

Soprane I

User manual



SRA INSTRUMENTS
210 rue des Sources
69280 Marcy l'Etoile
FRANCE

T : 04.78.44.29.47
F : 04.78.44.29.62
info@sra-instruments.com
www.sra-instruments.com

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1. Introduction

We assume that SOPRANE was correctly installed and parameterized.

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

We will assume later that SOPRANE was simply installed and parameterized, and that no analysis was performed.

The use of SOPRANE will require a number of steps:

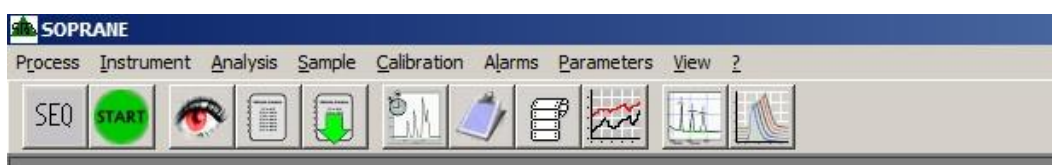
- First, we will visualize the various menus and we will check the possibility of establishing a dialogue with the analyzer,
 - We will create an analysis method,
 - We will create an analysis sequence,
 - We will carry out analyses,
 - From the chromatogram of an analysis, and directly, we will create a method of integration and a table of identification of the peaks,
 - We will see how to calibrate the apparatus,
 - We will program post-analytical calculations,
 - We will file the results,
 - We will print them,
 - We will visualize them graphically, in tendency,
 - We will discuss about the various possibilities of viewing,
 - We will program automatic regenerations of the columns.
-
- Finally, we will consider the possibilities of reprocessing analyzes and comparing chromatograms.

2. Beginning, Menus, Reading of the status

2.1 Start with Soprane

To run correctly, SOPRANE must know the configuration of the analyzer. If this configuration is unknown when launching Soprane, a message is displayed and the PGCSsetup program is automatically launched to read the configuration of the analyzer.

When starting (double click on the icon or menu START / Programs / SRA Instruments / SOPRANE), the software initializes itself and the main page of SOPRANE is shown:



SOPRANE manages the overall operation of the system and uses 2 external modules. One of these modules allows the processing of peak integration (component definitions, integration and calculations), the other module allows to compare analyzes and to follow the evolution of the concentrations as a function of time.



The following chapter describes the various menus of Soprane and the function of the icons.

2.2 The menus of Soprane

This is only an introduction to the different menus of SOPRANE; all details are given later in this manual.

Note that some sub-menus mentioned below may not appear on your screen depending on the basic options and those selected when configuring Soprane on your computer.

The **Process** menu has three sub-menus:

- Start analysis. It is used to start an analysis or an analyses sequence. Then, this sub-menu becomes Stop analysis and is used to stop an analysis.
- Print. Used to print the current window.
- Exit. Used, as the right top cross, to quit Soprane.

The **Instrument** menu has four sub-menus:

- Status. Used to show the status of the analyzer.
- Edit a method. Used to show and modify an analysis method.
- Send a method. Used to send the analytical parameters to the analyzer.
- Coupling. Used for μ GC-MS coupling in order to select the module coupled to the mass.

The **Analysis** menu has four sub-menus:

- Recall last analysis. Used to call the chromatogram, the method and the results of the last analysis.
- Batch processing. Used to apply the same treatment to several files.
- Process module. Used to load and access to the process module.
- Compare module. Used to load and access to the compare module.

The **Sample** menu has one sub-menu:

- Sequence table. Used to define a sequence of analyses (Only if several streams have been defined).

The **Calibration** menu has four sub-menus:

- Sequence table. Used to create an analysis sequence.
- Parameters. Used to modify the temporization between two analyses sequences.
- Batch calibration. Used to calibrate the method once the standard analyses have been performed.
- Display report. Used to display the calibration report.

The **Alarms** menu has two sub-menus:

- Acquit. Used to remove the consequences of an alarm or a defect.
- Parameters. Used to configure threshold alarms.

The **Parameters** menu has four sub-menus:

- Display and print. Used to select which variables will be displayed and/or printed at the end of an analysis.
- Trends. Used to define some trends and which has itself two sub-menus:
 - Property. Used to define the values and ranges of the trends window.
 - Delete trends. Used to delete trends filed values.
- Col. Bakeout (to be set in Soprane Setup). Use to bake out the columns.
- Configuration. Used to define what to do with the results of an analysis and which has itself four sub-menus:



- Calculation. Used to select or modify coefficients or calculations to do at the end of an analysis, if the calculation option is activated. It has itself six sub-menus:
 - o Complementary peak. Used to display the parameters for the calculation of a complementary peak.
 - o Calculation coefficients. Used to display the calculation coefficient table.
 - o Calculation 1 select. Used to display the calculation management window.
 - o Calculation 2 select. Used to display the calculation management window.
 - o Work sheet select. Used to parameter the calculation sheet.
 - o Select of specific calculations. Used to select a specific calculation.
- Results file (.DIF). Used to select the way to file results.
- User program. Used to define a user program.
- Output 4.20 mA. Used to define variables and ranges for 4-20mA outputs.

The **View** menu has eleven sub-menus: (plus the name of the windows opened)

- Chromatogram. Used to select and show the chromatogram(s) window.
- Results. Used to select and show the results window.
- Auxiliary. Used to display the window which allows to select a way of a VICI valve, for example, as well as the different sensors values which would have been configured in Soprane Setup (for example temperature and pressure).
- Analyses series. Used to select and show the analysis sequence window.
- Trends. Used to select and show the trends window.
- Cascade.
- Horizontal.
- Customized.
- Save windows positions. Used to memorize the position of the windows on the screen.
- Toolbar. Used to display or not the toolbar.
- Status bar. Used to display or not the status bar.

2.3 The icons of Soprane

Eleven icons are in the toolbar of Soprane.



From left to right, they are:

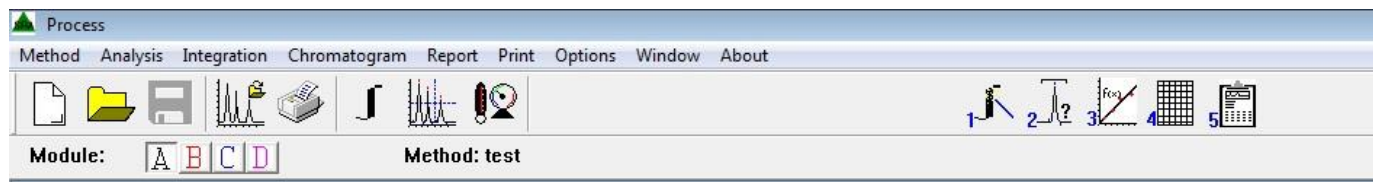
- Icon to write or modify an analysis sequence (shown only if several streams have been defined).
- Icon to start and stop an analysis or an analysis sequence.
- Icon to display the status of the analyzer.
- Icon to create and modify an analysis method.
- Icon to select and send a method to the analyzer.
- Icon to display the chromatogram(s).
- Icon to display the results window.
- Icon to display the analysis sequence window.
- Icon to display the trends window.
- Icon to access the process module.
- Icon to access the compare module.



2.4 The Process module

It is used for all that is related to peaks processing or re-processing and calibration.

Upon loading, the main screen is displayed:



2.5 The menus of the Process module

The **Method** menu has eight sub-menus:

- New method. Used to create a new analysis method.
- Open a method. Used to open an existing analysis method.
- Save. Used to save the method of the current window.
- Save as. Used to save the method of the current window under a new name.
- Save all. Used to save all the methods.
- Save archived method as. Used to save an archived method under a new name.
- Close all files. Used to close the windows and the associated files.
- Exit process.

The **Analysis** menu has three sub-menus:

- Load chromatogram. Used to load a filed chromatogram.
- Sample information. If a chromatogram has been loaded, used to access the sample information window related to this analysis.
- Analytical parameters used. If a chromatogram has been loaded, used to access the analytical parameters window related to this analysis.

The **Integration** menu has 18 sub-menus:

- Integrate. Used to re-integrate the chromatogram(s) and redo peaks identification and calculations.
- Identify peaks. Used to only redo peaks identification.
- Update calibration. Used to calibrate the system with the results of the on-going analysis.
- Options after integration. Used to configure the process during the acquisition.
- Optimal sensitivity. Used to determine the slope threshold value (slope sensitivity) to use at zero time.
- Manual baseline. Used to enter manual baseline setting.
- Edit events. Used to edit integration events.
- Modify events. Used to modify integration events.
- Events integration table. Used to create a components table from the analysis in memory.
- Display components table. Used to show the components table.
- Header of components table. Used to access the header of the components table.
- Build components table. Used to build a components table from what has been integrated.
- Undo manual baseline modification. Used to undo all manual baseline modifications.
- Control pallet. Used to display or not the control pallet.
- Manual baseline pallet. Used to display or not the manual baseline pallet.
- Events integration pallet. Used to display or not the events integration pallet.
- Edit free unit. Used to add concentration units specific to the user.



- Update retention time after integration. Used to allow automatic correction of the retention time at the end of each analysis.

The **Chromatogram** menu has six sub-menus:

- Display chromatogram. Used to display or not the chromatogram(s) window.
- Configuration of chromatogram view. Used to access the parameters of the chromatogram(s) window.
- Edit limits of chromatogram. Used to modify the limits of the chromatogram(s) display.
- Chromatogram on full scale. Used to display the entire chromatogram.
- Mode zoom. Used to allow zoom in a window.
- Thick (or thin) curve. Used to draw chromatogram(s) with a thick (or thin) curve.

The **Report** menu has five sub-menus:

- Report editor. Used to select what will appear in the final report.
- Set custom final report header. Used to customize the report header.
- Full report. Used to allow the display of the full report window.
- Report of integration parameters. Used to allow the display of the integration parameters report window.
- Report of components table. Used to allow the display of the components table report.

The **Print** menu has two sub-menus:

- Print. Used to print the current window.
- Print config. Used to define the print configuration.

The **Options** menu has five sub-menus:

- Edit, which has 5 sub-menus itself:
 - Cancel.
 - Cut.
 - Copy.
 - Paste.
 - Replace.
- Font. Used to select another font.
- Display, which has 4 sub-menus itself:
 - Tool bar. Used to display or not the tool bar.
 - Status bar. Used to display or not the status bar.
 - Mouse position. Use to display or not the mouse position.
 - Grid. Use to display or not the grid.
- Import/Export (Data point in ASCII). Used to import or export an analysis file, and which has itself 4 sub-menus:
 - Import EZChrom analyses.
 - Import a data file (ASCII).
 - Export analyses files (ASCII).
 - Export report in ASCII.
- Edit mathematics options. Used to subtract an analysis or to smooth a signal.

The **Window** menu has eleven sub-menus: (plus the name of the displayed windows).

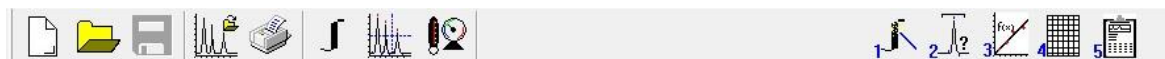
- Cascade.
- Tile horizontal.
- Tile vertical.
- Arrange icons.
- Refresh.



- Close all.
- Results table.
- Analytical parameters.
- Integration parameters.
- Display components table.
- Report editor.

2.6 The icons of the Process module

Thirteen icons are in the toolbar of the process module.



From left to right, they are:

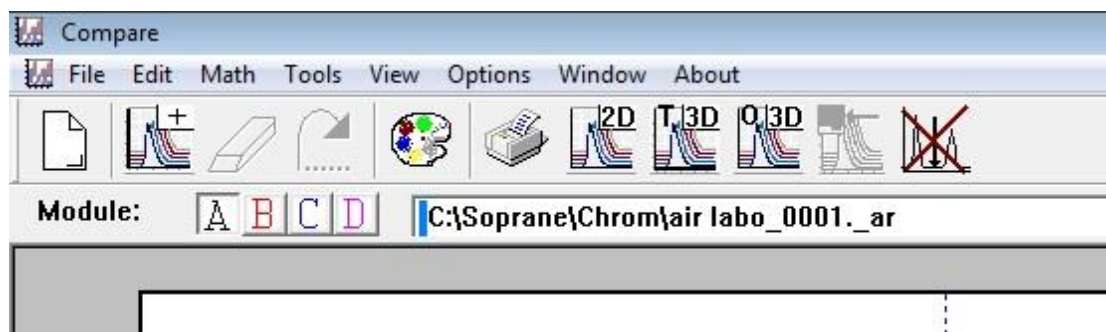
- Icon to create a new method.
- Icon to open an existing method.
- Icon to save files.
- Icon to load analysis results.
- Icon to print windows.
- Icon to integrate the chromatogram(s).
- Icon to view the chromatogram.
- Icon to view the analytical parameters used.
- Icon to access the integration parameters.
- Icon to access the components table.
- Icon to access the calibration results.
- Icon to access the results table.
- Icon to display the final report.

Under the tool bar, **Module:** A B C D allows the selection of the module whose analysis is then displayed.

2.7 The Compare module

The compare module is used to visualize and compare several chromatograms.

Upon loading, the main screen is displayed:



2.8 The menus of the Compare module

The **File** menu has eleven sub-menus:

- New. Used to open an empty window.
- Open. Used to open a filed window.
- Close. Used to close the current window.
- Save. Used to save the current window.
- Save as. Used to save the current window under a new name.
- Load. Used to simultaneously load up to 64 analyses in a window.
- Sequential load. Used to select up to 64 analyses and then display them one at a time.
- Save analysis as. Used to save the data.
- Print setup. Used to select parameters for the printer.
- Print. Used to print the current window.
- Exit Program. Used to close the compare module.

The **Edit** menu has four sub-menus:

- Undo. Used to undo the last action.
- Redo. Used to redo the last action.
- Copy.
- Chromatogram display limits. Used to modify the limits of the display.

The **Math** menu has six sub-menus:

- Difference. Used to display the difference between two curves.
- Sum. Used to display the sum of two curves.
- Ratio. Used to display the ratio of two curves.
- First derivative. Used to display the first derivative of a curve.
- Smooth. Used to smooth a curve.
- Scale. Used to modify the scale of a curve.

The **Tools** menu has four sub-menus:

- Zoom. Used to zoom a curve.
- Select. Used to select a specific curve.
- Move. Used to move a curve, with three possibilities: free, horizontal or vertical move.
- Stretch. Used to stretch a curve, with three possibilities: free, horizontal or vertical stretch.

The **View** menu has seven sub-menus:

- Toolbar. Used to display or not the toolbar.
- Channel bar. Used to display or not the channel bar.
- Status bar. Used to display or not the status bar.
- Pallet. Used to display or not the pallet.
- Mouse position. Used to display or not the mouse position.
- Gridline. Used to display or not the grid.
- Axes. Used to display or not the scale values on the axes.

The **Options** menu has six sub-menus:

- 2D. Used to display the curves in 2D mode.
- 3D transparent. Used to display the curves in 3D transparent mode.
- 3D opaque. Used to display the curves in 3D opaque mode.
- Display 3D panel. Used to display the window which allows to place the chromatograms in 3D.



- Zoom to same coordinates. Used to activate simultaneous zoom in several windows
- Font. Used to select font.

The **Window** menu has five sub-menus: (plus the name of the windows).

- Cascade.
- Horizontal tile.
- Vertical tile.
- Arrange icons.
- Refresh.

2.9 The icons of the Compare module

Eleven icons are in the toolbar of the compare module.



From left to right, they are:

- Icon to open a new window.
- Icon to open a filed window.
- Icon to undo.
- Icon to redo.
- Icon to display or not the pallet.
- Icon to print the current window.
- Icon to display the curves in 2D mode.
- Icon to display the curves in 3D transparent mode.
- Icon to display the curves in 3D opaque mode.
- Icon to display the window which allows to place the chromatograms in 3 D.
- Icon to deactivate the superposition of chromatograms done with the key combination Shift + Left click.

2.10 Reading of the status

When SOPRANE is launched, when a new method is sent to the analyzer, before to start analyses or before to stop SOPRANE and the analyzer, you must visualize the status of the analyzer. Is it "ready" for what is expected?

In addition, viewing status is the best way to ensure SOPRANE's ability to interact with the analyzer.

We have already seen that the "**Instrument / Status**" menu, as the icon symbolizing an eye, allows the reading of the status.

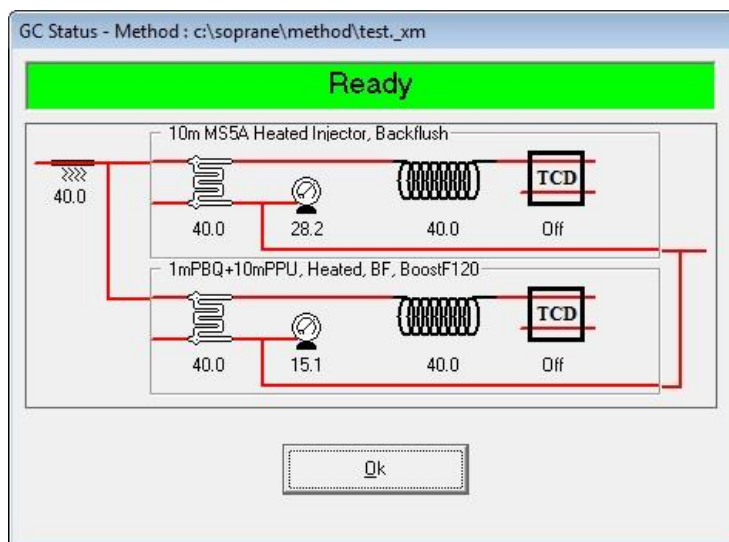
The window which opens indicates all that relates to the apparatus: number of modules, temperatures, pressure, and state of the detectors. The upper part of this window allows to see immediately whether the apparatus is operational (green background) or not (red background).



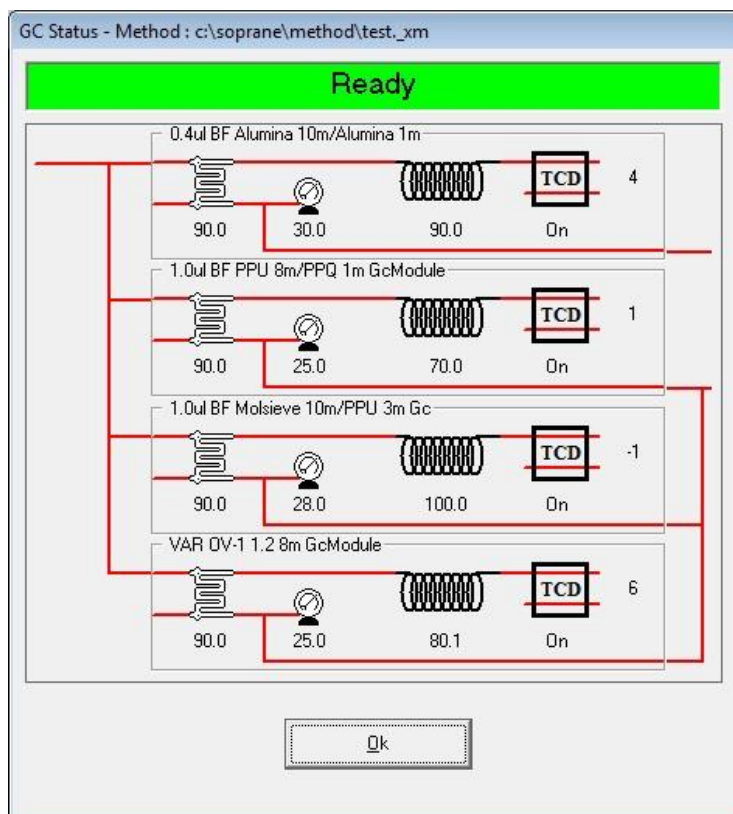
The screens corresponding to the status of different types of apparatus are presented below. They are relatively similar; we can just notice the following differences:

- The status of Micro GC 490 and Micro GC 3000 present more information concerning the columns than the M200 status.
- The status of Micro GC 3000 and M200 display a value on the right of the TCD corresponding to its auto-zero signal.

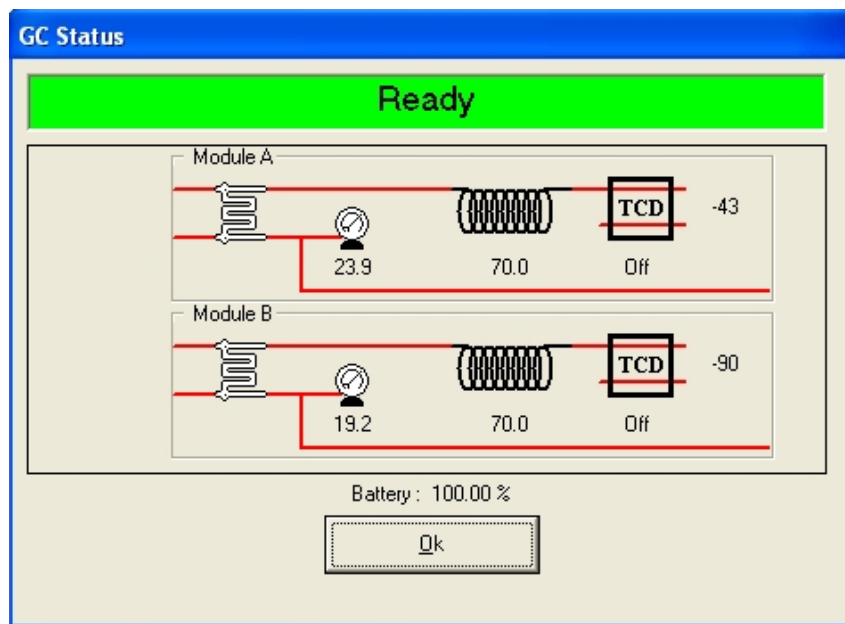
Status of a MicroGC 490:



Status of a MicroGC 3000:



Status of a M200:



3. Analysis methods

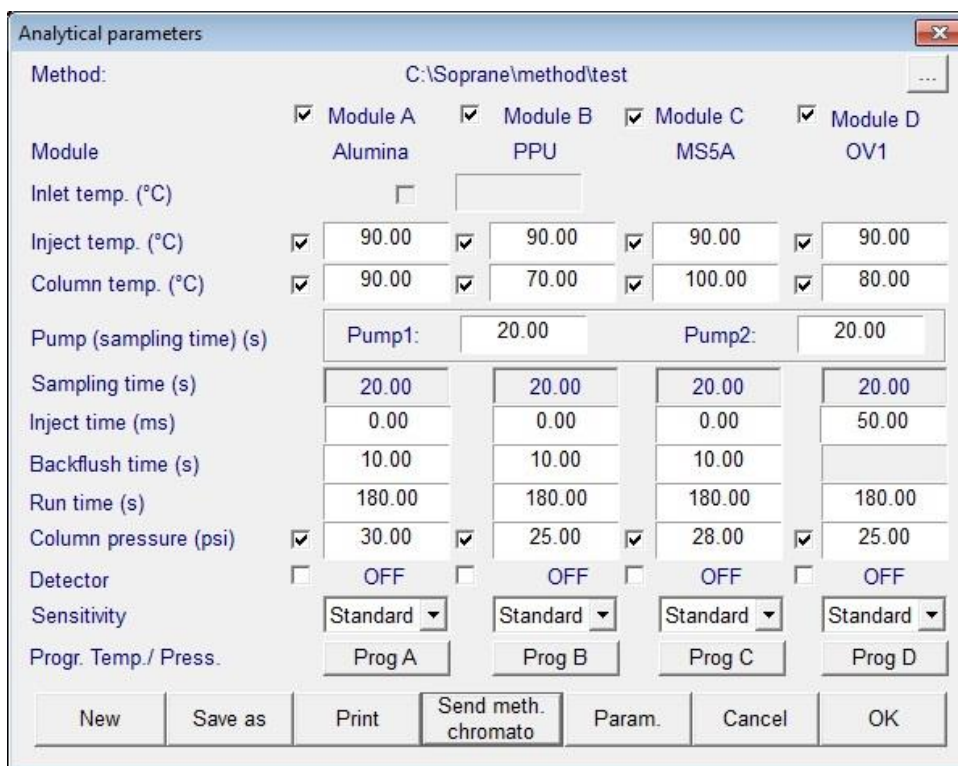
An analysis method regroups both analytical conditions, managed by SOPRANE, and integration and calibration parameters which will be configured in the Process module (see chapters 6 to 8).

3.1 Create and modify an analysis method

There are several ways to create an analysis method, depending if we start from new parameters or if we modify an existing method.

1. On the menu, click on **"Instrument / Edit a method"** or on the corresponding icon.
2. In the window displayed, you can proceed by different ways:
 - Modify the different analytical parameters displayed (example below for a Micro GC 3000) and click on "Save as".





Note: the definition of these parameters is presented in §3.4.

Or

- Click on **"New"** or **"New method"** (depending on the apparatus model). In the dialogue box, indicate the name chosen for the new method. No extension is required.

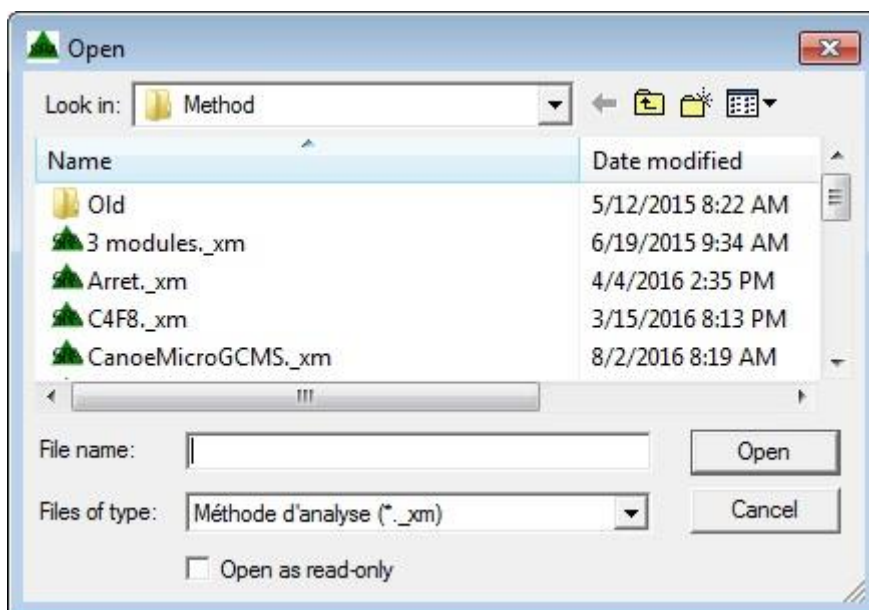


The window with analytical conditions is displayed, with default values. Set the analytical conditions and click on Ok.

Or

- Click on **"Open a method"** or on the button **"..."** depending on the apparatus model.
- Select the method and click on Open.







- Modify the analytical parameters and click on Ok.

3.2 Send a method to the analyzer

There are several ways to send an analysis method to the analyzer:

- Either from the analytical conditions window: 
 - Click on "**Send meth. chromat**" (for ex. when the method has just been created).
 - Click on "Open a method" or on the button "..." (Depending on the apparatus), select the method and click on "Send meth. chromat".
- Or:
 - Click on "**Instrument / Send a method**" or on the corresponding icon 
 - Select the desired method and click on Open.

3.3 The analytical conditions

The PGCSetup installation program allowed to configure SOPRANE according to the type of analyzer used: a Micro GC 490 or a Micro GC 3000 or a chromatograph M200.

The instruments being different, the visualization of the analyses methods will also be different.

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 μ GC 3000 and the M200 only, this duration can be set at zero for the back-flush injectors, in order 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 in order 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 is able to detect ppm as well as 100% of a compound.

Suppose we work with peaks heights, that is to say 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 μ 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 μ 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.

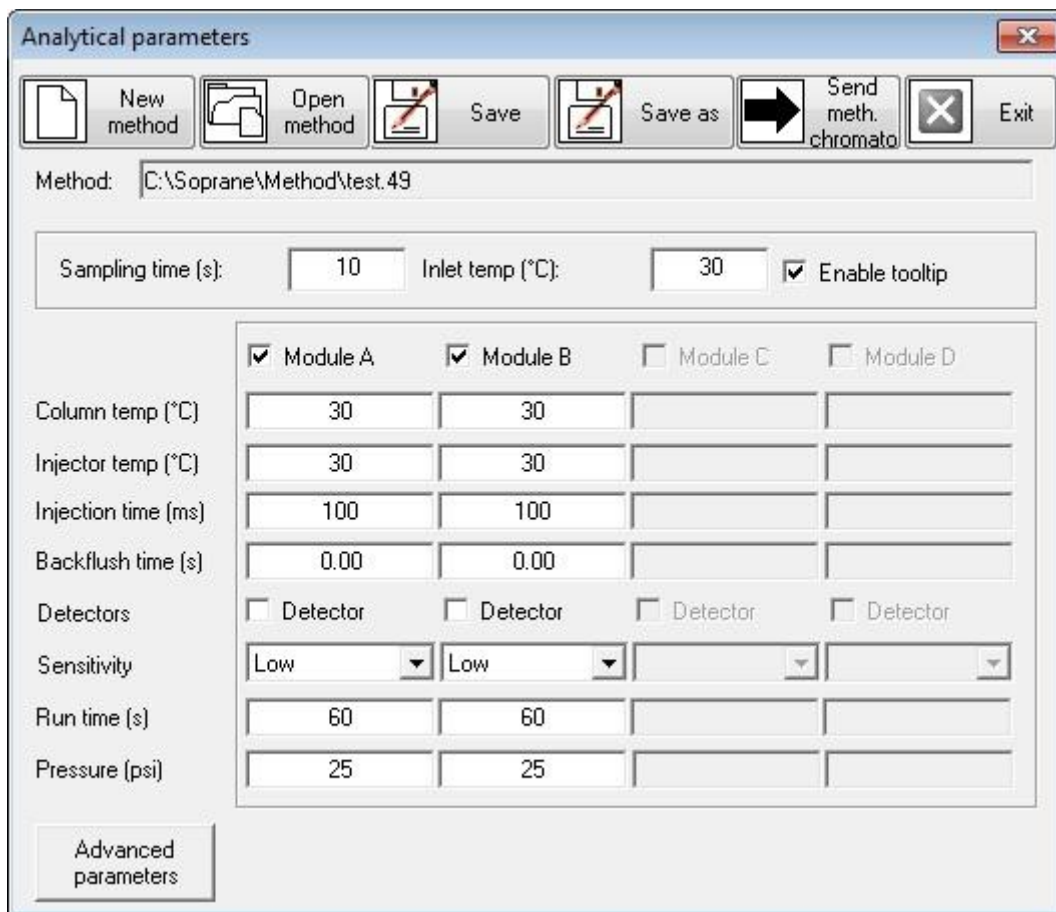
If you analyze compounds at ppm levels, the A/D conversion error becomes too important and it is better to minimize it by using a "high" sensitivity.

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.

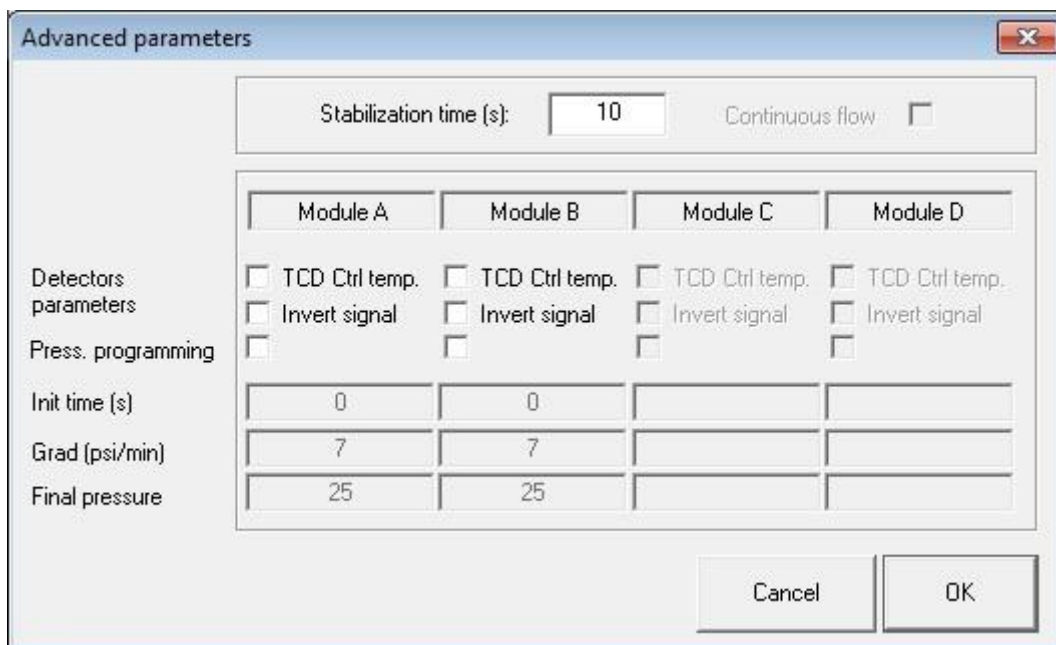
3.4 Driving of a Micro GC 490

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





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 Setup.
- **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.

3.5 Driving of a Micro GC 3000

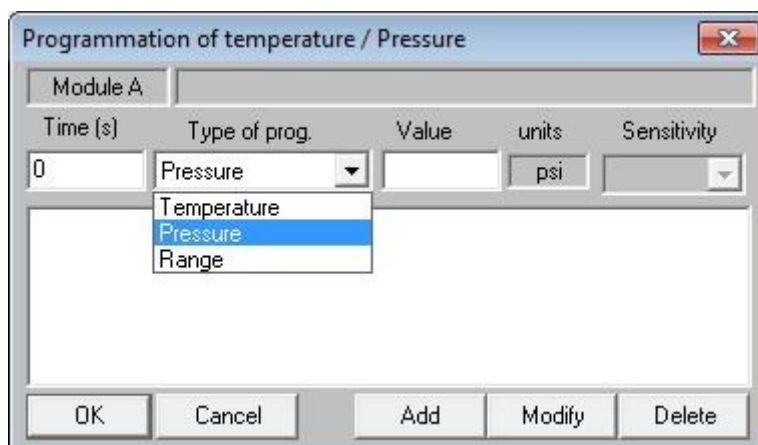
Here is the window in which analytical conditions for a Micro GC 3000 can be set:

Module	Alumina	PPU	MS5A	OV1
Inlet temp. (°C)	<input type="checkbox"/>			
Inject temp. (°C)	<input checked="" type="checkbox"/> 90.00	<input checked="" type="checkbox"/> 90.00	<input checked="" type="checkbox"/> 90.00	<input checked="" type="checkbox"/> 90.00
Column temp. (°C)	<input checked="" type="checkbox"/> 90.00	<input checked="" type="checkbox"/> 70.00	<input checked="" type="checkbox"/> 100.00	<input checked="" type="checkbox"/> 80.00
Pump (sampling time) (s)	Pump1: 20.00	Pump2: 20.00		
Sampling time (s)	20.00	20.00	20.00	20.00
Inject time (ms)	0.00	0.00	0.00	50.00
Backflush time (s)	10.00	10.00	10.00	
Run time (s)	180.00	180.00	180.00	180.00
Column pressure (psi)	<input checked="" type="checkbox"/> 30.00	<input checked="" type="checkbox"/> 25.00	<input checked="" type="checkbox"/> 28.00	<input checked="" type="checkbox"/> 25.00
Detector	<input type="checkbox"/> OFF	<input type="checkbox"/> OFF	<input type="checkbox"/> OFF	<input type="checkbox"/> OFF
Sensitivity	Standard	Standard	Standard	Standard
Progr. Temp./ Press.	Prog A	Prog B	Prog C	Prog D

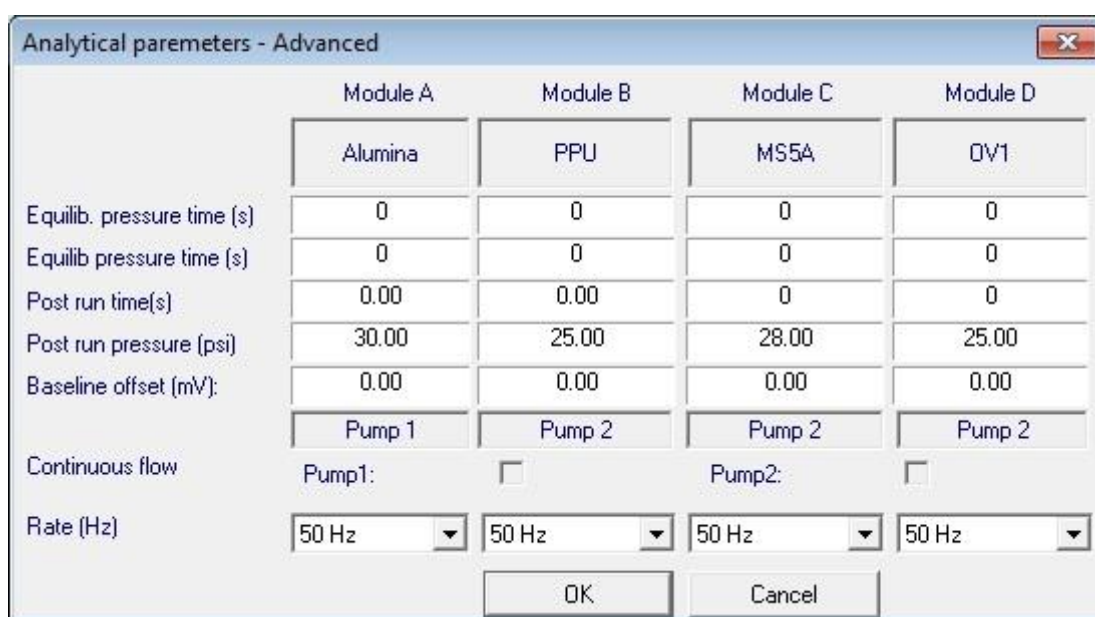
On this first screen of the analytical parameters, a set of buttons, named Prog A to Prog D, allows the writing of several programming steps in order to modify the values of temperature, pressure or sensitivity along the analysis.

These programming steps must be written in increasing times.





The button "Param." allows to reach a second screen:



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 taken into account. 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 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.

Baseline offset:

The value, expressed in millivolts, allows to shift the analysis signal in a direction or another.



The continuous flow:

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

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.

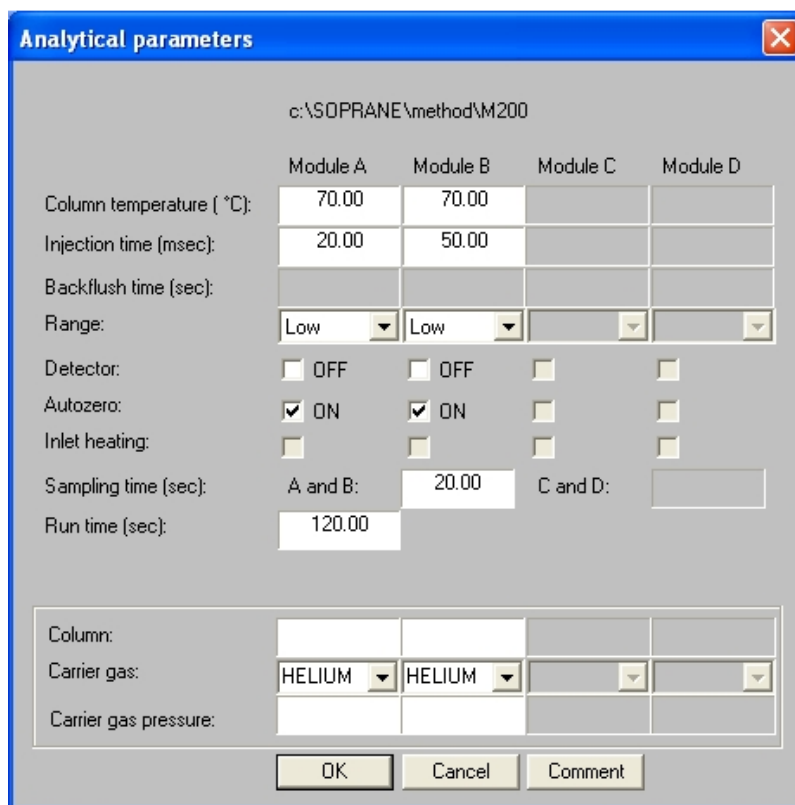
3.6 Driving of a M200

The display allowing visualization, editing or modification of all parameters of the analysis method is shown below.

The range of sensitivity the user may select is: low, mean or high.

The carrier gases are Hydrogen, Helium, Nitrogen or Argon.

The user has just to indicate the correct values for time and temperature.



3.7 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 also 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 13). 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. Analyses sequences

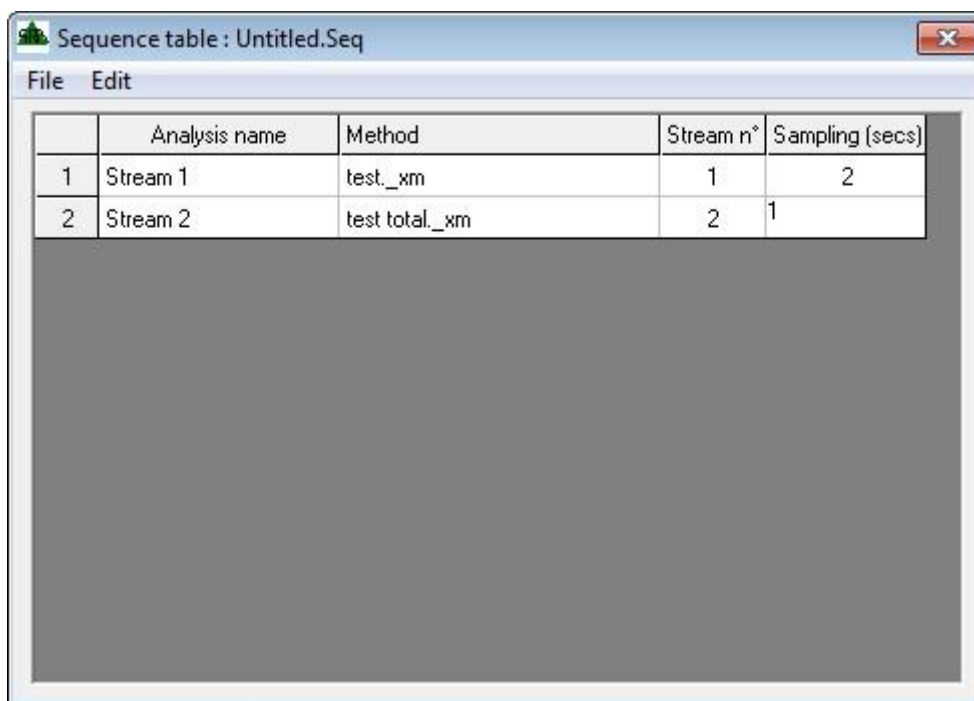
We have seen how to write (creation or modification) an analysis method and how to send it to the analyzer. The analyses sequence is useful when several methods are used because either we analyze several streams with different compositions or because we don't always work in the same operating conditions 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 considered to be more important than others.

The "**Sample / Sequence table**" menu allows to select the streams which will constitute the analyses sequence.





	Analysis name	Method	Stream n°	Sampling (secs)
1	Stream 1	test._xm	1	2
2	Stream 2	test total._xm	2	1

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 injection.

The analysis method already includes an injection loop sweeping duration, which corresponds to the pump management. Indeed, before injecting, it is necessary to make the sample circulate in the injection loop, which can require a pump to suck the sample.

The duration programmed here is before and does not concern the injection itself but the sample circulation. It corresponds to the sample selection.


When the stream selection valve is switched, it is necessary to sweep "residues" of the previous stream so that what will be injected will be representative of the sample to analyze. This requires a more or less long time depending on the sample, its characteristics, its flow rate and on the volume separating the sample selection valve from the injection valve.

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

If the sweeping duration exceeds the duration separating the end of the injection of the on-going analysis and the beginning of the following analysis, a temporization is implicitly added by SOPRANE.

5. Start and stop of the analyses



The menu "**Process / Start analysis**" of SOPRANE, as the icon **START** , allows the starting of the analyses.

It is then possible to start one or several analyses, an analyses sequence or the repetition of the same analyses sequence.



When requested, SOPRANE sends the analysis method and the analysis starts as soon as the chromatograph is stabilized under the necessary working conditions.

3 or 4 launching modes are accessible:

- **Analysis mode:**

In this window, it is possible to select the number of runs that we want to launch (up to 999), the analysis method, to give a name to the analyses series and to indicate a name for the folder (this latter will be automatically created).

You can also mention the sample name, the operator and the interval between each injection.

Check the box "Waiting for external start" if your Micro GC is coupled to an analysis instrument whose end of analysis will trigger the injection in the Micro GC.

Start of analysis

Start analysis

Analysis mode Number of runs: 1

Single sequence

Automatic mode

Calibration

Method: test_xm

Name: air labo

Path: C:\Soprane\Chrom

Sample name

Operator

Interval in minutes between injections: 0.00

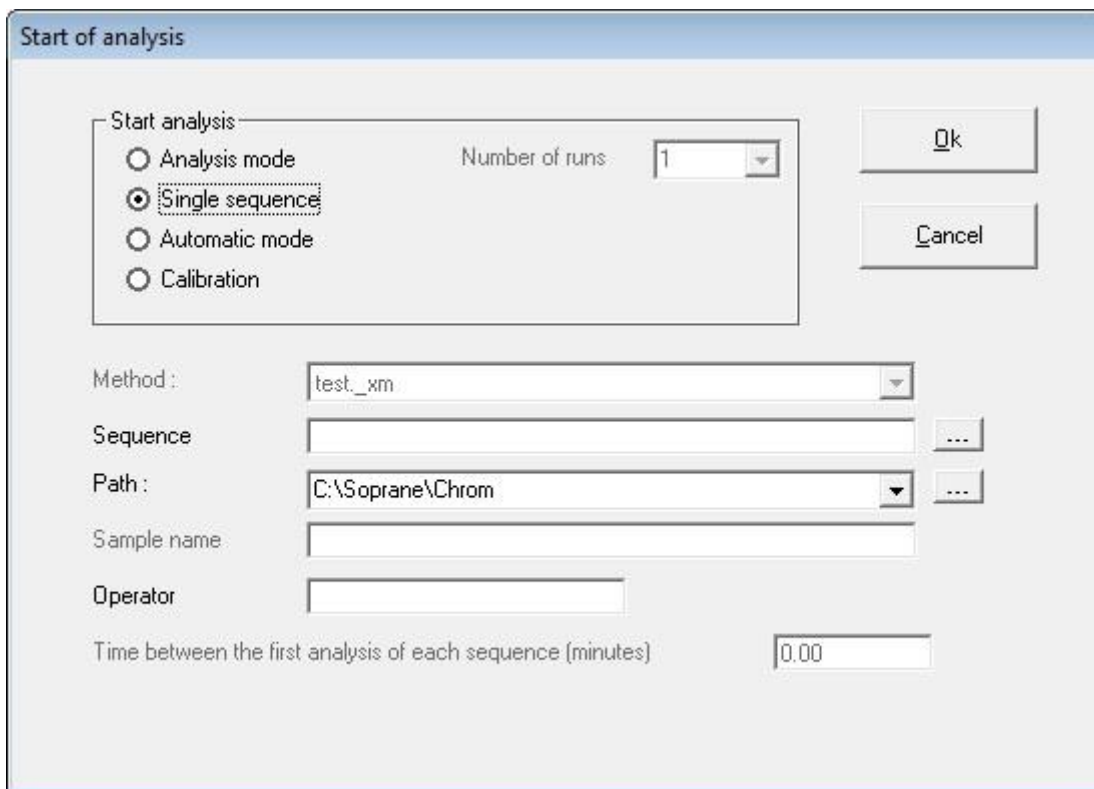
Ok

Cancel

- **Single sequence mode:**

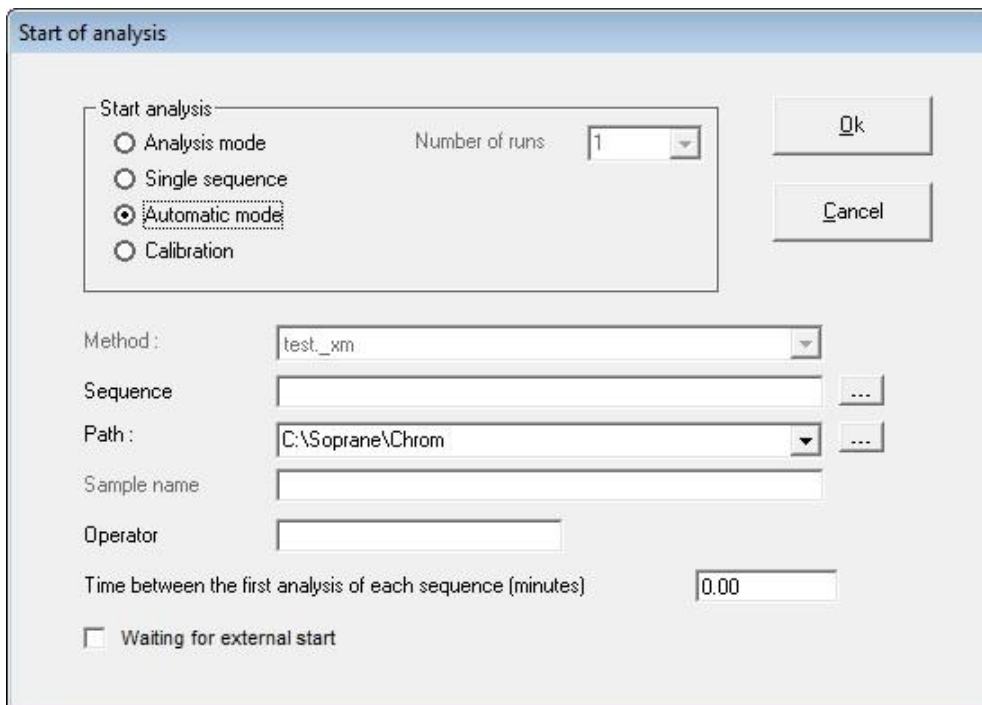
As the aim is to launch only one sequence, compared to the previous case, the number of runs, the method and the interval between the first analysis of each sequence are not accessible (grayed).





- Automatic mode:

As long as SOPRANE will be maintained in analysis, the same sequence will be indefinitely repeated. It may be necessary to respect a certain time before repeating the sequence thus you can specify the time (expressed in minutes) separating the injection times of the first analysis of two successive sequences.



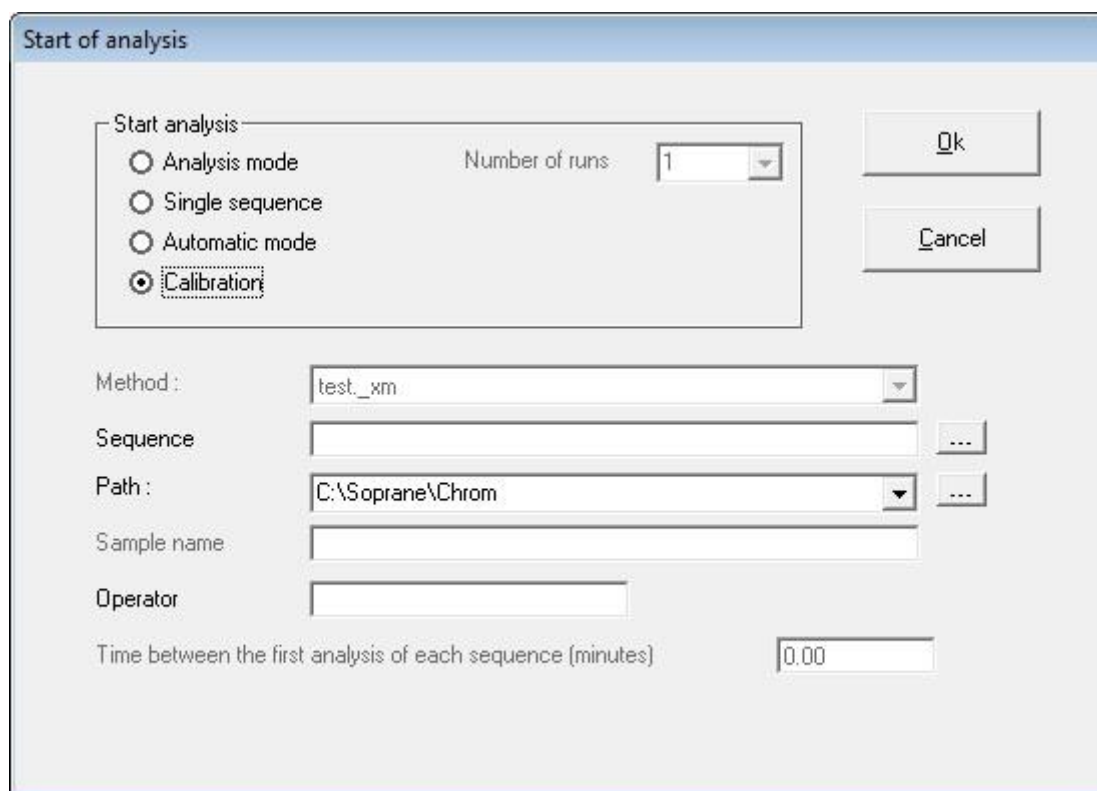
NOTE:

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

- **Calibration mode:**

This mode is displayed on the screen only if a standard has been previously defined when configuring the instrument in Soprane Setup.

For more details, see chapter 8 concerning calibration.



In the same way, the stop of an analyses cycle can be required by the menu "**Process / Stop**" or the icon



A dialog box asks for the confirmation of the demand and specifies that the effective stop will occur at the end of the analysis in progress.



6. Integration



The integration of a chromatogram is performed in the Process module, accessible via:



6.1 Integration methods

The integration method is a sub-part of the analysis method and is itself constituted of several parts:

- data specifying the treatment to perform
- data concerning the integration itself
- data concerning the sample
- a components table
- the potential indication concerning a mathematical treatment to use
- the reference of a potential user program to launch after the analysis.

When creating an analysis method in Soprane, some integration values by default are already associated to the analysis method.

Thus in practice, when we open the Process module to perform the integration, the analysis is displayed with the associated method and this is then that we will modify the integration values by default which will be saved in our analysis method.

However, it is all the same possible to create or open an integration method:

- To create a new integration method, select "**Method / New method**" or click on the icon "New".
- To open an existing integration method, select "**Method / Open a method**" or click on the icon "Open".

6.2 Integration events

The integration of a chromatogram needs 2 distinct processes:

- First it is necessary to detect the presence of peaks.
- In a second time you have to interpret the shape of these peaks in order 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: the peak width and the slope sensitivity.

The signal of analysis is measured at a frequency of 20, 50 or 100 Hz (as defined in the analysis method, for the μGC 3000). All the values are gathered in slices in order to have a process optimized according to the peak size. The grouping 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 to the sensitivity threshold value programmed by the user.



This process authorizes a rather important flexibility. Dividing by 2 or doubling the peak width will generally not lead to important 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 of 5 $\mu\text{V/s}$ allows, there too, the detection of "common" peaks.

To increase sensitivity, it is better to check first that the value used as peak width is correct. The best value is the mid-height estimated peak width. Then it is possible to adjust the sensitivity threshold.

6.3 Nature and values of integration events

The displayed chromatogram corresponds exactly to the signal used by the software for integration. If the signal is processed with high sensitivity (see analytical parameters in chapter 3.3) and that the analyzed compounds concentration is too high, the signal may be truncated. In such a case, the peak height or area will be false.

To obtain a good integration, it is thus necessary to modify the values of peak width and sensitivity threshold along the analysis. This is done by programming "Events".

Some events are related to peaks detection, others are used to define how the baseline has to be corrected, and the last ones are used to reject or to group peaks.

These events are described thereafter. For each event, we indicate the values and the representation on the chromatogram.

Peak detection: PD+, PD-

This event has 2 states ON, symbolized by PD+, and OFF, symbolized by PD-.

When the peak detection is ON, the system integrates the signal.

By default, this event is ON. It is up to the user to prohibit integration when it is wished (solvent rejection ...).

Negative peak detection: NPD+, NPD-

This event has 2 states ON, symbolized by NPD+, and OFF, symbolized by NPD-.

The event is OFF by default. When negative peak detection is ON, the system reverses its logic: a decreasing slope corresponds to a peak beginning, whereas an increasing slope marks the end of a peak and a possible return to baseline. The peak area is obviously expressed as a positive value.

The correct use of this event consists first to prohibit the peaks detection with an event PD OFF (see above), second to reverse the integration logic (NPD ON for negative peaks, NPD OFF for positive peaks), third to authorize the integration with an event PD ON. The two first events may be programmed at the same time, but the third event must be programmed at a later time.

Baseline detection: BD

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.



Slope absolute sensitivity: SAS

This event is the limit value expressed in $\mu\text{V/s}$ of the signal slope used to detect peaks or valleys between peaks.

The programmed value takes effect immediately, until another value replaces it.

Set absolute peak width: SAP

This event is the peak width value expressed in seconds used to detect peaks.

The programmed value takes effect immediately, until another value replaces it.

Set relative slope sensitivity: SRS

This event has 2 states Half and Double.

This event allows to multiply or divide by 2 the sensitivity threshold value used by the software. The new value remains active until a new value is attributed.

Peak relative width: SRP

In the same way, this event allows to double or divide by 2 the peak width value used by the software.

The new value remains active until a new value is attributed.

Force of baseline at next valley: FBN

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.

Force of baseline at all valleys: FBA+, FBA-

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 penetration: BP

This two states event is OFF by default.

It allows to authorize (ON) or to prohibit (OFF) that the baseline correction is carried out with a baseline which cuts the chromatogram.

Baseline split: BS

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

Peak group: PG

By default, this 3 states event (ON / ALL / OFF) has the value ALL.

It allows to activate one group, all the groups or no group for peaks. The baseline for a group is drawn in blue. When a group is started with the parameter PG ALL, the areas of all the peaks whose retention time is higher than the time of event PG ALL are added, until the programming of an event PG OFF or end of integration (PD OFF) or end of the analysis. The area thus obtained is assigned to the peak having the greatest individual area and the calculation of concentration is done with the response factor affected to this peak.

When a group is started with the parameter PG ON, the end of the group can also occur if the signal goes back to baseline, which leads to the creation of a new group (since we always are in peak grouping), and until normal end peak grouping as defined for PG ALL.



Skim peak detection: SKM

This event has 3 states (Tangent / Exponential / Off). It activates or deactivates tangential integration.

Shoulder peak detection: SPD

This two states event (ON / OFF) activates or deactivates the processing of a shoulder peak as a separated peak or not. The shoulder can be indifferently on the increasing or decreasing slope of the peak.

By default, this event is OFF and the two peaks will be processed as a single peak.

Peak Forcing: SP (Set Peak)

This two states event (ON / OFF) allows to impose the detection of peaks where the other parameters prove to be insufficient, because of the asymmetry of the peaks, of a too great disparity of the shape of the peak according to concentrations ratio...

When the parameter SP is activated (SP ON), the possible integration of a peak is immediately stopped with what is considered as a return to the baseline, even if it is not the case. A new peak is immediately begun, by considering starting from the baseline, even if it is not the case.

When the parameter SP is set OFF, the peak is stopped and the integration considers that the signal went back to the baseline.

The baseline correction on a peak integrated in SP mode is done in tangential mode. If points of valley are detected, it is not one peak but several ones and these peaks are separated by vertical lines (no integration on a trail for an integrated group of peaks in SP mode), the correction of baseline being the tangent to the group, possibly several tangents if a point of valley is on a level lower than the tangent to the group.

Note: The use of parameter SP was created to solve difficult cases. If one uses this parameter for a peak posing no problem the sensitivity will certainly have to be decreased (mainly by increasing SAP parameter or SAS parameter value) to avoid reacting to the least variation of the signal.

Minimum area reject : <AR


Maximum area reject : >AR

Minimum height reject : <HR

Maximum height reject : >HR

These four events receive directly their numerical values.

6.4 Events programming

When editing the integration part of an analysis method, the button  "integration parameters" allows to access to the integration events table.

Integration Information - C:\Soprane\method\testa		
Time	Type	Value
0.0	Absolute Slope	5.000000
0.0	Absolute Peak Width	0.500000

One moves in this table with the arrows of the numeric keypad or with the mouse. The lines of the table are automatically sorted on increasing retention times.

There does not exist any priority between 2 events considered at the same time: SOPRANE manages them simultaneously.


The addition of a line is done by a right-clicking in the "Time" column and a click on "Add a line".



The removal of a line in the events table is obtained by selecting the line (right click with the mouse in the "Time" column) and by removing it with the DELETE key or by clicking on "Delete line".

As we will see later in this chapter, another method, much more precise, consists in using a chromatogram and graphically positioning the events on this chromatogram.

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.

The menu "**Integration / Integrate**", just as the icon integrate  from the control pallet or from the toolbar or the tool of the manual baseline pallet allows to perform again the integration with the new set of parameters. The old values will be lost.

6.5 The graphical tools of the Process module

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 (μV) 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 (bottom of page) and it is possible to select each one of these modules by the buttons A, B, C and D not grayed located under the toolbar.

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

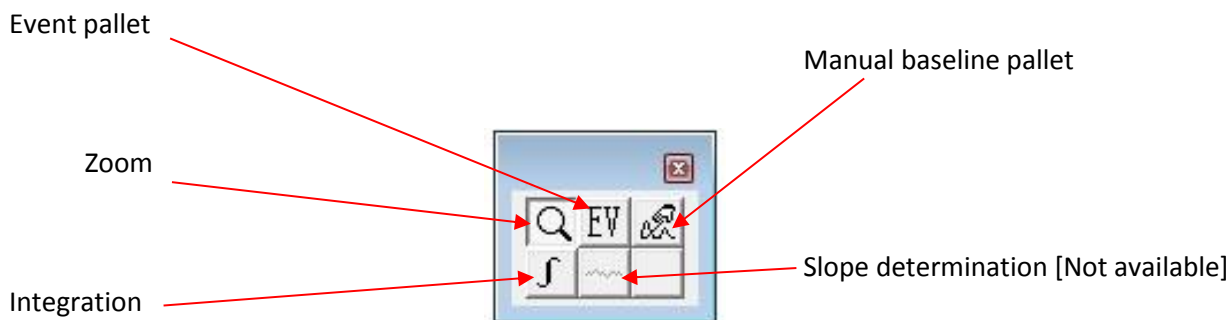
In this same bar, if a peak is integrated and that you place the mouse cursor on this peak, this peak area is indicated there.

6.5.1 Control pallet

A pallet of tools, known as "control pallet" is visualized. The menu "**integration / control pallet**" allows to show or hide it.

The commands accessible by this pallet of tools may also be reached by the menu integration.





NB: Some functionality, especially the manual baseline, are accessible only if the option is configured in Soprane Setup.

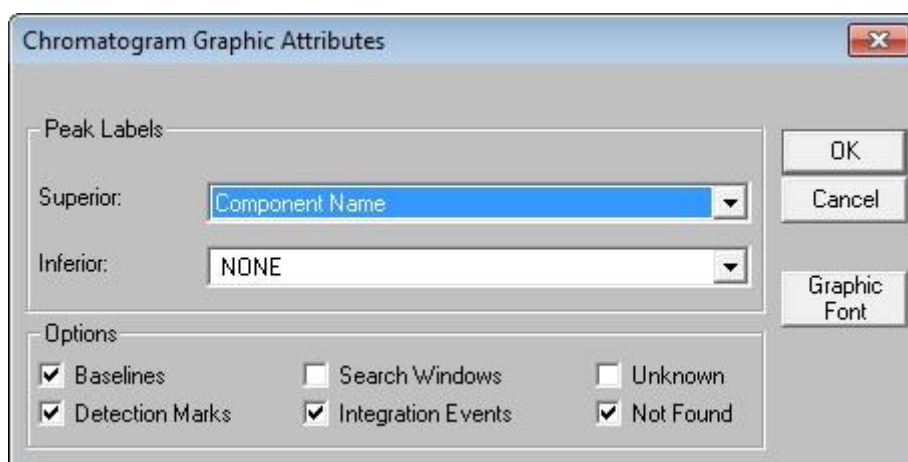
6.5.2 "Chromatogram" menu

The menu **"Chromatogram / Display chromatogram"** is useful to call the display of a chromatogram loaded in memory but not visualized.

The menu **"Chromatogram / configuration of chromatogram view"** allows the selection of what is interesting for the user.

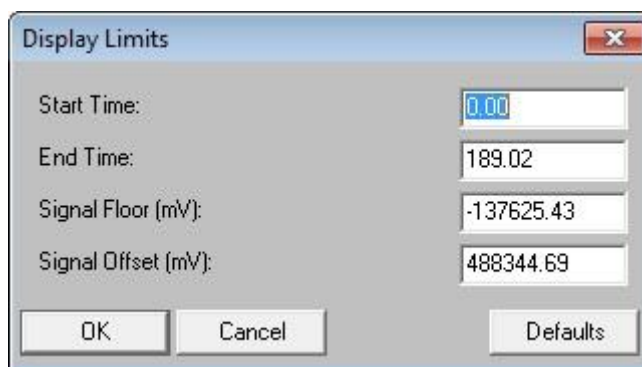
Normally each peak has its name indicated at the top. It is possible to display other values at the top or at the base of the peaks.

It is possible to indicate the baseline, the marks of beginning and end of peak, the size of the search window used to identify peaks, the integration events, to indicate the peaks seen but unknown and finally the peaks identified but not found.



The menu **"Chromatogram / edit limits of chromatogram"** is used to modify the limits: (time, offset and signal amplitude) of the representation of the chromatogram:





When the chromatogram is in the active window (menu "window" or menu "chromatogram / display chromatogram") different actions are possible with the keyboard and the mouse to move or to stretch the curves displayed or to modify their scale factor.

The zoom (control pallet tool or the toolbar icon) may be used several times consecutively to magnify a detail.

Actions related to what is shown:

The actions defined hereafter may be added, the result being memorized as scale factor or as current view display factor.

The Up Arrow is used to move the curve towards the top of the screen.

The Down Arrow is used to move the curve towards the bottom of the screen.

The Left Arrow is used to move the curve towards the left side of the screen.

The Right Arrow is used to move the curve towards the right side of the screen.

Page Up moves the curve of a quantity equal to a screen towards the bottom of the screen. This action is ignored as long as the chromatogram fills the whole screen since the displacement would result to visualize an empty screen.

Page Down moves the curve of a quantity equal to a screen towards the top of the screen. This action is ignored as long as the chromatogram fills the whole screen since the displacement would result to visualize an empty screen.

Control and Page Up moves the curve of a quantity equal to a screen towards the left side of the screen. This action is ignored as long as the chromatogram fills the whole screen since the displacement would result to visualize an empty screen.

Control and Page Down moves the curve of a quantity equal to a screen towards the right side of the screen. This action is ignored as long as the chromatogram fills the whole screen since the displacement would result to visualize an empty screen.

Control and the Up Arrow stretches the curve according to the signal axis, the zero value of the signal (theoretical value of the baseline in the absence of peak and drift) remaining positioned at the same place.



Control and the Down Arrow compresses the curve according to the signal axis, the zero value of the signal (theoretical value of the baseline in the absence of peak and drift) remaining positioned at the same place.

Control and the Left Arrow compresses the curve according to the time axis, the zero-time remaining positioned at the same place.

Control and the Right Arrow stretches the curve according to the time axis, the zero-time remaining positioned at the same place.

Actions to show another view:

The actions defined hereafter are used to create new views, to delete all of them or to go from view to view among the memorized views. Each of these views can be modified as indicated before.

The selection of a rectangle with the mouse (left button) is used to create a new view whose content will represent the part of the curve selected with the mouse.

Control and Home, as well as Shift and Home, creates a new view equivalent to the beginning view. The display is optimized so that the curve fills the whole view.

Home deletes all the views, excepted the first one. The modifications potentially brought on this first view are maintained and shown.

End is used to go to the last memorized view.

Shift and Page Up, as well as a double right click of the mouse, is used to show the preceding view, if it exists.

Shift and Page Down is used to show the next view, if it exists.

The menu "**Chromatogram / thick curve**" (or "**thin curve**") is used to modify the thickness of the line used to draw the chromatogram.

6.5.3 The zoom tool

The zoom tool (a magnifying glass) of the control pallet, as well as the equivalent icon in the toolbar, allows to magnify the chromatogram. It is enough to select a rectangle with the mouse (click on the left button maintained) and to release the button to modify the curve. This can be repeated several consecutive times. A double right click allows to make the opposite operation, going back each time to a zoom level.

It is also possible to use the arrow keys of the numeric pad to modify the position of the chromatogram on the screen, and/or the same keys with the key control pressed to stretch the chromatogram (All possible actions are described later in chapter 15-3).

6.5.4 Graphical edition of the integration events

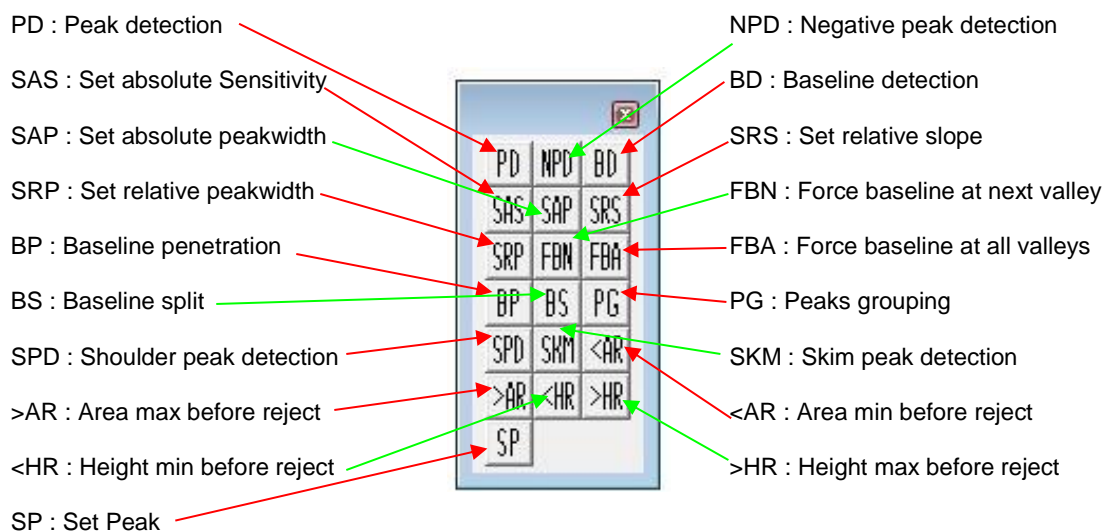
We saw how to write the integration events in the table. It can be faster to place them directly on the chromatogram. The examination of various chromatograms allows to define the zones where the peaks are expected. The zoom then allows a precise positioning of each event.

The menu "**Integration / Events integration pallet**", just as the icon "EV" of the control pallet, allows the visualization of the events pallet.



When visualized, the events pallet can be closed by a mouse click on the cross in right top of the pallet. The cursor symbolizing a hand noted EV shows that the tool "event" is active. A click on the zoom tool allows to deactivate the tool event.

The closing of the pallet does not remove the tool event (the cursor always symbolizes a hand). The tool events is inactive when one selects another tool (normally the zoom tool).



To position an event, it is enough to magnify the chromatogram until obtaining a correct visualization of the place where one wishes to insert the event, to select the event tool (click on the corresponding icon), to select the event which interests us (mouse left button pressed on the event icon) then to make it slide at the desired time (left button maintained pressed) and to drop it (left button released).

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

To delete an event, the easiest way is to remove it in the events table (see previous paragraph).

Sometimes, it is necessary to simply modify the time to which an event is programmed. In this case, it is enough to bring the cursor on the event and to seize it with the mouse left button. A vertical bar appears as soon as the mouse is moved. The event can be dragged then dropped down where it is wished. The change of the value may also be done directly in the table.

6.5.5 The manual baseline pallet

The events pallet modifies the events table and thus the method used. These modifications can be usable later on at the time of the analyses.

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.

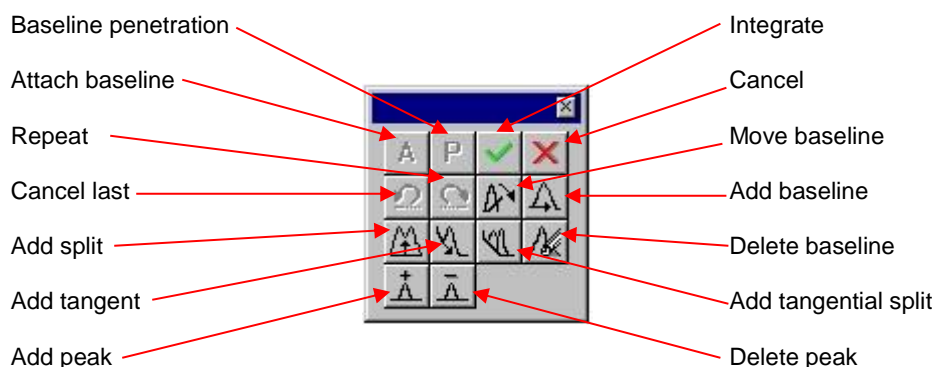
The menu "**Integration / Manual baseline pallet**", as well as the tool of the control pallet or of the toolbar symbolized by a mouse, allows to display the manual baseline pallet.

This pallet is closed using the cross located in its top on the right. The closing of the pallet removes also the tool manual baseline. When this tool is active, the cursor is symbolized by an arrow.



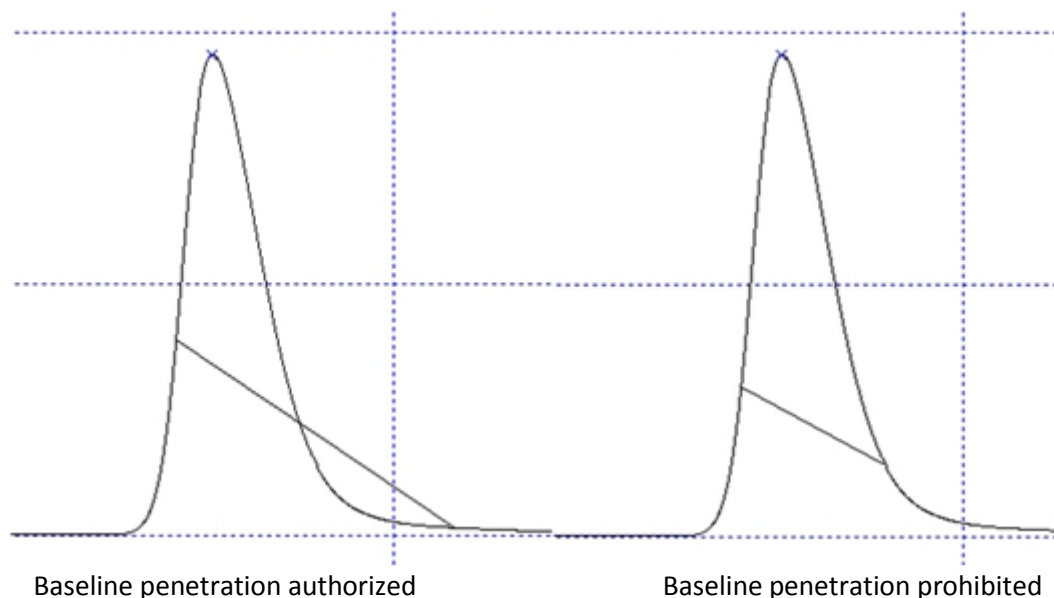
This tool allows to trace, to add or to move the baselines as desired and to modify the way the peaks are integrated.

To use it, it is enough to click on the tool, to bring the mouse to the starting point (beginning of the peak for example if a baseline is added), to press the left button of the mouse, to move the mouse on the point of arrival (end of the peak, in the preceding case) and to release the left button.



The tool for baseline penetration, symbolized by a "P", allows or prohibits that the baseline cuts the chromatogram and thus avoids adding a negative area to the peak (If the chromatogram is on both sides of a baseline, the area delimited by the signal and located under the baseline is counted negatively when correcting the baseline).

The defect is voluntarily magnified to show the impact of this tool



The menu **"Integration / Undo Manual baseline modification"** allows to remove all the modifications carried out. This menu is inactive if no manual correction has been made.



7. Peaks identification

The peaks integration being done, the aim is now to associate each peak to an eluted compound. The peaks identification is performed in the Process module.

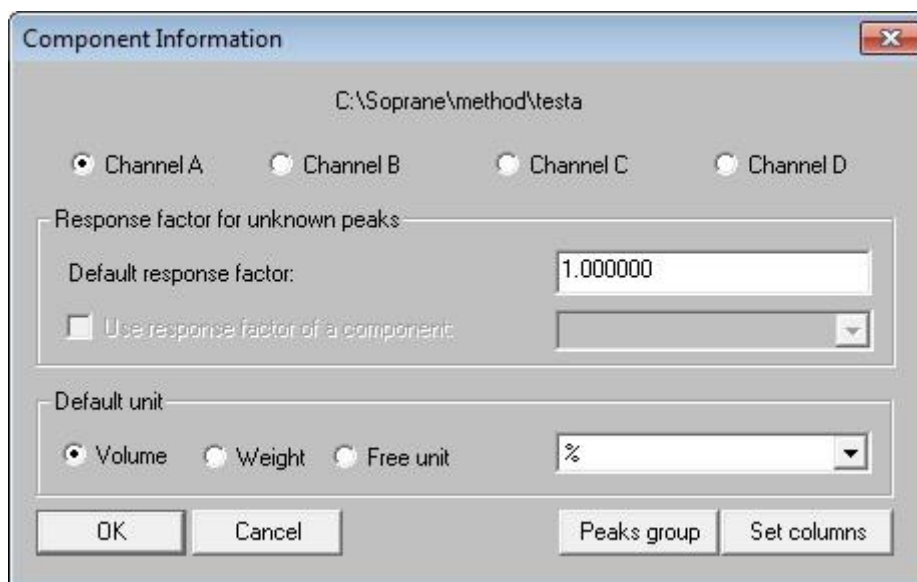
7.1 Components table

To reach the components table, click on the corresponding icon .

By default, we have a components table with predefined columns and units, but it can be modified. For this, select **"Integration / Header of components table"**.

Note: If no analysis has been made with the method, the components table is inaccessible.

The window displayed allows the programming of general information.



For each analytical module, it is thus possible to indicate:

- A response factor by default.
- A type of unit (volume, weight, free) and a unit (% , ppm, ppb) by default.

This display shows the concentration unit by default. The user has the possibility to add free units. This is done by the menu "Integration / Edit free unit".

This menu allows access to a screen allowing the editing of units in the form:



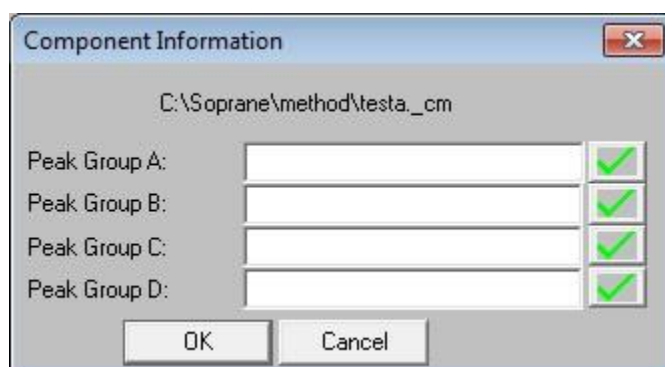


7.2 Peaks grouping

SOPRANE offers the possibility to gather peaks integrated separately in order to treat them later as only one peak.

When we will edit the components table, we will see that it is possible to define four groups of peaks identified by the letter A to D.

The button "Peaks group" allows to give a name to each one of the 4 groups of peaks. This may be done before or after the edition of the components table.



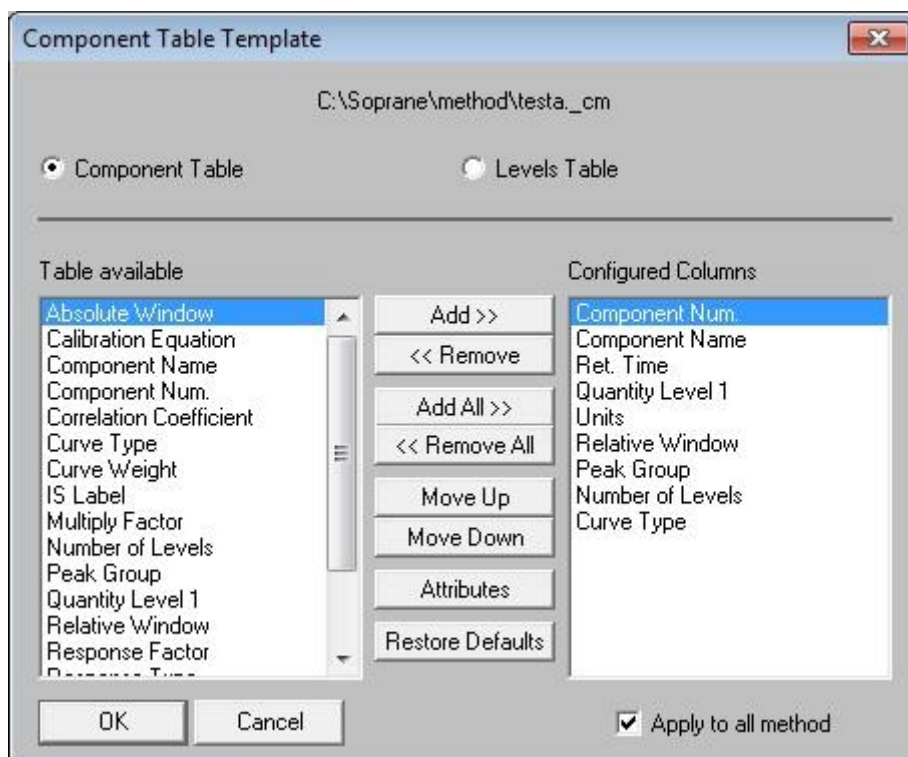
These peaks groups will be accessible only in the report of the Process module.

7.3 The columns of the components table

The components table can contain a lot of data. Some data are useful to a given user, others are not.

The button "Set columns" allows to reach a data sheet where one selects the nature of the columns which will be shown later on.





To the components table is associated a levels table which is similar. The part "components" relates to the peaks identification, the part "levels" relates to the calibration parameters.

Each column may be added, removed or be moved upwards or downwards.

A button "Attributes" also allows to modify the column name, the column width and various other similar parameters.

For the components table, the kind of columns viewable are:

The absolute 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 an absolute value.

The 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.

The component 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. It is under this name that the compound will be identified for post-analytical calculations or trends outputs for instance.

The component number: It is an identification number internally used by SOPRANE.

The 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.

The curve type: According to the number of points used to calibrate the response, it is possible to define several response 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, a curve of the second, third, fourth degree, exponential or a logarithmic curve may be defined.



The curve weight: It is the way to ponder the calibration curve. The software offers 9 possibilities based on the quantity: equal to 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.

The IS label: This column allows to define an Internal standard (Letter "I" followed by a reference letter) or to associate an internal standard to a peak (only the second letter).

The multiply factor: This coefficient acts like a multiplicative factor of the concentration.

The number of levels: It is the number of successive concentration values used to calibrate and determine the response curve for a given component.

The peak group: It is a flag (A, B, C or D) indicating which peaks, because they have the same flag, will be grouped for calculations. It is thus possible to define 4 groups of peaks. (Warning: they are not peaks integrated together with a common baseline correction; these peaks are integrated separately, or not, and then grouped only for calculations).

The quantity level 1: It is the component concentration.

The 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.

The response factor: It is the "traditional" response factor, i.e. corresponding to a line passing by origin.

The response type: The software allows to work indifferently with peaks area or height.

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

The RP label: This parameter allows to define a Reference Peak making easier the compound identification. To define the reference peak, one types the letter "R" and another letter which identifies the peak. To assign a peak reference to a compound, only type the second letter.

This process makes easier the identification of a peak difficult to find : its expected retention time will be corrected by applying a relative variation equal to the one observed on the reference peak (easy by its size to identify).

The units: It is the unit used to express the concentration value.

IMPORTANT NOTE:

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

For instance, let us 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 between 1 mn 42 seconds and 2 mn 18 seconds.

For the levels table, the kind of columns viewable are:



The amount: It is the amount of standard component for the considered level. It is possible to visualize the values obtained for each of the calibration measurements by a double click on this box.

The level: If the calibration is made with more than one standard stream, the level indicates which points correspond to the stream.

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

The area: It is the area or height value relating to that level of calibration.

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

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

Used: It 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 (X) or is not () used for this peak.

7.4 Display of the components table



The button "Components table" 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.

Number Component	Component Name	Time retention (Sec)	Quantity Level 1	Units of report	Relative Window (0 to runtime (seconds))	Peak Group	Levels	Curve Type
1	MeOH	43.84	1.000	%	5.00		1	Linear Through Zero
2	Acetone	56.34	100.000	ppmVol	5.00		1	Linear Through Zero

Level MeOH	Amount	Relative Tolerance (0 to runtime (seconds))	Area	Area / Amount	Used
1	1.0000	0.00	3923.00	3923.00	X

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 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 are 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 column heading ("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.

If the user has selected it by the menu "integration / update retention time after integration" the expected retention time will be corrected at the end of each analysis.

The second table relates to the calibration:

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" are to be informed.

On the bottom table (the levels table), the right border is thicker: when the mouse is over this border, the cursor is changed and offers the possibility to pull a window including the response curve display.

The screenshot shows a window titled 'Component Information - C:\Soprane\method\testsraa : MeOH*'. It contains two tables and a graph.

Number Component	Component Name	Time retention (Sec)	Quantity Level 1	Units of report	Relative Window (0 to runtime (seconds))	Peak Group	Levels	Curve Type
1	MeOH	43.84	1.000	%	5.00		1	Linear Through Zero
2	Acetone	56.34	100.000	ppmVol	5.00		1	Linear Through Zero

Level MeOH	Amount	Relative Tolerance (0 to runtime (seconds))	Area	Area / Amount	Used
1	1.0000	0.00	3923.00	3923.00	<input checked="" type="checkbox"/>

The graph shows a calibration curve with the equation $Y = 3922.990305x$. The x-axis is labeled 'Amount' and ranges from 0.00 to 1.00. The y-axis is labeled 'Area' and ranges from 0.00e3 to 4.00e3. A straight line passes through the origin (0,0) and the point (1.00, 3923.00).



SOPRANE avoids a tiresome programming to the user and allows him to save time by limiting the risks of error. The first time that one wants to edit the components table, SOPRANE has already in memory a chromatogram with integrated peaks.

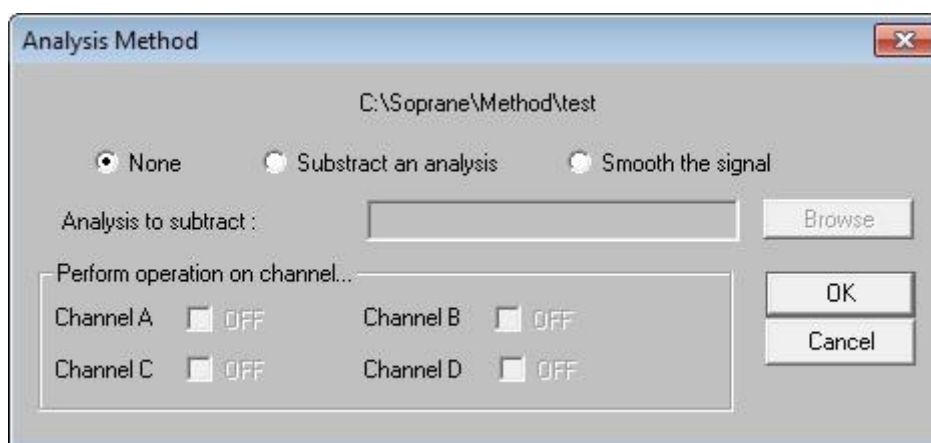
Instead of editing the components table from nothing, it is possible to ask SOPRANE to create this table with the parameters it holds. Then, it is only necessary to edit this table line by line to modify or remove data. In the process module, the creation of such a table is obtained by the menu "Integration / Build components table".

In the same way, if integration events are modified and that a new peak is integrated, SOPRANE can add it to the components table. For that, position the cursor on the peak and double right click with the mouse, the CTRL key being pressed.

7.5 The mathematical option

The menu "**Options / Edit mathematics options**" 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 from the analysis a reference chromatogram. 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.

The calculations are performed on the smoothed chromatogram or on the difference chromatogram, the original chromatogram being saved under another name in the same directory.



7.6 Reset peaks retention times

Not founding a peak can be a result, not from a failure in the peaks integration but from a failure in peaks identification (expected retention time not correct, window width too narrow ...).

The peaks identification is carried out using the expected retention times programmed in the components table and the absolute and relative search window values. If such an error is corrected, it is not necessary to perform again a calibration (the peaks area or height is not modified).

The menu "**Integration / Identify peaks**" allows to perform again the chromatogram peaks identification.

8. Calibration

Soprane 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 Soprane Setup 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.

8.1 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

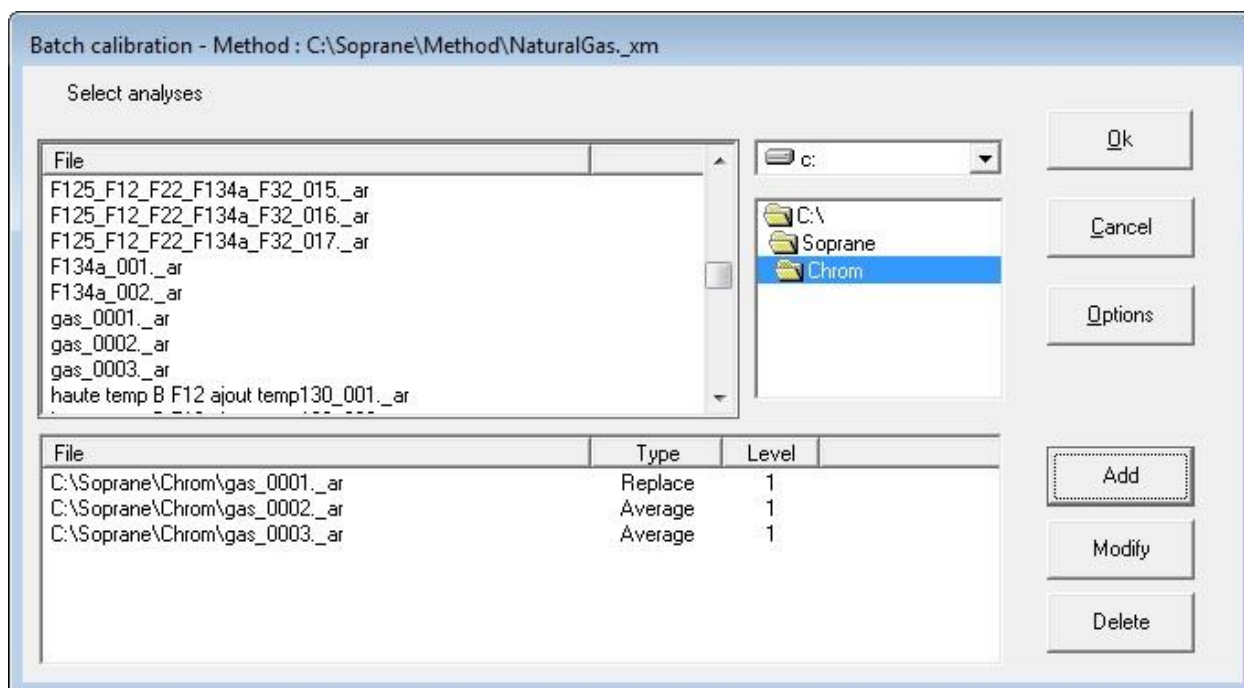
the display in the Calibration mode ; to select the component and to  directly inform the value of the surface. You can retrieve the value of this surface in the Results Table view .

8.2 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 via the "**Calibration / Calibration by reprocessing**" menu. First, you must select the method to be calibrated and then select the analysis files that will be used for this reprocessing. The "Details" button allows you to view the sample name, the analysis type and the calibrated level for a calibration.





When these files are selected, click the Add button.

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 Ok button.

You can then view the calibration report from the "**Calibration / Display 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.

8.3 Automatic calibration

We have indicated chapter 4 how to define an analysis sequence. In the same way, it is possible to define a calibration sequence. This option is available only if a calibration stream is defined in Soprane 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.

A first sub-menu "**Sequence table**" is used to define the calibration sequence in the same way we have define the analyses sequence.

	Analysis name	Method	Stream n°	Sampling (secs)	Type	Level
1	Standard 1	3 modules._xm	1	0	Blank	1
2	Standard 1	3 modules._xm	1	0	Replace	1
3	Standard 1	3 modules._xm	1	0	Average	1
4	Standard 1	3 modules._xm	1	0	Avera	1

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.

A second sub-menu "**Parameters**" is 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.

8.4 Calibration via the Launch menu

When you have defined a calibration sequence, you can launch this sequence directly from the "**Process / Start analysis**" menu. This solution is interesting especially if the standard selection is not automatic and thus manual.

8.5 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.

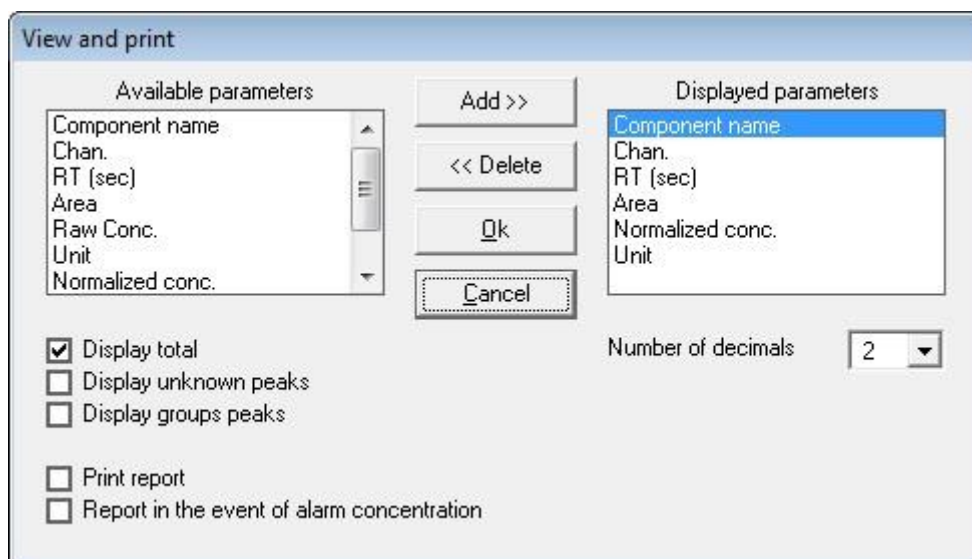
Generally: 1 Level = 1 cylinder

9. Results printing

9.1 View and print results

Chromatographic results may be displayed and printed according to several possibilities selected by the menu "**Parameters / Display and print**".





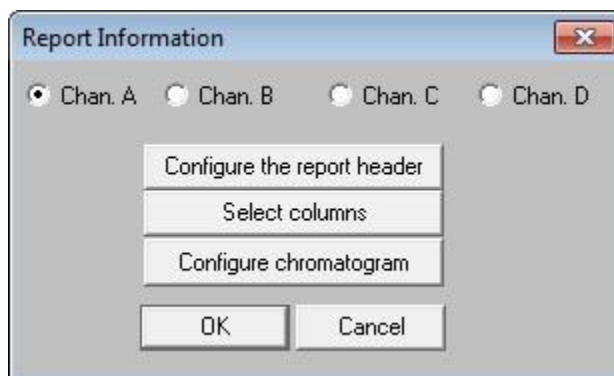
9.2 Creation of reports in the process module

The Process module allows to define all the reports one needs at the end of an analysis. These reports may be displayed and / or printed.

In the same way, any active window may be printed.

9.2.1 Configuring a report

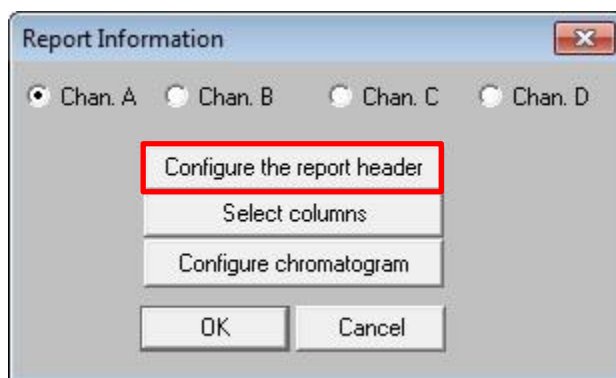
The menu "**Report / Report editor**" of the process module is used to modify the reports presentation. The window displayed offers the possibility to modify the header, the columns or the graphics of the sample report, the standard report or the report to export, for each of the channels A to D.



a) *The report header*

The button "Configure the report header" allows the access to another window used to define what is expected in the report.



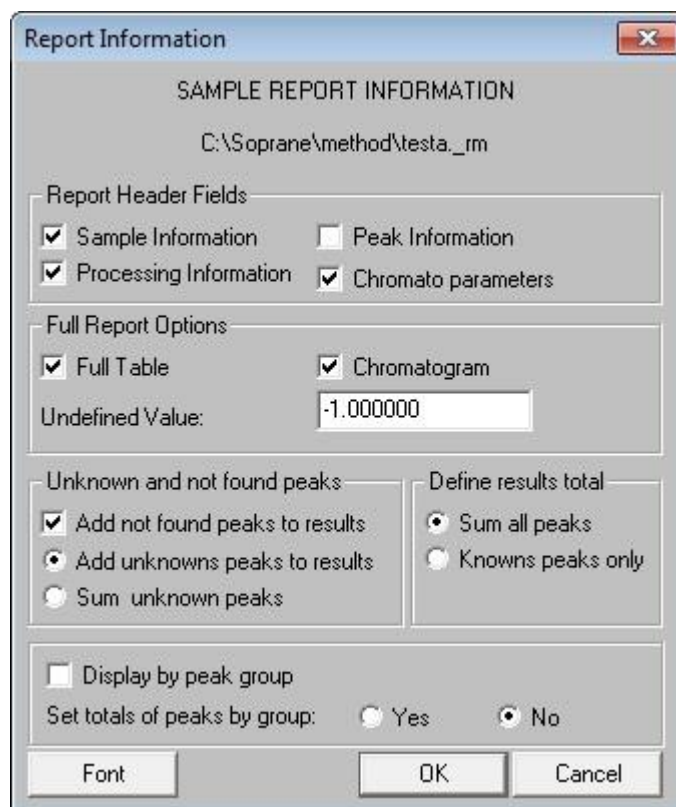


The user may choose, or not, to display (to print) any specific information related to peaks, sample, analyzer or even any comment.

The report may, or not, contain the chromatogram drawing.

Several possibilities can be used to manage unknown, or known but not found, peaks, for the total or for the groups of peaks.

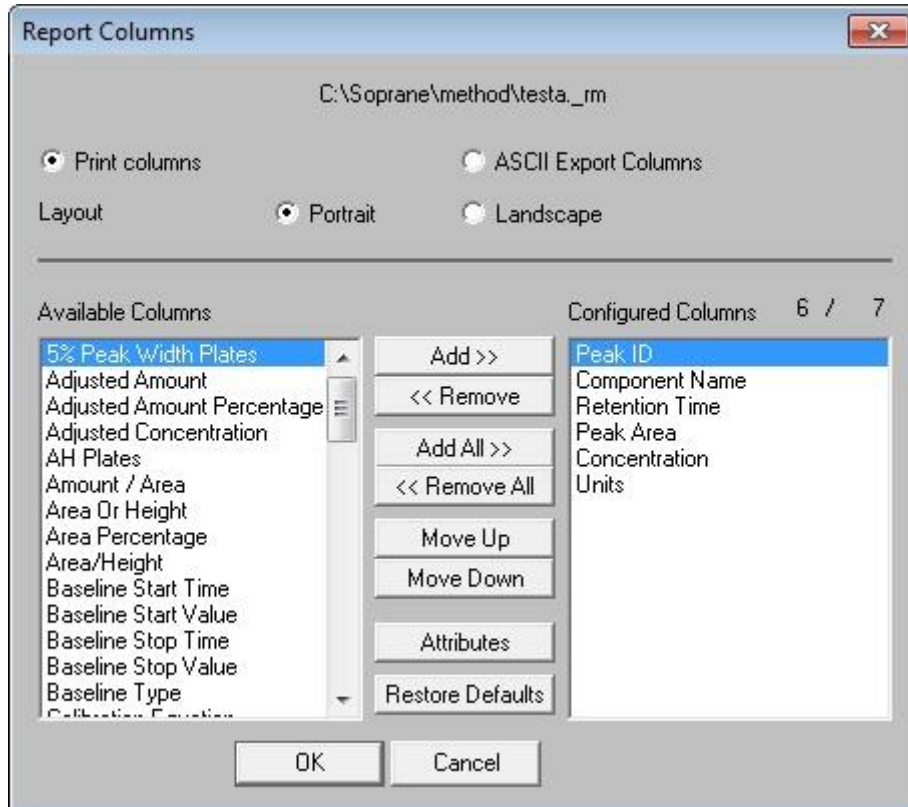
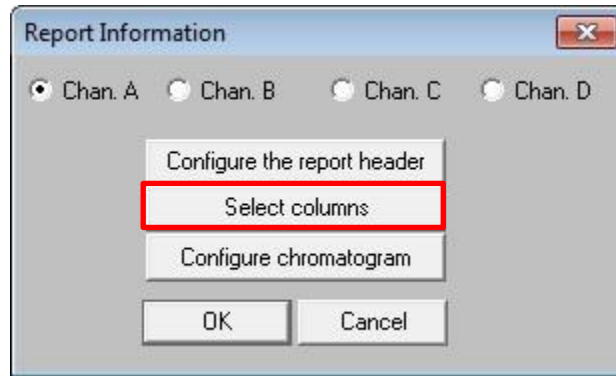
The screen allowing these definitions is shown below.



b) Report columns

The button "Select columns" allows the access to another window used to define what is expected in the report table.





On this screen, one selects the columns to print and the type of layout (portrait or landscape).

If in most cases it is enough to have the peak ID, the component name, the retention time, the peak area, the peak height, the adjusted amount and the concentration columns, all variables, and their corresponding column, needed by a user may be selected.

This screen allows the selection of what is interesting for the user.

Each peak may have two labels: a superior label and an inferior label. Generally, the component name is visualized at the top of the peak and there is nothing at the bottom.

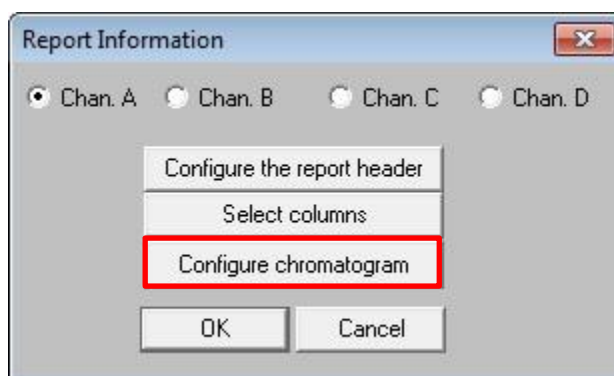


These two labels can be:

None,	Normalized concentration,
5% peak width plates,	Normalized height,
Adjusted amount,	Normalized original area,
Adjusted amount percentage,	Normalized original height,
Adjusted concentration,	Normalized raw amount,
AH plates,	Normalized area percentage,
Amount / area,	Original height percentage,
Area or height,	Original peak area,
Area percentage,	Original peak height,
Area / height,	Peak area,
Baseline start time,	Peak group name,
Baseline start value,	Peak height,
Baseline stop time,	Peak ID,
Baseline stop value,	Peak start time,
Baseline type,	Peak start type,
Calibration equation,	Peak start value,
Component name,	Peak stop time,
Concentration,	Peak stop type,
Concentration with unit,	Peak stop value,
Delta retention time,	Peak symmetry,
Expected retention time,	Peak tailing factor,
Half width plates,	Peak type,
Height / width,	Peak width,
Height percentage	Raw amount,
IS type,	Raw amount percentage,
Manually integrated,	Relative retention time,
Modified expected time,	Resolution FP,
Normalized adjusted amount,	Resolution USP,
Normalized area,	Response factor.

c) *Graphic representations*

The button "Configure chromatogram" allows the access to another window used to define what is expected on the graphics of the report.



Six options may be selected:

Baselines: allows or not the drawing of the baseline.

Detection marks: allows or not the drawing of integration marks.

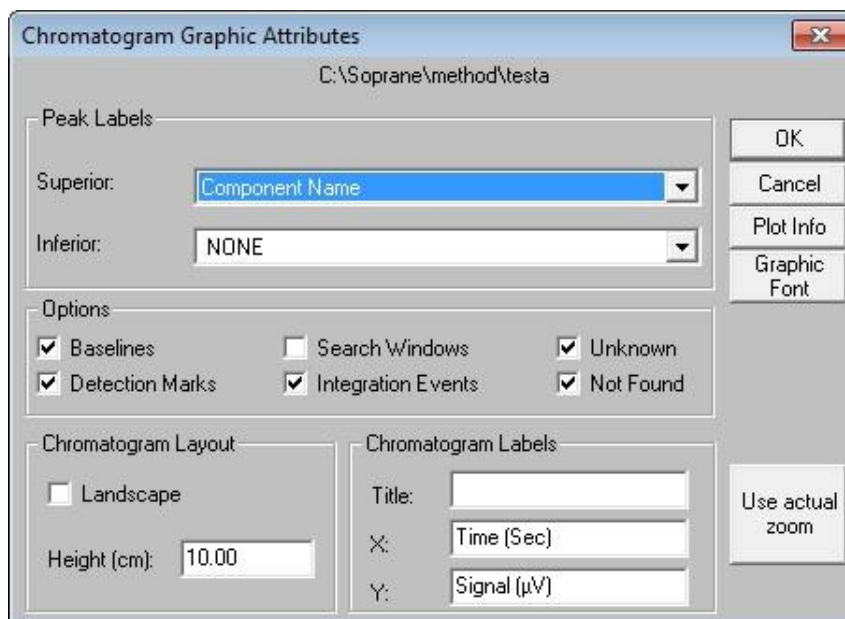
Search windows: allows or not the representation of the peaks search windows.

Integration events: allows or not the display of the integration events.

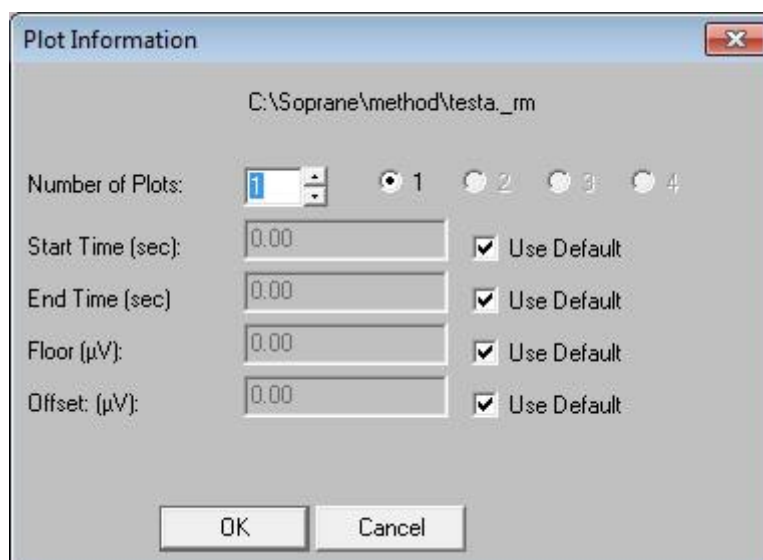
Unknown: allows or not the display of the indication "unknown" for a peak integrated but not identified.

Not found: allows or not the display of the indication "not found" for a peak expected but not integrated (and thus not identified).

These windows also allow to add text on the 2 chromatogram axes.



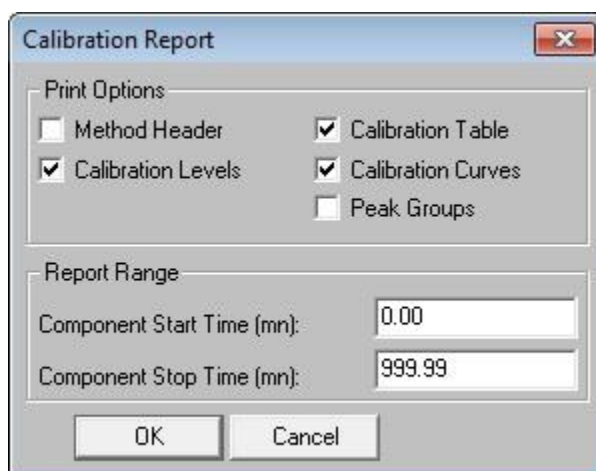
On the preceding screen related to the graphic representations of the reports, a button "Plot info" may be used to modify the view corresponding to each chromatogram.



9.2.2 Calibration report

The menu **"Report / Report of components table"** allows to define the desired data at the end of a calibration.

The window used to modify the report is:



9.3 Display and print of results from the process module

9.3.1 The menus "Report/full report" and "Report/report of integration parameters"

These menus respectively allow the window display of the full report and the window display of the report related to the integration parameters, this reports being defined as described previously.

When shown, these reports, alike any window, may be printed.

9.3.2 The menus "Print" and "Print config"

These menus are used to print the active window.

10. Displays and export of results

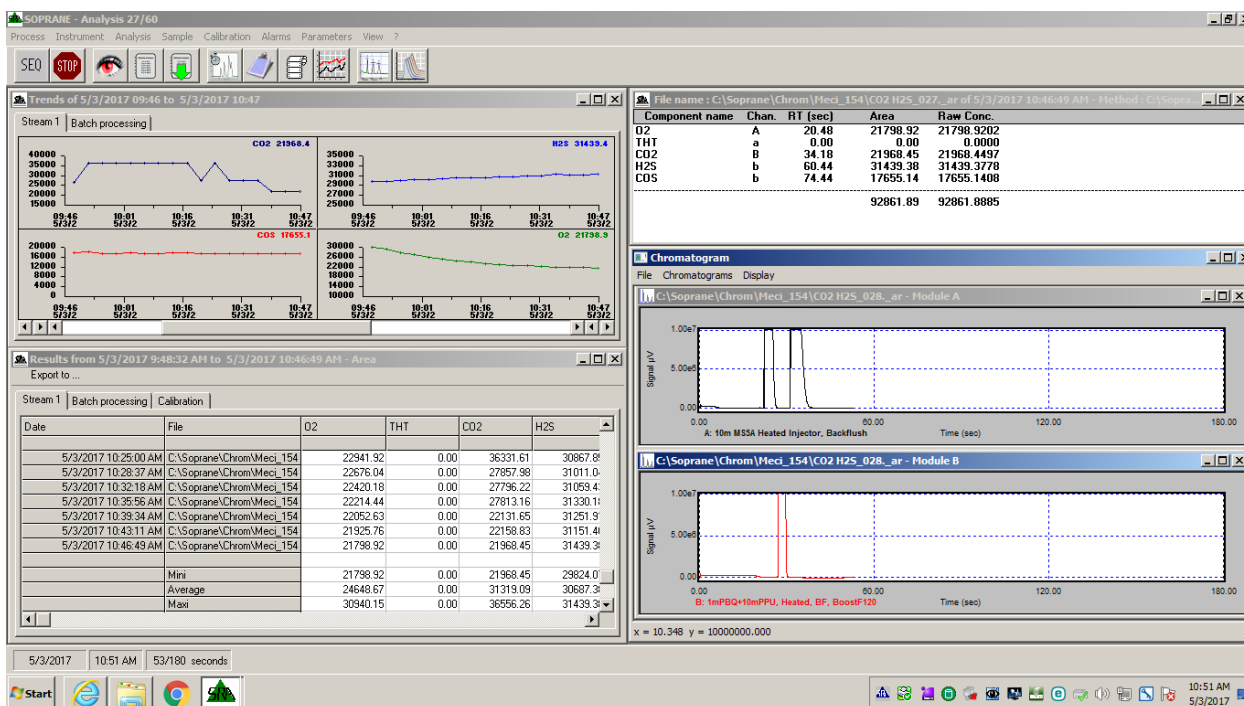
Under normal operation, SOPRANE allows the simultaneous display of 3 windows related to the analyses. These 3 windows allow the visualization of the results, of the analysis sequence in progress and of the trends. These windows can be resized, reduced or increased.

The display of a 4th window remains obviously possible if the user wants to view the chromatogram.

It is also possible to get to the Process module or the Compare module without hindering the course of the analyses.

The **"View"** menu allows to select each window to be displayed. It is also possible to display an auxiliary window to view the analog inputs and the selected analysis stream.





The 3 windows can be displayed in cascade mode (each window is slightly offset from the previous one), horizontal mode (the windows occupy the screen width and overlap vertically) or customized mode (the user places the window where he wants). Always by the means of the "View" menu, the nature and the position of the windows can be memorized so that SOPRANE can restore the display every time the program is started.

NOTE:

The option "Save windows positions" of the menu does not mean that SOPRANE will memorize the state in which one will leave the program. What is saved is the nature of the windows opened and their positions when the request is carried out and only at that time. When SOPRANE will be launched again, the windows will be automatically reopened and repositioned at the same place.



The window "Analyses sequence" offers the possibility to view the results stream by stream, or the result of a batch processing.

Date	File	O2	N2	CH4	CO2	C2	C3-c	iC4-c	nC4-c	C3-d	iC4-d	nC4-d	iCE
		%	%	%	%	%	%	%	%	%	%	%	%
31/01/2017 14:21:31	C:\Soprane\Ch	0.00	636.11	117131.80	7537.92	66250.38	3954.87	1177.86	682.69	62933.65	18803.02	11325.59	
31/01/2017 14:24:55	C:\Soprane\Ch	0.00	639.53	116812.09	7534.13	66541.79	4014.43	1141.92	669.02	62960.59	18810.96	11336.46	
31/01/2017 14:28:18	C:\Soprane\Ch	0.00	635.43	116880.39	7532.13	66475.00	3977.93	1163.12	687.18	62915.41	18801.38	11319.46	
31/01/2017 14:31:42	C:\Soprane\Ch	0.00	647.28	117151.07	7541.50	66349.89	4005.85	1167.05	678.44	62856.41	18777.65	11312.63	
31/01/2017 14:35:05	C:\Soprane\Ch	0.00	623.06	117161.48	7529.99	66287.29	3989.31	1163.53	682.61	62946.61	18810.88	11323.65	
31/01/2017 14:38:30	C:\Soprane\Ch	0.00	643.15	117131.60	7523.55	66194.07	3982.06	1170.76	684.43	62897.17	18793.59	11312.25	
31/01/2017 14:42:28	C:\Soprane\Ch	0.00	633.33	117170.96	7559.35	66309.49	3990.33	1158.44	680.54	61577.10	18789.24	11306.97	
31/01/2017 14:45:52	C:\Soprane\Ch	0.00	639.25	117071.51	7554.71	66118.61	4007.10	1171.55	684.11	62967.44	18797.74	11322.20	
31/01/2017 14:49:16	C:\Soprane\Ch	0.00	647.97	117090.49	7557.86	66586.62	4008.46	1159.31	687.19	62863.62	18773.14	11299.29	
31/01/2017 14:52:40	C:\Soprane\Ch	0.00	646.92	117274.65	7534.21	66149.47	3991.24	1162.10	686.21	62960.95	18808.37	11315.07	
31/01/2017 14:56:04	C:\Soprane\Ch	0.00	628.05	117242.17	7528.73	66358.66	4001.63	1161.54	674.41	62867.21	18778.44	11293.68	
31/01/2017 14:59:28	C:\Soprane\Ch	0.00	641.68	117175.07	7532.60	66361.45	3998.90	1153.25	681.95	62962.66	18815.02	11314.44	
31/01/2017 15:02:53	C:\Soprane\Ch	0.00	635.91	117306.52	7549.02	66460.26	4005.50	1184.37	675.11	62951.53	18809.08	11304.40	
31/01/2017 15:06:17	C:\Soprane\Ch	0.00	648.66	117371.26	7540.52	66355.21	4004.55	1166.76	666.74	62907.00	18794.51	11299.48	
31/01/2017 15:09:40	C:\Soprane\Ch	0.00	634.30	117262.54	7672.82	66407.45	3987.80	1168.31	675.56	62832.27	18770.85	11296.60	
31/01/2017 15:13:05	C:\Soprane\Ch	0.00	634.57	117175.23	7549.45	66471.20	3953.34	1172.95	681.62	62916.16	18796.32	11308.28	
	Mini	0.00	623.06	116812.09	7521.40	66118.61	3953.34	1141.92	666.74	61577.10	18770.85	11293.68	
	Average	0.00	638.31	117151.70	7546.45	66343.39	3990.78	1165.38	679.72	62845.82	18796.69	11313.96	
	Maxi	0.00	648.66	117371.26	7672.82	66586.62	4014.43	1184.37	687.19	63015.29	18827.22	11341.78	
	Rsd	0.00	1.05	0.11	0.43	0.19	0.42	0.78	0.85	0.49	0.08	0.11	

In this window "Results", it is possible to perform several operations:

- By positioning the mouse on a row and by right-clicking, it is possible to:
 - change the type of result
 - display the statistics (RSD)
 - access the processing module

Date	File	N2	CH4	CO2	C2H6	C3H8	iC4	iC5	C6	TBM	
		%	%	%	%	%	ppmVol	%	ppbVol	mg/m3	
24/11/2011 08:10:18	C:\Soprane\Chrom\PCS_Trentino_0015_ar	0.85	96.81	0.17	1.39	0.43	671.28	0.01	8.08	0.00	
24/11/2011 08:19:16	C:\Soprane\Chrom\PCS_Trentino_0016_ar	0.85	96.89	0.17	1.40	0.43	672.00	0.01	8.14	0.00	
24/11/2011 08:28:13	C:\Soprane\Chrom\PCS_Trentino_0017_ar	0.84	96.78	0.17	1.39	0.43	670.35	0.01	8.35	0.00	
24/11/2011 08:37:09	C:\Soprane\Chrom\PCS_Trentino_0018_ar	0.89	96.72	0.18	1.40	0.43	667.28	0.01	7.87	0.00	
24/11/2011 08:46:06	C:\Soprane\Chrom\PCS_Trentino_0019_ar	0.84	96.81	0.17	1.39	0.43	669.34	0.01	7.35	0.06	
24/11/2011 08:54:59	C:\Soprane\Chrom\PCS_Trentino_0020_ar	0.88	96.81	0.17	1.39	0.43	668.23	0.01	7.98	0.94	
24/11/2011 09:03:55	C:\Soprane\Chrom\PCS_Trentino_0021_ar	0.84	96.81	0.17	1.39	0.43	670.70	0.01	8.04	0.22	
24/11/2011 09:12:52	C:\Soprane\Chrom\PCS_Trentino_0022_ar	0.85	96.81	0.17	1.39	0.43	667.71	0.01	7.99	0.00	
24/11/2011 09:21:52	C:\Soprane\Chrom\PCS_Trentino_0023_ar	0.85	96.81	0.17	1.38	0.43	666.96	0.01	7.98	1.50	
24/11/2011 09:30:50	C:\Soprane\Chrom\PCS_Trentino_0024_ar	0.90	96.81	0.17	1.38	0.43	667.38	0.01	7.98	0.00	
24/11/2011 09:39:50	C:\Soprane\Chrom\PCS_Trentino_0025_ar	0.90	96.81	0.17	1.37	0.43	666.56	0.01	7.38	0.00	
24/11/2011 09:48:46	C:\Soprane\Chrom\PCS_Trentino_0026_ar	0.85	96.81	0.17	1.51	0.43	668.98	0.01	7.53	0.00	
24/11/2011 07:34:29	C:\Soprane\Chrom\PCS_Trentino_0011_ar	0.88	96.81	0.17	1.40	0.43	670.21	0.01	7.98	0.00	
24/11/2011 06:05:03	C:\Soprane\Chrom\PCS_Trentino_0001_ar	1.87	96.81	0.17	3.39	0.85	1383.06	0.05	91.06	0.00	
24/11/2011 06:13:59	C:\Soprane\Chrom\PCS_Trentino_0002_ar	2.00	96.81	0.17	3.40	0.85	1385.37	0.05	90.92	0.13	
24/11/2011 06:22:54	C:\Soprane\Chrom\PCS_Trentino_0003_ar	1.89	92.79	0.54	3.39	0.85	1398.54	0.05	91.79	0.00	
24/11/2011 06:31:50	C:\Soprane\Chrom\PCS_Trentino_0004_ar	2.00	92.78	0.55	3.39	0.85	1406.81	0.05	92.77	0.00	
24/11/2011 06:40:49	C:\Soprane\Chrom\PCS_Trentino_0005_ar	1.89	92.80	0.55	3.38	0.85	1397.52	0.05	99.67	0.00	
24/11/2011 06:49:47	C:\Soprane\Chrom\PCS_Trentino_0006_ar	1.89	92.73	0.55	3.38	0.85	1395.61	0.05	84.35	0.00	
24/11/2011 06:58:41	C:\Soprane\Chrom\PCS_Trentino_0007_ar	1.89	92.69	0.56	3.39	0.85	1393.47	0.05	96.35	0.00	
24/11/2011 07:07:37	C:\Soprane\Chrom\PCS_Trentino_0008_ar	1.89	92.67	0.55	3.37	0.85	1388.18	0.05	94.48	0.00	
24/11/2011 07:16:35	C:\Soprane\Chrom\PCS_Trentino_0009_ar	1.99	92.59	0.55	3.38	0.85	1390.09	0.05	94.15	0.00	
	Mini	0.83	92.59	0.17	1.37	0.43	666.56	0.01	7.35	0.00	
	Average	1.13	95.76	0.27	1.92	0.54	852.28	0.02	29.23	0.13	
	Maxi	2.00	97.07	0.56	3.40	0.85	1406.81	0.05	99.67	1.59	
	Rsd		41.05	1.82	61.86	44.76	33.90	36.65	86.60	125.80	280.58



- Double-clicking on a row allows to display the information concerning the analysis selected in the window "File name".

The screenshot shows the SOPRANE software interface. At the top, there is a menu bar with 'Process', 'Instrument', 'Analysis', 'Sample', 'Calibration', 'Alarms', 'Parameters', and 'View'. Below the menu bar is a toolbar with various icons. The main window displays a 'File name' window with the following data:

Component name	Chan.	RT (sec)	Area	Raw Conc.
N2		20.94	7589.78	0.89
CH4	a	21.96	63933.99	96.72
CO2	a	34.81	1818.17	0.18
C2H6	a	43.99	15121.39	1.40
C3H8	b	23.53	12701.49	0.43
iC4	b	27.24	2269.07	667.28
iC5	b	39.56	526.76	0.01
C6	b	114.05	350.42	7.87
TBM	c	0.00	0.00	0.00

Below this window, the main results table is visible, showing a grid of data for various components over time. The table has columns for Date, File, N2, CH4, CO2, C2H6, C3H8, iC4, iC5, C6, and TBM, with units like %, ppmVol, ppbVol, and mg/m3.

- Selecting several lines of analyses and then right-clicking allows to:
 - process analyses selected by clicking on Batch processing
 - use the selected analyses to perform a calibration by clicking on Batch calibration

The screenshot shows the 'Results from 24/11/2011 06:05:03 to 24/11/2011 09:48:46 - Raw Conc.' window. A context menu is open over a selected row, showing options like 'Copy', 'RT (sec)', 'Area', 'Raw Conc.', 'Display RSD', 'Batch processing', and 'Batch Calibration'. The table data is as follows:

Date	File	N2	CH4	CO2	C2H6	C3H8	iC4	iC5	C6	TBM	
		%	%	%	%	%	ppmVol	%	ppbVol	mg/m3	
24/11/2011 08:28:13	C:\Soprane\Chrom\PCS_Trentino_0017_ar		0.84	96.78	0.17	1.39	0.43	670.35	0.01	8.35	0.00
24/11/2011 08:37:09	C:\Soprane\Chrom\PCS_Trentino_0018_ar		0.89	96.72	0.18	1.40	0.43	667.28	0.01	7.87	0.00
24/11/2011 08:46:06	C:\Soprane\Chrom\PCS_Trentino_0019_ar		0.84	96.61	0.17	2.18	0.43	669.34	0.01	7.35	0.06
24/11/2011 08:54:59	C:\Soprane\Chrom\PCS_Trentino_0020_ar		0.88	96.69	0.17	1.39	0.43	668.23	0.01	7.98	0.84
24/11/2011 09:03:55	C:\Soprane\Chrom\PCS_Trentino_0021_ar		0.84	96.83	0.17	1.39	0.43	670.70	0.01	8.04	0.22
24/11/2011 09:12:52	C:\Soprane\Chrom\PCS_Trentino_0022_ar		0.85	96.86	0.17	1.39	0.43	667.71	0.01	7.99	0.00
24/11/2011 09:21:52	C:\Soprane\Chrom\PCS_Trentino_0023_ar		0.85	96.93	0.17	1.38	0.43	666.96	0.01	7.98	1.50
24/11/2011 09:30:50	C:\Soprane\Chrom\PCS_Trentino_0024_ar		0.90	96.98	0.17	1.38	0.43	667.38	0.01	7.98	0.00
24/11/2011 09:39:50	C:\Soprane\Chrom\PCS_Trentino_0025_ar		0.90	96.98	0.17	1.37	0.43	666.56	0.01	7.38	0.00
24/11/2011 09:48:46	C:\Soprane\Chrom\PCS_Trentino_0026_ar		0.85	97.07	0.17	1.51	0.43	668.98	0.01	7.93	0.00
24/11/2011 07:34:29	C:\Soprane\Chrom\PCS_Trentino_0011_ar		0.89	96.69	0.17	1.40	0.43	670.21	0.01	7.98	0.00
24/11/2011 06:05:03	C:\Soprane\Chrom\PCS_Trentino_0001_ar		1.87	92.76	0.54	3.39	0.85	1393.06	0.05	91.06	0.00
24/11/2011 06:13:59	C:\Soprane\Chrom\PCS_Trentino_0002_ar		2.00	92.88	0.55	3.40	0.85	1395.37	0.05	90.92	0.13
24/11/2011 06:22:54	C:\Soprane\Chrom\PCS_Trentino_0003_ar		1.89	92.79	0.54	3.39	0.85	1398.54	0.05	91.79	0.00
24/11/2011 06:31:50	C:\Soprane\Chrom\PCS_Trentino_0004_ar		2.00	92.78	0.55	3.39	0.85	1406.81	0.05	92.77	0.00
24/11/2011 06:40:49	C:\Soprane\Chrom\PCS_Trentino_0005_ar		1.89	92.80	0.55	3.3		1397.52	0.05	99.67	0.00
24/11/2011 06:49:47	C:\Soprane\Chrom\PCS_Trentino_0006_ar		1.89	92.73	0.55	3.3		1395.61	0.05	84.35	0.00
24/11/2011 06:58:41	C:\Soprane\Chrom\PCS_Trentino_0007_ar		1.89	92.69	0.56	3.3		1393.47	0.05	96.35	0.00
24/11/2011 07:07:37	C:\Soprane\Chrom\PCS_Trentino_0008_ar		1.89	92.67	0.55	3.3		1388.18	0.05	94.48	0.00
24/11/2011 07:16:35	C:\Soprane\Chrom\PCS_Trentino_0009_ar		1.99	92.59	0.55	3.3		1390.09	0.05	94.15	0.00
	Mini		0.83	92.59	0.17	1.37	0.43	666.56	0.01	7.35	0.00
	Average		1.13	95.76	0.27	1.92	0.54	852.28	0.02	29.23	0.13

- It is possible to delete components in the window "File name" in going in Soprane File Manager.

In the following example, we are going to remove the H2S column in the windows below:

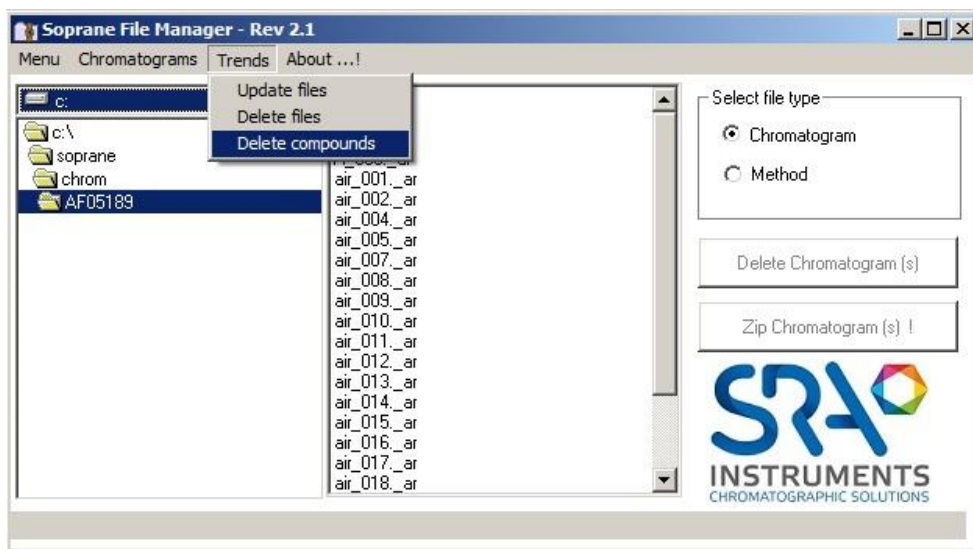


The screenshot shows the SOPRANE software interface. The top window displays a chromatogram analysis for file 'c:\soprane\chrom\AF05189\A_001_ar of 1/16/2017 12:05:56 PM'. Below this, a table shows the results for various components. The bottom window shows a summary table of results for multiple files.

Component name	Normalized	RT (sec)	Area	Raw Conc.	Unit	Chan
He	0.000000	0.00	0.00	0.000000	%	a
H2	0.000000	0.00	0.00	0.000000	%	a
O2	0.000000	0.00	0.00	0.000000	%	a
N2	0.000000	0.00	0.00	0.000000	%	a
CH4	0.000000	0.00	0.00	0.000000	%	a
Air	0.000000	0.00	0.00	0.000000	%	b
CH4	100.000000	23.31	1172.33	0.024378	%	b
CO2	0.000000	0.00	0.00	0.000000	%	b
H2S	0.000000	0.00	0.00	0.000000	%	b
Ethane	0.000000	0.00	0.00	0.000000	ppmVol	b
			100.000000	1172.33	0.024378	

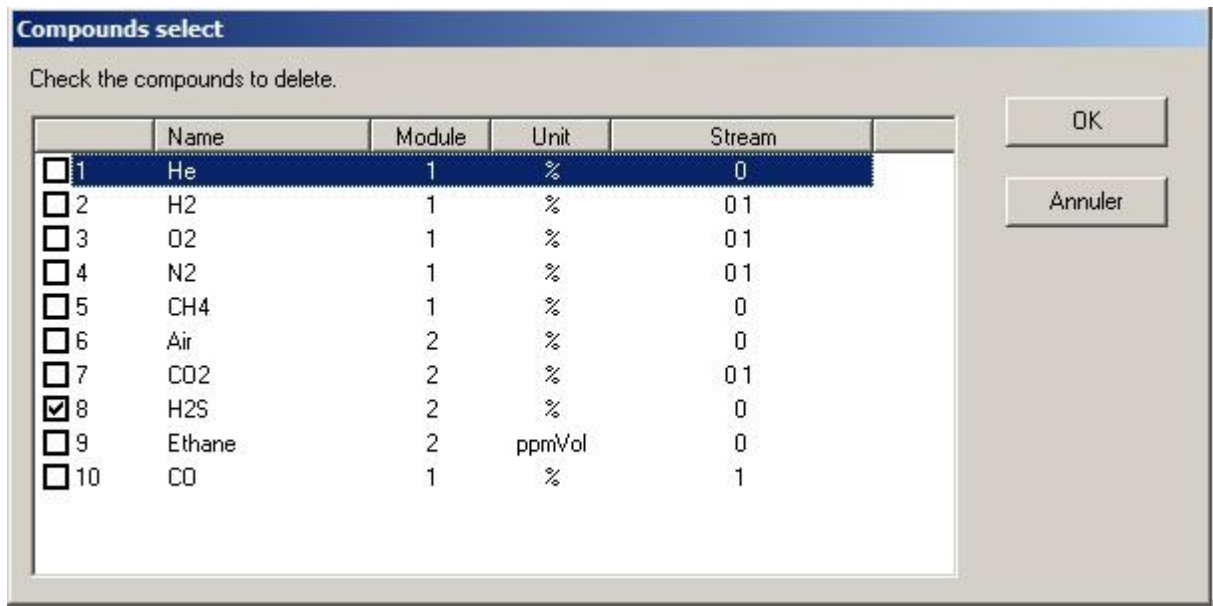
Date	File	He	H2	O2	N2	CH4	Air	CH4	CO2	H2S	Ethane
6/2017 12:05:56 PM	c:\soprane\chrom\AF05189\A_001_ar	0.00	0.00	0.00	0.00	0.00	0.00	23.31	0.00	0.00	0.00
6/2017 12:07:18 PM	c:\soprane\chrom\AF05189\A_002_ar	0.00	0.00	0.00	0.00	0.00	0.00	23.30	0.00	0.00	0.00
6/2017 12:33:43 PM	c:\soprane\chrom\AF05189\A_003_ar	0.00	0.00	0.00	0.00	0.00	20.04	0.00	0.00	0.00	0.00
6/2017 12:40:44 PM	c:\soprane\chrom\AF05189\A_005_ar	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
	Mini	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
	Average	0.00	0.00	0.00	0.00	0.00	5.01	11.65	0.00	0.00	0.00
	Maxi	0.00	0.00	0.00	0.00	0.00	20.04	23.31	0.00	0.00	0.00

For that, we open Soprane File Manager and we select **Trends/Delete compounds**.



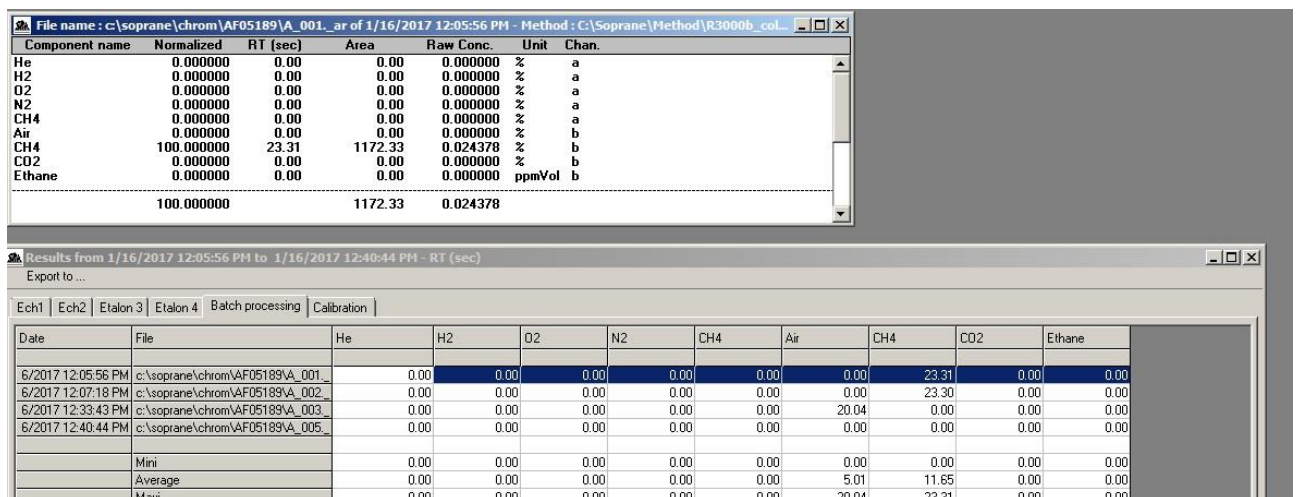
By clicking on Delete compounds, a window is displayed, in which components to be removed can be checked :





After having validated by clicking on Ok, we close File Manager and we go back to Soprane.

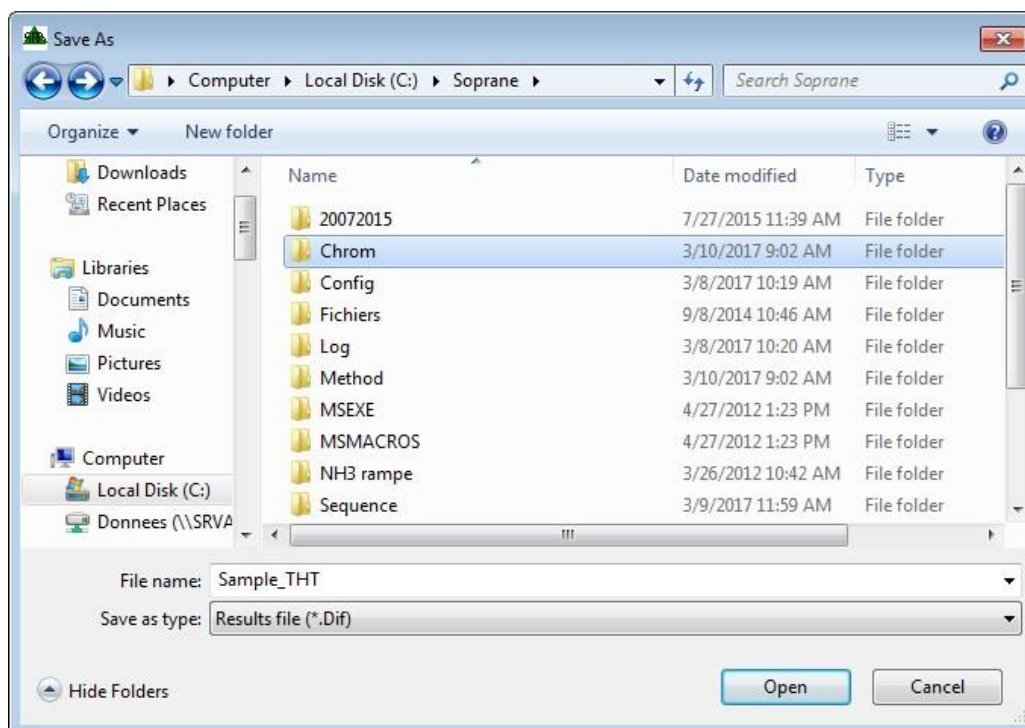
In Soprane, clicking on the "Results" window allows to update it, then clicking on the row of analysis that interests us is enough to display it in the window "File name".



At the top of this window there is a button used to export what is viewed to a .DIF file.

Any action on this button opens a new window to select the directory and the name of the file to be saved.





11. Post-analytical processing

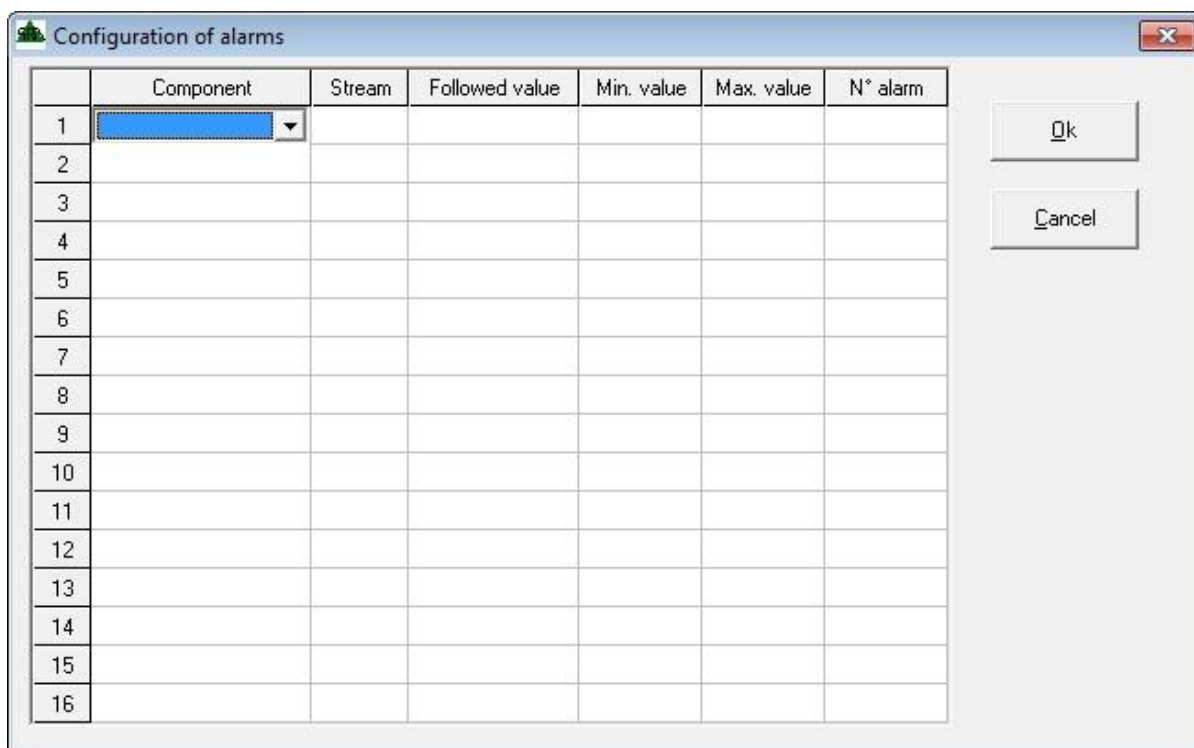
11.1 Alarms

SOPRANE offers the possibility to manage threshold alarms linked to components concentration. If relays have been defined (see Soprane I Configuration guide – chapter 2.3), 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 "**Alarms / Parameters**". 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, with 3 possibilities: the raw concentration, the normalized concentration or the mass concentration.
- The lower threshold value.
- The upper threshold value.
- The number of the relay associated with this alarm.





11.2 User program

SOPRANE offers the possibility to launch a program before or after the analysis via the menu "**Parameters / Configuration / User Program**".

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 § 6.1) that it was possible to access to a user program after the analysis (post-program).

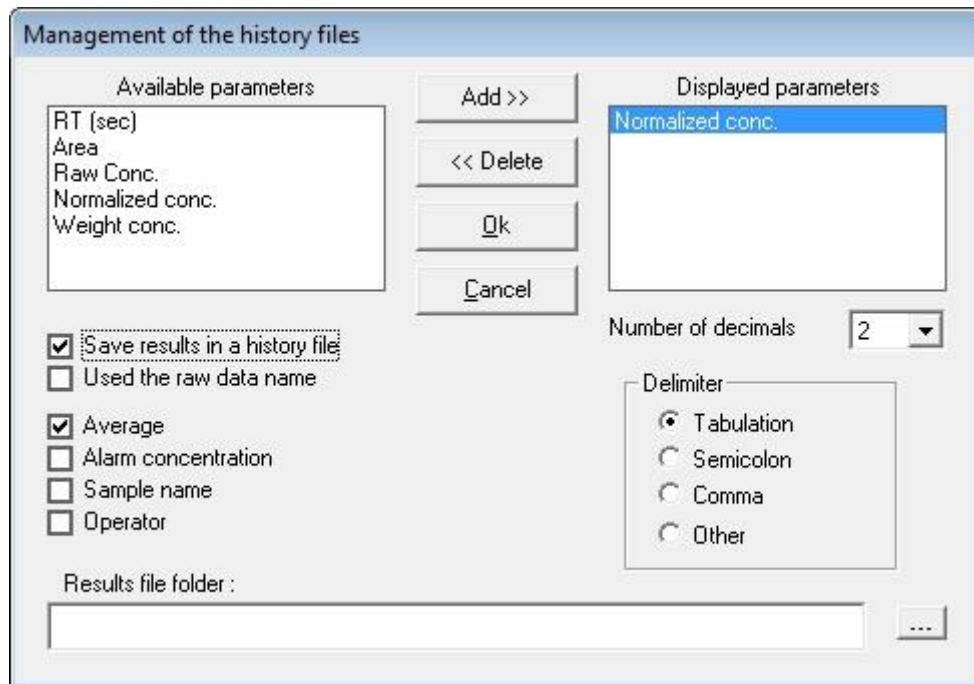


If necessary, a button, located at the left of the edit zone, is used to display directories and files and to directly select the user program.

11.3 Filing

SOPRANE allows to memorize 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.

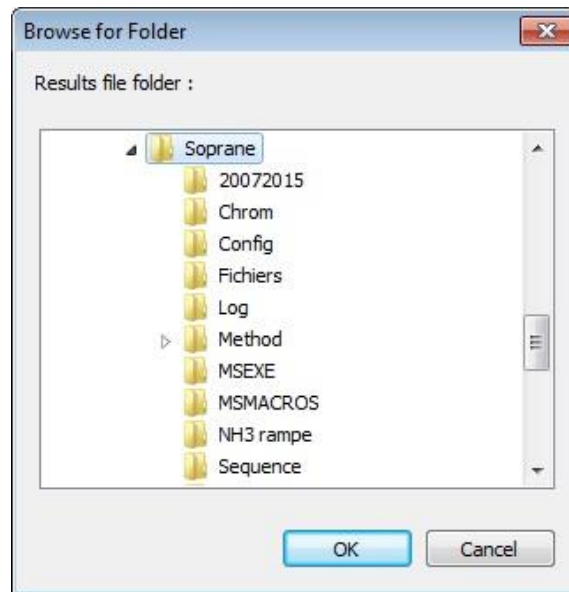
The menu **"Parameters / Configuration / Results files"** allows the display of a window where the name of the directory under which the results will be stored is indicated (Click on **"..."** at the bottom right).



You must check "Save results in a history file".

After clicking on "...", the window below is displayed. You can choose the folder.





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 and this for each stream. Such a file has the name yymmddVx.DIF or yymmddEx.DIF. "yymmdd" corresponds to the date (year, month, day), Vx or Ex represent the stream X of the analysis X or of the standard X.

NOTE:

1. The creation of a new file is done when storing whereas the date and the hour indicated in the file correspond to the injection moment. An analysis started one day can thus be stored in the file of the next day.

2. If the user asks for the display, possibly the printing, of the unknown components (Parameters / Display and printing), these unknown components will anyway be ignored when storing in the DIF file.

12. Trends and current outputs

12.1 Trends

SOPRANE allows to visualize the evolution of the concentrations or of the values computed on a time period.

The menu "**Parameters / Trends / Property**" allows to reach a group of data sheets used for the trends programming.

By selecting the first sheet, one will choose the name of the trends to visualize.



Trends name	Trends scales	Options
Trend n°1 :	<input type="text" value="CO2"/>	A
Trend n°2 :	<input type="text" value="CO2"/>	B
Trend n°3 :	<input type="text" value="None"/>	
Trend n°4 :	<input type="text" value="Acetone"/>	
Trend n°5 :	<input type="text" value="None"/>	
Trend n°6 :	<input type="text" value="None"/>	
Trend n°7 :	<input type="text" value="None"/>	
Trend n°8 :	<input type="text" value="None"/>	

Eight values can be visualized independently from each other (for instance, it is not necessary to use the tendency 4 to be able to use tendency 5). For each trend, a drop-down list allows to select the variable which will be visualized.

The reference of a variable which one wishes to visualize has obviously to be known by the system at the time when one programs its visualization. This explains why the access to the trends sheets will be denied as long as the user will not have programmed a minimum of data concerning the peaks identified in the analysis and the post-analytical calculations.

NOTE:

The identification of a peak is done by its name. If a peak name is changed, it will not be recognized any more on the trends sheet.

For example, you integrate a nitrogen peak whose name is N2 and you make the visualization in tendency of its concentration value. Then you change this N2 peak name to NITROGEN in the components table. You must then necessarily rewrite the request for visualization in tendency with this new name.

The second page relates to the output scales. For each of the 8 trends, it is possible to indicate a minimum value and a maximum value to take into account for the graphic representation. By default, these values are respectively 0 and 100.



Trends name	Min Scale	Max Scale
COS ppmVol	0	5
CO2 ppmVol	0	30000
Trend n°3	0	100
Acetone	0	100
Trend n°5	0	100
Trend n°6	0	100
Trend n°7	0	100
Trend n°8	0	100

The usable values can be in the range suggested by SOPRANE, which authorizes a maximum flexibility without risk of error, or can be directly written.

The unique constraint is that only entire positive numbers may be registered (neither dot, nor comma). The value of the minimum is inevitably lower than that of the maximum (the minimum is forced to zero if we attempt to impose a too high value).

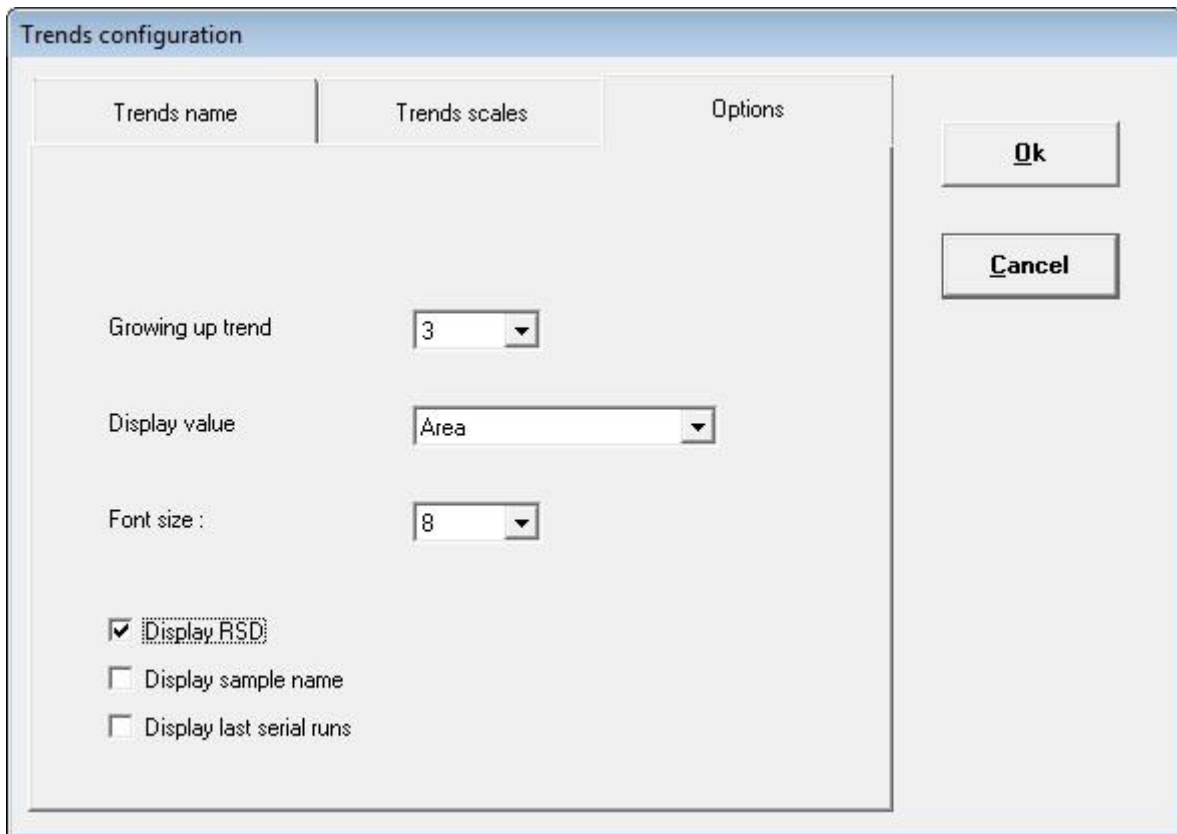
The last page "Options" allows you to define the time scale that you want to view.

By default, SOPRANE has selected a growing up trend display with visualization of the last hour. It is possible to keep this mode and to visualize up to 120 hours (5 days) of operation or all the analyses.

NOTE:

The visualized data are not those corresponding to "X" last hours of analysis but to the analyses of "X" last hours. If the apparatus were on standby, no result will be to visualize.

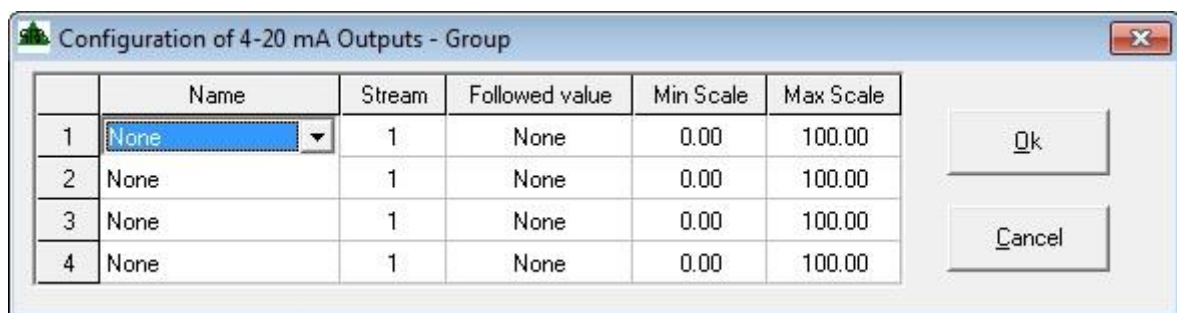




12.2 4-20 mA current outputs

For each group of current outputs, the user has to select which variable (name and stream) is sent and what is the output scale (minimum and maximum).

The display used for this programming is obtained by the menu **"Parameters / Configuration / Output 4-20 mA"**, available only if the option is unlocked in the Soprane protection key.



13. Columns bake out

When configuring SOPRANE (see Soprane I Configuration guide – Chapter 2.3) we possibly asked for the management of the columns bake out.



If such a request has been carried out, the menu "**Parameters**" of SOPRANE shows an option "**Col. Bakeout**".



This option works in the same way as the automatic calibration that is to say with priority upon the analyses sequence.

The bake out requires parameters different from those used to perform the analyses (higher column temperature, detector OFF), this is why we will indicate a bake out duration and the name of the method used to carry out the bake out.

Such a bake out can be performed during the night or the week-end and at the end you have an instrument ready to be used.

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.

If you don't want to launch a bake out, check the box "None".



Column bakeout programming

Bakeout management

None
 Now
 At end of sequence
 Programmed

Ok
Cancel

Date next bakeout (MM/DD/YY) : 07 / 12 / 2017

Time next bakeout (HH:MM:SS) : 16 : 50

Number of days between bakeouts : 0

Bakeout method : S05309rege._xm

Bakeout duration (mn) : 480

Post bakeout method : S05309._xm

Stabilization duration (mn) : 20

If you want to launch a bake out, there are 3 ways to proceed:

- It is possible to stop the analyses and to ask for an **immediate bake out**, by checking the box "**Now**" in the screen below.

You can choose the regeneration method and its duration (in min). If the duration is set to zero, the method is not loaded.

You can also choose a post-regeneration method and the stabilization duration (in min). In this case, when the bake out will be finished, the post-regeneration method will be sent to the analyzer even if the duration is set to zero.



- It is possible, by checking **"At end of sequence"**, to have a bake out which will be launched at the end of each sequence, whether the analyses are launched in sequence or automatic mode.

You can choose the bake out method, its duration (in min) as well as the post-regeneration method and its duration.

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

If the stabilization duration is set to zero, the post-regeneration method is loaded. If you are in automatic mode the analyses of the next sequence will start immediately.



- The 3rd way consists in **programming** the bake out at regular intervals. It is enough to indicate the date and the hour for the next bake out as well as the number of days separating 2 successive bake out (0 if only one bake out is needed). It is the same principle as previously for the methods and durations.

The scheduled bake out operates only if the analyses are launched in automatic mode.

When a bake out has to be performed, the automatic sequence is temporarily stopped and the bake out is performed. In this case, at the end of the bake out, the post bake out method is ignored and the method corresponding to the next analysis is sent to the chromatograph. Soprane waits then the necessary time to have a READY status and then the automatic sequence goes on.



14. Specific calculations

These specific calculations are available only if the key contains the specific calculations option.

14.1 Selection of the calculations

Depending on the options, SOPRANE allows different calculations.

These options allow:

- Natural Gas Analysis calculations,
- Customized calculations (15 calculations),
- GPL calculations,
- Combustion calculations,

Two sets of calculations may be used. It is thus possible to simultaneously calculate and manage the same parameters in different temperature conditions.

The menu "**Parameters / Configuration / Calculation / Calculation 1 select**" or "**Parameters / Configuration / Calculation / Calculation 2 select**" allows this programming.

Everyone is not concerned with this type of calculations and the possibilities offered only meet common needs.

The call of a user program allows to define other calculations possibilities.



NOTE:

It is normally required that the concentrations are normalized at 100% for a correct execution of calculations.

The user can select the unit in which the result will be expressed (when a unit is justified).

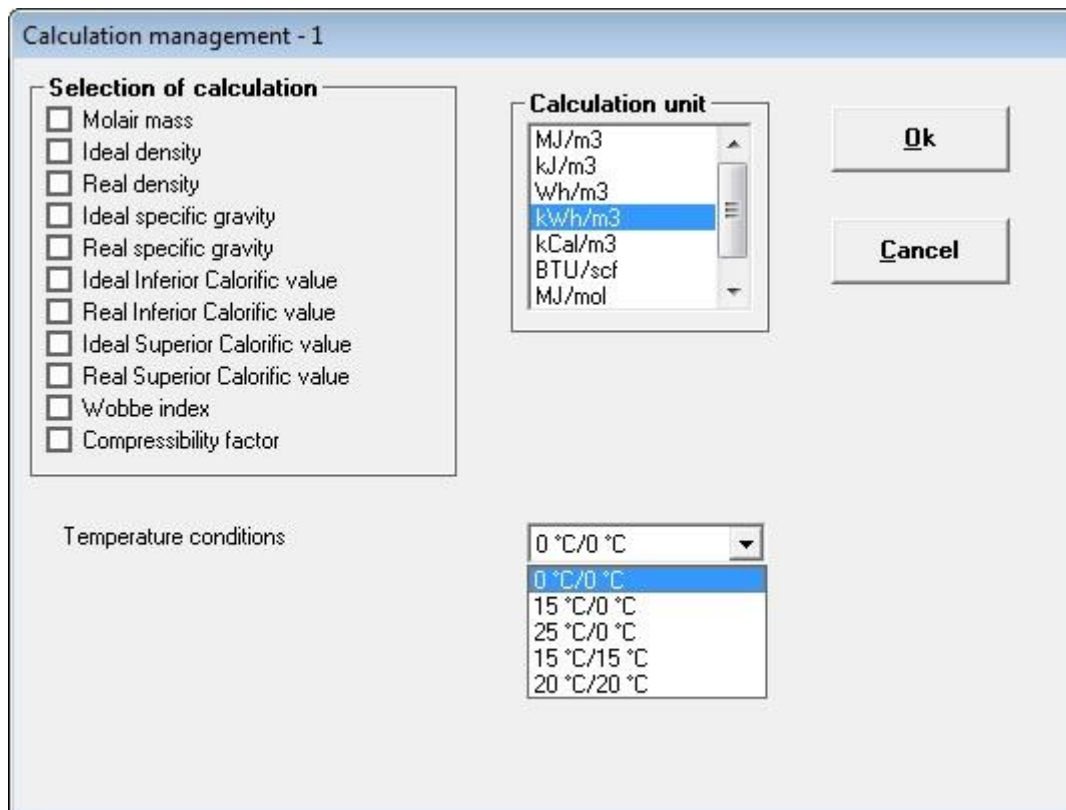
14.2 Specific calculations set for Natural Gas analysis

The menu "Parameters / Configuration / Calculation / Calculation 1 select" or "Parameters / Configuration / Calculation / Calculation 2 select" allows this programming.

A specific calculation set may be used in the case of NGA system.

The possible calculations are:

- The molar mass.
- The ideal density.
- The real density.
- The ideal specific gravity.
- The real specific gravity.
- The ideal inferior calorific value.
- The real inferior calorific value.
- The ideal superior calorific value.
- The real superior calorific value.
- The Wobbe index.
- The compressibility factor.



SOPRANE offers the possibility to go far beyond the standard concentration calculations and to carry out complementary calculations.

The menu "**Parameters / Configuration / Calculation / Calculation coefficients**" allows the setting of parameters used in further calculations. More comments on these calculations are given in appendix.

Calculation coeff. at 0 °C/0 °C

Coefficients

	Constituents	M (g/mol)	ICV MJ/m3	SCV MJ/m3	Z
1	He	4.003	0.000	0.000	1.00050
2	H2	2.016	10.777	12.788	1.00060
3	O2	31.999	0.000	0.000	0.99900
4	N2	28.014	0.000	0.000	0.99950
5	CH4	16.043	35.818	39.840	0.99760
6	CO	28.010	12.620	12.620	0.99930
7	CO2	44.010	0.000	0.000	0.99330
8	C2H4	28.054	59.040	63.060	0.99250
9	C2H6	30.070	63.760	69.790	0.99000
10	C3H6	42.081	85.940	91.980	0.98100
11	C3H8	44.097	91.180	99.220	0.97890
12	iC4	58.123	118.180	128.230	0.95800
13	nC4	58.123	118.610	128.660	0.95720
14	1-Butene	56.108	113.380	121.420	0.96500
15	Iso-Butene	56.108	112.630	120.670	0.96500
16	Cis-2-Butene	56.108	113.080	121.120	0.96100

Buttons: Ok, Cancel, Insert, Delete, Conditions

The default values are those of perfect components at 1.01325 bars according to standard ISO/DIS 6976:1995 and to the experimental standard X20-522.

A mouse click on the 'Coefficients' button allows to select a set of parameters. Inside this set of parameters, it is possible to modify the values.

A line may be inserted or deleted and a compound name may be modified.

BE CAREFUL: the name used here for the compound must be THE SAME as the one in the compounds table.

A 'Conditions' button is used to define the conditions you want to use to perform calculations. This assumes that you have values of all coefficients in these conditions.



Combustion and metering reference conditions (101.325 kPa)

Combustion temperature :	<input type="text" value="0.00"/>	<input type="button" value="Ok"/>
Reference temperature :	<input type="text" value="0.00"/>	
Temperature unit :	<input type="text" value="°C"/>	<input type="button" value="Cancel"/>
Air mass molaire :	<input type="text" value="28.9626"/>	
Air compressibility factor :	<input type="text" value="0.99941"/>	

The temperature values used in this window are reported in the preceding window and also in the two windows used to select the calculations.

14.3 Specific calculations set for GPL analysis

The menu "**Parameters / Configuration / Calculation / Calculation 1 select**" or "**Parameters / Configuration / Calculation / Calculation 2 select**" allows this programming.

A specific calculation set may be used in the case of GPL system.

In such a case, the possible calculations are:

- The total carbon
- The lower and upper calorific values
- The liquid density
- The liquid specific gravity
- The absolute vapor pressure at 37,5 °C, 40 °C, 50 °C and 70 °C
- The sums C3, C4, C5
- The sum of olefins
- The motor octane index
- The relative vapor pressure at 37,5 °C, 40 °C, 50 °C and 70 °C



Calculation management

Carbon total
 Lower calorific value
 Upper calorific value
 Liquid density
 Liquid spec. gravity
 Absolute Steam Pressure at 37.8°C
 Absolute Steam Pressure at 40°C
 Absolute Steam Pressure at 50°C
 Absolute Steam Pressure at 70°C
 Sum C3
 Sum C4
 Sum C5
 Olefine
 Moteur Octane Number
 Relative Steam Pressure at 37.8°C
 Relative Steam Pressure at 40°C
 Relative Steam Pressure at 50°C
 Relative Steam Pressure at 70°C

Calculation unit
 kj/100g Gas
 MJ/kg

Ok

Cancel

Temperature conditions
 0°C/0°C

Steam Pressure calculation
 % vol
 % mol
 % weight

Coefficients values

	Peak name	Nbr. Carbone	Coef. M Vol. kg/m3	Fact. PV 37.8°C kPa	Fact. PV 40°C kPa
1	CH4	1.00	0.00	0.00	0.00
2	C2H4	2.00	369.00	8106.00	8821.00
3	C2H6	2.00	375.76	5269.00	5611.00
4	C3H6	3.00	521.33	1570.00	1661.00
5	C3H8	3.00	507.30	1317.00	1352.00
6	iC4	4.00	562.98	507.00	531.00
7	nC4	4.00	584.06	355.00	377.00
8	1-Butene	4.00	601.15	415.00	457.00
9	Iso-Butene	4.00	600.50	426.00	467.00
10	Cis-2-Butene	4.00	627.20	314.00	337.00
11	Trans-2-Butene	4.00	610.00	340.00	365.00
12	1,2-Butadiene	4.00	658.00	0.00	272.00
13	1,3-Butadiene	4.00	627.30	405.00	436.00

Ok

Cancel

Insert

Add

Delete

14.4 Specific combustion calculations

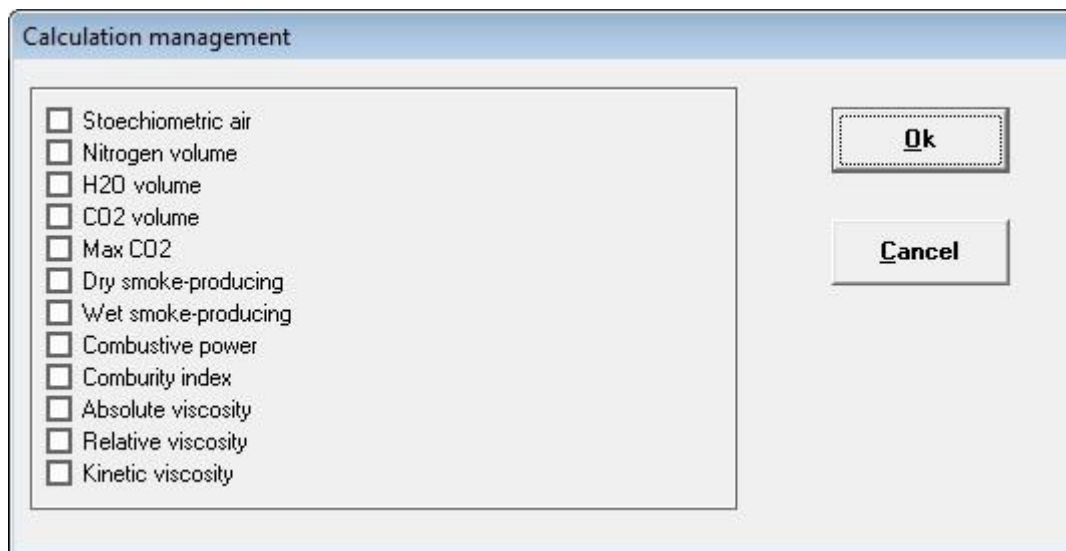
The menu "Parameters / Configuration / Calculation / Calculation 1 select" or "Parameters / Configuration / Calculation / Calculation 2 select" allows this programming.

The possible calculations are:

- The stoichiometric air
- The volume of nitrogen and CO₂
- The total water vapor



- The maximum CO₂
- The dry and wet fumes volumes
- The combustive power
- The combustibility index
- The absolute, relative and kinetic viscosities




	Peak name	H2O	CO2	O2	Comburity coef.
1	N2	0.00	0.00	0.00	0.00
2	CH4	2.00	1.00	2.00	9.54
3	CO2	0.00	1.00	0.00	0.00
4	C2H6	3.00	2.00	3.50	16.84
5	C3H8	4.00	3.00	5.00	24.37
6	iC4	5.00	4.00	6.50	32.41
7	nC4	5.00	4.00	6.50	32.41
8	iC5	6.00	5.00	8.00	40.87
9	nC5	6.00	5.00	8.00	40.87
10	neoC5	6.00	5.00	8.00	40.87
11	C6	7.00	6.00	9.50	50.00

15. Analyses reprocessing

The reprocessing is performed thanks to the Process module already presented when programming all that deals with integration, peaks identification or calibration (see chapters 6 to 8) or concerning the results printing (see chapter 9).



At any time, it is possible to call the process module and then to load a stored analysis file to modify or not its method, to change the integration, to redo peaks identification ...

The menu "**Analysis / Load Chromatogram**", as the icon representing 2 separated peaks , allows to select the chromatogram which one wishes to visualize.

This chromatogram was stored with its own analysis method.

The main tools, control pallet, integration events pallet, manual baseline pallet in the menu "Integration" have already been presented (see chapter 6.5).

Important note:

When working with the Process module, the user has the possibility to modify the method and to save this new method under its current name or under a new name.

For most software, when one loads a document "A" in memory and saves it under the name "B", we go on working with "B" in memory, that is to say all the modifications in memory will be written under the name "B" when saving on the disk.

The process module works differently. If a document "A" is loaded in memory and saved under the name "B", the memory is modified, but keeps its name "A" and a save operation will modify the source file "A".

16. Analyses comparisons

16.1 Compare module

From SOPRANE, the access to the module of comparison is obtained by the menu "**Analysis / Compare Module**", or, more directly, by the corresponding icon.



The Compare module is a powerful tool allowing the simultaneous visualization of several chromatograms. This allows to follow a phenomenon evolution during the analyses, for example a column degradation.

16.2 The menus "File / new" and "File / open"

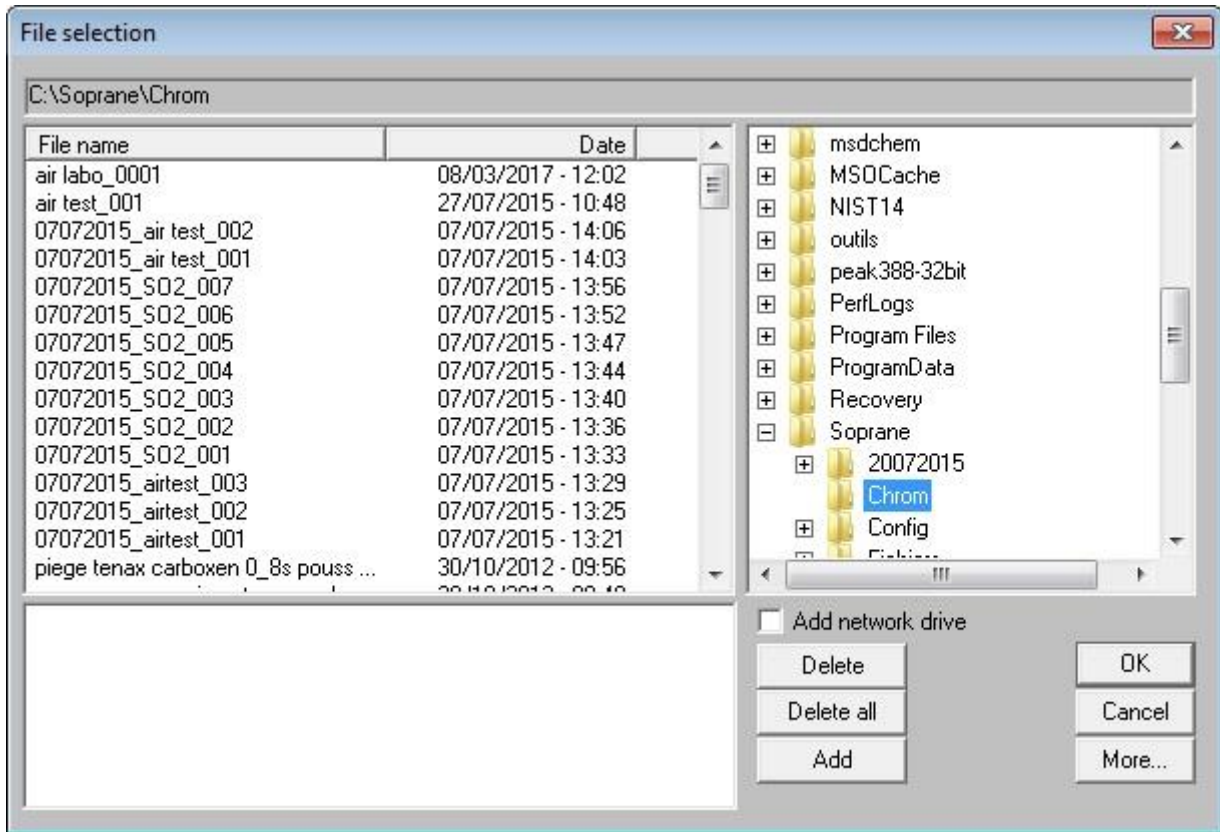
The compare module is a software in which one opens documents, each document containing from 1 (obviously, the comparison is more interesting beginning with 2) up to 64 analyses. Each document can be saved and opened again later on.

16.3 Choice for normal or sequential loading

The choice proposed allows the curves visualization either simultaneously or sequentially.

These two ways to load the analyses use the menu "**File / load**" or "**File / Sequential Load**". The displayed window allows the selection of the files to be visualized.

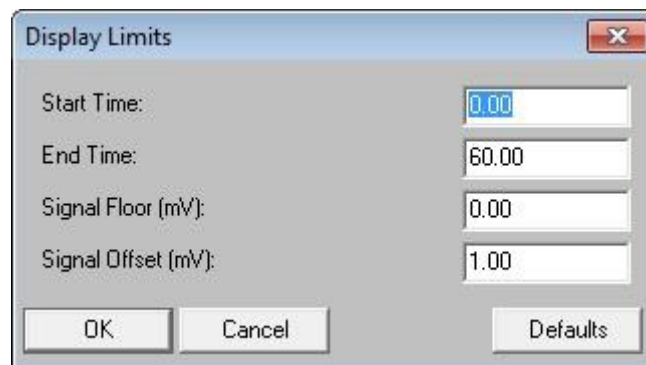




The user only needs to select one or more files (use of the keys shift and ctrl in connection with the mouse) and to ask for the addition of the selection by using the button "Add". In case of an error, the two buttons "Delete" and "Delete all" will be useful.

16.4 Editing the chromatogram display limits

The menu "Edit / chromatogram display limits" is useful to modify the screen.

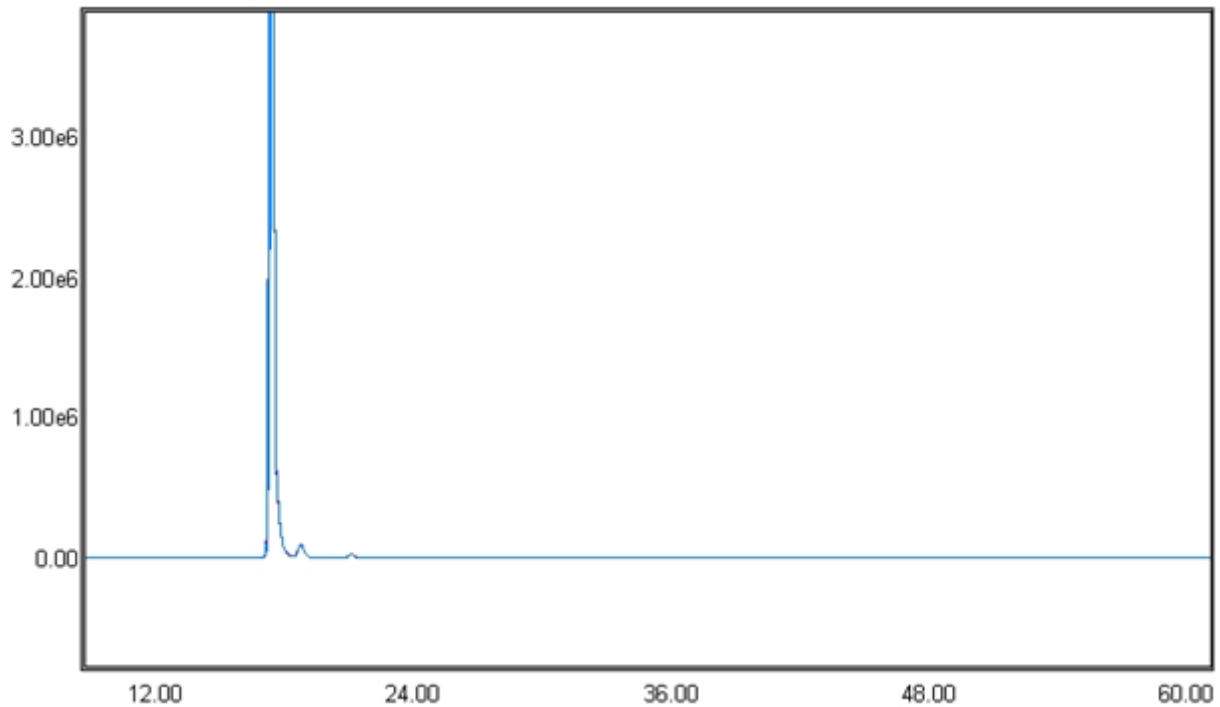


The zoom is also a way to correctly display the analyses.



16.5 2D, 3D and opaque 3D representations

By default, the chromatograms are visualized in 2D mode.



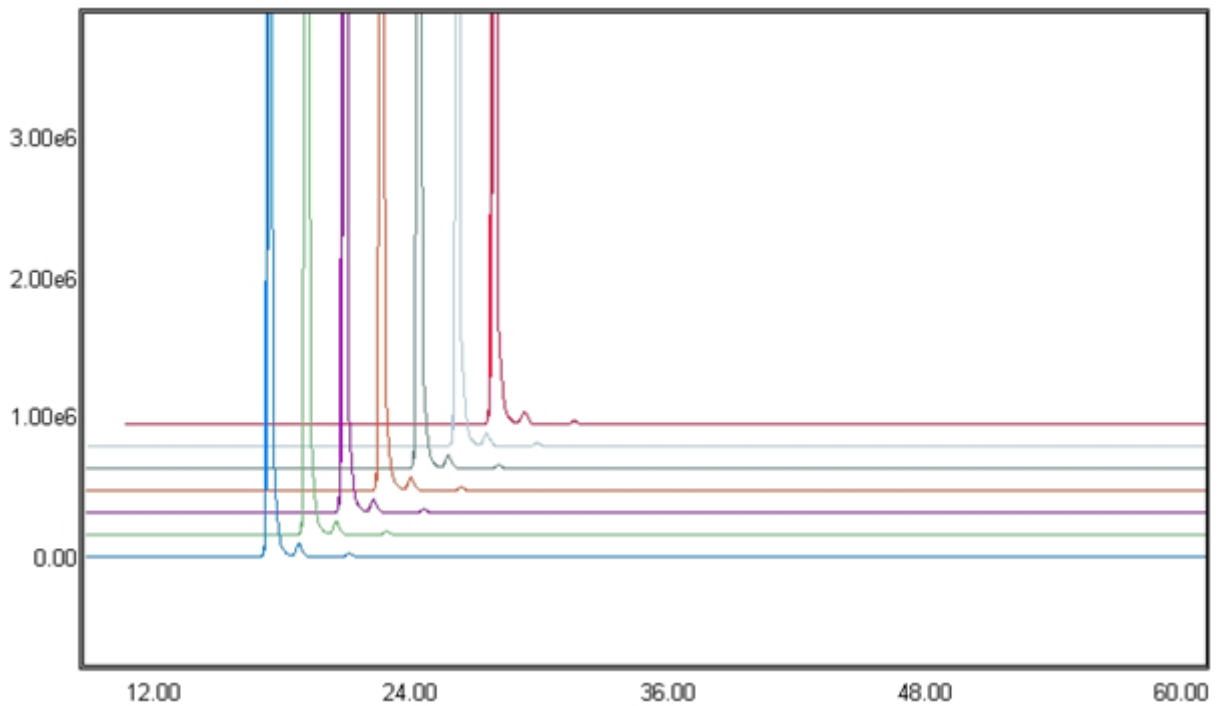
The menu "**Options / 2D, 3D Transparent or 3D Opaque**" allows to improve the display.

When one selects a 3D representation, transparent or opaque, it does not seem a lot of things occur. There is no more to do than to bring the mouse near the left lower corner of the display window, to maintain the ctrl key pressed and right click to see the difference.

Pressing the ctrl key allows to distinguish between an action of this type and a double right click corresponding to a zoom level cancel: the zoom tool is operational during the comparison of the chromatograms.

When right clicking while maintaining the ctrl key pressed, the compare module redraw the chromatograms on the screen so that the points origin of two successive chromatograms are spaced of an equal quantity, in distance and in direction, with the fifth of the vector separating the left lower corner of the display window and the cursor.

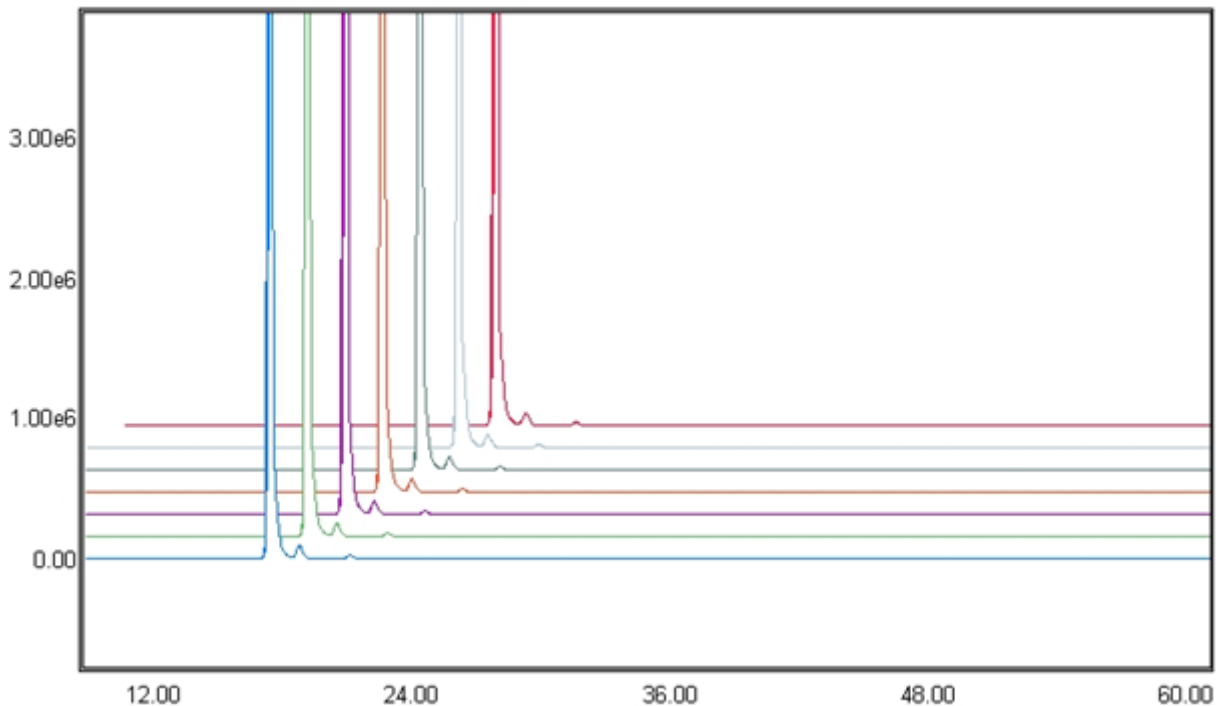




These chromatograms, corresponding to 7 analyses, are displayed in 3D transparent mode. If there is a lot of peaks in the analysis, even if we use of different colors, it may be difficult to visualize rapidly who is who.

If an opaque 3D representation, each chromatogram partially masks those which are behind it, whereas with transparent 3D, one "sees" through curves.

The same view, in 3D opaque mode is generally easier to understand.



16.6 Display options

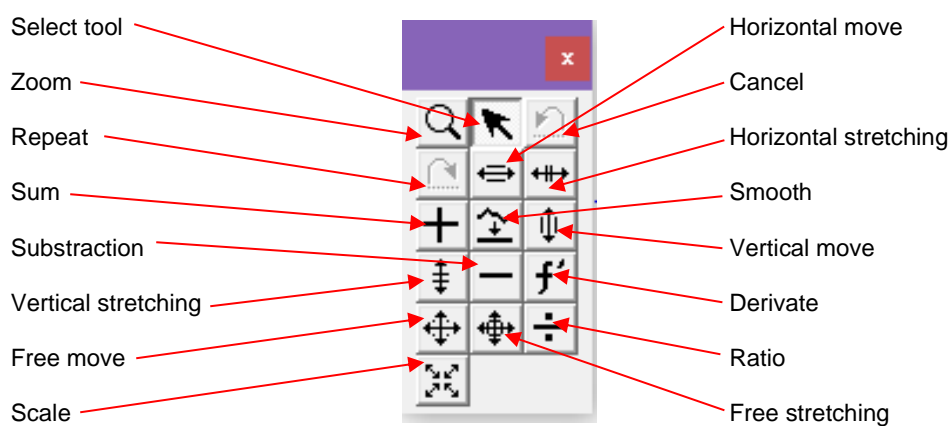
Normally all the options are selected to allow an easier work. The menus **"View / Mouse position, / Gridline and / Axes"** respectively allow to remove the mouse location indication in the status line, the screen background grid or the scales indication (time on the X axis and voltage on the Y axis).

16.7 Use of the tools pallet

The display, or the removal, of the pallet is obtained by the menu **"View / Pallet"** or by the icon of the toolbar



symbolizing a pallet.



The tools of the pallet are operational in 2D mode.

The pallet allows general operations, on a chromatogram or between 2 chromatograms. The same operations are obtained by the means of the menu **"Maths / Difference, / Sum, / Ratio, / 1st derivative, / Smooth or / Scale"**.

For a general operation (zoom, for example) it is enough to click on the icon of the tool to make it active.

An operation on a chromatogram (moving, stretching, scaling or first derivation) is also immediate: the tool is first selected, then one "takes" the chromatogram we want to apply the operation.

An operation on 2 chromatograms is done in 3 moves: first by selecting the first chromatogram (its reference is visualized in the list zone located above the visualization zone), then by selecting the tool, and finally by selecting the second chromatogram concerned by a mouse click.

Each time a chromatogram is selected, its reference is indicated inside the list zone located above the chromatogram window. It is also possible to do the opposite and to select a chromatogram using this list zone.

The tools "cancel" or "repeat" of the pallet, or the menus **"Edit / Undo"** or **"Edit / Redo"** may be used to remove or repeat only the last action.



16.8 The printing

The active window may be printed.

The menus **"File / print setup"** and **"File / print"** allow to configure the printer, to preview or to print the current window.

The icon symbolizing a printer may also be directly used to print the window.

17. File management

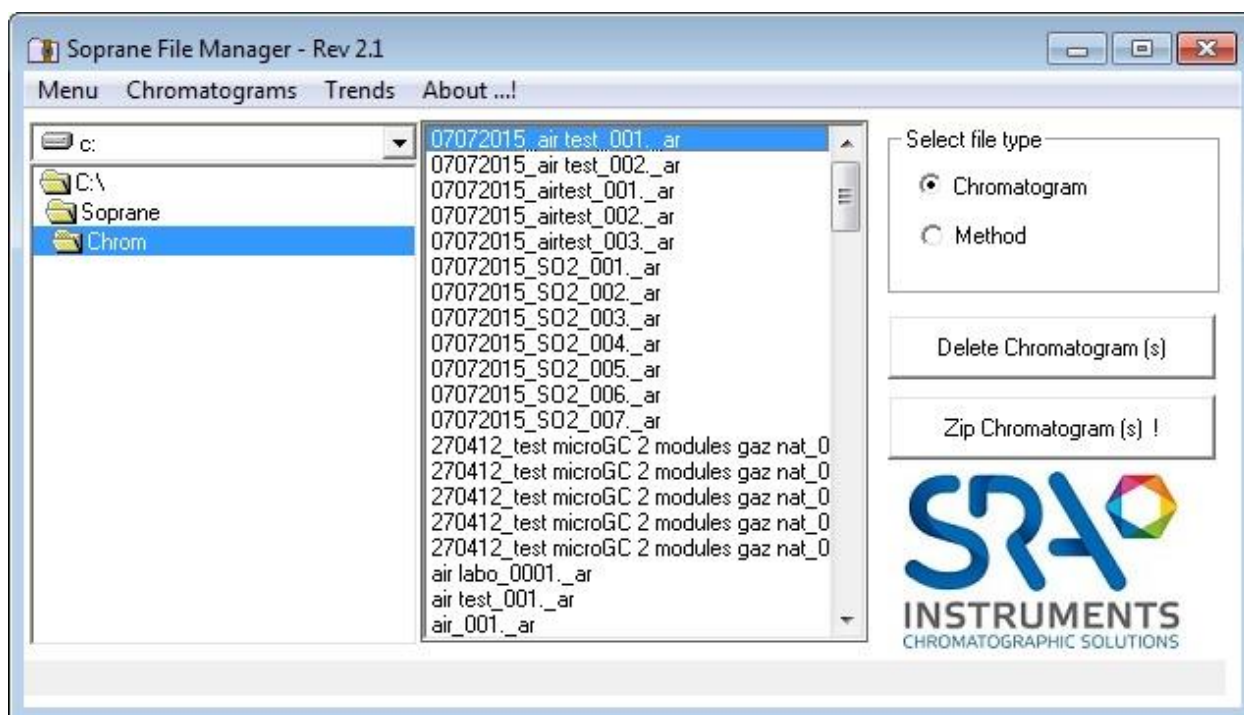
SOPRANE uses several files to memorize the analyzer configuration, the different analyses methods, the integration methods, the results...

Most of these files are interconnected, and the fact to move one of these files from a directory to another can cause problems.

The files management is facilitated thanks to the use of Soprane File Manager :



By clicking on the icon, the following window is displayed:



You can choose to carry out operations on chromatograms or methods, by selecting the type of files.

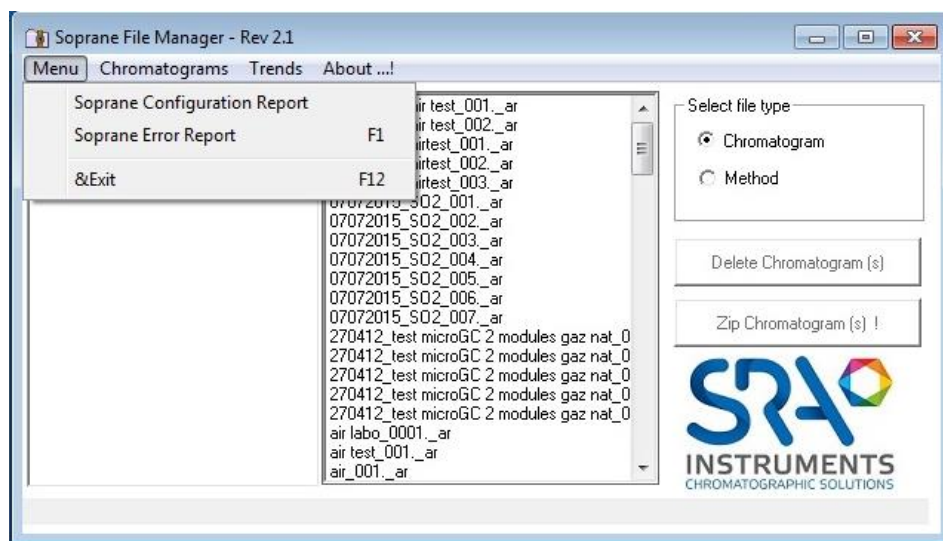
You can:

- Delete chromatograms or methods
- Compress chromatograms or methods under a .zip extension



In "Menu", you have also access to:

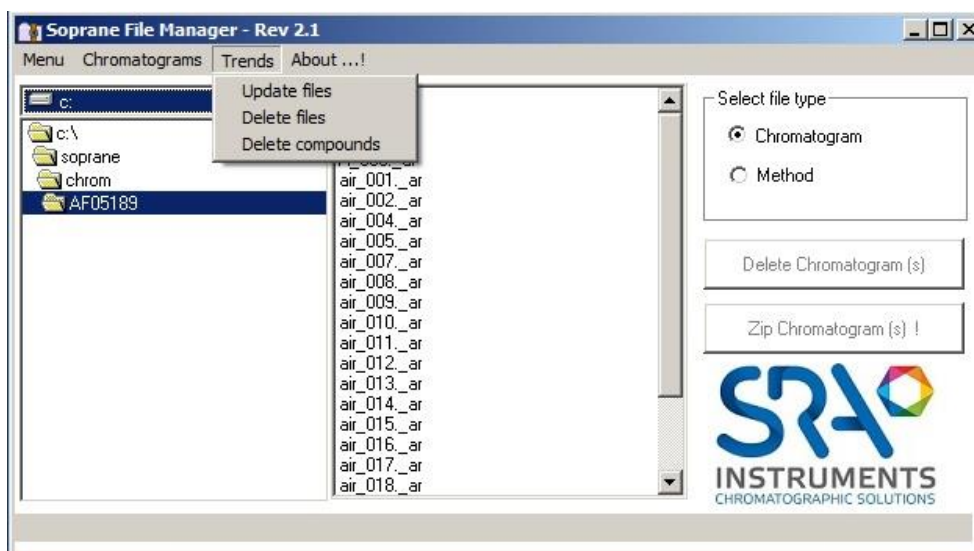
- The Soprane Configuration Report of your instrument
- The Soprane Error report, listing all the errors which occurred



When you call the after-sales service, it will be important to be able to provide these reports, in order to help solving the problem from a distance.

In the "Trends" menu, you can update files that you created with a previous version of Soprane and that you want to use with the current version.

You can also remove components (see chapter 10).



18. Calculations with Excel

An option from SOPRANE allows to establish the link with an EXCEL file to define any type of calculations. A few things are imposed, so that SOPRANE knows where to write and where to read the data.



If the option exists, the menu "Parameters" of SOPRANE allows to reach a screen of "Selection of worksheet".

Selection of work sheet

Name of the work sheet : C:\Soprane\Correction Axel.xls Ok

Name of the sheet : Feuil1 Cancel

Name of the component cell : Composant

Name of the results cell : Calculs

Name of the macro :

Export : Standard mode

The first line of this screen is the name 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 located in the column A: the first one is a cell with the text "Composant" and the second one with the text "Calculs".

If the realization of calculations requires the running of a macro, the name of this macro will be indicated in the fifth line.

Before to make calculations, SOPRANE prepares the worksheet.

For that, it seeks in column A the cell "Composant". It is assumed that the following lines correspond necessarily to the name of the components, such as they are known by SOPRANE (identification table programming). SOPRANE 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.

The EXCEL file carries out calculations and if programmed, SOPRANE activates the macro.

SOPRANE then seeks, in column A, a cell with the text "Calculs".



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.

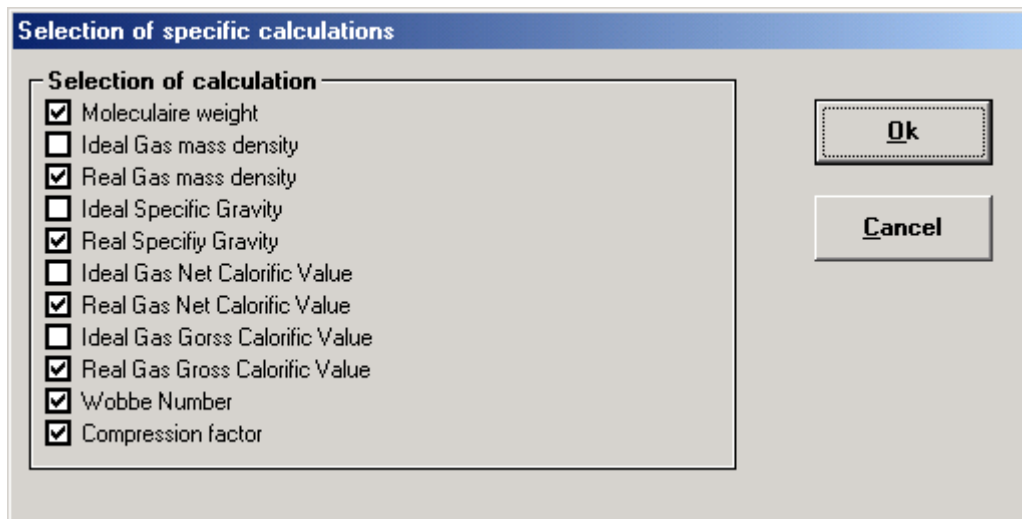
The other cells of the sheet are free for the user who may use them to store constants or calculation formulas.

When SOPRANE 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).

Component name	RT (sec)	Chan.	Raw Conc.	Area	Normalized	Mass.
Hydrogene	48.51	A	89.804	282079,582	39.081	
Oxygene	0.00	A	0.000	0.000	0.000	
Azote	71.01	A	27.607	8802,271	12.014	
Methane	0.00	A	0.000	0.000	0.000	
CO	0.00	A	0.000	0.000	0.000	
CO2	0.00	B	0.000	0.000	0.000	
Ethylene	0.00	B	0.000	0.000	0.000	
Ethane	82.60	B	1.724	14960,875	0.750	
H2S	137.01	b	0.523	4127,574	0.227	
Composant inconnu	147.99	b	5.256	5,256	2.287	
Propane	28.88	C	0.347	399,779	0.151	
Propylene	0.00	C	0.000	0.000	0.000	
iC4	0.00	C	0.000	0.000	0.000	
nC4	38.51	C	0.009	31,943	0.004	
Composant inconnu	40.32	c	43.250	43,250	18.821	
Trans-2-Butene	0.00	C	0.000	0.000	0.000	
1-Butene	0.00	C	0.000	0.000	0.000	
Iso-Butene	0.00	C	0.000	0.000	0.000	
Cis-2-Butene	0.00	C	0.000	0.000	0.000	
iC5	0.00	C	0.000	0.000	0.000	
nC5	70.11	C	0.015	77,333	0.006	
Composant inconnu	75.86	c	61.255	61,255	26.657	
1,3-Butadiene	0.00	C	0.000	0.000	0.000	
Pic 1	0.00	d	0.000	0.000	0.000	
			229.789	310589	100.000	
<hr/>						
Moleculaire weight :	10.278					
Real density :	0.4589					
Real Spe. Gravity :	0.3549					
Real Net CV :	16.65		MJ/m3			
Real Gross CV :	18.47		MJ/m3			
Wobbe :	52.04		MJ/m3			
Compressibility :	0.9993					

On the other hand, when SOPRANE indicates which calculations the user wishes to take into account, it uses the description of calculation such as defined in the column B of the EXCEL sheet.





The 2 following pages give a possible representation of an EXCEL sheet being used to carry out calculations such as defined above.

One will note the use of columns A, B and C for the writing of the concentrations starting from the line "Component name", as well as the use of the columns A, B, C, D and E for the reading of the calculated results starting from the line "Calculation Name".



Microsoft Excel - Calculs RGA Anglais.xls

Fichier Edition Affichage Insertion Format Outils Données Fenêtre eDocPrinter->PDF

Arial 8

L13C2 0

	1	2	3	4	5	6	7	8	9	10	11	12
	Component name	Component Amount	Component Normalized	Formule	Molar Mass		Hi 0/0 °C		Hs 0/0 °C		z 0°C, 101.325 kPa	
2	He	0,000	0,000	He	4,0026	0,0000	0,000	0,000	0,000	0,000	1,005	0,0000
3	Hydrogene	0,000	0,000	H2	2,0159	0,0000	10,777	0,000	12,788	0,000	1,006	0,0000
4	Oxygene	0,000	0,000	O2	31,9988	0,0000	0,000	0,000	0,000	0,000	0,999	0,0000
5	Azote	0,000	4,757	N2	28,0135	133,2602	0,000	0,000	0,000	0,000	1,000	0,1064
6	Methane	0,000	70,620	CH4	16,0430	1132,9567	35,818	2529,467	39,840	2813,501	0,998	3,4597
7	CO	0,000	0,000	CO	28,0100	0,0000	12,620	0,000	12,620	0,000	0,999	0,0000
8	CO2	0,000	0,170	CO2	44,0100	7,4817	0,000	0,000	0,000	0,000	0,993	0,0139
9	Ethane	0,000	6,510	C2H6	30,0700	195,7557	63,760	415,078	69,790	454,333	0,990	0,6510
10	Ethylene	0,000	0,000	C2H4	28,0540	0,0000	59,040	0,000	63,060	0,000	0,993	0,0000
11	Propane	0,000	17,096	C3H8	44,0970	753,8823	91,180	1558,813	99,220	1696,265	0,979	2,4833
12	Propylene	0,000	0,000	C3H6	42,0810	0,0000	85,940	0,000	91,980	0,000	0,981	0,0000
13	nC4	0,000	0,399	C4H10	58,1230	23,1911	118,610	47,325	128,660	51,335	0,957	0,0825
14	iC4	0,000	0,230	C4H10	58,1230	13,3683	118,180	27,181	128,230	29,493	0,958	0,0471
15	1-Butene	0,000	0,000	C4H8	56,1080	0,0000	113,380	0,000	121,420	0,000	0,965	0,0000
16	Iso-Butene	0,000	0,000	C4H8	56,1080	0,0000	112,630	0,000	120,670	0,000	0,965	0,0000
17	Cis-2-Butene	0,000	0,000	C4H8	56,1080	0,0000	113,080	0,000	121,120	0,000	0,961	0,0000
18	Trans-2-Butene	0,000	0,000	C4H8	56,1080	0,0000	112,910	0,000	120,960	0,000	0,961	0,0000
19	1,2-Butadiene	0,000	0,000	C4H6	54,0920	0,0000	109,840	0,000	115,870	0,000	0,955	0,0000
20	1,3-Butadiene	0,000	0,000	C4H6	54,0920	0,0000	107,470	0,000	113,510	0,000	0,966	0,0000
21	nC5	0,000	0,081	C5H12	72,1500	5,8442	146,000	11,826	158,070	12,804	0,918	0,0232
22	iC5	0,000	0,069	C5H12	72,1500	4,9784	145,690	10,053	157,760	10,885	0,937	0,0173
23	neo-pentane	0,000	0,000	C5H12	72,1500	0,0000	145,060	0,000	157,120	0,000	0,943	0,0000
24	C6	0,000	0,067	C6H14	86,1770	5,7739	173,450	11,621	187,530	12,565	0,892	0,0220
25	C7	0,000	0,000	C7H16	100,2040	0,0000	200,870	0,000	216,960	0,000	0,830	0,0000
26	C8	0,000	0,000	C8H18	114,2310	0,0000	228,280	0,000	246,380	0,000	0,742	0,0000
27	C9	0,000	0,000	C9H20	128,2580	0,0000	255,740	0,000	275,850	0,000	0,613	0,0000
28	C10	0,000	0,000	C10H22	142,2580	0,0000	283,160	0,000	305,290	0,000	0,434	0,0000
29	H2O	0,000	0,000	H2O	18,0153	0,0000	0,000	0,000	2,010	0,000	0,930	0,0000
30	Air					28,96260						0,99941
31												
32	Summation	0,000	99,999				2276,492		4611,365		5081,181	6,5

SRA INSTRUMENTS
210 rue des Sources
69280 Marcy l'Etoile
FRANCE

T : 04.78.44.29.47
F : 04.78.44.29.62
info@sra-instruments.com
www.sra-instruments.com

SA à Directoire et Conseil de
surveillance au capital de 150.000 €
RCS Lyon B 342 068 731
APE 4669B
SIRET: 342 068 731 00054
Code TVA FR 40342068731



	1	2	3	4	5	6	7	8	9	10	11	12	13
17	Cis-2-Butene	0,000	0,000	C4H8	56,1080	0,0000	113,080	0,000	121,120	0,000	0,961	0,0000	
18	Trans-2-Butene	0,000	0,000	C4H8	56,1080	0,0000	112,910	0,000	120,960	0,000	0,961	0,0000	
19	1,2-Butadiene	0,000	0,000	C4H6	54,0920	0,0000	109,840	0,000	115,870	0,000	0,955	0,0000	
20	1,3-Butadiene	0,000	0,000	C4H6	54,0920	0,0000	107,470	0,000	113,510	0,000	0,966	0,0000	
21	nC5	0,000	0,081	C5H12	72,1500	5,8442	146,000	11,826	158,070	12,804	0,918	0,0232	
22	iC5	0,000	0,069	C5H12	72,1500	4,9784	145,690	10,053	157,760	10,885	0,937	0,0173	
23	neo-pentane	0,000	0,000	C5H12	72,1500	0,0000	145,060	0,000	157,120	0,000	0,943	0,0000	
24	C6	0,000	0,067	C6H14	86,1770	5,7739	173,450	11,621	187,530	12,565	0,892	0,0220	
25	C7	0,000	0,000	C7H16	100,2040	0,0000	200,870	0,000	216,960	0,000	0,830	0,0000	
26	C8	0,000	0,000	C8H18	114,2310	0,0000	228,280	0,000	246,380	0,000	0,742	0,0000	
27	C9	0,000	0,000	C9H20	128,2580	0,0000	255,740	0,000	275,850	0,000	0,613	0,0000	
28	C10	0,000	0,000	C10H22	142,2580	0,0000	283,160	0,000	305,290	0,000	0,434	0,0000	
29	H2O	0,000	0,000	H2O	18,0153	0,0000	0,000	0,000	2,010	0,000	0,930	0,0000	
30	Air					28,96260						0,99941	
31													
32	Summation	0,000	99,999				2276,492		4611,365		5081,181		6,90
33													
34	Calculation Name	Calculation Text	Value at 0°	Unit	Decimals								
35	Moleculaire weight	Moleculaire weight	22,76492318		3								
36	Ideal density	Ideal Gas mass density	1,01565202		4								
37	Real density	Real Gas mass density	1,020519867		4								
38	Ideal Spe. Gravity	Ideal Specific Gravity	0,786011034		4								
39	Real Spe. Gravity	Real Specific Gravity	0,789312282		4								
40	Ideal Net CV	Ideal Gas Net Calorific Value	46,1136459	MJ/m3	2								
41	Real Net CV	Real Gas Net Calorific Value	46,33466075	MJ/m3	2								
42	Ideal Gorss CV	Ideal Gas Gorss Calorific Value	50,8118068	MJ/m3	2								
43	Real Gorss CV	Real Gas Gorss Calorific Value	51,05533914	MJ/m3	2								
44	Wobbe	Wobbe Number	64,68332029	MJ/m3	2								
45	Compressibility	Compression factor	0,995230032		4								
46													
47													

SRA INSTRUMENTS
210 rue des Sources
69280 Marcy l'Etoile
FRANCE

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19. Modbus

A specific software called SRAMODBUS, allows the exchange of data between the SOPRANE software 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.

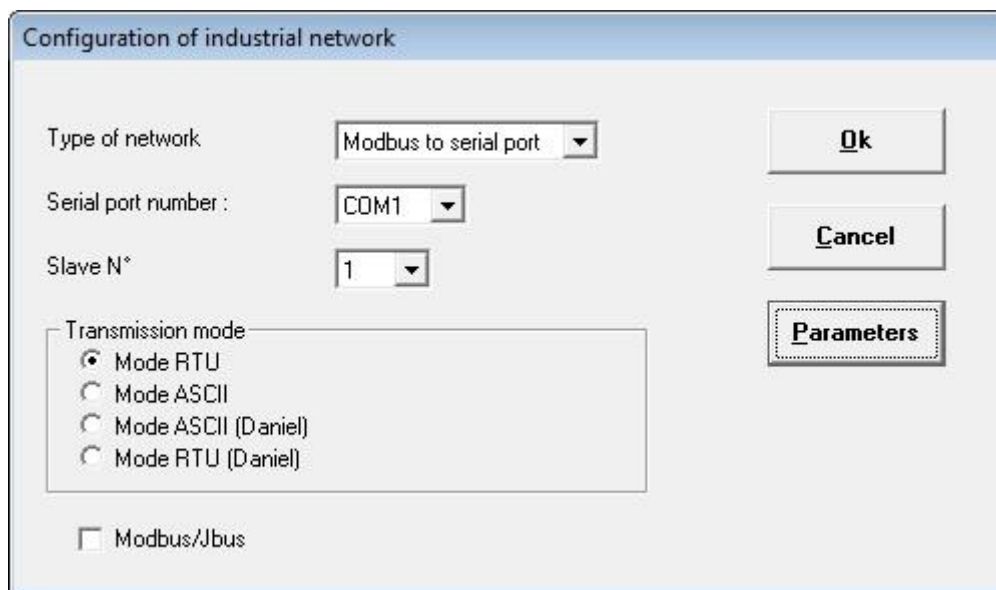
The data that can be exchanged are stored in an address table. The transmission protocol complies with a standard which consists in requesting or transmitting a question and in response the value of the variable located at a given address is transmitted.

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.

19.1 Hardware configuration

The PGCSETUP program allows to define this serial link configuration (see the configuration guide). The configuration Modbus window is shown only if the installation includes a Modbus option.



In this window:

- Choose the bus type, that is to say 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.



- 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 Ok button and quit Soprane Setup by confirming the saved changes.

NOTE:

The SRAMODBUS software is automatically launched after Windows initialization.

Consequently, the modification of the parameters will take effect only when Windows is started again.

19.2 Software configuration

Note: Before considering the configuration, it is better to perform some analyzes from Soprane, create the table of peaks and select the calculations if there are any. Thus, at each end of analysis, the SRAMODBUS software will retrieve the names of all these data and the configuration of the addresses will be facilitated.

The SRAMODBUS 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 SRAMODBUS software is running correctly, the SRA Instruments icon must be present in the notification area.



Double-click on the icon and click on **Restore**. The following window is opened:



The screenshot shows a window titled "SRA Instruments - Modbus comm..." with a menu bar containing "Configuration", "Display", and "About ...!". Below the menu bar is a table with three columns: "Address", "Name", and "Value". The table contains 24 rows, with the following data:

Address	Name	Value
1		
2	Life bit	28
3		
4		
5	Compounds alarm	0
6		
7		
8		
9		
10	Alarm	3
11		
12		
13		
14		
15		
16		
17		
18		
19		
20		
21		
22		
23		
24		

It is possible to give a variable name and a full scale value for each of the 8192 addresses that the database can handle.

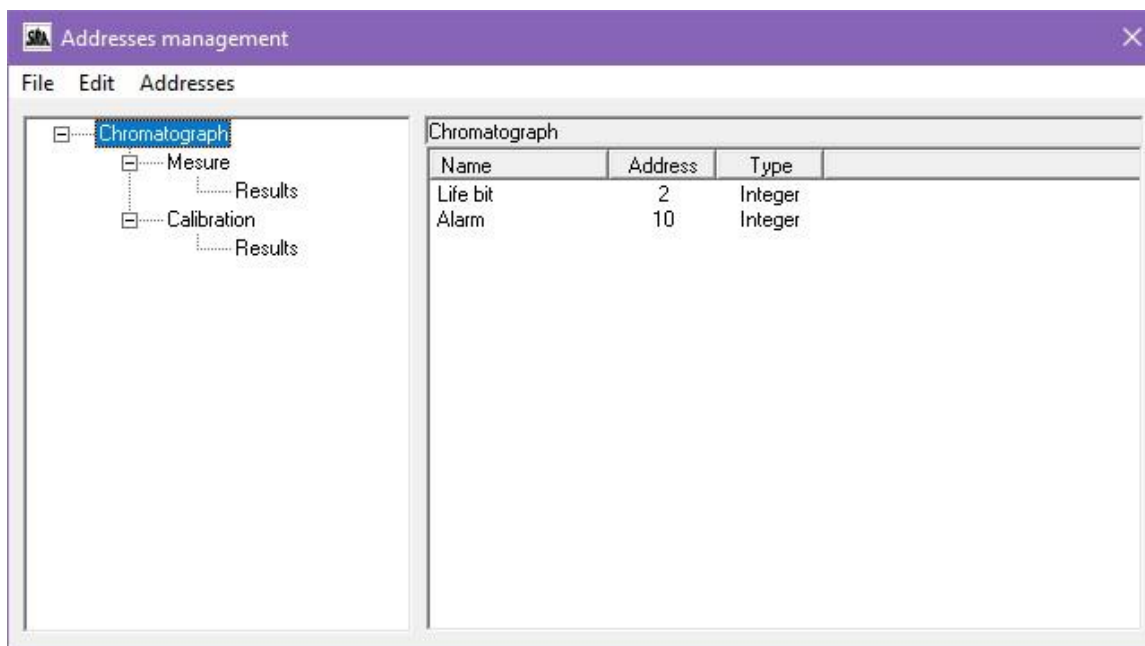
The data are separated in 3 levels:

- The system variables of the analyzer : "**Chromatograph**"
- The system variables of the analysis : "**Mesure / Calibration**"
- The values in relation with components and calculation : "**Results**"

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 SRAMODBUS software via the "**Configuration / Address**" menu.





In a first time, it is better to test whether the communication is correct (see Chapter 22 - Appendix concerning Modbus tests).

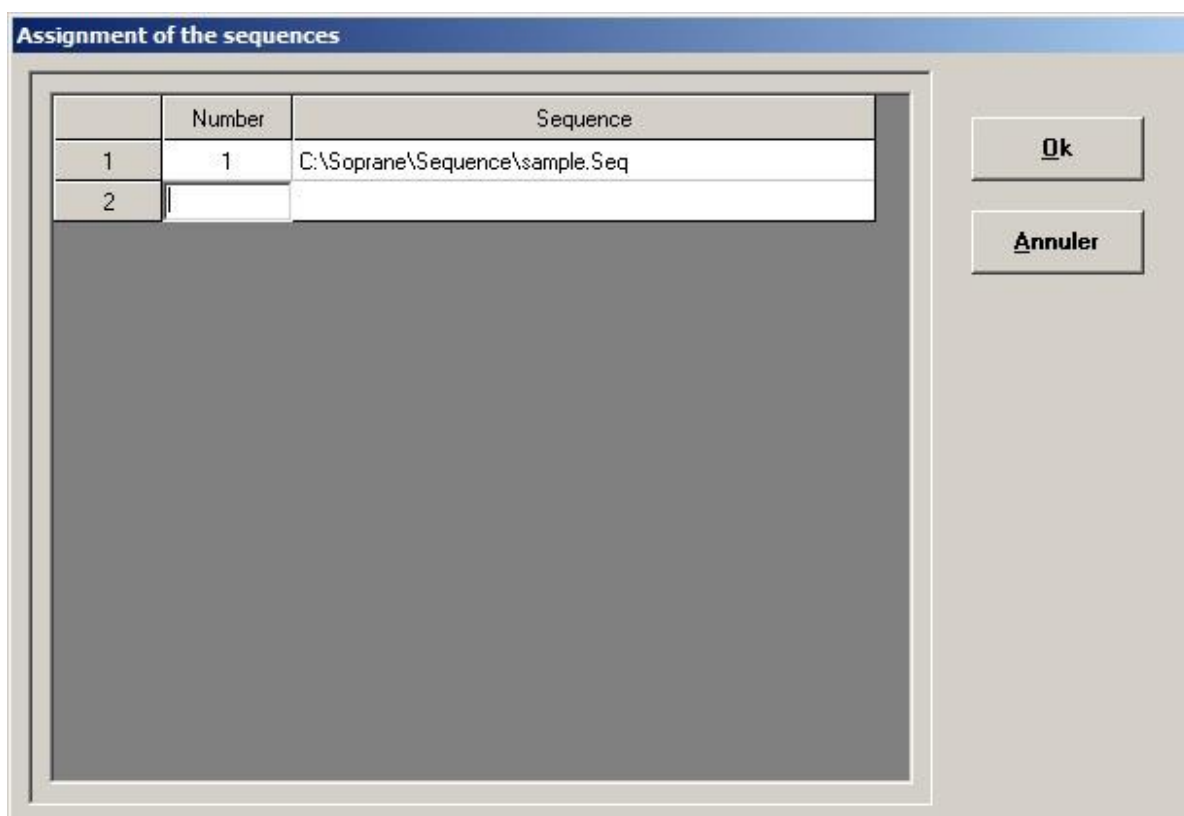
19.2.1 System variables of the analyzer

The variables that can be used are:

- **Stream flag:** in the case of a multi-stream application, this value indicates the number of the analyzed stream corresponding to the displayed results.
- **Analysis type:** this value indicates the type of analysis performed, either a measurement (0) or a calibration.
- **Alarm:** this value indicates the different alarms obtained during the analysis in the Soprane software. It can take several values, these values are obtained according to a combination of bits.
 - 0: no alarm
 - Bit 1: chromatograph default
 - Bit 2: cycle stopped
 - Bit 3: invalid or unknown method
 - Bit 4: defective connection with the chromatograph
 - Bit 5: unable to process results
 - Bit 6: sample flow rate default (option)
 - Bit 7: default with stream selector or multi-position valve (option)
 - Bit 8: default of concentration on one of the results
 - Bit 9: calibration default
- **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 cycle. It can take the following values:
 - 0: Wait
 - 1: Chromatograph ready test
 - 2: Waiting for start
 - 3: Waiting for injection
 - 4: Analysis in progress



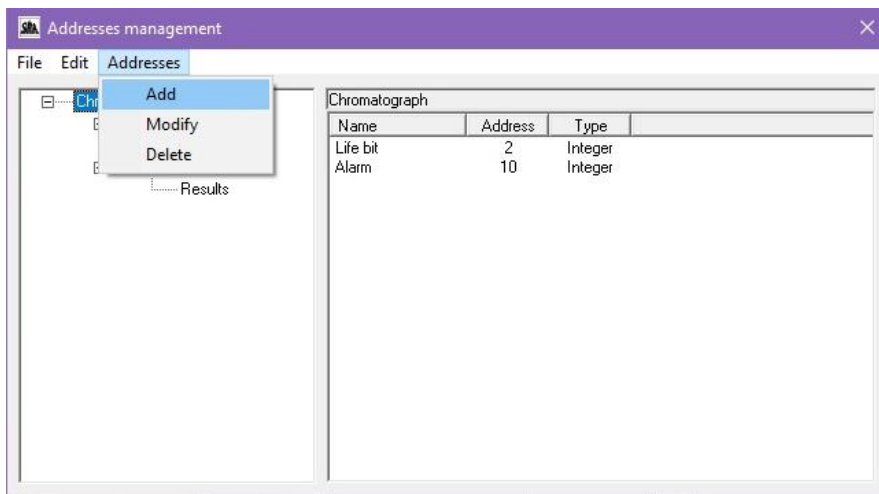
- 5: Recovering points
- 6: Post-processing
- 7: Analysis completed
- 8: Processing in progress
- 9: Calculation in progress
- 10: Bake out
- 11: Error processing
- **GC Ready:** this variable allows to know the state of the chromatograph. It can take the following values:
 - 0: default
 - 1: not ready
 - 2: ready
- **Start:** this variable is used to launch analyses via Soprane. 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 of analyses in single sequence mode.
 - 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 - Setup software via the menu "Options / Assignment of the sequences":



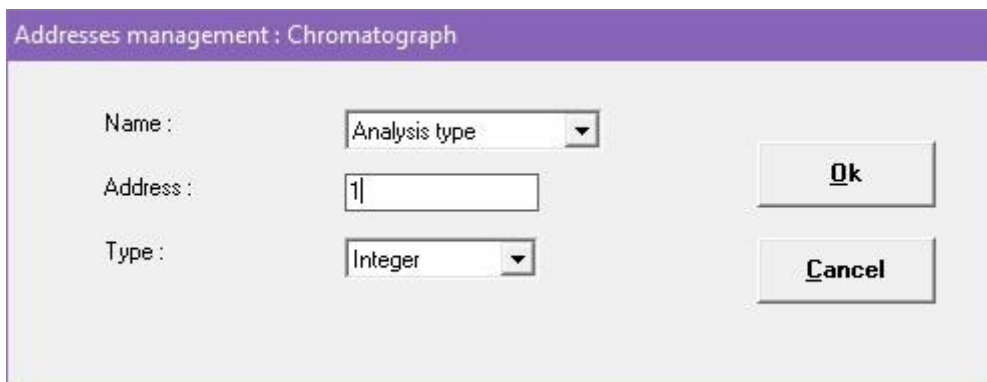
Note that if this variable has a value of zero, either the analyses are not launched or the analyses are stopped at the end of the current analysis.

To add these variables:

- Select "Chromatograph" by clicking on it
- In the menu bar, select "Addresses / Add"



- In the window that appears, select the name of the variable, type the address number and select the type (integer, long, float)



The notion of full scale is ignored for these variables.

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.



Addresses management : Chromatograph

Name :

Address :

Type :

19.2.2 System variables of the analysis

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 flag**: SRAModbus 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 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 "Mesure" or "Calibration"
- In the menu bar, select "Addresses / Add"
- In the window displayed, select the variable name, enter the address number and select the type (integer, long, float)

Addresses management : Chromatograph\Mesure

Name :

Address :

Type :

19.2.3 Values for components and calculations

SRAMODBUS offers the possibility to choose from a range of 6 values:

- Area



- Raw concentration
- Normalised concentration
- Weight concentration
- Calculation 1
- Calculation 2

To add these variables the principle is the same as previously:

- Click on "Results"
- In the menu bar, select "Addresses / Add"
- In the window that appears, select the name of the variable, type the address number and select the type (short integer, long integer, real)

The name of the component (which must be EXACTLY the same as what is programmed in the SOPRANE 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.

For the components, if you use the type 'Integer' or 'Long', the 'Coefficient' list is accessible. This coefficient 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. The value will then be multiplied by 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 "**Configuration / Options**" menu (see § 19.2.4).

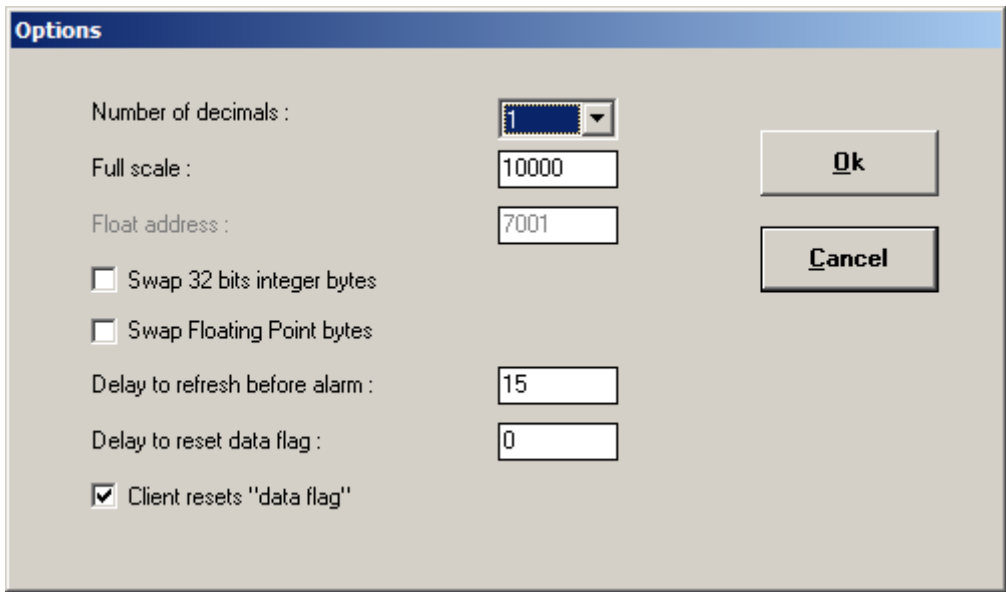
SOPRANE can perform post-analytical calculations. These calculations are, for example, the molar mass, the density, the specific gravity, the calorific capacities, etc. Two sets of calculations can be used, the calculations possibly being the same but carried out under different temperature or pressure conditions.

If the value corresponds to a calculation made in Soprane, it is necessary to select the value Calculation 1 or Calculation 2.

19.2.4 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, SRAMODBUS 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 restarts an analysis, the flag automatically returns to 0.





19.3 Display mode

The **"Display / Results"** menu displays the addresses corresponding to the results of the analyses.

The **"Display / Values"** menu displays the entire table of data stored in the database in the format of hexadecimal, integer or decimal values.

Address	Name	Value
1		
2	Life bit	28
3		
4		
5	Compounds alarm	0
6		
7		
8		
9		
10	Alarm	3
11		
12		
13		
14		
15		
16		
17		
18		
19		
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24		



20. Appendix I: integration parameters and errors

20.1 Comments about the integration

It is important to well understand how the integrator works and what effects may be caused by the use of 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 really due to a compound. Thus, during the peaks detection it is necessary to use correct detection parameters.

20.2 The peaks 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 in order 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's coordinates may be shown in the lower left corner of the window. These coordinates are directly expressed in microvolts and seconds.

Two remarks:

- The peak is assumed to be a Gaussian curve. In most cases, the peaks are asymmetric. If the peak is very asymmetric, the peak width must be shortened. The peak width may be also determined as being the time between the beginning and the top of the peak.
- The value programmed as peak width may be a few times more or less than the real value. The integration process is adaptable enough to give accurate results from an approximate parameter.

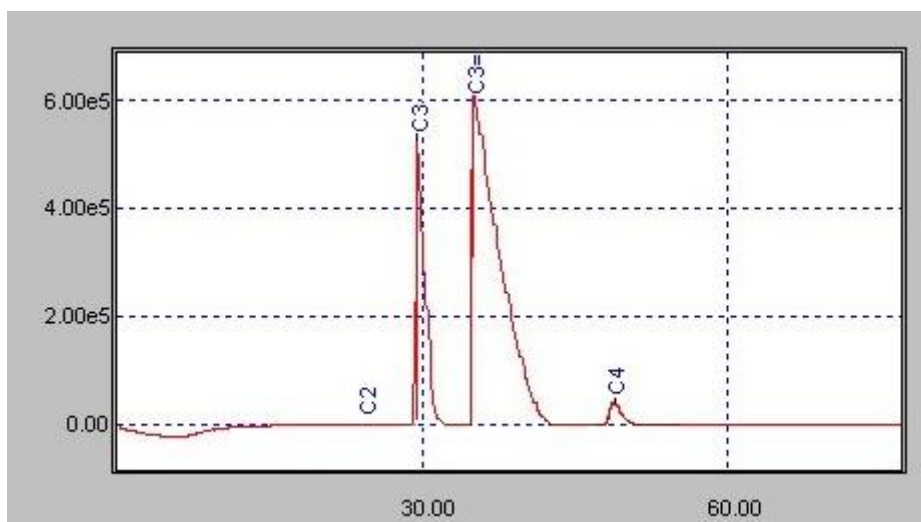
The threshold value or slope sensitivity must correspond to the reality. If this value is too high, the peaks are not detected or the baseline correction is not satisfying. If the value is too low, the noise is integrated. It is possible to determine an approximate value from the curve using the mouse and the coordinates of 2 points. The good value is close to the difference of the signal values divided by the difference of time values. There too, the integration process is adaptable.

If the concentration of the compounds may vary, it is preferable to try several values from several chromatograms before to select the good one. In this way, and because retention times may fluctuate when concentrations vary, these attempts will be useful to fix the times when the events have to be programmed.

20.3 Integration carried out with wrong parameters

On the chromatogram below, we want to integrate the peaks. They are very asymmetric and the peak referenced C3 for instance is one second wide at middle height but there is only 0.2 second from the beginning to the top.

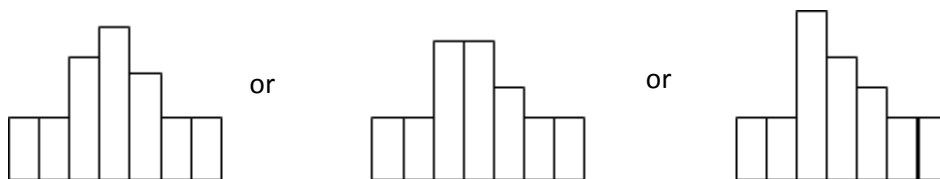
Thus, to detect correctly, with the best accuracy, the first part of the curve, the value of peak width to be programmed for the SAP parameters would be 0.2 seconds. If the peak was symmetric, this value would be 1 second.



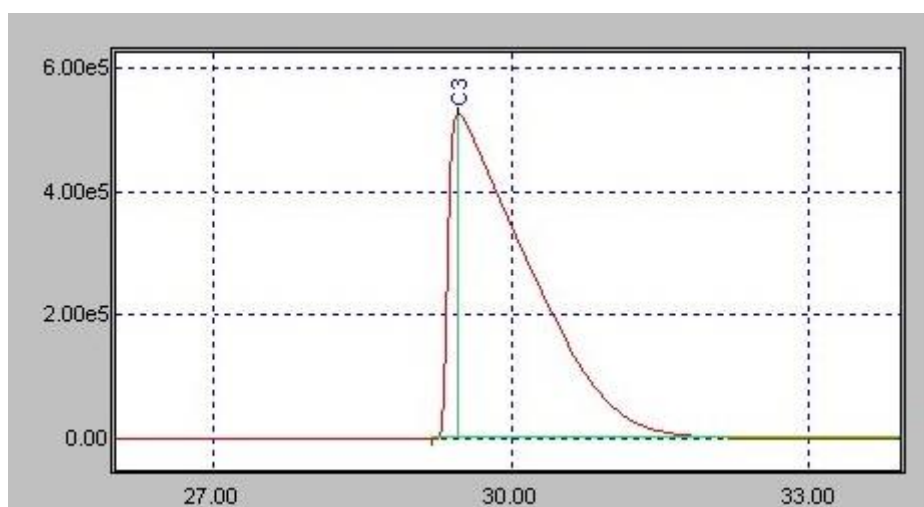
Suppose we program a far bigger value, for instance 4 seconds. We want to detect the peaks, thus, second mistake, we program the lowest possible value for the slope sensitivity, that is to say 0,001 $\mu\text{V/s}$.



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 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 second as SAP parameter. Due to the asymmetry, the best value would be 0.2 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.

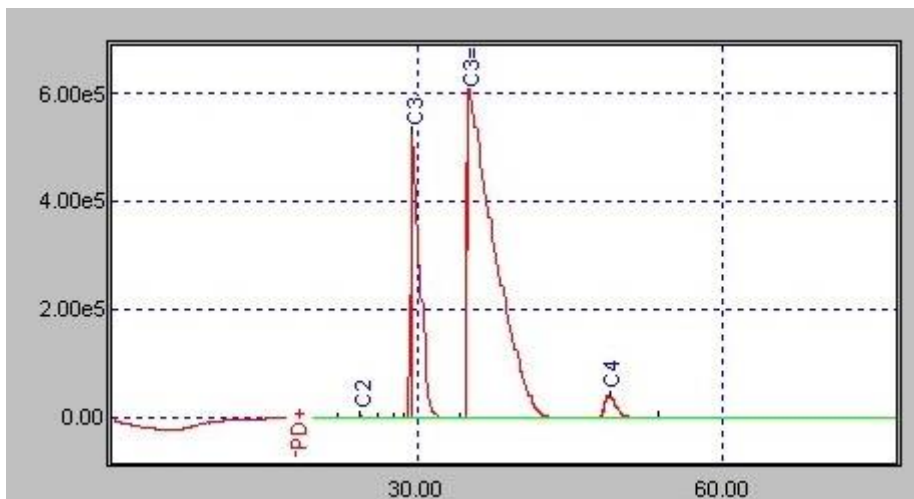
Two points is the minimum to ensure SOPRANE will always find an increasing signal during the first part of the peak.

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 (PD parameter ON) the system detects a peak and it is never able to go back to the baseline.

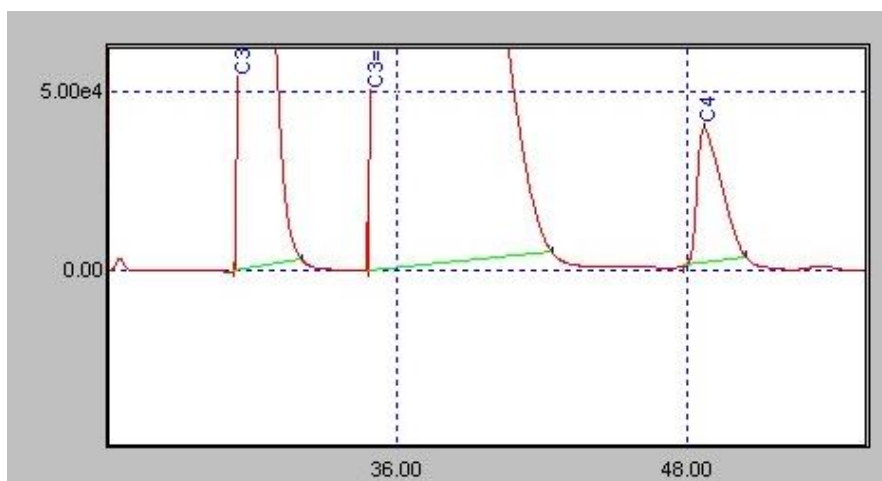




If we do the opposite and use a too high value for slope sensitivity, for instance 1000 $\mu\text{V/S}$, the peaks are correctly detected but SOPRANE considers to be back in the baseline state before the effective end of the peak.

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.

The chromatogram below has been integrated with these values.

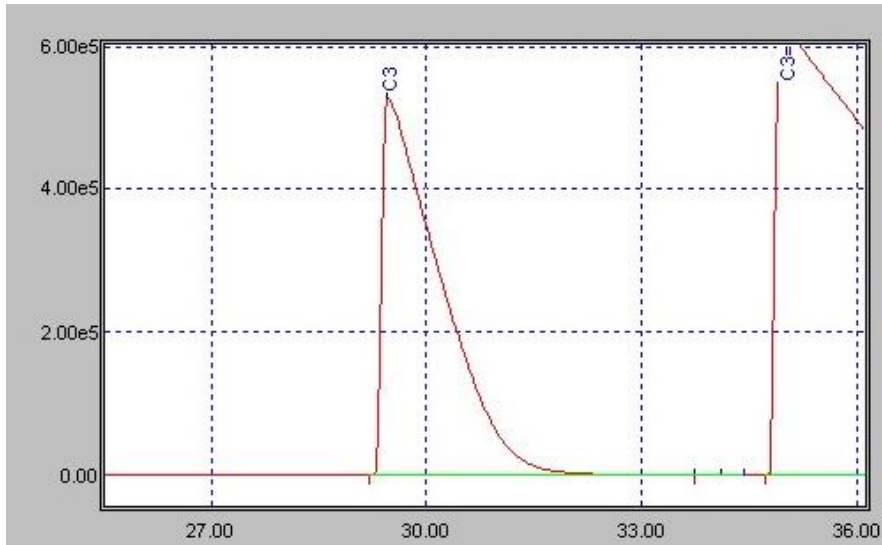


If the analyzer works with several streams and a wide range of concentrations, we will have to adjust the slope sensitivity parameter in order to have a good detection of the peaks in all cases.

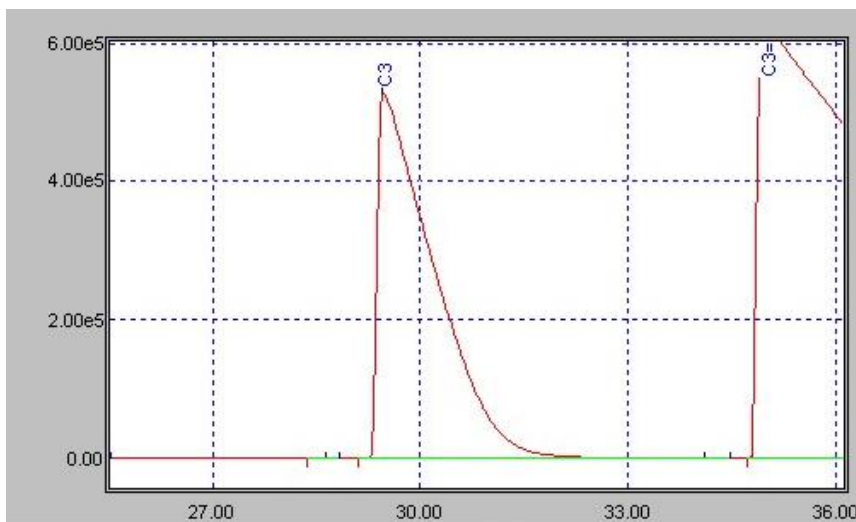
Different values of concentrations and of concentrations ratios give different results and we must ensure a good integration in all cases.

The same analysis has been integrated with different values to show the ability of SOPRANE to work correctly with values several times higher or lower than the good ones.





The integration of the chromatogram above has always been performed with a peak width of 1 second but using a slope sensitivity of 50 $\mu\text{V/s}$. The end of the peak C3 is detected at about 33.7 seconds.



This integration has always been performed with a peak width of 1 second and using a slope sensitivity of 5 $\mu\text{V/s}$. The end of the peak C3 is detected at about 34.1 seconds.

The difference with the precedent case is not significant.

If the concentration fluctuates, the best value may be 20 $\mu\text{V/s}$, depending on the expected concentrations range.



21. Appendix II: Recovery of an analysis and processing method from a chromatogram

In the case where a method has been erased by mistake, it is possible to recover the analytical part and the treatment part from a chromatogram.

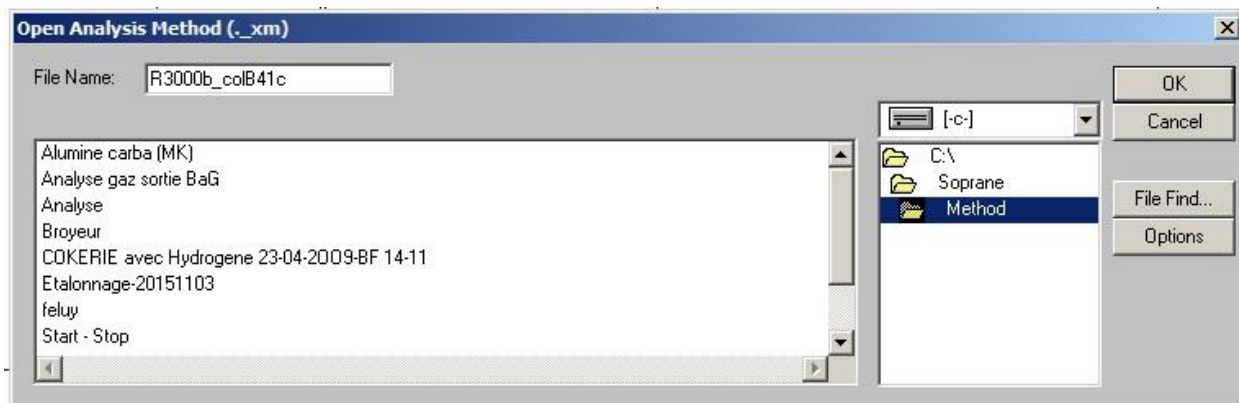
To do this, follow these instructions:

1. In the Soprane menu bar, click on the Processing module icon.
2. Click on the menu "**Analysis / Load chromatogram**" and select the chromatogram.
→ A message appears, indicating that the method does not exist.



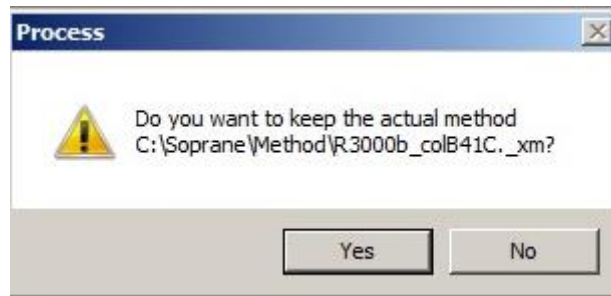
3. Click on **Ok**.
→ The chromatogram opens.
4. Click on the menu "**Method / Save archived method as**"

In the window displayed, fill in the field « File name » with the name you want to give to the method, then click on Ok.



5. Click on **Yes** in the window(s) successively displayed.
6. Click on the menu "**Method / Close all files**"
7. Click on the menu "**Method / Open a method**", select the method and click on Open.
8. Click on the menu "**Analysis / Load a chromatogram**"
→ The analysis is loaded and a message asking if you want to keep the method is displayed:





9. Click on **Yes**.
→ The method has been recovered.



22. Appendix III: Calculations

22.1 Comments about the calculations

The peaks integration leads to normalized concentrations values.

When using calculations, Soprane first calculates the molar mass of the sample by using the following formula:

$$M_{mol} = \sum_i^n CONC_i * M_{mol_i} / 100$$

Then, Soprane calculates the ideal density, the ideal specific gravity, the ideal inferior calorific value, the ideal superior calorific value and the compressibility factor of the stream according to the following formulas:

$$\text{Ideal Density} = \sum_i^n CONC_i * (M_{mol_i} * P / (R * T)) / 100$$

M_{mol_i} is the molar mass of each compound,

P is the pressure

R is the constant of perfect gases (8.31451)

T is the temperature in Kelvin degrees.

$$\text{Ideal Specific Gravity} = \sum_i^n CONC_i * M_{mol_i} / M_{molAir}$$

M_{mol_i} is the molar mass of each compound,

M_{molAir} is the air molar mass.

$$\text{Ideal ICV} = \sum_i^n CONC_i * P_{ci} / 100$$

P_{ci} is the inferior calorific value of each component expressed in MJ/m³.

$$\text{Ideal SCV} = \sum_i^n CONC_i * P_{cs_i} / 100$$

P_{cs_i} is the superior calorific value of each component expressed in MJ/m³.

$$Z_{sample} = 1 - (\sum_i^n CONC_i * (1 - Z_i))^{1/2}$$

Z_i is the compressibility factor of each component.

The software then calculates the real density, the real specific gravity, and the real inferior and superior calorific values from the compressibility factor of the sample.

$$\text{Real Density} = \text{Ideal density} / Z_{sample}$$

$$\text{Real Specific Gravity} = \text{Ideal Specific Gravity} * Z_{air} / Z_{sample}$$

Z_{air} is the compressibility factor of the air.

$$\text{Real ICV} = \text{Ideal ICV} / Z_{sample}$$

$$\text{Real SCV} = \text{Ideal SCV} / Z_{sample}$$

The Wobbe index is then determined. $\text{Wobbe} = \text{Real SCV} / (\text{Real Specific Gravity})^{1/2}$



22.2 Initial values used by Soprane

All values are those of perfect components at 0 °C, by volume at 0 °C and 1.01325 Bar according to the standard ISO/DIS 6976:1995 and the experimental standard X 20-522.

Air molar mass: $M_{molAir} = 28.9626$

Compressibility factor of the air: $Z_{air} = 0.99941$

Compound	Molar mass	PCI (MJ/m ³)	PCS (MJ/m ³)	Z
Helium	4,0026	0	0	1,0005
Hydrogen	2,0159	10,777	12,788	1,0006
Oxygen	31,9988	0	0	0,999
Nitrogen	28,0135	0	0	0,9995
Methane	16,043	35,818	39,84	0,9976
Carbon monoxyde	28,01	12,62	12,62	0,9993
Carbon dioxyde	44,01	0	0	0,9933
Ethylene	28,054	59,04	63,06	0,9925
Ethane	30,07	63,76	69,79	0,99
Propylene	42,081	85,94	91,98	0,981
Propane	44,097	91,18	99,22	0,9789
Iso-Butane	58,123	118,18	128,23	0,958
N-Butane	58,123	118,61	128,66	0,9572
1 Butene	56,108	113,08	121,42	0,965
Iso-Butene	56,108	112,63	120,67	0,965
Cis 2 Butene	56,108	113,08	121,12	0,961
Trans 2 Butene	56,108	112,91	120,96	0,961
1,2 Butadiene	54,092	109,84	115,87	0,955
1,3 Butadiene	54,092	107,47	113,51	0,966
Neo-Pentane	72,15	145,06	157,12	0,943
Iso-Pentane	72,15	145,69	157,76	0,937
N-Pentane	72,15	146	158,07	0,918
1-Pentene	70,134	140,8	150,86	0,938
Hexane	86,177	173,45	187,53	0,892
Heptane	100,2019	200,87	216,96	0,83
Octane	114,2285	228,28	246,38	0,742
Nonane	128,2285	255,74	275,85	0,613
Decane	142,2817	283,16	305,29	0,434
Water	18,056	0	0	0,93

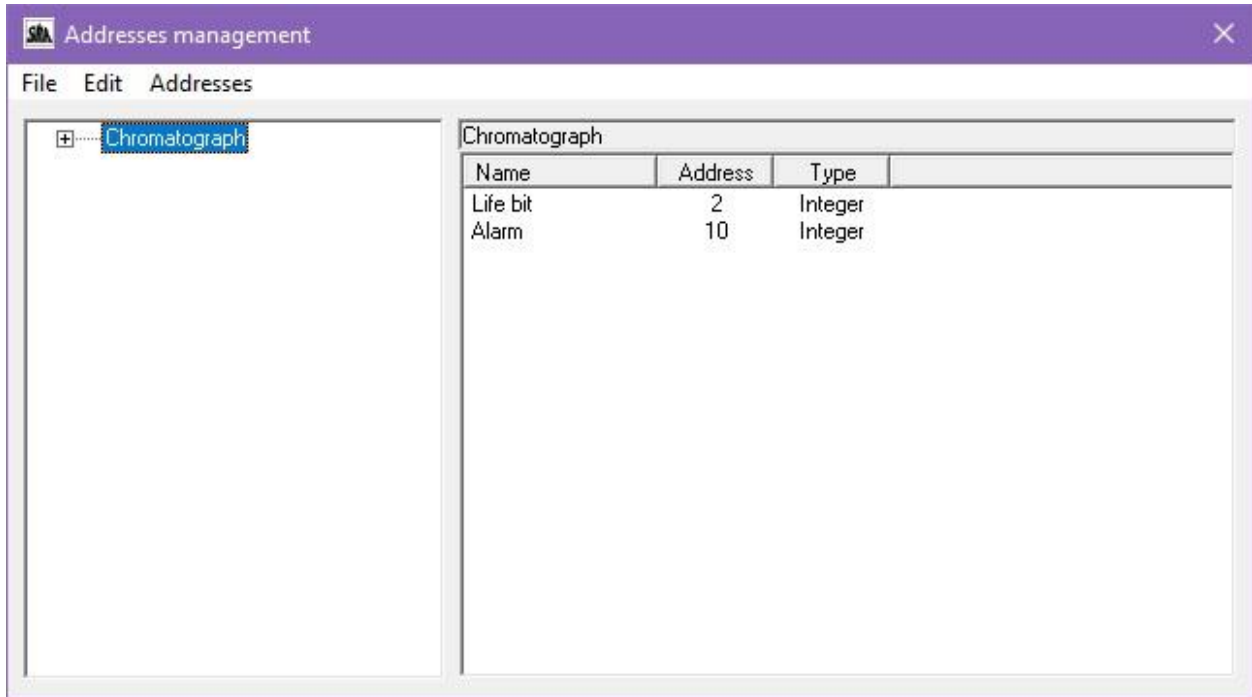


23. Appendix IV: Modbus tests

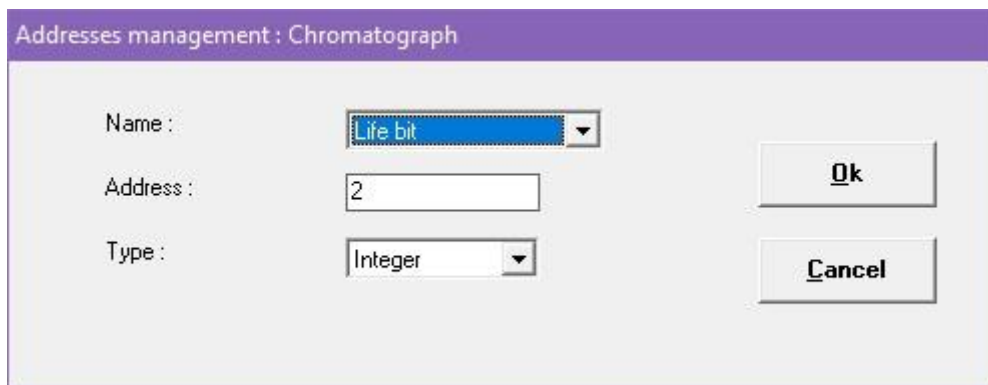
23.1 Communication tests

In a first time, it is better to test if the communication is correct.

Configure the life bit parameter at address 2 with the **"Configuration / Address"** menu.



Select **Chromatograph** and click on the **"Addresses / Add"** menu.



Select the following parameters and confirm with the Ok button.
Select the **"File / Save"** menu then **"File / Exit"** to return to the main screen.

From your supervisor:

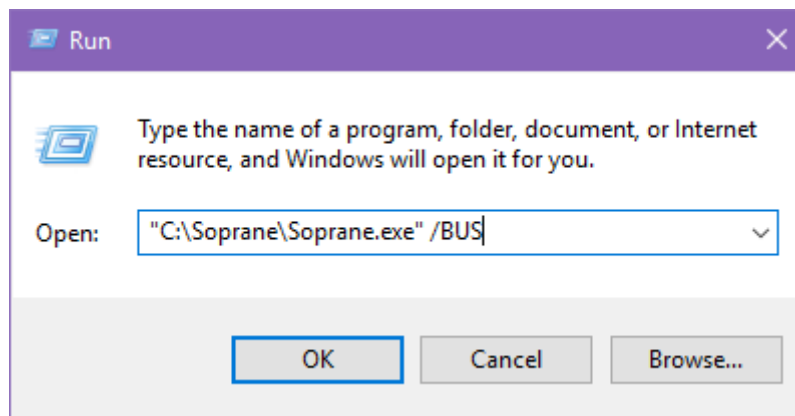


- Check that the configuration corresponds to the configuration defined in Soprane: communication medium, IP address if TCP/IP mode or communication protocol (speed, parity) and slave number if serial link.
- Program a Modbus reading of 3 first addresses in integer (addresses 1, 2 and 3). Indeed, in 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 refresh 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.

23.2 Tests of transmission of the values

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 from the Windows Run menu by entering the following line:



Then from Soprane, select the "**Analysis / Batch processing**" menu, select the method then the analysis and validate by Ok. The results are transmitted.

Be careful, if you launch Soprane each time this way, the results will be sent at each end of analysis and also at each reprocessing.



24. Appendix V: Comments on Soprane – Mass Hunter coupling

By default, Soprane allows you to be coupled with Agilent's Msd ChemStation software if it is installed on the same computer.

A special version of Soprane exists, 'Soprane-Coupling', which allows Soprane to be coupled with various software packages: Chemstation GC, Mass Hunter, Soprane. For the first two, it is necessary that these applications are installed on the same computer. For Soprane, it must be installed on another computer. In all cases, this coupling allows the results of the two software packages to be combined in a single report.

Please note: all the comments described below are also valid for installation of Soprane with the Msd ChemStation software. Only the 'Connection with Soprane' part is different because it is set by default with Soprane.

24.1 Coupling with Mass Hunter

Soprane can drive a M3000 Lan MicroGC, R3000 or Cp490 MicroGC and be linked to Mass Hunter software that drives either a 5977B MSD or a 5975T LTM-GC/MSD. It can also control a Solia MicroGC, which has the particularity of being able to connect the output of a module to the Agilent analyzer via a Valco Vici selection valve. In any case, Soprane launches the analyses on the MicroGC and Mass Hunter via an intermediate software. It is this software that retrieves Mass Hunter's results and transfers them to Soprane.

24.2 Software installation

Mass Hunter must be installed and configured first for the installation to be successful. Then, you must install Soprane Coupling version on the same computer.

The Soprane installation installs various macros in Mass Hunter and the intermediate software CpMsHunter.exe (SRA program). After this installation, it is necessary to restart Mass Hunter so that it considers the modifications made by the Soprane installation.

24.3 Link with Soprane

At Soprane level, the dialogue is carried out via DDE with the CpMsHunter software. It is therefore necessary to configure this dialog with PGCSepCp (SRA program) via the "**Instrument / Analyzer Coupling**" menu. The software checks the software installed on the computer.

The 'Coupling to Chemstation' option is only valid if the file ChemStation.ini is in the Windows directory. The 'Coupling Solia' option is only valid if the file MsdChem.ini is in the Windows directory.

The parameters are as follows:

- Application name: **CpMsHunter**
- Source field name: **System**
- Command parameter name: **MsCommand**



- Status parameter name: **MassStatus**

Modules selection

No coupling
 Coupling to Agilent ChemStation
 Coupling SOLIA
 Coupling with another analyzer

Source name : CpMsHunter
Topic name : System
Command item : MsCommand
Status item : MassStatus

Ok
Cancel

Please note, it is possible to couple Soprane to Mass Hunter using the 'Coupling with another analyzer' option and the same parameters. The difference is that the Solia option allows using the module selection valve to connect the MicroGC to the Mass and for the other option, the valve is not used, and the module selection will have to be done manually.

In the case of the 'Coupling Solia' option, the "**Modules selection**" menu is active.

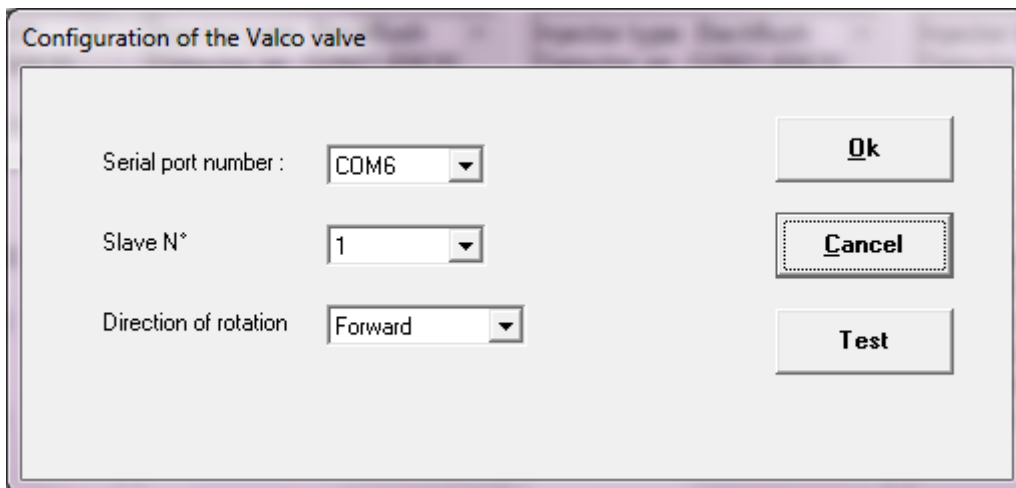
Modules selection

Position 1 : None
Position 2 : Backflush PPU 8m GcModule
Position 3 : 0.4ul BF Alumina 10m/Alumina 1m GcModule
Position 4 : VAR OV-1 2.0um 8m GcModule

Ok
Cancel

It is used to indicate the position of the valve used to connect a module to the Mass. Of course, it is also imperative that a Valco valve is configured via the "**Sampling / Valco Valve**" menu.

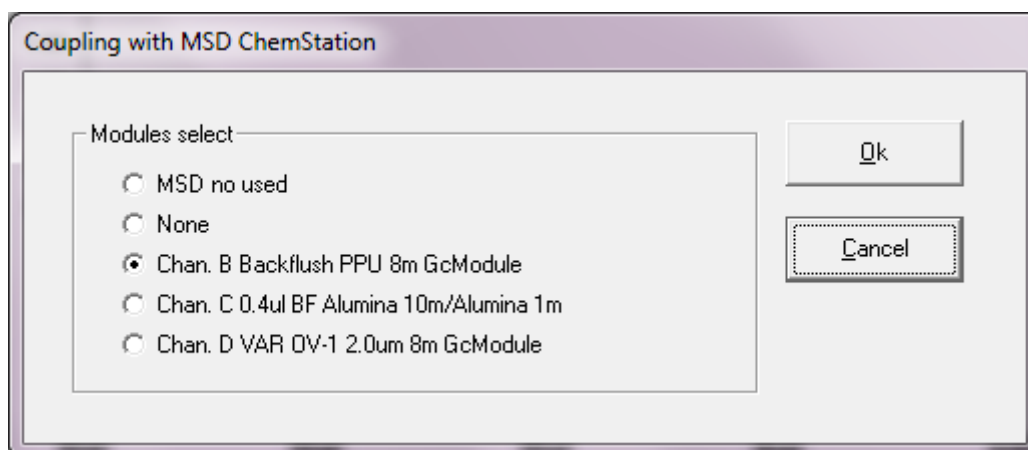




24.4 Use with Soprane

When the configuration has been completed, a **"Coupling"** menu is available in the **"Instrument"** menu.

In the case of a coupling with a Solia, a window is displayed to select the module to be connected to the Mass.



If a Valco valve has been configured, the module will be selected automatically.

The 'MSD no used' option allows you to use the Soprane software alone without a connection to Mass Hunter.

If the coupling is performed with another analyzer, clicking on the **"Coupling"** menu activates or deactivates the connection with the software.

In the case of a Solia coupling with a valve, it is also possible to create analysis sequences that allow to change the connected module, Chan. column.



Sequence table : C:\Soprane\Sequence\etal.Seq

	Analysis name	Method	Stream n°	Sampling (secs)	Chan.
1	bout B	So_UCB._xm	2	30	D
2	bout B	So_UCB._xm	2	30	D
3	bout B	So_UCB._xm	2	30	D

When starting the analyses with the Start button, you have several possibilities for working.

Start of analysis

Start analysis

- Analysis mode
- Single sequence
- Automatic mode
- Calibration

Number of runs: 3

Sampling (secs): 0

Method: So_Biogaz ppu._xm

Name: blc

Path: D:\Analyses\2017\SAV_171219

Sample name: air

Operator: sra

Interval in minutes between injections: 0.00

Waiting for external start

Only one MSD acquisition

Ok

Cancel



If you choose the 'Analysis mode', a checkbox 'Only one MSD acquisition' is valid.

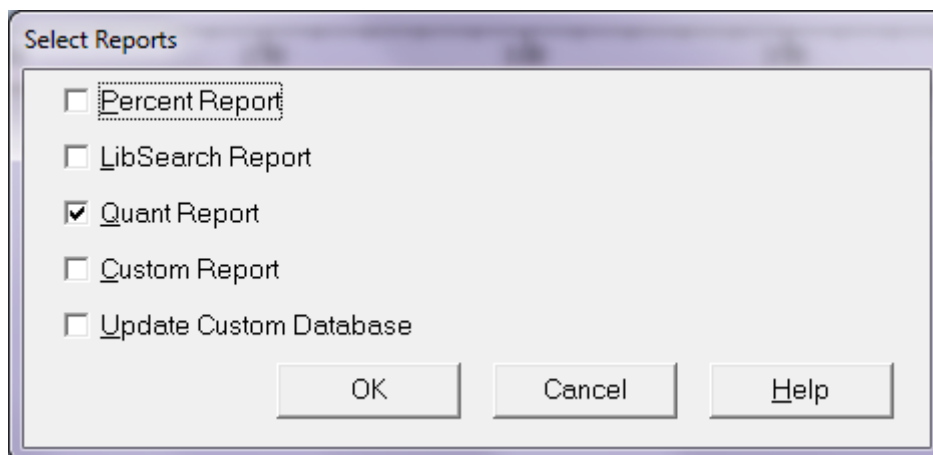
If it is unchecked, this will launch the number of analyses defined in the field 'Number of runs'. At the end of each analysis, Soprane will wait for the end of Mass Hunter's analysis to restart another one. In this case, it is preferable that the analysis time of the Mass be greater than or at least equal to the analysis time of the MicroGC. If checked, Soprane will run an analysis at Mass Hunter level and run analyses at MicroGC level as long as Mass Hunter analysis is running.

24.5 Use with Mass Hunter

When Mass Hunter is coupled with Soprane, it is possible to retrieve the results of this application **only if the analyses are processed with Data Analysis**. A common report can then be generated at Soprane level and Mass Hunter values will be integrated into Soprane's historical results files.

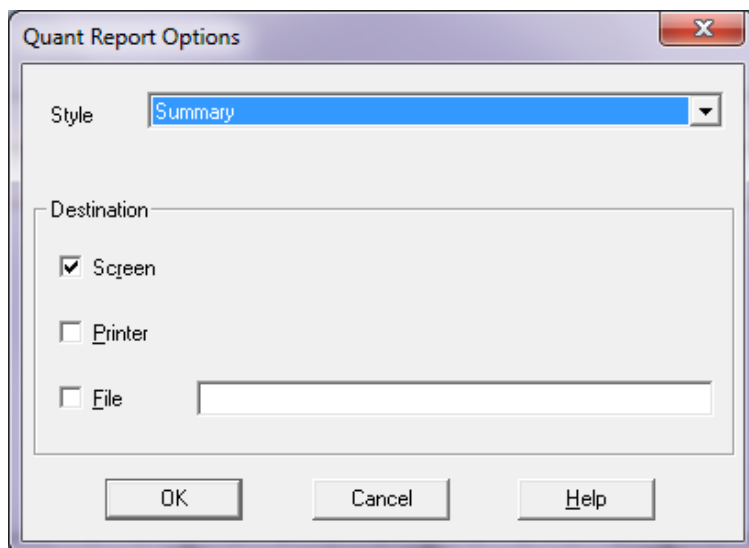
To obtain this transfer, it is necessary to set up the Mass Hunter method correctly to generate the results. This setting is made with the Data Analysis application.

Select the "**Method**" menu and then "**Edit Method**". The following window appears:

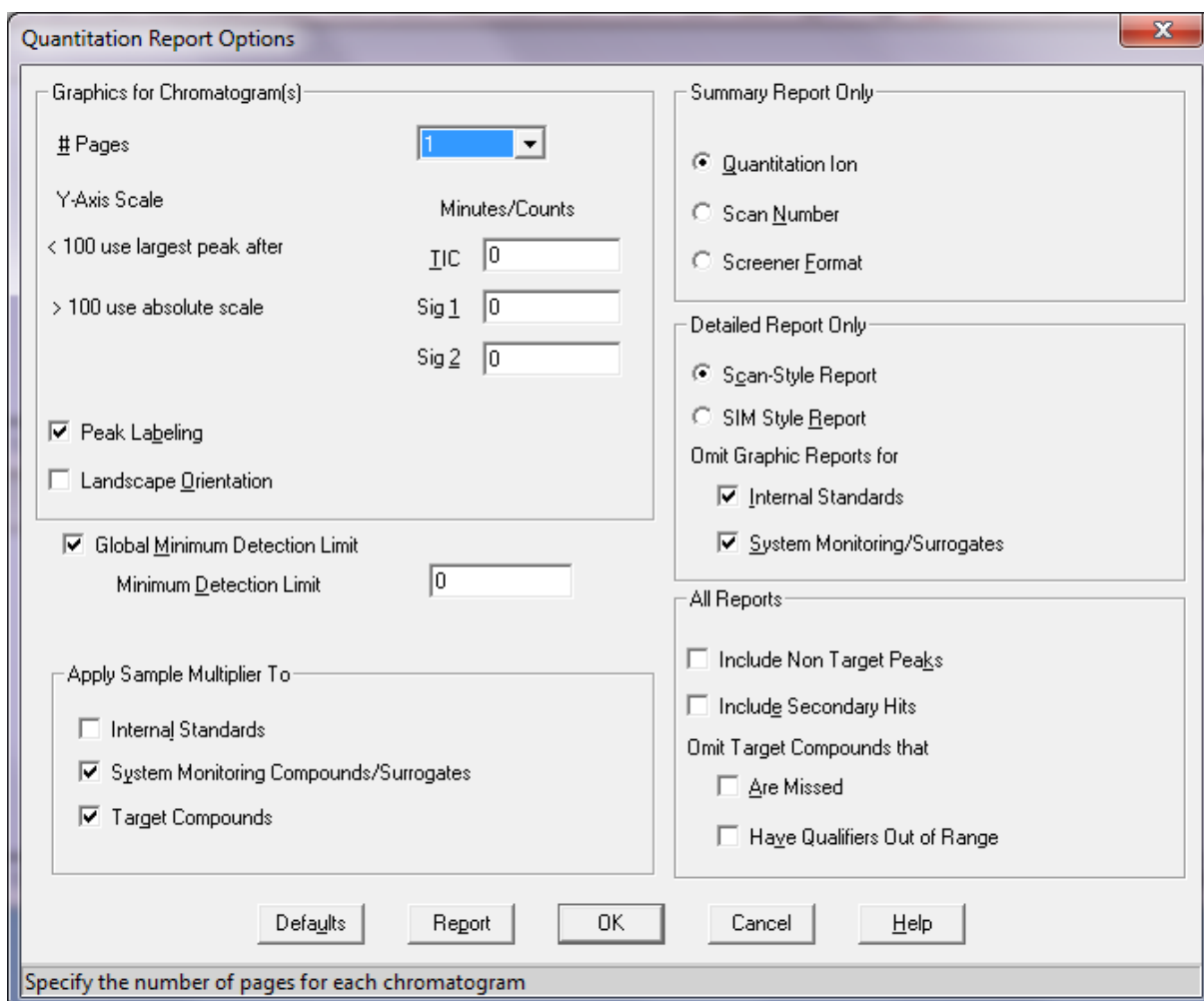


Select the 'Quant Report' checkbox and confirm with Ok, the following window appears.





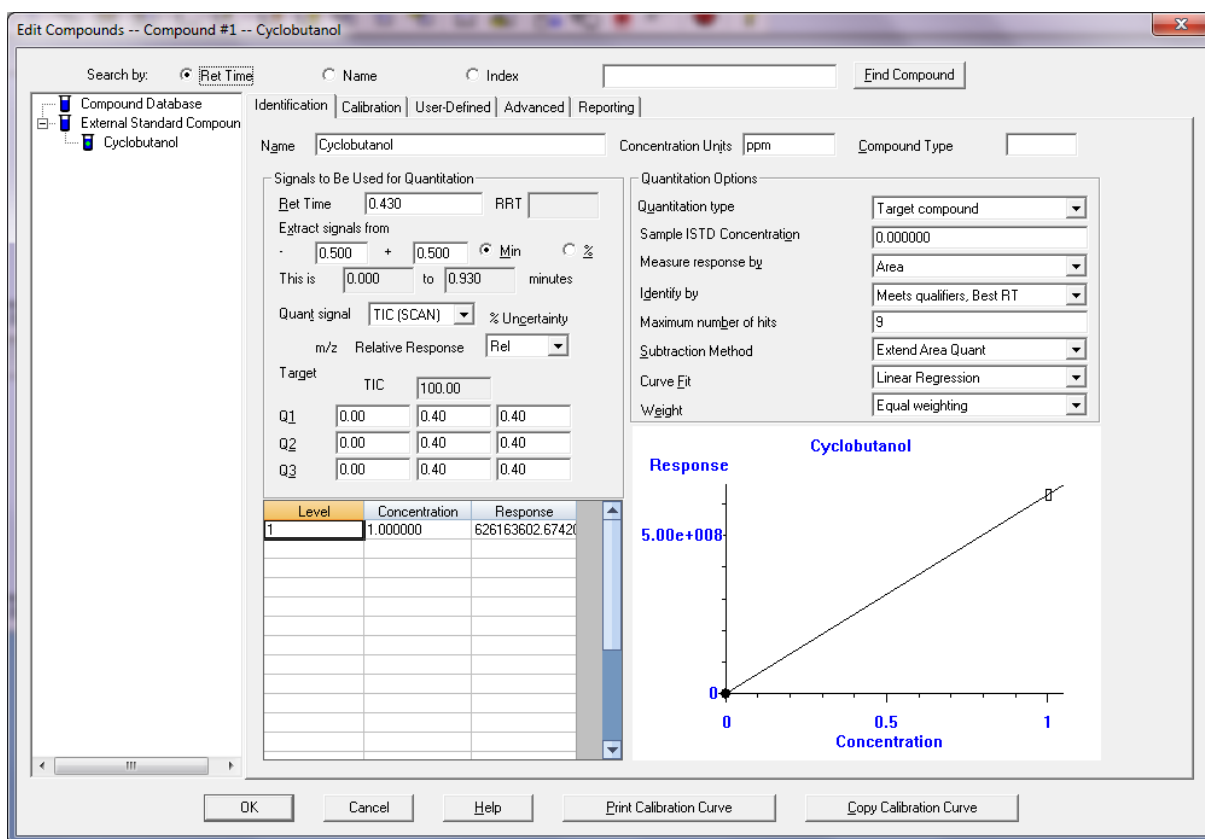
It is not necessary to check one of the boxes, validate by Ok, the following window is displayed.



Confirm with Ok and save the method to finish.



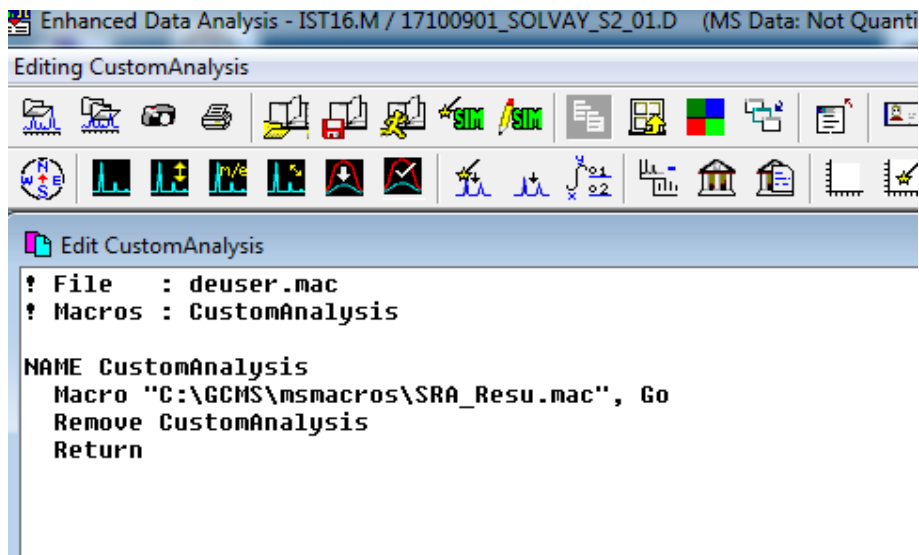
Then, it is necessary to create a table with at least one component. Select the **"Calibrate"** menu and select **"Edit Compounds"**.



Create a component by entering its various integration and quantification parameters, validate by Ok, and save the method to finish.

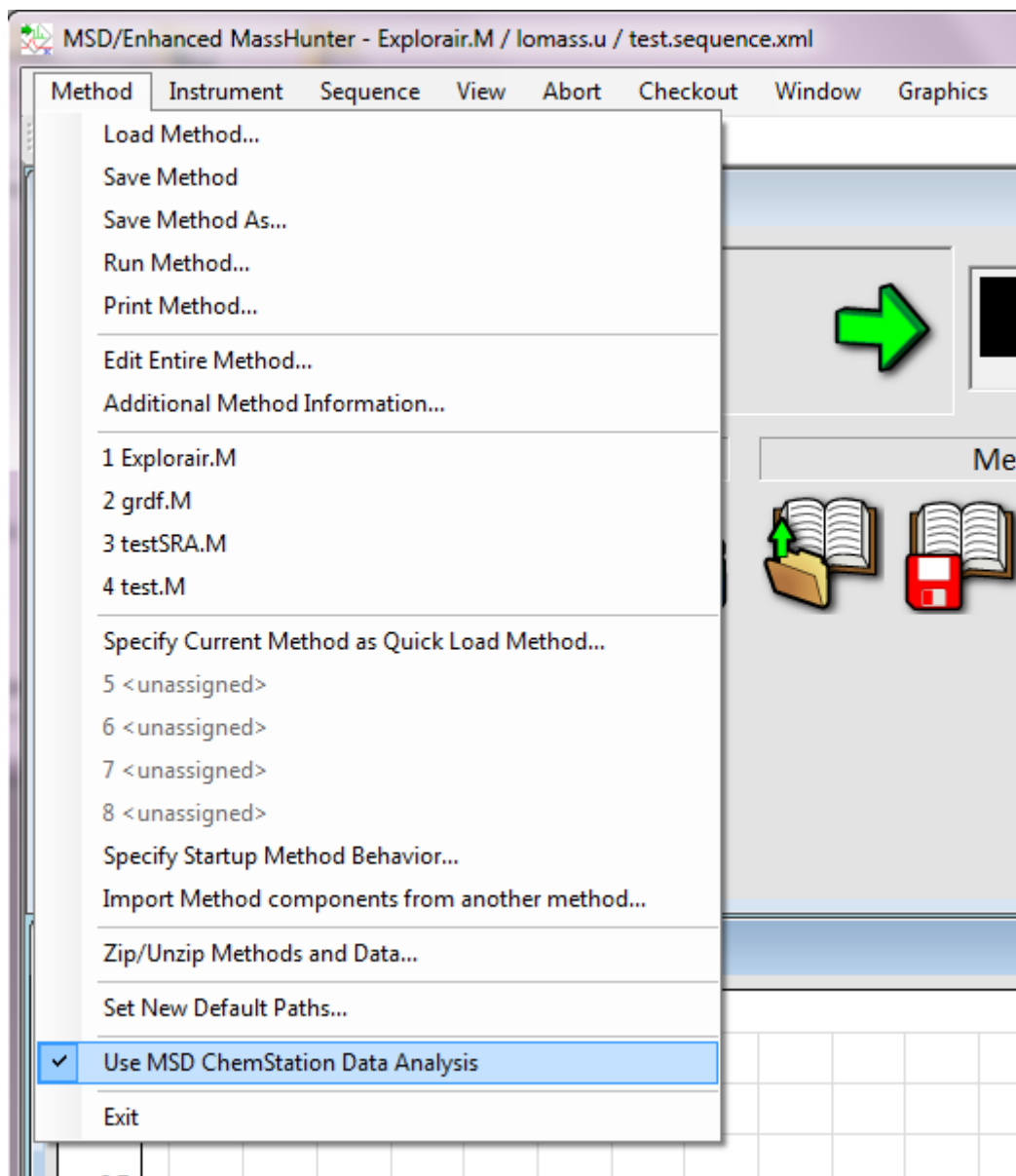
To finalize this setting at the level of Data Analysis, it is necessary to modify the 'CustomAnalysis' part of the method so that the macro that generates the results file is launched at the end of processing. This is done using the **"Transfer Data"** menu and **"Add Custom macro in method"**. The result of this action can be viewed using the **"Method"** menu and **"Edit CustomAnalysis"**.





Finally, to complete the parameterization of Mass Hunter, it is necessary to ask the GC-MS Acquisition application to use Data Analysis during processing. This action is activated when the "**Method / Use MSD ChemStation Data Analysis**" menu is checked.





When these actions are performed, the file 'SRA_Results.Txt' must be created at the end of each analysis in Mass Hunter's 'Executable' directory (C: \GCMS).

