



Mestrelab Research

# Gears SMA 3.1

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STARTING GUIDE



Document Number

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## Table of Contents

<b>1. THE WORKFLOW .....</b>	<b>3</b>
1.1. INPUT .....	3
1.2. PLUGINS.....	4
1.3. OUTPUT .....	9
<b>2. THE OUTPUT FOLDER.....</b>	<b>10</b>
2.1. THE HTML REPORT .....	10
2.2. THE ADVANCED REPORTS .....	11
<b>3. MNOVA GEARS RESULTS VIEWER .....</b>	<b>11</b>

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.

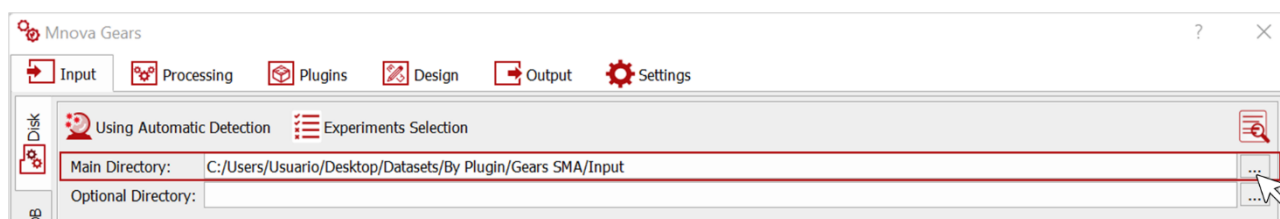
For Gears SMA analysis, you will mainly have to focus on three of the six available tabs to define your input, analysis plugin settings, and analysis output.




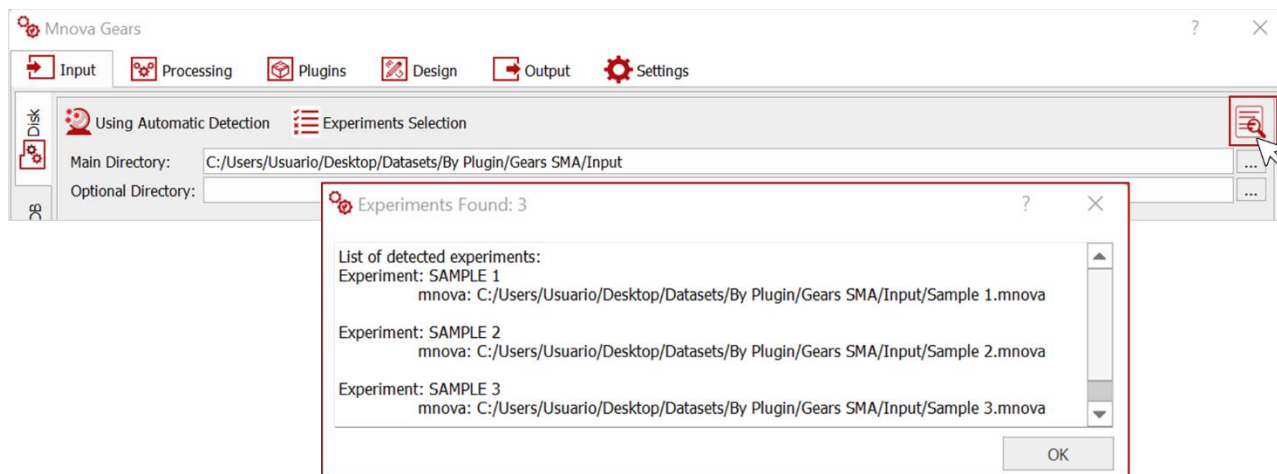
### 1.1. Input

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.



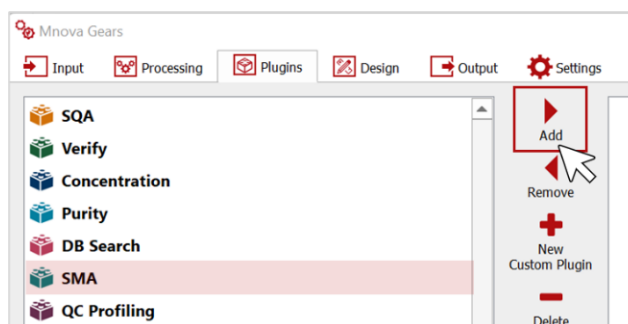
If your input data masks are well configured, Mgears can autodetect your data files  and list them in the dialog, as seen below. You can configure your data file extension(s) in the **Mask Manager** under the **Settings** tab, if needed.



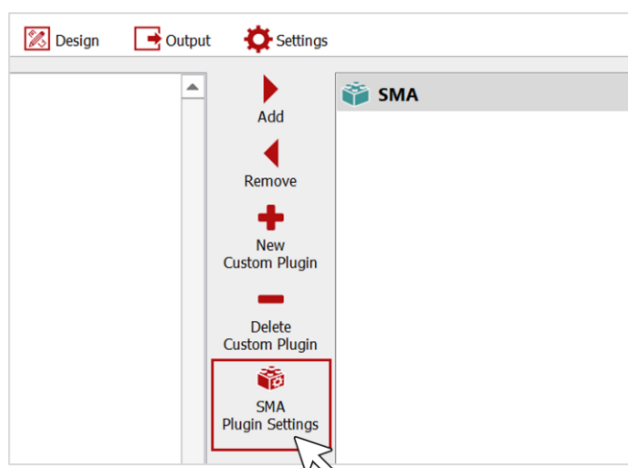
Advanced filtering options (using document modification/creation date, regular expressions, or a mapping file) can be applied to refine input detection from your selected directory. The use of these options is detailed in the [Mnova Gears Manual](#) and in our [Gears webinar part II](#).

## 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.

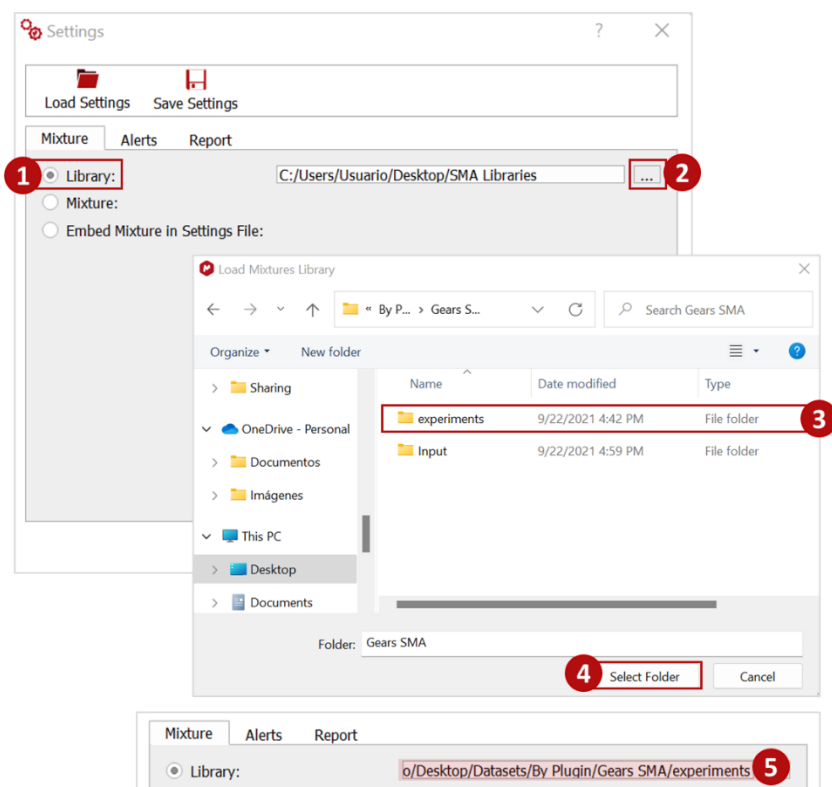


A three-tab dialog will open.

### 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

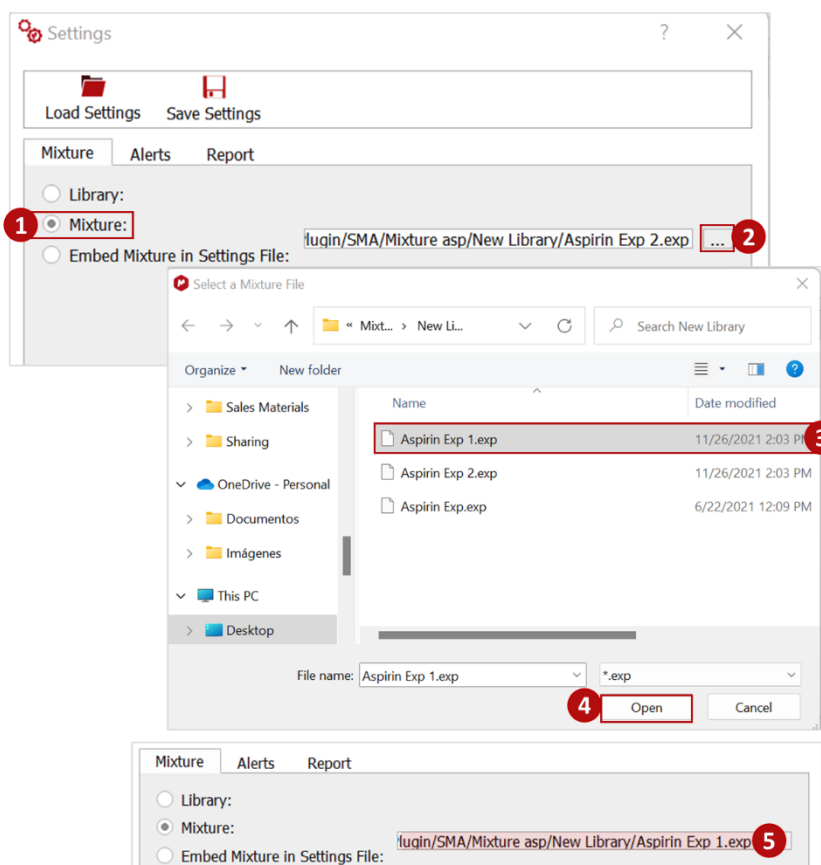
Parameter	Value
1 Data File Name	[Redacted]
2 Title	Aspirin_A2_neu_NOESY_01
3 Comment	RC:10.0 Experiment: Aspirin Ci

### Parameters table - Sample 3

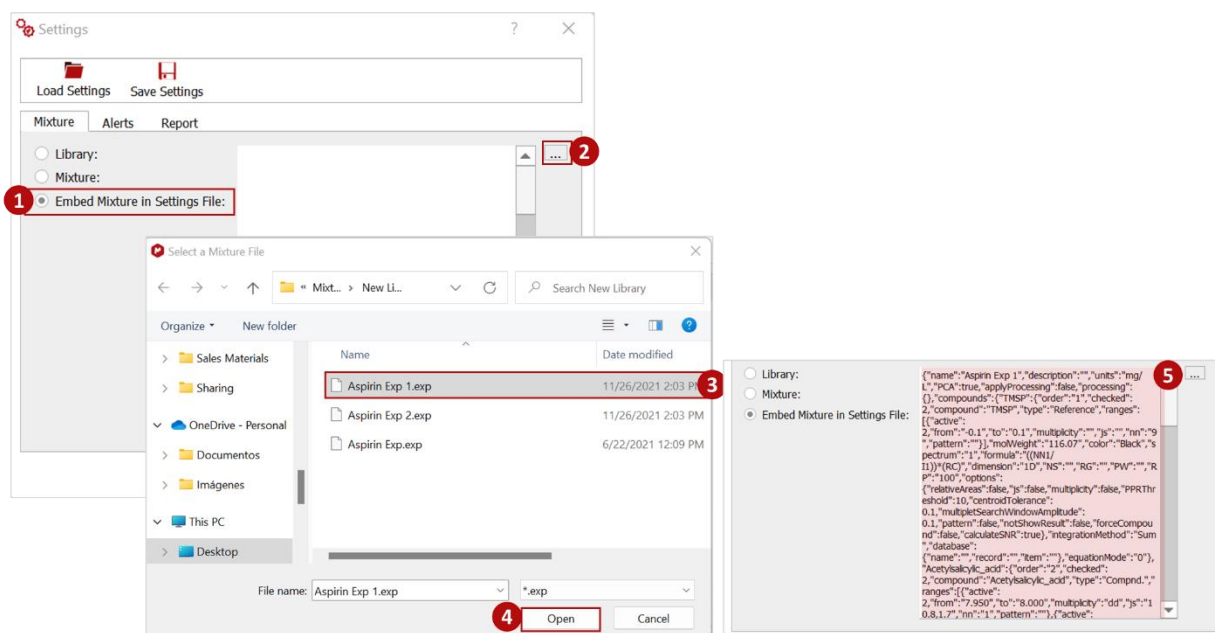
Parameter	Value
1 Data File Name	C:/Users/[Redacted]
2 Title	Solvents.154.1.1r
3 Comment	MIX: brucine_solvent

**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.



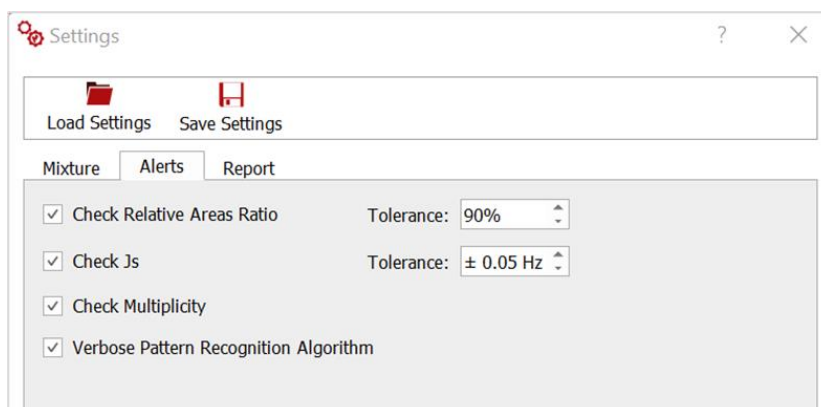
If you wish to embed mixture in the Mgears settings file, enable the **Embed Mixture in Settings File**, click on this button and upload the desired mixture file as shown below.



### 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:

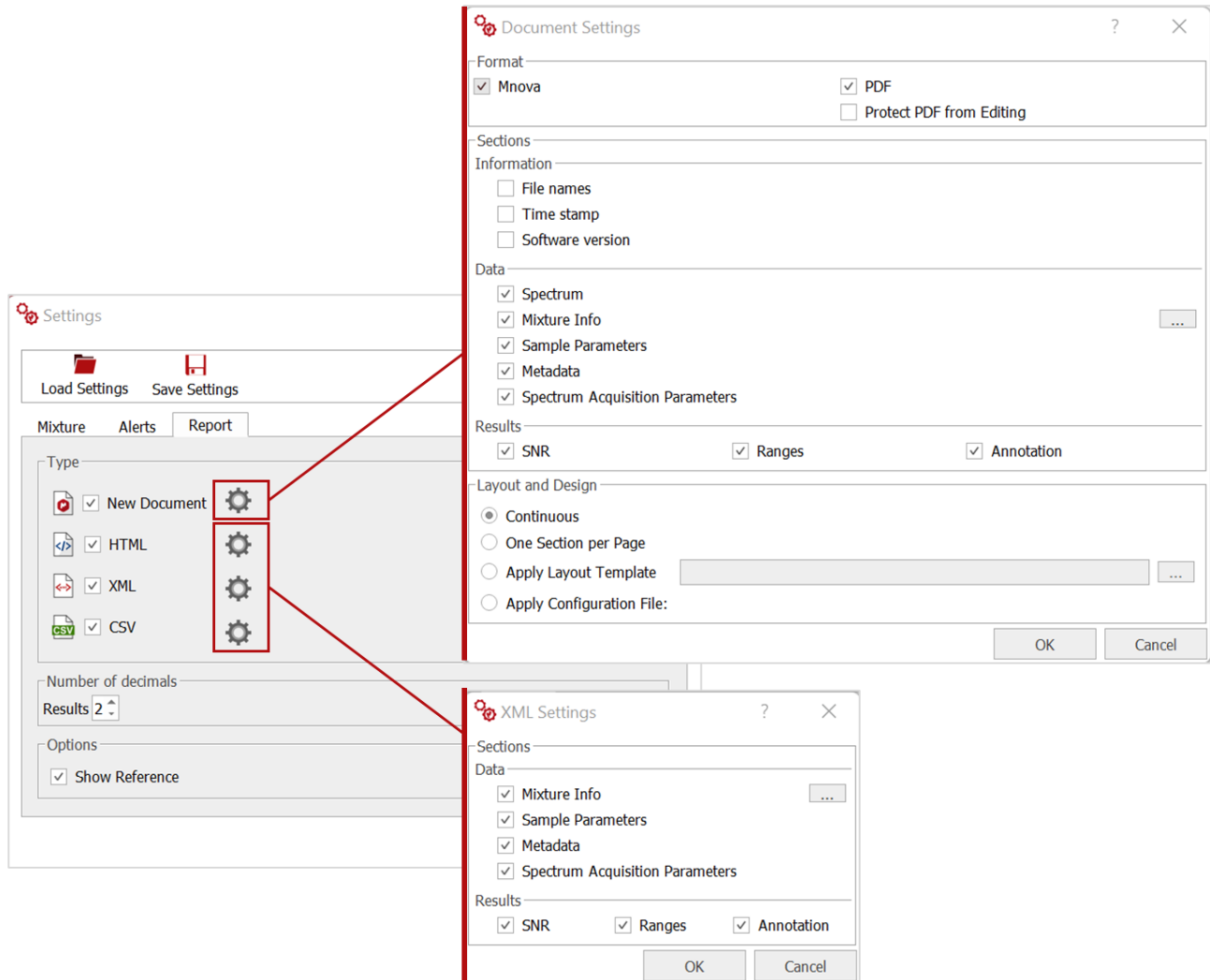
- **Check Relative Areas ratio:** to calculate the relative area ( $\text{Integral}_i / \text{NN}_i$ ) / ( $\text{Integral}_j / \text{NN}_j$ ) and compare it to the expected values (between  $1 - \text{tolerance}/100$  and  $1 + \text{tolerance}/100$ ). You can set the tolerance value in the dedicated 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

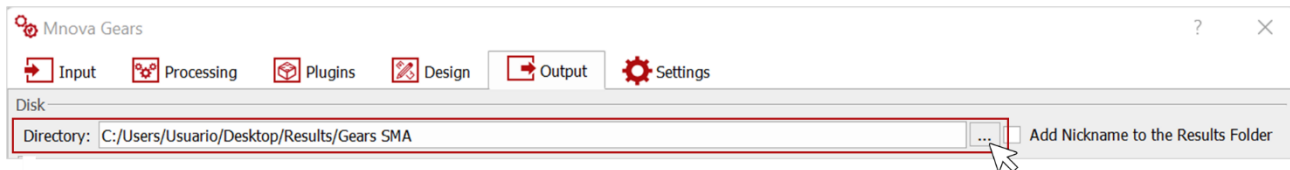
Gears SMA can generate advanced reports the same way Mnova SMA does. These reports can be customized in this **Report** tab. Here, you can check the types of reports you would like to have and configure the different sections that can be included. (For further details about the advanced reports, please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



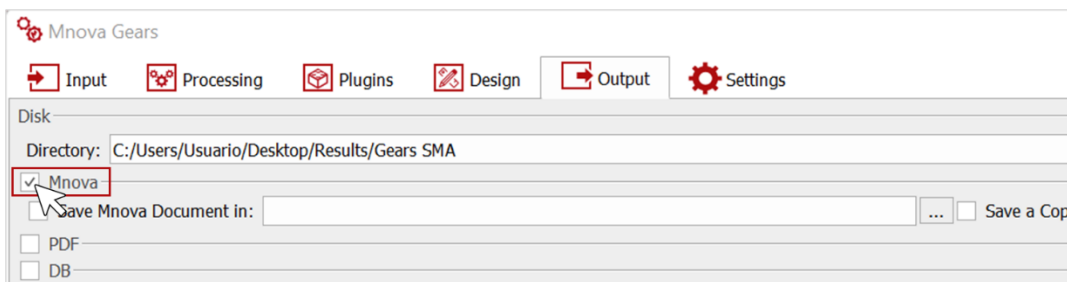
When you are happy with the setup, click on **OK** and go to the **Output** tab.

## 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](#).

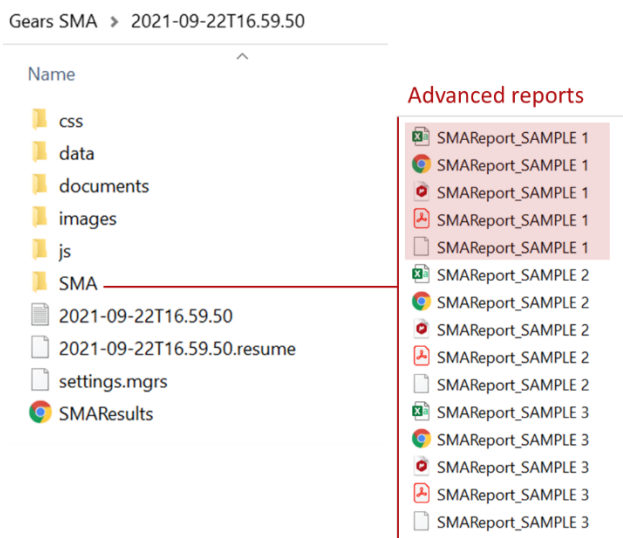


You can also choose to save your results to a database. To do so you will have to add the database connection credentials and connect. A new record will be created for each analyzed dataset (unless you decide to update existing ones!)

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.

MGEARS SMA RESULTS

### Parameters

Parameter	Value
Results Directory	C:/Users/Usuario/Desktop/Results/Gears SMA/2021-09-22T16.59.50
Started On	2021-09-22T16:59:50
Completed On	2021-09-22T17:01:01

### Detailed Results

Show  entries

Search:

#	Documents	Mnova Report	PDF Report	HTML Report	XML Report	CSV Report
1	SAMPLE 1.mnova	SMAReport_SAMPLE 1.mnova	SMAReport_SAMPLE 1.pdf	SMAReport_SAMPLE 1.html	SMAReport_SAMPLE 1.xml	SMAReport_SAMPLE 1.csv
2	SAMPLE 2.mnova	SMAReport_SAMPLE 2.mnova	SMAReport_SAMPLE 2.pdf	SMAReport_SAMPLE 2.html	SMAReport_SAMPLE 2.xml	SMAReport_SAMPLE 2.csv
3	SAMPLE 3.mnova	SMAReport_SAMPLE 3.mnova	SMAReport_SAMPLE 3.pdf	SMAReport_SAMPLE 3.html	SMAReport_SAMPLE 3.xml	SMAReport_SAMPLE 3.csv

Showing 1 to 3 of 3 entries

## 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](#).

**SMA REPORT**

Library: C:\Users\k\...\Desktop\Datasets\By plugin\Gears SMA\Experiments

Mixture name: Aspirin CI

Description: Determination of the levels of Acetylsalicylic acid, Ascorbic acid, Citric acid, Salicylic acid, Acetic acid Intermediate analysis

Units: mg/L

Compound List:

Checked	Compound	Type	Ranges	MolWeight	Spectrum	Formula	Dimension	Integration	Options
<input checked="" type="checkbox"/>	TMSP	Reference	From: 1.12 To: 1.12	116.0700	1	((NN1/1))*RC	1D	Sum	
<input checked="" type="checkbox"/>	Acetylsalicylic_acid	Compnd	From: 7.00 To: 8.00 From: 7.70 To: 8.00 From: 7.40 To: 8.00 From: 7.20 To: 8.00 From: 7.00 To: 8.00	180.1600	1	((((11/NN1)+(12/NN2)+(13/NN3)/(14/NN4)/4))*CCF	1D	Sum	Verbose Pattern Recognition Algorithm
<input checked="" type="checkbox"/>	Salicylic_acid	Compnd	From: 19.100 To: 19.100 From: 17.700 To: 19.100	138.1200	1	((((11/NN1)+(12/NN2)+(13/NN3)/(14/NN4)/4))*CCF	1D	Sum	Verbose Pattern Recognition Algorithm
<input checked="" type="checkbox"/>	Ascorbic_acid	Compnd	From: 4.00 To: 4.00 From: 4.00 To: 4.00	176.1300	1	((((11/NN1)+(12/NN2)+(13/NN3)/(14/NN4)/4))*CCF	1D	Sum	Verbose Pattern Recognition Algorithm
<input checked="" type="checkbox"/>	Acetic_acid	Compnd	From: 2.00 To: 2.00	60.0500	1	((11/NN1))*CCF	1D	Sum	
<input checked="" type="checkbox"/>	Citric_acid	Compnd	From: 3.00 To: 3.00 From: 3.00 To: 3.00	192.1300	1	((((11/NN1)+(12/NN2)+(13/NN3)/(14/NN4)/4))*CCF	1D	Sum	Verbose Pattern Recognition Algorithm

Sample Parameters:  
Reference Concentration: 10.0

Custom Parameters:

Metadata:

Spectrum Acquisition Parameters:

Data\_File\_Name: X:\2014\201403\01\Aspirin\_AZ\_mg\_NDEBY\_01

Title: Aspirin\_AZ\_mg\_NDEBY\_01

Comment: IC-10 Experiment Aspirin CI

Origin: Velion

Owner:

Site:

Instrument: velion

Autob:

Solvent: CH<sub>2</sub>Cl<sub>2</sub>

Temperature: 25

Public\_Requirement: NONE.VY

Experiment: ID

Probe: ID

Number\_of\_Scans: 128

Receiver\_Gain: 0

Resolution\_Delay: 3.5

Public\_Memory: 7.2

Precursor\_Frequency: 4.812103814403499

Acquisition\_Time: 2.00002

Acquisition\_Date: 2014-07-01T17:53:46

Modification\_Date: 2014-07-02T08:07:19

Class:

IRFAC:

Spectrometer\_Frequency: 590.5281593

Spectrum\_Method: 9615.3061028

Lowest\_Frequency: -1500.77522396

Noiseless: 0

Acquired\_Size: 24038

Spectral\_Size: 65536

Experiment: Aspirin CI

Chemical shift (ppm): 14 to -1

Peak labels: Salicylic\_acid\_2 (1.12), Acetylsalicylic\_acid\_2 (8.00), Acetylsalicylic\_acid\_3 (8.00), Acetylsalicylic\_acid\_3 (8.00), Salicylic\_acid\_1 (19.10), Salicylic\_acid\_3 (19.10), Ascorbic\_acid\_2 (4.00), Citric\_acid\_1 (3.00), Citric\_acid\_2 (3.00), Acetic\_acid (2.00), TMSP (1.12)

Compound	Result(mg/L)	DMF Mean (min, max)	Ranges
Acetylsalicylic_acid	242.564	2029.89 (1764.57, 2388.99)	From: 7.00 To: 8.00 From: 7.70 To: 8.00 From: 7.40 To: 8.00 From: 7.20 To: 8.00 From: 7.00 To: 8.00
Salicylic_acid	86.977	667.71 (480.76, 820.37)	From: 19.100 To: 19.100 From: 17.700 To: 19.100
Ascorbic_acid	169.318	1749.56 (880.24, 2618.88)	From: 4.000 To: 4.000 From: 4.000 To: 4.000
Acetic_acid	161.368	20128.17	From: 2.000 To: 2.000
Citric_acid	698.470	31227.02 (2061.61, 31652.43)	From: 3.000 To: 3.000 From: 3.000 To: 3.000

Compound	C	D	E	F	G	H	I	J	K	L
TMSP	1.12									
Acetylsalicylic_acid	7.00-8.00									
Salicylic_acid	19.100									
Ascorbic_acid	4.000									
Acetic_acid	2.000									
Citric_acid	3.000									

## 3. Mnova Gears Results Viewer

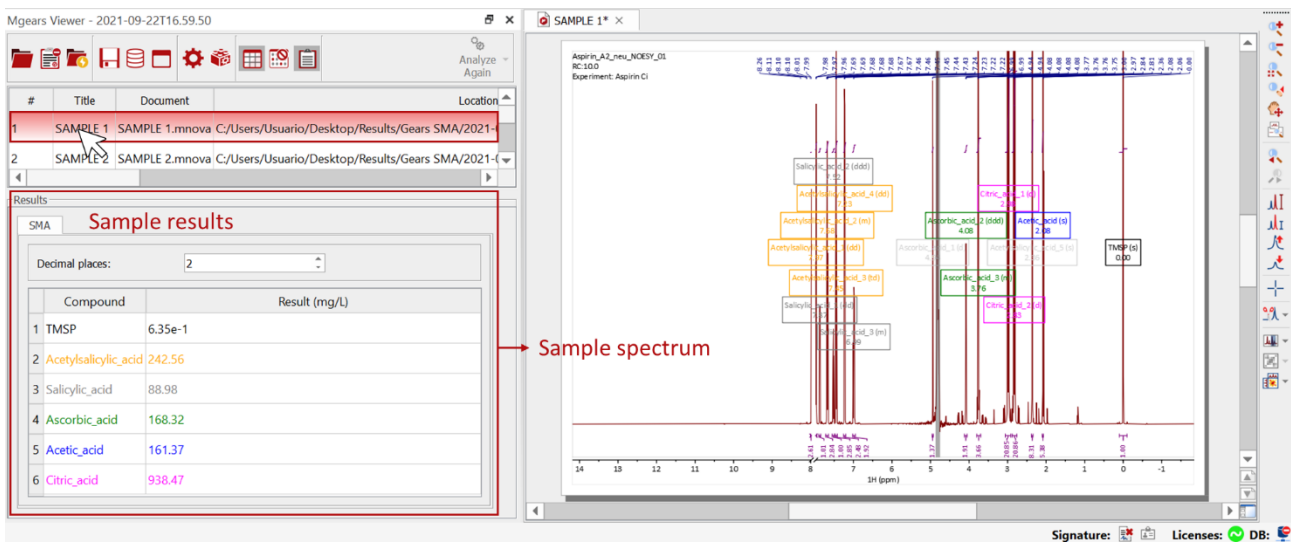
Open the **Mgears Results Viewer**, for a quick and convenient review of the results. Import your analysis results.

MestReNova

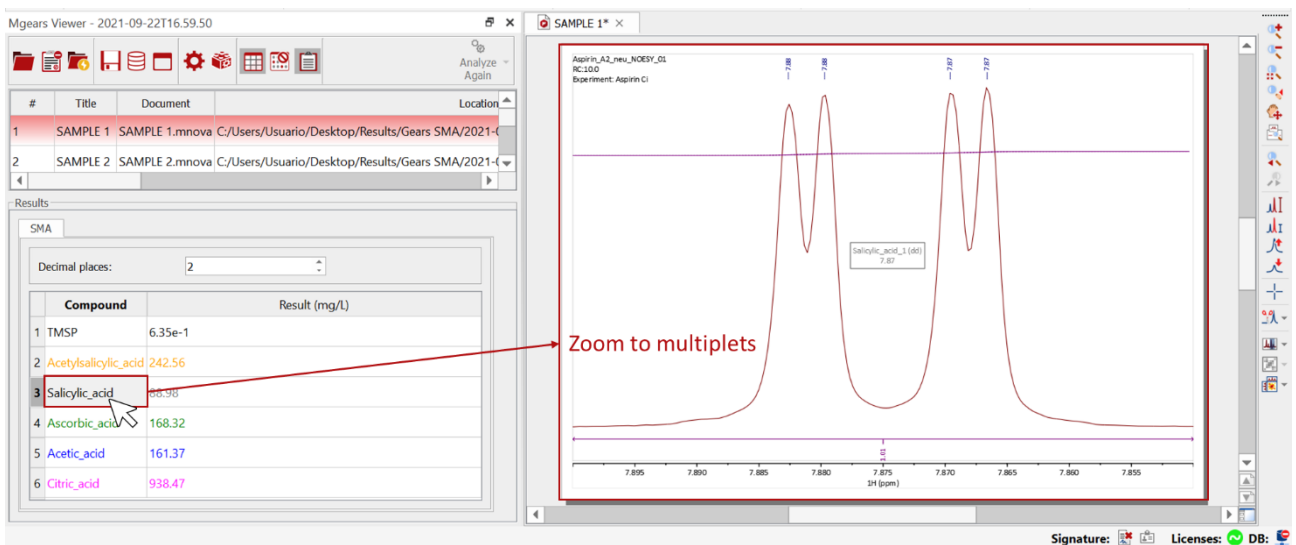
Elucidation Chemometrics Binding Automation

Mgears Mgears Viewer MyGears MyGears Workflows

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 screenshot shows the Mnova software interface with the Simple Mixture Analysis dialog box open. The dialog box has two tabs: 'Analysis Data' and 'Result'. The 'Analysis Data' tab is active, showing the following information:

- Mixture:** C:/Users/Usuario/Desktop/Datasets/By Plugin/Gears SMA/experime...
- Library:** experiments
- Name:** Aspirin CI
- Descriptor:** Determination of the levels of: Acetylsalicylic acid, Ascorbic acid, Citric acid, Salicylic acid, Acetic acid Intermediate analysis

Parameters are listed below:

- Standard:  Custom:
- Sample ID:
- Reference Concentration (RC): 1.0
- Sample Weight (SW) [mg]:
- Reference Weight (RW) [mg]:
- Number of Scans (NS):
- Receiver Gain (RG):
- Pulse Width (PW):
- Temperature (T):
- Spectral Width (SpecW):
- Spectral Size (SpecS):

A red box highlights the 'Load' icon (a red square with a white arrow) in the bottom right corner of the dialog box. The background shows the main Mnova interface with a table of results and a spectrum plot.

#	Compound	Result (mg/L)
1	TMSP	6.35e-1
2	Acetylsalicylic_acid	242.56
3	Salicylic_acid	88.98
4	Ascorbic_acid	168.32
5	Acetic_acid	161.37
6	Citric_acid	938.47

The loaded results can be revised and updated as required.

The screenshot shows the Mnova software interface with the Simple Mixture Analysis dialog box open. The 'Result' tab is active, displaying a table of results. A red box highlights the table, and a red arrow points from the table in the background to the table in the dialog.

#	Compound	Result (mg/L)	Annotation
1	<input checked="" type="checkbox"/> TMSP	6.35e-1	
2	<input checked="" type="checkbox"/> Acetylsalicylic_acid	242.56	
3	<input checked="" type="checkbox"/> Salicylic_acid	88.98	
4	<input checked="" type="checkbox"/> Ascorbic_acid	168.32	
5	<input checked="" type="checkbox"/> Acetic_acid	161.37	
6	<input checked="" type="checkbox"/> Citric_acid	938.47	

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.

**Exclude a multiplet from calculation**

#	Compound	Result (mg/L)	SNR
1	TMSP	6.35e-1	3571.00 (3571.00)
2	Acetylsalicylic_acid 249.14	2105.64 (1820.23)	0.00
3	Salicylic_acid 88.98	709.43 (495.87, 8)	
4	Ascorbic_acid 168.32	1804.80 (908.04, 4)	
5	Acetic_acid 161.37	20760.59 (20760.59)	

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.