Mestrelab Research

Gears SMA 3.1

STARTING GUIDE

Document Number

P/N 291 R2

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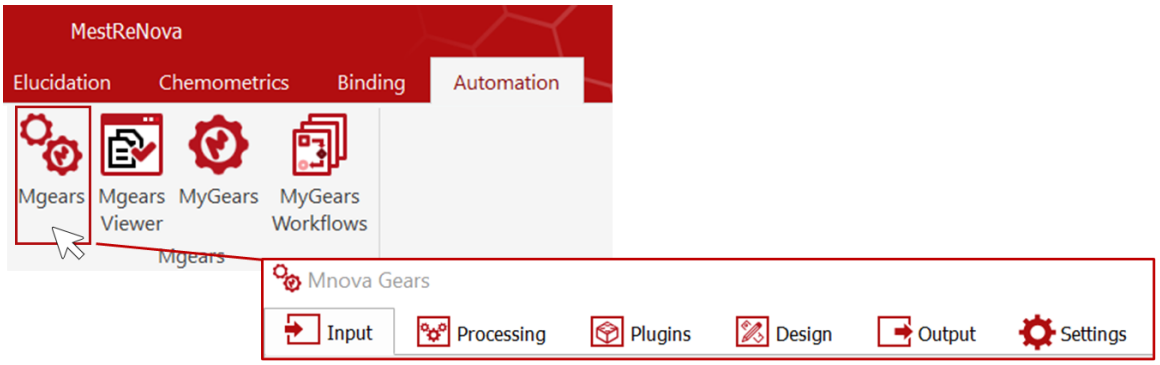
Gears SMA is the automated solution we provide to run mixture analyses in batch or real-time modes. Setting up such a workflow will require a number of preparatory steps in Mnova SMA, which means that you will need this plugin to be installed also. With Mnova SMA you will be able to create the library of experiments you want to use in your automated analysis. To do so, please follow the step-by-step guide published here.

Once your experiment library is ready for use, you can proceed and configure your SMA batch analysis in Mnova Gears.

1. The workflow

Launch Mgears from the Mnova **Automation** ribbon. The dialog with the usual six tabs will open.

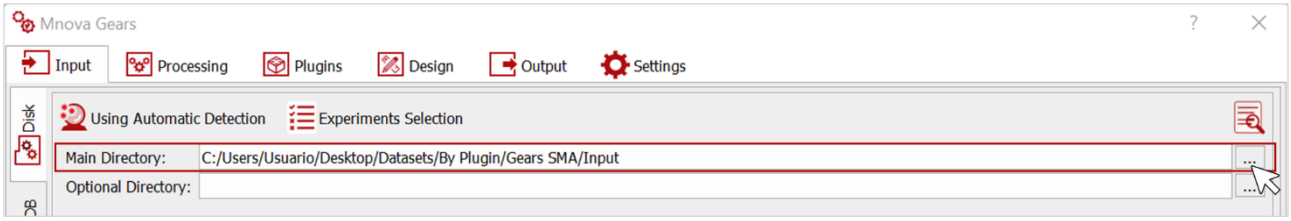
For Gears SMA analysis, you will mainly have to focus on three of the six available tabs to define your input, analysis plugin settings, and analysis output.



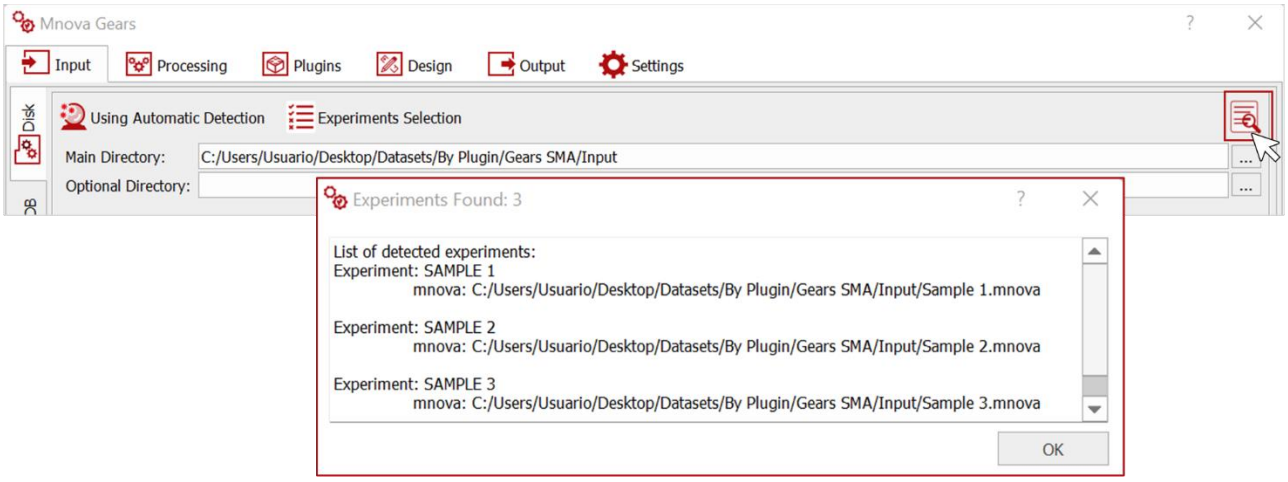
1.1.Input

In this example, we will run a batch analysis on data saved on our computer. However, Mgears can also read data from a database, or as it is acquired by your spectrometer in real time *(please refer to the Mnova Gears manual for more details about the configuration of these input types).*

Click on the ... button and select the folder containing the datasets to analyze.



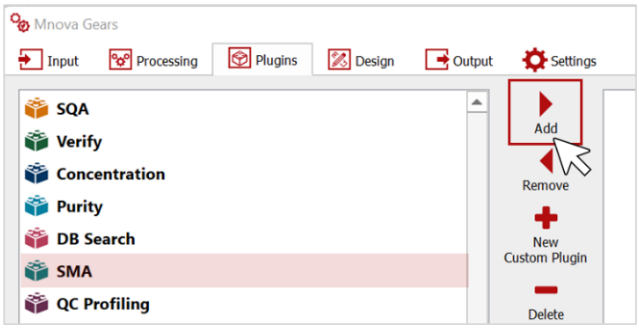
If your input data masks are well configured, Mgears can autodetect your data files and list them in the dialog, as seen below. You can configure your data file extension(s) in the **Mask Manager** under the **Settings** tab, if needed.



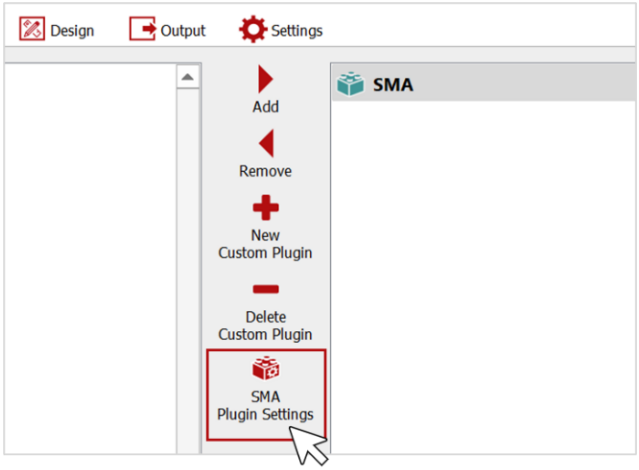
Advanced filtering options (using document modification/creation date, regular expressions, or a mapping file) can be applied to refine input detection from your selected directory. The use of these options is detailed in the Mnova Gears Manual and in our Gears webinar part II.

1.2. Plugins

In the **Plugins** section, select and add the SMA brick to your workflow.



Then, click on **SMA Plugin Settings** to configure analysis and reporting preferences.

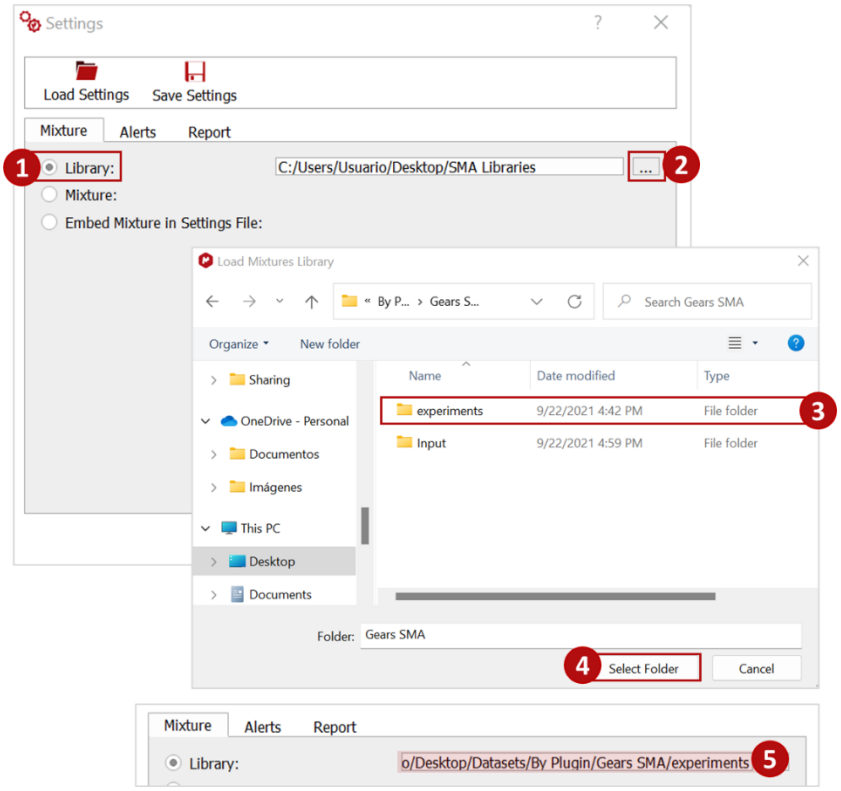


A three-tab dialog will open.

1.2.1. Mixture tab

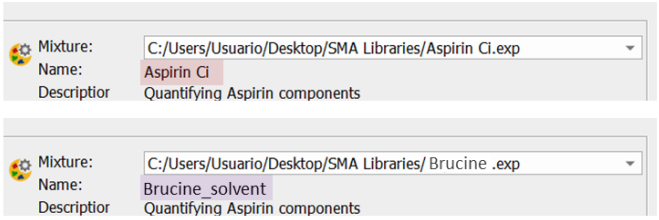
In this tab, you must define the analysis mixture(s) to be used.

When multiple mixtures are analyzed in the same run, a mixture library (with the different ".exp" files) must be selected. To select a library, enable the **Library** option, then click on this button ... and select the library from your directory as shown in the image below.

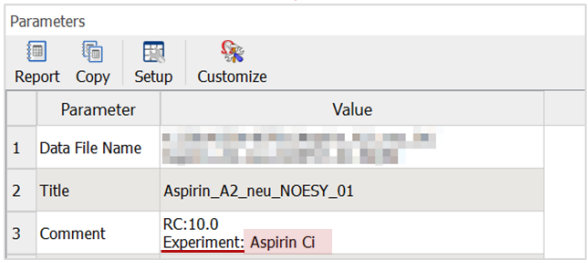


In this case, Gears SMA will need to retrieve the information about which experiment to apply for each sample from the parameters table of the input files. Therefore, a string with that information must be added in the comment field of the parameters table. See the example below, in which two samples require different mixture analyses: Sample 1 with “Aspirin Ci”, and Sample 2 with “brucine_solvent”.

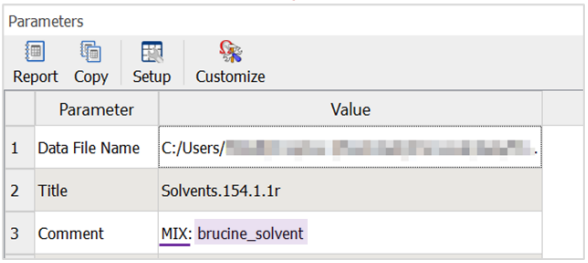
Selected Mixture



Parameters table - Sample 1

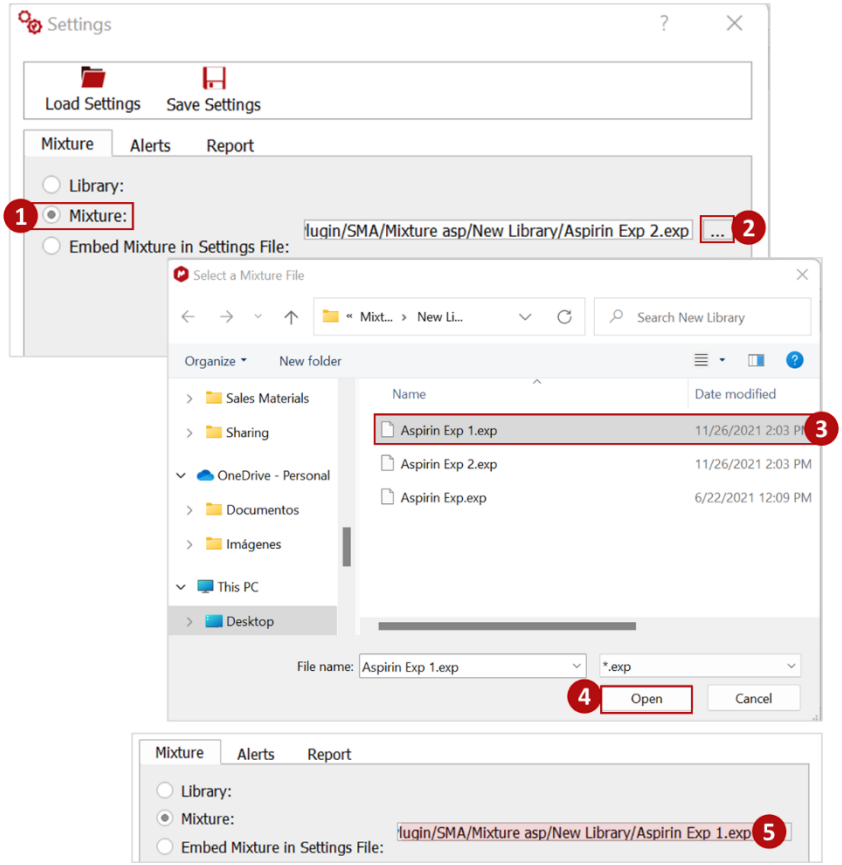


Parameters table - Sample 3

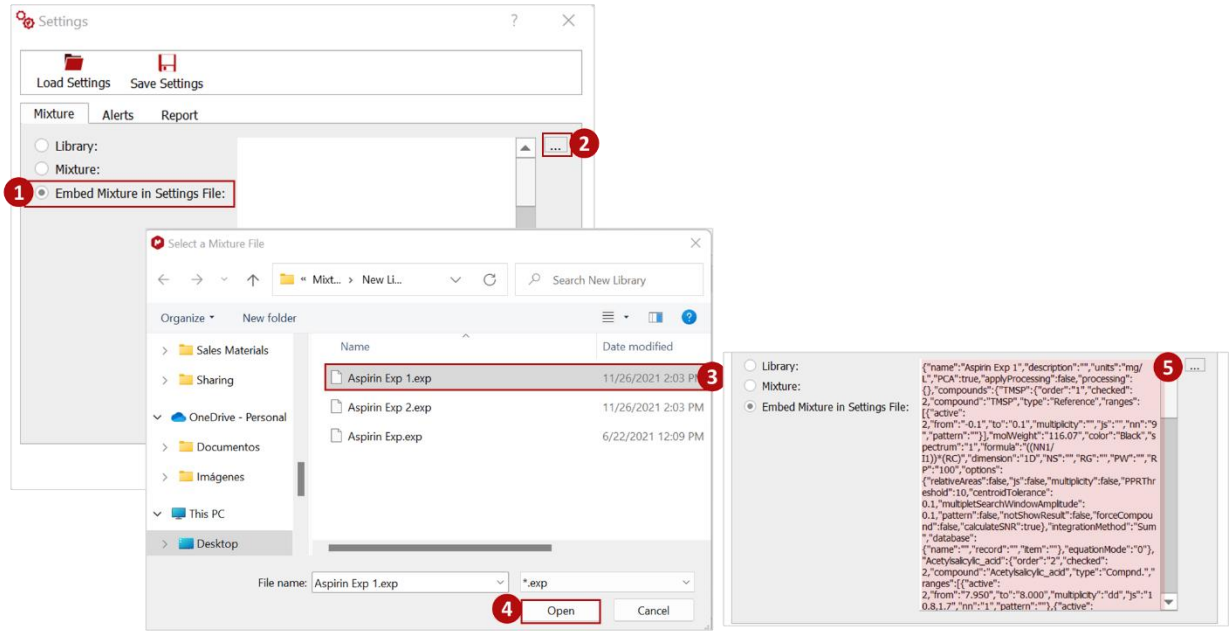


Note. The string is case-insensitive and can start with “Experiment”, “Exp”, “Mix”, or “Mixture” to designate the experiment/mixture to be used.

When all the samples must be analyzed using the same mixture, you can enable the **Mixture** option, click on this button ... and upload the desired mixture file as shown below.



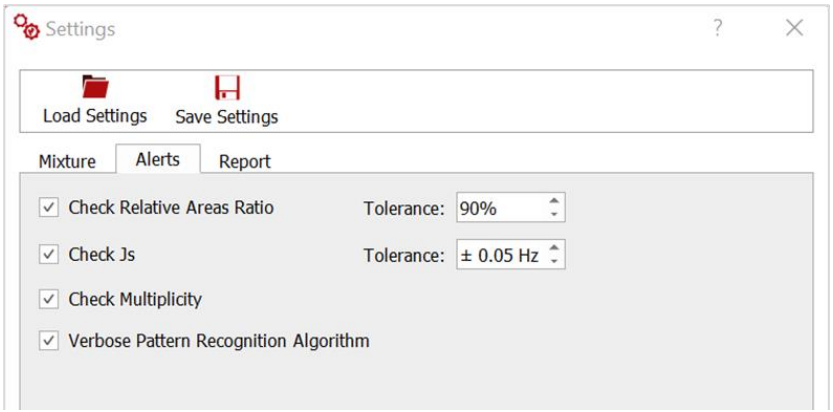
If you wish to embed mixture in the Mgears settings file, enable the **Embed Mixture in Settings File**, click on this button ... and upload the desired mixture file as shown below.



1.2.2. Alerts tab

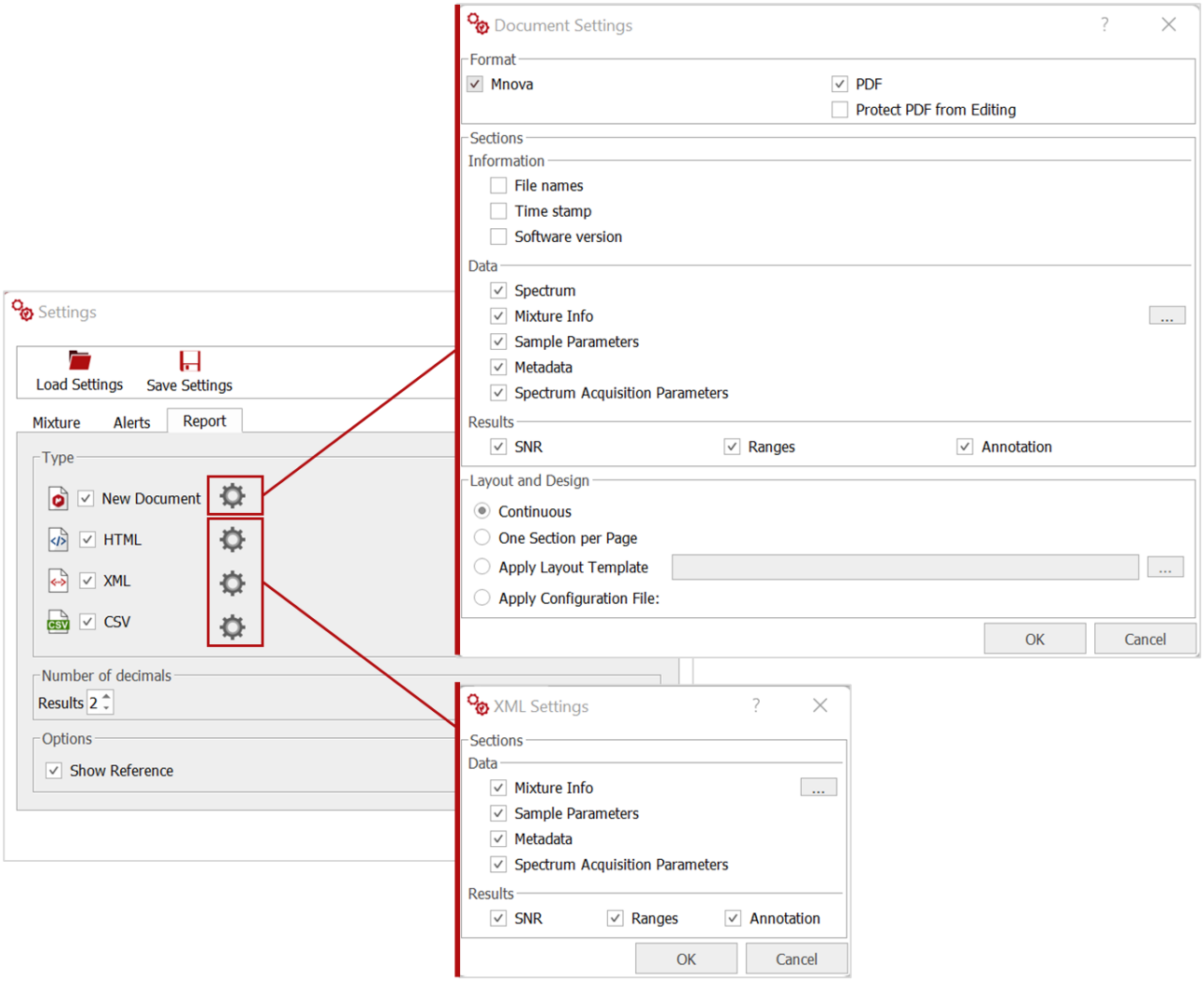
In the Alerts tab, you can configure the tests you want SMA to perform on your compounds. You can enable the:

- **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 compares it to the value defined by the user. You can set the tolerance value in the dedicated box.
- **Check Multiplicity:** to compare found multiplicities 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.



1.2.3. Report tab

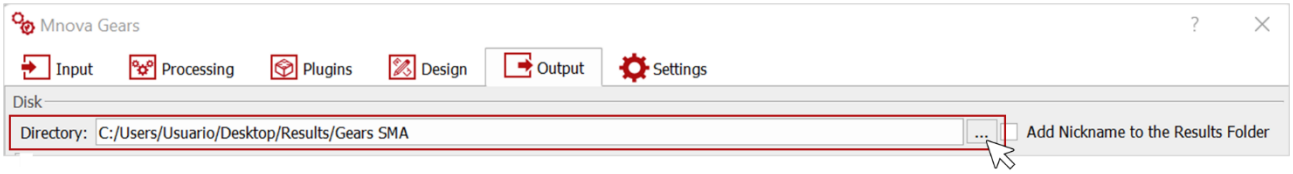
Gears SMA can generate advanced reports the same way Mnova SMA does. These reports can be customized in this **Report** tab. Here, you can check the types of reports you would like to have and configure the different sections that can be included. *(For further details about the advanced reports, please refer to the Mnova SMA manual).*



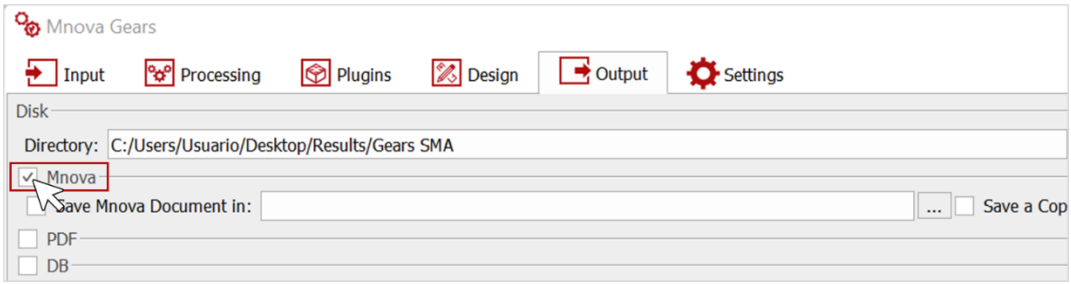
When you are happy with the setup, click on **OK** and go to the **Output** tab.

1.3.Output

Choose the directory in which you wish to save your analysis results.



Then, select the **Mnova** option to generate Mnova result files that can be opened with the **Gears results viewer.**

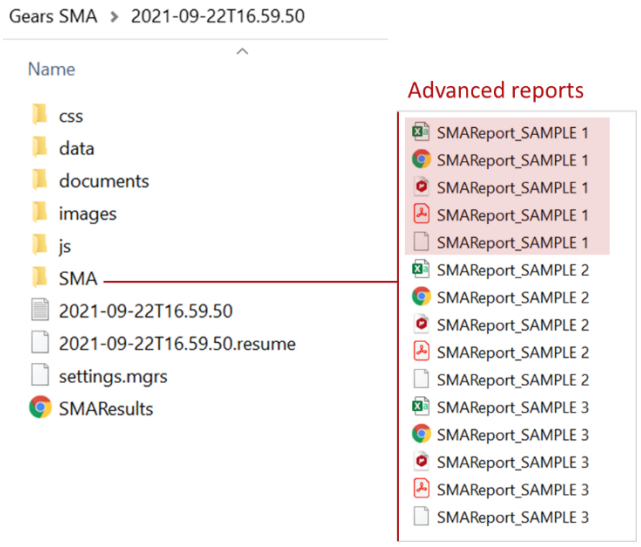


You can also choose to save your results to a database. To do so you will have to add the database connection credentials and connect. A new record will be created for each analyzed dataset (unless you decide to update existing ones!)

You are now ready to launch your analysis. Click on **Run** and let Mgears take care of the rest.

2. The output folder

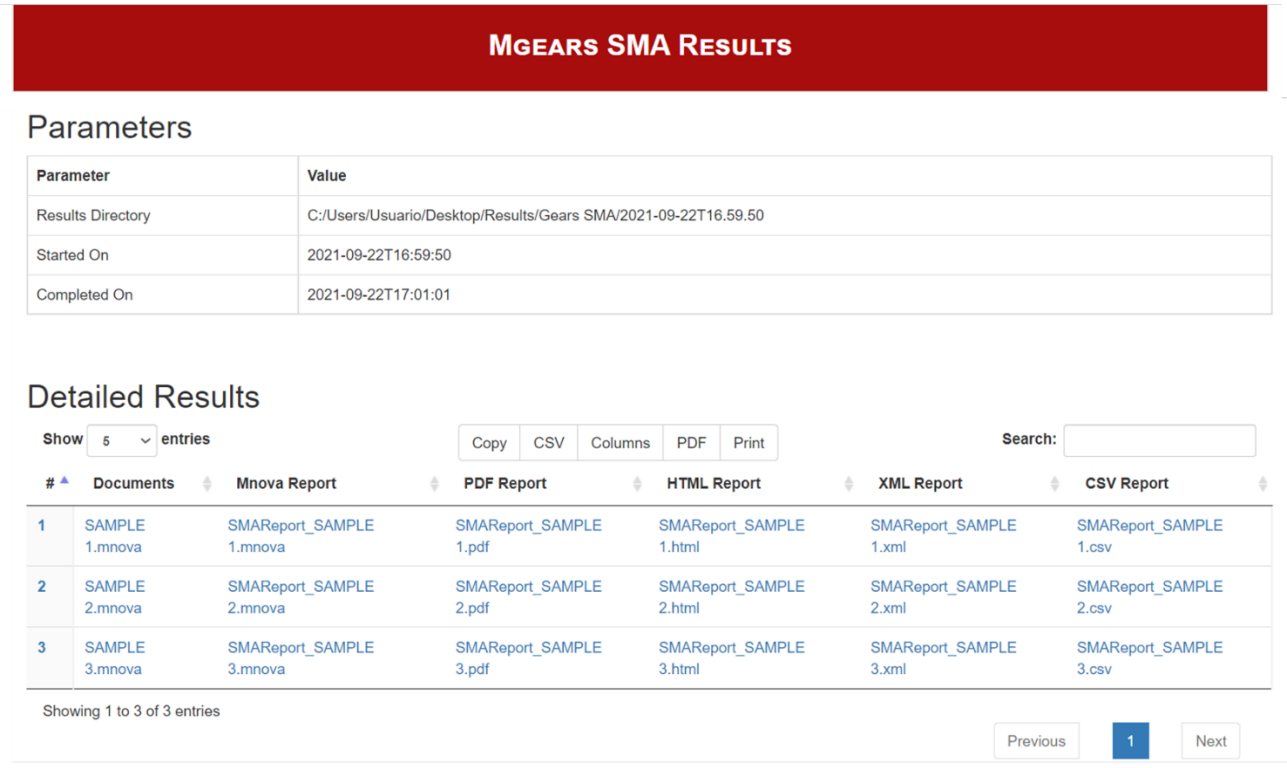
Once the evaluation is completed, the results of the analysis will be available at the directory you specified. The output folder, stamped with the date and time of your analysis, will contain all the output generated in the current evaluation including the configured advanced reports for each sample.



2.1.The HTML report

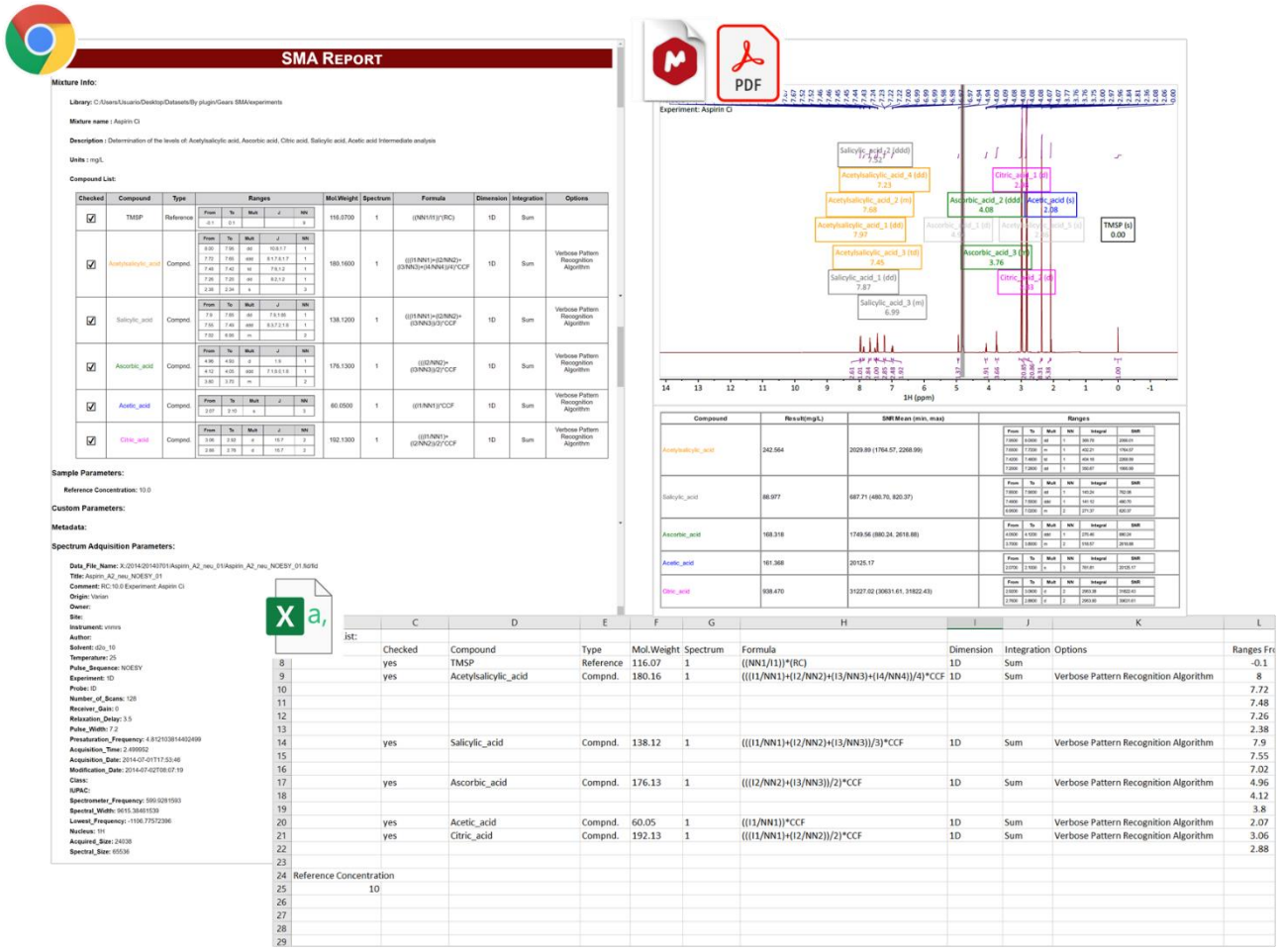
A global HTML report (named “SMAResults”) includes an overview of all samples and the generated reports. Each sample is reported on a different row with hyperlinks to the corresponding reports.

The HTML format allows you to change the display of the columns and adapt them to your preferences. You can then **Copy**, **Print**, or save the content into **CSV** or **PDF** formats.



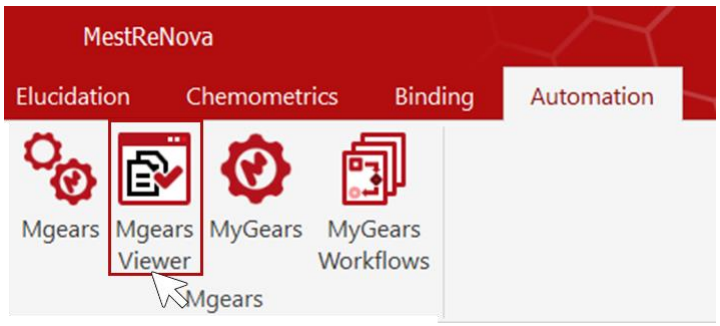
2.2.The advanced reports

The advanced reports are stored in a folder named SMA. The results for each sample include the mixture and calculation details for each component (ranges, multiplets, formulae, etc.), the analysis parameters, and the calculated concentrations. These can be displayed in an HTML, Mnova, or PDF file, and reported in a CSV as previously configured in the Report tab.

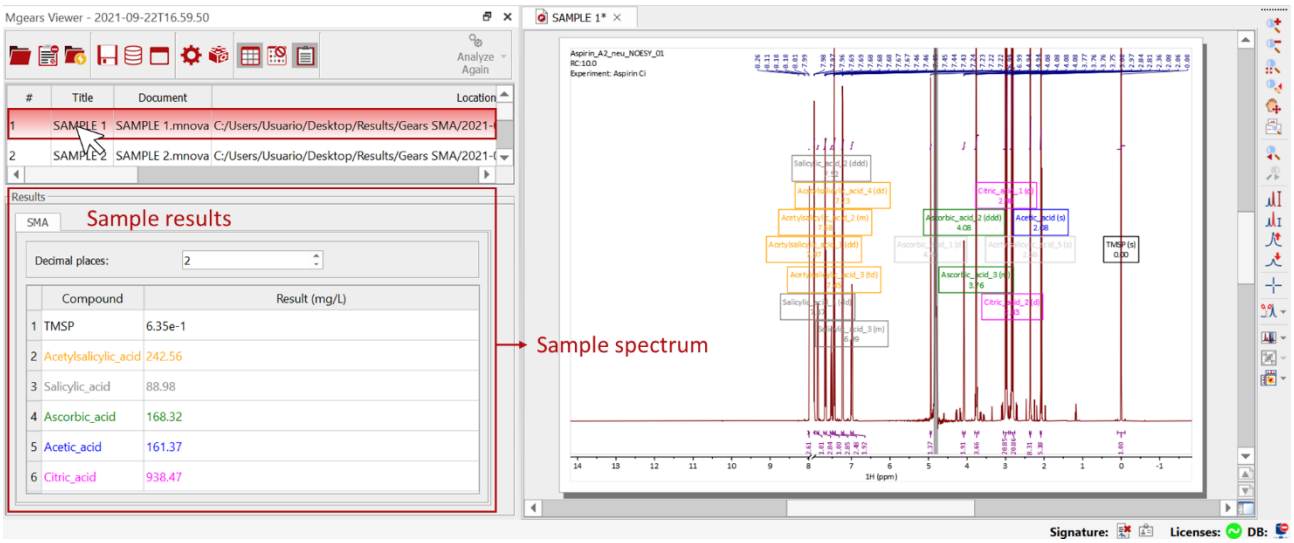


3. Mnova Gears Results Viewer

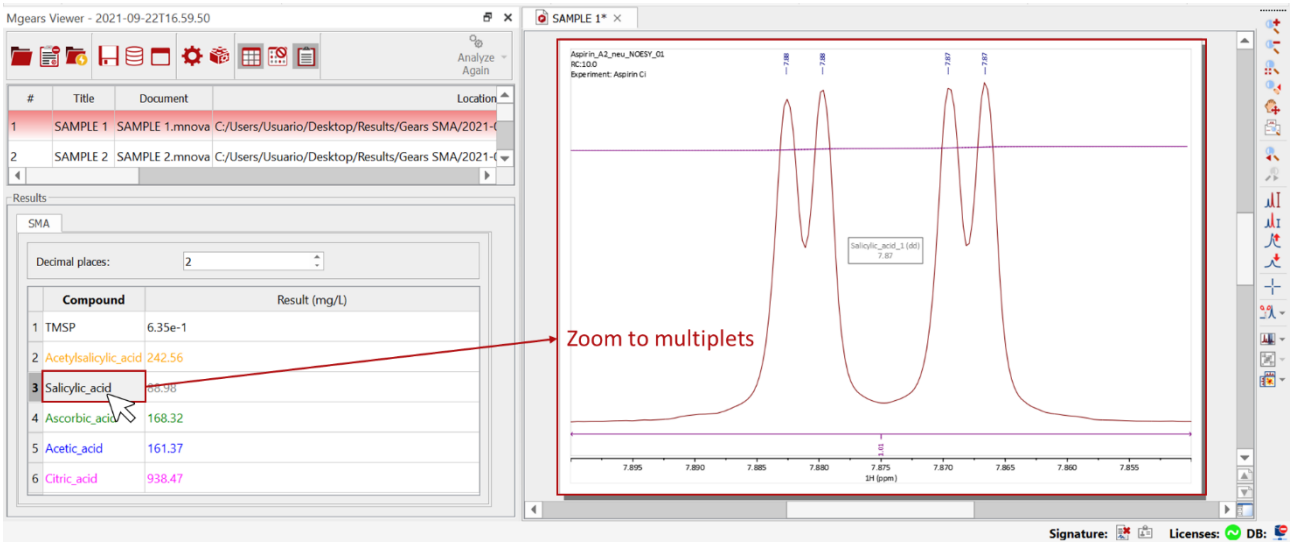
Open the **Mgears Results Viewer**, for a quick and convenient review of the results. Import your analysis results.



When the experiment is open, click on a specific dataset to view the corresponding results and spectrum. In the results table, each compound is displayed with a color - as configured in the mixture - or in grey if the result is invalid. The number of decimals for the concentration can be easily changed by editing the **Decimal place** box.

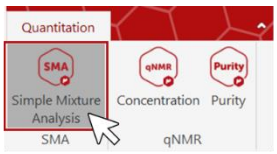


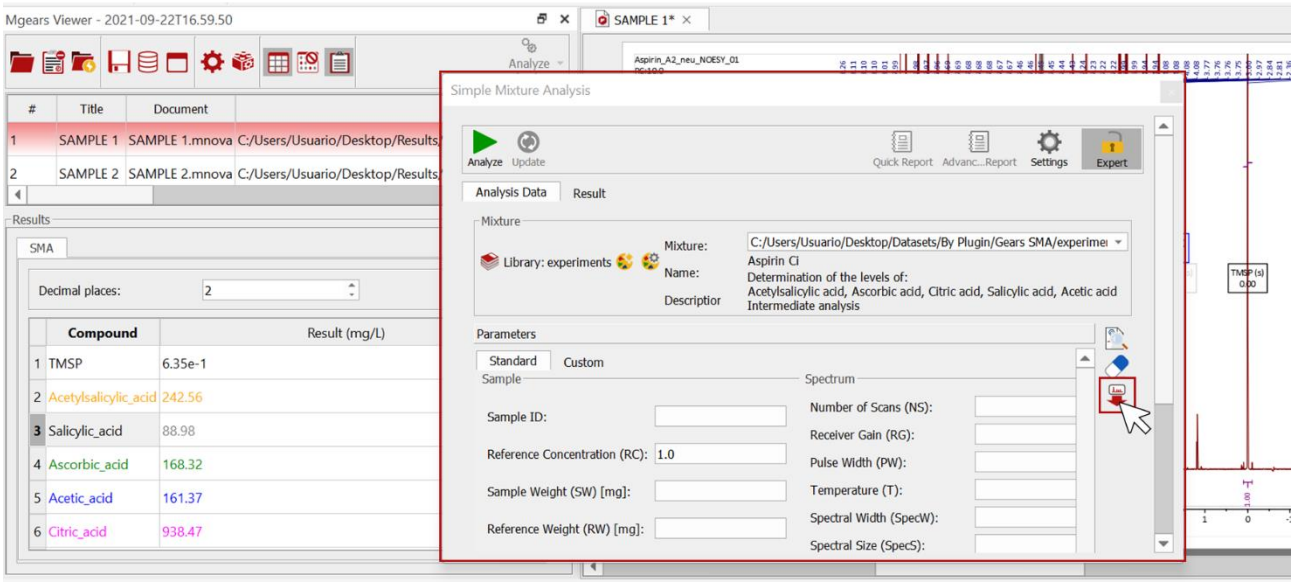
If you click on a compound, you can get a magnified view of one of its multiplets. You can then click again on the same compound to navigate among its other multiplets.



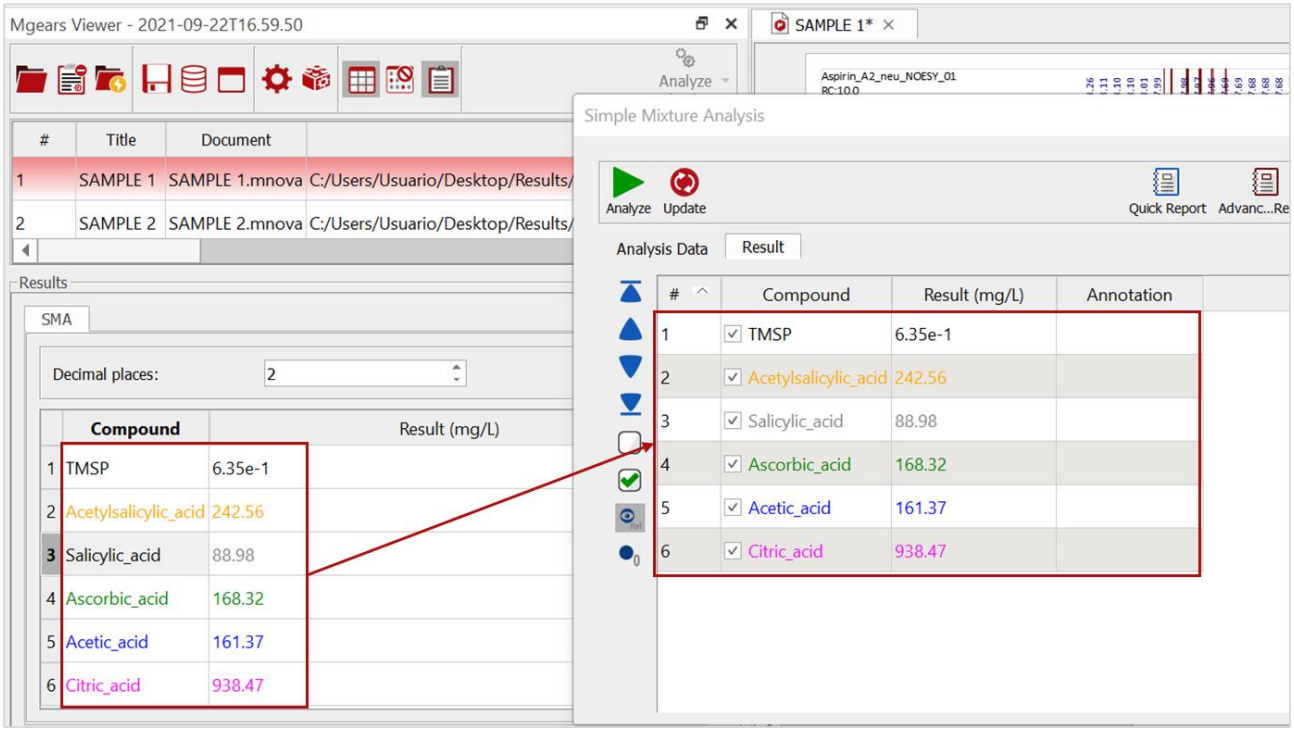
Since the SMA analysis is a complex one, the **Analyze Again** button is disabled in the Mgears Viewer, and the edition and re-analysis of samples must rather be done on a case-by-case basis using the Mnova SMA plugin.

To do so, go to the **Quantitation** tab in the Mnova upper ribbon and open the **Simple Mixture Analysis** plugin. Click on  to load the results of the active spectrum into the SMA dialog.

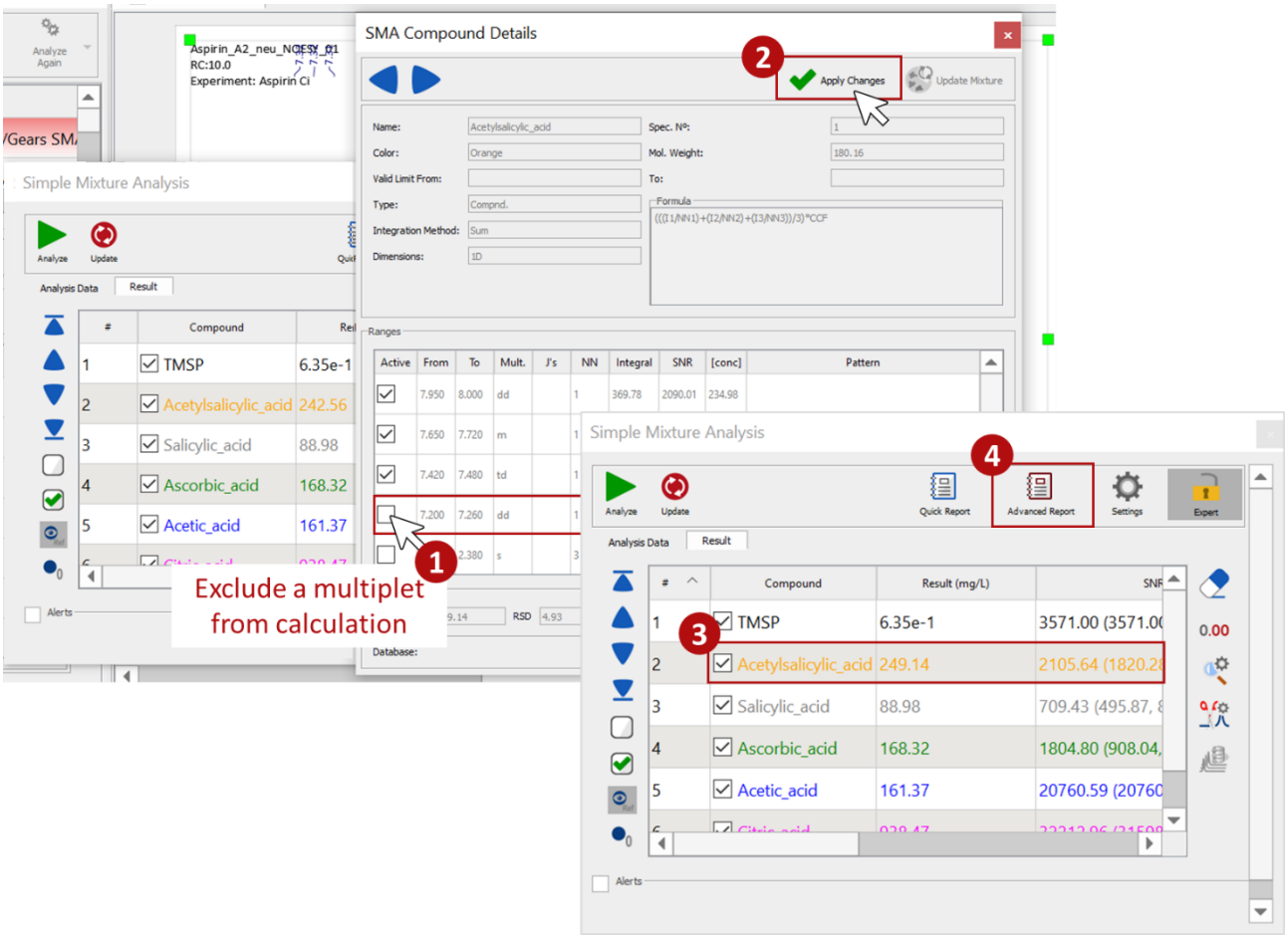




The loaded results can be revised and updated as required.



In the example below, a multiplet is excluded from the concentration calculation. After applying the changes, the concentration is automatically updated in the results table. New reports can therefore be generated using Mnova SMA.



Gears SMA is a perfect addition to your basic mixture analysis workflow which, with Mnova SMA, will allow you to speed up your analyses and reporting tasks.

Please refer to the Mnova Gears manual and the Mnova SMA manual for more details.