# **Metrohm IC Driver for OpenLab**



**Tutorial** 8.0102.8004EN / v6 / 2025-08-22





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# **Metrohm IC Driver for OpenLab**

1.0

## **Tutorial**

Technical Communication Metrohm AG CH-9100 Herisau

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Metrohm IC Driver for OpenLab

1 Overview

## 1 Overview

Metrohm IC Driver for OpenLab is a software driver for integrating Metrohm IC instruments in OpenLab 2.3 or higher.

Press F1 anywhere in the software to open the online help.

Metrohm IC Driver for OpenLab contains 3 different program areas.

- Control panel
- Acquisition
- Data analysis

## 1.1 Preconditions

The following preconditions must be fulfilled to ensure proper mode of operation:

- OpenLab is installed according to the Agilent instructions. Refer to the Agilent instructions for information concerning the minimum system requirements.
- The Metrohm IC Driver for OpenLab is installed according to the instructions (8.0102.8005EN Metrohm IC Driver for OpenLab Installation).



### NOTE

Refer to the OpenLab Help for further information about preconditions: **Getting Started** ▶ **Guides and Resources** ▶ **OpenLAB CDS** ▶ **Requirement Guide**.

## 1.2 Product versions

The product is available in the following versions:

Table 1 Product versions

Order number	Designation	Version feature
6.6080.100	Metrohm IC Driver for OpenLab	1.0

1.3 About the documentation

## 1.3 About the documentation



#### **NOTE**

Please read through this documentation carefully before putting the product into operation.

The documentation contains important information and warnings which you must follow in order to ensure safe operation of the product.

#### Symbols and conventions

The following icons and formatting may appear in this documentation:

[Next]	Button or key.
Work area / Properties	Menu paths in order to arrive at a particular position in the software.
File ► New	Menu or menu item
Method	Designations for names of parameters, menu items, tabs and dialog windows in the software.
	Carry out these steps in the sequence shown.
1	Instruction step
	The first number refers to the figure number, the second to the product part in the figure.
(5- <b>12</b> )	Cross-reference to figure legend

## 1.4 Terminology

For the understanding of this tutorial, it is important to define the terms **unit**, **module** and **instrument**.

A unit is a functional part of a module. Units are for example high-pressure pumps, injectors or degassers.

A module is an instrument with its own housing. A module consists of several units. Modules are for example 930/940/945 ICs, 858 Professional Sample Processors or 942 Extension Modules.

An instrument consists of several modules. An instrument contains all modules that are required for the analysis. An instrument is for example the combination of a 930 Compact IC Flex and an 858 Professional Sample Processor.

Instrument

Unit

Module

2 Control panel – Overview

## 2 Control panel – Overview

Open the **Control panel** to start OpenLab and the Metrohm IC Driver for OpenLab.

In the **Control panel**, the user can manage projects, instruments and administration settings.

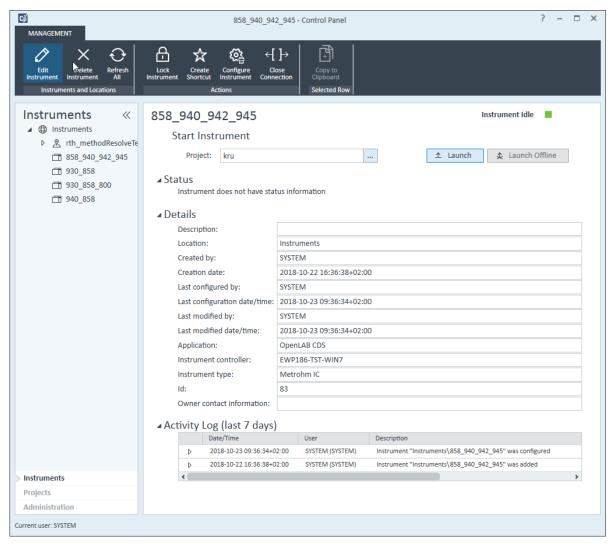


Figure 1 Control panel – Overview



#### **NOTE**

Refer to the OpenLab Help for information about administration, for example system configuration, licenses or diagnostics: **How**To ▶ OpenLAB CDS ▶ Control Panel ▶ Administration.

## 3 Creating a new project

To create a new project, go to **Control panel** ▶ **Projects**. Click on **Create** ▶ **Create Project**. Enter the following information:

- Name of the project
- Project folder path
   Click on **Browse** to select an existing project folder or create a new project folder.
- If project groups should be included in the project path, then check **Include project groups in project path**.
- Check OpenLAB CDS. This enables you to define CDS Settings, for example file locations or audit trail settings.

Click on **[OK]** to create the project.



#### **NOTE**

Refer to the OpenLab Help for information about creating and managing projects: **How To ▶ OpenLAB CDS ▶ Control Panel ▶ Projects**.

4 Creating a new instrument

## 4 Creating a new instrument

-----

To create a new instrument, go to **Control panel** ▶ **Instruments**. Click on **Create** ▶ **Create Instrument**. Enter the following information:

- Name of the instrument
- Instrument controller
   Select the desired instrument controller.
- Instrument type
   Metrohm IC
- Default project
   This is the location where the collected data is stored.
- If the instrument should always use the default project, then check always use default project with this instrument.
- The application is chosen automatically.

Click on **[OK]** to create the instrument.



#### **NOTE**

Refer to the OpenLab Help for further information about instruments: **How To ▶ OpenLAB CDS ▶ Control panel ▶ Instruments**.

## 5 Configuring the instrument

An instrument may maximally include the following modules:

- 2 x 930 Compact IC Flex, 940 Professional IC Vario or 945 Professional Detector Vario
  - Any combination of 940 Professional IC Vario, 930 Compact IC Flex and 945 Professional Detector is possible.
- 1 x 858 Professional Sample Processor
- 1 x 889 IC Sample Center
- 1 x 944 Professional UV/VIS Detector Vario or 947 Professional UV/VIS Detector Vario
- 1 x 941 Eluent Production Module
- 1 x IC Amperometric Detector per 930/940 IC
- The number of 942 Extension Modules Vario depends on the number of 940/945 ICs.
- The number of MSB devices (for example dosing units) depends on the number of available ports (according to the system configuration).
- 1 single quadrupole mass spectrometer from Agilent for IC-MS applications



#### **NOTE**

945 Professional Detectors behave in the same way as 930 and 940 ICs.



#### **NOTE**

You can only configure the instrument on Workstations (stand-alone systems) or on AICs (Agilent Instrument Controller). You cannot configure the instrument on clients or on servers.

You can configure the instrument either with automatic configuration or with manual configuration.



#### **NOTE**

Metrohm strongly recommends to configure the instrument with automatic configuration.

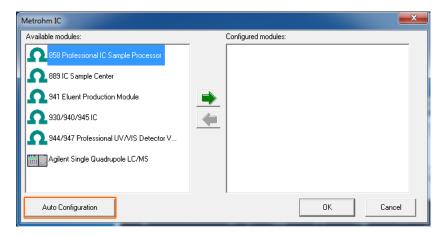
6

### **Automatic configuration**

-----

1 Click on Control panel ➤ Instruments ➤ Configure Instrument.

The Configuration window opens.



- 2 Click on [Auto Configuration].
- In the appearing window, click on **[OK]** to confirm that the driver should discover Metrohm instruments.

All connected modules are automatically recognized.

The **Post Auto Configuration** window appears.

- 4 To select the discovered modules, click on [Select All].
- 5 Click on [OK].



#### NOTE

If you click on **[Auto Configuration]** but do not want to select any modules to configure, then click on **[OK]** to abort.

Never click on **[Cancel]** or close the window. If you click on **[Cancel]** or close the window, then all modules are selected for the configuration.



#### **NOTE**

If you configure the instrument automatically, then the stirrer is deactivated by default. If you want to use the stirrer, then activate the stirrer in manual configuration of the 858 Professional Sample Processor (see chapter 5.2, page 12).

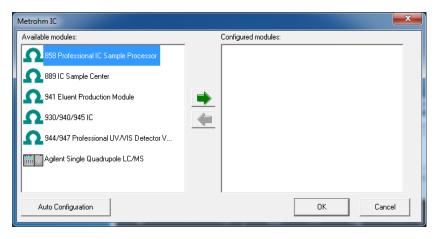
If you configure an instrument with a 941 Eluent Production Module automatically, then no level sensor is configured by default. Configure the rod length of the level sensors manually (see chapter 5.5, page 15).

#### **Manual configuration**

If it is not absolutely necessary, do not configure your instrument with manual configuration. Use automatic configuration instead of manual configuration.

1 Go to Control panel ► Instruments. Click on [Configure Instrument].

The **Configuration** window opens.



**2** Select a connected module from the **Available modules** window.



#### **NOTE**

In manual configuration, configure the modules in the following order:

- 1. 930/940/945 IC
- 2. 858 Professional Sample Processor
- 3. 889 IC Sample Center
- 4. 944/947 Professional UV/VIS Detector Vario
- 5. 941 Eluent Production Module

This is the same order as in automatic configuration. The order is relevant because you can only load a method if it was written on an instrument with the same order of modules.

- 3 Click on the green arrow to transfer the selected module from **Available modules** to **Configured modules**.
- **4** Double-click on a module to define the configuration settings.
- 5 If you want to deselect a module from **Configured modules**, then select the module and click on the red arrow.
- 6 Click on [OK].

After configuring the desired modules and defining the configuration settings, click on **[Launch]**.

The connection to the instrument is established. The **Acquisition** window opens.

To configure a new instrument or to disconnect the instrument, click on **[Close Connection]**.



#### **NOTE**

Refer to the OpenLab Help for further information about instrument configuration: **How To ▶ OpenLAB CDS ▶ Control panel ▶ Instruments**.

5.1 930/940/945 IC

### 5.1 930/940/945 IC



#### **NOTE**

Metrohm strongly recommends to configure the instrument with automatic configuration.

However, if you configure the instrument manually, proceed as follows.

#### Communication

Enter the following parameters:

- Device name
- Type ID
- Serial number

When you launch the instrument, Metrohm IC Driver for OpenLab checks the type ID and serial number. It is not possible to launch the instrument if the actual type ID or serial number do not match the configured type ID or serial number.

#### Options ▶

#### **Detectors**

Select the desired detectors from the drop-down list. The following detectors are available:

- Conductivity Detector
  - Click on [Configure] to set further parameters.
    - Cell Constant
    - Thermostat
- Amperometric Detector

You can configure 1 detector when using the 930 Compact IC Flex, the 945 Professional Detector Vario – Conductivity and the 945 Professional Detector Vario – Amperometry.

You can configure 2 detectors when using the 940 Professional IC Vario and the 945 Professional Detector Vario – Conductivity & Amperometry.

If you configure a 930 Compact IC Flex or a 940 Professional IC Vario with a detector, then the module runs through the following states at the start of a run: **Pre-run**, **Injecting**, **Run** 

If you configure a 930 Compact IC Flex or a 940 Professional IC Vario without a detector, then the module behaves in the same way as an 858 Professional Sample Processor. If you start a run, then the module skips the state **Injecting**. The module runs through the following states at the start of a run: **Pre-run**, **Run** 

#### MSB

Select the desired MSB devices from the drop-down lists. The following MSB devices are available:

770 Remote Box

10 ----

■ 800 Dosino

Click on **[Configure]** to set further parameters (see chapter 5.6, page 16).

#### Extension modules

-----

Select the desired extension modules from the drop-down list. The following extension modules are available:

- 942 Extension Module Vario ONE/Deg (2.942.1060)
- 942 Extension Module Vario SeS/PP (2.942.0500)

#### **Gradient Pumps**

For 940 ICs with 2 high-pressure pumps, it is possible to configure a gradient pump for a high-pressure gradient.

A high-pressure gradient can only be configured for **940 Professional ICs Vario** and for **942 Extensions Modules Vario** that are connected to a 940 Professional IC Vario. A high pressure gradient cannot be configured for 930 Compact ICs Flex.

Define the following parameters:

- Number of Pumps
   Define how many pumps the high-pressure gradient pump consists of.
- Pump A D
   Assign the high-pressure pumps to the gradient pump.

#### Dose-in gradient

For ICs with a high-pressure pump and a Dosino, it is possible to configure a gradient pump for a Dose-in gradient.

Define the following parameters:

- Pumps
  - Select a high-pressure pump that you want to use for the Dose-in gradient pump.
- Dosino

Assign a Dosino to the selected high-pressure pump.

#### Regeneration

For ICs with an MSM and a Dosino, it is possible to configure Dosino regeneration for the MSM.

Define the following parameters:

- MSM
  - Select an MSM to be regenerated by a Dosino.
- Dosino
- Assign a Dosino to the selected MSM.



#### NOTE

An instrument may maximally contain 1 high-pressure gradient pump, 1 Dose-in gradient pump and 1 Dosino for Dosino regeneration.



#### **NOTE**

A Dosino can be used either for a Dose-in gradient or for Dosino regeneration or as a normal Dosino or for eluent production in the 941 Eluent Production Module. A Dosino cannot be configured for several functions. A high-pressure pump can be used either for a high-pressure gradient or for a Dose-in gradient or as a normal high-pressure pump. A high-pressure pump cannot be configured for several functions.

-----



#### NOTE

If you want to use a Dosino for Dosino regeneration or a Dose-in gradient, then configure it for a 930/940 IC. It is not possible to use Dosinos at the 858 Professional Sample Processor for Dosino regeneration or Dose-in gradients.

If you want to use a Remote Box as an MSB device and configure it manually, then configure it for the 930/940/945 IC. It is not possible to select the Remote Box as an MSB device for the 858 Professional Sample Processor.

## **5.2** 858 Professional Sample Processor



#### NOTE

If you configure the instrument automatically, then the stirrer is deactivated by default. If you want to use the stirrer, then activate the stirrer in manual configuration of the 858 Professional Sample Processor.

#### Communication

Enter the following parameters:

- Device name
- Type ID
- Serial number

When you launch the instrument, Metrohm IC Driver for OpenLab checks the type ID and serial number. It is not possible to launch the instrument if the actual type ID or serial number do not match the configured type ID or serial number.

#### Options >

MSB

The 800 Dosino can be selected as an MSB device.

5 Configuring the instrument

Misc

-----

Click on [Configure] to set further parameters (see chapter 5.6, page 16).

Select the desired rack from the drop-down list.

Define whether you want to use a stirrer or not.

## 5.3 889 IC Sample Center



#### **NOTE**

Metrohm strongly recommends to configure the instrument with automatic configuration.

However, if you configure the instrument manually, proceed as follows.

#### Communication

Enter the following parameters:

- Device name
- Type ID
- Serial number

You cannot find the serial number of the 889 IC Sample Center on the module. Contact a Metrohm service engineer, if you need to know the serial number of your 889 IC Sample Center.

When you launch the instrument, Metrohm IC Driver for OpenLab checks the type ID and serial number. It is not possible to launch the instrument if the actual type ID or serial number do not match the configured type ID or serial number.

#### Options ▶

Misc

Enter the following parameters:

- Syringe volume
   Volume of the syringe.
- Buffer loop
   Volume of the buffer loop.
- Sample loop
   Volume of the sample loop of the injection valve.
- Needle to valve
   Whole volume, from the needle tip to the injection valve.

The syringe volume and the buffer loop volume have to match. Ensure that the volumes correspond to one of the following combinations:

- Syringe volume = 250 μL
   Buffer loop volume = 500 μL
- Syringe volume = 500 μL
   Buffer loop volume = 1'000 μL
- Syringe volume = 1'000 μL
   Buffer loop volume = 2'000 μL

#### Racks

Refer to the manual 8.889.8001 IC Sample Center for further information.

-----

- Left rack
   Select a rack type.
- Right rack
   Select a rack type.

Select the same rack type for both rack holders or a combination with **None** and any rack type.

The racks can also be changed in manual control (see chapter 12.1.3, page 77).

## 5.4 944/947 Professional UV/VIS Detector Vario



#### **NOTE**

Metrohm strongly recommends to configure the instrument with automatic configuration.

However, if you configure the instrument manually, proceed as follows.

#### Communication

Enter the following parameters:

- Device name
- Type ID
- Serial number

When you launch the instrument, Metrohm IC Driver for OpenLab checks the type ID and serial number. It is not possible to launch the instrument if the actual type ID or serial number do not match the configured type ID or serial number.



#### NOTE

In an instrument with a 944/947 Professional UV/VIS Detector Vario and an 858 Professional Sample Processor, connection problems may occur. In case of connection problems, reconfigure the instrument or establish a fresh connection.

5 Configuring the instrument

## 5.5 941 Eluent Production Module



#### **NOTE**

If you configure an instrument with a 941 Eluent Production Module automatically, then no level sensor is configured by default. Configure the rod length of the level sensors manually.

#### Communication

Enter the following parameters:

- Device name
- Type ID
- Serial number

When you launch the instrument, Metrohm IC Driver for OpenLab checks the type ID and serial number. It is not possible to launch the instrument if the actual type ID or serial number do not match the configured type ID or serial number.

#### **Options** ▶

#### **Rod length**

Select the rod length of the sensors. Always configure the level sensors manually. No level sensors are configured with **Auto Configuration**.

- Shor
  - A sensor with a short rod automatically goes into full mode.
- Long

A sensor with a long rod automatically goes into empty mode.

#### MSB

Select an 800 Dosino as an MSB device to produce eluent.

A sensor with 800 Dosino can only produce eluent, but not monitor the fill levels.

A sensor without 800 Dosino can only monitor the fill levels, but not produce eluent

Each MSB port is assigned to a sensor. This assignment is fixed and the user cannot change it.

- Sensor 1 No MSB connector
   It is not possible to configure an 800 Dosino for Sensor 1. Sensor 1 can only be used for monitoring.
- Sensor 2 MSB 2
- Sensor 3 MSB 3
- Sensor 4 MSB 4

Click on **[Configure]** to set parameters of the 800 Dosino (see chapter 5.6, page 16).

5.6 MSB devices

## 5.6 MSB devices



### **NOTE**

Metrohm strongly recommends to configure the instrument with automatic configuration.

However, if you configure the instrument manually, proceed as follows.

Dosing unit settings	
Serial Number	Enter the serial number of the 800 Dosino, not the serial number of the cylinder unit.
Volume	Volume of the cylinder.
	When you launch the instrument, Metrohm IC Driver for OpenLab checks the volume of the cylinder. An error is generated if the actual cylinder volume does not match the configured cylinder volume.
Tubing Parameters ►	Parameters for the tubing that is connected to the dosing unit.
	These parameters are important for the correct execution of the commands <b>Prepare</b> and <b>Empty</b> because they take the volumes of the tubing connections into account.
Port	Port to be used as the dosing port. Assign a port 1 - 4 to each dosing port.
Length (cm)	Length of the tubing on the dosing port.
Dosing Rate	Diameter of the dosing rate.
(mL/min)	The value depends on the volume of the cylinder unit. When the function is carried out, the dosing rate is automatically decreased to the highest possible value.
Preparation Parame- ters	Configure the parameters for preparing and emptying the dosing unit (see menu "Dosing unit ", page 47), (see menu "Empty", page 99).
	Dosing port through which the cylinder content is ejected during preparation and emptying.
	Dosing port for the <b>Prepare</b> and <b>Empty</b> commands is always <b>Dosing Port 1</b> .
Valve ►	
Rotation Direc-	Rotating direction of the valve disk.
tion	<ul> <li>Ascending</li> <li>The valve disk rotates in the direction of ascending port numbers.</li> </ul>

5 Configuring the instrument

	<ul> <li>Descending         The valve disk rotates in the direction of descending port numbers.     </li> <li>Automatic         The valve disk rotates in the direction with the shortest path.     </li> <li>Not Over         The valve disk does not cross the specified port during rotation.     </li> </ul>
Not Over	This field gets activated if you select the rotation direction <b>Not Over</b> .  This port is not crossed during rotation.

The Remote Box is also an MSB device but the Remote Box does not need to be configured.

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## 6 Acquisition window – Overview

The **Acquisition** window appears automatically after launching the instrument.

In the **Acquisition** window, the user can set the instrument parameters, monitor the instrument status and current runs, create methods, create time programs and acquire data.

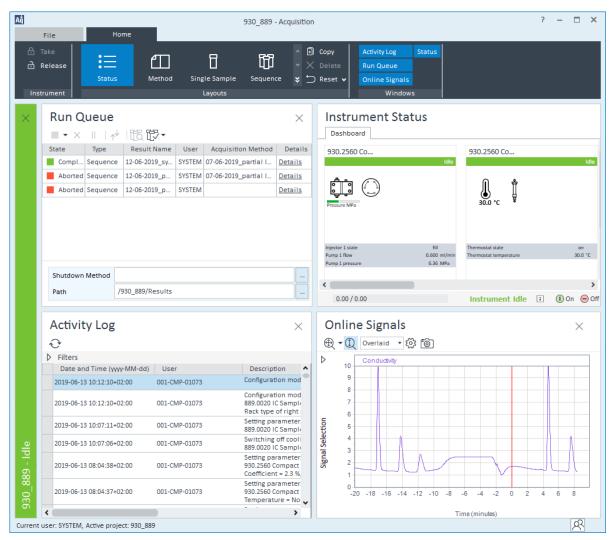


Figure 2 Acquisition window – Overview



#### **NOTE**

Refer to the OpenLab Help for further information about acquisition: **How To ▶ OpenLAB CDS ▶ Acquisition**.

7 Numbering of the units

## 7 Numbering of the units

If you set start parameters and time program commands, you have to select the index of the respective unit.

The numbering of each unit depends on its position in the daisy chain. The daisy chain defines how multiple modules are wired together in sequence.

- For 930/940/945 ICs this means: The upper unit always gets the number 1, the lower unit number 2 (for example for pumps and injectors).
- For extension modules this means: Only 1 extension module can be connected directly to the IC. The second extension module has to be connected to the first and the third to the second. The numbering of the units begins with the IC and continues with the extension modules according to their position in the daisy chain.
- For detectors this means: The sockets to plug in detectors are numbered. This number determines the index of a detector. Therefore, it is possible that only 1 detector is connected but labeled as **Detector 2** because it is plugged in socket 2.



#### NOTE

The numbering is fixed and cannot be changed manually.

In the status panels, the numbers of the units are not shown. Distinguish identical units by their position in the status panel.

Table 2 Numbering of the units in the status panel

1	3
2	4

### **Example dosing units:**

Numbering of the dosing units in the status panel. The instrument contains 3 dosing units that are connected to the 858 Professional Sample Processor.

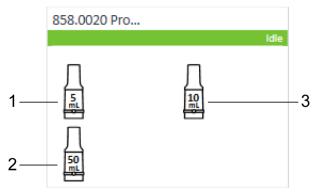


Figure 3 Numbering of the dosing units

## **Example high-pressure pumps:**

Numbering of the high-pressure pumps in the status panel. The instrument contains 2 high-pressure pumps that are connected to the 940 Professional IC Vario.



Figure 4 Numbering of the high-pressure pumps

8 Method

## 8 Method

Metrohm IC Driver for OpenLab distinguishes between 2 types of methods.

- Acquisition method
   Acquisition methods contain start parameters of the configured modules and a time program to define commands for the configured modules.
- Processing method
   A processing method contains information regarding data processing, for example information regarding analytes and their retention times, level of standards and integration parameters. Create and manage processing methods in the **Data analysis** window (see chapter 18, page 106).

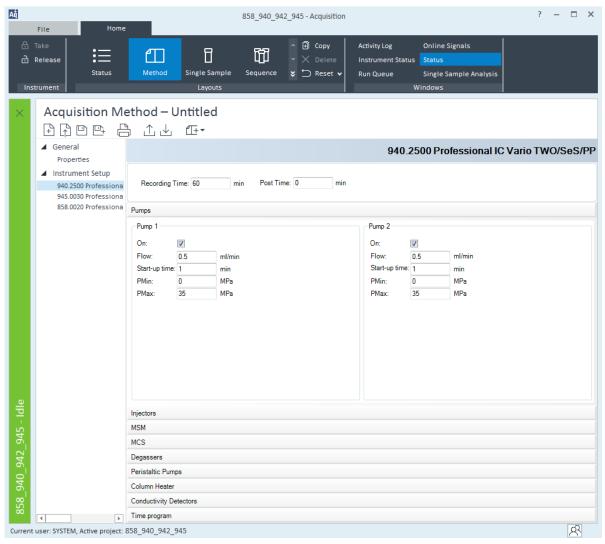


Figure 5 Acquisition method – Overview



#### **NOTE**

Refer to the OpenLab Help for further information about acquisition methods: **How To ▶ OpenLAB CDS ▶ Acquisition ▶ Acquisition methods**.

8 Method

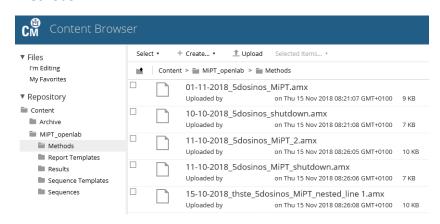
## 8.1 Acquisition method

The USB flash drive contains an acquisition method to analyze standard anions with sequential suppression. Proceed as follows to import the acquisition method:

## Importing an acquisition method

Connect to the **OpenLab Server** to open the content browser.

- 1 Go to Windows start ► Agilent Technologies ► OpenLAB Content Management ► Content Browser.
- 2 In the repository, navigate to your project. Open the folder **Methods**.



- 3 Click on 1 Upload .
- 4 Click on **[Browse]**. Navigate to the acquisition method on the USB flash drive (*Acquisition method\_IC\_Anions\_1.amx*). Click on **[Open]**.

Alternatively, load the method into the folder by using the drag-and-drop fuctionality.

The acquisition method is added to the folder **Methods** in the content browser.

You can open the method in the acquisition window (see chapter 8.1, page 23).

Metrohm IC Driver for OpenLab

8.1 Acquisition method



#### **NOTE**

If your OpenLab installation does not include content management, then copy the acquisition method from the USB flash drive with the installation files to a local folder for methods.

Proceed as follows to load the imported method:

### Loading an acquisition method

1 Go to Acquisition ► Home. Click on [Method].



- **3** Navigate to the folder where the method is stored.
- 4 Select a method. Click on [Open].
- **5** Adjust the method parameters if necessary. Synchronize time programs with events (see chapter 8.2, page 25) if necessary.

To start the acquisition method with start parameters and time program, run a single sample analysis or a sequence (see chapter 17, page 103).



### NOTE

To save time, run 2 commands in parallel. Activate the checkbox **Parallel**. While a command is being executed, the time program already continues with the next line. This option is possible for all time program commands of the dosing unit and for the time program command **Move**.

If the same unit is used for several commands at the same time, an error is generated, but not all units are stopped.

8 Method



#### **NOTE**

A sequence uses acquisition methods in the way they are when the method is submitted. It is not possible to apply changes to the acquisition method during a sequence. Start a new sequence to apply changes to the acquisition method.

## 8.2 Synchronizing events

Each module has its own time program. These time programs run in parallel but independently of each other. Synchronize time programs with the time program commands **Event Set**, **Event Wait** and **Event Reset**.

Match different events by labeling them with the same name.

There are 5 predefined names that can be selected in the drop-down list. It is also possible to define individual names.

#### Event set

**Event sets** trigger actions in other time program commands. An **event set** indicates the moment when another time program has to execute its commands.

As soon as the time program reaches the line with the **event set**, other time programs can see the **event set**.

#### Event wait

An **event wait** is always looking for **event sets** with the same name. If the **event wait** of a time program detects a corresponding **event set**, then the time program executes the commands that follow after the **event wait**.

#### Event reset

An **event reset** removes the corresponding **event set**. If you set an **event reset**, then the **event wait** keeps on looking for the corresponding **event set** and does not execute subsequent time program commands.

#### **Example**

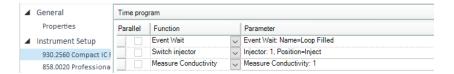
This example describes the synchronization of 2 time programs with events.

Both time programs start in parallel.

First, the sample processor transports the sample to the injector. Then the IC injects and starts measuring, while the sample processor rinses the needle. Therefore, the time program of the IC must wait until the sample processor has transported the sample to the injector.

8.2 Synchronizing events

### **Time program - 930 Compact IC Flex**



## 1 Event Wait: Name=Loop Filled

The time program of the IC is looking for an event set called **Loop Filled**.

When the event set **Loop Filled** is executed in the time program of the sample processor, the IC starts executing the commands in line 2 and line 3.

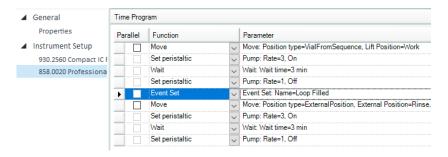
## 2 Switch injector

The IC switches the injector to the position Inject.

## **3 Measure Conductivity**

The conductivity detector of the IC starts recording the conductivity.

## **Time program - 858 Professional Sample Processor**



#### 1 Move

The sample processor moves to a position on the rack to take a sample.

## 2 Set peristaltic

The peristaltic pump of the sample processor starts on rate 3.

8 Method

#### 3 Wait

The time program of the sample processor waits for 3 minutes before it continues with the next line. During the waiting time, the peristaltic pump transports the sample to the injector.

#### 4 Set peristaltic

The peristaltic pump of the sample processor stops.

#### 5 Event Set: Name=Loop Filled

This event set matches the event wait of the IC because both events have the same name.

As soon as the time program of the IC reaches the line with the event wait command, the time program of the IC starts looking for the corresponding event set.

Now the IC starts executing the commands that follow the event wait command.

#### 6 Move

The sample processor moves to a position on the Liquid Handling Station.

#### 7 Set peristaltic

The peristaltic pump of the sample processor starts on rate 3.

#### 8 Wait

The time program of the sample processor waits for 3 minutes before it continues with the next line. During the waiting time, the needle is rinsed in the Liquid Handling Station.

#### 9 Set peristaltic

The peristaltic pump of the sample processor stops.

# 8.3 Equilibrating the instrument

Equilibrate the instrument with an equilibration method or with blank injections at the beginning of the sequence.

-----

#### **Running an equilibration method**

1 Enter the start parameters that you want to use for the measurement or load a method that contains the desired start parameters.

Click on 🕹 .

The instrument executes the start parameters. The instrument does not acquire data.

**3** Monitor the equilibration in **Online signals**.

#### **Running blank injections**

- 1 Create or open the sequence that you want to use for data acquisition.
- Add 1-3 lines with the sample type **Blank** at the beginning of the sequence. These vials can contain ultrapure water, for example.
- Do not add a processing method to these lines with the sample type **Blank**.

The results are excluded from data analysis. These results are not meaningful.

8 Method

#### 8.4 Shutdown method

A shutdown method is an acquisition method with the purpose to shut down the instrument.

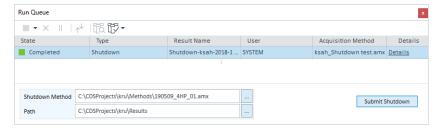
In a shutdown method, the instrument executes the start parameters but does not acquire data. Therefore, a shutdown method does not require a time program. A shutdown method cannot use information from the sequence table, for example the injection volume.

The USB flash drive contains a shutdown method (Shutdown method\_IC\_Anions.amx). Import the shutdown method in the same way as you imported the acquisition method (see chapter 8.1, page 23)

Proceed as follows to run a shutdown method:

#### Running a shutdown method

1 Go to the Run Queue.



**2** Click on [...].

A window to select a shutdown method appears.

- **3** Navigate to the folder where the method is stored.
- 4 Select a method. Click on [Open].
- 5 Click on [Submit Shutdown Run].

The shutdown method appears in the run queue and is executed.

8.5 Processing method



#### **NOTE**

Metrohm recommends to use shutdown methods without time program and with a recording time of 0 minutes.

If you use a method with time program as a shutdown method, then the time program is executed in the shutdown method. Time program commands that use information from the sequence cannot be used in the time program of a shutdown method.

Do **not** use the following commands in the time program of a shutdown method:

- Dosing unit commands Volume mode
  - Injection volume
    - Injection volume next sample
- Move Position type
  - Vial from Sequence
  - Next Vial from Sequence
  - Vial from Sequence +1
- Event wait



#### NOTE

If you submit a shutdown method, then the activity log may show an error message. This message is a notification to inform the user that no data is recorded and saved for this run. The shutdown method works correctly despite the message.

# 8.5 Processing method



#### **NOTE**

Refer to the OpenLab Help for further information about processing methods: How To ▶ OpenLAB CDS ▶ Data Analysis ▶ Working with Processing Methods.

30 ----

# 9 General description of parameters

#### 9.1 Manual control

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The status panels display the current state of the configured modules and enable the user to operate units manually. Status panels are located in the **Dashboard**.

The units of a module are shown in different status panels.

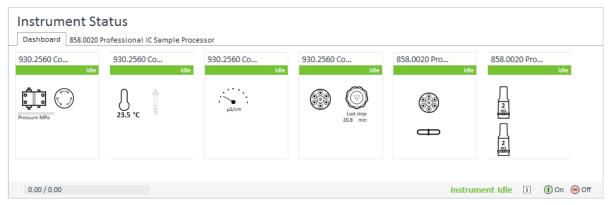


Figure 6 Dashboard – Overview

To open the **Dashboard**, go to **Acquisition** ▶ **Home**. Click on **[Status]**.



#### NOTE

All units of a module indicate the state of the module, not the state of the individual unit.

The state is displayed in the status panels and at the bottom of the dashboard. During initialization, the status panels display **Not Ready** but the dashboard already displays **Instrument Idle**. If the status panels and the dashboard display a different state, then the state of the status panels is relevant.

The status **Injecting** is not available for the 858 Professional Sample Processor and the 889 IC Sample Center. In an instrument that contains an IC and an autosampler, the autosampler is in status **Run** while the IC is in status **Injecting**.

9.1 Manual control



#### **NOTE**

An **[On]** button is located at the bottom of the **Dashboard**. This button has no functionality for Metrohm instruments. You cannot start the instrument with **[On]**. To start the instrument, send a method to the instrument or start units in manual control.

The same applies for the **[On]** and **[Off]** buttons on each status panel.

An **[Off]** button is located at the bottom of the **Dashboard**. Shut off the instrument with **[Off]**. The cooling of the 889 IC Sample Center is not switched off with the **[Off]** button. Switch off the cooling of the 889 IC Sample Center manually.

Click on in the bar at the top end of a status panel to display the current parameters.



Figure 7 Status panel of peristaltic pump and stirrer



Figure 8 Extended status panel of peristaltic pump and stirrer

Open the manual control of a unit by right-clicking on the respective icon in the status panel.

Always click on [Apply] to confirm changes in manual control.



#### **NOTE**

If the instrument goes offline, the status panels do not show the actual instrument state anymore. The status panels display the instrument state at the time the instrument was last online. The hardware does not switch off automatically if the instrument goes offline. To ensure that the hardware is off, switch off the hardware with the power-off button.

# 9.2 Start parameters

-----

Start parameters are sent to the units when you start the method.

To open the **Method** section, go to **Acquisition** ► **Home**. Click on [Method].

Click on a unit to set its start parameters. If the instrument contains 2 units of the same type (for example 2 high-pressure pumps), then the same menu appears for both units. The start parameters of both units can be set independently.

Define the length of the analysis in **Recording Time**. If you need additional time after recording the chromatogram, define it in **Post time**.

9.3 Time program

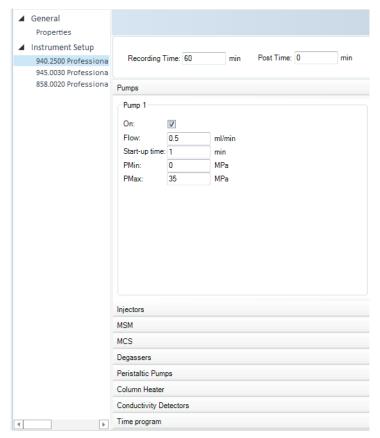


Figure 9 Start parameters – Overview

# 9.3 Time program

Write a time program to set the chronological order of actions during your measurement.

To write a time program, go to **Acquisition** ➤ **Home**. Click on **[Method]**. The last line of a module's method editor contains the time program.

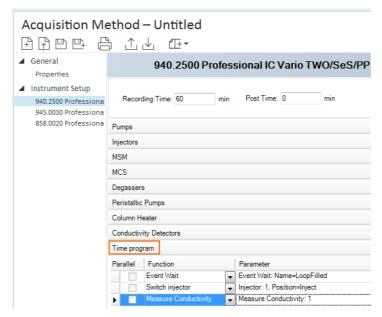


Figure 10 Time program – Overview

If several modules are configured (for example 940 Professional IC and 858 Professional Sample Processor), then each module has its own time program. Several modules can be synchronized with events.

To write a time program command, click on **[Add]**. Select a command in the drop-down list and define the command in the window that appears.

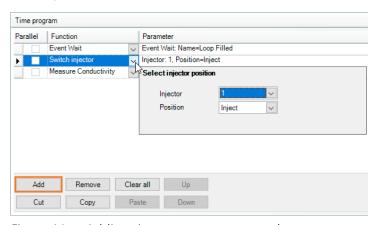


Figure 11 Adding time program commands

If the instrument contains a detector, the time program must contain a measure command, for example **Measure Conductivity** or **Measure Absorbance**. Otherwise, the instrument stays in the state **Injecting** and does never enter the state **Run**. If you do not want to acquire data during the run, then add a time program command **Measure Conductivity** at the end of the time program and define a recording time of 0 minutes.

Time program commands that are listed after a measure command in the time program must not take longer than the sum of recording time and post time. After the recording time and post time, the time program

9.3 Time program

is aborted even though not all time program commands have been executed. The recording time is equal to the measurement duration of measure commands in the time program.



#### **NOTE**

To save time, run 2 commands in parallel. Check the checkbox **Parallel**. While a command is being executed, the time program already continues with the next line. This option is possible for all time program commands of the dosing unit and for the time program command **Move**.

# 10 Parameters of the 930/940/945 IC and 942 Extension Module Vario

The 930 Compact IC Flex and 940 Professional IC Vario are ion chromatographs. The 930 Compact IC Flex and 940 Professional IC Vario are available in various product versions with different units.

With the 940 Professional IC Vario, it is possible to measure 2 channels (depending on the product version).

The 945 Professional Detector Vario is treated like an IC in the Metrohm IC Driver for OpenLab. The 945 Professional Detector Vario is a stand-alone detector for conductivity detection and/or amperometric detection. It can be combined with the 930 Compact IC Flex and 940 Professional IC Vario.

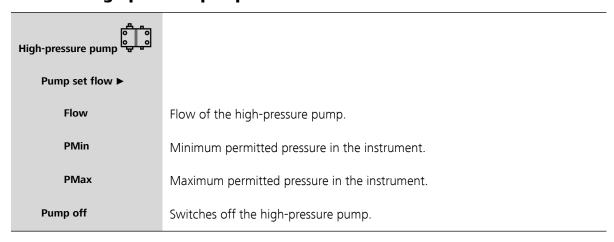
The 942 Extension Modules Vario are used to expand instruments with additional functions. The Metrohm IC Driver for OpenLab supports 2 product versions of the 942 Extension Module Vario:

- 942 Extension Module Vario ONE/Deg: Expands your instrument with an additional channel.
- 942 Extension Module Vario SeS/PP: Expands your instrument with sequential suppression.

#### 10.1 Manual control

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#### 10.1.1 High-pressure pump



10.1 Manual control

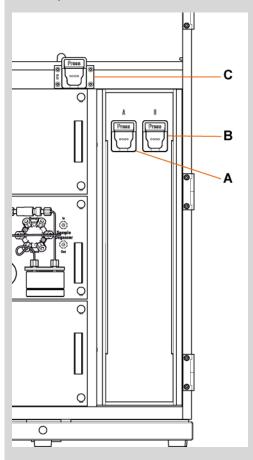


#### **NOTE**

Besides the PMax that is defined in the manual control, there is a PMax written on the column chip. If these values differ, then an error is generated as soon as the **lower** of these values is exceeded.

Each column holder is assigned to a high-pressure pump.

- Pump 1 Column holder A
- Pump 2 Column holder B
- Pump 3 Column holder C





#### **NOTE**

If the high-pressure pump is used for a Dose-in gradient, this is indicated with **D1** in the icon.



You can also define settings for the high-pressure pump in the start parameters (see chapter 10.2.1, page 48) and in the time program (see chapter 10.3.4, page 64).

#### 10.1.2 Injector

-----



**Injector Inject** 

Switches the valve to **Inject**.

Injector Fill

Switches the valve to Fill.

You can also define settings for the injector in the start parameters (see chapter 10.2.2, page 49) and in the time program (see chapter 10.3.1, page 63).

#### 10.1.3 MSM



MSM Step

The MSM steps. The time since the last step is reset.

With dosino regeneration, the default dosing rate of 1.0 mL/min is applied. It is not possible to change the dosing rate in manual control. If you want to use a different dosing rate, edit the dosing rate in the MSM start parameters (see menu "MSM 1", page 49) and send the method to the instrument.

MSM AutoStep ▶

Automatic stepping of the rotor to the next position starts.

Interval

Time interval between 2 sequential automatic rotor stepping operations.

With dosino regeneration, the default dosing rate of 1.0 mL/min is applied. It is not possible to change the dosing rate in manual control. If you want to use a different dosing rate, edit the dosing rate in the MSM start parameters (see menu "MSM 1", page 49) and send the method to the instrument.

MSM AutoStep off

Automatic stepping of the rotor to the next position stops.

10.1 Manual control



#### **NOTE**

If the MSM is regenerated by a Dosino, this is indicated with **M1** in the icon.



You can also define settings for the MSM in the start parameters (see chapter 10.2.3, page 49) and in the time program (see chapter 10.3.2, page 63).

#### 10.1.4 MCS

MCS	
MCS On	Switches on the MCS.
MCS Off	Switches off the MCS.

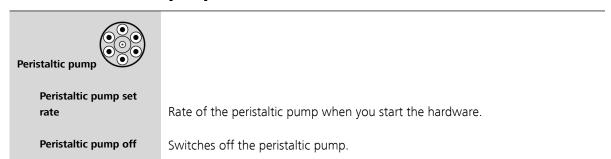
You can also define settings for the MCS in the start parameters (see chapter 10.2.4, page 50).

#### 10.1.5 Degasser

Degasser	
Degasser On	Switches on the degasser.
Degasser Off	Switches off the degasser.

You can also define settings for the degasser in the start parameters (see chapter 10.2.5, page 50).

#### 10.1.6 Peristaltic pump

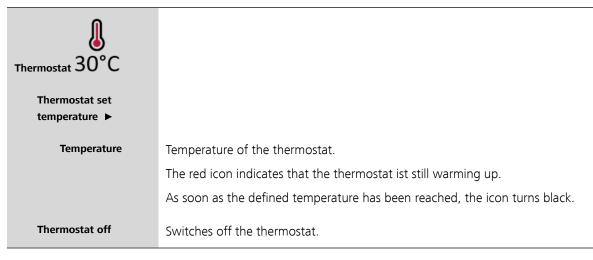


40 ----

You can also define settings for the peristaltic pump in the start parameters (see chapter 10.2.6, page 50) and in the time program (see chapter 10.3.3, page 64).

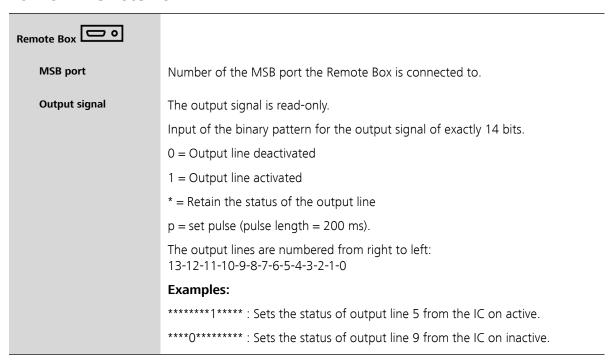
#### 10.1.7 Thermostat

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You can also define settings for the thermostat in the start parameters (see chapter 10.2.7, page 51).

#### 10.1.8 Remote Box



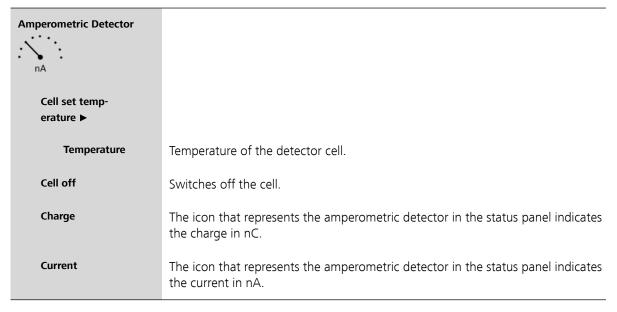
You can also define settings for the Remote Box in the time program (see chapter 10.3.5, page 64).

10.1 Manual control

## 10.1.9 Conductivity detector

You can define settings for the conductivity detector : in the start parameters (see chapter 10.2.8, page 51) and in the time program (see chapter 10.3.6, page 65).

#### 10.1.10 Amperometric detector



You can also define settings for the amperometric detector in the start parameters (see chapter 10.2.9, page 51) and in the time program (see chapter 10.3.7, page 66).

### 10.1.11 High-pressure gradient

High-pressure gradient	
A A	
pump Pressure MPa	
Pump set flow ▶	
Flow	Flow of the gradient pump.
PMin	Minimum permitted pressure in the instrument.
	The high-pressure gradient pump consists of several individual high-pressure pumps. If the pressure of 1 individual high-pressure pump falls below PMin, an error occurs.
PMax	Maximum permitted pressure in the instrument.

	The high-pressure gradient pump consists of several individual high-pressure pumps. If the pressure of 1 individual high-pressure pump exceeds PMax, an error occurs.	
Pump off	Switches off the gradient pump.	

The extended status panel displays the **Pump gradient flow**. The pump gradient flow is the sum of the flows of all pumps that are part of the high-pressure gradient. If the instrument also contains a Dose-in gradient, then the flow of the respective pump is shown below the pump icon and in the extended table as **Pump x flow**. The flow of the Dose-in gradient pump is not part of the pump gradient flow.

10.1 Manual control

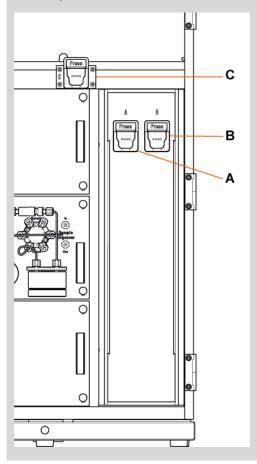


#### **NOTE**

Besides the PMax that is defined in the manual control, there is a PMax written on the column chip. If these values differ, then an error is generated as soon as the **lower** of these values is exceeded.

Each column holder is assigned to a high-pressure pump.

- Pump 1 Column holder A
- Pump 2 Column holder B
- Pump 3 Column holder C



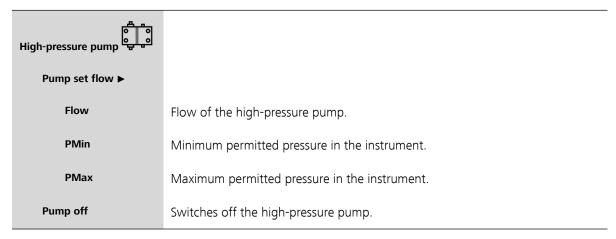
You can also define settings for the high-pressure gradient pump in the start parameters (see chapter 10.2.10, page 55) and in the time program (see chapter 10.3.8, page 66).

## 10.1.12 Dose-in gradient

-----

You can also define settings for the Dose-in gradient in the start parameters (see chapter 10.2.11, page 57) and in the time program (see chapter 10.3.9, page 67).

#### 10.1.12.1 High-pressure pump



Metrohm IC Driver for OpenLab

10.1 Manual control

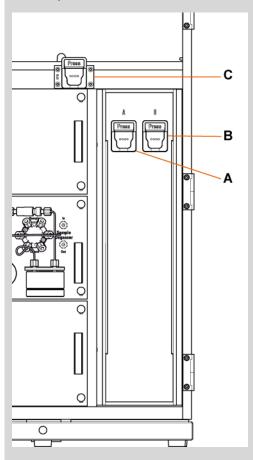


#### **NOTE**

Besides the PMax that is defined in the manual control, there is a PMax written on the column chip. If these values differ, then an error is generated as soon as the **lower** of these values is exceeded.

Each column holder is assigned to a high-pressure pump.

- Pump 1 Column holder A
- Pump 2 Column holder B
- Pump 3 Column holder C





#### **NOTE**

If the high-pressure pump is used for a Dose-in gradient, this is indicated with **D1** in the icon.



You can also define settings for the high-pressure pump in the start parameters (see chapter 10.2.1, page 48) and in the time program (see chapter 10.3.4, page 64).

#### 10.1.12.2 **Dosing unit**

-----

Dosing unit

Aspirate ► Aspirates the specified volume via the defined port. There is **no** automatic filling

beforehand or afterwards.

**Port** Port for aspirating the sample.

Rate for aspirating the sample.

**Volume** Volume to aspirate.

**Dosing ▶** Doses the specified volume via the defined port. There is automatic filling

beforehand or afterwards.

**Port** Port for dosing the sample.

Rate for dosing the sample.

**Filling Rate** Rate for filling the cylinder after dosing the sample.

**Volume** Volume to dose and fill in the cylinder.

**Empty** Empties the cylinder and all tubings of the dosing unit.

The parameters for emptying the dosing unit are defined in the configuration

(see menu "Dosing unit settings", page 16).

Fills the cylinder via the specified port.

**Port** Port for filling the cylinder.

Rate for filling the cylinder.

Move to exchange position ►

Fills the cylinder via the specified port first. Then rotates the valve disk to Port 2.

The dosing drive can be removed from the dosing unit.

**Port** Port for filling the cylinder.

Rate for filling the cylinder.

**Prepare**Rinses the cylinder and all tubings of the dosing unit with the solution that is

connected to the fill port.

The parameters for preparing the dosing unit are defined in the configuration (see menu "Dosing unit settings", page 16).

**Stop Dosino** 

Stops the dosing unit.



#### **NOTE**

If the Dosino is used for Dosino regeneration, this is indicated with **M1** in the icon.



If the Dosino is used for a Dose-in gradient, this is indicated with **D1** in the icon.



You can also define settings for the dosing unit in the time program (see chapter 15.2.1, page 98).

# 10.2 Start parameters

#### 10.2.1 High-pressure pump

Pump 1	
On	The high-pressure pump is switched on when you start the method.
Flow	Flow of the high-pressure pump when you start the method.
Start-up time	Define a start-up time for reaching the defined flow rate.
PMin	Minimum permitted pressure in the instrument when you start the method.
PMax	Maximum permitted pressure in the instrument when you start the method.



#### NOTE

If the pressure is below PMin or above PMax, an error is generated and the instrument is switched off.



#### **NOTE**

Besides the PMax that is defined in the start parameters, there is a PMax written on the column chip. If these values differ, then an error is generated as soon as the **lower** of both values is exceeded.

Each column holder is assigned to a high-pressure pump.

- Pump 1 Column holder A
- Pump 2 Column holder B
- Pump 3 Column holder C

See chapter 10.1.1, page 37 for an illustration of the column holders.

You can also define settings for the high-pressure pump in manual control (see chapter 10.1.1, page 37).

#### 10.2.2 Injector

-----

Injector 1	
	The injector index is not shown for the 889 IC Sample Center. The 889 IC Sample Center consists of only 1 injector.
Position	Position of the injector when the run starts.
	<ul> <li>Inject</li> <li>Switches the valve to Inject.</li> </ul>
	Fill Switches the valve to <b>Fill</b> .
	Maintain Current
	The valve maintains its current position.

You can also define settings for the injector in manual control (see chapter 10.1.2, page 39) and in the time program (see chapter 10.3.1, page 63).

#### 10.2.3 MSM

# Automatic stepping to next position during equilibration Interval Dosino regeneration ► If you enable this option, then automatic stepping of the rotor to the next position is initiated within the equilibrate mode and between injections. The time interval defined in the parameter interval is used. Time interval between 2 sequential automatic rotor stepping operations. If Dosino regeneration is configured, then it takes place automatically after each step of the rotor. This parameter is only shown if Dosino regeneration is configured.

49

Dosing device	The dosing device is defined in the configuration of the Dosino regeneration (see chapter 5.1, page 10).		
Solution ►	This parameters are only shown if Dosino regeneration is configured.		
Dosing Port	Port for dosing the regeneration solution.		
Volume	Volume of the regeneration solution.		
Time	Duration of the regeneration.		
Dosing rate	Dosing rate at which the MSM is regenerated. The dosing rate is automatical calculated from the <b>Volume</b> and <b>Time</b> .		
	This dosing rate is only applied to sequences and single sample analysis. If you send the current method to the instrument to equilibrate the instrument, then the default dosing rate of 1.0 mL/min is applied for the first MSM step. For all following MSM steps, the dosing rate from the method is applied.		
Fill Port	Port for filling the regeneration solution.		

You can also define settings for the MSM in manual control (see chapter 10.1.3, page 39) and in the time program (see chapter 10.3.2, page 63).

#### 10.2.4 MCS

MCS 1	
On	The MCS is switched on when you start the method.

You can also define settings for the degasser in manual control (see chapter 10.1.4, page 40).

#### 10.2.5 Degasser

Degasser 1	
On	The degasser is switched on when you start the method.

You can also define settings for the degasser in manual control (see chapter 10.1.5, page 40).

## 10.2.6 Peristaltic pump

Peristaltic pump 1	
On	The peristaltic pump is switched on when you start the method.
Rate	Rate of the peristaltic pump when you start the method.

You can also define settings for the peristaltic pump in manual control (see chapter 10.1.6, page 40) and in the time program (see chapter 10.3.3, page 64).

#### 10.2.7 Thermostat

-----

Thermostat	
On	The thermostat is switched on when you start the method.
Temperature	Temperature that is set for the thermostat when you start the method.
Wait for Stable Temperature	A run does not start before the set temperature has been reached and is stable.

You can also define settings for the thermostat in manual control (see chapter 10.1.7, page 41).

#### 10.2.8 Conductivity detector

Cond	luctivity	detector	1

Temperature Coefficient

The temperature coefficient corrects the measured conductivity of the detector at the operating temperature to the conductivity at the reference temperature.

**Polarity** 

**-** +





#### NOTE

The number of a detector refers to the number of the socket where the detector is plugged in. The number of a detector does not depend on the actual number of connected detectors. If the instrument contains 1 detector that is plugged in socket 2, then the detector is labeled as **Detector 2**.

You can also define settings for the conductivity detector in the time program (see chapter 10.3.6, page 65).

#### 10.2.9 Amperometric detector

#### **Amperoemtric Detectors**

**Cell State** 

- Or
  - The cell is switched on when you start the method.
- Off
   The cell is switched off when you start the method.

#### Mode Mode that is set when you start the method. Measurement with constant potential. Click on [Settings] to define further parameters for the mode DC. DC Potential Potential of the working electrode in comparison to the reference electrode. - Range Measuring range of the detector. - Damping If selected, disturbing influences are damped. Noise on the baseline is decreased. PAD Measurement with several potential steps. Click on [Settings] to define further parameters for the mode PAD. - Potential Profile Define the potential steps in the potential profile table (see chapter 10.2.9, page 51). All potential steps are shown in the graph. The measurement is marked with a red line in the graph. Duration Duration of the potential step. Range Measuring range of the detector. flexIPAD Measurement with flexible potential steps (levels, ramps) and integration. Click on [Settings] to define further parameters for the mode flexIPAD. - Potential Profile Define the potential steps in the potential profile table (see chapter 10.2.9, page 51). All potential steps are shown in the graph. The measurement is marked with a red line in the graph. Start Start time of the measurement within the profile. End Ending time point of the measurement within the profile. - Range Measuring range of the detector.

Temperature

Temperature that is set for the thermostat when you start the method.

Wait for stable Temperature

A run does not start before the set temperature has been reached and is stable.

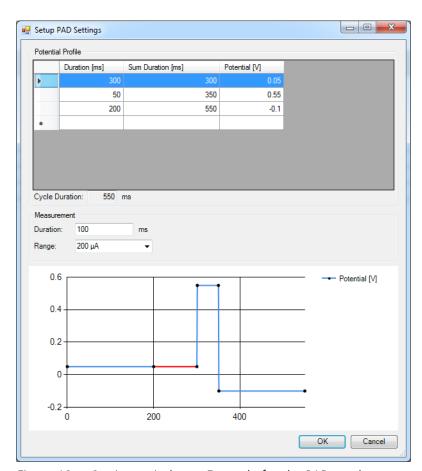


Figure 12 Settings window – Example for the PAD mode.

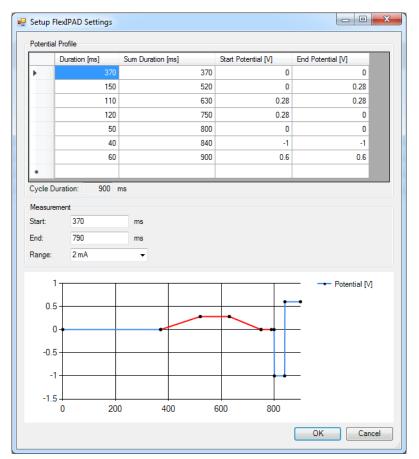


Figure 13 Settings window – Example for the flexIPAD mode.



#### **NOTE**

To start the system but switch on the amperometric cell later, use 2 different acquisition methods.

Use a method with the cell switched off to equilibrate the system.

Use a method with the cell switched on to acquire data.

Always equilibrate the system for at least 30 minutes before switching on the cell. Otherwise, the performance of the amperometric analysis is impaired.

You can also define settings for the amperometric detector in manual control (see chapter 10.1.10, page 42) and in the time program (see chapter 10.3.7, page 66).

# 10.2.10 High-pressure gradient

Gradient Pumps	
On	The high-pressure gradient pump is switched on when you start the method.
Flow	Flow of the high-pressure gradient pump when you start the method.
Start-up time	Define a start-up time for reaching the defined flow rate.
PMin	Minimum permitted pressure in the instrument when you start the method.
	The high-pressure gradient pump consists of several individual high-pressure pumps. If the pressure of 1 individual high-pressure pump falls below PMin, an error occurs.
PMax	Maximum permitted pressure in the instrument when you start the method.
	The high-pressure gradient pump consists of several individual high-pressure pumps. If the pressure of 1 individual high-pressure pump exceeds PMax, an error occurs.
Eluent A - D	Define the proportion in the mixing ratio for each eluent. Ensure that the total of all eluent proportions is 100%.
Gradient	Click on <b>[Gradient]</b> to define the gradient profile. Execute the gradient profile with the time program command <b>Start Gradient</b> . For each step in the gradient profile, define the following parameters:
	<ul> <li>Time         Moment when the gradient command is executed.</li> <li>Eluent A - D         Define the proportion in the mixing ratio for each eluent. Ensure that the total of all eluent proportions is 100%.</li> </ul>

#### Curve

Selection of the curve form with which the previous entry in the gradient table moves to the current entry.

- Linear

If the flow is not modified, then the proportion of eluent changes in a linear fashion.

If the flow and the proportion of the eluents is modified, then the proportion of the eluents and the flow change in a linear fashion. The mixing ratio changes in a nonlinear fashion.

- Step

If the flow is not modified, then the proportion of the eluent remains at its current value up to the point in time of the next command line. Then the proportion changes to the value of the next command line at once.

If the flow and the proportion of the eluents is modified, then the proportion of the eluents and the flow of the pump remain at their current value up to the point in time of the next command line. Then they change to the value of the next command line at once. The mixing ratio changes in the same way.

- Convex 1 4 / Concave 1 4
   If the flow is not modified, then the proportion of the eluent changes along the selected curve.
   If the flow and the proportion of the eluents is modified, then the flow changes along the selected curve. The proportion of eluents changes along the selected curve. The mixing ratio changes in a nonlinear fashion.
- Flow
   Flow rate at which the gradient step is executed.



#### **NOTE**

If the pressure is below PMin or above PMax, an error is generated and the instrument is switched off.



#### **NOTE**

Besides the PMax that is defined in the start parameters, there is a PMax written on the column chip. If these values differ, then an error is generated as soon as the **lower** of both values is exceeded.

Each column holder is assigned to a high-pressure pump.

- Pump 1 Column holder A
- Pump 2 Column holder B
- Pump 3 Column holder C

See *chapter 10.1.1*, page 37 for an illustration of the column holders.

You can also define settings for the high-pressure gradient pump in manual control (see chapter 10.1.11, page 42) and in the time program (see chapter 10.3.8, page 66).

## 10.2.11 Dose-in gradient

-----

Pumps	
On	The high-pressure pump is switched on when you start the method.
Flow	Flow of the high-pressure pump when you start the method.
Start-up time	Define a start-up time for reaching the defined flow rate.
PMin	Minimum permitted pressure in the instrument when you start the method.
PMax	Maximum permitted pressure in the instrument when you start the method.
Gradient	Click on <b>[Gradient]</b> to define the gradient profile. Execute the gradient profile with the time program command <b>Dose-in Gradient</b> . For each step in the gradient profile, define the following parameters:  Time  Moment when the gradient command is executed.
	<ul> <li>Ratio         Proportion in the mixing ratio from the Dosino to the flow of the high-pressure pump.     </li> <li>Curve         Selection of the curve form with which the previous entry in the gradient table moves to the current entry.         – Linear             The proportion of the eluent from the Dosino changes in a linear fashion.             – Step         </li> </ul>
	<ul> <li>Step         The proportion of the eluent from the Dosino remains at its current value up to the point in time of the next command line. Then the proportion changes to the value of the next command line at once.     </li> <li>Flow         Flow rate at which the gradient is executed.     </li> </ul>



#### NOTE

If the pressure is below PMin or above PMax, an error is generated and the instrument is switched off.



#### **NOTE**

Besides the PMax that is defined in the start parameters, there is a PMax written on the column chip. If these values differ, then an error is generated as soon as the **lower** of both values is exceeded.

Each column holder is assigned to a high-pressure pump.

- Pump 1 Column holder A
- Pump 2 Column holder B
- Pump 3 Column holder C

See *chapter 10.1.1, page 37* for an illustration of the column holders.

You can also define settings for the Dose-in gradient in manual control of the high-pressure pump (see chapter 10.1.1, page 37) and the dosing unit (see chapter 10.1.12.2, page 47) which are part of the Dose-in gradient and in the time program (see chapter 10.3.9, page 67).

# **10.2.12 Metrohm detectors with Agilent LC 1 - Instrument type**Combination of Agilent HPLC with Metrohm IC detectors:

In OpenLab CDS, it is possible to combine an Agilent LC / HPLC with a Metrohm IC detector (Conductivity / Amperometric) as a single instrument in OpenLab CDS software.



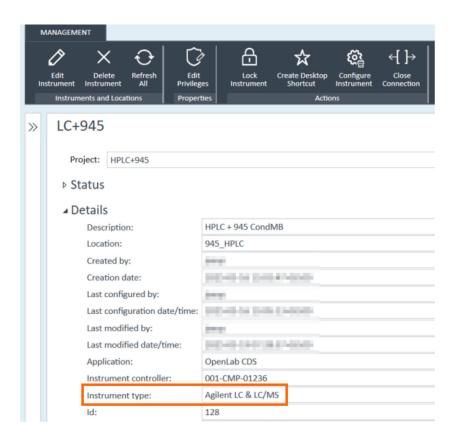
#### NOTE

For the standard setup (only Metrohm equipment without HPLC) please refer to chapter 2 (page 3) in this tutorial.

#### **Configuration of instruments in OpenLab:**

Pre-requisites:

- 66080100 Metrohm IC driver 1.0 for OpenLab CDS is installed. Check the installed version 1.0.9.24311.1 in Windows installed app.
- All modules are LAN / USB connected and switched on.
  - 1 Create an instrument and select instrument type Agilent LC & LC/MS.



2 On top menu, select "Configure".

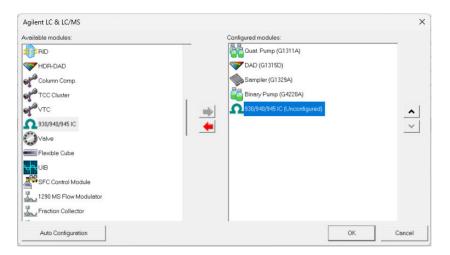


**3** Select auto-configuration to discover the Agilent instruments.

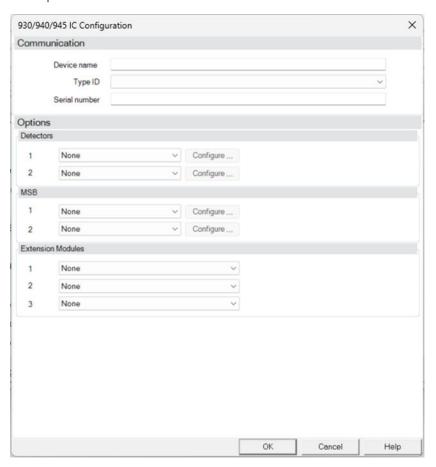


#### **NOTE**

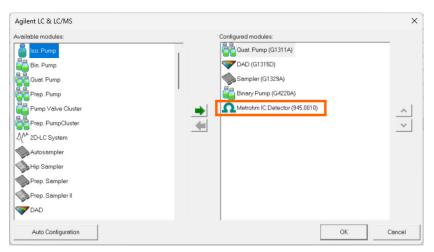
Please refer to the manufacturer to complete the required information.



- 4 Once Agilent modules are configured, select in the available modules the Metrohm 930 / 940 / 945. In the Configured modules list, appear as Unconfigured.
- Make left click on the unconfigured instruments and complete manually the fields with the requested information for Communication and Options.



The window indicates the configured modules (example with HPLC with Metrohm 2.945.0010):



- **7** Accept the windows with OK button.
- 8 Launch the instrument.
- **9** Create the acquisition method.



#### NOTE

If the instrument status is offline, please check the information introduced for the modules.

This special configuration of a Metrohm detector with Agilent HPLC can be only used in combination with an Agilent HPLC listed in the OpenLab configuration windows available modules.

For this combination, Metrohm available modules are 930, 940 or 945. Please, refer to the Released notes 8.0102.8007EN for the different module versions and limitations.

To configure only Metrohm modules without HPLC, please proceed as described in chapter 2, page 3 in this tutorial.

#### **Modules Synchronization:**

For the synchronization between the sample injection and the chromatogram acquisition it is necessary to use the remote lines of the modules with the corresponding interfaces.

Metrohm references for remote lines:

6.2148.010 - Remote Box MSB

• 6.2141.310 - Remote Cable Professional IC to MS Agilent (This cable needs adaptation. See instructions below.)

For the Agilent remote lines, there are two options, depending on the Agilent modules:

- Agilent instruments with **GPIO interface**.
- Agilent instruments with **ERI interface**.

# 1. Technical information with the Agilent General Purpose Interface (GPIO):

Table 3 Configuration for instruments with Agilent GPIO 9 - Pin Interface

Agilent GPIO remote interface	Metrohm remote box MSB
Connector A – 9 pin, male	Connector B – 25 pin, male (Connector B to be pin-adap- ted by user)
Pin 1 – Gray cable (Ground)	Pin 21 – White cable (Start)
Pin 3 – White cable (Start)	Pin 25 – Gray cable (Ground)

# 2. Technical information with Agilent ERI Enhanced Remote Interface:

**Connector A**: When using the Agilent reference cable 5188-8029 ERI to general purpose, no modification needed.

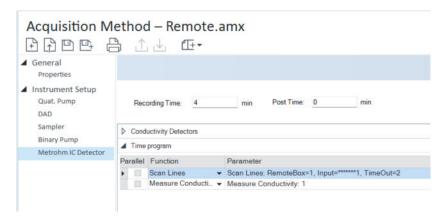
**Connector B**: needs modification.

Table 4 Configuration for instruments with Agilent ERI 15 - pin interface. Recommended reference cable Agilent 5188-8029 ERI for general purpose

Agilent ERI Connector A – D- Sub male 15 way to open end.	Metrohm remote box MSB  Connector B – 25 pin, male (Connector B to be pin-adapted by user)
Pin 7 – Blue cable (Start)	Pin 21 – Blue (Start)
Pin 10 – Violet cable (DGND)	Pin 25 – Violet cable (GND)

#### Acquisition method and time program in OpenLab CDS:

 Create an acquisition method and set up the parameters of the LC / HPLC modules. • In the instrument setup for the Metrohm IC module, the time program should contain a scan lines command. When the LC / HPLC makes the sample injection, a pulse will be sent to the Metrohm detector to synchronize the data acquisition (here in the example: "Measure Conductivity"):



# **10.3** Time program

## 10.3.1 Injector

-----

Switch injector	
Injector	Number of the injector.
	The number of the injector is not shown for the 889 IC Sample Center. The 889 IC Sample Center consists of only 1 injector.
Position	Position of the injector.  Inject Switches the valve to Inject. Fill Switches the valve to Fill.

You can also define settings for the injector in the start parameters (see chapter 10.2.2, page 49) and in manual control (see chapter 10.1.2, page 39).

#### 10.3.2 MSM

MSM Step	
Execution condition	The command is only run if the minium regeneration time has been reached or exceeded.
MSM	Number of the MSM.

10.3 Time program

Minimal regeneration	
time	Time that must have elapsed since the last stepping.

You can also define settings for the MSM in the start parameters (see chapter 10.2.3, page 49) and in manual control (see chapter 10.1.3, page 39).

## 10.3.3 Peristaltic pump

Set peristaltic	
Pump on	Switches on the peristaltic pump and sets the value for the pump rate.
Pump	Number of the peristaltic pump.
Rate	Rate of the peristaltic pump.

You can also define settings for the peristaltic pump in the start parameters (see chapter 10.2.6, page 50) and in manual control (see chapter 10.1.6, page 40).

## 10.3.4 High-pressure pump

Measure Pressure	
Pump	Number of the pump.

You can also define settings for the high-pressure pump in the start parameters (see chapter 10.2.1, page 48) and in manual control (see chapter 10.1.1, page 37).

## 10.3.5 Remote Box

Set Lines				
MSB port	Number of the MSB port the Remote Box is connected to.			
Output signal	The output signal is read-only.			
	Input of the binary pattern for the output signal of exactly 14 bits.			
	0 = Output line deactivated			
	1 = Output line activated			
	* = Retain the status of the output line			
	p = set pulse (pulse length = 200 ms).			
	The output lines are numbered from right to left: 13-12-11-10-9-8-7-6-5-4-3-2-1-0			

	Examples:			
	*******1*****: Sets the status of output line 5 from the IC on active.			
	****0********: Sets the status of output line 9 from the IC on inactive.			
Scan Lines				
MSB port	Number of the MSB port the Remote Box is connected to.			
Input signal	Input of the binary pattern for the output signal of exactly 8 bits.			
	0 = Output line deactivated			
	1 = Output line activated			
	* = Retain the status of the output line			
	The output lines are numbered from right to left: 7-6-5-4-3-2-1-0			
	Examples:			
	*****1**: Sets the status of output line 2 from the IC on active.			
	**0*****: Sets the status of output line 5 from the IC on inactive.			
Timeout	If <b>Timeout</b> is activated, then the time program is continued as soon as either the requested input signal has been received or the waiting time has expired. If the waiting time expires, the run is aborted.			
	If <b>Timeout</b> is not activated, then the time program waits indefinitely for an input signal.			

You can also define settings for the Remote Box in manual control (see chapter 10.1.8, page 41).

# 10.3.6 Conductivity detector

Measure Conductivity	
Detector	Number of the conductivity detector.
	The number of a detector refers to the number of the socket on the backside of the IC and not to the actual number of connected detectors. Therefore, it is possible that only 1 detector is connected but it is shown as <b>Detector 2</b> because it is plugged in socket 2.

10.3 Time program



#### **NOTE**

It is not possible to execute a time program that contains the command **Measure Conductivity** several times for the same conductivity detector.

Only the first **Measure Conductivity** command is executed. All subsequent **Measure Conductivity** commands are invalid. These commands are ignored but no error occurs.

You can also define settings for the conductivity detector in the start parameters (see chapter 10.2.8, page 51).

## 10.3.7 Amperometric detector

Measure Current	
Detector	Number of the detector.
Measure Charge	
Detector	Number of the detector.

You can also define settings for the UV/VIS detector in the start parameters (see chapter 10.2.9, page 51) and in manual control (see chapter 10.1.10, page 42).

## 10.3.8 High-pressure gradient

Start Gradient	
Start Gradient	Executes the gradient profile that was defined in the start parameters under <b>Settings</b> (see chapter 10.2.10, page 55).



#### NOTE

Ensure that the gradient is executed immediately after the injection. Therefore, the time program entry for **Start Gradient** must be placed immediately after the entry for **Switch injector** to fill position.

You can also define settings for the high-pressure gradient pump in the start parameters (see chapter 10.2.10, page 55) and in manual control (see chapter 10.1.11, page 42).

## 10.3.9 Dose-in gradient

-----

Executes the gradient profile that was defined in the start parameters.

MSB

**Dose-in Gradient** 

Select the MSB port to which the Dose-in gradient Dosino to be used is connected.



#### NOTE

Ensure that the gradient is executed immediately after the injection. Therefore, the time program entry for **Dose-in gradient** must be placed immediately after the entry for **Switch injector** to fill position.

You can also define settings for the Dose-in gradient in the start parameters (see chapter 10.2.11, page 57) and in manual control of the high-pressure pump (see chapter 10.1.1, page 37) and the dosing unit (see chapter 10.1.12.2, page 47) which are part of the Dose-in gradient.

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# 11 Parameters of the 858 Professional Sample Processor

The 858 Professional Sample Processor is conceived for preparing samples for ion chromatography.

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The equipment with a Swing Head with a robotic arm makes it possible to approach any given point on a sample rack. As a result, the number and sequencing of the samples on the sample rack is almost unlimited.

Optionally, you can combine the 858 Professional Sample Processor with a Liquid Handling Station to rinse the needle and dilute samples.

# 11.1 Configuring the lift positions

In the tab **858.xxxx Professional IC Sample Processor** of the **Instrument Status**, you can configure the lift positions of the 858 Professional Sample Processor.

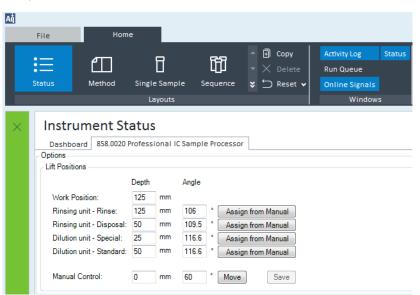


Figure 14 Configuring the lift positions

The external positions on the Liquid Handling Station depend on the exact position of the Liquid Handling Station. Therefore, these lift positions have to be configured individually for each instrument.

The following lift positions can be defined:

Work position
 Position for locations on the rack. You can adjust the immersion depth.

- Positions on the Liquid Handling Station. You can adjust the immersion depth and the angle.
  - Rinsing unit Rinse
  - Rinsing unit Disposal
  - Dilution unit Special
  - Dilution unit Standard

Dilution unit – Special and Dilution unit – Standard have the same angle setting. The difference between them lies in their immersion depths (work position).

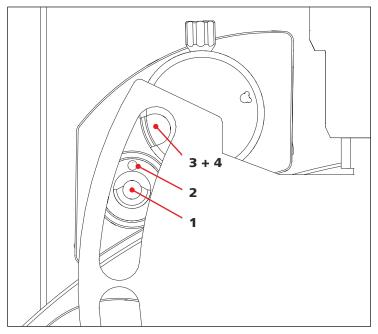


Figure 15 Positions on the Liquid Handling Station

1	Rinsing unit – Rinse	2	Rinsing unit – Disposal
3	Dilution unit – Special	4	Dilution unit – Standard

## **Example: Define the lift position Rinsing unit - Rinse**

- 1 Set the depth to 0 mm in **Manual Control**. Enter the estimated angle value for the lift position **Rinsing unit Rinse** in **Manual Control**.
- 2 Click on [Move].

The arm of the 858 Professional Sample Processor moves to the position that you entered in **Manual Control**.

Check whether the needle is centered over the position **Rinsing unit** – **Rinse**.

-----

- **4** Repeat steps 1-3 until you find the correct position.
- 5 Enter the desired depth for the lift position **Rinsing unit Rinse** in **Manual Control**.
- 6 Click on [Assign from Manual] next to Rinsing unit Rinse position to transfer the values from Manual Control to Rinsing unit Rinse.
- **7** Repeat this procedure for all positions on the Liquid Handling Station.



#### **NOTE**

Do not change the angle if the needle is positioned in the Liquid Handling Station or in a vial. Lift the needle above the rim of the Liquid Handling Station or any vial before executing a swing command. Otherwise, the needle collides with the Liquid Handling Station or a vial and the needle breaks.



#### NOTE

To deny access to the configuration of lift positions to some users, create an according user role or edit an existing user role. To create and edit user roles, go to **Control Panel** ► **Administration**. Deselect the following role privileges:

- Role type Project ➤ Acquisition Method ➤ Create and modify acquisition method
- Role type Instrument ➤ Instrument Management ➤ Manage instrument or location
- Role type Instrument ► Instrument Management ► Manage instrument or location access

Refer to the OpenLab Help for further information about user roles: How To ➤ OpenLAB CDS ➤ Control panel ➤ Administration ➤ Roles.

# 11.2 Manual control

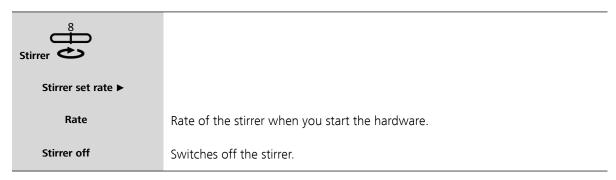
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## 11.2.1 858 Robotic arm and sample rack

Robotic arm and sample rack	
Move ►	
Position type	Type of target position.  Rack External Position
External posi- tion	Number of the external position.  This input field is only active if the position type <b>External position</b> is selected.
Vial	Number of the vial.  This input field is only active if the position type <b>Rack</b> is selected.
Lift position	<ul> <li>Home         Home position is always 0.</li> <li>Work         The sample is aspirated at this lift position.</li> <li>User Defined         The user can define an additional position.</li> </ul>
Depth	Immersion depth of the needle.  This input field is only active if the lift position <b>User defined</b> is selected.
Initialize Rack	Initializes the rack.

You can also define settings for the robotic arm and the sample rack in the time program (see chapter 11.4.1, page 73).

## 11.2.2 Stirrer



11.3 Start parameters

You can also define settings for the stirrer in the start parameters (see chapter 11.3.1, page 72) and in the time program (see chapter 11.4.2, page 74).

## 11.2.3 Peristaltic pump



Peristaltic pump set

rate

Rate of the peristaltic pump when you start the hardware.

Peristaltic pump off

Switches off the peristaltic pump.

You can also define settings for the peristaltic pump in the start parameters (see chapter 10.2.6, page 50) and in the time program (see chapter 10.3.3, page 64).

# 11.3 Start parameters

## 11.3.1 Stirrer

Stirrer	
On	The stirrer is switched on when you start the method.
Rate	Rate of the stirrer.

You can also define settings for the stirrer in manual control (see chapter 11.2.2, page 71) and in the time program (see chapter 11.4.2, page 74).

## 11.3.2 Peristaltic pump

Peristaltic pump 1	
On	The peristaltic pump is switched on when you start the method.
Rate	Rate of the peristaltic pump when you start the method.

You can also define settings for the peristaltic pump in manual control (see chapter 10.1.6, page 40) and in the time program (see chapter 10.3.3, page 64).

## 11.4 Time program

-----



#### **NOTE**

In the time program of the 858 Professional Sample Processor, you cannot define a recording time or post time. Therefore, ensure that the recording time and post time of the IC time program is long enough to cover all time program commands of the 858 Professional Sample Processor.

If the time program of the 858 Professional Sample Processor takes longer than the defined recording time and post time, the time program is stopped after the defined time.

## 11.4.1 858 Robotic arm and sample rack

#### Move

#### Position type

Type of target position.

- Vial from Sequence
- Vial from Method
- External Position
- Next Vial from Sequence

This position type allows to prepare the next sample in parallel. The sample processor moves to the vial position of the next line in the sequence. This position type can only be used if the next sample uses the same acquisition method as the current sample. Ensure that the sequences in the sequence table meet the requirements for the **Next Vial from Sequence** command.

Vial from Sequence +1

Use this function to calibrate an AnCat system, for example.

Define the vial position in the sequence table. With **Vial from Sequence** 

**+1** the autosampler automatically takes a sample from the vial that is defined in the sequence table and a sample from the subsequent vial. Example:

Define that the sample processor takes anion standard from vial 5. The sample processor automatically takes cation standard from vial 6.

#### **External Position**

Number of the external position.

Vial

Number of the vial.

#### Lift position

- Home Home position is always 0.
- Work

Work positions are defined in the **Instrument Status**, tab **858.xxxx Professional IC Sample Processor**.

The sample is aspirated at this lift position.

11.4 Time program

User Defined
 The user can define an additional position.

Depth

Immersion depth of the needle.

This input field is only active if the lift position **User Defined** is selected.



#### **NOTE**

If you create a single sample analysis or a sequence, you must select an injection source. If you want to use the **vial position** that is defined in the sequence, then select the following injection source:

- With an 858 Professional Sample Processor, select IC -Injection
   Valve or Sample Processor.
- With an 889 IC Sample Center, select Sample Center Injection Valve.

An error occurs if you select the injection source **External** or **No Injection/Instrument Blank** and the time program command **Vial from Sequence**, **Next Vial from Sequence** or **Vial from Sequence +1**.

You can also define settings for the robotic arm and sample rack in manual control (see chapter 11.2.1, page 71).

#### 11.4.2 Stirrer

Set stirrer	
Stirrer on	
Rate	Rate of the stirrer.



#### **NOTE**

To run a method with stirrer commands in the time program on an instrument without a configured stirrer, the commands for the stirrer need to be adapted.

If you run a method with commands for the stirrer on an instrument without stirrer, then the time program of the 858 Professional Sample Processor is deleted completely. To adjust a method with stirrer commands to run it on an instrument without stirrer, proceed as follows:

Activate the stirrer in the configuration of the 858 rofessional Sample Processor. Open the method. Remove the stirrer commands. Save the method. Now you can run the adapted method on an instrument without stirrer.

You can also define settings for the stirrer in the start parameters (see chapter 11.3.1, page 72) and in manual control (see chapter 11.2.2, page 71).

## 11.4.3 Peristaltic pump

-----

Set peristaltic	
Pump on	Switches on the peristaltic pump and sets the value for the pump rate.
Pump	Number of the peristaltic pump.
Rate	Rate of the peristaltic pump.

You can also define settings for the peristaltic pump in the start parameters (see chapter 10.2.6, page 50) and in manual control (see chapter 10.1.6, page 40).

12.1 Manual control

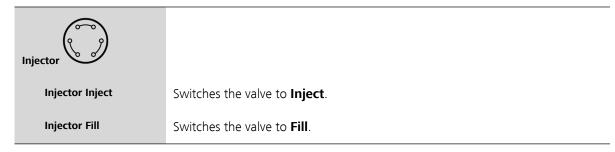
# 12 Parameters of the 889 IC Sample Center

The 889 IC Sample Center is a robust autosampler for high sample throughput and small sample volumes. The 889 IC Sample Center works according to the x-y-z principle and with high-resolution injection control for precise sample delivery.

The optional cooling function cools thermosensitive samples.

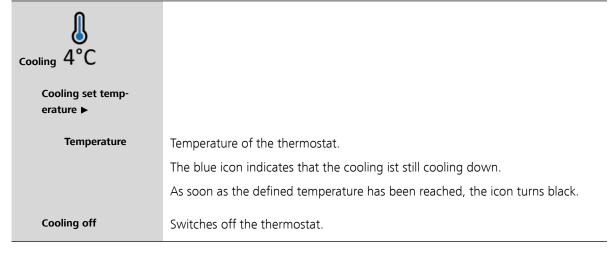
## 12.1 Manual control

## 12.1.1 Injector



You can also define settings for the injector in the start parameters (see chapter 10.2.2, page 49) and in the time program (see chapter 10.3.1, page 63).

## **12.1.2** Cooling



You can also define settings for the injector in the start parameters (see chapter 12.2.1, page 79).

## 12.1.3 889 Sample rack and needle

#### Sample rack and needle

-----



Move ▶

**Position type** Type of target position.

Rack

Wash Position

Waste Position

Rack • Left

Right

This input field is only active if the position type **Rack** is selected.

**Row** This input field is only active if the position type **Rack** is selected.

**Column** This input field is only active if the position type **Rack** is selected.

Needle • Home

The uppermost stop of the lift.

Work

The sample is aspirated at this lift position.

If the position type **Wash Position** or **Waste Position** is selected, then the

needle is always in **Work** position.

**Depth** Immersion depth of the needle.

This input field is only active if the position type **Rack** and the needle position

Work are selected.

**Home** The needle goes into **Home** position

Assign Racks ► Select the same rack type for both rack holders or a combination with None

and any rack type.

**Left rack** Select a rack type for the left rack.

**Right rack** Select a rack type for the right rack.

**Exchange Rack** Moves the rack to exchange position in order to exchange the racks.

**Exchange Needle** Moves the needle to exchange position in order to exchange the needle. For

more information about exchanging the needle, refer to 8.889.8001 Manual

889 IC Sample Center.

Remove both racks before moving the needle to exchange position.

12.1 Manual control

You can also define settings for the injector in the time program (see chapter 12.3.1, page 80).

# 12.1.4 889 Syringe, Compressor, Washing procedure

Syringe, Compressor, Washing procedure	
Syringe Fill ►	Fills the syringe completely via the specified port.
Port	Port for filling the syringe.
	<ul><li>Needle</li><li>Wash</li><li>Waste</li></ul>
Speed	Speed at which the syringe plunger is moved.
	<ul><li>Fast</li><li>Normal</li><li>Slow</li></ul>
	This input field is only active if the port <b>Needle</b> is selected.
Syringe Eject ►	Ejects the content of the syringe via the specified port.
Port	Port for ejecting the content of the syringe.
	<ul><li>Needle</li><li>Wash</li></ul>
	• Waste
Speed	Speed at which the syringe plunger is moved.
	■ Fast
	<ul><li>Normal</li><li>Slow</li></ul>
	This input field is only active if the port <b>Needle</b> is selected.
Syringe Aspirate ►	Aspirates the specified volume via the defined port.
Volume	Volume to aspirate. The maximum volume that can be aspirated depends on the current position of the syringe plunger.
Port	Port for aspirating the sample.
	<ul><li>Needle</li><li>Wash</li></ul>
	• Waste
Speed	Speed at which the syringe plunger is moved.
	<ul><li>Fast</li><li>Normal</li></ul>
	- Normal

	■ Slow
	This input field is only active if the port <b>Needle</b> is selected.
Syringe Dispense ▶	Dispenses the specified volume via the defined port.
Volume	Volume to dispense. The maximum volume that can be dispensed depends on the current position of the syringe plunger.
Port	Port for dispensing the sample.
	<ul><li>Needle</li><li>Wash</li><li>Waste</li></ul>
Speed	Speed at which the syringe plunger is moved.
	<ul><li>Fast</li><li>Normal</li><li>Slow</li></ul>
	This input field is only active if the port <b>Needle</b> is selected.
Compressor On	Switches on the compressor.
Compressor Off	Switches off the compressor.
Start Wash	Starts the washing procedure.
Stop Wash	Stops the washing procedure.
Reset	Resets the module.

You can also define settings for the syringe, compressor and washing procedure in the start parameters (see chapter 12.2.3, page 80) and in the time program (see chapter 12.3.3, page 82).

# 12.2 Start parameters

# **12.2.1** Cooling

Cooling	
On	The cooling is switched on when you start the method.
Temperature	Temperature that is set for the cooling when you start the method.
Wait for Stable Temperature	A run does not start before the set temperature has been reached and is stable.

12.3 Time program

You can also define settings for the cooling in manual control (see chapter 12.1.2, page 76).

## 12.2.2 Injector

Injector 1	
	The injector index is not shown for the 889 IC Sample Center. The 889 IC Sample Center consists of only 1 injector.
Position	Position of the injector when the run starts.
	<ul> <li>Inject         Switches the valve to Inject.</li> <li>Fill         Switches the valve to Fill.</li> <li>Maintain Current         The valve maintains its current position.</li> </ul>

You can also define settings for the injector in manual control (see chapter 10.1.2, page 39) and in the time program (see chapter 10.3.1, page 63).

## 12.2.3 Compressor

Compressor	
On	The compressor is switched on when you start the method.

# 12.3 Time program



#### **NOTE**

In the time program of the 889 IC Sample Center, you cannot define a recording time or post time. Therefore, ensure that the recording time and post time of the IC time program is long enough to cover all time program commands of the 889 IC Sample Center.

If the time program of the 889 IC Sample Center takes longer than the defined recording time and post time, the time program is stopped after the defined time.

## 12.3.1 889 Sample rack and needle

Move	
Position type	Type of target position.

- Wash
- Rack
- Waste
- Vial from Sequence
- Vial from Sequence +1

Use this function to calibrate an AnCat system, for example.

Define the vial position in the sequence table. With **Vial from Sequence** 

- +1 the autosampler automatically takes a sample from the vial that is defined in the sequence table and a sample from the subsequent vial.
- +1 is realized as follows:
  - Left rack, Position A1 +1 = Left rack, Position A2
  - Left rack, Position A8 +1 = Left rack, Position B1
  - Left rack, Position F8 +1 = Right rack, Position A1
  - Right rack, Position F8: +1 is not possible

Rack

-----

- Left
- Right

This input field is only active if the position type **Rack** is selected.

Row

This input field is only active if the position type **Rack** is selected.

Column

This input field is only active if the position type **Rack** is selected.

**Needle position** 

- Home
- Work

This input field is only active if the position type **Rack** is selected.

Depth

Immersion depth of the needle.

This input field is only active if the position type **Rack** and the needle position **Work** is selected.



#### **NOTE**

If you create a single sample analysis or a sequence, you must select an injection source. If you want to use the **vial position** that is defined in the sequence, then select the following injection source:

- With an 858 Professional Sample Processor, select IC -Injection
   Valve or Sample Processor.
- With an 889 IC Sample Center, select Sample Center Injection
   Valve.

An error occurs if you select the injection source **External** or **No Injection/Instrument Blank** and the time program command **Vial from Sequence**, **Next Vial from Sequence** or **Vial from Sequence** +1.

You can also define settings for the injector in manual control (see chapter 12.1.3, page 77).

12.3 Time program

# 12.3.2 Injector

Switch injector	
Injector	Number of the injector.
	The number of the injector is not shown for the 889 IC Sample Center. The 889 IC Sample Center consists of only 1 injector.
Position	Position of the injector.  Inject Switches the valve to Inject. Fill Switches the valve to Fill.

You can also define settings for the injector in the start parameters (see chapter 10.2.2, page 49) and in manual control (see chapter 10.1.2, page 39).

# 12.3.3 889 IC Sample Center

Full loop injection	
Rinsing volume	Volume for rinsing.
Needle height	Distance of the needle tip from the bottom of the vial.
Syringe Speed	Speed at which the syringe plunger is moved.  Slow Normal Fast
Air segment	If selected, then an air segment separates the sample from the content of the wash bottle (usually UPW).
Headspace pressure	If selected, then overpressure is channeled in through the air needle. This ensures that no air or steam bubbles form while aspirating the sample. Only select this option if you use vials with septa.
Wash after injection	If selected, then the washing procedure is carried out after the injection.
Partial loop injection	
Injection volume Input	<ul><li>From sample data</li><li>Injection volume</li></ul>
Injection volume	Define the injection volume manually.
	Maximum injection volume = 0.5 x sample loop volume

	The sample loop volume is defined in the configuration of the 889 IC Sample Center (see chapter 5.3, page 13).
	Refer to the manual 8.889.8001 IC Sample Center for further information regarding the injection volume.
	This input field is only active if the the injection volume input <b>Injection volume</b> is selected.
Rinsing volume	Volume for rinsing.
Needle height	Distance of the needle tip from the bottom of the vial.
Syringe Speed	Speed at which the syringe plunger is moved.
	<ul><li>Slow</li><li>Normal</li><li>Fast</li></ul>
Air segment	If selected, then an air segment separates the sample from the content of the wash bottle (usually UPW).
Headspace pressure	If selected, then overpressure is channeled in through the air needle. This ensures that no air or steam bubbles form while aspirating the sample. Only select this option if you use vials with septa.
Wash after injection	If selected, then the washing procedure is carried out after the injection.

Pickup	

### Injection volume Input

-----

- From sample data
- Injection volume

#### Injection volume

Define the injection volume manually.

Maximum injection volume = (sample loop volume - 3 x needle volume) / 2

The sample loop volume and needle volume are defined in the configuration of the 889 IC Sample Center (see chapter 5.3, page 13).

Refer to the manual 8.889.8001 IC Sample Center for further information regarding the injection volume.

This input field is only active if the the injection volume input **Injection volume** is selected.

### **Transport volume**

Volume of transport solution.

#### Needle height

Distance of the needle tip from the bottom of the vial.

#### **Syringe Speed**

Speed at which the syringe plunger is moved.

- Slow
- Normal

12.3 Time program

	■ Fast
Air segment	If selected, then an air segment separates the sample from the content of the wash bottle (usually UPW).
Headspace pressure	If selected, then overpressure is channeled in through the air needle. This ensures that no air or steam bubbles form while aspirating the sample. Only select this option if you use vials with septa.
Wash after injection	If selected, then the washing procedure is carried out after the injection.



#### **NOTE**

After injecting the sample, the 889 IC Sample Center automatically sets an event called **Injection Performed**. The corresponding event wait in the time program of the 930/940 IC must be entered manually. In the time program of the 930/940 IC, enter a command to start measuring after the event wait.

Wash	
	Performs the washing procedure.

You can also define settings for the washing procedure in manual control (see chapter 12.1.4, page 78).

# 12.3.4 Syringe

Syringe change port

The syringe valve port rotates to the selected position.  Needle Wash Waste
Port for filling the syringe.  Needle Wash Waste
Speed at which the syringe plunger is moved.  Slow Normal

	■ Fast
Eject	
Syringe Port	Port for ejecting the content of the syringe.
	<ul><li>Needle</li></ul>
	<ul><li>Wash</li><li>Waste</li></ul>
Syringe Speed	Speed at which the syringe plunger is moved.
	<ul><li>Slow</li><li>Normal</li></ul>
	■ Fast
Aspirate	
Volume	Volume to aspirate. The maximum volume that can be aspirated depends on the current position of the syringe plunger.
Syringe Port	Port for aspirating the sample.
	<ul> <li>Needle</li> </ul>
	<ul><li>Wash</li><li>Waste</li></ul>
Suringo Spood	Doub for annivation the county
Syringe Speed	Port for aspirating the sample.  • Slow
	<ul><li>Slow</li><li>Normal</li></ul>
	• Fast
Dispense	
Volume	Volume to dispense. The maximum volume that can be dispensed depends on the current position of the syringe plunger.
Syringe Port	Port for dispensing the sample.
	■ Needle
	<ul><li>Wash</li><li>Waste</li></ul>
Syringe Speed	Speed at which the syringe plunger is moved.
	• Slow

You can also define settings for the syringe in manual control (see chapter 12.1.4, page 78).

Normal Fast

13.1 UV/VIS lamp settings

# 13 Parameters of the 944/947 Professional UV/VIS Detector Vario

The 944 and 947 Professional UV/VIS Detectors Vario are independent modules for the photometric determination of light-absorbing substances in the UV/VIS range.

# 13.1 UV/VIS lamp settings



#### **CAUTION**

The lamp settings **must not** be adjusted except in the following cases:

- After first start-up, if the check of the intensity spectrum shows a cut-off.
- After the replacement of the UV lamp or VIS lamp, if the check of the intensity spectrum shows a cut-off.



#### **NOTE**

If you use the 947 Professional UV/VIS Detector Vario with a UV-lamp, then adjust the position of the UV-lamp after the initial start-up or after replacing the UV-lamp or VIS-lamp (see 809478001 Manual 947 Professional UV/VIS Detector Vario).

If you use the 944 Professional UV/VIS Detector Vario or the 947 Professional UV/VIS Detector Vario without UV-lamp, it is not necessary to adjust the UV lamp.



#### **NOTE**

Only users with rights to access the configuration can edit the settings in this tab.

Set the settings of the UV/VIS Detector in this tab. These parameters are used for every method. You only need to set them once.

Spectrum

Integration Duration

Time until the next reading of each diode in milliseconds.

## **Intensity Level** Intensity level of the VIS lamp.

-----

The input range of the intensity level for the **947** Professional UV/VIS Detector Vario is 2 ... 12.

If you enter a value that is > 8, a warning icon is displayed. Despite the warning icon, it is possible to set intensity level values up to 12. Ignore the warning icon.

**UV-Lamp Hours** Resets the recorded lamp hours of the UV lamp to 0.

Execute this step after replacing the UV lamp.

VIS-Lamp Hours Resets the recorded lamp hours of the VIS lamp to 0.

Execute this step after replacing the VIS lamp.

**Spectrum** Type of spectrum that will be displayed after clicking on **[View]**.

Baseline

The last baseline spectrum that has been recorded.

Intensity

Current intensity spectrum.

The spectrum does not refresh during auto-adjustment.

Absorbance

Current absorbance spectrum.

**Reset Baseline** Records a new baseline spectrum.

Auto Adjust The adjustment is carried out by a built-in algorithm of the instrument. The

algorithm calculates and sets optimized values for the **Integration Duration** 

and Intensity Level.

Intensity Monitor Toggles the live intensity spectrum on and off. If [Intensity Monitor] is toggled

on, then everything else in this window is inactive.

With the 947 Professional UV/VIS Detector Vario, the live intensity spectrum is needed to adjust the position of the UV lamp (see 809478001 Manual 947

Professional UV/VIS Detector Vario).

13.1 UV/VIS lamp settings

## Instrument Status

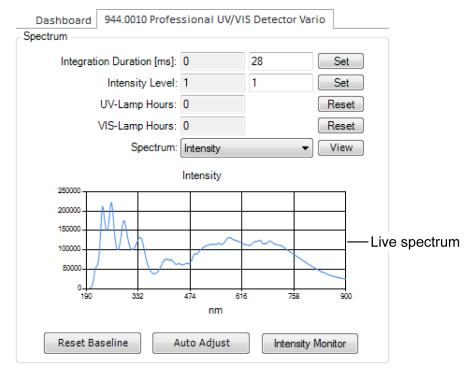


Figure 16 UV/VIS lamp settings

## **Adjust the lamp settings**

#### **Preconditions**

- The UV lamp has been on for at least 30 minutes.
- The flow-through cell is clean.
- The flow-through cell is rinsed with ultrapure water.
- The flow-through cell is free of air bubbles.
- The intensity spectrum has been checked and shows a cut-off.
- The lamp settings can be adjusted manually or automatically.

  To adjust the lamp settings automatically, click on [Auto Adjust].

  To adjust the lamp settings manually, conduct the following steps 2-3.
- **2** Enter the **Integration Duration**. Click on **[Set]**.
- 3 Enter the **Intensity Level**. Click on **[Set]**. A new intensity spectrum is displayed.



#### NOTE

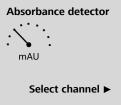
To deny access to the UV/VIS lamp settings to some users, create a corresponding user role or edit an existing user role. To create and edit user roles, go to **Control Panel ► Administration**. Deselect the following role privileges:

- Role type Project ➤ Acquisition Method ➤ Create and modify acquisition method
- Role type Instrument ➤ Instrument Management ➤ Manage instrument or location
- Role type Instrument ➤ Instrument Management ➤ Manage instrument or location access

Refer to the OpenLab Help for further information about user roles: How To ► OpenLAB CDS ► Control panel ► Administration ► Roles.

## 13.2 Manual control

#### 13.2.1 944/947 Professional UV/VIS Detector Vario



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Channel

Reset Baseline

Measuring channel in which the absorbance is measured.

Records a new baseline spectrum.



### NOTE

The time program of the 944/947 Professional UV/VIS Detector Vario does not include a **Reset Baseline** command. Therefore, Metrohm recommends to reset the baseline in manual control before starting a sequence.



Metrohm IC Driver for OpenLab

13.3 Start parameters

UV lamp On	Switches on the UV lamp.
UV lamp Off	Switches off the UV lamp.
VIS lamp	
VIS lamp On	Switches on the VIS lamp.
VIS lamp Off	Switches off the VIS lamp.

You can also define settings for the UV/VIS detector in the start parameters (see chapter 13.3.1, page 90) and in the time program (see chapter 13.4.1, page 91).

# **13.3 Start parameters**

## 13.3.1 944/947 Professional UV/VIS Detector Vario

UV Lamp	
On	The UV lamp is switched on when you start the method.
VIS Lamp	
On	The VIS lamp is switched on when you start the method.
Absorbance Detector	
Channels ►	For the 944 Professional UV/VIS Detector Vario and the 947 Professional UV/VIS Detector Vario <b>MW</b> , it is possible to choose 1 - 8 channels.
	For the 947 Professional UV/VIS Detector Vario <b>SW</b> , it is possible to choose 1 channel.
Wavelength	Wavelength of the selected channel.
Bandwidth	Subtracting and adding the bandwidth to the wavelength results in the actually measured wavelengths.
	Example:
	Wavelength = 390 nm; Bandwith = 5 nm
	The channel comprises the interval 385 - 395 nm.
	The absorbance is the average of all measured data points within the selected interval.

Measuring Duration	Measurement duration per data point.
Use Reference Chan- nel	The reference channel is optional. It corrects spectra by compensating lamp effects (drift, flicker).
Wavelength	Wavelength of the reference channel.
Bandwidth	Bandwidth of the reference channel.

You can also define settings for the UV/VIS detector in manual control (see chapter 13.2.1, page 89) and in the time program (see chapter 13.4.1, page 91).

# 13.4 Time program

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## 13.4.1 944/947 Professional UV/VIS Detector Vario

Measure Absorbance	
Channel	Measuring channel in which the absorbance is measured.
Measure Spectrum	
	Constantly measures spectra. The series of spectra results in 3D-data.



#### NOTE

The time program of the 944/947 Professional UV/VIS Detector Vario does not include a **Reset Baseline** command. Therefore, Metrohm recommends to reset the baseline in manual control (see menu "Absorbance detector", page 89) before starting a sequence.

You can also define settings for the UV/VIS detector in the start parameters (see chapter 13.3.1, page 90) and in manual control (see chapter 13.2.1, page 89).

14.1 Level sensor modes

# 14 Parameters of the 941 Eluent Production Module

The 941 Eluent Production Module allows you to produce eluent for your IC instrument from a concentrate and ultrapure water.

Thanks to the built-in Level Control, the module is capable of monitoring the liquid levels in up to 4 liquid containers with level sensors.

## 14.1 Level sensor modes

With the 941 Eluent Production Module, you can either monitor or produce eluent. These options are determined by the presence of an 800 Dosino.

You can use a level sensor in full mode or empty mode. These options are determined by the rod length.

Each combination of Production/Monitoring and Full mode/Empty mode is possible.

- Production Full
  - An 800 Dosino is configured for the level sensor. The level sensor is equipped with a short rod.
  - Eluent production takes place continuously. The production stops as soon as the defined eluent volume is produced or the liquid container is filled.
- Production Empty
  - An 800 Dosino is configured for the level sensor. The level sensor is equipped with a long rod.
  - Eluent production takes place in a batch process. If the liquid container gets empty, then the ongoing run is completed. After completing the run, the defined eluent volume is produced and the module waits until the waiting time has elapsed. Then the next run starts.
- Monitoring Full
  - No 800 Dosino is configured for the level sensor. The level sensor is equipped with a short rod.
  - The level sensor monitors the fill levels in liquid containers. A warning occurs as soon as the liquid container is full.
- Monitoring Empty
  - No 800 Dosino is configured for the level sensor. The level sensor is equipped with a long rod.
  - The level sensor monitors the fill levels in liquid containers. A warning occurs as soon as the liquid container is nearly empty.

## 14.2 Manual control

#### 14.2.1 941 Eluent Production Module

941 Eluent Production

-----

Module

Start eluent produc-

tion ▶

Starts eluent production with the following parameters:

Mode Shows the current mode of the level sensor. The mode is defined in the configu-

ration. The mode cannot be changed in manual control.

**Eluent volume** Volume of eluent to be produced.

This input field is only active if the mode **Production Empty** or **Production** 

**Full** is configured.

In the mode **Production Full**, eluent production stops if the liquid container is

full, even if the defined volume has not been reached yet.

**Dilution factor** Dilution factor of the eluent.

Aspirate ► Aspirates the specified volume via the defined port. There is **no** automatic filling

beforehand or afterwards.

**Port** Port for aspirating the sample.

Rate for aspirating the sample.

**Volume** Volume to aspirate.

**Dosing ►** Doses the specified volume via the defined port. There is automatic filling

beforehand or afterwards.

**Port** Port for dosing the sample.

Rate for dosing the sample.

**Filling Rate** Rate for filling the cylinder after dosing the sample.

**Volume** Volume to dose and fill in the cylinder.

Fills the cylinder via the specified port.

**Port** Port for filling the cylinder.

Rate for filling the cylinder.

14.3 Start parameters

Move to exchange position ▶	Fills the cylinder via the specified port first. Then rotates the valve disk to Port 2. The dosing drive can be removed from the dosing unit.
Port	Port for filling the cylinder.
Rate	Rate for filling the cylinder.
Stop eluent produc- tion	Stops eluent production.

You can also define settings for the 941 Eluent Production Module in the start parameters (see chapter 14.3.1, page 94).

# 14.3 Start parameters

## 14.3.1 941 Eluent Production Module

To start the eluent production with the defined start parameters, click on

# [ Language Send the current method to the instrument].

Sensors	
On	The level sensor is switched on when you start the method.
Mode	Shows the current mode of the level sensor.
	The mode is defined in the configuration. The mode cannot be changed in the start parameters.
Name	You can enter an individual name for each sensor.
Action	If a level sensor has the status not ok (empty mode = level sensor has no contact, full mode = level sensor has contact), then one of the following actions is triggered:
	<ul> <li>Record message         The activity log shows the message that a level sensor has the status not ok.</li> <li>Abort current run and sequence         The run is aborted. The instrument stops immediately. The activity log shows         the message that a level sensor has the status not ok.</li> <li>Complete current run and abort sequence         The current run is finished. Then the instrument stops. The activity log shows         the message that a level sensor has the status not ok.</li> </ul>
	This input field is only active if the mode <b>Monitoring Empty</b> or <b>Monitoring Full</b> is configured.
Dilution factor	Dilution factor of the eluent.

	This input field is only active if the mode <b>Production Empty</b> or <b>Production Full</b> is configured.
Eluent volume	Volume of eluent to be produced.
	This input field is only active if the mode <b>Production Empty</b> is configured.
Waiting time	Time that must elapse before the next run is started with the newly produced eluent. Slight concentration differences may occur between the old and the new eluent, resulting in an unstable baseline. Once the waiting time has elapsed, the chromatogram will be recorded again at a constant eluent concentration.
	This input field is only active if the mode <b>Production Empty</b> is configured.

You can also define settings for the 941 Eluent Production Module in manual control (see chapter 14.2.1, page 93).

15.1 Manual control

# 15 Parameters of the dosing unit

The dosing unit consists of an 800 Dosino that serves as dosing drive and a cylinder unit. The cylinder unit is available with 4 cylinder sizes: 5 mL, 10 mL, 20 mL and 50 mL.

Use the dosing unit for liquid handling tasks.

The 4 ports of the cylinder unit are designed for flexible use.

## 15.1 Manual control

## 15.1.1 Dosing unit

Dosing unit

Aspirate ► Aspirates the specified volume via the defined port. There is **no** automatic filling

beforehand or afterwards.

**Port** Port for aspirating the sample.

Rate for aspirating the sample.

**Volume** Volume to aspirate.

**Dosing** ► Doses the specified volume via the defined port. There is automatic filling

beforehand or afterwards.

**Port** Port for dosing the sample.

Rate for dosing the sample.

**Filling Rate** Rate for filling the cylinder after dosing the sample.

**Volume** Volume to dose and fill in the cylinder.

**Empty** Empties the cylinder and all tubings of the dosing unit.

The parameters for emptying the dosing unit are defined in the configuration

(see menu "Dosing unit settings", page 16).

Fills the cylinder via the specified port.

**Port** Port for filling the cylinder.

Rate	Rate for filling the cylinder.			
Move to exchange position ►	Fills the cylinder via the specified port first. Then rotates the valve disk to Port 2. The dosing drive can be removed from the dosing unit.			
Port	Port for filling the cylinder.			
Rate	Rate for filling the cylinder.			
Prepare	Rinses the cylinder and all tubings of the dosing unit with the solution that is connected to the fill port.			
	The parameters for preparing the dosing unit are defined in the configuration (see menu "Dosing unit settings", page 16).			
Stop Dosino	Stops the dosing unit.			



-----

## **NOTE**

If the Dosino is used for Dosino regeneration, this is indicated with **M1** in the icon.



If the Dosino is used for a Dose-in gradient, this is indicated with  ${\bf D1}$  in the icon.



You can also define settings for the dosing unit in the time program (see chapter 15.2.1, page 98).

15.2 Time program

# 15.2 Time program

## 15.2.1 Dosing unit

Aspirate				
	Aspirates the specified volume via the defined port. There is no automatic filling beforehand or afterwards.			
MSB	Number of the MSB port the dosing unit is connected to.			
Port	Port for aspirating the sample.			
Rate	Rate for aspirating the sample.			
Volume mode	<ul> <li>Select a volume mode from the drop-down list.</li> <li>from method</li> <li>Injection volume     The injection volume is defined in the sequence.</li> <li>Injection volume next sample     The injection volume is defined in the sequence.     This volume mode allows to prepare the next sample in parallel. The dosing unit takes the volume of the next line in the sequence while dosing the volume of the current line.</li> </ul>			
Volume	This input field is only active if the volume mode <b>from method</b> is selected.  User defined volume to aspirate.			

υ	o	s	е

MSB

Doses the specified volume via the defined port. There is automatic filling beforehand or afterwards.

Number of the MSB port the dosing unit is connected to.

**Port** Port for dosing the sample.

Rate for dosing the sample.

Filling rate Rate for filling the cylinder after dosing the sample.

**Volume mode** Select a volume mode from the drop-down list.

- from method
- Injection volume

The injection volume is defined in the sequence.

Volume	<ul> <li>Injection volume next sample         The injection volume is defined in the sequence.         This volume mode allows to prepare the next sample in parallel. The dosing unit takes the volume of the next line in the sequence while dosing the volume of the current line.     </li> <li>This input field is only active if the volume mode from method is selected.</li> <li>User defined volume to dose.</li> </ul>
	Oser defined volume to dose.
Eject to end volume	
	Ejects the entire content of the cylinder via the specified port.
MSB	Number of the MSB port the dosing unit is connected to.
Port	Port for ejecting the entire content of the cylinder.
Rate	Rate for ejecting the sample.
Fill	
	Fills the cylinder via the specified port.
MSB	Number of the MSB port the dosing unit is connected to.
Port	
Rate	Port for filling the cylinder.
nate	Rate for filling the cylinder.
Change port	
	The valve rotates to the specified port.
MSB	Number of the MSB port the dosing unit is connected to.
Port	The valve is switched to the defined port.
Empty	
	Empties the cylinder and all tubings of the dosing unit.
	Define the parameters for emptying the dosing unit in the configuration (see menu "Dosing unit settings", page 16).
MSB	Number of the MSB port the dosing unit is connected to.
Prepare	

15.2 Time program

Rinses the cylinder and all tubings of the dosing unit with the solution that is connected to the fill port.

Define the parameters for preparing the dosing unit in the configuration (see menu "Dosing unit settings", page 16).

MSB

Number of the MSB port the dosing unit is connected to.



## **NOTE**

If you create a single sample analysis or a sequence, you must select an injection source. If you want to use the **injection volume** that is defined in the sequence, then select the following injection source:

- With an 858 Professional Sample Processor, select IC -Injection
   Valve or Sample Processor.
- With an 889 IC Sample Center, select Sample Center Injection Valve.

An error occurs if you select the injection source **External** or **No Injection/Instrument Blank** and the time program command **Injection volume** or **Injection volume next sample**.

You can also define settings for the dosing unit in manual control (see chapter 10.1.12.2, page 47).

16 Online signals

# **16 Online signals**

The **Online Signals** section shows live data of the connected instruments.

The **Online Signals** function does not record data.

It is possible that the time axes of different signals do not coincide.

The moment when a time program starts measuring is displayed with a red line in **Online Signals**. If 2 detectors of a 2-channel instrument start measuring at a different time, then the following behavior applies: In the charts for the conductivity detectors, both of these moments are recorded at the same time. Actually, only the measurement for 1 detector starts at the recorded time. The measurement for the other detector starts later.

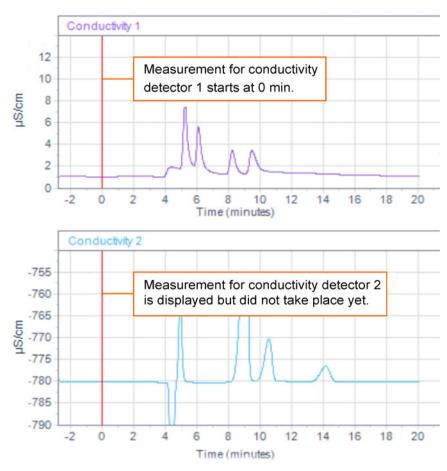


Figure 17 Display of conductivity measurement – Example



## **NOTE**

Refer to the OpenLab Help for further information about online signals: **How To ▶ OpenLAB CDS ▶ Acquisition ▶ Online Signals**.

17 Data acquisition

# 17 Data acquisition

OpenLab distinguishes between 2 kinds of data acquisition.

- Single sample analysis
   Only 1 sample is analyzed.
- Sequence

A series of samples is analyzed.

A sequence contains parameters of the run, for example sample type, acquisition method, processing method or injection source. These parameters can differ for each sample.



#### NOTE

Due to a bug in OpenLab 2.3, it is not possible to run single samples with an instrument that contains 2 ICs. With an instrument that contains 2 ICs, you can only run sequences.

(Tracking Number: CDS2ACQ-13525 250249)

This bug has been fixed in OpenLab 2.4. In OpenLab 2.4, it is possible to run single samples with an instrument that contains 2 ICs.

To create either a single sample analysis or a sequence, go to **Acquisition** ► **Home**. Click on **[Single Sample]** or **[Sequence]**.

Sequence creation templates facilitate the process of creating a sequence.

To create a new sequence with a sequence creation template, open the window **Sequence Creation Template**.

\_\_\_\_\_

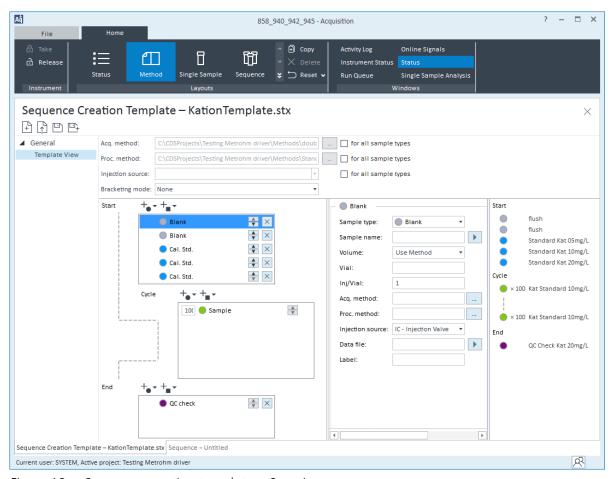


Figure 18 Sequence creation template – Overview



## **NOTE**

If you create a single sample analysis or a sequence, you must select an injection source. If you want to use the **vial position** that is defined in the sequence, then select the following injection source:

- With an 858 Professional Sample Processor, select IC Injection
   Valve or Sample Processor.
- With an 889 IC Sample Center, select Sample Center Injection Valve.



## NOTE

While you run a sequence, it is not possible to edit the current line and the next line of the sequence.

The **Run Queue** window shows information about current runs, for example state of a run, result name or acquisition method.

17 Data acquisition

The run queue can contain single samples and sequences. It is possible to place several single sample analyses in the run queue. A single sample can be submitted without waiting until the previous analysis is finished.



## NOTE

The **Fill Down** command in the sequence table can only be used with an instrument that contains an 858 Professional Sample Processor or an 889 IC Sample Center. To use the **Fill Down** command, choose the injection source **Sample Processor - Tower** with the 858 Professional Sample Processor or the injection source **IC Sample Center** with the 889 IC Sample Center for all sequences.



#### NOTE

Refer to the OpenLab Help for further information about acquiring single samples: **How To ▶ OpenLAB CDS ▶ Acquisition ▶ Single Sample**.

Refer to the OpenLab Help for further information about sequences:

How To ▶ OpenLAB CDS ▶ Acquisition ▶ Sequence.

# 18 Data analysis



## **NOTE**

Refer to the OpenLab Help for information about data analysis:

How To ▶ OpenLAB CDS ▶ Data analysis and Getting
Started ▶ Guides and Resources ▶ OpenLAB CDS ▶ Data analysis Reference Guide.

19 Reports

# 19 Reports

To open the report section, go to **Data analysis** ▶ **Reporting**.

You can create reports with report templates.

The USB flash drive contains a report template (*Ion chromatography example report.rdl*). Import the report template in the same way as you imported the acquisition method (*see chapter 8.1, page 23*). Import the report template to the folder **Report Templates** instead of **Methods**.

To edit the report template, open the template and click on **Editor**.

Define the content of reports with report items. Report items are snippets of information. Place all required report items with drag and drop in the report editor to compile a report template.

There are 3 driver specific report items.

- Instrument Modules
- Advanced Run Information
- Acquisition Method Information Multi Column

## **Instrument Modules**

This report contains the following information for each module:

- Name
- Part number
- Serial number
- Firmware version

This report item is located in **Report Items** ➤ **Instrument Information** ➤ **Instrument Modules**.

# Report Driver Related Info Module Type 858.0020 Professional IC Sample Processor System Part. No. Serial No. Firmware 5.858.0012

930.1560 2124

Figure 19 Instrument Modules – Report item

930.1560 Compact IC Flex SeS/PP/Deg

## **Advanced Run Information**

System

This report contains additional information about exchangeable hardware parts of the instrument, for example about analytical columns, dosinos or amperometric cells.

5.940.0101

This report item is located in **Report Items** ► **Samples** ► **Advanced Run Information**.

## **Report Driver Related Info**



## **Method Events**

ModuleNameValue930.1560 Compact IC Flex SeS/PP/DegDosinoDosino 19702; Dosing unit 2 ml930.1560 Compact IC Flex SeS/PP/DegDosinoDosino 21378; Dosing unit 20 ml930.1560 Compact IC Flex SeS/PP/DegType Metrosep A Supp 17 - 150/4.0; 0072.2077

## **Acquisition Method Information Multi Column**

This report item contains information regarding the method, the instrument modules and their configuration. This report item is located in

Report Items ► Method Information ► Acquisition Method Information Multi Column.

19 Reports -----

## Report Driver Related Info



190604\_rec19minDiG15minstep.amx Acquisition Method:

Path: C:\CDSProjects\kru\Results\MSMReg\_Doseln\M\_D-2019-06-06 16-48-39+02-00.rslt

## Method Information

C:\CDSProjects\kru\Methods\190604\_rec19minDiG15minstep.amx

Modified: 2019-06-06 15:55:35+02:00

Modifier: SYSTEM

Created: 2019-06-06 15:55:35+02:00

Creator: SYSTEM

Description:

2019-0606-1355-35702 Version:

## 858.0020 Professional IC Sample Processor

Peristaltic Pump On: Stirrer On:

Time Program:

Move:

Move: Position type=VialFromSequence, Lift Position=Work

Pump: Rate=2, On Set peristaltic: Wait: Wait time=2 min Wait:

Set peristaltic: Pump: Off

Event Set: Name=Injection Performed Event Set:

Move: Position type=VialFromMethod, Vial=36, Lift Position=Work Move: Move: Move: Position type=VialFromMethod, Vial=129, Lift Position=Work

Set peristaltic: Pump: Rate=2, On Wait: Wait: Wait time=2 min

Set peristaltic: Pump: Off

Module Display Name: 858.0020 Professional IC Sample Processor

Module Type:

## 930.1560 Compact IC Flex SeS/PP/Deg 0 min

Recording Time: 19 min MCS 1 On: Yes Conductivity Detector 1 2.3 %/°C Temperature Coefficient: Conductivity Detector 1 Polarity: + Degasser 1 On: Yes Injector 1 Position: Fill Peristaltic Pump 1 On: No 0.7 ml/min Pump 1 Flow: Pump 1 On: Pump 1 PMax: 18 MPa Pump 1 PMin: 0 MPa Pump 1 Start Time: 1 min MSM 1 On: MSM 1 Interval: 15 min Dosino Regeneration MSM 1: Dosino 1

Solution 1:

Post Time:

Dosing Port: Port1 Volume: 3.00 mL 15.0 min Time: Dosing Rate: 0.20 mL/min Fill Port: Dose-In Gradient Pump 1: Dosino 2 0 min Time: Ratio: 0 % Curve: Linear Time: 5.5 min Ratio: 0 % Curve: Linear Time: 6.5 min

C:\CDSProjects\kru\Report Templates\kru\_Acquisition method

Printed: 2019-06-20 13:28:37+02:00

Page 1 of 2

## **Report Driver Related Info**



Curve: Linear Time: 6.6 min Ratio: 80 % Step Curve: Time: 15 min Ratio: 80 % Curve: Step 0.7 mL/min Flow: Total Volume: 4.872001 mL

Time Program:

MSB=2, Port=2, Rate=66 Fill:

Event Wait: Name=Injection Performed

switch injector: Injector: Injector: 1, Position=Inject Measure Conductivity: Measure Conductivity: 1
Dose-in gradient: MSB=2
Module Display Name: Module Type:

Module Type: Injector: 1, Position=Inject

MSB=2 930.1560 Compact IC Flex SeS/PP/Deg

## **Method Properties**

Instrument Technique: Liquid Chromatography

Figure 20 Acquisition method multi column – Report item



## **NOTE**

Refer to the OpenLab Help for further information about reports: How **To** ► OpenLAB CDS ► Reporting.

20 Method resolve

## 20 Method resolve

If you load a method, then the Metrohm IC Driver for OpenLab checks whether the configured hardware corresponds to the instrument the method was written with.

It is possible to load a method that was written on an instrument with a different configuration. In this case, the Metrohm IC Driver for OpenLab resolves the differences between the instruments in the following way:

- If the configured instrument contains fewer modules than the instrument from the loaded method, then the entire modules are removed from the method.
- If the configured instrument contains more modules than the instrument from the loaded method, then the additional modules are added to the method. The start parameters are set to their default values.
   Adapt the start parameters if necessary. The time program is empty.
- If the configured instrument contains **fewer units** than the instrument from the loaded method, then the start parameters of the missing units are removed. A warning occurs in the time program if a time program command uses a non existing unit. The user has to resolve this difference manually by deleting or adapting the affected time program command.
- If the configured instrument contains **more units** than the instrument from the loaded method, then the default start parameters of the additional units are added. Adapt the start parameters if necessary.



## NOTE

If you write a method and change this method on an instrument with a different configuration afterwards, then the following behavior occurs: The parameters for the modules of the first instrument are still stored in the background of the method. If you load the method in an instrument with the same configuration as the first instrument, then the parameters that were defined in the original method are used again.

## 21 Recommendations

## **Configuration**

- An instrument may maximally include the following modules:
  - 2 x 930 Compact IC Flex, 940 Professional IC Vario or 945
     Professional Detector Vario
    - Any combination of 940 Professional IC Vario, 930 Compact IC Flex and 945 Professional Detector is possible.
  - 1 x 858 Professional Sample Processor
  - 1 x 889 IC Sample Center
  - 1 x 944 Professional UV/VIS Detector Vario or 947 Professional UV/VIS Detector Vario
  - 1 x 941 Eluent Production Module
  - 1 x IC Amperometric Detector per 930/940 IC
  - The number of 942 Extension Modules Vario depends on the number of 940/945 ICs.
  - The number of MSB devices (for example dosing units) depends on the number of available ports (according to the system configuration).
  - 1 single quadrupole mass spectrometer from Agilent for IC-MS applications
- Metrohm recommends to configure the instrument with automatic configuration.
- If you configure the instrument automatically, then the stirrer is deactivated by default. If you want to use the stirrer, then activate the stirrer in manual configuration of the 858 Professional Sample Processor (see chapter 5.2, page 12).
  - If you configure an instrument with a 941 Eluent Production Module automatically, then no level sensor is configured by default. Configure the rod length of the level sensors manually (see chapter 5.5, page 15)
- If you configure your instrument with manual configuration, configure the instrument in the following order:
  - 930/940/945 IC
  - 858 Professional Sample Processor
  - 889 IC Sample Center
  - 944/947 Professional UV/VIS Detector Vario
  - 941 Eluent Production Module

This is the same order as in automatic configuration. The order is relevant because you can only load a method if it was written on an instrument with the same order of modules.

21 Recommendations

• For manual configuration, the serial number is required. You cannot find the serial number of the 889 IC Sample Center on the module. Contact a Metrohm service engineer, if you need to know the serial number of your 889 IC Sample Center.

- The number of a detector refers to the number of the socket where the detector is plugged in. The number of a detector does not depend on the actual number of connected detectors. If the instrument contains 1 detector that is plugged in socket 2, then the detector is labeled as Detector 2.
- If you want to use a Remote Box as an MSB device, you have to configure the Remote Box for the 930/940/945 IC. It is not possible to select the Remote Box as an MSB device for the 858 Professional Sample Processor.
- A high-pressure gradient can only be configured for 940 Professional ICs Vario and for 942 Extensions Modules Vario that are connected to a 940 Professional IC Vario. A high pressure gradient cannot be configured for 930 Compact ICs Flex.
- An instrument may maximally contain 1 high-pressure gradient pump,
   1 Dose-in gradient pump and 1 Dosino for Dosino regeneration.

## **Status panels**

- In the status panels, all units of a module indicate the state of the module, not the state of the individual unit.
- The instrument status is displayed in the status panels and at the bottom of the dashboard. During initialization, the status panels display Not Ready but the dashboard already displays Instrument Idle. If the status panels and the dashboard display a different status, then the status of the status panels is relevant.
- The status **Injecting** is not available for the 858 Professional Sample Processor and the 889 IC Sample Center. In an instrument that contains an IC and an autosampler, the autosampler is in status **Run** while the IC is in status **Injecting**.
- It is possible to connect an extension module to a 945 Professional Detector Vario. In this case, the status panel displays the name of the detector as a title and not the name of the extension module.

## Method

- If the instrument contains several units of the same type, then the start parameters menu appears once for each unit. For example, if the instrument contains 2 peristaltic pumps, the start parameters menu of the peristaltic pump appears twice. The order of start parameter menus for several units of the same type is explained in *chapter 7*, page 19.
- With the command Parallel it is possible to execute several time program commands at the same time. If the same unit is used for several commands at the same time, an error is generated, but not all units are stopped.

- It is not possible to execute a time program that contains the command Measure Conductivity several times for the same conductivity detector
  - Only the first **Measure Conductivity** command is executed. All subsequent **Measure Conductivity** commands are invalid. These commands are ignored but no error occurs.
- For the 858 Professional Sample Processor and 889 IC Sample Center, you cannot define a recording time or post time. Therefore, ensure that the recording time and post time of the IC time program is long enough to cover all time program commands of the 858 Professional Sample Processor and the 889 IC Sample Center.
  If the time program of the 858 Professional Sample Processor takes longer than the defined recording time and post time, the time program is stopped after the defined time.
- The position type Next Vial from Sequence of the 858 Professional Sample Processor and the 889 IC Sample Center can only be used if the next sample uses the same acquisition method as the current sample. Ensure that the sequence in the sequence table meets the requirements of the Next Vial from Sequence command.
- Metrohm recommends to use shutdown methods without time program and with a recording time of 0 minutes.
  If you use a method with time program as a shutdown method, then the time program is executed in the shutdown method. Time program commands that use information from the sequence cannot be used in the time program of a shutdown method.

Do **not** use the following commands in the time program of a shutdown method:

- Dosing units commands Volume mode: Injection volume
- Dosing units commands Volume mode: Injection volume next sample
- Move Position type: Vial from Sequence
- Move Position type: Next Vial from Sequence
- Move Position type: Vial from Sequence +1
- Event Wait
- With instruments with a detector, it is not possible to execute a run without data acquisition. Always add a measure command to the time program. Otherwise, the instrument stays in the state **Injecting** and does never enter the state **Run**.
  - If you do not want to acquire data during the run, then add a time program command **Measure Conductivity** at the end of the time program and define a recording time of 0 minutes. As different detectors in an instrument can have different recording times, ensure that the recording time for each detector is properly adapted.
  - If an instrument does not contain a conductivity detector, then the instrument enters the **Run** state with the first acquisition command. In this case, the command **Measure Conductivity** is not needed.

21 Recommendations

In the MSM start parameters, the dosing rate for dosino regeneration is calculated from the parameters **Volume** and **Time**.
If you send the current method to the instrument to equilibrate the instrument, then the default dosing rate of 1.0 mL/min is applied for the first MSM step. For all following MSM steps, the dosing rate from the method is applied.

• If a module is in **Error** state and you send a method to the instrument, it may occur that the module remains in the **Error** state, but some units of the module work correctly. In this case, stop the run and press the **[Off]** button. Send the method to the instrument again. If the error remains, ensure that all modules are connected properly, close the instrument connection and launch the instrument again.

## **Data acquisition**

- If you create a single sample analysis or a sequence, you must select an
  injection source. If you want to use the **vial position** that is defined in
  the sequence, then select the following injection source:
  - With an 858 Professional Sample Processor, select IC -Injection
     Valve or Sample Processor.
  - With an 889 IC Sample Center, select Sample Center Injection Valve.

An error occurs if you select the injection source **External** or **No Injection/Instrument Blank** and the time program command **Vial from Sequence**, **Next Vial from Sequence** or **Vial from Sequence** +1.

- If you create a single sample analysis or a sequence, you must select an injection source. If you want to use the **injection volume** that is defined in the sequence, then select the following injection source:
  - With an 858 Professional Sample Processor, select IC -Injection
     Valve or Sample Processor.
  - With an 889 IC Sample Center, select Sample Center Injection Valve.

An error occurs if you select the injection source **External** or **No Injection/Instrument Blank** and the time program command **Injection volume** or **Injection volume next sample**.

- For Agilent instruments, you can run a pretreatment program for sample preparation. The pretreatment program is executed before the actual time program.
  - For Metrohm instruments, a pretreatment program does not exist.
- It is not possible to change the acquisition method during a run. If you want to change the acquisition method, finish the run, change the acquisition method and start a new run.
- While you run a sequence, it is not possible to edit the next line of the sequence.

- If a leak is detected during a sequence, the current sequence is aborted. The next sequence is started. At the start of the first run, the driver checks whether the instrument is still leaking. If the leak still exists, the sequence is also aborted. The driver repeats this procedure until all sequences have been aborted or the leak has been removed.
- The moment when a time program starts measuring is displayed with a red line in **Online Signals**. If 2 detectors of a 2-channel instrument start measuring at a different time, then the following behavior applies: In the charts for the conductivity detectors, both of these moments are recorded at the same time. Actually, only the measurement for 1 detector starts at the recorded time. The measurement for the other detector starts later.
- In online signals, it is possible that the time axes of different signals do not coincide.

## **Data analysis**

 In contrast to MagIC Net (the IC software from Metrohm), noise and drift of the conductivity detector are not measured in the time program. Noise and drift are determined with System Suitability Calculations. To calculate noise and drift, select Signal to noise in the processing method.

Refer to the OpenLab Help for further information System Suitability Calculations: How To ▶ OpenLAB CDS ▶ Data Analysis ▶ Calculations and Background References ▶ System Suitability Calculations.

22 Troubleshooting

# 22 Troubleshooting

## **Instrument errors**

If an error occurs during equilibration or during data acquisition, send the method to the instrument again. If the error persists, search the activity log (see "Log files", page 118). If necessary, send the log files to your Metrohm representative (see "Log files", page 118).

## **Connection problems**

In case of connection problems, proceed as follows to establish a stable connection:

## **Reconfigure the instrument**

- 1 Close the instrument connection with [Close Connection].
- Optionally delete the instrument and create a new instrument (see chapter 4, page 5).
- Configure the instrument again with automatic configuration (see "Automatic configuration", page 7) or with manual configuration (see "Manual configuration", page 8).
- 4 Launch the instrument again.

## **Establish a new connection**

Before executing this procedure, close OpenLab CDS, remove all connected modules from the PC and shut down the PC.

- 1 Start the PC.
- **2** Plug in the required modules.
- **3** Switch on the modules one after another.
- 4 Check whether the modules are available in the Windows Device Manager. This connection is mandatory.

5 Start OpenLab CDS and configure the instrument (see chapter 5, page 6).

## Several instruments on 1 PC

Execute this procedure if there are several instruments on 1 PC and the instruments do not get idle.

- 1 Close the instrument connections with [Close Connection].
- **2** Launch the instruments one after the other.
- **3** If the instruments still do not get idle, close the instrument connections again with **[Close Connection]**.
- 4 Launch the instruments one after the other again but change the launching order compared to the last attempt.
- **5** Repeat steps 3 and 4 until the instruments get idle.



#### **NOTE**

Especially with the 944 Professional UV/VIS Detector Vario, connection problems may occur.

If you try to reconnect the instrument after switching off the power or after disconnecting the USB plug, then the module is often not available in the Windows device manager.

## Log files

If a problem with your instrument occurs, then the activity log or the Metrohm log contain further information about the problem.

The activity log contains messages about errors and activities, for example executing parameters. The activity log states whether the logged activities were executed successfully or not. In case of a failure or an error, the activity log provides tips on how to solve the problem or possible reasons for the failure or error.

22 Troubleshooting

## **Searching the activity log**

- Access the activity log from the **Control panel** or the **Acquisition** window. Regarding the content of the activity log, it does not matter where you open it from.
  - There are 3 ways to access the activity log from the Control panel.
    - Click on [Projects], select a project and click on the icon to expand the activity log section.

    - Click on **Administration ► System Activity Log**.
  - To access the activity log from the Acquisition window, click on Home ➤ Windows ➤ Activity Log.
- 2 In the activity log, click on **[Filters]**.

The filter menu is expanded.

- **3** Filter the messages by date, description and time period.
- **4** See if there is a message that provides more information about your problem.



#### **NOTE**

The error messages are displayed in red letters.

If you were not able to solve the problem, send the activity log and the Metrohm log files to your Metrohm representative. Proceed as follows.

## Sending the activity log to your Metrohm representative

1 Click on Control panel ► Administration ► Export ► Export Detailed.

Save the activity log to your computer.

**2** E-mail the activity log to your Metrohm representative.

## **Sending the Metrohm log to your Metrohm representative**

- 1 Copy the folder **C:\temp\Metrohm\log**.
- **2** E-mail the folder as a .zip file to your Metrohm representative.

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