



Mestrelab Research

Mnova SMA 3.1

USER MANUAL



Document Number

P/N 283 R2

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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.

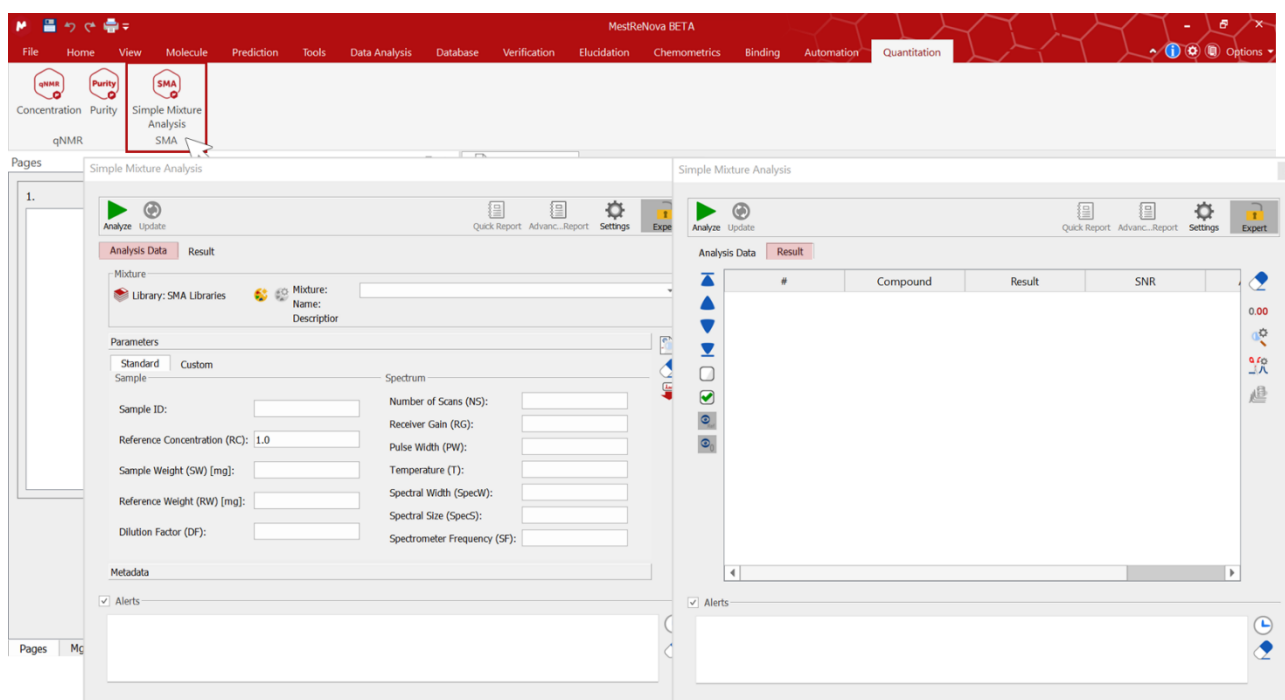
In this manual, we describe all the features provided by the Mnova SMA plugin.

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 sample
	Update result
	Configure SMA analysis settings
	Create a quick report with result
	Create an advanced report with result
	Lock Expert mode
	Activate Expert mode

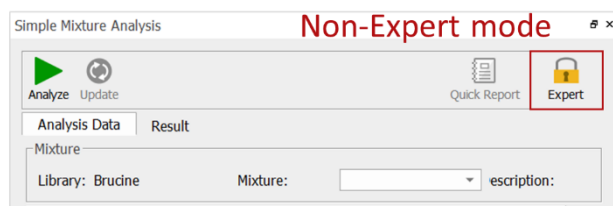
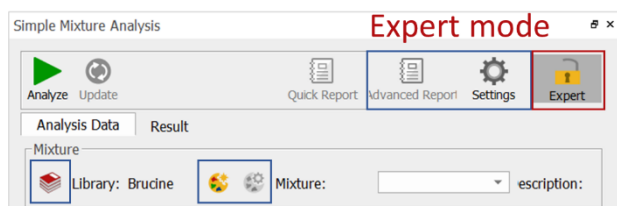
Analysis Data Tab

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
	Show/hide Reference results
	Show/hide results with no valid multiplets
	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

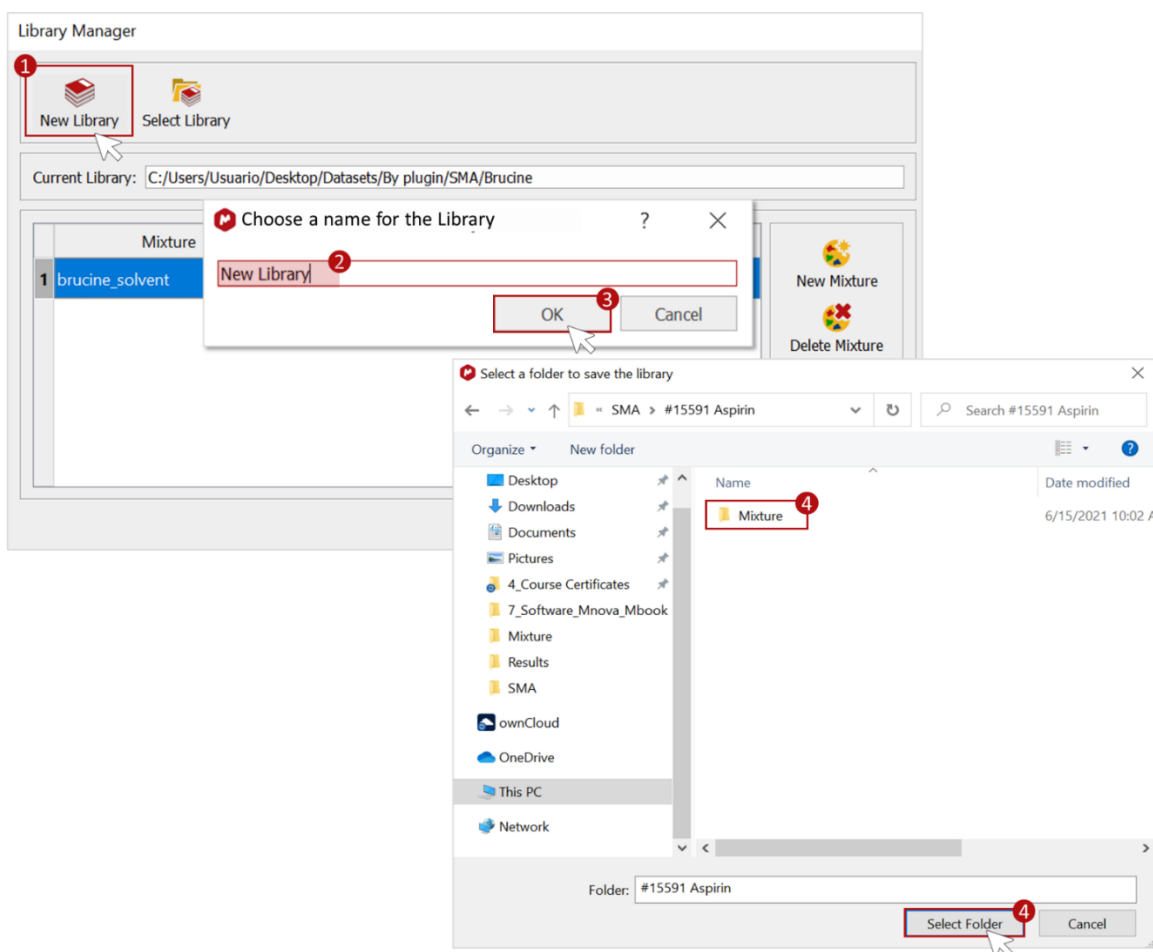
SMA analysis requires a valid mixture/experiment (“.exp” file). Developed and validated methods can be stored in libraries for future use and can easily be shared with other users. It is possible to create an unlimited number of different experiments and save them to either pre-existing or new libraries.

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.

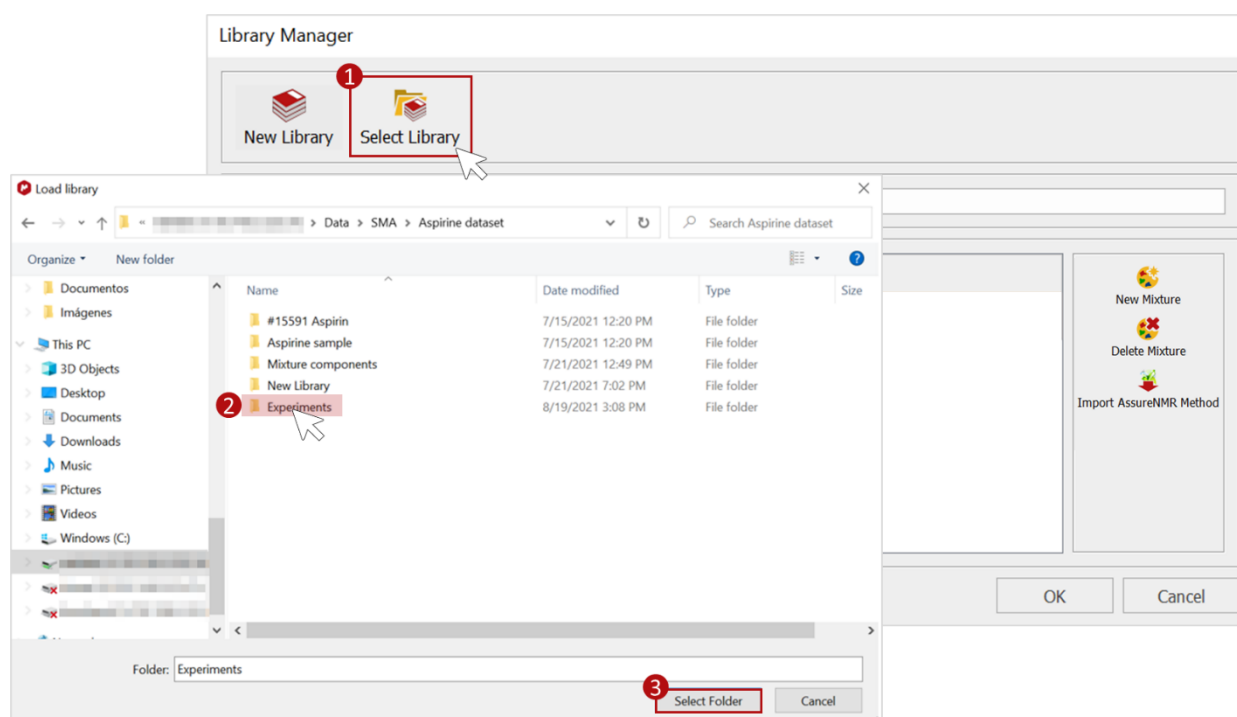


You can now click on **New Mixture** to create a new experiment (refer to [section 3.4](#)).

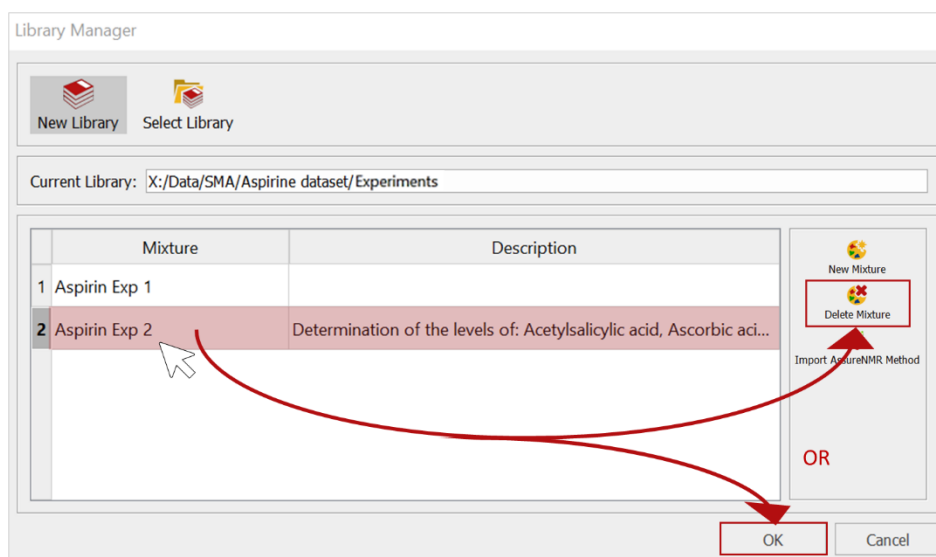
3.2. Selecting a previously created Library

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**.



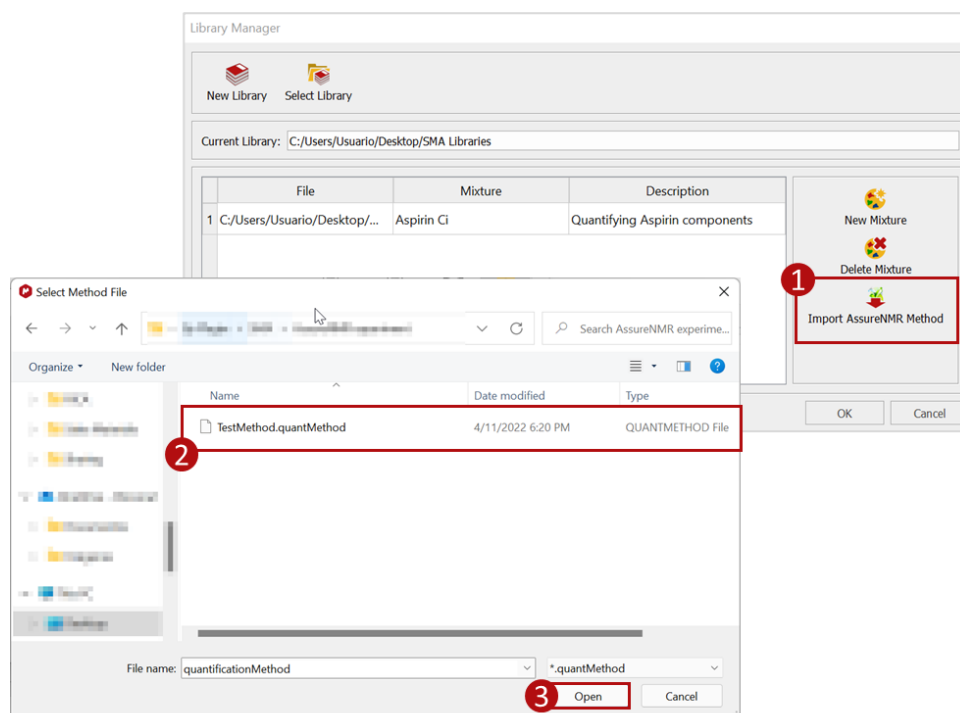
You can now select an experiment from the open library and hit **OK** to use it for your analysis, or even delete a previously added mixture by clicking on **Delete Mixture**.



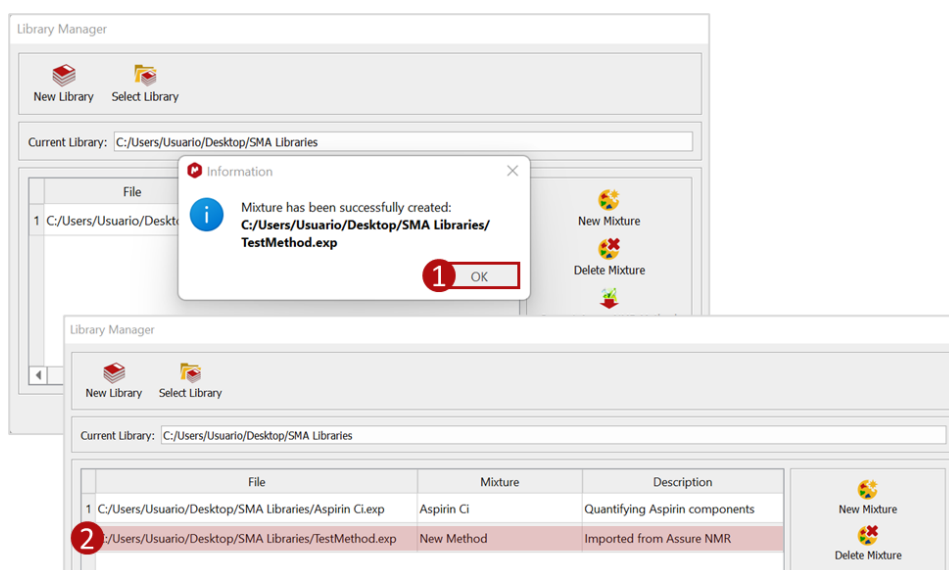
Otherwise, you can **Import an AssureNMR Method**, as explained in [section 3.3](#), or create a **New Mixture** by following the steps described in [section 3.4](#).

3.3.Importing an AssureNMR Method

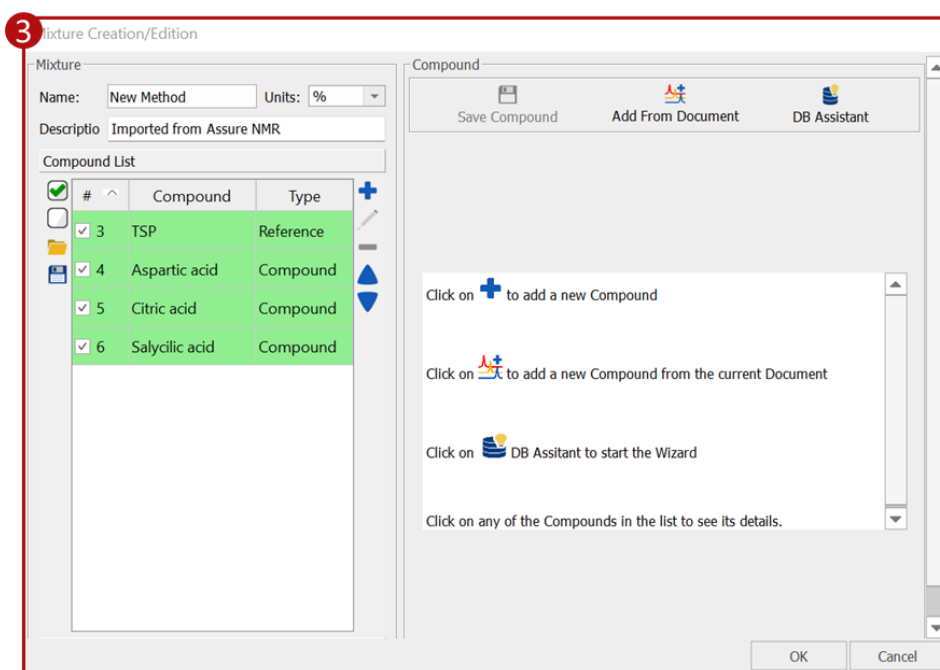
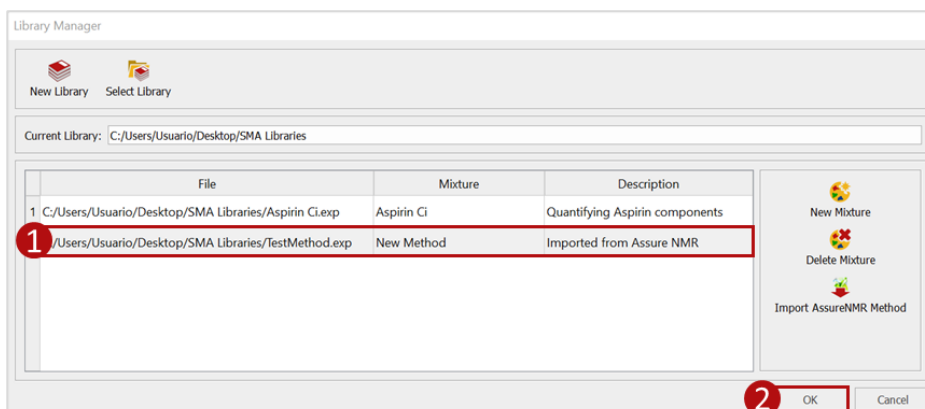
To import an AssureNMR method, press the **Import AssureNMR Method** button and select the “*.quantMethod” file from your directory. Click on **Open**.



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.

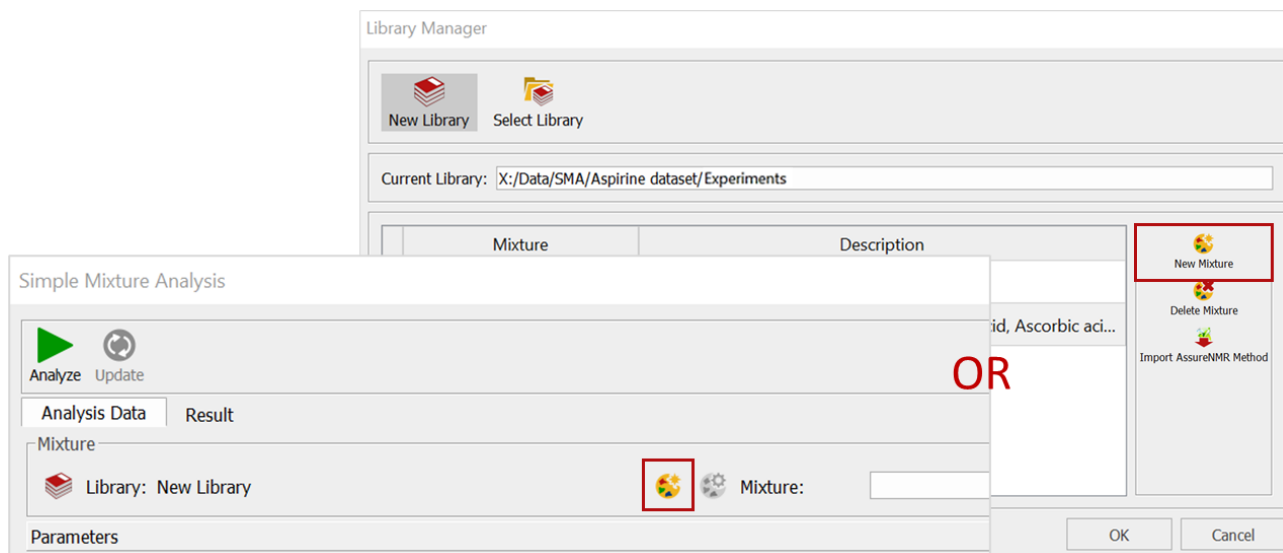


Notes about imported AssureNMR experiments:

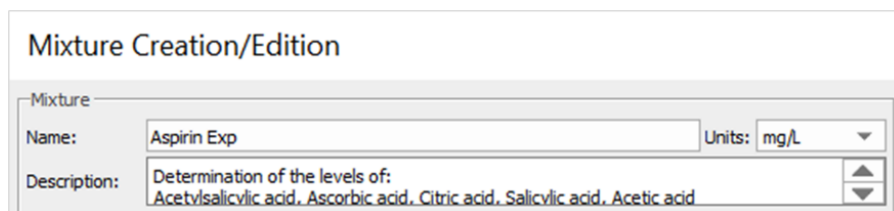
- The generated “.exp” file name matches the original AssureNMR method file name.
- The **Mixture** name is set to “New Method” and the **Description** to “Imported from Assure NMR”.
- The **Calculations**, **PCA**, and **Processing** options are all unchecked by default.
- The “Std. Concentration Eq.” 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.

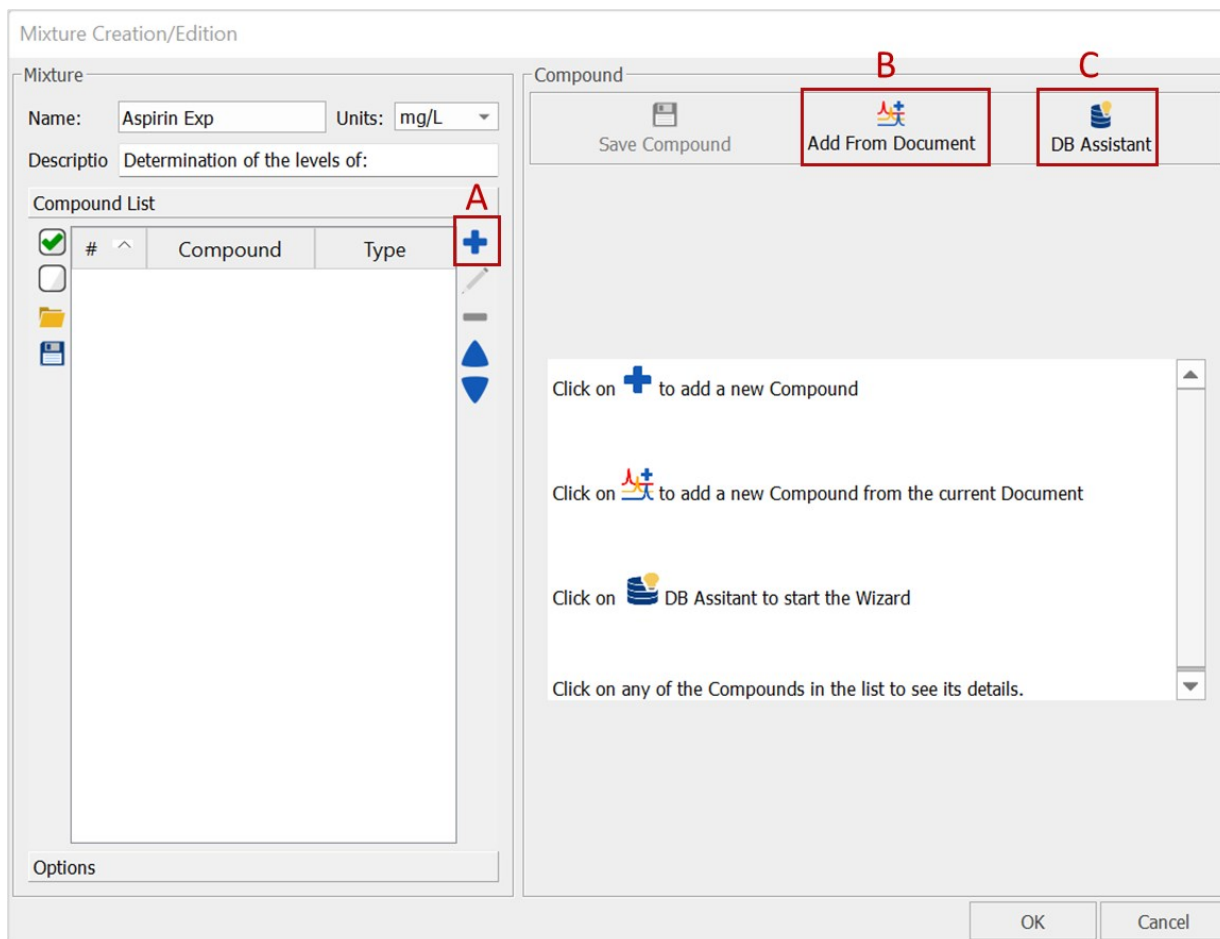


The **Mixture Creation/Edition** dialog will open. Add a name and short description for your experiment.




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

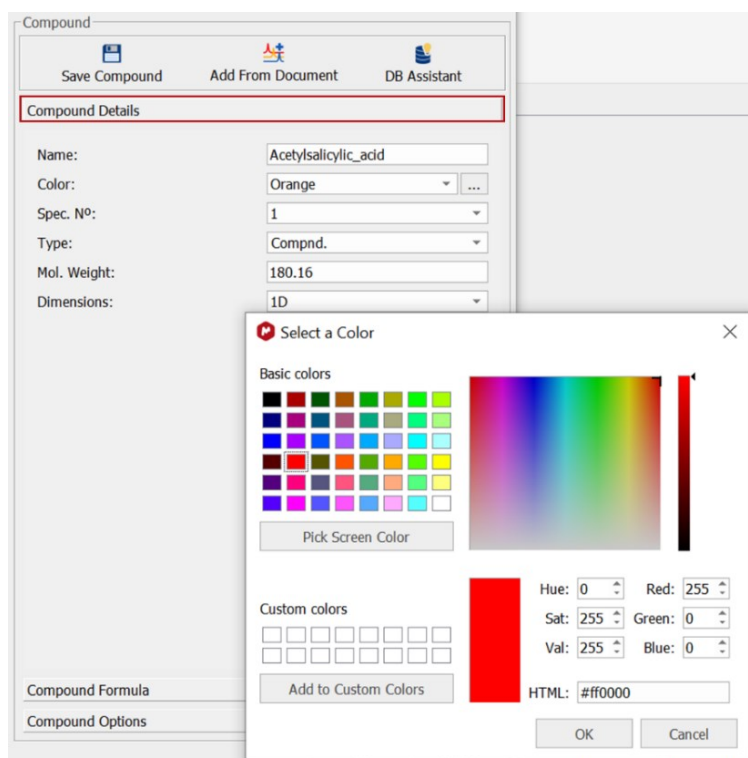


A. Manual addition of mixture compounds

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.

Compound

Save Compound Add From Document DB Assistant

Compound Details

Name: TMSP

Color: Black

Type: Reference

Reference Type: Reference

Mol. Weight: 116.07

Dimensions: 1D

Spec. N°: 1

Reference Spectrum Acquisition Parameters

Number of Scans (NSR):

Receiver Gain (RGR):

Pulse Width (PWR):

Temperature (TR):

Spectral Size (SpecSR):

Spectral Width (SpecWR):

Dilution Factor (DFR):

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.

Reference Type: External PULCON

Mol. Weight: 116.07

Dimensions: 1D

Spectrum File: Jsuario/Desktop/Datasets/Mnova docs/ExternalRef.mnova

Reference Spectrum Acquisition Parameters

Number of Scans (NSR): 8

Receiver Gain (RGR): 38

Pulse Width (PWR): 6

Temperature (TR): 29

Spectral Size (SpecSR): 16384

Spectral Width (SpecWR): 4801.34437643

Dilution Factor (DFR):

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

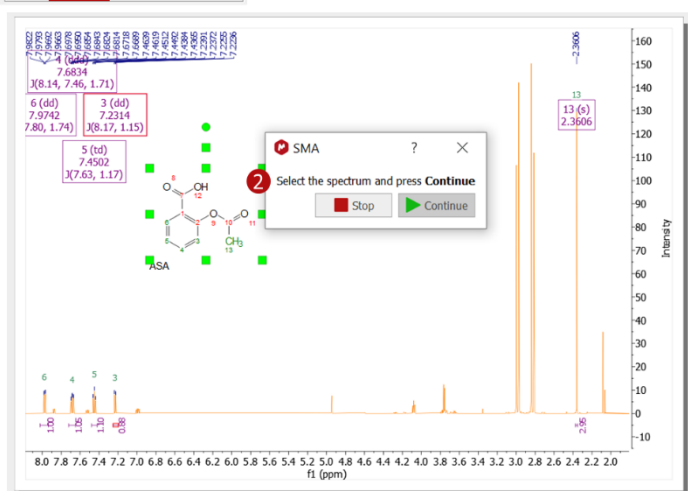
A.2. Compound formula

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.

Add ranges from current Spectrum



Automatically



Add ranges from current Spectrum

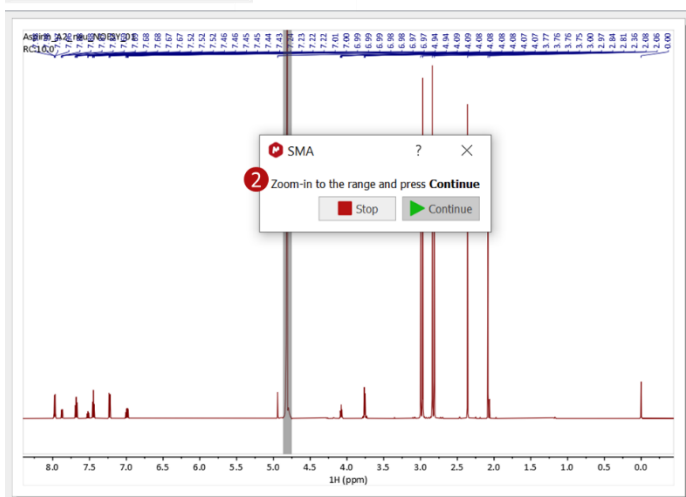
Pattern Recognition

Active	From	To	Mult.	J's	NN	Pattern
<input checked="" type="checkbox"/>	8.00	7.95	dd	10.8,1.7	1	
<input checked="" type="checkbox"/>	7.72	7.65	ddd	8.1,7.8,1.7	1	
<input checked="" type="checkbox"/>	7.48	7.42	td	7.6,1.2	1	
<input checked="" type="checkbox"/>	7.26	7.20	dd	8.2,1.2	1	

Add ranges from current Spectrum



Manually

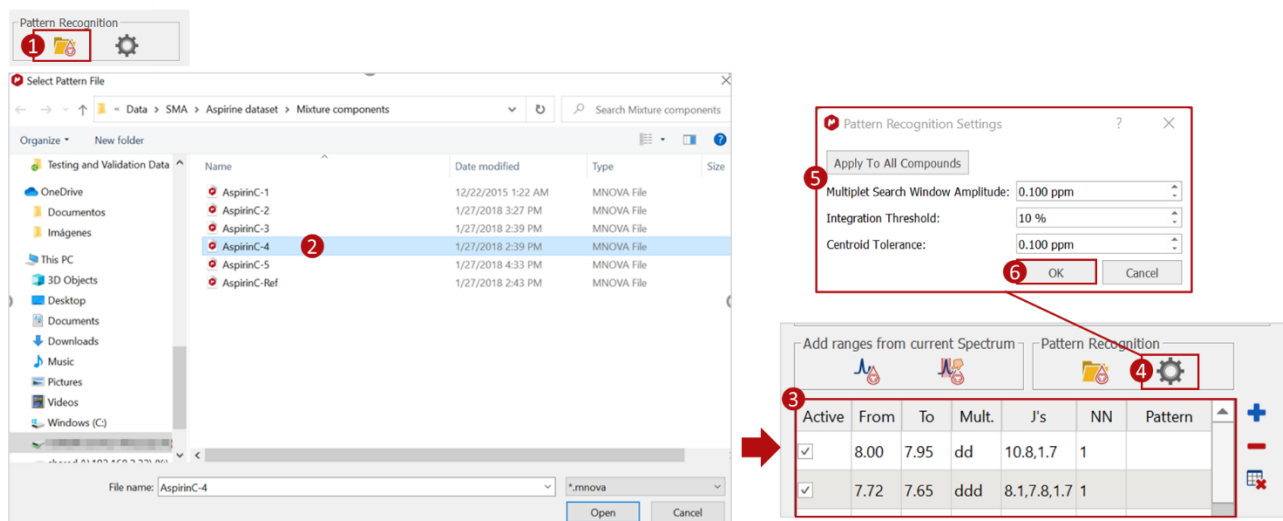


Add ranges from current Spectrum

Pattern Recognition

Active	From	To	Mult.	J's	NN	Pattern
<input checked="" type="checkbox"/>	8.00	7.95	dd	10.8,1.7	1	
<input checked="" type="checkbox"/>	7.72	7.65	ddd	8.1,7.8,1.7	1	
<input checked="" type="checkbox"/>	7.48	7.42	td	7.6,1.2	1	
<input checked="" type="checkbox"/>	7.26	7.20	dd	8.2,1.2	1	

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.

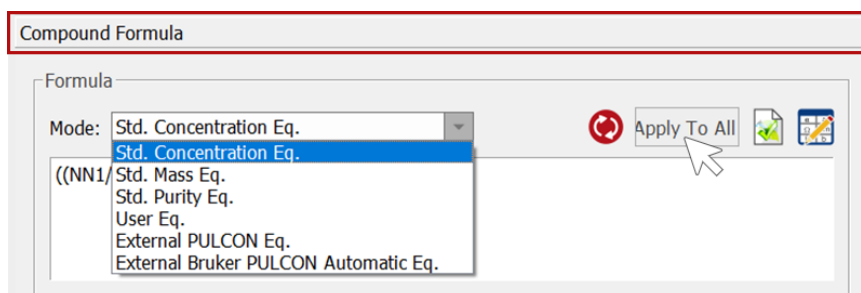


The **Pattern Recognition Settings** include:

- 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.

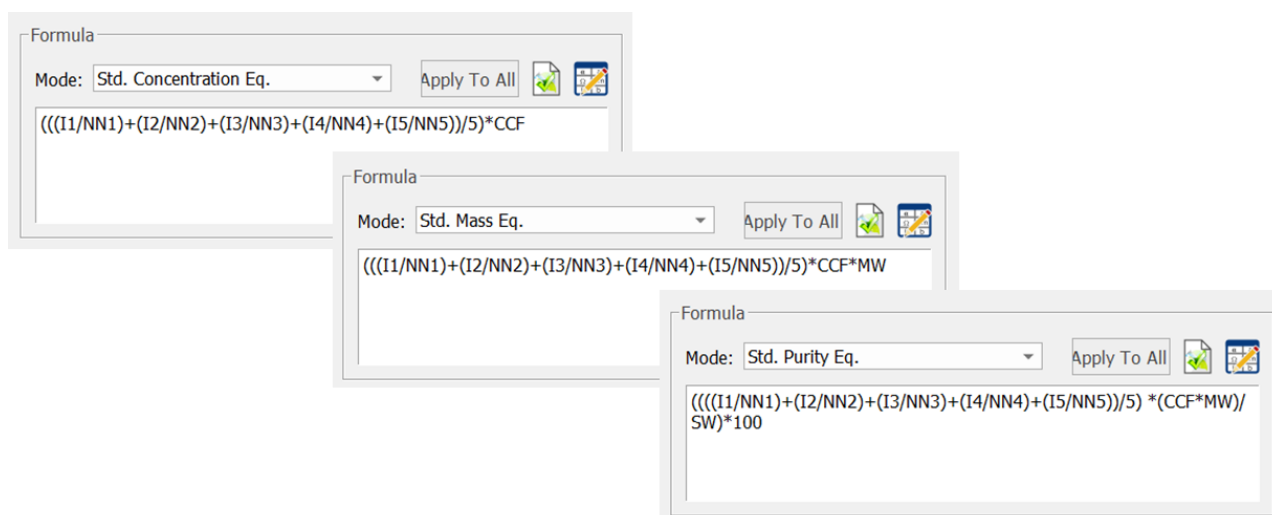
Once you have configured these parameters, you can apply them to all the compounds in the mixture.

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.

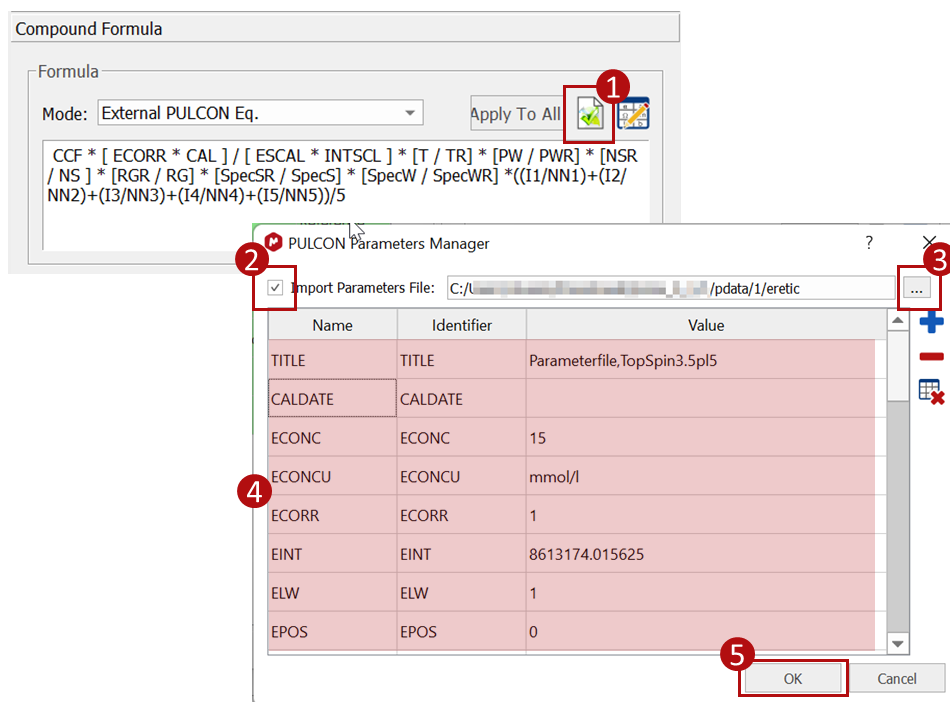


A.2.2. External PULCON equation

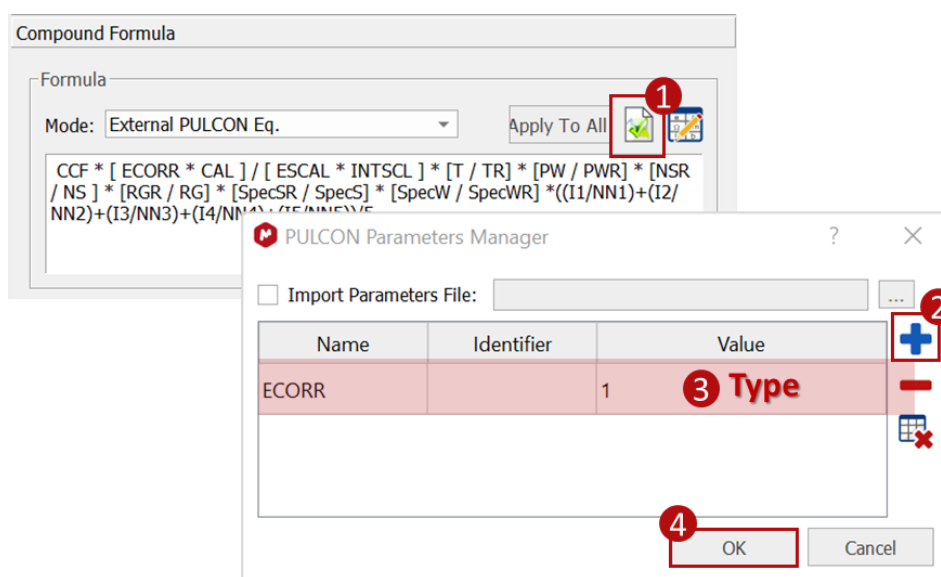
When using an **External PULCON equation** for quantitation, PULCON parameters must be provided (via an “eretic” file or manually) to correctly apply the equation.

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.

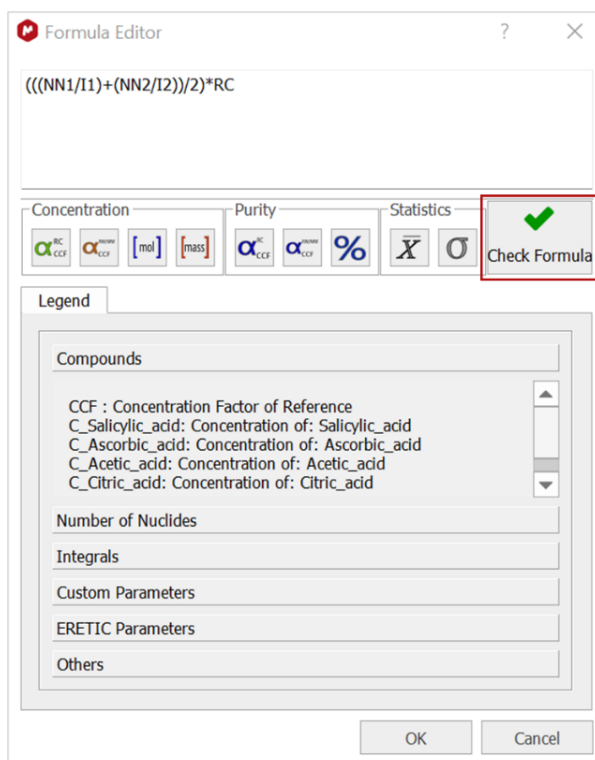
Click **OK** to save your changes. The **External PULCON equation** is now correctly defined.

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

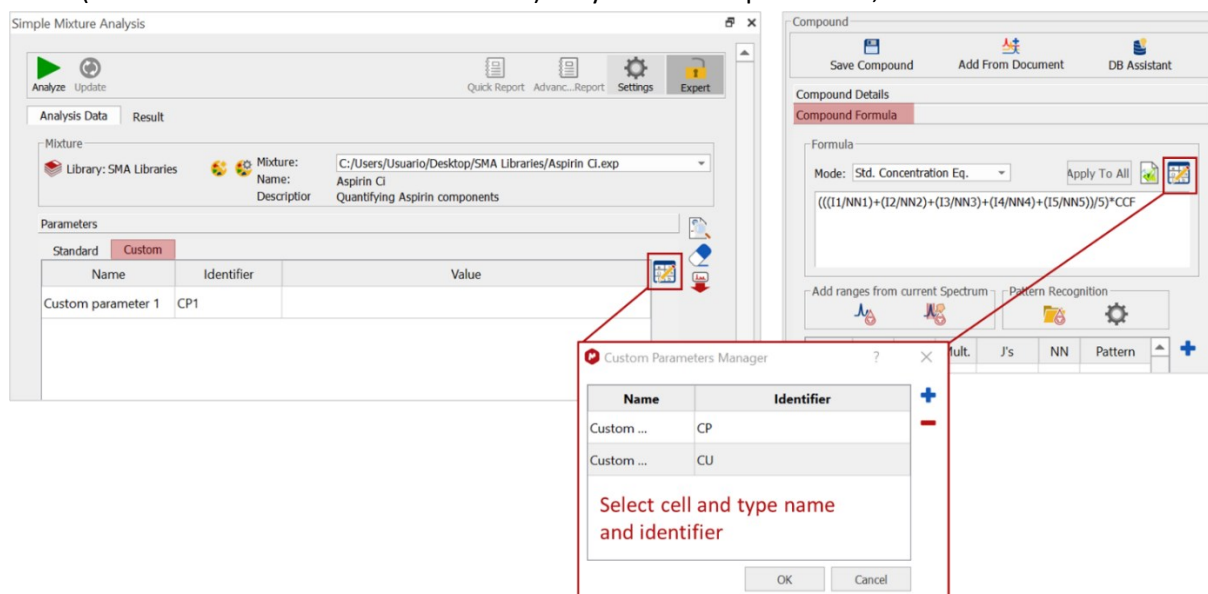
To add your own formula, choose the **User Equation** mode; the **Formula Editor** will open. Use the available buttons to type and check your formula for errors. You can read more about the [formula editor](#) in our associated blog post.



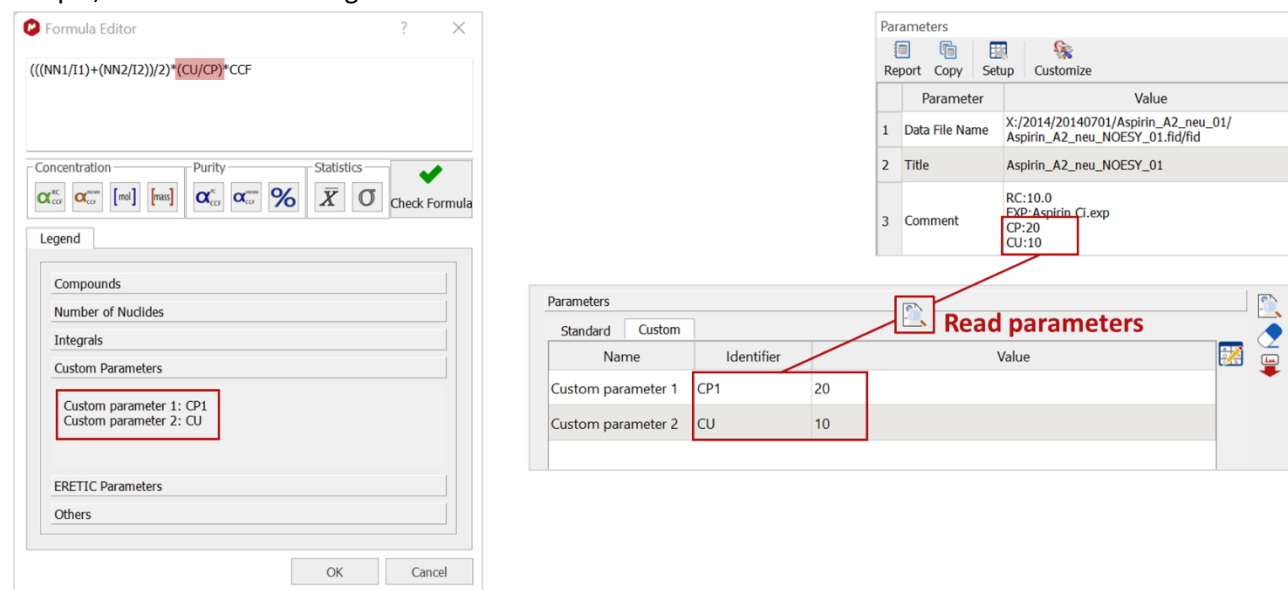
Note that you can also define custom or PULCON parameters to be used in the equation for the concentration calculation.

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**.

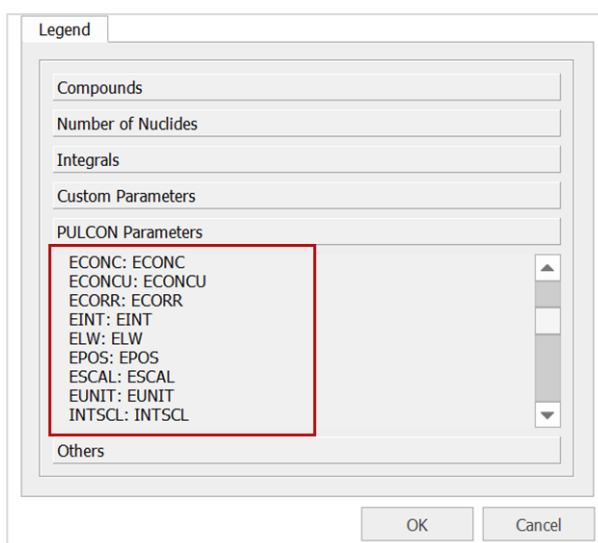


The custom parameters are now added to the **Custom** table and to the **Formula editor** and can be used in the equation. **Values** for custom parameters can be added manually or read from the **Parameters** table of the sample, as shown in the image below.



PULCON Parameters

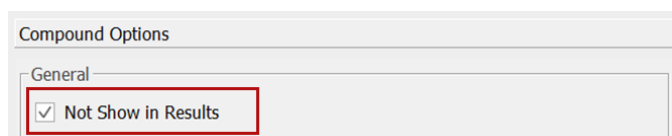
How one defines PULCON parameters is described [above](#). The PULCON parameters are added to the **Formula editor**, as seen in the image below, and can be used to complete the user custom equation.



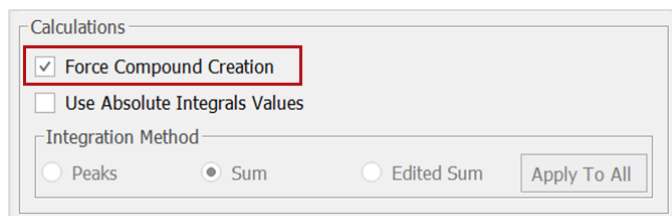
A.3. Compound options

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.

Calculations

Force Compound Creation

Use Absolute Integrals Values

Integration Method

Peaks Sum Edited Sum

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


Calculations

Force Compound Creation

Use Absolute Integrals Values

Integration Method

Peaks Sum Edited Sum

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

Mixture Creation/Edition

Mixture

Name: Aspirin Exp Units: mg/L

Description: Determination of the levels of:

Compound List

#	Compound	Type
1	TMSP	Reference
2	Acetylsalicylic_acid	Compnd.

Compound

Compound Details

Compound Formula

Compound Options

General

Do not show in Results

Calculations

Force Compound Creation

Use Absolute Integrals Values

Integration Method

Peaks Sum Edited Sum

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.

Multiple Mnova documents

OR

One Mnova document with multiple pages

The screenshot shows the Mnova interface. At the top, there are several document windows: AspirinC-1*, AspirinC-2, AspirinC-3, AspirinC-4, AspirinC-5, and AspirinC-Ref. Below these, a main window displays a spectrum with peaks labeled A, B, and C. The chemical structure of Salicylic acid is shown on the left. The spectrum has an x-axis labeled 'ft (ppm)' ranging from 8.4 to 6.4 and a y-axis labeled 'Intensity' ranging from -1 to 19. Peak A is at 7.8766 ppm (dd), peak B is at 7.5241 ppm (ddd), and peak C is at 6.9925 ppm (m). A 'Pages' panel on the right shows three pages of spectra, each with a small chemical structure and peak labels.

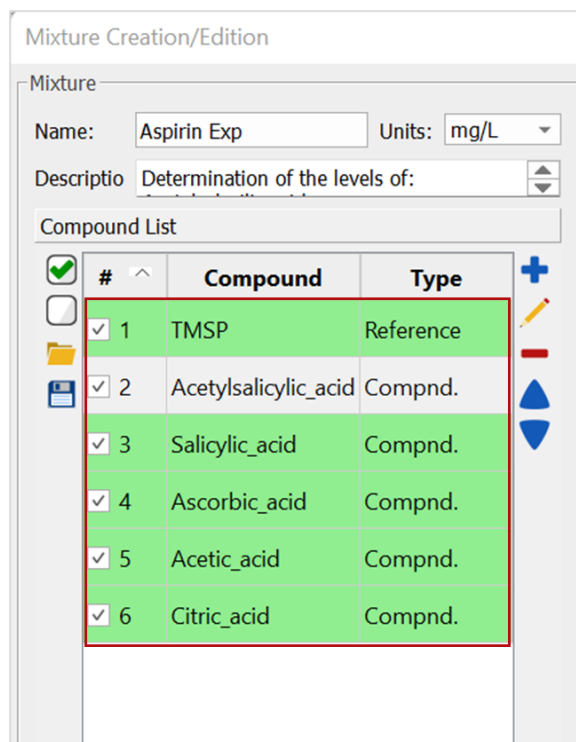
Select the Mnova document or Mnova document pages with the compounds you wish to add, then click on



to import the compound's details into the **SMA Mixture Creation/Edition** panel.

The screenshot shows the 'SMA Mixture Creation/Edition' panel. The 'Compound' section has three buttons: 'Save Compound', 'Add From Document' (highlighted with a red box and a mouse cursor), and 'DB Assistant'. Below these buttons, there are instructions: 'Click on + to add a new Compound', 'Click on [icon] to add a new Compound from the current Document', 'Click on [icon] DB Assistant to start the Wizard', and 'Click on any of the Compounds in the list to see their details.' The background shows a spectrum with intensity on the y-axis (ranging from -10 to -160) and chemical structures on the right.

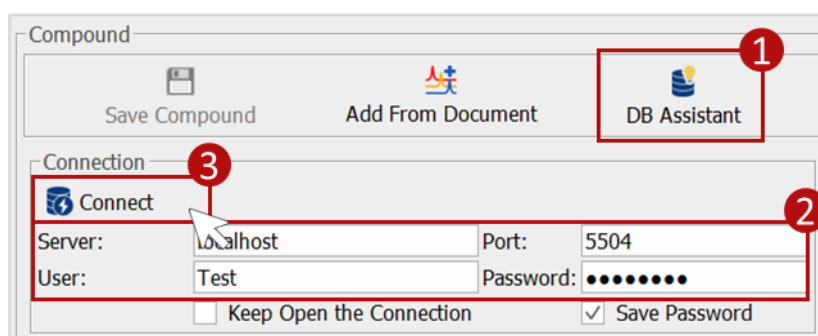
The added compounds will appear in the **Compound List**, as shown below.



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

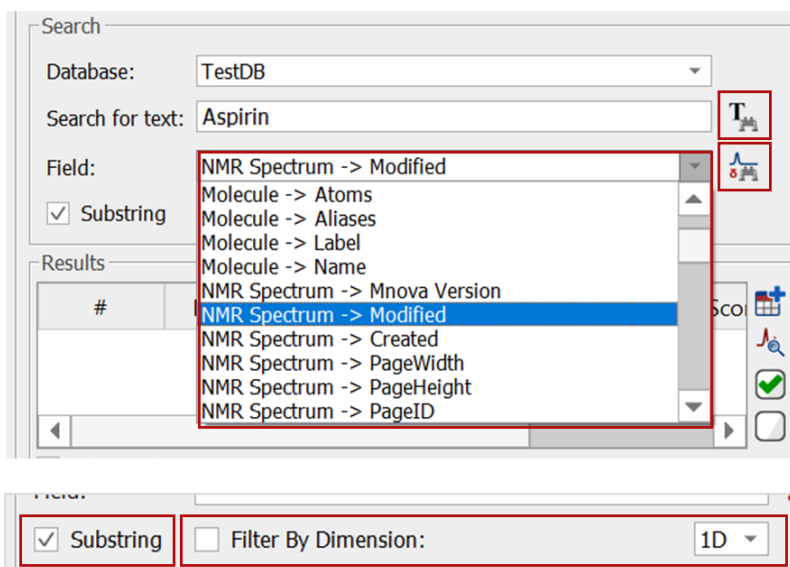
Launch the **DB assistant** by clicking on . Enter the server connection details, then click on **Connect**.




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

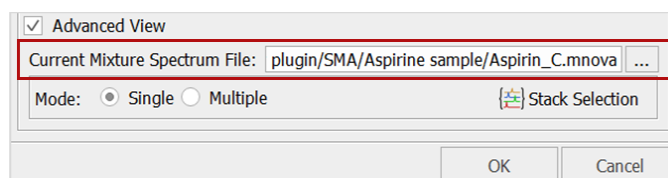
Choose the DB you want to search, then type the text and click on to search. You can also search your database by multiplets/peaks. To do so, open a spectrum in Mnova, then click on the button.

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



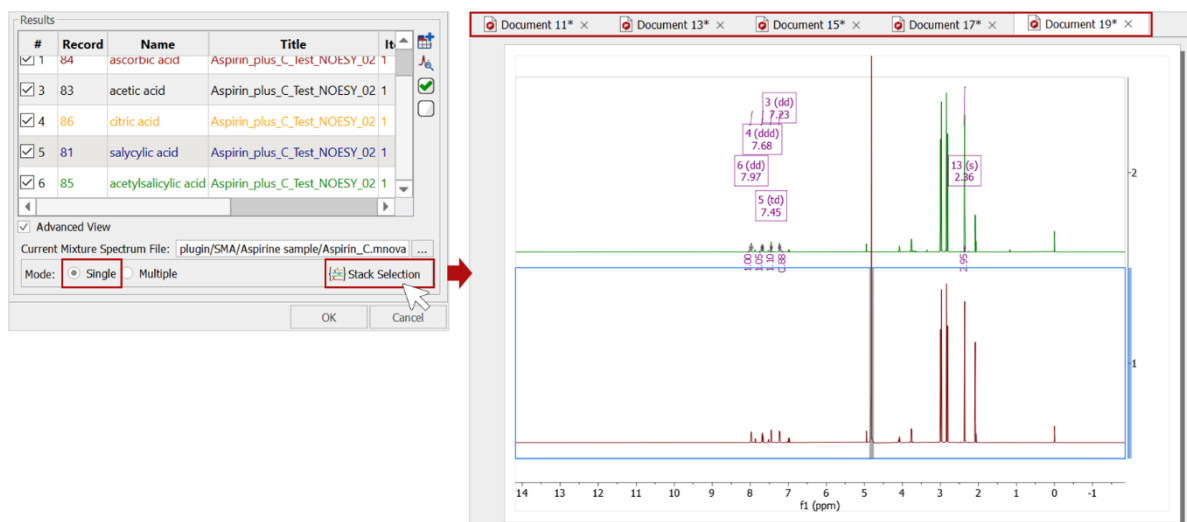
The search hits will appear in the **Results** section. You can double click on a database record to open and view it, or you can select more than one record and click on the zoom button  to open them all at once.

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).

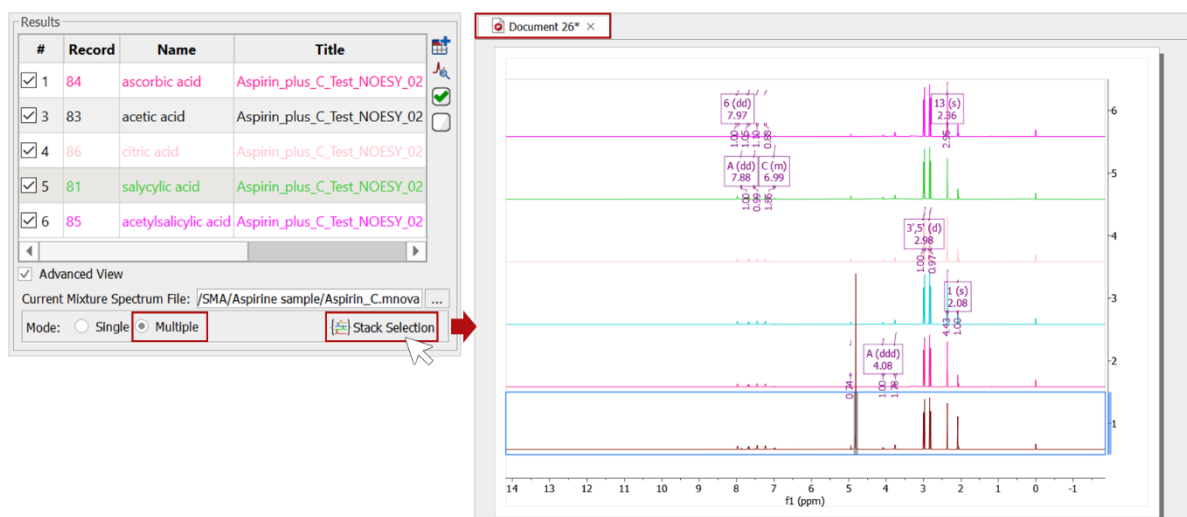


This option is available in the **Advanced View** panel (hidden by default) and offers two stacking modes:

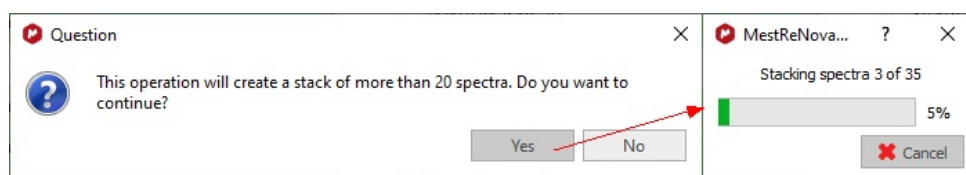
- The **Single** mode: stacks spectra one by one with the base analyte spectrum. A new Mnova document is generated with the stacked spectra for every selected record.




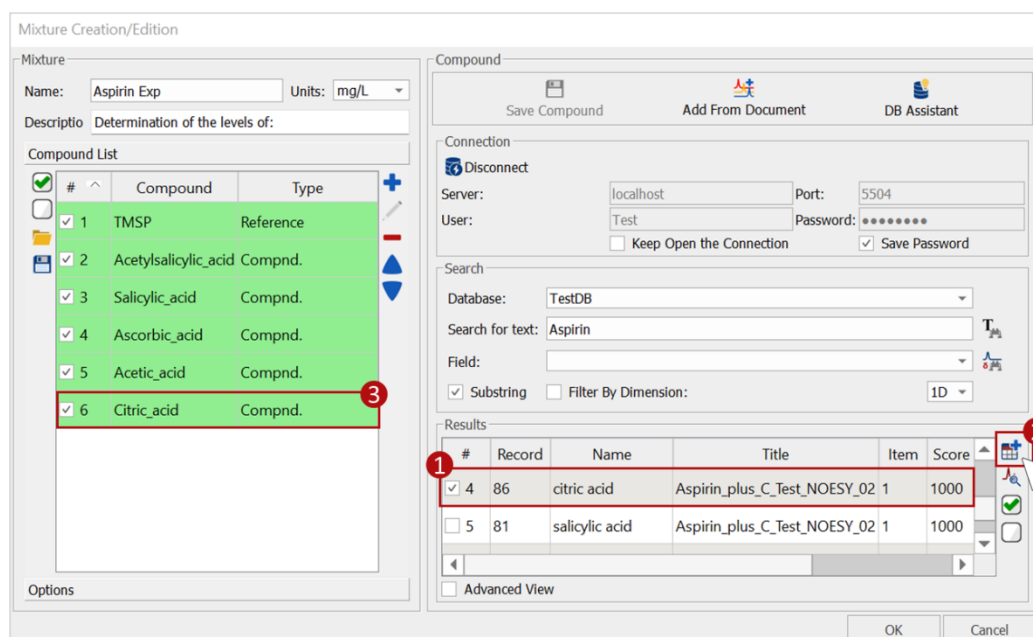
- The **Multiple** mode: stacks all spectra together.



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.

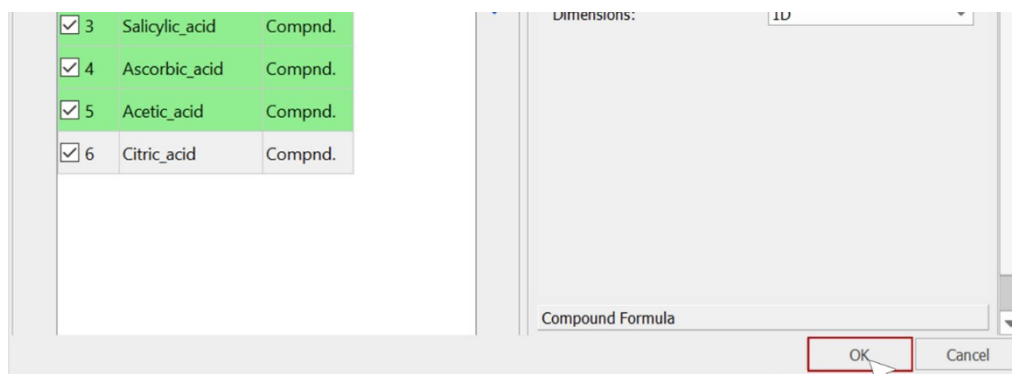


Now select the compound(s) you want to add to your mixture and click on  to add it (them) to the **Compound List**.



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

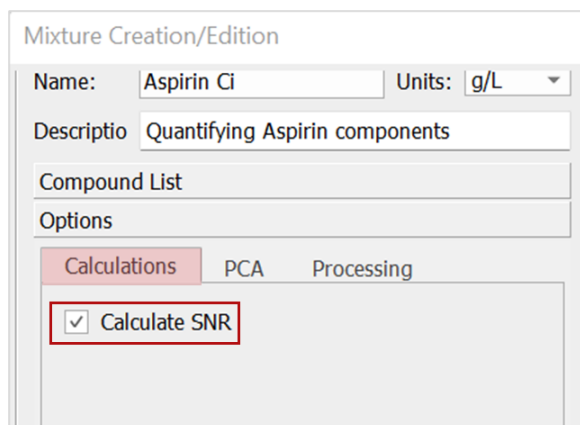
Once all your mixture compounds are added, you can save your mixture/experiment by clicking **OK**.



3.5. Configuring experiment options

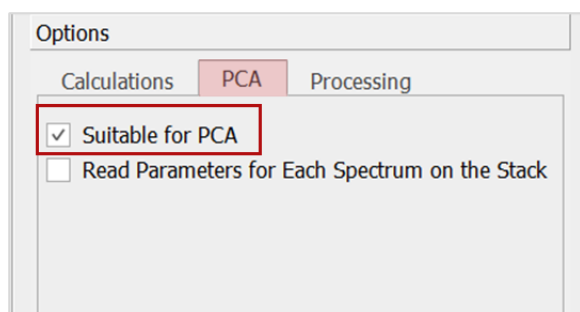
In the **Calculations** tab, you can enable the option to **Calculate SNR**. When enabled, the SNR value will be calculated and included in the results table.

Note that SNR will only be calculated for 1D spectra



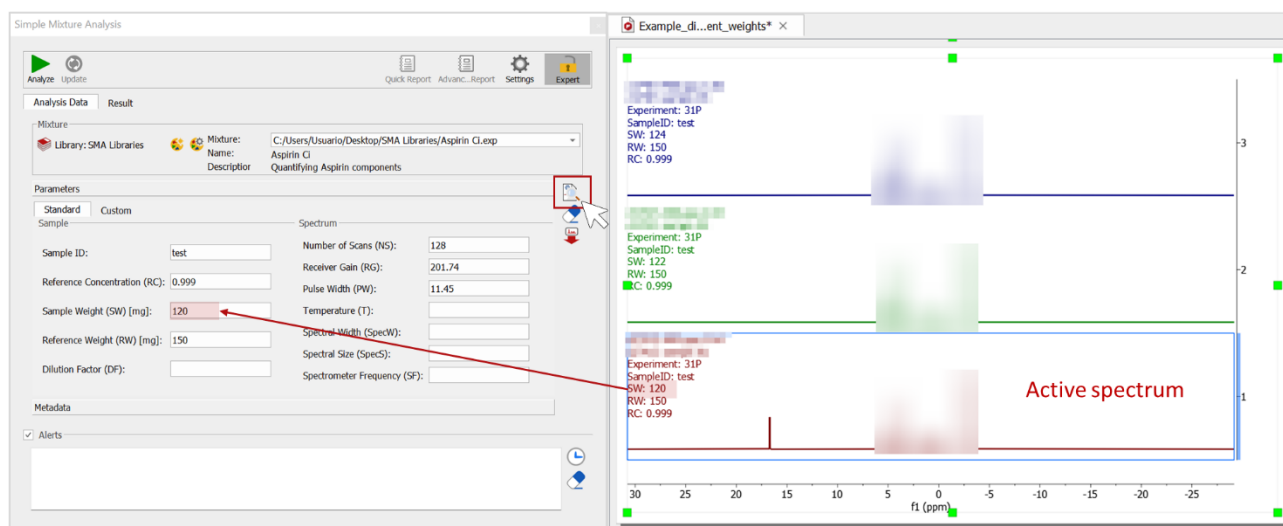
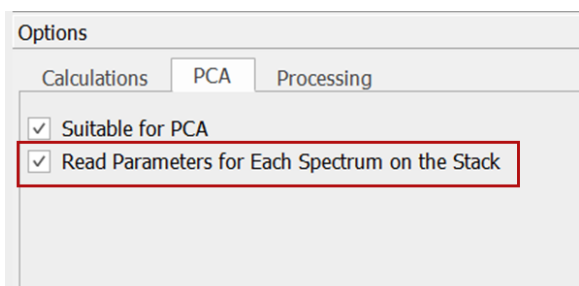
The screenshot shows the 'Mixture Creation/Edition' dialog box. The 'Name' field is 'Aspirin Ci' and 'Units' is 'g/L'. The 'Description' is 'Quantifying Aspirin components'. The 'Options' section is expanded to the 'Calculations' tab, where the 'Calculate SNR' checkbox is checked and highlighted with a red box.


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)**.

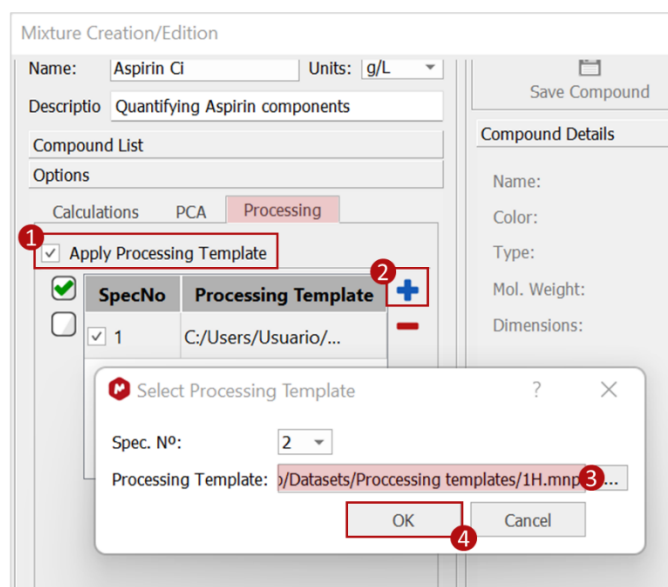


The screenshot shows the 'Options' dialog box with the 'PCA' tab selected. The 'Suitable for PCA' checkbox is checked and highlighted with a red box. The 'Read Parameters for Each Spectrum on the Stack' checkbox is unchecked.

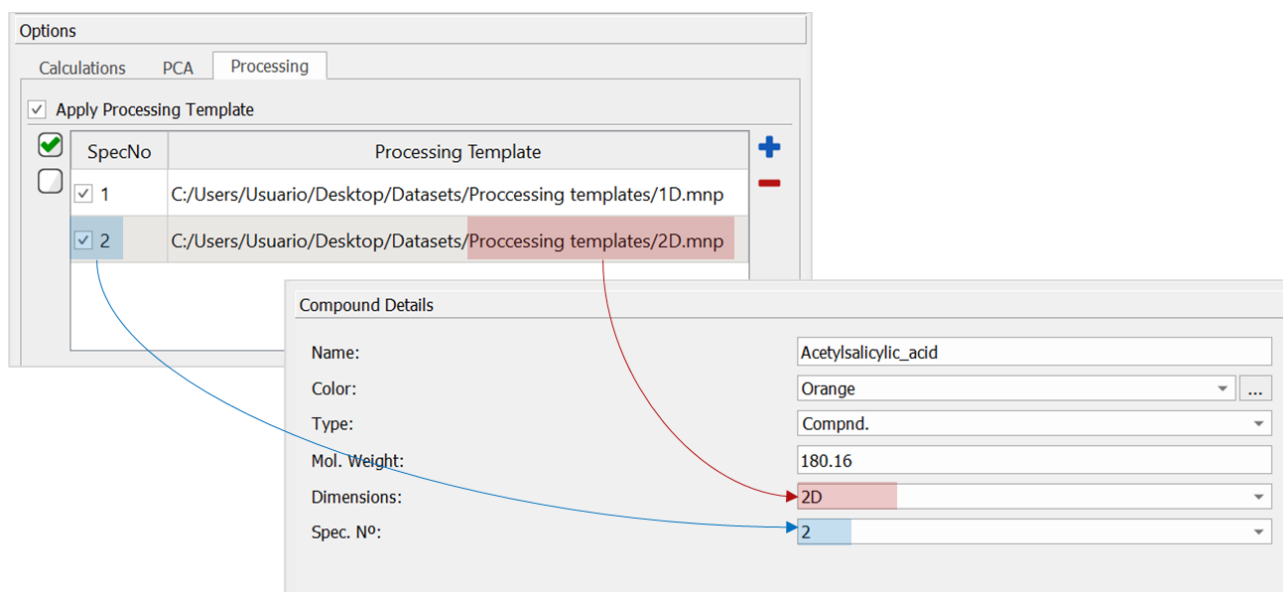
When performing a PCA analysis with a stack of spectra, the option to **Read parameters for each spectrum on the stack** is also available. If enabled, SMA will update the parameters for each spectrum calculation from the comments field in the parameters table of the sample. The updated parameters can 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.



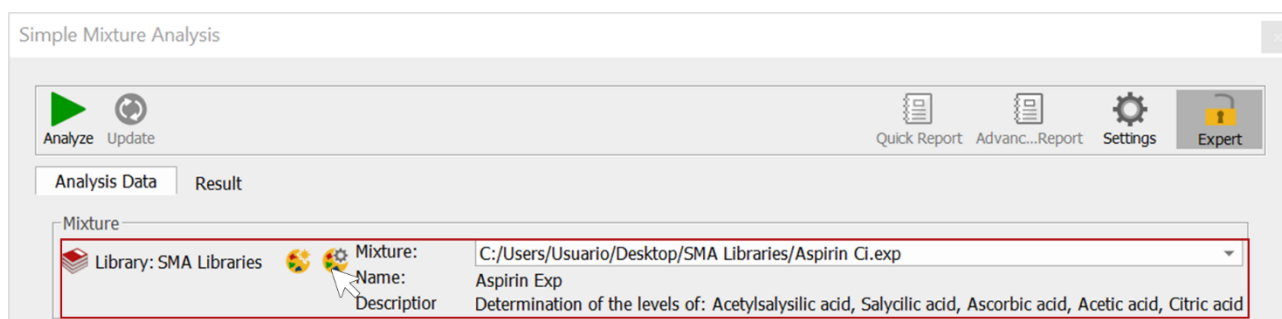
When a mixture includes components with different types of nuclei and/or dimensions, it is possible to add a processing template for each. In such cases, a different spectrum number (**SpecNo**) must be attributed to each processing templates. In the example below, the 2D processing template will be 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.



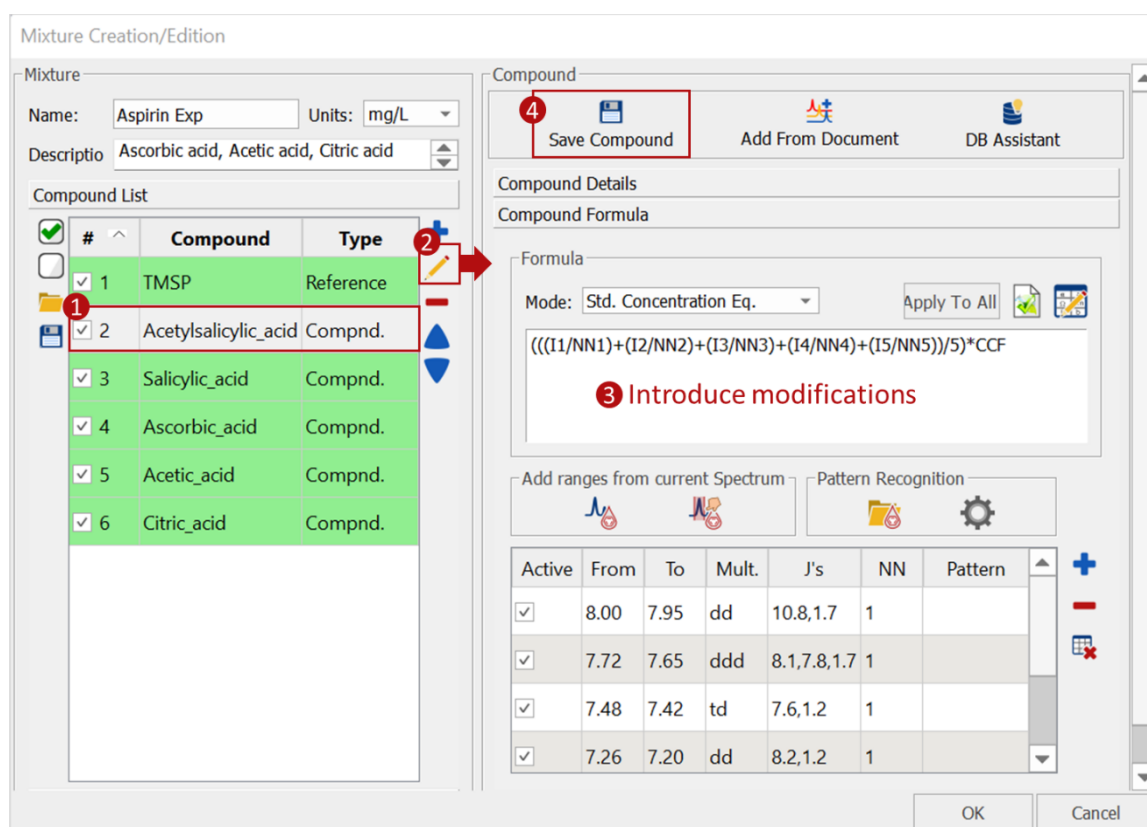
Finally, you can check or uncheck table rows to delete processing templates .



3.6.Reviewing/editing the mixture details

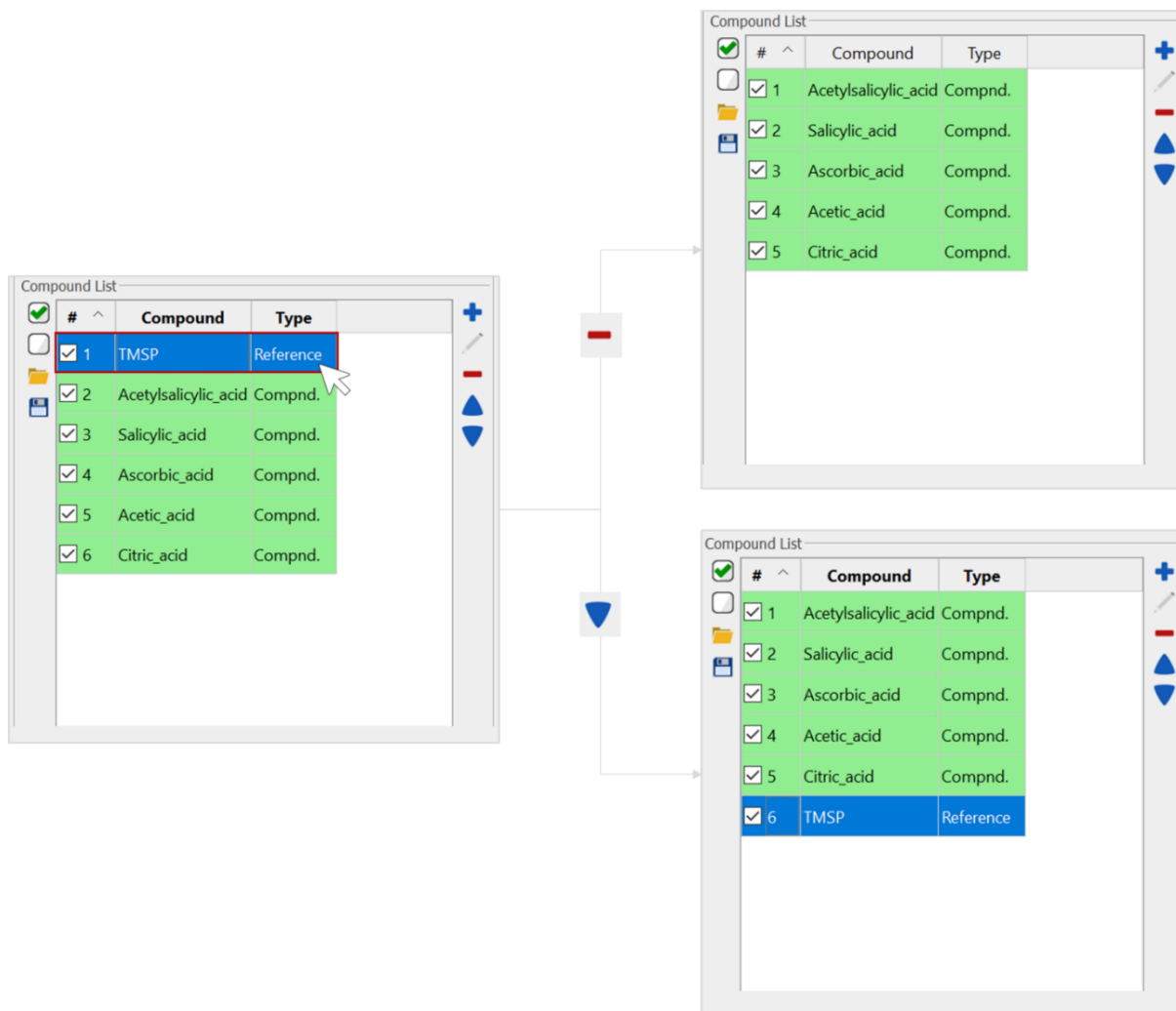
Your library and selected mixture are now displayed in the SMA panel. You can open your experiment to edit **Mixture** and **Compound** details by clicking on this button



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.



The diagram illustrates the modification of a compound list through three sequential states:

- Initial State:** A 'Compound List' window containing six entries:

#	Compound	Type
1	TMSP	Reference
2	Acetylsalicylic_acid	Compnd.
3	Salicylic_acid	Compnd.
4	Ascorbic_acid	Compnd.
5	Acetic_acid	Compnd.
6	Citric_acid	Compnd.
- Deletion:** A minus sign icon is shown next to the first entry, indicating its removal.
- Reordering:** An up/down arrow icon is shown next to the sixth entry, indicating its movement to the top of the list.

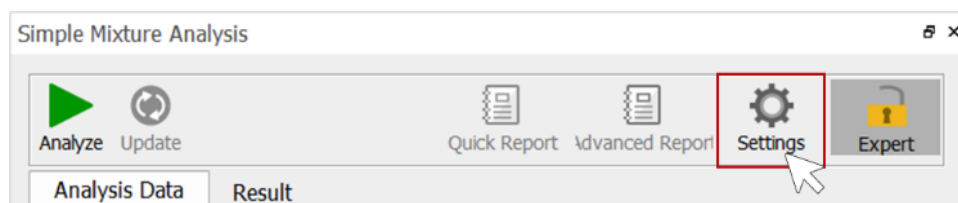
The final state of the 'Compound List' window is:

#	Compound	Type
1	Acetylsalicylic_acid	Compnd.
2	Salicylic_acid	Compnd.
3	Ascorbic_acid	Compnd.
4	Acetic_acid	Compnd.
5	Citric_acid	Compnd.
6	TMSP	Reference

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

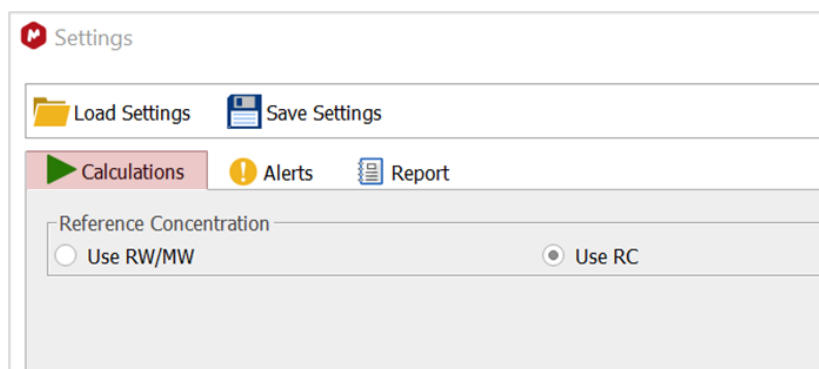
4. SMA general settings

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.

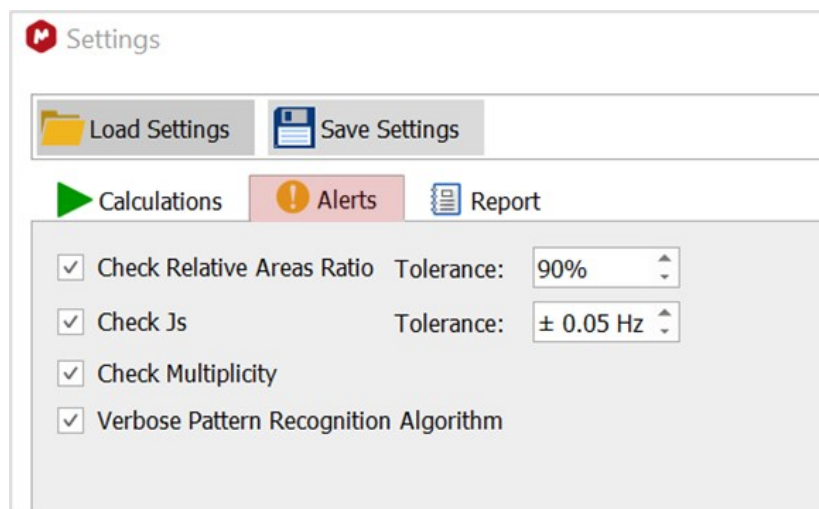


4.2. The Alerts tab

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.

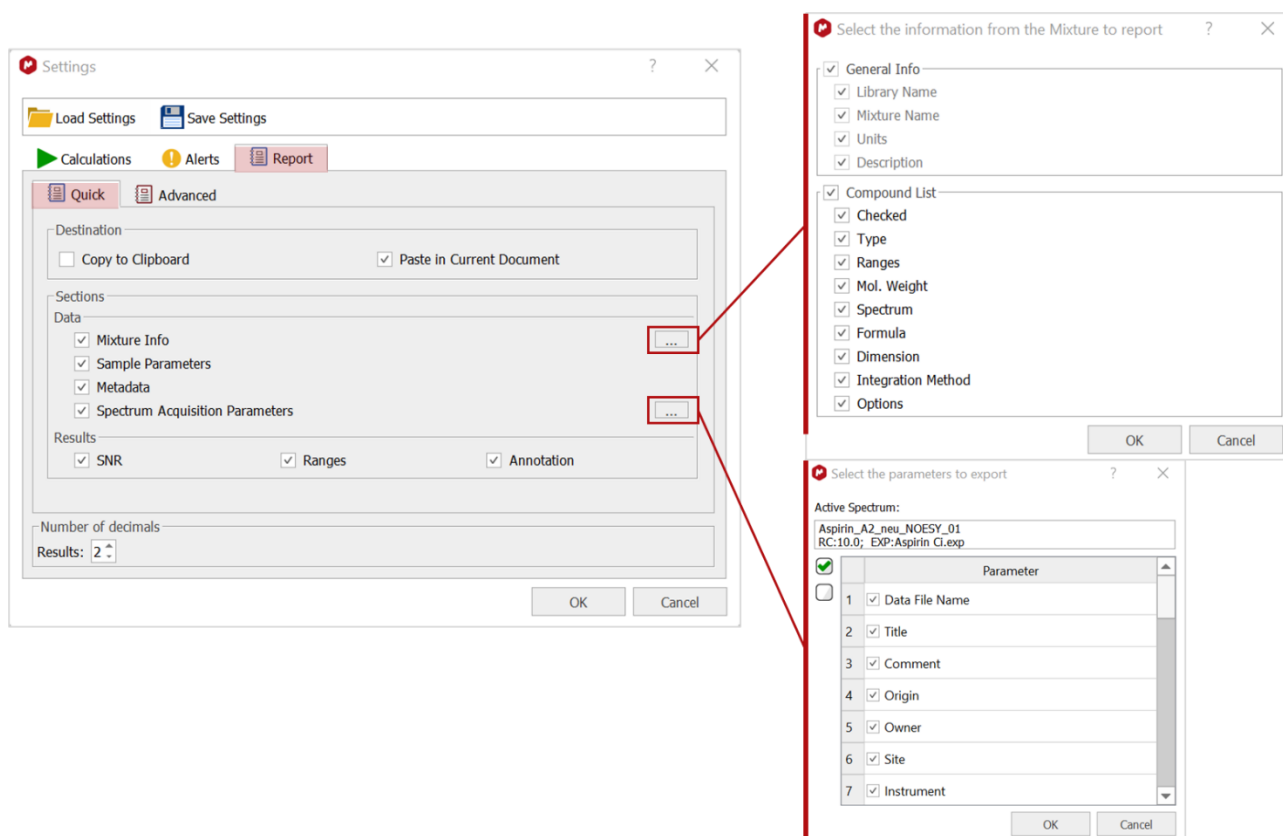
A. Quick Reports

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

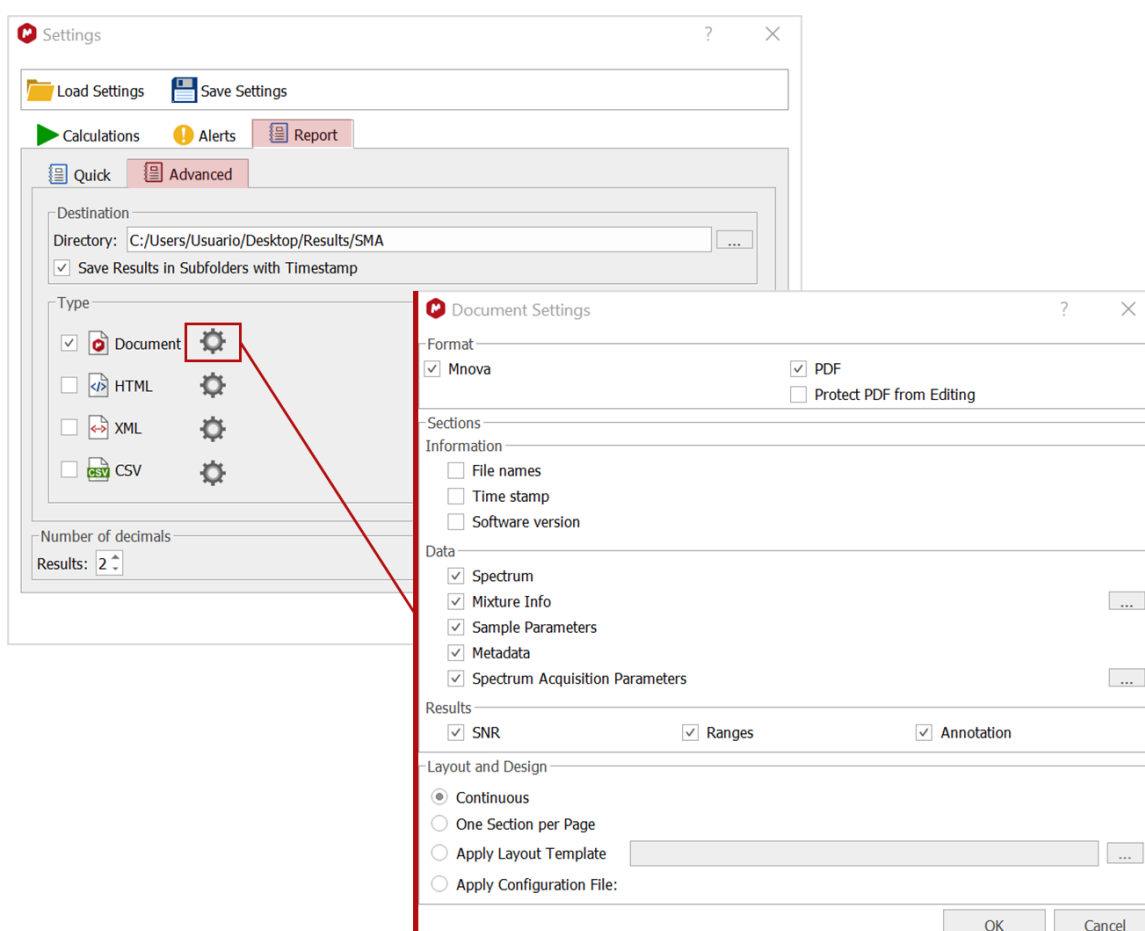
On the other hand, **Advanced reports** are extent reports with complete information about the experiment's parameters and results. Various types of advanced reports are available and customizable (PDF, Mnova, HTML, XML, CSV). Advanced reports can be saved in the directory of your choice.

Mnova and PDF reports configuration:

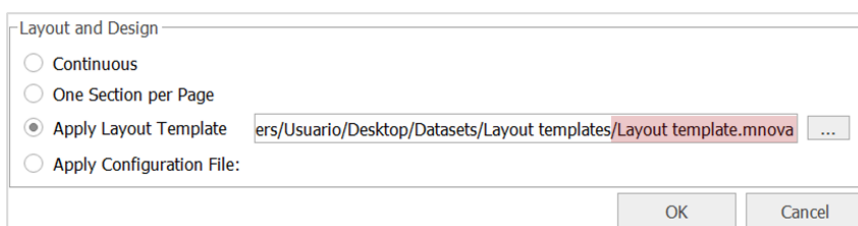
Both Mnova and PDF reports can be generated, and PDF reports can be protected from editing.

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.

1 Apply Configuration File:

- Default
- Custom

2 Download

3 Name

- ConfigurationFile.json
- Template_CompoundList_FirstPage.mnova
- Template_CompoundList_OtherPages.mnova
- Template_Logo_SMA.mnova
- Template_Metadata.mnova
- Template_Results.mnova
- Template_SampleParameters.mnova
- Template_Signatures.mnova
- Template_Spectrum.mnova
- Template_SpectrumAcquisitionParameters.mnova
- Template_TitleInfo.mnova

3 Edit and Save

```

{
  "filename": "C:/Users/Usuario/Desktop/Work/Issues/20099_test/Example5/Configuration/Template_Results.mnova",
  "apply": "true",
  "applyToSection": "Results",
  "applyToPage": "Others",
  "pageSettings": {
    "footer": {
      "alignment": "66",
      "macro": "{pageIndex}/{pageCount}",
      "foregroundColor": "#000000",
      "visible": "true",
      "opacity": "0.7",
      "font": {
        "family": "Arial",
        "size": 10,
        "bold": false,
        "italic": false,
        "underline": false
      }
    }
  }
}

```

4 Custom /Usuario/Desktop/Datasets/By Plugin/SMA/MyConfigurationFile.json

Use Custom Configuration file

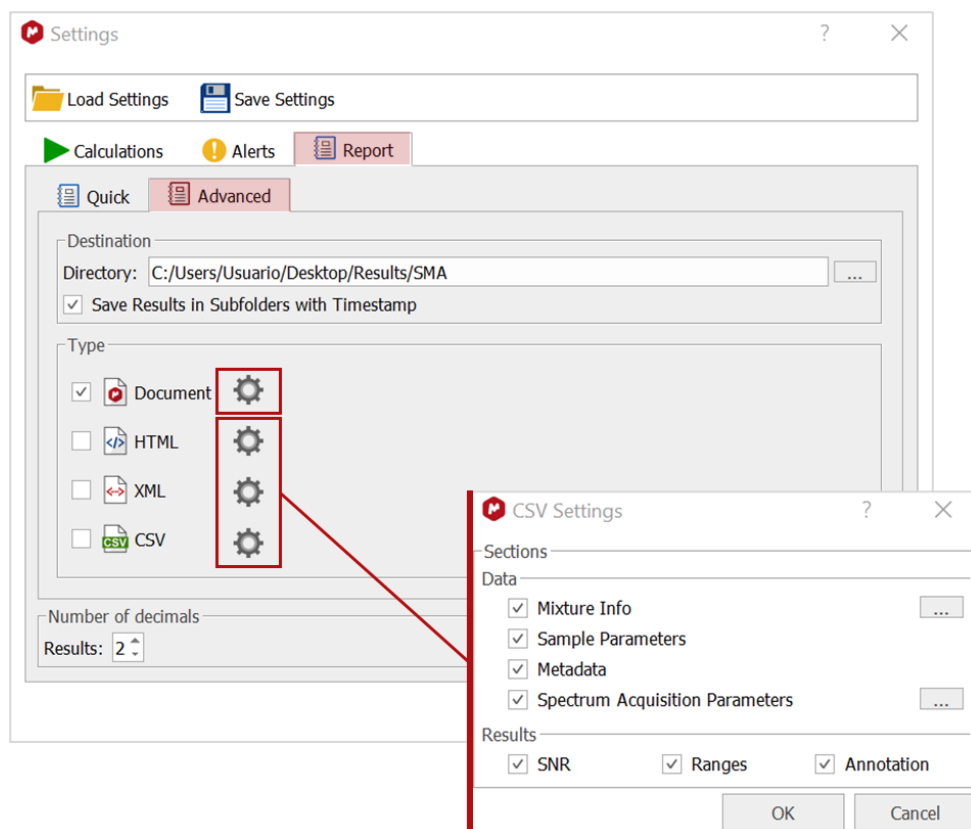
Layout and Design

- Continuous
- One Section per Page
- Apply Layout Template
- Apply Configuration File:
 - Default
 - Custom

OK Cancel

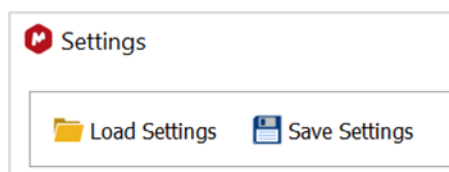
HTML, XML, and CSV report configuration

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 .

Simple Mixture Analysis

Library: SMA Libraries Mixture: C:/Users/Usuario/Desktop/SMA Libraries/Aspirin Cl.exp
 Name: Aspirin Exp
 Descriptor: Determination of the levels of: Acetylsalicylic acid, Salicylic acid, Ascorbic acid, Acetic acid, Citric acid

Parameters

Standard Custom

Sample

Read from sample's parameters table and filled automatically

Spectrum

Sample ID:		Number of Scans (NS):	128
Reference Concentration (RC):	10.0	Receiver Gain (RG):	0
Sample Weight (SW) [mg]:	500	Pulse Width (PW):	7.2
Reference Weight (RW) [mg]:	2.4	Temperature (T):	25
Dilution Factor (DF):		Spectral Width (SpecW):	9615.38461539
		Spectral Size (SpecS):	65536
		Spectrometer Frequency (SF):	599.9281593

Metadata

Sample's parameters table

Parameters	
Parameter	Value
1 Data File Name	X:/2014/20140701/Aspirin_A2_neu_01/Aspirin_A2_neu_NOESY_01.fid/fid
2 Title	Aspirin_A2_neu_NOESY_01
3 Comment	RC:10.0; SW:500; RW:2.4
4 Solvent	d2o_10
5 Temperature	25.0
6 Pulse Sequence	NOESY
7 Experiment	1D
8 Number of Scans	128
9 Receiver Gain	0
10 Relaxation Delay	3.5000
11 Pulse Width	7.2000

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.

Parameters	
Parameter	Value
1 Data File Name	X:/2014/20140701/Aspirin_A2_neu_01/Aspirin_A2_neu_NOESY_01.fid/fid
2 Title	Aspirin_A2_neu_NOESY_01
3 Comment	RC:10.0; SW:500; RW:2.4; EXP:Aspirin Exp

6. SMA results

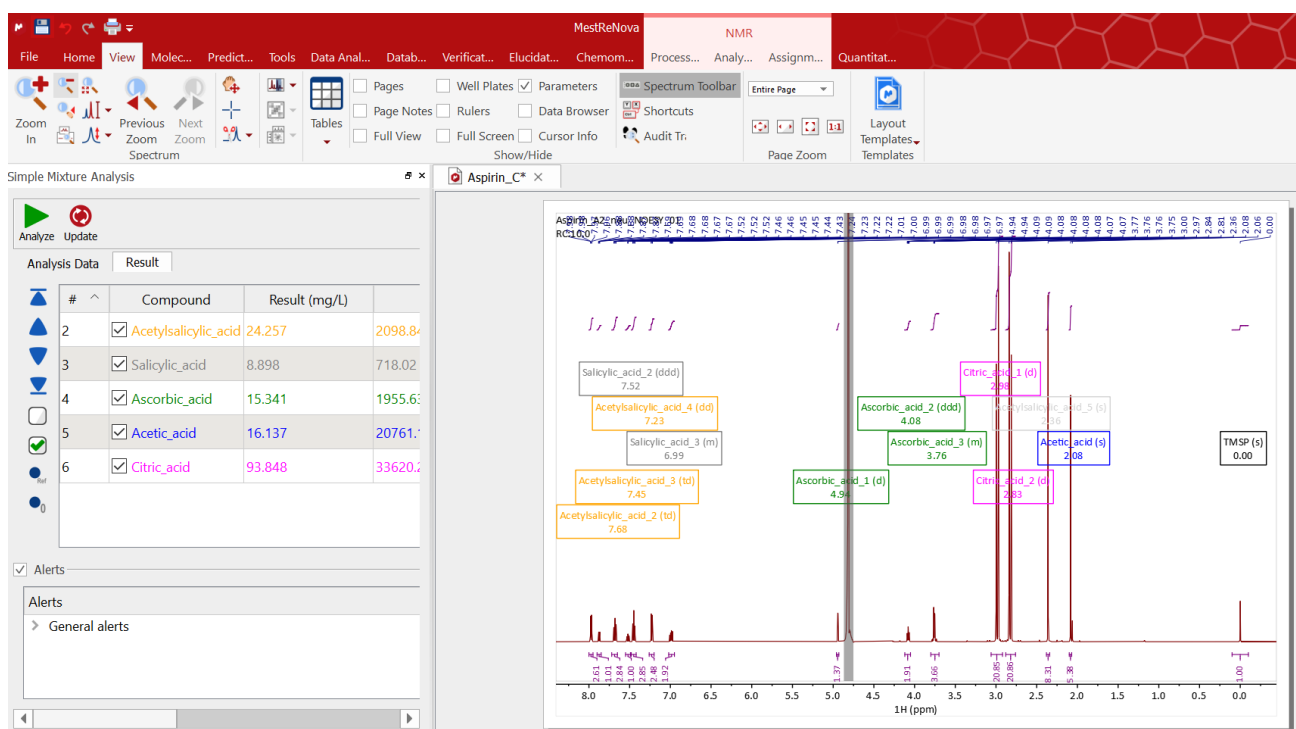
Once the analysis is complete, results are automatically displayed in the **Results** tab.

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.

Simple Mixture Analysis

Analyze Update

Analysis Data Result

#	Compound	Result (mg/L)	SNR	Annotation
2	Acetylsalicylic_acid	0	NC	
3	Salicylic_acid	8.897	613.92 (422.89, 746.74)	
4	Ascorbic_acid	15.340	1672.10 (740.89, 2313.00)	
5	Acetic_acid	16.136	17751.11 (17751.11, 17751.11)	
6	Citric_acid	93.840	28745.88 (28143.49, 29348.27)	

Alerts

- General alerts
- Compound_Acetylsalicylic_acid
- Compound_Salicylic_acid
- Compound_Ascorbic_acid

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

Alerts

By compound

- Compound_Acetylsalicylic_acid
- Compound_Ascorbic_acid
 - Relative areas ratio 2.78 between multiplet Ascorbic_acid_2 and multiplet Ascorbic_acid_1 is not the expected: Expected value in range [0.10-1.90]
 - Relative areas ratio 2.67 between multiplet Ascorbic_acid_3 and multiplet Ascorbic_acid_1 is not the expected: Expected value in range [0.10-1.90]
- Compound_Citric_acid
- General alerts

By time

Alerts

```
[12:17:57]: Error evaluating Custom Parameter
[12:17:57]: An identifier is required for the custom parameter
[12:17:57]: The Multiplicity of the multiplet Citric_acid_1 [3.06, 2.92] is d and it was expected to be m
[12:17:57]: Relative areas ratio 2.67 between multiplet Ascorbic_acid_3 and multiplet Ascorbic_acid_1 is not the expected: Expected value in range [0.10-1.90]
[12:17:57]: Relative areas ratio 2.78 between multiplet Ascorbic_acid_2 and multiplet Ascorbic_acid_1 is not the expected: Expected value in range [0.10-1.90]
[12:17:57]: The list of Js of the multiplet Acetylsalicylic_acid_4 [7.26, 7.20] is not the expected
[12:17:57]: The list of Js of the multiplet Acetylsalicylic_acid_2 [7.72, 7.65] is not the expected
[12:17:57]: The list of Js of the multiplet Acetylsalicylic_acid_1 [8.00, 7.95] is not the expected
```

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.

Default order



#	Compound	Result (mM)	SNR
1	Acetic_acid	16.13	32961.71 (32961.71, 32961.71)
2	Acetylsalicylic_acid	24.38	11752.85 (3049.81, 45400.00)
3	Ascorbic_acid	15.33	3100.76 (1373.47, 4288.00)
4	Citric_acid	93.79	53133.59 (52202.16, 54044.00)
5	Salicylic_acid	8.89	1134.38 (783.87, 1373.11)

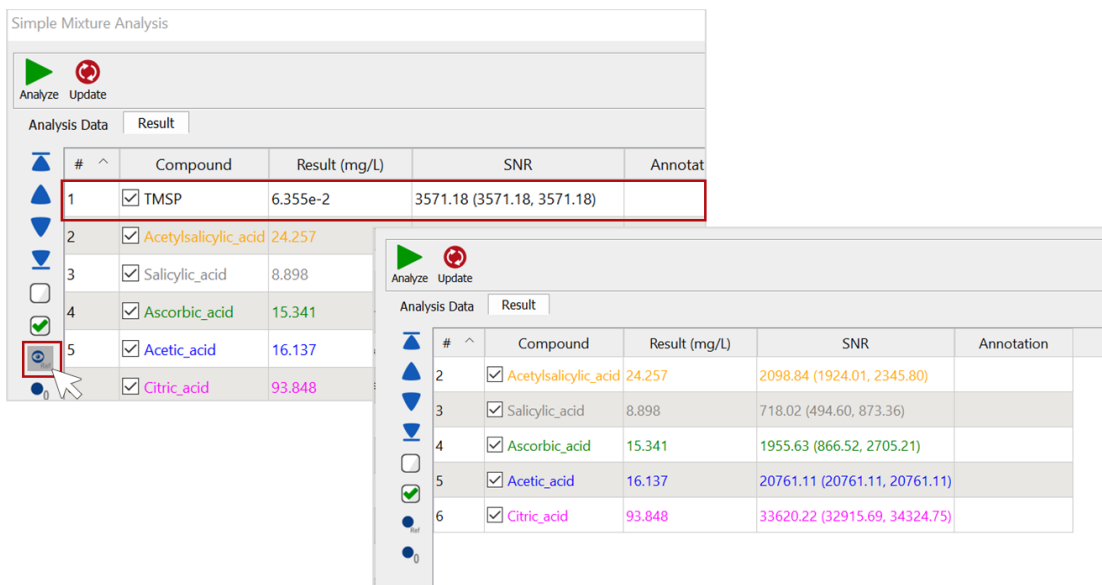
By concentration


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.

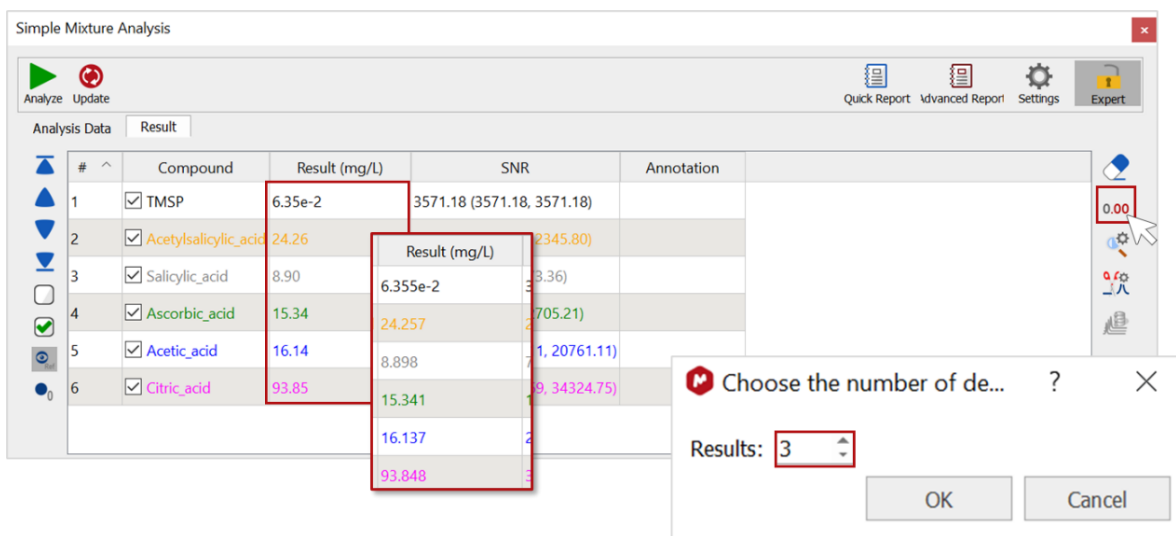
Simple Mixture Analysis


#	Compound	Result (mg/L)	SNR	Annotation
1	TMSP	6.35e-2	3571.18 (3571.18, 3571.18)	
2	Acetylsalicylic_acid	24.26	2098.84 (1924.01, 2345.80)	
3	Salicylic_acid	8.90	718.02 (494.60, 873.36)	
4	Ascorbic_acid	15.34	1955.63 (866.52, 2705.21)	
5	Acetic_acid	16.14	20761.11 (20761.11, 20761.11)	
6	Citric_acid	93.85	33620.22 (32915.69, 34324.75)	

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  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.

The screenshot shows the 'Analysis Data' window with a table of compounds and a zoomed-in NMR spectrum. The table lists the following compounds and their results:

#	Compound	Result (mM)	SNR
1	Acetic_acid	16.13	32961.71 (32961.71, 32961.71)
2	Acetylsalicylic_acid	24.38	11752.85 (3049.81, 4549.81)
3	Ascorbic_acid	15.33	3100.76 (1373.47, 4288.47)
4	Citric_acid	93.79	53133.59 (52202.16, 54064.02)
5	Salicylic_acid	8.89	1124.39 (783.97, 1470.81)

The zoomed-in NMR spectrum shows two multiplets: Acetylsalicylic_acid_1 (dd) at 7.97 ppm and Salicylic_acid_1 (dd) at 7.87 ppm. A '20X Zoom applied' label is visible on the spectrum.

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

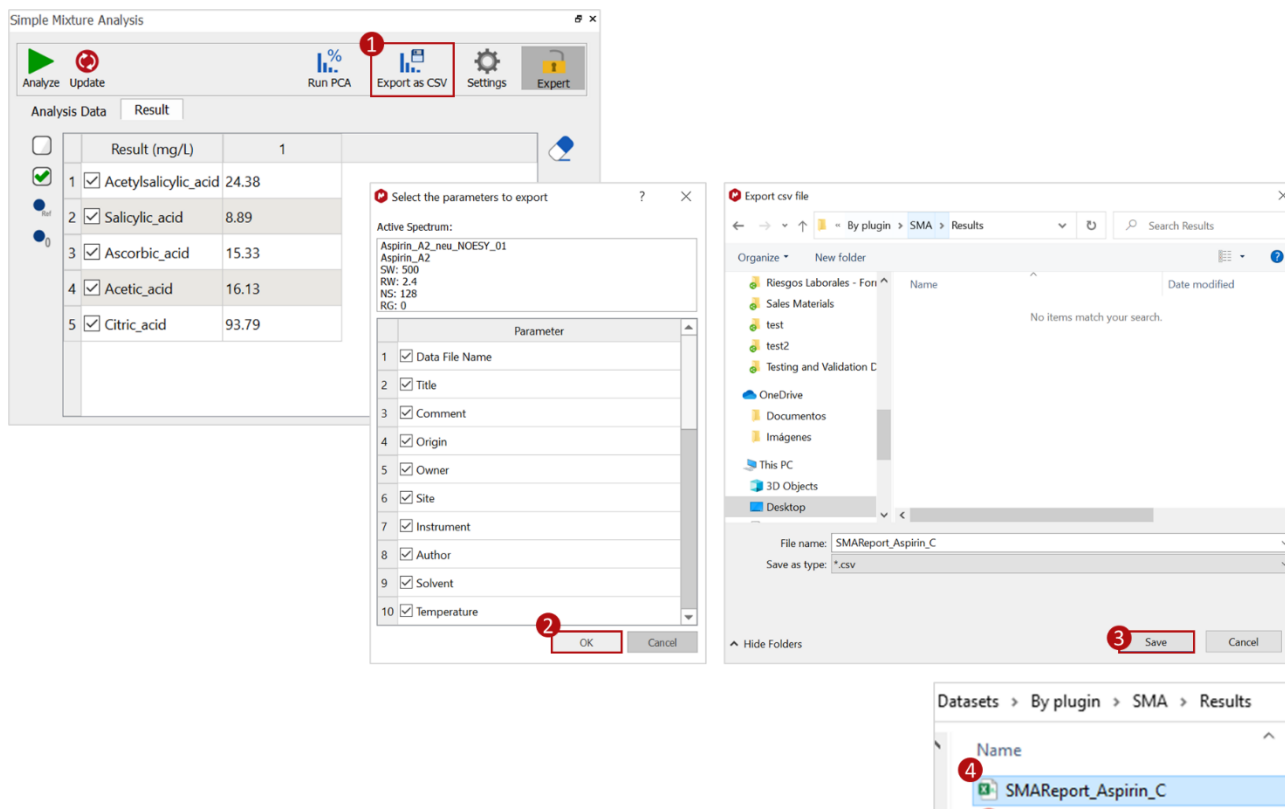
When running an experiment that is "Suitable for PCA", the SMA dialog will present two buttons that will allow you to run the PCA and export the associated data to a CSV file. **A license for the Chemometrics plugin must be obtained to perform a PCA.**

The screenshot shows the 'Simple Mixture Analysis' dialog box. The 'Run PCA' and 'Export as CSV' buttons are highlighted with a red box. The 'Analysis Data' window shows the following table:

Result (mg/L)	1
1	Acetylsalicylic_acid 24.38
2	Salicylic_acid 8.89
3	Ascorbic_acid 15.33
4	Acetic_acid 16.13
5	Citric_acid 93.79

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.

The screenshot illustrates the process of updating multiplet ranges in the SMA software. It is divided into three main parts:

- Initial Results Table:** A table showing the initial analysis results. The compound 'Acetylsalicylic acid' is highlighted in orange, and its multiplet ranges are listed in the 'Ranges' table below. A red circle '1' points to the 'Acetylsalicylic acid' row in the main table, with the text 'Double-click' next to it.
- SMA Compound Details Dialog:** A dialog box opens for 'Acetylsalicylic acid'. It contains fields for Name, Color, Valid Limit, Type, Integration Method, and Dimensions. Below these is a 'Ranges' table with columns: Active, From, To, Mult., J's, NN, Integral, SNR, [conc], and Pattern. A red circle '2' points to the 'Active' checkbox for the range 2.340-2.380. A red circle '3' points to the 'Apply Changes' button.
- Progress Dialog and Updated Results:** A progress dialog titled 'Analyzing Mixture...' shows a progress bar at 83% and a 'Cancel' button. A red circle '4' points to the progress bar. Below this, the updated 'Simple Mixture Analysis' window shows the results table with 'Acetylsalicylic acid' now having a result of 24.38 and SNR of 11752.85. A red circle '5' points to this updated result.

#	Compound	Result (mg/L)	SNR
1	TMSP	6.35e-2	5616.89 (5616.89, 5616.89)
2	Acetylsalicylic acid	24.24	3334.97 (3049.81, 3680.88)
3	Salicylic acid	8.89	1134.38 (783.87, 1373.12)
4	Ascorbic acid	15.33	3100.76 (1373.47, 4288.80)

Active	From	To	Mult.	J's	NN	Integral	SNR	[conc]	Pattern
<input checked="" type="checkbox"/>	7.950	8.000	dd		1	369.80	3423.35	23.49	
<input checked="" type="checkbox"/>	7.650	7.720	td		1	402.18	3049.81	25.54	
<input checked="" type="checkbox"/>	7.420	7.480	td		1	404.14	3680.88	25.67	
<input checked="" type="checkbox"/>	7.200	7.260	dd		1	350.60	3185.82	22.27	
<input checked="" type="checkbox"/>	2.340	2.380	s		3	1177.48	45424.37	24.93	

#	Compound	Result (mg/L)	SNR
1	TMSP	6.35e-2	5616.89 (5616.89, 5616.89)
2	Acetylsalicylic acid	24.38	11752.85 (3049.81, 45424.37)
3	Salicylic acid	8.89	1134.38 (783.87, 1373.12)
4	Ascorbic acid	15.33	3100.76 (1373.47, 4288.80)
5	Acetic acid	16.13	32961.71 (32961.71, 32961.71)
6	Citric acid	93.79	53133.59 (52202.16, 54065.02)

Once you have applied changes 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.

Mixture Creation/Edition

Name: Aspirin Exp Units: mg/L

Description: Ascorbic acid, Acetic acid, Citric acid

Compound List

#	Compound	Type
1	TMS	Reference
2	Acetylsalicylic acid	Compnd.
3	Salicylic acid	Compnd.
4	Ascorbic acid	Compnd.
5	Acetic acid	Compnd.
6	Citric acid	Compnd.

Formula: $\frac{((1/NN1)+(12/NN2)+(13/NN3)+(14/NN4)+(15/NN5))/5}{5} \times CCF$

Active

From	To	Mult.	J's	NN	Pattern
7.420	7.480	td	7.6,1.2	1	
7.200	7.260	dd	8.2,1.2	1	
2.340	2.380	s		3	

Multiplet range included

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.

Aspirin* x

SMA REPORT

Sample Parameters:

- Reference Concentration: 1.0
- Sample Weight: 500
- Reference Weight: 2.4

Custom Parameters:

- PYR: 0

Results:

Compound	Result(mg/L)	SNR Mean (min, max)	Ranges						Annotations
			From	To	Mult	NN	Integral	SNR	
Acetylsalicylic acid	24.384	7408.63 (1924.01, 28647.82)	7.9500	8.0000	dd	1	369.78	2158.89	
			7.0500	7.7200	td	1	402.21	1924.01	
			7.4200	7.4800	td	1	404.18	2345.80	
			7.2000	7.2600	dd	1	350.67	1966.64	
			2.3400	2.3800	s	3	1177.53	28647.82	
Salicylic acid	8.896	718.02 (494.60, 873.36)	7.8500	7.9000	dd	1	143.25	785.11	
			7.4900	7.5500	ddd	1	141.12	494.60	
			6.9500	7.0200	m	2	271.37	873.36	
Ascorbic acid	15.341	1955.63 (866.52, 2705.21)	4.9300	4.9800	d	1	184.50	2295.17	
			4.0500	4.1200	ddd	1	270.46	866.52	
			3.7000	3.8000	m	2	518.57	2705.21	
Acetic acid	16.137	20761.11	2.0700	2.1000	s	3	761.81	20761.11	
Citric acid	83.848	33620.22 (32915.69, 34324.75)	2.9200	3.0600	d	2	2893.39	32915.69	
			2.7600	2.8800	d	2	2893.90	34324.75	






1. Aspirin_A2_neu_NOESY_01

2.

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.

SMA > Results

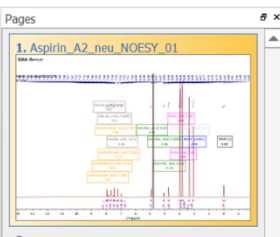
Name

-  SMAReport_Aspirin_C
-  SMAReport_Aspirin_C
-  SMAReport_Aspirin_C
-  SMAReport_Aspirin_C
-  SMAReport_Aspirin_C



You can find examples of such advanced reports below:

Mnova report



On different pages

2.

Mixture Info
Library Name: Aspirin Exp
Description: Determination of the levels of Acetylsalicylic acid, Ascorbic acid, Citric acid, Salicylic acid and Intermediate analysis
Units: mg/L

Compound List

Checked	Compound	Type	Reference	From	To	Int	Options	Mol Weight	Spectrum	Formula	Dimension	Integration	Options
<input checked="" type="checkbox"/>	TMSP	Reference		From	To	Int	Options	116.070	1	(NN1)/1P	1D	Sum	
<input checked="" type="checkbox"/>	Acetylsalicylic_acid	Compnd.		From	To	Int	Options	180.150	1	(((111)/NN1)/N1)/2CP	1D	Sum	
<input checked="" type="checkbox"/>	Salicylic_acid	Compnd.		From	To	Int	Options	138.120	1	(((111)/NN1)/N1)/2CP	1D	Sum	
<input checked="" type="checkbox"/>	Ascorbic_acid	Compnd.		From	To	Int	Options	176.130	1	(((111)/NN1)/N1)/2CP	1D	Sum	
<input checked="" type="checkbox"/>	Acetic_acid	Compnd.		From	To	Int	Options	60.050	1	(111)/1CP	1D	Sum	
<input checked="" type="checkbox"/>	Citric_acid	Compnd.		From	To	Int	Options	192.130	1	(((111)/NN1)/N1)/2CP	1D	Sum	

3.

Compound	Result (mg/L)	SMR Mean (m/z, m/e)	From	To	Int	Options	Annotations
Acetylsalicylic_acid	24.25P	2055.84 (1934.01, 2345.80)	From	To	Int	Options	
Salicylic_acid	5.899	716.02 (494.00, 873.36)	From	To	Int	Options	
Ascorbic_acid	15.541	1855.63 (866.52, 2756.21)	From	To	Int	Options	
Citric_acid	16.137	20761.11	From	To	Int	Options	

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 of	Ascorbic acid	Citric acid	Salicylic acid	Acetic acid											
4	Intermediate analysis	mg/L																	
5		Compound List:																	
6			Checked	Compound	Type	Mol.Weight	Spectrum	Formula	Dimension	Integration	Options	Ranges	Frc	Ranges	Mt	Ranges	J	Ranges	NN
7			yes	TMSP	Reference	116.07		1 (((111)/NN1))	1D	Sum	Verbose P	-0.1	0.1					9	
8			yes	Acetylsalicylic_acid	Compnd.	180.16		1 (((111)/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						
13			yes	Salicylic_acid	Compnd.	138.12		1 (((111)/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						
16			yes	Ascorbic_acid	Compnd.	176.13		1 (((111)/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						
19			yes	Acetic_acid	Compnd.	60.05		1 (((111)/NN1))	1D	Sum	Verbose P	2.07	2.1 s						
20			yes	Citric_acid	Compnd.	192.13		1 (((111)/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
			From	To	Mult	J	NN						
<input checked="" type="checkbox"/>	TMSP	Reference	-0.1	0.1				116.0700	1	((1N11))^(RC)	1D	Sum	
<input checked="" type="checkbox"/>	Acetylsalicylic_acid	Compnd	7.950	8.000	00	10.8,1.7	1	180.1600	1	(((1NN1)+(2NN2)+(3NN3)+(4NN4))/4)^CCF	1D	Sum	Verbose Pattern Recognition Algorithm
			7.650	7.720	00	8.1,8.1,7	1						
			7.420	7.480	10	7.6,1.2	1						
			7.200	7.260	00	8.2,1.2	1						
<input checked="" type="checkbox"/>	Salicylic_acid	Compnd	7.9	7.85	00	7.9,1.85	1	138.1200	1	(((1NN1)+(2NN2)+(3NN3))/3)^CCF	1D	Sum	Verbose Pattern Recognition Algorithm
			7.55	7.49	000	8.3,7.2,1.8	1						
			7.02	6.95	m		2						
<input checked="" type="checkbox"/>	Ascorbic_acid	Compnd	4.96	4.93	d	1.9	1	176.1300	1	(((1NN1)+(2NN2)+(3NN3))/3)^CCF	1D	Sum	Verbose Pattern Recognition Algorithm
			4.12	4.05	000	7.1,6.1,8	1						
			3.80	3.70	m		2						
<input checked="" type="checkbox"/>	Acetic_acid	Compnd	2.07	2.10	s		3	60.0500	1	((1NN1))^CCF	1D	Sum	Verbose Pattern Recognition Algorithm
<input checked="" type="checkbox"/>	Citric_acid	Compnd	3.06	2.82	d	15.7	2	192.1300	1	(((1NN1)+(2NN2))/2)^CCF	1D	Sum	Verbose Pattern Recognition Algorithm
			2.88	2.76	d	15.7	2						

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
 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: (6f8ace83-c3ba-49fb-ac9e-a6d5eb862d56)
 IUPAC:
 Spectrometer_Frequency: 599.9281593
 Spectral_Width: 9015.38461539
 Lowest_Frequency: -1106.77572396
 Nucleus: 1H
 Acquired_Size: 24038
 Spectral_Size: 65536

Results:

Compound	Result(mg/L)	SNR Mean (min, max)	Ranges						Annotations
			From	To	Mult	NN	Integral	SNR	
TMSP	6.351e-2	5616.89	-0.1000	0.1000	s	9	141.71	5616.89	
Acetylsalicylic_acid	24.240	3334.97 (3049.81, 3680.88)	7.9500	8.0000	00	1	369.80	3423.35	
			7.6500	7.7200	10	1	402.18	3049.81	
			7.4200	7.4800	10	1	404.14	3680.88	
			7.2000	7.2600	00	1	350.60	3185.82	
Salicylic_acid	8.891	1134.38 (783.87, 1373.12)	7.9500	7.9000	00	1	143.26	1246.16	
			7.4927	7.5500	000	1	141.01	783.87	
			6.9500	7.0200	m	2	271.42	1373.12	
Ascorbic_acid	15.332	3100.76 (1373.47, 4288.80)	4.9300	4.9000	d	1	194.45	3640.00	
			4.9500	4.1200	000	1	270.52	1373.47	
			3.7000	3.8000	00	2	518.59	4288.80	
Acetic_acid	16.128	32961.71	2.0700	2.1000	s	3	761.85	32961.71	
Citric_acid	93.793	53133.59 (52202.16, 54065.02)	2.8200	3.0600	d	2	2953.41	52202.16	
			2.7600	2.8800	d	2	2953.94	54065.02	