Mestrelab Research

Gears MS Scan 1.0

STARTING GUIDE

Document Number

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Contents

For researchers working with LCMS data in the field of metabolomics, a common task is to quantify the masses found within a certain retention time window. Such an analysis can be unexpectedly difficult in instrument vendor software, especially when the list of masses is long or the number of samples large. MS Scan is a plugin for Mnova Gears that has been developed to solve this problem, it automatically extracts mass spectra and corresponding chromatograms from a batch of TIC (total ion current) files. The software:

- reads a TIC from an input document
- extracts up to three mass spectra in the previously set Retention Time ranges
- it then reads the peaks, extracts the chromatograms, and quantifies peaks for each of the masses that pass the specified threshold.

MS Scan generates automatic reports with results that can be easily reviewed and edited via the Mgears viewer.

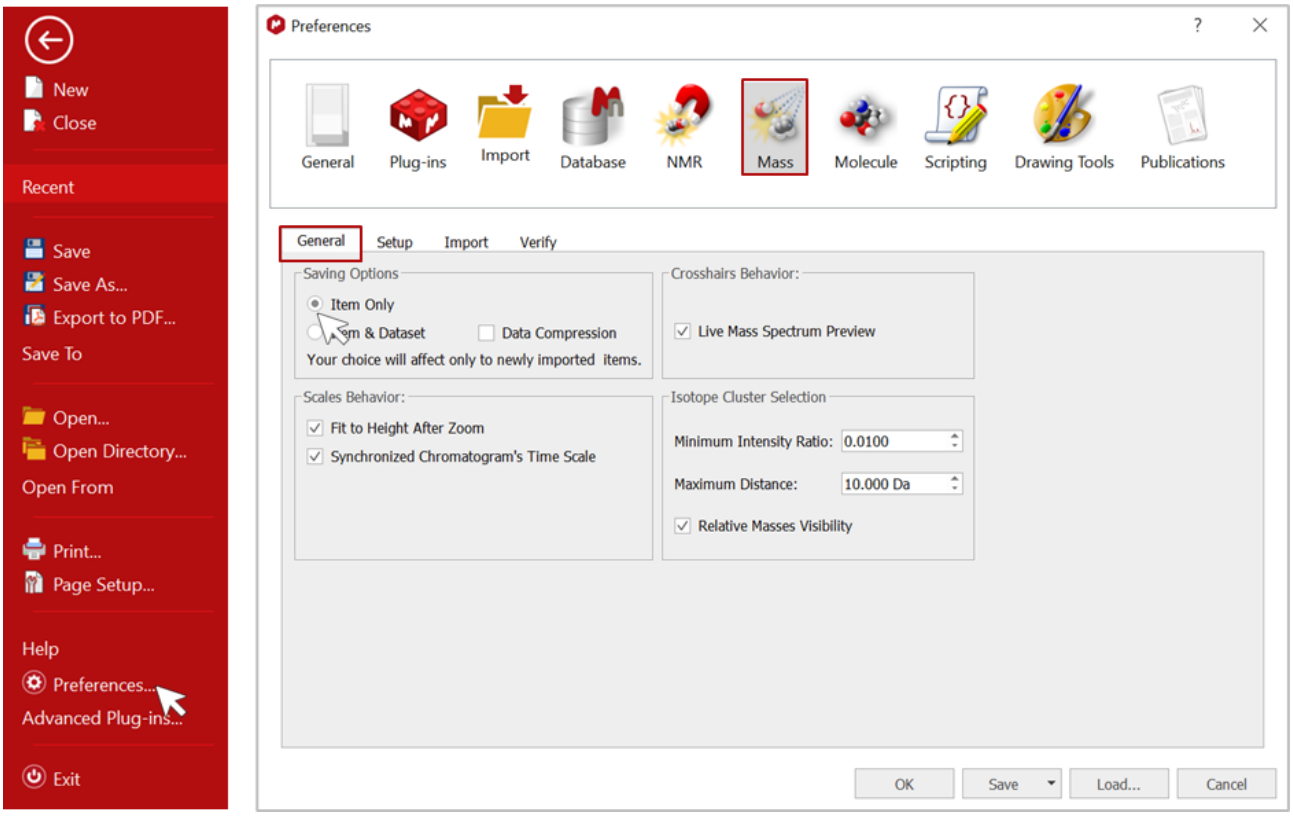
This document is intended to help you configure and run a typical MS Scan analysis. For more details about Mgears options, please refer to the Mgears manual.

So, let´s get you started!

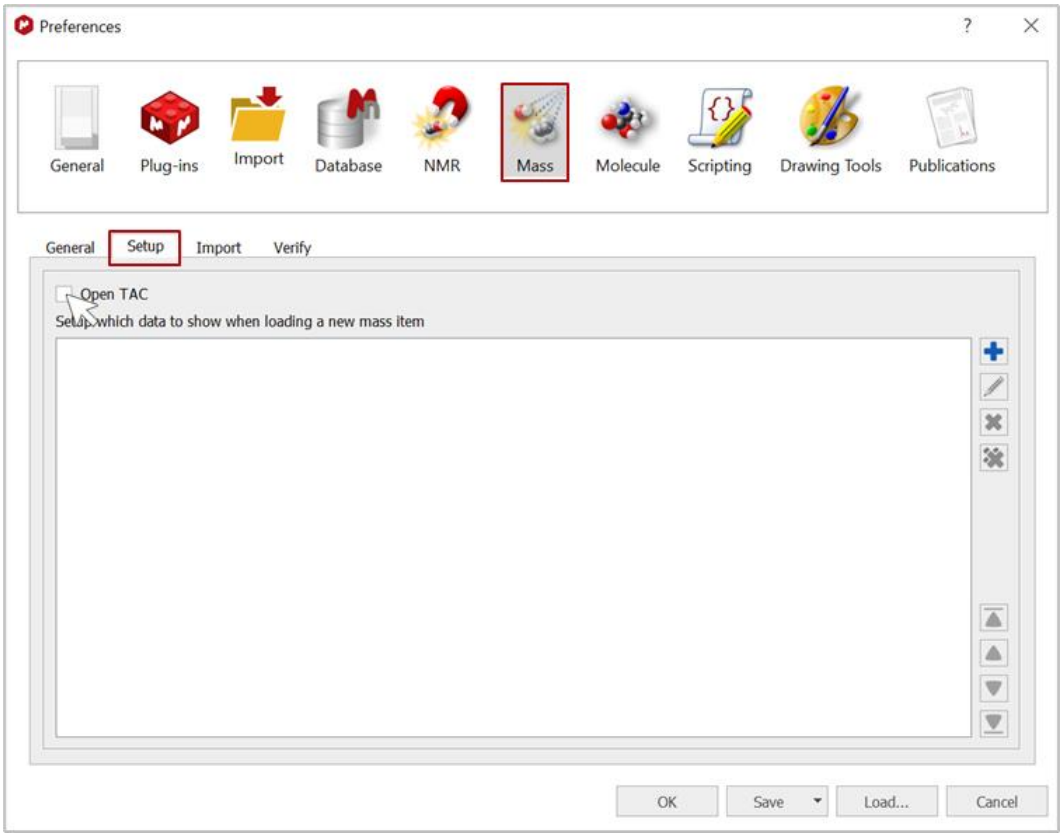
1. The Workflow

Before starting your analysis, go to Mnova **File** > **Preferences** > **Mass** to configure the mass analysis preferences. MS Scan creates quite a lot of graphics, so it is highly recommended to save the Mnova results with the minimum possible “weight”.

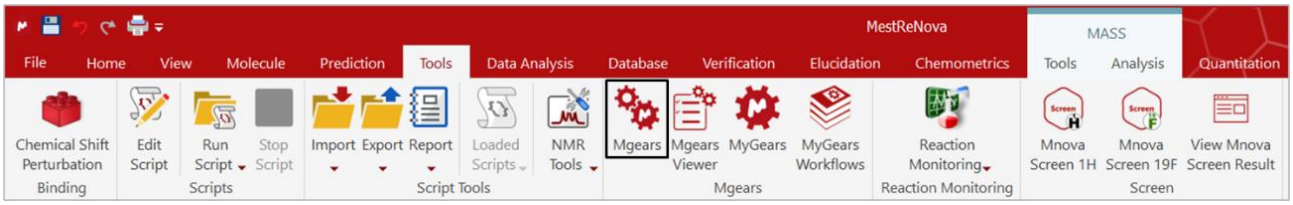
To do so, in the **General** tab > **Saving Options**, check the **Item Only** option to save the minimum data required.



In the **Setup** tab, uncheck the **Open TAC** option to avoid opening the PDA total absorbance chromatogram at the top of each document.



Now launch Mgears from the **Tools** ribbon.

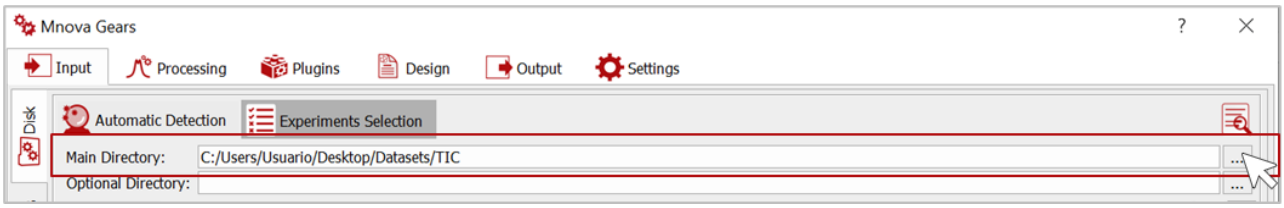


The MS Scan analysis follows the general Mgears workflow based on the five-step setup.

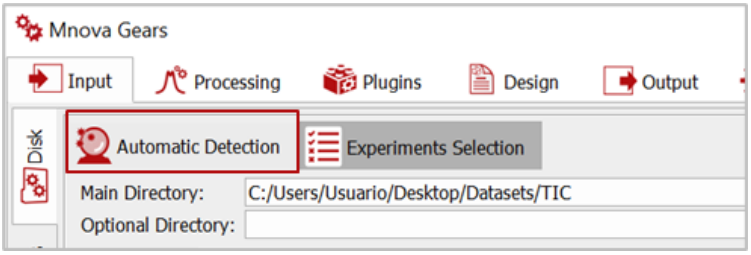
1.1. Input

First, in the **Input** tab, select the data files for analysis by Mgears. Input files can come from **Disk** directories, a database (**DB**), or from **Real-Time** acquisition. These modes are detailed in the Mnova Gears manual.

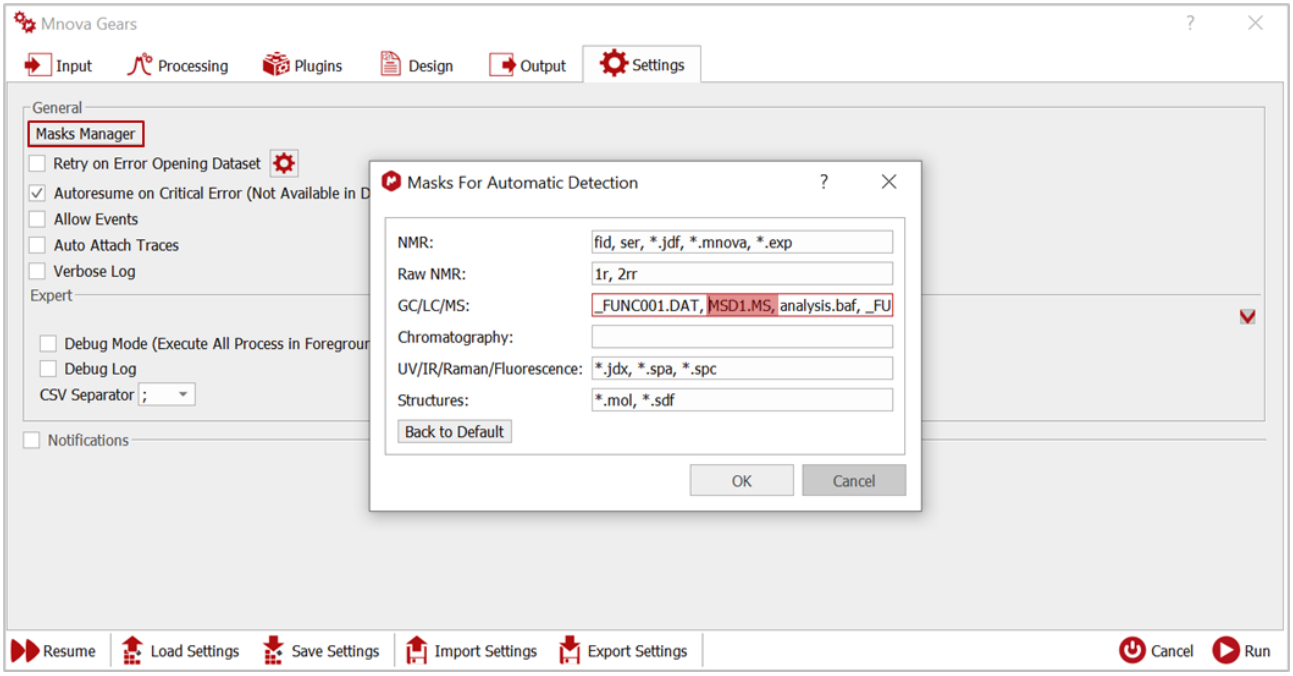
In this guide, we will use data from a **Disk** directory. So, in the **Disk** section, click on ... and choose the directory from which your MS data files will be retrieved.



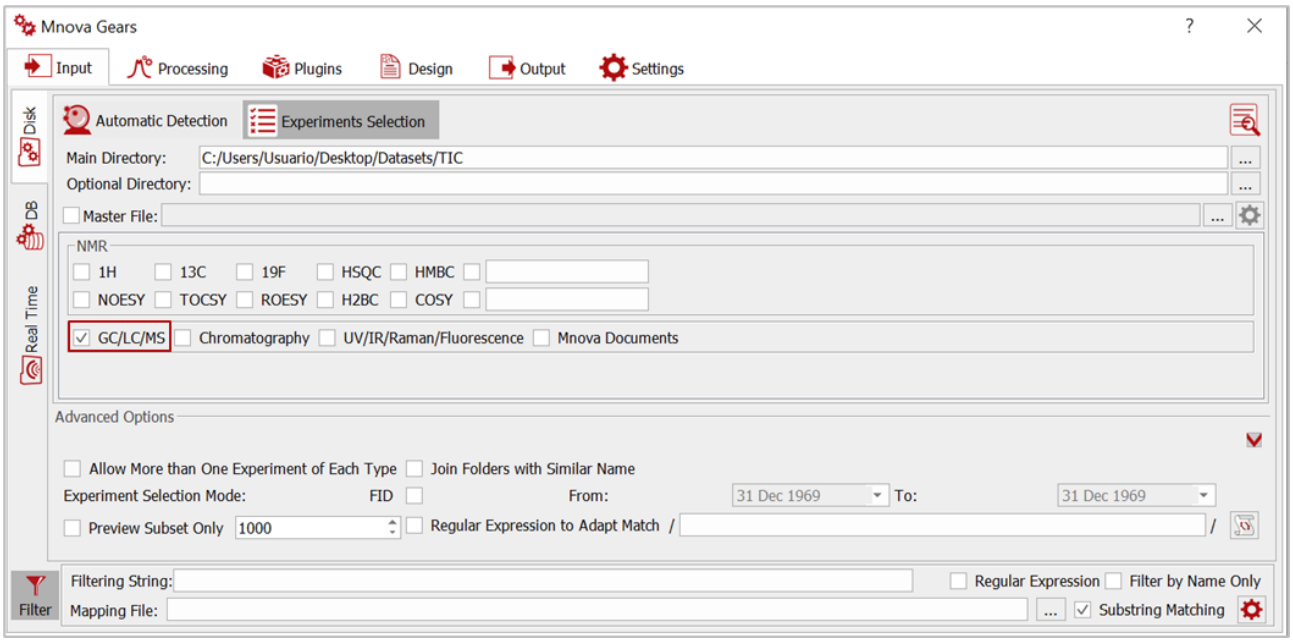
Use the **Automatic Detection** mode, with which Mgears will use the saved masks to find experiment files.



Watch out! Your dataset masks ("MSD1.MS" in this example) must be correctly configured to be recognized by Mgears. Go the **Settings** tab and click on the **Mask Manager** button to view current masks. If your file mask is not entered, you can simply type it and click on **OK** to save the changes.

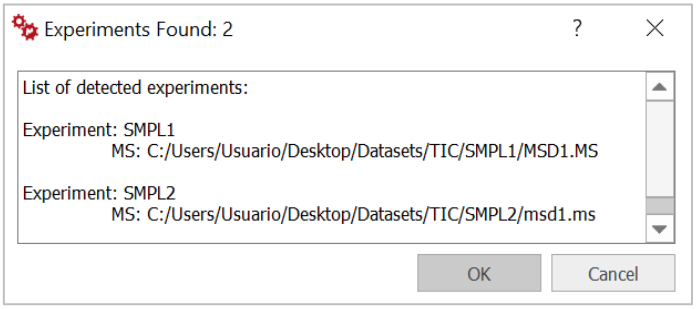


Going back to the **Input** section, you can click on **Experiments Selection** and check the **GC/LC/MS** experiment type to avoid Mgears attempting to recognize and analyze other types of experiment files.



If needed, configure the **Advanced Options** or use the **Filtering Options** to refine the detection of your input data files.

Top Tip! Before moving to the next step, you can use the **Automatic inspection** button to check if the detected experiments correspond to your selection criteria.

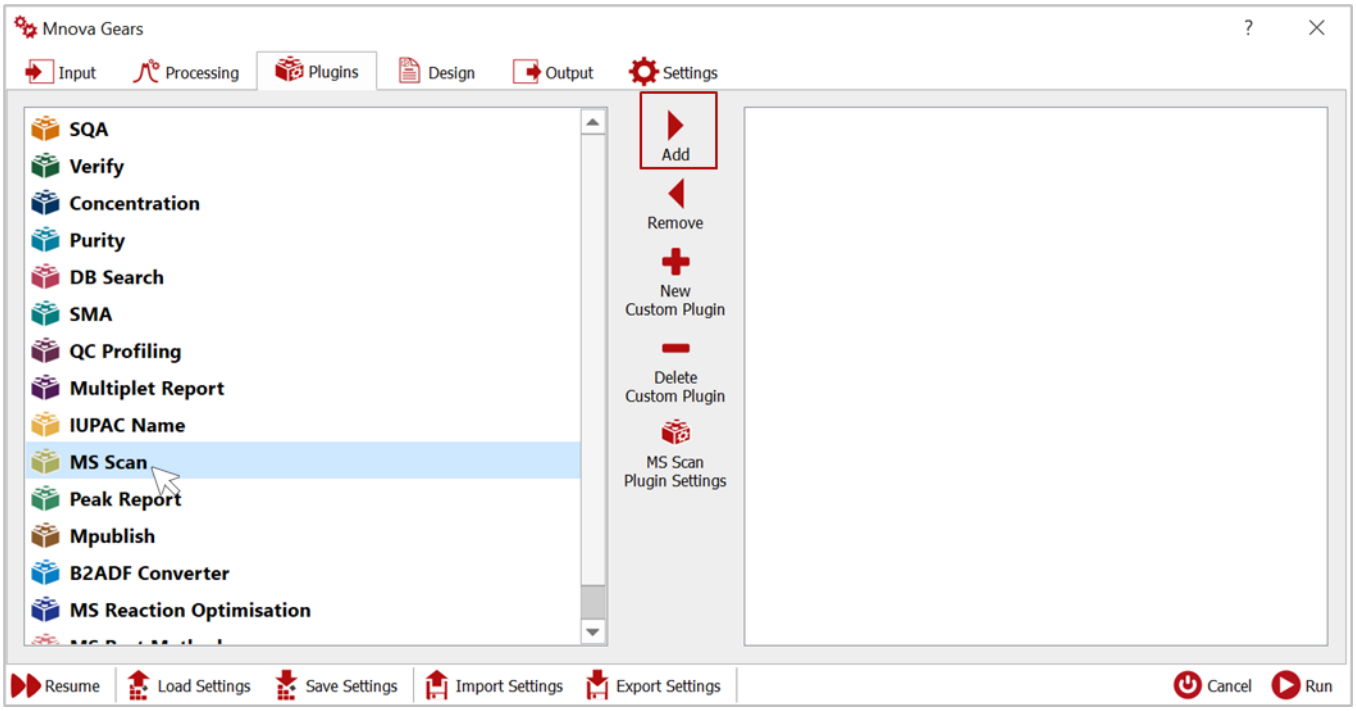


1.2. Processing

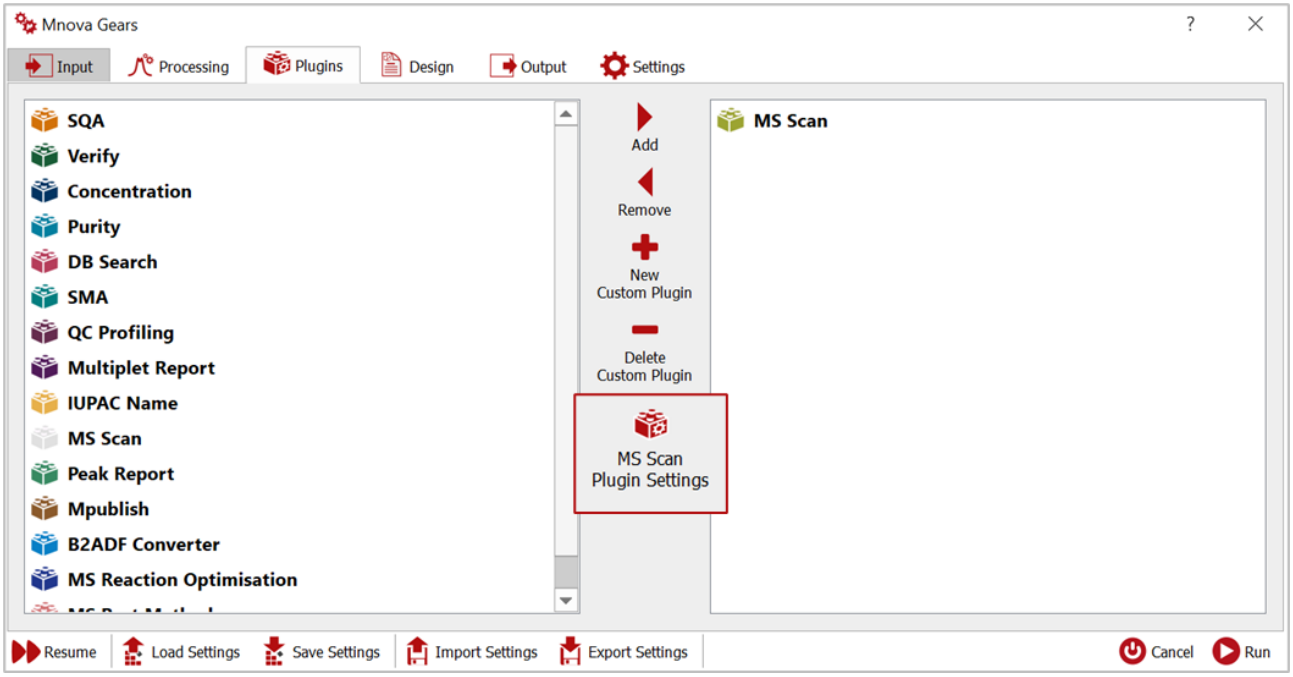
In the **Processing** tab, you can upload a processing script to apply your own customized processing settings *(please refer to the Mnova Gears manual for more details about this option).*

1.3. Plugins

In the **Plugins** tab, select and add the MS Scan plugin.



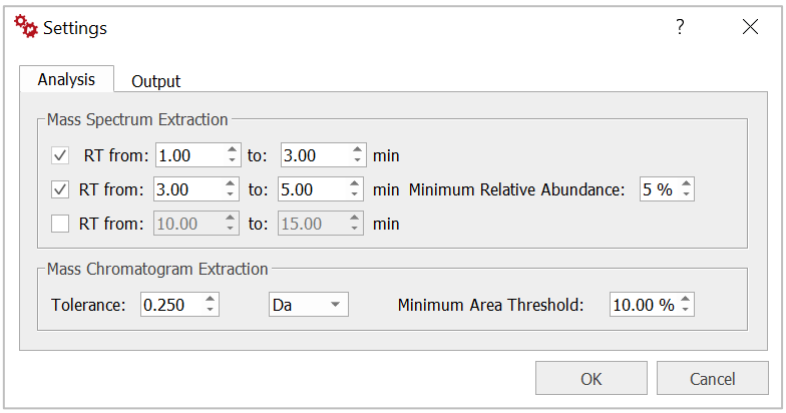
The added plugin will appear on the right-hand side of the dialog. You should now click on **MS Scan Plugin Settings** to configure the **Analysis** and **Output** parameters.



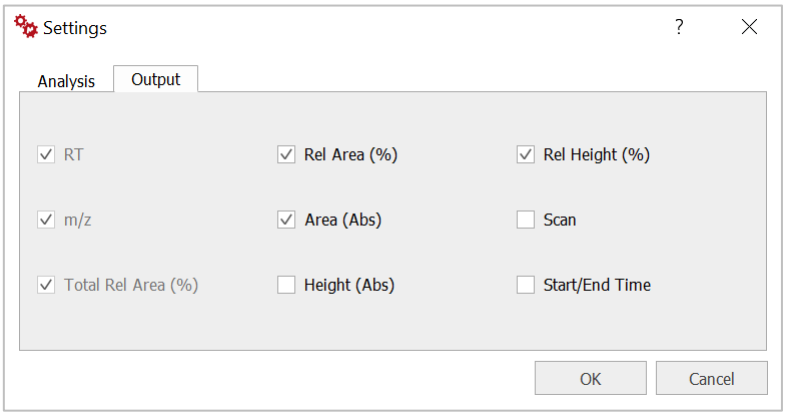
A **Settings** dialog will appear. In the **Analysis** tab, you should choose the mass spectrum **Retention time** (**RT**) ranges from which you want to extract chromatograms. You can enter up to three RT ranges.

You should also define the **Minimum Relative Abundance** % for the Mass spectrum extraction.

You can then choose the **Tolerance** and **Minimum Area Threshold** for the peaks of the mass chromatogram extraction.

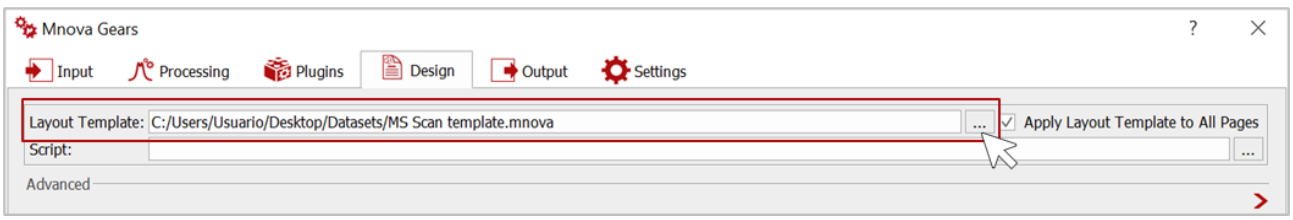


In the **Output** tab, you can configure the variables to display in the CSV and HTML result files that will be automatically generated by Mgears. The **RT**, **m/z**, and **Total Relative Area** of the peaks are included in the reports by default, whereas other parameters, such as **Relative area**, peak **Height**, etc., are entirely optional.



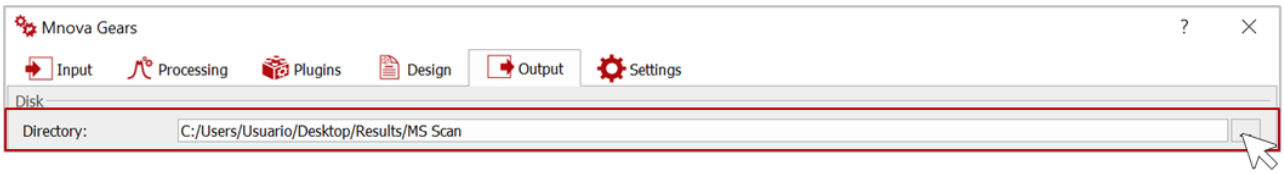
1.4. Design

In the **Design** tab, you can upload an Mnova layout templates or a Script to produce a final customized report.



1.5. Output

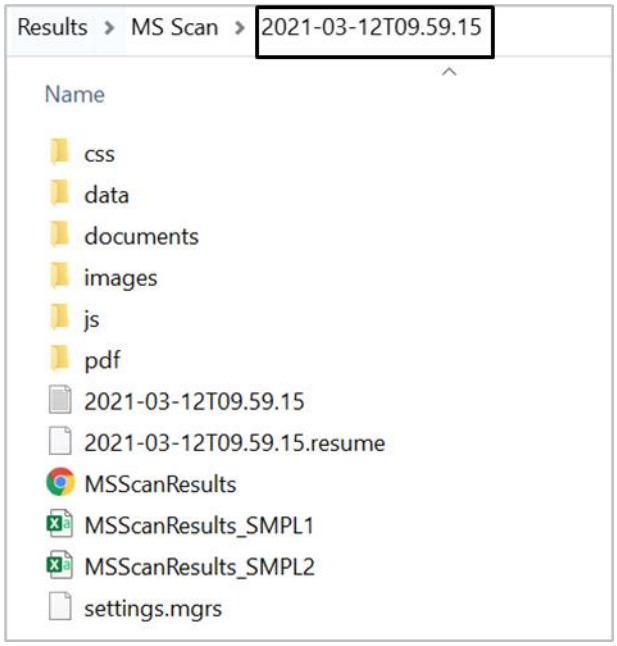
In the **Output** tab, click on ... and choose a directory in which to save your analysis results.



As for all Mgears plugins, you can also choose to create an Mnova or PDF document with your results and save your results to a connected DB.

2. The output folder

The results folder, which is named according to the date and time at which your analysis was run, is saved under the directory specified previously. This folder contains all the output generated in the current evaluation.



MS Scan results and analysis parameters are reported:

- in a CSV document:

Tolerance [Da]	Minimum Relative Abudance [%]	Minimum Area Threshold [%]			
0.25	5	10			
m/z [Da]	RT [min]	Total Rel Area [%]	Rel Area [%]	Abs Area	Rel Height [%]
537.3	1.28	10.09	100	14523	100
552.2	1.96	70.13	100	100985.5	100
568	1.4	0.84	73.99	1216	58.06
568	2.66	0.3	26.01	427.5	41.94
614	1.76	16.77	100	24147.5	100
537.3	4.24	0.14	48.38	198.112	49.36
537.3	4.66	0.15	51.62	211.4	50.64
552.2	3.2	0.11	28.65	162	17.4
552.2	3.48	0.08	20.34	115	18.62
552.2	4.46	0.13	32.63	184.5	24.41
552.2	4.5	0.07	18.39	104	39.56
568	3.94	0.05	10.94	75	50.08
568	4.14	0.42	89.06	610.5	49.92
614	3.22	0.16	22.79	234.5	25.58
614	3.66	0.24	33.14	341	31.82
614	3.9	0.19	27.11	279	21.87
614	4.2	0.12	16.96	174.5	20.73

- and in an HTML file:

Mgears MSScan Results

Parameters

Parameter	Value
Results Directory	C:/Users/Usuario/Desktop/Results/MS Scan/2021-03-12T09.59.15
Started On	2021-03-12T09:59:15
Completed On	2021-03-12T09:59:20
Minimum Relative Abundance	5%
Tolerance	0.25 Da
Minimum Area Threshold	10.00 %

Detailed Results

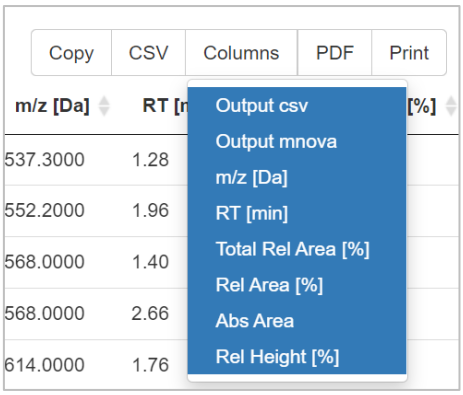
Show 100 entries Copy CSV Columns PDF Print Search:

Output csv	Output mnova	m/z [Da]	RT [min]	Total Rel Area [%]	Rel Area [%]	Abs Area	Rel Height [%]
MSScanResults_SMPL1.csv	SMPL1.mnova	537.3000	1.28	10.09	100.00	14523.000	100.00
MSScanResults_SMPL1.csv	SMPL1.mnova	552.2000	1.96	70.13	100.00	100985.500	100.00
MSScanResults_SMPL1.csv	SMPL1.mnova	568.0000	1.40	0.84	73.99	1216.000	58.06
MSScanResults_SMPL1.csv	SMPL1.mnova	568.0000	2.66	0.30	26.01	427.500	41.94
MSScanResults_SMPL1.csv	SMPL1.mnova	614.0000	1.76	16.77	100.00	24147.500	100.00
MSScanResults_SMPL1.csv	SMPL1.mnova	537.3000	4.24	0.14	48.38	198.112	49.36
MSScanResults_SMPL1.csv	SMPL1.mnova	537.3000	4.66	0.15	51.62	211.400	50.64
MSScanResults_SMPL1.csv	SMPL1.mnova	552.2000	3.20	0.11	28.65	162.000	17.40
MSScanResults_SMPL1.csv	SMPL1.mnova	552.2000	3.48	0.08	20.34	115.000	18.62
MSScanResults_SMPL1.csv	SMPL1.mnova	552.2000	4.46	0.13	32.63	184.500	24.41
MSScanResults_SMPL1.csv	SMPL1.mnova	552.2000	4.50	0.07	18.39	104.000	39.56

Each row in the CSV and HTML reports represents an extracted chromatogram peak with its m/z, RT, and Total Rel Area (%). Rel Area (%), Abs Area, and Rel Height (%) are also displayed for each peak, as previously defined in the plugin settings in this example.

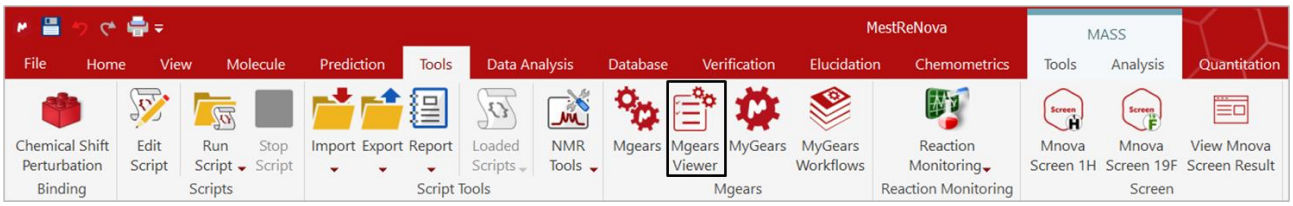
You will also find links to the CSV and Mnova results in the HTML report.

The advantage of this type of report is that it allows you to change the display of the **Columns** and adapt them to your preferences, then **Copy**, **Print**, or save your results into **CSV** or **PDF** format.

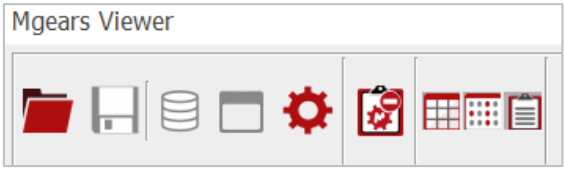


3. Results review with the Mgears Viewer

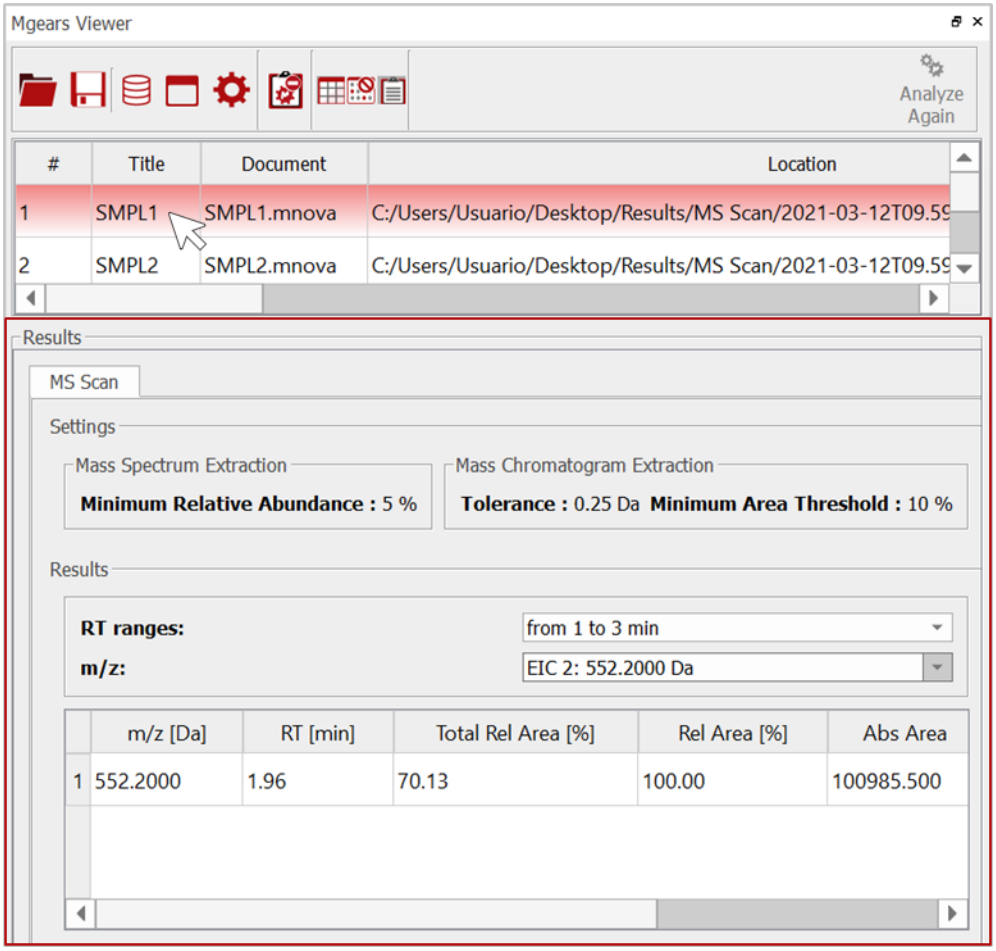
MS Scan is compatible with the **Mgears Viewer**, which allows you to review your results. Start this example by opening the **Mgears Viewer** from the **Tools** section in Mnova:



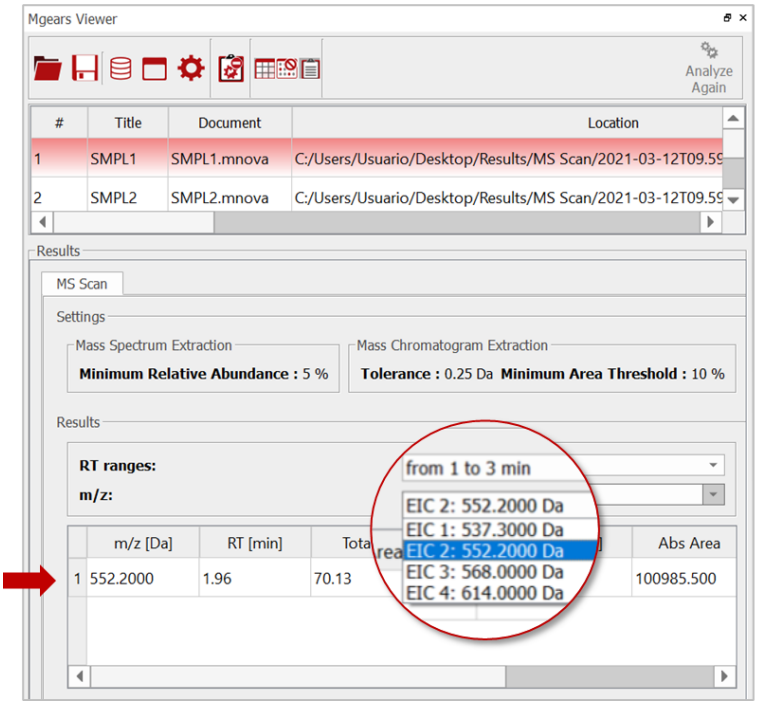
Click on  and select the MS Scan analysis output folder.

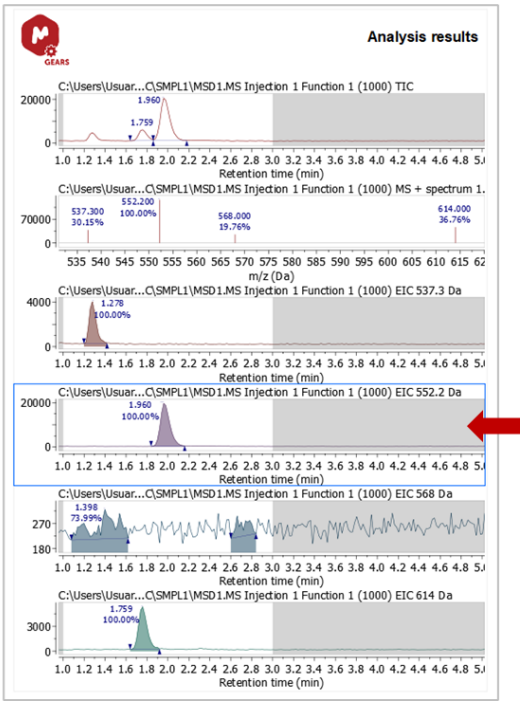


The experiment results will be loaded in the **Mgears Viewer** dialog. Select a sample in the table or well plate. The detailed results will appear in the **Results** section, and the corresponding Mnova document will open.



In the **Results** section, you can select the **RT range** and **m/z** you want to inspect. Detailed results are displayed in the table below, and the corresponding extracted-ion chromatogram (EIC) plot is set as active in the Mnova document.





You can review your results, change peaks colors, etc., using the standard tools from Mnova, then save the changes by clicking on **Save** .

Note that, in this version of MS Scan (1.0), the **Analyze Again** option is not available, therefore a recalculation cannot be performed.

For more details on the Mnova Gears options, please refer to the Mnova Gears manual.