Mestrelab Research

Mnova SMA 3.1

USER MANUAL

Document Number

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1. Introduction

The Simple Mixture Analysis (SMA) plugin is a simple and versatile tool for the quantitation of mixtures of components via NMR. It allows the development and storage of methods for the rapid and consistent analysis of samples. SMA also includes advanced reporting options, result visualization and reviewing capabilities, and a system of alerts to automatically highlight potential errors.

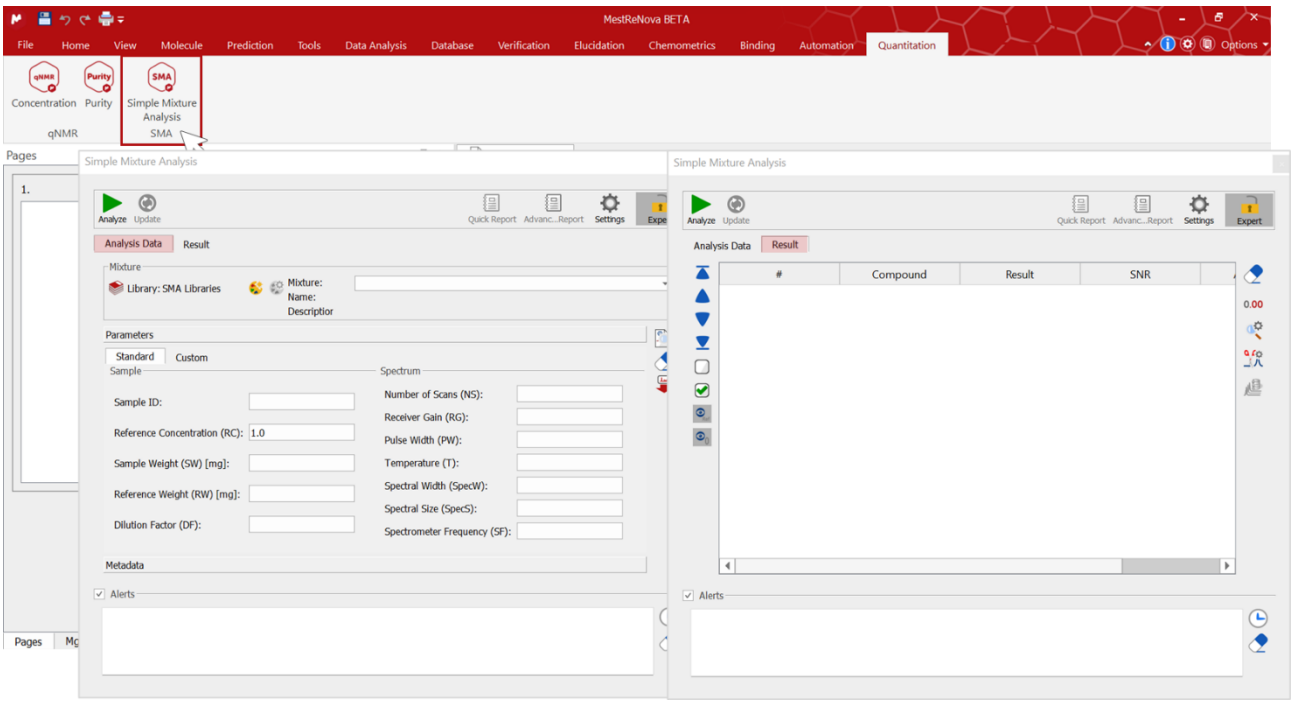
In this manual, we describe all the features provided by the Mnova SMA plugin.

2. SMA dialog

The SMA plugin is found under the **Quantitation** tab in the Mnova software's upper ribbon.

When opened, the SMA dialog presents the main buttons used to **Analyze** and **Update** results, generate **Quick Reports** and **Advanced Reports**, and configure the general analysis **Settings** at the top of the screen. Below, the two associated tabs are shown:

- The **Analysis Data** tab, where you will define the experiment to use, your sample and spectrum parameters, and certain other metadata related to the current analysis
- The **Results** tab, in which you will review your analysis results and receive appropriate alerts about errors (should they occur) and tests (when configured).



All the available action buttons are described below:

Simple Mixture Analysis dialog

Button	Description
Analyze	Analyze sample
Update	Update result
Settings	Configure SMA analysis settings
Quick Report	Create a quick report with result
Advanced Report	Create an advanced report with result
Expert	Lock Expert mode
Expert	Activate Expert mode

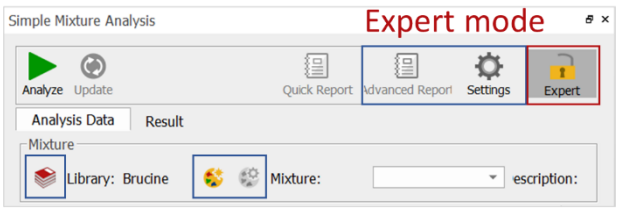
Analysis Data Tab

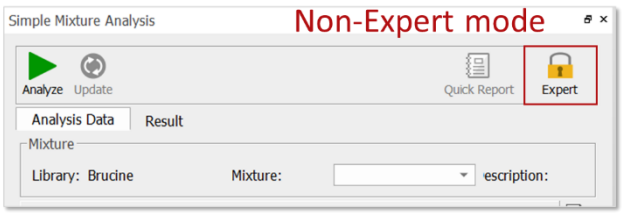
Button	Description
	Open Library manager
	Create a new mixture
	Edit mixture
	Read Sample´s parameters
	Clear parameters and metadata
	Load results saved in the active document
	Group alerts by time or compound
	Clear alerts
	Open custom parameters manager

Results Tab

Button	Description
	Zoom on first compound to view detailed result
	Zoom on previous compound
	Zoom on next compound
	Zoom on last compound
	Uncheck all displayed results
	Check all displayed results
Ref	Show/hide Reference results
0	Show/hide results with no valid multiplets
0.00	Change number of decimals
	Modify zoom factor on the spectrum
	Smart cuts of areas between the multiplets
	Stack compound spectra from DB

The **Expert** mode gives access to all of the SMA plugin's features. It allows expert chemists to set up an experiment's SOPs and define analysis settings. Locking the **Expert** mode will hide these functionalities, as can be seen in the image below.





3. SMA analysis setup

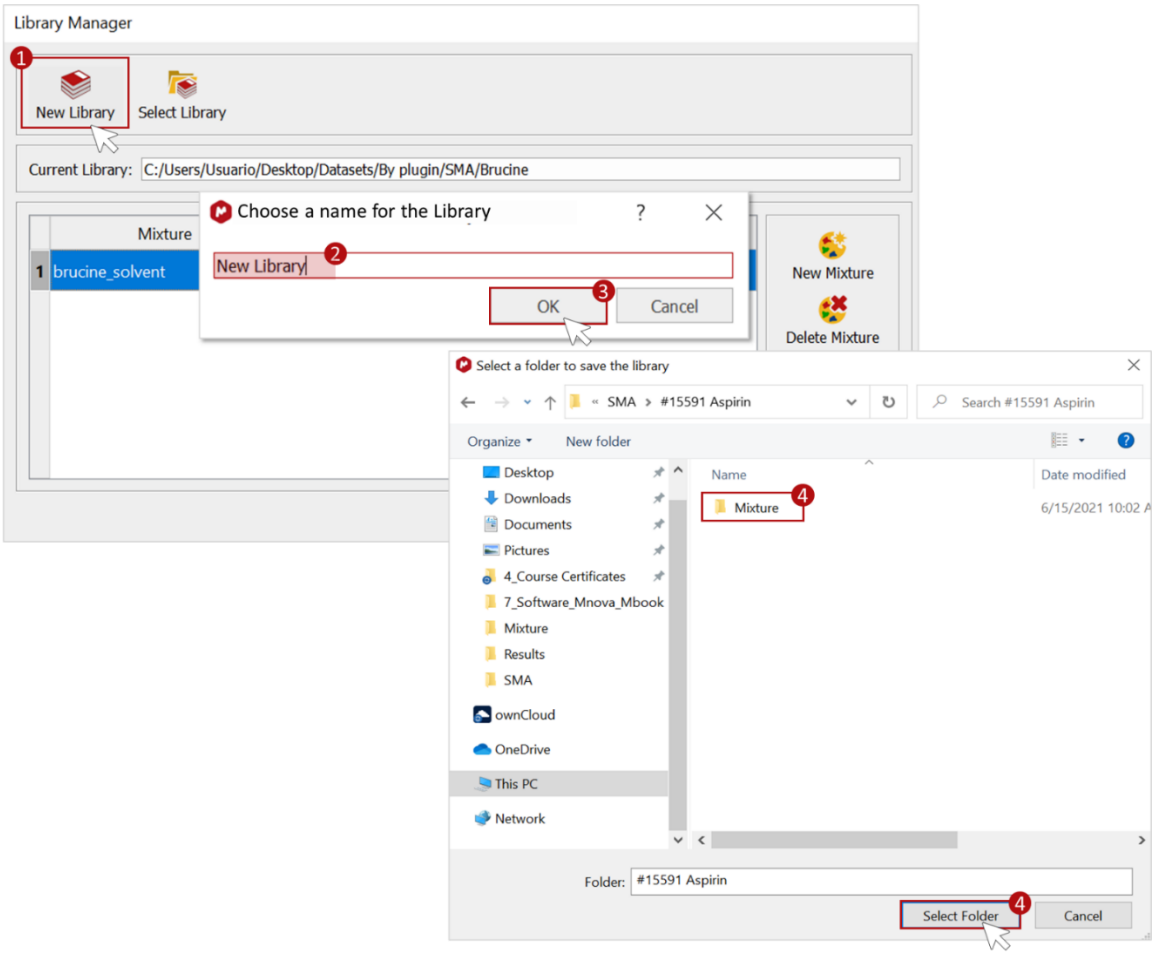
SMA analysis requires a valid mixture/experiment (".exp" file). Developed and validated methods can be stored in libraries for future use and can easily be shared with other users. It is possible to create an unlimited number of different experiments and save them to either pre-existing or new libraries.

3.1. Creating a new library

In the **Simple Mixture Analysis dialog**, click on  to open the **Library Manager**.

1. Click on **New Library**
2. Choose a name for the library
3. Click on **OK**
4. Select the folder in which you want to save the library
5. Hit **OK**

Your new library is created in the location specified.

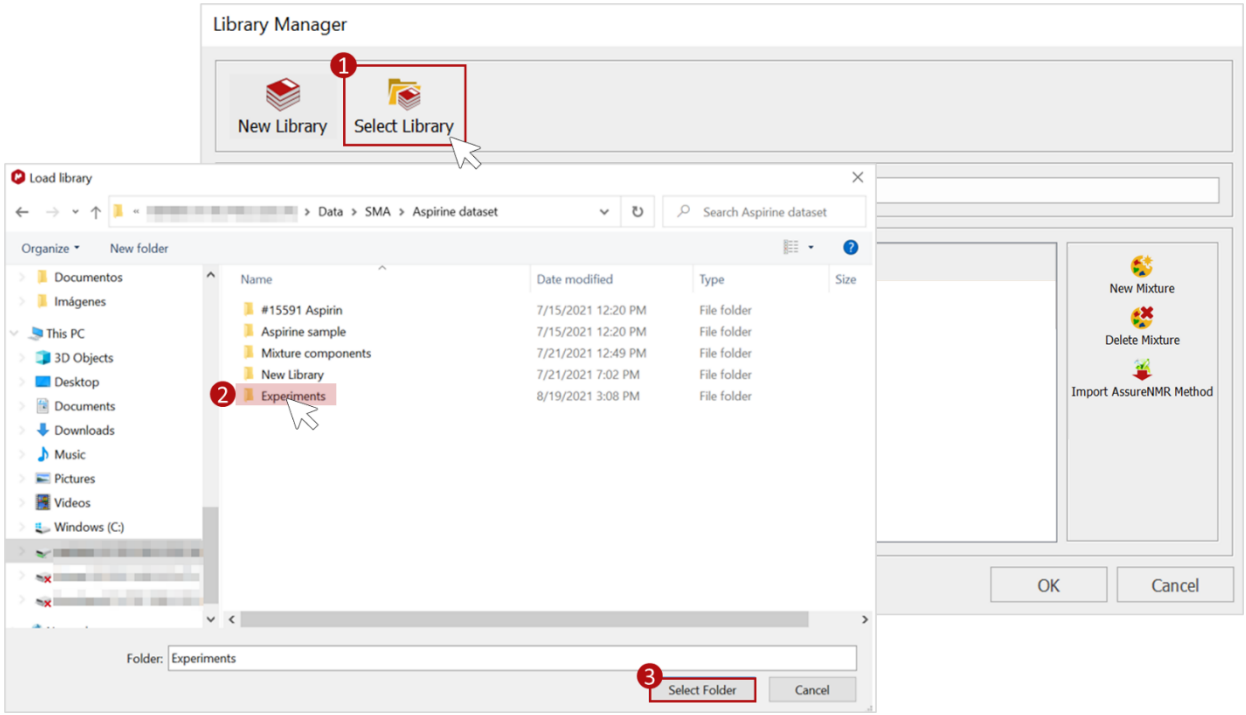


You can now click on **New Mixture**  to create a new experiment (refer to section 3.4).

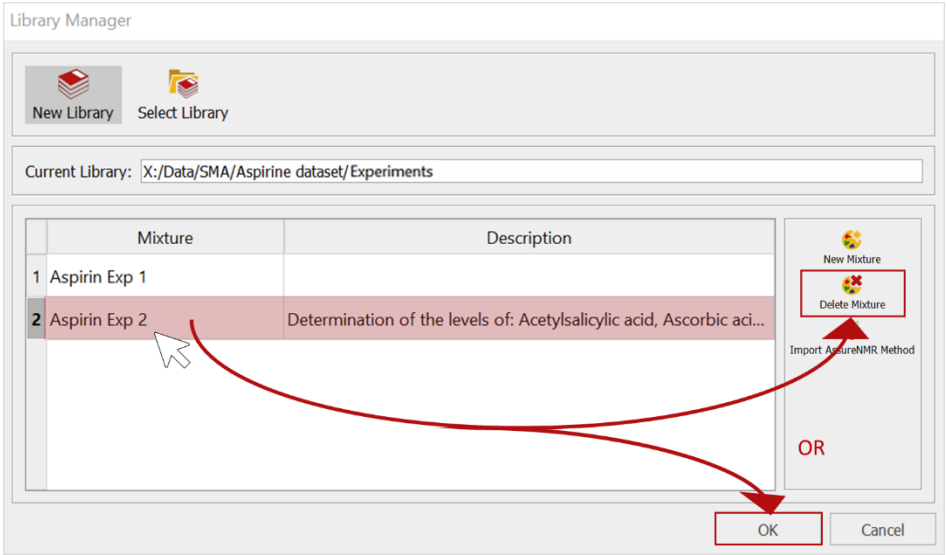
3.2.Selecting a previously created Library

In the **Simple Mixture Analysis** dialog, click on  to open the **Library Manager**.

1. Click on **Select Library**
2. Choose the location of the library you have already saved, or where you want to save your new experiment
3. **Select Folder**.



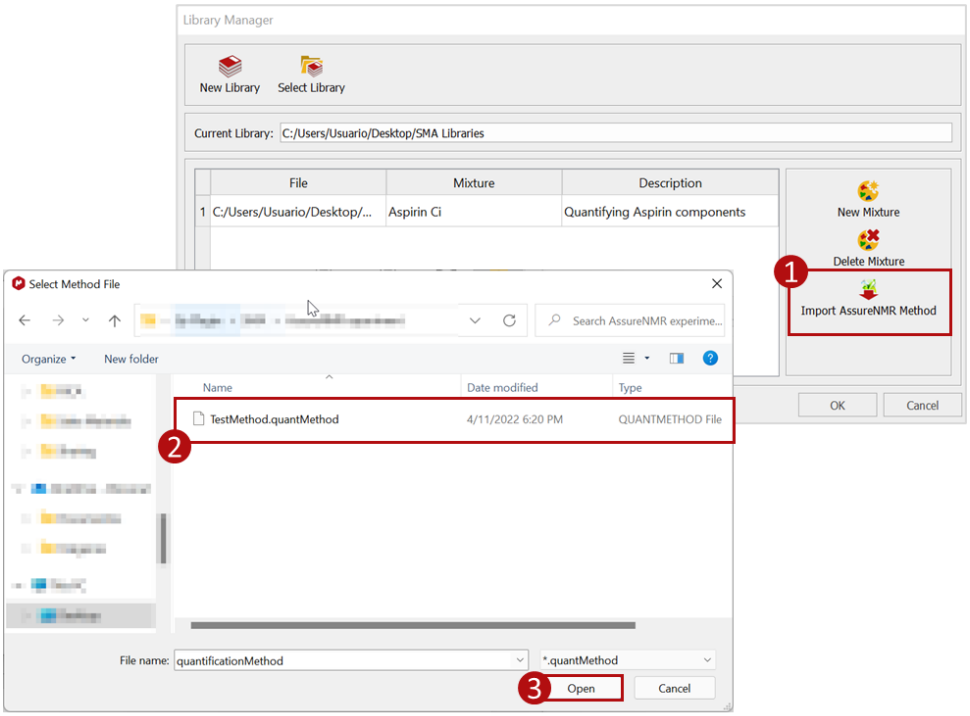
You can now select an experiment from the open library and hit **OK** to use it for your analysis, or even delete a previously added mixture by clicking on **Delete Mixture**.



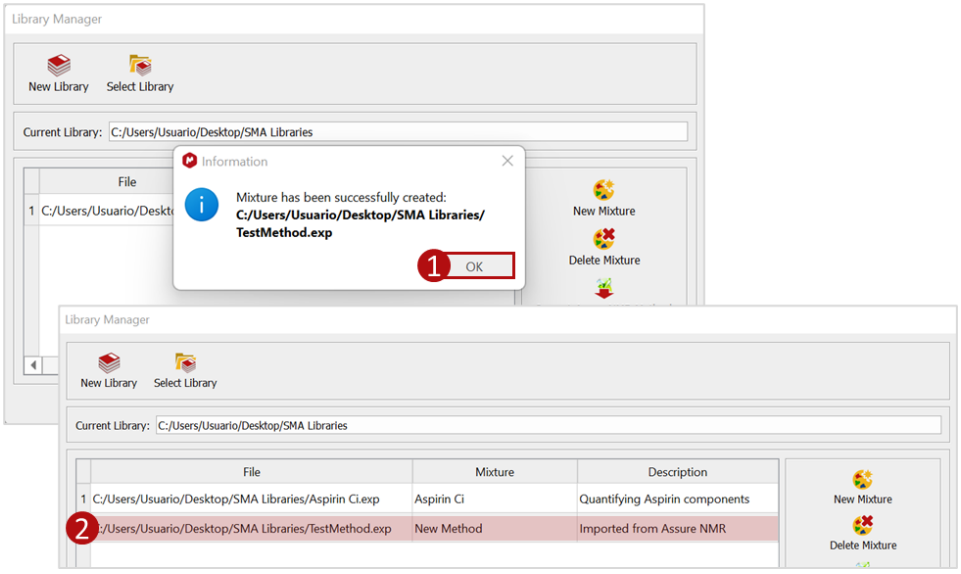
Otherwise, you can **Import an AssureNMR Method**, as explained in section 3.3, or create a **New Mixture** by following the steps described in section 3.4.

3.3.Importing an AssureNMR Method

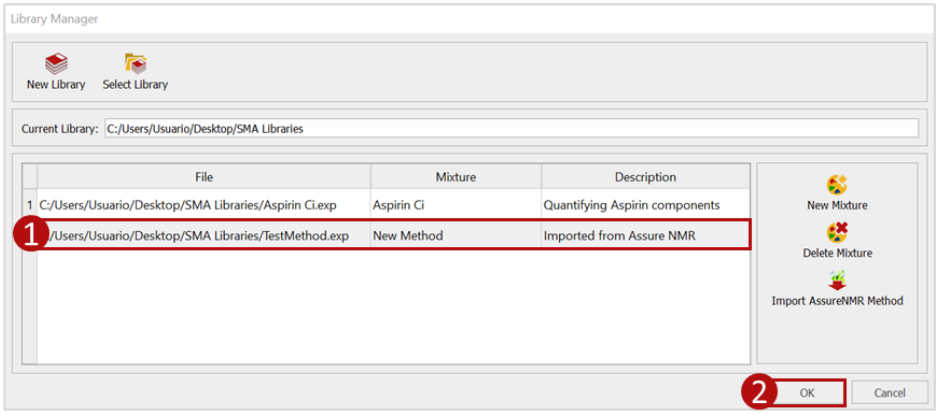
To import an AssureNMR method, press the **Import AssureNMR Method** button and select the "*.quantMethod" file from your directory. Click on **Open**.

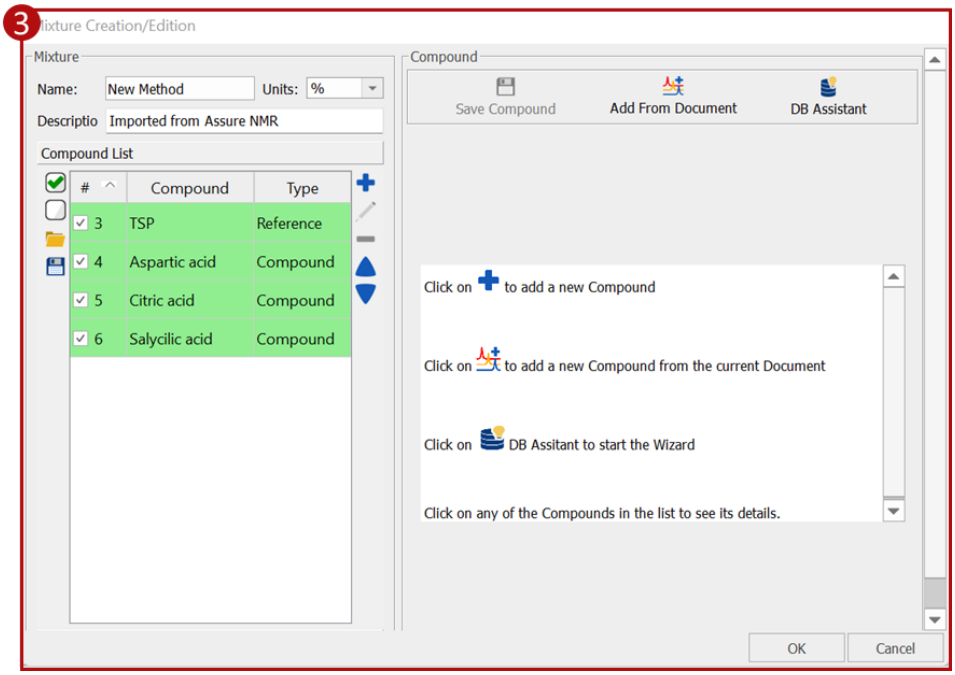


SMA will convert the AssureNMR Method into and ".exp" file that can be correctly read and run using Mnova SMA. A message will appear when the conversion is complete. Click on **OK**. The AssureNMR mixture will appear in the library table as seen below.



You can now select the mixture and press **OK** to open the **Mixture Creation/Edition** dialog and edit it, or to otherwise simply use it for your analysis.



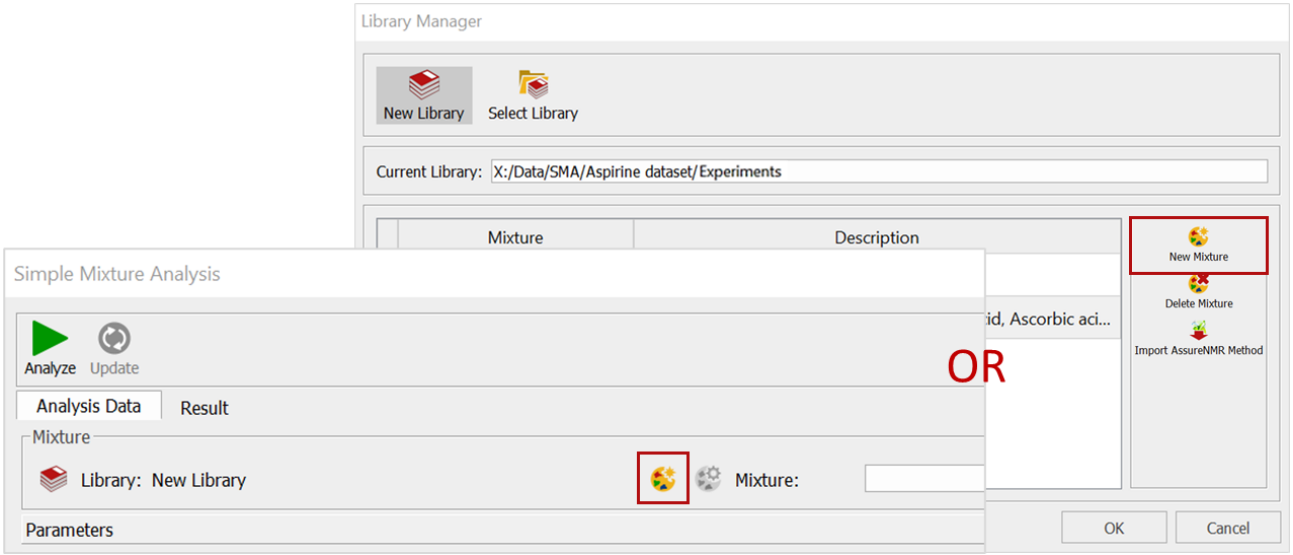


Notes about imported AssureNMR experiments:

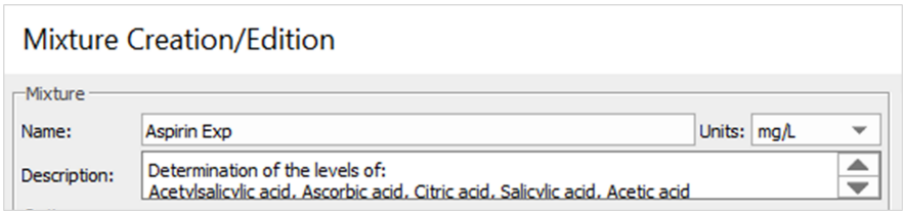
- The generated ".exp" file name matches the original AssureNMR method file name.
- The **Mixture** name is set to "New Method" and the **Description** to "Imported from Assure NMR".
- The **Calculations**, **PCA**, and **Processing** options are all unchecked by default.
- The "Std. Concentration Eq." is set as the default **Formula** for 1D NMR methods and generated automatically for each compound; for 2D methods, the default **Formula** would be the "User Eq" and must be manually entered by the user.
- The "Sum" integration method is set by default for all the compounds.

3.4. Creating a new mixture/experiments

To add a new mixture/experiment to your library, use the **New Mixture** button in the **Library Manager** or in the **Simple Mixture Analysis** panel.



The **Mixture Creation/Edition** dialog will open. Add a name and short description for your experiment.

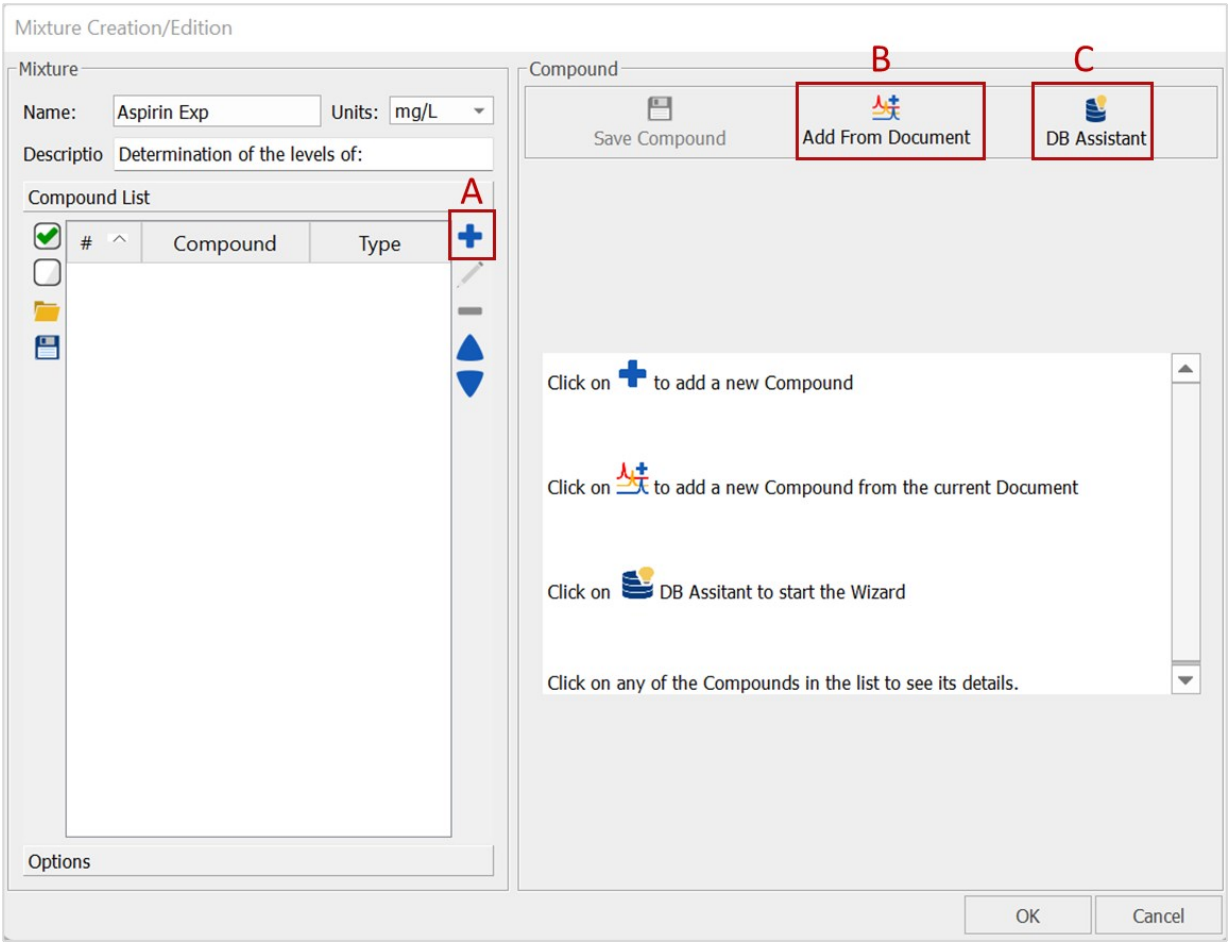


Mixture compounds can be added in one of three ways:

A. Manually, by entering compound details piecemeal

B. Automatically, from an open Mnova document

C. Using the DB assistant

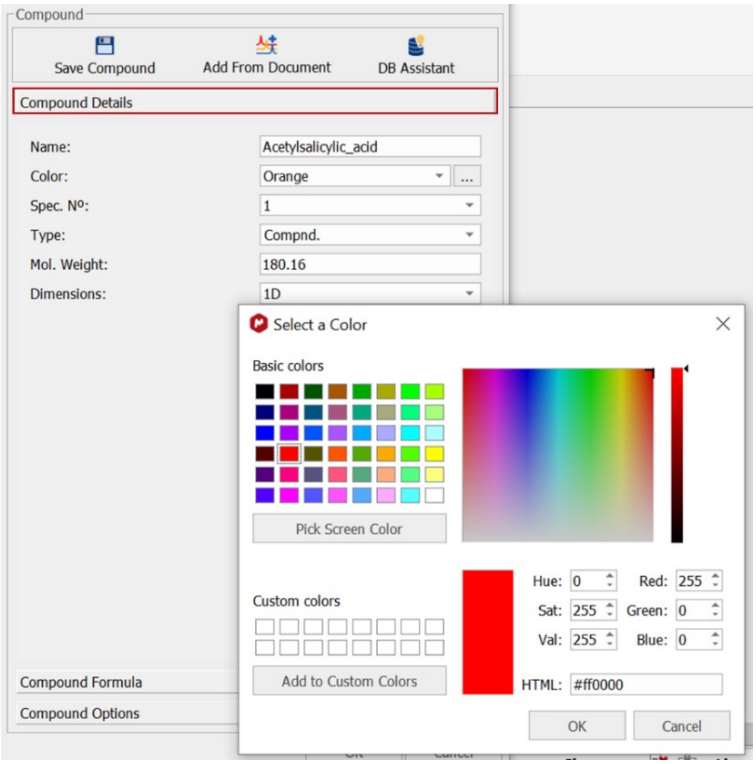


A. Manual addition of mixture compounds

Click on the  button to add a new compound, then fill in the compound's information.

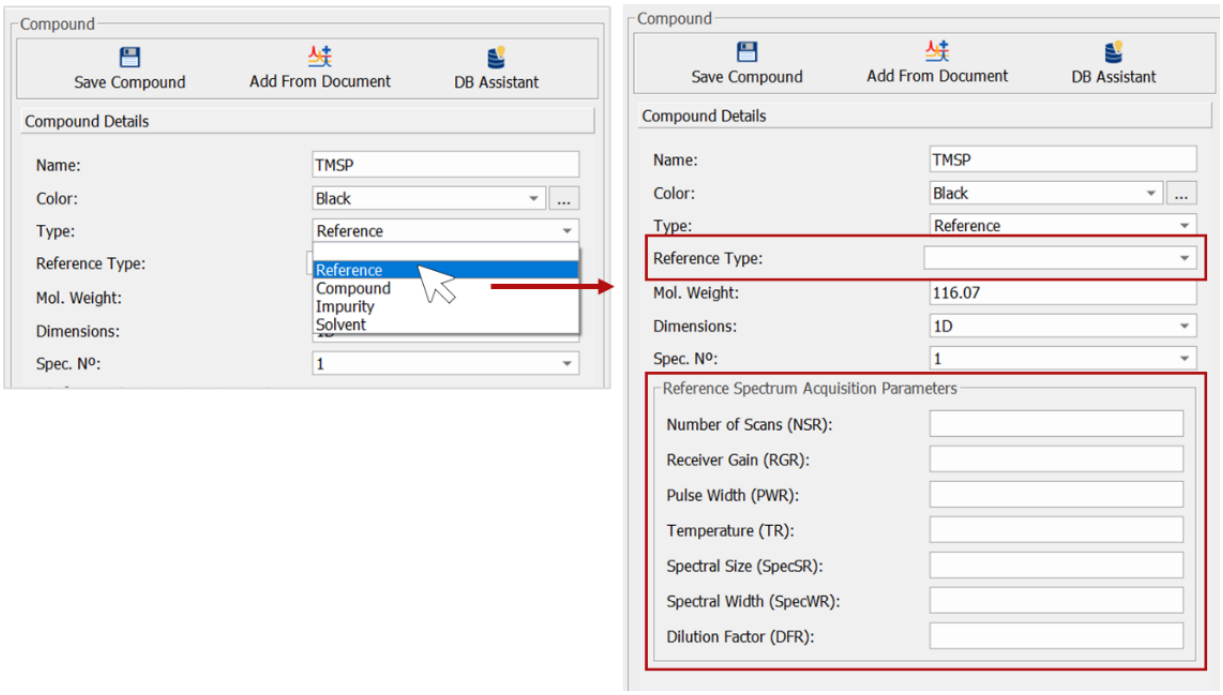
A.1. Compound details

In the **Compound details** section, enter the compound **Name**, **Type** (Reference, Compound, Impurity, or solvent), **Molecular weight**, and NMR **dimension**. Then, choose a **Color** from the available color palette to use in the display of the results.

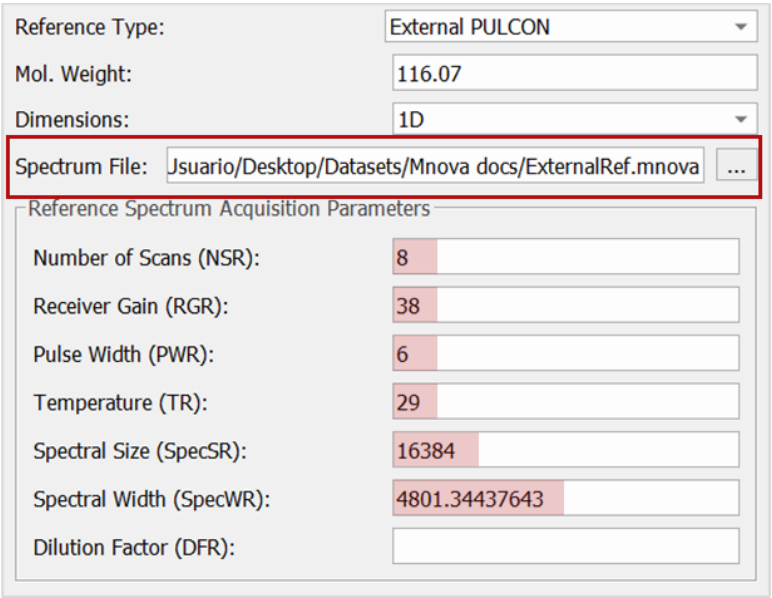


When adding a **Reference** to a mixture, a new bloc of fields appears to allow you to choose the **Reference type** and fill in the **Reference Spectrum Acquisition Parameters**.

When using an **Internal Reference**, these parameter fields can be completed manually.



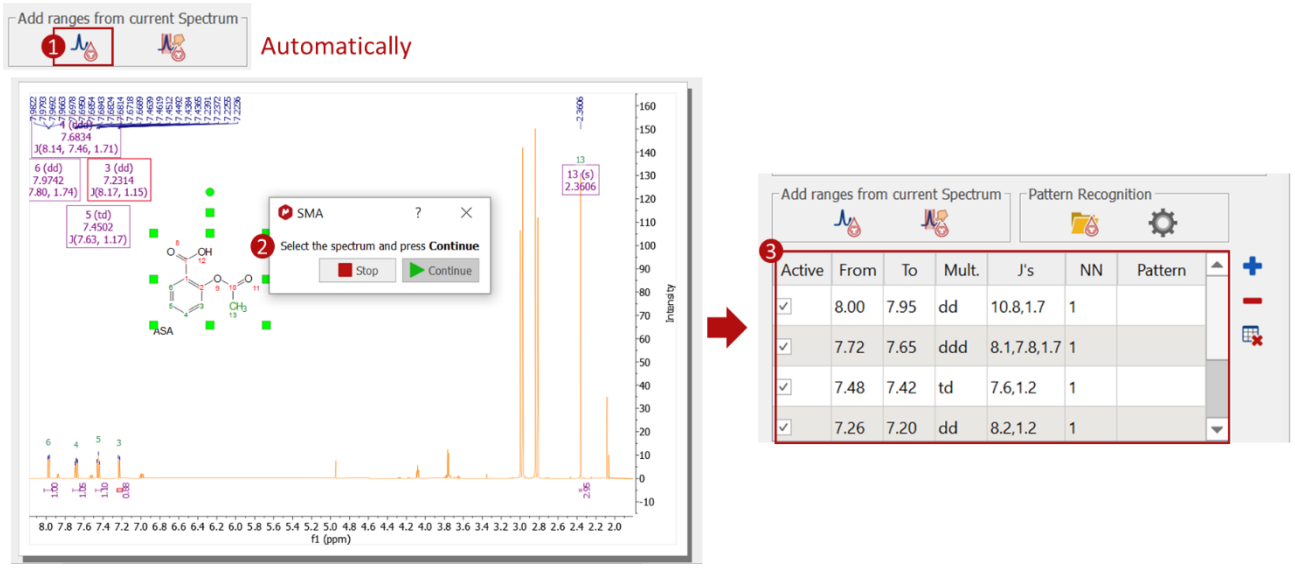
When using an **External PULCON** reference, you must define the path in which your reference spectrum can be found. The **Reference Spectrum Acquisition Parameters** are then automatically completed with the information available in the spectrum file.

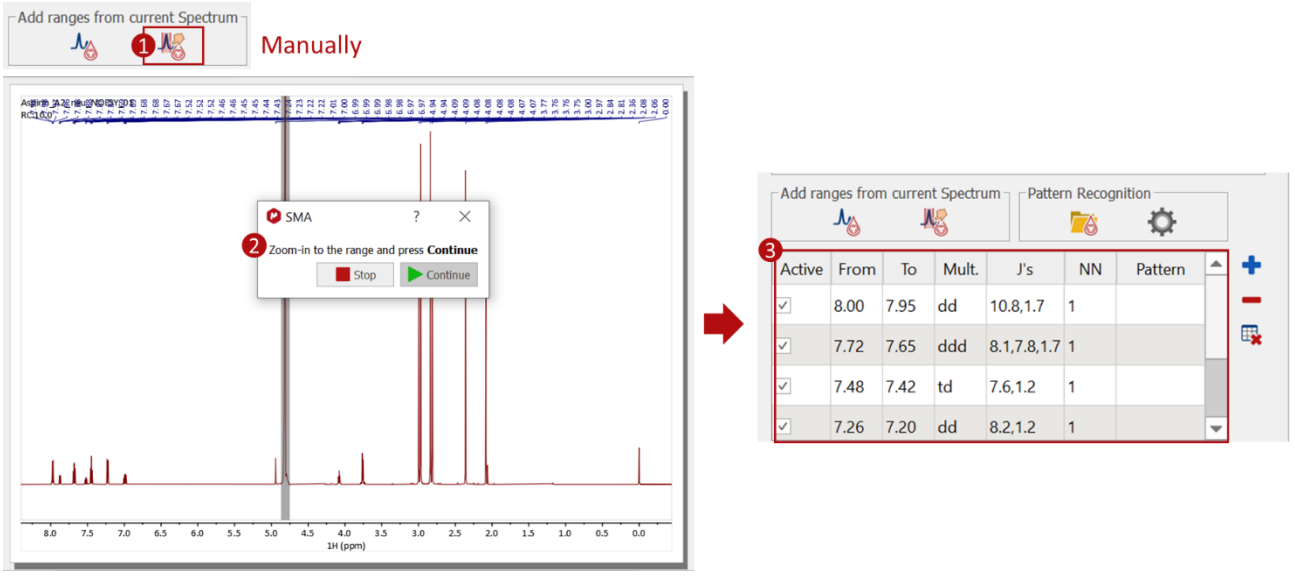


When using an **External Bruker PULCON automatic** reference, the **Reference Spectrum Acquisition Parameters** are automatically parsed from the eretic file.

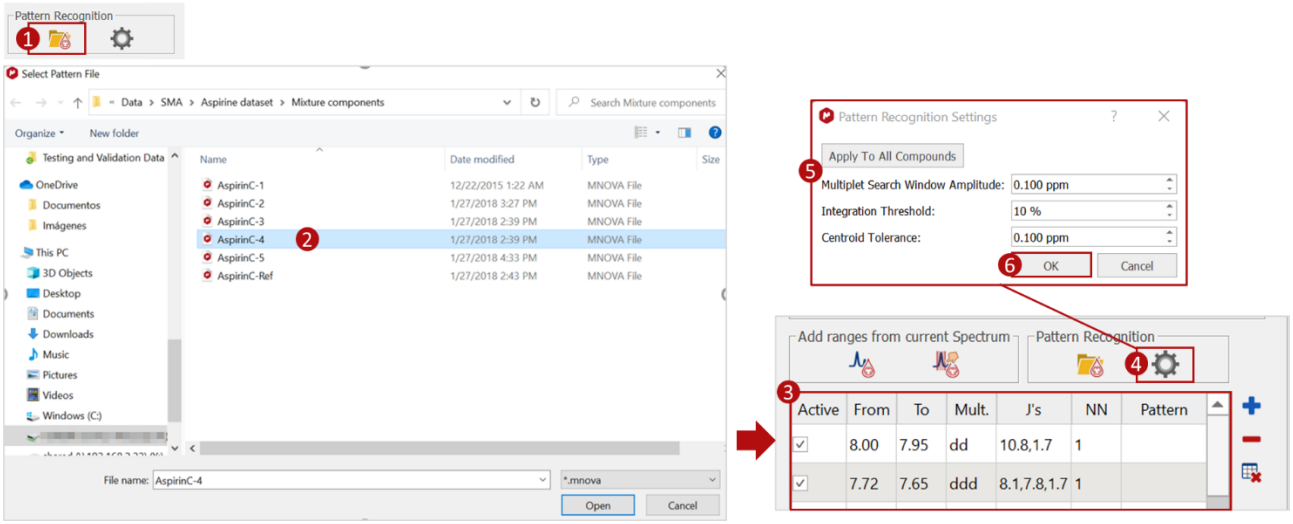
A.2. Compound formula

In the **Compound Formula** section, you should add your compound's multiplet(s) chemical shift range(s) and the Number of Nuclides (NN) required for the calculation. These ranges can either be added manually or imported from an active spectrum or a document. Follow the steps in the images below in each case.





Another possibility is to run a **Peak Pattern Recognition** to find a multiplet pattern in your 1D spectrum when peaks overlap. In this case, a spectrum of the pure compound and a set of parameters must be provided to be used as a reference for the Pattern Recognition.



The **Pattern Recognition Settings** include:

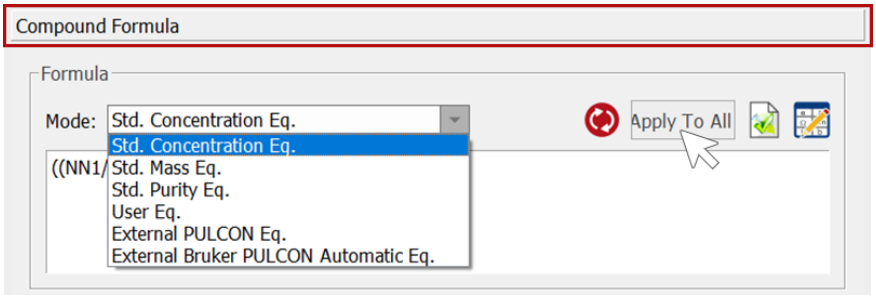
- The **Multiplet Search Window Amplitude:** to determine the amplitude, in ppm, of the peak search window for the mixture multiplet. The search window will be the range of the Pattern Multiplet extended by the amplitude: (from_pattern+amplitude, to_pattern-amplitude). For example, the search window for the first multiplet in the example above, where amplitude is set to 0.1000 ppm, would be [8.022 + 0.1, 7.935 – 0.1].

- **The Integration Threshold:** to define the limiting percentage of the total area of the peaks within a scale of search window.

- **The Centroid Tolerance:** to determine the distance between the centroid of the reference pattern multiplet and the multiplet to be considered by the tool. The higher the tolerance, the greater the number of matches that might occur.

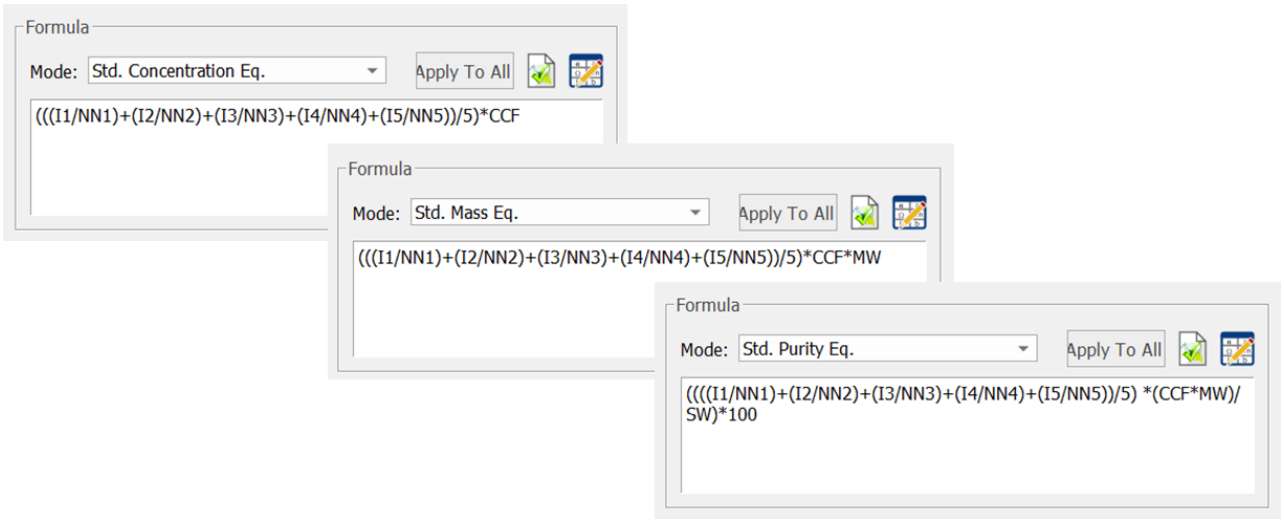
Once you have configured these parameters, you can apply them to all the compounds in the mixture.

Next, you must determine the equation to use for quantification. You can either choose one of the three hard-coded formulae available for Concentration, Mass % and Purity, add your own formula, or select an External PULCON equation to be applied. In any case, by clicking **Apply to all** you can apply the formula you choose to all the mixture components. Otherwise, you must add a formula for each compound separately.



A.2.1. Std. Concentration, Std. Mass, or Std. Purity equations

When applying one of the hard-coded concentration, mass, or purity formulae, the equation is automatically generated with the multiplets and retrieved spectrum parameters, as shown below.

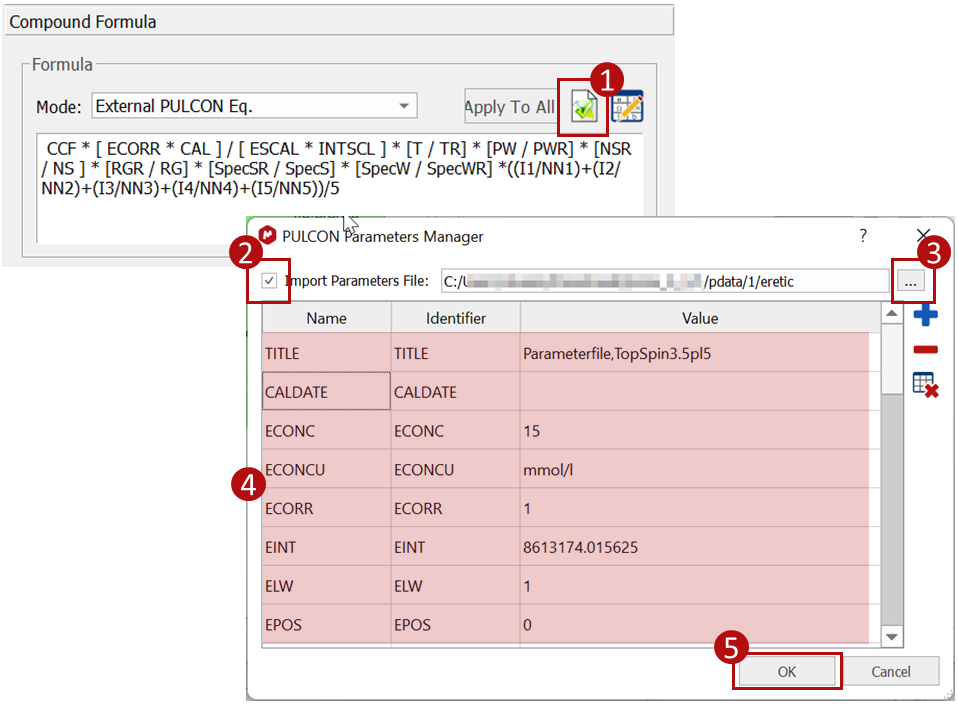


A.2.2. External PULCON equation

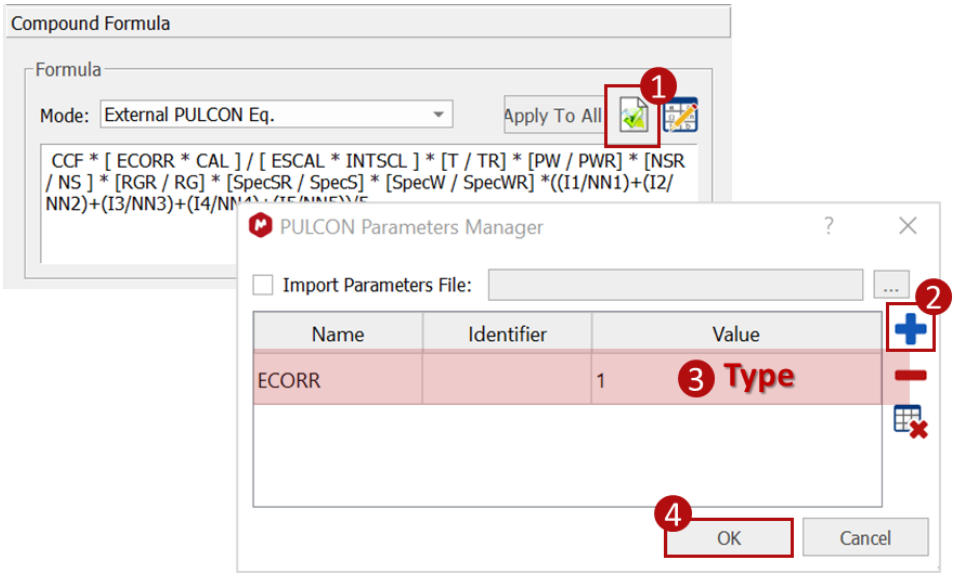
When using an **External PULCON equation** for quantitation, PULCON parameters must be provided (via an "eretic" file or manually) to correctly apply the equation.

Click on this button  to open the **PULCON Parameters Manager**:

- Enable and import the "eretic" file included in the raw data folder. The parameters are retrieved and displayed in the table, as seen in the image below.



– Otherwise, press the **Add** button and type the parameters **Name** and **Value** manually.



You can remove parameters from this table using the **Remove** button.

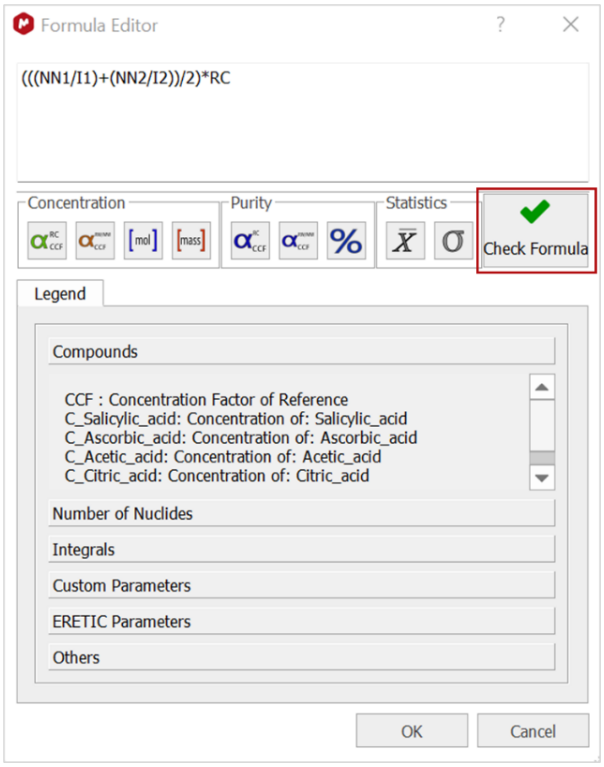
Click **OK** to save your changes. The **External PULCON equation** is now correctly defined.

A.2.3. External Bruker PULCON automatic equation

When using an **External Bruker PULCON automatic equation** for quantitation, PULCON parameters are automatically read from the raw data files and no further configuration is needed.

A.2.4. User equation

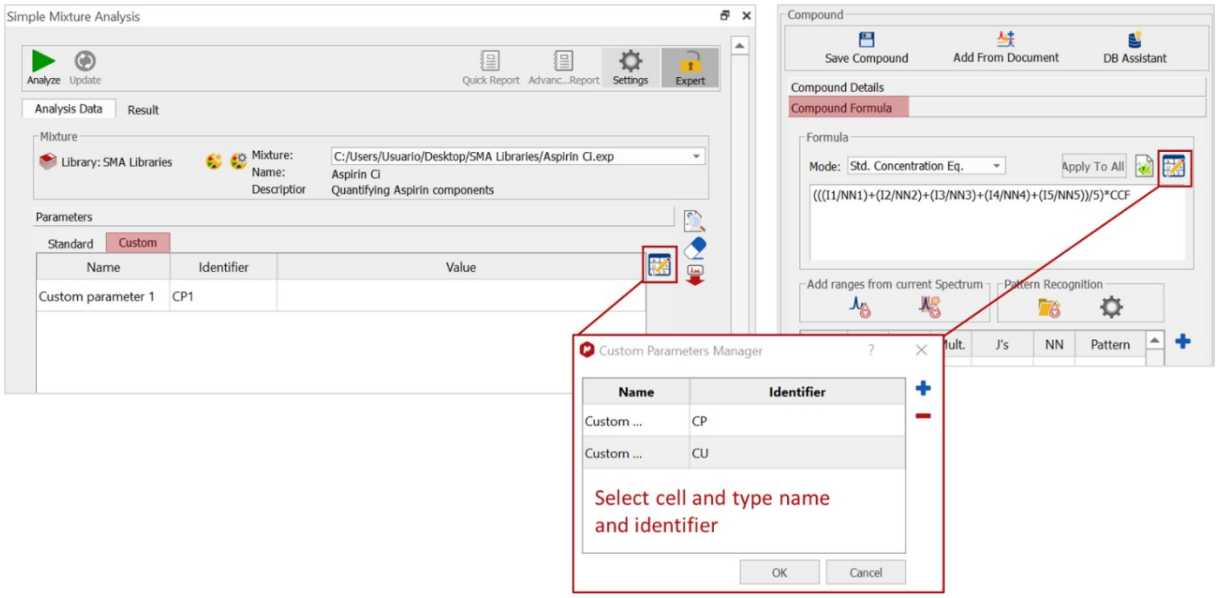
To add your own formula, choose the **User Equation** mode; the **Formula Editor** will open. Use the available buttons to type and check your formula for errors. You can read more about the formula editor in our associated blog post.



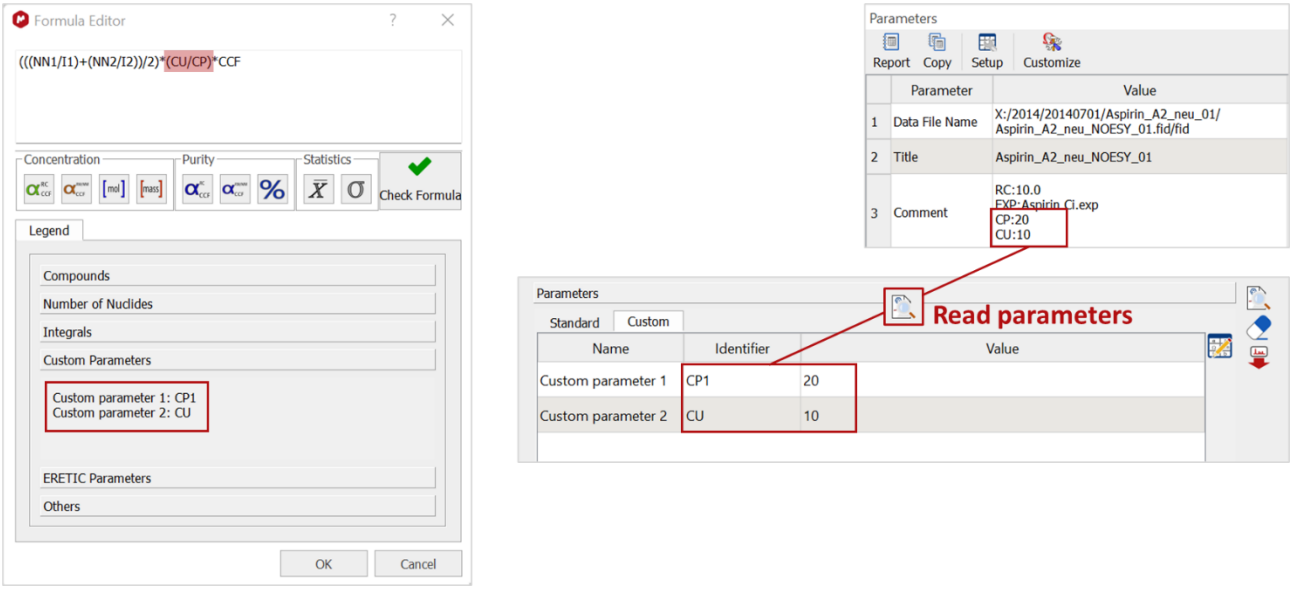
Note that you can also define custom or PULCON parameters to be used in the equation for the concentration calculation.

Custom Parameters

Defining custom parameters can either be achieved from the **SMA** main dialog in the **Custom** tab, or from the **Mixture Creation/Edition** tab in the **Compound Formula** section. Click on this button,  , to open the **Custom Parameters Manager**, then on  to add a new row in the table. Select the cell and type a name and an identifier (a nomenclature to use in the formula) for your custom parameter, then click **OK**.

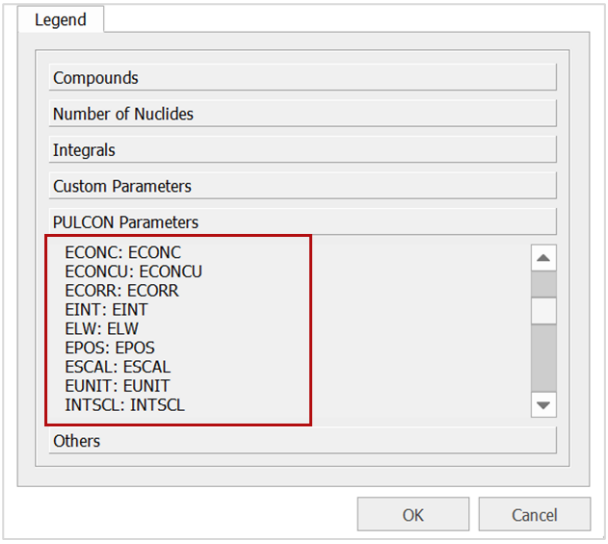


The custom parameters are now added to the **Custom** table and to the **Formula editor** and can be used in the equation. **Values** for custom parameters can be added manually or read from the **Parameters** table of the sample, as shown in the image below.



PUCLON Parameters

How one defines PULCON parameters is described above. The PULCON parameters are added to the **Formula editor**, as seen in the image below, and can be used to complete the user custom equation.

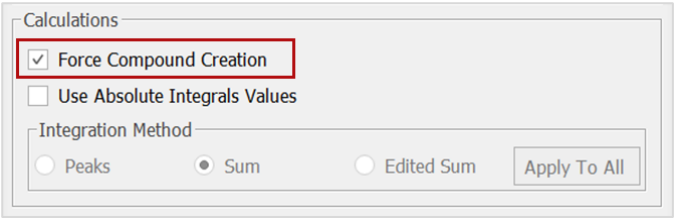


A.3. Compound options

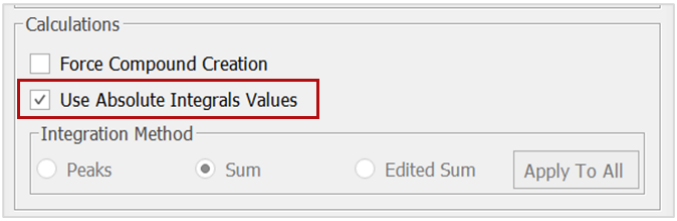
In this section, you can configure the following calculations and analysis options:

- **Not Show in results:** if checked, the results of the analysis will not be displayed in the **Results** tab. This is particularly useful when you want to use the integrals of a certain *compound A* to calculate the concentration of another *compound B* of the mixture, but you are not interested in the quantification of *compound A* itself.

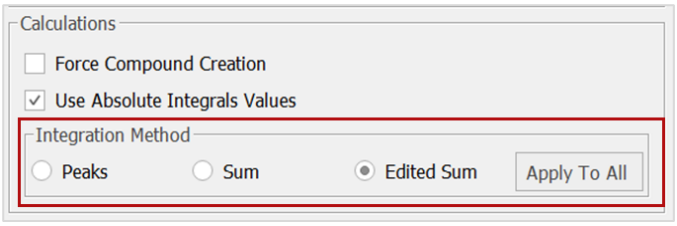
- **Force compound creation:** if checked, a compound will be created, even if no peaks were found in the defined ranges. This "fake" compound will be visible in the results table, and alert messages about the creation of peaks will be displayed so that you can review the spectrum and fix the problem manually.



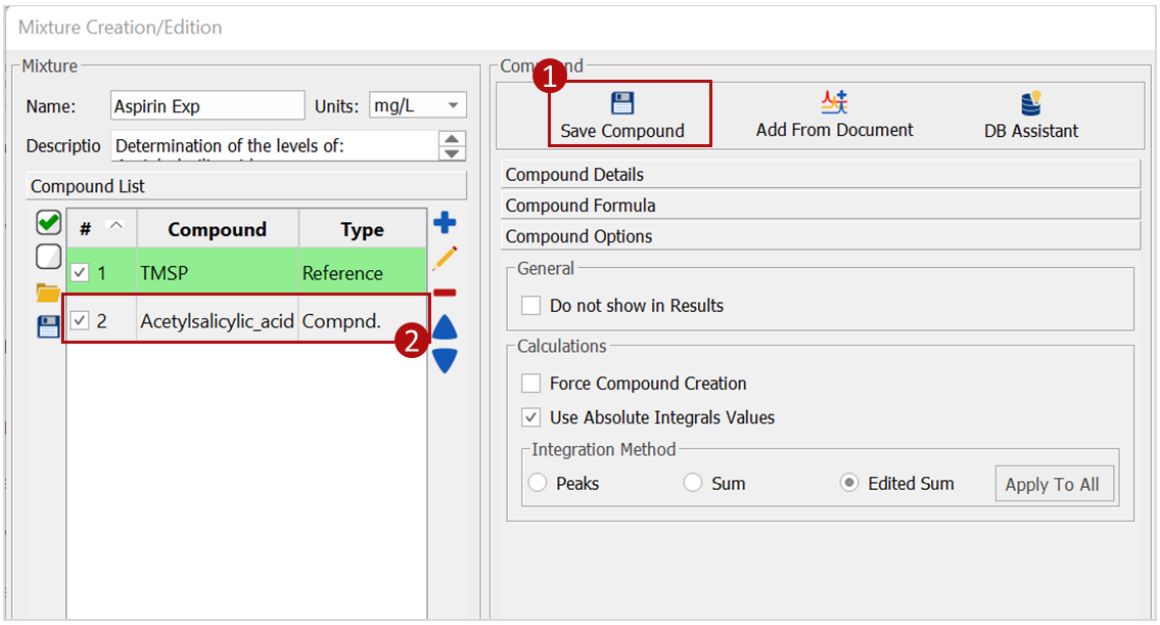
- Enable/disable the **Use of absolute values** for integrals.



- **Integration method:** choose the integration method and apply it to all compounds, if needed.

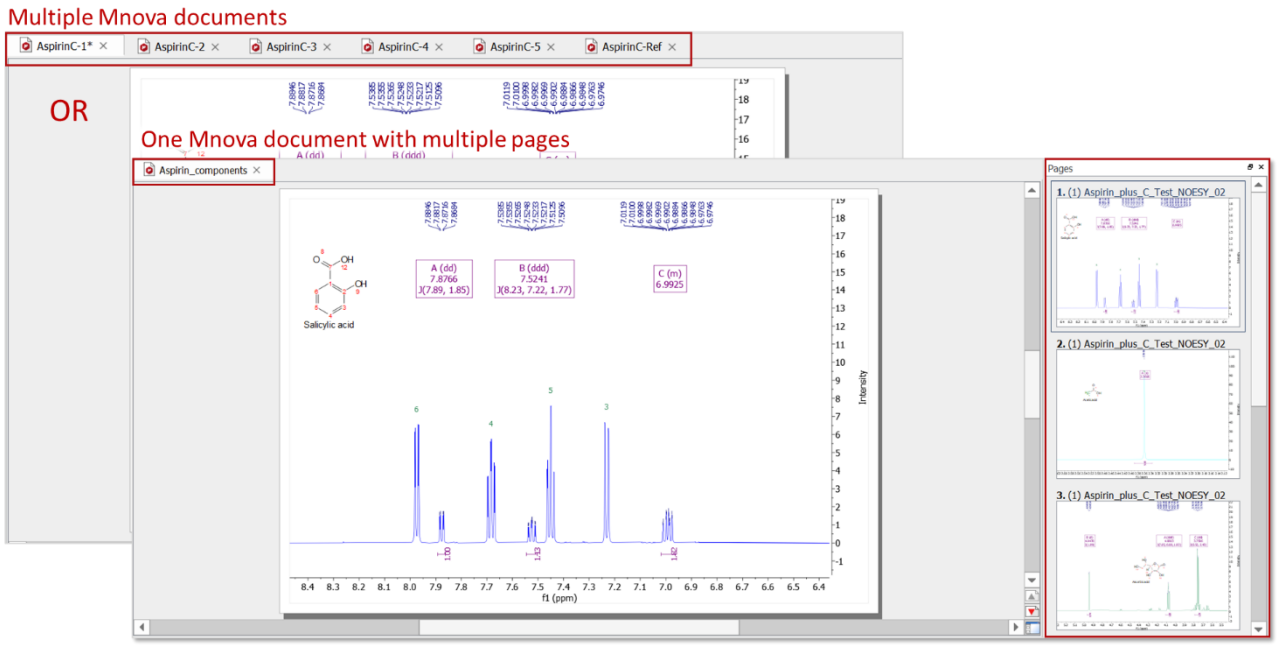


- Once all the required information is entered, press this button, , to save the compound to the **Compound List**, as shown below.

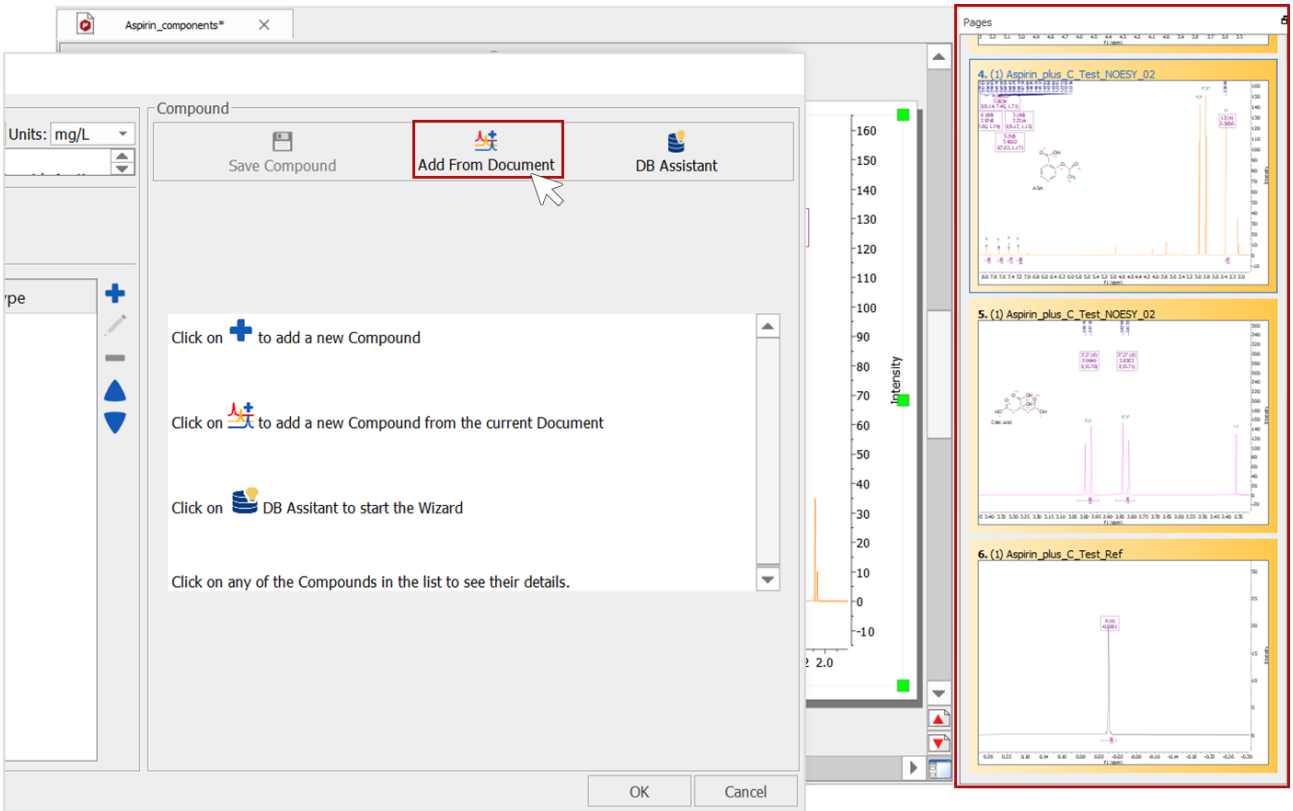


B. Adding mixture compounds from an Mnova document

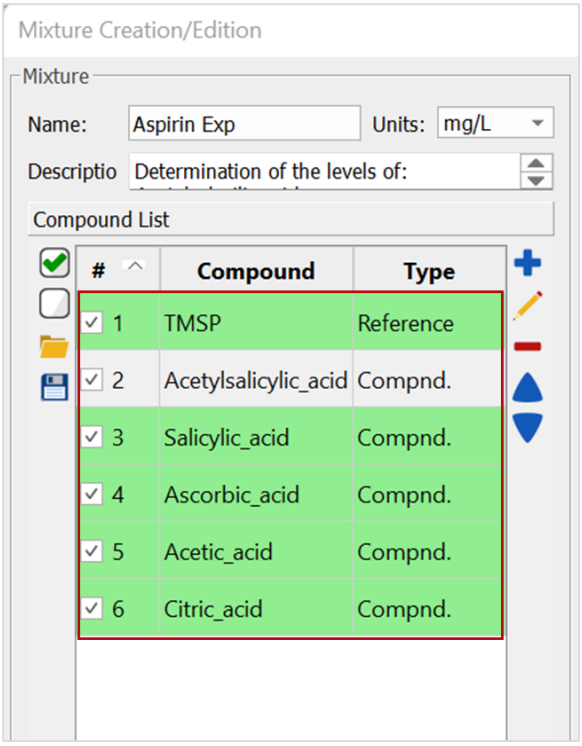
Open your mixture component files in Mnova. You can either have them saved in separate files or grouped on several pages in a single Mnova file.



Select the Mnova document or Mnova document pages with the compounds you wish to add, then click on  to import the compound's details into the **SMA Mixture Creation/Edition** panel.



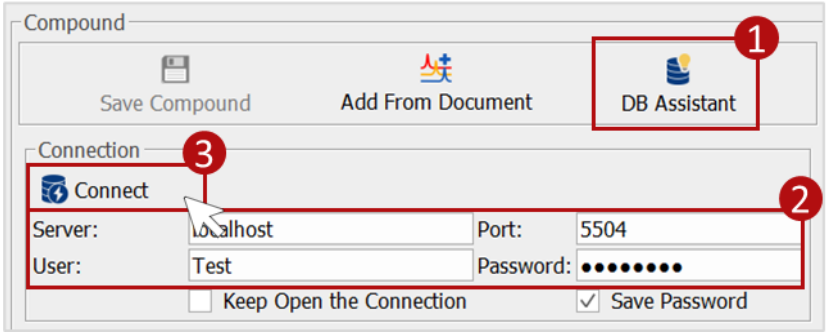
The added compounds will appear in the **Compound List**, as shown below.



You can now select any compound from the list and **Edit** its details, as detailed in sections A.1.-A.3.

C. Using the DB assistant to add mixture compounds

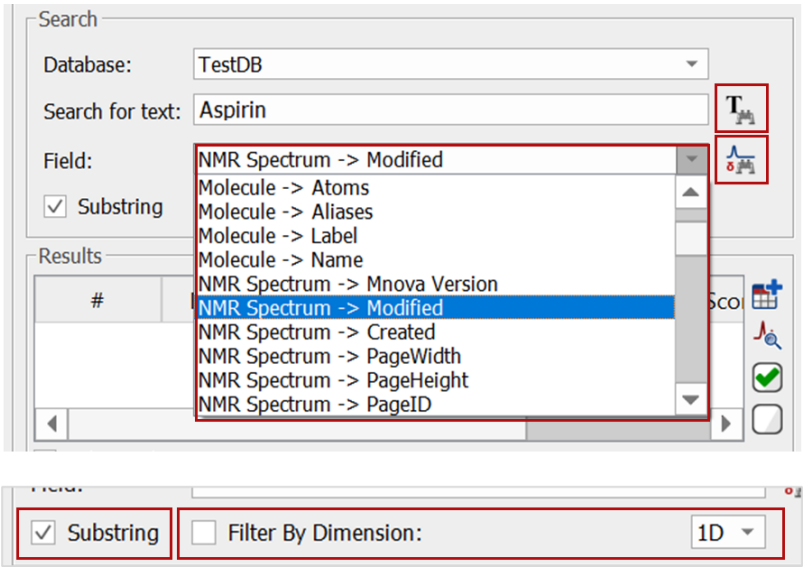
Launch the **DB assistant** by clicking on . Enter the server connection details, then click on **Connect**.



Check the **Keep Open the connection** or the **Save Password** options, if needed.

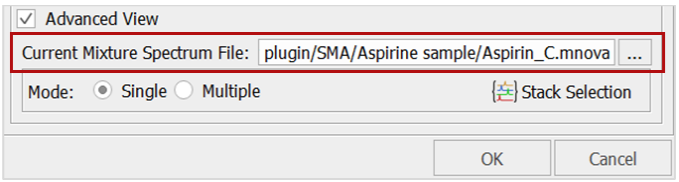
Choose the DB you want to search, then type the text and click on to search. You can also search your database by multiplets/peaks. To do so, open a spectrum in Mnova, then click on the button.

A search can be performed for a specific database field and/or by substrings. Results can be filtered by dimension (1D or 2D).



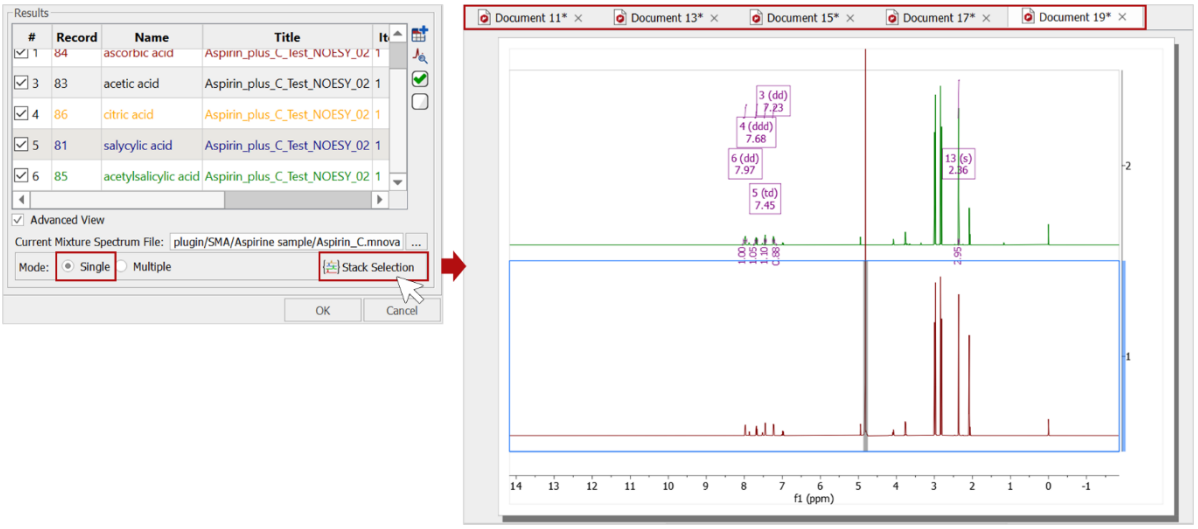
The search hits will appear in the **Results** section. You can double click on a database record to open and view it, or you can select more than one record and click on the zoom button to open them all at once.

To help you select the hit spectrum that best fits your analysis, you can stack database hits with the analyte spectrum (open with Mnova or select in the **Current Mixture Spectrum File** box).

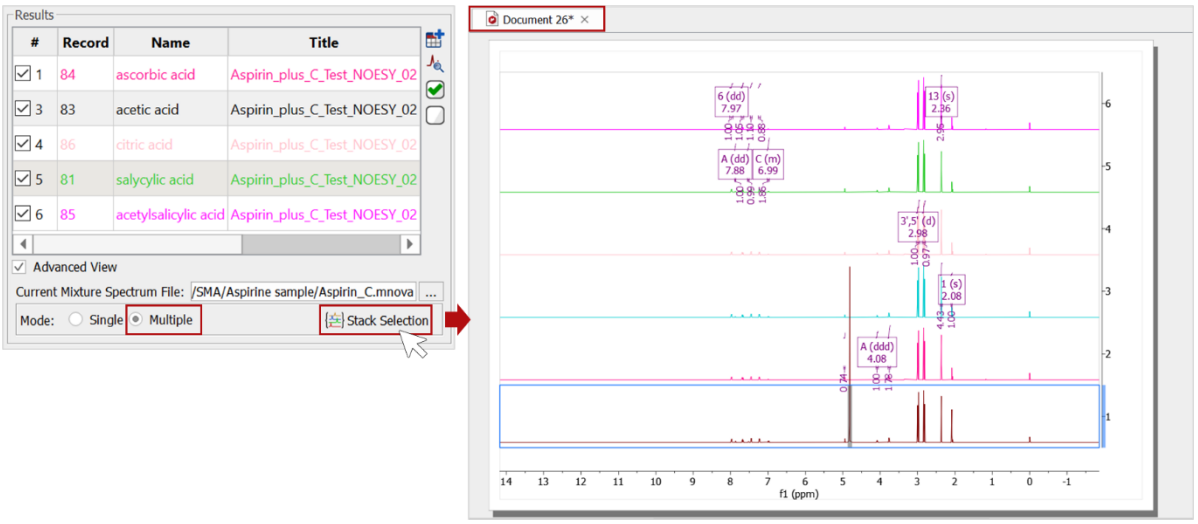


This option is available in the **Advanced View** panel (hidden by default) and offers two stacking modes:

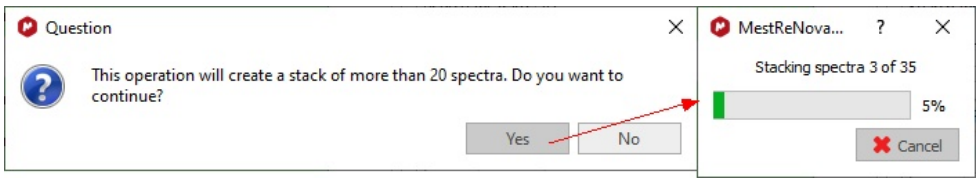
- The **Single** mode: stacks spectra one by one with the base analyte spectrum. A new Mnova document is generated with the stacked spectra for every selected record.



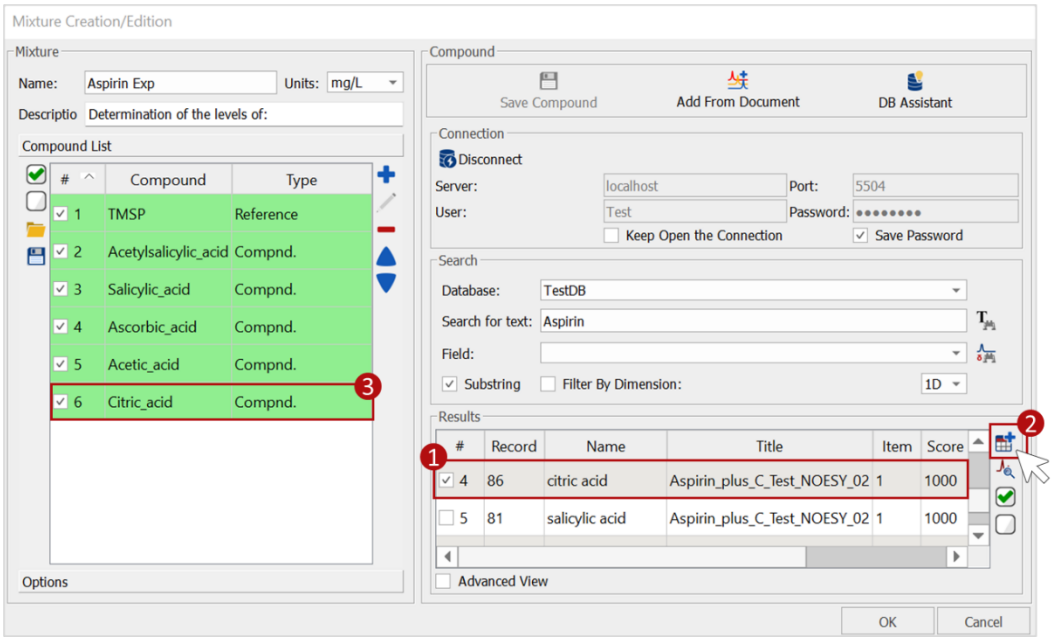
- The **Multiple** mode: stacks all spectra together.



Note that when attempting to stack more than 20 items, a warning message is displayed indicating that the stack will contain more than 20 spectra.

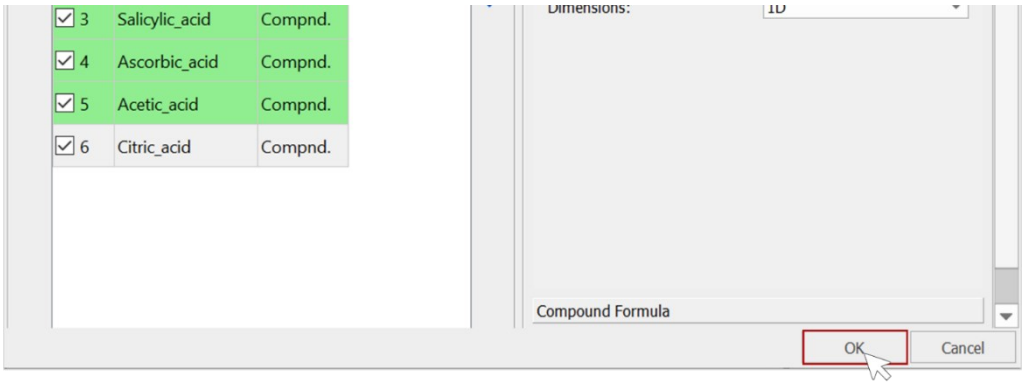


Now select the compound(s) you want to add to your mixture and click on  to add it (them) to the **Compound List**.



You can select any compound from the list and **Edit**  its details, as detailed in sections A.1.-A.3.

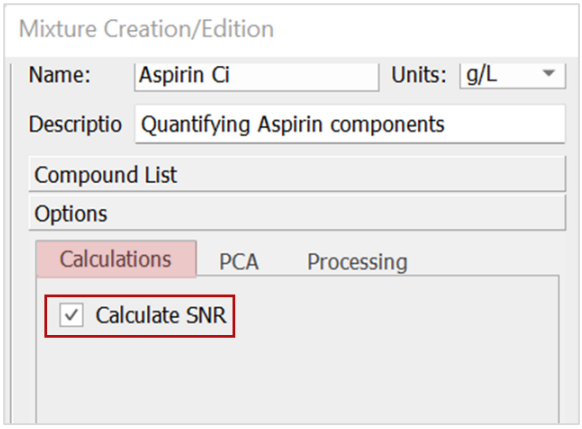
Once all your mixture compounds are added, you can save your mixture/experiment by clicking **OK**.



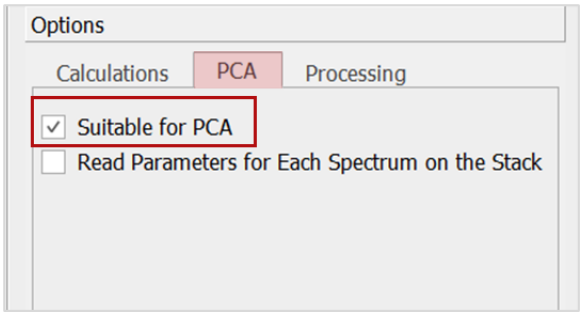
3.5. Configuring experiment options

In the **Calculations** tab, you can enable the option to **Calculate SNR**. When enabled, the SNR value will be calculated and included in the results table.

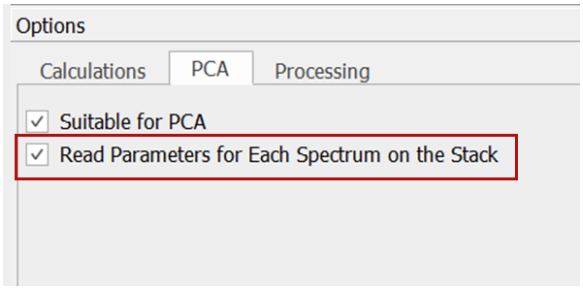
Note that SNR will only be calculated for 1D spectra

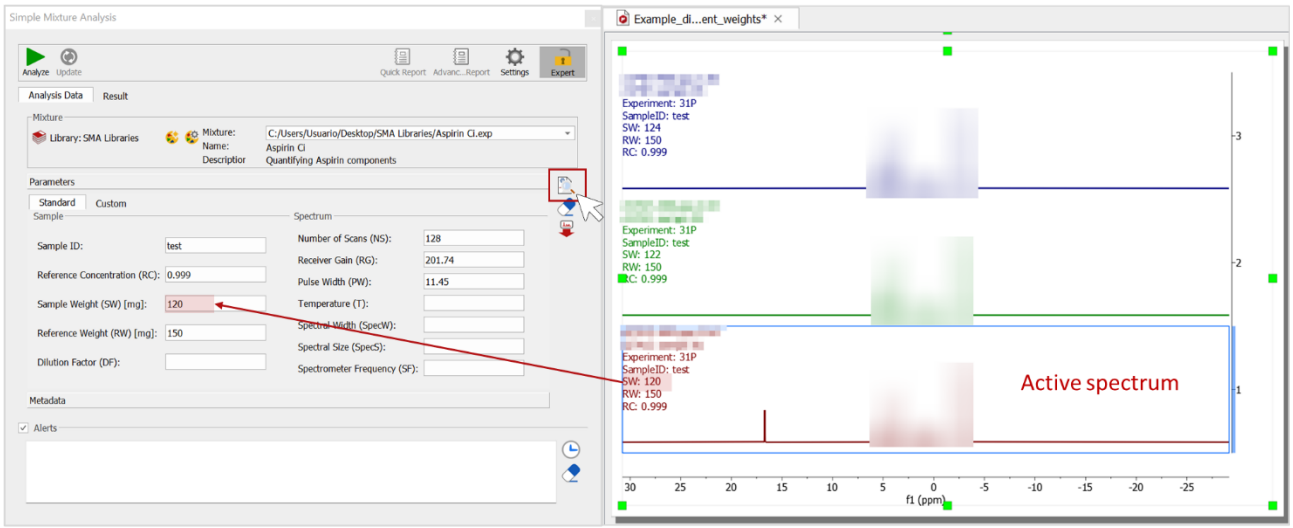


In the **PCA** tab, check the **Suitable for PCA** option if you want to retrieve the SMA results in a format suitable for a subsequent **principal component analysis** (PCA).

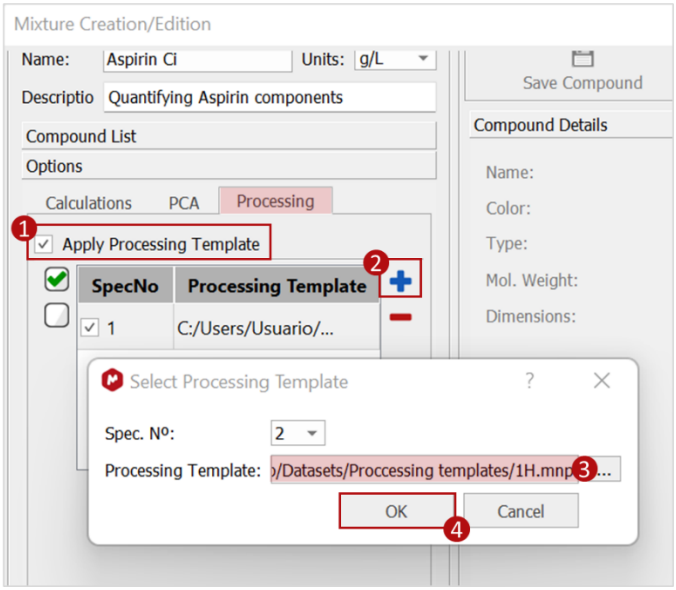


When performing a PCA analysis with a stack of spectra, the option to **Read parameters for each spectrum on the stack** is also available. If enabled, SMA will update the parameters for each spectrum calculation from the comments field in the parameters table of the sample. The updated parameters can include the Reference Weight (RW), Sample Weight (SW), Reference Concentration (RC), Dilution Factor (DF), Number of Scans (NS), Pulse Width (PW), and Receiver Gain (RG).

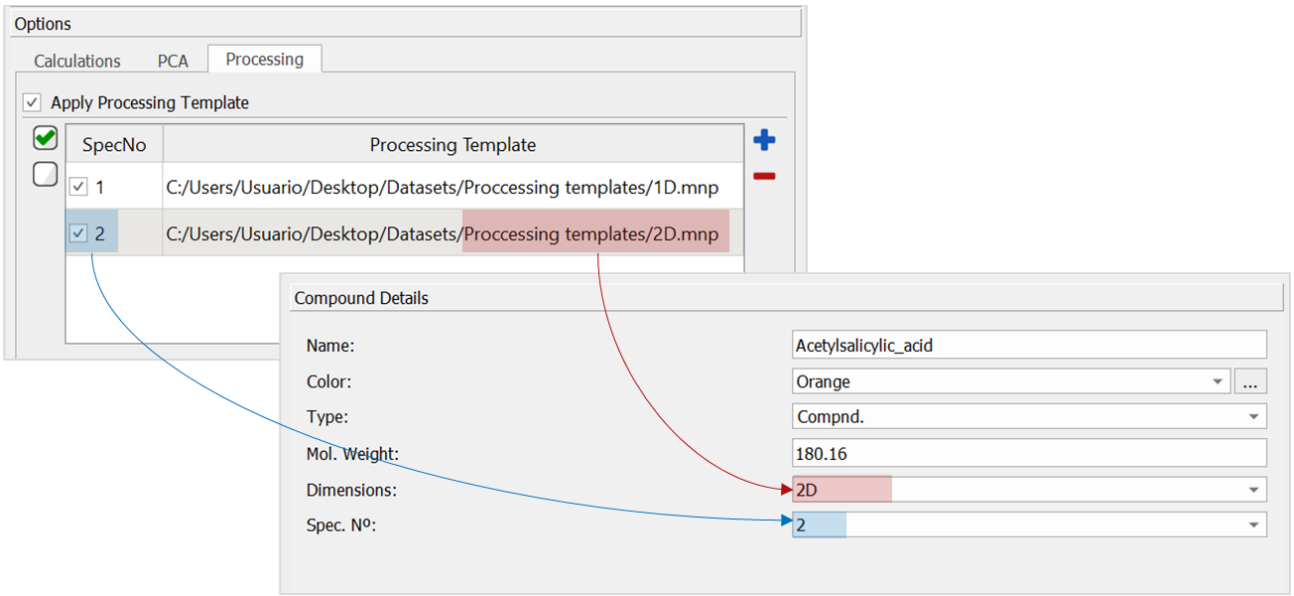




In the **Processing** tab, check the option **Apply a Processing Template** if you wish to add one or more processing templates for use in the current experiment. When you click on the blue cross button,  , a new dialog will open. Select and add the **Processing template** from your directories then hit **OK**. The added template will be listed in the table, as seen in the image below, and will be applied to the spectrum number 2.



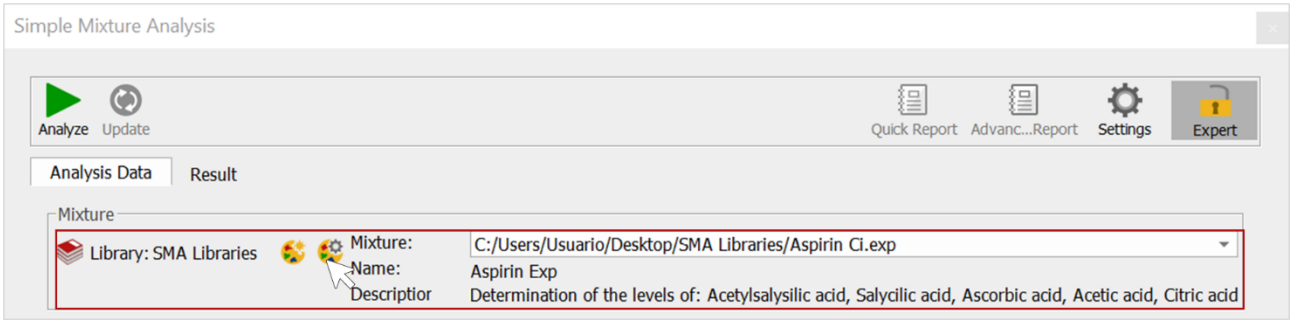
When a mixture includes components with different types of nuclei and/or dimensions, it is possible to add a processing template for each. In such cases, a different spectrum number (**SpecNo**) must be attributed to each processing templates. In the example below, the 2D processing template will be applied to spectrum number 2 - of the Mnova document in hand - which includes the Salicylic acid 2D spectrum, whereas the 1D processing template will be applied to the other mixture components with a 1D spectrum.



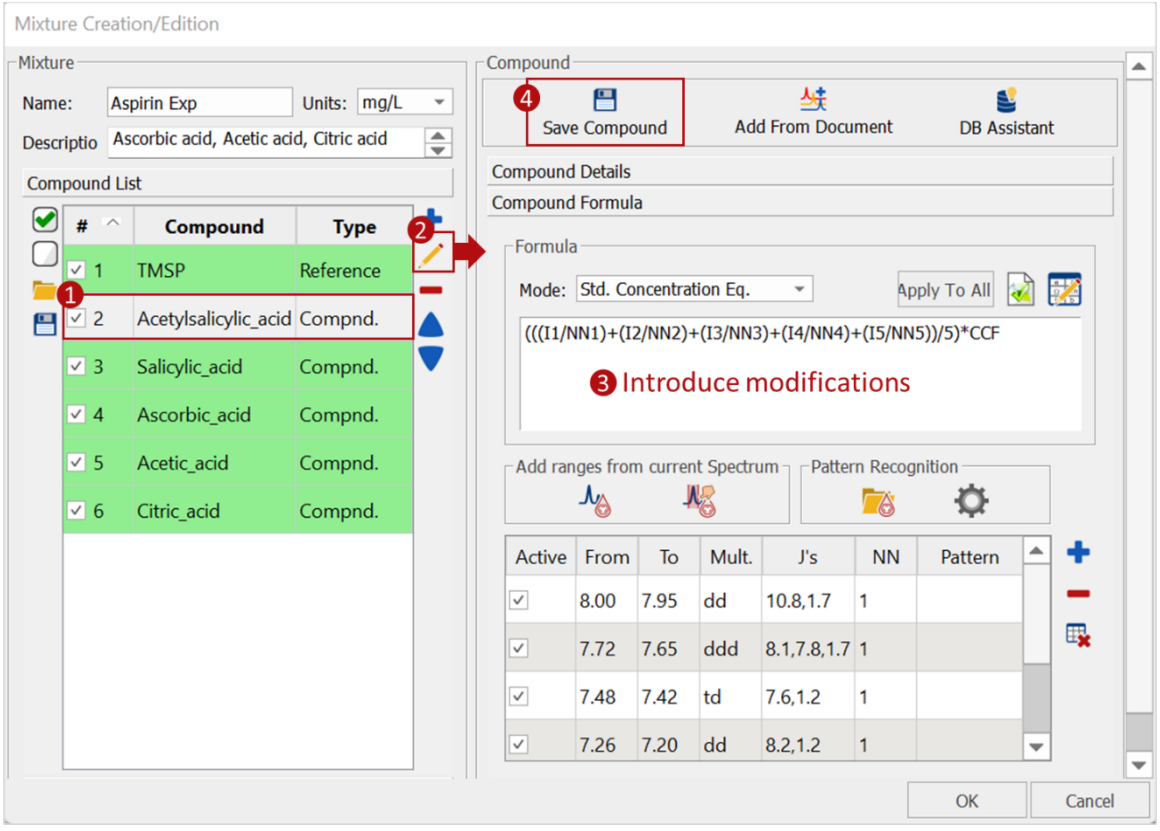
Finally, you can check or uncheck table rows to delete processing templates .

3.6. Reviewing/editing the mixture details

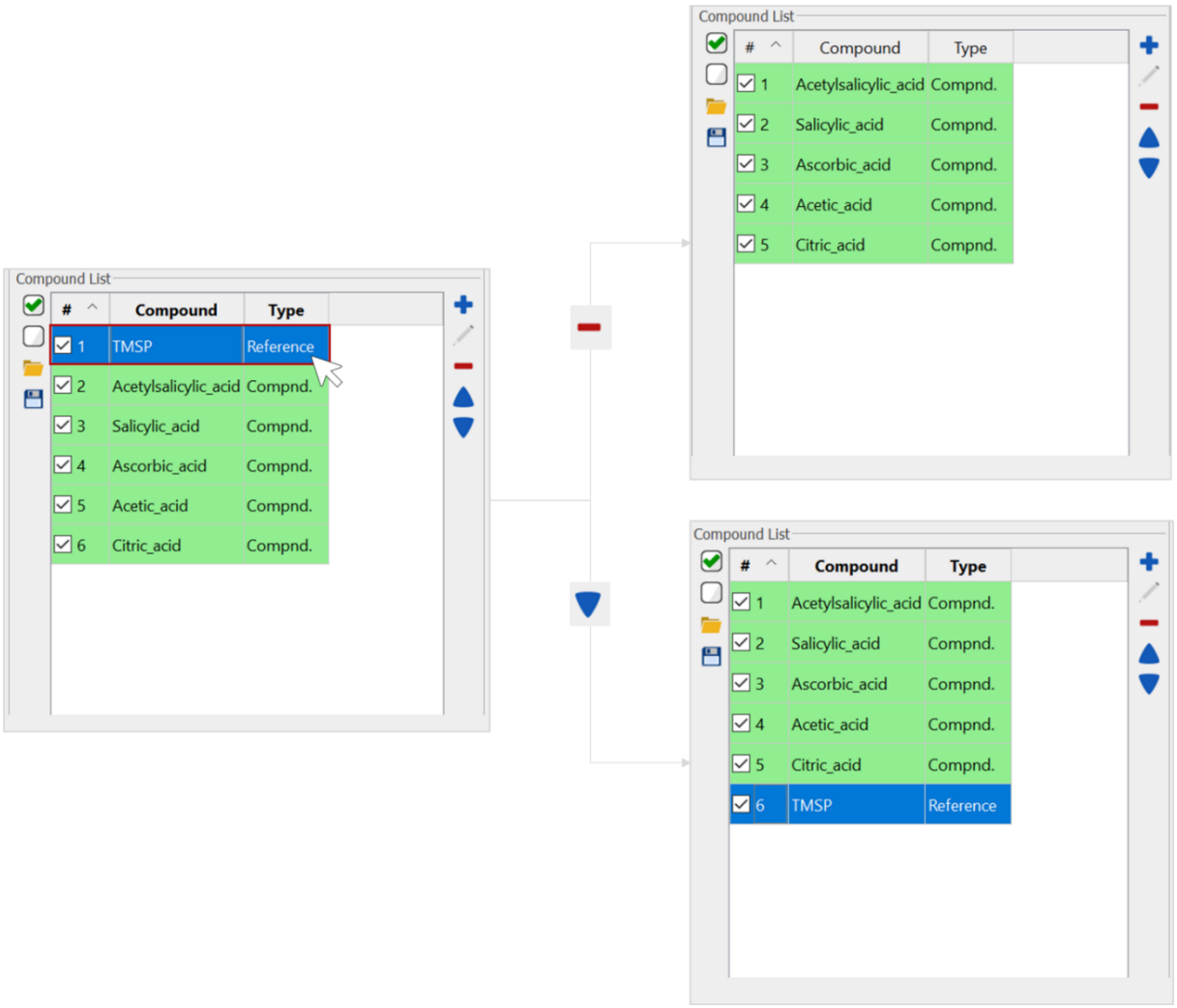
Your library and selected mixture are now displayed in the SMA panel. You can open your experiment to edit **Mixture** and **Compound** details by clicking on this button .



Select a compound and hit the **Edit** button . The **Compound** details section is accordingly activated and becomes editable. Make any modifications you want, then save them by clicking on this button: .



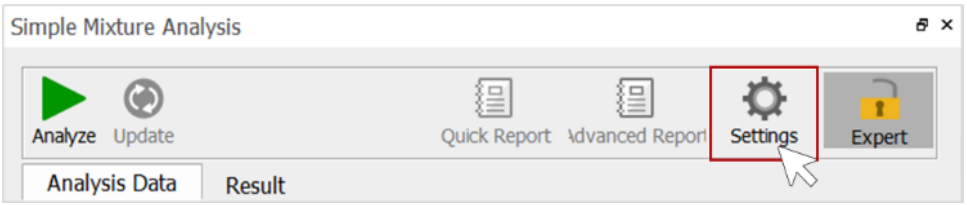
You can also select and delete a previously added compound, or select and change priority with . The analysis will be performed in the order you define.



Click on **OK** to save your modifications.

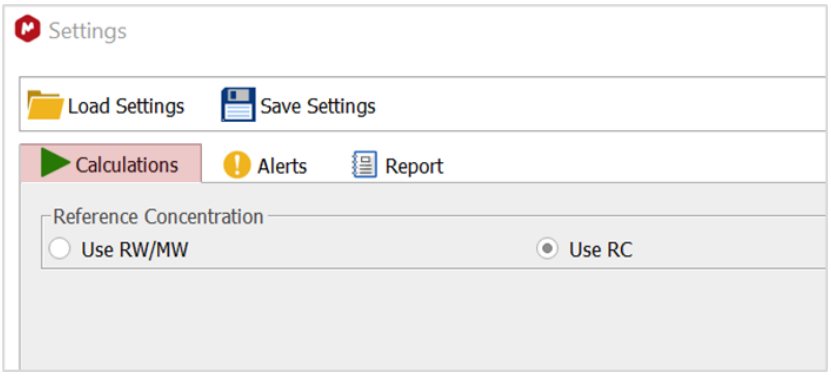
4. SMA general settings

Before proceeding with the analysis of the samples, you might want to configure some general calculations and reporting settings. To do so, click on the **Settings** icon in the **Simple Mixture Analysis** window. A new dialog will open with two tabs: **Calculations** and **Report**.



4.1. The Calculations tab

In this tab, you can indicate whether the Reference Concentration (RC) or the Reference Weight (RW) and Molecular Weight (MW) (RW/MW) will be used for calculation. RC and RW values can either be present in the parameters table of the sample or manually entered by the user in the SMA panel.

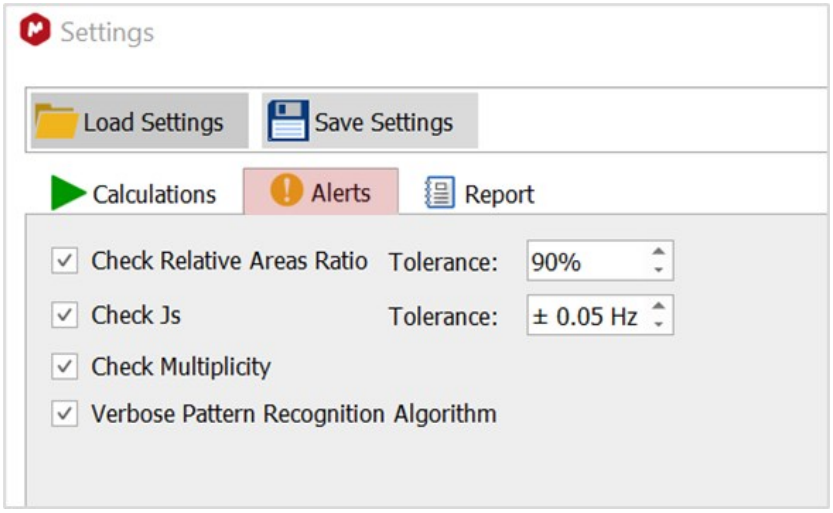


4.2. The Alerts tab

When running an analysis, SMA can run various tests and report on possible associated errors via the alerts window. In this tab, you can configure the tests you want to perform on your compounds. You can enable the following:

- **Check Relative Areas ratio:** to calculate the relative area (Integral_i/NN_i) / (Integral_j/NN_j) and compare it to the expected values (between 1-tolerance/100 and 1+tolerance/100). You can set the tolerance value in the dedicated box.
- **Check Js:** to calculate the Js value for a certain multiplet and compare it to that defined by the user. You can set the tolerance in the dedicated box.
- **Check Multiplicity:** to compare multiplicities found to those defined by the user in the Mixture.

- **Verbose Pattern Recognition Algorithm:** to display information about the search and search results when using the pattern recognition tool.



4.3.The Report tab

In this tab, quick and advanced reports can be customized.

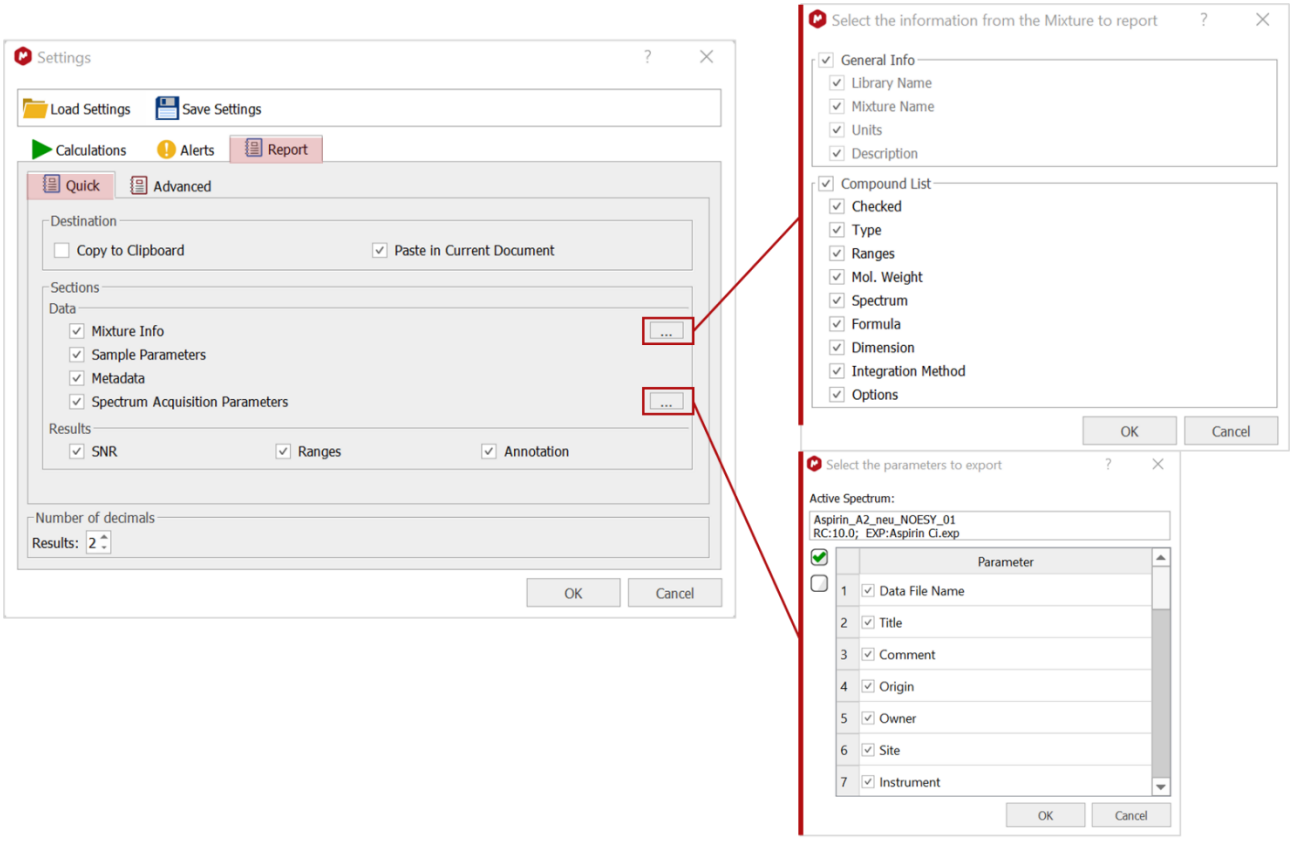
A. Quick Reports

Quick reports are concise text reports that can be quickly pasted into the Mnova document or copied to the clipboard.

Report sections can include data (**Mixture info**, **Sample parameters**, **Metadata**, **Spectrum acquisition parameters**) and results (**SNR**, **Ranges**, **Annotations**), and are fully customizable.

When **Spectrum Acquisition Parameters** is checked, make sure you have an open Mnova document to retrieve and display the available parameters for selection.

The number of decimals to be used in the reported results can also be chosen in this section.



See an example of a **Quick Report** in section 6.4.

B. Advanced Reports

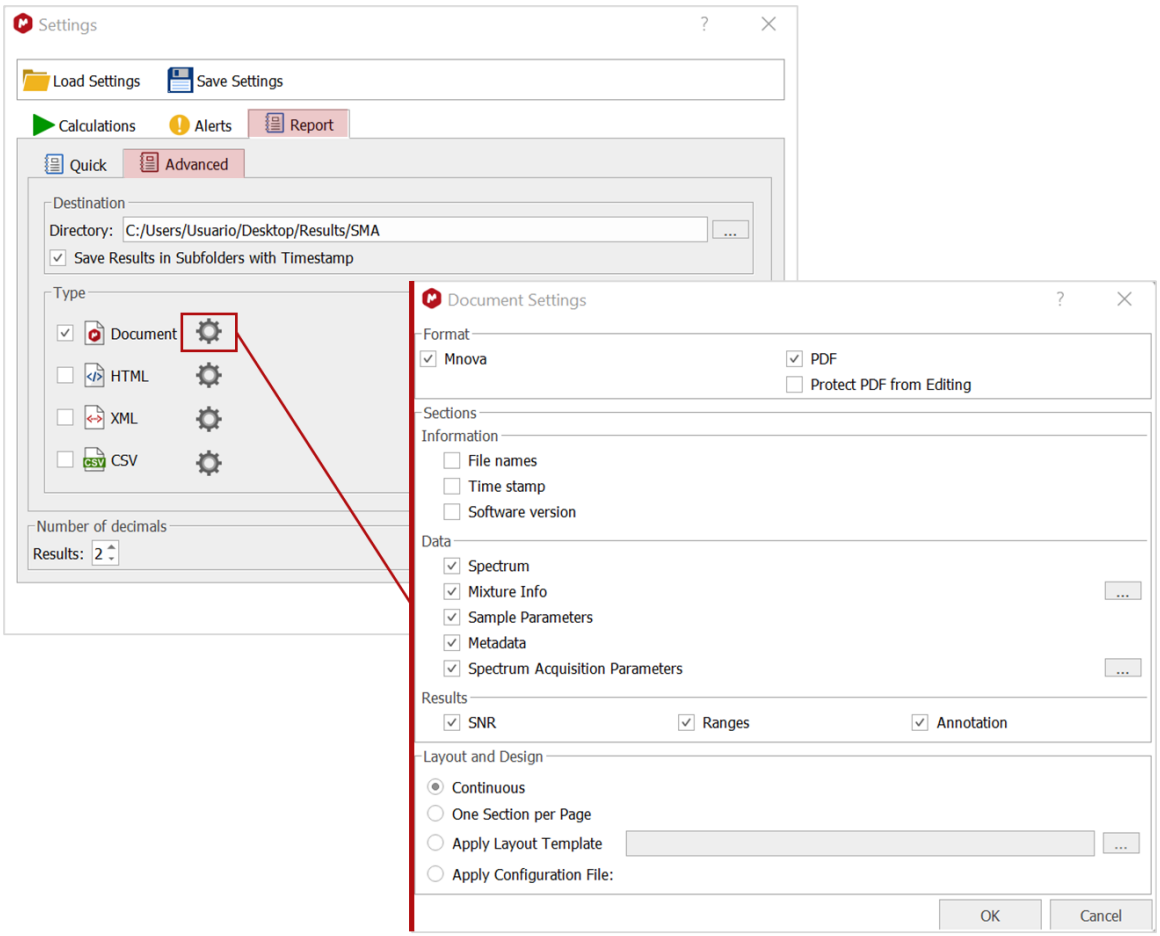
On the other hand, **Advanced reports** are extent reports with complete information about the experiment´s parameters and results. Various types of advanced reports are available and customizable (PDF, Mnova, HTML, XML, CSV). Advanced reports can be saved in the directory of your choice.

Mnova and PDF reports configuration:

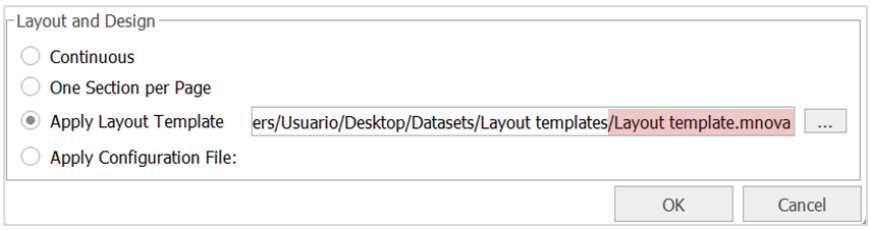
Both Mnova and PDF reports can be generated, and PDF reports can be protected from editing.

General information about **File names**, **Time stamp** and **Software version** can be included along with data (**Mixture info**, **Samples parameters**, **Metadata**, **Spectrum acquisition parameters**) and results (**SNR**, **Ranges**, **Annotations**).

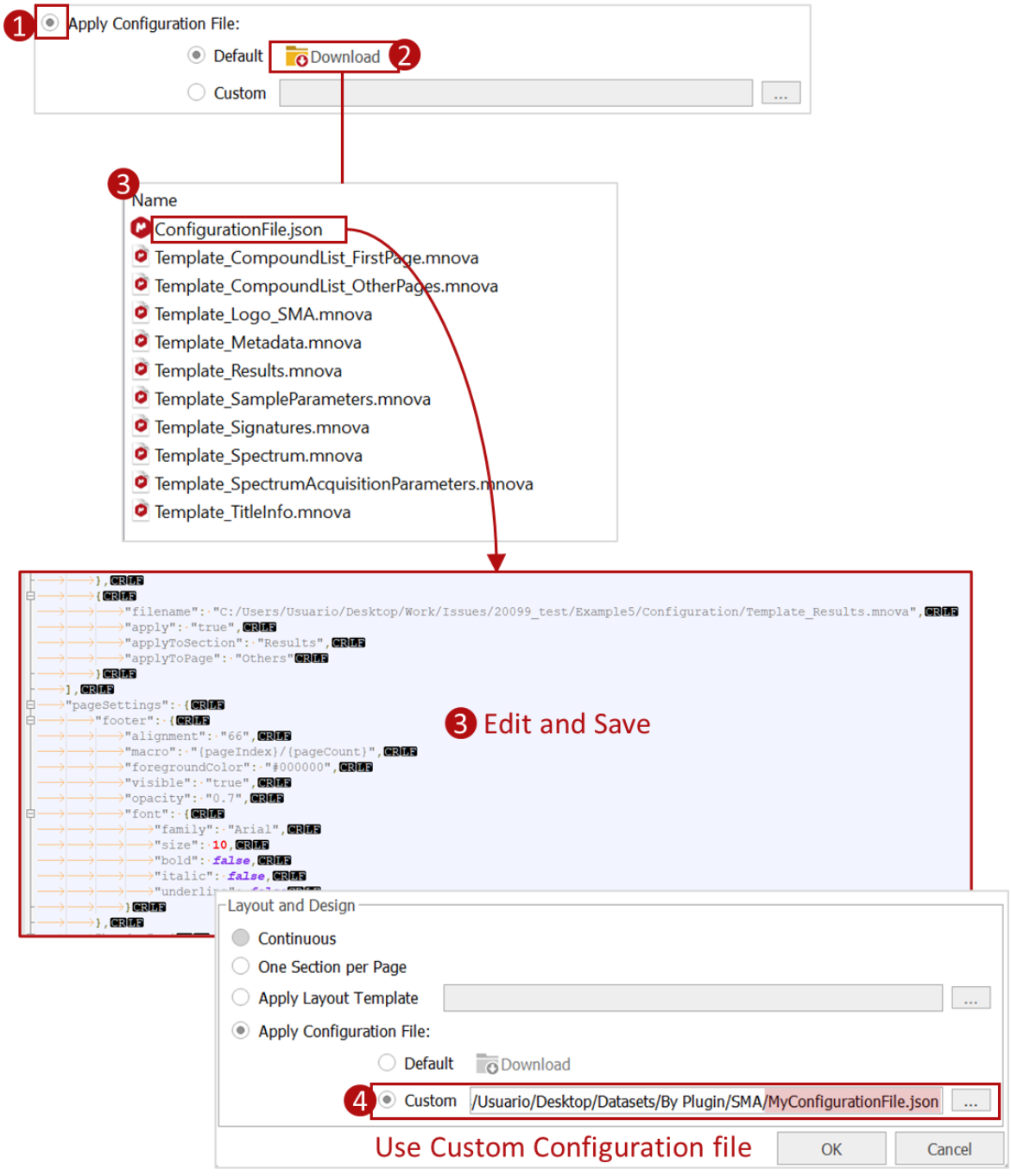
Default (**Continuous** or **One Section per Page**) or custom (**Layout Template** or **Configuration File**) layouts and designs can be applied to both Mnova and PDF reports.



Layout templates (".mnova") can be easily generated with Mnova itself and loaded for use in SMA.

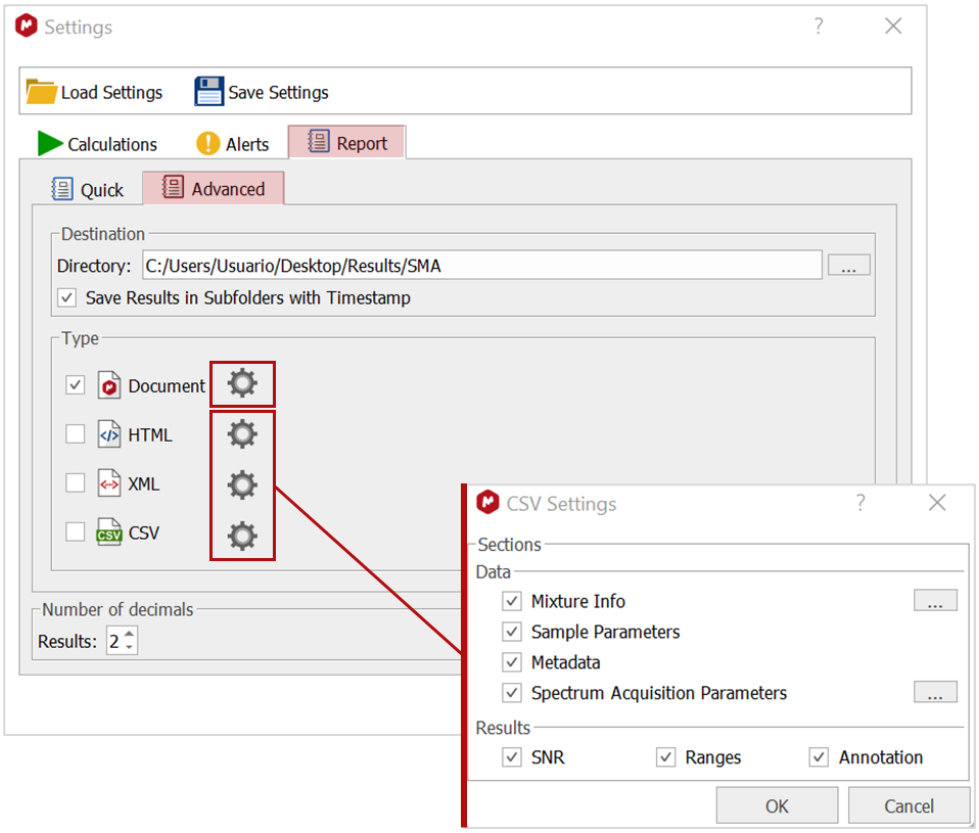


Configuration files (".json") can be customized based on a default file available for download, then saved and loaded for use.



HTML, XML, and CSV report configuration

Report sections can include data (**Mixture info**, **Sample parameters**, **Metadata**, **Spectrum acquisition parameters**) and results (**SNR**, **Ranges**, **Annotations**) and are fully customizable.



See examples of **Advanced Reports** in section 6.4.

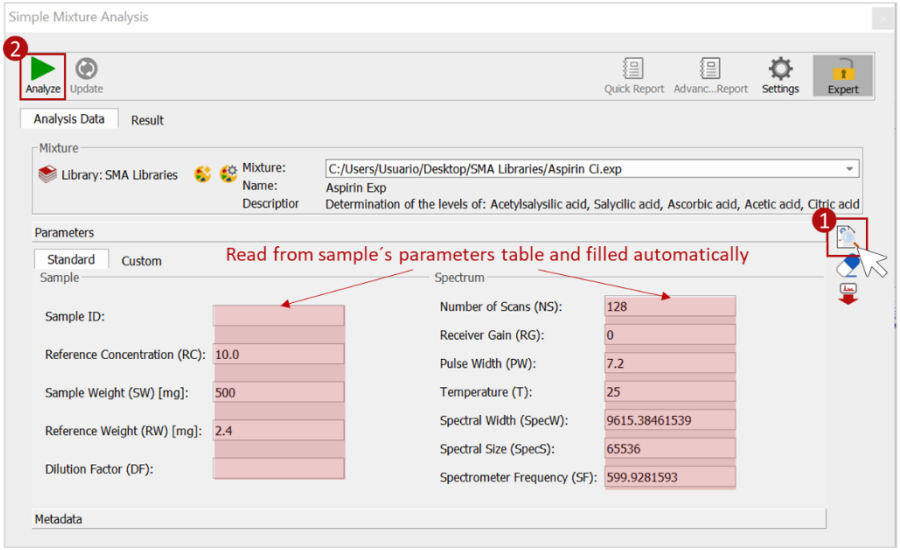
Note that you can **Save** your settings and easily **Load** them for future analyses.

When you have finished the configuration, click on **OK** to confirm your choices.

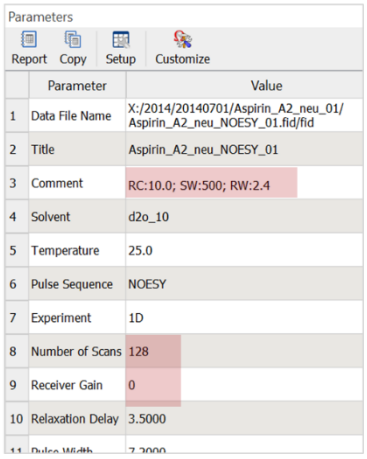
5. SMA sample analysis

Once you have selected a mixture (experiment) and configured your analysis preferences, running an SMA analysis becomes very easy. You first need to open your sample spectrum in Mnova, then click on the magnifying glass button to read your sample parameters. The sample's parameters table will be automatically completed. If the dataset does not include this metadata (in the comment field of the parameters table), the user will be required to fill the table fields manually.

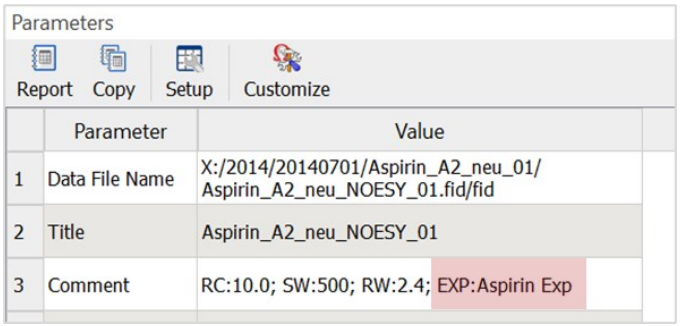
You can now analyze your sample by clicking on this button Analyze.



Sample´s parameters table



Note that you can also specify the mixture name on the comments field of the parameters table of your sample. The corresponding mixture is then loaded when the Read parameters button is used. The string to indicate the mixture name is case-insensitive and can start with "Experiment", "Exp", "Mix", or "Mixture", followed by the name of the experiment/mixture to be used.



6. SMA results

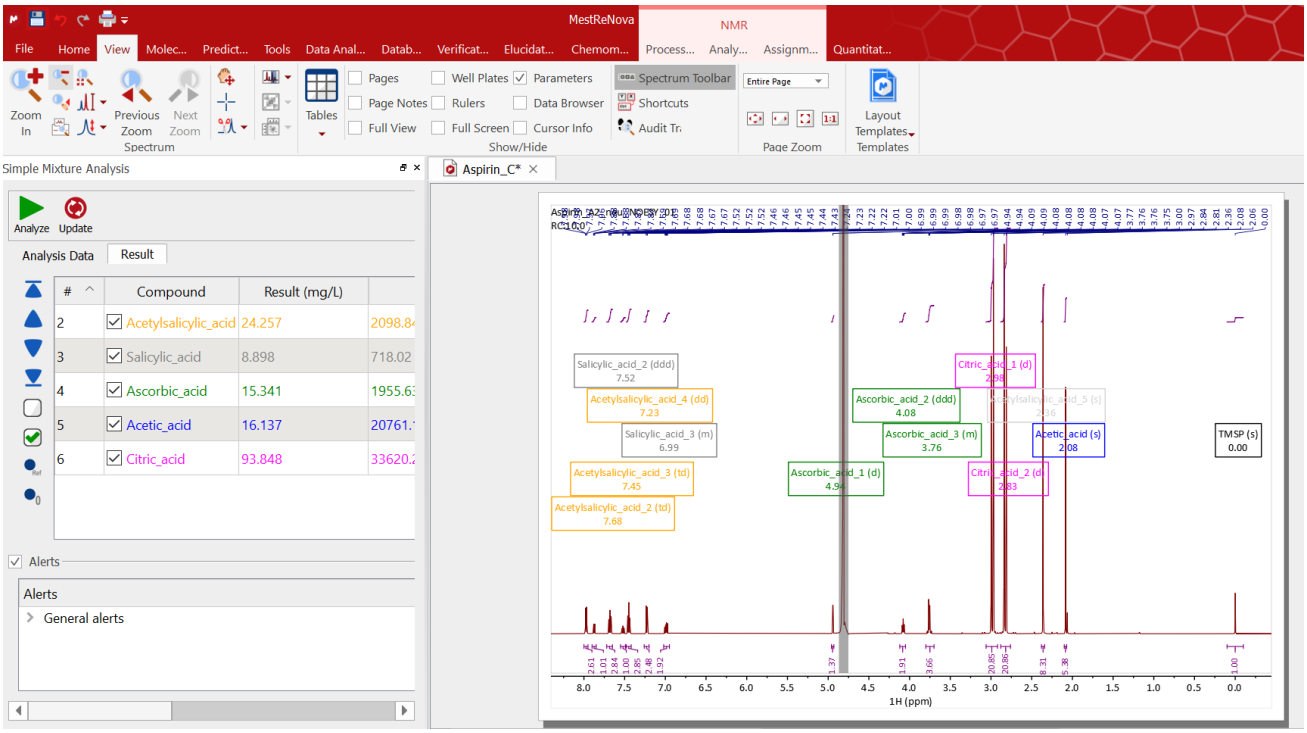
Once the analysis is complete, results are automatically displayed in the **Results** tab.

SMA results can also be loaded from an active document by clicking on this button  . The results and related information (Mixture Information, Calculation Settings, Standard Parameters, Metadata) are accordingly pasted into the SMA panel and a library is generated in the default directory that facilitates the sharing of results for review and repetition of the analysis using the same mixture.

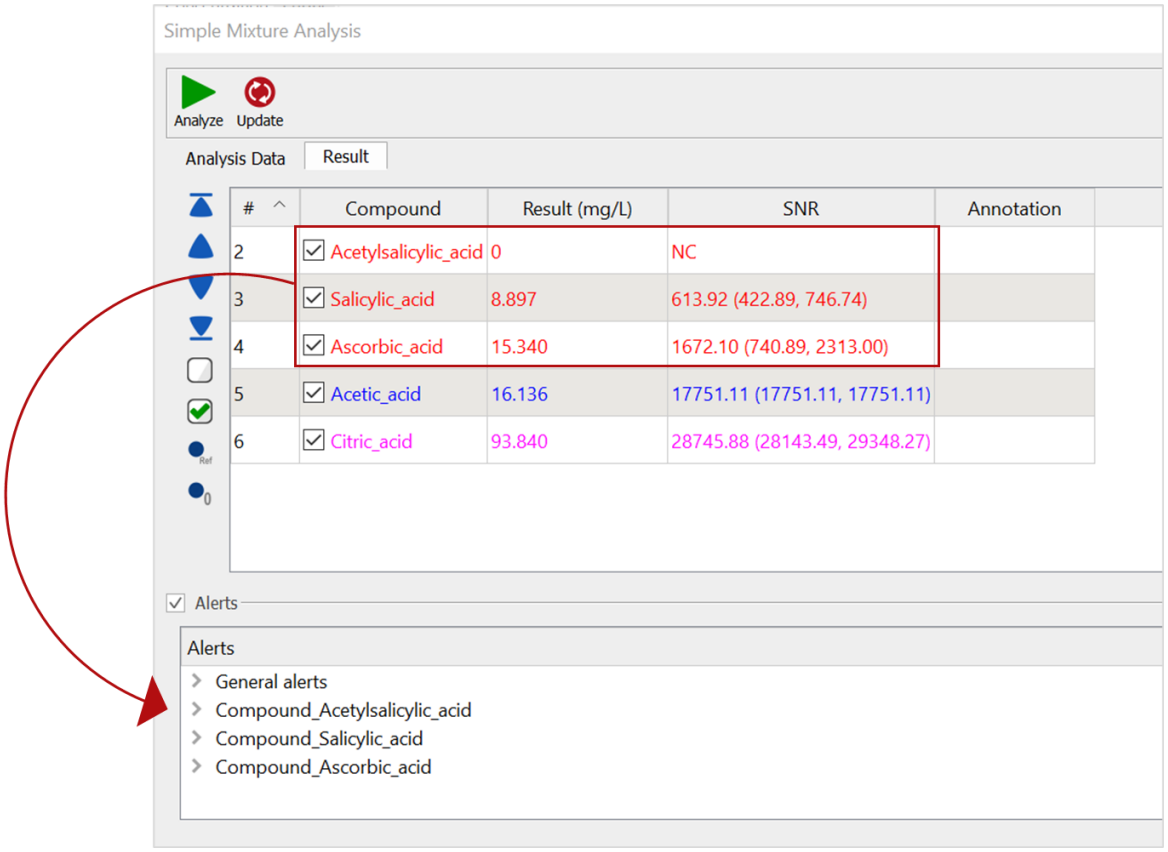
Note that when running an automated Batch or RT SMA analysis with Gears SMA, individual sample results can also be loaded into the SMA results tab for revision.

6.1. The results table

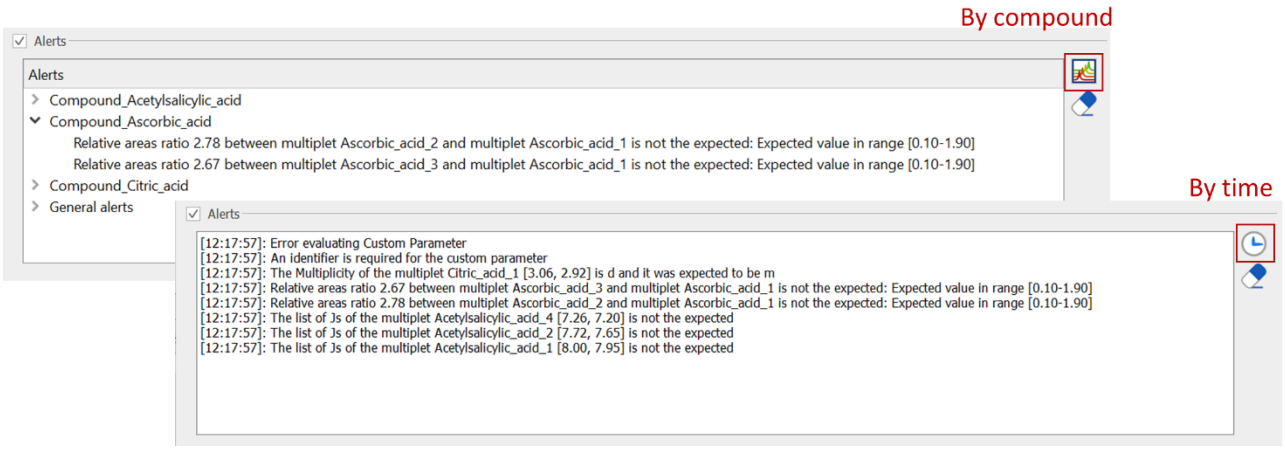
Your results will be displayed in the **Results** tab as follows. Mixture components will be colored in the results table and in the spectrum as specified in the experiment options.



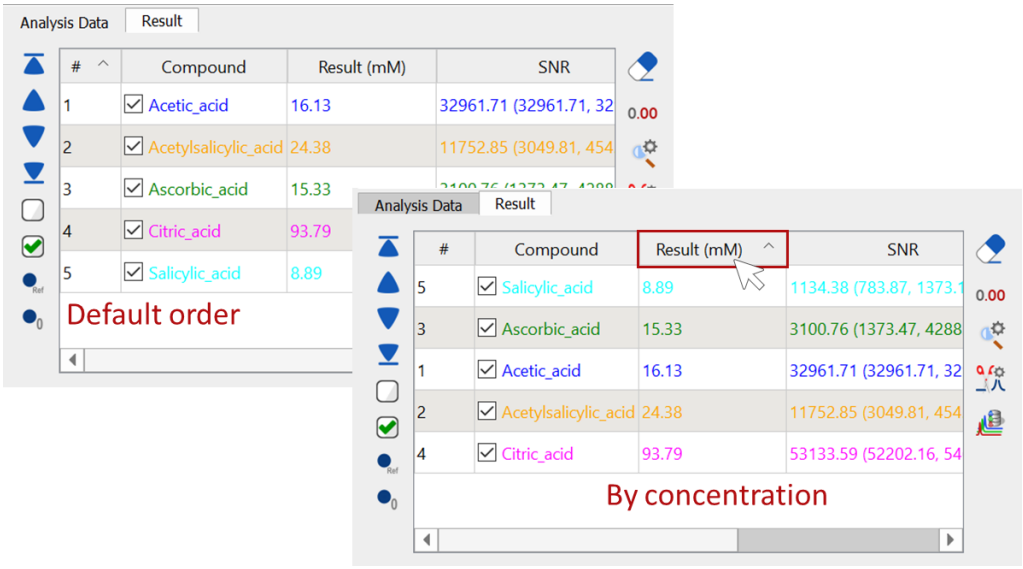
A compound that is recolored "red" in the results table might be causing errors to occur, so remember to check the warning messages appearing in the Alerts section.



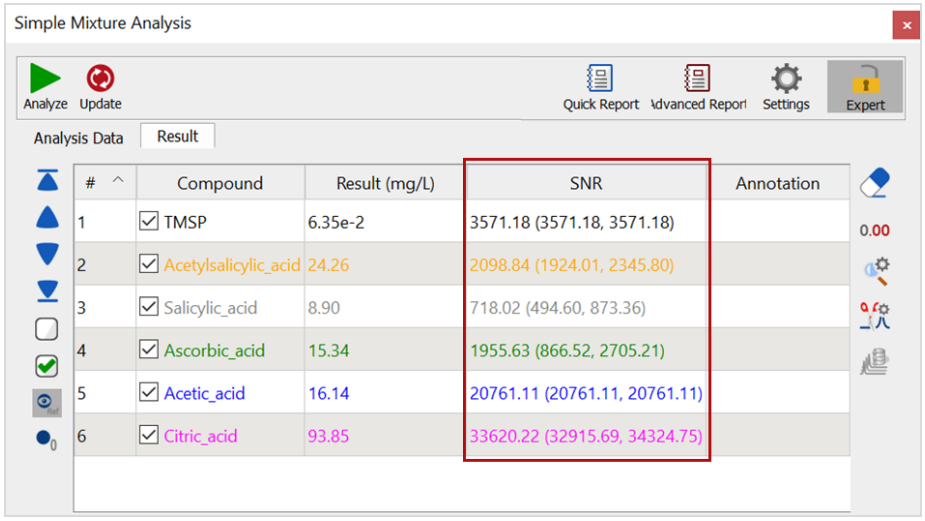
The alerts can be displayed by **Compound** or by **Time** .



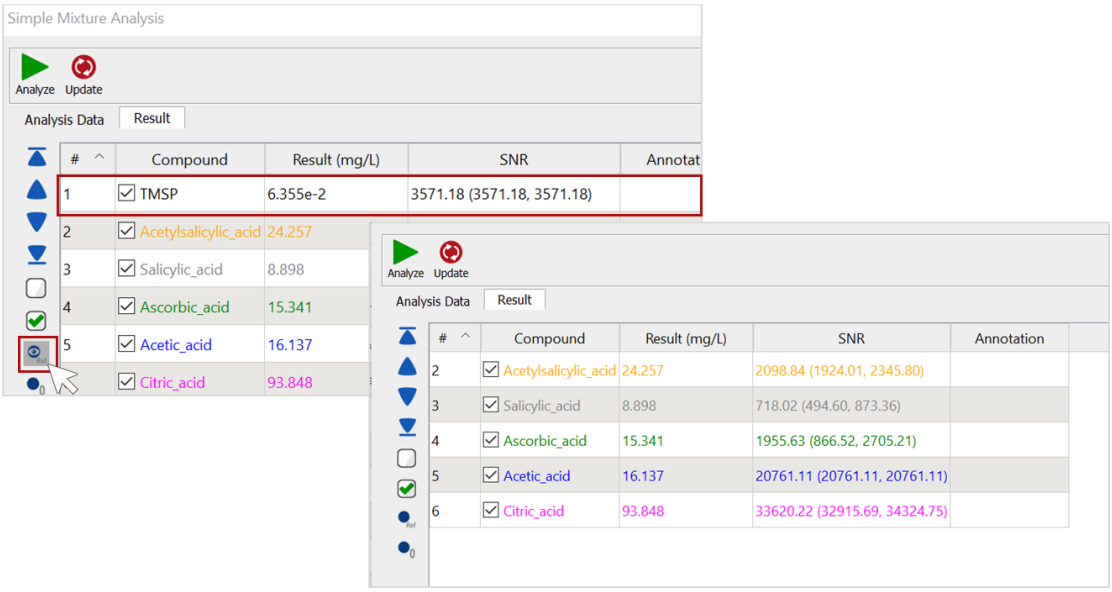
By default, compounds are displayed in the same order they have been assigned in the mixture panel. You can change this order to alphabetical or by increasing concentration, etc., by clicking on the headers of the results table.



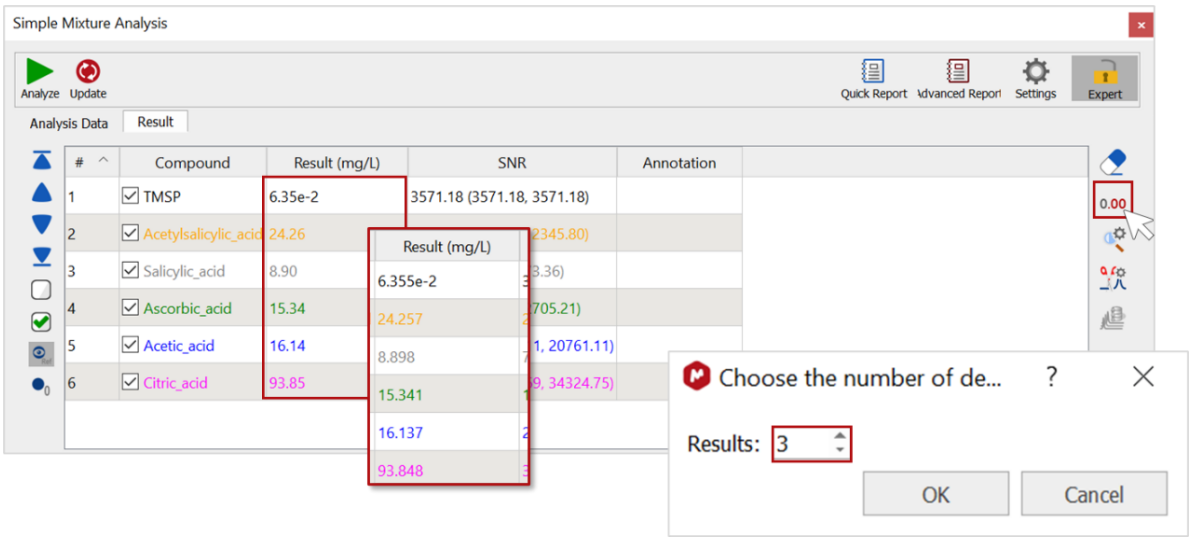
When the **Calculate SNR** option is enabled for the SMA experiment, a column with the SNR value and range is added to the results table. If the compound involves several multiplets, the SNR is the average of the individual values of such for each multiplet. The SNR is automatically recalculated if changes are made in the multiplets selection.



You can also show/hide the results with no valid multiplet or the results of the reference compound , as shown in the image below.

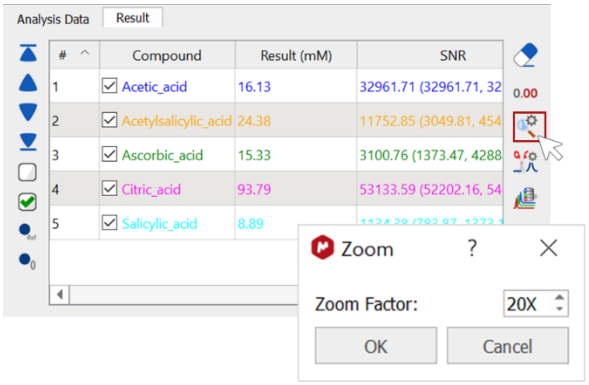


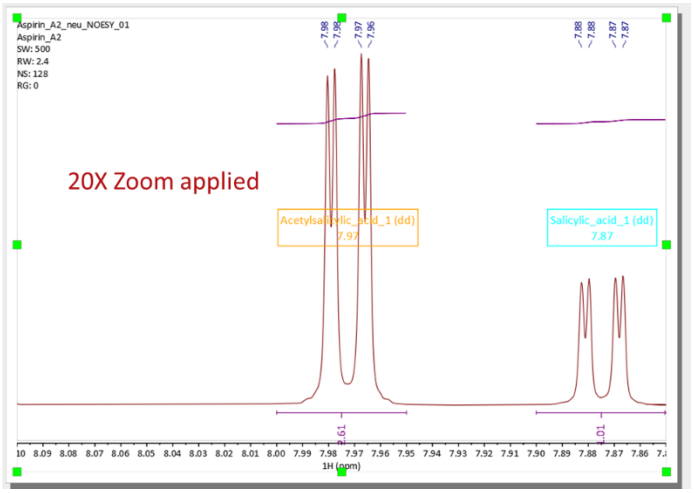
With the 0.00 button you can change the number of decimals used in the results table.



Use the **Smart cuts** tool to perform cuts in the areas between the multiplets. All cuts are restored when pressing the same button again.

The blue arrows allow you to navigate between the compounds. A view of the first multiplet in each compound can thus be obtained. To change the zoom factor on the viewed spectra you can click on the button to change the zoom value.

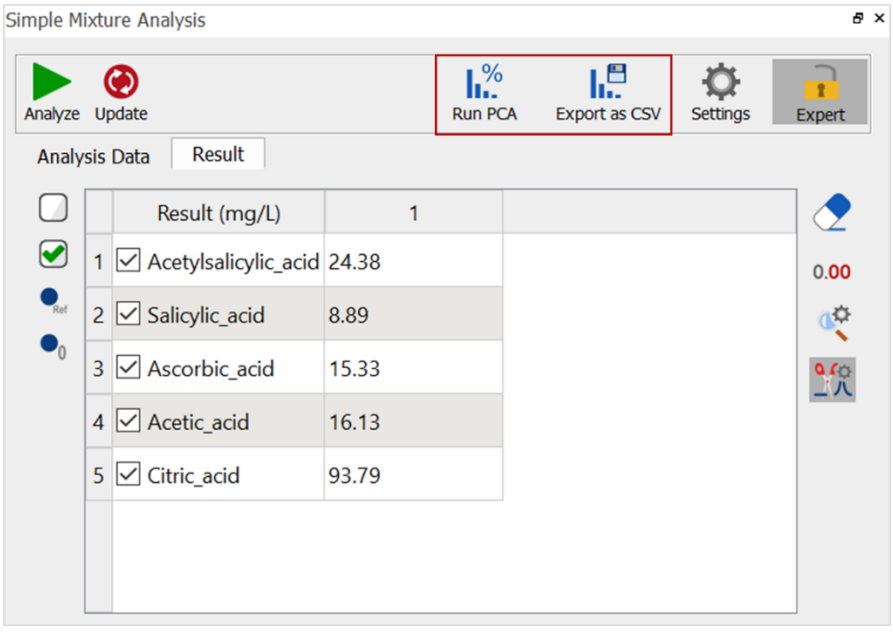




When mixture components come from a database (mixture created with database assistant), it is possible to stack analyte spectra with database records to review the spectral profile by clicking on the icon.

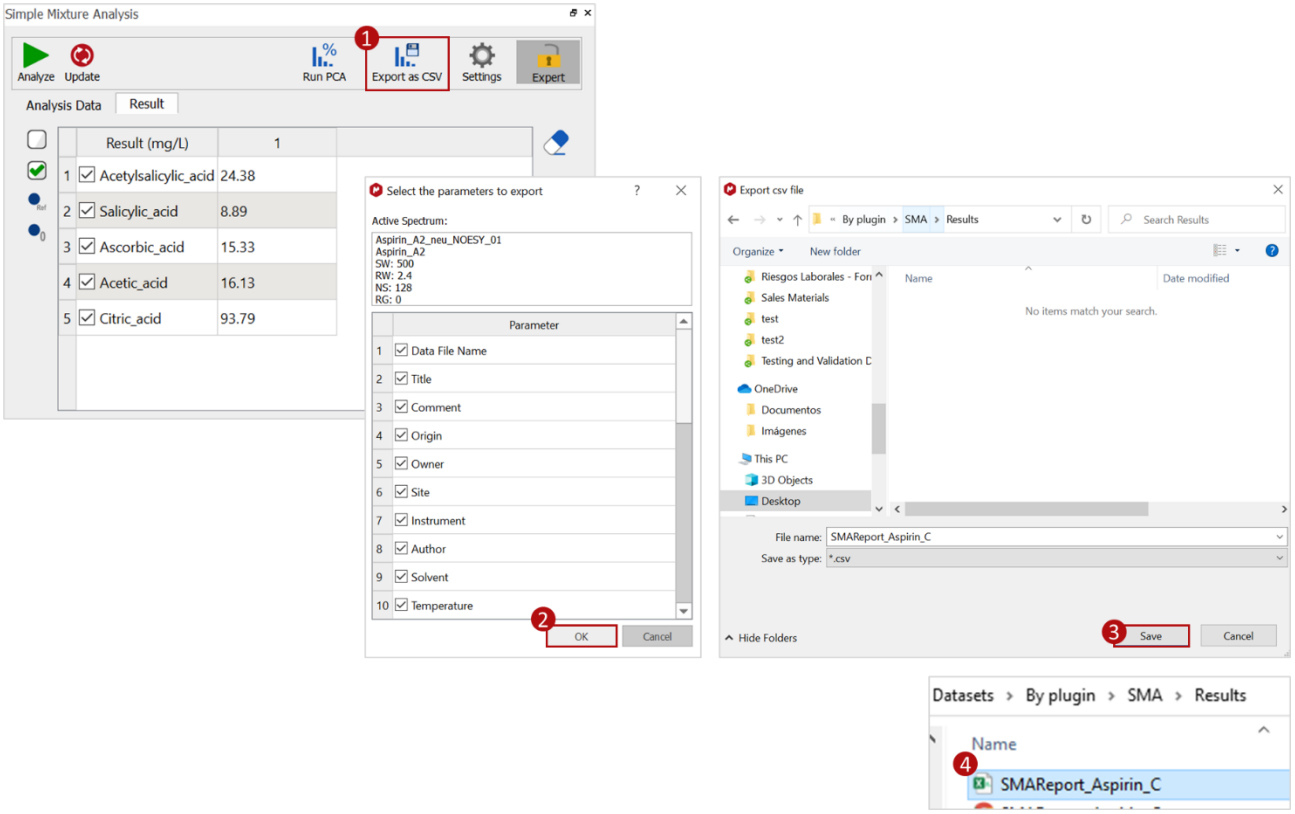
6.2. Experiment suitable for PCA

When running an experiment that is "Suitable for PCA", the SMA dialog will present two buttons that will allow you to run the PCA and export the associated data to a CSV file. ***A license for the Chemometrics plugin must be obtained to perform a PCA.***



If you click on **Run PCA**, a dialog with the original SMA data will open. *Please refer to the Mnova manual for more details about the PCA study.*

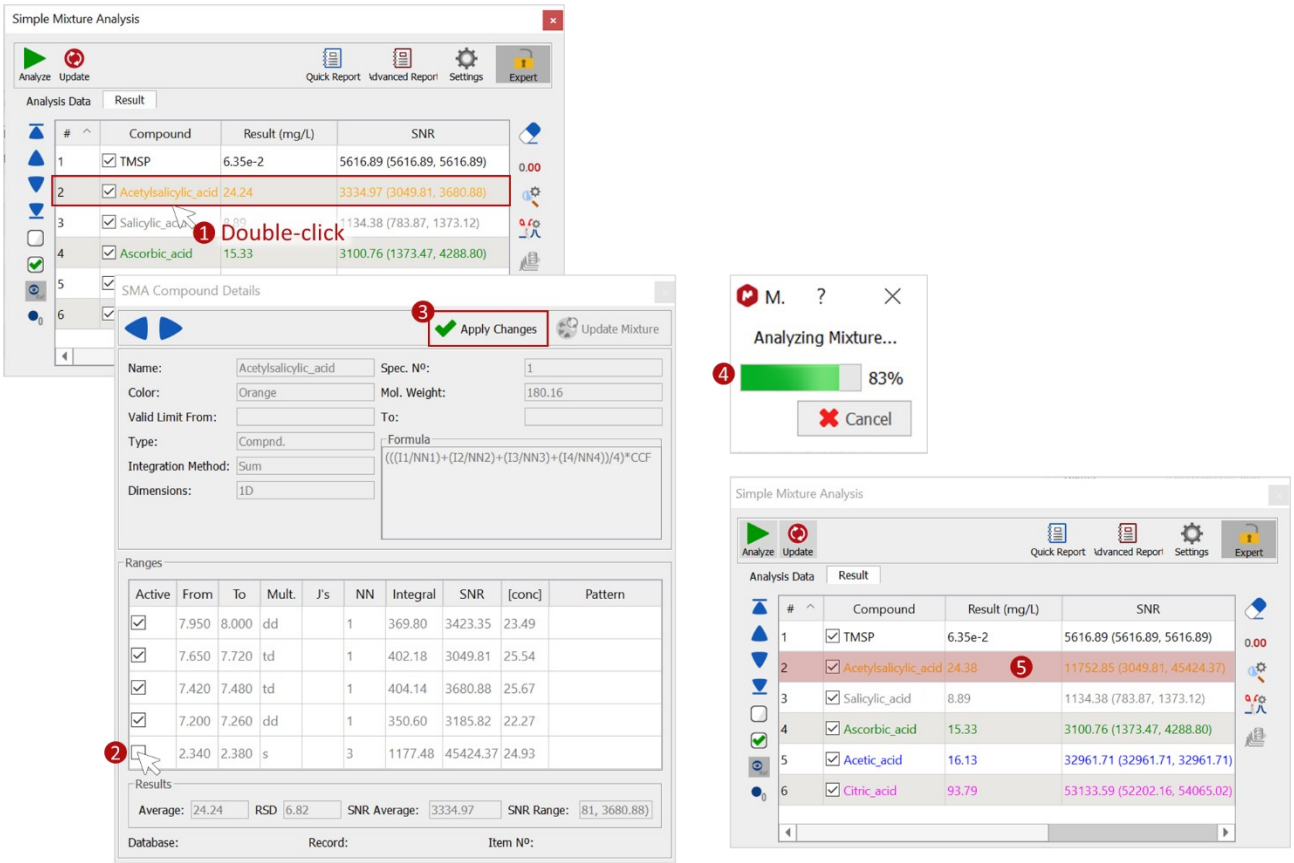
When you click on **Export as CSV**, a new dialog with a set of parameters to choose from is opened. Select the rows you want to include in the CSV, then hit **OK** and save your report to the directory of your choice.



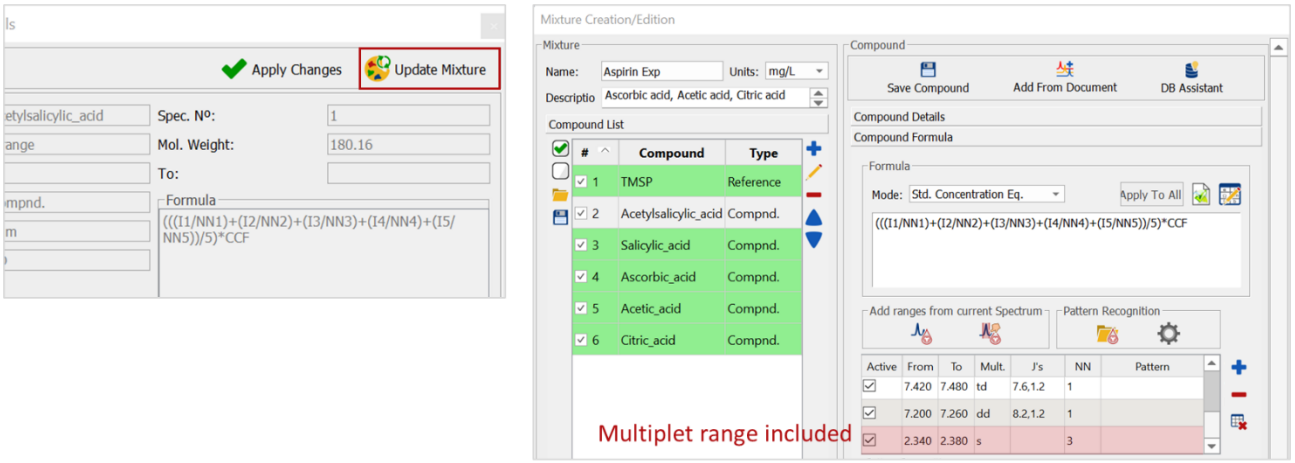
6.3. Revision and update

SMA results can be easily revised and updated. For instance, you can adjust the multiplet ranges on the spectrum and click on the **Update** button to redo the analysis. This can be very useful if peak positions vary slightly from sample to sample.

You can also update the multiplet ranges used for the calculation. To do so, double-click on the compound of interest in the results table. The SMA Compound detail dialog will open. Check/uncheck the ranges you want to include/exclude, respectively, then **Apply changes**. The mixture will therefore be reanalyzed and the results updated in the results table.

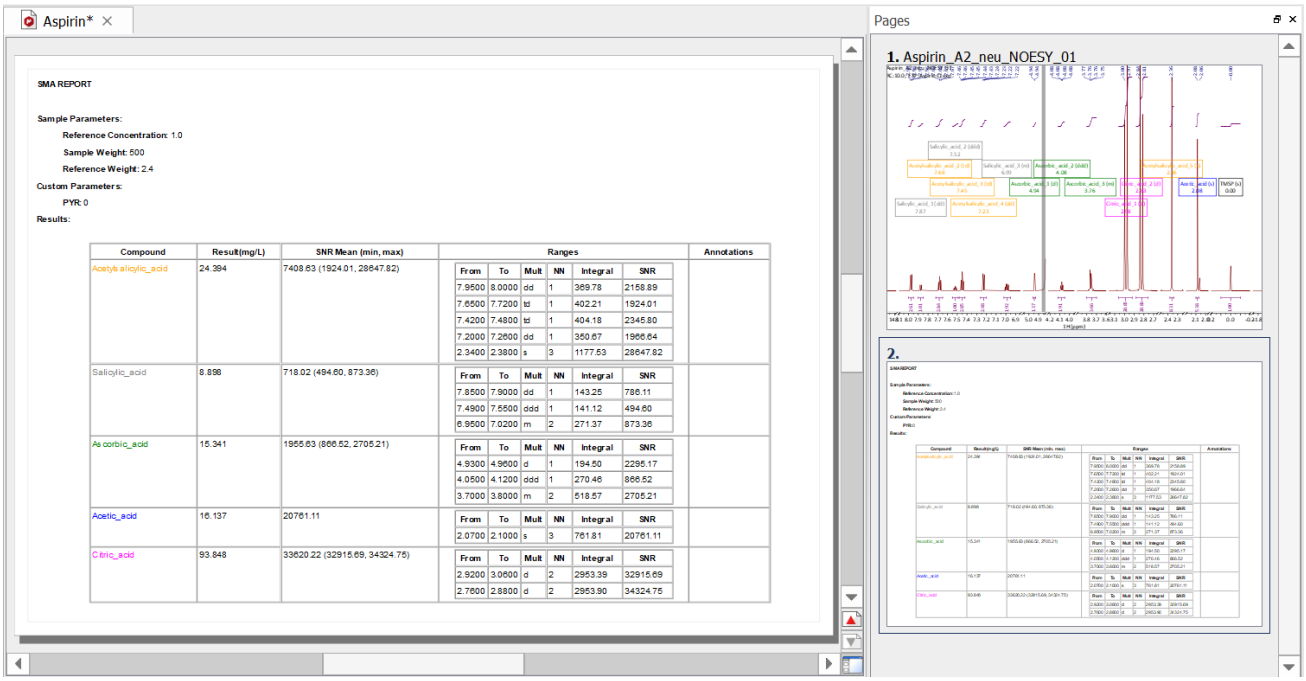


Once you have applied changed to a compound, the **Update Mixture** button will become active and will allow you to save those changes to the mixture used for the analysis.

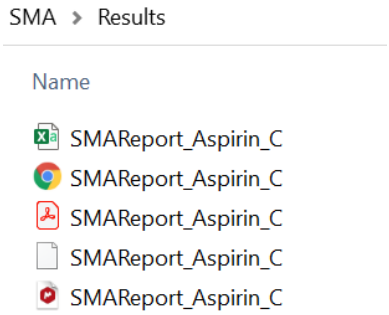


6.4. Reporting

Click on **Quick Report** to generate the report type you configured in the **Settings** > **Report** > **Quick** menu item. An example of a quick report pasted into an Mnova document is provided below.

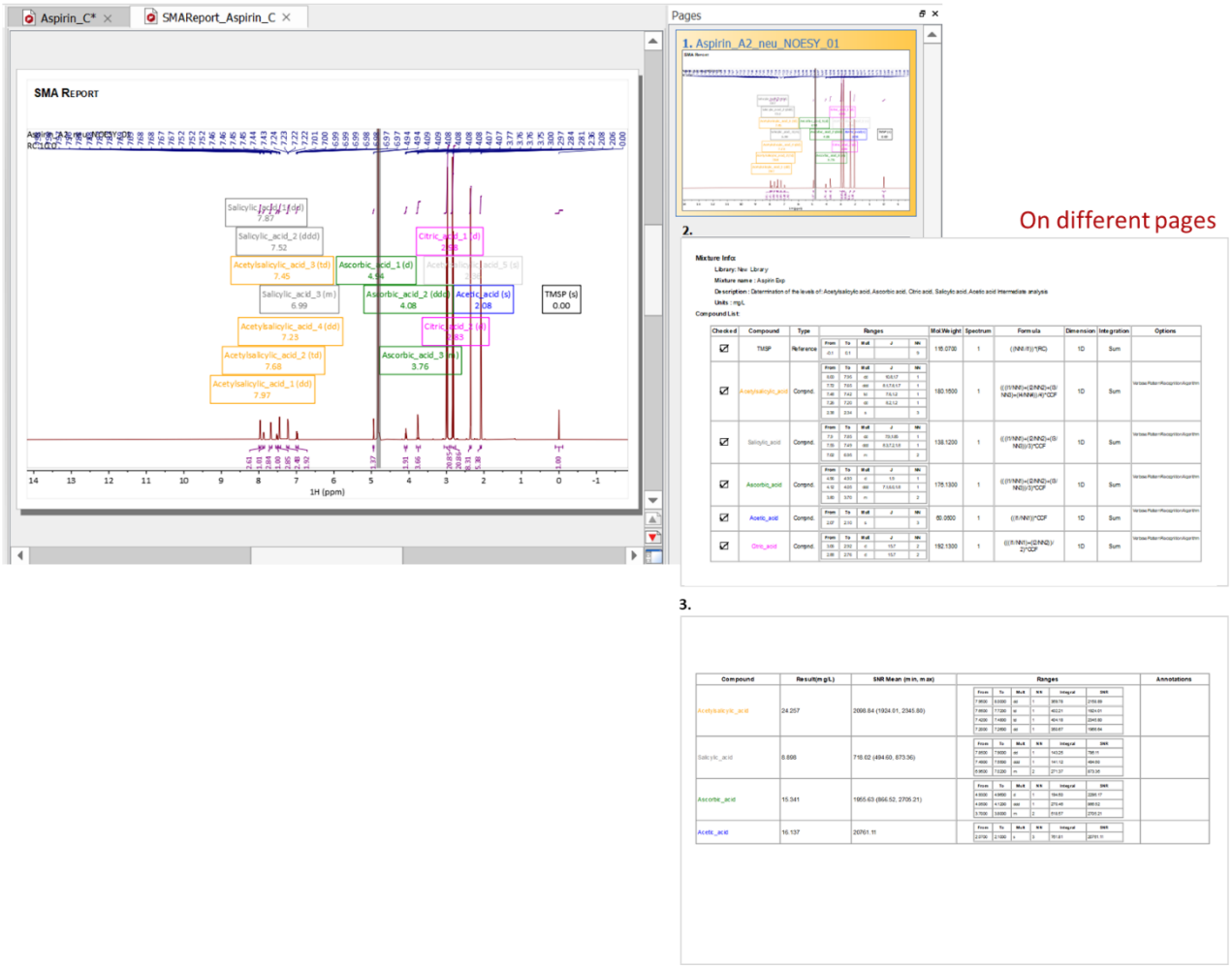


Click on **Advanced reports** to generate the output files you configured in the **Settings** > **Report** > **Advanced** menu item. All associated files will be saved in the directory you specified.



You can find examples of such advanced reports below:

Mnova report



CSV report

	A	B	C	D	E	F	G	H	I	J	K	L	M	N	O	P	Q	R	S
1	**Mixture Info:**																		
2		Library	**Mixture name**	**Description**	**Units**														
3		New Library	Aspirin Exp	Determination o	Ascorbic acid	Citric acid	Salicylic a	Acetic acid											
4	**Intermediate analysis**	mg/L																	
5		Compound List:																	
6			**Checked**	**Compound**	**Type**	**Mol.Weight**	**Spectrum**	**Formula**	**Dimensior**	**Integratio**	**Options**	**Ranges Fr**	**Ranges To**	**Ranges Mu**	**Ranges J**	**Ranges NN**			
7			yes	TMSP	Reference	116.07	1	((NN1/I1))	1D	Sum		-0.1	0.1			9			
8			yes	Acetylsalicylic_a	Compnd.	180.16	1	(((I1/NN1)	1D	Sum	Verbose P	8	7.95	dd	10.8	1.7	1		
9												7.72	7.65	ddd	8.1	7.8	1.7	1	
10												7.48	7.42	td	7.6	1.2	1		
11												7.26	7.2	dd	8.2	1.2	1		
12												2.38	2.34	s		3			
13			yes	Salicylic_acid	Compnd.	138.12	1	(((I1/NN1)	1D	Sum	Verbose P	7.9	7.85	dd	7.9	1.85	1		
14												7.55	7.49	ddd	8.3	7.2	1.8	1	
15												7.02	6.95	m		2			
16			yes	Ascorbic_acid	Compnd.	176.13	1	(((I1/NN1)	1D	Sum	Verbose P	4.96	4.93	d	1.9	1			
17												4.12	4.05	ddd	7.1	6	1.8	1	
18												3.8	3.7	m		2			
19			yes	Acetic_acid	Compnd.	60.05	1	(((I1/NN1))	1D	Sum	Verbose P	2.07	2.1	s		3			
20			yes	Citric_acid	Compnd.	192.13	1	(((I1/NN1)	1D	Sum	Verbose P	3.06	2.92	d	15.7	2			
21												2.88	2.76	d	15.7	2			
22	**Sample Parameters:**																		
23		Reference Concentration																	
24		1																	
25	**Custom Parameters:**																		
26																			
27																			
28	**Metadata:**																		
29																			

HTML report

SMA Report

Mixture Info:

Library: New Library

Mixture name : Aspirin Exp 1

Description :

Units : mg/L

Compound List:

Checked	Compound	Type	Ranges	Mol.Weight	Spectrum	Formula	Dimension	Integration	Options
☑	TMSP	Reference	From: -0.1, To: 0.1, Mult: , J: , NN: 9	116.0700	1	((NN1/I1))*(RC)	1D	Sum	
☑	Acetylsalicylic_acid	Compnd	From: 7.950, To: 8.000, Mult: dd, J: 10.8,1.7, NN: 1 From: 7.650, To: 7.720, Mult: ddd, J: 8.1,7.8,1.7, NN: 1 From: 7.420, To: 7.480, Mult: td, J: 7.6,1.2, NN: 1 From: 7.200, To: 7.260, Mult: dd, J: 8.2,1.2, NN: 1 From: 2.340, To: 2.380, Mult: s, J: , NN: 3	180.1600	1	(((I1/NN1)+(I2/NN2)+(I3/NN3)+(I4/NN4))/4)*CCF	1D	Sum	Verbose Pattern Recognition Algorithm
☑	Salicylic_acid	Compnd	From: 7.9, To: 7.85, Mult: dd, J: 7.9,1.85, NN: 1 From: 7.55, To: 7.49, Mult: ddd, J: 8.3,7.2,1.8, NN: 1 From: 7.02, To: 6.95, Mult: m, J: , NN: 2	138.1200	1	(((I1/NN1)+(I2/NN2)+(I3/NN3))/3)*CCF	1D	Sum	Verbose Pattern Recognition Algorithm
☑	Ascorbic_acid	Compnd	From: 4.95, To: 4.93, Mult: d, J: 1.9, NN: 1 From: 4.12, To: 4.05, Mult: ddd, J: 7.1,6.0,1.8, NN: 1 From: 3.80, To: 3.70, Mult: m, J: , NN: 2	176.1300	1	(((I1/NN1)+(I2/NN2)+(I3/NN3))/3)*CCF	1D	Sum	Verbose Pattern Recognition Algorithm
☑	Acetic_acid	Compnd	From: 2.07, To: 2.10, Mult: s, J: , NN: 3	60.0500	1	((I1/NN1))*CCF	1D	Sum	Verbose Pattern Recognition Algorithm
☑	Citric_acid	Compnd	From: 3.06, To: 2.92, Mult: d, J: 15.7, NN: 2 From: 2.88, To: 2.76, Mult: d, J: 15.7, NN: 2	192.1300	1	(((I1/NN1)+(I2/NN2))/2)*CCF	1D	Sum	Verbose Pattern Recognition Algorithm

Sample Parameters:

Reference Concentration: 1.0

Custom Parameters:

Metadata:

Spectrum Adquisition Parameters:

Data_File_Name: X:/2014/20140701/Aspirin_A2_neu_01/Aspirin_A2_neu_NOESY_01.fid/fid
Title: Aspirin_A2_neu_NOESY_01
Comment: Aspirin_A2 SW: 500 RW: 2.4 NS: 128 RG: 0
Origin: Varian
Owner:
Site:
Instrument: vnmrs
Author:
Solvent: d2o_10
Temperature: 25
Pulse_Sequence: NOESY
Experiment: 1D
Probe: ID
Number_of_Scans: 128
Receiver_Gain: 0
Relaxation_Delay: 3.5
Pulse_Width: 7.2
Presaturation_Frequency: 4.812103814402499
Acquisition_Time: 2.499952
Acquisition_Date: 2014-07-01T17:53:46
Modification_Date: 2014-07-02T08:07:19
Class: {6ffface83-c3ba-4d6b-acf6-a6d5bb862db6}
IUPAC:
Spectrometer_Frequency: 599.9281593
Spectral_Width: 9615.38461539
Lowest_Frequency: -1106.77572396
Nucleus: 1H
Acquired_Size: 24038
Spectral_Size: 65536

Results:

Compound	Result(mg/L)	SNR Mean (min, max)	Ranges	Annotations
TMSP	6.351e-2	5616.89	From: -0.1000, To: 0.1000, Mult: s, NN: 9, Integral: 141.71, SNR: 5616.89	
Acetylsalicylic_acid	24.240	3334.97 (3049.81, 3680.88)	From: 7.9500, To: 8.0000, Mult: dd, NN: 1, Integral: 369.80, SNR: 3423.35 From: 7.6500, To: 7.7200, Mult: td, NN: 1, Integral: 402.18, SNR: 3049.81 From: 7.4200, To: 7.4800, Mult: td, NN: 1, Integral: 404.14, SNR: 3680.88 From: 7.2000, To: 7.2600, Mult: dd, NN: 1, Integral: 350.60, SNR: 3185.82	
Salicylic_acid	8.891	1134.38 (783.87, 1373.12)	From: 7.8500, To: 7.9000, Mult: dd, NN: 1, Integral: 143.26, SNR: 1246.16 From: 7.4927, To: 7.5500, Mult: ddd, NN: 1, Integral: 141.01, SNR: 783.87 From: 6.9500, To: 7.0200, Mult: m, NN: 2, Integral: 271.42, SNR: 1373.12	
Ascorbic_acid	15.332	3100.76 (1373.47, 4288.80)	From: 4.9300, To: 4.9600, Mult: d, NN: 1, Integral: 194.45, SNR: 3640.00 From: 4.0500, To: 4.1200, Mult: ddd, NN: 1, Integral: 279.52, SNR: 1373.47 From: 3.7000, To: 3.8000, Mult: dd, NN: 2, Integral: 518.59, SNR: 4288.80	
Acetic_acid	16.128	32961.71	From: 2.0700, To: 2.1000, Mult: s, NN: 3, Integral: 761.85, SNR: 32961.71	
Citric_acid	93.793	53133.59 (52202.16, 54065.02)	From: 2.9200, To: 3.0600, Mult: d, NN: 2, Integral: 2953.41, SNR: 52202.16 From: 2.7600, To: 2.8800, Mult: d, NN: 2, Integral: 2953.94, SNR: 54065.02	