instruction for processing a sample. It contains all the components that are necessary to record a chromatogram. These include:

- Devices and their start parameters
- Time program
- Parameters for the evaluation of the chromatograms
- Result definitions

The method described in this tutorial is created using a method template that is predefined in ***MagIC Net***. A method template contains the most common component names, their retention times, the measured quantity (surface or height) for the evaluation of the peaks and the way in which the calibration curve is to be fitted.

The ***MagIC Net*** installation contains some sample methods. The sample methods are stored in the following folder by default: C:\Programs (x86)\Metrohm\MagIC Net\examples\methods. The sample methods can be imported and adapted to the application to be carried out *(see Quick guide MagIC Net How to adapt a method - 8.102.8078)*.

To use methods that were created in an older version of ***MagIC Net***, see the following document: *Quick guide MagIC Net How to adapt a method - 8.102.8078*

3.1 Methode for manual injection

3.1.1 Creating a new method

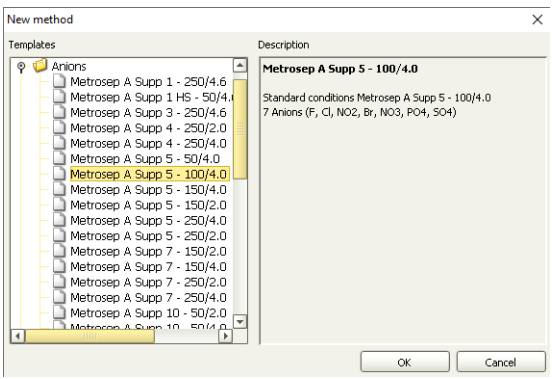
Creating a method

1 Click on the icon for the **Method** program part.

2 Open the **New method** dialog using the **File ► New…** menu.

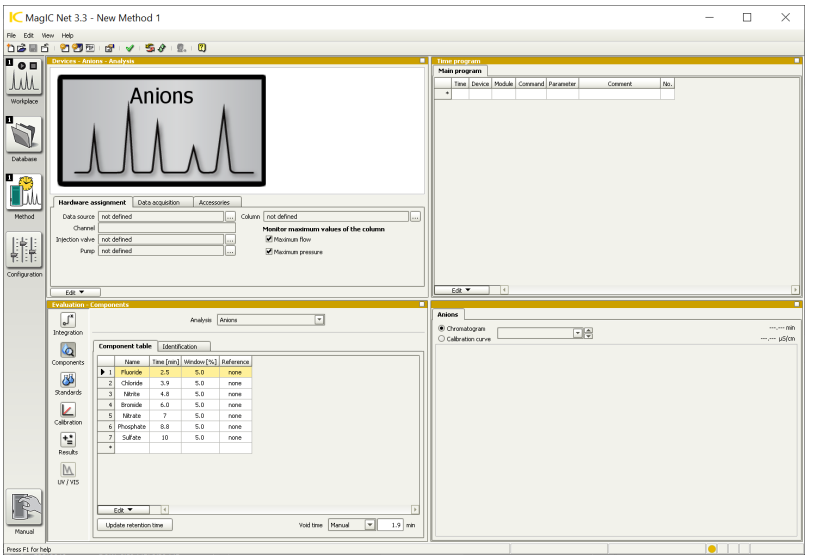
3 Under **Templates**, on the left part of the window, highlight **Anions ► Metrosep A Supp 5 - 100/4.0** and confirm with **[OK]**.

The method template opens.



The symbol of the **Anions** analysis method is displayed in the **Devices** subwindow. The **Evaluation - Components**

subwindow shows the component table with the ions of the method template and their retention times.



The **Method** program part has a total of 4 subwindows:

Devices	Visualization of the devices that are assigned to the method and the analysis.
Time program	Representation of the time program.
Evaluation	The subwindow contains the areas **Integration**, **Components**, **Standards**, **Calibration** and **Results**.
Chromatograms	Display of the chromatograms of the last determination that was recorded with this method, the chromatograms of the standards that are used for the calibration of the samples and the calibration curves.

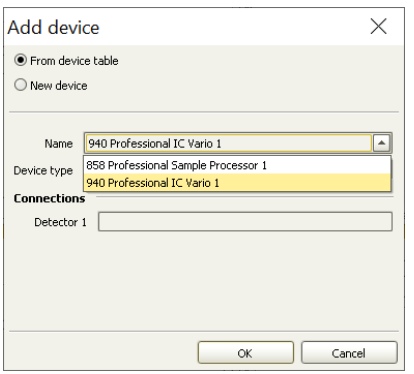
3.1.2 Defining devices and start parameters

Assembling devices

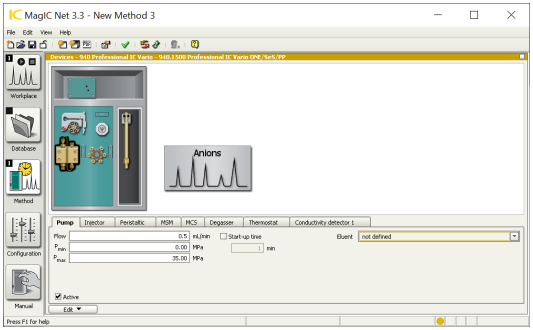
1 In the **Devices** subwindow, click on the menu **Edit ▶ Add ▶ Device**.

2 In the **Add device** dialog, select the **From device table** option.

3 Select the **940 Professional IC Vario 1** device in the **Name** field and click on **[OK]**.



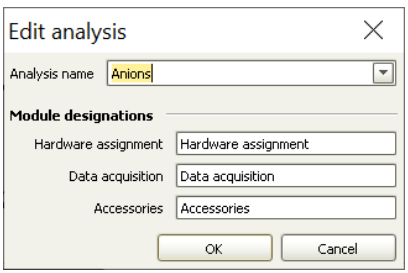
The image of the **940 Professional IC Vario** appears in the upper part of the **Devices** subwindow.



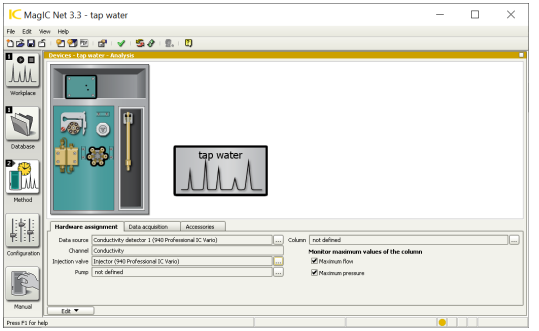
Changing the analysis name (optional)

1 Click on the icon of the **Anions** analysis in the upper part of the **Devices** subwindow.

2 Open the **Edit analysis** dialog using the **Edit ▶ Edit** menu.



3 In the **Analysis name** field, enter the new name **Tap water** and confirm with **[OK]**.



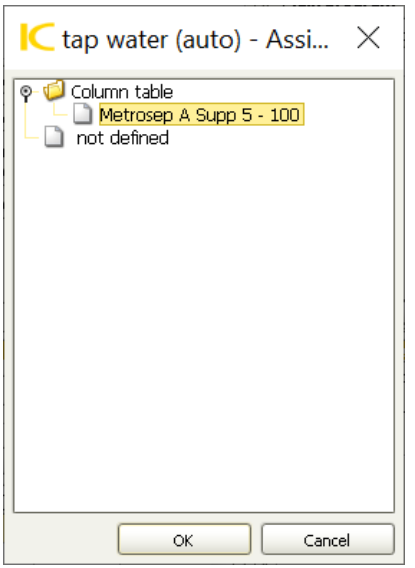
Defining the parameters for the analysis

1 Click on the **Tap water** icon.

2 **Editing the Hardware assignment tab**

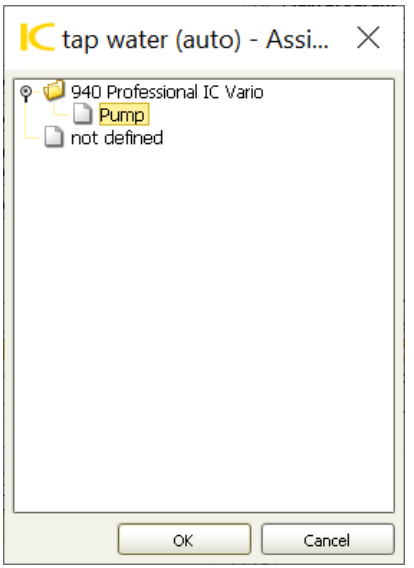
- Select the **Hardware assignment** tab.
- In the **Data source** field, click on the ... button.
- In the **Tap water - Assign data source** dialog under **940 Professional IC Vario 1 > Conductivity detector 1**, highlight the entry **Conductivity** and click on **[OK]**.
- In the **Channel** field, **Conductivity** is entered automatically.
- Click on the ... button in the **Injection valve** field.
- In the **Tap water-assign injection valve** dialog under **940 Professional IC Vario 1**, highlight the entry **Injector** and click on **[OK]**.
- Click on the ... button in the **Column** field.

- In the **Tap water - Assign column** dialog under **Column table**, highlight the entry of the assigned column **Metrosep A Supp 5 - 100** and click on **[OK]**.

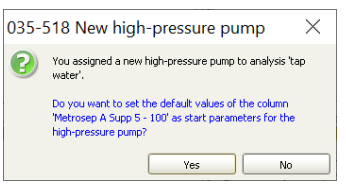


- Click on the button in the **Pump** field.

- In the **Tap water - Assign pump** dialog under **940 Professional IC Vario 1**, highlight the entry **Pump** and click on **[OK]**.



- Confirm the message **New high-pressure pump** with **[Yes]**.



The default parameters of the column are applied to the start parameters of the pump.

3 Editing the Data acquisition tab

- Select the **Data acquisition** tab.
- In the **Recording time** field, enter a time of **15 min**.

4 **Editing the Accessories tab**

- Select the **Accessories** tab.
- Click on the **[Add]** button.
- In the selection list of the **Add accessory** dialog, select the **H_2SO_4 pump tubing**.
- Click on **[OK]**.

The pump tubing is entered in the accessories table. The pump tubing connection is added to the table in the same way.

Defining the parameters for the IC device

1 Click on the image of the **940 Professional IC Vario 1**.

The tabs of the **940 Professional IC Vario 1** modules appear and can be edited.

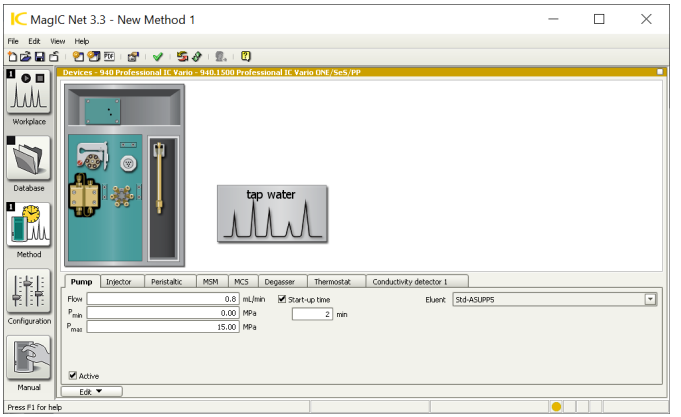
NOTICE

The **Active** check box needs to be activated so that a module can be used in a method (default setting).

2 **Editing the Pump tab**

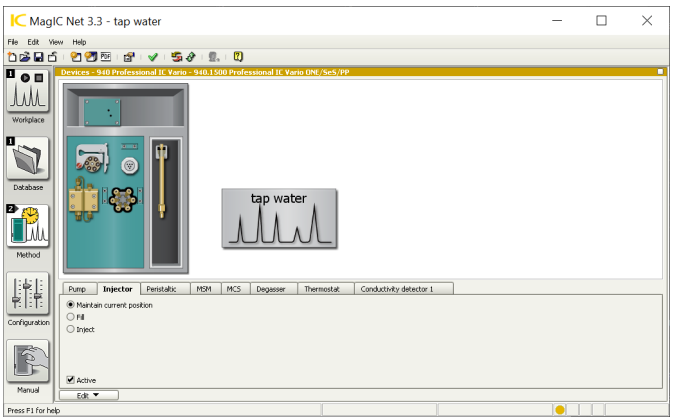
- Select the **Pump** tab (or click on the symbol of the pump).
- The values of the fields **Flow**, **P_{min}**, **P_{max}** and **Start-up time** are read automatically.

- Use the **Eluent** selection list to select the previously defined eluent **Std-ASUPP5**.



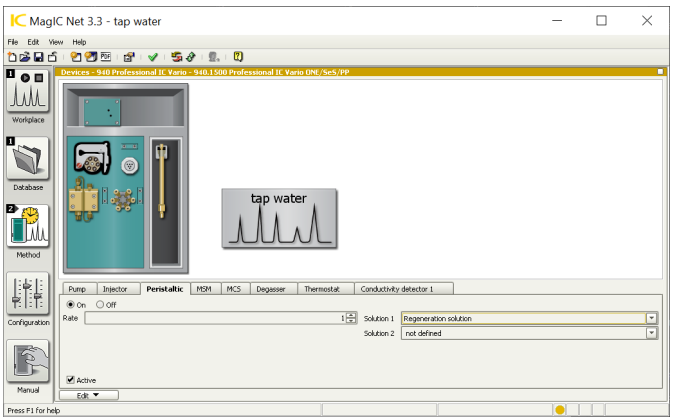
3 Editing the Injector tab

- Select the **Injector** tab (or click on the symbol of the injector).
- Accept the default settings.



4 Editing the Peristaltic tab

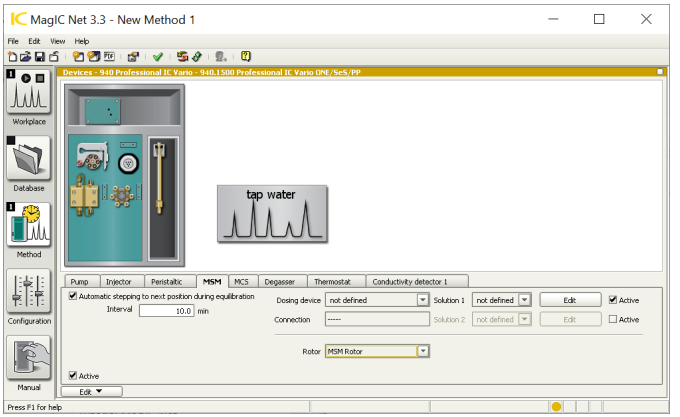
- Select the **Peristaltic** tab (or click on the symbol of the peristaltic pump).
- Activate the **On** option.
- In the **Rate** field, enter the value **1**.
  (There are 7 speed levels, with 6 revolutions/min per level.)
- In the selection list **Solution 1**, select the solution **MSM regeneration solution H_2SO_4**.



5 Editing the MSM tab

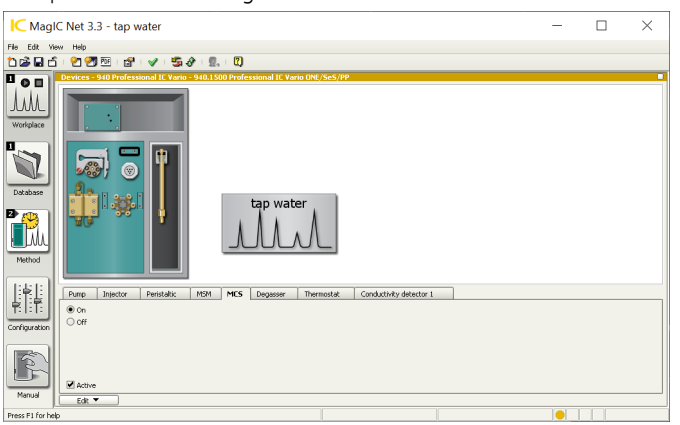
- Select the **MSM** tab (or click on the symbol of the MSM).

- Accept the default settings.
  The automatic stepping to next position every 10 minutes should be activated. The check box for Dosino regeneration can be deactivated if the suppressor is regenerated using a peristaltic pump.



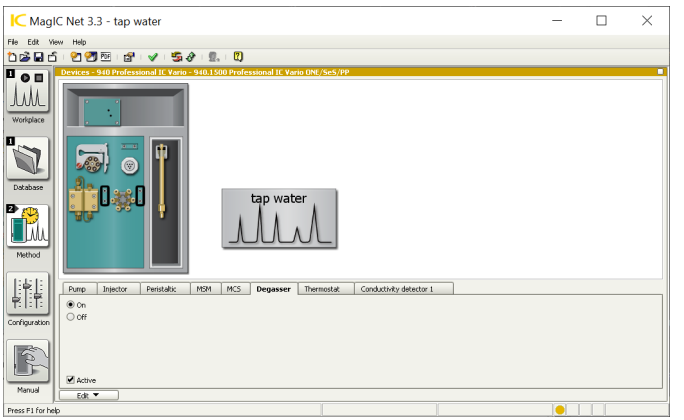
6 Editing the MCS tab

- Select the **MCS** tab (or click on the symbol of the MCS).
- Accept the default settings.



7 Editing the Degasser tab

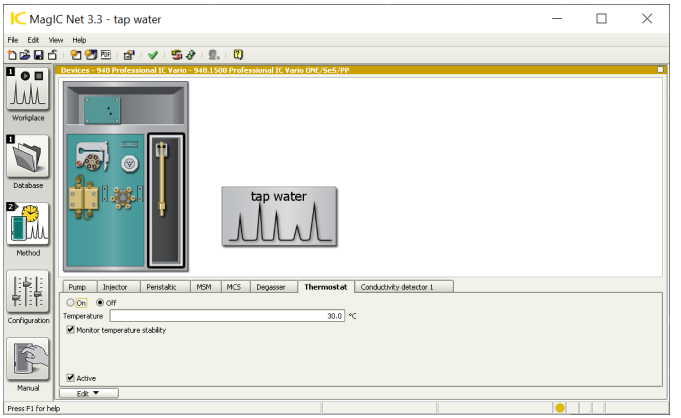
- Select the **Degasser** tab (or click on the symbol of the degasser).
- Accept the default settings.



8 Editing the Thermostat tab

- Select the **Thermostat** tab (or click on the symbol of the Thermostat).

- Switch on the column thermostat and deactivate **Monitor temperature stability**.



9 Editing the Conductivity detector 1 tab

- Select the **Conductivity detector 1** tab (or click on the symbol of the detector).
- Accept the default settings.

3.1.3 Time program

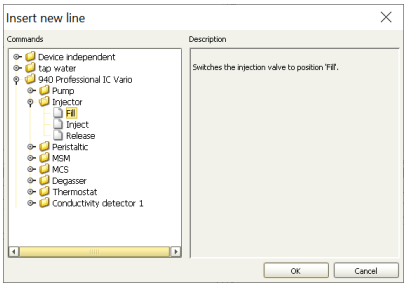
The time program is part of every method. It is a step by step description of how a sample is processed. The time program is created in the **Time program** subwindow of the **Method** program part.

Defining the time program

1 Setting the injection valve to Fill

- Open the **Insert new line** dialog via the **Edit ► New** menu.

- Select **940 Professional IC Vario ► Injector ► Fill** in the left part of the window under Commands.

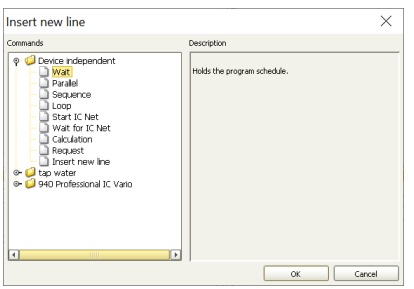


- Confirm with **[OK]**.
  The **940 Professional IC Vario - Injector - Fill** dialog is opened.
- Accept the time entry **0** min.
- Confirm with **[OK]**.

2 Interrupting the program

The program is stopped to manually fill the injection valve.

- Highlight the bottom row of the time program. Open the **Insert new line** dialog via the **Edit ► New** menu.
- Select **Device independent ► Wait** in the left part of the window under Commands.

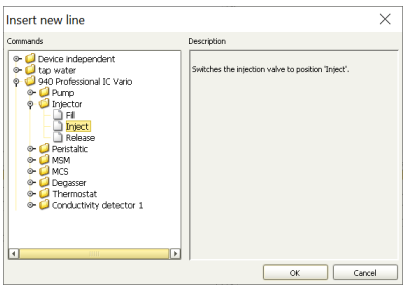


- Confirm with **[OK]**.
  The **Wait** dialog opens.
- Highlight the **Stop program and wait for [Continue]** option.

- Click on the button and enter a text for the message, for example: Fill the sample loop with the solution that is to be injected and then click on **[Continue]**.
- Confirm twice with **[OK]**.

3 Setting the injection valve to Inject

- Highlight the bottom row of the time program. Open the **Insert new line** dialog via the **Edit ► New** menu.
- Select **940 Professional IC Vario ► Injector ► Inject** in the left part of the window under Commands.

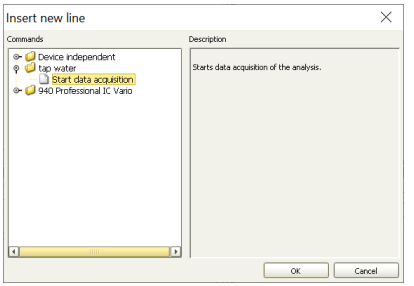


- Confirm with **[OK]**.
  The **940 Professional IC Vario - Injector - Inject** dialog is opened.
- Accept the time entry **0** min.
- Confirm with **[OK]**.

4 Starting the data acquisition

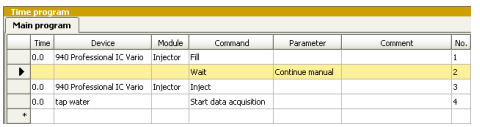
- Open the **Insert new line** dialog via the **Edit ► New** menu.

- Select **Tap water ▶ Start data acquisition** in the left part of the window under Commands.



- Confirm with **[OK]**.
  The **Tap water - Start data acquisition** dialog opens.
- Accept the time entry **0** min.
- Confirm with **[OK]**.

The complete time program to fill the injection valve manually looks as follows:



Time program

Main program

	Time	Device	Module	Command	Parameter	Comment	No.
	0.0	940 Professional IC Vario	Injector	Fill			1
▶				Wait	Continue manual		2
	0.0	940 Professional IC Vario	Injector	Inject			3
	0.0	tap water		Start data acquisition			4
*							

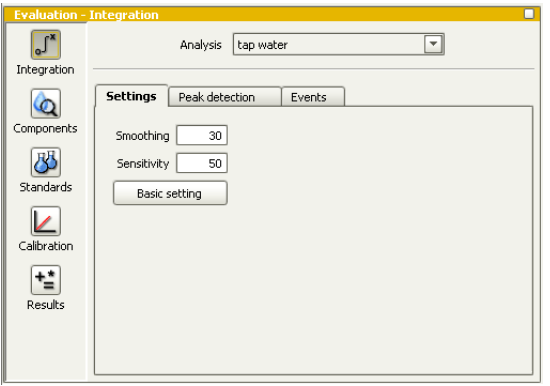
3.1.4 Evaluation

The parameters for the evaluation of the chromatograms are defined under **Evaluation**. Each analysis has its own set of evaluation parameters.

Integration

The integration parameters are defined in the method template.

1 Click on the **Integration** button.



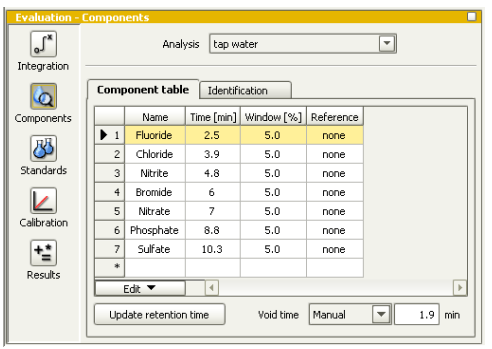
The analysis name **Tap water** is automatically entered in the **Analysis** selection list.

The entries on the **Properties**, **Peak detection** and **Results** tabs are automatically transferred.

Components

The components and the parameters for the identification are defined in the method template.

1 Click on the **Components** button.



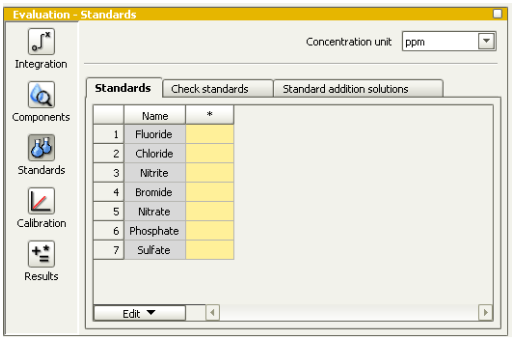
2 The entries on the **Component table** and **Identification** tabs are transferred.

Standards

The concentrations of the components in the standard solutions are displayed in the Standards area.

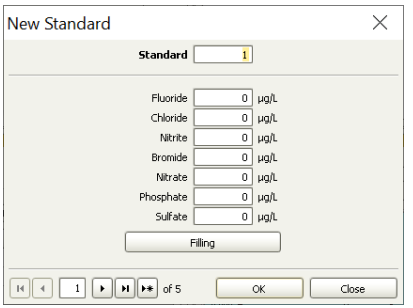
1 Click on the **Standards** button.

All the components that are defined in the method template are listed in the standards table.



2 Select the **ppm** option in the **Concentration unit** field.

3 Open the **New standard** dialog via the **Edit ▶ New** menu on the **Standards** tab.

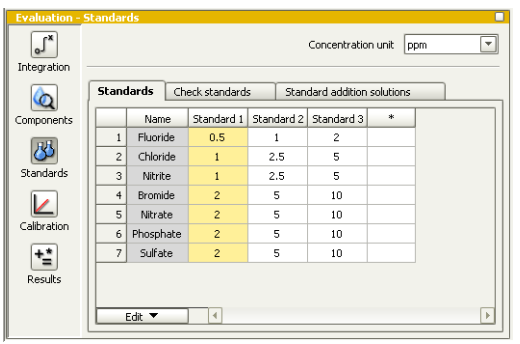


4 Enter the concentration value **0.5** in the **Fluoride** field. Enter the value **1** in the **Chloride** and **Nitrite** fields and the value **2** in the **Bromide**, **Nitrate**, **Phosphate** and **Sulfate** fields.

5 Click on ▸ to open the next standard.

6 Repeat the steps **3** to **5** to enter the concentrations of standard 2 and standard 3. The number of the next standard is automatically entered in the **Standard** field. The concentration of the components in standard 2 and standard 3 are displayed in the following table:

Table with the standard concentrations:



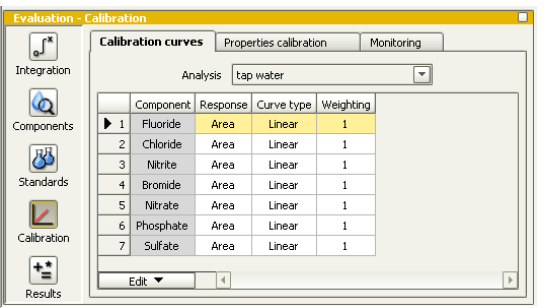
	Name	Standard 1	Standard 2	Standard 3	*
1	Fluoride	0.5	1	2	
2	Chloride	1	2.5	5	
3	Nitrite	1	2.5	5	
4	Bromide	2	5	10	
5	Nitrate	2	5	10	
6	Phosphate	2	5	10	
7	Sulfate	2	5	10	

Calibration

The calibration is carried out according to the method of the external standard. The peak areas in the chromatogram of an unknow sample are compared to the peak areas of the components of a standard solution with a known concentration. The calibration method is defined in the method template.

1 Click on the **Calibration** button.

2 Select the **Calibration curve** tab.



The component name, measured quantity, curve type and the weighting are defined in the method template. The table can be edited row by row. Either via the **Edit ▶ Edit** menu or by double-clicking on a row which opens the **Calibration curve** dialog of the corresponding component.

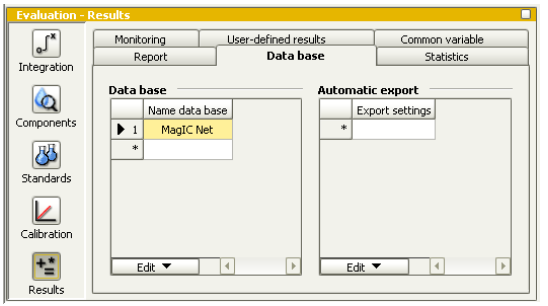
Results

The results of the determinations are stored in the default database **MagIC Net** (additional databases can be defined). You can

also define that a report is generated once the evaluation is finished.

1 Storing results in the database

- Click on the **Results** button.

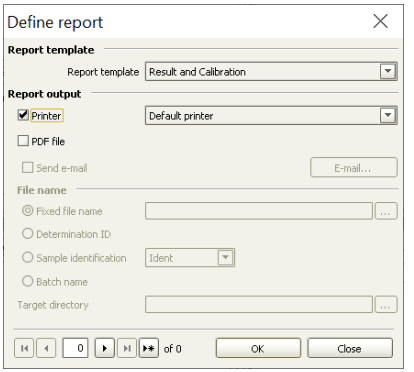


- Select the **Database** tab.
- In the **Database** area, select the database in which the determination data is to be stored. The database **MagIC Net** is set by default. Additional databases can be created in the database manager in the **Database** area.

2 Printing results (optional)

- Select the **Report** tab.
- Open the **Define report** dialog via the **Edit ► New...** menu.
- Highlight the template **Result and Calibration** in the **Report template** list box.
- In the **Report output** area, activate the **Printer** check box.

- Select a printer in the **Printer** selection list.



- Confirm with **[OK]**.

You also have the possibility to create your own report template *(see chapter 5.4, page 101)*.

3.1.5 Saving a method

Saving a method

After having entered all relevant parameters for the method, save the method as follows:

1. Open the **Save method** dialog using the **File ► Save as...** menu.

2. Enter the name **Tap water** for the method in the **Method name** field.

3. Click on **[Save]**.

3.2 Method with Sample Processor

Creating a method for a determination with a Sample Processor differs from the method for a manual injection only in the following points:

- Defining devices and start parameters
- Time program

3.2.1 Creating a new method

(see chapter 3.1.1, page 25)

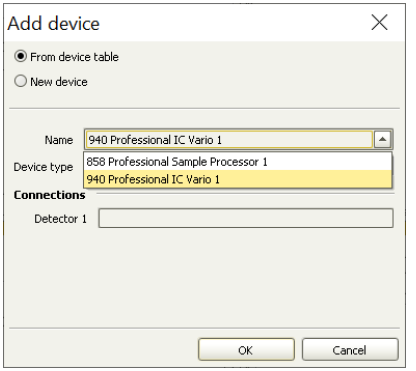
3.2.2 Defining devices and start parameters

Assembling devices

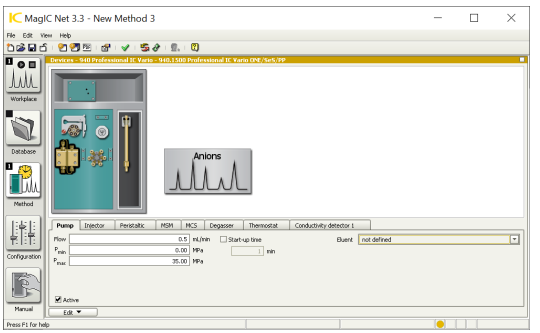
1. In the **Devices** subwindow, click on the menu **Edit ► Add ► Device**.

2. In the **Add device** dialog, select the **From device table** option.

3. Select the **940 Professional IC Vario** device in the **Name** field and click on **[OK]**.



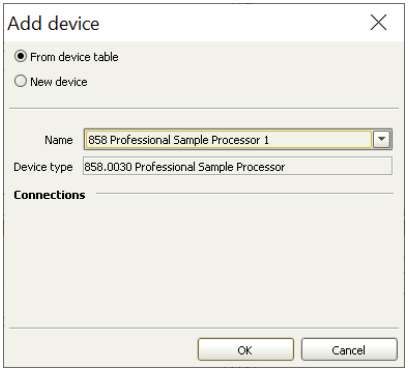
The image of the **940 Professional IC Vario** appears in the upper part of the **Devices** subwindow.



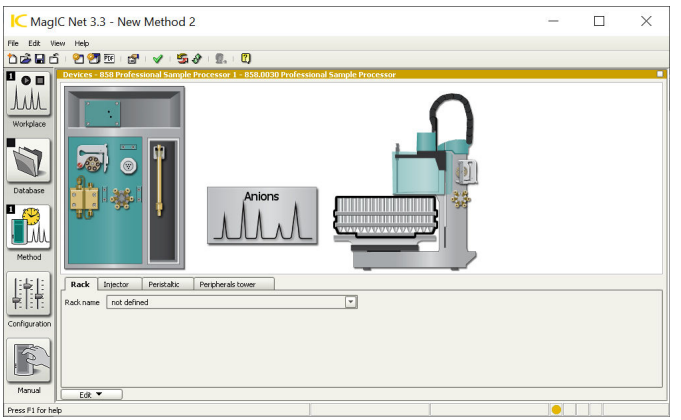
4 In the **Devices** subwindow, click on the menu **Edit ► Add ► Device**.

5 In the **Add device** dialog, select the **From device table** option.

6 Select the **858 Professional Sample Processor** device in the **Name** field and click on **[OK]**.



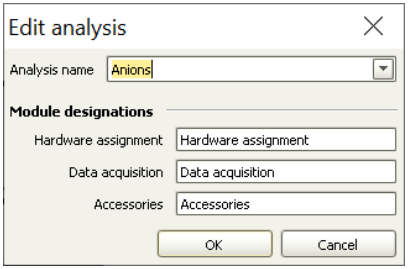
The image of the **858 Professional Sample Processor** appears in the upper part of the **Devices** subwindow.



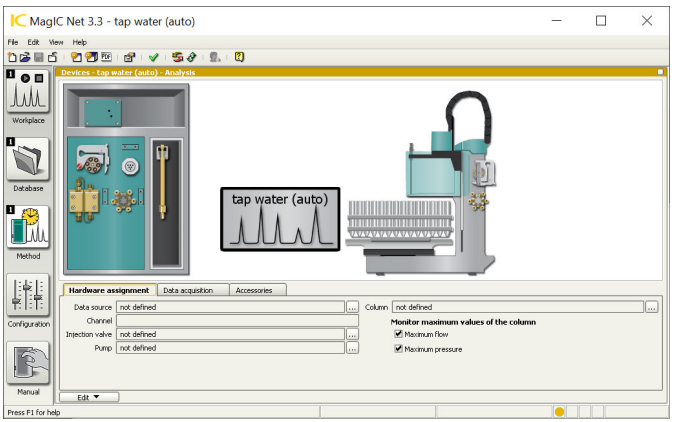
Changing the analysis name (optional)

1 Click on the icon of the **Anions** analysis in the upper part of the **Devices** subwindow.

2 Open the **Edit analysis** dialog using the **Edit ► Edit** menu.



3 In the **Analysis name** field, enter the new name **Tap water (auto)** and confirm with **[OK]**.



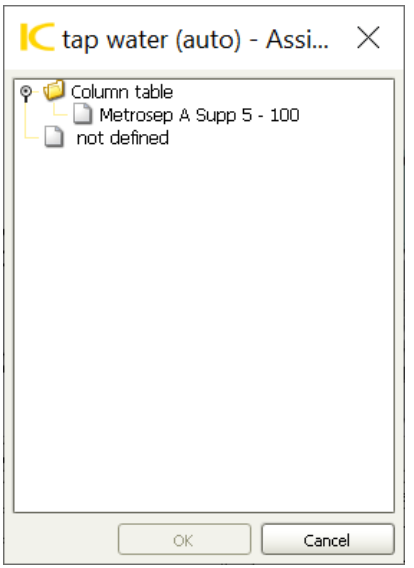
Defining the parameters for the analysis

1 Click on the **Tap water (auto)** icon.

2 **Editing the Hardware assignment tab**

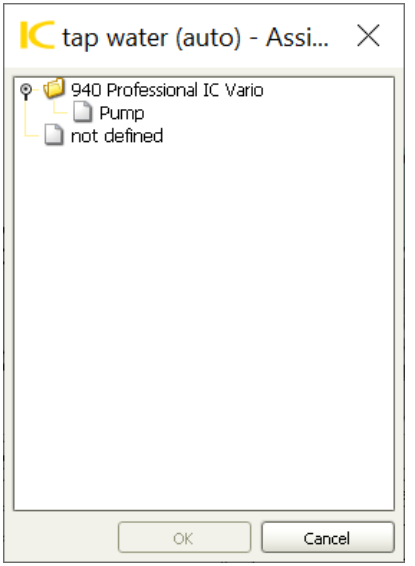
- Select the **Hardware assignment** tab.
- In the **Data source** field, click on the ... button.

- In the **Tap water (auto) - Assign data source** dialog under **940 Professional IC Vario ▶ Conductivity detector 1**, highlight the entry **Conductivity** and click on **[OK]**.
- In the **Channel** field, **Conductivity** is entered automatically.
- Click on the ... button in the **Injection valve** field.
- In the **Tap water (auto) - Assign injection valve** dialog under **940 Professional IC Vario**, highlight the entry **Injector** and click on **[OK]**.
- Click on the ... button in the **Column** field.
- In the **Tap water (auto) - Assign column** dialog under **Column table**, highlight the entry of **Metrosep A Supp 5 - 100** and click on **[OK]**.

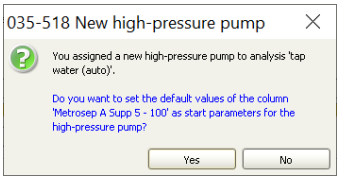


- Click on the ... button in the **Pump** field.

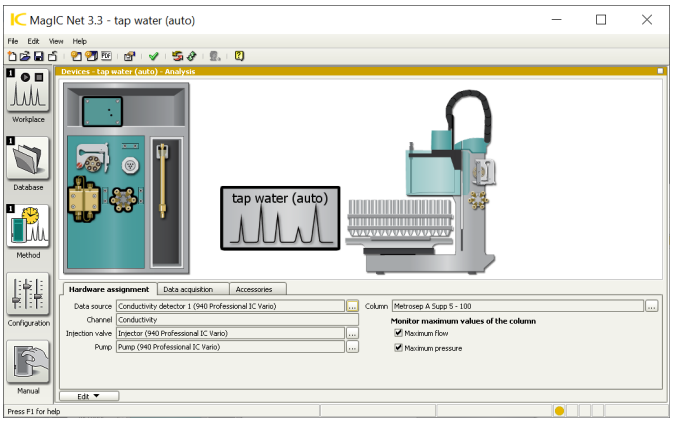
- In the **Tap water (auto) - Assign pump** dialog under **940 Professional IC Vario**, highlight the entry **Pump** and click on **[OK]**.



- Confirm the message **New high-pressure pump** with **[Yes]**.



The default parameters of the column are applied to the start parameters of the pump.
The **Hardware assignment** tab looks as follows:



3 Editing the Data acquisition tab

- Select the **Data acquisition** tab.
- In the **Recording time** field, enter a time of **15 min**.

4 Editing the Accessories tab

- Select the **Accessories** tab.
- Click on the **[Add]** button.
- In the selection list of the **Add accessory** dialog, select the H_2SO_4 pump tubing.
- Click on **[OK]**.

The pump tubing is entered in the accessories table.

The pump tubing connection can be added in the same way *(see chapter 2.6, page 18)*.

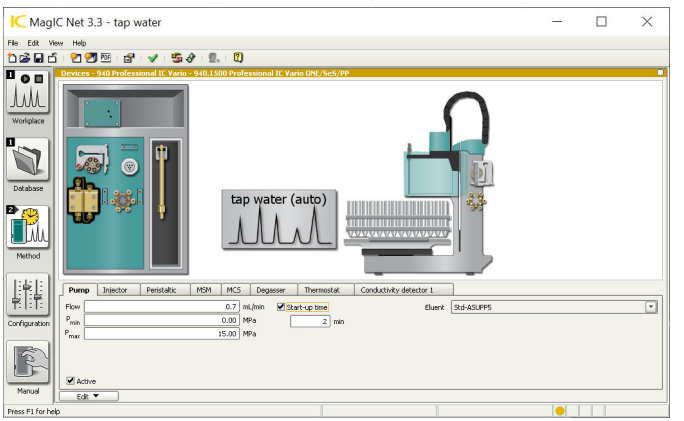
Defining the parameters for the IC device

1 Click on the image of the **940 Professional IC Vario**.

The tabs of the **940 Professional IC Vario** modules appear and can be edited.

2 **Editing the Pump tab**

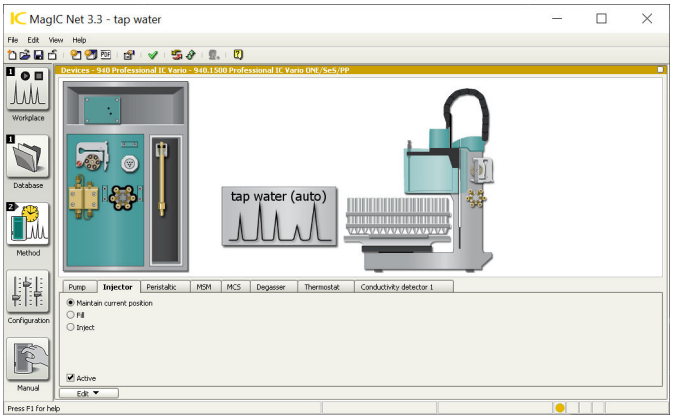
- Select the **Pump** tab (or click on the symbol of the pump).
- The values of the fields **Flow**, **P_{min}**, **P_{max}** and **Start-up time** are read automatically.
- Use the **Eluent** selection list to select the previously defined eluent **Std-ASUPP5**.



3 **Editing the Injector tab**

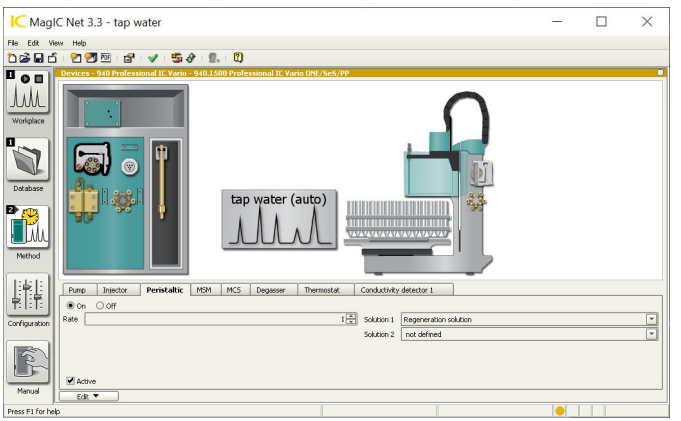
- Select the **Injector** tab (or click on the symbol of the injector).

- Accept the default settings.



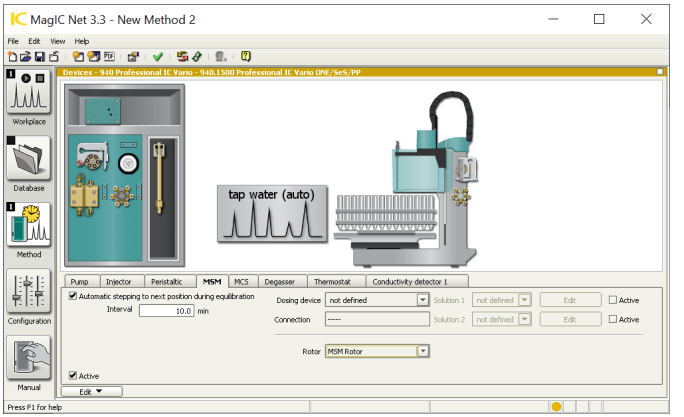
4 Editing the Peristaltic tab

- Select the **Peristaltic** tab (or click on the symbol of the peristaltic pump).
- Activate the **On** option.
- In the **Rate** field, enter the value **1**.
  (There are 7 speed levels, with 6 revolutions/min per level.)
- In the selection list **Solution 1**, select the solution **MSM regeneration solution H_2SO_4**.



5 Editing the MSM tab

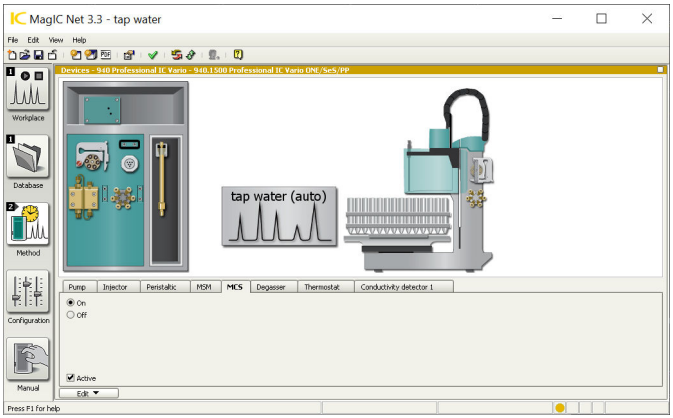
- Select the **MSM** tab (or click on the symbol of the MSM).
- Accept the default settings. The check box for Dosino regeneration can be deactivated if the suppressor is regenerated using a peristaltic pump.



6 Editing the MCS tab

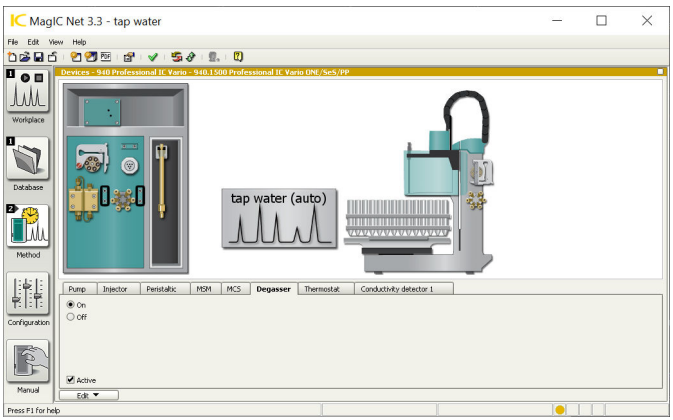
- Select the **MCS** tab (or click on the symbol of the MCS).

- Accept the default settings.



7 Editing the Degasser tab

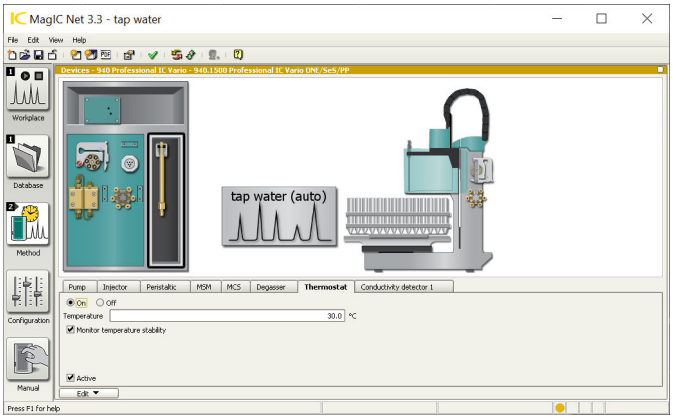
- Select the **Degasser** tab (or click on the symbol of the degasser).
- Accept the default settings.



8 Editing the Thermostat tab

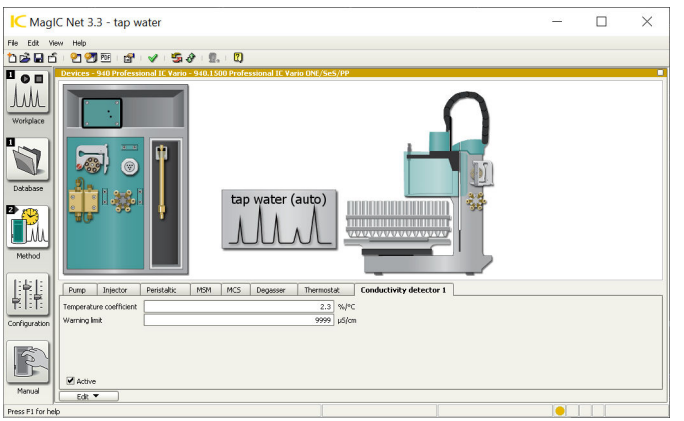
- Select the **Thermostat** tab (or click on the symbol of the column thermostat).

- Switch on the thermostat and deactivate the **Monitor temperature stability** check box.



9 Editing the Conductivity detector 1 tab

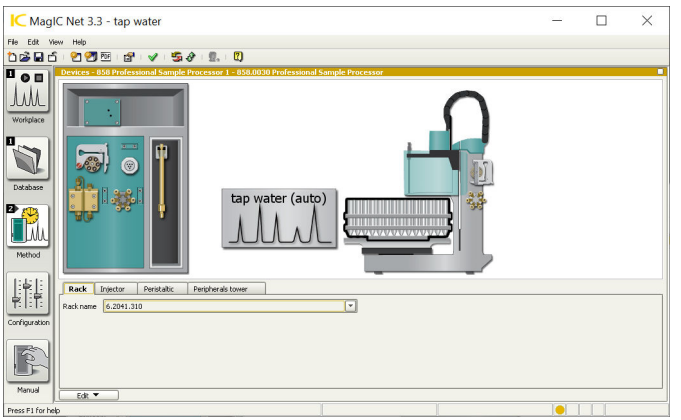
- Select the **Conductivity detector 1** tab (or click on the symbol of the conductivity detector).
- Accept the default settings.



Defining the parameters for the Sample Processor

1 Editing the Rack tab

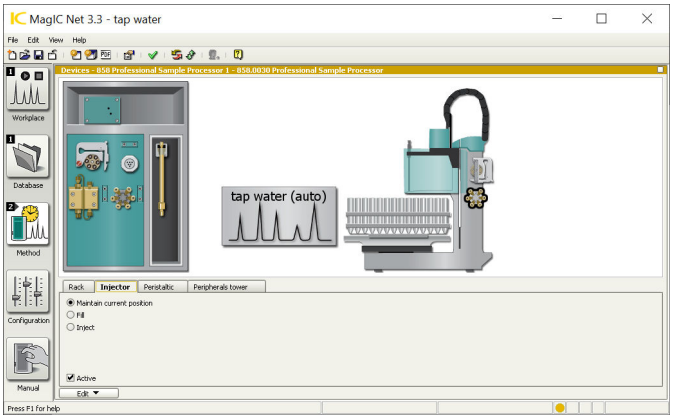
- Select the **Rack** tab.
- Select the number of the rack in the **Rack name** selection list.



2 Editing the Injector tab

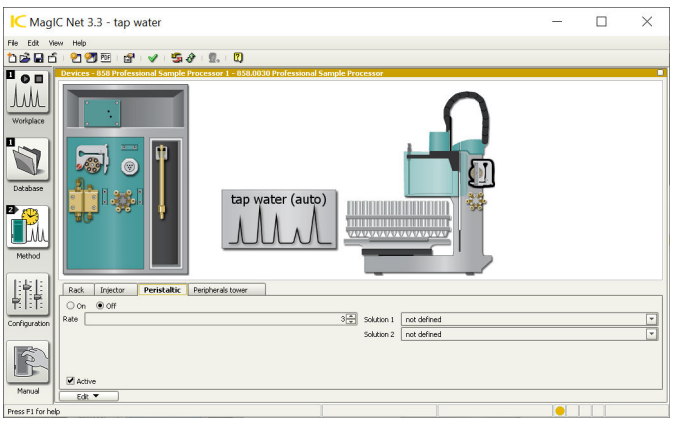
- Select the **Injector** tab.

- Deactivate the injector.



3 Editing the Peristaltic tab

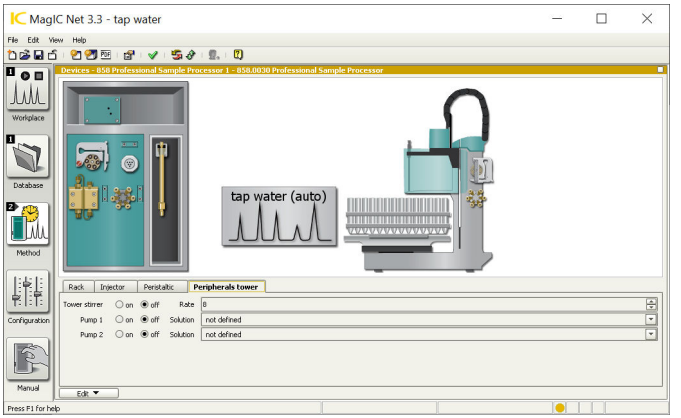
- Select the **Peristaltic** tab.
- Enable the **Off** radio button.



4 Editing the Peripherals tower tab

- Select the **Peripherals tower** tab.

The settings are applied because no other instruments are used.



3.2.3 Time program

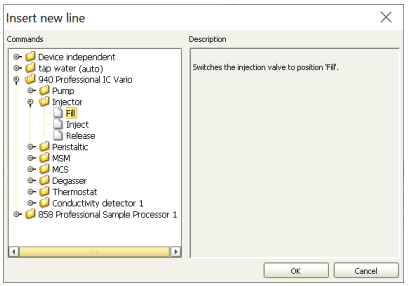
The time program is part of every method. It is a step by step description of how a sample is processed. The time program is created in the **Time program** subwindow of the **Method** program part. In contrast to a manual method, the time program for an automated process of determinations contains additional commands for the Sample Processor.

Defining the time program

1 Setting the injection valve to Fill

- Open the **Insert new line** dialog via the **Edit ► New** menu.

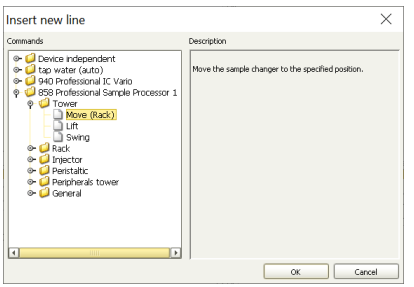
- Select **940 Professional IC Vario ► Injector ► Fill** in the left part of the window under Commands.



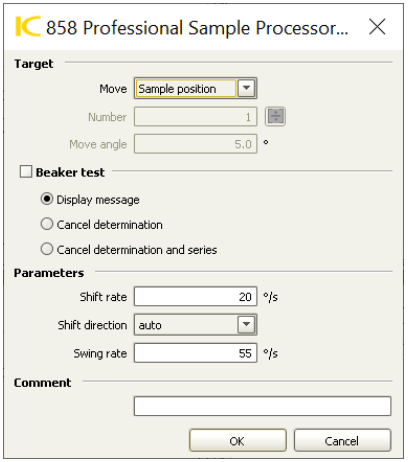
- Confirm with **[OK]**.
  The **940 Professional IC Vario - Injector - Fill** dialog is opened.
- Accept the time entry **0** min.
- Confirm with **[OK]**.

2 Moving to a sample position

- Highlight the bottom row of the time program. Open the **Insert new line** dialog via the **Edit ► New** menu.
- Select **858 Professional Sample Processor ► Tower ► Move (Rack)** in the left part of the window under Commands.



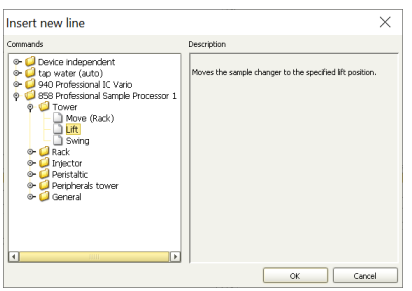
- Confirm with **[OK]**.
  The **858 Professional Sample Processor - Tower - Move (Rack)** dialog is opened.



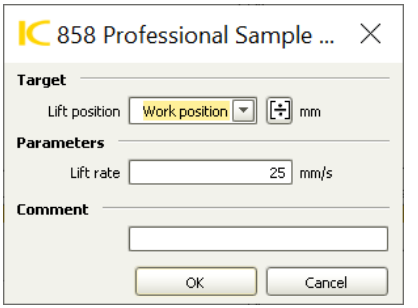
- Accept the values in the fields.
- Confirm with **[OK]**.

3 Immersing the aspiration needle into the sample

- Highlight the bottom row of the time program. Open the **Insert new line** dialog via the **Edit ▶ New** menu.
- Select **858 Professional Sample Processor ▶ Tower ▶ Lift** in the left part of the window under Commands.



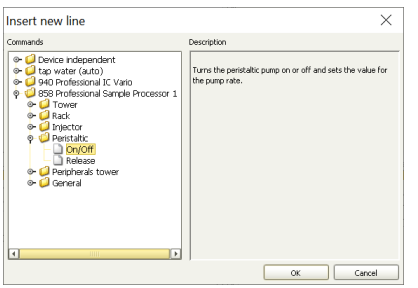
- Confirm with **[OK]**.
  The **858 Professional Sample Processor - Tower - Lift** dialog is opened.
- Select the **Work position** entry in the **Lift position** selection list.



- Confirm with **[OK]**.

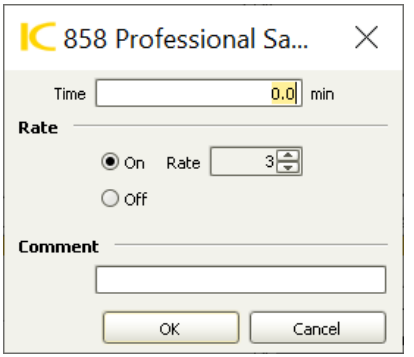
4 Filling the injection valve with sample

- Open the **Insert new line** dialog via the **Edit ▶ New** menu.
- Select **858 Professional Sample Processor ▶ Peristaltic ▶ On/Off** in the left part of the window under Commands.



- Confirm with **[OK]**.
  The **858 Professional Sample Processor - Peristaltic - On/Off** dialog is opened.
- Accept the time entry **0** min in the **Time** field.

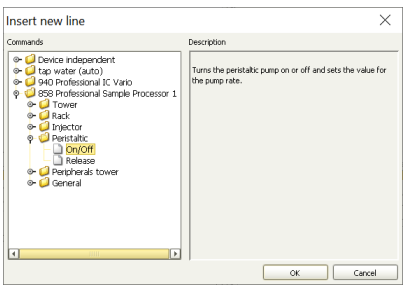
- Accept the values in the other fields, too.



- Confirm with **[OK]**.

5 Deactivating the peristaltic pump of the Sample Processor

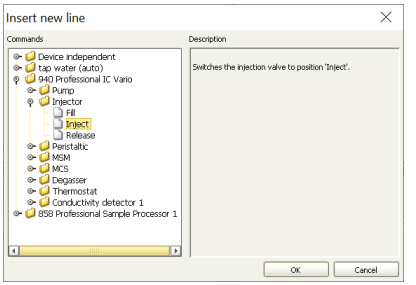
- Open the **Insert new line** dialog via the **Edit ► New** menu.
- Select **858 Professional Sample Processor ► Peristaltic ► On/Off** in the left part of the window under Commands.



- Confirm with **[OK]**.
  The **858 Professional Sample Processor - Peristaltic - On/Off** dialog is opened.
- Enter the time entry **2.5** in the **Time** field.
- Select the option **Off** in the **Rate** area.
- Confirm with **[OK]**.

6 Setting the injection valve to Inject

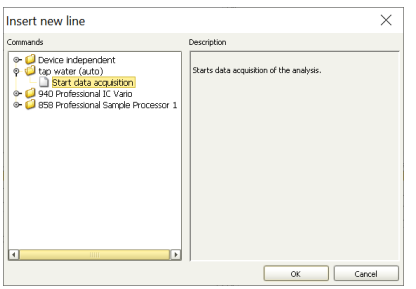
- Open the **Insert new line** dialog via the **Edit ▶ New** menu.
- Select **940 Professional IC Vario ▶ Injector ▶ Inject** in the left part of the window under Commands.



- Confirm with **[OK]**.
  The **940 Professional IC Vario - Injector - Inject** dialog is opened.
- Enter the value **2.5** in the **Time** field.
- Confirm with **[OK]**.

7 Starting the data acquisition

- Highlight the bottom row of the time program. Open the **Insert new line** dialog via the **Edit ▶ New** menu.
- Select **tap water (auto) ▶ Start data acquisition** in the left part of the window under Commands.

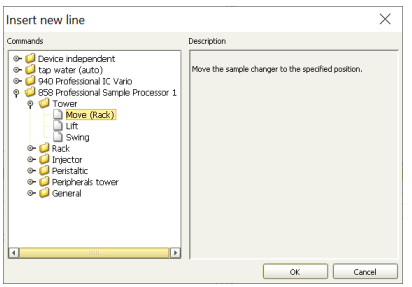


- Confirm with **[OK]**.
  The **Tap water (auto) - Start data acquisition** dialog opens.
- Enter the value **2.5** in the **Time** field.
- Confirm with **[OK]**.

8 Moving to the position of the special beaker

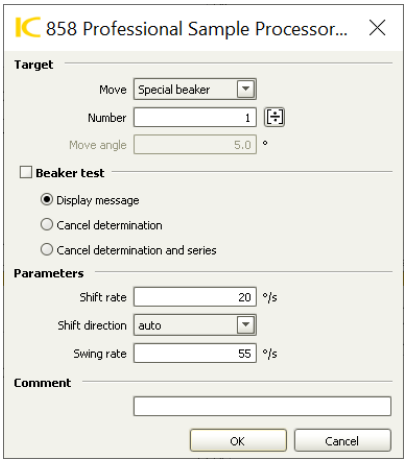
Special beakers have a large volume (e.g. 250 mL) and usually contain the rinsing solution. It is preferable to set these beakers at high rack positions in order to be able to begin sample series at position 1. The lift positions have to be assigned to the special beakers separately.

- Open the **Insert new line** dialog via the **Edit ► New** menu.
- Select **858 Professional Sample Processor ► Tower ► Move (Rack)** in the left part of the window under Commands.



- Confirm with **[OK]**.
  The **858 Professional Sample Processor - Tower - Move (Rack)** dialog is opened.

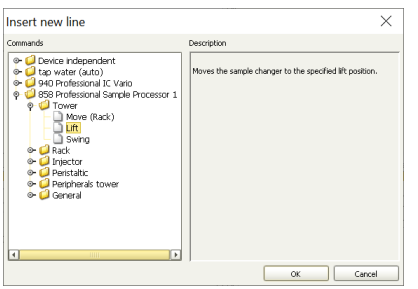
- Select the **Special beaker** entry in the **Move** selection list and enter the value **1** in the **Number** field.



- Confirm with **[OK]**.

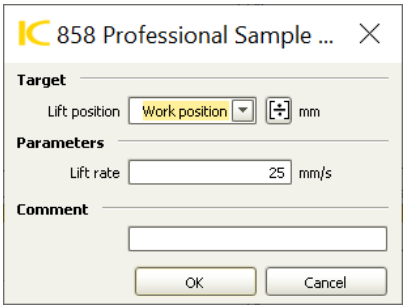
9 Immersing the aspiration needle into the special beaker

- Open the **Insert new line** dialog via the **Edit ▶ New** menu.
- Select **858 Professional Sample Processor ▶ Tower ▶ Lift** in the left part of the window under Commands.



- Confirm with **[OK]**.
  The **858 Professional Sample Processor - Tower - Lift** dialog is opened.

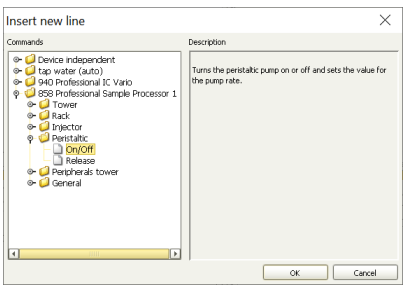
- Select the **Work position** entry in the **Lift position** selection list.



- Confirm with **[OK]**.

10 Switching on Rinse

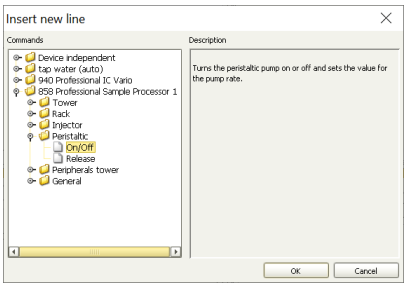
- Open the **Insert new line** dialog via the **Edit ▶ New** menu.
- Select **858 Professional Sample Processor ▶ Peristaltic ▶ On/Off** in the left part of the window under Commands.



- Confirm with **[OK]**.
  The **858 Professional Sample Processor - Peristaltic - On/Off** dialog is opened.
- Accept the time entry **0** min in the **Time** field.
- Accept the values in the other fields, too.
- Confirm with **[OK]**.

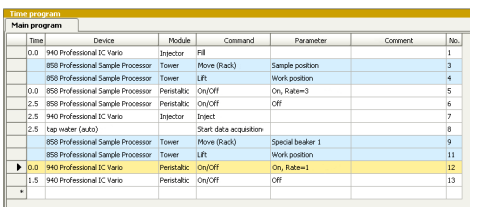
11 Switching off Rinse

- Open the **Insert new line** dialog via the **Edit ▶ New** menu.
- Select **858 Professional Sample Processor ▶ Peristaltic ▶ On/Off** in the left part of the window under Commands.



- Confirm with **[OK]**.
  The **858 Professional Sample Processor - Peristaltic - On/Off** dialog is opened.
- Enter the value **1.5** in the **Time** field.
- Select the option **Off** in the **Rate** area.
- Confirm with **[OK]**.

The complete time program looks as follows:



Time program

Main program

Time	Device	Module	Command	Parameter	Comment	No.
0.0	940 Professional IC Vario	Injector	Fill			1
	858 Professional Sample Processor	Tower	Move (Rack)	Sample position		3
	858 Professional Sample Processor	Tower	Lift	Work position		4
0.0	858 Professional Sample Processor	Peristaltic	On/Off	On, Rate=3		5
2.5	858 Professional Sample Processor	Peristaltic	On/Off	Off		6
2.5	940 Professional IC Vario	Injector	Inject			7
2.5	tap water (auto)		Start data acquisition			8
	858 Professional Sample Processor	Tower	Move (Rack)	Special beaker 1		9
	858 Professional Sample Processor	Tower	Lift	Work position		11
0.0	940 Professional IC Vario	Peristaltic	On/Off	On, Rate=1		12
1.5	940 Professional IC Vario	Peristaltic	On/Off	Off		13

3.2.4 Evaluation

(see chapter 3.1.4, page 40)

3.2.5 Saving a method

Saving a method

After having entered all relevant parameters for the method, save the method as follows:

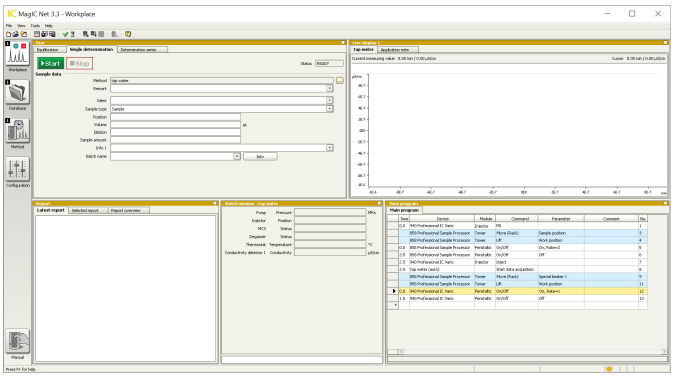
1. Open the **Save method** dialog using the **File ▶ Save as…** menu.
2. Enter the name **Tap water (auto)** for the method in the **Method name** field.
3. Click on **[Save]**.

4 Carrying out the determination

In this section you will learn how to:

- check the retention times of analytes
- enter sample data
- measure standards and samples.

These steps are performed in the **Workplace** program part. The following subwindows are available:



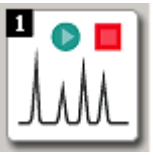
Run	Controlling runs and managing the sample data
Live display 1	Display of the chromatogram during the analysis
Report	Display of the reports of analyses
Watch window	Information on the method and the associated instruments
Time program	Visualization of the run of the method
Live display 2	Display of a second chromatogram that runs in parallel

The subwindows to be displayed can be determined with the icon or via the **View ► Change layout...** menu item.

4.1 Equilibration

Starting the equilibration

Before the analysis is carried out, the IC instrument has to be equilibrated for about 30 minutes until the baseline is stable.



1. Switch to the **Workplace** program part.

2. Select the **Equilibration** tab in the **Run** subwindow.

3. Click on the ... button in the **Method** field.

4. Highlight the method **Tap water** or **Tap water (auto)** in the **Open method** dialog.

   If several method groups already exist, the group to which the method was saved must first be selected in the **Method group** list box.

5. Click on **[Start HW]**.

The recording of the baseline starts. Once the baseline is stable, the measurement can be started (after about 30 minutes).

4.2 Manually adjusting retention times

To check and edit the retention times for the 7 components fluoride, chloride, nitrite, bromide, nitrate, phosphate und sulfate which are stored in the method, the mean standard is measured in a single measurement.

Single measurement of a standard

1. Switch to the **Workplace** program part.

2. In the **Run** subwindow, select the **Single determination** tab.

3. Select the method **Tap water** or **Tap water (auto)** in the **Open method** field.

4. Select **Standard 2** in the **Sample type** selection list.

5. **Entering sample data**

   Enter the following values in the fields:

   - In the **Ident** field the name **Standard 2**.
   - In the **Position** field the value **1**.
   - In the **Volume** field the value **20**.
   - In the **Dilution** field the value **1**.
   - In the **Sample amount** field the value **1**.
   - In the **Batch name** field, select the batch **Batch 1**.

6. Click the **[Start]** button.

   The determination is started and the time program is worked through.

7 If a method with manual injection is used:

- Fill the injector manually as soon as the fill message appears.
- Confirm the message with **[Continue]**.

Correction of the retention times

Compare the retention times from the chromatogram with the times in the method template. If there are discrepancies, enter the new retention times from the chromatogram in the component table. There are 2 options to do this:

- Adjust the retention times in the **Method** program part. This approach is described in the following steps.
- Adjust the retention times in the **Workplace** program part under **Live display ► Analysis name ► Evaluation parameters ► Live modifications - Evaluation** (see *MagIC Net online help - Live display - Adjusting evaluation parameters*).

1 Change to the **Method** program part.

2 Click on the **Edit ► Update** menu.

3 In the **Evaluation** subwindow, click on the **[Components]** button and select the **Component table** tab.

4 Click on the row with the component of which the retention time is to be corrected.

5 Drag the blue line to the relevant peak in the **Chromatograms** subwindow.

6 In the **Evaluation** subwindow, click on the **[Update retention time]** button.

The retention time from the chromatogram is transferred to the component table.

7 Repeat steps **4** to **6** for all the components that need adjusting.

8 Save the method via the **File ► Save...** menu item or by clicking on the icon.

4.3 Measuring standards and samples manually

Standards

1 Switch to the **Workplace** program part.

2 In the **Run** subwindow, select the **Single determination** tab.

3 Check that the **Tap water** method is selected in the **Method** field.

4 Select **Standard 1** in the **Sample type** selection list.

5 **Entering sample data**

Enter the following values in the fields:

- In the **Ident** field the name **Standard 1**.
- In the **Position** field the value **1**.
- In the **Volume** field the value **20**.

- In the **Dilution** field the value **1**.
- In the **Sample amount** field the value **1**.
- In the **Batch name** field the batch **Batch 1**.

6 Click the **[Start]** button.

The determination is started and the time program is worked through.

Rows highlighted in red show the current program step, rows in gray show the completed program steps.

7 If a method with manual injection is used:

- Fill the injector manually with a syringe as soon as the fill message appears.
- Confirm the message with **[Continue]**.

The data acquisition is started and the determination runs until the end.

Steps **4** to **7** are repeated for the measurement of standard 2 and standard 3. Select **Standard 2** or **Standard 3** in the **Sample type** selection list and enter the name **Standard 2** or **Standard 3** in the **Ident** field.

The recording of the current chromatogram can be viewed in the **Live display** subwindow.

Information on the method and the associated instruments are displayed in the **Watch window** subwindow. This display can be personalized. To do so, right-click in the **Watch window**. Select the **Properties Watch window** menu item. Personalize the display according to your preferences and confirm the settings with **[OK]**.

Sample

1 Select the **Sample** entry in the **Sample type** selection list.

2 **Entering sample data**

Enter the following values in the fields:

- In the **Ident** field, enter the name **Tap water**.
- In the **Position** field the value **1**.
- In the **Volume** field the value **20**.
- In the **Dilution** field the value **1**.
- In the **Batch name** field, select the batch **Batch 1**.

3 Click the **[Start]** button.

The determination is started and the time program is worked through.

4 If a method with manual injection is used:

- Fill the injector manually with tap water as soon as the fill message appears.
- Confirm the message with **[Continue]**.

5 After measuring all the samples and standards, switch off the instrument. To do so, select the **Equilibration** tab and click on **[Stop HW]**.

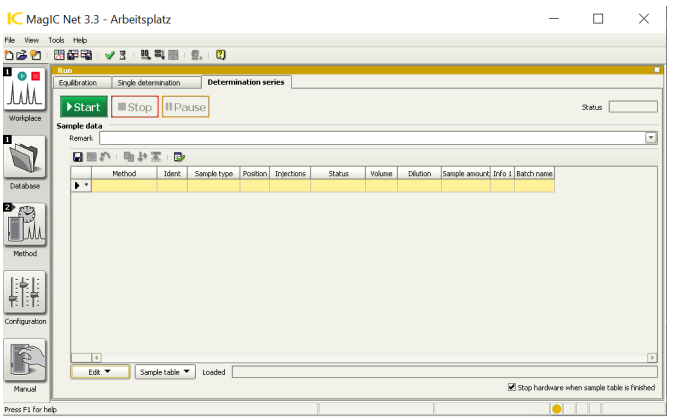
4.4 Measuring standards and samples automatically

Like with a manual measurement, the IC instrument is first equilibrated *(see chapter 4.1, page 73)* and the retention times are adjusted *(see chapter 4.2, page 74)*. Then the sample table is created and the standards and the sample are measured.

Creating a sample table

1 Switch to the **Workplace** program part.

2 In the **Run** subwindow, select the **Determination series** tab.



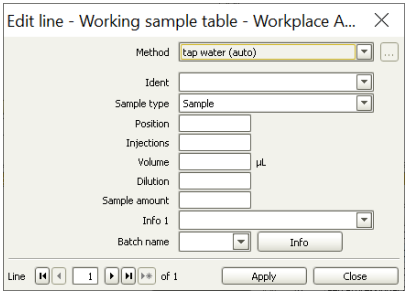
3 Open the **Edit line - Workplace sample table** dialog using the **Edit ▶ Edit line** menu.

4 Click on the [...] button in the **Method** field.

Highlight the method name **Tap water (auto)** in the table and click on **[Open]**.

If several method groups already exist, the group to which the method belongs must first be selected in the **Method group** list box.

Tap water (auto) is automatically entered in the **Method** field.



5 Entering values for standard 1

Enter the following values in the fields:

- In the **Ident** field the name **Standard 1**.
- Select **Standard 1** in the **Sample type** selection list.
- In the **Position** field the value **1**.
- In the **Injections** field the value **1**.
- In the **Volume** field the value **20**.
- In the **Dilution** field the value **1**.
- In the **Batch name** field the batch **Batch 1**.
- Click on **[Apply]**.

The values are written into the first line of the sample table.

6 Entering values for standard 2

- Click on the ▸ button in the **Line** field.

The next higher value is automatically entered in the **Position** field. The values for standard 1 are also automatically applied in the fields **Injection**, **Volume**, **Dilution**, **Sample amount** and **Batch name**.

- In the **Ident** field, enter the name **Standard 2**.
- Select **Standard 2** in the **Sample type** selection list.
- Click on **[Apply]**.

7 Entering values for standard 3

Follow step **6** as described above to enter standard 3:

- In the **Ident** field, enter the name **Standard 3**.
- Select **Standard 3** in the **Sample type** selection list.
- Click on **[Apply]**.

8 Entering the values for the sample

Follow step **6** as described above to enter the sample data:

- In the **Ident** field, enter the name **Tap water**.
- Select the **Sample** entry in the **Sample type** selection list.
- Click on **[Apply]**.
- Once all the data for the standards and the sample are entered, click on the **[Close]** button and return to the **Determination series** tab.

9 Stopping the hardware

- Activate the **Stop hardware when sample table is finished** check box.

NOTICE

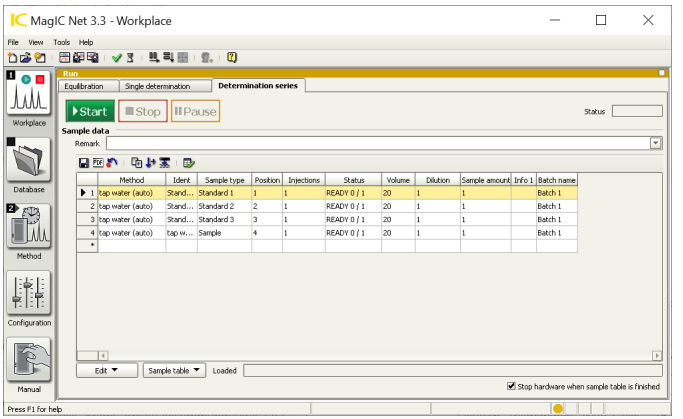
The **Stop hardware when sample table is finished** check box must be activated if the instruments are to be automatically switched off after the measurements are completed (e.g. if measurements take place over night).

10 Saving the sample table

- Open the **Save sample table** dialog using the **Sample table ► Save as...** menu.
- In the **Name** field, enter the name **Tap water sample**.

- Click on **[Save]**.

The complete table with standards and sample looks as follows:



11 **Checking the determination series**

- Carry out the **run test** for the method with the **Tools ▶ Run test** menu item or the icon. This checks the sample table as well as the necessary hardware.
  Alternatively, in case only the sample data was adjusted, the sample table test can be carried out with the **[Sample table] ▶ Sample table test...** menu item or the icon. This only checks if all the sample data is correct.

Measuring standards and samples

1 Fill the samples in sample vials and place them on the rack according to the sample table that you created. Fill the rinsing beaker with ultrapure water and place it on the rack.

2 Click on the **[Start]** button on the **Determination series** tab.

First, the chromatograms of the 3 standards are measured and then the chromatogram of the sample. The recording of a chromatogram can be viewed in the **Live display** subwindow.

The current rack position and various IC parameters such as conductivity, pressure, flow, degasser are displayed in the **Watch window** subwindow. This display can be personalized. To do so, right-click in the **Watch window**. Select the **Properties Watch window** menu item. Personalize the display according to your preferences and confirm the settings with **[OK]**.

Samples that are being processed at the time are highlighted in red, completed samples are gray.

5 Actions in the database

The **Database** program part contains the following subwindows:

- **Determination overview**
  Determinations are displayed in the **Determination overview** subwindow where they can also be viewed.
- **Results**
  A table with the components and their concentrations, retention times etc. is displayed in the **Results** subwindow.
- **Curves 1 - 5**
  In the **Curves 1 - 5** subwindows, either the chromatogram and the calibration curve, the flow or the pressure are displayed.
- The **Information** subwindow is used to display data on the sample, the instruments etc. in their respective tabs.

5.1 Viewing determinations

You have multiple options for selecting and viewing your determinations:

- Sorting according to column
- Finding via a quick filter
- Finding with a special filter
- Via the **Search** menu
- Select via a batch (user-defined filter)

Sorting

1 Click on the icon for the **Database** program part.

2 Open the database in which your data is saved.

3 First click in the table with all the data sets on the column heading according to which the table is to be sorted.

The table is sorted according to the selected column in ascending order.

4 Click again on the same column title.

The table is sorted according to the selected column in descending order.

Quick filter

1 Click on the icon or use the **Determinations ► Filter ► Quick filter** menu.

The cursor turns into a special filter symbol. When navigating within the table, the cells in which the cursor is located will have a yellow background.

2 Place the cursor in a cell that is to serve as a filter criterion and double-click with the left mouse button.

The data sets are filtered according to the content of the selected table field. The quick filter can be applied again within the filtered table.

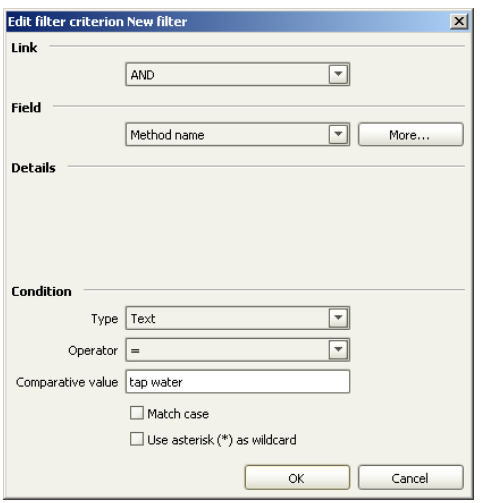
3 To remove the filter, use the **Determinations ▶ Filter ▶ Remove filter** menu or click on the icon.

Special filter

The special filter allows you to specify the filter conditions in detail.

1 Open the corresponding dialog using the **Determinations ▶ Filter ▶ Special filter** menu.

2 Use the **Edit ▶ Edit line** menu to open the **Edit 'New filter' filter criterion** dialog.



3 Click on the **[More...]** button in the **Field** section and select the **Method name** entry under the **Method ► Identification** dialog.

4 Enter the method name **Tap water** in the **Comparative value** field and click on **[OK]**.

5 In the **Special filter** dialog, click on the **[Use filter]** button and close the window.

A table containing all of the data sets for the **Tap water** method appears in the **Determination overview** subwindow.

The data of a highlighted data set appears in the other subwindows.

Searching

This function enables you to search for determinations with a specific user.

1 Open the **Search - Database 'MagIC Net'** dialog using the **Determinations ► Search** menu.

2 Click on the **[More...]** button in the **Search in** section and select the **User (short name)** entry under the **Determination ► Recording** dialog.

3 Enter your short name in the **Search term** field.

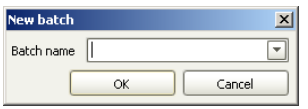
4 Click on **[Search next]**.

The first line corresponding to the search term is highlighted.

Batch (user-defined filter)

1 Creating a new batch

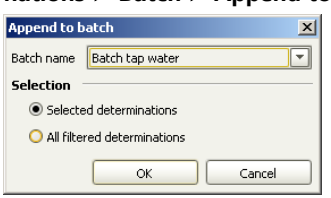
- Open the **New Batch** dialog via the **Determinations ▶ Batch ▶ New batch** menu.



- Enter the name **Anions** in the **Batch name** field.
- Click on **[OK]**.

2 Adding determinations to batch

- Highlight the data sets in the table which are to be added to the batch.
- Open the **Append to batch** dialog via the **Determinations ▶ Batch ▶ Append to batch** menu.



- Select the name **Batch tap water** in the **Batch name** list box.
  Data sets can also be added to a batch that was created in the **Workplace**. To do this, select the name of the corresponding batch in the **Batch name** list box.
- Enable the **Selected determinations** option.
- Click on **[OK]**.

The data sets selected in the determination overview are added to the batch and can be selected again at any given time.

A maximum of 500 data sets can be added to a batch.

3 Opening a batch

Select the required batch in the **Batch** selection window in the **Determination overview** subwindow.

All the data sets that were appended to the batch are displayed.

4 Deleting a batch

- Open the **Delete batch** dialog via the **Determinations ► Batch ► Delete batch** menu.

- Select the name **Batch tap water** in the **Batch name** list box.
- Click on **[OK]**.

The batch is deleted from the database.

5 Deleting the applied filters

Special filters or quick filters that are currently used and a selected batch can be removed via the **Determinations ► Filter ► Remove filter** menu. All data sets are displayed again.

5.2 Viewing results

There are several possibilities to view and display the results, chromatograms and curves. The following options are described in this chapter:

- Displaying **Results**.
- Zooming into areas on the chromatogram with the mouse or via a dialog.
- Changing the display of the chromatograms.
- Displaying the calibration curve.
- Displaying the detail overview for several determinations.
- Overlaying curves.

Displaying the results

Various parameters are displayed in the **Results** subwindow.

1 Click on the required data set in the **Determination overview** subwindow.

The parameters of the selected data set are displayed in the **Results** subwindow.

2 The parameters of the table can be set in the **Properties result window** dialog.

Open the **Properties result window** dialog by double-clicking the field of the result view or via the **View ► Properties ► Results properties** menu.

3 Click on the required parameter in the **Available columns** selection list. Move the selected parameter with the >> key to the list **Displayed columns**.

4 Repeat step 3 for each required parameter.

5 Click on **[OK]** to close the **Result window properties**.

The selected parameters are displayed in the **Results** subwindow.

Zooming into areas on the chromatogram with the mouse

Individual areas of a chromatogram can be displayed in magnified form using the zoom function.

1 Highlight a data set in the overview table.

The associated chromatogram is displayed in the **Curves 1** subwindow.

2 With the left mouse button held down, drag a rectangle over the area that is to be magnified.

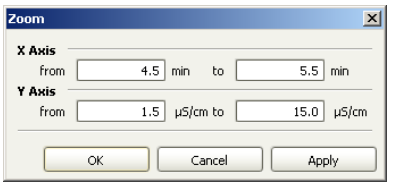
Zooming into areas on the chromatogram via a dialog

1 Highlight a data set in the overview table.

The associated chromatogram is displayed in the **Curves 1** subwindow.

2 Right-click on the chromatogram.

3 Open the **Zoom** dialog for entering the zoom range using the **Zoom** context menu.



4 In the **X Axis** area, enter the value **4.5** in the **from** field and the value **5.5** in the **to** field.

5 Click on **[OK]**.

As an example, the peak of nitrite is displayed in magnified form.

Restoring down selected areas on the chromatogram

1 Right-click on the chromatogram. Click on **Unzoom** in the context menu.

2 Alternatively, the display can be restored by double-clicking into the chromatogram.

The chromatogram is displayed in its original size.

Changing the display of the chromatograms

You have the option to edit the properties of a chromatogram. You can change the display of the chromatogram, the axis labeling or the labeling in the chromatograms. Below you will change

the labeling for the peaks and the axes in the chromatogram. Proceed as follows:

1 Changing the labeling for the peaks

- Right-click on the chromatogram.
- Select the **Properties** menu item.
- Select the **Chromatogram** tab.
- Deactivate the **Retention time** check box and activate the **Concentration** check box.
- Click on **[OK]**.

2 Changing the axis label

- Right-click on the chromatogram.
- Select the **Properties** menu item.
- Select the **Axes** tab in the **Properties - Graphics** dialog.
- Click in the **X Axis** area in the **Axis label** field and enter the **retention time**.
- Click in the **Y Axis** area in the **Axis label** field and enter the **Conductivity**.
- Click on **[OK]**.

Displaying a calibration curve

1 Highlight a data set in the overview table.

2 In **Subwindow Curves 1**, select the **Calibration curve** option.

3 Select the **Nitrite** entry in the **Components** selection list.

The calibration curve of **Nitrite** and the calibration function are displayed.

Displaying details

1. Highlight the required determinations in the **Determination overview** subwindow.

2. Open the **Open detail overview** dialog using the **Determinations ► Detail overview...** menu.

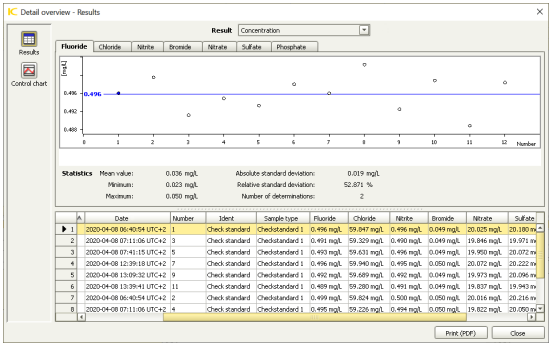
3. Select the **Selected determinations** option.

4. Confirm the selection in the **Open detail overview** dialog with **[OK]**.

   Details about the selected determinations are displayed in the **Detail view - Results** dialog.

5. Select the **Concentration** option in the **Result** selection list. For each component there is a tab. Select the tab for the required component.

   The concentration of the selected component is displayed in a diagram for the required determinations. The concentrations of all the components can be viewed in the list of all the determinations.



6 Create a PDF file of the curve overlay if needed. Click on **[Print (PDF)]** to do so.

The **Print result overview (PDF)** dialog opens.

7 Select the required components and the required format in the **Print result overview (PDF)** dialog.

Close the **Print result overview (PDF)** dialog with **[OK]**.

A PDF file is created.

8 Close the **Detail view - Results** dialog with **[Close]**.

Overlaying curves

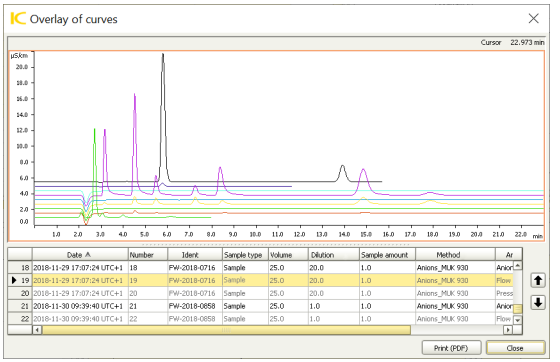
1 Highlight the required determinations in the **Determination overview** subwindow.

2 Open the **Overlay curves** dialog using the **Determinations ▶ Overlay curves...** menu.

3 Select the **Selected determinations** option.

4 Close the **Overlay curves** dialog with **[OK]**.

The **Overlay of curves** dialog displays the curve overlay of the selected determinations.



5 Create a PDF file of the curve overlay if needed. Click on **[Print (PDF)]** to do so.

The **Print curves overview (PDF)** dialog opens.

6 Select the required format in the **Print curves overview (PDF)** dialog.

Close the **Print curves overview (PDF)** dialog with **[OK]**.

A PDF file is created.

7 Close the **Overlay of curves** dialog with **[Close]**.

5.3 Reprocessing determinations

When reprocessing determinations, sample data, evaluation parameters and the curve evaluation can be changed and the results recalculated.

Example 1 describes the evaluation of the peak height instead of the evaluation of the peak area which is defined in the method template.

Example 2 describes the adjustment of the integration parameters.

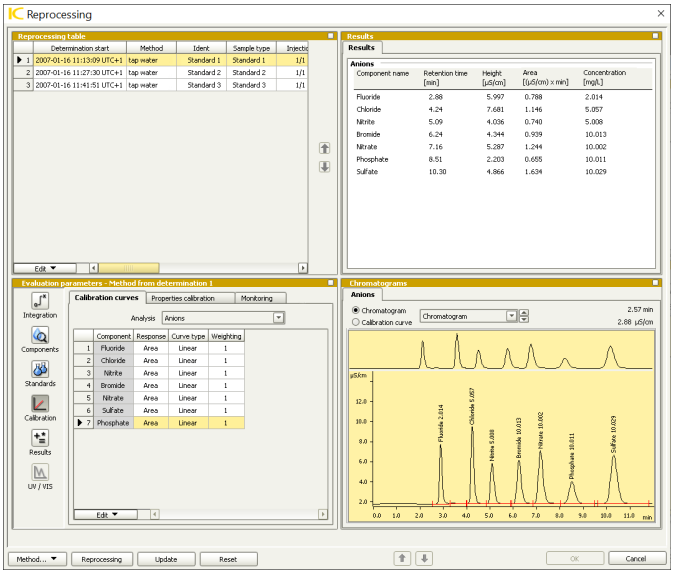
Detail view - Calibration

Example for the adjustment of the calibration.

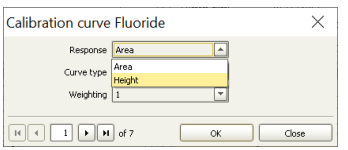
1 Reprocessing the calibration curve

- Highlight the 3 standards in the **Determination overview** subwindow.
- Open the corresponding dialog via the **Determinations ► Reprocess...** menu.
- Click on the **[Calibration]** button in the **Evaluation parameters** subwindow.
- Select the **Calibration curves** tab.

- Highlight the first component (fluoride) in the table.



- Open the **Calibration curve fluoride** dialog using the **Edit ► Edit** menu:

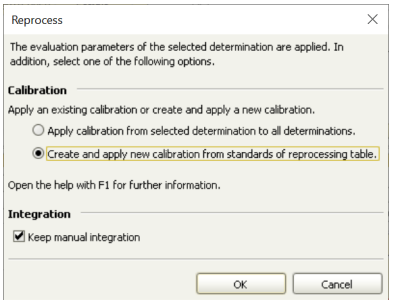


- Select **Height** as a new parameter in the **Response** field and click on **[OK]**.
- Accept the new measured quantity for all the components in the table via the **Edit ► Take over settings for all components** menu.
- Click on **[Update]**.

The calibration curves of the 3 standards are recalculated.

2 Open the **Reprocessing** dialog using the **[Reprocess]** button.

Select the **Create and apply new calibration from standards of reprocessing table.** option.



During the reprocessing new calibrations are created from the standards. To do this, the evaluation parameters of the highlighted determination are used. The reprocessing table is run through from top to bottom.

3 Close the **Reprocessing** dialog with **[OK]**.

The modified data is saved.

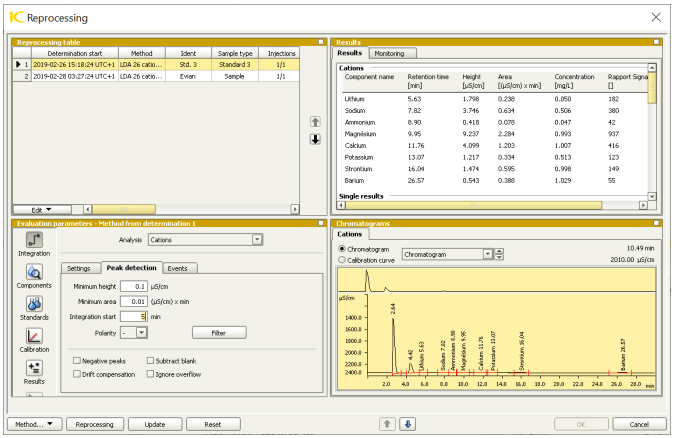
Detail view - Integration

Example for the adjustment of the integration parameters.

1 **Reprocessing the integration parameters**

- Highlight standard 3 and a sample in the **Determination overview** subwindow.
- Open the corresponding dialog via the **Determinations ► Reprocess...** menu.
- Click on the **[Integration]** button in the **Evaluation parameters** subwindow.
- Select the **Peak detection** tab.

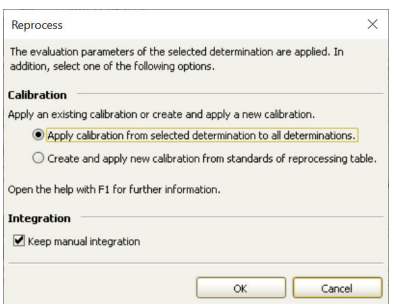
- The injection peak is not of interest. Therefore, set the **Integration start** to **5** min.



The peak data of the standard is recalculated. Click on **[Update]** to view the effects that the adjusted integration start has.

2 Open the **Reprocessing** dialog using the **[Reprocess]** button.

Select the **Apply calibration from selected determination to all determinations.** option.



The calibration (standard chromatograms, calibration points and calibration curves) of the highlighted determination is

used during reprocessing for the calibration of all determinations in the table.

3 Check in the updated sample chromatogram if the change of the integration time is correct.

4 Close the **Reprocessing** dialog with **[OK]**.

The modified data is saved.

5.4 Creating a report template

To create a report with the analysis results, you can adjust an existing report template or define a new report template.

Below you adjust an existing report template with a calibration curve. In addition, you create a new report template with a result table and the chromatogram of the tap water sample.

Adjusting the report template for the calibration curve

1
- Open the **Open report template** dialog using the **Tools ► Report template ► Open...** menu.
- Highlight the **Result and Calibration** report template.
- Click on **[Open]**.
- Click on the ▸ button to change to page 2.
- Open the **Properties - Calibration curve field** dialog by double-clicking on the **Calibration curve** field.

If the properties are not changed, the calibration curves of all the components in the report are displayed. To display individual calibration curves in the report, e.g. only of nitrate, continue with step 2.

2

- Enter the component **Nitrate** (as an example) in the **Component** list box.
- In the **Curve display** area of the **Properties - Calibration curve field** dialog, select the **from database** option.
- Click on **[OK]**.
- Open the **Report preview** window using the **File ► Page preview** menu. The **Report preview** window shows a preview of the report with the selected data.

3

- If all the properties displayed in the **Report preview** window are correct, open the **Save report template** dialog via the **File ► Save as...** menu.
- In the **Save report template** dialog, enter the name **Calibration curve** in the **Name** field.
- Click on **[Save]**.

Creating a new report template for a result table/ chromatogram

1 **Creating a result table**

- Open the **Report template - New form report** dialog via the **Tools ► Report template ► New ► Form report** menu.
- Highlight the **Result and Calibration** report template.
- Click on **[Open]**.
- Click on the **Curve + result table** icon in the toolbar.
- Place the cursor, which now has the shape of a cross, in the report template and create the required area with the left mouse button held down.

The **Properties - Curve + result table field** dialog opens.

2

- Enter the sample name **Tap water** in the **Analysis** field.
- Click on the **Result** button.
- Highlight the **Resolution** entry in the **Available results** list and move it to the **Displayed results** list with the [>>] button.
- Highlight **Resolution** and click on **[Decimal place]**.
- Select the value **1** in the **Number of decimals - Resolution** dialog.
  Enter the value **2** for the decimal places of the **Concentration**.
- Click on **[OK]**.

3

- Confirm the message **Save template** with **[Yes]** and close the **Report template - New form report** dialog.
- In the **Save report template** dialog, enter the name **Results** in the **Name** field.
- Click on **[Save]**.

5.5 Printing a report

Printing calibration curves

1 Highlight the row of standard 3 in the **Determination overview** subwindow.

2 Open the **Report output** dialog via the **File ► Print ► Report...** menu.

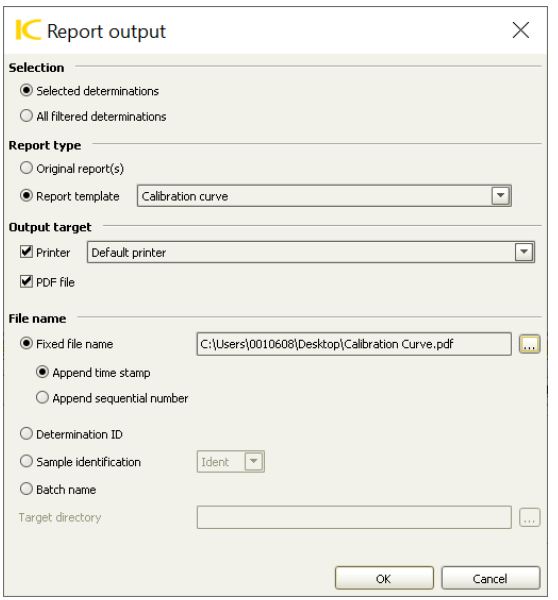
3 Highlight the **Selected determination** option in the **Selection** area.

4 In the **Report type** area, highlight the **Report template** option and select the **Calibration curve** report template.

5 In the **Output target** area, deactivate the **Printer** check box and activate the **PDF file** check box.

6 Click on the ... icon in the **File name** area. In the **Select file for report** dialog, enter the name **Calibration curve** in the **File name** field and select a suitable path to save the file.

7 Click on **[OK]**.



8 Close the **Report output** dialog with **[OK]**.

Printing the result table/chromatogram

1 Highlight the row with the **Tap water** entry in the **Determination overview** subwindow.

2 Open the **Report output** dialog via the **File ► Print ► Report...** menu.

3 Highlight the **Selected determinations** option in the **Selection** area.

4 In the **Report type** area, highlight the **Report template** option and select the **Results** report template.

5 In the **Output target** area, deactivate the **Printer** check box and activate the **PDF file** check box.

6 Click on the ... button, enter the name **Sample** in the **File name** field in the **Save as** dialog, and select a suitable path to save the file.