

# Soprane II

## Documentation



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# 1. Introduction

SOPRANE II is a chromatography software (Chromatography Data System). It is more particularly dedicated to micro-chromatograph (MicroGC) and to on-line analysis. The software can support several instruments (up to 4) as well as sampling systems.

Here are the available features:

- Define a sequence of analyses using multiple streams and several methods of analysis (see chapter [Methods and sequences](#)).
- Automate sending of analytical methods to the different modules of the analyzer, (see chapter [Methods and sequences](#)).
- Acquire the signals and perform the integration at the end of the analysis, (see chapters [Analyzes management](#) and [Process](#))
- Determine the concentrations and other calculations, (see chapter [Process](#))
- To do regular calibrations (see chapter [Calibration sequence management](#))
- Archive the results,
- Print or visualize them under various forms,
- Communicate with third-party applications (or automatons) for the sending of results of the analysis (4-20 mA, relays, link Modbus, ...).

The first part of this manual defines how to configure SOPRANE II.

Some items described in this manual do not correspond to the definition of the "hardware" of your specific analyzer and are therefore not accessible.

SOPRANE II uses a USB key (micro size) for the management of licenses. If the USB license is not connected, SOPRANE II will lock after a few seconds. This key contains information about the analyzer(s), the communication modes (4-20mA, Modbus...), the specific calculations and many others.

Two operations will be necessary before being able to use SOPRANE II: first, to install the software on your computer, then to define the options you're concerned with, among the possibilities offered by your equipment and to consequently configure the installation.

See also:

[Installation](#)

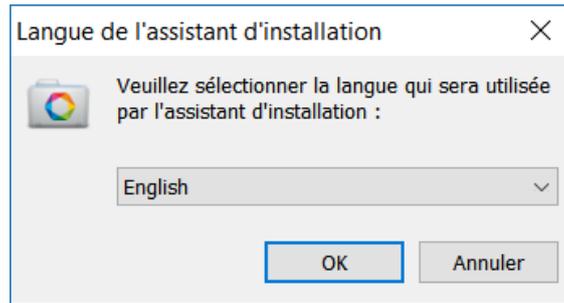
## 2. Installation

SOPRANE II installation package includes this manual and a USB key to install on a USB port of the computer.

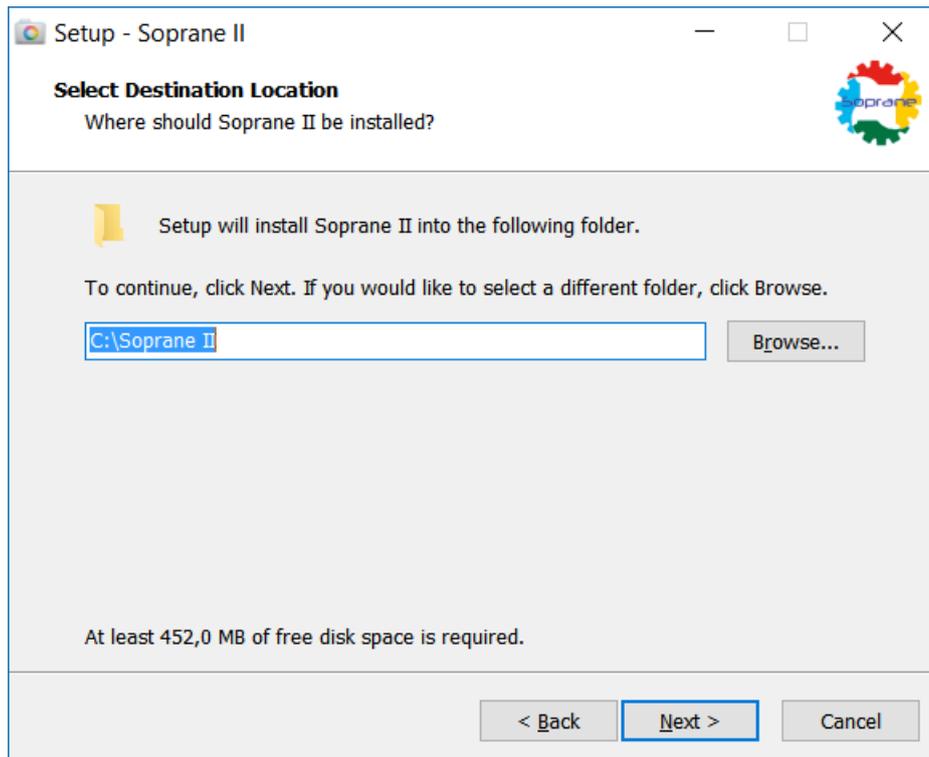
Insert the SOPRANE II USB key on a USB port and start the installation of the software.

In the window which opens, select the language which will be used by the installation wizard.





Once the language has been selected, choose the folder in which SOPRANE II will be installed.



The key delivered with SOPRANE II has a double purpose: to define the configuration specific to the analyzer and its device (and the use needed), and to control the software license to prevent from any fraudulent use.

The installation of the software thus requires installing the key driver. If it is already installed (because of a prior installation), it is not necessary to reinstall it.

After having installed SOPRANE II, you must configure the application (analyzers, inputs / outputs, directories etc...). Each of these items are available only if the option is present in the license provided with the installation media USB.

See the chapter:

[Analyzer configuration](#)

[Creation](#)

[Analyzer creation with network connection](#)

[Analyzer creation with serial connection](#)



[Selection](#)

[Close an analyzer](#)

[Display configuration](#)

### 3. Analyzer configuration

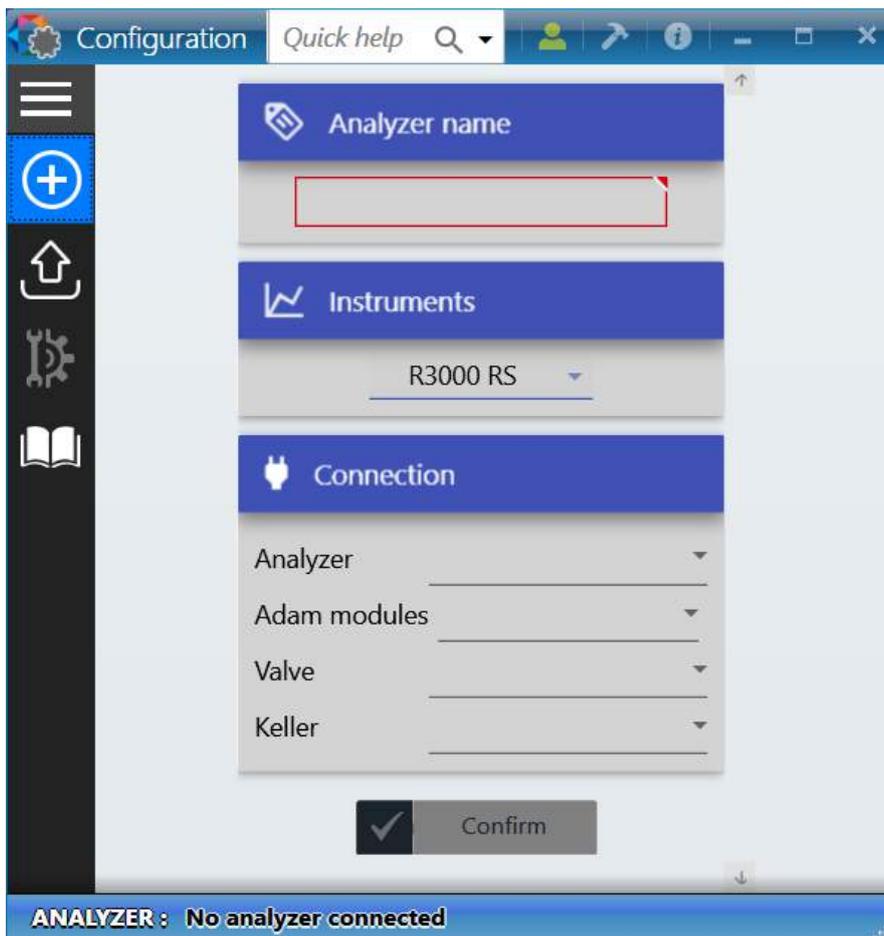


The management of an analyzer configuration is handled by the **Configuration** application present in the SOPRANE II's installation folder. This software can be launched with the command Start / Programs / SRA Instruments / Soprane II Configuration.

Each analyzer is defined by a profile. It is composed as follows:

- A name (name of the analyzer)
- The analyzer type: MicroGC R3000 (series), M3000 (LAN) Inficon, Agilent 490 (LAN) , ...
- The address of the analyzer communication port. COM1, 2... for a serial port, 10.1.1.XXX for an IP address. This address must be selected or written in the field "Analyzer" on the panel "Connection".
- The address of the serial port to communicate with the inputs / outputs modules (field "Adam modules").
- The address of the serial port to pilot VALCO valves (field "Valve").
- The address of the serial port to pilot one or more TES module (field "TES").

Once launched, the first display will propose to create an instrument.



The instrument can be a MicroGC SRA R3000, a MicroGC Inficon 3000, a MicroGC Inficon Fusion, a MicroGC Agilent 490. SOPRANE II can communicate with the analyzers via Ethernet (LAN) or a serial port (RS232). Depending on the information in the USB license, the transmission mode may be restricted to only one type of connection.

To go further, see also the chapters:

#### Creation

[Analyzer creation with network connection](#)

[Analyzer creation with serial connection](#)

#### Selection

[Close an analyzer](#)

[Display configuration](#)

#### Instrument

[Changing communication ports](#)

[Rename an instrument](#)

[Remove an instrument](#)

#### Hardware

[Sampling configuration](#)

[Valco valves](#)

[Electro-valves](#)

[Management of logic inputs and outputs](#)

[Sampling by electro-valves](#)

[Pump sampling management](#)

[Alarms](#)

[Information GC ready](#)

[External start](#)

[Auxiliary pump](#)

[Start analysis command](#)

[Start sequence command](#)

[Control flow sample](#)

[Test of the inputs and outputs](#)

[Logic inputs](#)

[Logic outputs](#)

[Analog inputs](#)

[Test 4-20mA modules](#)

[Valves test](#)

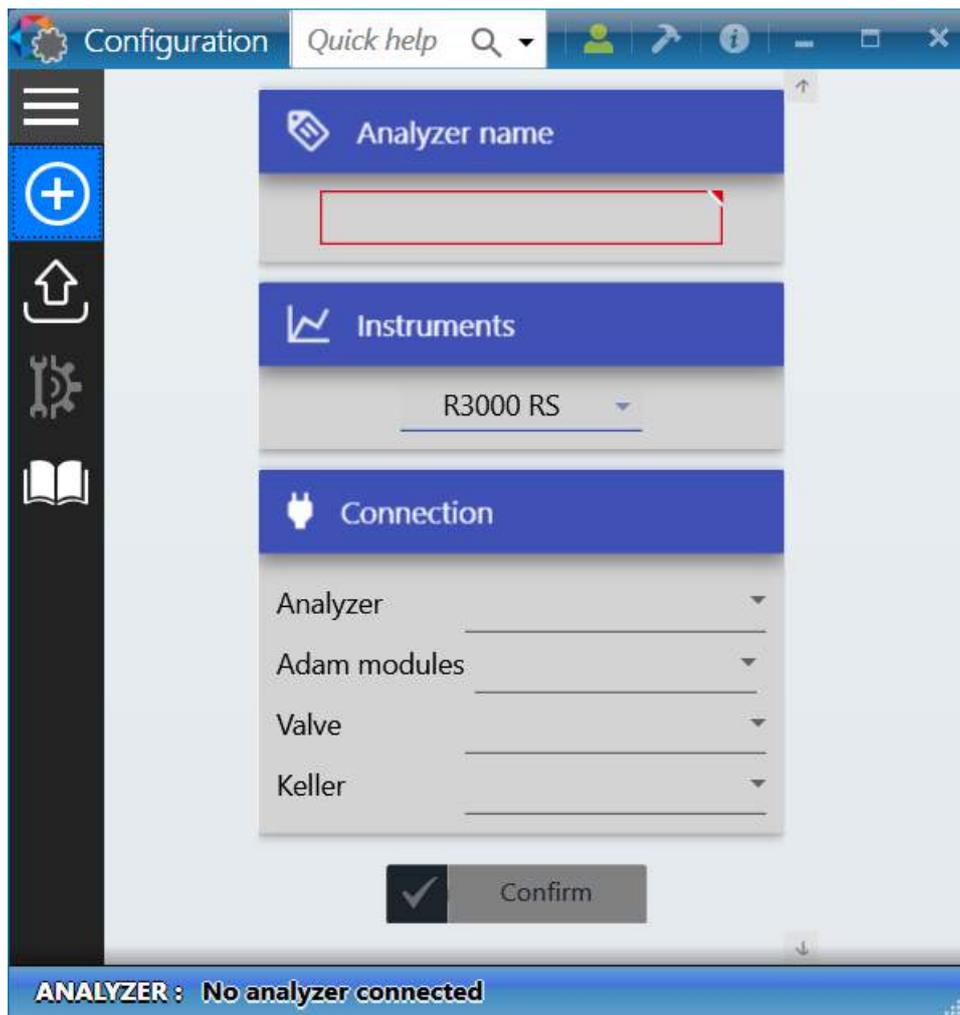
[Carrier gas selection](#)

## 3.1. Creation

SOPRANE II allows to create as many analyzers as desired. The number of instruments specified in the USB license defines the number of analyzers that can be used at the same time. To create an analyzer, click the

button  **Create an analyzer.**





Several types of instrument are available:

- R 3000:  $\mu$ GC SRA a series connection type RS232 (max of the RS232 cable length  $\sim$  20 m).
- M 3000:  $\mu$ GC Inficon 3000 with a network connection, does not require a computer near the chromatograph.
- Agilent 490:  $\mu$ GC Agilent 490 with a network connection, does not require a computer near the chromatograph.

All definitions of connection external modules such as Adam modules, valves and TES modules will be made from this display.

To create an instrument, just enter the name of the instrument, its type, the communication port and if necessary the connection to the external modules (Adam modules, Keller sensor and valves).

When the data are validated, the program tests the existence of an analyzer at the specified address and the possibility to communicate.

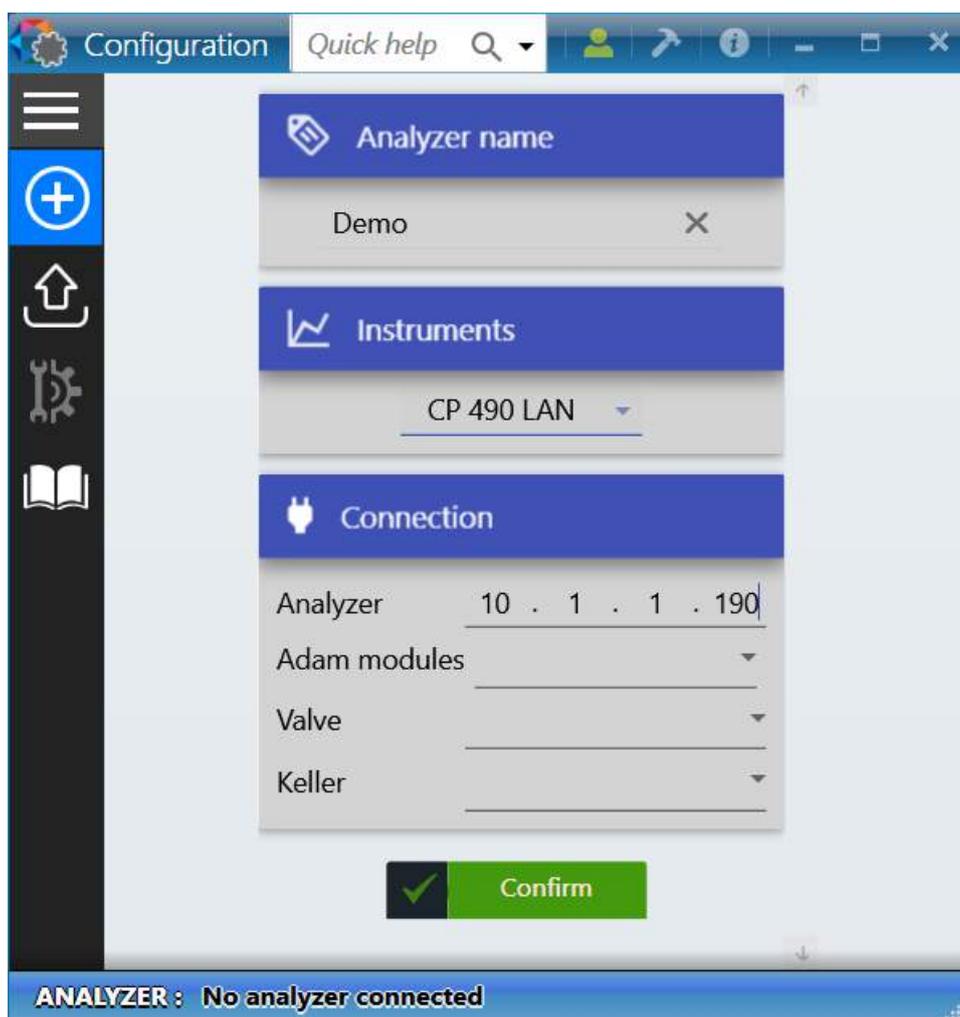


To see how to create an analyzer with a network connection see chapter: [Analyzer creation with network connection](#)

To see how to create an analyzer with a serial connection see chapter: [Analyzer creation with serial connection](#)

### 3.1.1. Analyzer creation with network connection

The case we are considering corresponds to a network connection, in this case, the IP address of the analyzer will be requested:



Without further specification, the chromatographs are delivered initialized to address 192.168.100.100 for Agilent 490 and 10.1.1.1.101 for M3000Lan.

If it is necessary to change this address of the analyzer, the simplest way consists in establishing a direct connection between the computer and the analyzer (TCP/IP connection), using your Web browser and going to the home page of the analyzer.

This is done by directly typing the IP address, 10.1.1.190 (or other if changed) inside the address bar of the web browser as indicated in the next figure.



The analyzer homepage offers several possibilities: read and modify the IP configuration, read the status of the GC and several utilities, to define, for example, the carrier gas used on the analyzer.

The only use we need here is the modification of the IP address.

The screenshot shows a web browser window with the URL 10.1.1.190. The page title is "490 Micro GC" and it features the Agilent Technologies logo. The main content area is titled "Status: Instrument - Overview" and displays the following information:

- Instrument Information:**
  - Instrument name: microgc
  - Site info
  - Instrument serial number: 123
  - GC Time: 23-11-2000 05:29:57
  - Solution: \*
- GC Status:**

	Channel 1		Channel 2	
	Setpoint	Actual	Setpoint	Actual
Column description	20m MS5A Heated Injector, Backflush		10m PPU, Heated Injector, BF, Ultimetel	
Carrier gas	Helium		Helium	
Channel serial number	655240		16235002	
Column temperature [°C]	100.0	100.0	80.0	80.0
Injector temperature [°C]	90.0	90.1	90.0	90.0
Column pressure [kPa]	193.1	193.1	193.1	193.3
Auto zero [mV]		-50.1		-5.7

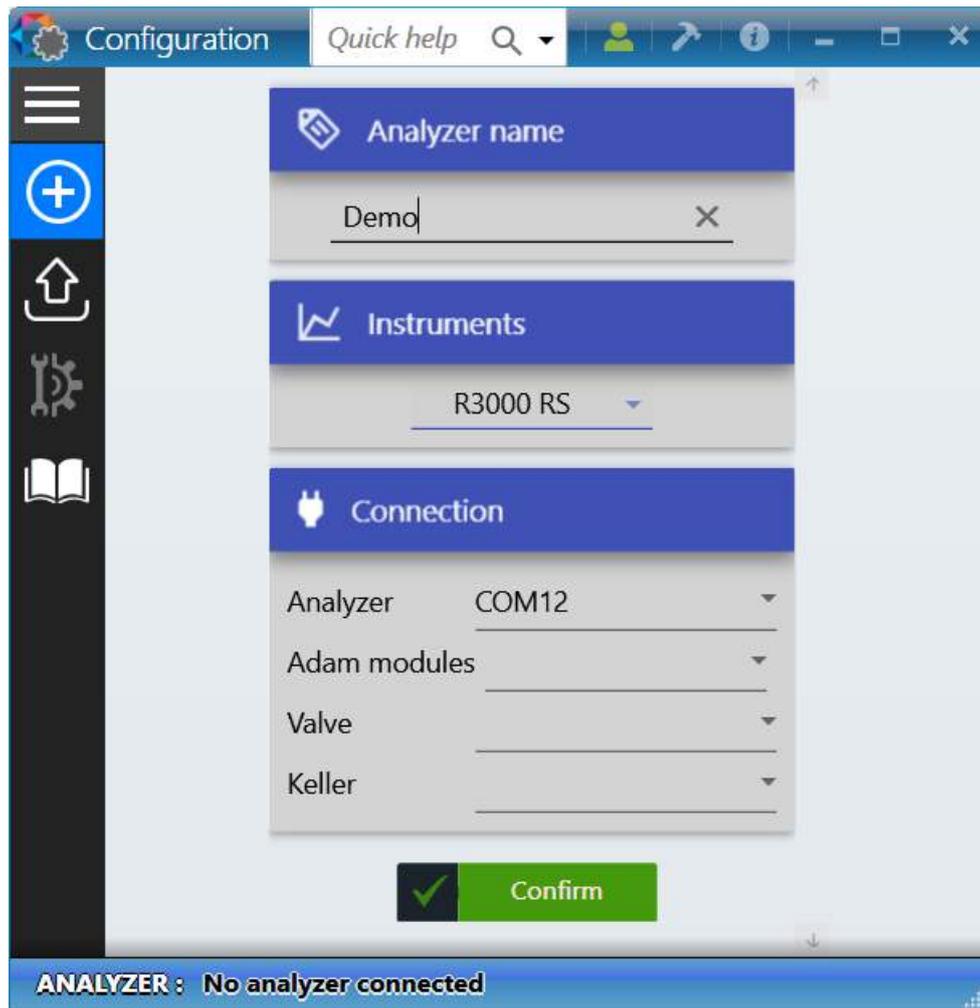
On the left side, there is a navigation menu with categories: Status (Instrument Status, Statistics, Firmware), Control (Identify, Reset), Configuration (Network, Wireless Network, Date & Time, Names), Maintenance (Update, Fieldcase, Diagnostics), and Support (Agilent.com, User manual).

### 3.1.2. Analyzer creation with serial connection

The case we are examining is that of a serial connection with a  $\mu$ GC R3000 RS, in this case, the software asks for the serial port number to use to communicate with the analyzer.

The software asks for the number of the serial port used to communicate with the analyzer.

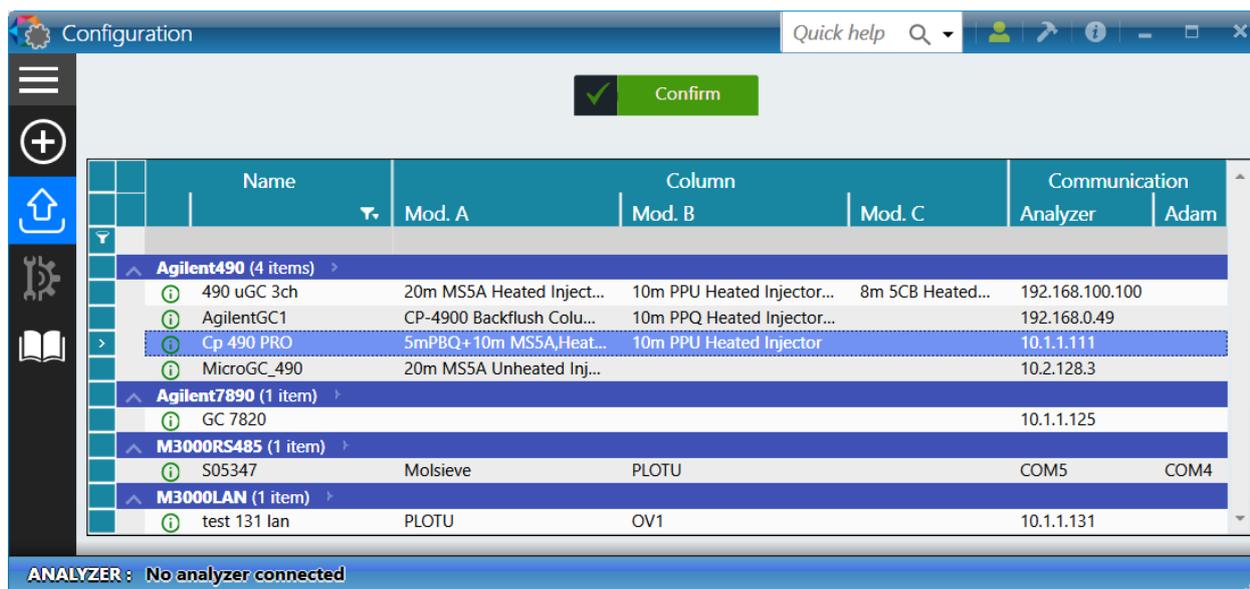




### 3.2. Selection

To load, or change an analyzer, click the button  **Select analyzer**.





	Name	Column		Communication	
		Mod. A	Mod. B	Mod. C	Analyzer
Agilent490 (4 items)					
	490 uGC 3ch	20m MS5A Heated Inject...	10m PPU Heated Injector...	8m 5CB Heated...	192.168.100.100
	AgilentGC1	CP-4900 Backflush Colu...	10m PPQ Heated Injector...		192.168.0.49
	Cp 490 PRO	5mPBQ+10m MS5A.Heat...	10m PPU Heated Injector		10.1.1.111
	MicroGC_490	20m MS5A Unheated Inj...			10.2.128.3
Agilent7890 (1 item)					
	GC 7820				10.1.1.125
M3000RS485 (1 item)					
	S05347	Molsieve	PLOTU		COM5 COM4
M3000LAN (1 item)					
	test 131 lan	PLOTU	OV1		10.1.1.131

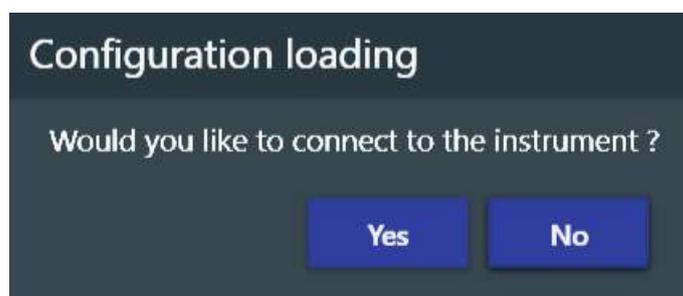
**ANALYZER : No analyzer connected**

Each line represents an analyzer (their configuration is saved in a database).

By clicking on one of them, or selecting with the arrows, information about this configuration appears.

- The name of the instrument.
- The type of the instrument.
- The type of column by module.
- The description of the different connections of the instrument.

To select the instrument, click on the confirmation button, then the configuration will be loaded. A display asks if you want to connect to the instrument, or only view the configuration. In the latter case, no change will be allowed.

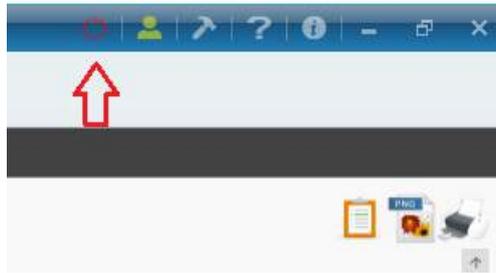


In all cases, the configuration will be displayed (see chapter [Display configuration](#) for more details).

### 3.3. Close an analyzer

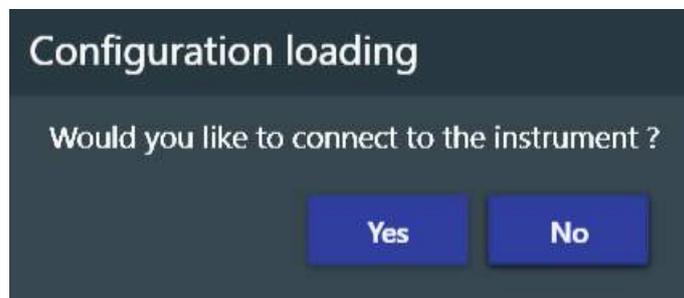
Closing an analyzer can be done by clicking on the icon  located in the upper left on the title bar, or by exiting the application.





### 3.4. Display configuration

Once the analyzer has been selected, a window asks if you want to connect to the instrument, or only display configuration (without modification).



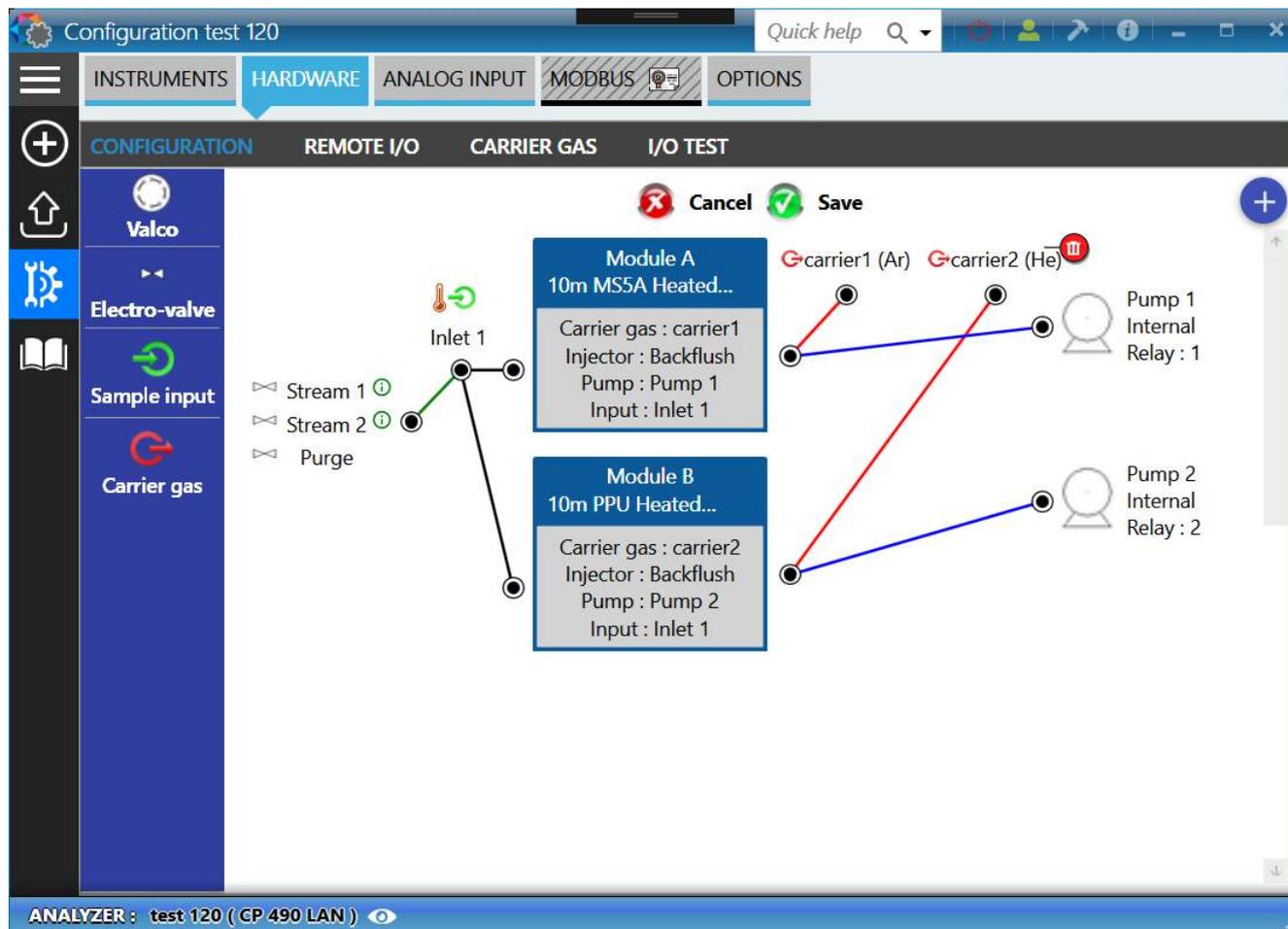
Two views are available:

The first display is the "graphical" visualization of the analyzer with a summary of all the items present in the configuration.



To access, click on the **Configuration** icon , and then click on the tab **Hardware** and **Configuration**.



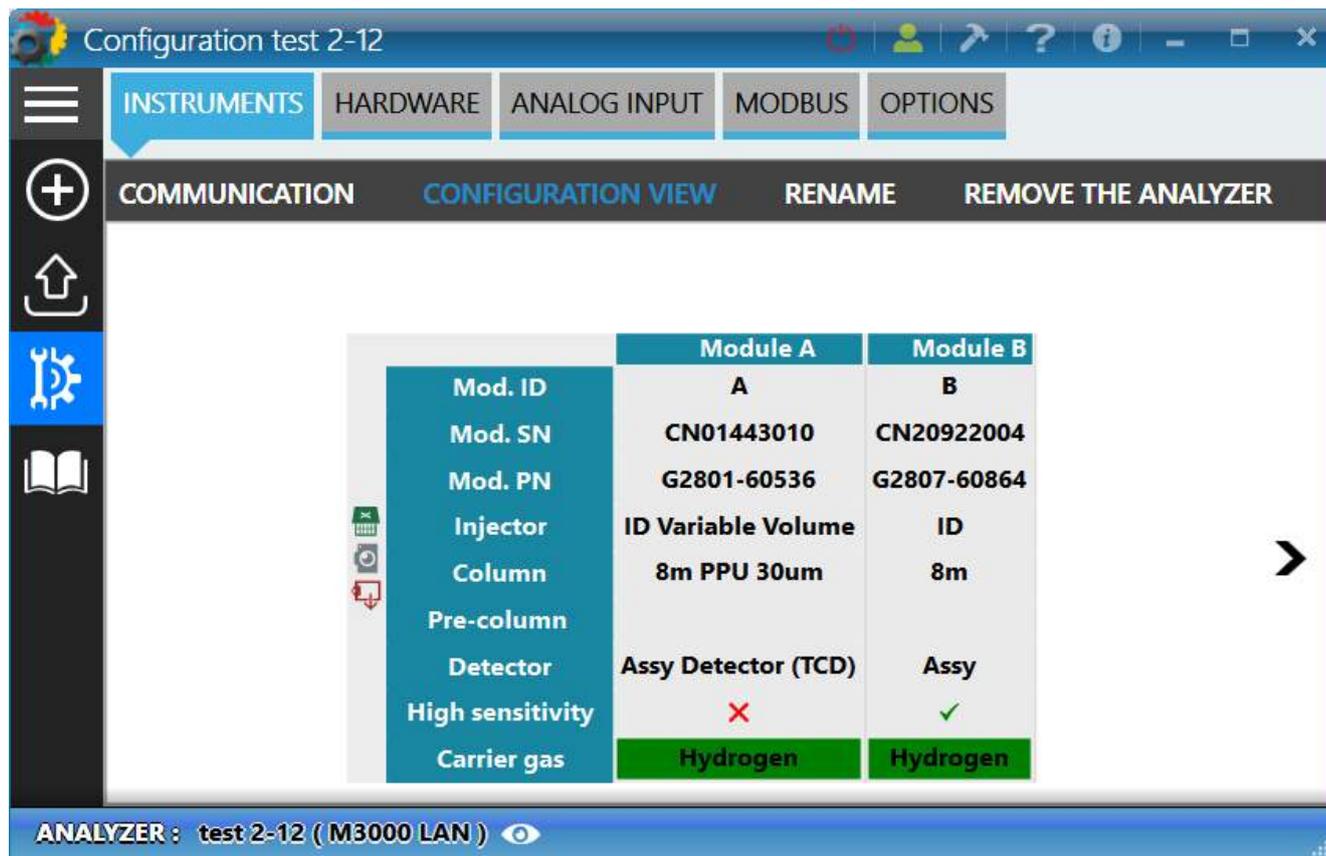


The middle part of the view shows all the items connected to analytical module(s) such as pumps, valves, sample inputs...

The definition of additional hardware elements is also possible at this place of the software, see chapter [Hardware](#).

Another more detailed view is also available by selecting the tab **Instrument** and **Display configuration**.





Note:

On the status bar at the bottom of the window, the icon  (besides the instrument name), allows you to view the configuration at any time, this icon is also available on SOPRANE II.

### 3.5. Instrument

See also:

- [Changing communication ports](#)
- [Rename an instrument](#)
- [Remove an instrument](#)

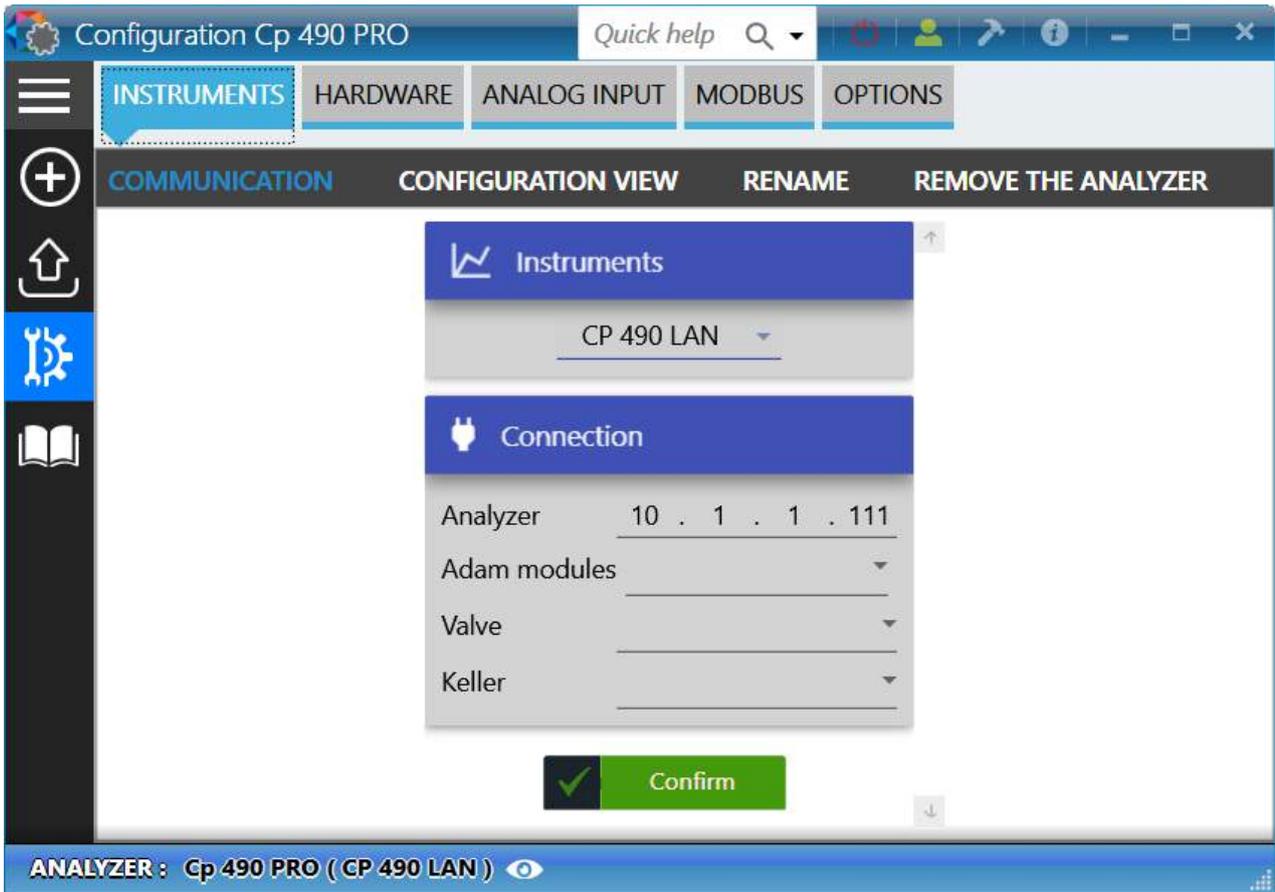
#### 3.5.1. Changing communication ports

To change the communication ports of an instrument, you must first connect to it.

Once connected, follow the path: "Configuration  > Instruments > Communication".

The display allows you to change the instrument type, the communication port to this instrument, as well as the connections to I/O modules, the valves and Keller modules.



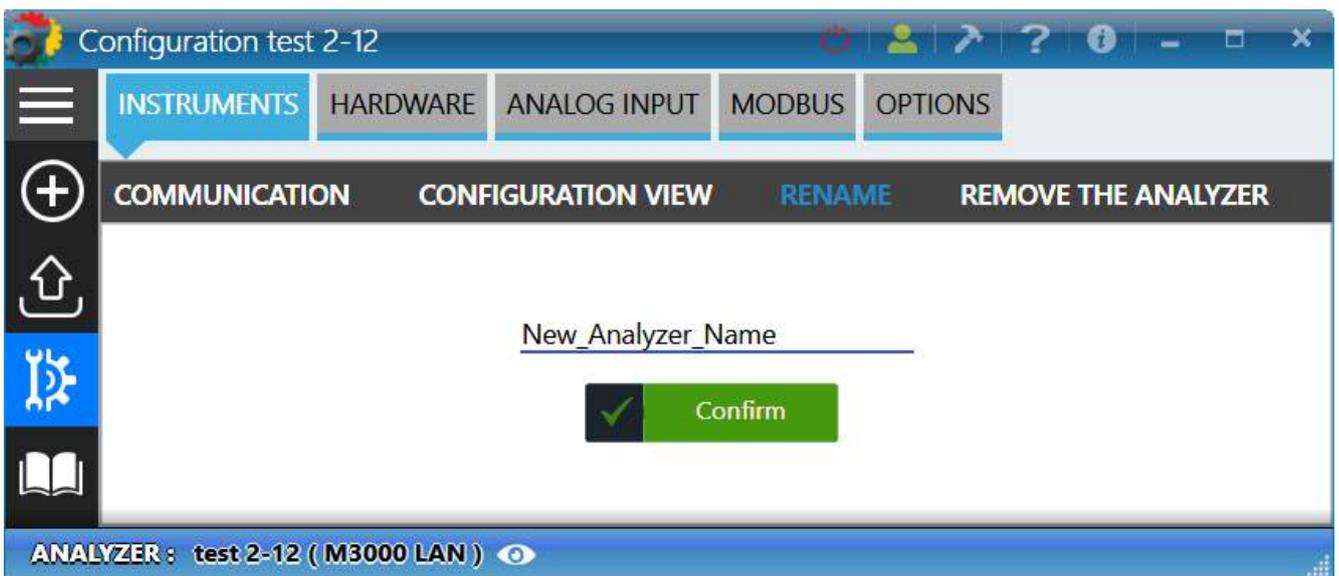


### 3.5.2. Rename an instrument

To rename an analyzer, you must first connect to it. Once connected, follow the following path:

"Configuration  > Instruments > Rename "".

Type the new name for the instrument then click on "Confirm".



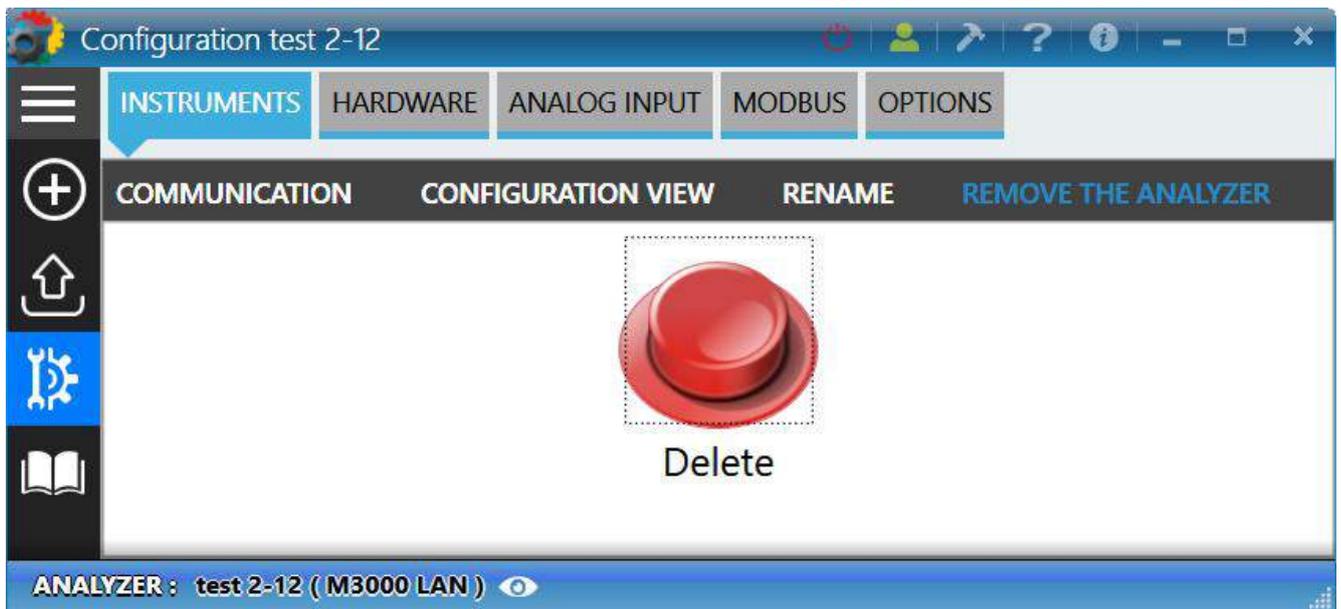
### 3.5.3. Remove an instrument

To remove an analyzer, you must first connect to it. Once connected, follow the following path:

"**Configuration**  > **Instruments** > **Remove the analyzer**".  
Click on the red button to remove the instrument.



Removing an analyzer removes methods and analyses performed with the instrument.



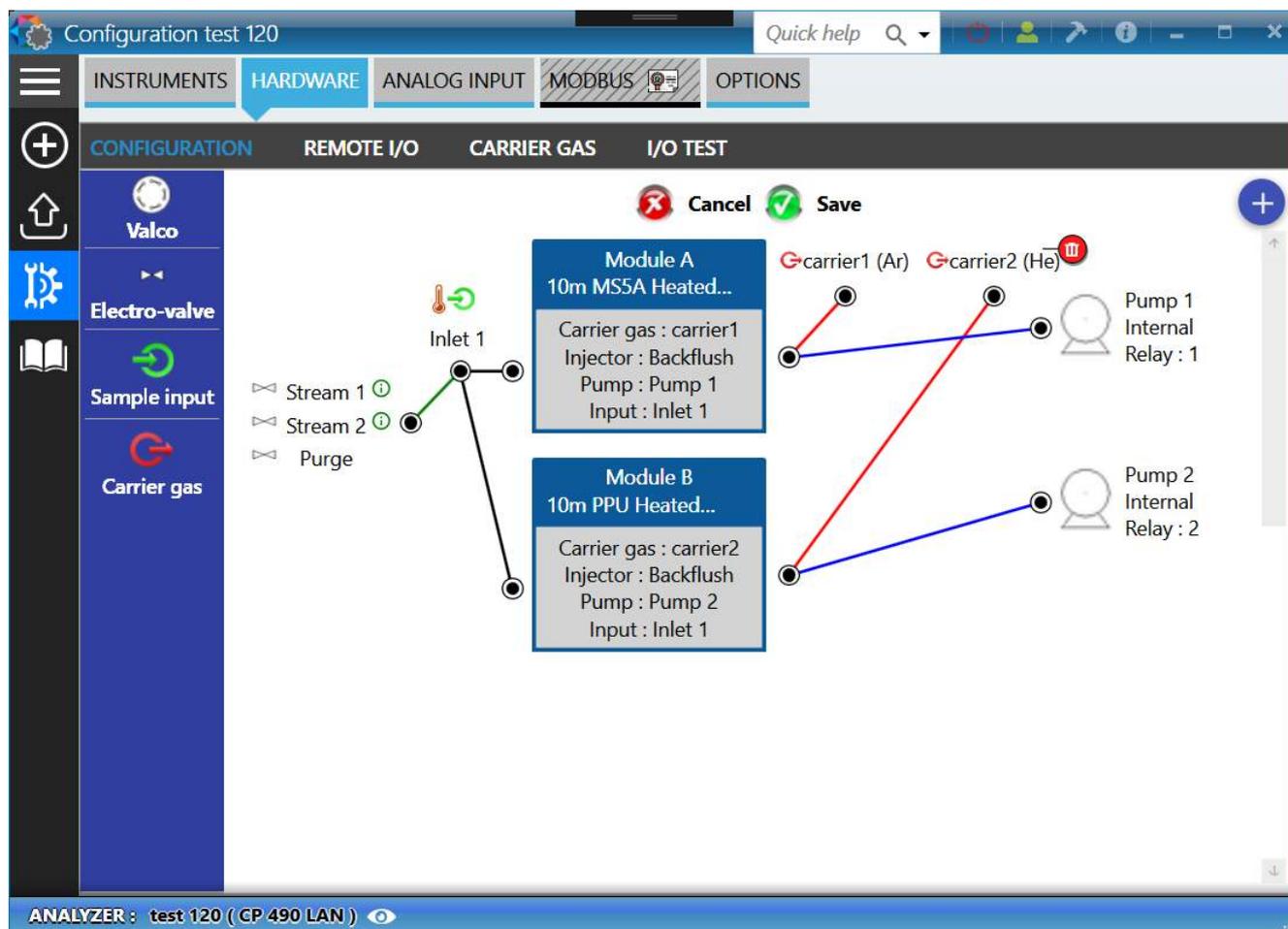
## 3.6. Hardware

It is necessary to define the hardware to be used to carry out the analyzes: how to dialog with the analyzer, how many flows to manage, how they are selected, do we use inputs / outputs, ...

The USB license connected to the computer contains a definition of the installation. It is necessary to configure these options to be able to use them.

To change the "Hardware" configuration, follow the path: "**Configuration**  > **Hardware** > **Configuration**".





This menu shows the configuration of the instrument.

- **Management of the sampling channels**

The sampling channels are managed by the button  for the Valco valve selection or by the button  for the sampling by electro-valves.

The total number of streams used (streams to be analyzed and calibration streams not differentiated, value from 1 to 16 streams), which will be standard streams and the way in which these streams will be selected (set of electro-valves, a BCD coded multi-positions valve or a multi-positions valve with parallel entry).

See also the chapter [Sampling configuration](#) to find out how to properly set sampling channels.

- **Auxiliary pump**

It indicates the presence of an auxiliary pump (button ) which will allow the stop of the pump before or after injection, or permanent aspiration of the sample. The device used to drive the pump may be either a relay of the remote module or one the two embedded relays of the MicroGC (if present).

See also chapter [Auxiliary pump](#) to learn how to configure the auxiliary pump.



- **Sample inputs**

The definition of the sample inputs  allows to determine which input is connected to which module.

*Note:*

*The icon is displayed as an indication, this does not change the configuration of the instrument.*

- **Pump**

Allows a quick sampling of compounds. The sampling pumps are indicated with the icon , we define which module drives which pump. Changing pumps is only enabled on the R3000 MicroGC. For other instruments, pumps are displayed for information only.

To learn how to configure pumps, see also chapter [Sampling pump management](#).

- **Carrier gas inputs**

Nitrogen, Argon, Helium or hydrogen can be used. To add a carrier gas input, click on the button . By default, the carrier gas is Argon.

*Note:*

*By moving the mouse over an element, the icon  allows to remove the item if needed.*

See also:

[Sampling configuration](#)

[Valco valves](#)

[Electro-valves](#)

[Management of logic inputs and outputs](#)

[Sampling by electro-valves](#)

[Pump sampling management](#)

[Alarms](#)

[Information GC ready](#)

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[Logic inputs](#)

[Logic outputs](#)

[Analog inputs](#)

[Test 4-20mA modules](#)

[Valves test](#)

[Carrier gas selection](#)

### 3.6.1. Sampling configuration

SOPRANE II allows to control up to 16 sampling channels, either by electro-valves or by multi-position valve. The multi-position valves can be managed either by reading in BCD and move step by step, or by reading and



positioning in BCD or by Valco type valve controlled by serial connection. In the case of using the BCD, your computer must be equipped with a logical inputs/outputs card.

See also:

- [Valco valves](#)
- [Electro-valves](#)

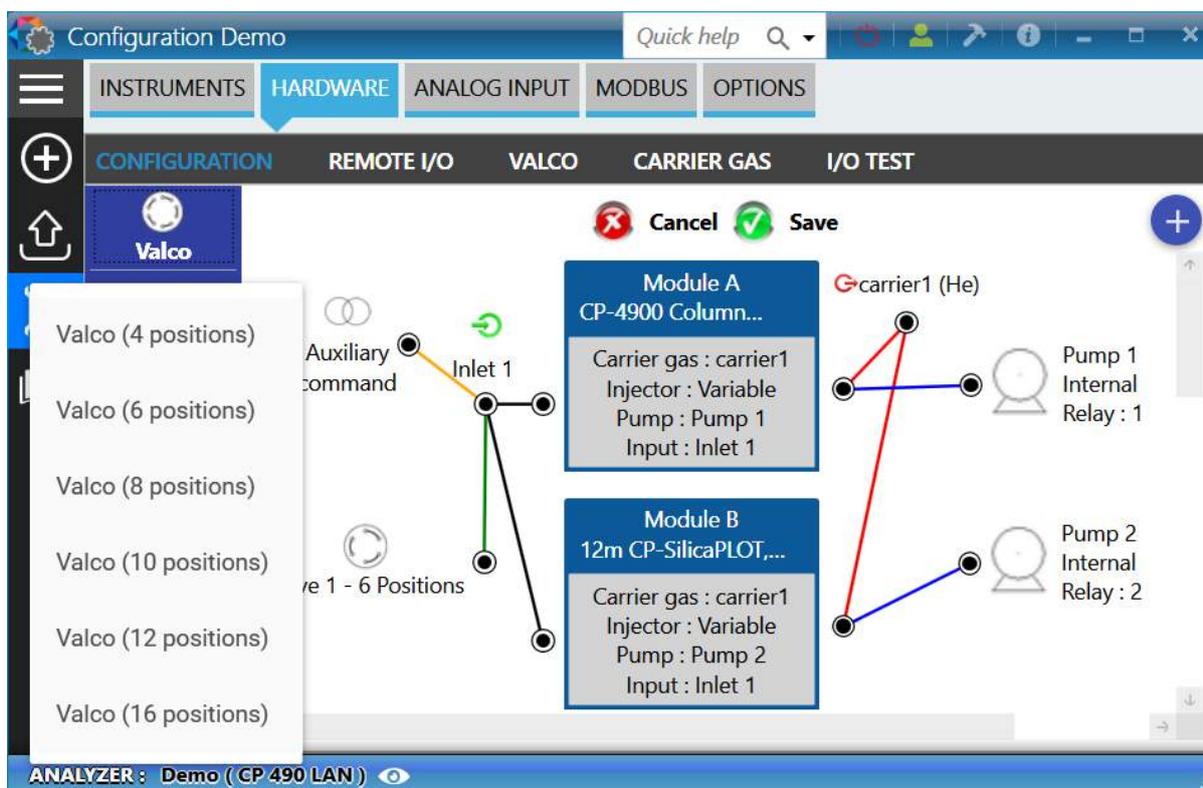
### a) Valco valves

To define the selection of the sampling channels by Valco valve, follow the following path: "**Configuration**  > **Hardware** > **Configuration**".

The window that is displayed allows to define the Valco valve type to use, as well as the number of channels.

By clicking on the button , a menu with the different types of Valco appears. The different choices are:

- Valco 4 positions
- Valco 6 positions
- Valco 8 positions
- Valco 10 positions
- Valco 12 positions
- Valco 16 positions



*Note:*

By moving the mouse over an element, the icon  allows to remove the item if needed.



Once the Valco is correctly added to the graphic, to configure each stream follow the path "**Configuration**



> **Hardware** > **Valco** ".

On the next window, you can define:

- The name of the stream
- The valve
- The valve positions
- If the stream is the purge stream (selected after injection or an analysis)
- If the auxiliary pump is activated when the stream is selected

	Name	Valve	Position	Purge	Auxiliary pump activation
<input checked="" type="checkbox"/>	Stream 1	Valve 1 - 6 Positions	1	<input type="radio"/>	<input checked="" type="checkbox"/>
<input checked="" type="checkbox"/>	Stream 2	Valve 1 - 6 Positions	2	<input checked="" type="radio"/>	<input checked="" type="checkbox"/>
<input checked="" type="checkbox"/>	Stream 3	Valve 1 - 6 Positions	3	<input type="radio"/>	<input checked="" type="checkbox"/>
<input checked="" type="checkbox"/>	Stream 4	Valve 1 - 6 Positions	4	<input type="radio"/>	<input checked="" type="checkbox"/>
<input checked="" type="checkbox"/>	Stream 5	Valve 1 - 6 Positions	5	<input type="radio"/>	<input checked="" type="checkbox"/>
<input checked="" type="checkbox"/>	Stream 6	Valve 1 - 6 Positions	6	<input type="radio"/>	<input checked="" type="checkbox"/>

### b) Electro-valves

To define the selection of the sampling channels by electro-valve, follow the following path: "**Configuration**



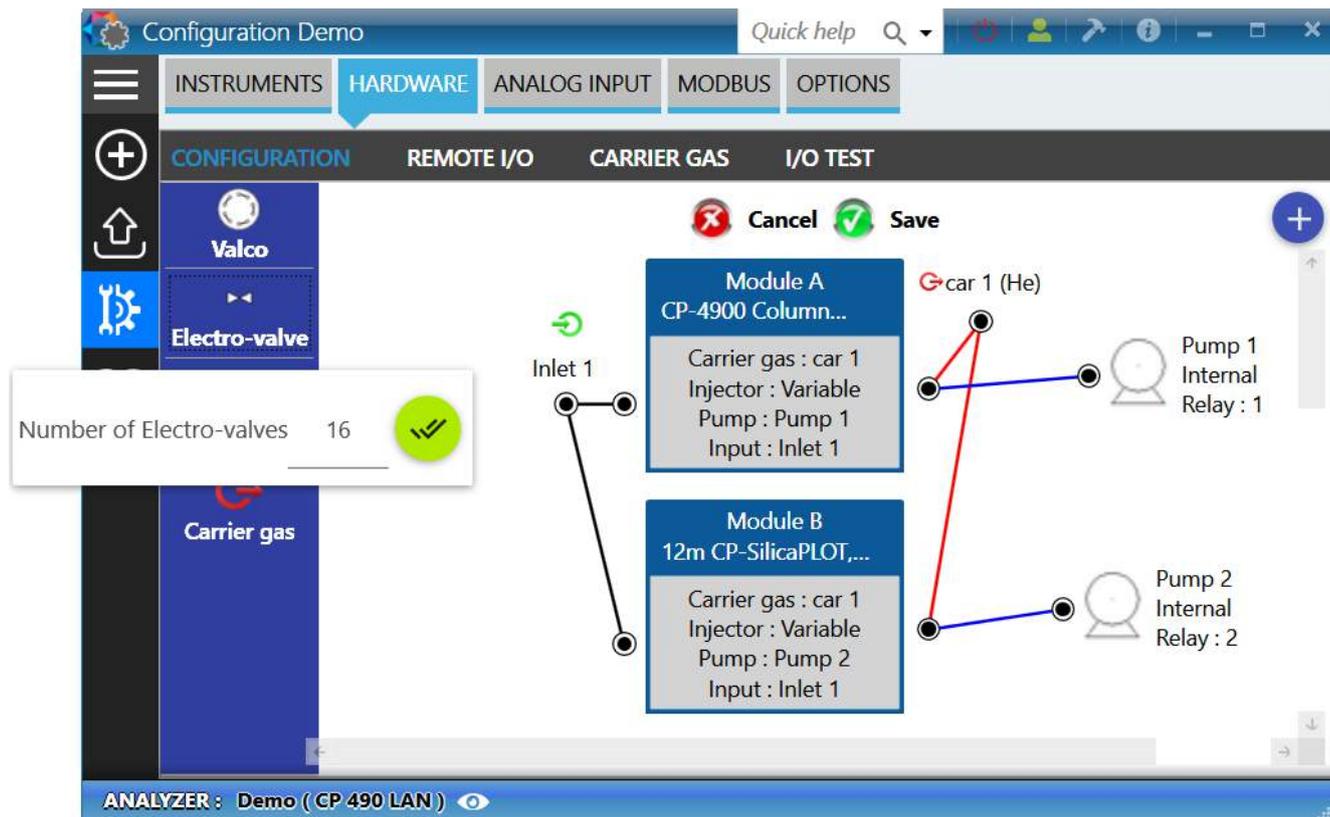
> **Hardware** > **Configuration** ".

The window displayed enables the definition of the number of sampling channels.

By clicking on the button  a menu allows to define the number of channels.

To configure each of the channels see chapter [Sampling by electro-valves](#).





*Note:*

By moving the mouse over an element, the icon  allows to remove the item if needed.

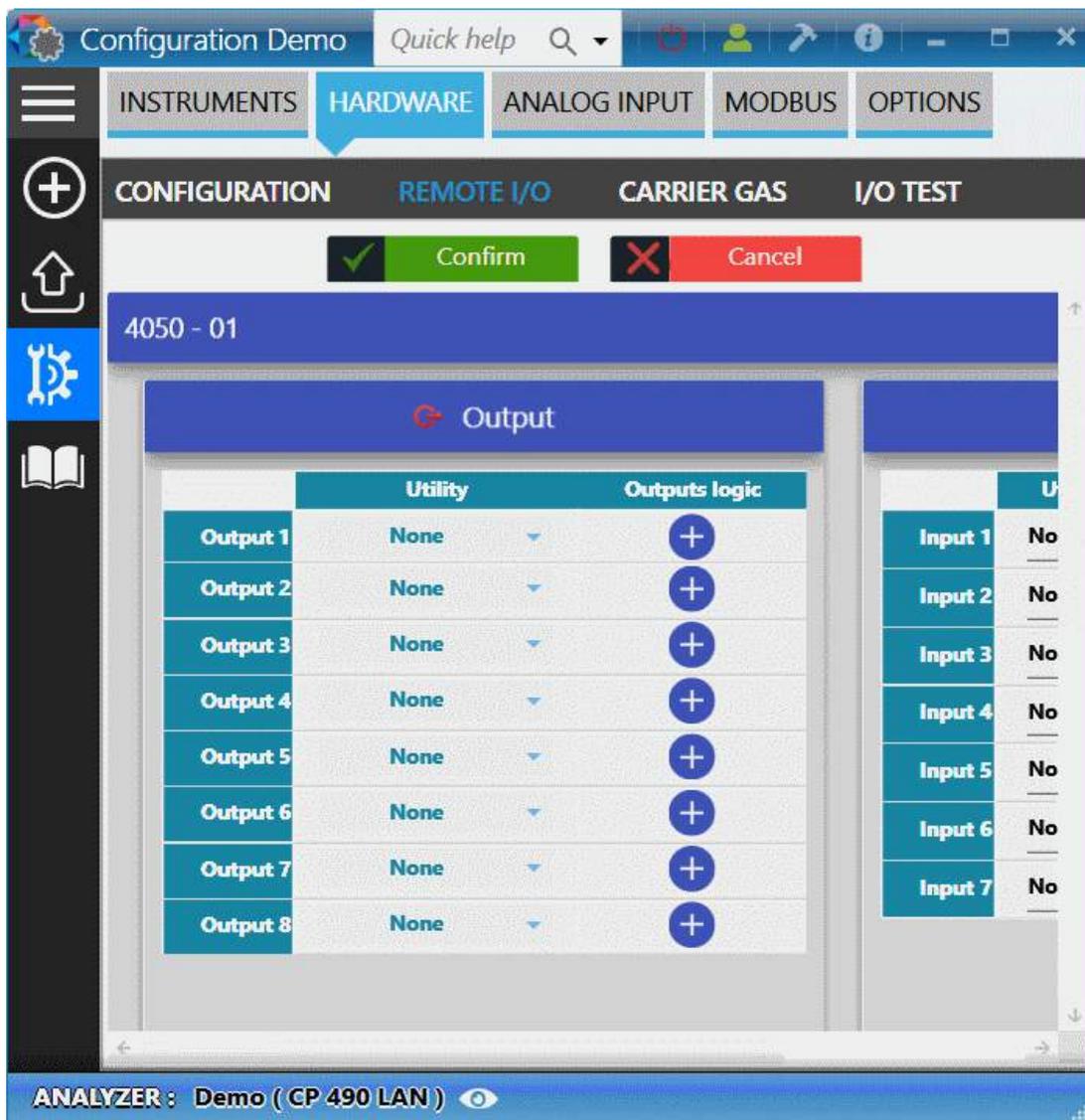
### 3.6.2. Management of logical inputs and outputs

The use of relays is defined by the remote I/O management. To access to it, follow the path: "**Configuration**

 > **Hardware** > **Remote I/O** "

The application detects each module and regroups them by names, separating the inputs and outputs.





All the possible uses of the outputs are:

- Pump: defines a pump to a relay.
- Sample: defines a sampling channel to a relay.
- Alarm: defines an alarm to a relay.
- Information GC ready: when the status of the instrument is ready, activates the relay.
- External start : when the relay is activated, starts the analysis.
- Auxiliary command : Select the auxiliary pump mode.
- None



All the possible uses of the entries are:

- Starting analysis: when the input is activated, starts the analysis.
- Start sequence: when the input is activated, starts an analysis sequence.
- The sample flow control: when the input is activated, activates the sample flow control alarm.
- None

Each input or output can have a positive logic (relay activated when there is a contact) or a negative one (relay activated when no contact is detected).

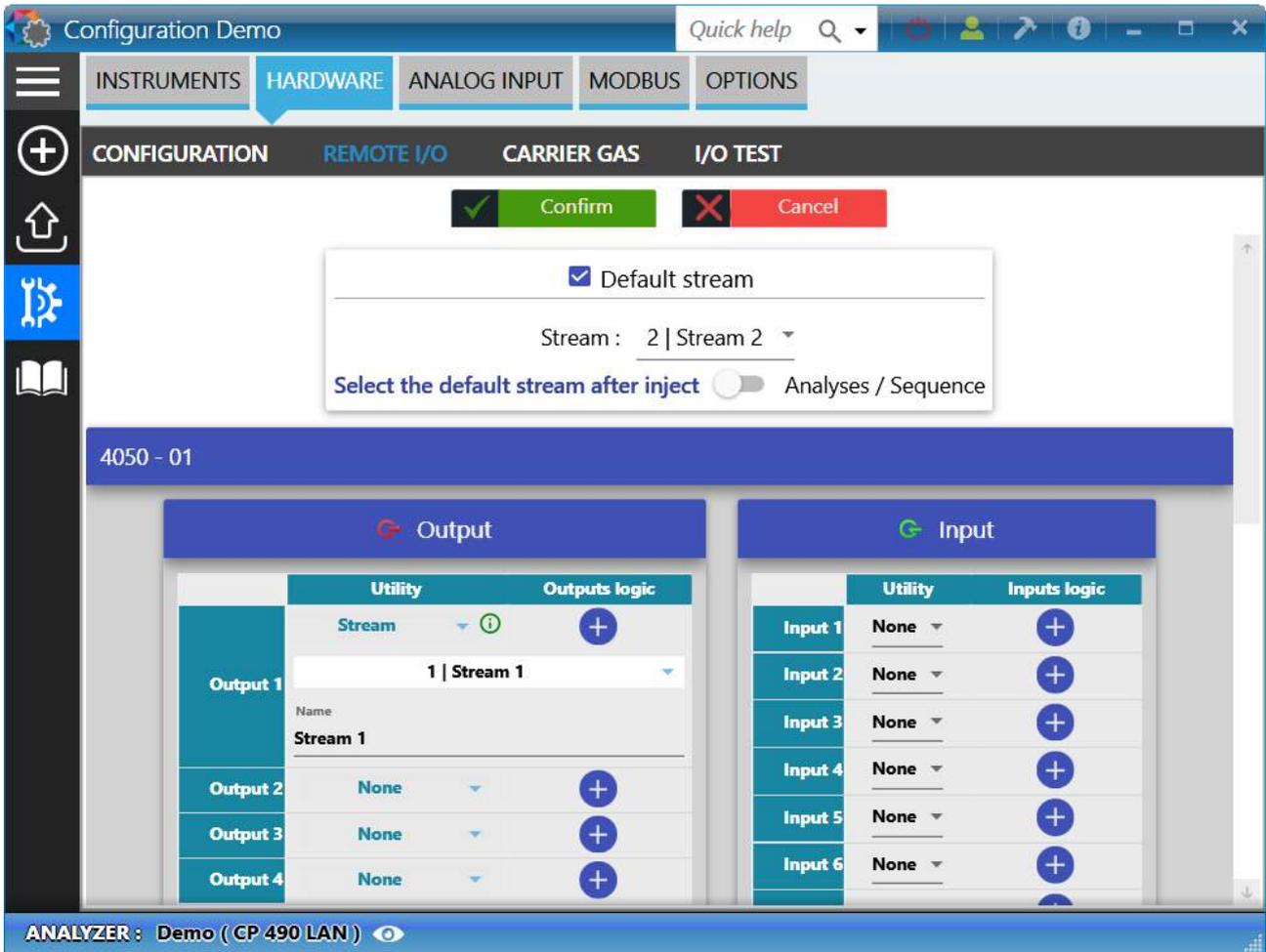
See also:

[Sampling by electro-valves](#)  
[Pump sampling management](#)  
[Alarms](#)  
[Information GC ready](#)  
[External start](#)  
[Auxiliary pump](#)  
[Start analysis command](#)  
[Start sequence command](#)  
[Control flow sample](#)

#### ***a) Sampling management by electro-valve***

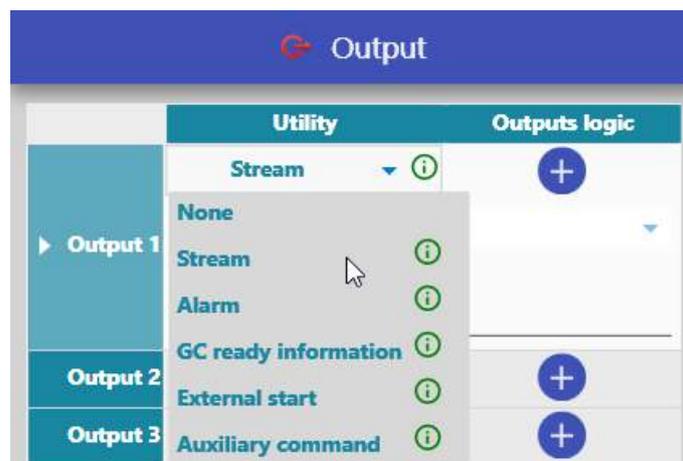
To manage the stream selection, actions described in the chapter [Hardware](#) must have been performed. The following example corresponds to the configuration of a R3000 instrument, but the display is the same for all instruments.





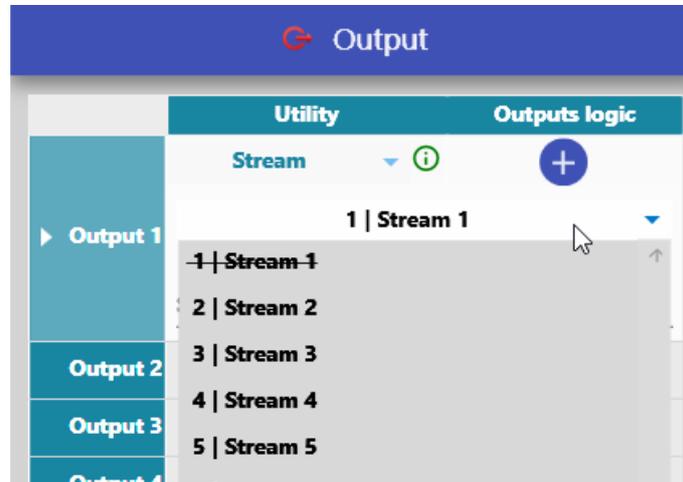
If relays are available (via Adam modules or remote relays in the MicroGC), the stream selection is available. To assign a stream to a relay follow these steps:

1. Selection of the stream utility

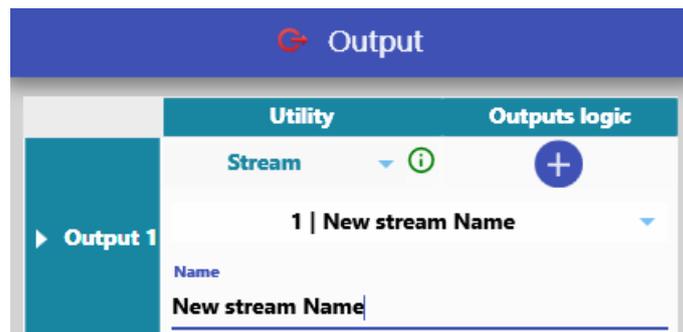


## 2. Selection of the corresponding stream

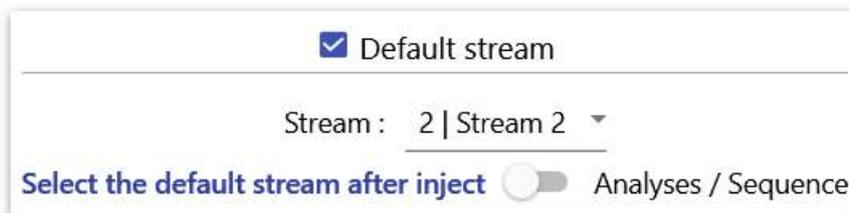
The number of streams has been determined according to the configuration in the [Hardware](#) chapter. A drop-down list contains all available streams.



Once selected, the field **Name** allows you to change the name of the stream.



You also could define a default stream, if checked, the default stream will be selected after each analyses/sequence or if you prefer after each injection.



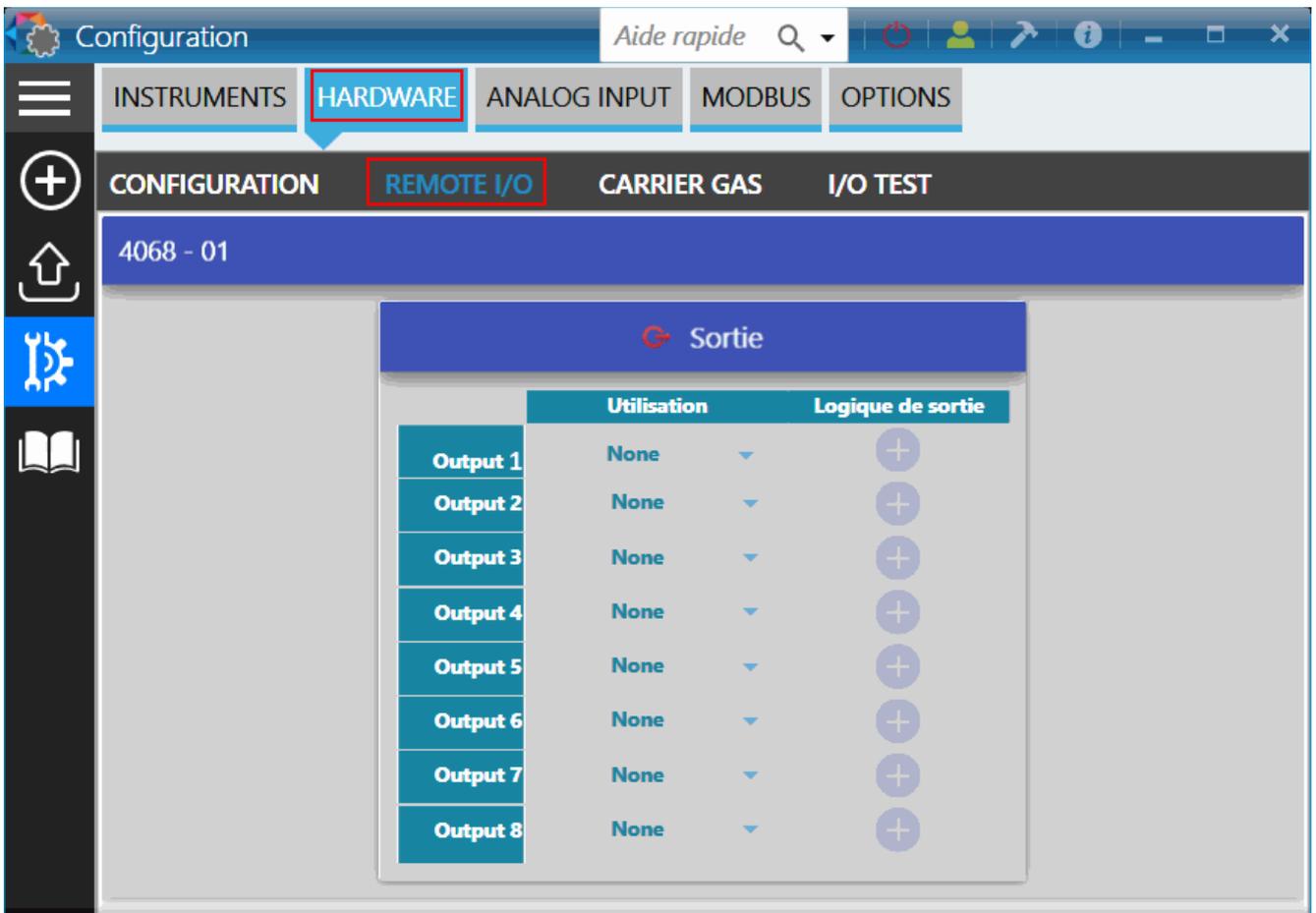
**b) Sampling pump management**

To add and to manage the sampling pumps, actions described in the chapter [Hardware](#) must have been performed.

Sampling pumps are either managed by the analyzer itself (Inficon 3000 LAN, Inficon Fusion, Agilent 490) or by Adam modules (M3000 Rs485).

In the case they are managed internally, the modification of these pumps will not be possible, they will be displayed for your information.

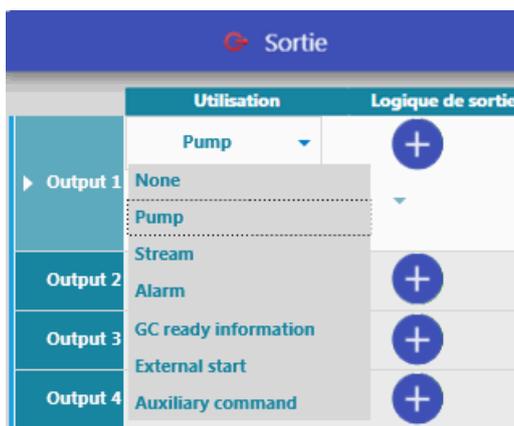
Otherwise we will have the following view:



In the case the module Adam has outputs, the selection of the pump is available. To assign a pump to a relay follow these steps:



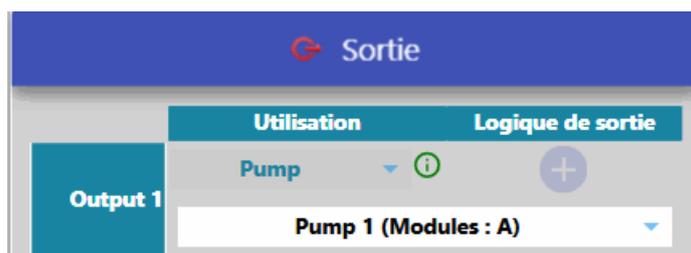
### 1. Selection of the pump utility



### 2. Selection of the corresponding pump

Pumps have been determined according to the configuration in the [Hardware](#) chapter. A drop-down list contains all available pumps. (in the following example there is only pump 1)

Once selected, connected modules are displayed for information purposes.



#### c) Alarms

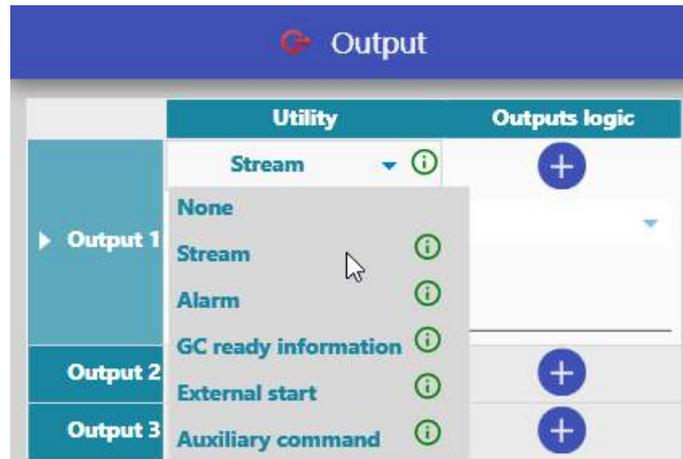
Outputs can be assigned to alarms which, if activated, will generate a default in SOPRANE II software.

To assign an alarm to a relay, follow the following path: **Configuration**  **Hardware** > **Configuration** > **Remote I/O**". If logical outputs are available, the alarm selection will then be available.

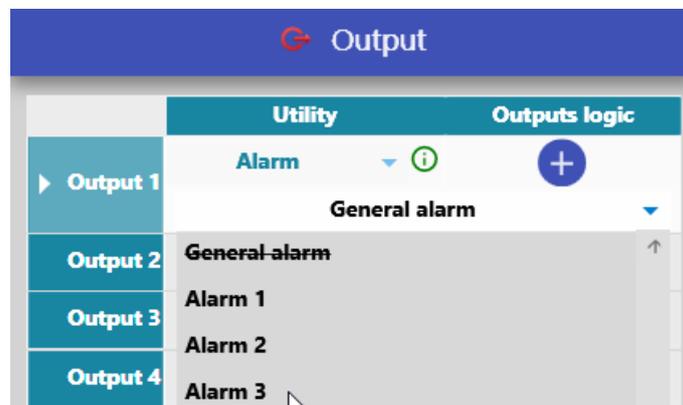
To assign an alarm, follow these steps:



1. Selection of the alarm utility



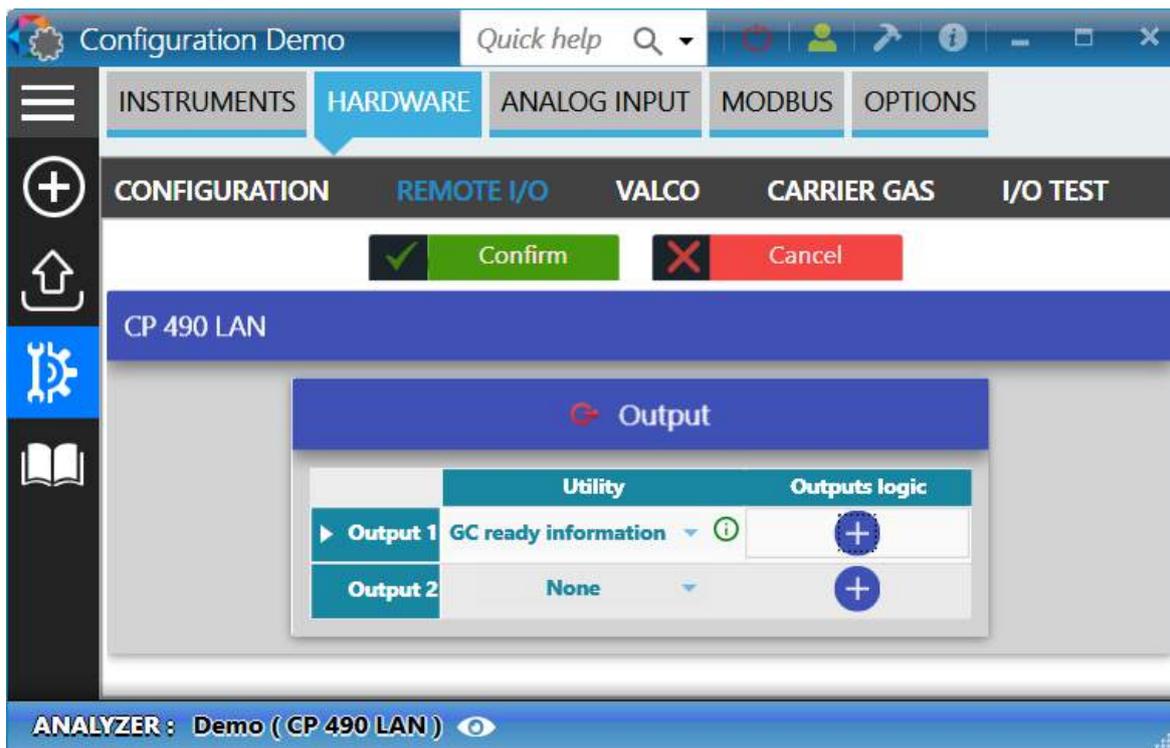
2. Selection of the corresponding alarm



**d) Information GC ready**

SOPRANE II offers the possibility to activate a relay when the analysis has started. For this, follow the following path: "**Configuration**> **Hardware**> **Configuration**> **Remote I/O**". If logical outputs are available, the option will be available.



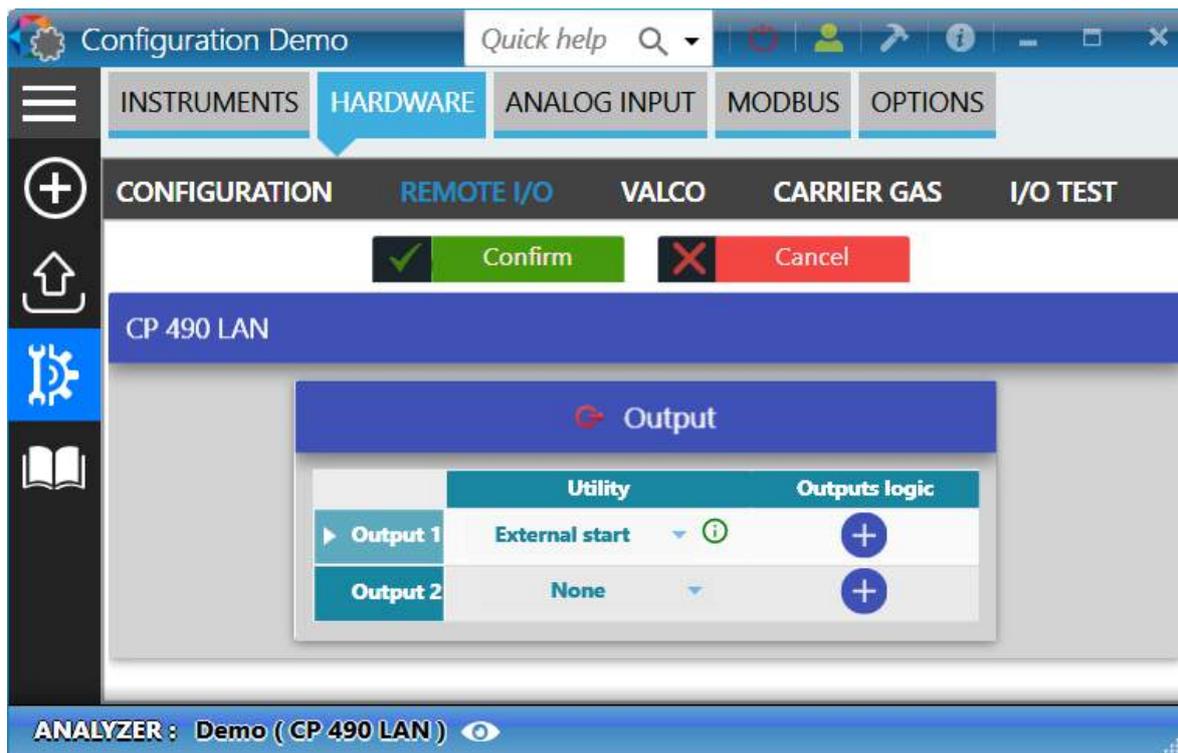


**e) External start**

The external start output allows an external device to start an analysis on the analyzer.

To activate the option, follow the path: "Configuration  Hardware > Configuration > Remote I/O". If logical outputs are available, the option will be available.



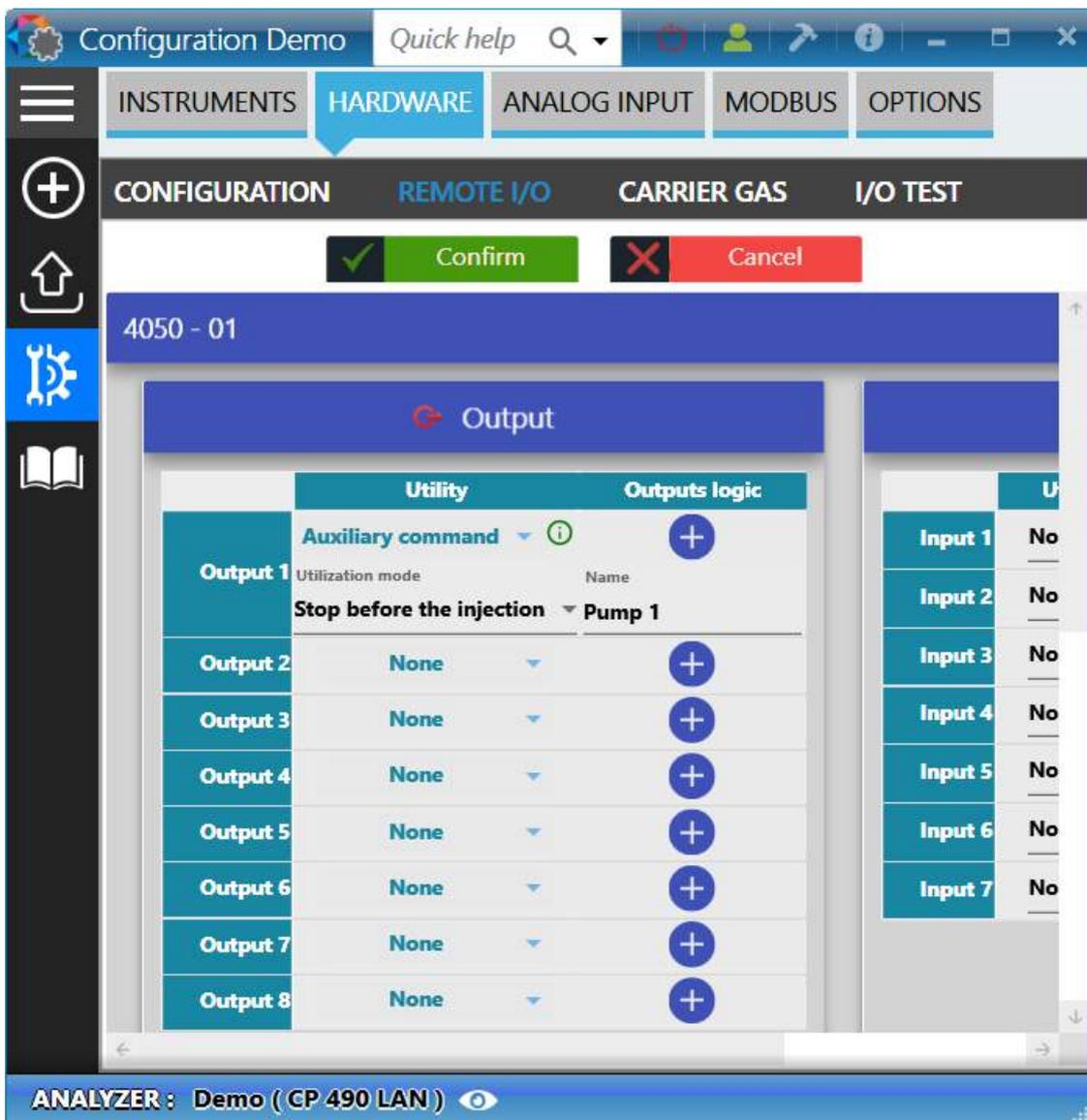


**f) Auxiliary pump**

The auxiliary control command allows to specify the management of a possible auxiliary pump: reference of the relay associated with its driving, choice to stop the pump before or after injection, or permanent aspiration of the sample.

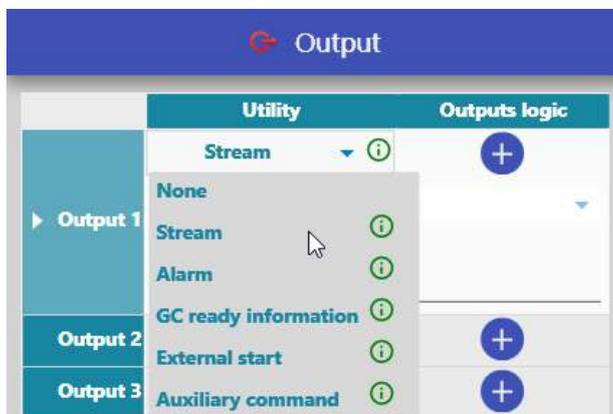
To activate the option, follow the following path: "Configuration  > Hardware > Configuration > Remote I/O". If logical outputs are available, the option will then be available.





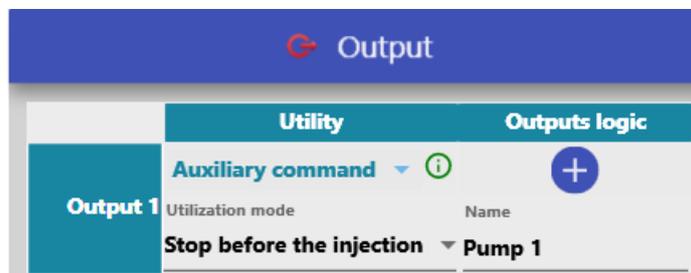
To use the auxiliary command, follow these steps:

1. Selection of the auxiliary control utility



## 2. Selection of the operating mode

Once the option is selected, the choice to stop the pump can be done **before** or **after injection** or **permanent aspiration** of the sample.



**None** mode is useful if we have set up a pump and that we want to put it on standby for some time or if we want to drive it by DDE.

**Stop before injection**, this means that the pump will start when changing streams and that it will stop just before we send the start command to the MicroGC. It is better, in this case, to schedule a scanning time.

**Stop after injection**, this means that the pump stops at the beginning of the acquisition (after the injection of the MicroGC).

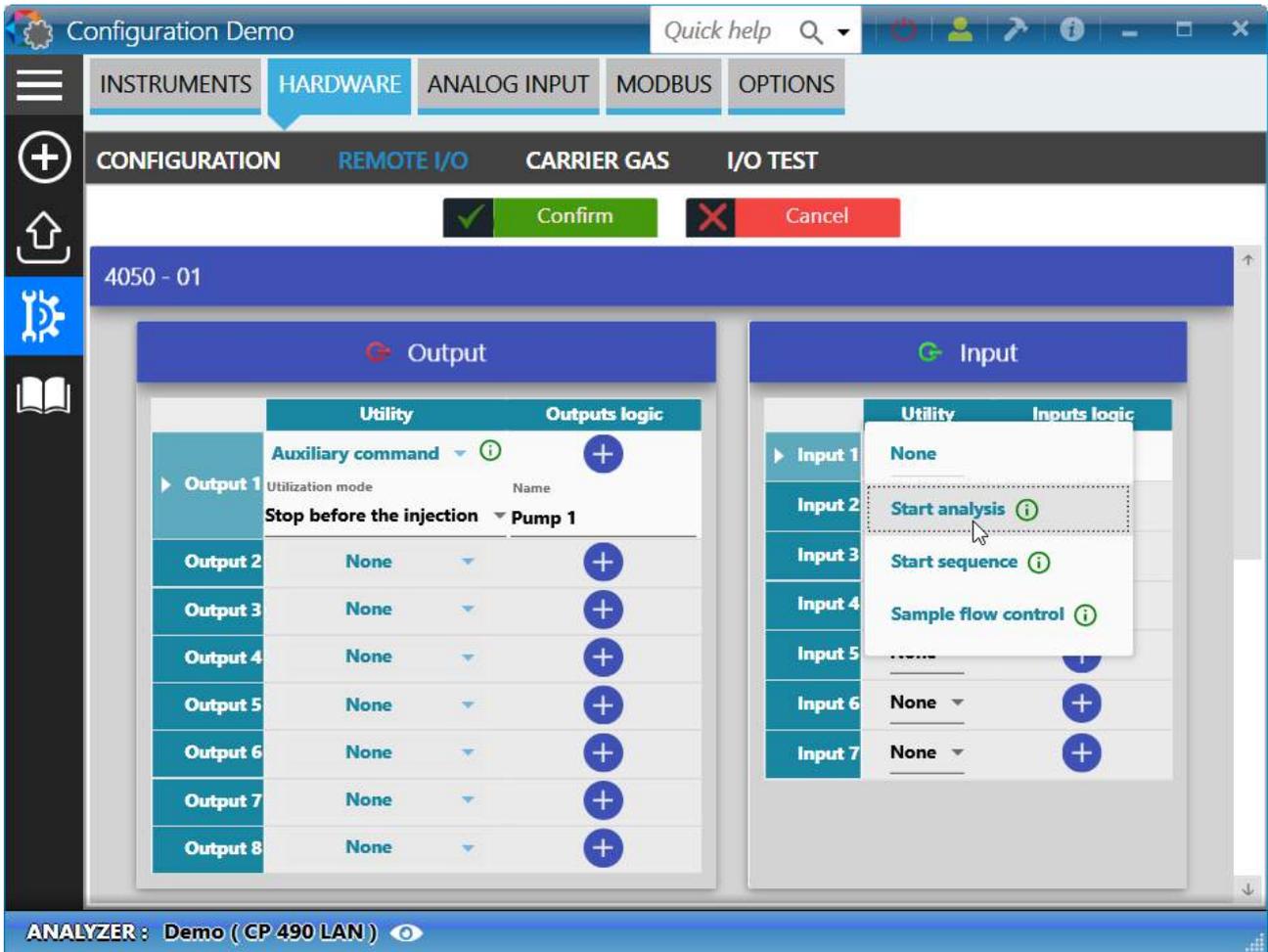
In **Manual** mode, the auxiliary is activated according to the Event table.

### ***g) Start analysis command***

Managing this input starting signal enables to start sampling and then analyzing when the logical input is triggered.

To activate the option, follow the following path: "**Configuration**  **> Hardware > Configuration > Remote I/O**". If logical inputs are available, the option will be available.



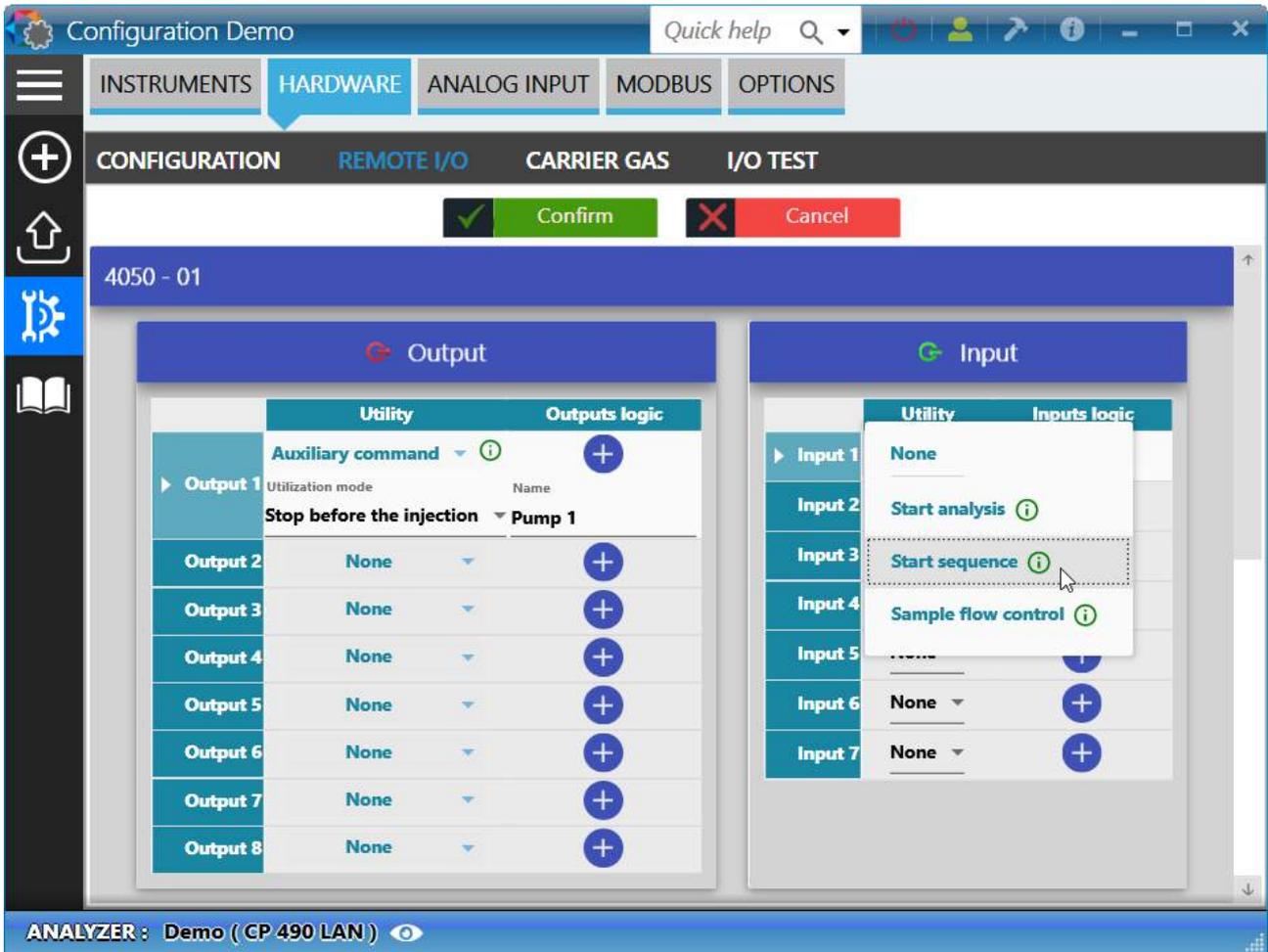


### ***h) Start sequence command***

Managing this input starting signal enables to start the last executed sequence when the logical input is triggered.

To activate the option, follow the following path: "Configuration  > Hardware > Configuration > Remote I/O". If logical inputs are available, the option will be available.





***i) Sample flow control***

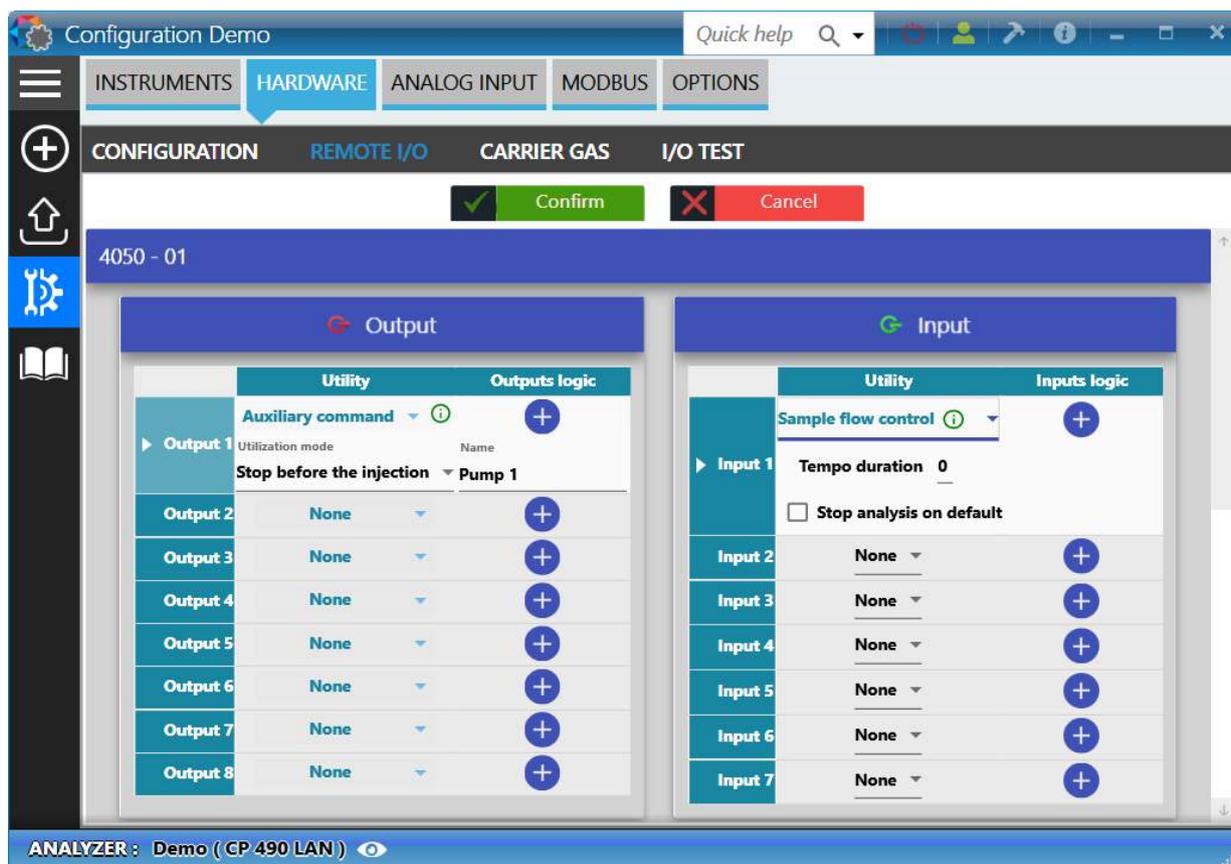
The control flow sample may be used to detect a problem with the sample.

If the sampling system is equipped with a rotameter with level contacts, this feature is used to manage a defect associated with the analyzer defect.

Because pressure variations may occur, the user may define a temporization before this false value is considered as a defect.

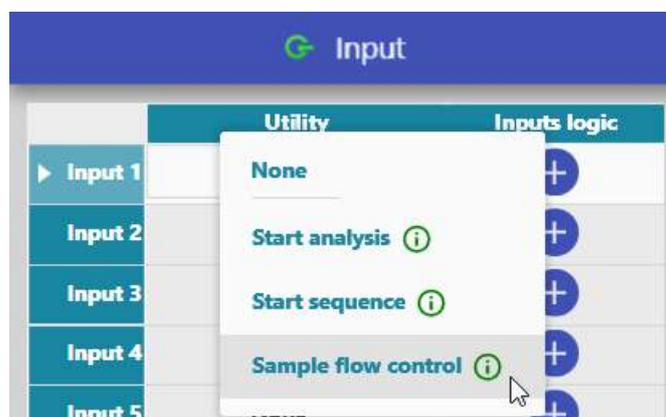
To activate the option, follow the following path: "Configuration  Hardware > Configuration > Remote I/O". If the logical inputs are available, the option will be available.





To use the sample flow control command, follow these steps:

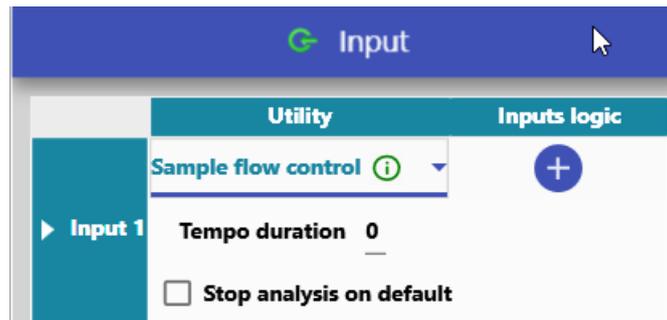
1. Selection of the auxiliary control utility



2. Definition of the default variables.

In case of default, SOPRANE II will wait for a period defined by the field **Tempo duration**, and will allow again a command. Analyses can be completely stopped if the option is checked.





### 3.6.3. Test of the inputs and outputs

See also:

[Logical inputs](#)

[Logical outputs](#)

[Analog inputs](#)

[Test 4-20mA modules](#)

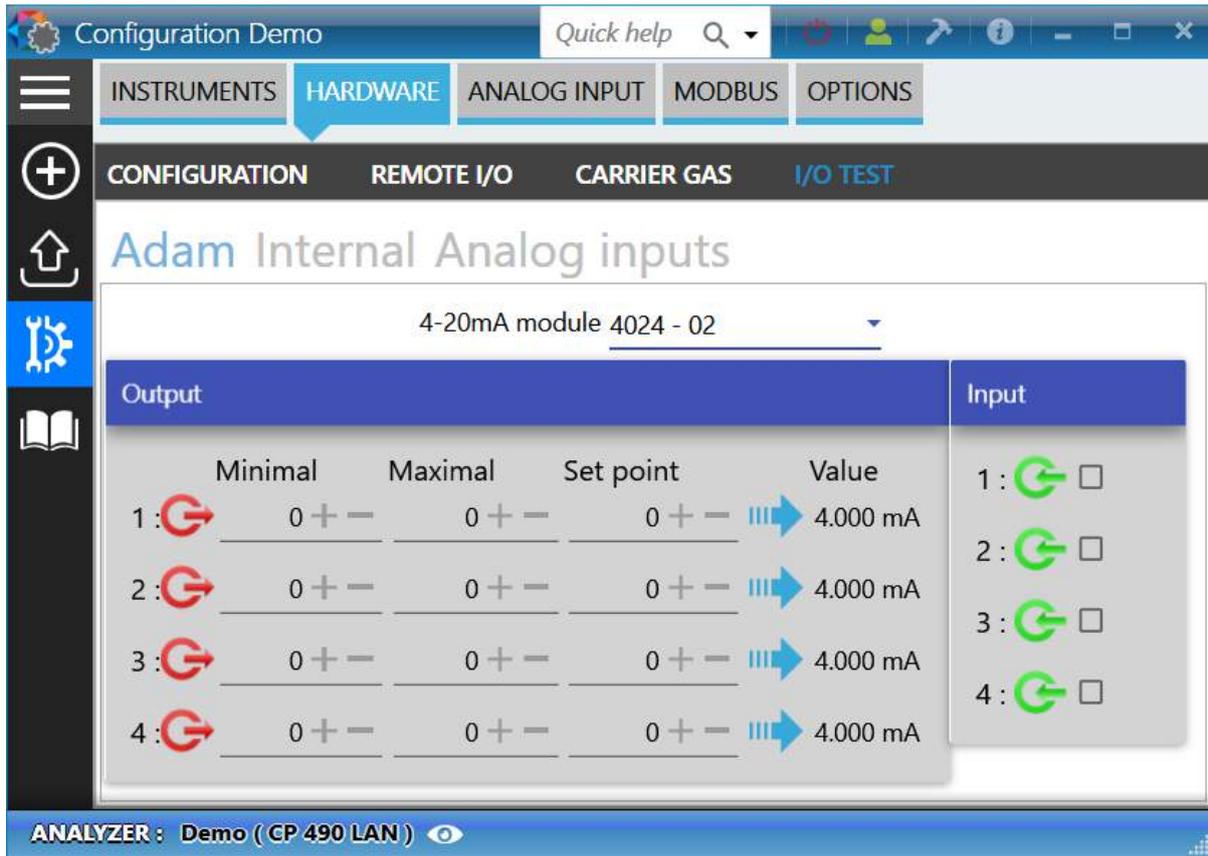
[Valves test](#)

#### ***a) Logical inputs***

To test the logical inputs, follow the following path: "Configuration  > Hardware > I/O Test".

In the following example, we are connected to a CP490 instrument with a Lan connection, the outputs reading will be done by an Adam 4024 module, the following view is exactly the same for any logical input device.





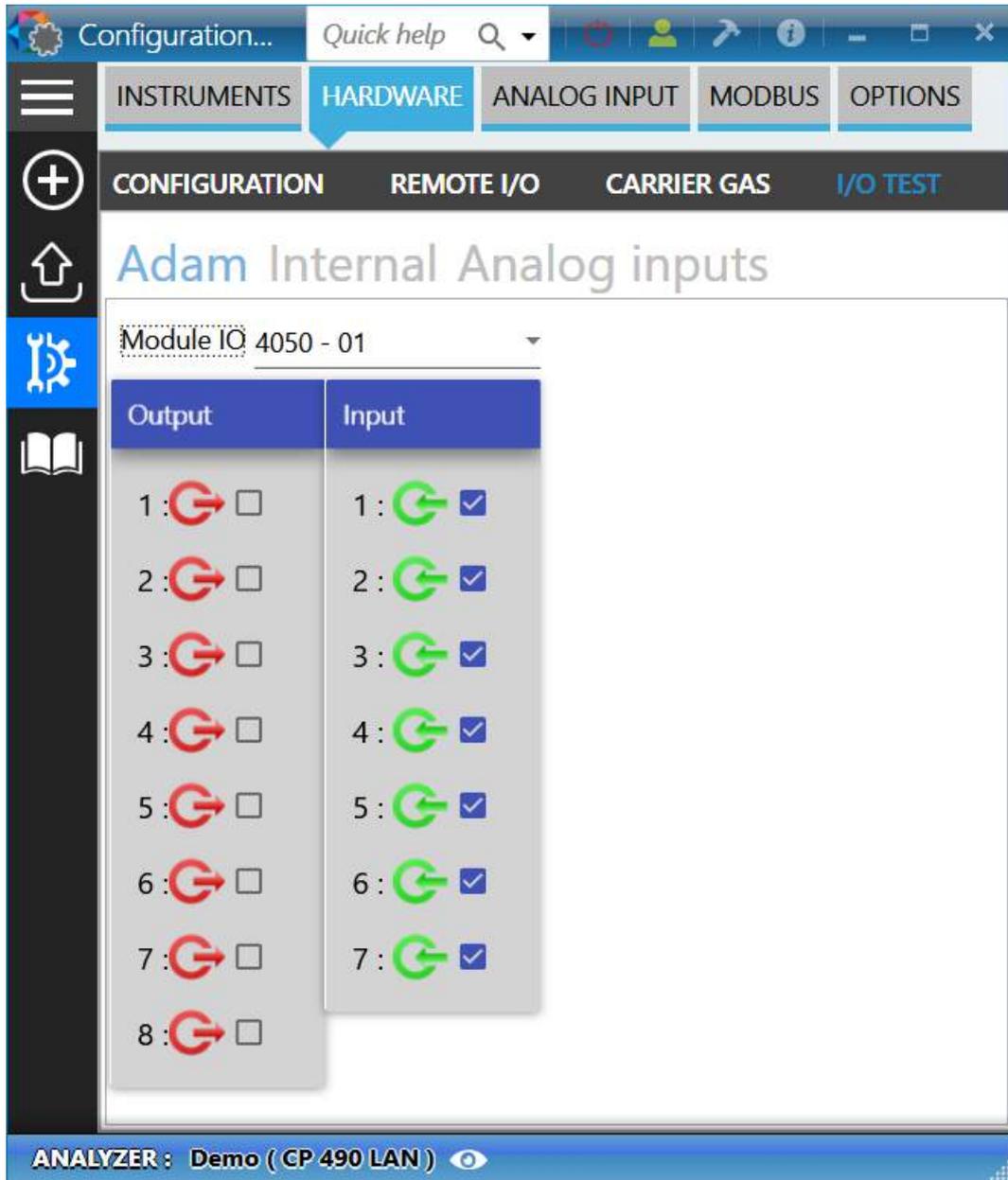
Let us focus only on logical inputs. The module contains 4 inputs, which cannot be modified by software and which display the current outputs status.



**b) Logical outputs**

To test the logical outputs, follow the following path: "**Configuration**  **Hardware > I/O Test**".

In the following example, we are connected to an CP490 instrument with a Lan connection, the outputs reading will be done by an Adam 4050 module, the following view is exactly the same for any logical output device.



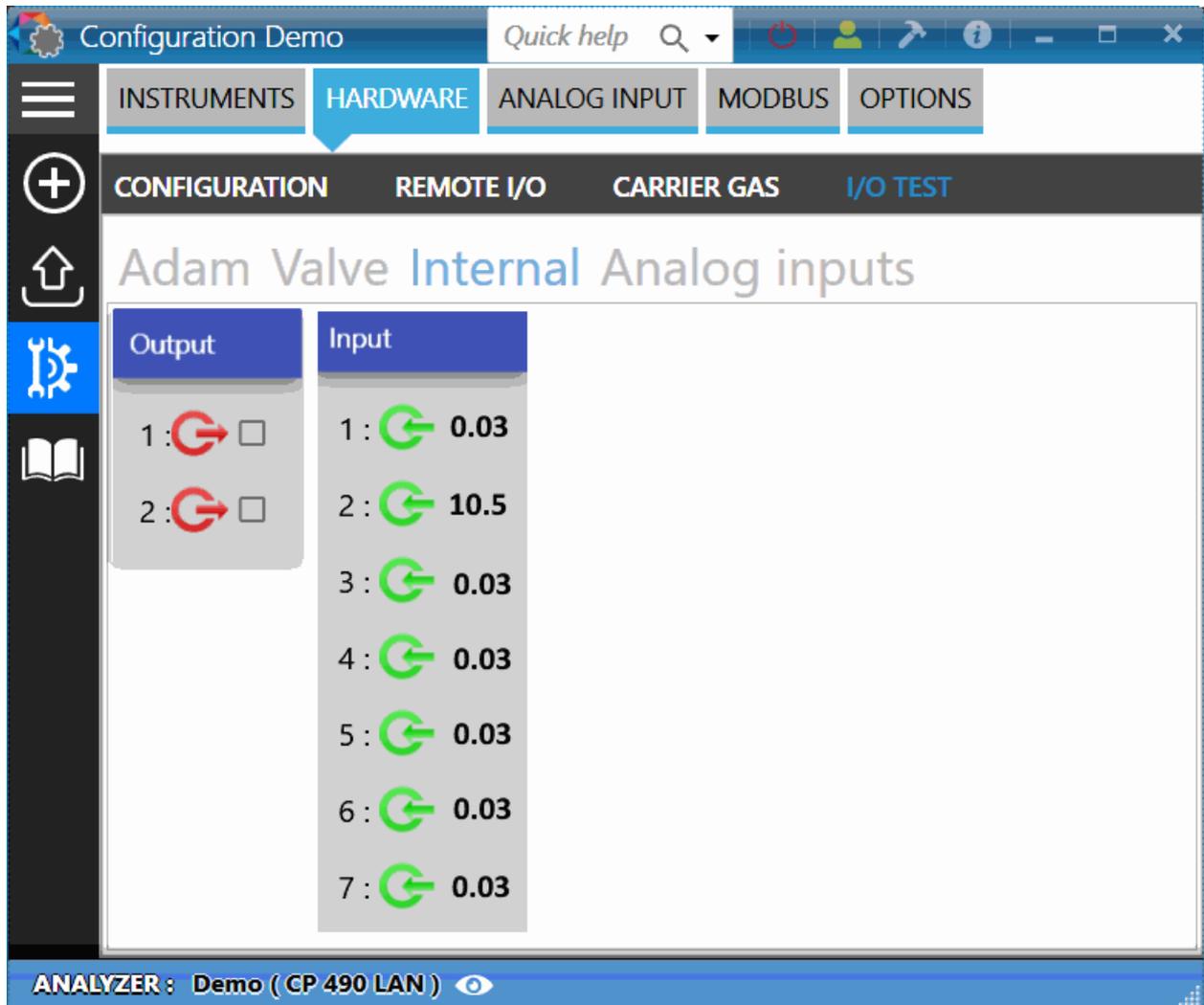
In the previous view, the software will read the status of each output and will change the state if the user turns the output on or off.



**c) Analog inputs**

To test the analog inputs, follow the following path: "Configuration  > Hardware > I/O Test".

In following example, we are connected to an Agilent 490 instrument.



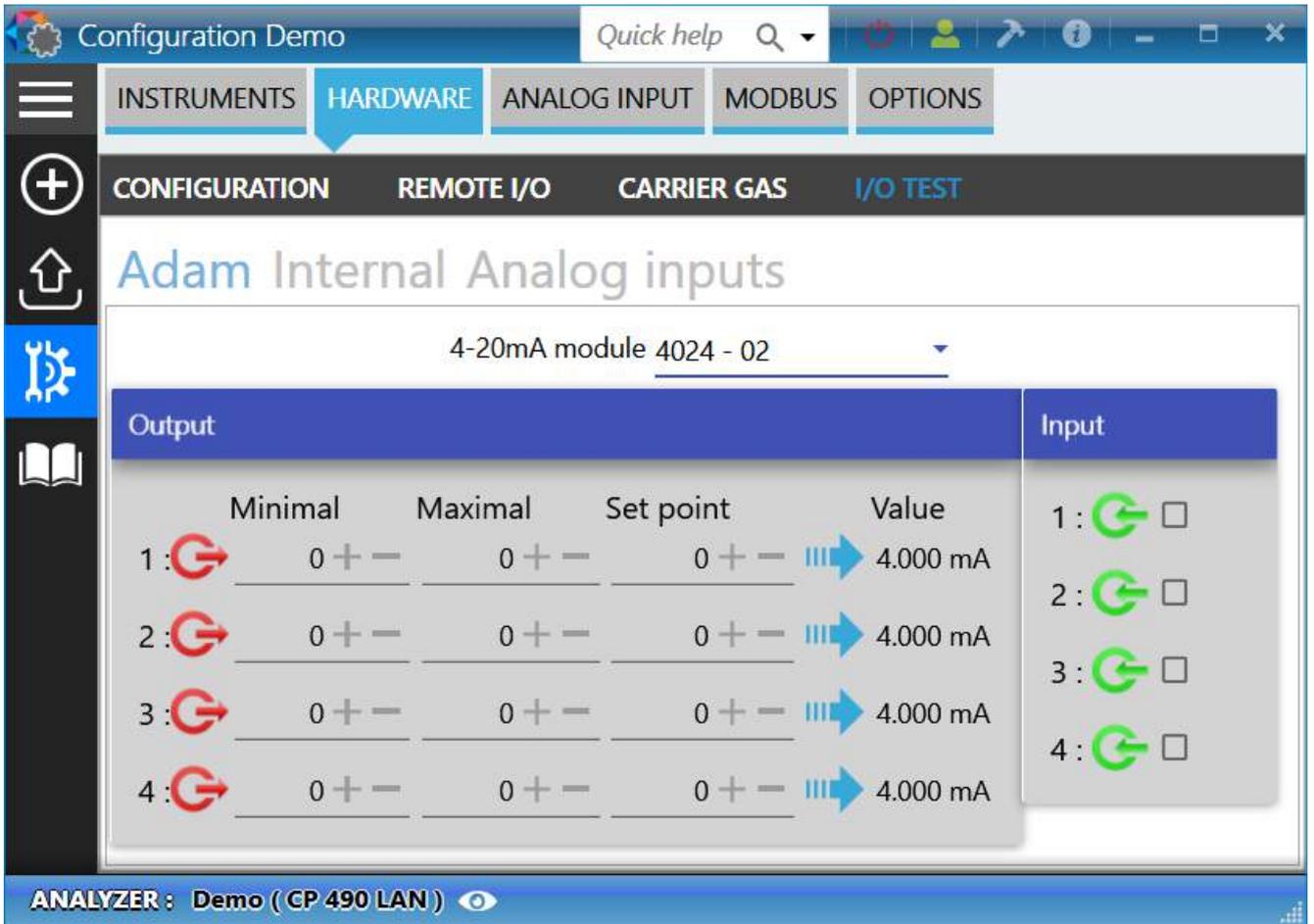
**d) Test 4-20mA modules**

The management of the 4-20mA modules is an option that is only allowed if the 4-20mA option in the license is enabled.

To test the 4-20mA modules, follow the following path: "Configuration  > Hardware > I/O Test".

The 4-20mA modules have 4 analog outputs and 4 logical inputs.





1. Analog outputs

Output				
	Minimal	Maximal	Set point	Value
1 :	0 + -	0 + -	0 + -	4.000 mA
2 :	0 + -	0 + -	0 + -	4.000 mA
3 :	0 + -	0 + -	0 + -	8.020 mA
4 :	0 + -	0 + -	0 + -	12.920 mA

For each output a minimum, a maximum and a set-point are proposed, the value is defined according to these three parameters.

Change one of these parameters to change the value.



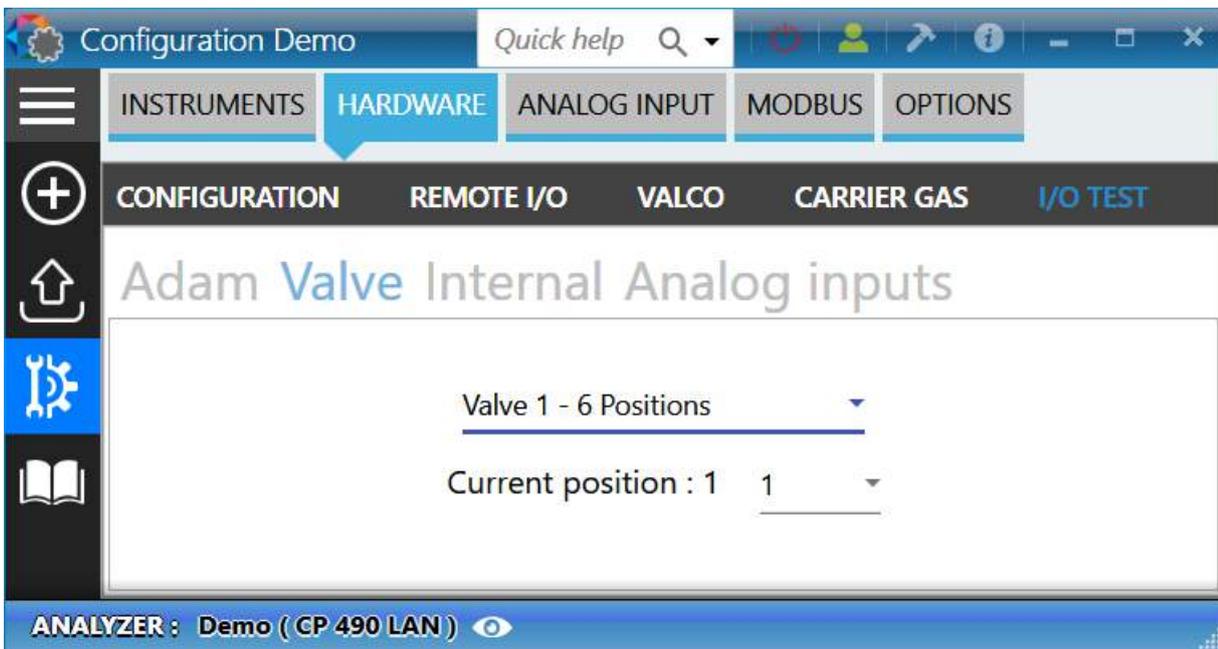
## 2. Logical inputs



The logical inputs cannot be changed by software; they display the current state of the outputs.

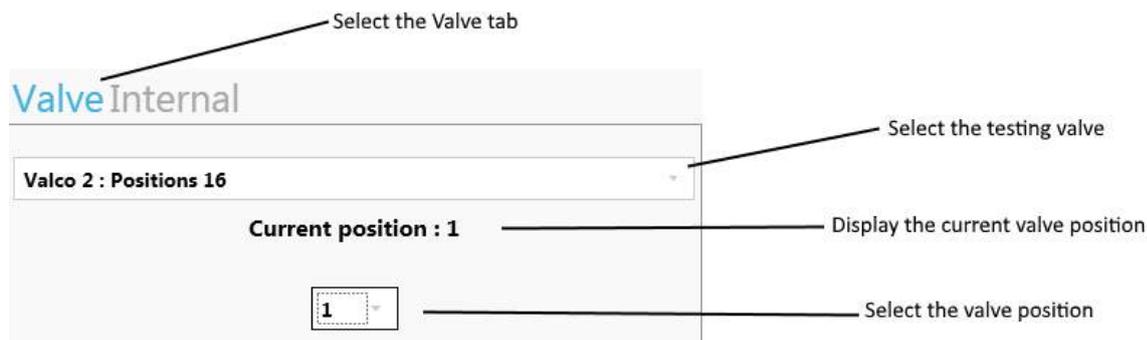
### e) Valves test

To test the valves, follow the following path: "**Configuration**  > **Hardware** > **I/O Test**".



Here is the description of the different elements:





### 3.6.4. Carrier gas selection

The different carrier gases which can be used for  $\mu$ GC/GC are:

- Argon
- Nitrogen
- Helium
- Hydrogen

Their quality is essential for the proper functioning of your analyzer.

**Important note:**

**The use of Helium as a carrier gas with the MicroGC configured in Argon or Nitrogen reduces the response by a factor of 10, and reverses the peaks without further impact.**

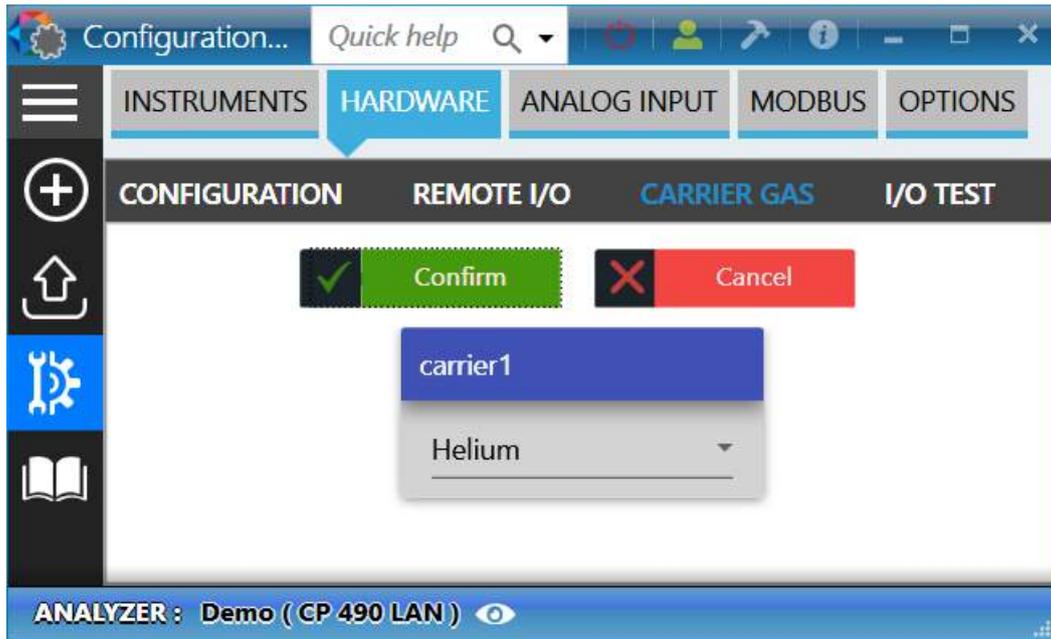
**The use of Argon as a carrier gas with a configuration in nitrogen or helium has the effect of irreversibly damaging the detector.**

To add the carrier gases, actions described in the chapter [Hardware](#) must first be performed.



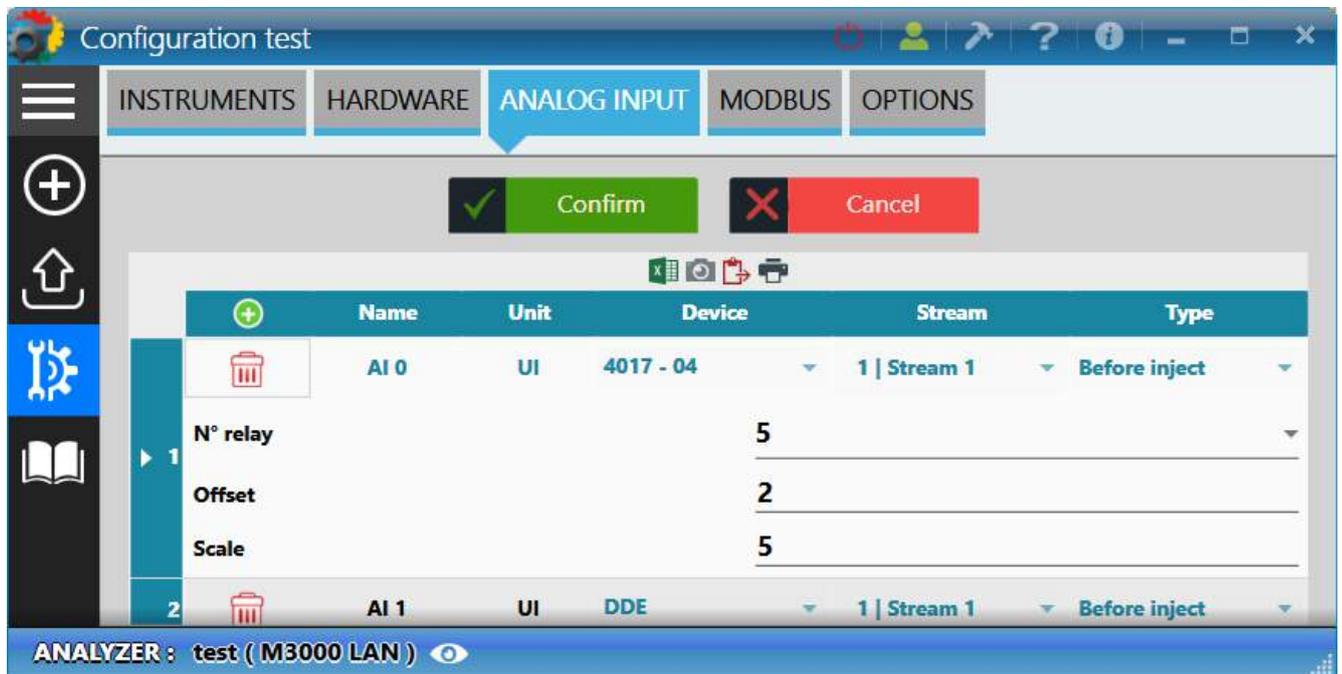
Then follow the following path: "Configuration  Hardware > Configuration > Carrier gas".





### 3.7. Analog input management

SOPRANE II can read analog inputs during the analysis and integrate them to the results at the end of the acquisition. To do this, you must (for each input used) enter a name, a unit, select the I/O device and the scales.



To add an analog input, click on the button  , default values will be added. Values can be changed in the table above. To delete a line, click on the button .



Analog parameters:

- **Name:** The name identifying the analog input.
- **Unit:** Unit of value of the analog input.
- **Device:** Acquisition device of the analog input (embedded module or external module).
- **Stream:** Sampling stream associated with the analog input.
- **Type:** Indicates when the value will be read (before sampling or before injection).

In addition to these main values, additional values may be entered according to the device:

- **Embedded I/O or Adam modules**

	AI 0	UI	4017 - 04	▼	1   Stream 1	▼	Before inject	▼
<b>N° relay</b>				5				
<b>Offset</b>				2				
<b>Scale</b>				5				

- **DDE (Dynamic Data Exchange)**

DDE is used for the dynamic exchange of data between applications, it doesn't require additional data.

	AI 1	UI	DDE	▼	1   Stream 1	▼	Before inject	▼
---	------	----	-----	---	--------------	---	---------------	---

- **BronkHorst**

Bronkhorst is a variety of flow-meter/mass-controller. To communicate with this device, an ID number (Slave) is required.

	AI 2	UI	BronkHorst	▼	1   Stream 1	▼	Before inject	▼
<b>Slave</b>				1				



- **TES**

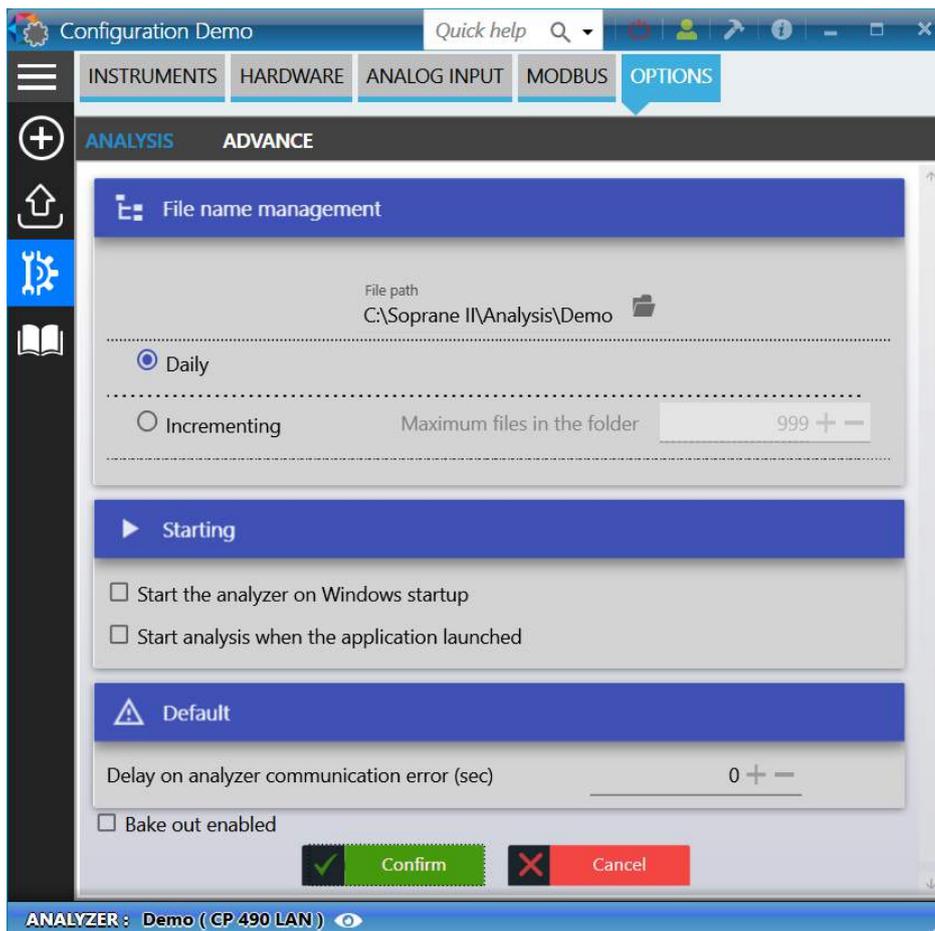
The TES module is an input/output module using a Modbus RS485 connection in asynchronous slave mode.

	<b>AI 3</b>	<b>UI</b>	<b>TES</b>	▼	<b>1   Stream 1</b>	▼	<b>Before inject</b>	▼
<b>Module</b>								
<b>N° relay</b>	<b>1</b>							
<b>Offset</b>	<b>2</b>							
<b>Scale</b>	<b>5</b>							

### 3.8. Options management

To access the options, follow the following path: "Configuration  > Options".

#### 3.8.1. "Analysis" tab



**File management** section:

- Management mode: either a daily management based on the date (1 folder per day), or a rotating management with the indication of the maximum number of analyses to be saved (all analyses in the same folder).
- The location of the results files.

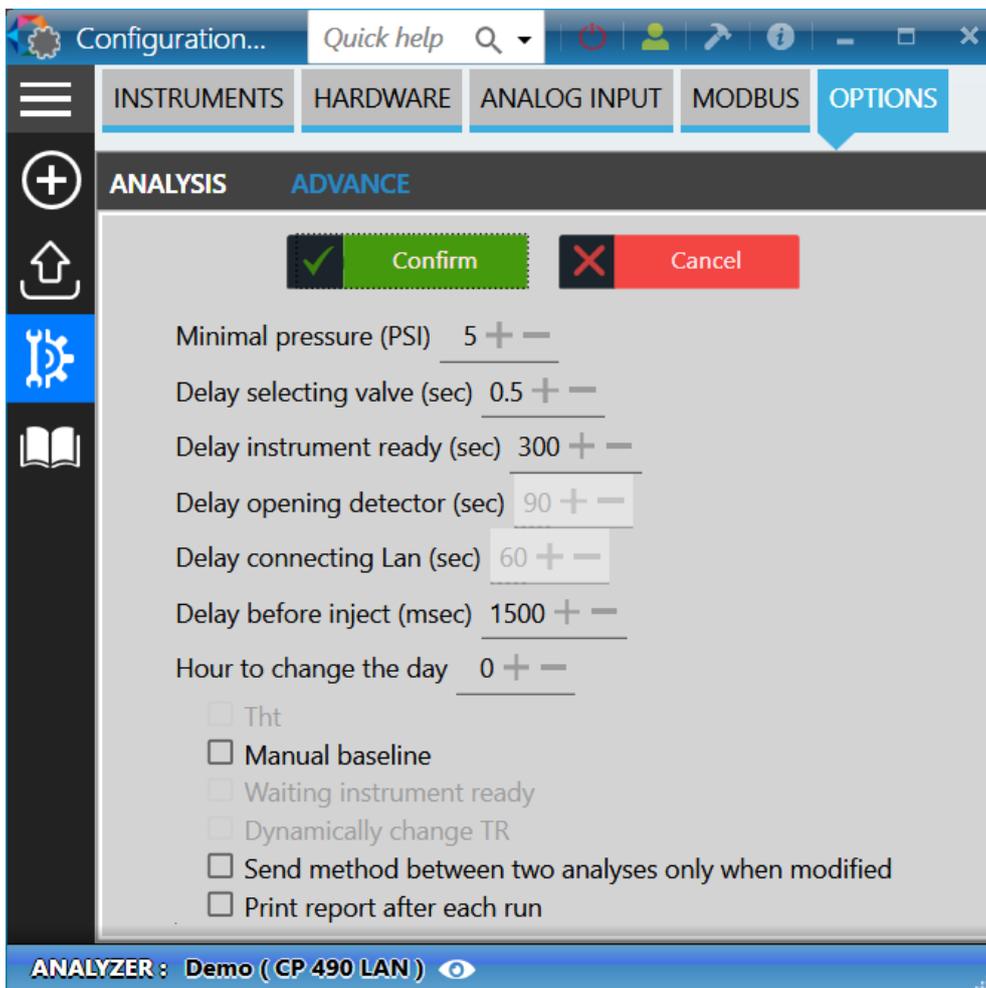
**Start** section:

- Starts when the computer starts.
- Start of analysis when the software starts.

**Default** section:

- The duration of the purge and waiting for a ready signal. This is the duration (normally 300 seconds) during which the communication with the analyzer is prohibited due to a default. Being in purge, the analyzer cannot work during this time.
- Activate (or not) the regeneration of analytical columns.

**3.8.2. "Advance" tab**



The **minimal pressure** corresponds to minimal pressure to set in the method.

The **Delay selecting valve** value (in seconds) is the time taken by the valve to change the position.

The **Delay instrument ready** value (in seconds) is the duration before generating an alarm if the status is not ready.

The **Delay opening detector** value (sec) is the time before the detectors can be switched on after a method is sent.

The **time for the change of day** setting is the time to create a new folder when saving analyses. If the management of the results files is not in daily mode, this setting has no effect.

**Manual baseline** enables to manually edit baseline in the Process tab (see chapter [Manual baseline](#)).

If the parameter "**Send method between two analyses only when modified**" is checked, the method will be send only when the method is edited, otherwise the method will be send before each run.

If the parameter "**Print the report**" is checked, the report will be printed after each run.

## 4. Using Soprane II

At this point, we assume that SOPRANE II has been correctly installed and configured, as it has been defined previously (see chapter [Analyzer configuration](#)).

In most cases, SOPRANE II is delivered to you installed. In this case, your version of SOPRANE II was used to check the operation of your analyzer, and thus filed results, analyses methods and analyses sequences are already on your hard disk.

We will suppose here that SOPRANE II has only been installed and configured, and that no analysis has been carried out.

The use of SOPRANE II will require many steps:

- First, we will have a look at the different menus and we will check the possibility to establish a connection with the analyzer (see chapter [Menus](#)),
- We will create an analysis method (see chapter [Analytical methods management](#)),
- We will create an analysis sequence (see chapter [Analysis sequences management](#)),
- We will carry out analyses (see chapter [Analyzes management](#)),
- From the chromatogram of an analysis, and directly, we will create an integration method and an identification table of the peaks (see chapter [Process](#)),
- We will see how to calibrate the instrument (see chapter [Calibration](#)),
- We will program post-analytical calculations (see chapter [Post-analytics calculations](#)),
- We will visualize results graphically, in tendency (see section [Trends](#)),
- We will program automatic regenerations of the columns (see chapter [Bake-out management](#)).
- Finally, we will consider the possibilities to reprocess the analyses and to compare chromatograms (see chapter [Comparisons](#)).



## 4.1. Menus

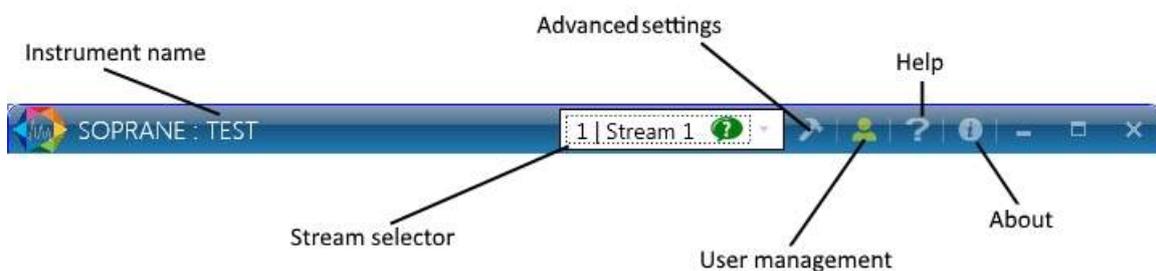
To run correctly, SOPRANE II must know the configuration of the analyzer. If this configuration is unknown when launching SOPRANE II, a message is displayed.

This is the main page for SOPRANE II:



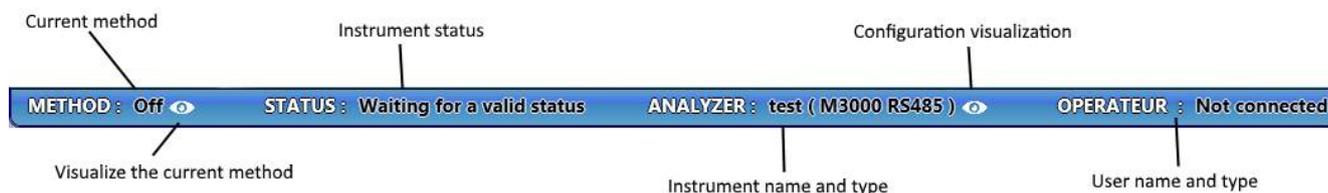
The important elements to be considered are

- The title bar



- The status bar

The status bar continuously displays the important parameters of the instrument.



- Menus

The following chapters describe the different menus of SOPRANE II and the function of the icons.

- [Analyzes](#)
- [Process](#)
- [Logs](#)
- [Users](#)

### 4.1.1. Analyzes



The **Analyzes** menu has ten possible actions:

1. Start or stop an analysis (or a sequence)

When the icon displays , start an analysis or a sequence is possible. If the icon is  there is an ongoing analysis and the stop is then possible.

See chapter [Analyzes management](#) to find out how to start an analysis.

2. Status display

Reads the instrument status. It can be of different colors to indicate the status:



The reading of the status is not available (the configuration is not initialized).



The analyzer is not operational to run analyzes.





The analyzer is operational to run analyzes.



The analyzer is running an analysis.

For detail on the status display see chapter: [Status](#)

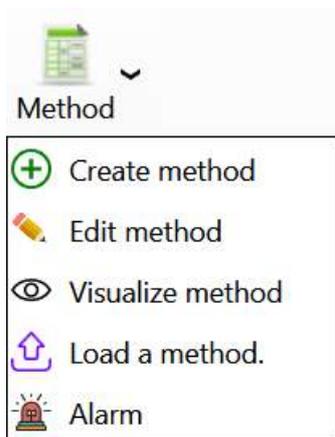
### 3. Real time display



Displays the real-time signal of the analyzer running an analysis.

To see in detail the display of the real-time signal see chapter: [Real time](#)

### 4. Edition or sending of a method

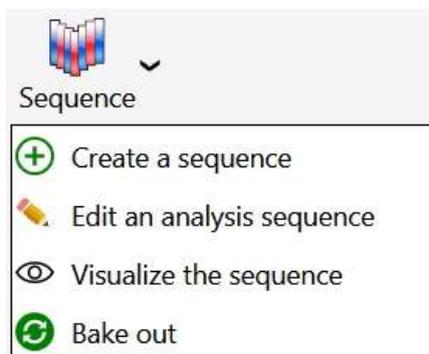


Allows to create, edit, save or load a method.

To see how to edit a method see chapter: [Analytical methods management](#)

Alarm could be defined and connected to a relay, see chapter [Alarms component](#).

### 5. Edition of a sequence.

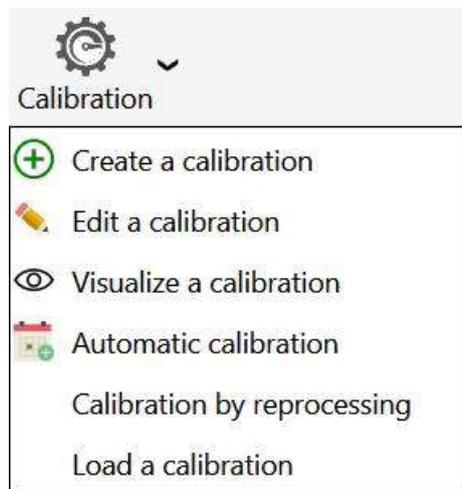


Allows to create, edit, save or visualize a sequence.

To see how to edit a sequence see chapter: [Analysis sequences management](#)

To see how to bake out your column see chapter: [Bake-out management](#)

## 6. Edition or programming of a calibration



Allows to create, edit, save or visualize a calibration method. Can also program a calibration.

Note: Last two items are only available when the result is visible.

To see how to edit a calibration method see chapter: [Calibration sequence management](#)

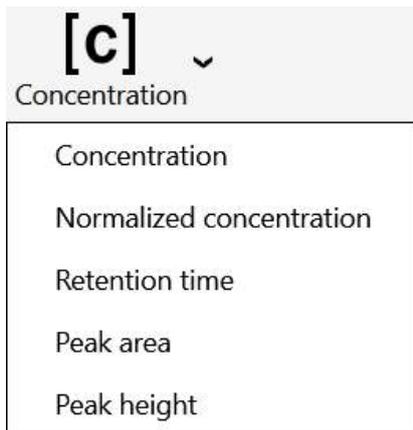
## 7. Results management

The button Results  is used to select and display the results.

See chapter for more details on the display of the results: [Results](#)

## 8. Select the visualized result value





By clicking on the menu, visualized results will be updated according to the selected type of result.

To see details, see chapter [Results](#).

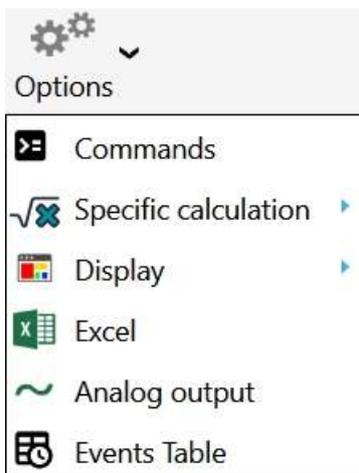
### 9. Trends

SOPRANE II allows to visualize the evolution of the concentrations or of the values computed on a period (See chapter [Trends](#))

### 10. Comparison of analyzes

The button  is used to open the executable of comparison and overlay of analyzes. For more details on the comparison of analysis see chapter: [Comparisons](#)

### 11. Options



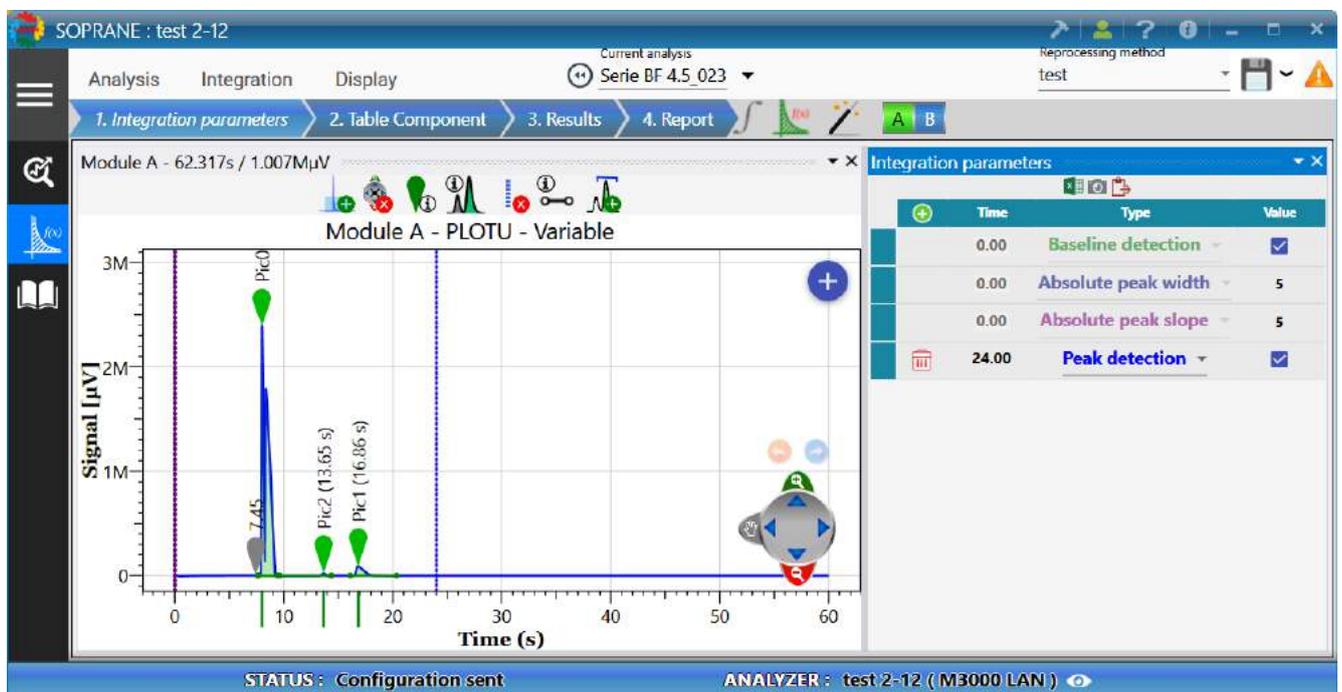
By clicking on the option menu, you will be able to:

- Configure pre and post command (see chapter [Pre and Post command](#))
- Configure specific calculation (see chapter [Post-analytics calculations](#))
- Configure the result display
- Save automatically your results to an Excel file (see chapter [Excel calculation](#))
- Send result to analog outputs (see chapter [Send results through analogical outputs](#))
- Configure a pre-analysis event table (see chapter [Analysis event table](#))

### 4.1.2. Process

The process module is used to create an integration method and everything concerning the processing or reprocessing of the peaks.

For more details on the process of an analysis see chapter: [Process](#)



### 4.1.3. Logs

Allows the display and the management of the logs.

Application logging offers three types of logs:

- [Action log](#), allows you to indicate all the main actions performed by the user.
- [Alarms log](#), displays all alarms that have been triggered.
- [Errors log](#), to locate errors (rather intended for the developer).
- [Event log](#), displays all Soprane II crashes
- [Calibrations history](#), display the history of calibration

For more details, see chapter: [Logs management](#)



### 4.1.4. Users

This tab is available only if the user is an administrator.

For more details on user's management see chapter: [Users management](#)

See also:

[User login](#)

[User creation](#)

[Remove a user](#)

[Change password](#)

[User access](#)

## 4.2. Reading the status

When SOPRANE II is launched, when a new method is sent to the analyzer, before starting analyses or before stopping SOPRANE II and the analyzer, we will visualize the status of the analyzer. Is it "ready" for what is expected ?

Moreover, it is the best way to make sure that SOPRANE II can communicate with the analyzer.

There are several places where these status indications can be found; see the following chapters:

[Status bar](#)

[Title bar](#)

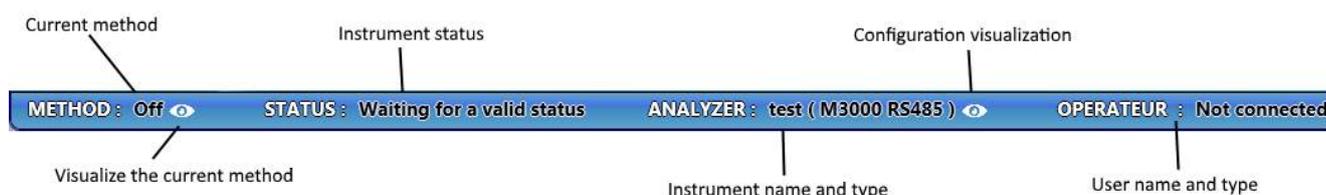
[Eye](#)

### 4.2.1. Status bar

SOPRANE II allows to know at any time the state in which the analyzer is.

This information is in the horizontal bar at the bottom of the SOPRANE II main screen.

The information given is as follows:



When the cursor is moved to the field corresponding to the analyzer, additional information on the analyzer configuration appears.

Module	A	B
Detector	TCD	TCD
Column	PLOTU	Molsieve

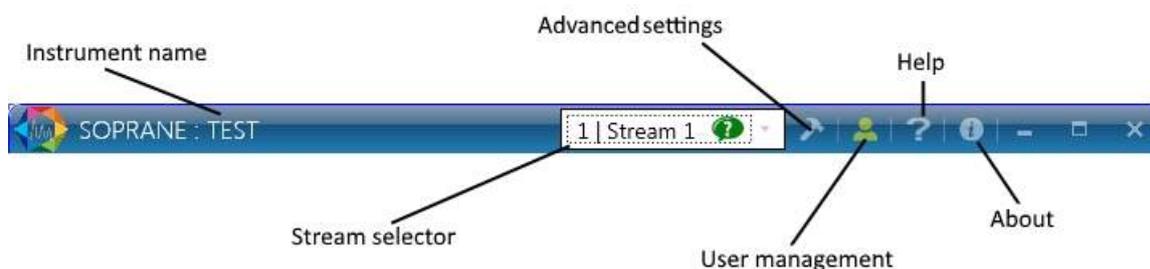


When the cursor is moved over the field corresponding to the method, additional information about the current method appears.

	Module A	Module B
Sampling temperature (°C)	90	90
Injector Heating (°C)	50	50
Column temperature (°C)	50	50
Detector	×	×

### 4.2.2. Title bar

The title bar is an important element to know about the instrument state.



### 4.2.3. Eye

The button representing an eye in the "Analysis" tab, allows the reading of the status. When blinking, the visualization of the status is available.

It can be of different colors to indicate status:



The status reading is not available (configuration is not loaded).



The analyzer is not operational to launch an analysis.



The analyzer is operational to launch an analysis.



The analyzer is analyzing.

### 4.2.4. Status

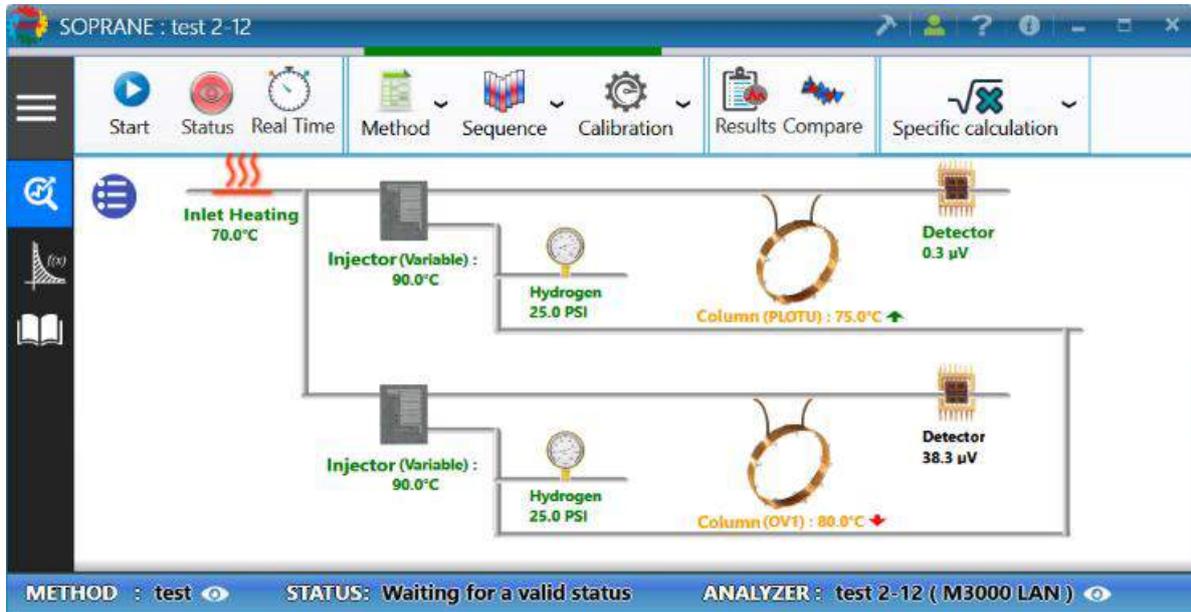
The display shows everything about the device: number of modules, temperature, pressure, detector status. The upper part of the window allows to see immediately whether the module is operational (green background) or not (red background).

Module A - Column : PLOTU - Injector : Variable : Module is ready.

Module B - Column : Molsieve - Injector : Variable : Module is not ready.



In the following example, the instrument is a M3000 with a network connection, the display remains the same depending on the instrument.



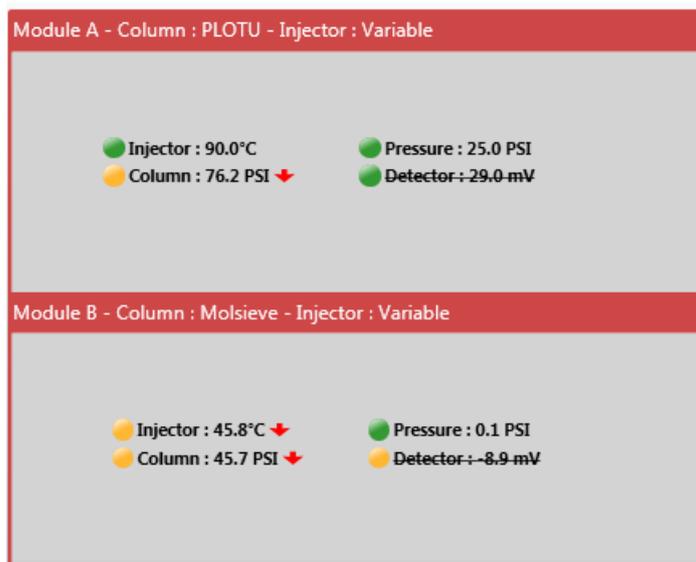
In the case an element has not reached its set-point, it means it is not ready. The text will be in **Orange**

(example column  )

If the set-point has been reached, the writing will be in **green** (example Carrier gas pressure  ). In the case the element is not activated it will be in **black** (example detector  ).

Another simple visualization of the status is possible by clicking on the button  and on the button  to return to the graphical visualization.





In both views, when the mouse cursor moves over an item in the Status or Visual part, additional information appears as the current status, set-point, or value of the item.

## 4.3. Methods and sequences

See also:

[Analytical methods management](#)

[Operative conditions](#)

[CP490 operating conditions](#)

[M3000 Operative conditions](#)

[Loading an analytical method](#)

[The 4 useful methods](#)

[Analysis sequences management](#)

[Bake-out management](#)

[Calibration sequence management](#)

[Automatic calibration](#)

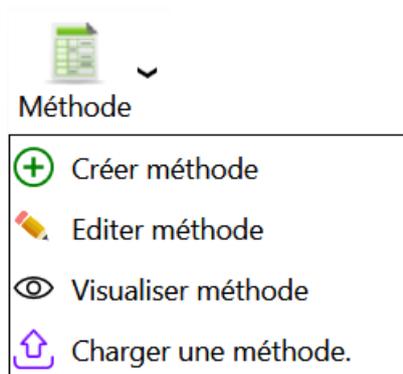
### 4.3.1. Analytical methods management

SOPRANE II offers the possibility to directly visualize and modify an existing analysis method.

Excepted for the first one (because the first time, it will be necessary to create also an integration method, a components table, ... and that has to be done with the process module), SOPRANE II also allows to create an analysis method.

To access methods, go to the **Analysis** tab, and click the button below:





See also:

[Operative conditions](#)

[M3000 Operative conditions](#)

[CP490 operating conditions](#)

[Loading an analytical method](#)

[The 4 useful methods](#)

### ***a) Operating conditions***

Once connected to an instrument, the management of methods is available.

The display allows to view, edit or modify all the parameters of the analytical method.

- To create a method, go to the tab **Analysis** and click on **Create method**.
- To modify or edit a method, go to the tab **Analysis** and click on **Edit method**.
- To load a method, go to the tab **Analysis** and click on **Load method**.

The installation program **Configuration**



allowed to configure SOPRANE II according to the type of analyzer used.

These devices being different, the analyzes methods will also be different.

To see the operating conditions edition for devices of type **M3000** see chapter: [M3000 Operating conditions](#)

To see the operating conditions edition for devices of type **CP490/Varian 4900** see chapter: [CP490 operating conditions](#)

Here are the different parameters you can have access to in the method:

For each analytical module (we will consider only module A, the information to provide being similar for modules B, C and D), you have to provide 2 types of data:

- Check boxes. They correspond to ON/OFF states.
- Numerical values.

### **Inlet temperature:**

It represents the connection tube between the incoming sample and the injector. If this inlet must be heated, a valid temperature, expressed in degree Celsius must be programmed.



### **Injector and column heating:**

The principle is the same. These heating are generally necessary.

### **Sampling time:**

Before injecting the sample, it is necessary that the sample circulates in the injection loop. The user indicates a value, expressed in seconds, during which the pump will be activated to suck the sample and make it circulate. The duration required for this sweeping depends on the distance the sample has to go.

### **The injection time:**

It is the duration, expressed in milliseconds, during which the injection valve will be active. A too low value doesn't bring a good reproducibility; we will use 50 ms as a default value. For the  $\mu$ GC 3000, this duration can be set at zero for the back-flush injectors, to obtain a better reproducibility as the injector is not linked anymore with time. For samples containing traces compounds, this value can be increased.

### **The backflush time:**

It is the time (reference zero at injection), expressed in seconds, at which the gas flow will be reversed in the pre-column to protect the analytical system from a possible pollution with heavy compounds.

For the Micro GC 490, if this value is set at zero, the backflush is never activated, at the opposite of the other instruments for which all the compounds are backflushed if this value is set at zero.

### **The run time:**

It corresponds to the duration of an analysis; it is expressed in seconds.

### **The column pressure:**

The box must be checked, or a value indicated, so that the carrier gas circulates in the column with a pressure at the head of the column equal to the value indicated and expressed in PSI.

### **Detector:**

The check box allows to switch on or remove the detector bridge current.

### **Sensitivity:**

It is possible to select different values for the gain of the amplifier (see paragraphs on the driving of each instrument).

The choice of sensitivity allows to define the amplifier management for sensitivity going from low to high.

### **IMPORTANT NOTE:**

We have just said that the sensitivity parameter can take different values and that this allows to manage the gain of the amplifier.

The detector is very sensitive and can detect ppm as well as 100% of a compound.

Suppose we work with peaks heights, we measure the signal difference between the top of the peak and the value of the baseline (we suppose here that the baseline level is the same before and after the peak).

Let us suppose that the signal is about 2 volts for a peak corresponding to 100% of product. For one ppm, the signal will be about 2  $\mu$ V.

When working in "standard" sensibility, the AD converter of the amplifier gives a point for a 5 nV variation in input. So, we will have about 400 points for a voltage variation of 2  $\mu$ V.



Let us suppose now that the maximal error made by the converter during conversion is about 10 points. We could have an error of 10 points on the top of the peak, but also on the baseline level, thus a total error of 20 for a value of 400.

If we program a "high" sensitivity, the signal is now amplified by a factor ten before the conversion and the value is divided by ten after conversion.

The error is now of 20 for a value of 4000, and after division by ten, the error due to the analog to digital conversion is 2 for 400. Ten times better!

Of course, the maximum signal of the detector which can be treated by the converter is not about 10 volts but about 1 volt (this signal is multiplied by 10 before conversion) and if we inject 100% of compound with "high" sensitivity, the signal at the converter input will be too high and the output will be saturated.

**CONCLUSION:** if a compound concentration is about a few percent or more, use the "standard" sensitivity and the conversion error will be negligible.

If you analyze compounds at ppm levels, the A/D conversion error becomes too important and it is better to minimize it by using a "high" sensitivity.

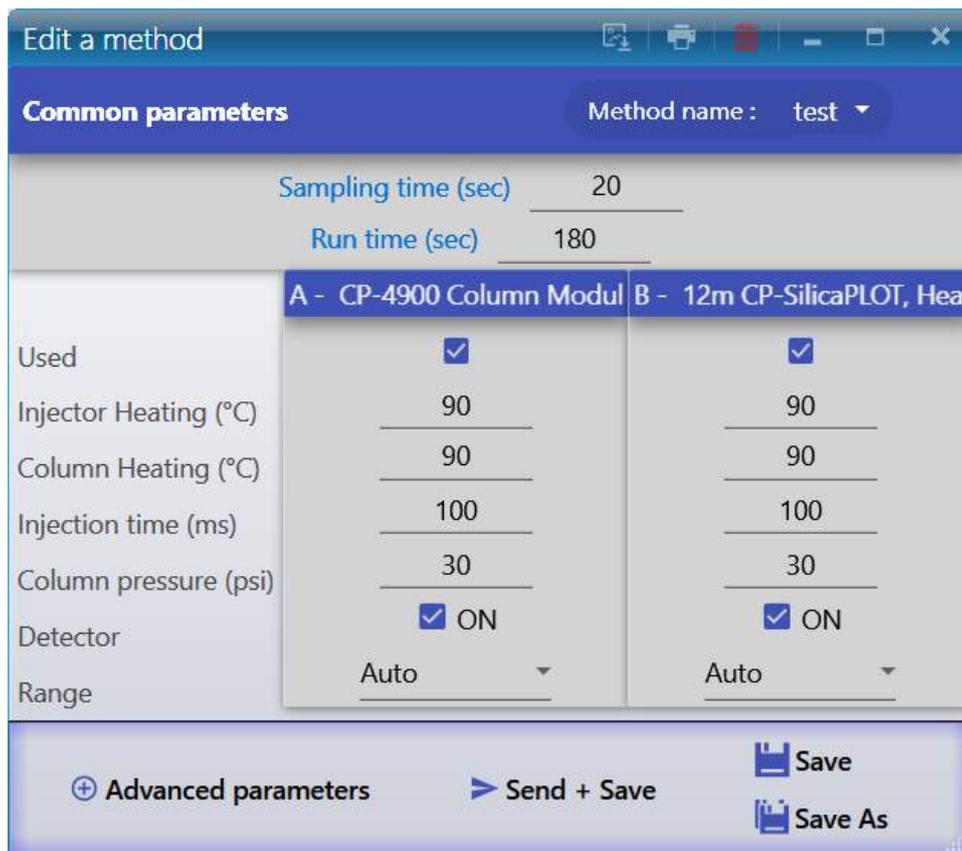
The button "Param." or "Advanced parameters" allows to open a second sheet of parameters, which will be mentioned in the following paragraphs, because they vary from one analyzer to another.

#### a) 1. CP490 operating conditions

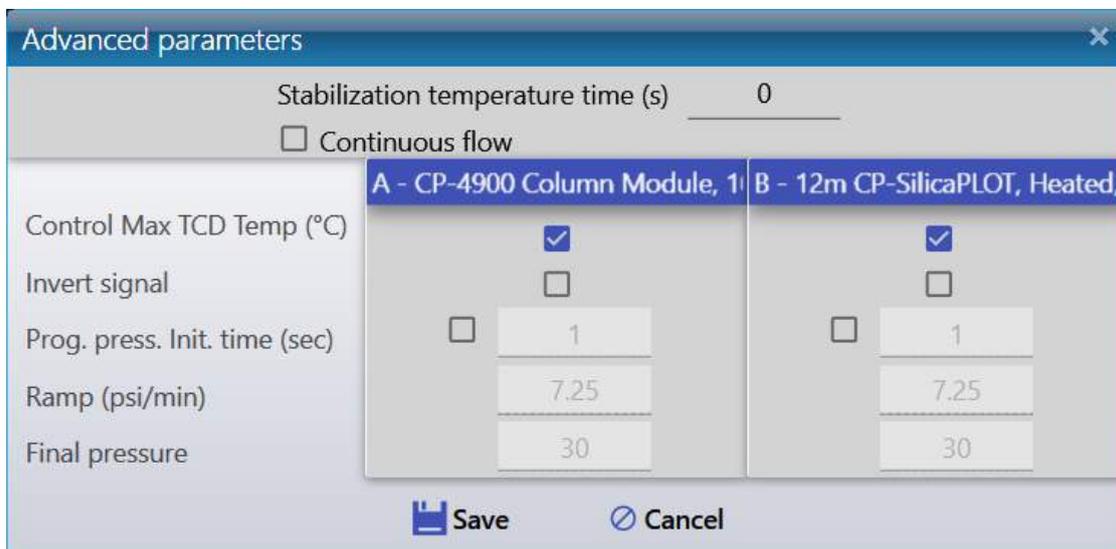
Here is the window in which analytical conditions for a Micro GC 490 can be set:

See chapter [Operating conditions](#), to have information about each parameter.





The button "Advanced parameters" allows to reach a second screen:



- The **stabilization time** corresponds to the duration of latency before the micro GC switches to "ready"
- **Continuous flow**: If this box is checked, the pump is deactivated since the sample circulates "continuously" in the injection loop, the continuous flow can be activated only in SOPRANE II Setup (see chapter [Control flow sample](#)).

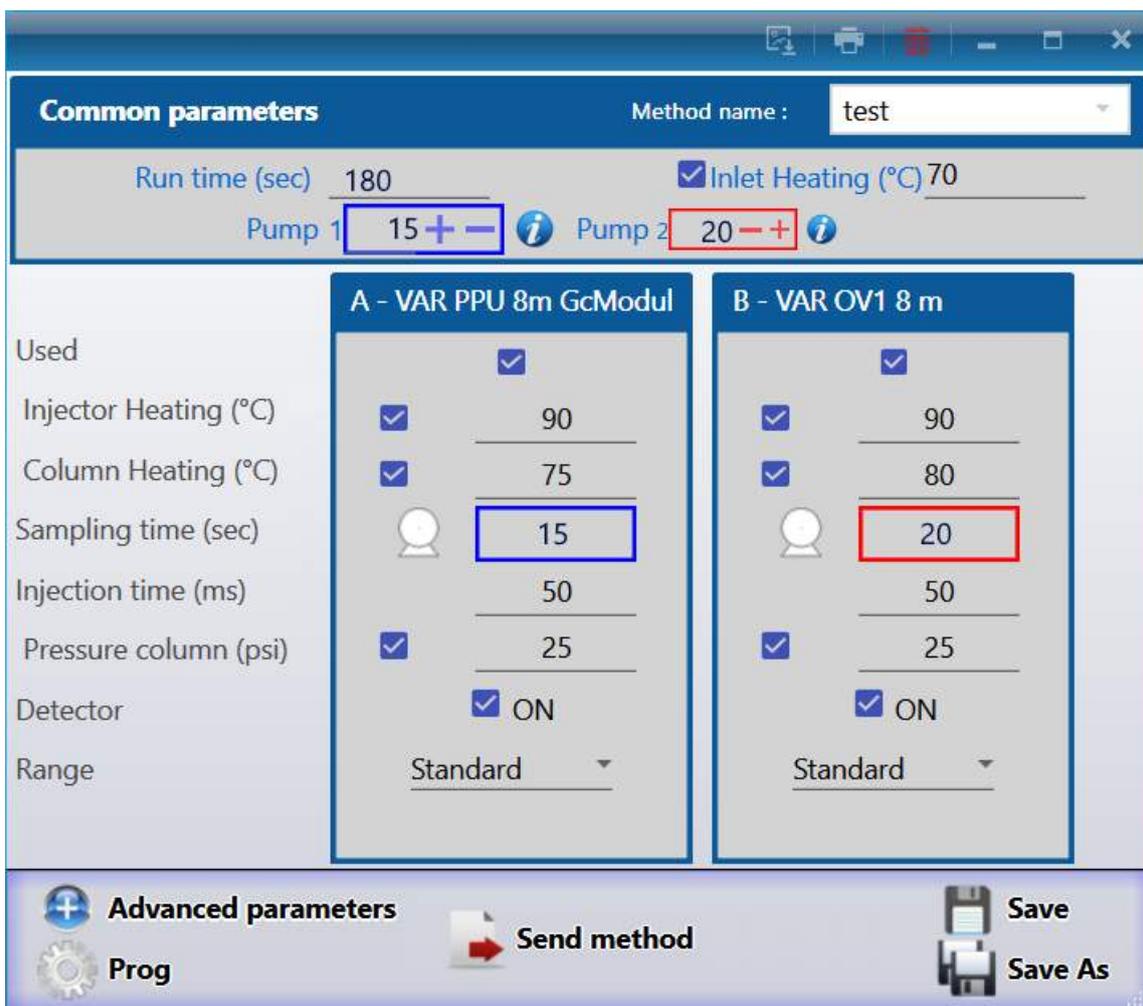


- **TCD Ctrl temp.:** TCD temperature control, if the TCD heats due to a wrong carrier gases configuration, for example, a security switches off the TCD.
- **Invert signal:** allows to invert the signal when using Argon or Nitrogen gas.
- **Press. programming:** allows to program the pressure if needed.

a) **2. M3000 operating conditions**

Here is the window in which analytical conditions for a Micro GC 3000 can be set:  
The following display is identical for Lan and series M3000 instruments.

See chapter [Operating conditions](#), to have information about each parameter.

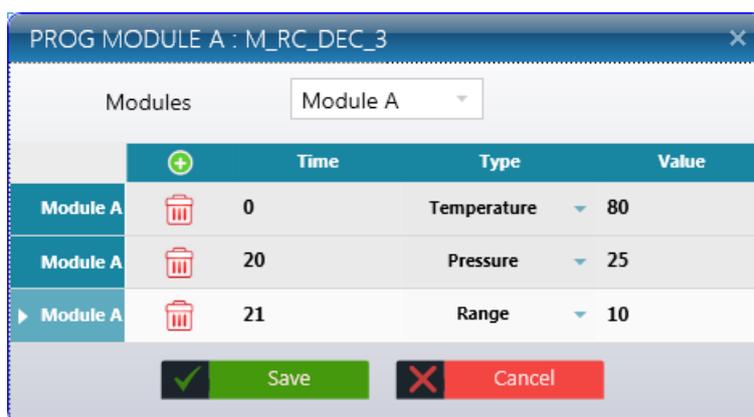


On the first screen of the operating conditions, a button, named Prog , allows to write several steps of programming to modify the values of temperature, pressure or sensibility during the analysis.

• **Programming**

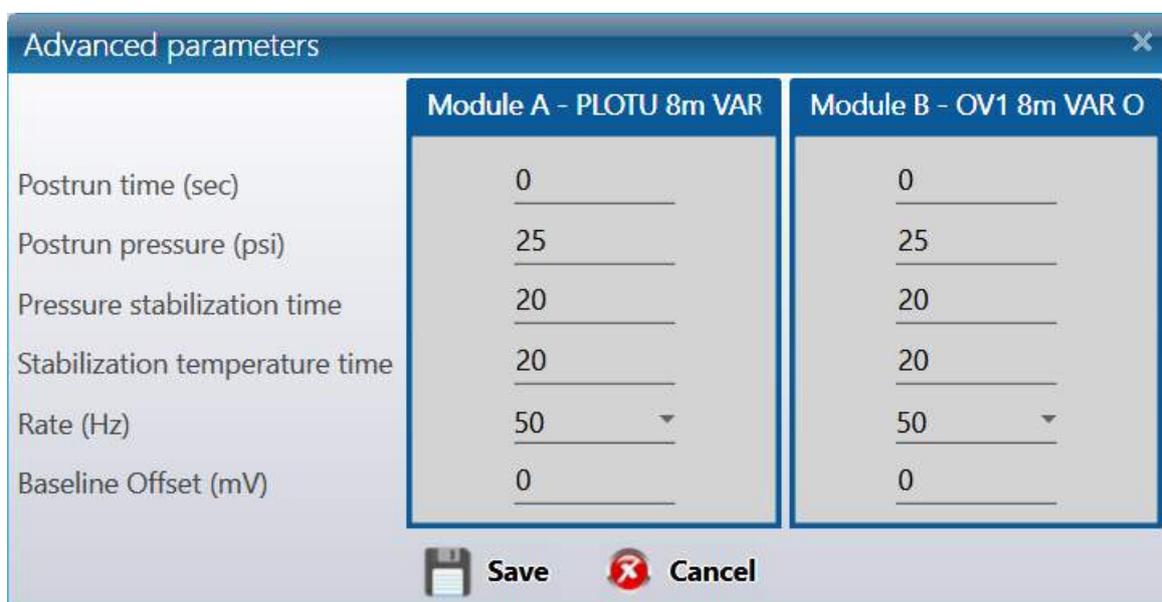
All these steps of programming must be written by increasing times.





• **Advanced settings**

The button  **Advanced parameters** allows to reach a second information screen.



**The post-run time and pressure:**

They allow, when it is necessary, to avoid waiting too long for the elution of a heavy compound not analyzed. At the end of the analysis, the carrier gas pressure at the head of column is adjusted with the value indicated here (normally higher than the pressure used during the analysis) and this value is maintained during the time indicated as post-run value.

**The temperature or pressure equilibrium times:**

They are the durations, expressed in seconds, aiming at limiting the defaults management. If a setting is modified, the new instruction cannot be immediately considered. The value programmed here corresponds to the duration during which the normal difference between the real value and the new setting is not managed as a default.

Note: the temperature equilibrium times have to be entered in the second line.



The **stabilization time** corresponds to the duration of latency before the micro GC switches to "ready"

**The rate:** It is the signal sampling frequency, expressed in Hz. It is possible to choose to measure the signal 20, 50 or 100 times per second.

**The continuous flow:**

If this box is checked, the pump is deactivated since the sample circulates "continuously" in the injection loop.

**Baseline offset:**

The value, expressed in millivolts, allows to shift the analysis signal in a direction or another. When all these screens are validated, SOPRANE II proposes to save the modifications carried out.

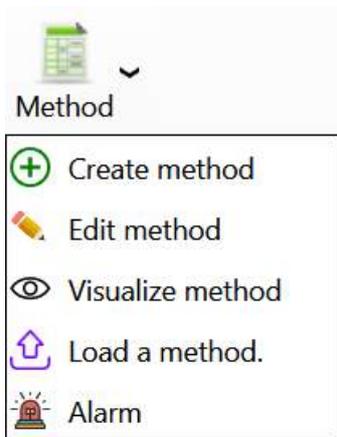
A method is not only made of operating conditions, but also of integration parameters and events, of compounds identification data, of reports, ...

For now, we can create and modify operative conditions of several methods corresponding to several streams.

To see how to set a sequence of analysis see chapter: [Analysis sequences management](#).

***b) Loading an analytical method***

The loading of a method is accessible in the tab "**Analysis** or click on **method**".



Na...	Inlet	Injector		Column		Pressure		Injection		Detector	
		Mod. A	Mod. B	Mod. A	Mod. B	Mod. A	Mod. B	Mod. A	Mod. B	Mod. A	Mod. B
off	70,0 °C	90,0 °C	90,0 °C	75,0 °C	80,0 °C	5,0 PSI	5,0 PSI	50 ms	50 ms	OFF	OFF
off 1	70,0 °C	90,0 °C	90,0 °C	75,0 °C	80,0 °C	5,0 PSI	5,0 PSI	50 ms	50 ms	OFF	OFF
test	70,0 °C	90,0 °C	90,0 °C	75,0 °C	80,0 °C	25,0 PSI	25,0 PSI	50 ms	50 ms	ON	ON
test_1	70,0 °C	90,0 °C	90,0 °C	75,0 °C	80,0 °C	25,0 PSI	25,0 PSI	50 ms	50 ms	ON	ON

To validate the selection of the method, press on the button **Confirm**, and the method will be loaded.

### c) The 4 useful methods

Whatever the type of instrument you use, it is necessary to create the 4 following methods:

- ✓ **Start/Stop method:** only carrier gases circulate in the analyzer but the columns are not heated, the temperatures are set below 50°C. This method will then be used when starting and shutting down the instrument.
- ✓ **Standby method:** the carrier gases circulate; the columns are heated but the detectors are switched off. This method will be used after the Start/Stop method and when one wants to let the analyzer under conditions (Pressure and temperature) stabilized awaiting analysis.
- ✓ **Analysis method:** the carrier gases circulate; the columns are heated and the detectors are switched on.
- ✓ **Bake-out method:** it is a method used to regenerate columns (see chapter [Bake-out management](#)). The temperature is higher, the pressure slightly increased and the detectors are switched off.

Before switching off the analyzer, and for security reasons concerning columns, it is better to send the Start/Stop method and to wait that the columns reach a temperature below 50°C.

### 4.3.2. Analysis sequences management

We have seen how to write (creation or modification) an analysis method and how to send it to the analyzer (see chapter [Analytical methods management](#)).

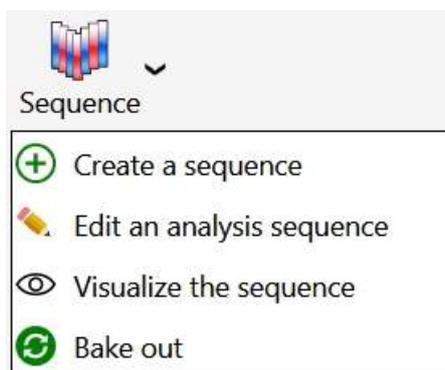
The analyses sequence is useful when several methods are used because either we analyze several streams with different compositions or because we don't always work in the same operating conditions for example.

We want to perform cyclic analyses. It is thus necessary to define which streams will be analyzed, which analysis method will be used for that, how long it will be necessary to wait before injection, ...

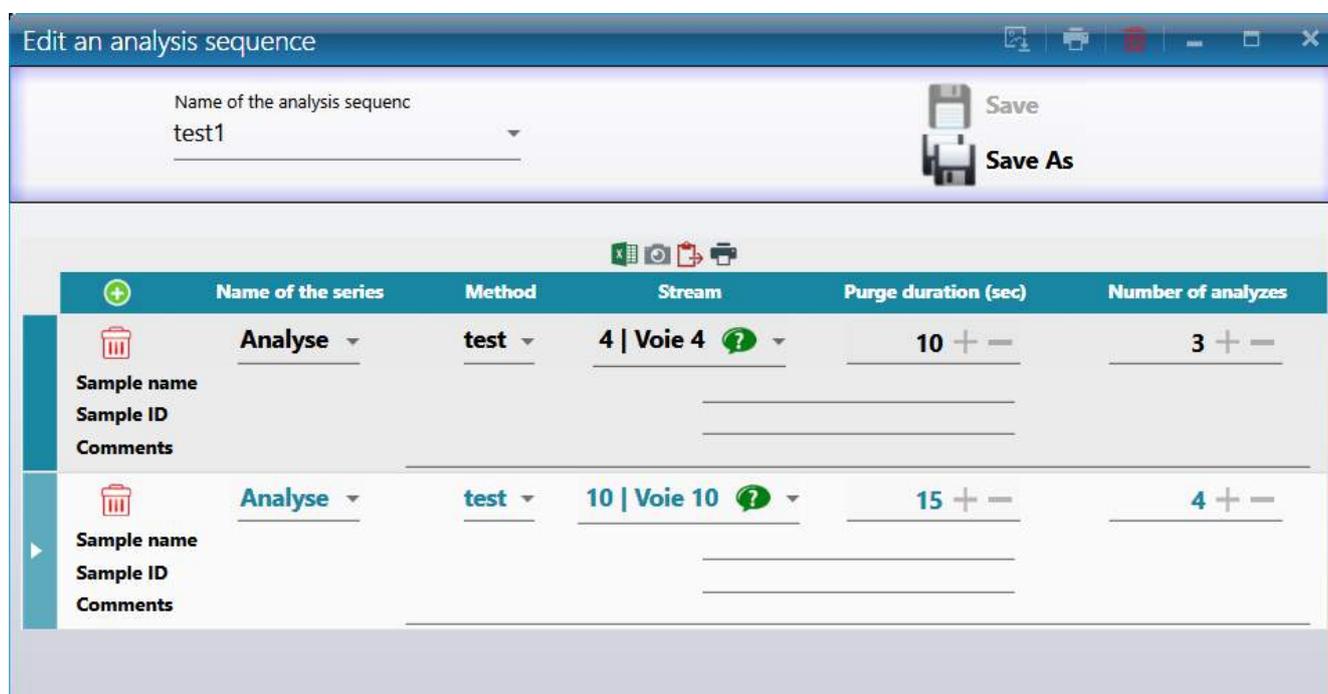
We suppose that the chromatograph allows the analysis of several streams. These streams can be selected by campaign (only analyses of one stream are carried out) or sequentially, all streams having the same analysis frequency or some being more important than others.



To access to the sequences edition, go to the **Analysis** tab and click on the next button.



The following window will appear:



In this table, it is possible to **define analyses by giving them a name**, to **select an analysis method** (a list box shows the different methods), to indicate **which stream is concerned** (another list box is used to select it) and to specify the minimal duration (expressed in seconds) of the sampling before any injection.

The analysis method already comprises one duration of sweeping of the injection loop, which corresponds to the pump management. Indeed, before carrying out the injection, it is necessary to make circulate the sample in the injection loop, but it is also necessary to have something representative of the sample, which needs to select the stream and perhaps to actuate another pump and wait a minimal duration.

The **duration of purge time** indicated here is before the injection loop and does not concern the injection itself but the flow as a whole. It corresponds to the selection of the stream.

When the stream selection valve is commutated, it is necessary to sweep "residues" of the preceding stream so that what is injected is representative of the stream to analyze, which requires a more or less important



duration, function of the sample, of its characteristics, of the flow and the volume separating the stream selection valve from the injection valve.

The value thus programmed (value in seconds) will allow SOPRANE II to anticipate the following analysis and to select next stream early enough to ensure an adequate sweeping of it.

If the duration of sweeping exceeds the duration separating the end of the injection of the analysis in progress and the beginning of the following analysis, a time delay is implicitly added by SOPRANE II.

Note:

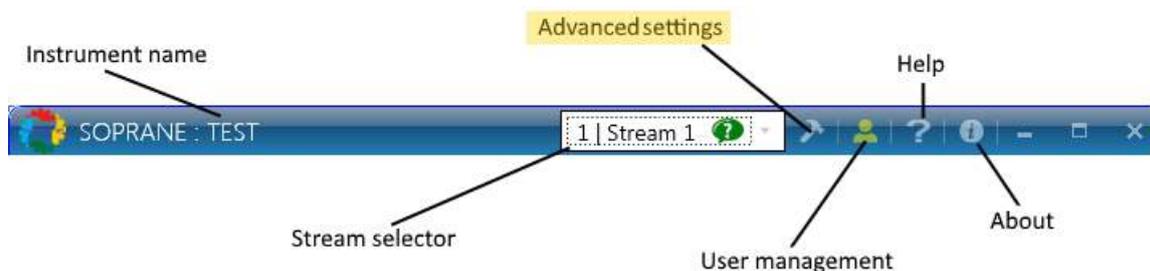
An analyses sequence can of course include the reference of a stream defined elsewhere as used for calibration. Keep in mind that it is an analyses sequence, which means that these standards will be analyzed as any other samples and will lead to the calculation of concentrations.

To see how to edit a calibration sequence, see the chapter [Calibration sequence management](#).

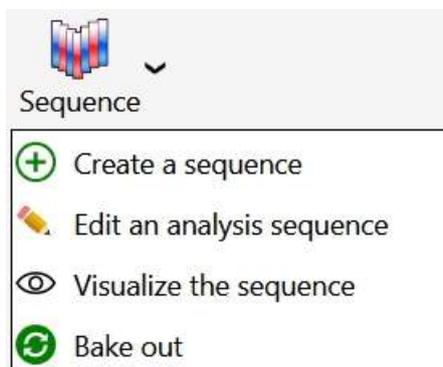
### Bake-out management

When configuring SOPRANE II (see chapter [Analyzer configuration](#)) the management of the regeneration of the columns could be set (see chapter [Options management](#)).

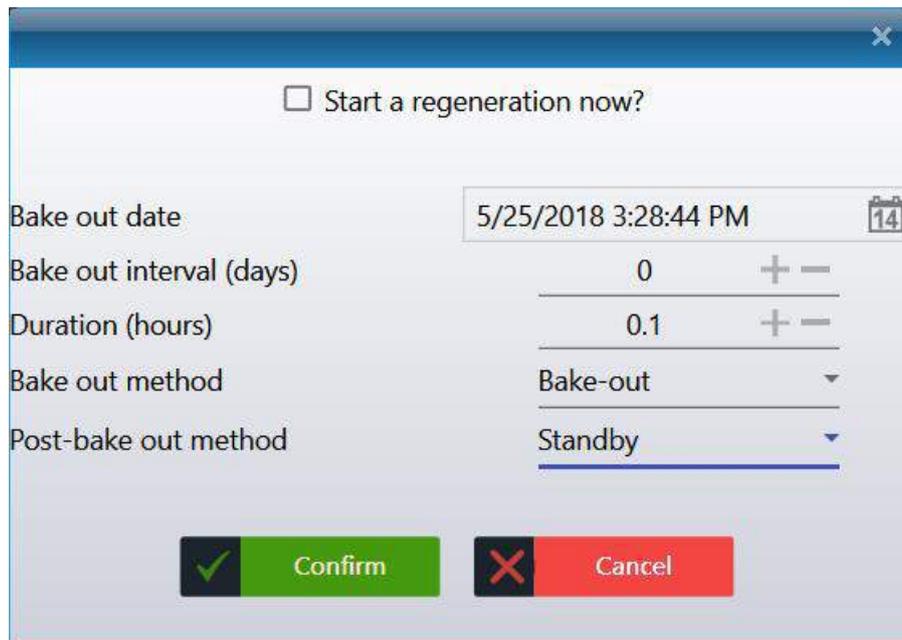
If such a request was made, click on "Advanced settings"  of SOPRANE II.



The "Regeneration column." option will be available. This option works in the same way as the automatic calibration that is to say it has priority on an on-going analyses sequence.



Below is the window that will open.



It is sufficient to indicate the **date and time of the next bake out** and the **number of days between two successive bake out** (0 if only one bake out is to be carried out).

Bake out requires parameters (higher column temperature, detector OFF) different from those used for analysis, therefore a **bake out duration** and the **name of a method to be used to carry out the regenerations** should be indicated.

Finally, a **post regeneration method** must be indicated.

There are 2 ways to proceed with bake out. It is possible to stop the analyses and request an immediate bake out or to program this bake out so that it can be carried out a little later.

In this case, when the bake out is completed, the post regeneration method will be sent to the analyzer. This post-regeneration method is similar to the methods used to perform the analyses but with the detectors OFF. Such regeneration can be carried out during the night or the weekend, and at the end the user has a device ready for use.

The second way is to program the bake out at regular intervals and then start an analysis sequence. When a bake out is to be carried out, the sequence is temporarily interrupted. At the end of bake out, the post regeneration method is ignored and the method corresponding to the next analysis is sent to the analyzer. SOPRANE II then waits for the necessary time to have a READY status for the analyzer, then the sequence returns to its normal course.

The post-regeneration allows to decrease the temperature after the bake out. The post-regeneration method can then be used as a method of end of sequence because it allows to load a method without carrying out analyses.

If the bake out duration is set to zero, the regeneration method is not loaded and only the post-regeneration is loaded.



### 4.3.3. Calibration sequences management

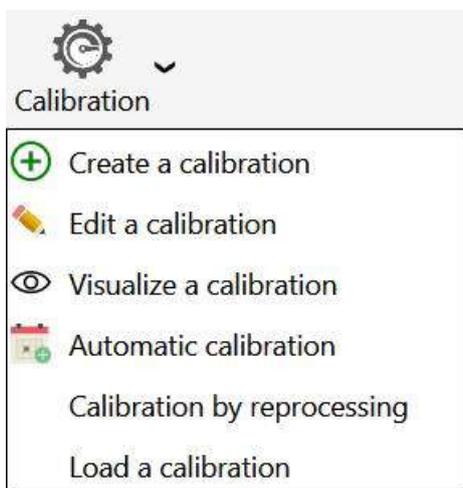
Before being able to create a calibration sequence, you must have first created an analysis method (see chapter [Analytical methods management](#)).

Several analysis methods may be written because we analyze several streams with different compositions, because we don't work in the same operating conditions, ...

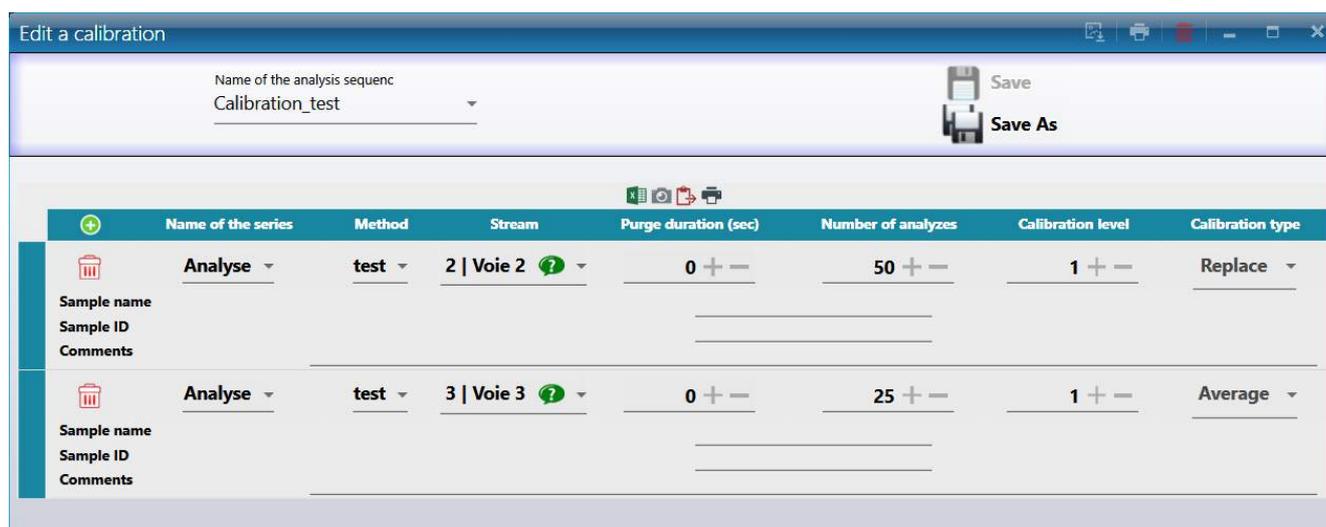
We want to perform cyclic analyses. It is thus necessary to define which streams will be analyzed, which analysis methods will be used for that, how long it will be necessary to wait before any injection, ...

We suppose that the chromatograph allows the analysis of several streams. These streams can be selected by campaign (only analyses of one stream are carried out) or sequentially, all streams being swept the same manner, or some being more important than others...

To access to calibration sequences, go to the **Analysis** tab and click on the next button.



The following window will appear:



In this table, it is possible to **define analyses by giving them a name**, to **select an analysis method** (a list box shows the different methods), to indicate **which stream is concerned** (another list box is used to select it) and to specify the minimal sampling duration (expressed in seconds) before any injection and the number of repetitions of this step.

These are the same settings as when editing a sequence (see chapter [Analysis sequences management](#)), you must also add the reference of a stream defined elsewhere as used for calibration. It should be kept in mind that this is an analyzes sequence, which means that these standards will then be analyzed like any other sample and will give rise to the calculation of concentrations. The calibration type will also be entered.

Information concerning the sample can be added. These values are the sample name, its ID and a comment if necessary.

The analysis method already comprises one duration of sweeping of the injection loop, which corresponds to the pump management. Indeed, before carrying out the injection, it is necessary to make circulate the sample in the injection loop, but it is also necessary to have something representative of the sample, which needs to select the stream and perhaps to actuate another pump and wait a minimal duration.

The **duration of purge time** indicated here is before the injection loop and does not concern the injection itself but the flow as a whole. It corresponds to the selection of the stream.

When the stream selection valve is commutated, it is necessary to sweep "the remainders" of the preceding stream so that what is injected is representative of the stream to analyze, which requires a more or less important duration, function of the sample, of its characteristics, of the flow and the volume separating the stream selection valve from the injection valve.

The value thus programmed (value in seconds) will allow SOPRANE II to anticipate the following analysis and to select next stream early enough to ensure an adequate sweeping of it.

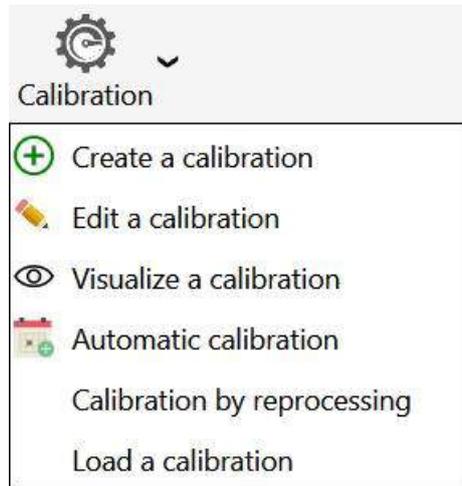
If the duration of sweeping exceeds the duration separating the end of the injection of the analysis in progress and the beginning of the following analysis, a time delay is implicitly added by SOPRANE II.

Calibrations history could be visualized (see chapter [Calibration history](#)).

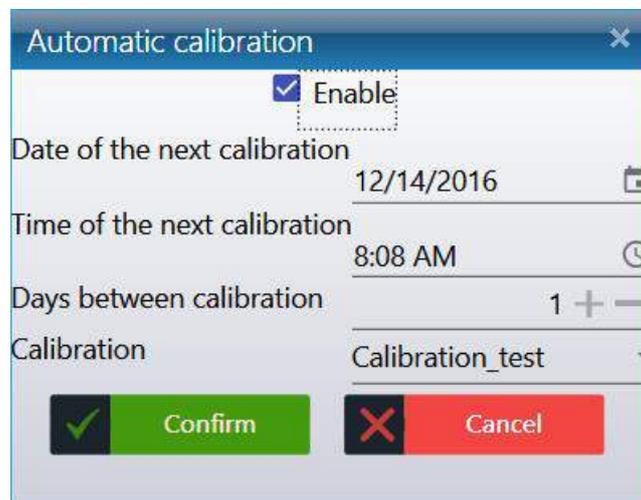
## Automatic calibration

To access to automatic calibration, go to the **Analysis** tab and click on the calibration button and then select the **Automatic calibration**.





The following window will appear:



First, the automatic calibration, must be **activated**, if it is disabled the calibration will not occur.

If it is requested for an automatic calibration, it is necessary to define the **date** and **time** for the first automatic calibration, and then the **number of days** (0-999) before any next automatic calibration. The value 0 days between calibrations is used to do one and only one automatic calibration: the others are prohibited.

**The automatic calibration will only be done with a start-up in automatic mode.**

Calibrations history could be visualized (see chapter [Calibration history](#)).

## 4.4. Analyzes management

[Reading the status](#)

[Status bar](#)

[Title bar](#)

[Eye](#)



## [Analyzes](#)

[Real time](#)

[Start an analysis](#)

[Start a sequence](#)

[Start a calibration](#)

## [Analyses results](#)

[Series of analyses](#)

[Results of an analysis](#)

[Trends](#)

[Batch reprocessing](#)

[Calibration by reprocessing](#)

### 4.4.1. Analyses

The "Start" button  on the "**Analyzes**" tab allows to start analyzes according to the sequence that has been programmed.

When such a request is made, SOPRANE II sends the analysis method and the analysis starts as soon as the chromatograph is stabilized under the required operating conditions.

In the same way, stopping a cycle of analyzes can be requested by the button symbolizing a STOP panel. For security reasons, a dialog box allows to confirm (or not) the request and specifies that the effective stop will occur at the end of the current analysis.

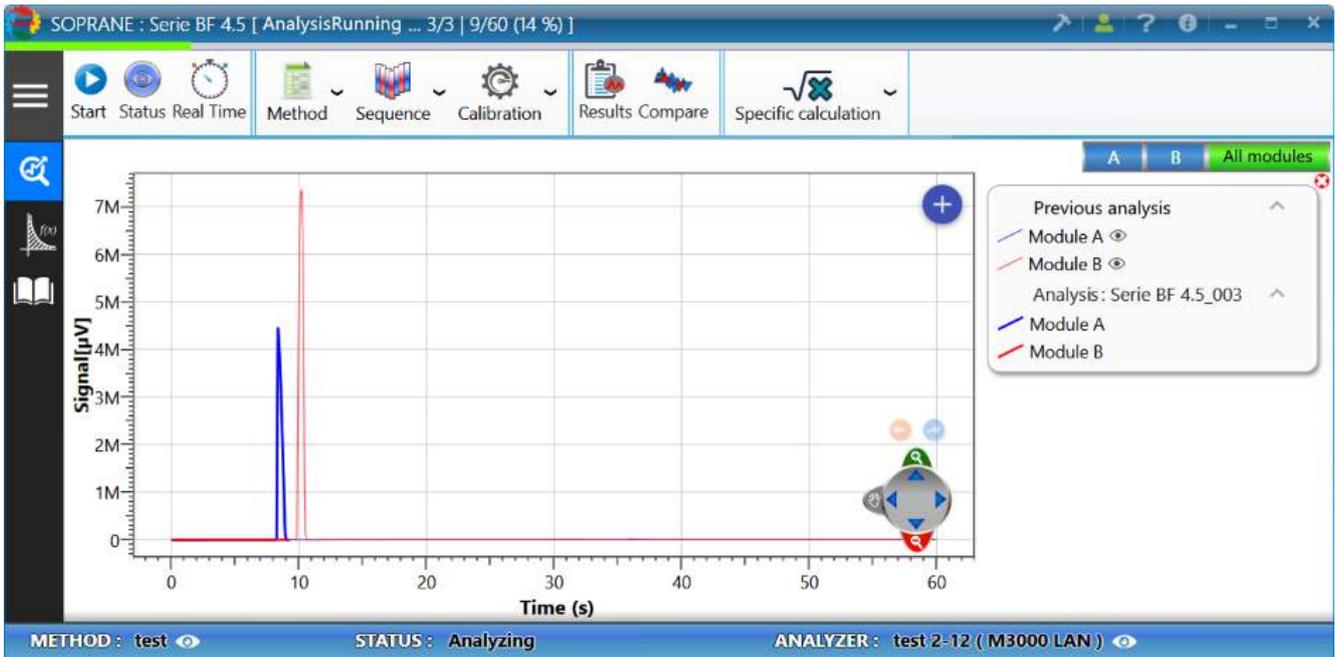
Three modes of analysis are possible:

- Analysis: To launch a defined number of analyzes using the same method (see chapter [Start an analysis](#)).
- Sequence: To launch an analyses sequence (see chapter [Start a sequence](#)).
- Calibration: To launch a calibration sequence (see [Start a calibration](#)).

#### ***a) Real time***

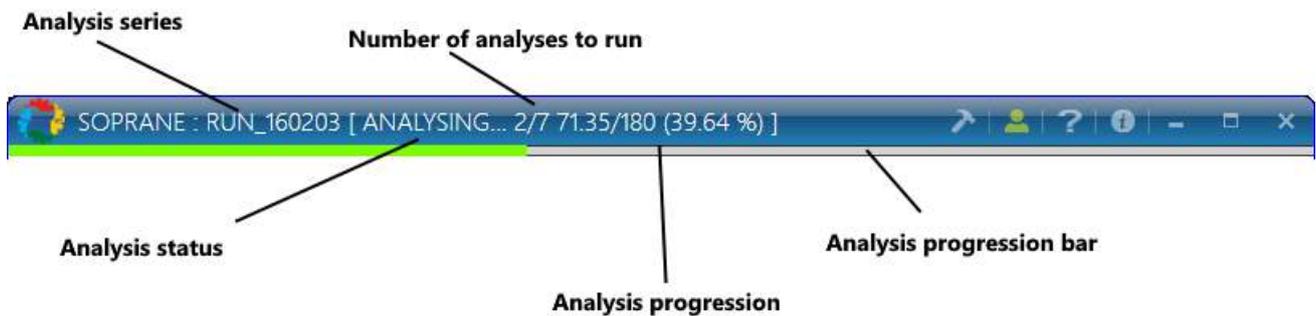
When an analysis is running, the following display is displayed:



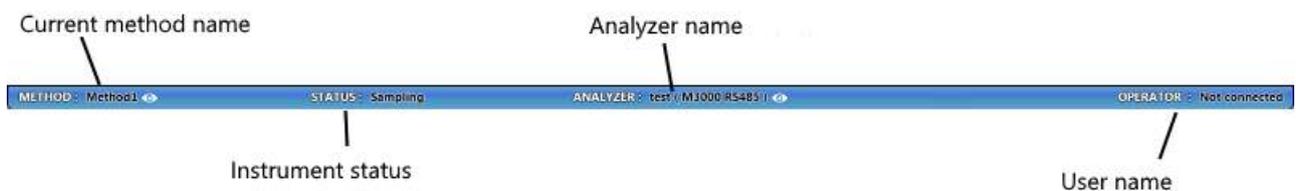


There are several elements to take into account to know the progress of the analysis:

1. The title bar



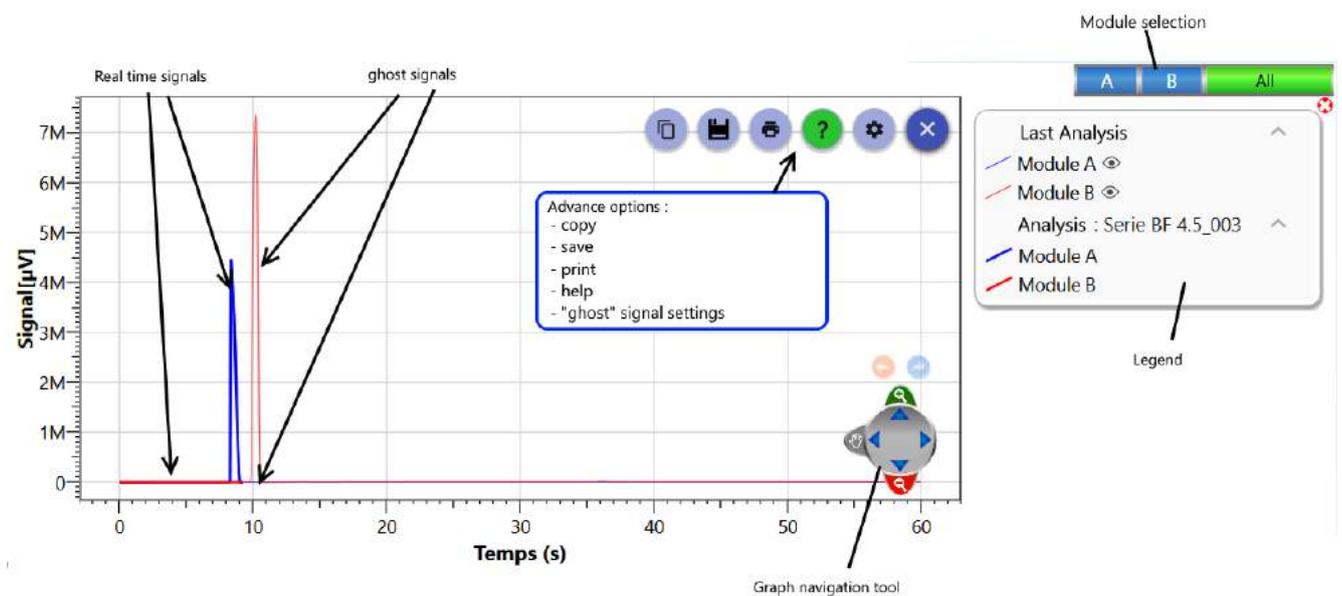
2. The status bar



### 3. The real-time signal

During an analysis, SOPRANE II displays the signal received from the detectors. By default, all the modules are displayed on the same graph, the selection of the module to be displayed can be modified by clicking on the name of the corresponding module.

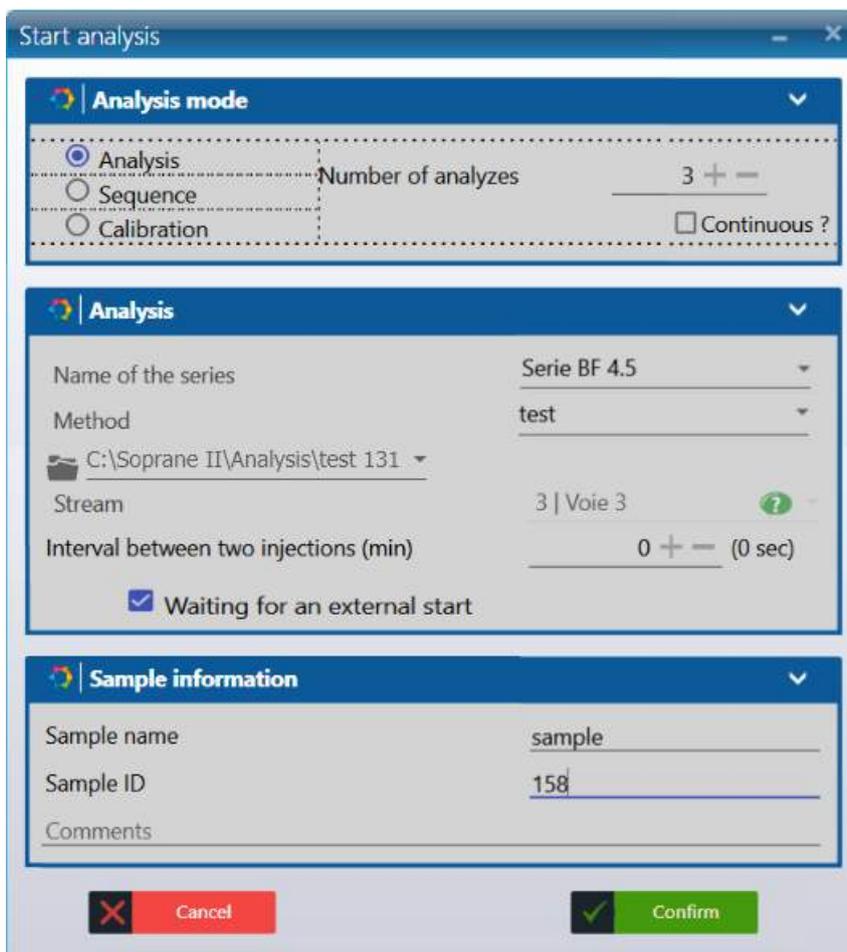
The graph offers the possibility to compare the real-time signal with the previous analysis. To remove the previous signal, click on  and to display it again click on the button .



The real-time signal offers the possibility to move and zoom on the graph. For more information see chapter [Chart](#).

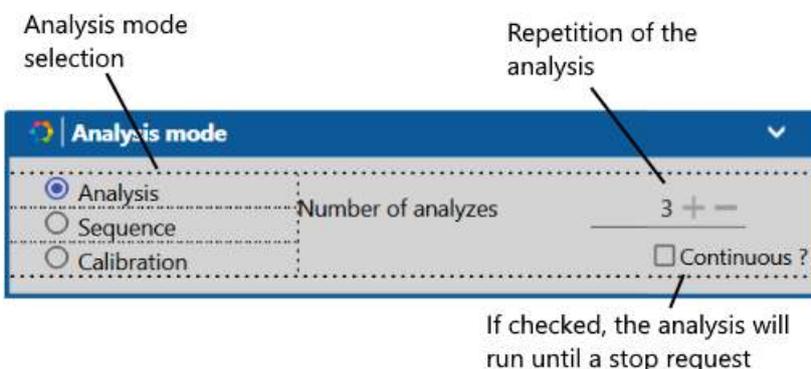


**b) Start an analysis**

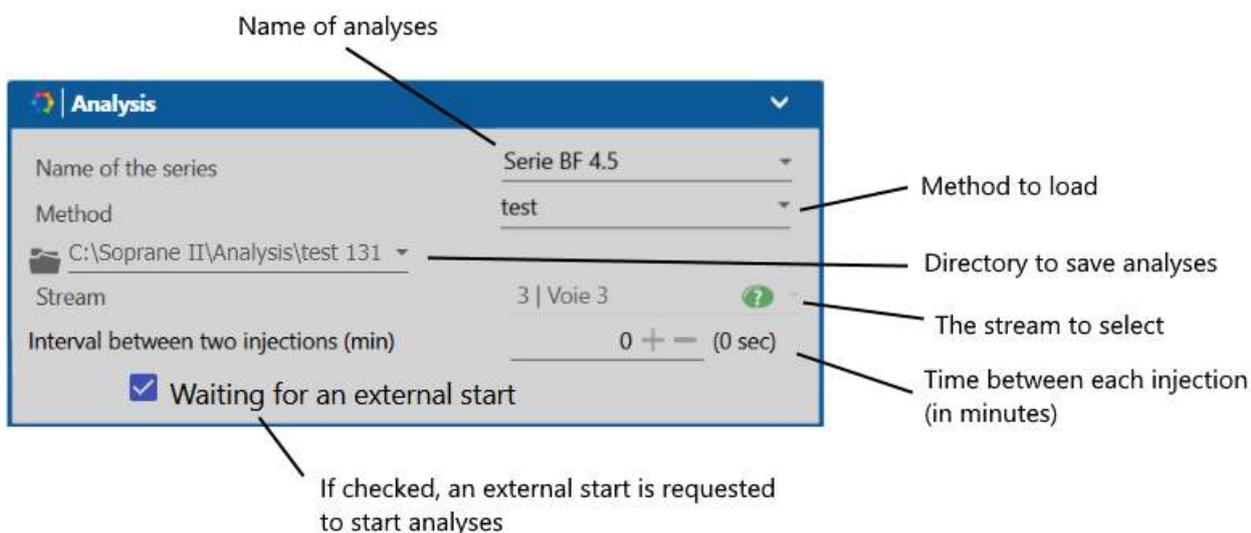


Before starting one (or several) analyze(s), it will be necessary to fill in several fields:

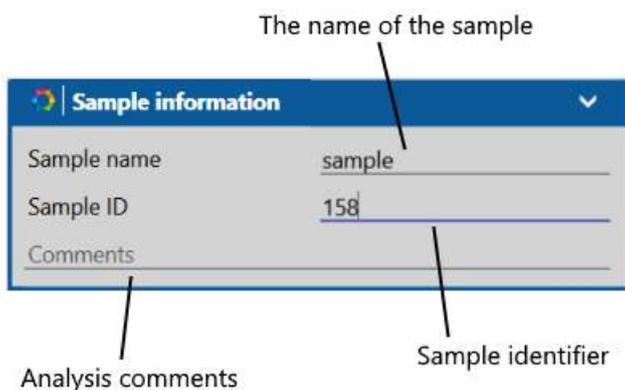
1. Analysis mode



## 2. Analysis information



## 3. Sample information



Note: The icon  allows you to enlarge or reduce the corresponding panel.

Once all the information is filled in, the analysis will start at confirmation.

To go further, see chapter [Real time](#).

See also chapters [Start a sequence](#) and [Start a calibration](#).

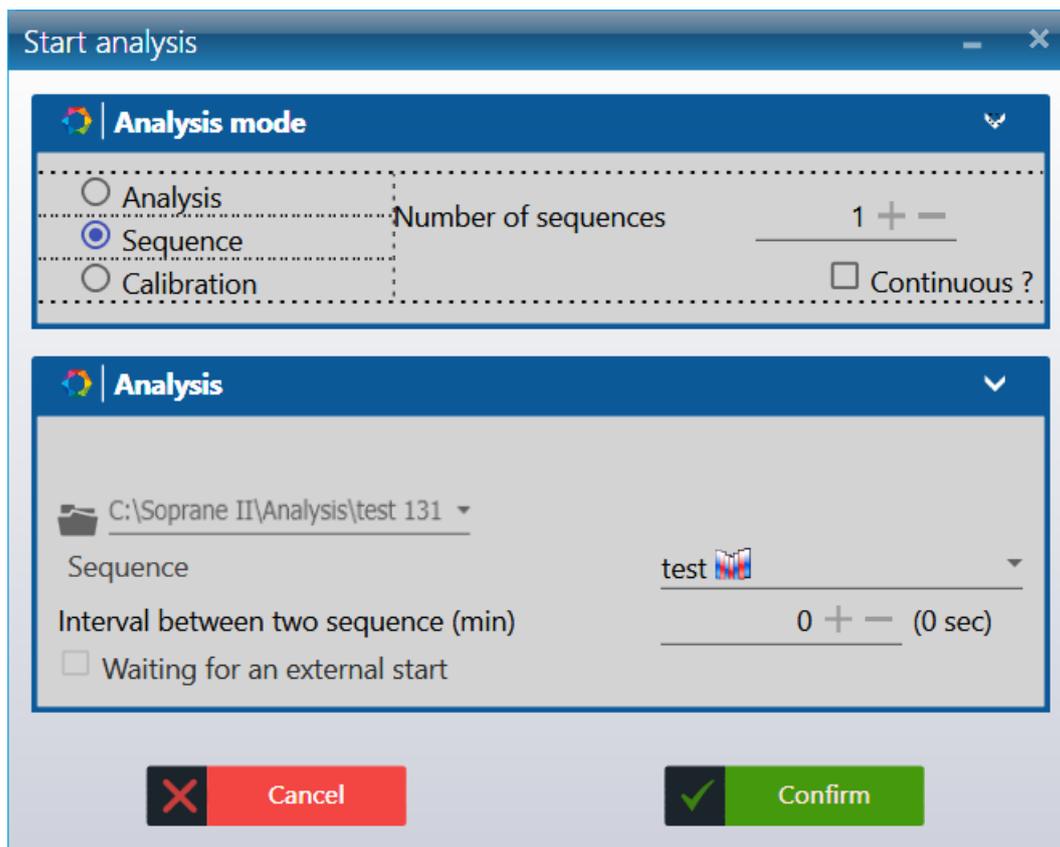
To see how to create a method see chapter [Analytical methods management](#).



**c) Start a sequence**

We suppose that the chromatograph allows the analysis of several streams. These streams can be selected by campaign (only analyses of one stream are carried out) or sequentially, all streams having the same analysis frequency, or some being more important than others.

An analyses sequence may of course include the reference of a stream defined elsewhere as being used for calibration. It should be kept in mind that this is a sequence of analyzes, which means that these standards will be then analyzed as any other samples and will lead to calculation of concentrations.

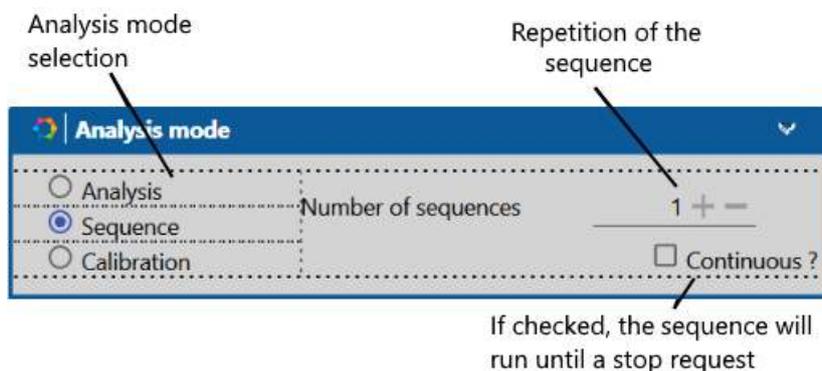


The **Sequence** field is used to load a sequence of analyzes (This assumes that several streams have been defined).

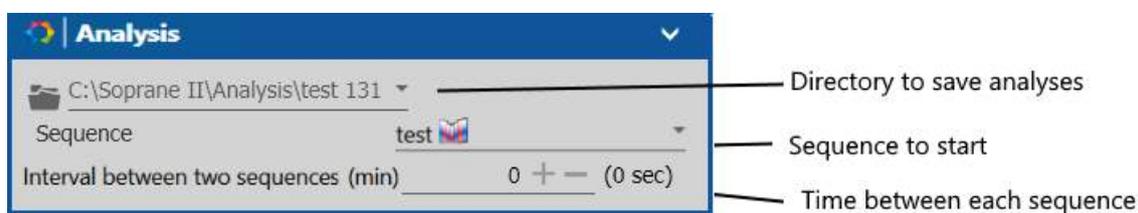
Before launching one (or several) sequence(s), it will be necessary to fill in several fields:



## 1. Sequence mode



## 2. Sequence information



**Note:** The icon  allows you to enlarge or reduce the corresponding panel.

Once all the information is filled in, the analysis will start at confirmation.

To go further, see chapter [Real time](#).

See also chapters [Start an analysis](#) and [Start a calibration](#).

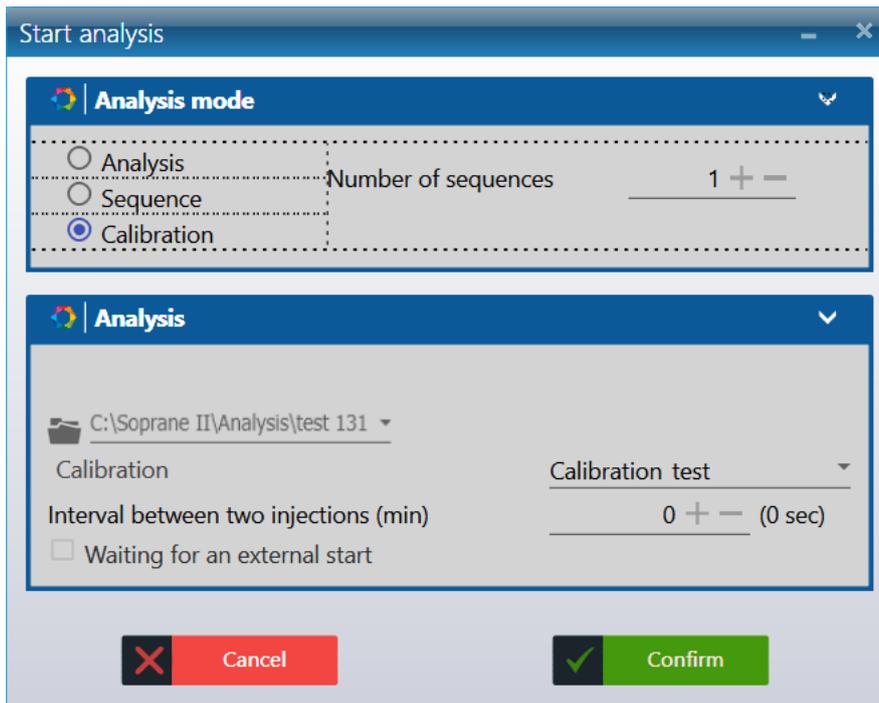
To see how to create a method see chapter [Analytical methods management](#). See chapter [Analysis sequences management](#) to create a sequence.

### **d) Start a calibration**

We suppose that the chromatograph allows the analysis of several streams. These streams can be selected by campaign (only analyses of one stream are carried out) or sequentially, all streams having the same analysis frequency, or some being more important than others.

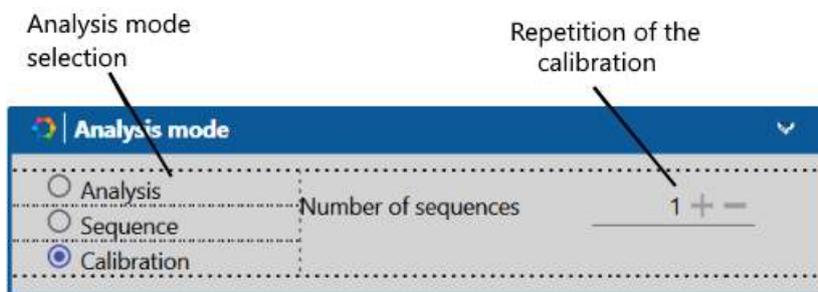
Unlike an analyses sequence, at the end of an analysis, the standards will then be analyzed and will give rise to the calculation of concentrations.



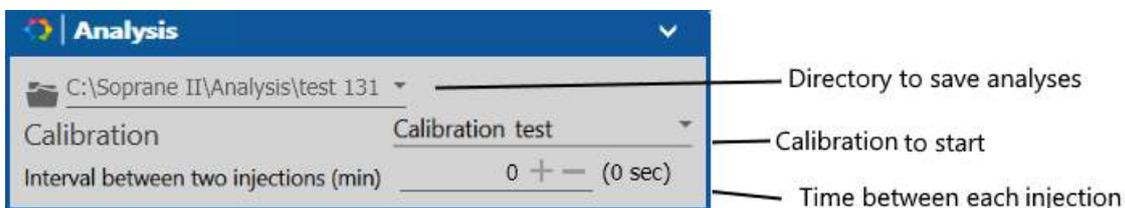


Before launching one (or several) calibration(s), it will be necessary to fill in several fields:

1. Calibration mode



2. Calibration information



Note: The icon  allows you to enlarge or reduce the corresponding panel.

Once all the information is filled in, the analysis will start at confirmation.

To go further, see chapter [Real time](#).

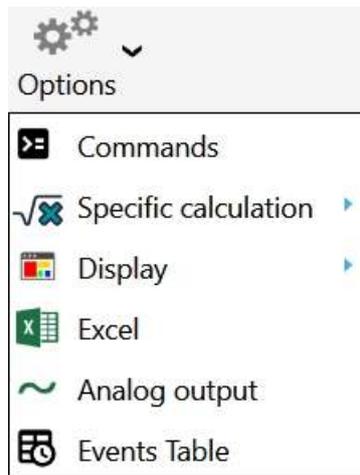


See also chapters [Start an analysis](#) and [Start a sequence](#).

To see how to create a method see chapter [Analytical methods management](#), see chapter [Analysis sequences management](#).

### ***e) Analysis events table***

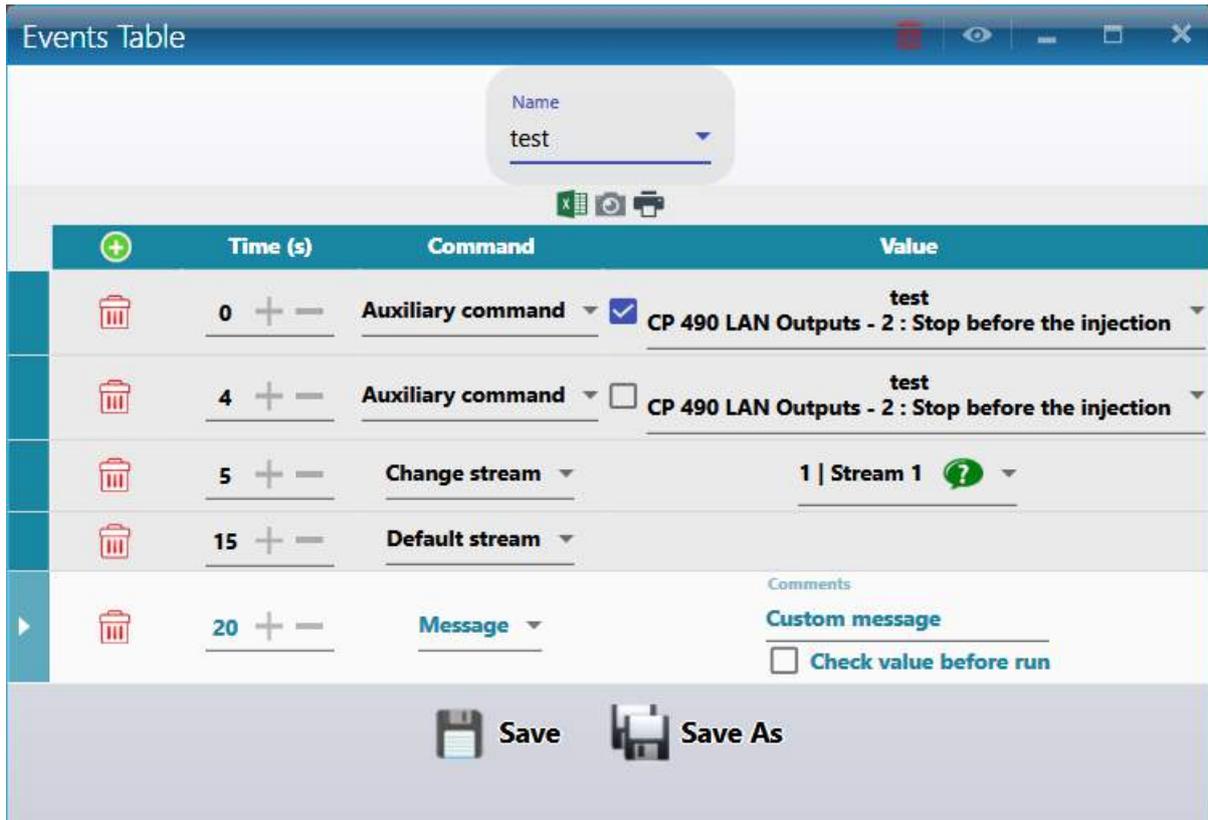
Soprane II allows to control various commands before and after injection such as auxiliary pump activation, stream selection. These commands are accessible via the "**Options\Events table**" menu.



For each event, here are the steps you must indicate:

- The starting time of the event
- The command (None, Auxiliary command, change stream, select the default stream, custom message and read analog input)
- The command value (could be different if you change the command type)





Soprane II will automatically start the analysis at the end of the event sequence.

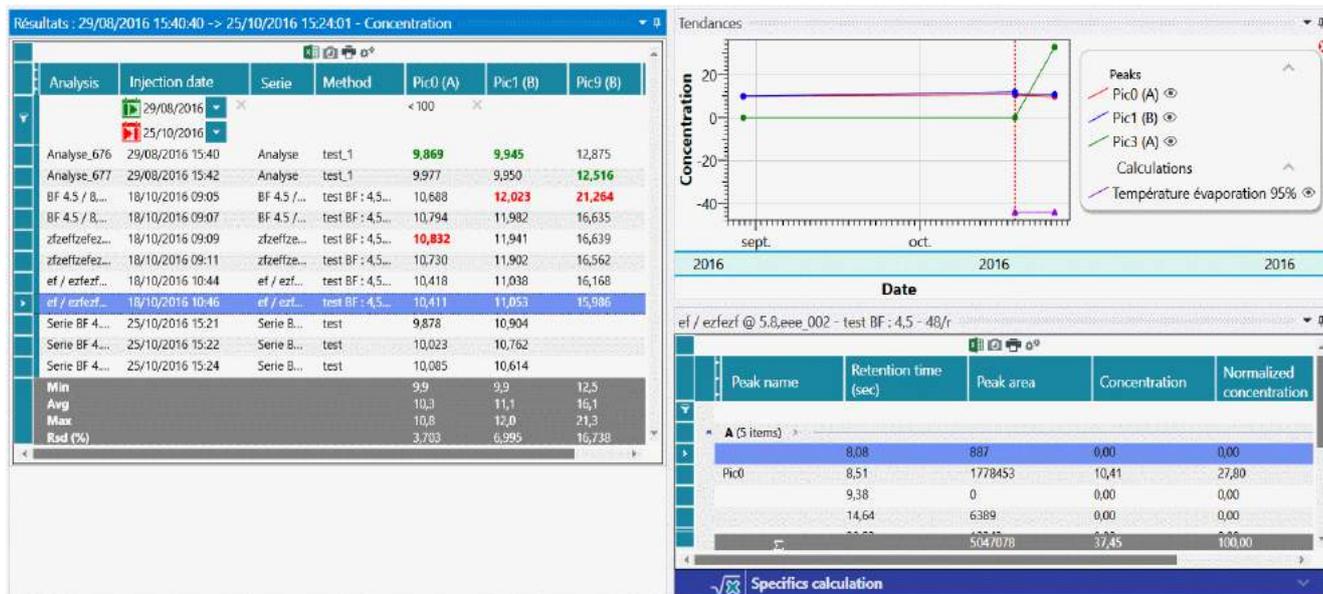
Once the configuration of the event table is finished, save it and select the event table in the pre-command (see chapter [Pre and Post command](#))

#### 4.4.2. Analyses results

In normal operation, SOPRANE II allows simultaneous visualization of 3 windows related to analyzes.

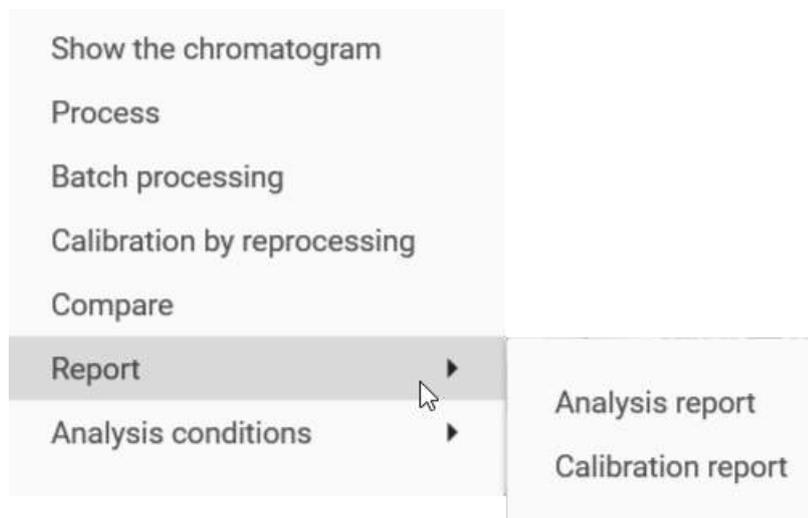
These 3 windows allow the visualization of the **results of all analyzes**, of the **selected analysis** and of the **trends**. These windows can be resized, minimized, or restored.

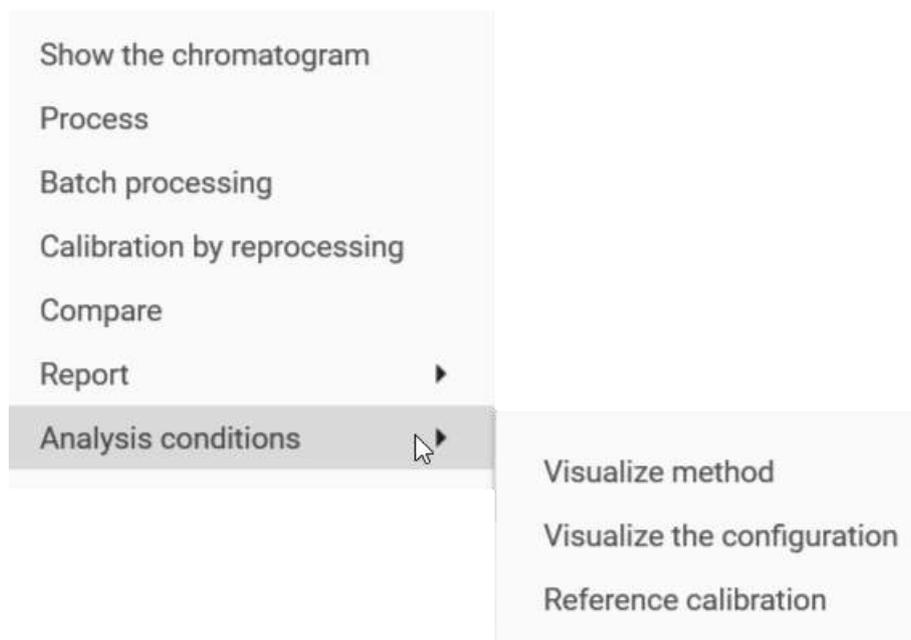




### 1. Description of menus

The "Action" menu allows to perform some operations according to the selection of the analyzes in the analysis table. The same actions are possible by right clicking on the analysis results table (For further details, see Heading [Quick actions](#)).





The different operations are:

- **Show the chromatogram**: Open the chromatogram with the integration parameters in another window (the shortcut is double click on the result line) (Available only if a single result is selected)
- **Process**: Loads the selected analysis into the processing part. (Available only if a single analysis is selected, see [Process](#))
- **Batch Processing**: Retrieves each selected analysis with a specified method. (See [Batch reprocessing](#)).
- **Calibration by reprocessing**: Calibrates all analyzes selected with a specified method. (See [Calibration by reprocessing](#))
- **Compare**: Opens the Analytics Comparison tool (see the [Comparisons](#) chapter).
- **Report**: Displays reports (Available only if a single result is selected, see [Report](#))
  - Analysis report: Displays the analysis report (Available only if a single scan is selected, see [Report](#))
  - Calibration report: Displays the calibration report (if a calibration has been done) (see chapter [Calibration report](#))
- **Analysis conditions**: Available only if a single analysis is selected; here are the different possible operations:
  - Displays the injection method parameters.
  - Displays the analyzer configuration during injection.
  - Displays the calibration reference (see chapter [Reference calibration](#)).

The menu "**Trend**", offers the possibility to add new trends and to configure them (see chapter [Trends](#)).

The last menu "**Options**", offers the possibility to configure the nature and position of windows. They can be memorized so that SOPRANE II can restore the display each time the program is started.

## 2. Description of the different display modes

Values in the data tables as well as the trends are displayed only under one mode at the same time. The selection of the mode will be done by selecting it in the list proposed at the top in the center of the window.



Here are the different display modes:

- The **Results table** mode displays all the analyzes with the results at the end of the injection.
- The **Reprocessing** mode displays all the analyzes that have been reprocessed.
- The **Calibration** mode displays all the analyzes that have been calibrated by reprocessing.

3. Description of the different results to be displayed

The main table as well as the trends only focus on one type of result. The change of the result to be displayed will be done by selecting it from the list in the top right of the window.

Here are the different values which can be displayed:

- Concentration
- Standardized Concentration
- Retention time (in seconds)
- Peak area
- Peak Height

To see in detail the operation of these three windows, see the following chapters:

[Series of analyses](#)

[Results of an analysis](#)

[Trends](#)

To go further, see also:

[Quick Actions](#)

[Process](#)

[Batch reprocessing](#)

[Calibration by reprocessing](#)

[Comparisons](#)

[Report](#)

***a) Series of analyses***

The "**Analysis series**" window offers the possibility to see the results of analyzes, reprocessing or calibration.



Results : 8/29/2016 3:40:40 PM -> 11/4/2016 4:14:06 PM - Concentration

Analysis	Injection date	Serie	Method	Pic0...	Pic1 (
	01/01/2015			<100	
	11/17/2016				
Analyse_676	8/29/2016 3:40 PM	Analyse	test_1	9.869	9.945
Analyse_677	8/29/2016 3:42 PM	Analyse	test_1	9.977	9.950
BF 4.5 / 8,4...	10/18/2016 9:05...	BF 4.5 / 8,...	test BF : 4,5...	10.688	12.023
BF 4.5 / 8,4...	10/18/2016 9:07...	BF 4.5 / 8,...	test BF : 4,5...	10.794	11.982
zfzeffzefez_001	10/18/2016 9:09...	zfzeffzefez	test BF : 4,5...	10.832	11.941
zfzeffzefez_002	10/18/2016 9:11...	zfzeffzefez	test BF : 4,5...	10.730	11.902
ef / ezfezf @...	10/18/2016 10:44...	ef / ezfezf...	test BF : 4,5...	10.418	11.038
ef / ezfezf @...	10/18/2016 10:46...	ef / ezfezf...	test BF : 4,5...	10.411	11.053
Serie BF 4.5_0...	10/25/2016 3:21...	Serie BF 4.5	test	9.878	10.904
Serie BF 4.5_0...	10/25/2016 3:22...	Serie BF 4.5	test	10.023	10.762
Min				9.9	9.4
Avg				10.1	10.1
Max				10.8	12.0
Rsd (%)				2.820	9.653

The top of this window presents several buttons . (See chapter [Exporting data from data table](#) for more details).

It is possible to open the **processing** tool or the **comparison** tool but also to **reprocess** or **re-calibrate** analyzes without hindering the sequence on-going. If only one analysis is selected, the analysis report can be consulted as well as the analysis conditions (method, analyzer configuration and reference calibration).

To do this, simply select one (or several) analyze(s) at the same time in the table, right-click (or via the Action menu) and the following context menu will appear:



Analysis	Serie	Injection date	Pic0 (A)	Pic3 (A)	Type
		01/01/2015			
		12/14/2016			
8,4 @f_684	8,4 @f	10/18/2016 9:05 AM	10.688		Replace
Analyse 675	Analyse	8/28/2016 3:40 PM	9.869		Average
Analyse			9.977	0.000	Average
8,4 @f			10.794	0.000	Average
zfzeffze			10.832		Average
zfzeffze			10.730		Average
ezfezf			10.418		Average
ezfezf			10.411		Average
Serie BF			9.892		Average
Serie BF			10.037	0.000	Average

The different operations are:

- **Show the chromatogram**: Open the chromatogram with the integration parameters in another window (the shortcut is double click on the result line) (Available only if a single result is selected)
- **Process**: Loads the selected analysis into the processing part. (Available only if a single analysis is selected, see [Process](#))
- **Batch Processing**: Retrieves each selected analysis with a specified method. (See [Batch reprocessing](#)).
- **Calibration by reprocessing**: Calibrates all analyzes selected with a specified method. (See [Calibration by reprocessing](#))
- **Compare**: Opens the Analytics Comparison tool (see the [Comparisons](#) chapter).
- **Report**: Displays reports (Available only if a single result is selected, see [Report](#))
  - Analysis report: Displays the analysis report (Available only if a single scan is selected, see [Report](#))
  - Calibration report: Displays the calibration report (if a calibration has been done) (see chapter [Calibration report](#))
- **Analysis conditions**: Available only if a single analysis is selected; here are the different possible operations:
  - Displays the injection method parameters.
  - Displays the analyzer configuration during injection.
  - Displays the calibration reference (see chapter [Reference calibration](#)).

The table displays all the peaks existing in the method's components table, and detects the minimum, maximum, average values and the RSD value in % (Variation coefficient).

The minimum values are displayed in **green** and the maximum ones in **red**.



The analysis selected in this table will be indicated by a vertical bar in the trend chart (see chapter [Trends](#)) and will modify the information contained in the results table (see [Results of an analysis](#) chapter).

The table contains by default all the series of analyzes carried out, it is possible to perform filtering (see chapter [Filter data](#)).

See also:

- [Trends](#)
- [Results of an analysis](#)

**b) Results of an analysis**

The following table shows the results of the analysis selected in the analysis series table (see chapter [Series of analyses](#)).

The title of the table indicates the analysis name and the analytical method used.

etalon 1000ppm_002 - Méthode air					
	Peak name	TR (sec)	Area	Concentration	Normalized [c]
▲ A (4 items) ▶					
>	He	51.67 sec	10744 µV.s	0.0000 ppm	0.00 %
	H2	55.43 sec	17657 µV.s	0.0000 ppm	0.00 %
	O2	74.54 sec	342858 µV.s	20.6325 %	20.38 %
	N2	96.68 sec	1108252 µV.s	80.6197 %	79.62 %
▲ B (25 items) ▶					
	Pic6	22.28 sec	4673604 µV.s	0.0000 %	0.00 %
	CH4	25.89 sec	5876 µV.s	0.0000 ppm	0.00 %
		26.89 sec	0 µV.s	0.0000 %	0.00 %
		27.47 sec	0 µV.s	0.0000 %	0.00 %
		27.58 sec	0 µV.s	0.0000 %	0.00 %
	CO2	72.02 sec	808 µV.s	0.0000 ppm	0.00 %

The displayed values are:

- Peak name
- Retention time
- Area
- Raw Concentration
- Standardized Concentration
- Unit
- Name of Peak Group

The peak selected in this table will highlight the peak in the trend graph (see chapter [Trends](#)).

The top of this window presents several buttons . (See section [Exporting data from data table](#) for more details).

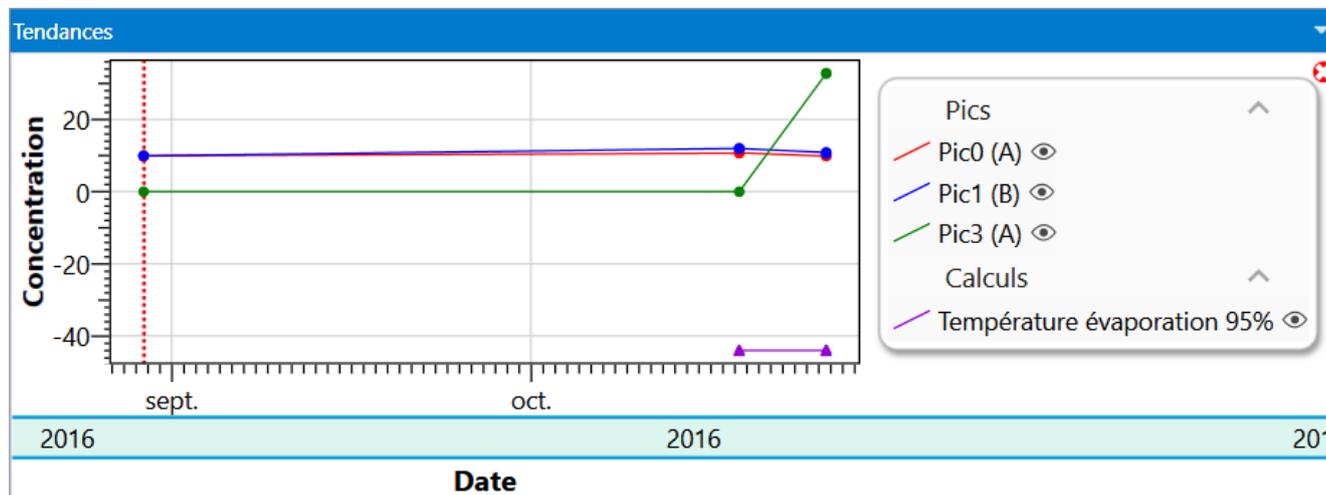
The table contains by default all the series of analyzes carried out, it is possible to perform filtering (see chapter [Filter data](#)).



**c) Trends**

**1. Description**

In normal operation, SOPRANE II allows simultaneous visualization of 4 windows related to the analyzes and allows to visualize the evolution of values or calculated values over a period.



These 4 windows allow the visualization of the chromatogram, the results, the current analysis sequence and the trends. These windows can be resized, minimized, or restored.

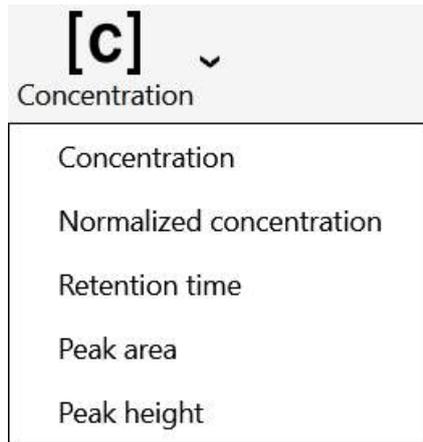
Peaks, calculations and analog inputs can be viewed independently of each other. Access to trend sheets is prohibited until the user has scheduled a minimum of data concerning the peaks identified in the analysis and the post-analytical calculations.

The identification of a peak is done by its name and the module. If the name of a peak is changed, it will no longer be recognized on the trend sheets. So, for example, I integrate a nitrogen peak whose name is N2 and I use the trend viewing of its concentration value.

I change the name of this peak from N2 to AZOTE in the constituent table. It is necessary for me to rewrite the demand for visualization in trend under this new name.

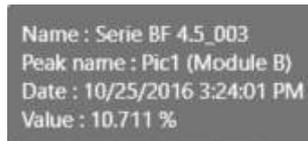
The horizontal axis represents the injection date of the analysis, the vertical axis corresponds to the value you have chosen to display. To change the value to display, select the Results menu, the following pop-up window will appear.





On the graph, a point represents an analysis value, the red vertical bar represents the location of the analysis selected in the analysis series table (see chapter [Series of analyses](#)). If you click on an analysis point, the analysis selected in the analysis series table will be changed.

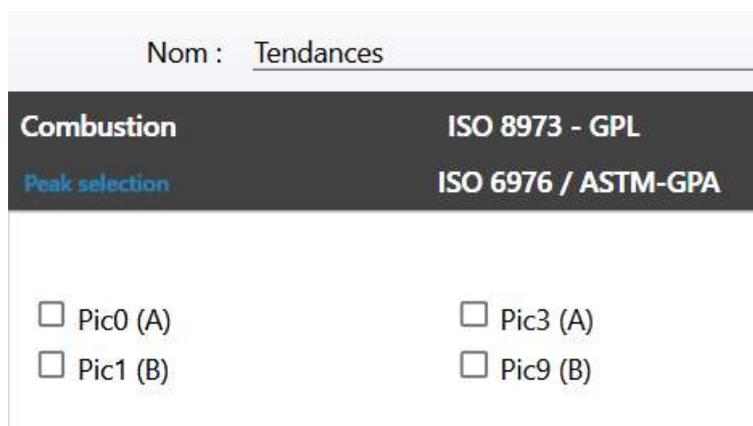
A tool-tip appears when the cursor is above a trend point.



## 2. Trends configuration

The "**Options / Trend Configuration**" menu allows to access to a property sheet used for trend programming. The "**Option / Add New Trend**" menu will open the same type of window.

### Peak Selection



Analog input selection

ISO 6976 / ASTM-GPA	Combustion	ISO 8973 - GPL
<b>Peak selection</b>	<b>Analog inputs</b>	
<input checked="" type="checkbox"/> AI 0	<input checked="" type="checkbox"/> AI 1	
<input checked="" type="checkbox"/> AI 2		

Calculations ISO 6976 + ASTM-GPA

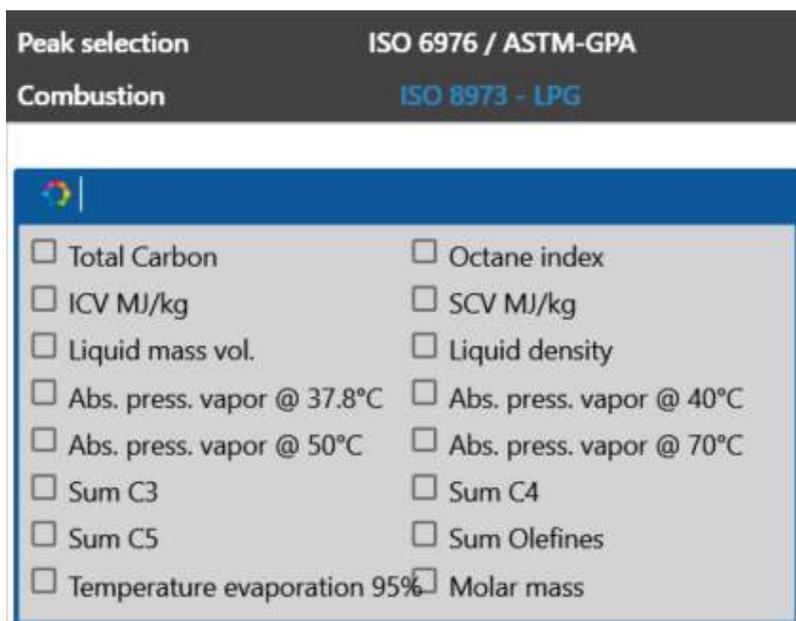
Combustion	ISO 8973 - LPG
<b>Peak selection</b>	<b>ISO 6976 / ASTM-GPA</b>
<input type="checkbox"/> Molar mass	<input type="checkbox"/> Ideal mass vol.
<input type="checkbox"/> Real mass vol.	<input type="checkbox"/> Ideal density
<input type="checkbox"/> Real density	<input type="checkbox"/> Ideal LHV
<input type="checkbox"/> Real LHV	<input type="checkbox"/> Ideal HHV
<input type="checkbox"/> Real HHV	<input type="checkbox"/> Wobbe index
<input type="checkbox"/> Ideal Wobbe index	<input type="checkbox"/> Fact. of compression

Combustion calculations

Peak selection	ISO 6976 / ASTM-GPA
<b>Combustion</b>	<b>ISO 8973 - LPG</b>
<input type="checkbox"/> Air stoichiometric	<input type="checkbox"/> Volume H2O
<input type="checkbox"/> Volume Nitrogen	<input type="checkbox"/> CO2 Max
<input type="checkbox"/> Volume CO2	<input type="checkbox"/> Wet smoking
<input type="checkbox"/> Dry smoking	<input type="checkbox"/> Index of comburty
<input type="checkbox"/> Combustive power	



ISO 8973 - LPG calculations

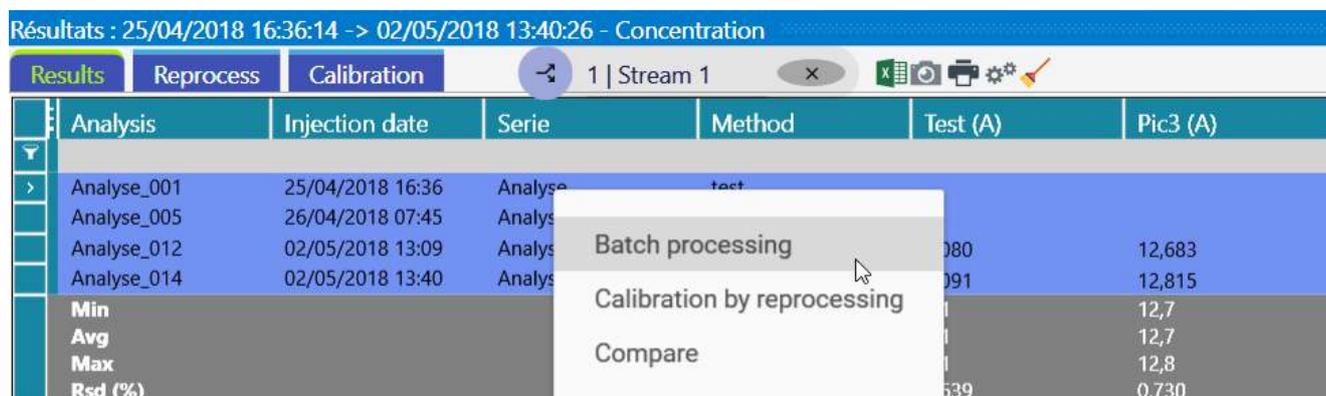


Note:

The option "Saving windows positions" in the menu does not mean that SOPRANE II will save the state defined when exiting the program. What is saved is the nature and position of the windows when requested. When SOPRANE II will be launched again, the windows will automatically be reopened and repositioned at the same place.

**d) Batch reprocessing**

Batch reprocessing consists in performing again integration calculations, identification and post-analysis calculations for several analyzes at a time. Once the operation has been completed, the reprocessing table will display the analyzes with the updated results values. The trend window is also updated.



The first step consists in selecting the analyzes to be reprocessed, then right click on the analyzes and click on **Reprocessing** (or with the menu **Results> Reprocessing**).

Once the reprocessing has been requested, a window will appear proposing you to select an integration method.

Once the method has been chosen, each of the analyzes will be integrated with the indicated method. The reprocessing table and the trend chart will be updated.

*Note:*

*If an analysis has been updated in the processing part (see the chapter [Process](#)), the results of the table are automatically updated; there will be no need to re-process to update the values.*

**e) Calibration by reprocessing**

Calibration by reprocessing consists in performing again integration calculations, identification, calibration and post-analysis calculations for several analyzes at a time. Once the operation has been completed, the calibration table will display the analyzes with the updated results values. The trend window is also updated.

Résultats : 25/04/2018 16:36:14 -> 02/05/2018 13:40:26 - Concentration

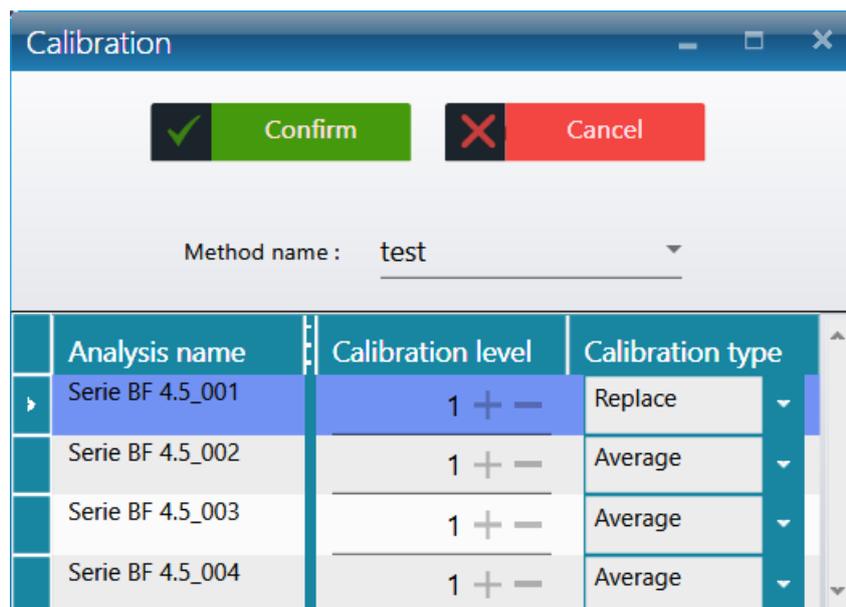
Analysis	Injection date	Serie	Method	Test (A)
Analyse_001	25/04/2018 16:36	Analyse	test	
Analyse_005	26/04		test	
Analyse_012	02/05		test	0,080
Analyse_014	02/05		test	0,091
Min				0,1
Avg				0,1
Max				0,1
Rsd (%)				8,639

Context menu options: Batch processing, Calibration by reprocessing, Compare

The first step consists in selecting the analyzes to calibrate, then right-click on the analyzes and click on **Calibration by reprocessing** (or with the menu **Action> Calibration by reprocessing**).

Once the calibration by reprocessing has been requested, the following window will appear, proposing you to select an integration method and for each of the selected analyzes, to choose the **calibration level** and the **type of calibration** to be performed.





The different types of calibration are:

**Blank:** The analysis is defined as a blank to be ignored. This allows to rinse and wait for stabilization after passing a new standard.

**Replace:** This analysis replaces everything known for this level and is therefore the first measure of a possible series that will be averaged.

**Average:** This analysis is used to average the known data for this level, so that each measure keeps the same importance.

**Weighted:** This analysis is used to average the known data for this level, so that each analysis counts as much as all previous ones.

Once validated, each of the analyzes will be calibrated with the requested parameters and the indicated method. The calibration table and the trend chart will be updated.

For more information on calibration, see the chapter [Calibration](#).

*NOTE:*

If an analysis has been updated in the processing part (see the chapter [Process](#)), the results of the table are automatically updated; there will be no need to repeat a calibration by reprocessing to update the values.

**f) Quick actions**

Quick actions are available either via the **Action** menu on the **Results** page, or by right-clicking on the results table.



Analysis	Serie	Injection date	Pic0 (A)	Pic3 (A)	Type
		01/01/2015			
		12/14/2016			
8,4 @f_684	8,4 @f	10/18/2016 9:05 AM	10.688		Replace
Analyse 576	Analyse	8/29/2016 3:40 PM	9.869		Average
Analyse			9.977	0.000	Average
8,4 @f			10.794	0.000	Average
zfzeffe			10.832		Average
zfzeffe			10.730		Average
ezfezf			10.418		Average
ezfezf			10.411		Average
Serie BF			9.892		Average
Serie BF			10.037	0.000	Average

The different operations are:

- **Show the chromatogram**: Open the chromatogram with the integration parameters in another window (the shortcut is double click on the result line) (Available only if a single result is selected)
- **Process**: Loads the selected analysis into the processing part. (Available only if a single analysis is selected, see [Process](#))
- **Batch Processing**: Retrieves each selected analysis with a specified method. (See [Batch reprocessing](#)).
- **Calibration by reprocessing**: Calibrates all analyzes selected with a specified method. (See [Calibration by reprocessing](#))
- **Compare**: Opens the Analytics Comparison tool (see the [Comparisons](#) chapter).
- **Report**: Displays reports (Available only if a single result is selected, see [Report](#))
  - Analysis report: Displays the analysis report (Available only if a single scan is selected, see [Report](#))
  - Calibration report: Displays the calibration report (if a calibration has been done) (see chapter [Calibration report](#))
- **Analysis conditions**: Available only if a single analysis is selected; here are the different possible operations:
  - Displays the injection method parameters.
  - Displays the analyzer configuration during injection.
  - Displays the calibration reference (see chapter [Reference calibration](#)).



## 4.5. Process

The integration of a chromatogram is performed in the Process module, accessible via the "Process" tab.

See sections:

### [Integration management](#)

#### [Principle of integration](#)

##### [Events affecting the integration](#)

###### [Peak detection](#)

###### [Negative peak detection](#)

###### [Absolute peak width](#)

###### [Absolute sensitivity threshold](#)

###### [Relative peak width](#)

###### [Relative sensitivity threshold](#)

###### [Force integration](#)

##### [Events affecting the baseline](#)

###### [Baseline detection](#)

###### [Forcing of baseline at next valley](#)

###### [Forcing of baseline at all valleys](#)

###### [Baseline split](#)

###### [Baseline penetration](#)

###### [Shoulder peak detection](#)

###### [Peak group](#)

##### [Rejection events](#)

###### [Minimum area rejection](#)

###### [Maximum area rejection](#)

###### [Minimum height rejection](#)

###### [Maximum height rejection](#)

### [Identification management](#)

#### [Peaks references](#)

#### [Forcing](#)

#### [General case](#)

#### [Optimization of the process](#)

### [Calibration](#)

#### [The principle of the calibration](#)

#### [Response curves](#)

#### [Calibration rejection](#)

### 4.5.1. Principles

#### ***a) Integration***

It is important to well understand how the integrator works and what effects may be caused by using the wrong parameters or integration events.



During the analysis, the signal is sampled at a sufficient rate to keep a good accuracy. The frequency (20, 50 or 100 Hz) at which this sampling is performed is indicated in the analysis method. All the values are stored in a database for real-time display, integration or further reprocessing.

The integration is performed in several steps:

- First, the signal is examined to detect all points where "something" occurs. It is the beginning of a peak, it is the top, it is the end. At this moment, a table is memorized with all the data concerning the detected peaks.
- Second, these detected peaks are inspected in detail according to the will of the user. Does any beginning or end of a detected peak correspond to a baseline or a valley? Is it necessary to group the peak with the preceding one or the next one? Where is it pertinent to place the baseline? Is it necessary to reject the peak ?, ...
- Third, all the calculations used to determine the area, the height, the beginning time, the beginning value, the retention time, ... are performed and the results are stored in a table of integrated peaks.

Another process is then activated to identify the peaks and to determine concentrations or response factors.

The peaks detection is the most important part of the integration process. If you don't detect the peaks, it is useless to try to correct their area. If you detect peaks where there is only background noise the problem is similar: you won't be able to ensure that the concentration value obtained is due to a compound. Thus, during the peaks detection it is necessary to use correct detection parameters.

## 1. Peak detection

The peaks detection uses a mathematical algorithm based on the calculation of the first and second derivatives of the signal.

Because it is not necessary to have the same precision as during the acquisition, and mainly to eliminate the noise, the values obtained during the acquisition (slices of 1/20th, 1/50th or 1/100th of second) are grouped in wider slices. The calculations of the mathematical function are made from these wider slices and they need a more or less important number of these slices.

Each time the user set ON the peak detection (Programming of the event PD, [Peak Detection](#)), or modify the peak width (Programming of the event SAP, Set [Absolute Peak width](#), or the event SRP, Set [Relative Peak width](#)), or modify the slope sensitivity (Programming of the event SAS, Set [Absolute Sensitivity](#), or the event SRS, Set [Relative Sensitivity](#)) the system determines the width of the wide slices and the number of these slices to use during next calculations.

The algorithm is optimized when the system has enough values to see variations of the curve without spending time to make useless calculations.

The main parameter is the peak width and a "correct" value is the width expressed in seconds and measured at mid-height.

It is easy to determine this peak width: the mouse coordinates can be viewed in the lower left corner of the window. These coordinates are directly expressed in microvolts and seconds.

Two remarks:

- The peak is supposed to be a Gauss curve. In most cases, the peak is asymmetric. If the peak is very asymmetrical, the peak width parameter should be reduced. This parameter can also be the time value between the start and the top of the peak.



- The value retained may be several times larger or smaller than the actual value. The integration process is flexible enough to lead to a correct result from an approximate parameter.

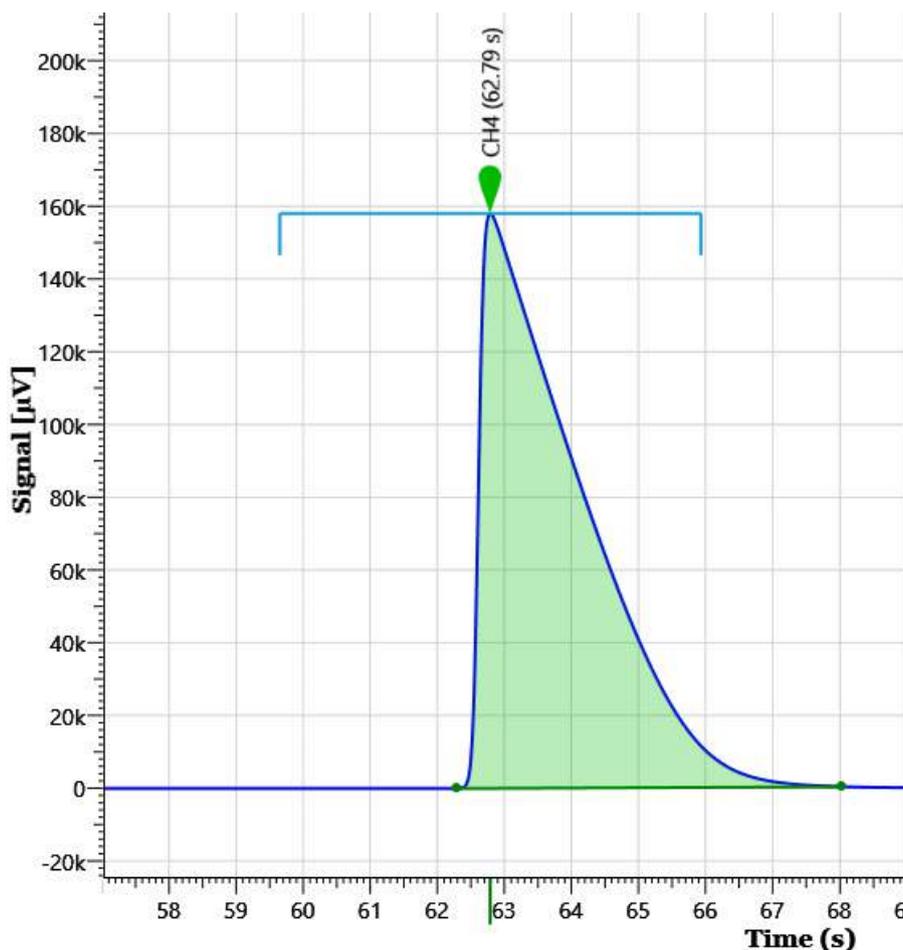
The threshold value or slope sensitivity must correspond to the reality. If this value is too high, peaks are not detected or baseline correction is not satisfactory. If it is too low, the noise is integrated. It is possible to determine an approximate value from the curve using the mouse and the coordinates of 2 points. The correct value is close to the ratio of signal difference to time difference. Here too, the integration process is able to adapt.

If the concentration of a component may vary, it is preferable to try several values from several chromatograms before imposing a value. In this way, and since retention times can fluctuate when concentrations vary, these tests will be useful in determining the times at which events should be scheduled.

## 2. Integration carried out with wrong parameters

On the chromatogram below, we want to integrate the peak CH4. This is very asymmetric peak, it is 1.5-second-wide at middle height but only 0.3 second from the beginning to the top.

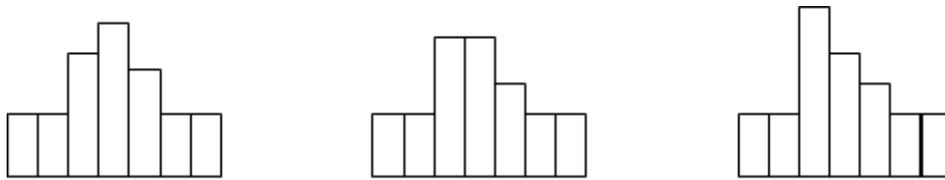
Thus, to detect correctly, with the best accuracy, the first part of the curve, the value of peak width to be programmed for the "[peak width](#)" parameters would be 0.3 seconds. If the peak was symmetric, this value would be 1.5 second.



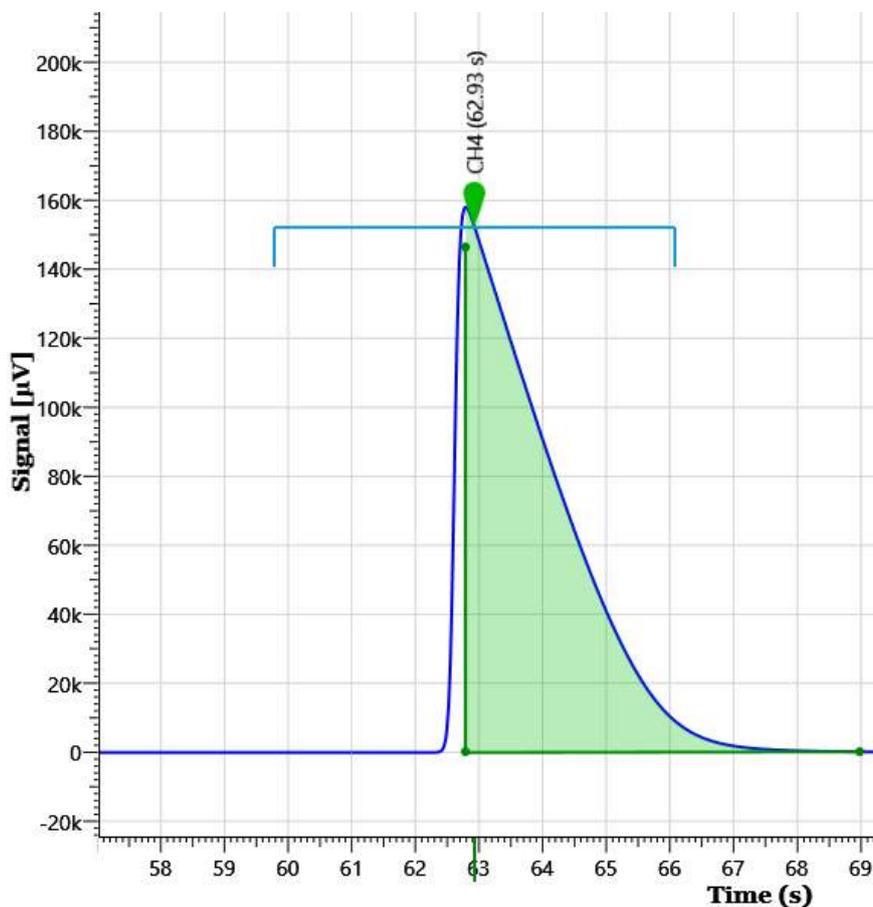
Suppose we program a far bigger value, for instance 4 seconds. We want to detect the peaks, thus, second mistake, we program the lowest possible value for the slope sensitivity, 0,001 µV/s.



With these values the integration process uses only 3 or 4 values to represent the peak. The system is very sensitive but, due to the fluctuations of the retention time, the peak may be represented like one of the following pictures:



In most cases, SOPRANE II will be able to detect correctly the beginning, the top and the end of the peak, but sometimes the process considers the top as a baseline and divides the peak in two unresolved peaks with the same retention time.



The first thing to do when we encounter this unexpected kind of integration is to verify the parameters values and more specifically the peak width and the slope sensitivity.

We will use now an "acceptable" value of 1.5 second as "[Absolute peak width](#)" parameter. Due to the asymmetry, the best value would be 0.3 seconds for the first part of the peak (from the beginning to the top) and 2 seconds for the second part (from the top to the end). One second seems to be a good compromise because with this value we are sure to see 2 points during the first part of the peak: after grouping, the width of the slices is about 1/10th of the value programmed as peak width.



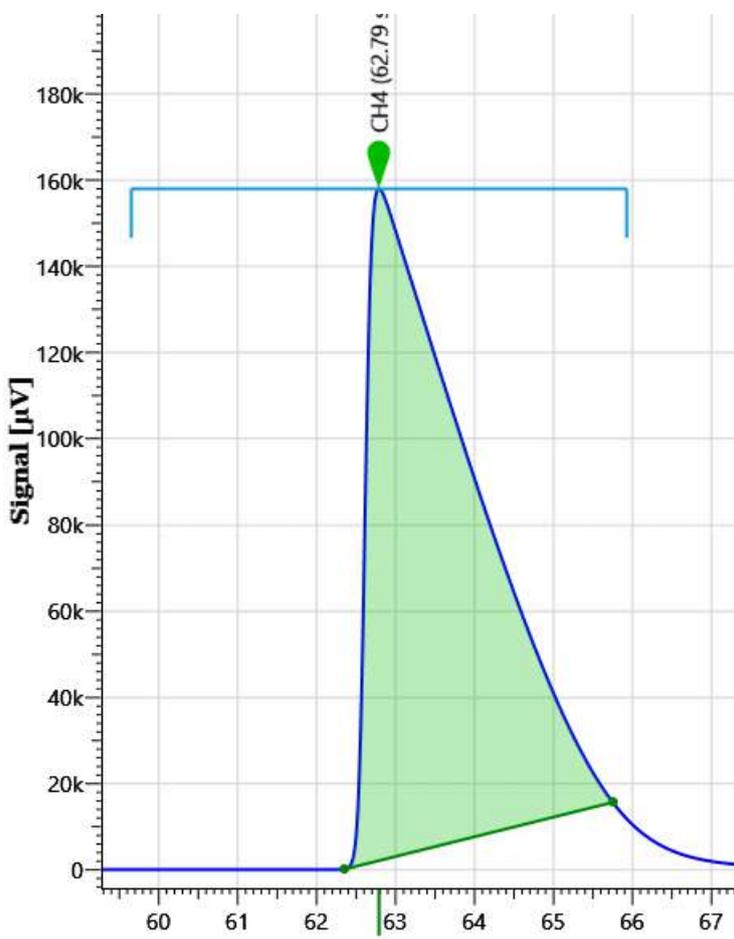
Two points is the minimum to ensure SOPRANE II will always find an increasing signal during the first part of the peak.

If the slope sensitivity is the lowest possible value, it is quite impossible to find the baseline. Any variation of the signal is a peak.

The chromatogram there after has been integrated with these values.

As soon as the integration is authorized ([Peak detection](#) parameter ON) the system detects a peak and it is never able to go back to the baseline.

If we do the opposite and use a too high value for [slope sensitivity](#), for instance 100  $\mu\text{V/S}$ , the peak is correctly detected but SOPRANE II considers to be back in the baseline state before the effective end of the peak. The fact that the peaks are correctly detected is the consequence of the asymmetry which leads to a very high slope when the peak begins. With a peak more symmetric a similar defect would have been observed at the beginning of the peak.



If the analyzer works with several streams and a wide range of concentrations, we will have to adjust the slope sensitivity parameter to have a good detection of the peaks in all cases.

Different values of concentrations and of concentrations ratios give different results and we must ensure a good integration in all cases.



To obtain a good integration, it is necessary to change the values of peak width and sensitivity threshold during the analysis. This is achieved by scheduling events.

Some events deal with peaks detection, others include baseline correction mode, and the latter are used to reject peaks.

See chapters:

[Events affecting the integration](#)

[Peak detection](#)

[Negative peak detection](#)

[Absolute peak width](#)

[Absolute sensitivity threshold](#)

[Relative peak width](#)

[Relative sensitivity threshold](#)

[Force integration](#)

[Events affecting the baseline](#)

[Baseline detection](#)

[Forcing of baseline at next valley](#)

[Forcing of baseline at all valleys](#)

[Baseline split](#)

[Baseline penetration](#)

[Shoulder peak detection](#)

[Peak group](#)

[Rejection events](#)

[Minimum area rejection](#)

[Maximum area rejection](#)

[Minimum height rejection](#)

[Maximum height rejection](#)

**a) 1. Events affecting the integration**

See chapters:

[Peak detection](#)

[Negative peak detection](#)

[Absolute peak width](#)

[Absolute sensitivity threshold](#)

[Relative peak width](#)

[Relative sensitivity threshold](#)

[Force integration](#)

**Peak detection**

Because it is not necessary to integrate all the peaks from the beginning of the injection until the end of the analysis and because spurious peaks can be the consequence, for example, of the switching of a valve, an event allows to disable the integration.

By default, integration is active.

Be careful, the software considers to be at the baseline when integration becomes allowed or when it becomes prohibited, and the part of the peak that would be before or after would simply be ignored.



### **Negative peak detection**

Sometimes a peak is negative, and in this case the working logic must be reversed. The Negative Peak Detection event fulfills this role.

By default, the event is disabled and the software expects positive peaks.

Be careful, this event is complementary to the event allowing integration. To avoid unwanted interpretations, if the signal is not in the "baseline" state when reversing the working logic, it is often preferable to prohibit the integration (which forces recognition of the Baseline), to reverse the logic, and then to re-enable the integration.

### **Absolute peak width**

This event allows the grouping of points into slices used for the integration calculations. The value, expressed in seconds, is the width at mid-height or the time interval between the start and the top of the peak.

By default, the software uses a value of 0.5 seconds.

### **Absolute slope sensitivity**

This event corresponds to the slope expressed in  $\mu\text{V/s}$  and allows to fix the detection threshold of the significant elements (start or end of peak, top or valley, shoulder).

By default, the software uses a value of 5  $\mu\text{V/S}$ .

### **Relative peak width**

The peaks width increases as the retention time increases. The interest is rather limited, but instead of managing several events, we can seek to refine a first event and then consider that at a given time we will double its value, that at another time we will multiply again by two, ...

The Peak width relative value event allows, when programmed as active, to double the peak width value. It allows, when programmed as inactive, to divide by two the peak width value.

### **Relative slope sensitivity**

Similarly, if the peaks width increases, the slope varies too.

The Relative sensitivity threshold value event, when programmed as active, to double the absolute slope value. It allows, when programmed as inactive, to divide by two the absolute slope value.

### **Force integration**

In many cases, an analysis of an isolated sample will not only be performed.

Very often, the analyzer will operate continuously to monitor changes in the concentrations of one or more streams.

The parameters values will then be defined To allow the integration of mixtures which can be very different, with retention times that will fluctuate, with peaks that will be well separated, with peak asymmetry ratios which can evolve.

Some cases, such as strongly asymmetric peaks and low concentrations, can show the limits of integration: the number of points is not sufficient to characterize something.



One way out is to force integration. The mechanisms described above remain active, but since the software knows that there is a very high probability that a peak will be present, it is much more tolerant and concludes that a peak occurs when it sees level variations.

The Force integration event allows to delimit a time window where integration is facilitated.

A peak being integrated is stopped when entering in such a window. Likewise, the end of a possible peak being processed is imposed when emerging from the window.

Warning: if the peak width already allows a relatively easy integration, the use of the Force integration event makes it possible to detect the smallest variations like as many peaks badly separated. When using the **Force integration** event, it may be necessary to increase the peak width value to limit this phenomenon.

## a) 2. Events affecting the baseline

[Baseline detection](#)

[Forcing of baseline at next valley](#)

[Forcing of baseline at all valleys](#)

[Baseline split](#)

[Baseline penetration](#)

[Shoulder peak detection](#)

[Peak group](#)

### **Baseline detection**

This event has 2 states ON and OFF.

The use of this event allows to prohibit the return recognition to baseline at the end of a peak integration. The event is ON by default, which means that the integrator searches for, and may find, a return to the baseline at the end of a peak or a group of peaks.

From the moment it is used (it then becomes OFF), and until one re-uses it (go back to ON), all the peaks are considered as belonging to one single and only one single group of peaks.

The return to baseline will thus occur only after the second use of the parameter.

If the end of the analysis occurs before the effective return to baseline, possibly because the event is used only one time, the last "low point" of the chromatogram is assumed to be a return to baseline.

The event is active by default.

### **Forcing of baseline at next valley**

This two states event is OFF by default.

Use of this event forces the software to consider the first next valley point as being a return to baseline. This recognition of baseline inhibits the process, without the need to program an OFF state for the event

### **Forcing of baseline at all valleys**

This two states event is OFF by default.

Use of this event forces the software to consider all next valley points as being returns to baseline. This baseline recognition at each valley goes on until the end of the analysis or the programming of an OFF value for this event



### **Baseline split**

This two states event is OFF by default. It allows to force the software to trace a baseline common for all the peaks.

### **Baseline penetration**

Normally the baseline is tangential to an isolated peak or a group of peaks and the peak or the group is located integrally on only one side of the baseline.

A peak located in the time window where the Baseline penetration event is active can have its start and its end on both sides of the baseline.

Be careful, in such a case, the part below the baseline is removed from the part above.  
The event is inactive by default.

### **Shoulder peak detection**

A peak can also be pressed to another. This is called a peak on the shoulder.

The slope can grow, for example, then continue to grow more slowly or even be canceled and then grow again to reach a top. There is neither decrease nor valley to separate the two peaks, just an inflection point.

A similar phenomenon can also occur on the decreasing slope of a peak.

The Shoulder peak detection event detects this phenomenon within the time window where it is active.

The event is inactive by default.

### **Peak grouping**

This event allows to define a time window where all the peaks, isolated or not, will be grouped in a single peak for the calculation of the response coefficients or the calculation of the concentration.

The area of the group of peaks will be equal to the sum of the individual surfaces. The height of the group of peaks will be equal to the sum of the individual heights. The retention time of the peak grouping will be equal to the half-sum window start time plus window end time or end of analysis. These values will be arbitrarily assigned to the peak the closest to the retention time thus determined. To ensure the identification, it will be enough to take the time middle and a window covering the whole zone. A peak detected at the beginning, the middle or the end of the window will be recognized.

The event is inactive by default.

## **a) 3. Rejection events**

Despite all precautions, peaks could be detected where there is only background noise or a parasite. It may be interesting to ignore peaks that do not meet one of the following criteria.

See the following chapters:

[Minimum area rejection](#)

[Maximum area rejection](#)

[Minimum height rejection](#)

[Maximum height rejection](#)

### **Minimum area rejection**

A peak is rejected if its surface is less than the value that this event has at the time found as retention time.  
The default value is 0.

### **Maximum area rejection**

A peak is rejected if its surface is greater than the value that this event has at the time found as retention



time.

The default value is 10 power 100.

#### **Minimum height rejection**

A peak is rejected if its height is lower than the value that this event has at the time found as retention time. The default value is 0.

#### **Maximum height rejection**

A peak is rejected if its height is greater than the value that this event has at the time found as retention time.

The default value is 10 power 100.

### **b) Identification**

Identification is the process by which a peak corresponds to a constituent.

Identification is based on the retention time and an identification window.

The identification window is defined with a time interval situated on either side of the retention time and consisting of a constant part (fixed window) and a part proportional to the retention time (Variable window or relative window).

Assume an expected peak at the retention time of 50 seconds with a fixed window of 2 seconds and a variable window of 10%.

The time interval will be equal to 2 seconds plus 10% of 50 seconds thus a total of 7 seconds and any peak whose actual retention time is between 43 seconds and 57 seconds could be identified as the expected peak.

The problem of identification is the choice of the peak when several possible candidates are inside the identification window.

The software allows a maximum of 10 peaks inside an identification window.

It also considers the order in which the peaks are expected. Assume an already identified peak A and the searching of a peak B in a window containing several peaks including peak A. If the expected retention time of peak B is lower (higher) than the one of peak A, the searching inside the window will be limited to peaks whose real retention time is lower (higher) than the one of peak A.

#### **b) 1. Peaks references**

Identification can be more hampered because retention times fluctuate, forcing users to choose wider identification windows.

This is true, but often the retention times fluctuate in the same way for all the peaks and the analysis includes one or more peak(s) easy to identify because they are properly isolated.

This is also true in the case of columns requiring regular regeneration. In this case, the identification windows are enlarged to compensate the gradual drift of the values.

It is convenient to use a wide window to identify an isolated peak (we can also force the identification of this peak, as we will see later), to define this peak as a reference peak (it is assigned a letter from A to Z to represent it), then to say that some other peaks use this reference peak (remember the identifier A to Z). In this case, the software considers that the retention times shift in the same way and the referenced peak will be searched in a window centered on a time equal to the expected retention time for this peak, divided by the expected retention time for the reference peak and multiplied by the retention time found for the reference peak. This allows to use narrower searching windows, thus to reduce the number of peaks likely to be in a searching window.



Although this does not add much, a peak can use as a reference a peak that uses itself a reference peak that uses itself... and so on.

In case several references are used, the identification process assumes that the same peak could not be found in the searching window of several reference peaks (reference peaks sufficiently distinct from each other) and the attribution of peaks is done in the processing order without handling this type of error.

The identification program indicates an error in case of looping leading to an impossibility of processing, of the type peak x serves as reference for the peak y which serves as reference for the peak x. The error is reported but it does not lead to blockage and the peaks concerned are identified as normal peaks.

If a peak is defined as a reference but is not used as such, it will simply be identified as a priority according to the peaks reference identification process, without leading to an error.

Similarly, if a peak uses an undefined reference, the reference will be ignored without the error being reported.

## **b) 2. Forcing**

When several peaks are present in a searching window, the software calculates a note considering the importance of the peak (peak majority) and its position in the window (peak the closest to the center) and then takes the peak whose sum of the 2 notes is the highest.

Identification forcing consists of ignoring one of the two processes.

The field of the constituents table used to define the forcing is set at the value 0 in the absence of forcing (default value), the value 1 to force the largest peak or 2 if we want to force the peak the closest to the center.

### 1. The most important peak

When the peaks are sufficiently separated, one can hope to have only one peak per window and consider that the other peaks are only traces or noise. It seems logical to say that the main peak is the product to be identified.

This can lead to errors when working with peak height. An interfering peak may have a significant height, taller than that of the analyzed product, while having a very low surface area.

If the peaks are insufficiently isolated and the retention times tend to fluctuate, the identification windows of two neighboring components may overlap and a single window may have peaks similar in heights or surfaces.

The field of the constituents table allowing to define the forcing has the value 1 if one wants to force the most important peak.

### 2. The closest to center

This other way of proceeding consists in considering that the retention time of the constituents is precisely known and that the peak the closest to the center of the window (and therefore to the time at which it is expected) is the best candidate.

This seems logical but does not consider that the retention time of a product is modified by the constituents concentration having a close retention time: a high concentration product tends to repel a lower concentration product.

The field of the constituents table allowing to define the forcing has the value 2 if one wants to force the



peak the closest to the center.

### **b) 3. General case**

Synthesizing these two conceptions means that they both exist and that it is better to use them both. When several peaks are present in a window, we determine for each of them a note function of their size and a note function of their deviation from the center of the window then the sum of these two notes is used to choose the peak to identify.

The size-related score is obtained by looking for the main peak and by dividing the height or area of each peak by the height or area of the major peak. The scores obtained are therefore between 0 and 1. The note linked to the position relative to the center of the window is obtained by dividing the shortest distance between the middle of the window and a top by the actual distance between the middle of the window and the top of each peak. Here again, a score between 0 and 1 is obtained.

The peak with the highest sum will be the major peak located near the center of the window.

### **b) 4. Optimization of the process**

Identifications of reference peaks and forcing peaks occur by increasing times.

The identification program starts by identifying the reference peaks, managing a possible reference level (reference peak that uses a reference peak, which uses...). Reference peaks can be identified with or without forcing.

The forcing peaks not defined as reference peaks are then identified.

The remaining peaks are then identified globally. After setting the note for each peak in each window, the program calculates all possible combinations according to the peaks order, including this of the peaks already identified.

The program then retains the combination with the highest score (sum of individual scores).

### ***c) Calibration***

SOPRANE II offers several calibration possibilities:

- Manual calibration
- Calibration by reprocessing
- Automatic calibration
- Calibration via the Launch menu

The Calibration menu is present only if one or several streams has or have been defined.

The "Configuration" program allows you to define the total number of streams as well as the number of calibration streams. If no calibration stream has been indicated, the menu does not exist.

#### **1. Manual calibration**

Manual calibration consists in directly modifying the response coefficients of the method by the processing module. It is therefore sufficient to start the processing interface, to load an analysis carried out on the



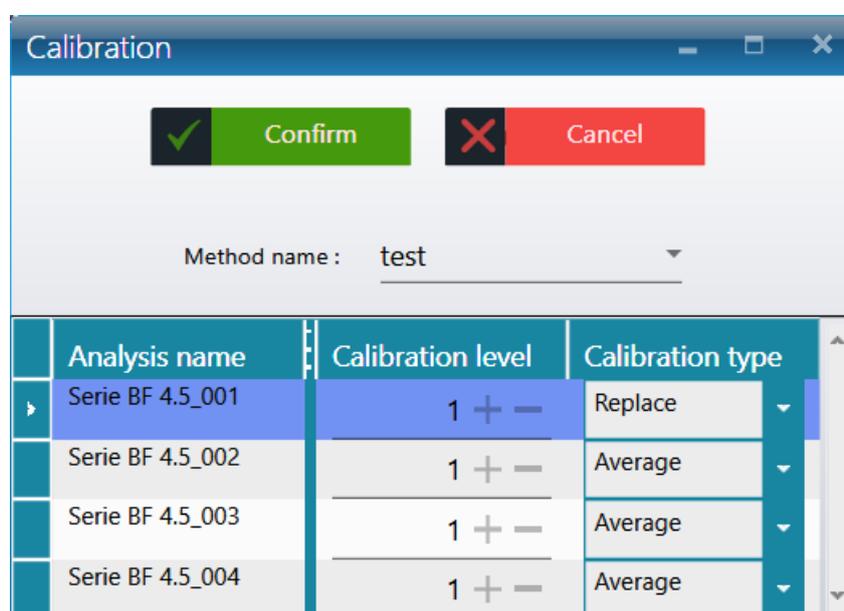
standard gas and to load the method associated with this analysis, to select the analytical module, to select the display in the Calibration mode (see chapter [Calibration table](#)), to select the component and to directly inform the value of the surface. You can retrieve the value of this surface in the Results Table view (see chapter [Results table](#)).

## 2. Calibration by reprocessing

You can perform a calibration by reprocessing when you have completed a series of analyzes and verified that they have been correctly integrated and identified (for example, tests carried out in the case of an audit).

Calibration by reprocessing is available in SOPRANE II via the main **Analysis** tab "**Calibration / Calibration by reprocessing**" menu (see chapter [Calibration by reprocessing](#)).

First, you must select the method to be calibrated and then select the analysis that will be used for this reprocessing.



When these analyses are selected, right click the select "**Calibration by reprocessing**". For each analysis, the software asks you what type of action you want to achieve and on what level.

There are 4 types of action for the calibration:

- **Replace:** the response coefficients stored in the method are replaced by the coefficients calculated during this analysis.
- **Average:** the software calculates an average between the response coefficients stored in the method and those obtained during this analysis. The result of this average is then stored in the method. (Arithmetic average).
- **Weighted:** the software calculates an average between the response coefficients stored in the method and those obtained during this analysis by weighing more or less the old coefficients. The result of this average is then stored in the method. (Geometric average).
- **Blank:** no modification of the response coefficients is done. This type of analysis is used to purge the lines or to perform the calibration checks without modifying the method.



To start the calibration by reprocessing, just click on the **Confirm** button.

You can then view the calibration report if you select a single analysis, right click and select "**Report > Calibration report**" menu.

The method is saved automatically.

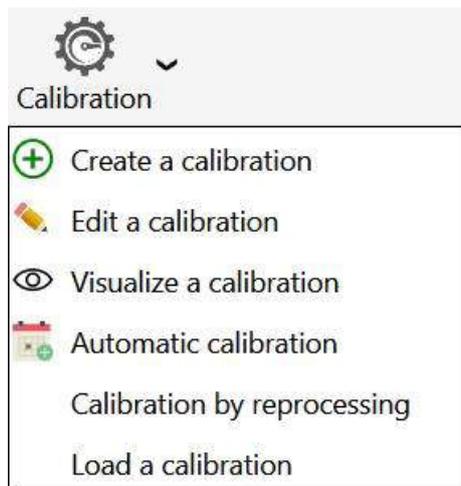
As far as it is possible and to verify the results before modifying the method, we recommend this method.

### 3. Automatic calibration

We have indicated chapter [Analysis sequences management](#) how to define an analysis sequence. In the same way, it is possible to define a calibration sequence (see chapter [Calibration sequence management](#)). This option is available only if a calibration stream is defined in SOPRANE II Setup, this type of calibration is mainly used when the instrument is equipped with a stream selector.

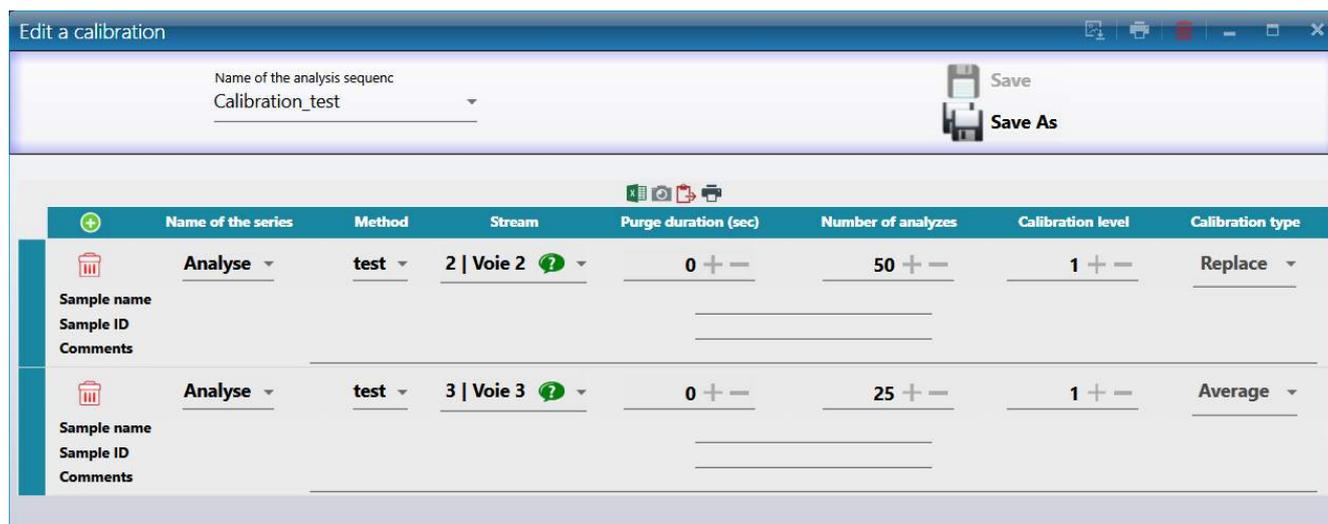
The calibration can be automatically triggered, and its programming has priority on the course of the analyses sequence.

The drop-down menu "**Calibration**" is used to define the calibration sequence in the same way we have define the analyses sequence.

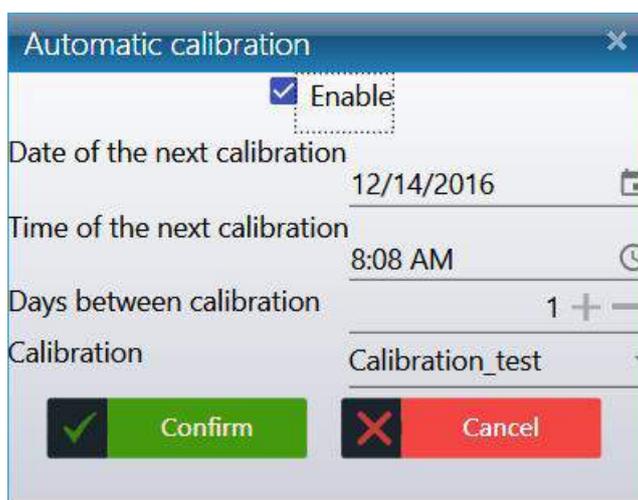


Compared with the analyses sequence table, two columns are added. The first one, type, is used to define which type of calibration will be used for the new calibration. The second one is the level of calibration, necessary when several points are used to define a response curve.





The action types have been defined in the previous paragraph. The drop-down menu "Calibration" can also define an "Automatic calibration" used to define a request for an automatic calibration and, in this case, the frequency of the calibrations.



If it is requested for an automatic calibration, it is necessary to define the date and time for the first automatic calibration, and then the number of days (0-999) before any next automatic calibration. The value 0 day between 2 calibrations is used to do one and only one automatic calibration: the others are prohibited.

**CAUTION:** The calibration is launched only when this analyzer is running, in automatic mode.

#### 4. Calibration via the Launch menu

When you have defined a calibration sequence, you can launch this sequence directly from the "Analysis / Start" menu. This solution is interesting especially if the standard selection is not automatic and thus manual. (see chapter [Start a calibration](#))



## 5. Calibration levels

Frequently the standard cylinders used do not contain all the components and, in this case, it is necessary to have several cylinders to calibrate all the method compounds.

If all the standard concentrations of these different cylinders are mentioned as level 1, most probably you will encounter calibration problems. Indeed, if in a cylinder one of the compounds is not present and that for some reason, there is an artifact or baseline shift leading to a peak detection at this compound expected time, this peak area will replace this compound standard area which will make the calibration wrong. To solve this problem, the software offers the possibility to use several calibration levels. So, for a cylinder, a calibration level will have to be used and for another cylinder, a second level will have to be used. The level selection will be done via the option “used” which will have to be checked depending on the level mentioned.

### Generally: 1 Level = 1 cylinder

Calibrations history could be visualized (see chapter [Calibrations history](#)).

#### c) 1. The principle of the calibration

Chromatography is an analysis method which proceeds by comparison: a known quantity of a product is analyzed and the area or height of the corresponding peak is measured. When an unknown quantity of the same product is analyzed, the inverse operation is carried out: the peak area or height is measured and the quantity is deduced therefrom.

The main question is therefore to know how the detector behaves when a constituent goes through it.

The TCD (Thermal Conductivity Detector), or  $\mu$ TCD in the case of  $\mu$ GC, offers the advantage of being a very linear detector over a wide concentration range.

The FID (Flame Ionization Detector) remains a detector whose response is linear but over a more restricted concentration range.

In many cases, the detector response can be assimilated to a straight line passing through the origin. It will sometimes be necessary to consider that the answer is a straight line that does not pass through the origin or that it is a curve.

It will always be preferable to use one or more standards whose concentration(s) are close to the quantity that we want to analyze.

#### c) 2. Response curves

One or several standards are required to calibrate an analyzer and a given standard may not contain all the components analyzed on an apparatus.

SOPRANE II proposes "calibration levels" and a calculation method will have to define all the usable levels, specifying for each constituent whether it is present or not at a given level, and if so, in which amount.

For a given constituent, a calibration sequence will have to use a minimum number of levels used, function of the equation desired for the response curve.

One point is required to define a straight line passing through the origin, 2 points to define any straight line, and so on.



Several points superior to the minimum will allow an improvement of the response with the searching of the optimal curve according to a process to be defined.

The response curve equation given by SOPRANE II always represents the peak area or height expressed as a function of the concentration.

Straight line passing through the origin:

There is only one unknown and only one standard level is required.

Straight line not passing through the origin:

There are 2 unknowns and two levels are necessary.

Straight line not passing through the origin but with a straight line passing through the origin for the concentration values lower than the lowest concentration used during the calibration:

There are 2 unknowns and two levels are required.

Quadratic (curve of degree 2):

There are 3 unknowns and three levels are required.

Cubic (curve of degree 3):

There are 4 unknowns and four levels are required.

Curve of degree 4:

There are 5 unknowns and five levels are required.

Exponential:

There are 2 unknowns and two levels are necessary.

Logarithmic:

There are 2 unknowns and two levels are necessary.

Optimization of the response:

If, for a given constituent, we use a number of levels greater than the minimum number required, SOPRANE II will use all the points and will define the optimal response by applying the least squares method.

The user has the choice to define the variable to be used for this optimization.

The correction is defined by:

- Equal: the importance of the points is the same,
- Quantity: the importance of the points is proportional to the quantity of product,
- Inverted quantity: the importance of the points is inversely proportional to the quantity of product,
- Quantity square: the importance of the points is proportional to the square of the quantity of product,
- Inverted square quantity: the importance of the points is inversely proportional to the square of the quantity of product,
- Logarithm of quantity: the importance of the points is proportional to the logarithm of the quantity of product,
- Logarithm of the inverted quantity: the importance of the points is inversely proportional to the logarithm of the quantity of product,
- Logarithm of the squared quantity: the importance of the points is proportional to the square of the logarithm of the quantity of product,
- Logarithm of the inverted squared quantity: the importance of the points is inversely proportional to the



square of the logarithm of the quantity of product.

### c) 3. Calibration rejection

The calibration of an analyzer can have serious consequences, especially if it is calibration performed automatically. SOPRANE II therefore provides the possibility to validate a minimum of things and, possibly, to reject the calibration of one or more constituents.

Generally, a calibration sequence uses several measurements carried out on one or several standards. For each analysis of each standard (SOPRANE II proposes calibration levels, used or not for a given constituent, to define the standards), it is possible to specify how the result of the measurement should be used.

Each measure can be described as:

- **Blank:** The analysis is defined as a blank to be ignored. This allows to rinse and wait for stabilization after passing through a new standard.
- **Replace:** This analysis replaces everything known for this level and is therefore the first measure of a possible series that will be averaged.
- **Average:** This analysis is used to average the known data for this level, so that each measure keeps the same importance.
- **Weighted:** This analysis is used to average the known data for this level, so that each analysis counts as much as all previous ones.

When performing an automatic calibration (initiating a calibration sequence) or a calibration by reprocessing several stored analyzes, we fix a process which will allow to calculate response equations only when the last analysis of the last level will be treated. It is only at this stage that SOPRANE II will consider verifying, constituent by constituent, the calibration validity according to the maximum deviation provided by the user for this constituent.

4 cases are possible:

- The maximum permissible variation is 0%. A zero deviation has no meaning, but this 0% deviation value indicates that no validation of the results is required. This value is to be used when the method has never been calibrated or when it is known that the previous calibration can not be a reliable reference.
- The maximum permissible variation is x% and the difference between the calibration result and the data stored during the previous calibration is below x%. The calibration of this component is validated. The previous data is lost and replaced by the calibration data that has just been performed.
- The maximum permissible variation is x%, the difference between the calibration result and the data stored during the previous calibration is greater than x% and the standard amounts present at the levels for which this "defect" is observed are not the same as during the previous calibration (amount variation greater than 1%). There is no evidence of a lack of reproducibility, but the question can be asked. SOPRANE II accepts this component calibration but reports the problem so that the user can re-calibrate if necessary.
- The maximum permissible variation is x%, the difference between the calibration result and the data stored during the previous calibration is greater than x% and the standard amounts present at the levels for which this "defect" is observed are the same as during the previous calibration. The variation in response is abnormal and SOPRANE II rejects the calibration. Rejection is reported and SOPRANE II keeps on working with the previous calibration values.

Another validity check is then carried out to confirm that the response curve of each constituent is an



increasing function.

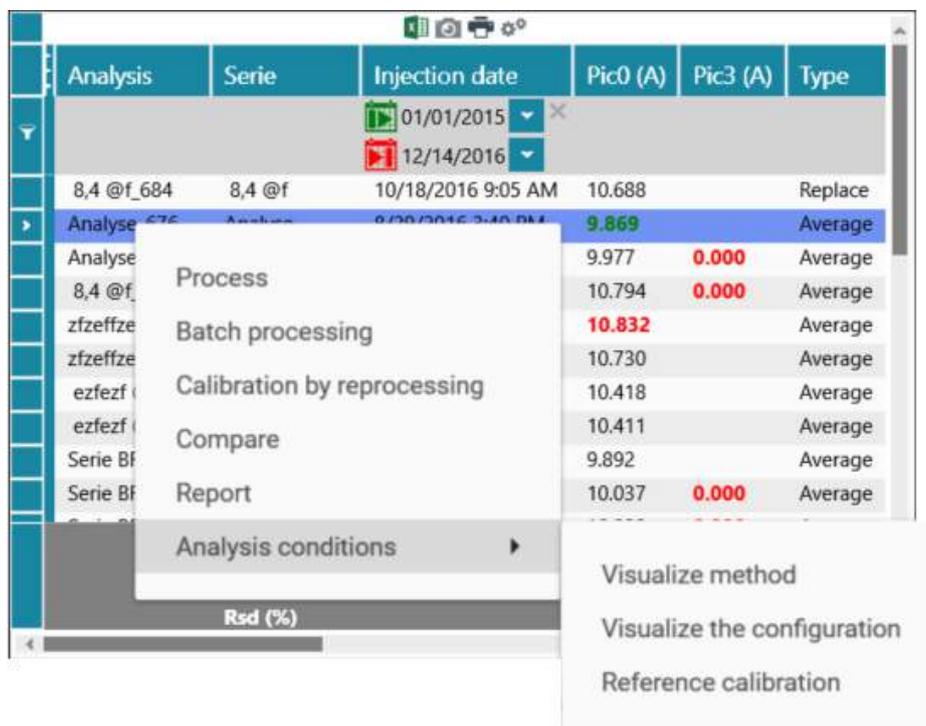
SOPRANE II therefore performs, when necessary, a verification of this growth between the minimum and maximum concentration values used to carry out the calibration but also between zero and the lowest concentration value or between the highest concentration value and 10 times this value. A possible defect, whose probability is extremely low, will be reported but will not result in the calibration rejection.

### c) 4. Reference calibration

The reference calibration is the last calibration used to get the current results.

The reference calibration is available from several ways:

The first one is from the result (or reprocessing/calibration) table: Select a single analysis and right click, then expand "**Analysis conditions**" and select "**Reference calibration**"



The second way is from the **Process** tab: Select the "**Calibration**" menu and click on "**Reference calibration**".

On the first tab, a result table will be visualized:



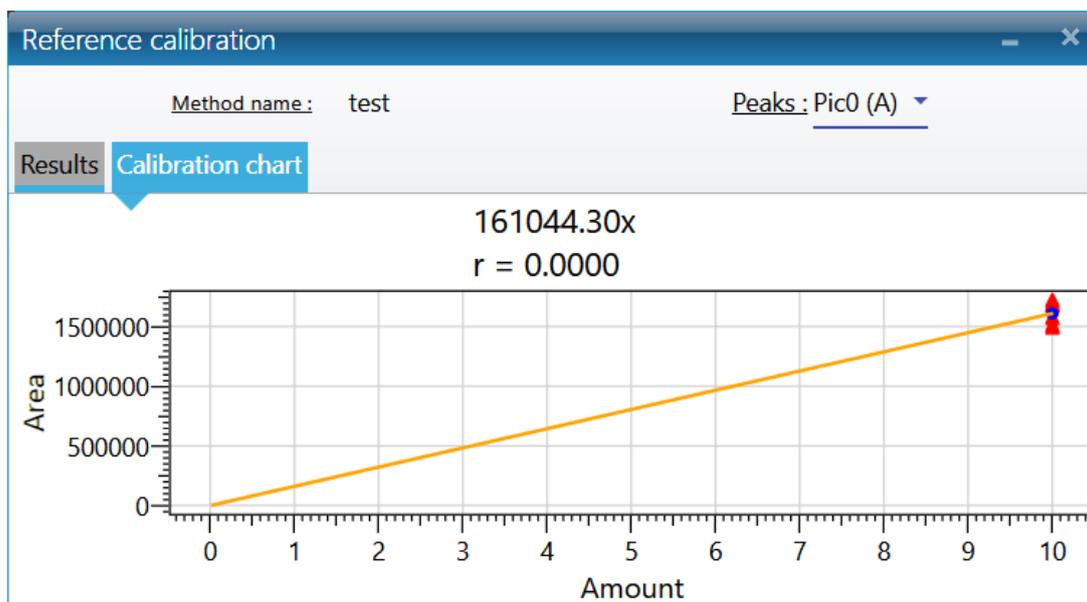
Reference calibration

Method name : test Results : Concentration

Results Calibration chart

Analysis name	Level	Type	Pic0 (A)	Pic1 (A)	Pic2 (A)	Pic3 (B)	Pic4 (B)
Analysis_198	1	Replace	10.000	10.000	10.000	10.000	10.000
Analysis_193	1	Average	10.000	10.000	10.000	10.000	10.000
Analysis_194	1	Average	10.000	10.000	10.000	10.000	10.000
Analysis_195	1	Average	10.000	10.000	10.000	10.000	10.000
Analysis_196	1	Average	10.000	10.000	10.000	10.000	10.000
Analysis_197	1	Average	10.000	10.000	10.000	10.000	10.000

On the second tab, a calibration chart for all peaks will be visualized:



See also chapter [Calibrations history](#) and [Calibration report](#).

### c) 5. Calibration report

The calibration report is available from several ways:

The first one is from the result (or reprocessing/calibration) table. Select a single analysis and right click. Expand "Analysis conditions" and select "calibration report"

The second way is from the Process tab. Select the "Calibration" menu and click on "Calibration report".



The screenshot displays the 'Reference calibration - test' window in the SRA INSTRUMENTS software. The interface is split into two main panels. The left panel shows a 'Calibration report' for 'Soprane II' dated '04.06.2018'. It includes a 'Component table' with two tables of analysis results (Pico (A) and Pico (B)) and an 'Integration parameters' table. The right panel shows two calibration graphs: 'Pico (A)' and 'Pico (B)'. Both graphs plot 'Area' against 'Amount' and show a linear relationship with a regression line. The 'Pico (A)' graph has a regression equation of  $y = 101044.37x$  and  $r = 0.9999$ . The 'Pico (B)' graph has a regression equation of  $y = 91299x$  and  $r = 0.9999$ .

**Calibration report**  
 Calibration date: 15/01/2018 2:02:42 PM Method: test

**Component table**

Analysis name	Level	Type	Pico (A)		Pico (A)		Pico (A)	
			Area	Concentration	Area	Concentration	Area	Concentration
Analysis_198	1	Replicat	1077192 µV.s	10.000 %	1016 µV.s	10.000 %	12993 µV.s	10.000 %
Analysis_198	1	Average	1492344 µV.s	10.000 %	1028 µV.s	10.000 %	13359 µV.s	10.000 %
Analysis_194	1	Average	1510497 µV.s	10.000 %	822 µV.s	10.000 %	13590 µV.s	10.000 %
Analysis_195	1	Average	1575795 µV.s	10.000 %	956 µV.s	10.000 %	14228 µV.s	10.000 %
Analysis_196	1	Average	1688912 µV.s	10.000 %	984 µV.s	10.000 %	15034 µV.s	10.000 %
Analysis_197	1	Average	1719815 µV.s	10.000 %	1020 µV.s	10.000 %	15468 µV.s	10.000 %

Analysis name	Level	Type	Pico (B)		Pico (B)	
			Area	Concentration	Area	Concentration
Analysis_198	1	Replicat	2729249 µV.s	10.000 %	1866 µV.s	10.000 %
Analysis_198	1	Average	2720614 µV.s	10.000 %	2115 µV.s	10.000 %
Analysis_194	1	Average	2721968 µV.s	10.000 %	1683 µV.s	10.000 %
Analysis_195	1	Average	2722368 µV.s	10.000 %	1889 µV.s	10.000 %
Analysis_196	1	Average	2724199 µV.s	10.000 %	1815 µV.s	10.000 %
Analysis_197	1	Average	2722764 µV.s	10.000 %	1888 µV.s	10.000 %

**Integration parameters**

Module	Time	Type	Value
A	0.00	Baseline detection	ON
A	0.00	Absolute peak width	0.5
A	0.00	Absolute peak slope	5
B	0.00	Baseline detection	ON
B	0.00	Absolute peak width	0.2
B	0.00	Absolute peak slope	2

Of course, you can edit the report, see chapter [Report](#).

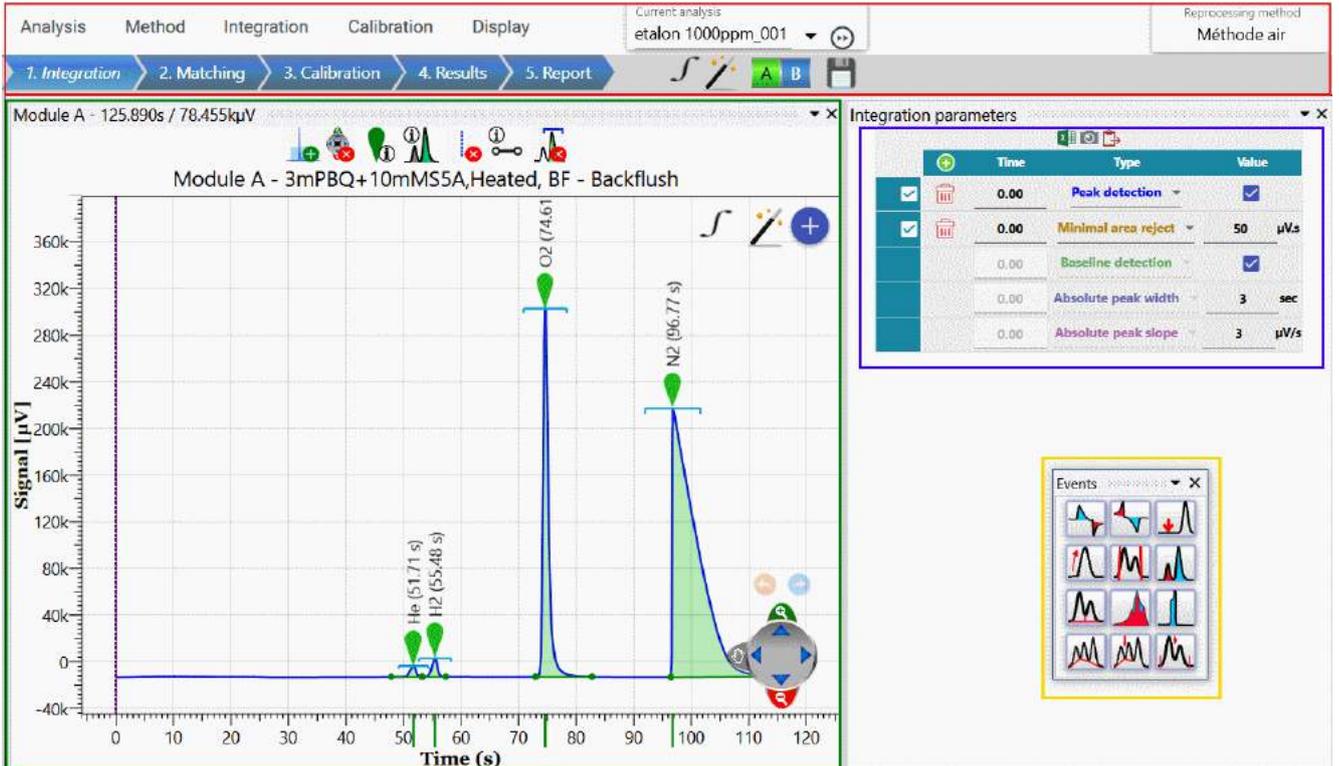
See also chapter [Reference calibration](#) and [Calibrations history](#).

### 4.5.2. Integration management

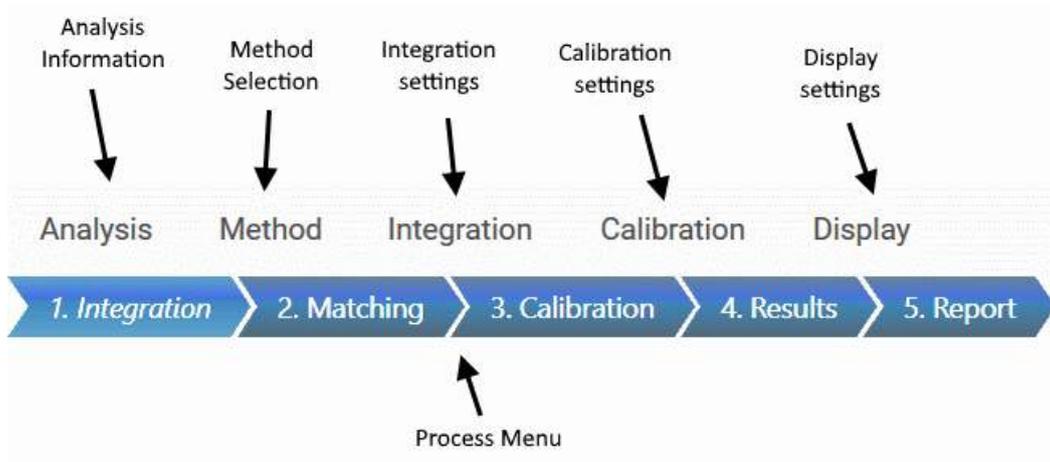
The "Integration parameter" page is divided into 4 parts:

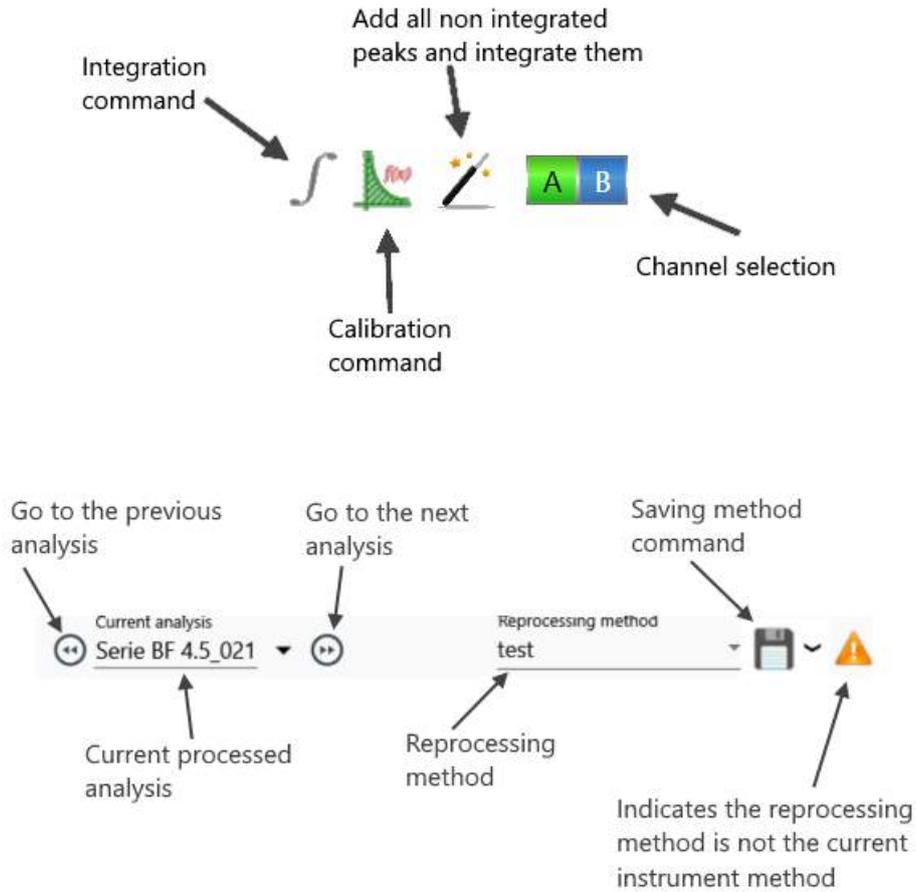
- Menu & Commands
- Graphic
- Table of events
- Palette



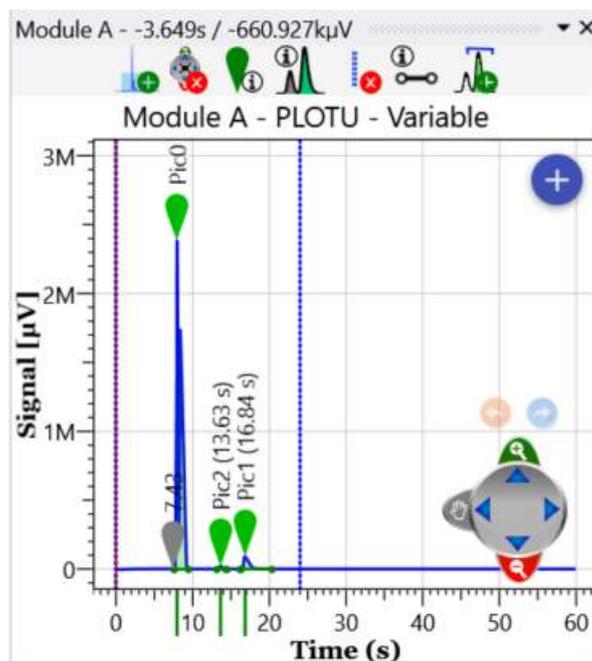


### 1. Menu & Commands





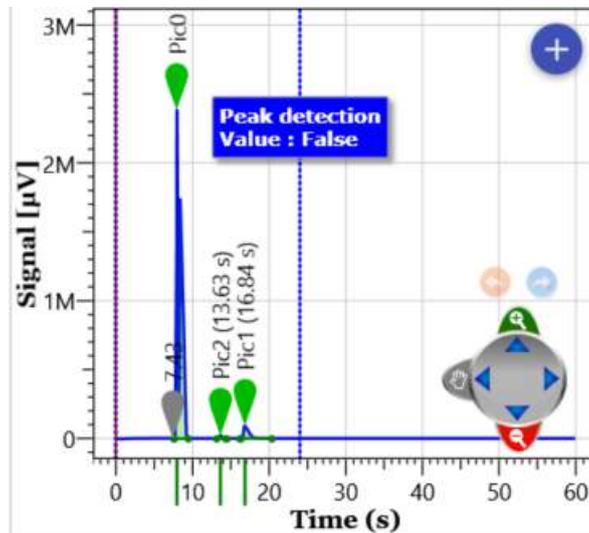
**2. Graphic**



The graphic gives access to the integrated signal and to all the events added by the user.

Each vertical line represents an event of the integration table with a corresponding color.

When the mouse cursor is over the event line, the event name appears and the line can be moved.



For more information concerning the browsing on the chart, see the chapter [Chart](#).

### 3. Events table

	+	Time	Type	Value
		0.00	Baseline detection	<input checked="" type="checkbox"/>
		0.00	Absolute peak width	3 sec
		0.00	Absolute peak slope	3 µV/s
<input checked="" type="checkbox"/>	<input type="checkbox"/>	0.00	Peak detection	<input checked="" type="checkbox"/>
<input checked="" type="checkbox"/>	<input type="checkbox"/>	0.00	Minimal area reject	50 µV.s

Integration events can be added with the integration table. Each row in this table allows to add a vertical line on the graph, with the color corresponding to the event.

A line can be added or deleted in two different ways. Either by clicking on the icon  (the icon  will delete the line) or by right clicking that will display a menu that will propose these possibilities. Graphically, position the mouse cursor over an event line and press the "delete" key.

The different expected values are:

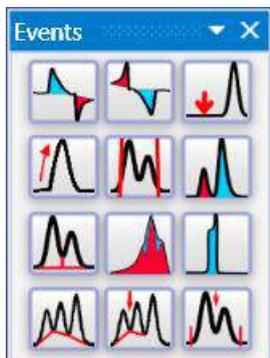
- The time
- The type of event
- The value (which can be a numeric value or a check value).



To see the integration events list, see the chapter [Integration](#).

For more information on the edition of the integration parameters, see chapter: [Integration settings](#)

#### 4. Palette



Events can also be added by this small palette. Each icon represents an event. The displacement with the mouse cursor over one of the icons display its detailed description.

For more information on the palette see chapter [Chromatogram](#).

To see the integration events list, see the chapter [Integration](#).

##### **a) Integration settings**

The integration of a chromatogram needs 2 distinct processes: first it is necessary to detect the presence of peaks; in a second time, you must interpret the shape of these peaks to be able to apply various methods of baseline correction.

The integration events meet these 2 needs.

Two parameters are important to detect the peaks and their form: these are the peak width and the slope sensitivity.

The signal of analysis is measured at a rate of 20, 50 or 100 Hz (as defined in the analysis method). All these values are then gathered in slices to have an optimized process depending on the size peak. The regrouping is carried out according to the peak width value programmed by the user, which then allows a follow-up of the signal by comparing the slope with the sensitivity threshold value programmed by the user.

This process authorizes a rather important flexibility. To divide by 2 or to double the peak width will generally not lead to significant modifications of the result. It is however judicious to use values in connection with reality.

The peak width default value of 0.5 second allows the correct integration of peaks with a short retention time.

The sensitivity threshold default value equal to 5  $\mu\text{V}/\text{s}$  allows too the detection of "common" peaks.

To increase sensibility, it is better to first check that the peak width is correct. The best value is the peak width estimated at mid height. Then it is possible to adjust the sensitivity threshold. An idea of the correct value may be directly red on the chromatogram: the mean slope for a peak is the difference between the top and bottom signal values divided by the time difference between the top and the beginning of the peak.

When editing the integration part of an analysis method, the first step is to edit "integration parameters".



	+	Time	Type	Value
		0.00	Baseline detection	<input checked="" type="checkbox"/>
		0.00	Absolute peak width	3 sec
		0.00	Absolute peak slope	3 $\mu\text{V/s}$
<input checked="" type="checkbox"/>		0.00	Peak detection	<input checked="" type="checkbox"/>
<input checked="" type="checkbox"/>		0.00	Minimal area reject	50 $\mu\text{V.s}$

One moves in this table with the arrows of the numeric keypad or with the mouse. The rows of the table are automatically sorted in increasing times during editing.

There is no priority between 2 events planned at the same time: SOPRANE II manages them simultaneously.

Integration events can be added through the integration table. Each row in this table adds a vertical line on the graph, of the color corresponding to the event.

A line can be added or deleted in two different ways. The first is by clicking on the icon  (the icon  will delete the line) or by right clicking that will display a menu that will propose these possibilities. Graphically, position the mouse cursor over an event line and press the "delete" key.

The different expected values are:

- Enable the event
- The event time
- The type of event
- The value, which can be a numeric value or a check value.

If we modify the integration parameters, or the integration events, or if we manually change the baseline, it is necessary to re-integrate the peaks.

Another method, much more precise, consists in using a chromatogram and graphically positioning the events on this chromatogram (see chapter [Graphical tools](#)).

To see the list of integration events, see the chapter [Integration](#).

### ***b) Graphical tools***

To simplify the work, the process module makes a great use of graphical tools.

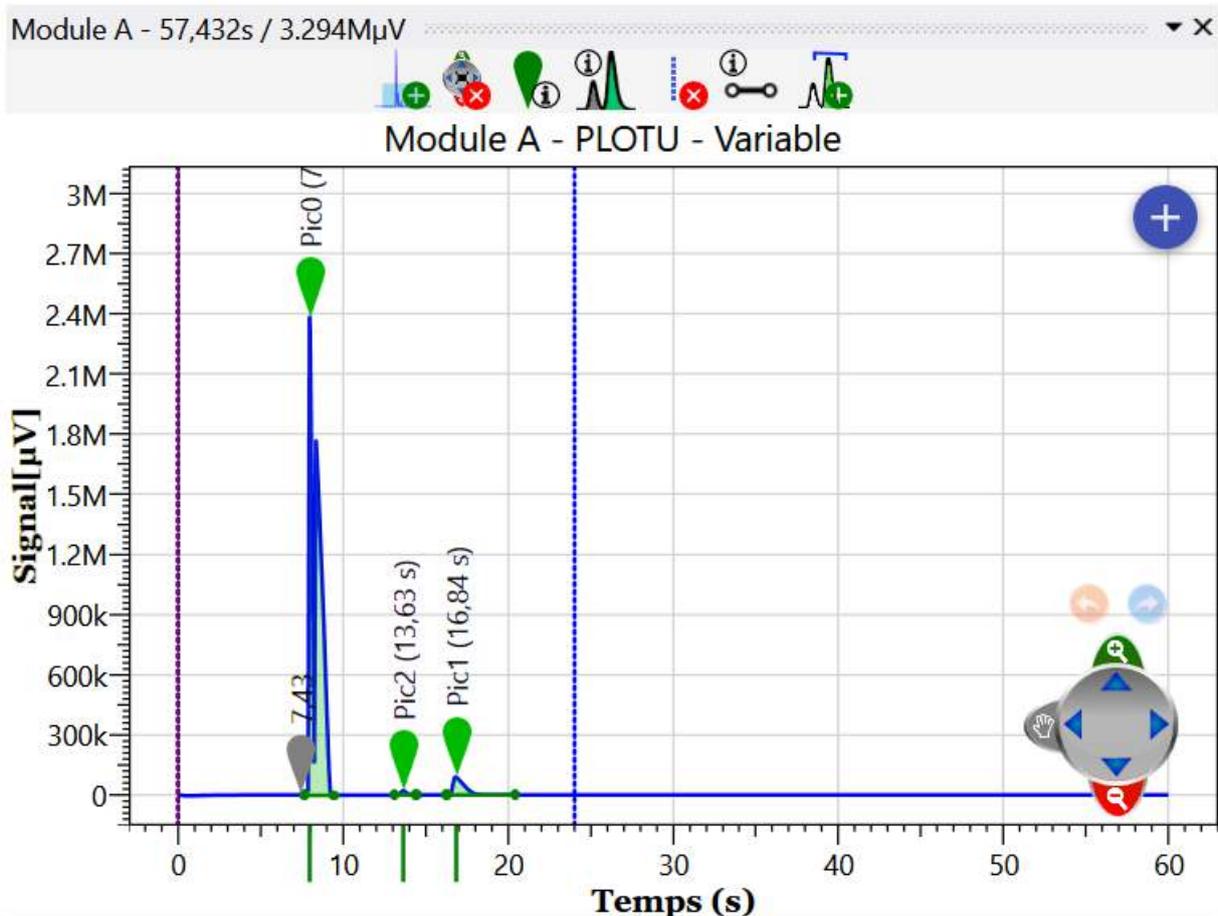
Inside the process module, the chromatogram is represented with time (expressed in seconds) in abscissa and the signal value ( $\mu\text{V}$ ) in ordinate.

If several modules (A, B, C and D) equip the analyzer, the indication of their existence is indicated in the channel bar on the visualized window (top of page) and it is possible to select each one of these modules by the buttons A, B, C and D located under the toolbar.

The position of the mouse (value of X in seconds, value of Y in  $\mu\text{V}$ ) is indicated in the status bar at the bottom left. A chromatogram point can thus be localized with an extreme precision.



Here is an example of a graphic in the processing part.

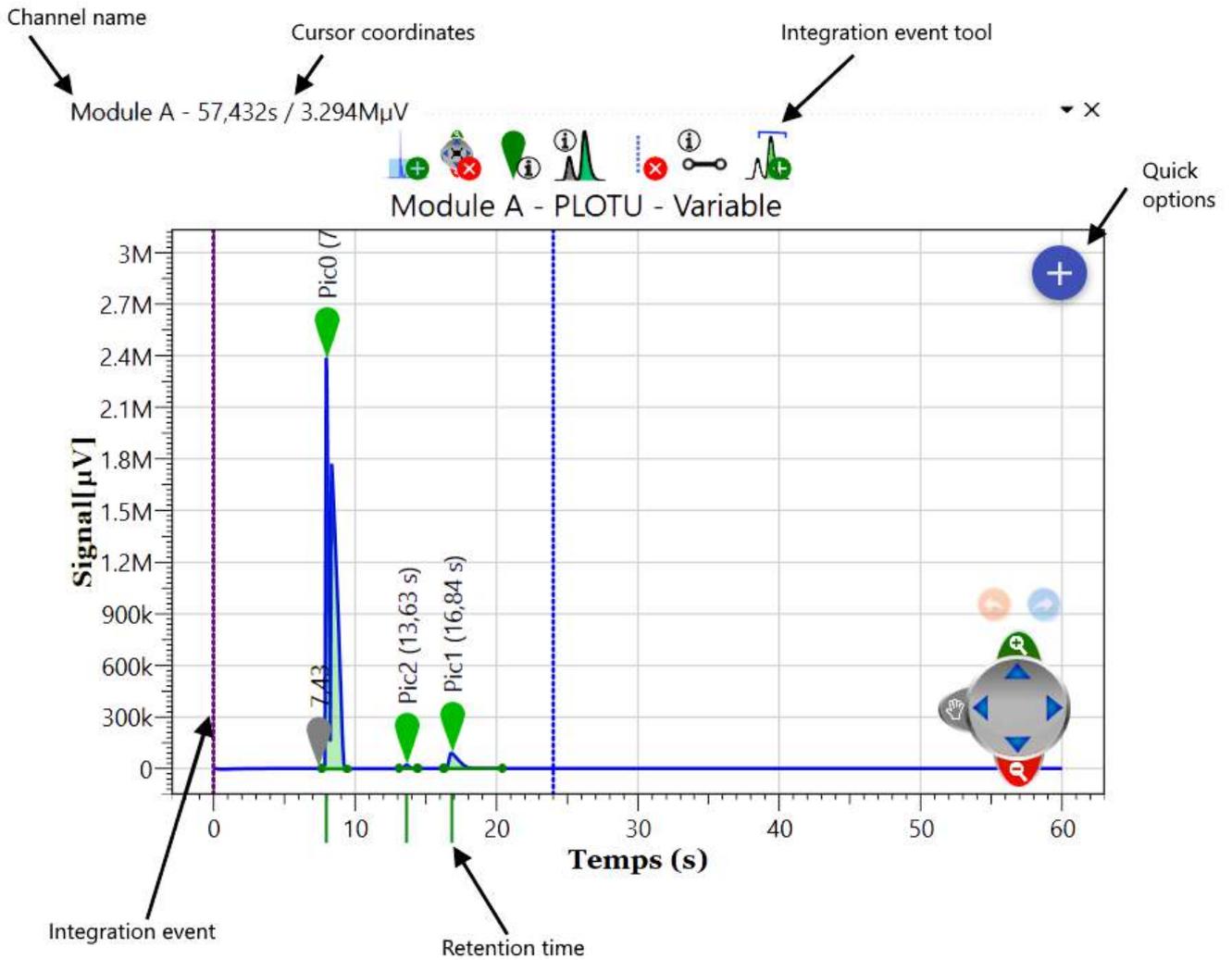


In this chapter we will see in detail each of the important elements concerning the chromatogram.

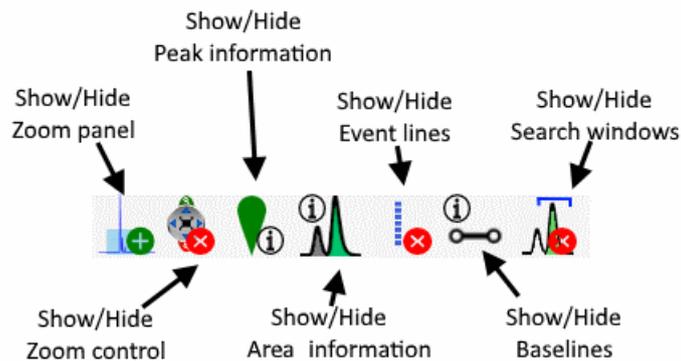
### 1. Graphic

The graph is an important visual element for the visualization of the chromatogram, but also for quick visualization of the integration elements.



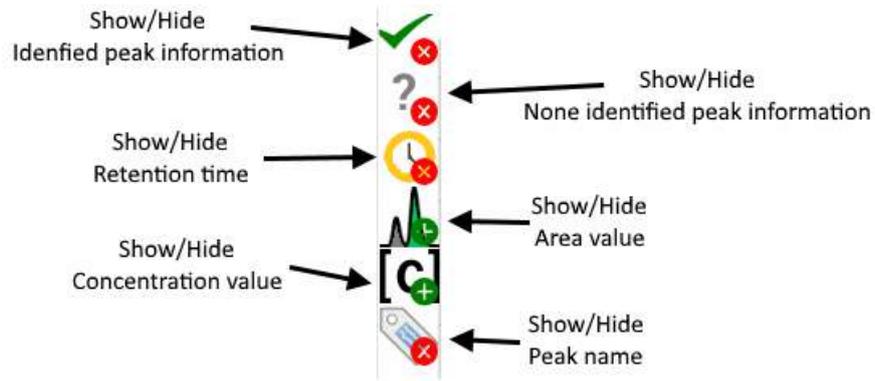


Here's the description of each graphical event information

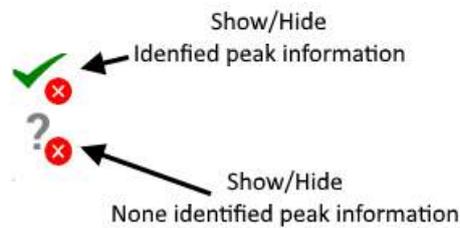


If you click on "**peak information**", you will be able to change the description of the peak, see description below:

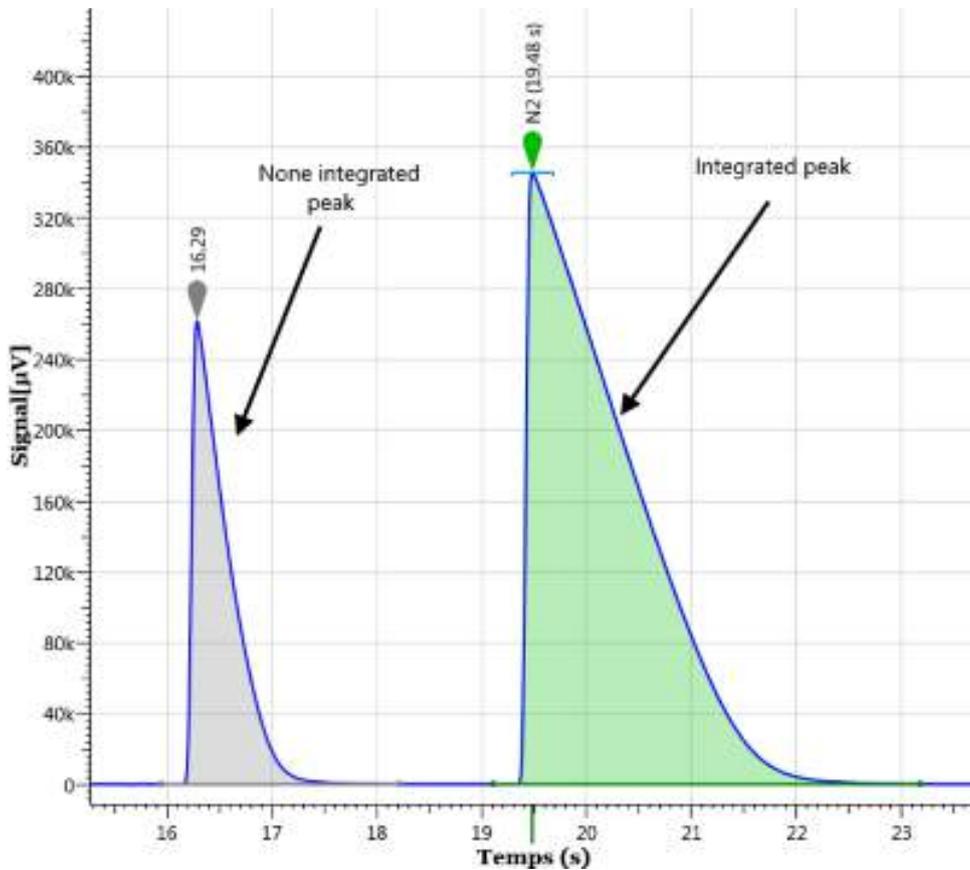




If you click on "area information" or "baseline information", you will be able to change the visibility of the parameter, see description below:

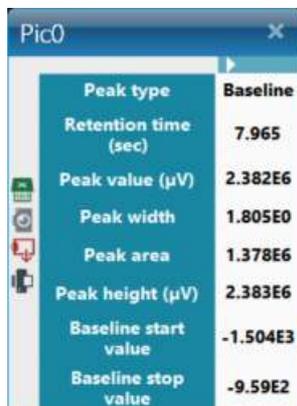


Here's below the visualization of a none identified peak, and an identified peak:



There is a useful shortcut to know to add a peak; just make **Ctrl+left** click and the peak will be added at the cursor location. A drag-drop from the peak to the array of components will also add the peak.

A double click on the icon  or  display the information about the peak as in the display below.



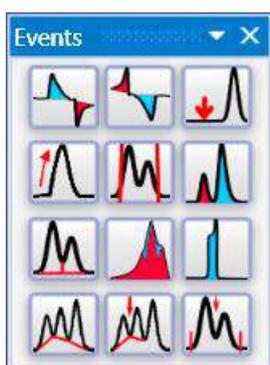
Peak type	Baseline
Retention time (sec)	7.965
Peak value (µV)	2.382E6
Peak width	1.805E0
Peak area	1.378E6
Peak height (µV)	2.383E6
Baseline start value	-1.504E3
Baseline stop value	-9.59E2

For more information about the chromatogram navigation see chapter [Chart](#).

## 2. Palette

The [Integration settings](#) chapter describes how to directly add the integration events to the table. It may be faster to place them directly on the chromatogram. The examination of various chromatograms allows to define the zones where the peaks are expected. The zoom allows a precise positioning of each event.

To display the integration palette, click on the menu "Display / Show the palette of integration events". When viewed, the events palette can be closed with a mouse click on the cross on the top right of the palette. Closing the palette does not remove the event tool (the cursor always represents a hand). The event tool is disabled when you select another, normally the zoom tool.



Events can also be added by this small palette. Each icon represents an event; the displacement over one of the icons will display its detailed description.

Here is the list of the shortcuts available in the palette:

- : Positive peak detection (see section [Peak detection](#))
- : Negative peak detection (see section [Negative peak detection](#))



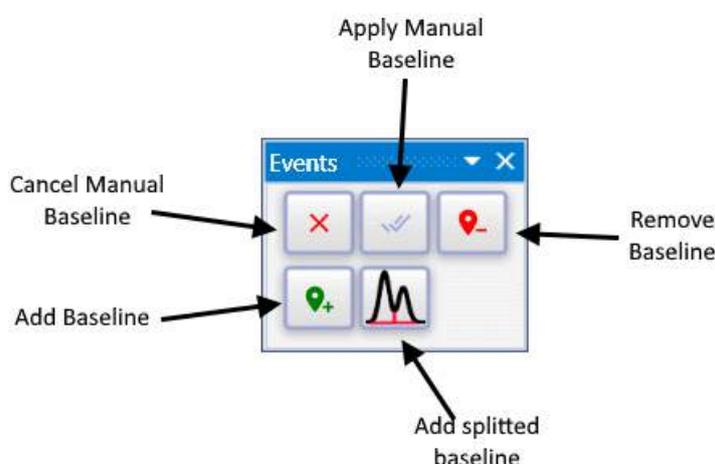
- : Baseline detection (see section [Baseline detection](#))
- : Absolute sensitivity threshold (see section [Absolute slope sensitivity](#))
- : Absolute value of peak width (see section [Absolute peak width](#))
- : Minimal area rejection (see section [Minimum area rejection](#))
- : Baseline split (see section [Baseline split](#))
- : Peak grouping (see section [Peak group](#))
- : Shoulder peak detection (see section [Shoulder peak detection](#))
- : Forcing of baseline on all valleys (see section [Forcing of baseline at all valleys](#))
- : Forcing of baseline on the next valley (see section [Forcing of baseline at next valley](#))
- : Force integration (see section [Force integration](#))

To position an event, simply zoom the chromatogram until you get a correct view of the location where you want to insert the event, select the event tool (click on the icon), enter the event that interests us (left mouse button pressed on the icon of the event), click on the desired time.

A window allows to display, and in case of error to modify, the nature of the event, the time and the value or state of the event.

To delete an event, the easiest way is to edit the events table (see chapter [Integration settings](#)). Sometimes it is simply necessary to change the time at which an event is scheduled. In this case, just move the cursor to the event and enter it with the left mouse button. A vertical bar appears as soon as the mouse is moved. The event can then be added where desired. A change of value can also be written directly in the event table.

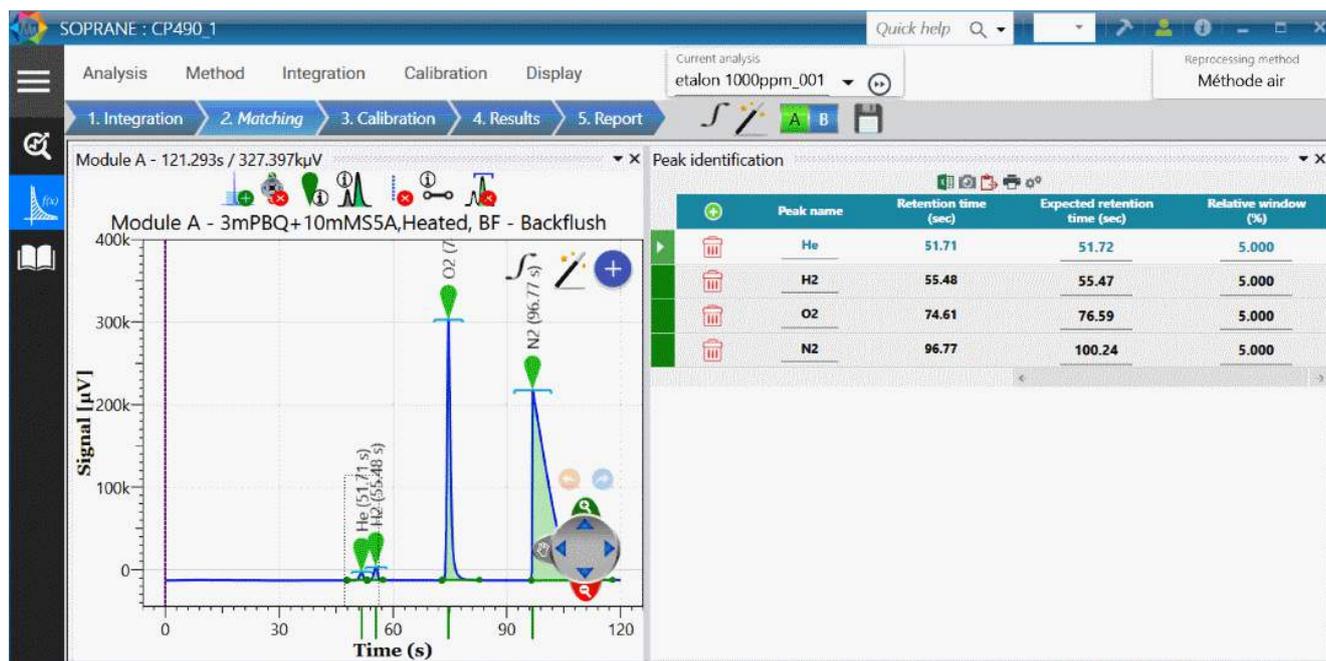
If the manual baseline is enabled, the following palette will be visible:



See chapter [Options management](#), to know how to active the "Manual baseline", and see chapter [Manual baseline](#) to know how to use the feature.



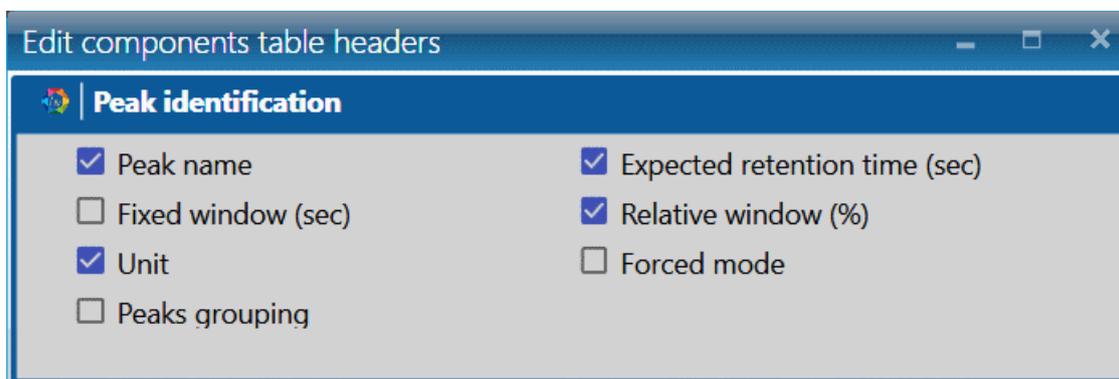
### c) Components table



If no analysis has been performed with the method being edited, the components table is inaccessible.

#### 1. The components table columns :

The components table can contain a wide variety of data. Some will be useful to a user, others will not. The button  allows to reach a selection screen of the columns that will be displayed later.



The columns to be visualized are:

**Peak name:** It is the name of the component. The name programmed here is used as a reference to identify the peak in the other modules of SOPRANE II. It is under this name that the component will be identified for post-analytical calculations or for trends for instance.

**Expected retention time:** It is the expected retention time expressed in seconds. This value is used as a reference for the components identification.



**Absolute window:** It is a time window taken before and after the expected retention time and during which the software tries to identify the peak. This window value is expressed under the form of an absolute value of time.

**Relative window:** It is a time window taken before and after the expected retention time during which the software tries to identify the peak. This value of window is expressed under the form of a percentage of the expected retention time.

**Units:** It is the unit used to express the concentration value.

**Response type:** The software allows to work with peaks area or height.

**Peaks grouping:** It is a flag (A, B, C or D) indicating which peaks, because they have the same flag, will be grouped for the calculations. 4 groups of peaks can then be defined. (Be careful: these are not peaks integrated together, with a common baseline; these peaks are integrated separately, or not, and then grouped only during the calculations).

**IMPORTANT NOTE:**

Both absolute and relative window values are cumulative. The time window used to search and identify the peaks is the sum of the two programmed values.

If we consider a peak whose estimated retention time is 2 minutes (120 seconds), with a relative window of 10% (12 seconds) and an absolute window of 0,1 minute (6 seconds).

The peak will be identified if during an analysis its retention time is comprised between 1 min 42 seconds and 2 min 18 seconds.

2. Components table:

The components table allows the edition of each of the constituents to be analyzed.

	+	Peak name	Retention time (sec)	Expected retention time (sec)	Relative window (%)
	🗑️	He	51.67	51.72	5.000
	🗑️	H2	55.43	55.47	5.000
▶	🗑️	O2	74.54	76.59	5.000
	🗑️	N2	96.68	100.24	5.000

The button allows the addition of a new line, will delete the line.

One or several lines can be selected, just like in a conventional word processor, by positioning the mouse in front of each line. Pressing the DELETE key will delete the selected lines.

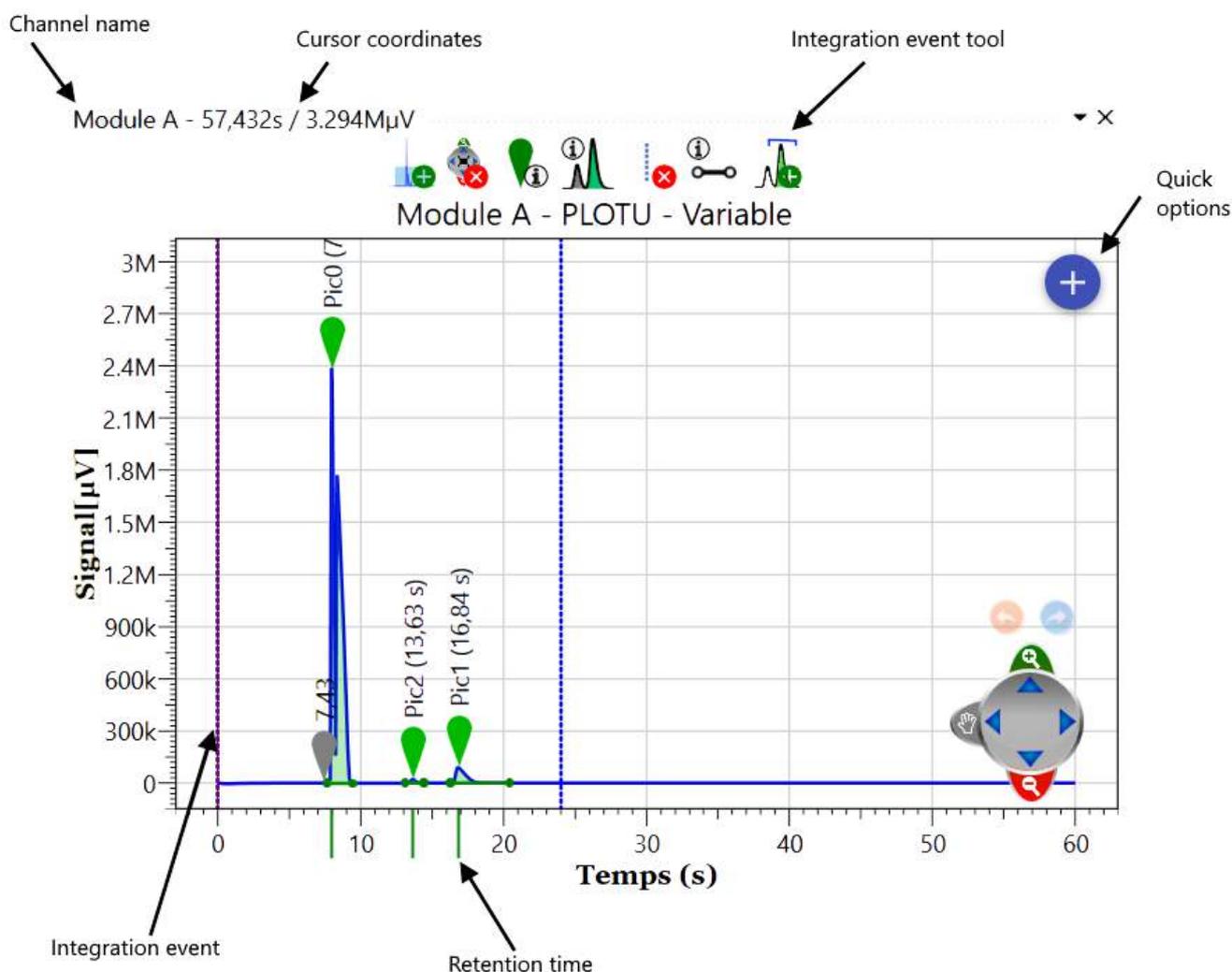


It is possible to test a complete line by carrying out a double click in the left margin of each line. The component data are checked and a window indicates if all is correct, if data are missing or if an information is wrong.

If the option **"Update retention time after integration"** is activated, the expected retention time will be updated after each analysis or integration.

If the option **"Update retention time after calibration"** is activated, the expected retention time will be updated after each calibration. (see chapter [Retention time update](#)).

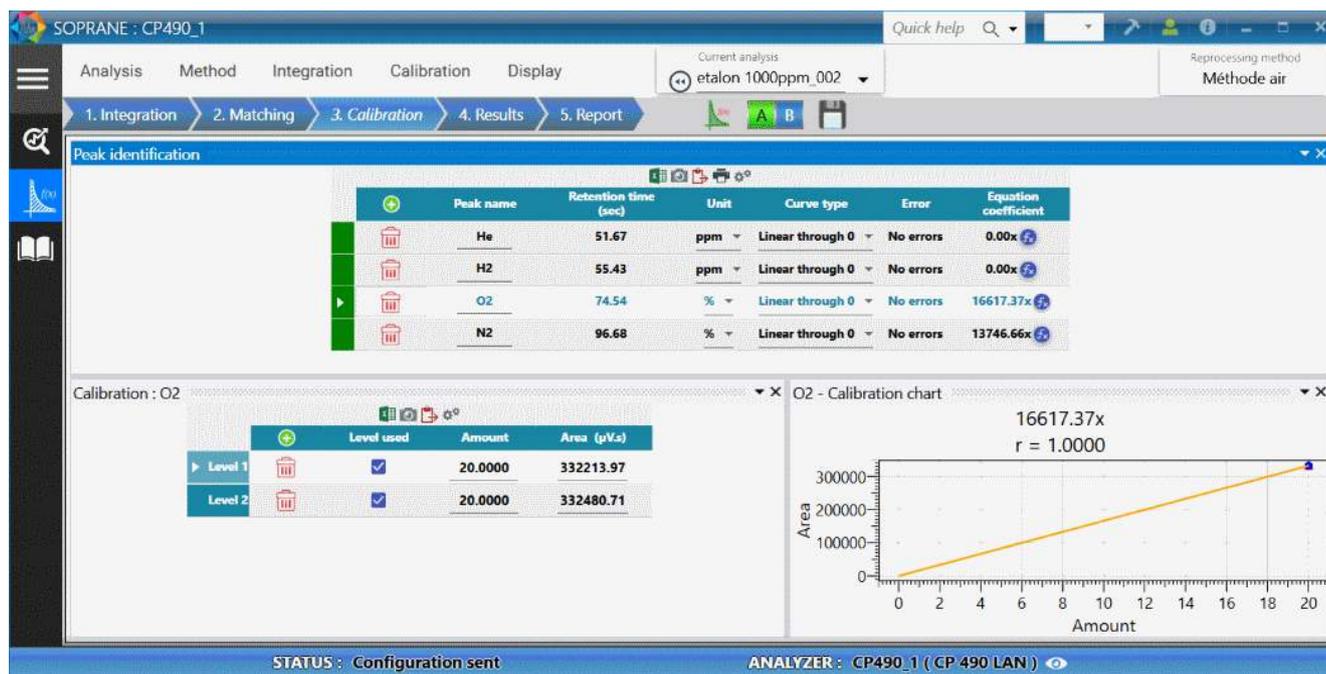
### 3. Graphic



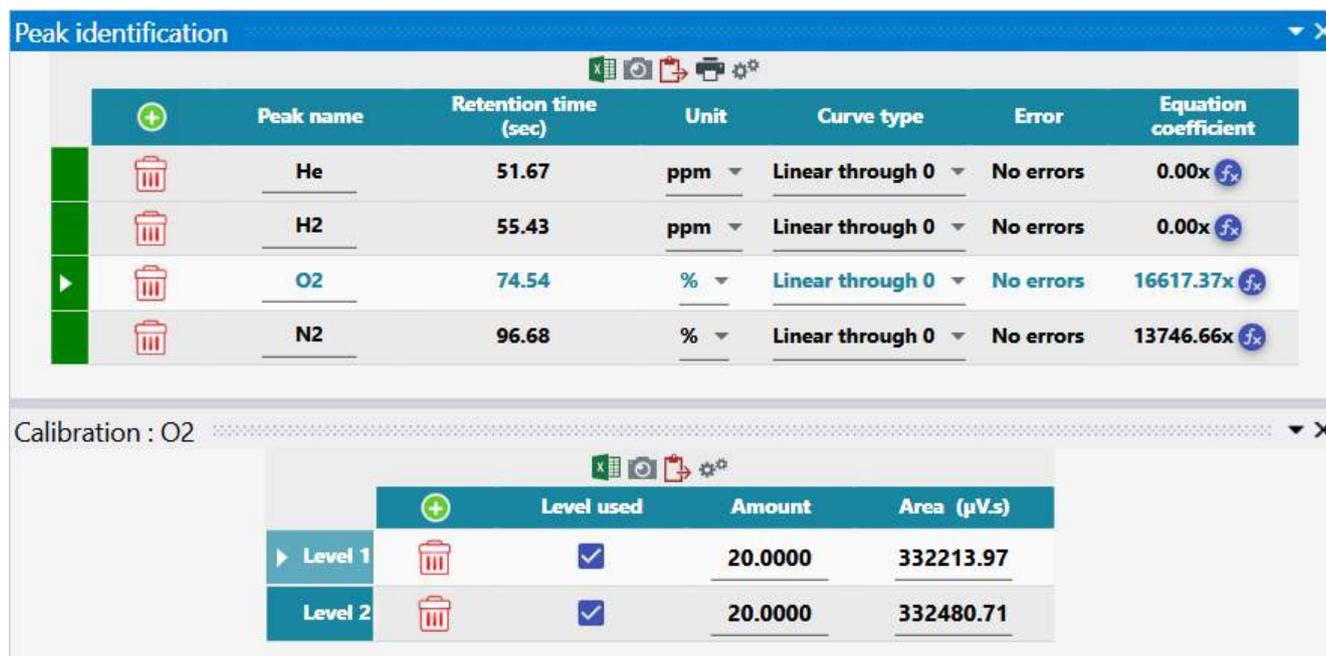
#### d) Calibration table

The menu **"3. Calibration"** allows to display and program the values necessary for the identification and the calculation of the response factors or of the concentrations of each component to be analyzed.





Two tables are visualized:



One can move inside these 2 tables using the arrows of the numeric keypad or the mouse. The change to the next box when the cursor is in the box at the bottom right of the table, as well as the change to the next line when the cursor is in the last line, allows the addition of a new line.

One or several line(s) can be selected, as in all classical word processor, by positioning the mouse in front of each line. An action on the delete key then allows the removal of these lines.



The top table relates to the peaks and their identification. The insertion of a line was not considered: a line can be added and SOPRANE II sorts the lines according to the retention time.

It is possible to test the validity of a complete line by carrying out a double click in the left margin of each line. The component data are checked and a window indicates that all is correct, or that information is missing or that one is erroneous.

If the response curve is not a line passing by the origin, several coefficients will be required to define it. The column "curve type" allows to define the general equation of the curve visualized in the column "Calibration equation". When one clicks in this last column on the box intersecting with the line on which one wishes to intervene, the box becomes grayed and is selected. A click on the button "fx" ("Calibration equation") allows the opening of a window to edit the coefficients. The coefficients A, B, C, D and possibly E are indicated, knowing that A represents the coefficient of lowest exponent, B the following... and E the coefficient of highest exponent.

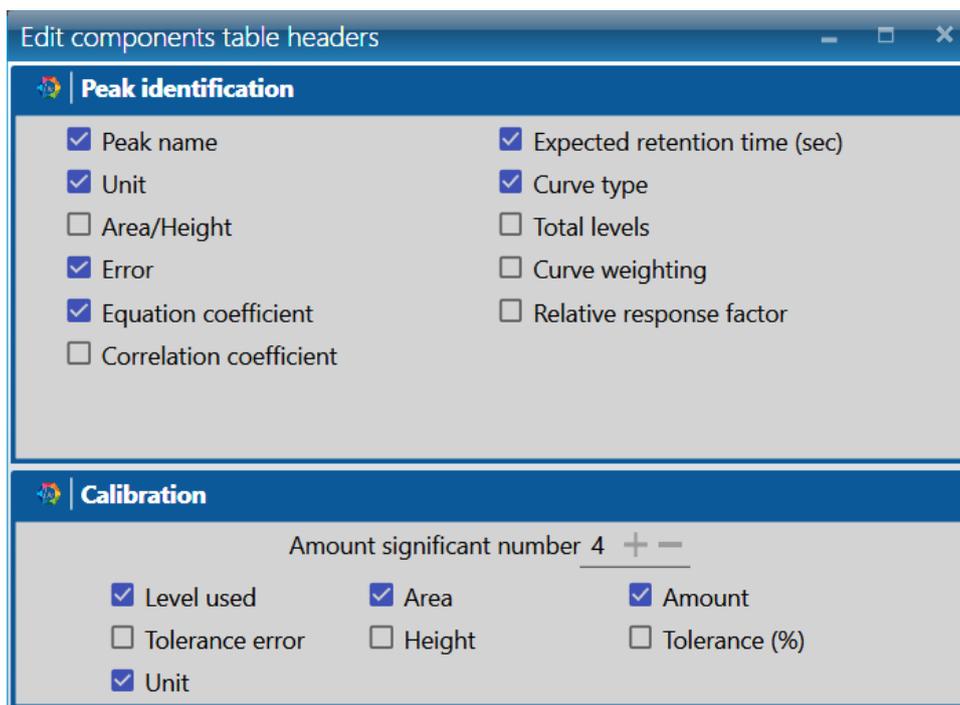
An equation of the second degree is thus defined by:  $Cx^2 + Bx + A$

In this first table, the user indicates the retention time of each component as well as two time windows, one relative, the other absolute, used to identify the peak. The peak identification window is the sum of the 2 programmed values.

The second table relates to the calibration levels:

For each peak selected in the top table, a levels table must be defined to specify the calibration conditions.

The level, the amount, the relative tolerance and the flag "used" have to be informed.



For the calibration table, the columns to be visualized are:

**Peak name:** It is the name of the component. The name programmed here is used as a reference to identify the peak in the other modules of SOPRANE II. It is under this name that the component will be identified for post-analytical calculations or for trends for instance.



**Retention time:** It is the retention time expressed in seconds. This value is used as a reference for the components identification.

**Units:** It is the unit used to express the concentration value.

**Curve type:** Depending on the number of points used to define the curve, it is possible to define several types of curves. One point allows to define a line passing by the origin. Two points define a line not passing by the origin. In the same way, we can define a curve of the second, third or fourth degree, an exponential or a logarithmic curve.

**Number of levels:** It is the number of successive concentration values used during calibration to determine the response curve for a given component.

**Error:** The calibration error description

**Curve weight:** It is the way to weight the calibration curve. The software offers 9 possibilities based on the quantity: equal to the quantity, proportional to the quantity, to inverse of the quantity, to the square of the quantity, to the inverse of the square of the quantity, to the logarithm of the quantity, to the inverse of the logarithm of the quantity, to the square of the logarithm of the quantity, to the inverse of the square of the logarithm of the quantity.

**Calibration equation:** If the response curve is not a line passing by origin, the equation of the curve, with its coefficients, will be visualized here.

**Response factor:** It is the "traditional" response factor, i.e. corresponding to a response curve passing by origin.

**Correlation coefficient:** The response curve is extrapolated from several points. This coefficient gives an indication on the quality of the calibration curve. The closest to 1 is the coefficient, the closest to the points defining it is the calibration curve.

For the level table, the columns to be visualized are:

**The amount significant numbers:** This is the number of significant number the amount value will have.

**The flag "used":** This is a flag specifying that this level is used for this component. A simple click in this zone allows to indicate that this level is used or not for this peak.

**The area:** This is the area or height peak value relative to that level of calibration.

**The amount:** This is the quantity of standard compound for the specific level.

**The relative tolerance:** That is the maximum variation accepted before to reject a calibration value.

**The height:** This is the height of standard compound for the specific level.

**The area / amount:** This is the ratio corresponding to the response factor in the case of a response curve passing by the origin.



**The standard deviation:** This is the variation observed for this level.

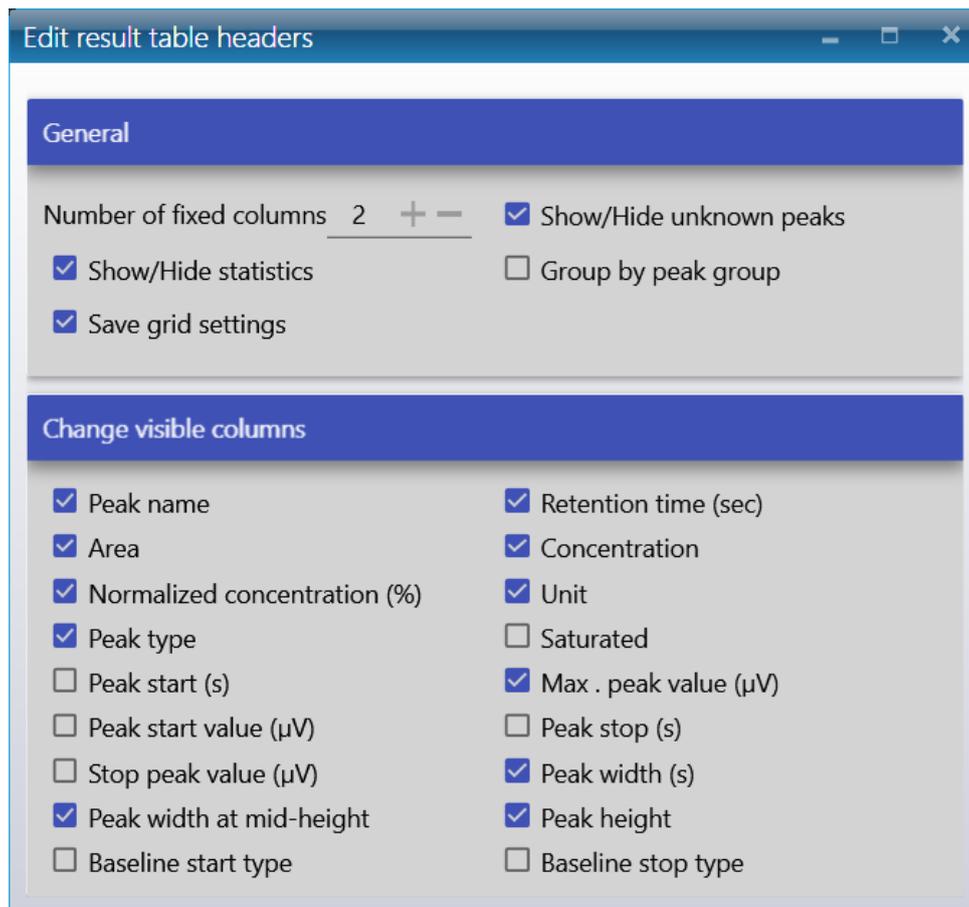
**e) Results table**

The results table can contain a wide variety of data. Some will be useful to a user, others will not. The button  allows to reach a selection screen of the columns that will be displayed later.



Module	Peak name	Retention time (sec)	Peak area	Concentration	Normalized concentration (%)	Unit	Peak type	Peak
A		7.43	15528.16	0.00	0.00	%	Baseline	915
A	Pic0	7.96	1377770.36	10.00	25.00	%	Baseline	2.38
A	Pic2	13.63	7901.64	10.00	25.00	%	Baseline	20.8
A	Pic1	16.84	69145.84	10.00	25.00	%	Baseline	88.0
B		8.91	55.28	0.00	0.00	%	Baseline	2.61
B	Pic3	9.74	2748224.19	10.00	25.00	%	Baseline	6.48
B		11.02	269.15	0.00	0.00	%	Baseline	958
B		11.57	308.83	0.00	0.00	%	Baseline	1.39
B		12.23	131.54	0.00	0.00	%	Baseline	1.14
Σ			4219334.99	40.00	100.00			





**f) Report**

The "Calculation" part allows to define all the reports that may be needed at the end of an analysis. These reports can be displayed or printed.



**Soprane II : CP490\_1** Quick help

Analysis: Current analysis: **etalon 1000ppm\_002** | Reprocessing method: **Méthode air**

1. Integration | 2. Matching | 3. Calibration | 4. Results | 5. Report

Modules: **A B** | Template: **Complete**

**Soprane II : 29.05.2018**

Analysis name: etalon 1000ppm\_002 | Injection date: 05/23/2018 14:39:17 | Method: Méthode air  
 File path: C:\Soprane II\Analysis\CP490\_1\msd\180523\etalon 1000ppm\_002.jca | Instrument.SN: 1806035

**Chromatogram**

Module A - 3mPBPQ+10mMS2A\_Heated\_BI - Backflush | Module B - 10m FPU Heated Injector - Variable

**Integration parameters**

Module	Time	Type	Value
A	0.00	Peak detection	ON
A	0.00	Minimal area reject	50
A	0.00	Baseline detection	ON
A	0.00	Absolute peak width	3
A	0.00	Absolute peak slope	3
B	0.00	Peak detection	ON
B	0.00	Maximal height reject	1E+04M
B	0.00	Baseline detection	ON
B	0.00	Absolute peak width	3
B	0.00	Absolute peak slope	3
B	70.00	Force peak	ON

**Results**

Module	Peak name	Retention time (s)	Concentration	Normalized concentration (%)	Unit	Peak width (s)
A	He	51.67	0	0	ppm	3.645
A	Hz	55.429	0	0	ppm	4.035
A	Oz	74.543	20.833	20.377	%	9.89
A	Nz	96.676	80.62	79.623	%	21.68

**Table 1 (Right Panel):**

Module	Peak name	Peak width at half-height	Peak area	Baseline start type	Baseline stop type	Peak start (s)
A	He	1.095	30743.892	Start	Split	49.65
A	Hz	1.042	17656.82	Split	Stop	53.285
A	Oz	0.912	342828.191	Start	Stop	72.91
A	Nz	4.411	1108231.682	Start	Stop	96.37
B	Pic6	1.063	4572694.342	Start	Stop	21.28
B	CH4	1.075	5876.895	Split baseline	Stop	24.74
B		0.025	0.006	Start	Stop	26.82
B		0	0.005	Start	Stop	27.43
B		0.029	0.009	Start	Stop	27.58
B	CO2	1.276	867.886	Start	Stop	70.11
B		0.029	0.025	Start	Stop	110.52
B		0.022	0.004	Start	Stop	110.52
B		0.027	0.007	Start	Stop	110.52
B		0.054	0.014	Start	Stop	110.71
B		0.067	0.029	Start	Stop	110.82

Page 1 / 3 | Page 2 / 3

STATUS : Configuration sent | ANALYZER : CP490\_1 ( CP 490 LAN )

The report is largely configurable; we can set the report visualization as well as its content.

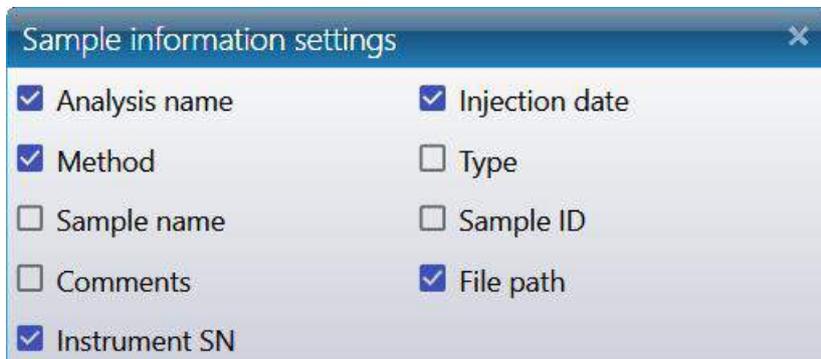
Set the report display:

- : Print
- : Copy the active selection
- : Zoom in and zoom out
- : View full size report
- : View report based on width
- : Show entire page
- : View Report on Two Pages



Set the report content:

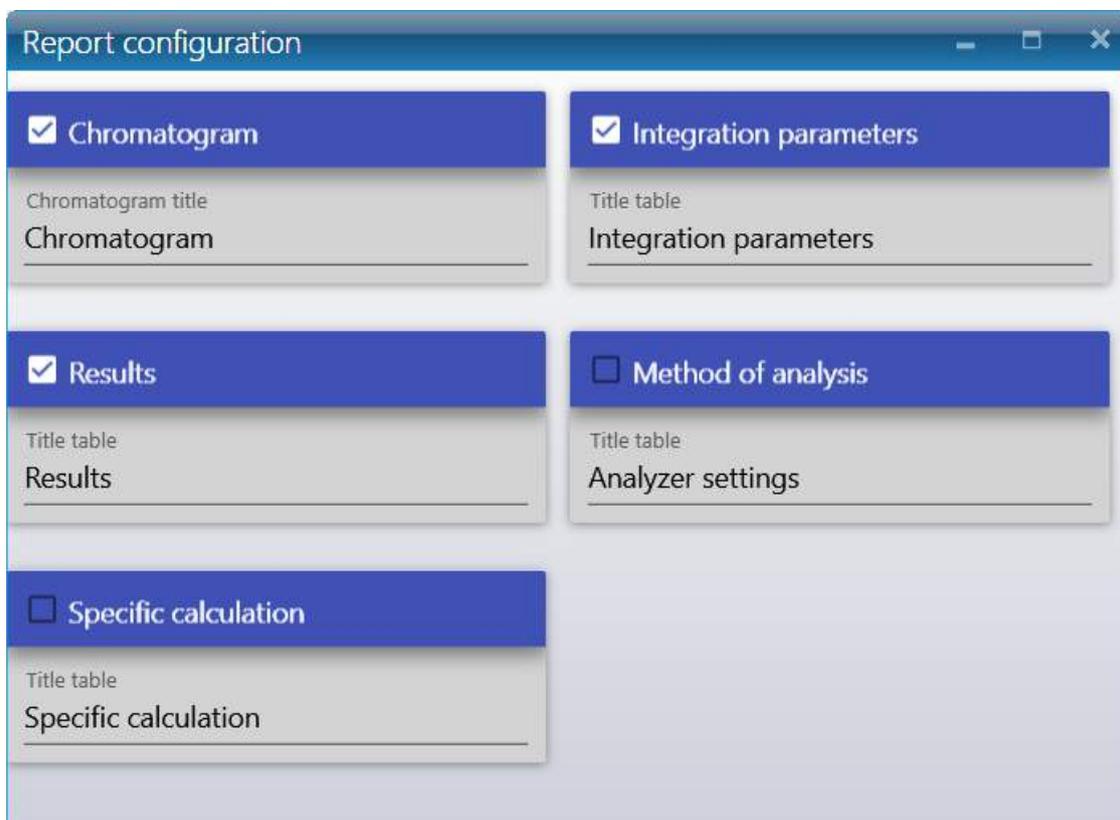
- Edit sample information :



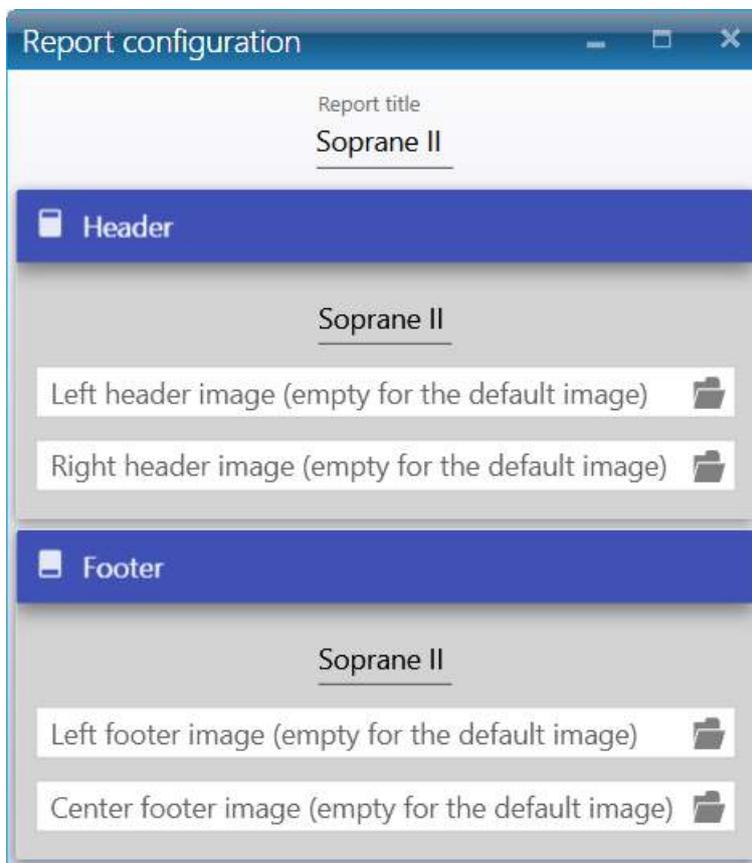
-  Report configuration

There are 5 parts in the report: the chromatogram, the integration parameters, the components table, and the analysis method and specific calculation.

Each of these parts can be visible or not, and their titles are modifiable.



- : Editing headers and footers



By clicking on the icon  a window will ask to choose an image to replace the existing one.

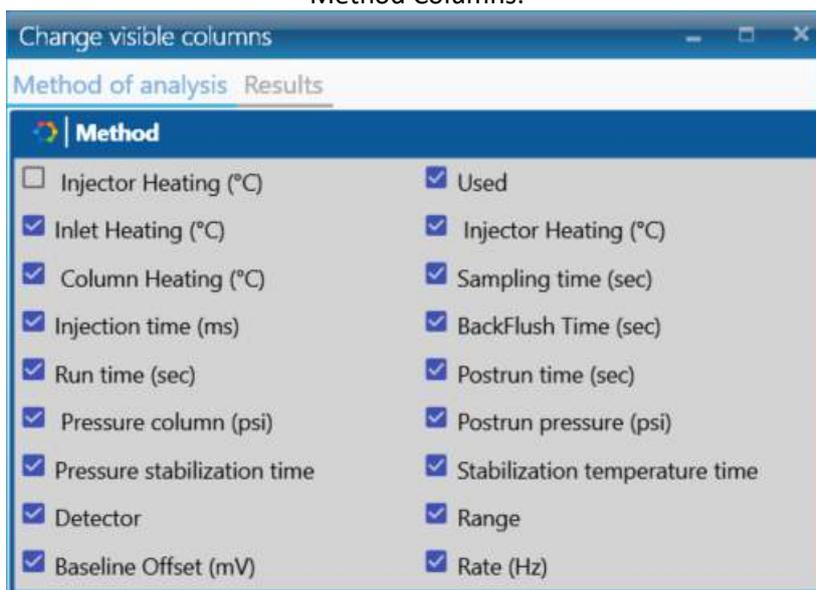
If the field is empty, the default images will be added.

-  Change the report orientation (Landscape or Portrait)
-  Change columns in tables

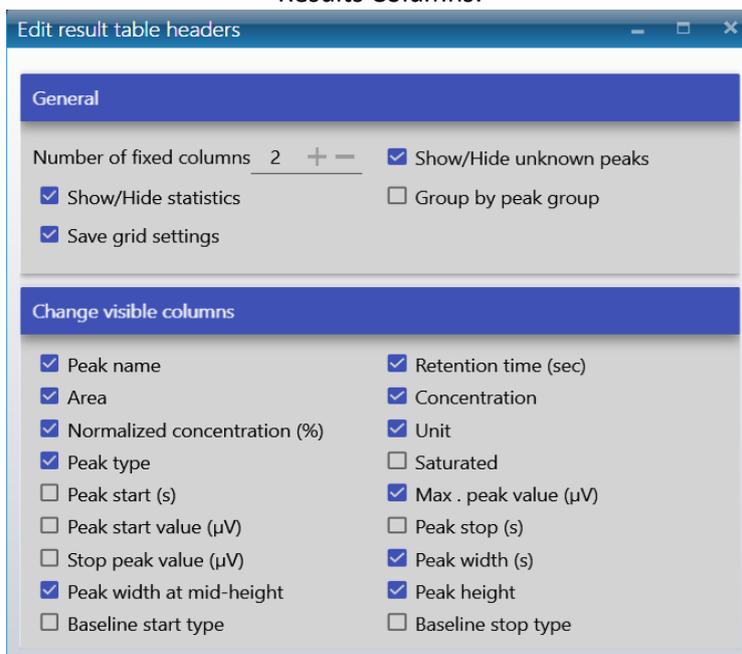
If in most of the cases we are satisfied with the columns **ID peak, constituent name, retention time, peak area, peak height, adjusted quantity and concentration**, all variables, and their corresponding column, that a user would need may be selected.



Method Columns:



Results Columns:



-  Create a custom report from a Word document (see chapter [Report Template](#))
-  Refresh the report
-  It is possible to view the active module, but also to have a single report for all the selected modules.

**NOTE:** The visible part of the chromatogram corresponds to the zoom of the chromatogram in the "Integration or Identification" part.



## f) 1. Report template

Soprane II offers the possibility to create your custom report from a template Word document.

1. Create a Word document template, with all the information you want to be presented. This document is a normal Word file that could include text, pictures, graphics... .
2. You must fill this document with keywords (see the list of keywords after the example).
3. Soprane II will read the document and check if the document has some keywords and will replace each keyword by the desired value.

Here's an example of a Word document template:

# Repair and Control report



Please find in the following document the description of work and tests carried out on your analyzer:

## 1. INSTRUMENT:

Chromatograph type: **[InstrumentType]**  
Serial number: **[InstrumentSN]**  
Software: **[Software]**

## 2. CONFIGURATION:

The [NbModules] channels of the chromatograph are configured as follows:

Channel	Signal	Carrier gas	Injector	Column	Detector
A	1	[CarrierGas1]	[InjectorType1]	[ColumnType1]	[DetectorType1]
B	2	[CarrierGas2]	[InjectorType2]	[ColumnType2]	[DetectorType2]

**[Configuration]**

## 3. REPAIR:

## 4. TESTS AND ANALYSES:

### Method:

**[Method]**

### Natural gas mixture analysis:

**[Chromatogram1]**

**[Chromatogram2]**

Base line stability → OK  
Sensitivity → OK  
Resolution → OK



Words between brackets are keywords; these keywords will be replaced by Soprane II with the expected result values.

Here's an example of the result file:

Page 1:

## Repair and Control report



Please find in the following document the description of work and tests carried out on your analyzer:

### 1. INSTRUMENT:

Chromatograph type: **CP 490 LAN**  
 Serial number: **123**  
 Software: **Soprane II (1.1.491)**

### 2. CONFIGURATION:

The 2 channels of the chromatograph are configured as follows:

Channel	Signal	Carrier gas	Injector	Column	Detector
A	1	Helium	Variable	CP-4900 Column Module, 10m PPQ Heated In	TCD
B	2	Helium	Variable	12m CP-SilicaPLOT, Heated, UM	TCD

	Module A	Module B
Mod. SN	51079	16515012
Mod. PN	740143	35810077
Heated injector	✓	✓
Max inj. temp.	110	110
Min inj. temp.	30	30
Column	CP-4900 Column Module, 10m PPQ Heated In	12m CP-SilicaPLOT, Heated, UM
Injector type	Variable	Variable
Max col. temp.	180	180
Min col. temp.	30	30
Carrier gas	Helium	Helium
Detector type	TCD	TCD
Mode of pressure control	EPC	EPC



**3. REPAIR:**

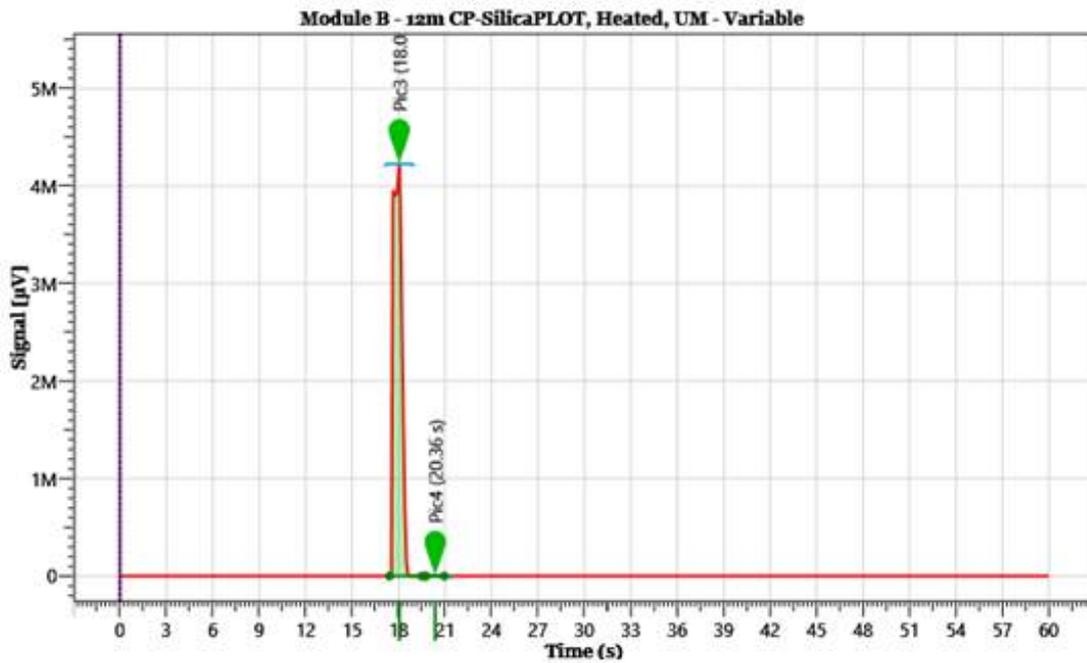
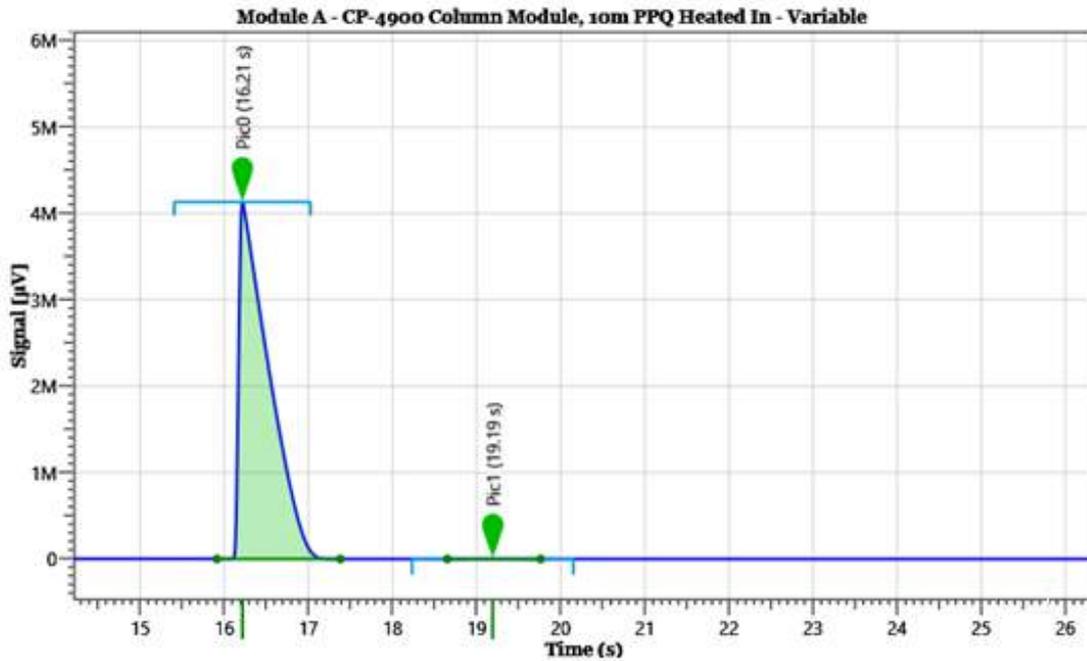
**4. TESTS AND ANALYSES:**

**Method:**

Common parameters		
Sampling time (sec)	20	
Run time (sec)	60	
	A - CP-4900 Column Module, 10	B - 12m CP-SilicaPLOT, Heated, l
Used	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>
Injector Heating (°C)	90	90
Column Heating (°C)	90	90
Injection time (ms)	100	100
Column pressure (psi)	30	30
Detector	<input checked="" type="checkbox"/> ON	<input checked="" type="checkbox"/> ON
Range	Auto	Auto

**Natural gas mixture analysis:**





Base line stability → OK  
Sensitivity → OK  
Resolution → OK

The only thing to know is which keywords to use, here's the list of all keywords:



## 1. Image keywords

[Method] : Import the analytical method

[Configuration] : Import the instrument configuration

[ResultTable] : Import the analysis result table

[Chromatogram{moduleIndicator}]: Import the chromatogram according to the module indicator number (example [Chromatogram1] for the module A)

## 2. Text keywords

### //Global values

[DateNow]: Write the date of the report generation

[Software] : Write the software used with the current version

### //Instrument settings

[InstrumentSN] : Write the instrument serial number

[NbPump] : Write the number of pumps installed

[NbModules] : Write the number of installed modules

[InstrumentType] : Write the instrument type (example CP490, M3000 Lan...)

### // Global Method

[NbRuns] : Write the number of runs made with the current analysis method

[TotalRunTime] : Write the total run time in seconds made with the current analysis method

[LastRun] : Write the last injection date made with the current analysis method

### //Result

[AnalysisDate] : Write the analysis injection date

[AnalysisName] : Write the analysis name

[AnalysisSerie]: Write the series name

[AnalysisMethod] : Write the analytical method name

[AnalysisPath] : Write the path of the result file

[AnalyzerName] : Write the analyzer name

[SampleType] : Write the sample type (Blank, Sample, Standard)

[CalibrationLevel] : Write the calibration level

[Stream] : Write the analyzed stream

### //Module configuration

[ModuleSN{moduleIndicator}] : Write the module serial number (example [Chromatogram1] for the module A)

[ModulePN{moduleIndicator}] : Write the module part number (example [ModulePN1] for the module A)

[InjectorHeated{moduleIndicator}] : Write "True" if the injector is heated otherwise "False" (example [InjectorHeated1] for the module A)

[InjectorTempMin{moduleIndicator}] : Write the minimal injector temperature (example [InjectorTempMin1] for the module A)

[InjectorTempMax{moduleIndicator}] : Write the maximal injector temperature (example [InjectorTempMax1] for the module A)

[ColumnType{moduleIndicator}] : Write the column type (example [ColumnType1] for the module A)

[HasBackflush{moduleIndicator}] : Write "True" if the instrument has a backflush column otherwise "False" (example [HasBackflush1] for the module A)

[ColumnTempMin{moduleIndicator}] : Write the minimal column temperature(example [ColumnTempMin1]



for the module A)

**[ColumnTempMax{moduleIndicator}]** : Write the maximal column temperature(example **[ColumnTempMax1]** for the module A)

**[CarrierGas{moduleIndicator}]** : Write the carrier used for the specified module (example **[CarrierGas1]** for the module A)

**[DetectorType{moduleIndicator}]** : Write the detector type used for the specified module (example **[DetectorType1]** for the module A)

**[InjectorType{moduleIndicator}]** : Write the injector type used for the specified module (example **[InjectorType1]** for the module A)

**[ChannelEnabled{moduleIndicator}]** : Write if the module is used (example **[ChannelEnabled1]** for the module A)

**[InjectorTemp{moduleIndicator}]** : Write the injector temperature used for the specified module (example **[InjectorTemp1]** for the module A)

**[ColumnTemp{moduleIndicator}]** : Write the column temperature used for the specified module (example **[CColumnTemp1]** for the module A)

**[InjectTime{moduleIndicator}]** : Write the injection time used for the specified module (example **[InjectTime1]** for the module A)

**[BackflushTime{moduleIndicator}]** : Write the backflush time used for the specified module (example **[BackflushTime1]** for the module A)

**[AnalysisTime{moduleIndicator}]** : Write the analysis time used for the specified module (example **[AnalysisTime1]** for the module A)

**[RampRate{moduleIndicator}]** : Write the ramp rate used for the specified module (example **[RampRate1]** for the module A)

**[Pressure{moduleIndicator}]** : Write the pressure in PSI used for the specified module (example **[Pressure1]** for the module A)

**[TCD{moduleIndicator}]** : Write if the detector is activated for the specified module (example **[TCD1]** for the module A)

**[Range{moduleIndicator}]** : Write the signal range used for the specified module (example **[Range1]** for the module A)

**[Rate{moduleIndicator}]** : Write the signal rate used for the specified module (example **[Rate1]** for the module A)

**[SampleTime{moduleIndicator}]** : Write the sample time used for the specified module (example **[SampleTime1]** for the module A)

**[InletTemp{moduleIndicator}]** : Write the inlet temperature used for the specified module (example **[InletTemp1]** for the module A)

**[ContinuousFlow{moduleIndicator}]** : Write if the continuous flow is used for the specified module (example **[ContinuousFlow1]** for the module A)

To generate a custom report, go to "**Process > 5. Report**" and click on the following icon :

The path of the original template file and the final report must be filled. Click on the validation button to generate the report.

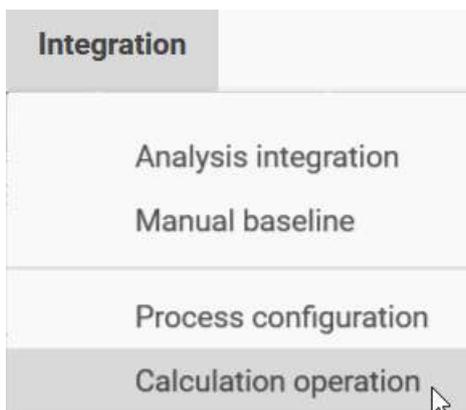




**g) Process settings**

**g) 1. Mathematical options**

The **"Integration / Calculation operation"** menu allows to reach a window where are defined the mathematical treatments to be done at the end of the analysis.

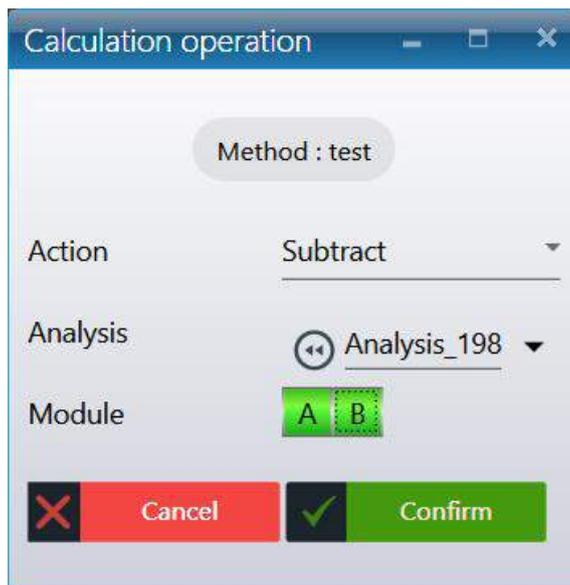


The window displayed offers the possibility to subtract or reduce the background noise on a module.

Two options are proposed.

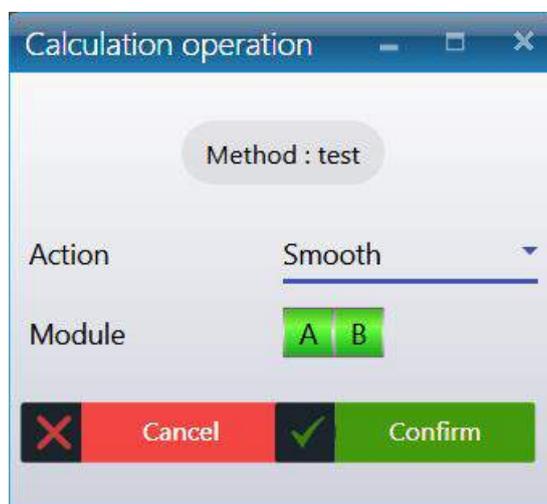
The first option allows to subtract a reference chromatogram from the analysis.





The calculations are about the difference between the 2 curves.  
In this case, the user selects the channel(s) on which this subtraction has to be made and calculations are carried out on the difference between the 2 curves.  
This treatment is interesting for instance when analyzing ppm of a component alone in a solvent and located on the trailing peak. The subtraction of an analysis of the pure solvent gives a more accurate peak, easier to integrate.

The second option consists in smoothing the chromatogram before treatment.



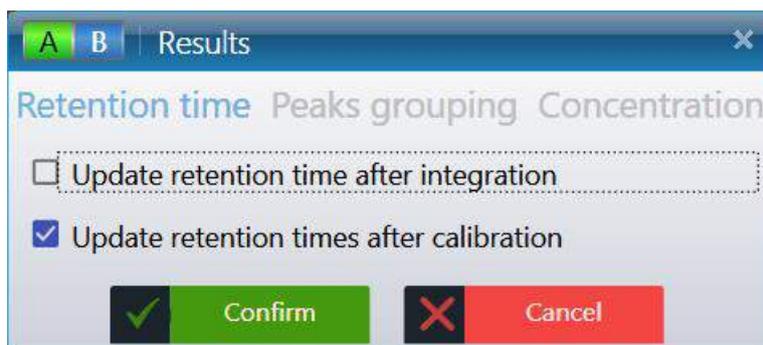
There too, the user selects the channel(s) on which this action has to be performed.  
Smoothing is not necessary to have a better integration. In most cases, the use of correct values for integration parameters allows a good integration of a noisy chromatogram.



### g) 2. Retention time update

The fact of not finding a peak may not be due to a lack of integration of the peaks but to a lack of identification of the peaks (non-compliant expected retention time, search window too narrow, ...). Peak identification is performed from the retention time programmed in the component table and the absolute and relative search window values. If one corrects such an error, it is not necessary to redo a calibration: the surface or the height of the peaks did not vary.

The menu "**Integration / Process configuration**" makes it possible to redo the identification of the peaks of the chromatogram.



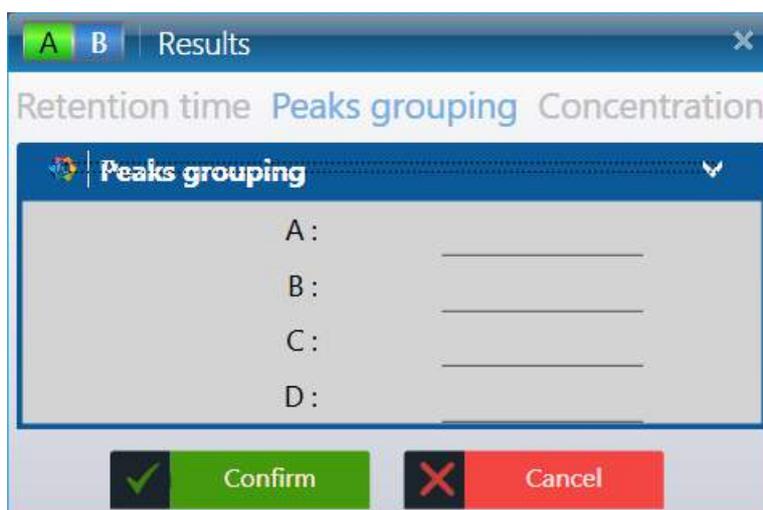
### g) 3. Peaks grouping

SOPRANE II offers the possibility to group separately integrated peaks so that they can be treated later as one and the same peak.

When we will edit the components table, we will see that it is possible to define 4 groups of peaks identified by the letters A to D.

To name each of these 4 groups of peaks, click on the **Integration** menu. To configure the processing part, click **Process configuration**.

This can be done before or after the components table edition.

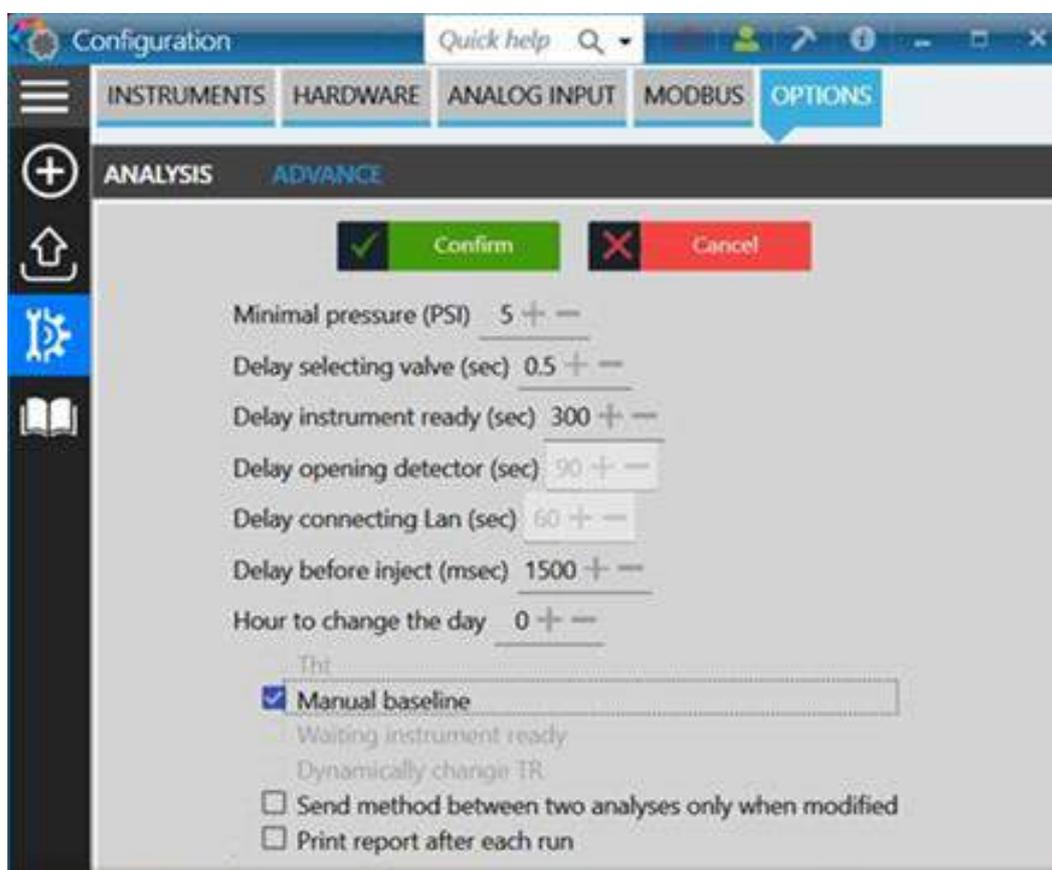


#### g) 4. Manual baseline

Sometimes, it may be necessary to go even further on a particular chromatogram and to impose a baseline correction which is normally impossible to be obtained with the integration events. These modifications are then specific of this chromatogram and do not have to be written in the analysis method.

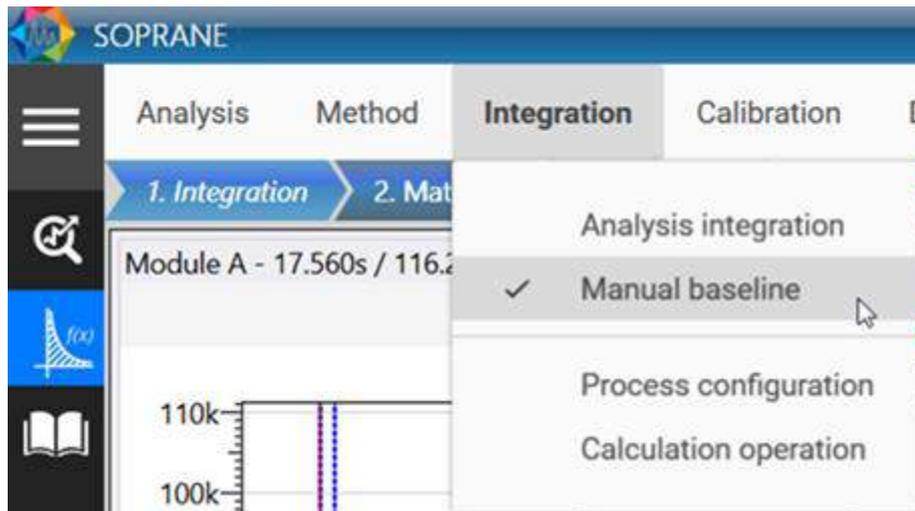
To activate the manual baseline, follow the next procedure:

1. Close Soprane II
2. Open the Configuration
3. Select the instrument
4. Go to the Option tab and select “Advance”
5. Check the option “Manual baseline”
6. Click on Confirm



7. Close the Configuration
8. Open the instrument with Soprane II
9. Go to the Process tab
10. On the “Integration” menu, check “Manual baseline”

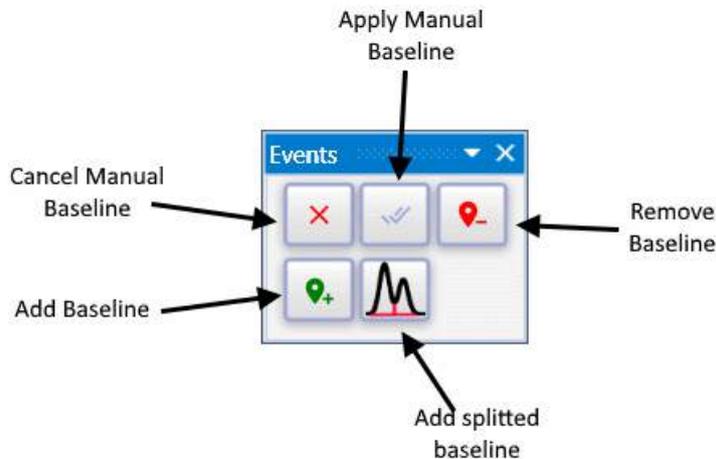




With the manual baseline feature, you will be able to add/remove and modify a baseline, and add a baseline split.

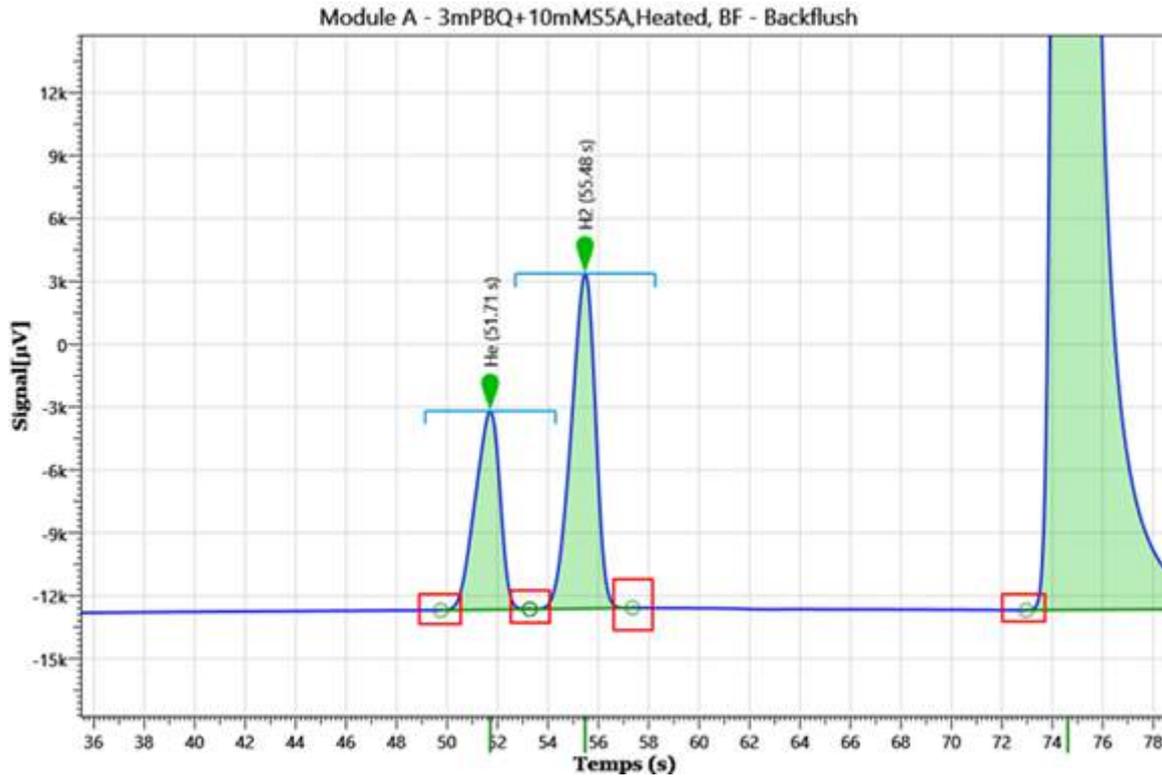
Be careful, manual baseline is not saved with the method, it is a feature to adjust results, so if you perform a batch processing or an integration, manual baselines will be cleared.

If the manual baseline is enabled, the following palette will be visible:



Once the "manual baseline" parameter is checked in the configuration and in the process part, you should have the beginnings and ends of the baseline surrounded (see image below). You can move these baselines by clicking on the circle while keeping the mouse pressed.



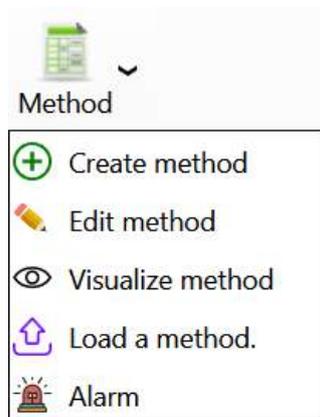


## 4.6. Post-analytical processing

### 4.6.1. Component alarms

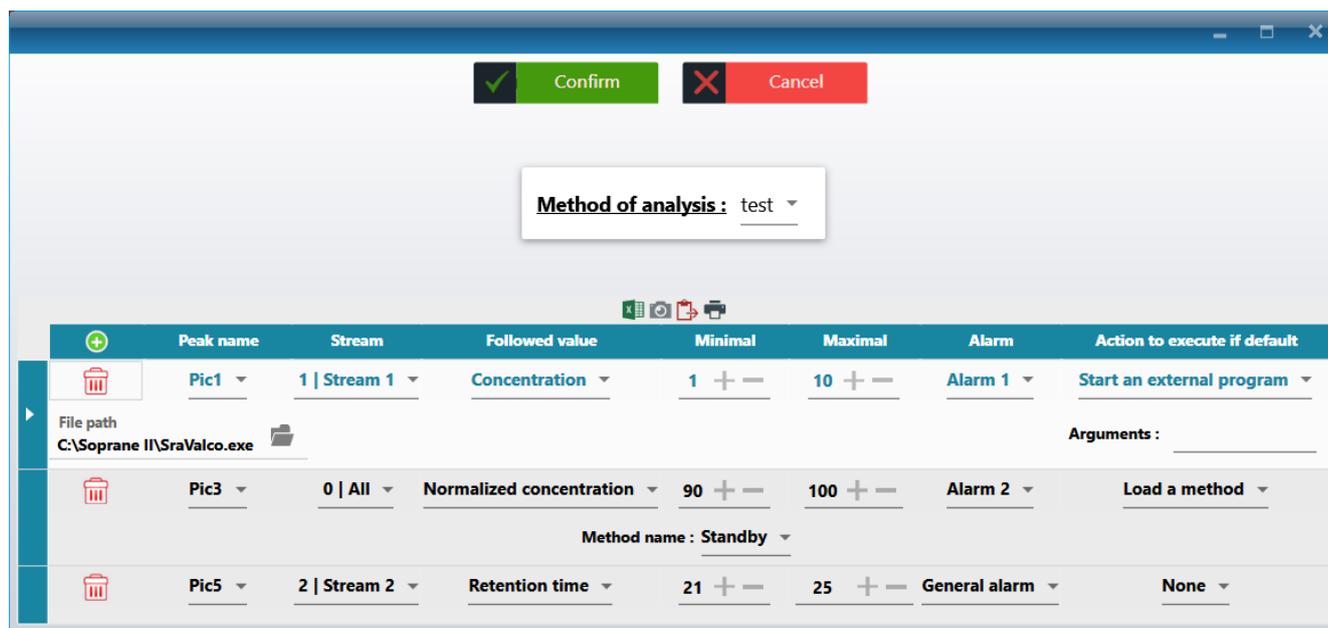
SOPRANE II offers the possibility to manage threshold alarms linked to components concentration. If relays have been defined (see chapter [Alarms](#)), 16 alarms are available. A relay output is generally used to indicate an analyzer defect. The other relays may be used for these threshold alarms.

Select "**Method / Alarms**".



For each of the alarms you must indicate:

- The monitored component reference (a drop-down list is used to avoid any error).
- The stream on which this component is monitored.
- The variable used for this default (raw concentration, normalized concentration, peak area or height).
- The lower threshold value.
- The upper threshold value.
- The number of the relay associated with this alarm.
- The action to execute if default (optional)



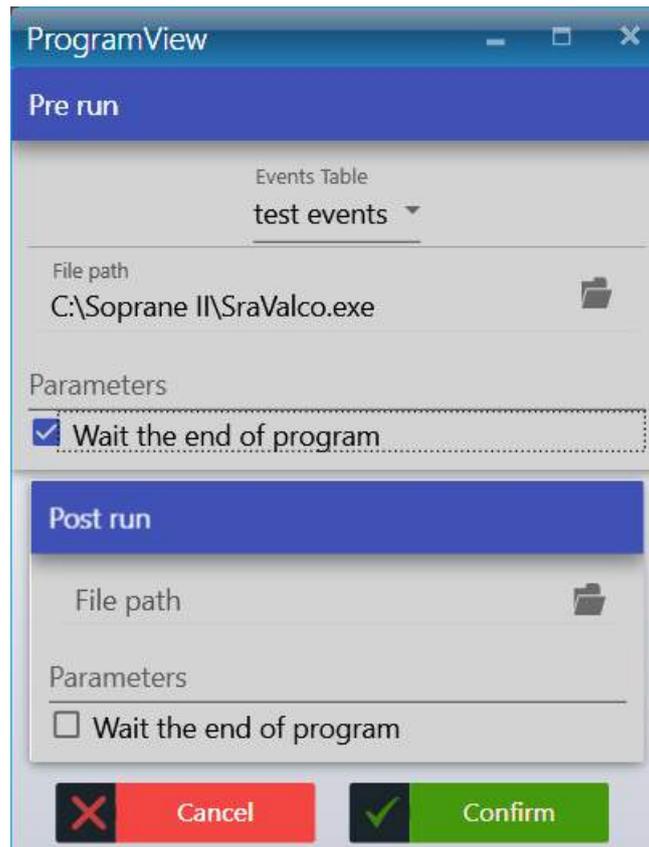
#### 4.6.2. Pre and post command

SOPRANE II offers the possibility to launch a program before or after the analysis via the **"Options / Program"** menu.

It is possible to launch a program before the injection and to wait or not the end of the execution of this program. If this option is unchecked, the injection cycle goes on and the pre-run program can lead to a Start of the MicroGC. If this option is checked, the injection cycle is stopped for the whole duration of the pre-run program (eg external pump).

We have mentioned (see chapter [Analysis event table](#)) that it was possible to start a custom event table (to switch stream, activate relays...) before the analysis (pre-run).





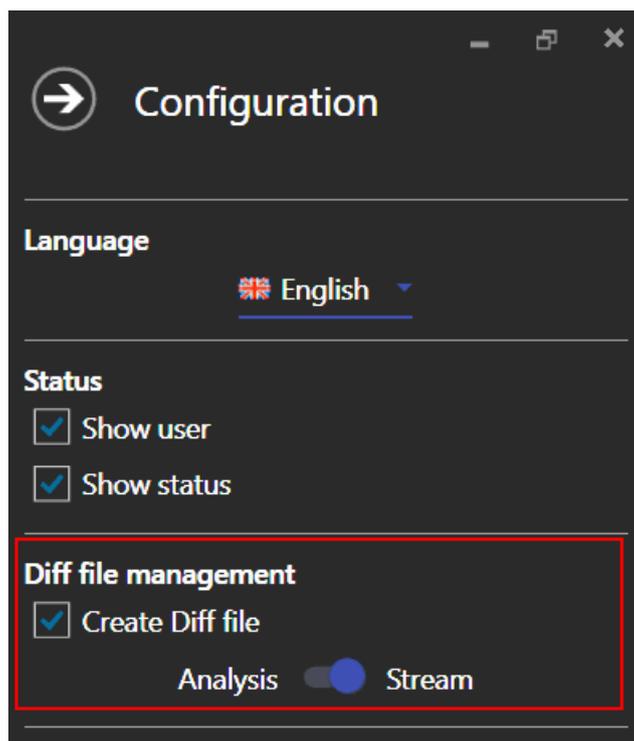
If necessary, a button, located at the right of the edit zone, is used to display directories and files and to directly select the user program.

### 4.6.3. Archiving

SOPRANE II allows to save the analyses results in files directly exploitable by a spreadsheet (DIFF extension). These files are also viewable in a text editor. The fields, whose value is in ASCII, are separated by a tabulation and the analyses by a line return.

The menu "**Parameters / Configuration / Results files**" allows the display of a flyout window where the name of the directory under which the results will be stored is indicated.





The data stored in these files are:

- The date and the hour of the analysis.
- The file name.
- The area and the concentration of the peaks (normalized or not, according to what was programmed).
- The sum of the concentrations (if this option were required).
- The post-analytical calculations eventually needed.

A new file is automatically generated each day (if daily management see chapter [Options management](#)). The file name will be name of the series if the field "Analysis" is checked otherwise, it will be named as the stream name.

## 4.7. Specific calculations

The analysis method, as described above (see chapters [Methods and sequences](#) and [Integration management](#)), is sufficient for all the ordinary calculations of chromatography.

SOPRANE II offers the possibility to go much further than the simple concentration calculations and to carry out complementary calculations. Specific calculation options are available if they are enabled in the license. (ISO 6976 calculations, LPG calculations, Combustion calculations, Annex calculations, Excel calculations).

The default values are those of perfect components at 1.01325 bars in compliance with ISO/DIS 6976:2016 and experimental standard X20-522.

The components detected and identified in the analysis are considered only if the name has a match in the reference tables.



#### 4.7.1. Calculations of the calorific value of natural gas (ISO 6976:2016)

Specific calculations reports according to ISO 6976:2016 can be generated at the end of the analysis. It is possible to create these reports with a series of calculations, a specific unit for PCI, PCS, and different temperature conditions.

##### a) Selection of calculations

The selection of calculations can be found in the "Analysis" tab, "Specific calculations" menu, "Calculations selection" command. 5 reports can be defined at each end of the analysis.

To define calculations "ISO 6976:2016", click "+" to add calculations (maximum 5) and "-" to reduce the number of reports.



For each calculation you can:

- Activate the calculation (tick "Used"). This action will allow the creation of the report at the end of the analysis. If the "Used" box is unchecked, the calculation parameters will be considered, but the report will not be created at the end of the analysis.
- Define the temperature conditions. The ISO6976 standard can be applied at specific temperature conditions. Select the desired temperature conditions.
- Select the unit for PCI and PCS calculation.
- Select the calculations to perform.

**These calculations are applicable only from standardized concentrations. Note that the unknown and not present components in the ISO6976 reference table are considered in the calculations of the standardized concentrations (and thus of the calculations of the standard). To exclude them, you must untick the display of the unknown components of the report and do not activate the compounds (outside the ISO6976 specification) of the component table of the method used.**

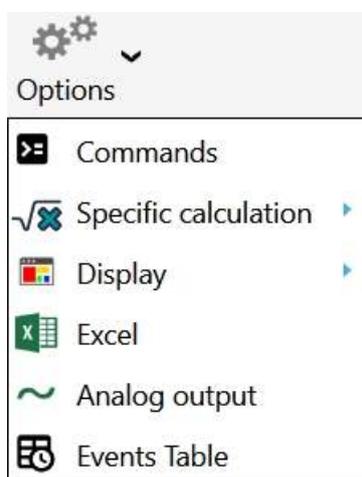
Note:

The Wobbe index and the compression factor will not be calculated if the selected unit is "Btu / scf", "MJ / mol", "kJ / mol".

### ***b) Definition of reference values***

The ISO 6976:2016 reference coefficients table is stored in the file "iso6976-2016.coef" (in the SOPRANE II installation directory).

To edit the values, go to the "Analysis" tab and click on the drop-down menu "Option" and select "Specific calculations" menu and click on the "Coefficients table" command.



The ISO 6976:2016 reference coefficients table can be found in the section of the tab "ISO6976 Natural gas".

The editor is under the form of a table containing the reference coefficients, a list containing the temperature and reference conditions specified in the ISO 6976 standard and a panel of commands.



Coefficients tables					
Iso 6976:2016		Combustion	ISO 8973:1999 - LPG		
	+	Component	Molar mass	SCV	Summation factor
1		CH4	16.042	892.920	0.049
2		C2H6	30.069	1564.350	0.100
3		C3H8	44.096	2224.030	0.147
4		nC4	58.122	2883.350	0.202
5		iC4	58.122	2874.210	0.189
6		nC5	72.149	3542.910	0.259
7		iC5	72.149	3536.010	0.246
8		neoC5	72.149	3521.750	0.225
9		nC6	86.175	4203.240	0.332
10		iC6	86.175	4195.640	0.311

**Temp. of reference**

T° Ref Combustion  
0°C

T° Ref Measuring  
0°C

**≡+ Insert**

**↺ Restore**

**⊗ Nb atoms**

**Ref coefficients of Air**

**💾 Save**

The table is composed of the columns "**Component**", "**Molecular mass**", "**SCV**" and "**Summation factor**". For each reference compound you will find its molar mass, reference SCV as a function of reference temperature conditions as well as the summation factor which also varies according to the reference conditions.

You can remove a component by clicking on the button . To add a component, click on . A new line will be added at the end of the table. To insert a component into the table at a specific position, click in a cell of the component which will take over the new component, then click on the "**Insert**" command. Enter the name and reference coefficients of this component and save the information by clicking on the "**Save**" button.

The user can redefine his own reference values for each temperature and reference condition. These values will be stored in the current analyzer database. At any time, the user can restore the original values by clicking on the "**Restore**" button.

If you change the temperature conditions (from 0°C / 0°C to 15°C / 0°C for example), the coefficients table will be updated according to this information. The SCV, and summation factors are different depending on the temperature conditions.

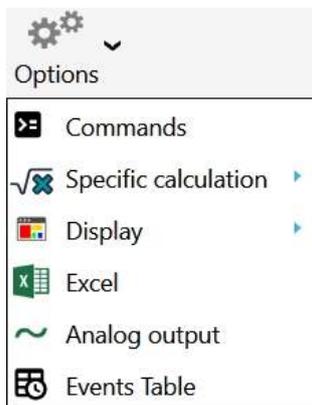
To restore the original table, click on the "**Restore**" command in the Coefficients Table window. SOPRANE II will display the coefficient values of the file "iso6976-2016.coef". Click on the button "Yes" to reset the analyzer reference coefficients.



### 4.7.2. LPG calculations (ISO 8973)

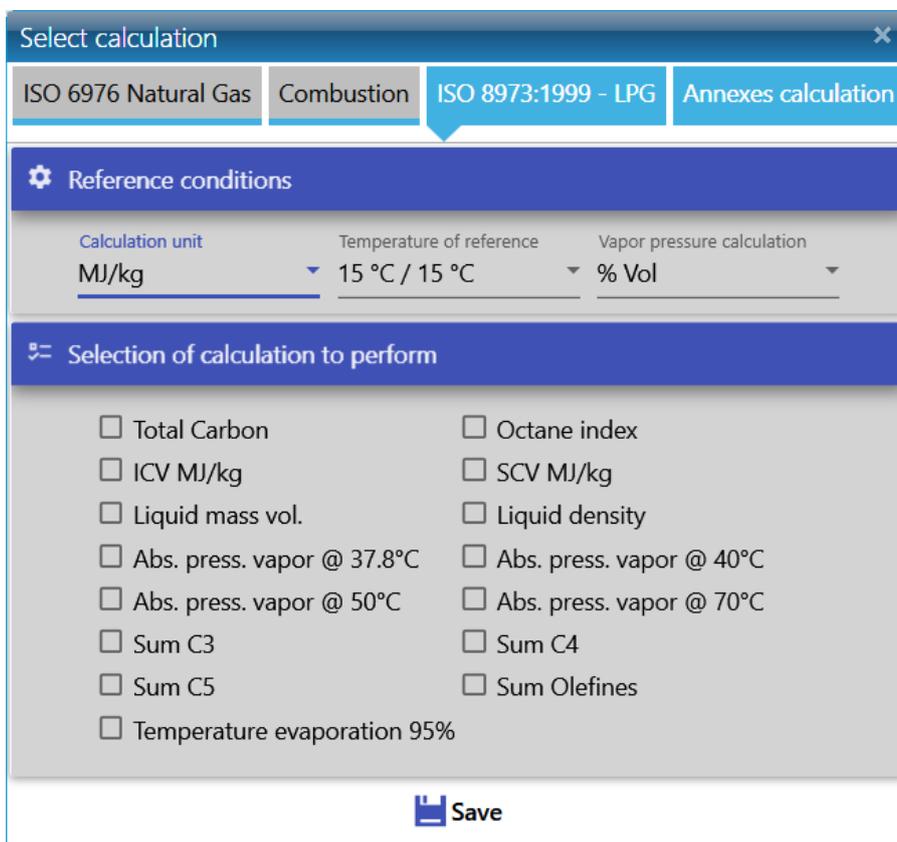
In the case of LPG analyzes, SOPRANE II can display a results report in appliance with the ISO 8973 standard. The user selects the reference parameters as well as the calculations to be carried out and the results will be generated at each end of the analysis.

To set the report, go to "**Analysis > Option > Specific calculations > Select calculations**" command. Click on the "ISO 8973 - LPG" tab to display the reference parameters.



#### a) Selection of calculations

The "ISO 8973 - LPG" tab displays the ISO 8973 calculation options. Select the basic parameters (calculation unit, reference temperature and concentration unit) and select the calculations to be carried out.

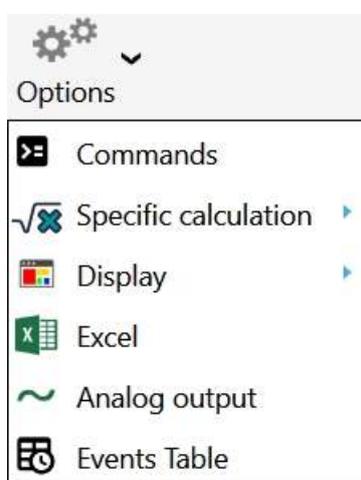


These calculations are applicable only with the standardized concentrations of the components of the analysis. The components unknown and not present in the reference table are considered in the calculations of the normalized concentrations (and thus of the calculations of the standard). To exclude them, you must untick the display of unknown components in the report and do not activate the compounds (out of specification) in the components table of the method being used.

The results will be displayed in a specific section of the final report that will be generated at each end of the analysis.

### b) Definition of reference values

The ISO 8973 reference coefficients table is stored in the "gpl.coef" file (in the SOPRANE II installation directory). To edit the values, go to "**Analysis > Option > Specific calculations > Coefficients table**".



Coefficients tables								
Iso 6976:2016		Combustion		ISO 8973:1999 - LPG				
	+	Component	Molar mass	Nb carbon	Sum C3	Sum C4	Sum C5	Coef. M Vol
1	🗑️	CH4	16.043	1	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	0
2	🗑️	C2H4	28.054	2	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	369
3	🗑️	C2H6	30.07	2	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	375.76
4	🗑️	C3H6	42.081	3	<input checked="" type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	521.33
5	🗑️	C3H8	44.097	3	<input checked="" type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	507.3
6	🗑️	iC4	58.123	4	<input type="checkbox"/>	<input checked="" type="checkbox"/>	<input type="checkbox"/>	562.98
7	🗑️	nC4	58.123	4	<input type="checkbox"/>	<input checked="" type="checkbox"/>	<input type="checkbox"/>	584.06
8	🗑️	1-Butene	56.108	4	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	601.15
9	🗑️	Iso-Butene	56.108	4	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	600.5
10	🗑️	Cis-2-Butene	56.108	4	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	627.2



The ISO 8973 standard reference coefficients table can be found in the section of the "ISO 8973 - LPG" tab.

The editor is presented under the form of a table containing the reference coefficients, a list containing the temperature and reference conditions indicated in the standard and a panel of commands.

The table is composed of the columns "Component", "Molar mass", "Nb carbon", "Sum C3" "Sum C4", "Sum C5", and "Coef M Vol", "Press abs Vapor @ 37.8, 50 and 70°C ", " Olefins "and" Octane index factor ".

You can remove a component by clicking on the button . To add a component, click on . A new line will be added at the end of the table. To insert a component into the table at a specific position, click in a cell of the component which will take over the new component, and then click on the "Insert a component" command. Enter the name and reference coefficients of this component and save the information by clicking on the "Save" button.

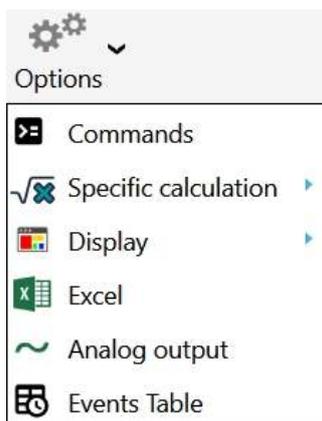
The user can redefine his own reference values for each temperature and reference condition. These values will be stored in the current analyzer database. At any time, the user can restore the original values by clicking on the button "Restore the original coefficients". This action will empty the current table (specific to the analyzer) and insert the default values of the gpl.coef file.

The user can also update this file from the current table.

### 4.7.3. Combustion calculations

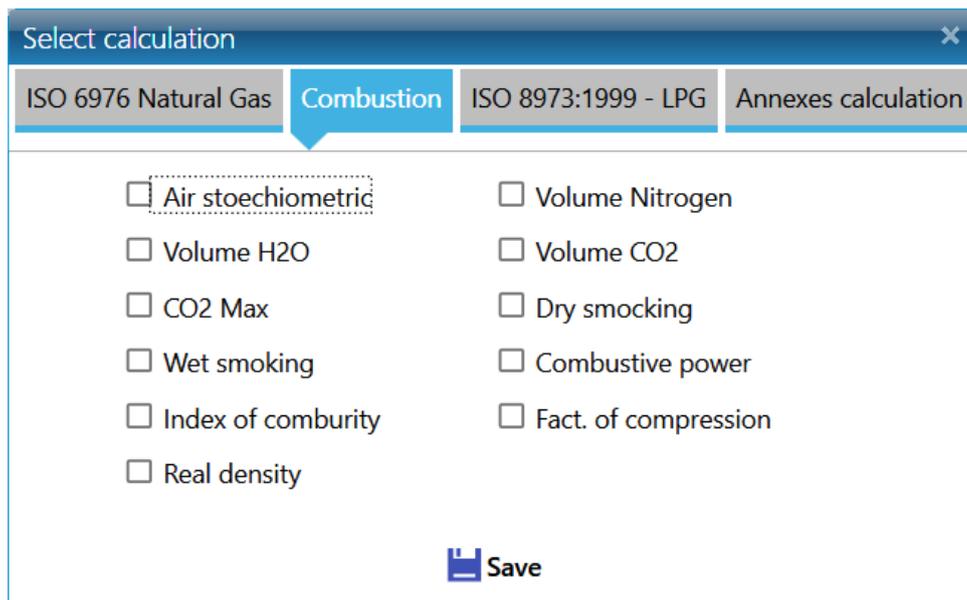
Increased attention given to the quality of combustion emissions and high cost of energy impose a greater interest in the optimization of the combustion in boilers and burners in general. The relationship between air and fuel, combustion products, are critical parameters that need to be monitored and controlled.

Soprane II carries out the combustion calculations and generates a report at the end of the analysis. Select the calculations to be integrated in the final report by going to the "**Analysis > Options > Specific calculation > Select calculations**".



In the calculation selection window, click on the "Combustion" tab and then check the calculations to be carried out. For these calculations, there are no reference coefficients.



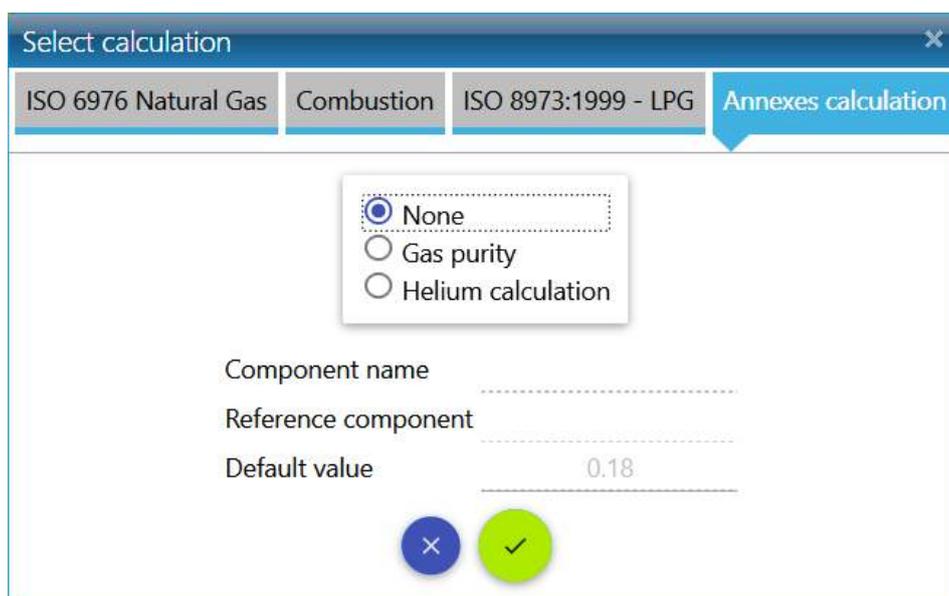


#### 4.7.4. Additional calculations

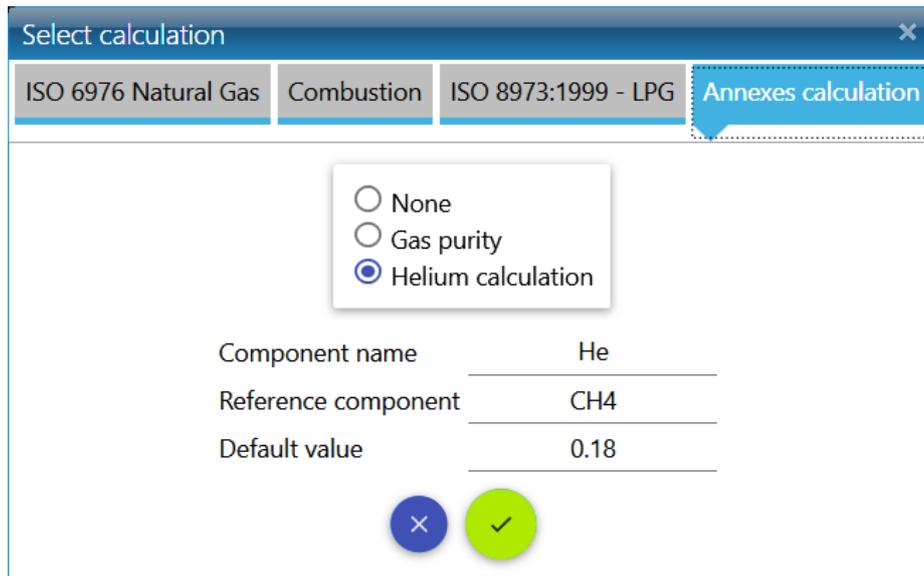
Other specific calculations can be applied to the analyzes results. For this, go to the tab "Annexes calculation". Check the box that corresponds to the calculation to be carried out. If you do not want to make calculations, check the box "None".

##### a) Gas purity

The gas purity is calculated with the standardized concentrations. The concentration of the referenced component (in this case helium) is calculated by sub-straying at 100 the sum of the standardized concentrations of all the other compounds of the analysis. If units are different from %, a calculation is applied to the standardized concentration to set it back to %.



**b) Helium calculation**



The Helium estimation is related to ISO 6976 and Natural Gas Analysis, it must be added to the ISO 6976 Calculation Option.

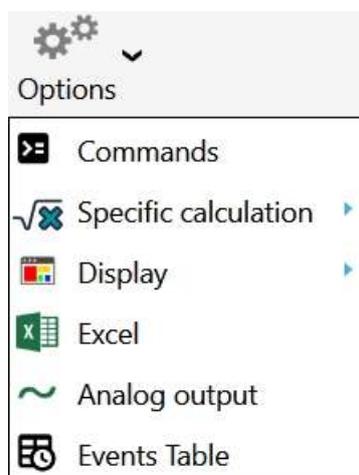
Helium is naturally present in Natural Gas, but is not measured by conventional GC analyzer (as Helium is used by carrier gas).

This option is used to calculate the Helium concentration, estimating it from the measured CH4 concentration.

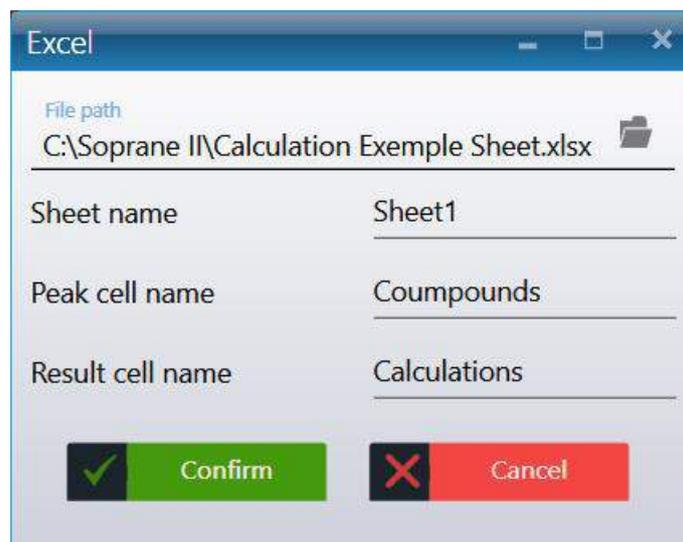
**4.7.5. Excel calculation**

A SOPRANE II option allows to establish the link with an EXCEL file to define any type of calculations. A few things are imposed, so that SOPRANE II knows where to write and where to read the data.

If the option exists, click on the drop-down menu "**Options**" and select "**Excel**"



The following window will appear:



The first line of this screen is the file path of the EXCEL file.

An EXCEL file can comprise several sheets, thus the second line corresponds to the reference of the sheet used for the data exchanges.

Two benchmarks are necessary and are in the column A: the first one is a cell with the text "**Compounds**" and the second one with the text "**Calculations**".

Before to make calculations, SOPRANE II prepares the worksheet.

For that, it seeks in column A the cell "**Compounds**". It is assumed that the following lines correspond necessarily to the name of the components, such as they are known by SOPRANE II (identification table programming). SOPRANE II may identify each component by this way.

Every time a component is found, its raw concentration is written in the same line, in the column B, then its normalized concentration, always in the same line in column C.

SOPRANE II then seeks, in column A, a cell with the text "**Calculations**".

The results calculated by the EXCEL sheet must necessarily be in the following lines, according to the following format:

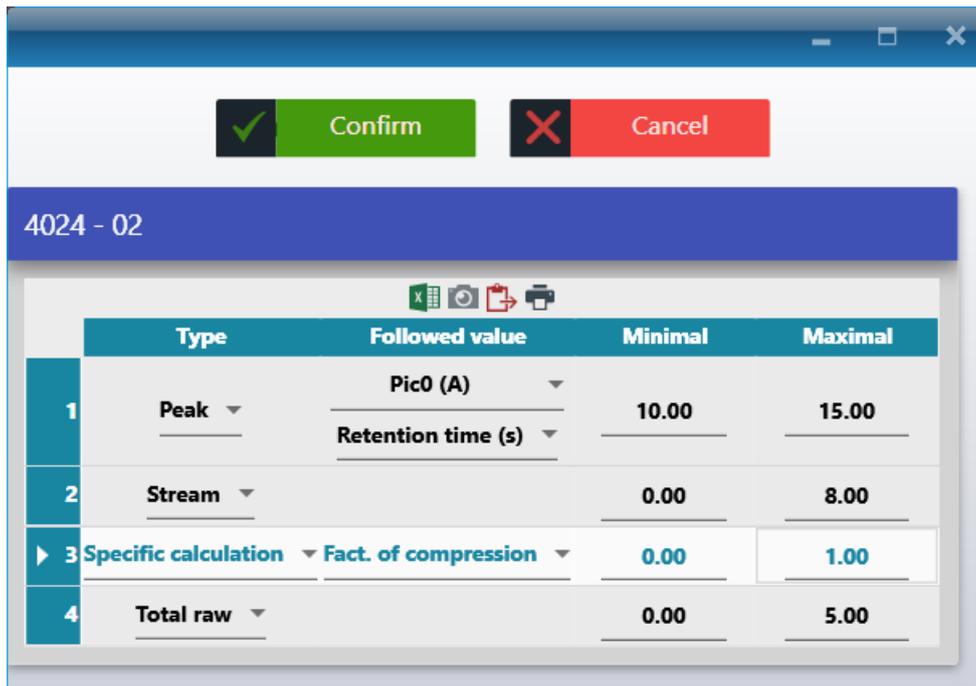
- Column A: name of the result
- Column B: description
- Column C: numerical value
- Column D: units
- Column E: number of decimals of the result.

The other cells of the sheet are free for the user who may use them to store constants or calculation formulas.

When SOPRANE II prints the result of an analysis, or when one wants to send the result of a calculation on a trend or a 4-20 mA output, calculation is referred by its name (Column A).







Here's the list of the different types of values that can be sent:

- Peak value (it needs to select the followed peak and which result to send (Retention time, Concentration, Area...))
- Current stream
- Specific calculation (need to select which type of calculation)
- Total raw

#### 4.8.2. Modbus

A specific software called SRA.Soprane.Modbus, allows the exchange of data between Soprane II and another computer via a Modbus industrial network.

Thus, the results of an analysis can be fully transmitted: date, time, stream, measurement or calibration, concentrations, calculation results.

The data that can be exchanged are stored in an address table. The transmission protocol complies with a standard which consists in requesting or transmitting a question and in response the value of the variable located at a given address is transmitted.

You simply have to define a table of exchange defining the variables that you want to read, their address and their format.

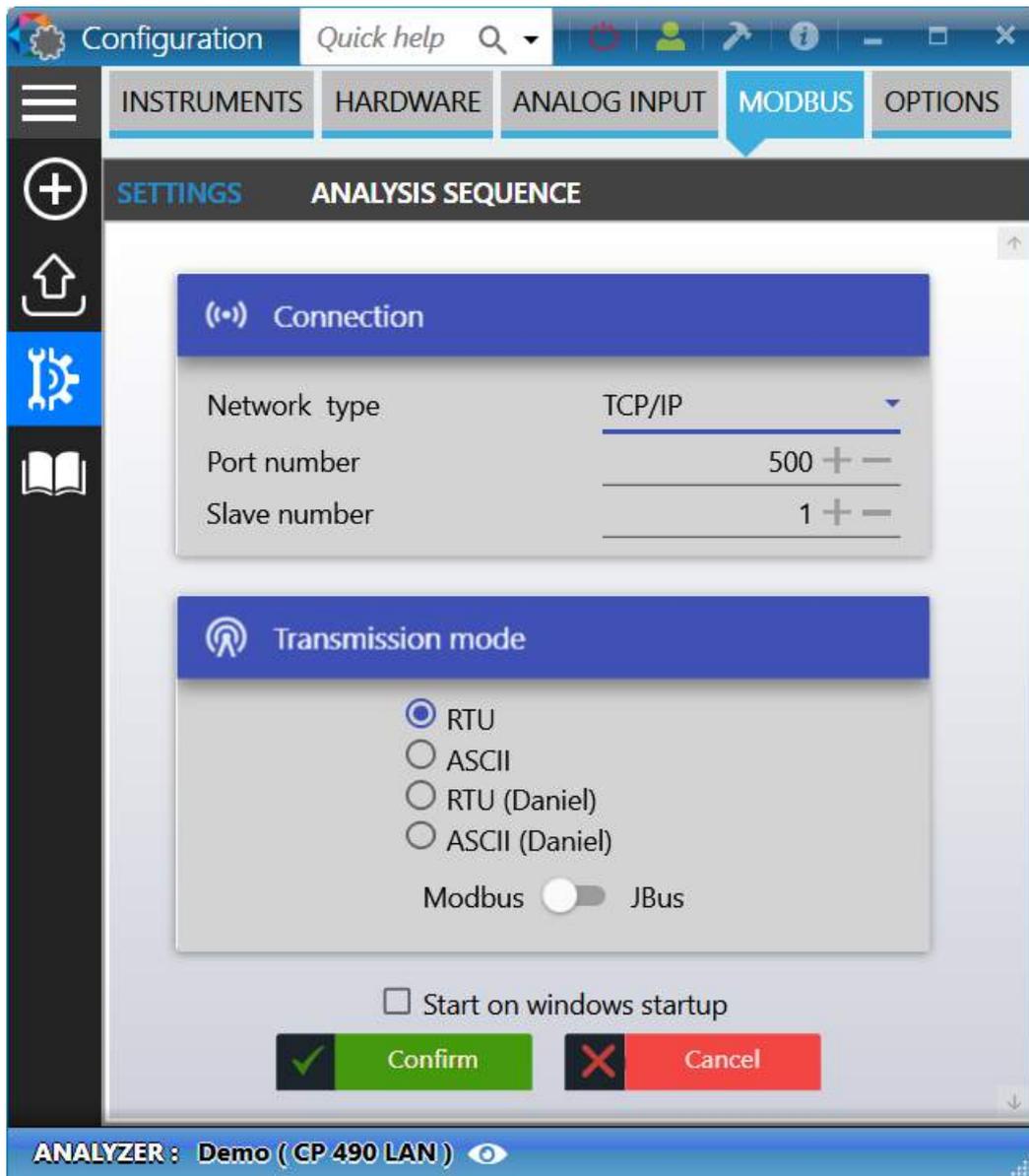
It is therefore necessary to first define the hardware configuration and to determine the address where any data will be written.

##### a) Hardware configuration

The configuration program allows to define this serial link configuration.

The configuration Modbus window is shown only if the installation includes a Modbus option.





In this window:

- Choose the bus type, the communication protocol to interact with the remote system.
  - If you choose Modbus to serial port, select the serial port used. In this case, the "Parameters" button is used to view and modify the transmission parameters (speed, number of bits, parity, number of stop bits, control type).
  - If you choose Modbus to TCP/IP, keep the 502 value for the port number.
- Indicate a slave number for SOPRANE II.
- Select a transmission mode.
- Choose to use a Modbus/Jbus transmission protocol.

By default, keep the transmission mode in RTU mode and the Modbus/Jbus unchecked.

Validate with the "Confirm" button and quit SOPRANE II Setup by confirming the saved changes.



**NOTE:**

The MODBUS software is automatically launched after Windows initialization. Consequently, the modification of the parameters will take effect only when Windows is started again.

**b) Software configuration**

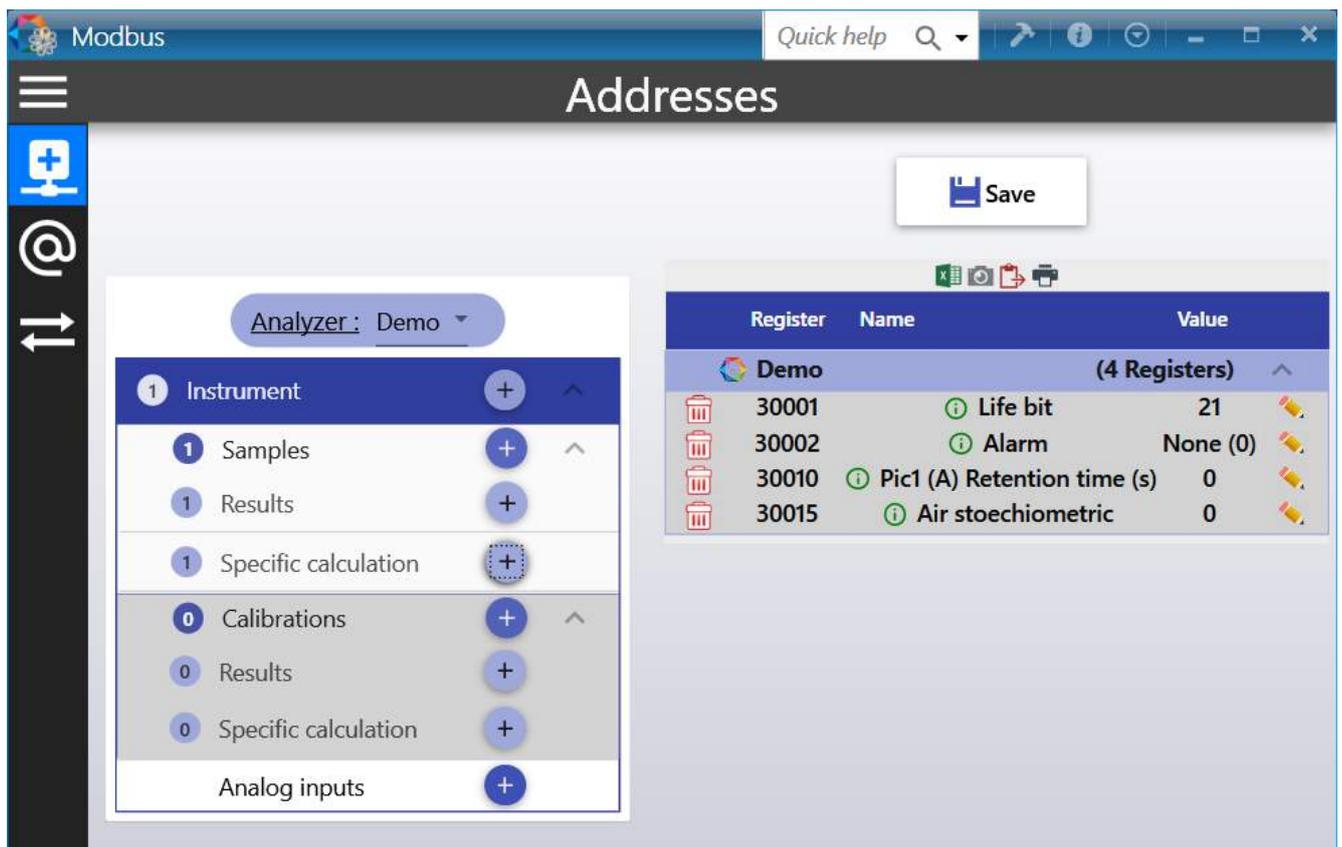
*Note: Before considering the configuration, it is better to perform some analyzes with Soprane II, create the table of peaks and select the calculations if there are any. Thus, at each end of analysis, the MODBUS software will retrieve the names of all these data and the configuration of the addresses will be facilitated.*

The MODBUS software is used to assign an address and a scale factor for each variable. This software is running as a background task and, under normal functioning, its window is not shown.

If the MODBUS software is running correctly, the SRA Instruments icon must be present in the notification area.



Double-click on the icon and click on **Open**. The following window is opened:



The data are separated in 5 levels:

- The system variables of the analyzer: "**Instrument**"
- The system variables of the analysis: "**Samples / Calibrations**"
- The values in relation with components: "**Results**"
- The values in relation with calculation: "**Specific calculation**"
- The values in relation with analog inputs: "**Analog inputs**"

For each data transferred an address and a type of value are assigned and for the results, a coefficient when submitted as an integer (short or real).

This setting is performed directly in the MODBUS software via the "**Addresses**" tab.

In a first time, it is better to test whether the communication is correct (see Chapter [Modbus Test](#)).

The "**Raw data**" tab contains all Modbus values in four different tables. Two tables store on/off discrete values (coils) and two store numerical values (registers). The coils and registers each have a read-only table and read-write table. Each table has 9999 values. Each coil or contact is 1 bit and assigned a data address between 0000 and 270E. Each register is 1 word = 16 bits = 2 bytes and has data address between 0000 and 270E.

The "**Communication**" tab contains all Modbus transmission and receptions.

## b) 1. Instrument variables

The variables that can be used are:

- **Selected stream:** in the case of a multi-stream application, this value indicates the current selected stream.
- **Inject top:** this value is set at 1 each time an analysis is started.
- **Analysis type:** this value indicates the type of analysis performed (0 = blank, 1 = sample, 2 = standard).
- **Alarm:** this value indicates the different alarms obtained during the analysis in the SOPRANE II software. It can take several values; these values are obtained according to a combination of bits.
  - 0: no alarm
  - 1: chromatograph default
  - 2: cycle stopped
  - 4: invalid or unknown method
  - 8: defective connection with the chromatograph
  - 16: unable to process results
  - 32: sample flow rate default (option)
  - 64: default with stream selector or multi-position valve (option)
- **Life bit:** this variable is used to monitor the transmission. Its value is updated every second.
- **Status:** this variable is used to monitor the Soprane II cycle. It can take the following values:
  - 0: Wait
  - 1: Chromatograph ready
  - 2: Waiting for start
  - 3: Waiting for injection (sampling)
  - 4: Analysis in progress



- 5: Recovering points
- 6: Analysis completed
- 7: Bake out
- 8: Error processing
- **GC Ready:** this variable allows to know the state of the chromatograph. It can take the following values:
  - 0: not ready
  - 1: ready
  - 2: default
- **Start:** this variable is used to launch analyses via SOPRANE II. It can take several values:
  - 0: No analysis requested, or cycle stopped after the current analysis.
  - 1: Start of analyses in simple analysis mode.
  - 2: Start a single sequence.
  - 3: Start of analyses in automatic mode.
  - 4: Start of analyses in calibration mode.
- **Run time:** indicates at time  $t$ , the time elapsed since the start of the analysis.
- **Sequence/number:** this variable is used to indicate the number of analyses requested in the case of an analysis request type 1. For the other types, it indicates the number of the sequence that we want to carry out. This assignment is carried out in the SOPRANE II - Setup software via the menu "Modbus / Analysis sequence":

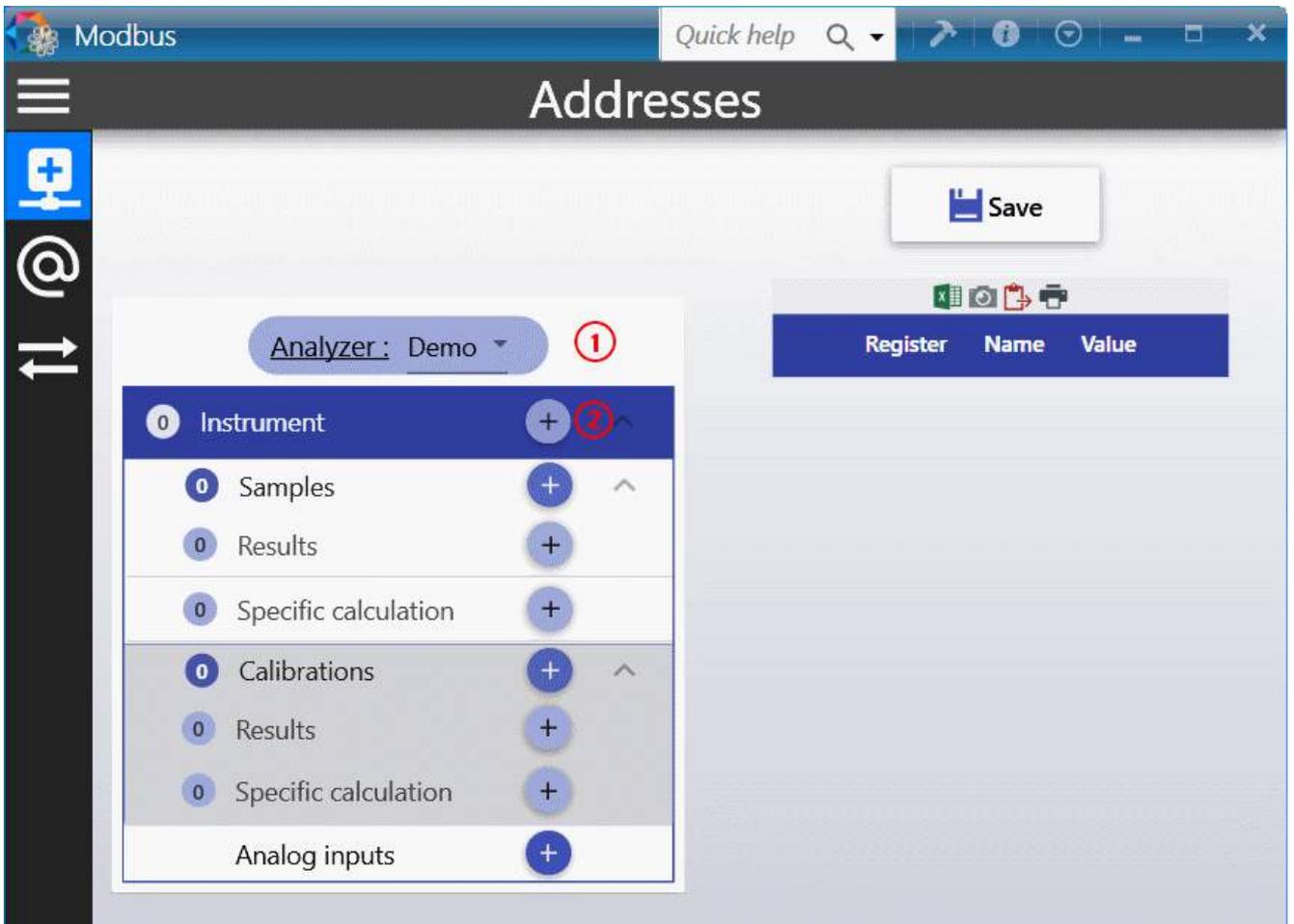


Note that if this variable has a value of zero, either the analyses are not launched or the analyses are stopped at the end of the current analysis.

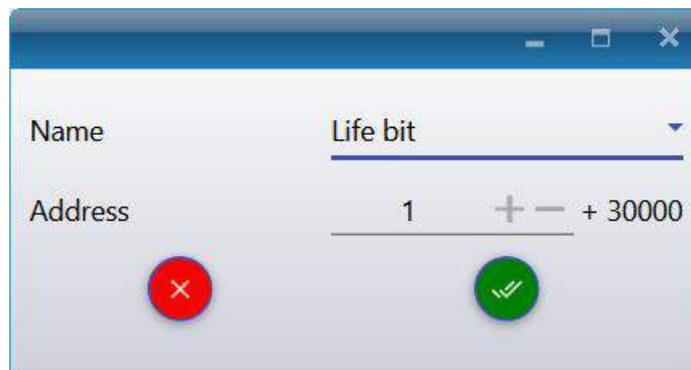


To add these variables:

- Select the analyzer
- Click on the add button of the parameter Instrument



- In the window that appears, select the variable, type the address number.



To launch analyses, simply put a value in the Analysis and Sequence/Number variable. The analyses are performed as long as the value of the Analysis variable is not changed and null. You can change the sequence number at will.



## b) 2. Sample/Calibration values

The variables that can be used are:

- **The year** of the analysis
- **The month** of the analysis
- **The day** of the analysis
- **The hour** of the analysis
- **The minutes** of the analysis
- **The seconds** of the analysis
- **The data ready flag:** Modbus uses this variable and passes it to 1 to indicate that the results of the analysis are available. It is up to the remote computer to reset it to 0 when it has read these values.
- **The compounds alarm:** the value of this variable is decomposed into 16 bits. If a SOPRANE II alarm is triggered, the bit corresponding to this alarm will be active.

To add these variables the principle is the same as previously:

- Click on Add in "Samples" or "Calibration" mode
- In the menu bar, select "Addresses / Add"
- In the window displayed, select the variable, enter the address number

## b) 3. Result values

MODBUS offers the possibility to choose among this range of values:

- Area
- Raw concentration
- Normalized concentration
- Height
- Retention time

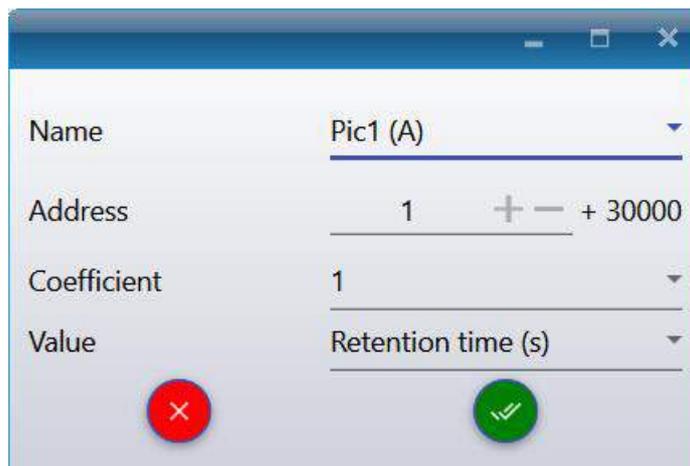
To add these variables the principle is the same as previously:

- Select the analyzer
- Click on "Results"
- In the window that appears, select the component name, the address number, the coefficient and select the type of value.

The name of the component (which must be EXACTLY the same as what is programmed in the SOPRANE II component table) must be entered in the combo box.

If you have done analyses before and that the components are correctly identified, the list of components will be available.





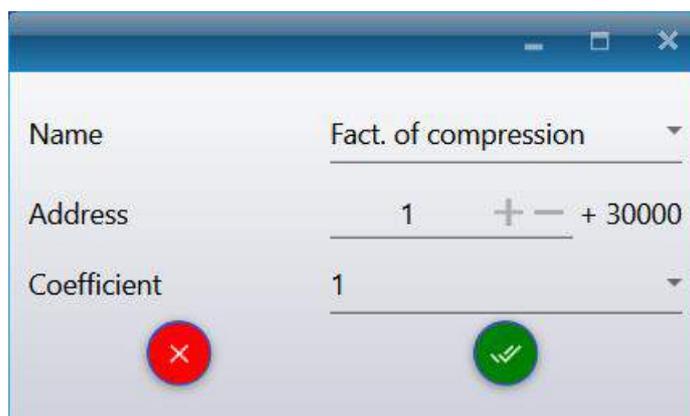
The coefficient parameter is used to transfer the decimals of the value. Indeed, the values transmitted with this choice of 'type' are always integer values and therefore the decimals are deleted. For example, if you want to have two digits after the decimal point, the trick is to set the coefficient to 100 before sending and it will be enough to divide by 100 the value received to obtain a value with two decimals. **Caution, the maximum value sent cannot exceed 65535 with the type 'integer'** so it is necessary to correctly configure this coefficient according to the unit of the component. This maximum value can be changed with the 'Full scale' value in the "Settings" menu (the "hammer" icon on the top right of the window) (see chapter [Modbus options](#)).

**b) 4. Specific calculation values**

SOPRANE II can perform post-analytical calculations. These calculations are, for example, the molar mass, the density, the specific gravity, the calorific capacities, etc. Two sets of calculations can be used, the calculations possibly being the same but carried out under different temperature or pressure conditions.

To add these variables the principle is the same as previously:

- Select the analyzer
- Click on "Specific calculation"
- In the window that appears, select the value, the address number and the coefficient.



The coefficient parameter is used to transfer the decimals of the value. Indeed, the values transmitted with this choice of 'type' are always integer values and therefore the decimals are deleted. For example, if you



want to have two digits after the decimal point, the trick is to set the coefficient to 100 before sending and it will be enough to divide by 100 the value received to obtain a value with two decimals. **Caution, the maximum value sent cannot exceed 65535 with the type 'integer'** so it is necessary to correctly configure this coefficient according to the unit of the component. This maximum value can be changed with the 'Full scale' value in the "**Settings**" menu (the "hammer" icon on the top right of the window) (see chapter [Modbus options](#)).

## b) 5. Analog input values

To add these variables the principle is the same as previously:

- Select the analyzer
- Click on "Analog values"
- In the window that appears, select the analog input name, the address number and the coefficient.

The name of the analog value (which must be EXACTLY the same as what is programmed in the configuration (see chapter [Analog input management](#))) must be entered in the combo box.

The coefficient parameter is used to transfer the decimals of the value. Indeed, the values transmitted with this choice of 'type' are always integer values and therefore the decimals are deleted. For example, if you want to have two digits after the decimal point, the trick is to set the coefficient to 100 before sending and it will be enough to divide by 100 the value received to obtain a value with two decimals. **Caution, the maximum value sent cannot exceed 65535 with the type 'integer'** so it is necessary to correctly configure this coefficient according to the unit of the component. This maximum value can be changed with the 'Full scale' value in the "**Settings**" menu (the "hammer" icon on the top right of the window) (see chapter [Modbus options](#)).

## c) Modbus Test

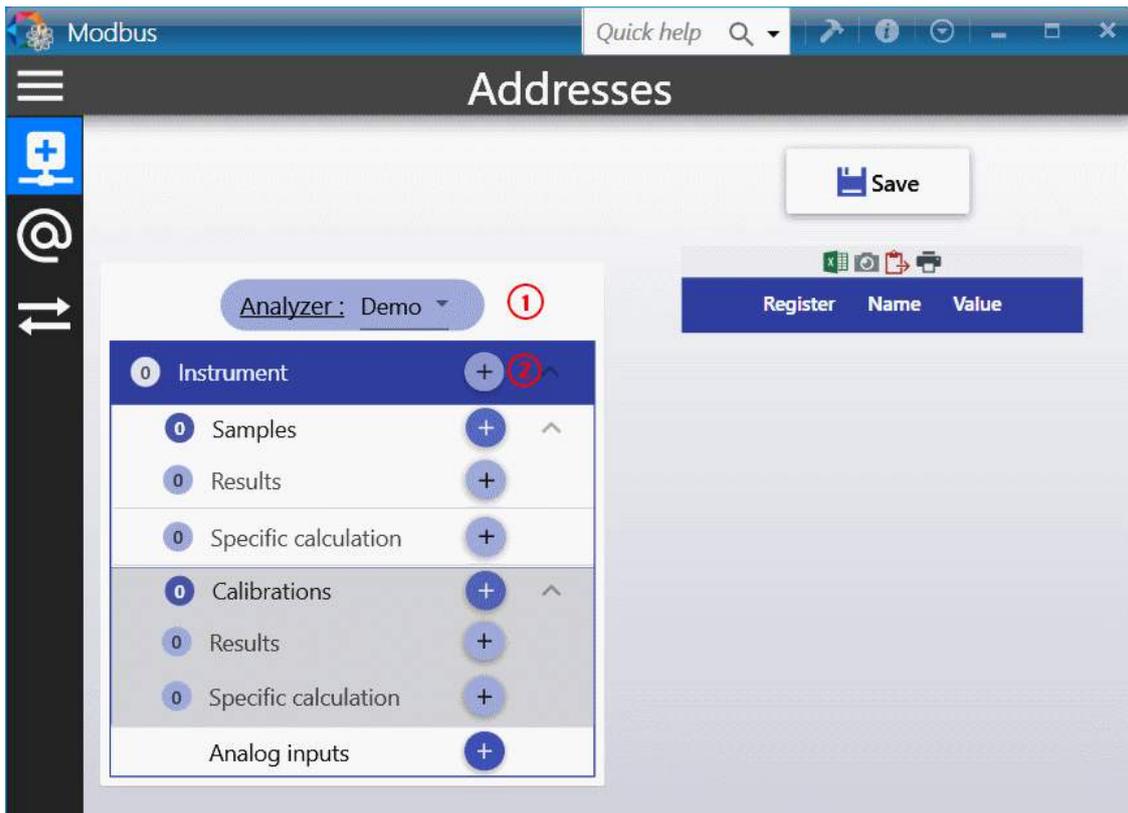
### 1. Communication tests

In a first time, it is better to test if the communication is correct.

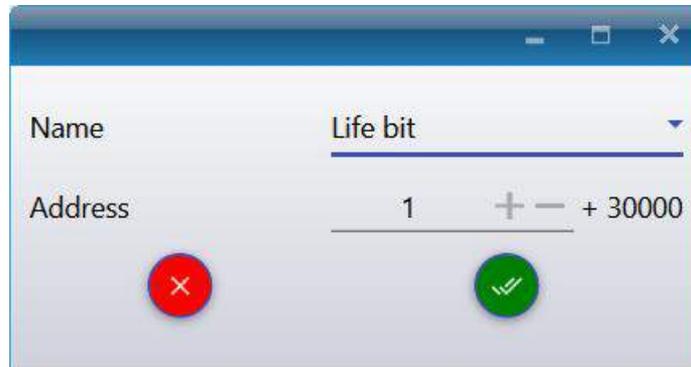
Configure the life bit parameter at address 1 with the "**Addresses**" menu.

Select **Instrument** and click on the "**Add**" button.





Select the following parameters and confirm with the validation button.



From the main Modbus screen, click on "Save".

From your supervisor:

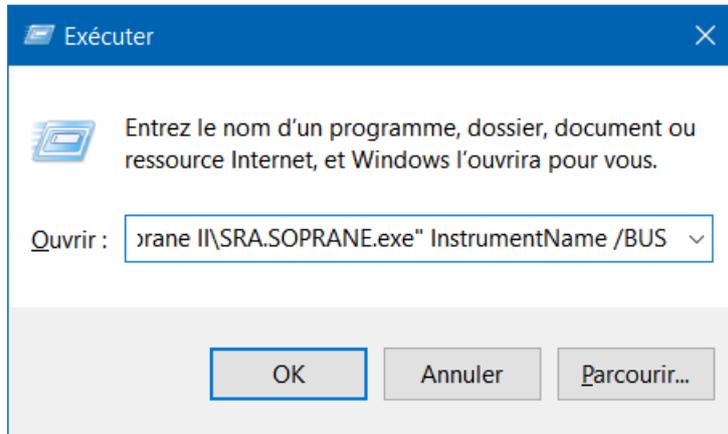
- Check that the configuration corresponds to the configuration defined in SOPRANE II: communication medium, IP address if TCP/IP mode or communication protocol (speed, parity) and slave number if serial link.
- Program a Modbus reading of 3 first addresses in integer (addresses 1, 2 and 3). Indeed, in some cases, there may be an offset of an address and therefore by defining a reading frame as well, this will enable you to check if the address numbers match. It is better to provide a rather long refreshing time (> 100 ms or even every second) because the values evolve only after each analysis and so this function does not use too many resources on the PC.

If the reading is correct, then the configuration of the addresses can be envisaged.



## 2. Value transmissions

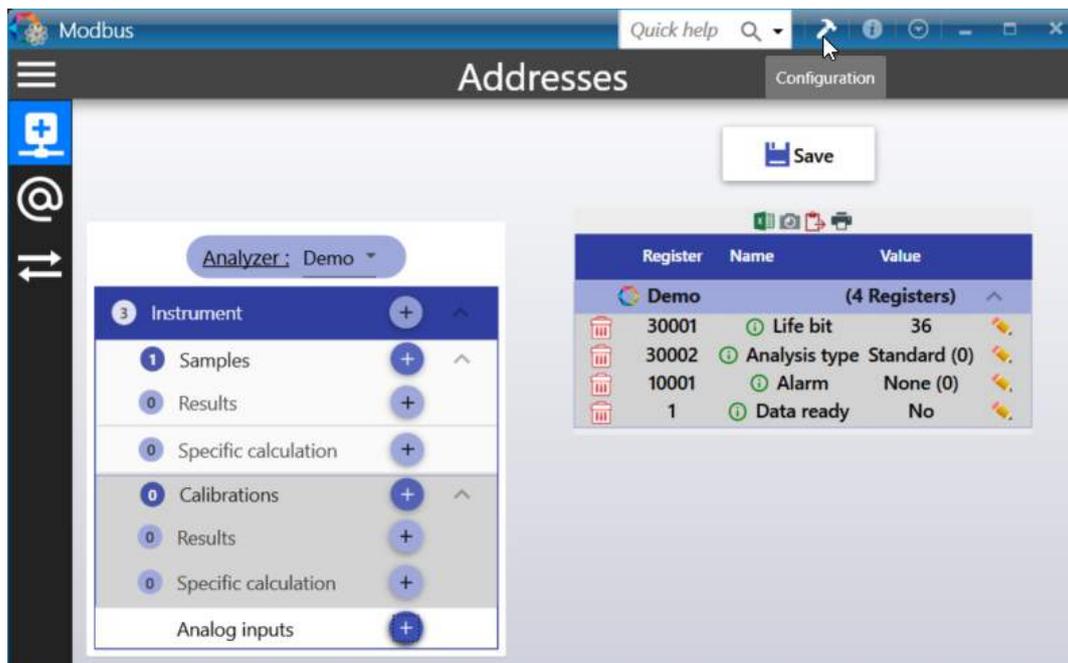
The results of the analyses are sent at each end of analysis. Unfortunately, this is not practical during the communication tests. There is a possibility to send the results after each reprocessing of analyses. For this, it is necessary to launch Soprane II from the Windows Run menu by entering the following line: "C:\Soprane II\SRA.SOPRANE.exe" InstrumentName /BUS (the Soprane II path between quotes followed by the name of the instrument and the parameter /BUS)



Then from the result table of Soprane II, select several analyses, right click and select "Batch processing", select the method then the analysis and validate (see chapter [Batch reprocessing](#)). The results are transmitted.

**Be careful, if you launch Soprane II each time this way, the results will be sent at each end of analysis and also at each reprocessing.**

### d) Modbus options



- **Number of decimals:** allows you to set the number of decimal places to be displayed for the display of all the values in the main window of the software.
- **Full scale:** In RTU mode, and if the format of the values is 16-bit integer it is necessary to specify a full-scale value that is used to convert the data to 0-10000 or 0-65535 scale. In this mode, the value representing the constituent, or the calculation is transmitted after being converted to a number in the range 0-10000 or 0-65535.  
Let us assume a component with a concentration of 5. The programmed scale value is assumed to be 20. Here we select a scale of 10000, which means that 20 becomes 10000. The value transmitted to the host computer will be 2500.
- **Float address:** If you have chosen to transmit the results in ASCII mode (Daniel mode), the values are not converted. The software then asks for a real variable address. SRAMODBUS considers that all addresses below this address correspond to integer variables (stored on 16 bits), and all higher addresses correspond to real variables stored on 32 bits.
- **Swap 32 bits integer bytes:** if the option is checked, the low weight and the high weight of the values transmitted in the 32-bit integer format are inverted.
- **Swap Floating Point bytes:** if the option is checked, the low weight and the high weight of the values transmitted in the real format are inverted.
- **Delay to refresh before alarm:** If the values are not refreshed after this time, MODBUS will raise an alarm for no refresh.
- **Delay to reset data flag:** at the end of the analysis, the data flag changes to 1. After the set delay, the flag returns to 0. If the delay is 0, this option is not enabled.
- **Client resets "data flag":** if the option is checked, it is up to the client to set the data flag to 0. Otherwise, when SOPRANE II restarts an analysis, the flag automatically returns to 0.

## 4.9. Chart

The graphic is a very useful element to display a signal, it also offers a wide range of features like zoom on a signal or axis, moving on the graph...

### 1. Zoom in / Zoom out

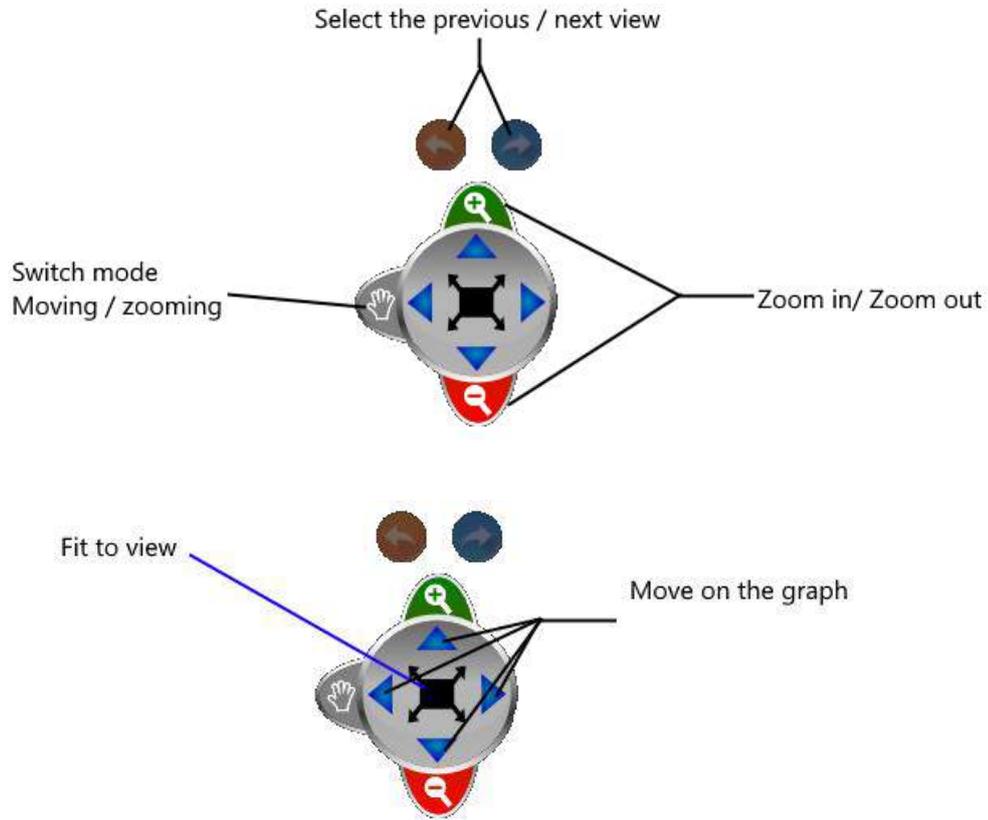
- Scroll the mouse wheel on the graph to zoom in / zoom out
- Select an area of the chart
  
- Scroll the mouse wheel on the horizontal axis to horizontally zoom in / zoom out horizontally
- Scroll the mouse wheel on the vertical axis to zoom in / zoom out vertically
- Double right click on the horizontal or vertical axis to zoom
- Double left click on the horizontal or vertical axis to zoom out

### 2. Navigation

- Drag the mouse over the horizontal or vertical axis to move on the graph
- Ctrl + Drag the mouse to move on the graph



### 3. Palette



### 4. Shortcuts

- F11: Screenshot of the graphic in the clipboard
- Ctrl + S: Saves the graphic in image format

## 4.10. Use of data tables

### 4.10.1. Exporting data from data table

In most of the tables, data can be exported at any time.

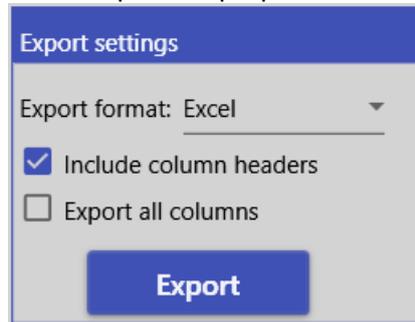
The following buttons      allow different export actions.

- : Exports data in an exploitable format by Excel, CSV or a printable file (see chapters [Export to Excel](#), [Export to Csv](#), [Export to Xps](#) and [Export to Diff](#) for more details).
- : Copies the table in the clipboard in image format.
- : Copies the table values in the clipboard.
- : Proposes a print preview and prints the results if desired.
- : Displays a configuration window for the corresponding table.



### a) Export to Excel

By clicking on the button , a window will open and propose a list of formats to be exported. Choose Excel.



An option allows to include column headers; if this option is unchecked, the columns will have no title.

See the following chapters for more export options:

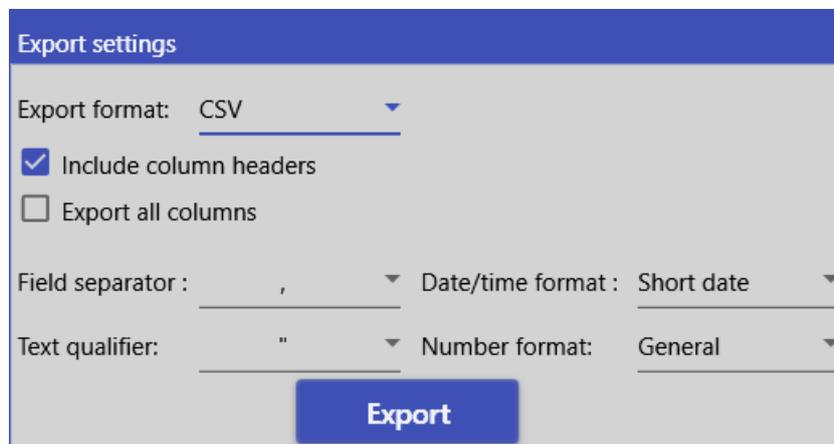
[Export to Csv](#)

[Export to Xps](#)

[Export to Diff](#)

### b) Export to Csv

By clicking on the button , a window will open and propose a list of formats to be exported. Choose CSV.



An option allows to include the column headers; if this option is unchecked, the columns will have no title.

The choice of the column separator offers the following choices:

- ; (semicolon)
- , (Comma)
- Tab

The different types of text delimiters are double quote (") or single quote (') characters.



Several date formats are available:

- Short date (day/month/year)
- Full Date (example Tuesday, October 18, 2016)
- Full date and short time (example Tuesday 18 October 2016 09:05)
- Full date and long time (example Tuesday 18 October 2016 09:05:45)
- Short date and short hour (example 18/10/2016 09:05)
- Short date and long time (example 18/10/2016 09:05:45)
- Month and day
- Year and month

The different digital formats can be of different types:

- General (most compact format)
- Fixed point (full and decimal digits with an optional negative sign)
- Scientific (Exponential)
- Two decimals
- Three decimals

See the following chapters for more export options:

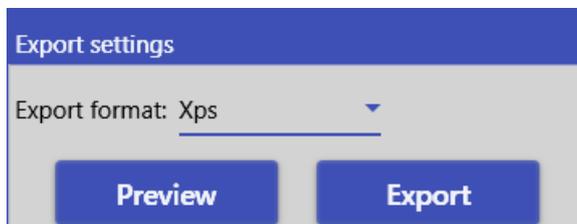
[Export to Excel](#)

[Export to Xps](#)

[Export to Diff](#)

**c) Export to Xps**

By clicking on the button , a window will open and propose a list of formats to be exported. Choose XPS. A preview is available before export.



See the following chapters for more export options:

[Export to Excel](#)

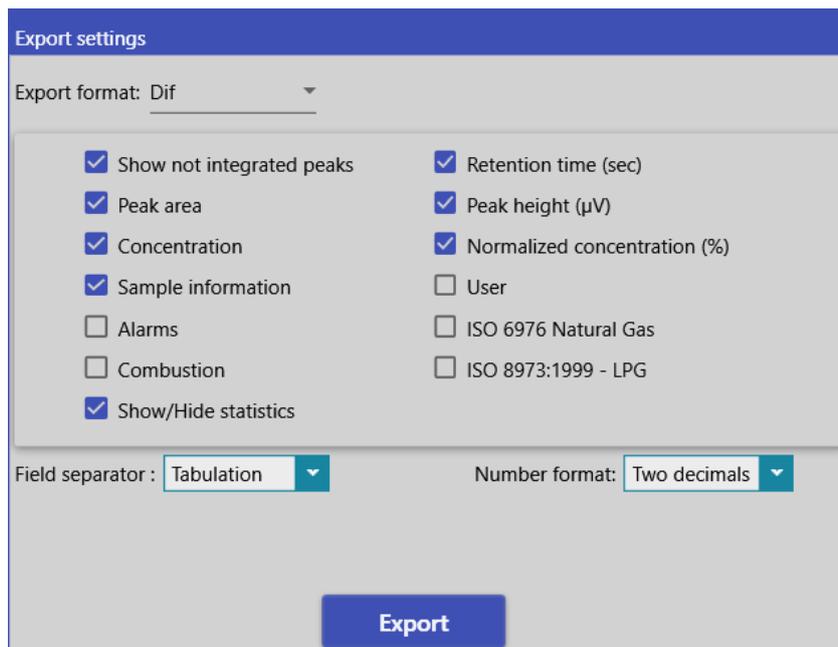
[Export to Csv](#)

[Export to Diff](#)

**d) Export to Diff**

By clicking on the button , a window will open and propose a list of formats to be exported. Choose Diff.





SOPRANE II allows to save the analyses results in files directly exploitable by a spreadsheet (DIF extension). These files are also viewable in a text editor. The fields, whose value is in ASCII, are separated by a tabulation and the analyses by a line return.

See the following chapters for more export options:

[Export to Excel](#)

[Export to Csv](#)

[Export to Xps](#)

#### 4.10.2. Filter data

##### *a) Automatic filtering*

Most of the tables in SOPRANE II have the ability to filter columns directly at the table level like an Excel spreadsheet.

By default, when automatic filtering is enabled, a drop down that displays the associated column's distinct values. Through this drop down, the auto-filter values that are used to automatically filter the data items can be modified.



Analysis	Injection date	Serie	Method	Pic0...	Pic1
	01/01/2015				
	11/17/2016				
Analyse_676	8/29/2016 3:40 PM	Analyse			
Analyse_677	8/29/2016 3:42 PM	Analyse			
Serie BF 4.5_001	10/25/2016 3:21...	Serie BF 4			
Serie BF 4.5_002	10/25/2016 3:22...	Serie BF 4			
Serie BF 4.5_003	10/25/2016 3:24...	Serie BF 4			
Serie BF 4.5_004	11/3/2016 3:39 PM	Serie BF 4			
Serie BF 4.5_005	11/3/2016 3:41 PM	Serie BF 4			
Serie BF 4.5_006	11/3/2016 3:57 PM	Serie BF 4			

**b) Customized filtering**

Customized filtering represents a row in which values can be entered to filter the items in the corresponding columns.

When a single value is entered in a cell, the elements of the corresponding column are filtered according to the filtering criterion.

For example, in the following table, only the series of analyzes containing the "Air" field are displayed.

Analyse	Date d'injection	Série
		Air
16020402_Air_001	2/4/2016 5:17	16020402_Air
16020402_Air_002	2/4/2016 5:19	16020402_Air
16020402_Air_003	2/4/2016 5:21	16020402_Air
16020402 Air 004	2/4/2016 5:23	16020402 Air

The filtering criterion can be indicated by prefixing the value with the desired operator (see table below).



- Relational Filtering Criteria

Symbol	Description	Example
<>	Filters the items to display only those that <b>are different from the specified value.</b>	<>Test
*(Operator precedes value)	Filters the items to display only those that <b>end with the specified value.</b>	*Test*
=	Filters the items to display only those that <b>are equal to the specified value.</b>	=Test
>	Filters the items to display only those that <b>are greater than the specified value.</b>	> 50
>=	Filters the items to display only those that <b>are greater than or equal to the specified value.</b>	>=50
<	Filters the items to display only those that <b>are inferior to the specified value.</b>	<50
<=	Filters the items to display only those that <b>are inferior or equal to the specified value.</b>	<=50
*(Followed by a value)	Filters the items to display only those that <b>start with the specified value.</b>	*Test

For example, if **5** is specified as a filter, all elements in the column (assuming that the column contains numeric data) will be automatically filtered to display only those with a value of 5. If all values are lower than 5, the **lower** operator must precede the filter value: **<5**. In addition, to filter items that begin with a given string, use the **\*** key preceded by a value (for example, [**value \***]); to filter items that end with this value, use the **\*** key followed by a value (for example, [**\* value**]).

The following example shows how to display only the series "16020402\_Air", simply add "=".

Analyse	Date d'injection	Série
		=16020402_Air
16020402_Air_001	2/4/2016 5:17	16020402_Air
16020402_Air_002	2/4/2016 5:19	16020402_Air
16020402_Air_003	2/4/2016 5:21	16020402_Air
16020402_Air_004	2/4/2016 5:23	16020402_Air

- Conditional filters

Filter	Description	Example
<b>AND</b>	Includes all data according to the <b>AND</b>	[Hello <b>AND</b> world]
<b>NOT</b>	Excludes all data according to <b>NOT</b>	[ <b>NOT</b> 5]
<b>OR</b>	Includes all data according to <b>OR</b>	[Hello <b>OR</b> Goodbye]

The items in a column can be filtered according to more than one value by separating those values with the **AND** or **OR** conditional operators. These operators, which must be in uppercase, are used in conjunction with both relational and conditional filters to apply multiple filtering criteria to a column's items.



For example, to filter string items which include both words [Hello] and [world], the words would need to be separated by the AND operator: [Hello AND world].

The NOT conditional operator can also be used to exclude a specific value.

For example, to exclude only the value [5], [NOT 5] can be specified as the filter criterion. If more than one value is to be excluded, then the NOT operator needs to precede both values. For example, [NOT 5 AND NOT 7] will include all values with the exception of 5 and 7.

*With the exception of the conditional operators (i.e., AND, NOT, OR), all extra white space preceding or following an operator will automatically be trimmed.*

As a general example, the following table contains two filters.

The first is in the Serie column, which displays only the series containing the "Analysis" or "BF 4.5" field. The second filter is at the column Pic0 (A) which only displays values greater than 30.

Analysis	Injection date	Serie	Method	Pic0...	Pic1 (B)
	07/21/2016	Analyse OR BF 4.5		<30	
	11/29/2016				
Analyse_676	8/29/2016 3:40 PM	Analyse	test_1	9.869	9.945
Analyse_677	8/29/2016 3:42 PM	Analyse	test_1	9.977	9.950
BF 4.5 / 8,4 @f_684	10/18/2016 9:05...	BF 4.5 / 8,4 @f	test BF : 4,5...	10.688	12.023
BF 4.5 / 8,4 @f_685	10/18/2016 9:07...	BF 4.5 / 8,4 @f	test BF : 4,5...	10.794	11.982
Serie BF 4.5_001	10/25/2016 3:21...	Serie BF 4.5	test	9.878	10.904
Serie BF 4.5_002	10/25/2016 3:22...	Serie BF 4.5	test	10.023	10.762

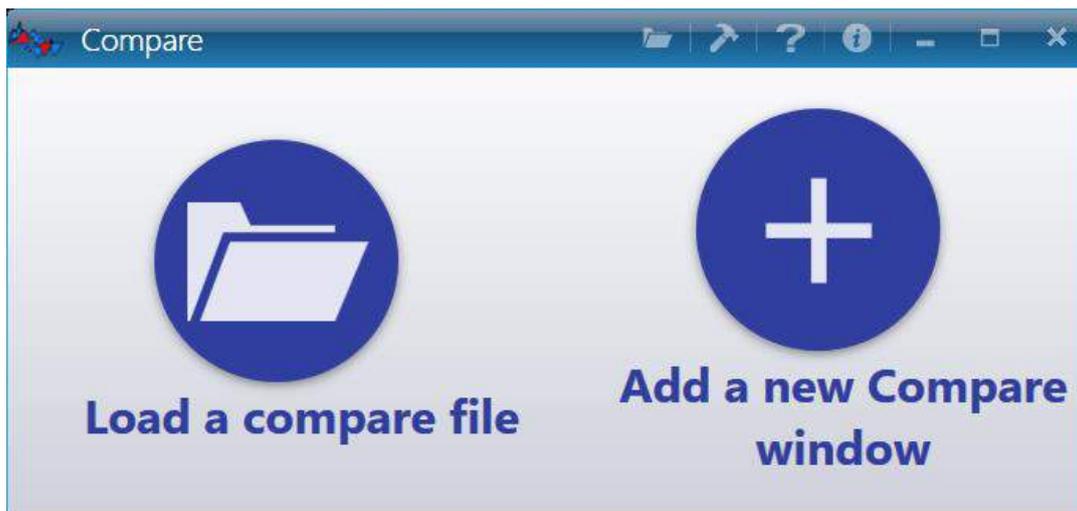
## 5. Comparison of analyzes

The comparison module is used to visualize and compare several chromatograms. This allows to follow the evolution of a phenomenon during the analyzes, possibly the degradation of the columns.

The comparison module is a software in which one opens documents, each document consisting of 1 (the interest starting at 2) to 64 analyzes.

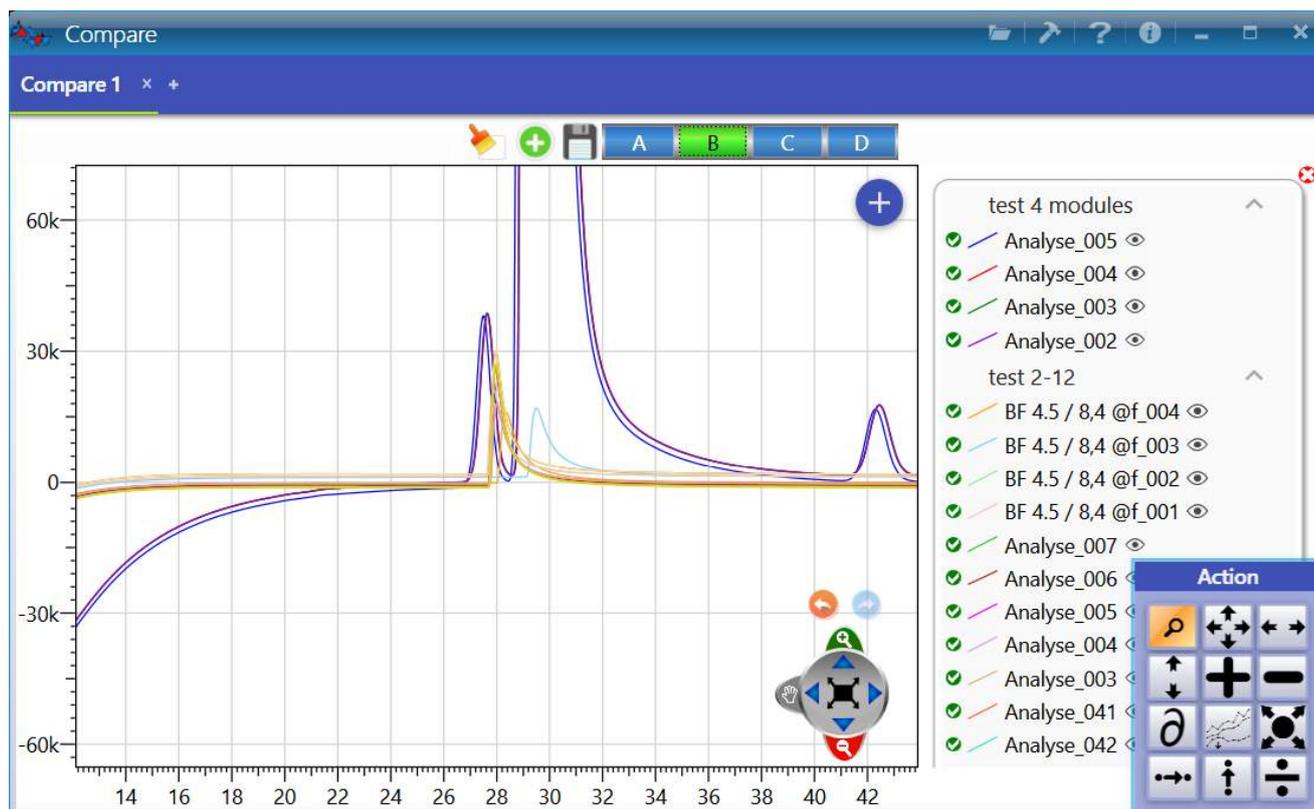
When loading, the main screen is displayed:





Two choices are offered: the first is to load a previously saved analysis comparison file and the second is to start from an empty window and to add the desired analyzes.

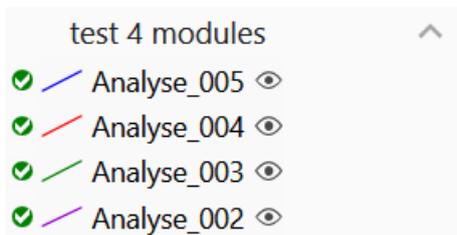
When the loading has been enabled, all the chromatograms are visualized simultaneously on the displayed document.



Each chromatogram has its own color, which allows to differentiate them. The name of this chromatogram is displayed in the legend of the graph.



By passing the cursor over one of these analyzes, the curve will be bolded to better differentiate it from the others.



To allow graphical operations on some analyzes, you must select them. The icon  indicates that the analysis allows these operations on this analysis while the icon  indicates that any operation will be ignored on this analysis.

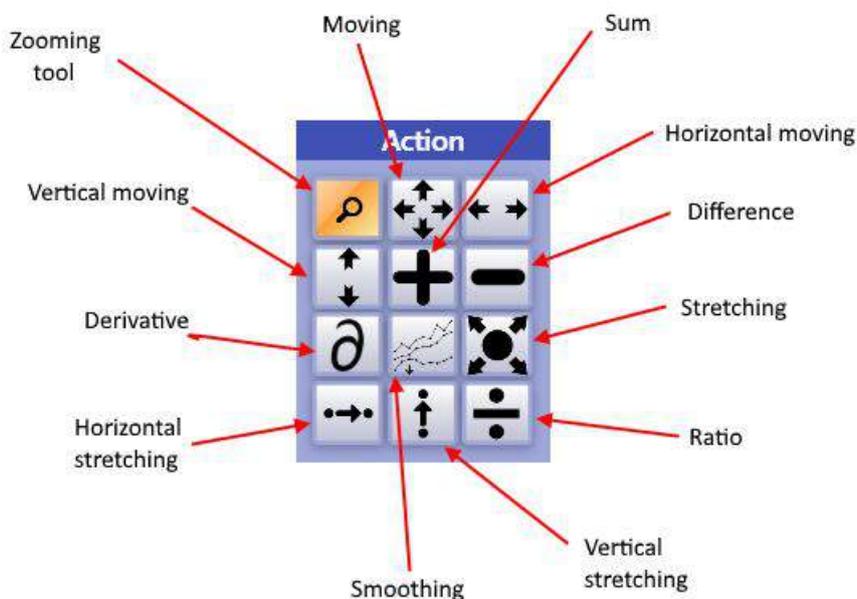
To do not display an analysis, simply click on the icon  the analysis will be hidden (a hidden analysis will have the following icon ).

The module bar allows the display of the chromatograms of each module that equip the analyzer with a single mouse click on the corresponding letter A to D.

Each document can be saved and reopened later.

The zoom tool is also a way to properly view the analyzes (see chapter [Graphic](#) for more details).

The palette allows general operations concerning a chromatogram or involving two chromatograms.



For a general operation (zoom, for example), just click on the icon of the tool to make it active.

An operation on a chromatogram (displacement, stretching, scaling or first derivative) is also immediate: the tool is first selected and then the chromatogram to which the operation is to be applied is "captured".



An operation involving 2 chromatograms is carried out in 3 steps: the chromatograms are first selected in the legend, then the tool is selected and then a click on the graph will apply the operation.

## 6. Users management

There are three levels of identification. The first is the **Operator** level, which is the one with the most restricted use. The next level is the **Service** level, whose access is almost complete but does not allow as much rights as that of the **Administrator** level, which has all the possible accesses, in addition to manage the accesses of the other mentioned levels.

By default, when SOPRANE II is started, the level is set to "Operator".

To access users management, the icon  is available at the top left of the title bar.

**To go further, see the chapters:**

[User login](#)

[User creation](#)

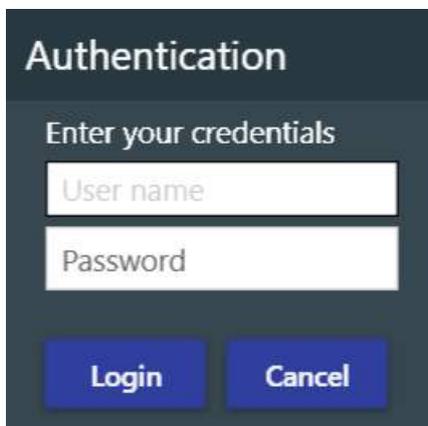
[Remove a user](#)

[Change password](#)

[User access](#)

### 6.1. User login

To identify yourself, the icon  is available at the top left of the title bar.



The image shows a dark-themed authentication dialog box titled "Authentication". It contains the text "Enter your credentials" above two input fields: "User name" and "Password". At the bottom, there are two buttons: "Login" and "Cancel".

Two pieces of information are required:

- The user name
- The password

Once this two information are valid, the user will be selected.

For the following chapters, the user must be authenticated as an **administrator**.



To go further, see the chapters:

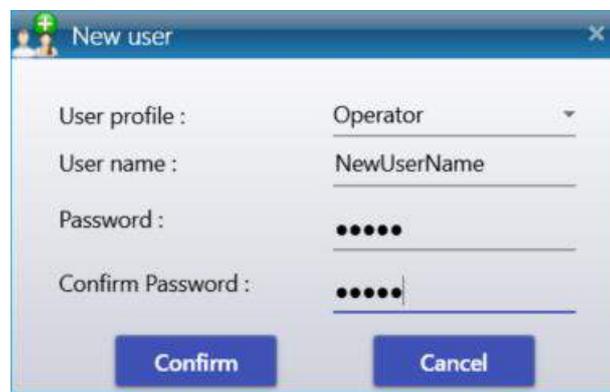
- [User creation](#)
- [Remove a user](#)
- [Change password](#)
- [User access](#)

## 6.2. User creation

Adding a user is possible only if an **Administrator** is already logged in (see chapter [User login](#) to login).

Once the administrator is logged in, go to the **User** tab  and click on **Add User** .

The next page will open.



User information are:

- The user profile
- The user name
- The password

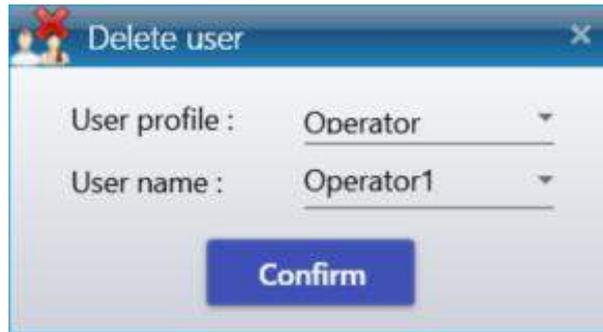
## 6.3. Remove a user

Adding a user is possible only if an **Administrator** is already logged in (see chapter [User login](#) to login).

Once the administrator is logged in, go to the **User** tab  and click on **Delete User** .

The next page will open and propose to select the information concerning the user to delete.





The fields to be filled in are:

- The user profile
- The user name

## 6.4. Change password

The modification of the user password is possible only if an **Administrator** is already logged in (see chapter [User login](#) to login).

Once the administrator is logged in, go to the **User** tab  and click on **Change Password** .

By clicking on "**Change password**", a new window opens proposing to fill in the fields concerning the password:

- The current password
- The new password
- Confirm new password



## 6.5. User access

User access management is allowed only for an **Administrator** (see chapter [User login](#) to login).

Once the administrator is logged in, go to the **User** tab  and then click either on **Operator**  or **Service** .

Each check mark represents an action of SOPRANE II. If the check-mark is ticked, the user will have the right to perform the action otherwise it will be locked.

Configuration	Analysis	Method of analysis	Analysis sequence	Calibration	Process	Logs
<input checked="" type="checkbox"/> Create an analyzer <input checked="" type="checkbox"/> Select analyzer <input checked="" type="checkbox"/> Visualize the configuration <input checked="" type="checkbox"/> Read the configuration <input checked="" type="checkbox"/> Configuration <input checked="" type="checkbox"/> Valve <input checked="" type="checkbox"/> Auxiliary pump <input checked="" type="checkbox"/> Flow <input checked="" type="checkbox"/> Analysis option <input checked="" type="checkbox"/> Alarms <input checked="" type="checkbox"/> Analog inputs <input checked="" type="checkbox"/> Relay <input checked="" type="checkbox"/> Sampling Configurations <input checked="" type="checkbox"/> Stream management <input checked="" type="checkbox"/> 4-20mA module <input checked="" type="checkbox"/> Modbus	<input checked="" type="checkbox"/> Start analysis <input checked="" type="checkbox"/> Visualize analysis results. <input checked="" type="checkbox"/> Visualize analysis trends <input checked="" type="checkbox"/> Real Time <input checked="" type="checkbox"/> Process <input checked="" type="checkbox"/> Compare	<input checked="" type="checkbox"/> Create method <input checked="" type="checkbox"/> Edit a method <input checked="" type="checkbox"/> Load a method.	<input checked="" type="checkbox"/> Create a sequence <input checked="" type="checkbox"/> Edit an analysis sequence	<input checked="" type="checkbox"/> Create a calibration <input checked="" type="checkbox"/> Edit a calibration <input checked="" type="checkbox"/> Automatic calibration	<input checked="" type="checkbox"/> Integration <input checked="" type="checkbox"/> Calibration <input checked="" type="checkbox"/> Matching <input checked="" type="checkbox"/> Table Component <input checked="" type="checkbox"/> Calculations	<input checked="" type="checkbox"/> Visualize action log <input checked="" type="checkbox"/> Visualize Errors logs. <input checked="" type="checkbox"/> Visualize Alarms logs.

## 7. Maintenance

### 7.1. Backflush time adjustment

#### 7.1.1. What is the backflush ?

When developing the method, an important step is to set the backflush time. The main goal of the backflush system is to protect the analytical column. The most common situation where the backflush system is encountered is when using a Molsieve 5Å column (MS5A). This will be the only case discussed in this chapter.

The Molsieve 5Å column is dedicated to the analysis of permanent gases (He, H<sub>2</sub>, Ar/O<sub>2</sub>, N<sub>2</sub>, CH<sub>4</sub> and CO). If heavier compounds are injected into the MS5A column, the stationary phase will lose its efficiency and its separation power will decrease rapidly. To protect this column against heavy compounds, in particular CO<sub>2</sub>, H<sub>2</sub>O and H<sub>2</sub>S, a pre-column is installed between the injector and the analytical column (MS5A).

After the injection, there are two steps:

- "Fore flush" mode: the carrier gas passes through the injector, then the pre-column and finally



through the analytical column.

- "backflush" mode: the carrier gas arrives between the pre-column and the analytical column.

During the "fore flush" mode, the molecules of the sample are injected into the pre-column where a first separation takes place. The light compounds not retained thus not separated (He, H<sub>2</sub>, Ar/O<sub>2</sub>, CO) leave the pre-column first, followed immediately thereafter by CH<sub>4</sub>. Only then the heavy compounds go out.

When the "backflush" mode is activated, the compounds that have had time to exit the pre-column continue their way to the detector and are separated in the analytical column. Compounds that are still in the pre-column are backflushed.

A well-adjusted backflush time is a backflush time long enough to allow all compounds of interest (He, H<sub>2</sub>, Ar/O<sub>2</sub>, N<sub>2</sub>, CH<sub>4</sub> and CO) to pass through and short enough to backflush heavy compounds that could damage the analytical column.

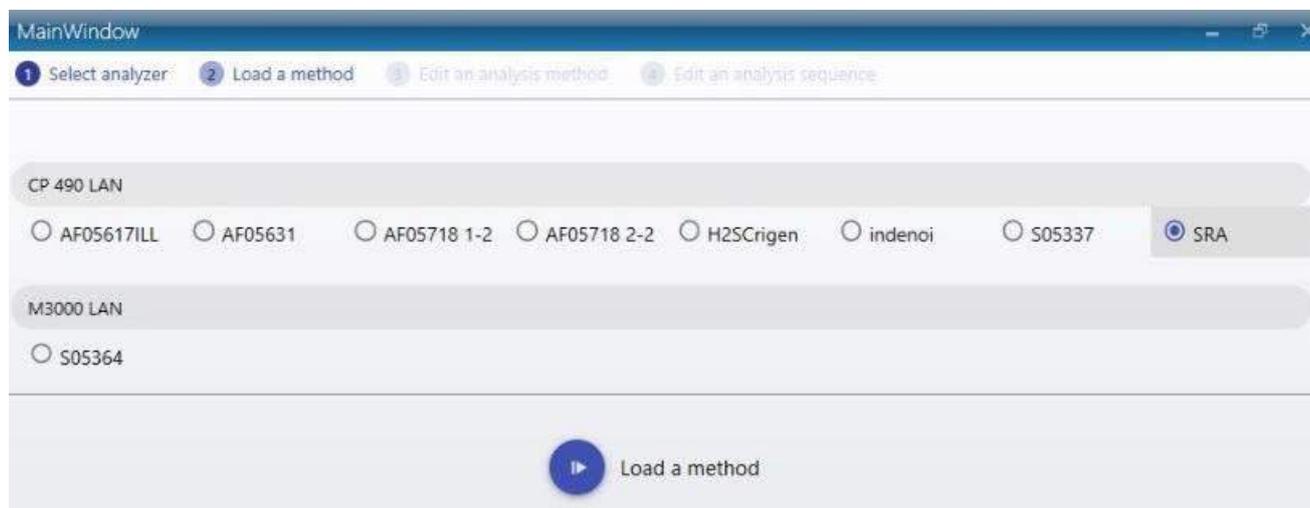
### 7.1.2. How to adjust the backflush time with Soprane II ?

#### **! Important note:**

**The backflush time must be adjusted after defining the temperature, carrier gas pressure and injection time. If one of these parameters is changed, the backflush time must be adjusted again.**

A dedicated tool has been developed to help the customer adjust the backflush time.

1. Open " SRA.Soprane.BackflushMethodGenerator.exe" in "C:\Soprane II".
2. Select the analyzer and click on "Load a method":

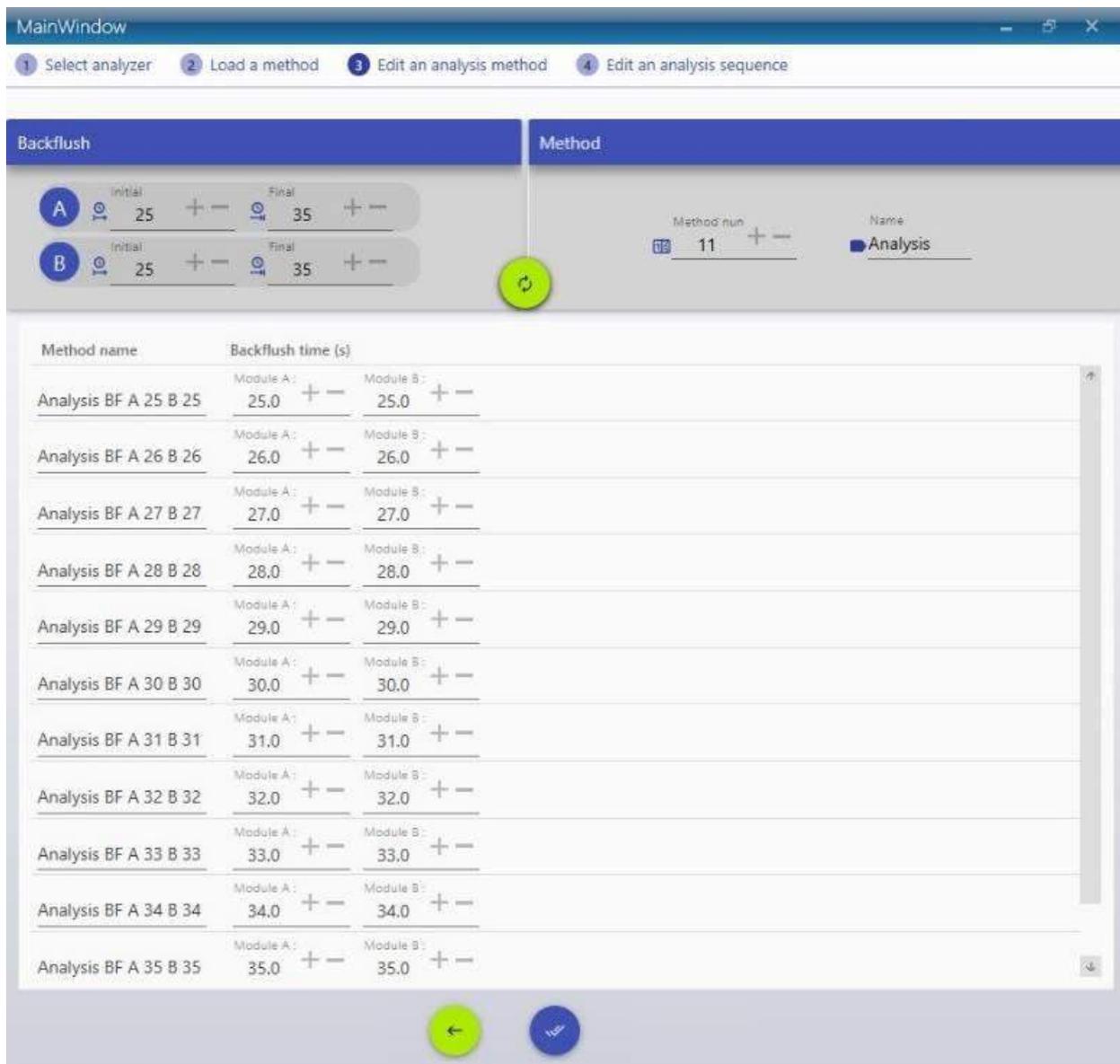


3. Select the analytical method to develop:



Name	Inlet	Injector				Column				Pressure				Injection				Detector			
		Mod. A	Mod. B	Mod. C	Mod. D	Mod. A	Mod. B	Mod. C	Mod. D	Mod. A	Mod. B	Mod. C	Mod. D	Mod. A	Mod. B	Mod. C	Mod. D	Mod. A	Mod. B	Mod. C	Mod. D
Start Stop	50.0 °C	50.0 °C	50.0 °C	50.0 °C	50.0 °C	50.0 °C	50.0 °C	50.0 °C	50.0 °C	7.0 PSI	7.0 PSI	7.0 PSI	7.0 PSI	0 ms	0 ms	50 ms	50 ms	OFF	OFF	OFF	OFF
Regeneration	90.0 °C	95.0 °C	95.0 °C	95.0 °C	95.0 °C	160.0 °C	160.0 °C	180.0 °C	180.0 °C	35.0 PSI	35.0 PSI	35.0 PSI	35.0 PSI	0 ms	0 ms	50 ms	50 ms	OFF	OFF	OFF	OFF
Standby	90.0 °C	95.0 °C	95.0 °C	95.0 °C	95.0 °C	110.0 °C	110.0 °C	75.0 °C	75.0 °C	28.0 PSI	28.0 PSI	28.0 PSI	28.0 PSI	0 ms	0 ms	50 ms	50 ms	OFF	OFF	OFF	OFF
Analysis	100.0 °C	95.0 °C	95.0 °C	95.0 °C	95.0 °C	110.0 °C	110.0 °C	75.0 °C	75.0 °C	28.0 PSI	28.0 PSI	28.0 PSI	28.0 PSI	30 ms	50 ms	50 ms	50 ms	ON	ON	ON	ON

4. Select an initial and a final backflush time for the channels equipped with a backflush system.
5. Select the number of method to run. For a first estimation, try to have a step of 1 second between two backflush times (for example: initial backflush time = 5 seconds, final backflush time = 10 seconds, method run = 6).
6. Define a name for the series of analyses.
7. Click on  to generate automatically methods with different backflush times.



**Backflush**

Channel A: Initial 25, Final 35

Channel B: Initial 25, Final 35

**Method**

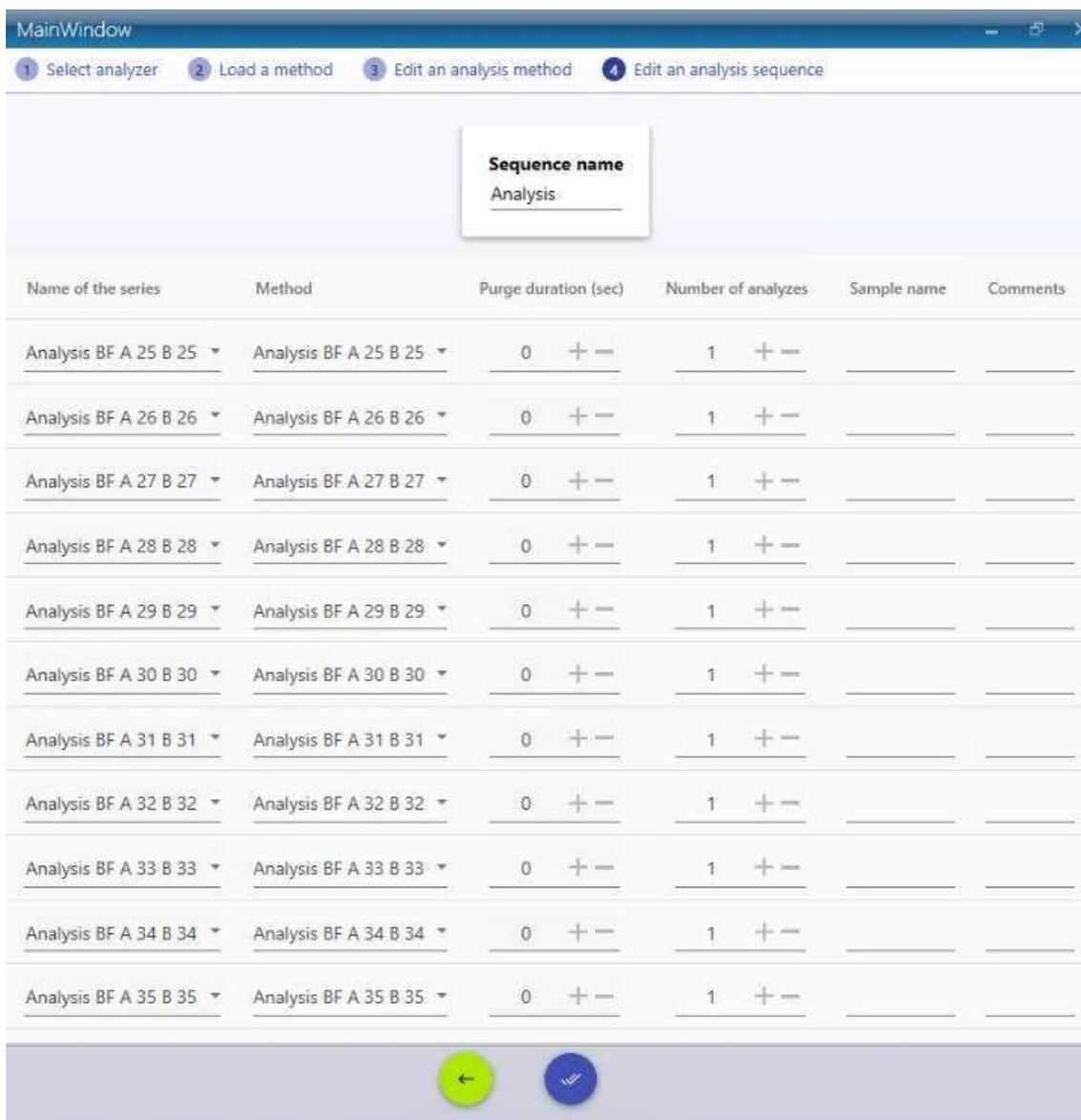
Method run: 11

Name: Analysis

Method name	Backflush time (s)	
Analysis BF A 25 B 25	Module A: 25.0	Module B: 25.0
Analysis BF A 26 B 26	Module A: 26.0	Module B: 26.0
Analysis BF A 27 B 27	Module A: 27.0	Module B: 27.0
Analysis BF A 28 B 28	Module A: 28.0	Module B: 28.0
Analysis BF A 29 B 29	Module A: 29.0	Module B: 29.0
Analysis BF A 30 B 30	Module A: 30.0	Module B: 30.0
Analysis BF A 31 B 31	Module A: 31.0	Module B: 31.0
Analysis BF A 32 B 32	Module A: 32.0	Module B: 32.0
Analysis BF A 33 B 33	Module A: 33.0	Module B: 33.0
Analysis BF A 34 B 34	Module A: 34.0	Module B: 34.0
Analysis BF A 35 B 35	Module A: 35.0	Module B: 35.0



8. Click on  to create automatically a sequence of analysis with one analysis for each method previously generated.
9. Give a name to this sequence and click on  :

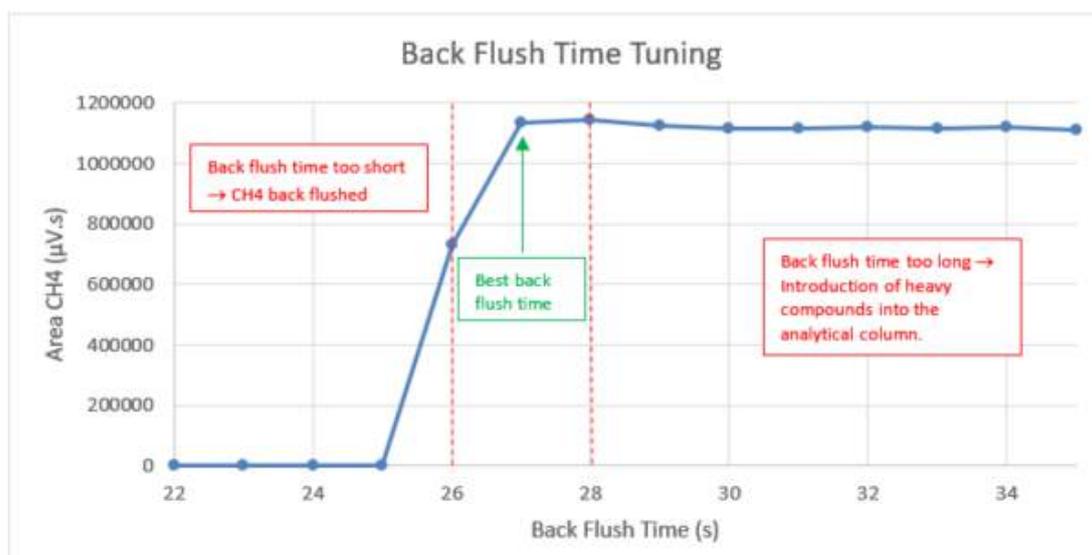


10. Connect a standard containing CH<sub>4</sub> to the Micro GC, open Soprane II, click on "Start" and launch the previously generated sequence (see chapter [Start a sequence](#)):

After a few minutes, you will obtain chromatograms with different backflush times:

11. Open them one by one in Process, place your mouse on the peak of CH<sub>4</sub> and record its area:
12. In an Excel file, write the area of peak of CH<sub>4</sub> in function of the backflush time and draw the corresponding curve:





13. Adjust the backflush time precisely at more or less 0.1 second.
14. Apply the same method as previously but create a sequence with a step of 0.1 second. For the previous example, start at 26 seconds and finish at 28 seconds with a step of 0.1 second.

## 7.2. File management

When exchanging data between two computers (usually from the user's computer to an SRA Instruments computer when requesting help to solve an analytical or integration problem): what are the files associated with the analyzes or the methods necessary for the whole functioning?

SOPRANE II uses several files to store the analyzer configuration, the different analysis methods, the integration methods, the results, ...

These files are, for the most part, linked to each other and moving one of these files from one directory to another can have unfortunate consequences.

To export and import data, the best way is to use the specially designed **File Manager**  utility. It allows you to copy, delete, move files, export or import them. The File Manager tool is in the SOPRANE II installation directory.

See chapter [Export data](#) to export data

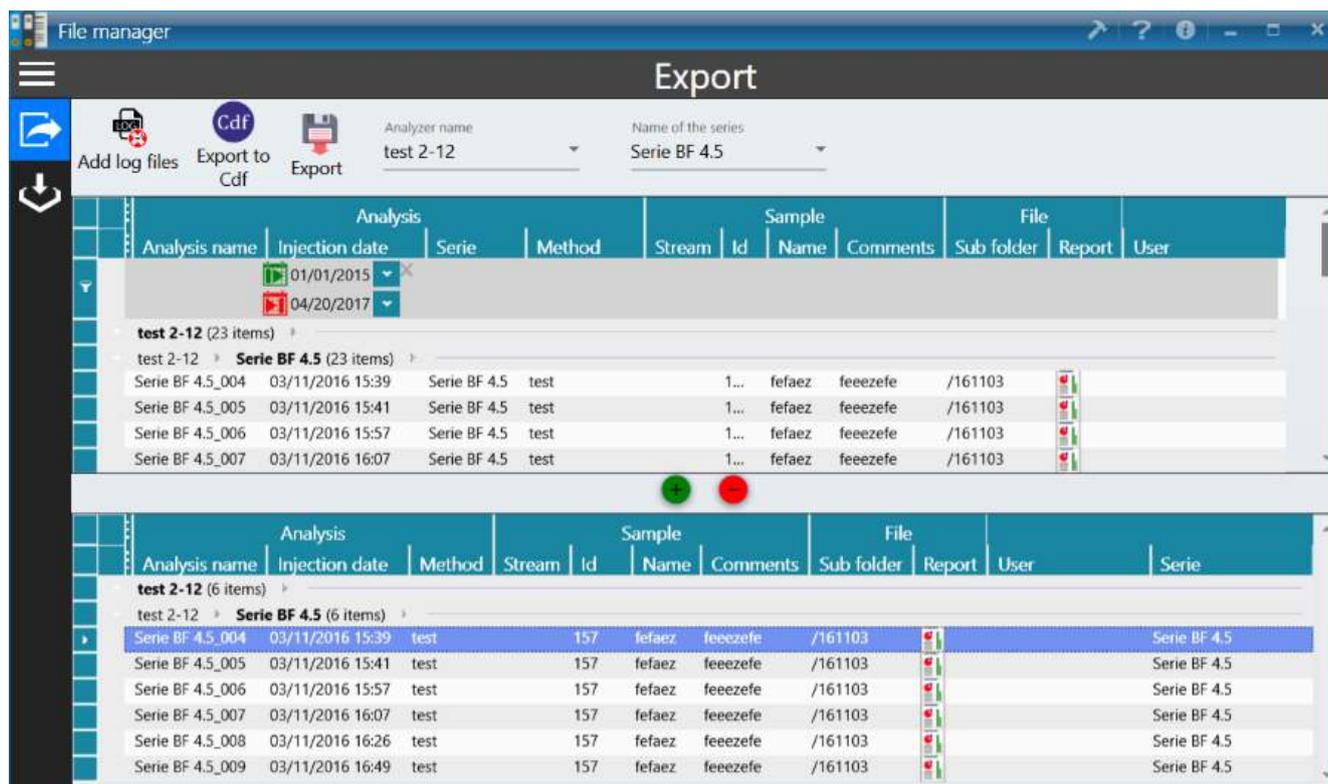
See chapter [Import data](#) to import data

### 7.2.1. Export data

It may be useful to send some data such as analyses, methods; that's why the **File Manager**  tool is very useful.

When loading, the main screen is displayed:





By default, the **export** mode is activated, the first data table contains all the analyzes corresponding to the selected analyzer and series.

These analyzes can be added by selecting them and by clicking on the button . Once added, the analyzes will be displayed in the second table below containing all the analyzes that will have to be exported. To remove one or several analyzes, just click on the button .

Log files can be added to the export by clicking on the button .

The export option in Cdf (or Aia)  allows to convert the selected analyzes into this format readable by other chromatography software.

To compress the data, click the **Export** button. Then select the location of the data.

Note:

To facilitate the search of analyzes to be exported, the two tables in this view can be filtered and sorted (for more information see the chapter [Use of data tables](#)).

**7.2.2. Import data**

The import allows you to create a new analyzer with all the corresponding analyzes and methods. To do this, all you have to do is to locate and open the file with the **.szip** extension by clicking on the load button .



**IMPORTANT NOTE:**

When importing, SOPRANE II copies the configuration file and therefore deletes the one that was used. This has no consequence when exchanging with SRA Instruments since the imported configuration file (if SRA Instruments returns you corrected files) is a copy of your own configuration file.

If you export data to a computer that is working with another analyzer, its configuration file will be destroyed.

The following display will then be displayed:

Analysis		Sample			File					
Analysis name	Injection date	Serie	Method	Stream	Id	Name	Comments	Sub folder	Report	User
	01/01/2015									
	04/20/2017									
test 2-12 (6 items)										
test 2-12 Serie BF 4.5 (6 items)										
Serie BF 4.5_004	03/11/2016 15:39	Serie BF 4.5	test		157	fefaez	feeezefe	/161103		
Serie BF 4.5_005	03/11/2016 15:41	Serie BF 4.5	test		157	fefaez	feeezefe	/161103		
Serie BF 4.5_006	03/11/2016 15:57	Serie BF 4.5	test		157	fefaez	feeezefe	/161103		
Serie BF 4.5_007	03/11/2016 16:07	Serie BF 4.5	test		157	fefaez	feeezefe	/161103		
Serie BF 4.5_008	03/11/2016 16:26	Serie BF 4.5	test		157	fefaez	feeezefe	/161103		
Serie BF 4.5_009	03/11/2016 16:49	Serie BF 4.5	test		157	fefaez	feeezefe	/161103		

All the analyzes of the loaded file will be listed in the table of the previous display. These are the analyzes to be imported.

The following window proposes to edit the analyzers, analyzes or methods names ; for that, click on the button .

Analyzer settings

Confirm Cancel

test 2-12

Analyzer name : M3000 Lan 131

File path C:\Soprane II

All series Methods

Analyse BF 4.5 / 8,4 @f test off test\_1

test BF : 4,5 - 48/r

test 4 modules

Analyzer name : M3000 Rs test

File path C:\Soprane II

All series Methods

Analyse test



Once validated, the information in the table will be updated.

The import will be done by clicking on **Import**. Once the import is successful, a new analyzer will be created as well as its shortcut on the desktop.

## 7.3. Logs management

Application logging offers three types of logs:

- [Action log](#), allows you to indicate all the main actions performed by the user.
- [Alarms log](#), displays all alarms that have been triggered.
- [Errors log](#), allows to locate errors during a crash (rather intended to the developer).
- [Event log](#) contains all the crashes information of Soprane II
- [Calibrations history](#) contains all calibration made with Soprane II.

### 7.3.1. Actions log

The Actions Log event table is available on the "**Logs**" tab and contains all the events that SOPRANE II has detected.

The table contains the following information:

- **Date:** The date of the event.
- **Profile:** User Profile (Administrator, Service or Operator)
- **User:** User name
- **Action:** Action performed

The table columns can be sorted and filtered. Selected rows can be deleted (either by the "**delete**" key, or by clicking on the button  or via the context menu).

Events can also be archived by clicking on the icon ; a file with the current date will then be created.

### 7.3.2. Alarms log

The Alarms Log event table is available in the "**Logs**" tab and contains all the alarms that have been triggered.

The table contains the following information:

- **Date:** The date of the alarm triggering.
- **Peak name:** The name of the peak corresponding to the alarm.
- **Minimum:** Minimum scale before the alarm is triggered.
- **Maximum:** Maximum scale before the alarm is triggered.
- **Value:** the value when the alarm is triggered.



- **Device:** Device name assigned to the alarm.

The table columns can be sorted and filtered. Selected rows can be deleted (either by the "delete" key, or by clicking on the button  or via the context menu).

Events can also be archived by clicking on the icon ; a file with the current date will be created.

### 7.3.3. Errors log

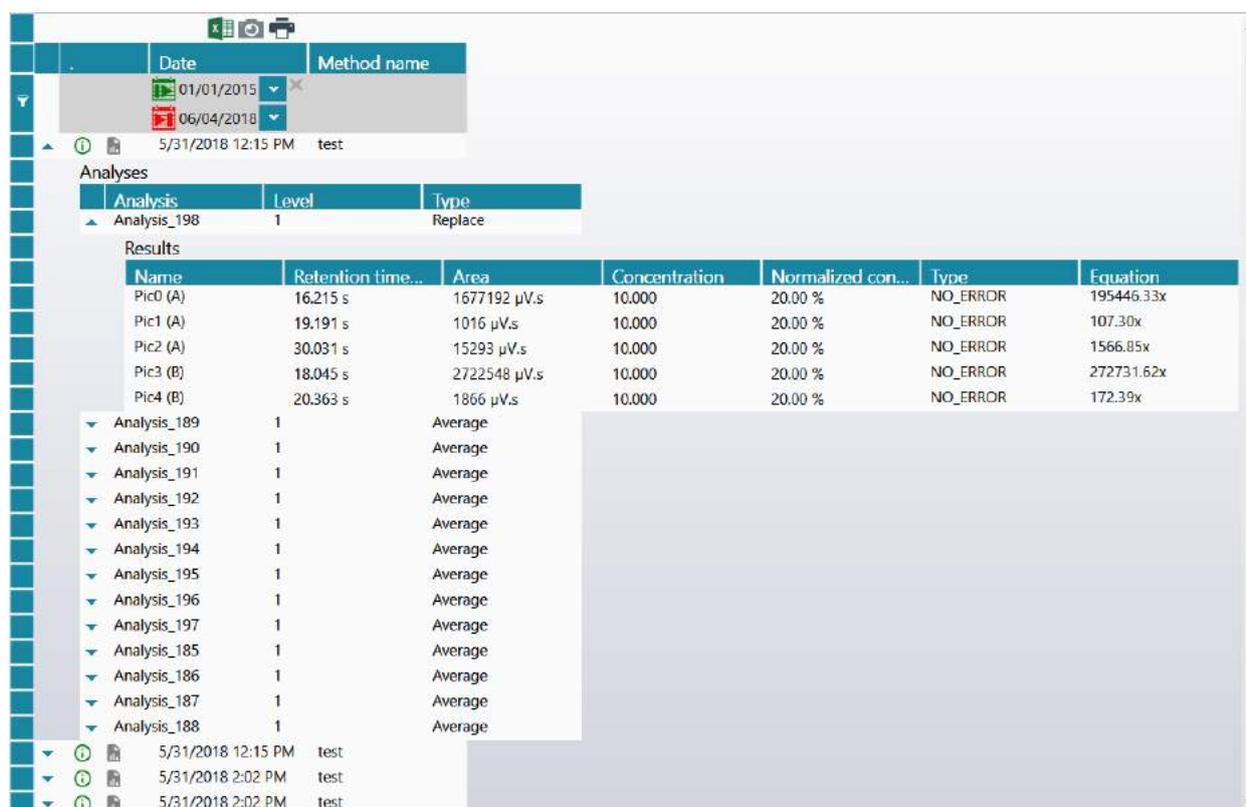
The Errors Log event table is available in the "Logs" tab and contains all the errors which have been detected. This information is intended to developers.

### 7.3.4. Event log

The Event Log table is available in the "Logs" tab and contains all the crashes information of Soprane II. This information is intended to developers.

### 7.3.5. Calibrations history

The Calibrations history table is available in the "Logs" tab and contains all calibration made with Soprane II.



Analysis	Level	Type
Analysis_198	1	Replace

Name	Retention time...	Area	Concentration	Normalized con...	Type	Equation
Pic0 (A)	16.215 s	1677192 µV.s	10.000	20.00 %	NO_ERROR	195446.33x
Pic1 (A)	19.191 s	1016 µV.s	10.000	20.00 %	NO_ERROR	107.30x
Pic2 (A)	30.031 s	15293 µV.s	10.000	20.00 %	NO_ERROR	1566.85x
Pic3 (B)	18.045 s	2722548 µV.s	10.000	20.00 %	NO_ERROR	272731.62x
Pic4 (B)	20.363 s	1866 µV.s	10.000	20.00 %	NO_ERROR	172.39x

Note: The two small icons   will allow you to view the calibration results and the calibration report (see chapter [Reference calibration](#) and [Calibration report](#)).



## 8. Appendix : Driving a Solia from Soprane II

Soprane II, when combined with MassHunter GC-MS Acquisition and Chemstation Data Analysis, enables the MicroGC/MS SOLIA coupling to be controlled.

### 8.1. Installation

Communication between Soprane II, MassHunter and Chemstation Data Analysis is carried out via computer macros. These macros are automatically deployed in the MassHunter and Chemstation Data Analysis tree structure when Soprane II is installed. It is therefore necessary to install Agilent softwares before installing Soprane II.

Install Chemstation Data Analysis and then Soprane II as administrator and following the recommended settings.

### 8.2. Instrument configuration

#### 8.2.1. Creating the Solia instrument in Soprane II

The screenshot shows the 'Instruments' configuration window in Soprane II. The window has a blue header with a graph icon and the text 'Instruments'. Below the header is a dropdown menu showing 'CP 490 LAN'. Underneath is a 'Connection' section with a plug icon and the text 'Connection'. This section contains several fields: 'Analyzer' with the value '10 . 1 . 1 . 101', 'Adam modules' with a dropdown arrow, 'Valve' with a dropdown arrow, 'Solia' with the value '490 - 2' and a dropdown arrow, and 'Keller' with a dropdown arrow. At the bottom of the window is a green button with a checkmark icon and the text 'Confirm'.

From Soprane Configurator, create a new analyzer by clicking on the "+" icon. Then enter the IP address of the instrument. Select "490 - 2" for the Solia category (as shown in the image above).

#### 8.2.2. Creating the MSD instrument in Agilent GCMS Configuration

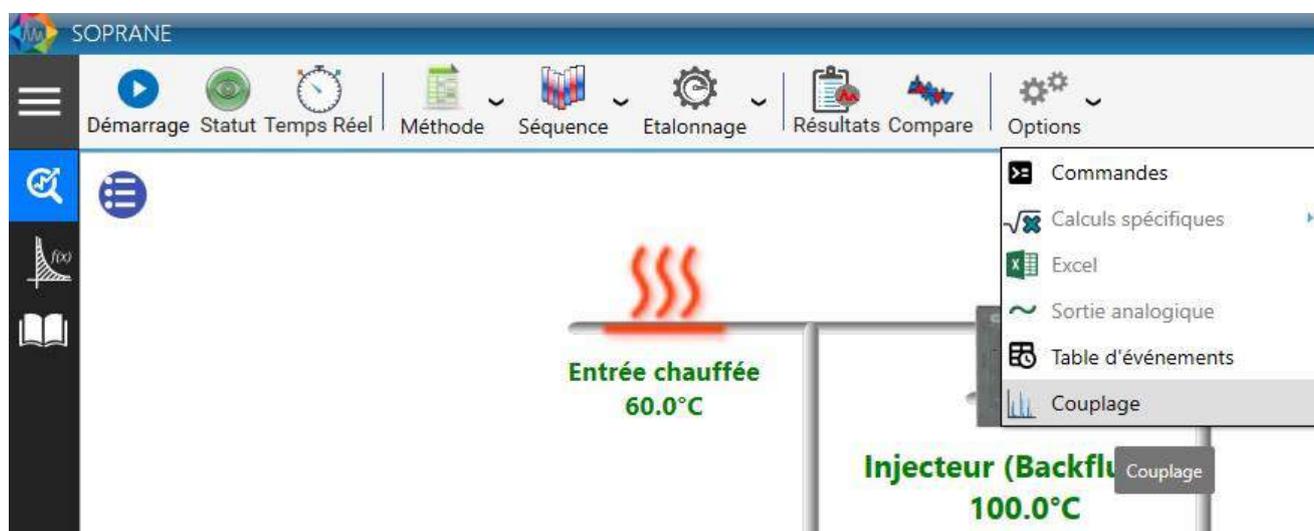
- Start Agilent GCMS Configuration as an administrator
- Select the instrument number to be configured (default is "1")
- Fill in the name of the instrument (for example "MSD") and the identity (ID) of the laboratory (optional)



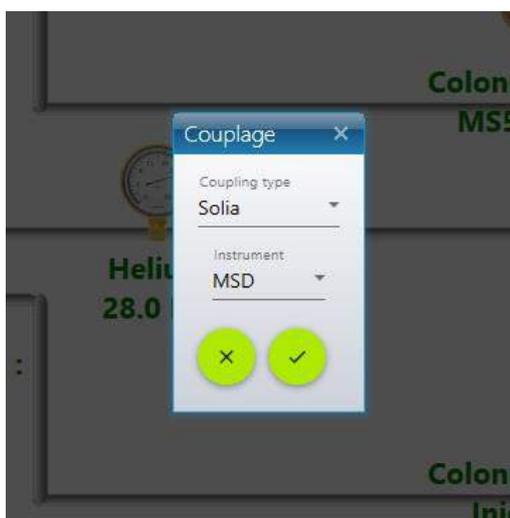
- Select the MSD model
- Enter the IP address of the MSD. The IP address of the instrument is displayed on the screen inside the top cover of the MSD.
- Specify the polarity of the quadrupole in "DC Polarity". This information is located inside the top cover ("Pos" or "Neg")
- Select "None" for the GC model
- Select "Workflow mode: Enhanced".

### 8.3. Configuration of the coupling

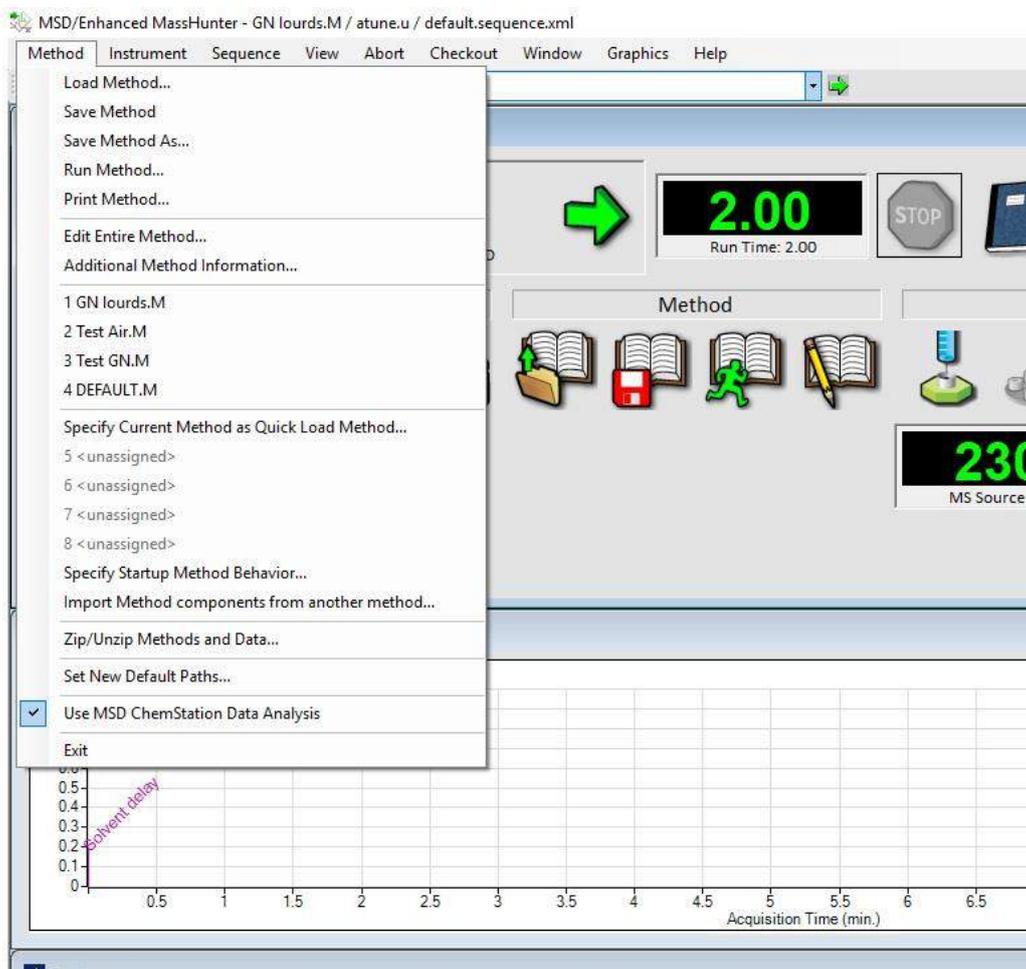
In order to drive the coupling, it is necessary to configure the coupling in each of the software packages. In Soprane II, the activation of the coupling is done from the "option" tab and then "coupling".



A window will then open. Select "Solia" and then the name of the MS instrument created in the Agilent GCMS configurator, as below:



In MassHunter, check the line "Use MSD ChemStation Data Analysis" in the "Method" menu.

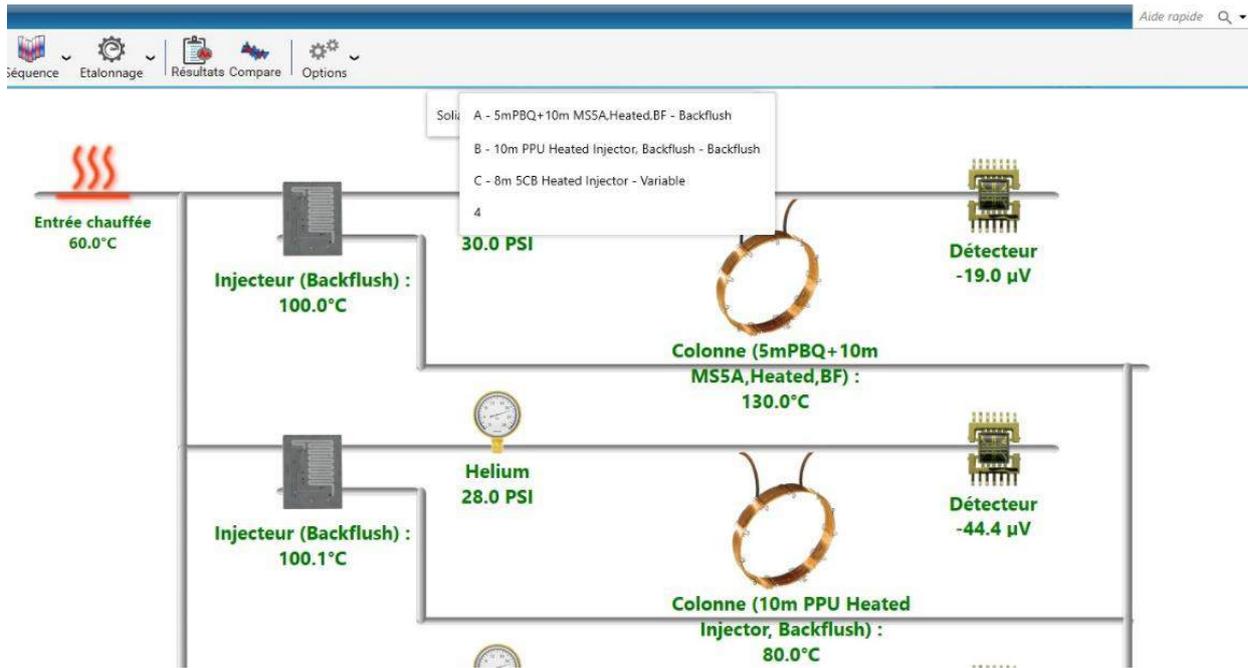


## 8.4. Controlling the Solia

Once these configuration requirements have been completed, it is possible to control the channel selection valve between the  $\mu$ GC modules and the MS detector. There are several ways to change the position of this valve.

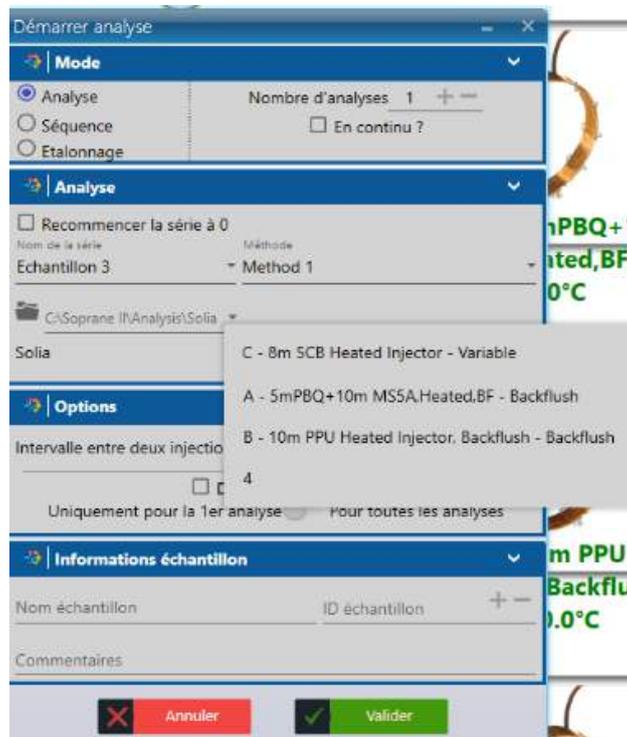
From the "Status" tab, by clicking on the bar above the diagram:





The names of the different modules are displayed on the screen. Click on the module to be coupled to the MS detector.

When starting analyses, in the "Start" tab:



When writing an analysis sequence: the valve position will change between the analyses and during the sequence, in order to couple the desired µGC module to the MS detector for each analysis:





### 8.4.1. Creating an analysis method

A Solia analysis method includes a Soprane analysis method and a MassHunter analysis method.

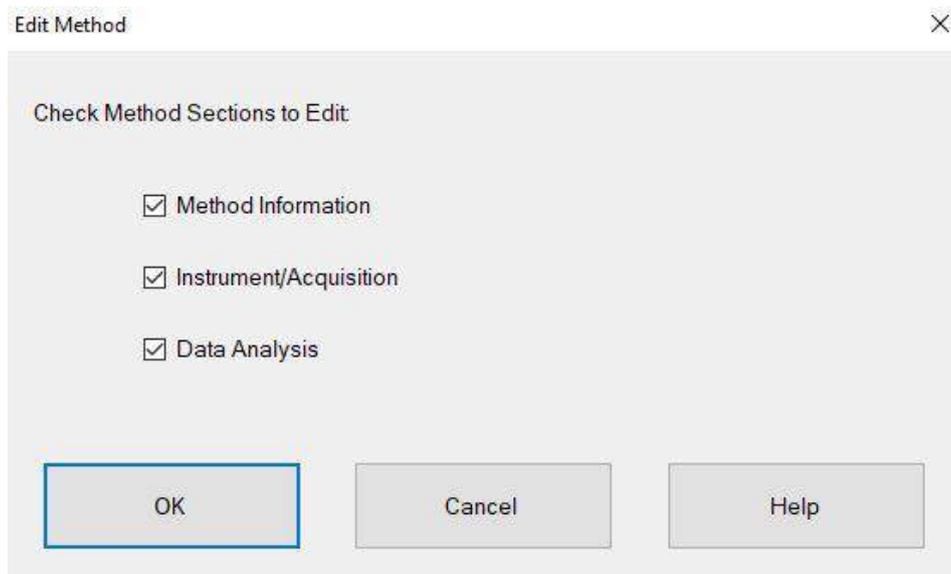
### 8.4.2. Creating a Soprane II analysis method

Refer to Chapter 4.3.1.

### 8.4.3. Creating a MassHunter analysis method

From the "File" tab, save the method under the desired name. Then edit the method.

Check all three boxes:



Check "Data Acquisition" and "Data Analysis":

Method Information

Method Comments:

Save Copy of Method With Data

Method Sections to Run

Pre-Run Macros/Commands

Instrument Control:  Browse...

Data Analysis:  Browse...

Data Acquisition

Data Analysis

Post-Run Macros/Commands

Instrument Control:  Browse...

Data Analysis:  Browse...

OK Cancel Help

Select "Sample Inlet: Other/None" and "Injection Source: External Device".

Inlet and Injection Parameters

Sample Inlet: Other/None

Injection Source: External Device

Use MS

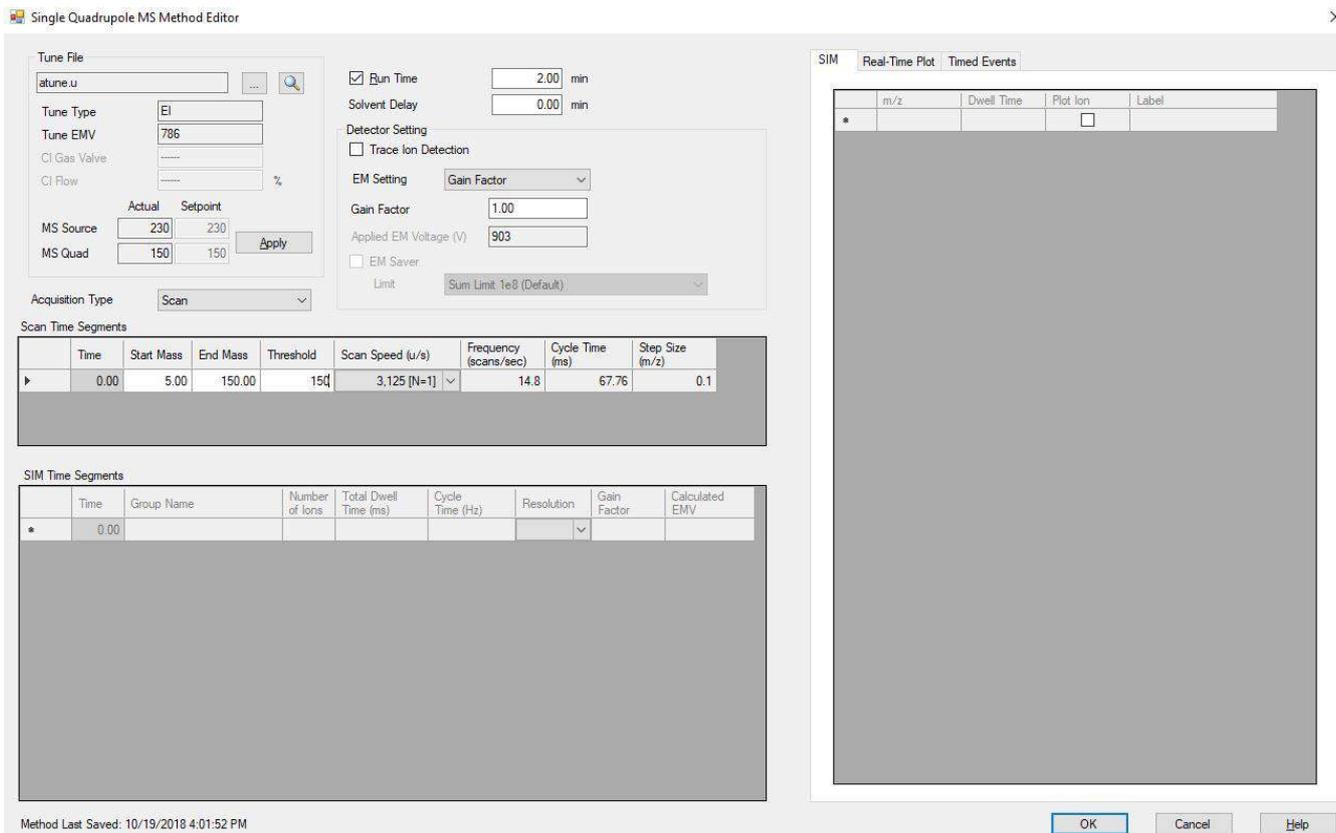
Inlet Location:  Front  Rear

MS Connected to:  Front  Rear

OK Cancel Help

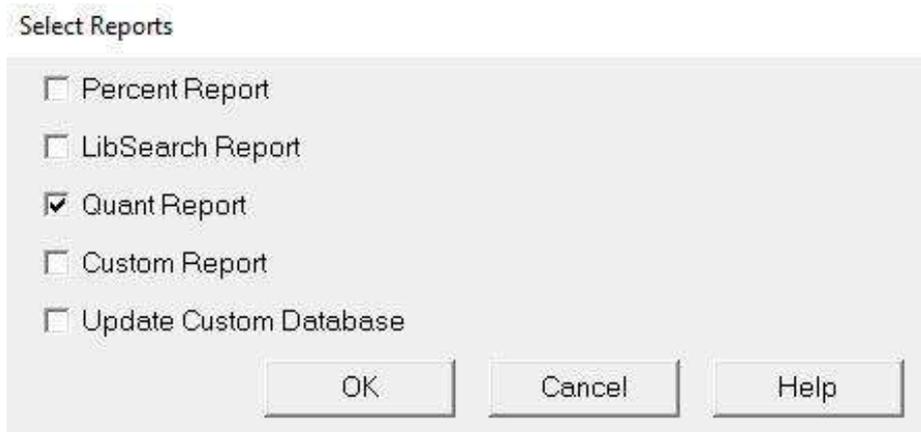


Define MS parameters :



**SRA recommends the above default settings, which should be modified according to the application. The Run Time must be equal to or greater than the Soprane II analysis time.**

Check "Quant Report" (essential for the transmission of results to Soprane II) and save the method.



## 8.5. Results processing

Soprane II offers the possibility to combine all  $\mu$ GC (TCD detection) and MS results in a same table, as shown below.

Analyse	Date d'injection	Série	Méthode...	$\mu$ GC results							MSD results					SOLIA Mo...
				C1 (A)	C2 (B)	C3 (B)	rC4 (C)	rC4 (C)	rC5 (C)	rC5 (C)	Total brut	C5 (MSD)	2methylC5 (MSD)	rC4 (MSD)	rC4 (MSD)	
Gaz_002	19/10/2018 11:53	Gaz	Test BF	10,012	1,002	1,001	1,031	1,036	1,034	1,040	16,157	1,389	1,385	1,403	1,385	C - 8m 5CB...
Gaz_003	19/10/2018 11:56	Gaz	Test BF	10,021	1,002	1,003	1,031	1,037	1,035	1,040	16,169	1,395	1,397	1,421	1,403	C - 8m 5CB...
Gaz_004	19/10/2018 11:58	Gaz	Test BF	10,014	1,002	1,003	1,030	1,035	1,033	1,038	16,156	1,408	1,409	1,431	1,412	C - 8m 5CB...
Gaz_005	19/10/2018 12:01	Gaz	Test BF	10,035	1,003	1,003	1,030	1,035	1,033	1,038	16,175	1,418	1,422	1,439	1,419	C - 8m 5CB...
Gaz_006	19/10/2018 12:04	Gaz	Test BF	10,041	1,003	1,003	1,031	1,037	1,035	1,039	16,188	1,429	1,430	1,448	1,427	C - 8m 5CB...
Gaz_007	19/10/2018 12:07	Gaz	Test BF	10,044	1,003	1,003	1,031	1,037	1,036	1,038	16,191	1,434	1,435	1,455	1,434	C - 8m 5CB...
Gaz_008	19/10/2018 12:09	Gaz	Test BF	10,021	1,002	1,002	1,031	1,038	1,035	1,041	16,171	1,447	1,442	1,455	1,442	C - 8m 5CB...
Gaz_009	19/10/2018 12:12	Gaz	Test BF	10,022	1,003	1,003	1,030	1,037	1,035	1,038	16,169	1,448	1,447	1,463	1,444	C - 8m 5CB...
Gaz_010	19/10/2018 12:17	Gaz	Test BF	10,024	1,002	1,002	1,030	1,036	1,034	1,038	16,185	1,454	1,447	1,470	1,449	C - 8m 5CB...
Min				10,012	1,002	1,001	1,030	1,035	1,033	1,038	16,156	1,389	1,385	1,403	1,385	
Avg				10,026	1,002	1,003	1,031	1,036	1,035	1,039	16,171	1,425	1,424	1,454	1,424	
Max				10,044	1,003	1,003	1,031	1,038	1,036	1,041	16,191	1,454	1,447	1,470	1,449	
Std (D)				0,114	0,036	0,070	0,036	0,084	0,091	0,110	0,075	1,641	1,575	1,496	1,400	

The table above groups the TCD results of the  $\mu$ GC modules (indicated by the letters (A), (B) and (C)), as well as the MSD results.

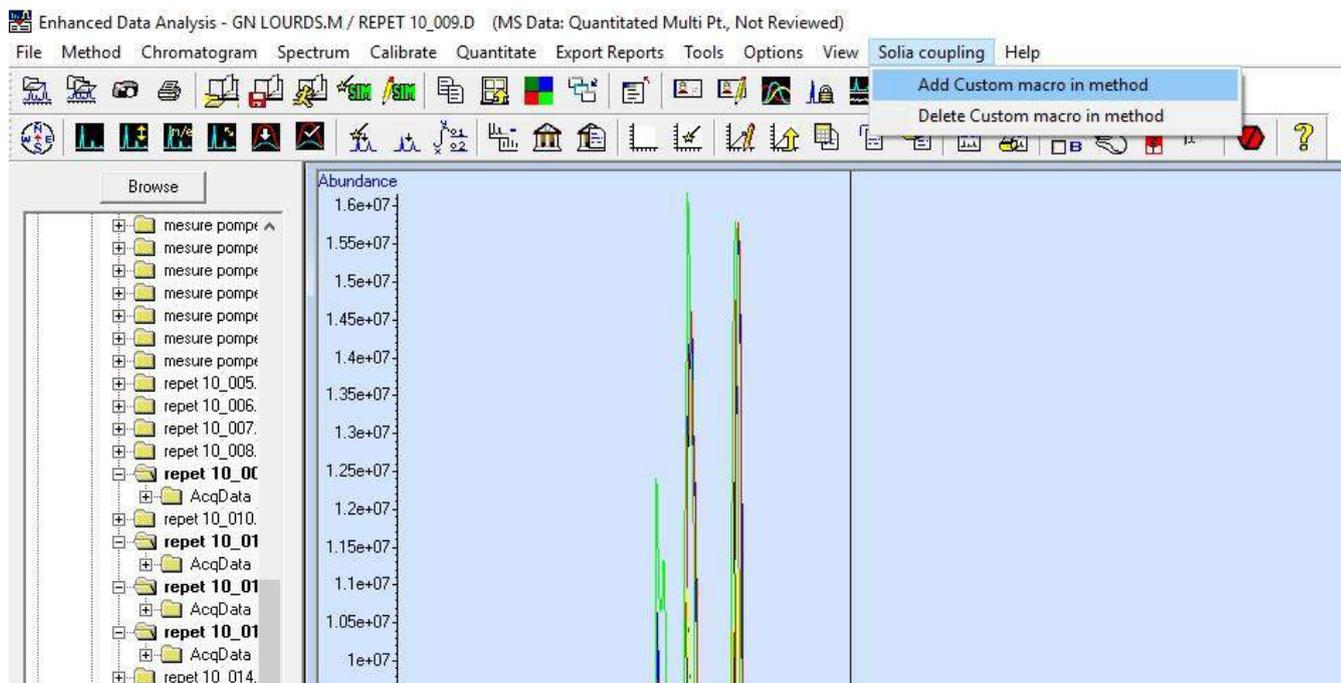
### 8.5.1. Creating a Soprane II processing method

Refer to Chapter 4.5.

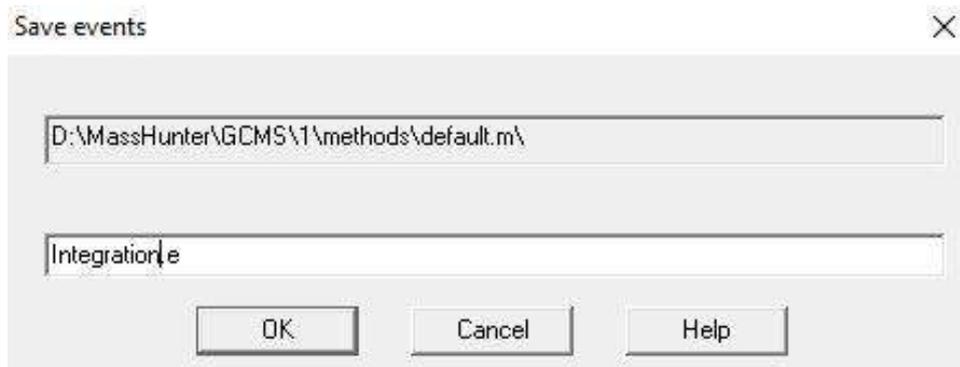
### 8.5.2. Creating a Chemstation Data Analysis processing method

Open Chemstation Data Analysis and load the acquisition method used. The processing method must be the same as the acquisition method for the results to be transmitted to Soprane II.

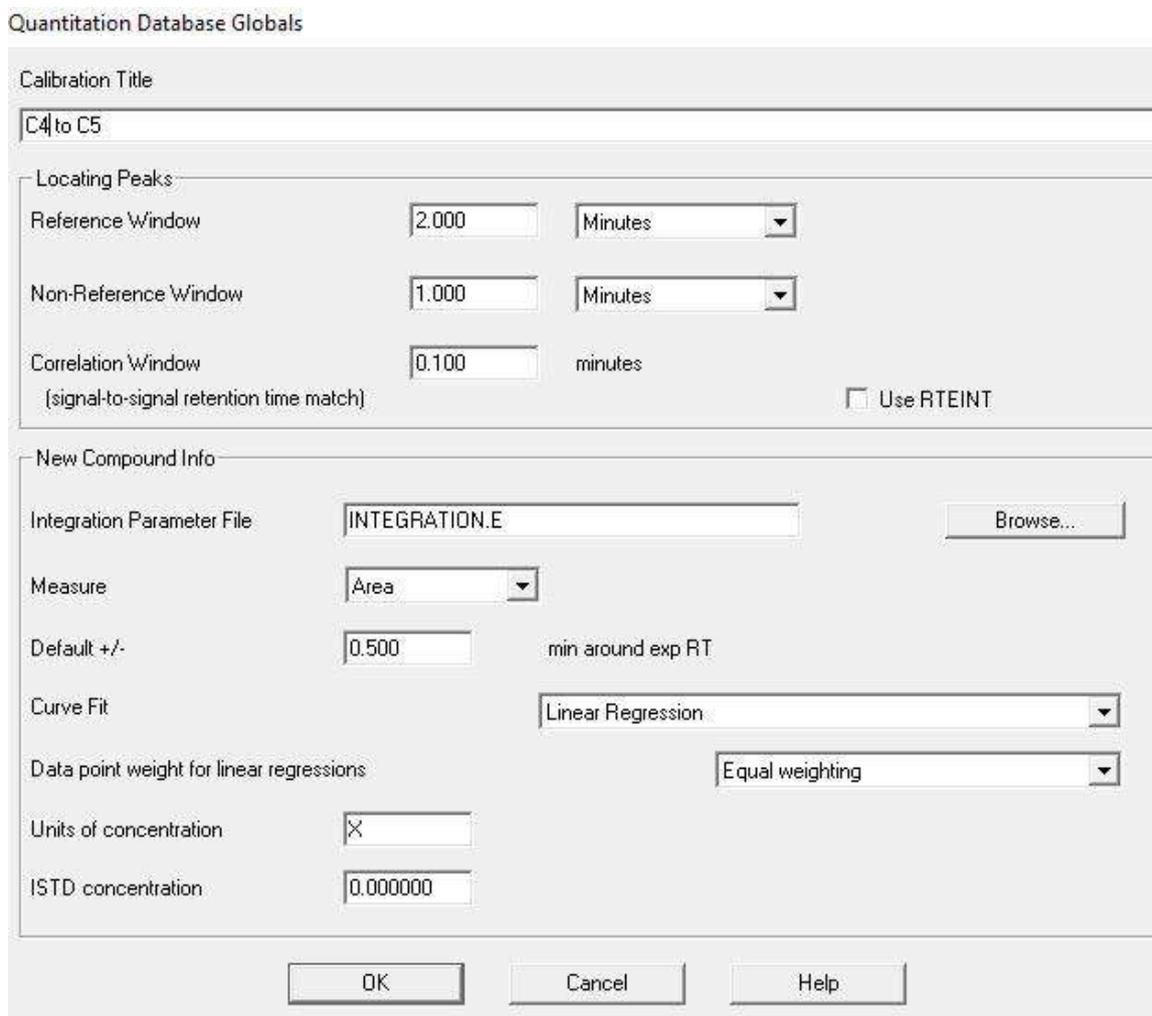
In the "Solia Coupling" tab of Chemstation Data Analysis, click on "Add Custom macro in method".



From the "Chromatogram" tab, click on "AutoIntegrate" and then modify the integration parameters in "MS Signal Integration parameters" if necessary. Then save the integration parameters under the desired name:



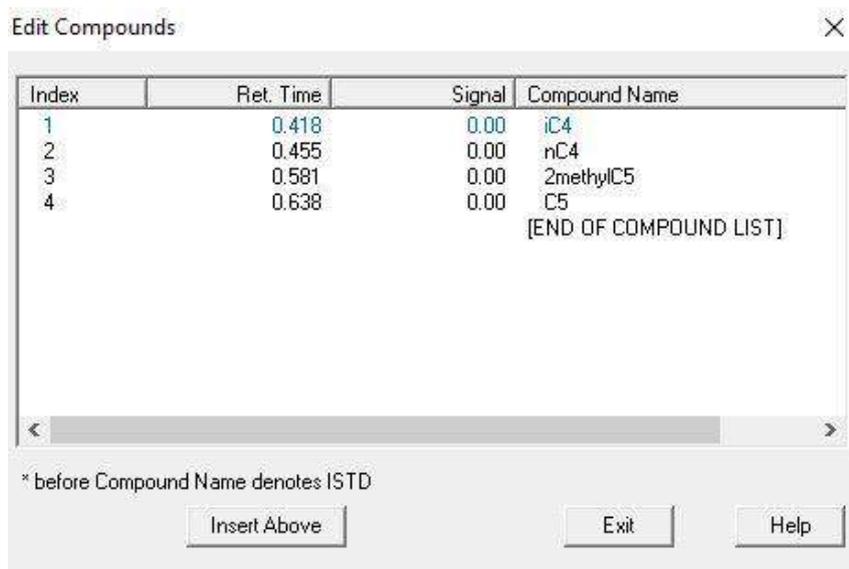
From the Calibration tab, click on "Set Up Quantitation".



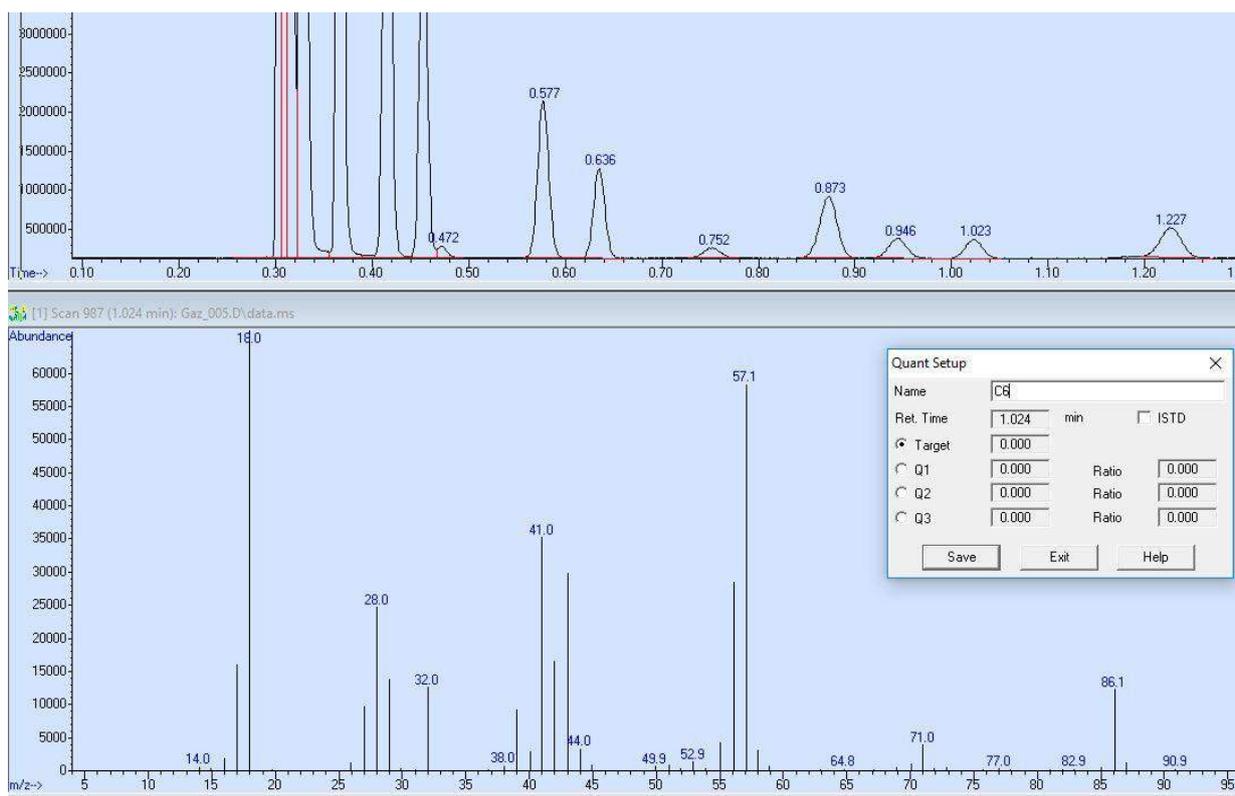
Fill in the fields "Calibration Title", "Integration Parameter File" (click on browse and load the previously saved integration file) and "Units of concentration". Uncheck "Use RTEINT" and click on OK.



The following window allows you to add the desired compounds to the calibration table. Click on "Insert Above".



Right double-click on the chromatographic peak's apex to be added to define its retention time in the calibration. Define the name of the compound.



At this stage, it is also possible to select target ions used for quantification. To do this, click simultaneously on the left click and right click on the m/z peak of the mass spectrum to be considered.



Click on "Save" to move to the next compound, and on "Exit" when all the compounds have been added to the table.

Fill in the fields "Compound concentration" and "New Level ID".

Update Calibration

Calibration Data File (Selection ignored by Sequence):  
C:\Soprane II\Analysis\Solia\181019\Gaz\_005.D

Add Level (supply new Calibration Level ID)

Compound Concentration: 1.0

ISTD Concentration: 0.000000

Update Level (select existing Calibration Level ID)

Responses  Average  Replace

Retention Times  Average  Replace

Replace Qualifier Ion Relative Responses

Update Mass Assignments

Delete Level (select existing Calibration Level ID)

Level IDs

New Level ID: 1

Existing Level ID: 1

Do Update Cancel Help



