MagIC Net

Metrohm
Ion analysis

Tutorial

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Although all the information given in this documentation has been checked with great care, errors cannot be entirely excluded. Should you notice any mistakes please send us your comments using the address given above.

Documentation in additional languages can be found on *http://products.metrohm.com* under **Literature/Technical documentation**.

Table of contents

1 Introduction

1.1 Structure of the tutorial

The present tutorial guides you through your first steps with the software ***MagIC Net***. You will be introduced to the most important operating features by recording a chromatogram. The introduction will involve determining the concentration of the anions F^-, Cl^-, NO_2^-, Br^-, NO_3^-, PO_4^{3-} and SO_4^{2-} in tap water. An 850 Professional IC Anion MCS and a Metrosep A Supp 5 column with integrated chip are used in the determinations.

The tutorial is arranged in four parts:

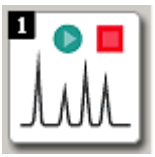
- Configuring hardware which is managed by the system and used in the method
- Method for performing a determination
- Performing the determination
- Evaluating the determination, reprocessing and printing out a report

You will be shown how the determination is performed using a simple system with manual injection. We shall also describe a determination using an automated system with sample changer.

1.2 Program description

MagIC Net comprises the following program parts:

Workplace



- Opening/Closing Workplaces
- Entering sample data
- Starting individual determinations and series of samples
- Live visualization of chromatograms and system parameters (Watch Window)

Database

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

Method

- Entering the device combination used and its parameters
- Definition of the time program
- Entering the integration parameters
- Entering the analytes
- Result definition

Configuration

- Information on devices, columns, eluents, accessories, solutions, common variables and rack data
- User administration
- Security settings
- Program administration

Manual Control

- Manual control of a workplace
- Manual control of all devices

1.3 Visualization conventions

The following symbols and formats will be used in this documentation:

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

2 Configuration

The Metrohm devices connected to the PC via a USB connector are automatically recognized when the program is started, as are the devices (dosinos, stirrers, pumps, remote box) connected to MSB connectors of USB devices. Metrohm devices and external devices connected to the PC via an RS232 connector must be added manually to the device table.

All hardware components used in a method must be saved in the program part **Configuration**. This can include:

- Devices (850 Professional IC, 858 Professional Sample Processor etc.)
- Columns
- Eluents
- Accessories (Pump tubing, pump tubing connections etc.)
- Solutions
- Common variables
- Rack data

2.1 Starting the software

Note

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

Starting MagIC Net

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

2 Enter user name and password and click on **[OK]**.

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

The dialog window of the program part **Configuration** is opened. A total of seven subwindows can be displayed:

Devices	Shows the automatically recognized and manually added devices.
Columns	Shows the data of automatically recognized and manually recorded columns.
Eluent	Shows the data for the eluents.
Accessories	Shows the data of automatically recognized and manually added accessories.
Solutions	Shows the data of automatically recognized solutions in a dosing unit and solutions added manually.
Rack Data	Shows the data of automatically recognized Metrohm sample racks and manually imported Metrohm sample racks.
Common variables	Shows the data of all common variables.

2.2 Configuring devices

Proceed as follows to start the **850 Professional IC Anion MCS** for the first time:

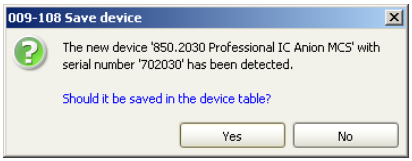
Connecting 850 Professional IC

1 **Connecting instrument**

Connect device to the PC using a USB cable.

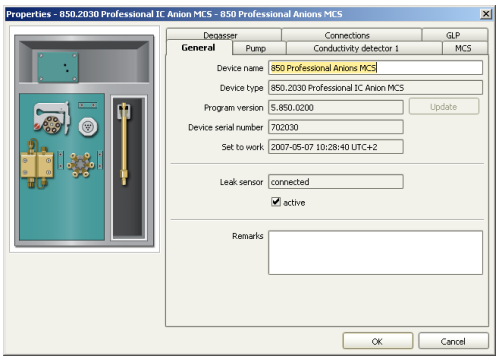
2 Switching on device

The device parameters of the **850 Professional IC Anion MCS** are automatically recognized.



3 Saving device in the table

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



4 Checking properties

Check the data in the **Properties** dialog window and close with **[OK]**.

The **850 Professional IC Anion MCS** is entered in the device list in the **Devices** subwindow.

5 Changing device name (optional)

Proceed as follows to give your device another name:

- In the device table, double click on the line with the entry **850 Professional IC Anion MCS**.
- Select the **General** tab.
- Enter the new name in the **Device name** field.
- Close the dialog window with **[OK]**.

If you perform your determinations with a sample changer, you will first of all have to connect the device.

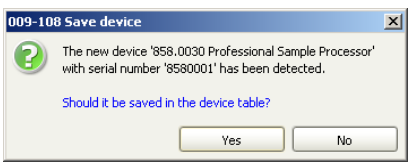
Connecting 858 Professional Sample Processor

1 Connecting instrument

Connect device to the PC using a USB cable.

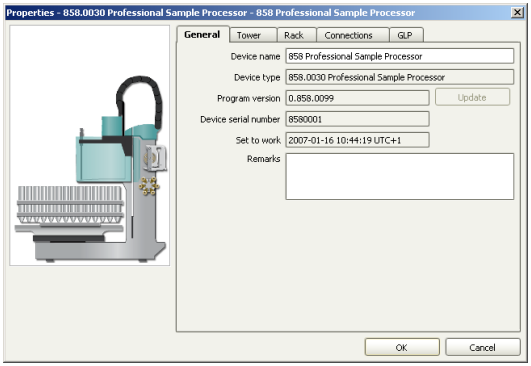
2 Switching on device

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



3 Saving device in the table

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



4 Define rack parameters

- Select the tab **Rack**.
  The number of the default rack, 6.2041.440, must be entered in the **Rack name** field.
- Click on the **[Rack Data]** button.
- Select the **Lift positions** tab.
- Use the **Work position** field to enter the value **125**.
- Select the **Special beaker** tab.
- Click on **[Edit]** and open the **Special beaker 1** dialog window.
- Use the **Rack position** field to enter the value **149**.
- Use the **Work position of tower 1** to enter the value **125**.

Close all dialog windows with **[OK]**.

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

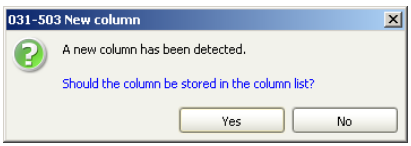
2.3 Configuring column

Columns with chip

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

1 **Inserting column in holder**

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



2 **Saving column in the table**

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

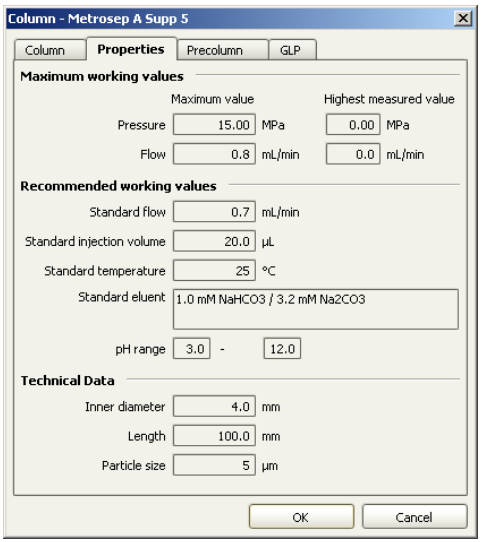
The column is entered in the column table in the subwindow **Columns**.

3 **Editing Column tab**

In the **Column - Metrosep A Supp 5** dialog field in the **Column** tab use the **Column name** field to enter the name **A Supp 5**.

4 **Editing Properties tab**

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



5 Editing Precolumn tab

Activate the **Use precolumn** check box.

Simultaneously to the activation, the system defines that the precolumn is to be monitored together with the column.

6 Monitoring tab

Note

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

- Use the **Determinations** field to enter the value **500** (example) and activate the **Monitoring** check box.
- Use the **Working hours** field to enter the value **72** (example) and activate the **Monitoring** check box.

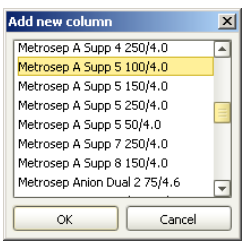
- For the **Determinations** and **Working hours** of the **precolumn** enter the same limit values as for the column, and activate the check box for monitoring it. The precolumn is monitored in the same way as the column.
- In the **Message** area, activate the **Acoustic signal** check box.

Column without chip

If you use a column without a chip, this must first of all be configured. Use the **[Edit]** menu in the **Columns** subwindow for this. In the case of known columns, several parameters are automatically entered, while with unknown columns these parameters have to be taken from the column information sheet and entered.

1 Add column

Use the **Edit ▸ New...** menu to open the **Add new column** dialog window.



2 Selecting column

Highlight the column **Metrosep A Supp 5** in the list and click on **[OK]**.

The **Column - Metrosep A Supp 5** dialog window is opened.

3 Editing column

Note

Only the name has to be entered for Metrohm columns.

- Select the **Column** tab
- Use the **Column name** field to enter the name **Metrosep A Supp 5**.
- In the **Set to work** field click on the button … and select the date of first use.
  The **Column type** and **Order number** fields are automatically filled in for known columns.
  The entries in the **Serial number**, **Batch number** and **Comment** fields are optional.

4 Editing Properties tab

If the columns are known, the values for pressure flow etc. are automatically entered. If the columns are unknown, the values have to be taken from the column information sheet and entered.

5 Editing Precolumn tab

The fields are filled in automatically if the columns are known. If the columns are unknown, the values have to be taken from the column information sheet and entered.

Proceed as follows to enter the date of first use:

- Select the **Precolumn** tab.
- Activate the **Use precolumn** check box.
- Click on the button … of the **Set to work** field.
- Select the date and confirm with **[OK]**.

6 **Editing GLP tab (optional)**

This tab only has to be edited if monitoring in accordance with GLP 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.
- Use the **GLP test interval** field to enter the value **100** The date of the next GLP test is automatically entered in the **Next GLP test** field.
- In the **Message** area, activate the **Acoustic signal** check box.
- In the **Action** area, activate the **Display message** option.
- Close the dialog window by clicking on **[OK]**.

2.4 Defining eluent

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

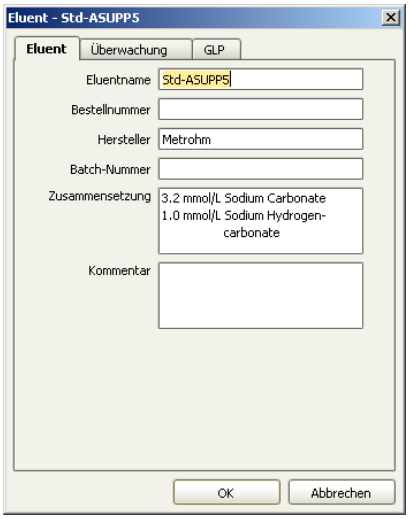
1 Use the **Edit ▸ New...** menu to open the **Eluent** dialog window.

2 **Eluent properties**

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

Field	Input
Eluent name	Std-ASUPP5
Order number	optional
Manufacturer	optional
Batch number	optional

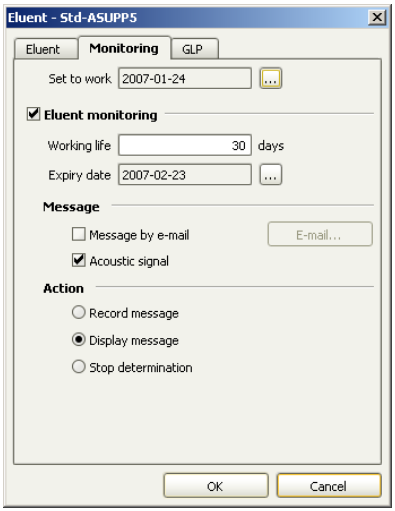
Composition	3.2 mmol/L sodium carbonate, 1.0 mmol/L sodium hydrogen carbonate
Comment	optional



3 Editing Monitoring tab

- Select the **Monitoring** tab.
- The date of the first use is automatically entered when entering the eluent.
- Activate the **Eluent monitoring** check box.
- Use the **Working life** field to enter the value **30** (the working life depends on the eluent).
  If you click on the button ... the date will automatically be entered in the **Expiry date** field.
- In the **Message** area, activate the **Acoustic signal** check box.

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



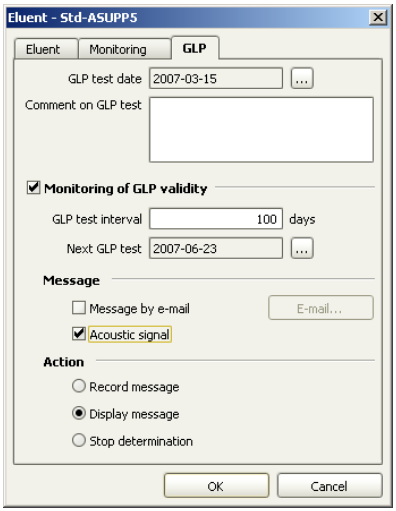
- Close the dialog window by clicking on **[OK]**.

4 Editing 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.
- Use the **GLP test interval** field to enter the value **100**.

  If you click on the button ... the date will automatically be entered in the **Next GLP test** field.
- In the **Message** area, activate the **Acoustic signal** check box.

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



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

2.5 Adding solutions

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

1 Use the **Edit** ▸ **New** menu to open the **Solution** dialog window.

2 Edit the **Solution** tab

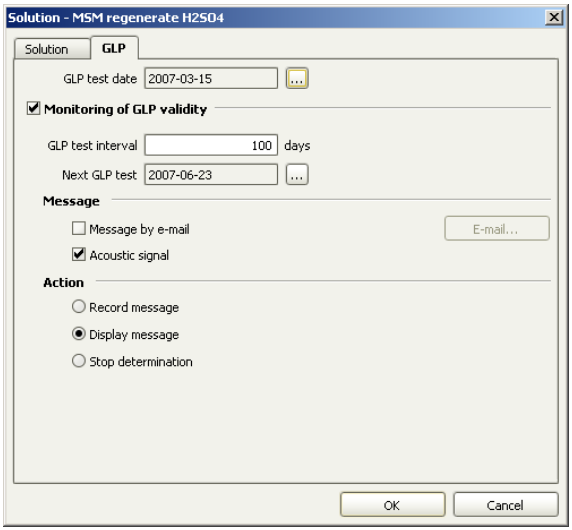
- Use the **Solution name** field to enter the name **H_2O**.
- Use the **Concentration** field to enter the concentration value **100** and select the concentration unit **%** in the list field.
- In the **Production date** field, click on the … in the toolbar.

- Select the date and conform with **[OK]**.
- Activate the **Solution monitoring** check box.
- Use the **Working life** field to enter the value **100**.
  If you click on the button ... the date will automatically be entered in the **Expiry date** field.
- In the **Message** area, activate the **Acoustic signal** check box.
- In the **Action** area, activate the **Display message** option.
- Close the dialog window by clicking on **[OK]**.

3 Editing 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.
- Use the **GLP test interval** field to enter the value **100**.
  If you click on the button ... the date will automatically be entered in the **Expiry date** field.
- In the **Message** area, activate the **Acoustic signal** check box.

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



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

The second solution with the name **MSM regeneration solution H_2SO_4** is entered in the same way.

2.6 Adding accessories

Accessories must always be added and configured manually. The individual steps are executed in the **Accessories** subwindow.

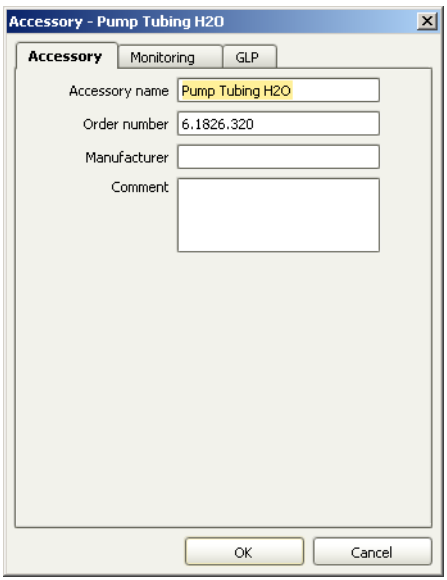
Two pump tubings and one pump tubing connection with security device and filter are added. The pump tubing connection with inline filter is used to protect the separation column and suppressor from potential contamination from the eluents or rinsing solution.

Adding new accessories

1 Use the **Process** ▸ **New** menu to open the **Accessory** dialog window.

2 In the **Accessory** tab, use the **Accessory name** field to enter the name **Pump Tubing H_2O**.

3 Enter the number **6.1826.320** in the **Order number** field.



4 Select the **Monitoring** tab.

5 Activate the **Accessory monitoring** check box.

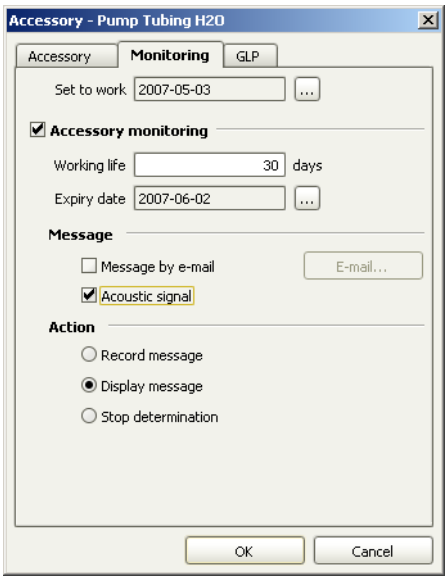
6 In the **Working life** field enter the value **30**.

7 In the **Expiry date** click on the … button.

The expiry date is entered automatically.

8 In the **Message** area, activate the **Acoustic signal** check box.

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



Repeat steps **1** bis **9** in order to add a second pump tubing and a pump tubing connection. The accessory name of the second tubing is **Pump Tubing H_2SO_4**. The **Pump tubing connection with security device and filter** has the order number **6.2821.120**.

3 Creating method

A method is a procedural specification for processing a sample. It comprises all elements which are needed to record a chromatogram. These include:

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

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

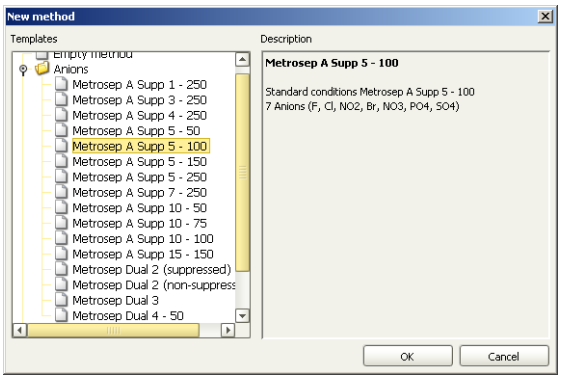
3.1 Method for manual injection

3.1.1 Creating new method

Creating method

1 Click on the symbol of the program part **Method**.

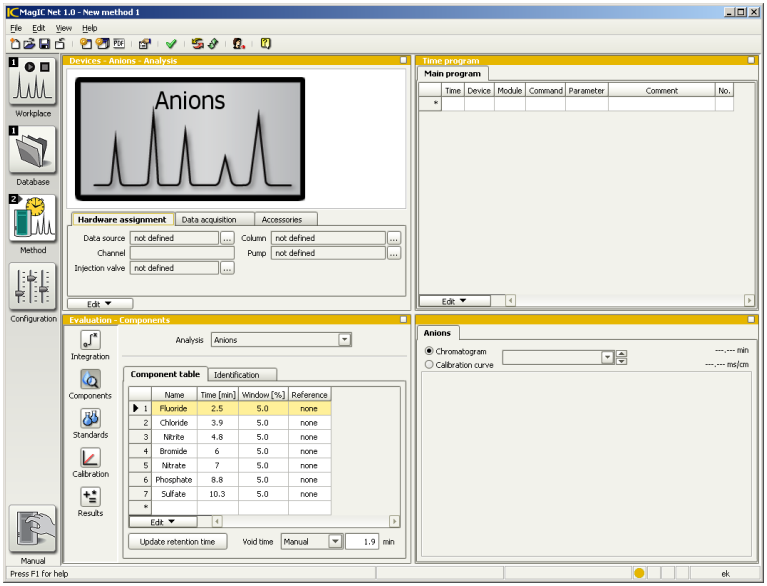
2 Use the menu **File ▸ New...** to open the **New method** dialog window.



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

The method template is opened.

The **Devices** subwindow shows the symbol of the analysis method **Anions**. The **Evaluation - Components** subwindow shows the component table with the ions of the method template and their retention times.



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

Devices	Visualization of the devices assigned to the method and the analysis.
Time Program	Visualization of the time program.
Evaluation	The subwindow consists of the areas **Integration**, **Components**, **Standards**, **Calibration** and **Results**.
Chromatograms	Shows the chromatograms of the last determination recorded with this method, the chromatograms of the standard which are used for calibrating the samples, and those of the calibration curves.

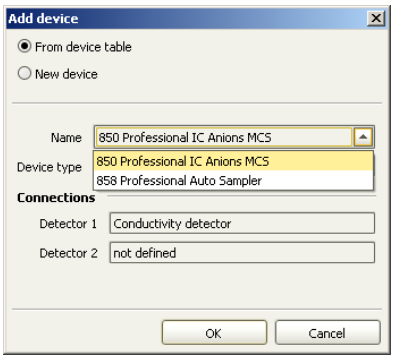
3.1.2 Defining devices and their start parameters

Putting together devices

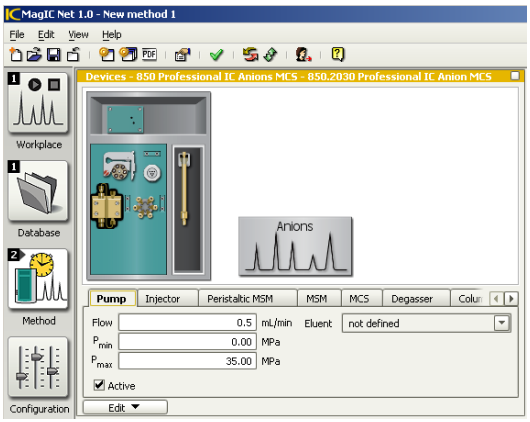
1 In the **Devices** subwindow, click in the menu **Edit** ▸ **Add** ▸ **Device**.

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

3 In the **Name** field, select the device **850 Professional IC Anion MCS** and click on **[OK]**.



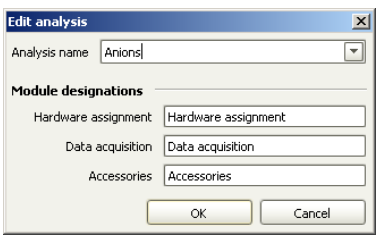
The top of the **Devices** subwindow will display the figure of the **850 Professional IC Anion MCS**.



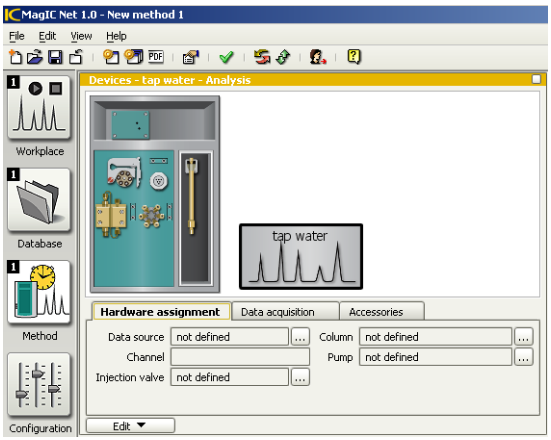
Changing analysis name (optional)

1 In the top of the **Devices** subwindow, click on the symbol of the **Anions** analysis.

2 Use the **Edit** ▸ **Edit** menu to open the **Edit analysis** dialog window.



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



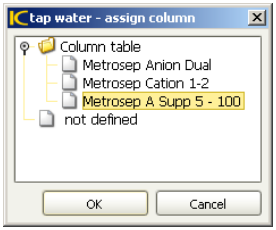
Defining parameters for analysis

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

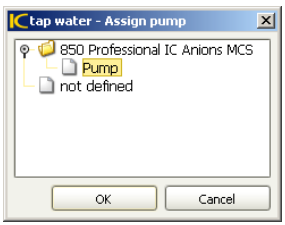
2 **Editing Hardware assignment tab**

- Select the **Hardware assignment** tab.
- In the **Data source** field, click on the … button.
- In the **Tap water-assign data source** dialog window under **850 Professional IC Anion MCS > Conductivity detector 1**, highlight the entry **Conductivity** and click on **[OK]**.
- In the **Channel** field, **Conductivity** is automatically entered.
- In the **Injection valve** field click on the … button.
- In the **Tap water-assign injection valve** dialog window under **850 Professional IC Anion MCS** highlight the entry **Injector** and click on **[OK]**.
- In the **Column** field click on the … button.

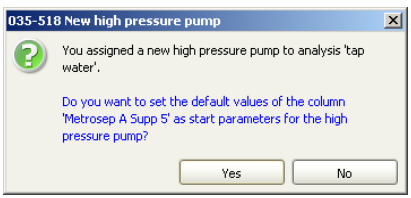
- In the **Tap water-assign column** dialog window under **Column table**, highlight the entry **Metrosep A Supp 5** and click on **[OK]**.



- In the **Pump** field clock on the ... button.
- In the **Tap water-assign pump** dialog window under **850 Professional IC Anion MCS** highlight the entry **Pump** and click on **[OK]**.



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



3 Editing Data acquisition tab

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

4 Editing Accessories tab

- Select the **Accessories** tab.

- Click on the **[Add]** button.
- In the list box of the **Add accessory** dialog window, select the pump tubing H_2O.
- Click on **[OK]**.

The pump tubing is entered in the accessories table. The pump tubing H_2SO_4 and pump tubing connection with security device and filter are added to the table in the same way.

Defining parameters for IC device

1 Click on the symbol of the **850 Professional IC Anion MCS**.

The tabs of the **850 Professional IC Anion MCS** modules appear and can be edited.

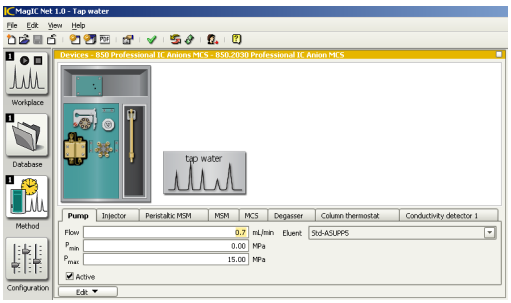
Note

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

2 **Editing Pump tab**

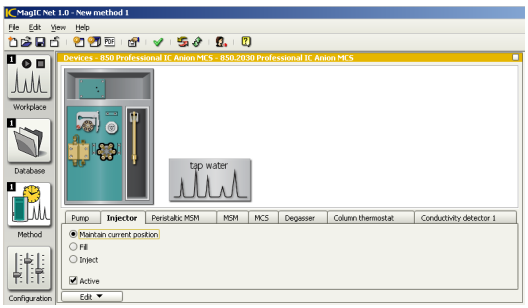
- Select the **Pump** tab (or click on the symbol of the pump).
- The values of the fields **Flow**, $\mathbf{P_{min}}$ and $\mathbf{P_{max}}$ are read in automatically.

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



3 Editing Injector tab

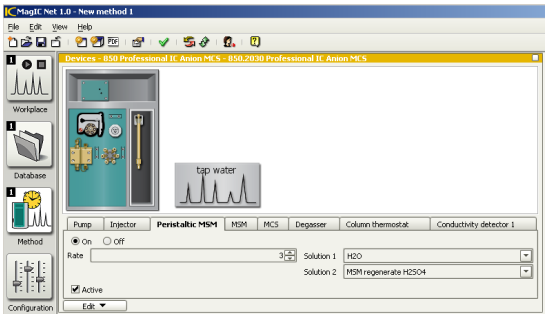
- Select the **Injector** tab (or click on the symbol of the injector).
- Accept the default settings.



4 Editing Peristaltic MSM tab

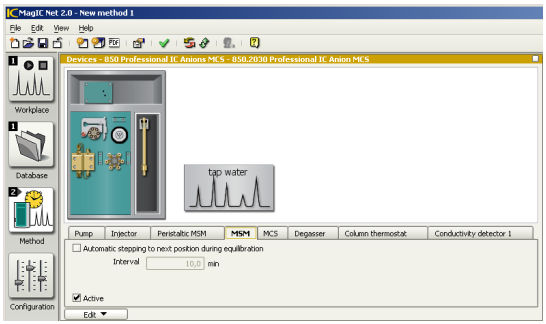
- Select the **Peristaltic MSM** tab (or click on the symbol of the peristaltic MSM).
- Activate the **On** option.
- In the **Rate** field, accept the value **3**.
  (There are 7 speed levels, with 6 revolutions/min per level.)
- Use the **Solution 1** list box to select the solution **H_2O**.

- Use the **Solution 2** list box to select the solution **MSM regeneration solution H_2SO_4**.



5 Editing MSM tab

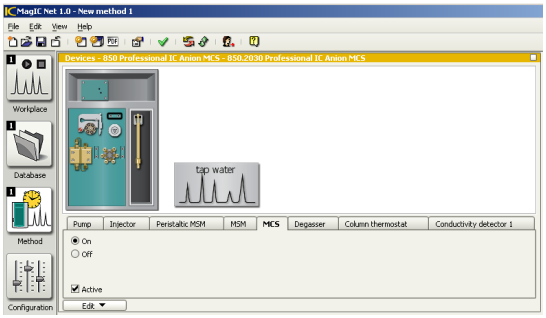
- Select the **MSM** tab (or click on the symbol of the MSM).
- Accept the default setting.



6 Editing MCS tab

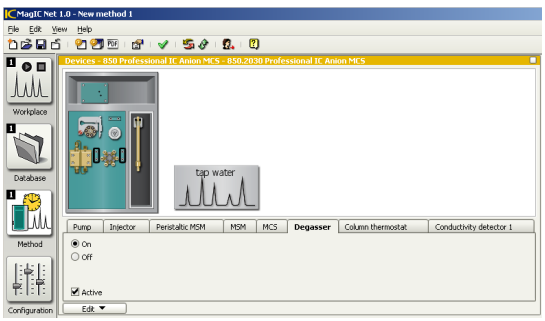
- Select the **MCS** tab (or click on the symbol of the MCS).

- Accept the default settings.



7 Editing Degasser tab

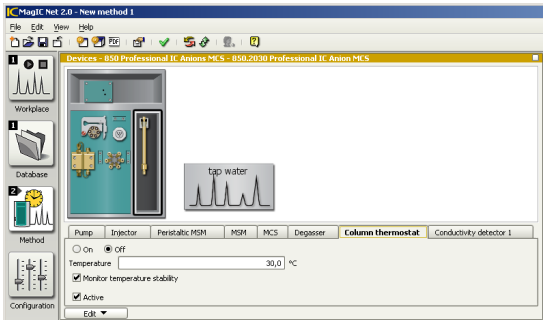
- Select the **Degasser** tab (or click on the symbol of the degasser).
- Accept the default settings.



8 Editing Column thermostat tab

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

- Accept the default settings.



9 Editing Conductivity detector 1 tab

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

3.1.3 Time program

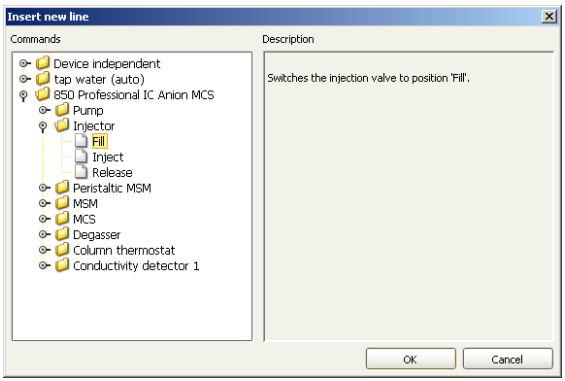
The time program is a component of each method. It provides a step by step description of the sequence for processing a sample. The time program is compiled in the **Time program** subwindow of the program part **Method**.

Defining time program

1 Switching injection valve to fill

- Use the **Edit** ▸ **New** menu to open the **Insert new line** dialog window.

- Select **850 Professional IC Anion MCS ▸ Injector ▸ Fill** in the left of the window under commands.

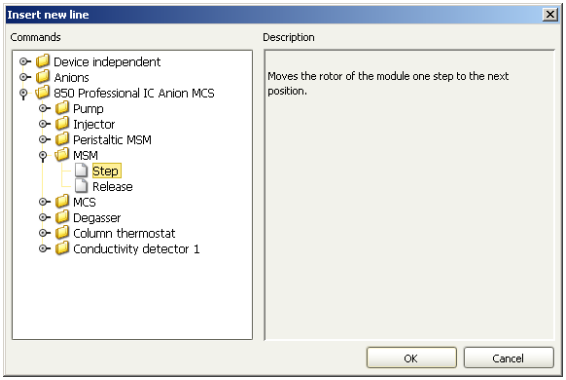


- Confirm with **[OK]**.
  The dialog window **850 Professional IC Anion MCS - Injector - Fill** is opened.
- Accept the time data **0** min.
- Confirm with **[OK]**.

2 Switching MSM to next position

- Use the **Edit ▸ New** menu to open the **Insert new line** dialog window.

- Select **850 Professional IC Anion MCS ▸ MSM ▸ Step** In the left of the window under commands.



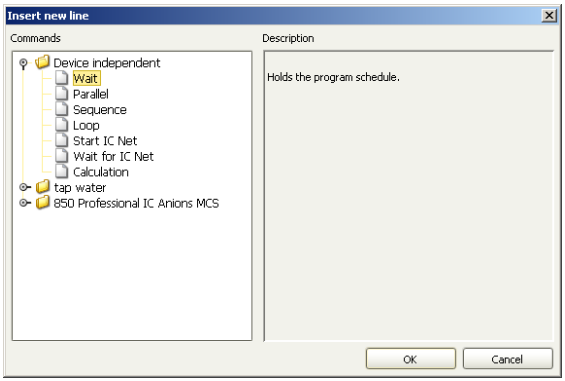
- Confirm with **[OK]**.
  The dialog window **850 Professional IC Anion MCS - MSM - Step**.
- Accept the time data **0** min.
- Confirm with **[OK]**.

3 Interrupting program

The program is stopped in order to fill the injection valve manually.

- Use the **Edit ▸ New** menu to open the **Insert new line** dialog window.

- Select **Device-independent ▸ Wait** In the left of the window under commands.

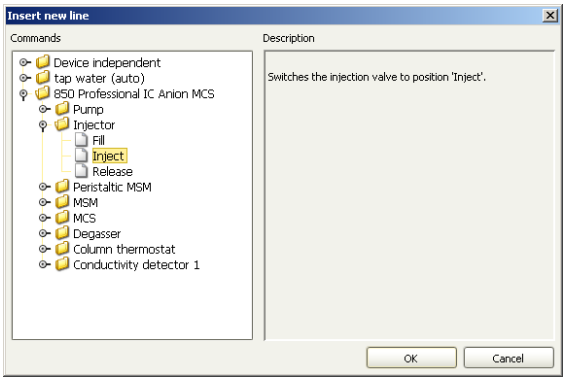


- Confirm with **[OK]**.
  The dialog window **Wait** opens.
- Highlight the option **Stop program and waiting for [Continue]**.
- Click on the button  and enter a text for the message.
- Confirm twice with **[OK]**.

4 Switching injection valve to inject

- Use the **Edit ▸ New** menu to open the **Insert new line** dialog window.

- Select **850 Professional IC Anion MCS ▸ Injector ▸ Inject** in the left of the window under commands.

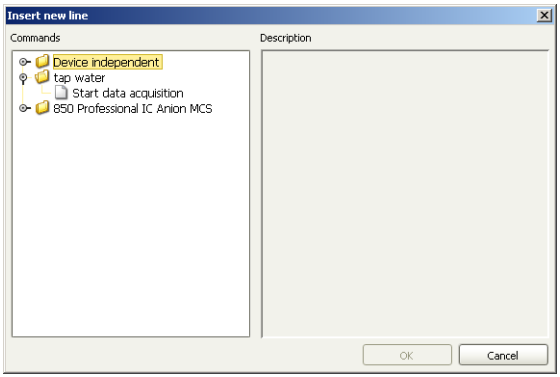


- Confirm with **[OK]**.
  The dialog window **850 Professional IC Anion MCS - Injector - Inject** is opened.
- Accept the time data **0** min.
- Confirm with **[OK]**.

5 Starting data acquisition

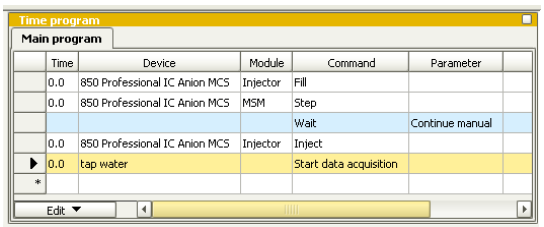
- Use the **Edit ▸ New** menu to open the **Insert new line** dialog window.

- Select **850 Professional IC Anion MCS ▸ Tap water ▸ Start data acquisition** in the left of the window under commands.



- Confirm with **[OK]**.
  The dialog window **850 Professional IC Anion MCS - Tap water - Start data acquisition** is opened.
- Accept the time data **0** min.
- Confirm with **[OK]**.

The complete time program for manual filling of the injection valve appears as follows:



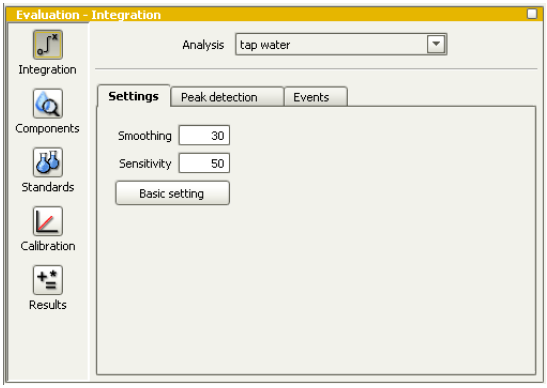
3.1.4 Evaluation

The parameters for evaluating the chromatograms are defined in the **Evaluation** subwindow. 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.



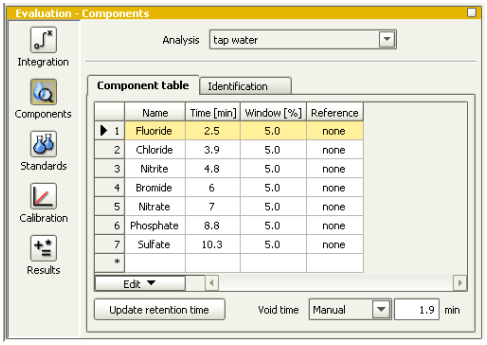
In the **Analysis** list box, the analysis name **Tap water** is automatically entered.

The entries in the tabs **Settings**, **Peak detection** and **Events** are accepted.

Components

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

1 Click on the **Components** button.



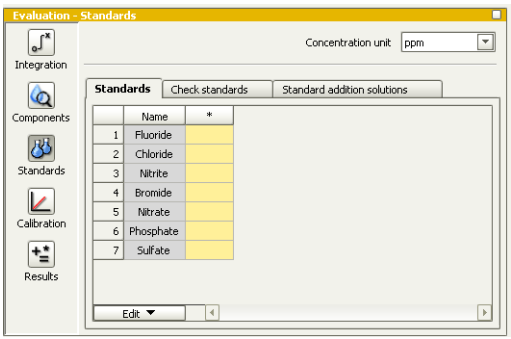
2 The entries in the tabs **Component table** and **Identification** are accepted.

Standards

In the Standards area, the concentrations of the components are indicated in the standard solutions.

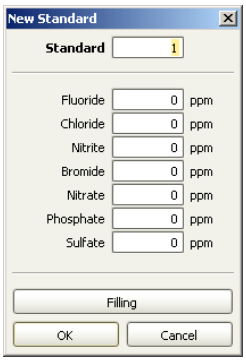
1 Click on the **Standards** button.

The Standard Table lists all the components defined in the method template.



2 In the **Concentration unit** field, select the **ppm** option.

3 In the **Standards** tab, use the **Edit** ▸ **New** menu to open the **New Standard** dialog window.

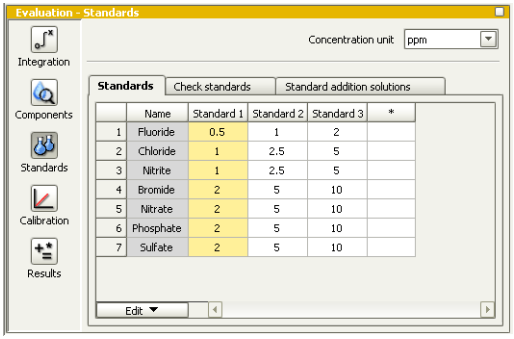


4 In the **Fluoride** field, enter the concentration value **0.5**. In each of the fields **Chloride** and **Nitrite** enter **1** as a value, and in each of the fields **Bromide**, **Nitrate**, **Phosphate** and **Sulfate** enter the value **2**.

5 Click on **[OK]**.

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

Table with the standard concentrations

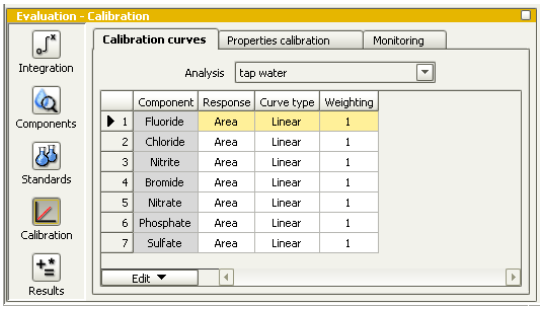


Calibration

The calibration is performed after the method of the external standards. The peak areas in the chromatogram of an unknown sample are compared with the peak values of the components of a standard solution with known concentrations. The calibration method is specified in the method template.

1 Click on the **Calibration** button.

2 Select the **Calibration curves** tab.



The component names, measured quantity, curve type and evaluation are specified in the method template. The table

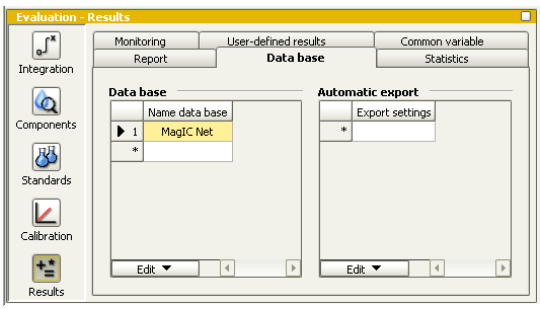
can be edited line by line. Either via the **Edit** ▸ **Edit** menu or by double clicking on a line, which opens the **Calibration curve** dialog window of the corresponding component.

Results

The results of the determinations are saved in the standard database **MagIC** (further databases can be defined). You can also indicate that a report is to be generated once the evaluation is complete.

1 Saving results in database

- Click on the **Results** button.

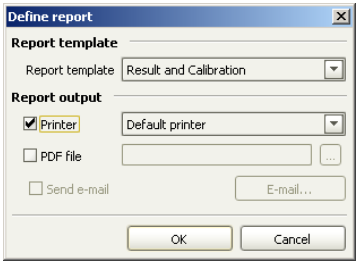


- Select the **Database** tab.
- In the **Database** area, select the database in which the determination data are to be saved. The **MagIC Net** database is indicated by default.

2 Printing out results

- Select the **Report** tab.
- Use the **Edit** ▸ **New** menu to open the **Define report** dialog window.
- In the **Report template** list box, highlight the **Result and Calibration** template.

- In the **Report output** area, activate the **Printer** list box.
- Select a printer in the **Printer** list box.



- Confirm with **[OK]**.

You also have the option of creating your own report template *(see Chapter 5.4, page 91)*.

3.1.5 Saving method

Saving method

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

1. Use the **File ▸ Save as...** menu to open the **Save method** dialog window.
2. In the **Method name** field, enter **Tap water** as the name for the method.
3. Click on **[Save]**.

3.2 Method with sample processor

The way a method for a determination with a sample processor is compiled only differs from the method for a manual injection in respect to the following points:

- Defining devices and their start parameters
- Time program

3.2.1 Creating new method

(see Chapter 3.1.1, page 21)

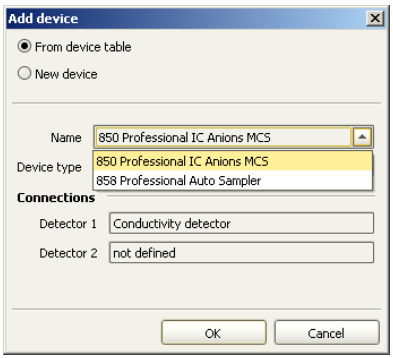
3.2.2 Defining devices and their start parameters

Putting together devices

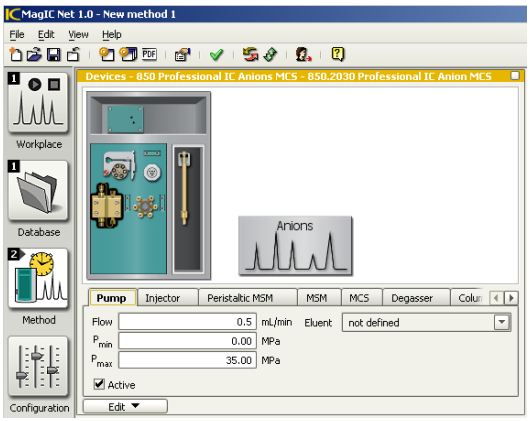
1. In the **Devices** subwindow, click in the menu **Edit** ▸ **Add** ▸ **Device**.

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

3. In the **Name** field, select the device **850 Professional IC Anion MCS** and click on **[OK]**.



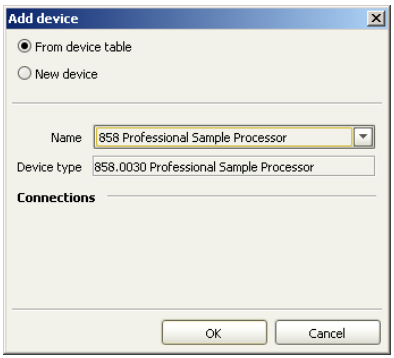
The top of the **Devices** subwindow will display the figure of the **850 Professional IC Anion MCS**.



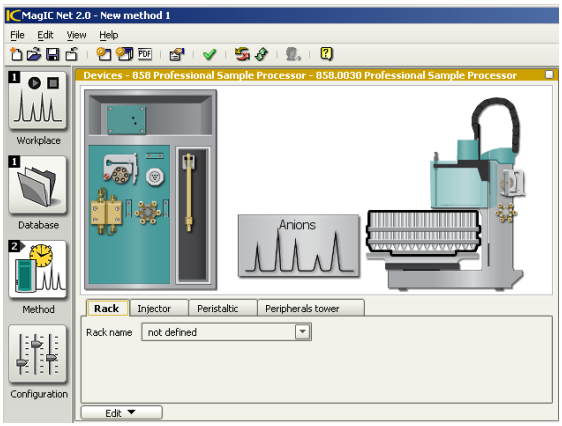
4 In the **Devices** subwindow, click in the menu **Edit ▸ Add ▸ Device**.

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

6 In the **Name** field, select the device **858 Professional Sample Processor** and click on **[OK]**.



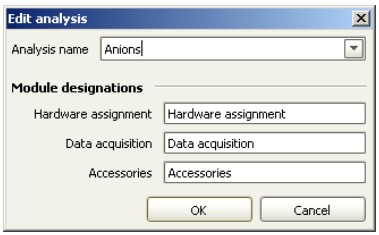
The top of the **Devices** subwindow will display the symbol of the **858 Professional Sample Processor**.



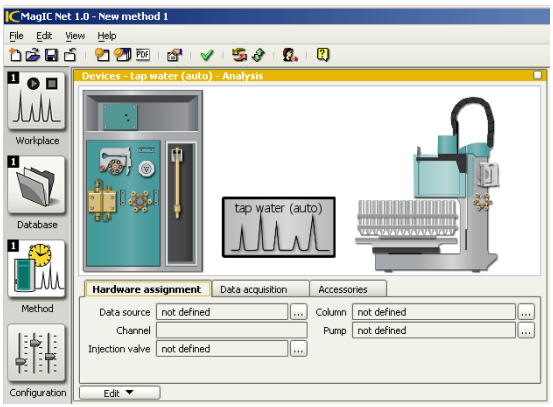
Changing analysis name (optional)

1 In the top of the **Devices** subwindow, click on the symbol of the **Anions** analysis.

2 Use the **Edit** ▸ **Edit** menu to open the **Edit analysis** dialog window.



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



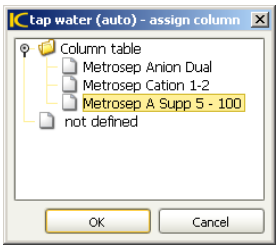
Defining parameters for analysis

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

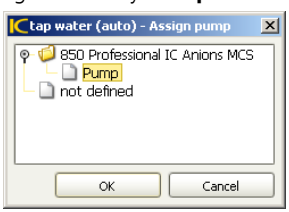
2 **Editing Hardware assignment tab**

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

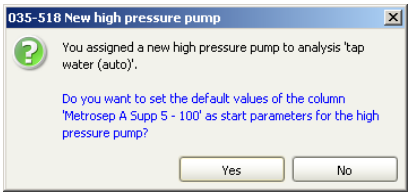
- In the **Tap water (auto)-assign data source** dialog window, under **850 Professional IC Anion MCS ▸ Conductivity detector 1** highlight the entry **Conductivity** and click on **[OK]**.
- In the **Channel** field, **Conductivity** is entered automatically.
- In the **Injection Valve** field click on the … button.
- In the **Tap water (auto)-assign injection valve** dialog window, under **850 Professional IC Anion MCS** highlight the entry **Injector** and click on **[OK]**.
- In the **Column** field click on the … button.
- In the **Tap water (auto)-assign column** dialog window, under **Column table** highlight the entry **Metrosep A Supp 5** and click on **[OK]**.



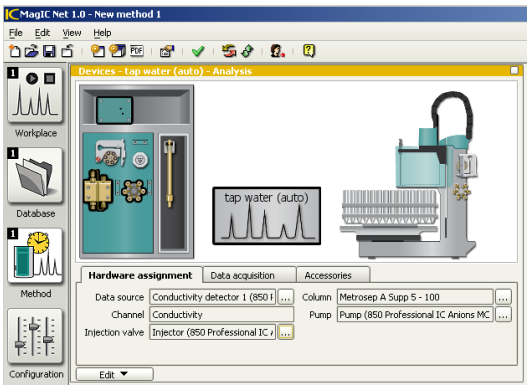
- In the **Pump** field click on the … button.
- In the **Tap water (auto)-assign pump** dialog window, under **850 Professional IC Anion MCS** highlight the entry **Pump** and click on **[OK]**.



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



The **Hardware assignment** tab appears as follows:



3 Editing Data acquisition tab

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

4 Editing Accessories tab

- Select the **Accessories** tab.
- Click on the **[Add]** button.
- In the list box of the **Add accessory** dialog window, select the pump tubing H_2O.
- Click on **[OK]**.

The pump tubing is entered in the accessories table. The pump tubing H_2SO_4 and the pump tubing connection with

security device and filter are added to the table in the same way.

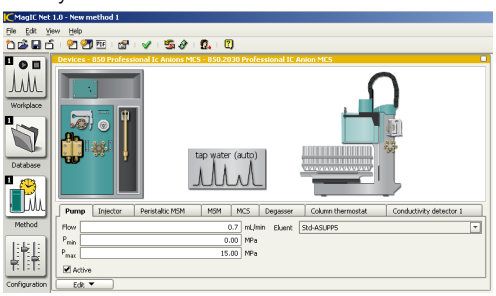
Defining parameters for IC device

1 Click on the symbol of the **850 Pofessional IC Anion MCS**.

The tabs of the **850 Professional IC Anion MCS** modules appear and can be edited.

2 **Editing Pump tab**

- Select the **Pump** tab (or click on the symbol of the pump).
- The values of the fields **Flow**, $\mathbf{P_{min}}$ and $\mathbf{P_{max}}$ are read in automatically.
- Use the **Eluent** list box to select the **Std-ASUPP5** previously defined.

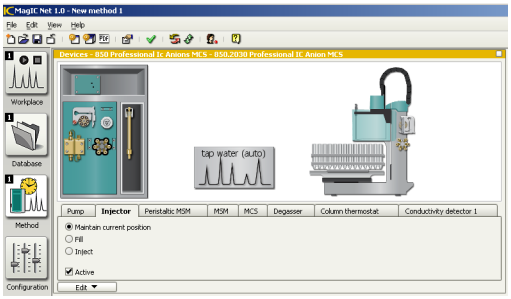


- Activate the **Active** check box.

3 **Editing Injector tab**

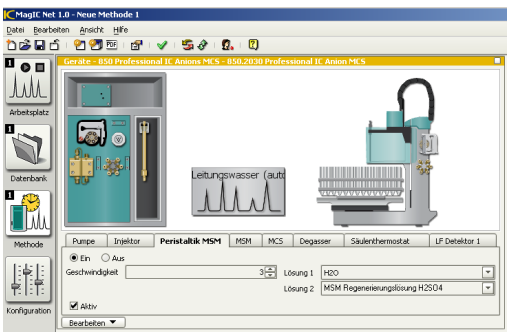
- Select the **Injector** tab (or click on the symbol of the injector).

- Accept the default settings.



4 Editing Peristaltic MSM tab

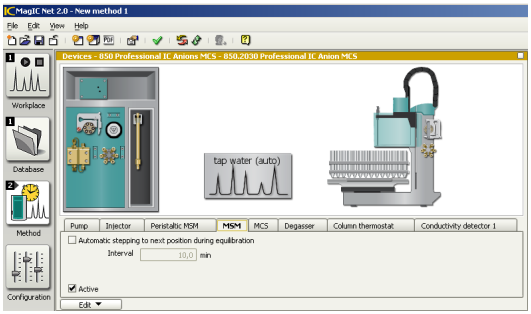
- Select the **Peristaltic MSM** tab (or click on the symbol of the peristaltic MSM).
- Activate the **On** option.
- Accept the value 3 in the **Rate** list box.
  (There are 7 speed levels, with 6 revolutions/min per level.)
- Use the **Solution 1** list box to select the solution **H_2O**.
- Use the **Solution 2** list box to select the solution **MSM regeneration solution H_2SO_4**.



5 Editing MSM tab

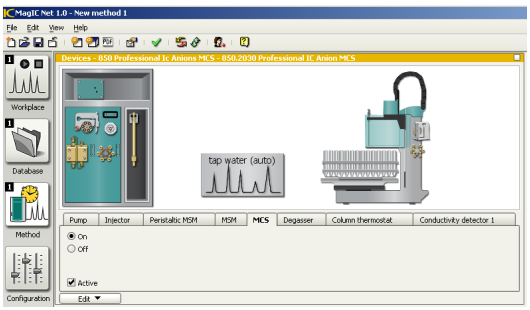
- Select the **MSM** tab (or click on the symbol of the MSM).

- Accept the default settings.



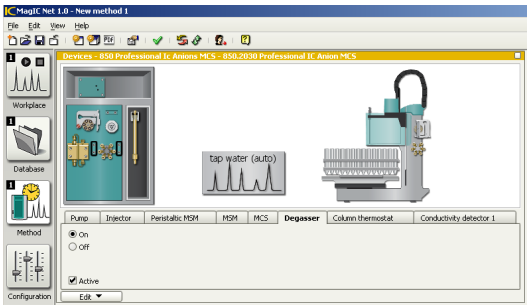
6 Editing MCS tab

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



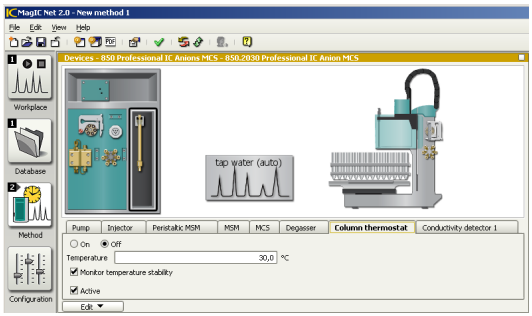
7 Editing Degasser tab

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

- 

8 Editing Column thermostat tab

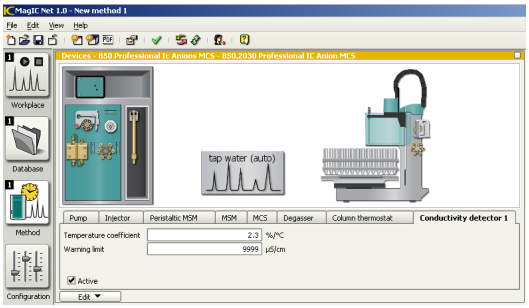
- Select the **Column thermostat** tab (or click on the symbol of the column thermostat).
- Accept the default settings.



9 Editing Conductivity detector 1 tab

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

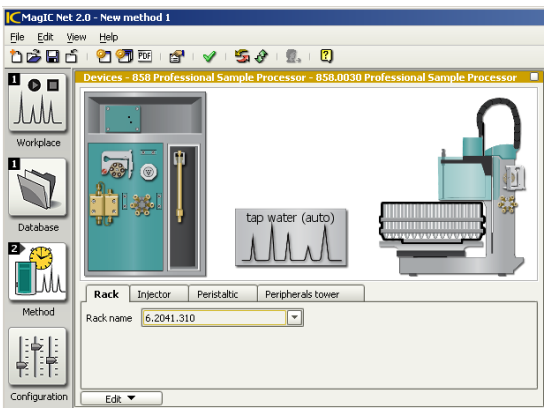
- Accept the default settings.



Defining parameters for sample processor

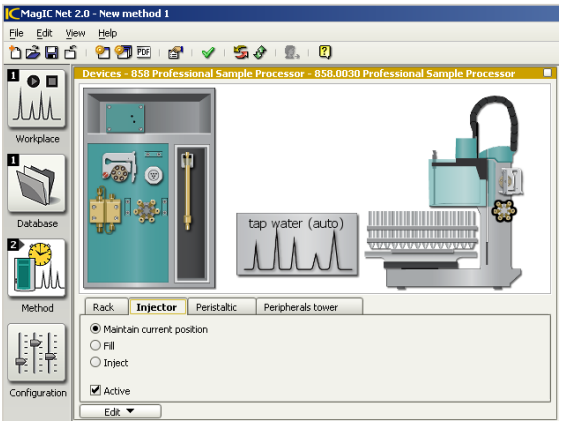
1 Edit Rack tab

- Select the **Rack** tab.
- Use the **Rack name** list box to select the number of the rack.



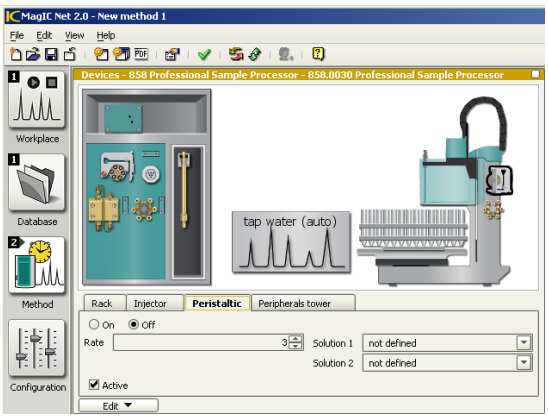
2 Editing Injector tab

- Select the **Injector** tab.
- Accept the default settings.



3 Editing Peristaltic tab

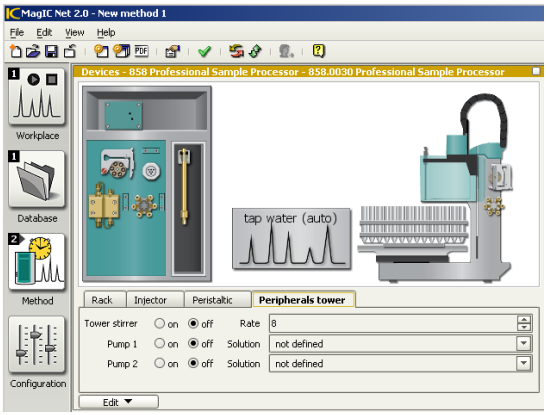
- Select the **Peristaltic** tab.
- Activate the **Off** option.



4 Editing Peripherals tower tab

- Select the **Peripherals tower** tab.

The settings are accepted, as no further devices are used.



3.2.3 Time program

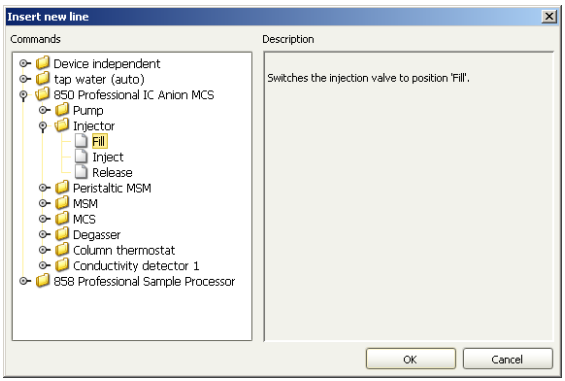
The time program is a component of each method. It provides a step by step description of the sequence for processing a sample. The time program is compiled in the **Time program** subwindow of the program part **Method**. The time program for an automated sequence of determinations contains additional commands for the sample processor, in contrast to a manual method.

Defining time program

1 Switching injection valve to fill

- Use the **Edit** ▸ **New** menu to open the **Insert new line** dialog window.

- Select **850 Professional IC Anion MCS ▸ Injector ▸ Fill** in the left of the window under commands.

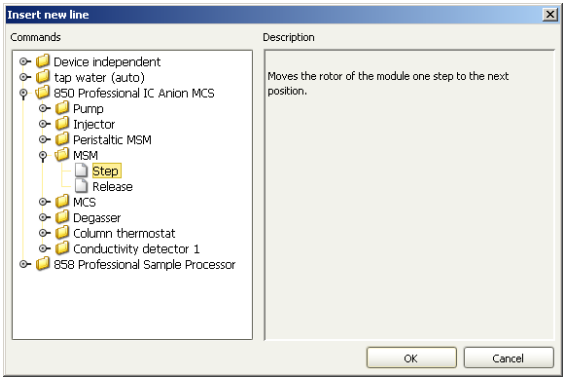


- Confirm with **[OK]**.
  The dialog window **850 Professional IC Anion MCS - Injector - Fill** is opened.
- Accept the time data **0** min.
- Confirm with **[OK]**.

2 Switching MSM to next position

- Use the **Edit ▸ New** menu to open the **Insert new line** dialog window.

- Select **850 Professional IC Anion MCS ▸ MSM ▸ Step** In the left of the window under commands.

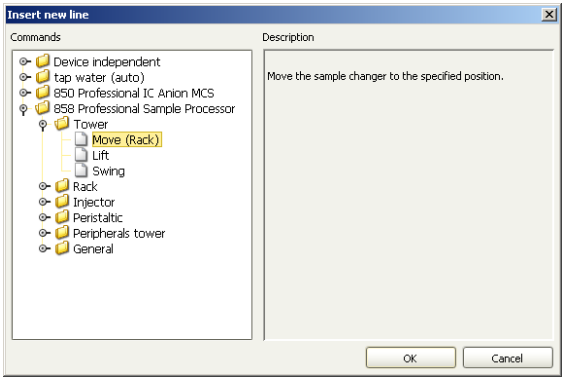


- Confirm with **[OK]**.
  The dialog window **850 Professional IC Anion MCS - MSM - Step** is opened.
- In the **Time** field, accept the time data **0** min.
- Confirm with **[OK]**.

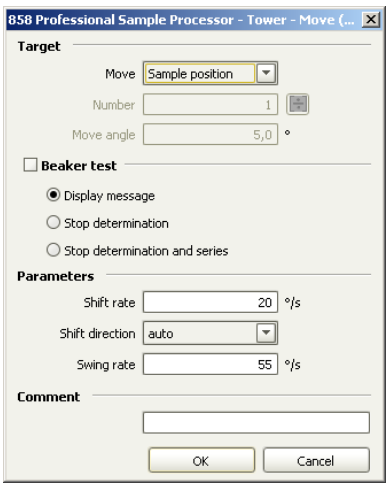
3 Moving to sample position

- Use the **Edit ▸ New** menu to open the **Insert new line** dialog window.

- Select **858 Professional Sample Processor ▸ Tower ▸ Move (Rack)** in the left of the menu under commands.



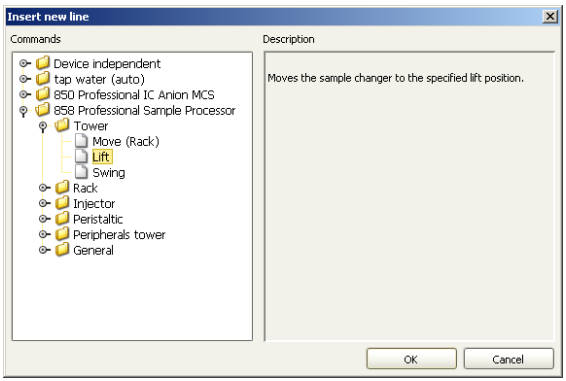
- Confirm with **[OK]**.
  The dialog window **858 Professional Sample Processor - Tower - Move (Rack)** opens.



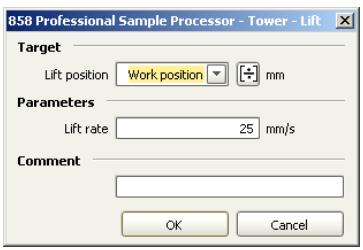
- Accept the field values.
- Confirm with **[OK]**.

4 Dipping aspiration needle in sample

- Use the **Edit** ▸ **New** menu to open the **Insert new line** dialog window.
- Select **858 Professional Sample Processor** ▸ **Tower** ▸ **Lift** in the left of the menu under commands.



- Confirm with **[OK]**.
  The dialog window **858 Professional Sample Processor - Tower - Lift** opens.
- Use the **Lift position** list box to select the entry **Work position**.

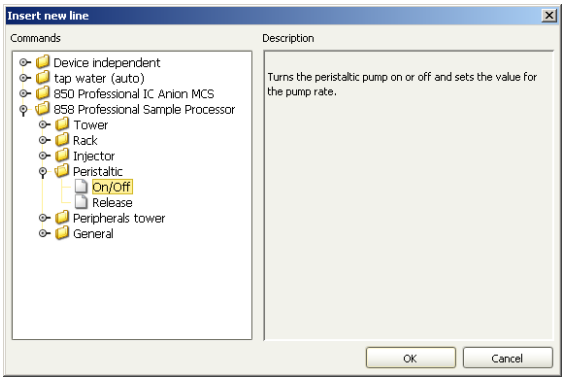


- Confirm with **[OK]**.

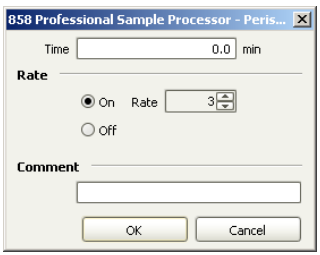
5 Filling injection valve with sample

- Use the **Edit** ▸ **New** menu to open the **Insert new line** dialog window.

- Select **858 Professional Sample Processor ▸ Peristaltic ▸ On/Off** in the left of the menu under commands.



- Confirm with **[OK]**.
  The dialog window **858 Professional Sample Processor - Peristaltic - On/Off** opens.
- In the **Time** field, accept the time data **0** min.
- Also accept the other field values.

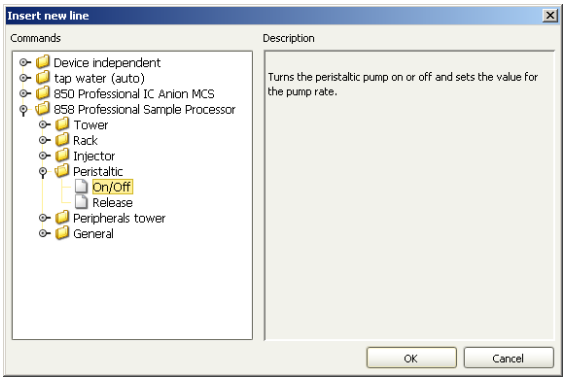


- Confirm with **[OK]**.

6 Switching off peristaltic pump of the sample processor

- Use the **Edit ▸ New** menu to open the **Insert new line** dialog window.

- Select **858 Professional Sample Processor ▸ Peristaltic ▸ On/Off** in the left of the menu under commands.

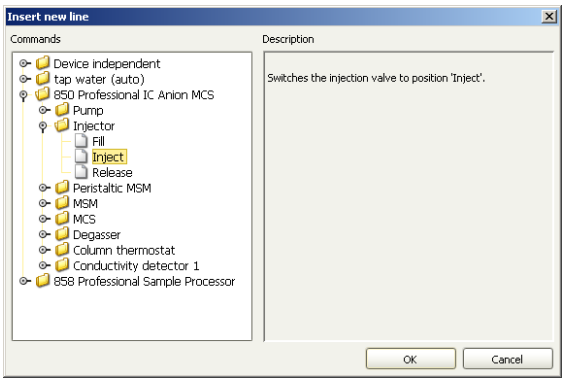


- Confirm with **[OK]**.
  The dialog window **858 Professional Sample Processor - Peristaltic - On/Off** opens.
- Use the **Time** field to enter the time data **2.5**.
- In the **Rate** area, select the option **Off**.
- Confirm with **[OK]**.

7 Switching injection valve to inject

- Use the **Edit ▸ New** menu to open the **Insert new line** dialog window.

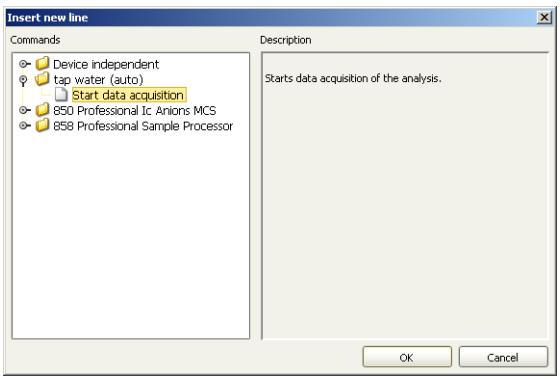
- Select **850 Professional IC Anion MCS ▸ Injector ▸ Inject** in the left of the menu under commands.



- Confirm with **[OK]**.
  The dialog window **850 Professional IC Anion MCS - Injector - Inject** is opened.
- Use the **Time** field to enter the value **2.5**.
- Confirm with **[OK]**.

8 Starting data acquisition

- Use the **Edit ▸ New** menu to open the **Insert new line** dialog window.
- Select **Tap Water (auto) ▸ Start Data acquisition** in the left of the menu under commands.



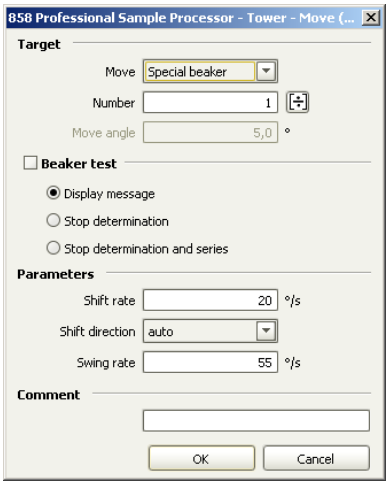
- Confirm with **[OK]**.
  The dialog window **850 Professional IC Anion MCS - Tap Water (auto) - Start Data Recording** opens.
- Use the **Time** field to enter the value **2.5**.
- Confirm with **[OK]**.

9 Moving to special beaker position

The so-called special beakers have a large volume (e.g. 250 mL) and mostly contain the rinsing solution. These beakers are preferably set at high rack positions so that sample series can start from rack position 1. Lift positions must be separately assigned for special beakers. Lift positions must be separately assigned for special beakers.

- Use the **Edit ▸ New** menu to open the **Insert new line** dialog window.
- Select **858 Professional Sample Processor ▸ Tower ▸ Move (Rack)** in the left of the menu under commands.
- Confirm with **[OK]**.
  The dialog window **858 Professional Sample Processor - Tower - Move (Rack)** opens.

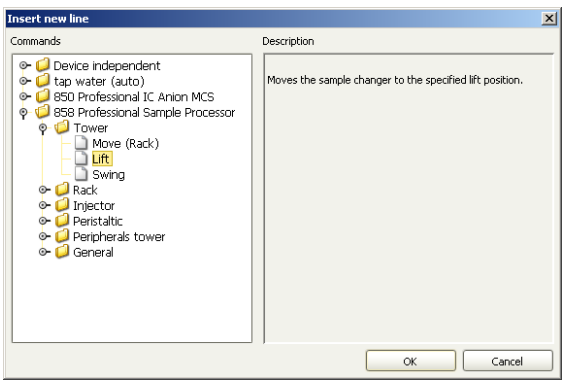
- Use the **Move** list box to select the entry **Special beaker** and the **Number** field to enter the value **1**.



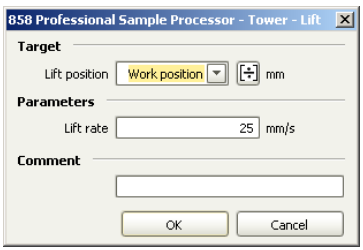
- Confirm with **[OK]**.

10 Dipping aspiration needle in special beaker

- Use the **Edit ▸ New** menu to open the **Insert new line** dialog window.
- Select **858 Professional Sample Processor ▸ Tower ▸ Lift** in the left of the menu under commands.



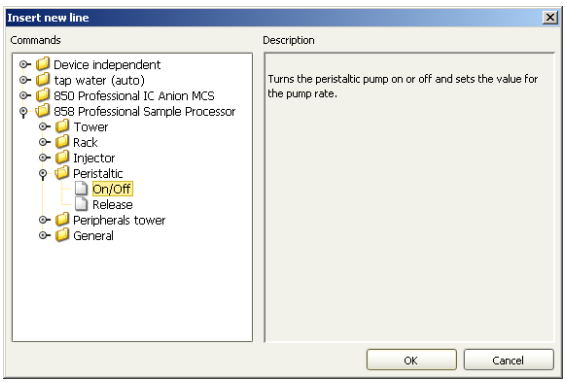
- Confirm with **[OK]**.
  The dialog window **858 Professional Sample Processor - Tower - Lift** opens.
- Use the **Lift position** list box to select the entry **Work position**.



- Confirm with **[OK]**.

11 Switching on rinsing

- Use the **Edit** ▸ **New** menu to open the **Insert new line** dialog window.
- Select **858 Professional Sample Processor** ▸ **Peristaltic** ▸ **On/Off** in the left of the menu under commands.

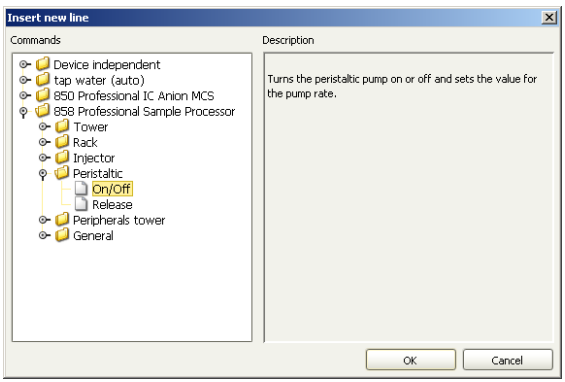


- Confirm with **[OK]**.
  The dialog window **858 Professional Sample Processor - Peristaltic - On/Off** opens.
- Use the **Time** field to accept the time data **0** min.

- Also accept the other field values.
- Confirm with **[OK]**.

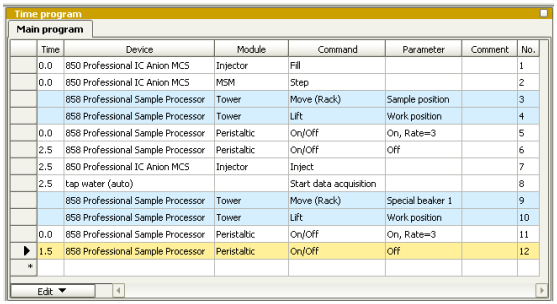
12 Switching off rinsing

- Use the **Edit** ▸ **New** menu to open the **Insert new line** dialog window.
- Select **858 Professional Sample Processor** ▸ **Peristaltic** ▸ **On/Off** in the left of the menu under commands.



- Confirm with **[OK]**.
  The dialog window **858 Professional Sample Processor - Peristaltic - On/Off** opens.
- Use the **Time** field to enter the value **1.5**.
- In the **Rate** area, select the option **Off**.
- Confirm with **[OK]**.

The complete time program appears as follows:



3.2.4 Evaluation

(see Chapter 3.1.4, page 37)

3.2.5 Saving method

Saving method

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

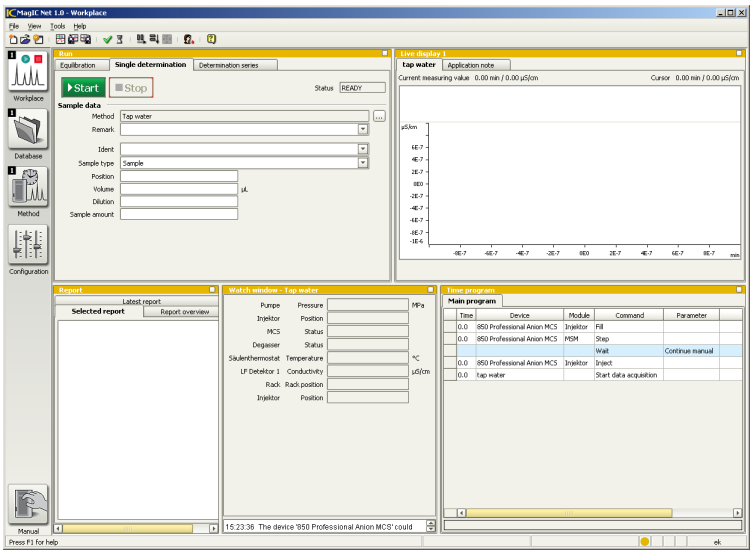
1. Use the **File ▸ Save as...** menu to open the **Save method** dialog window.
2. In the **Method name** enter **Tap water (auto)** as a name for the method.
3. Click on **[Save]**.

4 Performing the determination

In this section you will learn how to:

- Check retention times of the analytes
- Enter sample data
- Measure standards and samples.

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



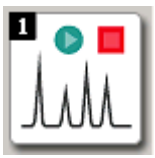
Run	Control of processes and management of the sample data
Live display 1	Visualization of the chromatogram during the analysis
Report	Displays the reports of analyses
Watch window	Information on the methods and associated devices
Time Program	Visualization of the method execution

Live display 2 Visualization of a second chromatogram running in parallel

4.1 Equilibration

Starting equilibration

Before the analysis is carried out, the IC device must be balanced for around 30 minutes until the baseline is stable.



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

2 Use the **Run** subwindow to select the **Equilibration** tab.

3 In the **Method** field, click on the … button.

4 In the **Open method** dialog window, highlight the method **Tap water**.

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

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

Recording of the baseline begins. As soon as the baseline is stable, the measurement can be started (after approx. 30 min).

Preparing suppressor manually

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

2 Select **Workplace** list box and highlight the **850 Professional IC Anions MCS** in the left part of the window.

3 Select the **MSM** tab.

4 Click on the **[Next]** button.

5 Click on the **[Next]** button again after 10 min.

6 Repeat step **5** twice again.

This ensures that all three chambers of the suppressor are regenerated.

4.2 Measuring standards and samples manually.

Standards

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

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

3 In the **Method** field, check whether the **Tap water** method is selected.

4 Use the **Sample type** list box to select **Standard 1**.

5 **Enter sample data**

Enter the following values in the fields:

- Use the **Ident** field to enter the name **Standard 1**.
- Use the **Position** field to enter the value **1**.
- Use the **Volume** field to enter the value **20**.
- Use the **Dilution** field to enter the value **1**.
- Use the **Sample amount** field to enter the value **1**.

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

The determination is started and the time program executed for manual determination

Lines highlighted in red show the current program stage, lines highlighted in blue show the processed program stage.

7 As soon as the message for filling appears, fill the injector manually.

8 Confirm the massage with **[Next]**.

The data recording is started and the determination executed to the end.

Repeat steps **4** to **8** for the measurements of standard 2 and standard 3. The **Sample type** list box is used to select **Standard 2** or **Standard 3** and the **Ident** field is used to enter the name **Standard 2** or **Standard 3**.

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

Information on the methods and associated devices is displayed in the **Watch window** subwindow.

Sample

1 Use the **Sample type** list box to select the entry **Sample**.

2 **Enter Sample data**

Enter the following values in the fields:

- Use the **Ident** field to enter the name **Tap water**.
- Use the **Position** field to enter the value **1**.
- Use the **Volume** field to enter the value **20**.
- Use the **Dilution** field to enter the value **1**.
- Use the **Sample amount** field to enter the value **1**.

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

The determination is started and the time program executed for manual determination.

4 As soon as the message for filling appears, fill the injector manually.

5 Confirm the massage with **[Next]**.

The data recording is started and the determination executed to the end.

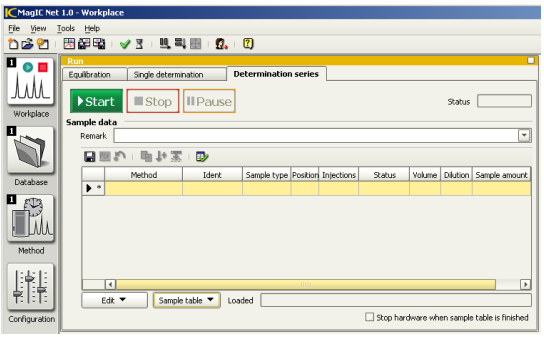
4.3 Measuring standards and samples automatically

Just as for a manual measurement, the IC device is first of all balanced *(see Chapter 4.1, page 70)*. The sample table is then created and the sample measured.

Creating new sample table

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

2 Use the **Run** subwindow to select the **Determination series** tab.



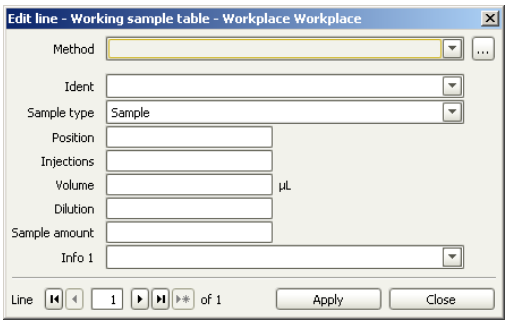
3 Use the **Edit** ▸ **Edit line** menu to open the dialog window **Edit line - Working sample table - Workplace**.

4 In the **Method** field, click on the … button.

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

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

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



5 Entering values for Standard 1

Enter the following values in the fields:

- Use the **Ident** field to enter the name **Standard 1**.
- Use the **Sample type** list box to select **Standard 1**.
- Use the **Position** field to enter the value **1**.
- Use the **Injections** field to enter the value **1**.
- Use the **Volume** field to enter the value **20**.
- Use the **Dilution** field to enter the value **1**.
- Use the **Sample amount** field to enter the value **1**.
- Click on **[Apply]**.

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

6 Entering values for Standard 2

- In the **Line** field click on the ▶ button.

The next higher value is automatically entered in the **Position** field. The values of standard 1 are automatically accepted in the **Injection**, **Volume**, **Dilution** and **Sample amount** fields.

- Use the **Ident** field to enter the name **Standard 2**.
- Use the **Sample type** list box to select **Standard 2**.
- Click on **[Apply]**.

7 Entering values for Standard 3

To enter standard 3, proceed in the same way as for step 6:

- Use the **Ident** field to enter the name **Standard 3**.
- Use the **Sample type** list box to select **Standard 3**.

8 Entering values for sample

To enter sample data, proceed in the same way as for step **5**:

- Use the **Ident** field to enter the name **Tap water**.
- Use the **Sample type** list box to select the entry **Sample**.
- Once all the data for the standards and the sample have been entered, click on the **[Close]** button and return to the **Determination series** tab.

9 Stopping hardware

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

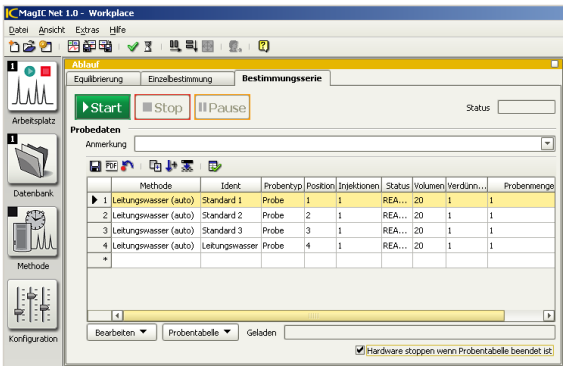
Note

The check box **Stop hardware when sample table is finished** must be activated if the devices are to be switched off after completion of the measurements (e.g. when measuring over night).

10 **Saving sample table**

- Use the **Sample table ▸ Save as...** to open the **Save sample table** dialog window.
- Use the **Name** field to enter the name **Tap water sample**.
- Click on **[Save]**.

The complete table with standards and sample appears as follows:



Measuring standards and samples

1 In the **Determination series** tab, click on the **[Start]** button.

The chromatograms of the three standards are then measured, followed by those of the sample. The current chromatogram recording can be tracked in the **Live display** subwindow. The current rack position as well as various IC parameters, such as conductivity, pressure, flow, degasser etc. are displayed in the **Watch window - tap water** subwindow.

Samples undergoing processing are highlighted in red, while measured samples are highlighted in blue.

4.4 Modifying retention times manually

In order to check and eventually modify the retention times of the seven components fluoride, chloride, nitrite, bromide, nitrate, phosphate and sulfate (specified in the method), the mean standard is measured in a single measurement.

Single measurement of a standard

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

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

3 Use the **Method** field to select the method **Tap water**.

4 Use the **Sample type** list box to select **Standard 2**.

5 **Enter sample data**

Enter the following values in the fields:

- Use the **Ident** field to enter the name **Standard 2**.
- Use the **Position** field to enter the value **1**.
- Use the **Volume** field to enter the value **20**.
- Use the **Dilution** field to enter the value **1**.
- Use the **Sample amount** field to enter the value **1**.

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

The determination is started and the time program executed for manual determination.

7 As soon as the message for filling appears, fill the injector manually.

8 Confirm the massage with **[Next]**.

The data recording is started and the determination executed to the end.

Correcting the retention times

Compare the retention times from the chromatogram with those in the method template. If there are deviations, enter the new retention times from the chromatogram into the component table as follows:

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

2 Click on the **Edit** ▸ **Refresh**.

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

4 Click on the line with the component whose retention time is to be corrected.

5 Click in the peak belonging to this 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 to be corrected.

5 Editing determinations

5.1 Viewing determinations

You have several options for selecting and viewing your determinations:

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

Sorting

1 Click on the symbol of the program part **Database**.

2 First click on the heading of the column for sorting in the table with all the databases.

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

3 Click again on the same column title.

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

Quick filter

1 Click on the menu **Determinations ▸ Filter ▸ Quick filter**.

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 serving as a filter criterion and click with the left mouse button.

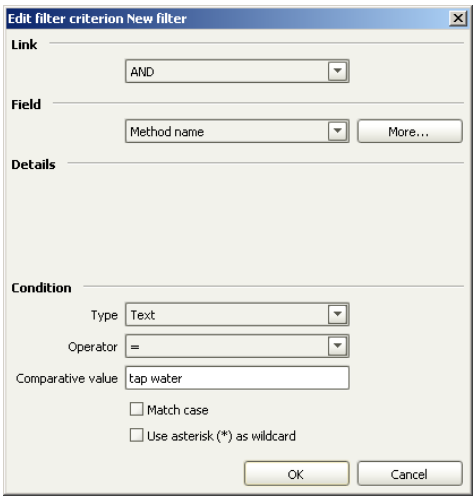
The datasets are filtered according to the content of the required table field. The quick filter can be applied again within the filtered table.

Special filter

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

1 Open the corresponding dialog window via the **Determinations ▸ Filter ▸ Special filter** menu.

2 Use the **Edit ▸ Edit line** menu to open the dialog window **Edit filter criterion New filter**.



3 In the **Field** list box, highlight the entry **Method name**.

4 Use the **Comparison value** field to enter the method name **Tap water** and click on **[OK]**.

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

The **Determination overview** subwindow then displays the table with all the datasets of the **Tap water** method.

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

The **Results** subwindow then displays a table with the components, their concentrations, retention times etc. The parameters of the table can be brought together in the **Properties result window** dialog window. It is opened by double clicking in the field of the results display or the menu **View ▸ Properties ▸ Properties Results**.

The chromatograms and the calibration curve are shown in the **Curves 1** subwindow.

Data of the sample, the devices etc., can be displayed in the **Information** subwindow via the individual tabs.

Search

1 Use the **Determinations** ▸ **Search** menu to open the **Search - Database 'MagIC Net'** dialog window.

2 In the **Search in** list box, highlight the entry **User (short name)**.

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

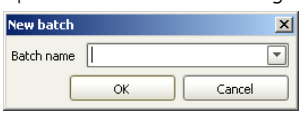
4 Click on **[Search next]**.

The first line corresponding to the search term is highlighted.

Batch (user-defined filter)

1 **Create batch**

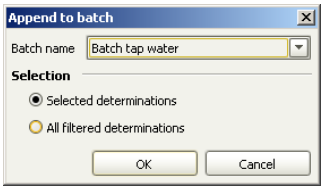
- Use the **Determinations** ▸ **Batch** ▸ **New batch** to open the **New batch** dialog window.



- In the **Batch name** field, enter the name **Batch tap water**.
- Click on **[OK]**.

2 Add determinations to batch

- Highlight the datasets in the table, which are to be added to the batch.
- Use the **Determinations ▸ Batch ▸ Append to batch** menu to open the **Append to batch** dialog window.



- In the **Batch name** list box, select the name **Batch tap water**.
- Higlight the option **Selected determinations**.
- Click on **[OK]**.

The datasets selected in the Determination overview are added to the batch and are available for selection at any time.

3 Deleting batch

- Use the **Determinations ▸ Batch ▸ Delete batch** menu to open the **Delete batch** dialog window.

- In the **Batch name** list box, select the name **Batch tap water**.
- Click on **[OK]**.

The batch is deleted from the database.

4 **Delete applied filter**

The **Determinations** ▸ **Filter** ▸ **Remove filter** menu is used to remove a special or quick filter currently applied and to remove a selected batch. All datasets are displayed again.

5.2 Viewing results

Zoom with mouse

The zoom function can be used to magnify individual areas of a chromatogram.

1 Highlight a dataset in the overview table.

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

2 Zoom in on the area to be magnified while keeping the left mouse button pressed.

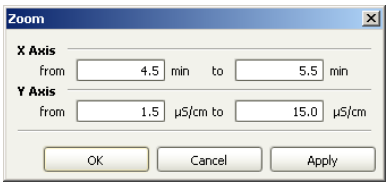
Zoom with dialog

1 Highlight a dataset in the Overview Table.

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

2 Click in the chromatogram with the right mouse button.

3 The **Zoom** context menu can be used to open the **Zoom** dialog window for entering the zoom range.



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

5 Click on **[OK]**.

The peak of nitrite is zoomed in.

Unzoom

1 Click in the chromatogram with the right mouse button.

2 Click on the context menu **Unzoom**.

The chromatogram is shown in its original size.

Changing the chromatogram visualization

You have the option of editing the properties of a chromatogram. You can change the visualization of the chromatogram, the labeling of the axes or the labeling in the chromatograms. Afterwards change the labeling of the peaks and the axes in the chromatogram. Proceed as follows:

1 **Changing peak labeling**

- Click in the chromatogram with the right mouse button.
- Select the menu item **Properties**.
- Select the **Chromatogram** tab.

- Activate the **Retention time** check box and deactivate the **Concentration** check box.
- Click on **[OK]**.

2 **Changing axis labeling**

- Click in the chromatogram with the right mouse button.
- Select the menu item **Properties**.
- In the **Properties - Graphics** dialog window, select the **Axes** tab.
- In the **X axis** area, click in the **Axis label** field, and enter **Retention time**.
- In the **Y axis** area, click in the **Axis label** field and enter **Conductivity**.
- Click on **[OK]**.

Visualizing calibration curve

1 Highlight a dataset in the overview table.

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

3 In the **Component** list box, select the entry **Nitrite**.

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

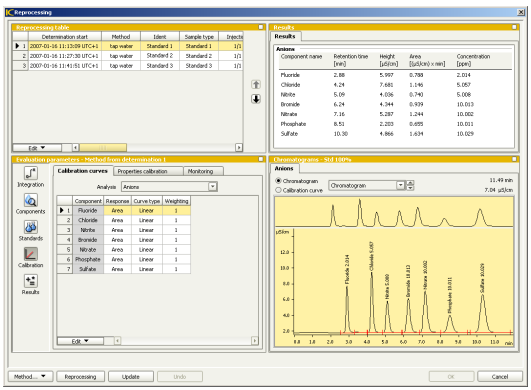
5.3 Reprocessing determinations

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

As an example, the evaluation over the peak height is described instead of over the peak area, which is defined in the method template.

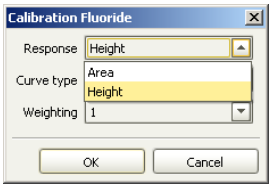
1 Reprocessing calibration curve

- Highlight the three standards in the **Determination overview** subwindow.
- Use the **Determinations** ▸ **Reprocess...** menu to open the corresponding dialog window.



- In the **Evaluation parameters** subwindow, click on the **[Calibration]** button.
- Select the **Calibration curves** tab.
- Highlight the first component (fluoride) in the table.

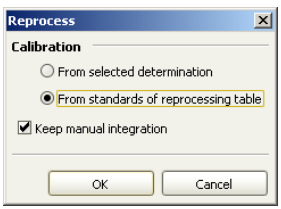
- Use the **Edit** ▸ **Edit** menu to open the **Calibration curve Fluoride** dialog window:



- In the **Response** field, select **Height** as a new parameter and click on **[OK]**.
- Use the **Edit** ▸ **Take over settings for all components** menu to accept the new measured quantity (response) for all components in the table.
  Repeat steps 5 to 8 for standard 2 and standard 3.
- Click on **[Update]**.

The calibration curves of the three standards are recalculated.

2 Open the Reprocess dialog window via the **[Reprocessing]** button.



3 Click on **[OK]**.

5.4 Create new report template

In order to create a report with the results of the analysis, you first of all have to define a report template. In the following you create:

- A report template for the calibration curve of the standard
- A report template with the result table and the chromatogram of the sample **Tap water**

Report template for calibration curve

1 ▪ Use the **Tools** ▸ **Report templates** ▸ **New** ▸ **Form report** menu to open the **Report template - New form report** dialog window.

- Click on the **Calibration curve** icon  in the toolbar.
- Place the mouse cursor (which now has the form of a cross) in the report template and create the required area by keeping the left mouse button pressed down. The **Properties - Calibration curve field** dialog window is opened.
- In the **Analysis** list box, enter **Standard 2** as an example.
- In the **Component** list box, enter the component **Nitrate** as an example.
- In the **Curve view** area of the **Properties - Calibration curve field** dialog window, select the **from database** option.
- Click on **[OK]**.
- Close the **Report Template - New form report** dialog window and confirm the **Save template** message with **[Yes]**.
- In the **Save report template** dialog window, use the **Name** field to enter the name **Calibration curve**.

- Click on **[Save]**.

Report template for result table/chromatogram

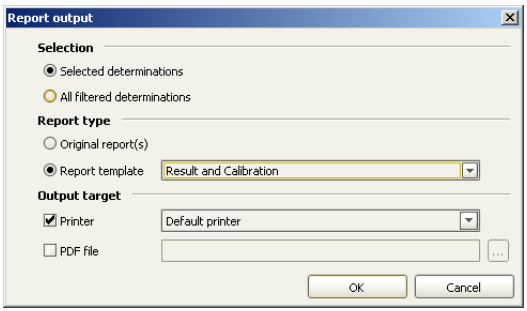
1 Creating result table

- Click on the **Curve + result table** icon  in the toolbar.
- Place the mouse cursor (which now has the form of a cross) in the report template and create the required area by keeping the left mouse button pressed down.
- In the **Properties Curve + result table field** dialog window, use the **Analysis** field to enter the sample name **Tap water**.
- Click on the **Result** button.
- In the **Available results** list, highlight the entry **Component name** and use the  key to move to the **Displayed results** list.
  The **Retention time**, **Area** and **Concentration** are added to the list in the same way.
- Highlight **Retention time** and click on **[Number of decimals]**.
- In the **Number of decimals - Retention time** dialog window, select the value **2**.
  For the decimal places of the **Area** and **Concentration** also enter the value **2**.
- Click on **[OK]**.
- Close the **Report template - New form report** dialog window and confirm the **Save template** message with **[Yes]**.
- In the **Save report template** dialog window use the **Name** field to enter the name **Results**.
- Click on **[Save]**.

5.5 Printing report

Printing calibration curve

1. In the **Determination overview** subwindow, highlight the line of standard 3.
2. Use the **File** ▸ **Print** ▸ **Report...** menu to open the **Report output** dialog window.
3. In the **Selection** area, highlight the **Selected determinations** option.
4. In the **Report type** area, highlight the **Report template** option and select the **Result and Calibration** report template.
5. In the **Output line** area, deactivate the **Printer** check box activate the **PDF file** check box.
6. The symbol … and in the **Save as** dialog window, use the **File name** field to enter the name **Calibration curve**.
7. Click on **[Save]**.



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

Printing results table/chromatogram

1 In the **Determination overview** subwindow, highlight the line with the entry **Tap water**.

2 Use the **File** ▸ **Print** ▸ **Report...** menu to open the **Report output** dialog window.

3 In the **Selection** area, highlight the **Selected determinations** option.

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

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

6 Click on the button … and in the **Save as** dialog window, use the **File name** field to enter the name **Sample**.