Mestrelab Research

Mnova Gears 2.5

USER MANUAL

Document Number

P/N 236 R3

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1. Introduction

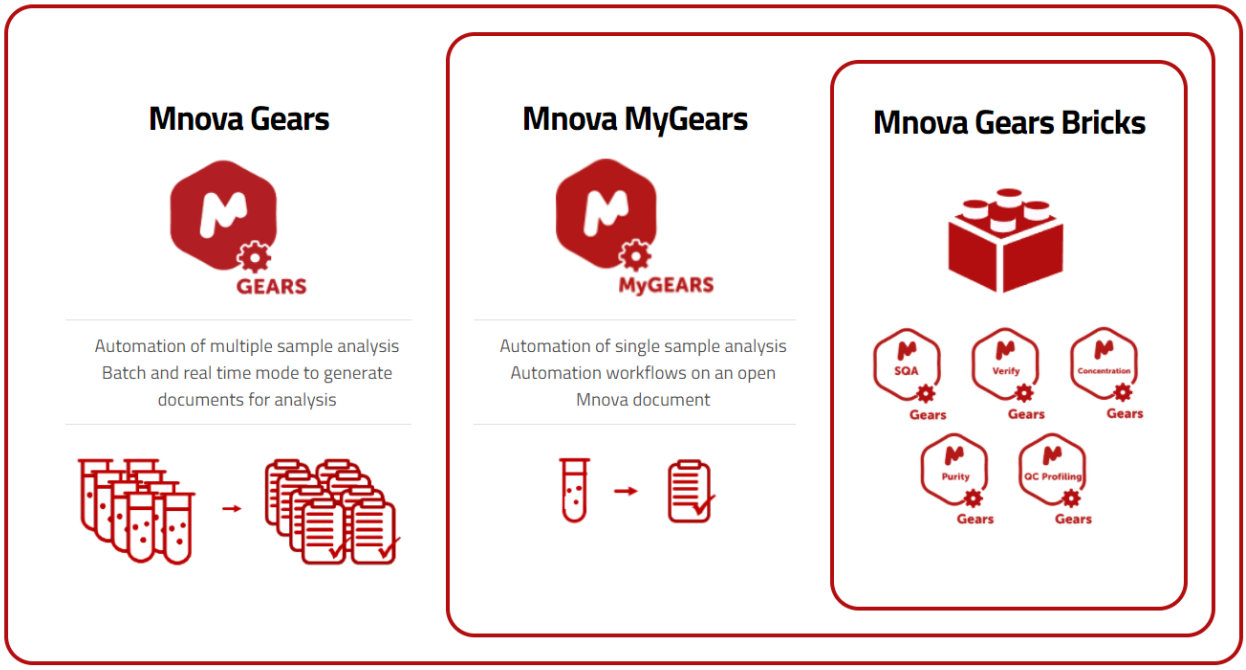
Mnova Gears is a software suite that can be used to build automation workflows for your analytical data analyses (NMR, MS, IR, etc.). It is built around the concept of plugins called “bricks” that execute specific tasks in a fully automatic mode from data pickup and processing to results reporting, saving, and databasing. In addition to full automation, Mnova Gears allows for the customization of every step in your workflow to adapt it to your specific needs.

Mnova Gears comes in two flavors:

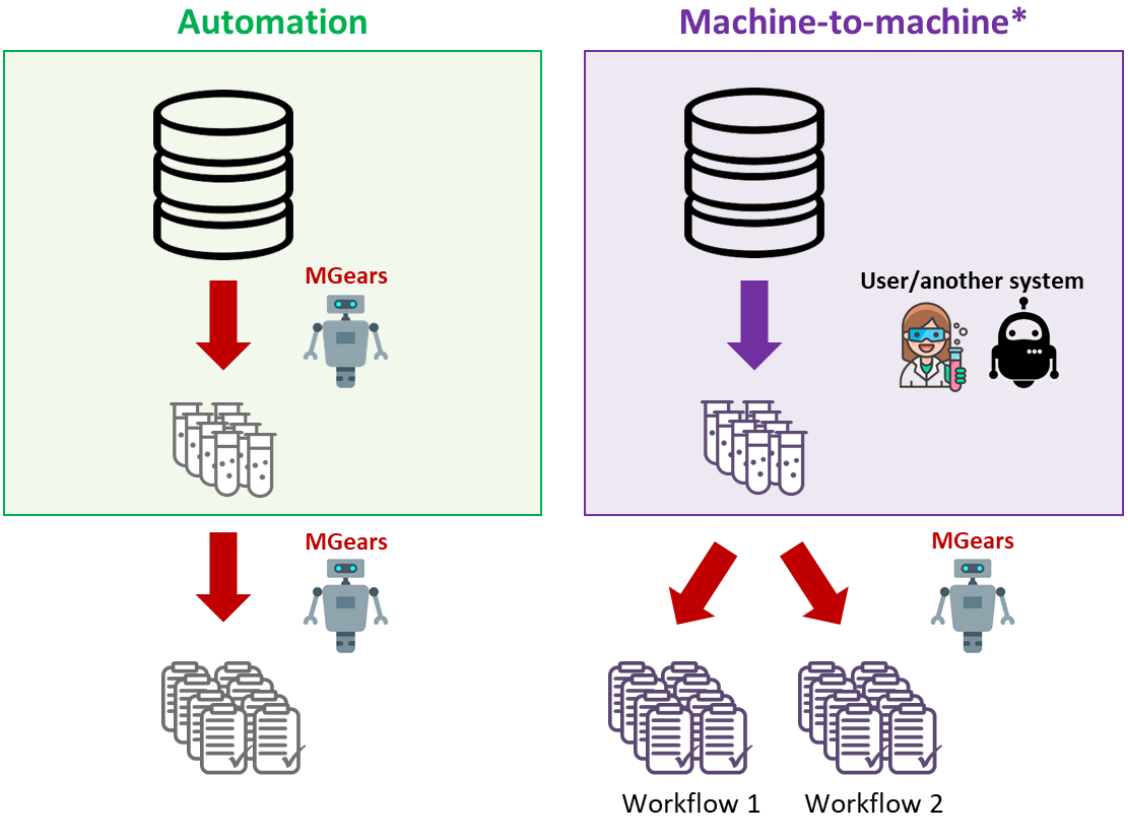
- The **Mnova Gears** product, suitable for the processing large datasets in batches or in real time.
- The **Mnova MyGears** product, that allows you to build and run workflows based on single samples. MyGears is best suited to small-scale analyses, where the overhead of manually opening data is not significant but the benefits of automating processing and reporting are hugely so.

Several **Mnova Gears bricks** are currently available that can be used as standalone components or in combination in a workflow.

Please check our website page for more details about available bricks and don´t hesitate to contact us to discuss your custom automations!



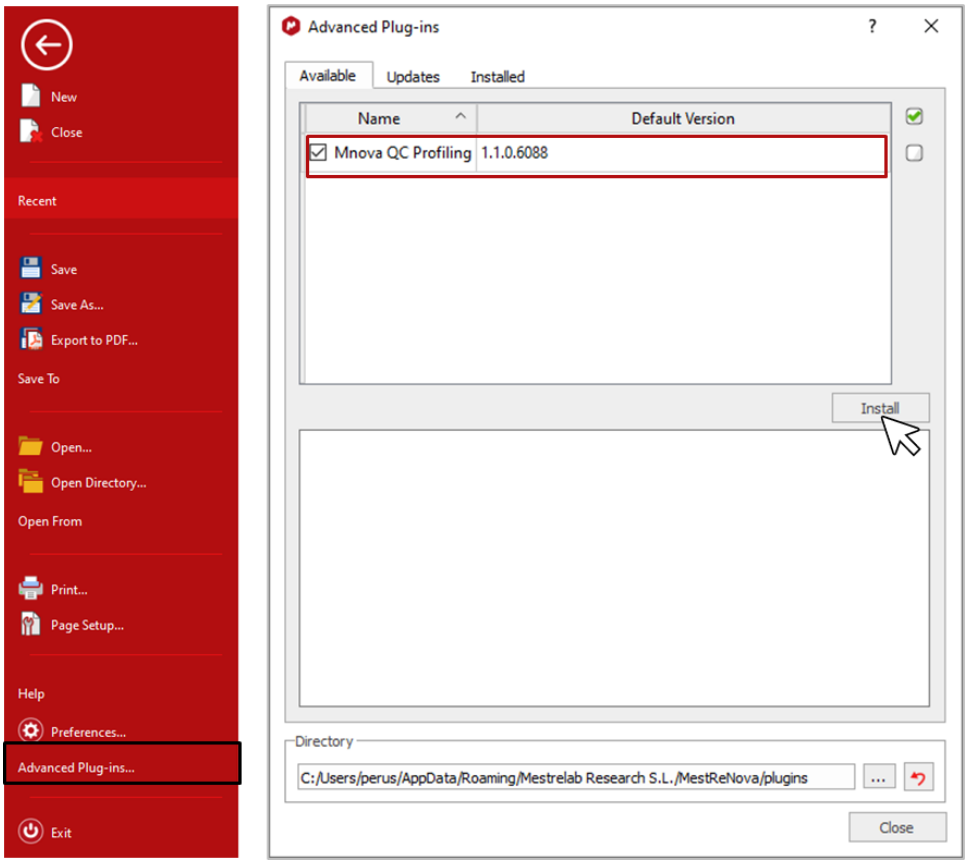
Apart from running automated workflows, Mnova Gears allows you to operate in a machine-to-machine mode* which means that you can run one or several workflows on your datasets with minimal human intervention. In this case, datafiles and workflow parameters must be provided by the user or an external program so that Mgears can operate on them.



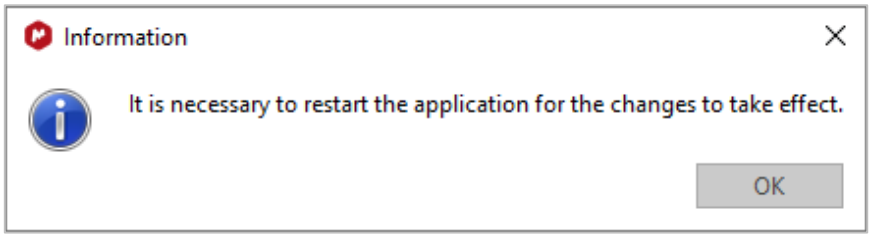
**Requires Machine-to-machine license*

2. Installation

Once you receive your software or plugin license, open Mnova and drag-and-drop your license file into the application. Then, go to the **File** tab > **Advanced Plug-ins.** A new window will open. In the **Available** tab, select the **Mnova Gears plugin** and click on **Install**.

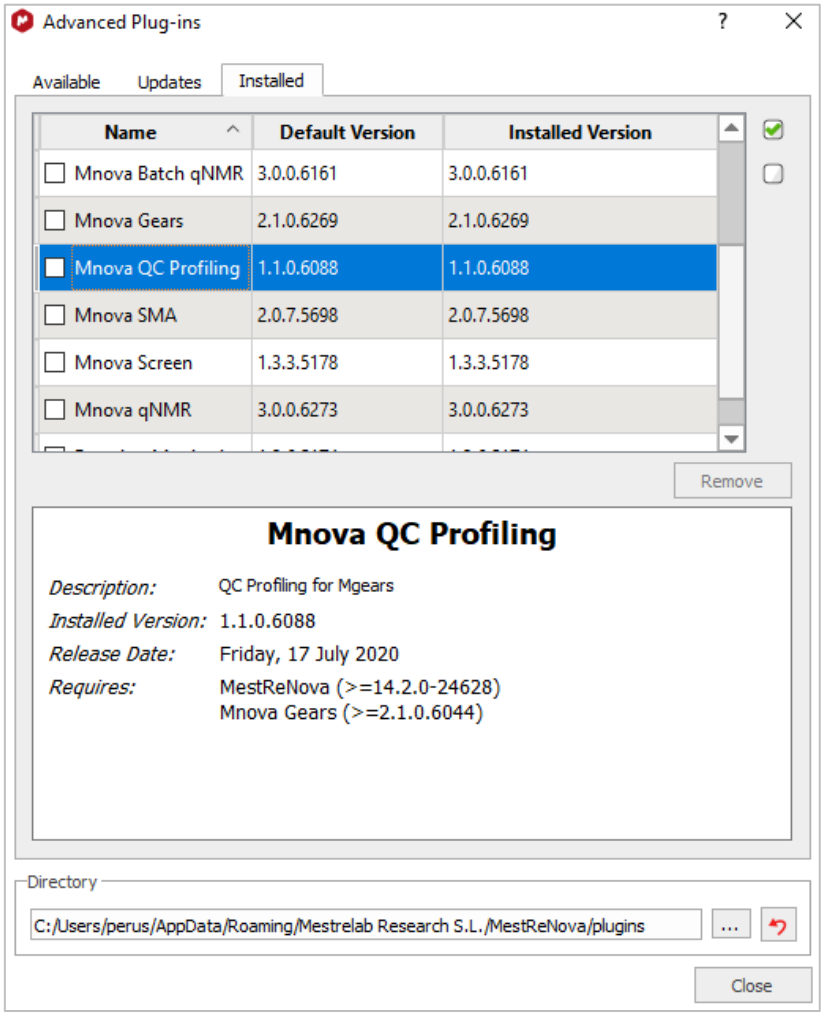


A window will open to prompt you to restart the application. Click on **OK**.

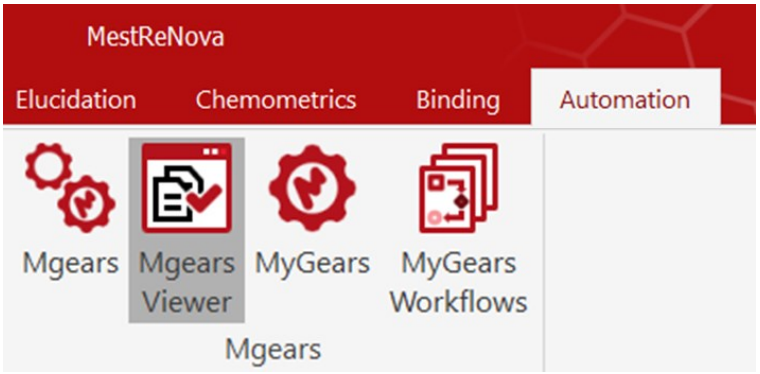


Close **Mnova** and open it again.

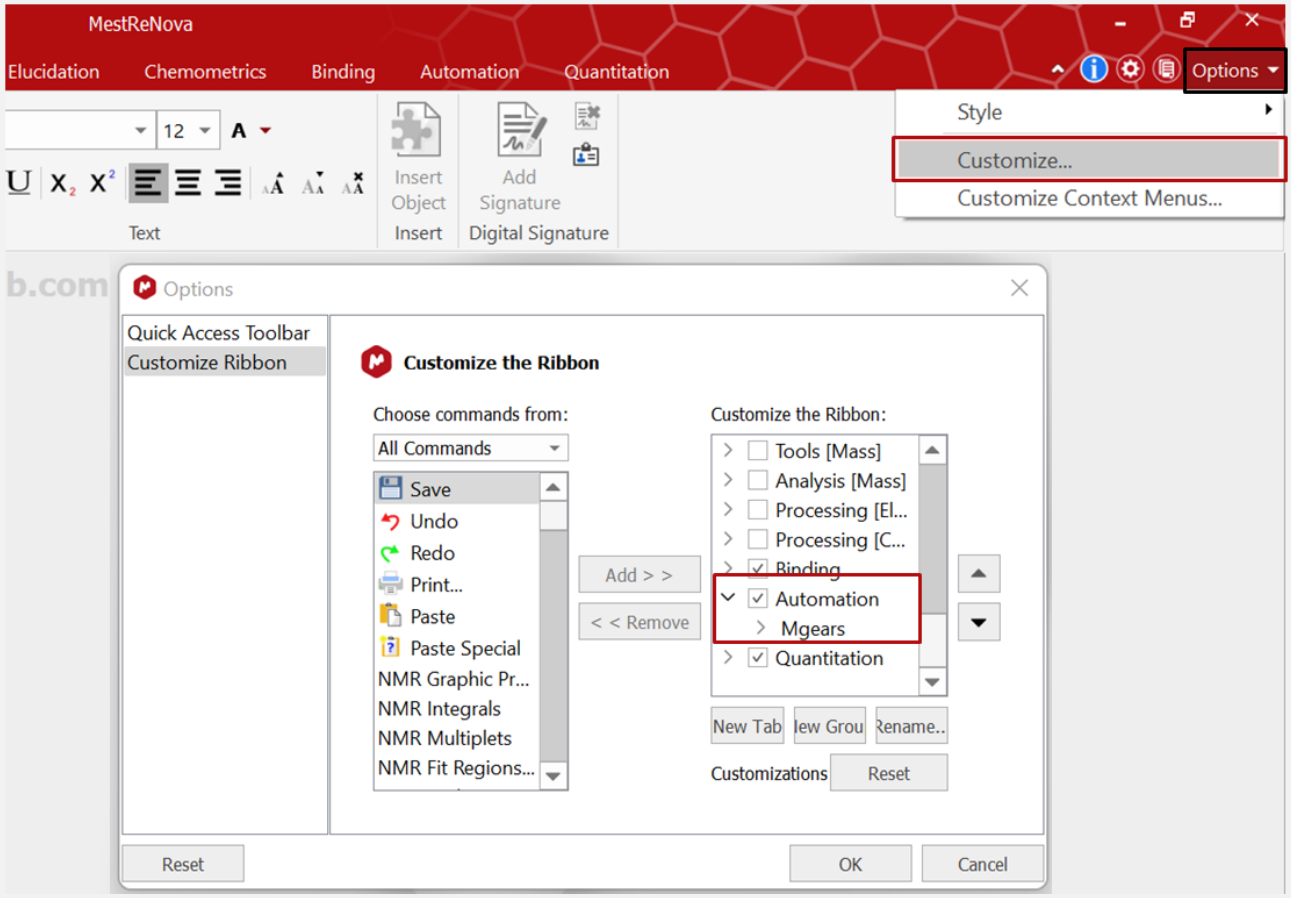
Check that the plugin has been installed correctly. All installed plugins will be listed in the **Installed** tab (**File** > **Advanced Plug-ins).**



If installation has been successful, you will find Mgears, Mgears Viewer, MyGears and MyGears Workflows in the Mnova ribbon under the **Automation** section.



Note. If the **Automation** tab is not visible in the Mnova Ribbon, go to **Options**>**Customize**..., and manually add **Automation** to the ribbon.



3. Mgears dialog

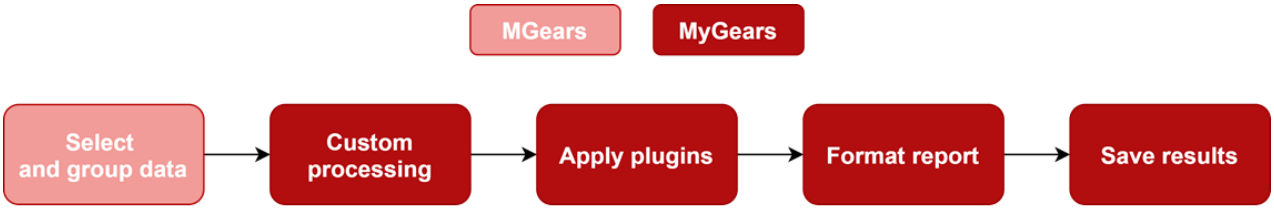
The Mgears dialog has a simple and straightforward design that includes:

- six tabs, each allowing the setup of a single part of the workflow
- a set of commands to control analysis

Tab	Description
Input	Choose analysis input
Processing	Customize processing or enable advised processing
Plugins	Select analysis plugins and configure plugin settings
Design	Apply layout template to your Mnova analysis result
Output	Choose repository to save your data and output files
Settings	Configure Mgears general settings

Command	Description
Resume	Load resume file and restart data processing
Load Settings	Load all mgears settings from OS registry
Save Settings	Save all mgears settings to the OS registry
Import Settings	Load all mgears settings from file
Export Settings	Save all mgears settings into a file
Cancel	Close mgears
Run	Start the automation

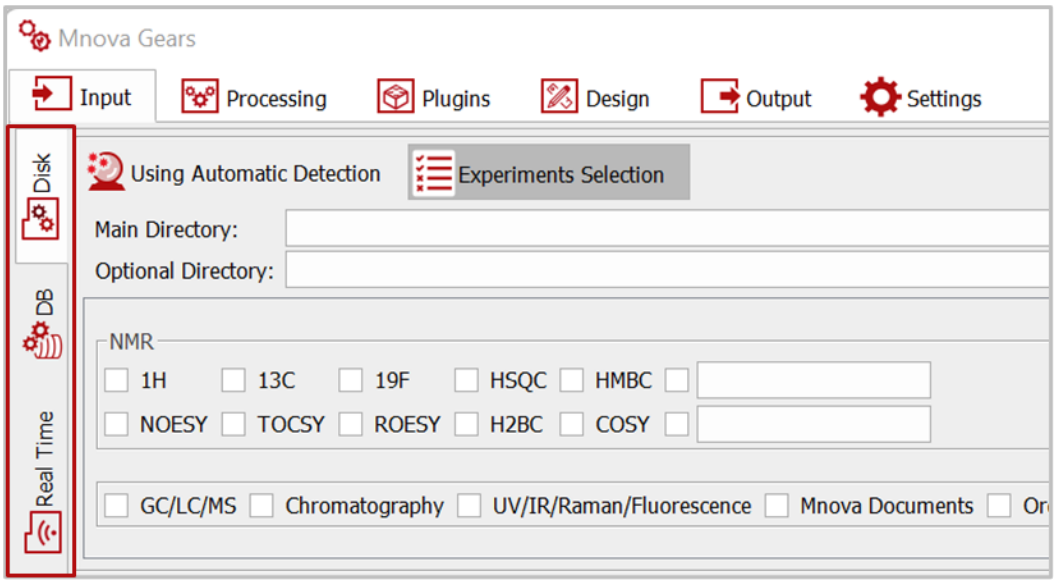
As represented by the dialog sections, a full Mgears workflow will start with the selection of the input data and then go to the rest of the processing, analysis, and reporting configuration. Alternatively, when using MyGears, the workflow starts a step further on, at the processing tab, since the user should already have the relevant data file opened in Mnova.



In the following sections, we will detail each tab of the Mgears dialog and the many configuration options each tab offers.

3.1. Input

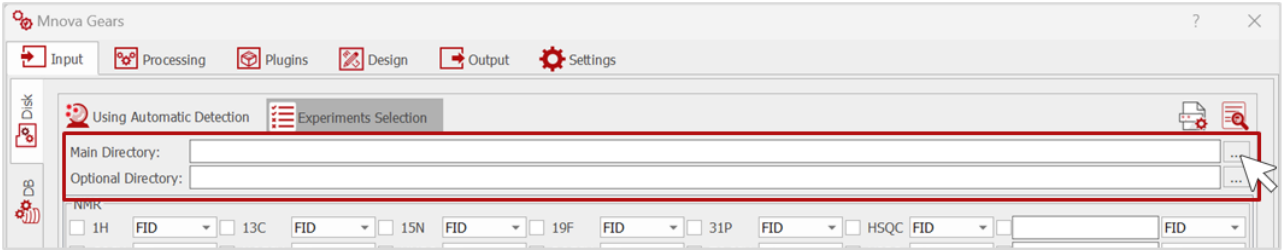
Mgears can handle input data saved on **Disk** directories, in a database (**DB**), or acquired in **Real Time** from a disk or from a network drive. These three modes are visible on the left-hand side of the Mgears dialog.



Each mode has a specific configuration that will allow you to adapt Mgears to your data and handle your analysis appropriately.

3.1.1. Data from disk

To analyze input data from your **Disk,** click on ... and select the **Main directory** in which your data files are saved. If part of your input data is saved in another folder, you can additionally select and add that folder in the **Optional directory**.



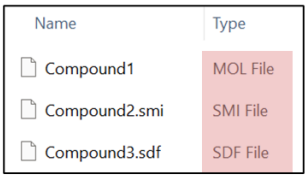
3.1.1.1. Mask manager

Click on this  button to open the **Mask Manager** where you can edit and add new masks for your experiment files to be automatically detected by Mgears. The following default masks are available:

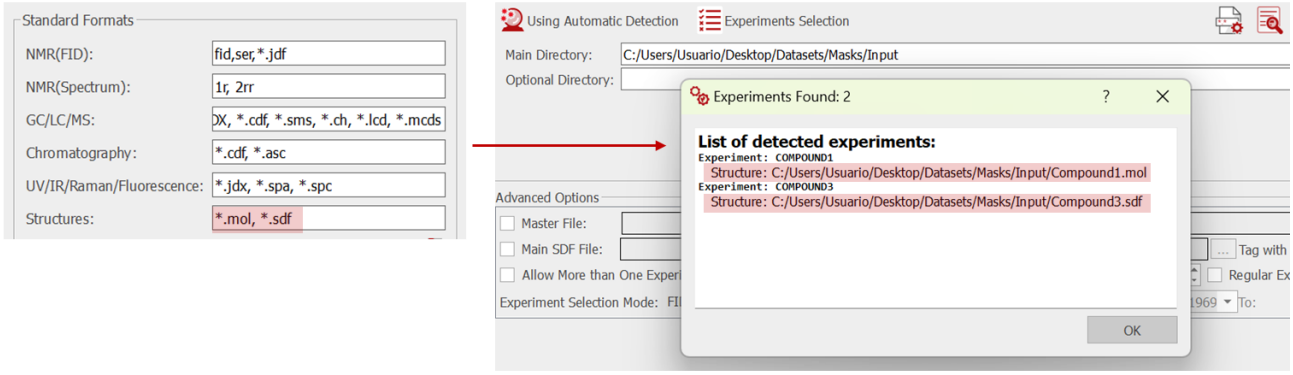
- **NMR (FID):** fid,ser,*.jdf
- **NMR (Spectrum):** 1r, 2rr
- **LC/GC/MS:** _FUNC001.DAT, MSD1.MS, analysis.baf, _FUNC001.IDX, *.cdf, *.sms, *.ch, *.lcd, *.mcds
- **Chromatography:** *.cdf, *.asc
- **UV/IR/Raman/Fluorescence:** *.jdx, *.spa, *.spc
- **Structures:** *.mol, *.sdf

If your data mask is not in the list above, type it in the corresponding box for the experiment type then click **OK** to save your changes. See example in the image below.

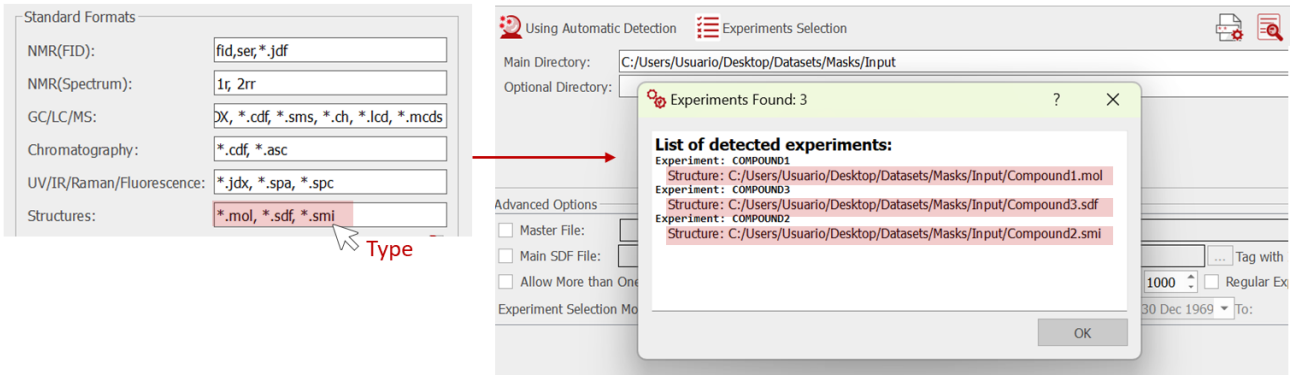
Input



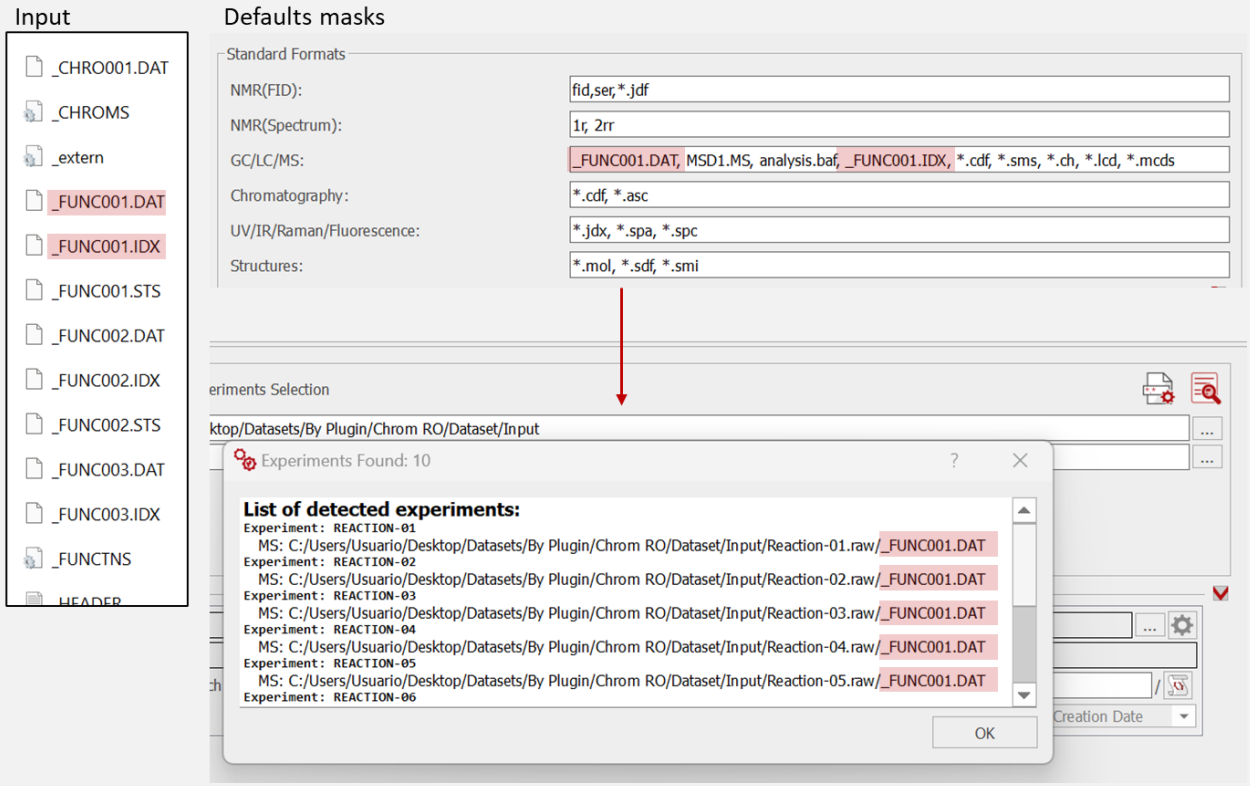
Defaults masks



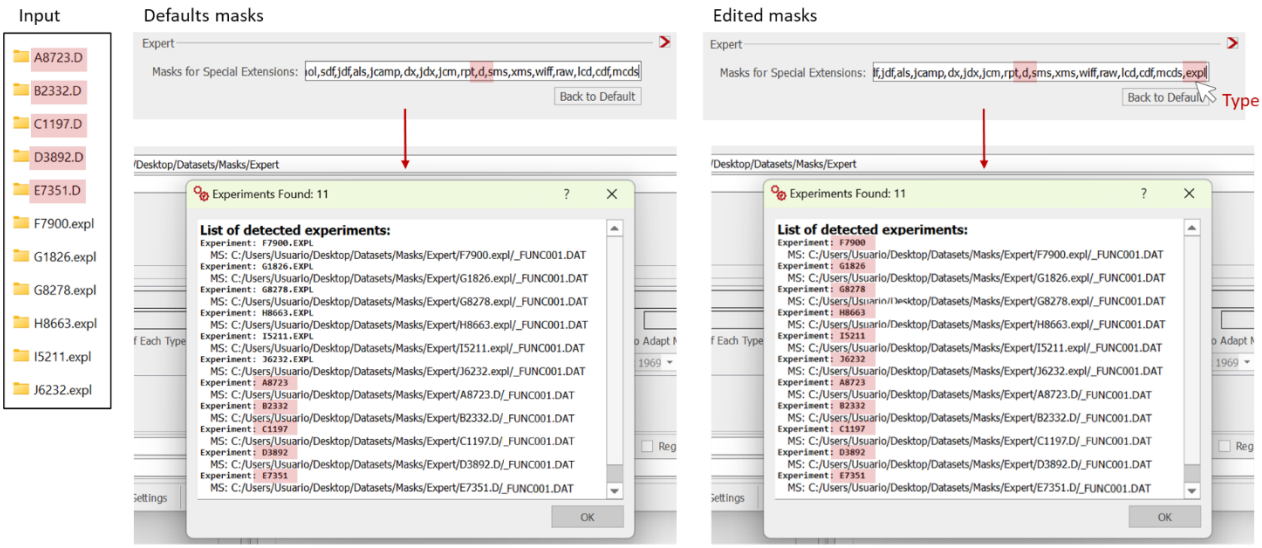
Edited masks



Note. When your dataset contains multiple files for the same experiment that are matched with the declared masks (for instance, "_FUNC001.DAT" and "_FUNC001.IDX"), Mgears will detect one occurrence and discard the other matches so that you don't get the same experiment duplicated.

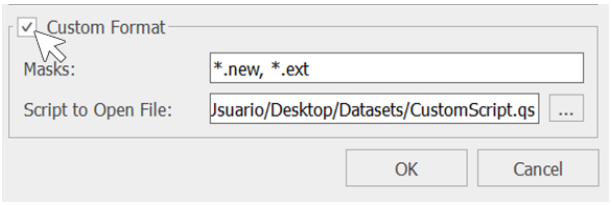


If the data file or folder incorporates both the experiment name and the extension (e.g., files named "C923-m3.raw" or a folder named "A8723.D"), Mgears is capable of identifying the extension and excluding it from the experiment name. This functionality is facilitated by the list of masks accessible in the expert settings section. You have the flexibility to modify the default list and include your specific extensions, as illustrated in the image below.

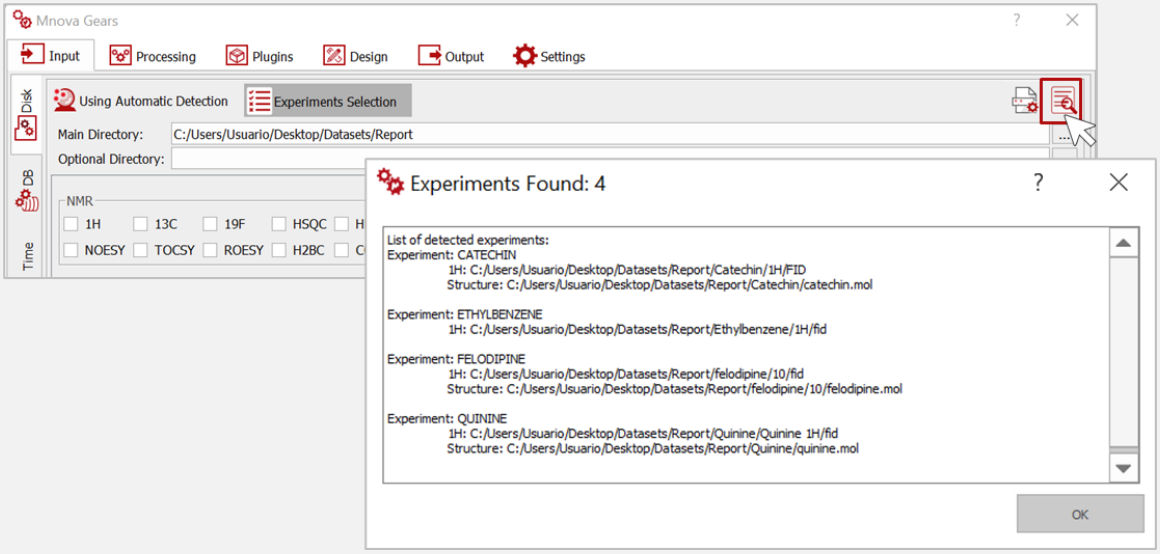


To undo any changes you introduce, you can click on **Back to Default** and then on **OK**.

It is also possible to use a custom script to open any file with Mgears. To do so, you must enable the **Custom Format** option, type your data folder masks, and upload the script by clicking on ... . The script will be executed when a file matches one of the masks added.



Top Tip! Whenever you select your input data you can use the **Automatic inspection** button to preview the detected data in your directories that will be used by Mgears to execute the analysis.



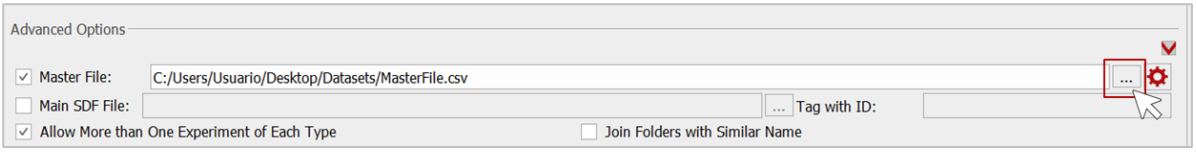
3.1.1.2. Advanced options

Several advanced options are available to give you more flexibility at the time of selecting your input data:

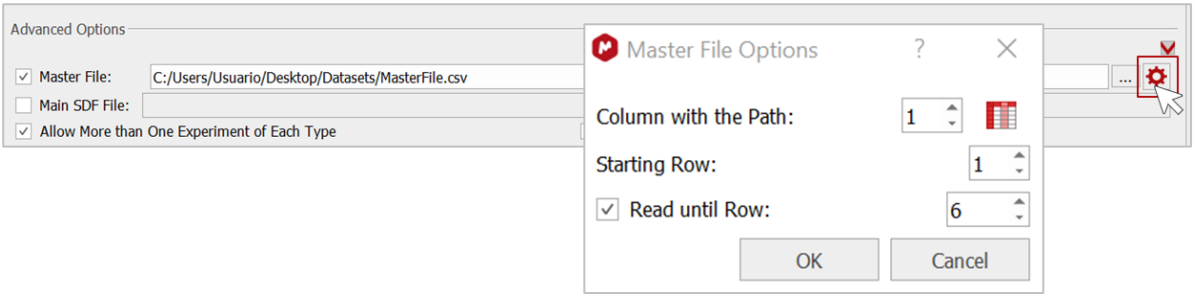
- **Master file:** If datasets are saved at different locations on the disk, it is possible to use a **Master file** with the list of paths to the directories with spectra and molecule files. A master file can be a .txt or a .csv file with an absolute path on each row.

```
C:\Users\Downloads\16089\subset_1\SDH-0001_1_04_12_18_DMSO_1.raw
C:\Users\Downloads\16089\subset_1\SDH-0001_1_04_12_18_PBS_2.raw
C:\Users\Downloads\16089\subset_1\SDH-0001_1_04_12_18_PBS_3.raw
C:\Users\Downloads\16089\subset_1\SDH-0001_1_04_12_18_PBS_4.raw
C:\Users\Downloads\16089\subset_1\SDH-0002_1_04_12_18_DMSO_1.raw
C:\Users\Downloads\16089\subset_1\SDH-0002_1_04_12_18_PBS_2.raw
C:\Users\Downloads\16089\subset_1\SDH-0002_1_04_12_18_PBS_3.raw
C:\Users\Downloads\16089\subset_1\SDH-0002_1_04_12_18_PBS_4.raw
```

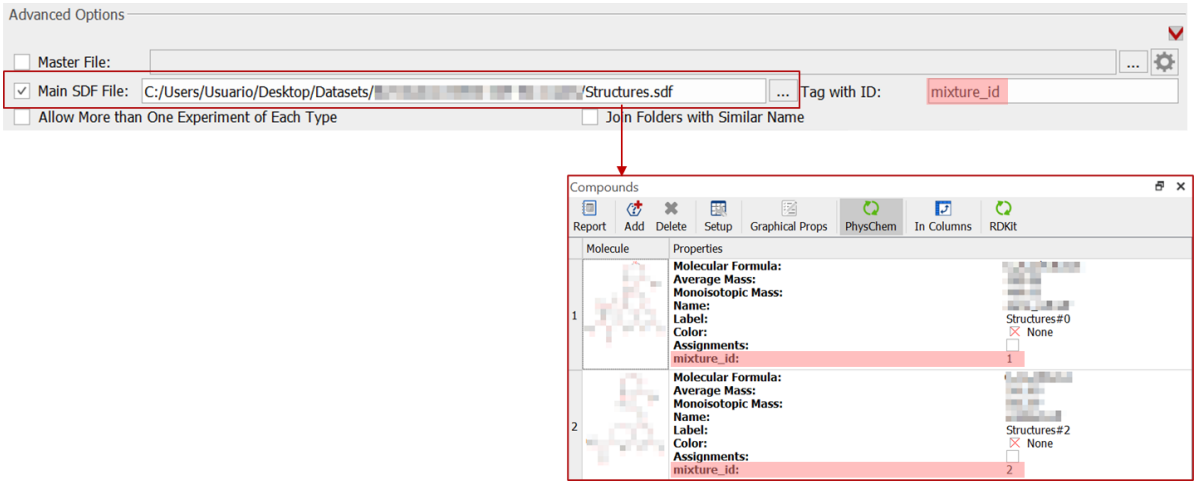
Tick the **Master file** option then click on ... to add your master file.



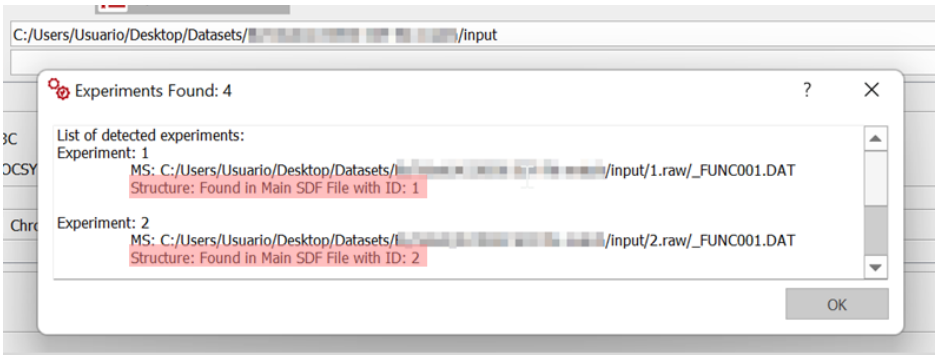
In the **Master file options** dialog, you can configure a set of basic features to give some flexibility to the input. You can indicate which column contains the path and set the starting and end row to read the data in the master file.



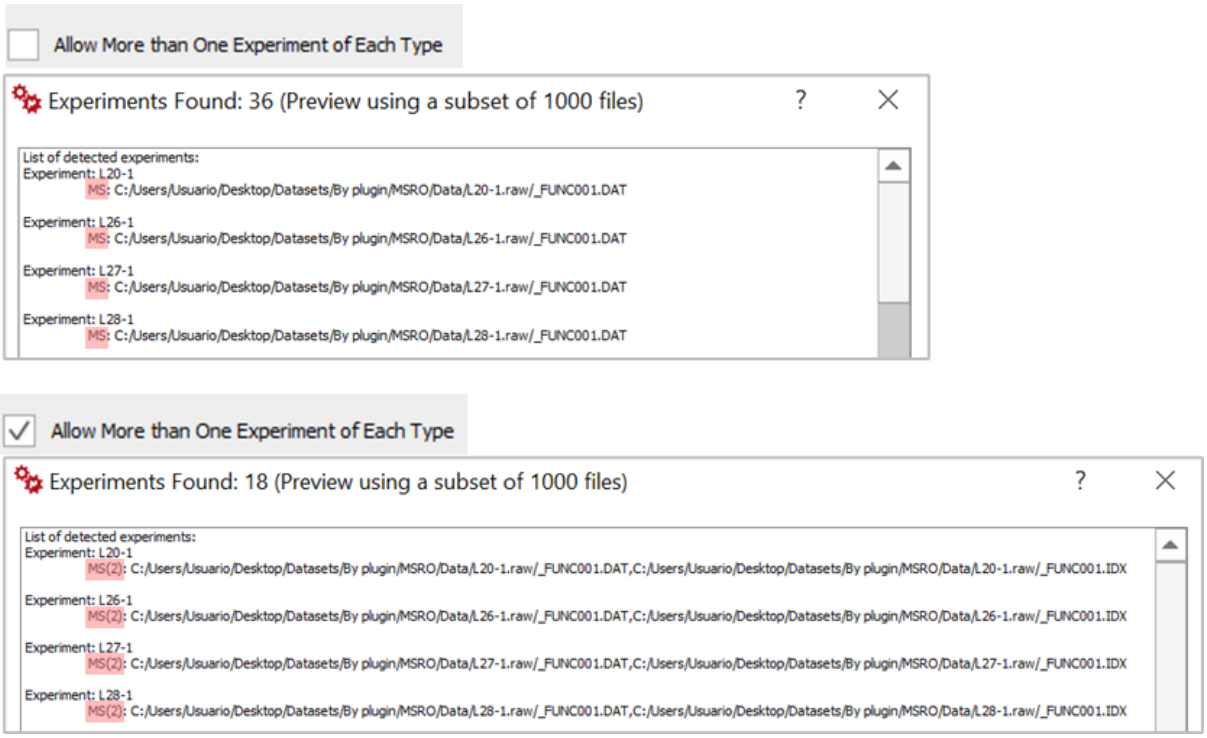
- **Main SDF File:** If you have all the molecular structures saved in a single SDF file, you can unable this option to automatically match each molecule to the corresponding datafile analyzed in a batch. Matching is done using a tag that is added to each molecule ("*mixture_id*" in the example below). Enable the **Main SDF File** option and upload your SDF file, then type the **Tag with ID** to be used.



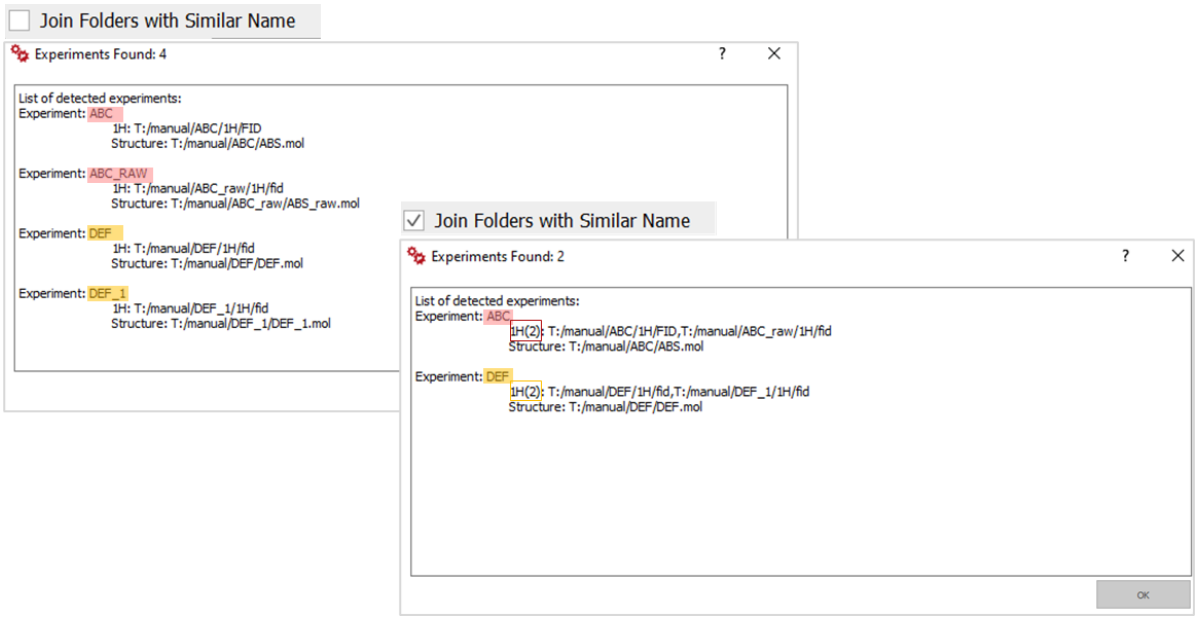
Mgears detects and matches each structure with the corresponding datafile.



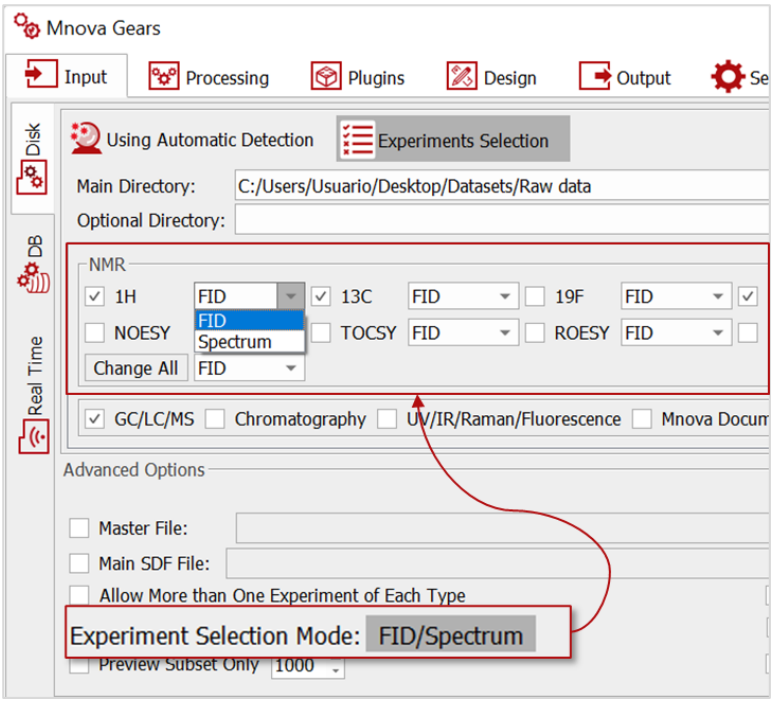
- **Allow more than one experiment of each type:** Activate this option when you want Mgears to detect several experiments of the same type in a document. In the example below, two MS raw datafiles are detected in each group.



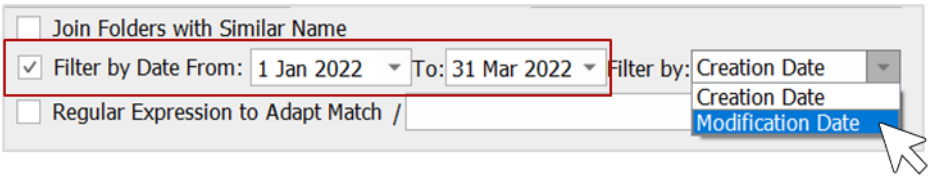
- **Join folders with similar name:** This option is used to join spectra with similar starting names within the same group. If enabled, Mgears will detect repetitions or small variations in the data folder names. For instance, if there is a group “ABC” and a new spectrum is found named “ABC_raw”, it will be included in the “ABC” group because the start of the new file’s name, “ABC”, matches the previous group name.



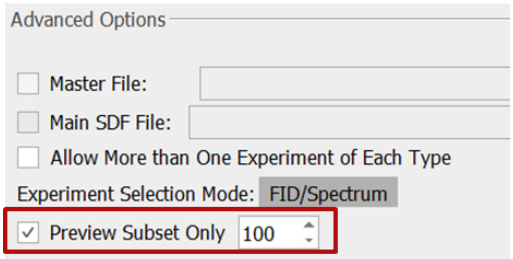
- **Experiment Selection Mode:** Choose this option if you want to detect raw data files only (**FID**) or both raw and processed data files (**FID/Spectrum**). When the **FID/Spectrum** mode is enabled, it is possible to manually select which data files to use for each type of experiment, as seen below:

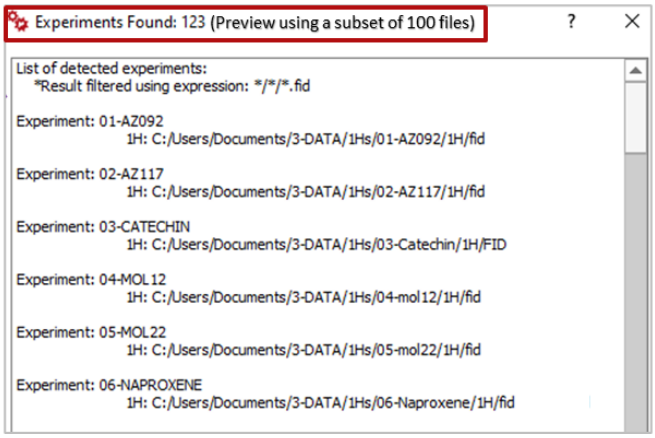


- **Select data files dates:** Activate this option to detect data files created or modified between two specific dates. You can choose to filter by file **Creation** or **Modification** date.

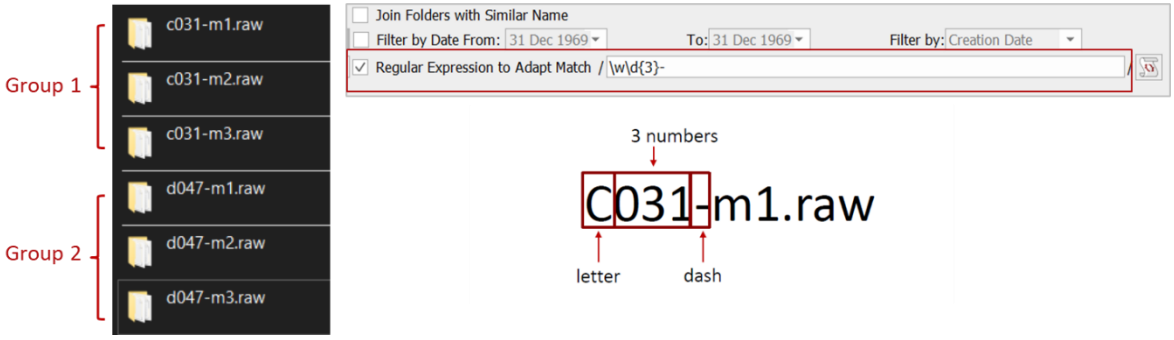


- **Preview Subset Only:** Activating this feature allows you to choose the number of files you want to visualize in the **Automatic inspection** dialog  . This option is checked by default and uses 1000 as its default value. When unchecked, all detected files are visualized.

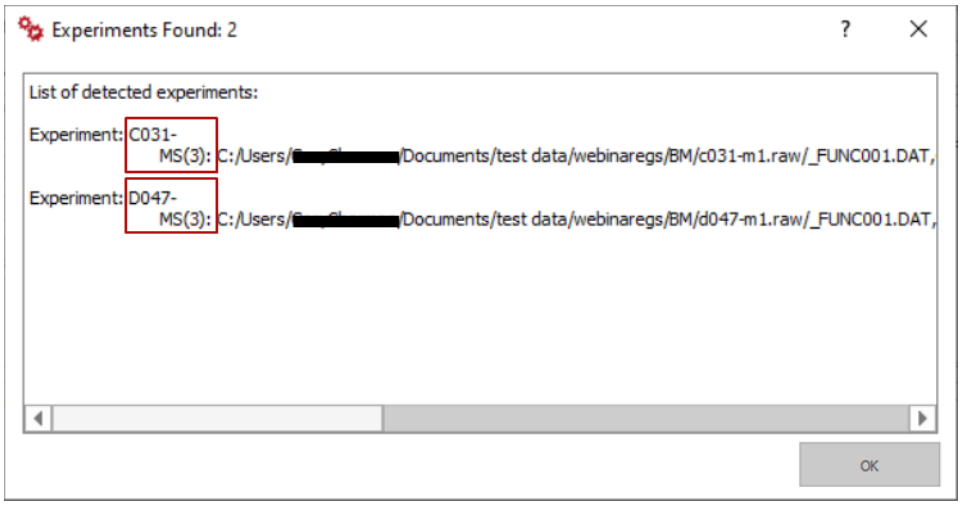




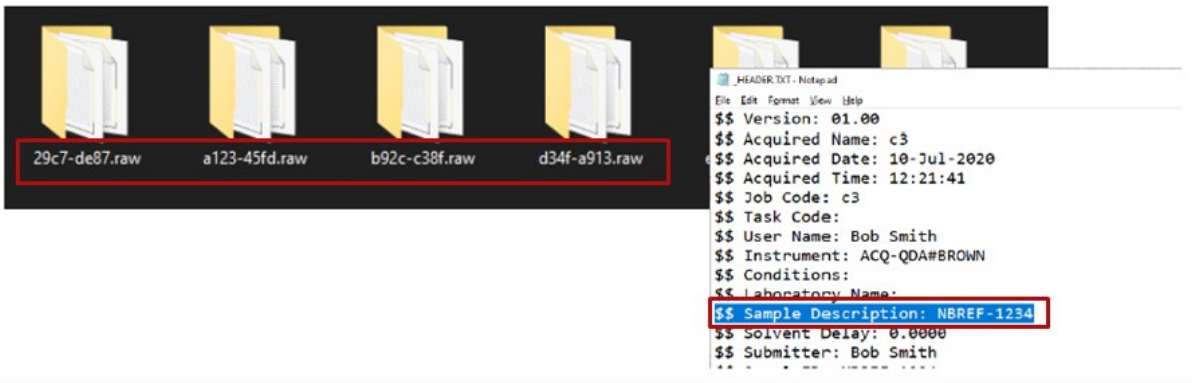
- **Regular Expression to Adapt match:** Check this option if you need to group samples with only a part of the file name matching. The regular expression you type will be used to capture the common part of the string in the names of the files detected, which will then be grouped in a single experiment.

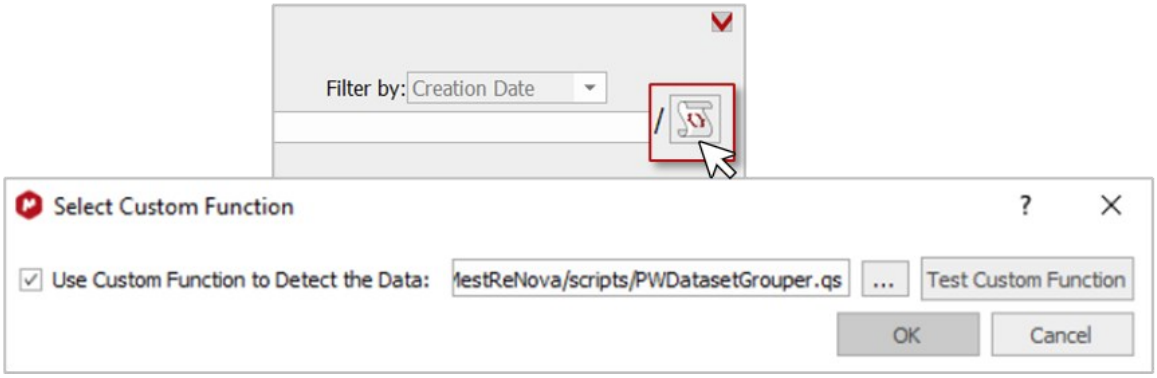


Use the **Automatic inspection** button  to check how Mgears has grouped the detected data.



- **Use Custom function:** Check this option and upload a custom script to replace the default grouping algorithm used by Mgears. This is particularly useful when your data files names are not easy to group (for instance, when the file name is an ID generated automatically by the instrument).
  You can contact our team for advice and support.



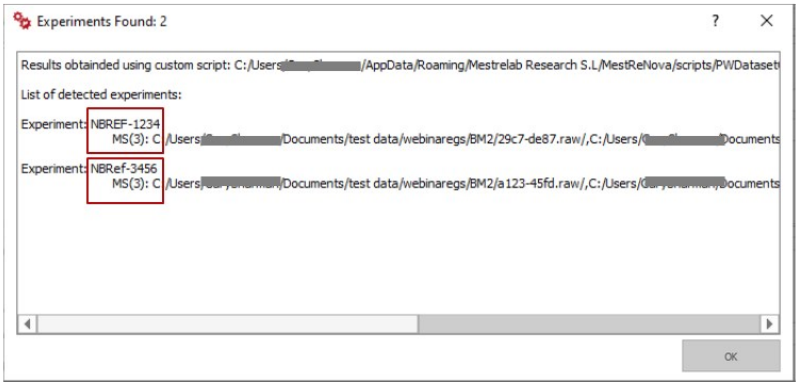


A simple script of about ~20 lines long can allow Mgears to:

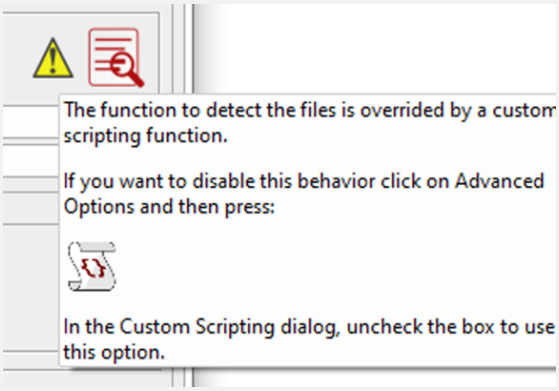
- Find all the header files in the specified directory from settings
- Read the “sample description”
- Create a group for each unique sample ID
- Add relevant samples to this ID

Use the **Automatic inspection** button to check how Mgears has grouped the detected data.

```
function PWDatasetGrouper(aSettings) {
    //basedir for search of datasets
    var basedir = aSettings.path;
    var dir = Dir(basedir);
    //find all _header.txt files
    var datasets = dir.entryListAdv("*.raw/_HEADER.TXT");
    var results = {};
    var names = [];
    for (var i = 0; i < datasets.length; i++) {
        var f = new File(datasets[i]);
        f.open(File.ReadOnly);
        var s = new TextStream(f);
        var line;
        do {
            line = s.readLine();
            //read sample description field
            if (line.indexOf("$$ Sample Description:") != -1) {
                var sname = line.substring(22).trim();
                if (!includes(names, sname)) {
                    names.push(sname);
                    var a = {};
                    a.MS = [];
                    results[sname] = a;
                    results[sname].MS.push(datasets[i].replace("_HEADER.TXT", ""));
                } else {
                    results[sname].MS.push(datasets[i].replace("_HEADER.TXT", ""));
                }
            }
        } while (!s.atEnd());
        try {
            f.close();
        } catch (e) {}
    }
    return results;
}
```



Watch out! When using a custom function, a **Warning** symbol appears next to the **Automatic inspection** button with a tooltip indicating that a custom scripting function is active.



3.1.1.3. Filtering options

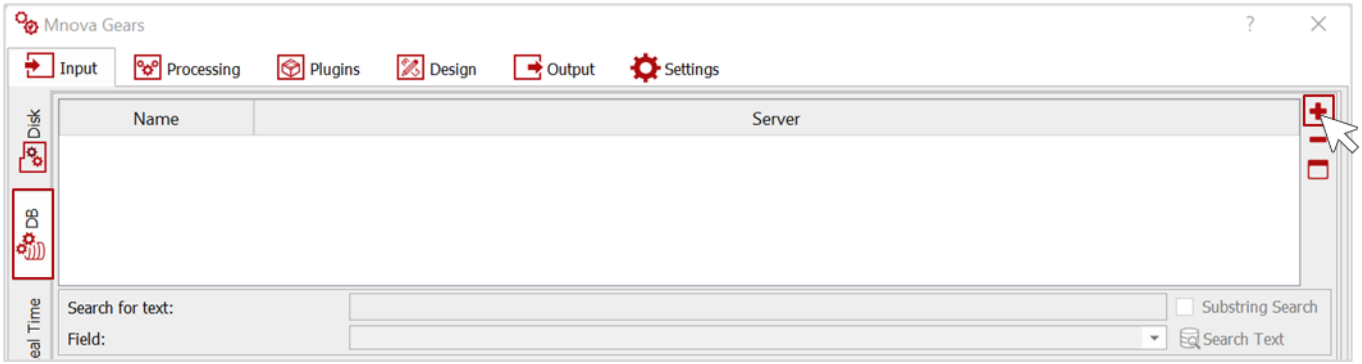
A **Filtering string** or a **Mapping file** can be used to filter your input data from the disk. *Please refer to section 3.1.4.*

Watch out! Advanced filtering will be disabled (hidden) while working with a Master file.

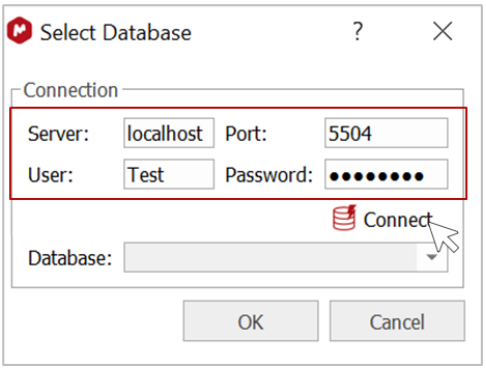
3.1.2. Data from database

Input data can also be retrieved from one or more Mnova spectral **Databases** (DB). In this mode, a list of spectra can be retrieved via a number of search terms for database fields.

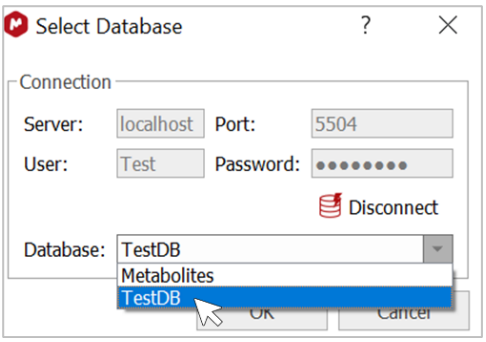
In the **DB** section, click on  to add a DB.



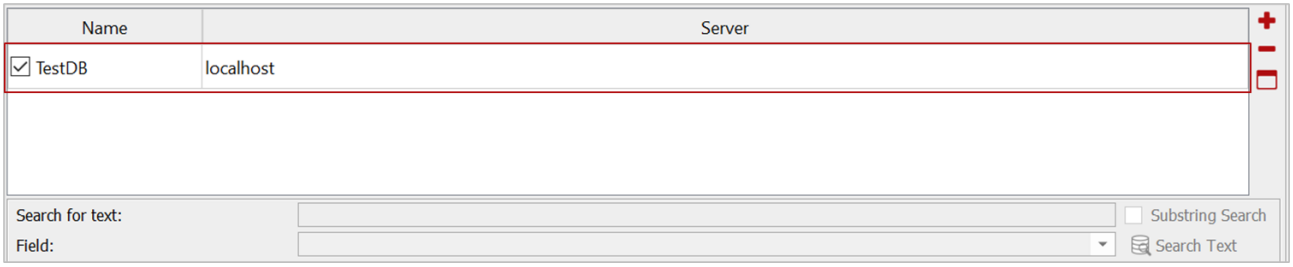
A dialog will appear. Enter the **Server** name, **Port**, **User**, and **Password**, then click on **Connect**.



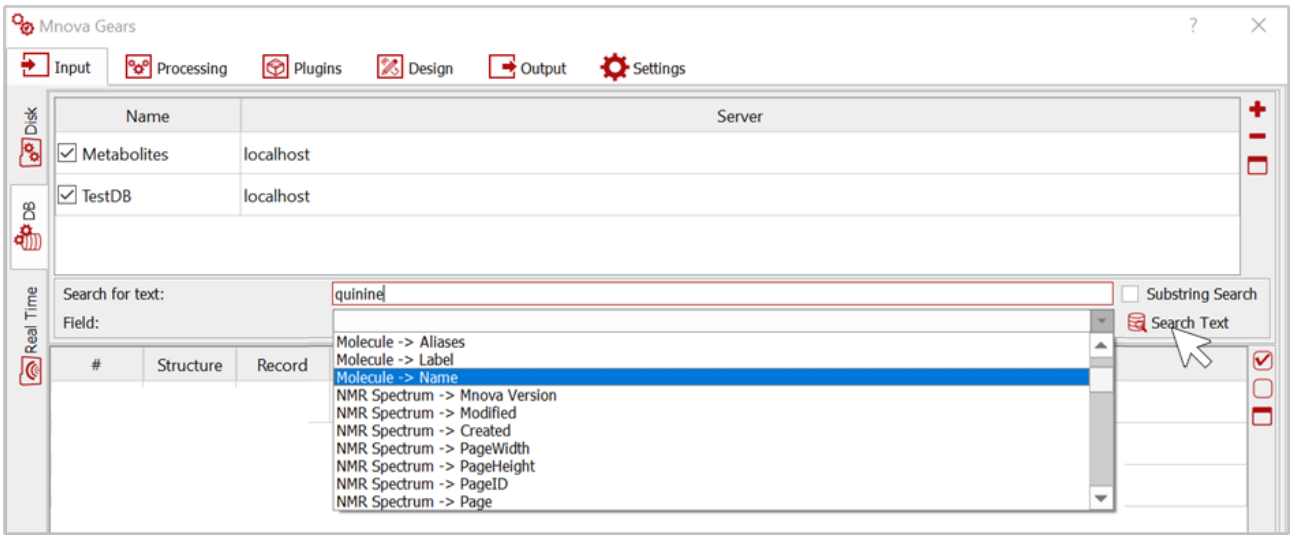
Once you have connected successfully to the server, select the **Database** containing your input data and click on **OK**.



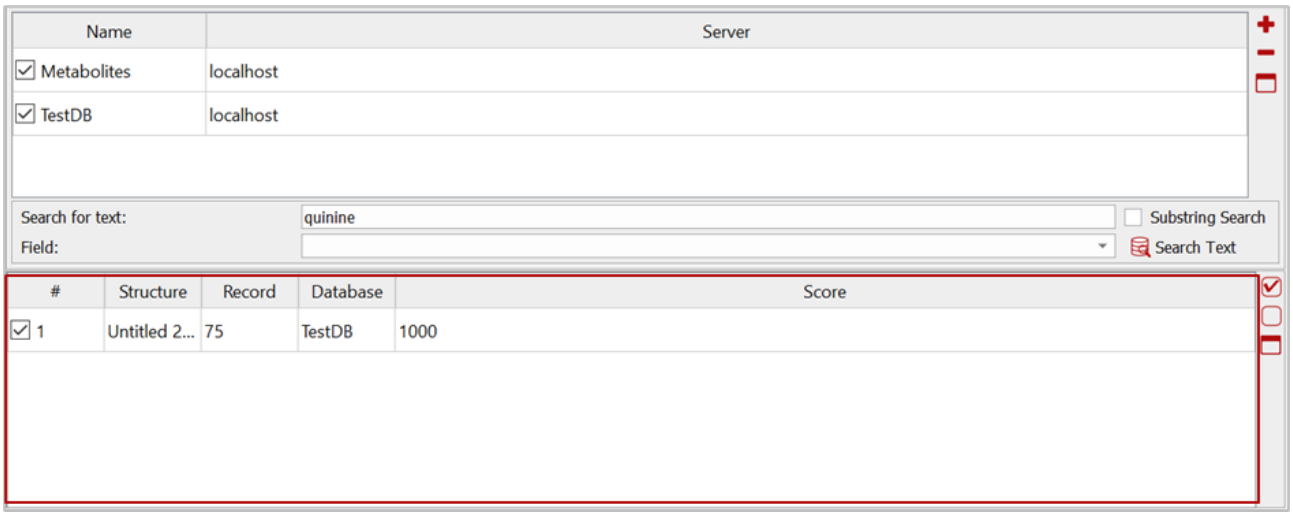
The selected database will appear in the table as seen in the image below. Click again on  to add another database if needed, or on to delete a previously added database.



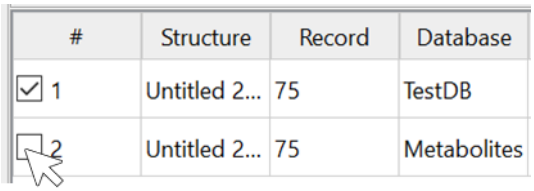
It is possible to **Search for text** in the database. Type the text in the dedicated box then click on **Search Text**. You can optionally select a specific **Field** in the database for your search. In this example, two databases are searched by **Molecule name**. You can disable the search in one of these two databases by unchecking the corresponding box.



The search results will appear in the table below with the **Record** number and **Database** in which they were saved.



If your search results include many records, you can exclude the records you don't want to use in your analysis by unticking the corresponding checkbox.



You can also use these buttons,  ,  , and  , to **Check all** and **Uncheck all**, or **Clear** the results table, respectively.

Enable the **Substring Search** option to perform a search using substrings.

3.1.2.1. Filtering options

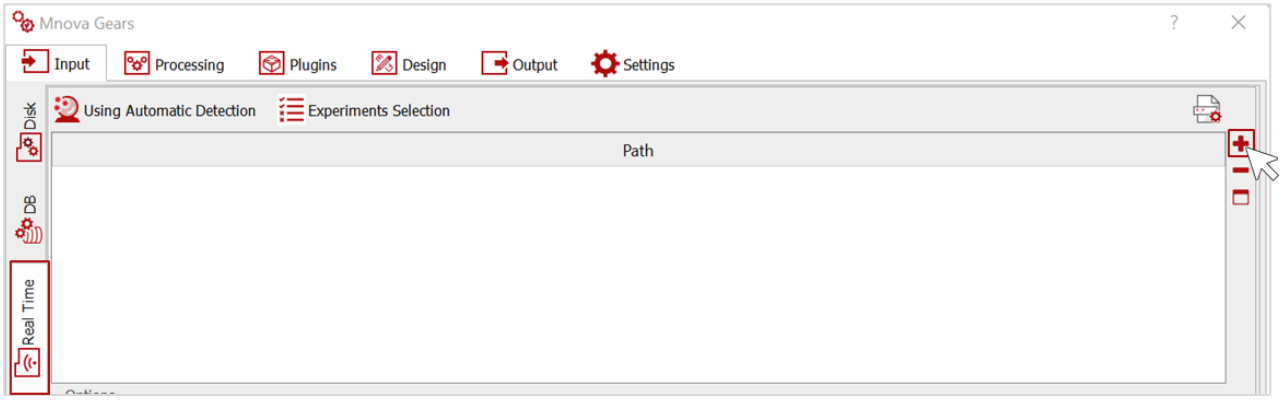
A **Mapping file** can be used to filter input data from a DB. *Please refer to section 3.1.4.*

Watch out! When using the DB mode, the filtering options override the manual selection of data files, and therefore Mgears will disable the list of records if the Filter mode is selected.

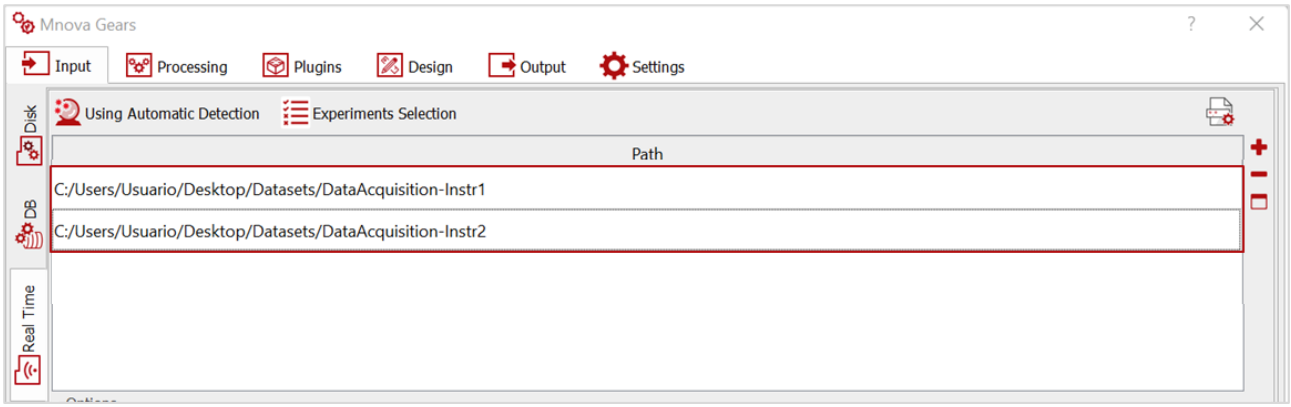
3.1.3. Data acquired in real time

Input data can also be analyzed as soon as it is acquired. With the **Real time** (RT) mode, Mgears will watch (Listener) a set of folders for incoming data and operate on it as it arrives (or optionally when all expected parts of a set are ready). The RT input mode can help improve productivity by taking care of all the routine analysis before the user even interacts with the data.

The settings for the listener can be selected under the **Real Time** tab. Click on  to add the folder paths you want Mgears to watch. It is also possible to use URLs from networks that are visible to the system.

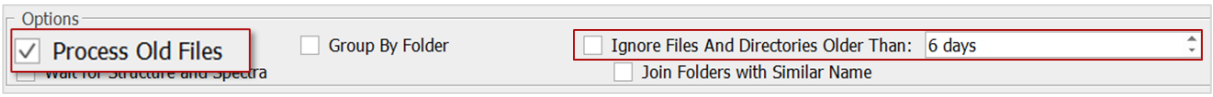


You can add one or more paths. These will appear in the table as seen below. You can **Delete** a path or **Clear** the whole table by clicking on or  , respectively.

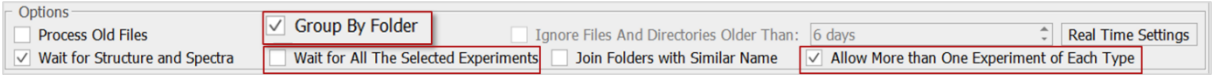


3.1.3.1. Options

- **Process old files:** If checked, all files already present in the directory will be processed. In this case you can choose to **Ignore Files and Directories older than** a certain time.



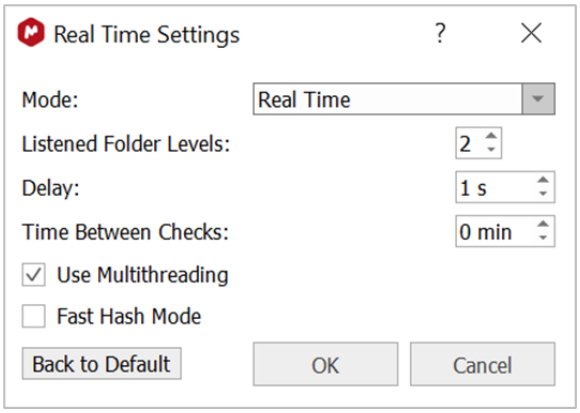
- **Group by folder:** Enable this option to group spectra with similar folder names into a unique Mnova results document. Two other options are configurable in this case: **Wait for all the Selected experiments** to process them together (otherwise experiment files are processed once available in the watched folder)**,** and **Allow more than one experiment of Each type.** Also, in this case, **Filtering** options are made available.



- **Wait for Structure and Spectra:** This option will prompt Mgears to wait for at least one structure and one spectrum before processing an experiment.

- **Join Folders with similar name:** This option is used to join spectra with similar starting names within the same group. If enabled, Mgears will detect repetitions or small variations in the data folder names. For instance, if there is a group "ABC" and a new spectrum is found named "ABC-1" or "ABC_raw", it will be included in the "ABC" group, because the start of the new file name, "ABC", matches the previous group name. *Please refer to section* *3.1.1.2.*

- **Real Time settings:** By clicking on this button, a dialog will open to allow you to set the folder listener's settings.



Real-time acquisition can be performed in two modes:

- The **Real Time** mode, in which the listener will rely on the operating system (OS) to determine when changes happen in the listened directories. Such changes in the file system are therefore immediately reported to the user. With this mode, the listened folders can also be periodically checked for modifications every X minutes (X is the time set in the **Time Between Checks** option). This is useful when working with network shared units because, depending on the configuration, the OS may not report the changes correctly/in time.

- The **Timer** mode, in which the listener will check the directories every "X" minutes to detect changes ("X" is the time set in the **Time Between Checks** option). With this option, the listener will generally consume fewer system resources.

Another configurable setting is the **Listened folder Levels** value, which corresponds to the directory tree level that the listener will reach to look for modified files. When set to zero (0), the listener will only look in the top directory. Note that your folders' architecture and size may affect the performance.

The **Delay** value corresponds to the number of seconds that the system will wait to check whether the modifications in a specific file have finished.

Finally, you can check the **Multithreading** option if you want the listener try to use several threads when creating the file cache, which will increase the performance of the system; and the **Fast Hash Mode** if you want the listener to only use the modification date of the file when looking for changes.

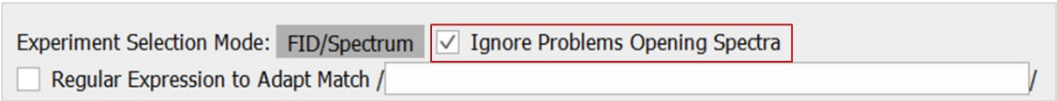
3.1.3.2. Advanced options

- **Experiment Selection Mode:** Choose this option if you want to detect raw data files only (**FID**) or both raw and processed data files (**FID/Spectrum**). When the **FID/Spectrum** mode is enabled, it is possible to manually select which data files to detect for each type of experiment.

- **Regular Expression to Adapt match:** This option will allow you to group samples when only part of the file name matches. The regular expression you type will be used to capture the common part of the string in the names of the files detected and group them in a single experiment. *Please refer to section 3.1.1.2.*

- **Allow Reprocessing Custom Format File:** When working with custom format files, this option allows you to reprocess a custom file after making changes. If this option is disabled, Mgears will discard a previously processed file and won't reprocess it.

- **Ignore Problem Opening spectra:** Sometimes Mnova will return an error when opening a file even though the file has loaded correctly. By enabling this option, you can force Mgears to ignore problems detected by Mnova and use the file anyway, otherwise Mgears will not use the affected spectrum.



3.1.3.3. Filtering options

A **Filtering string** or a **Mapping file** can only be used when the **Group by Folder** option has been enabled. *Please refer to section 3.1.4.*

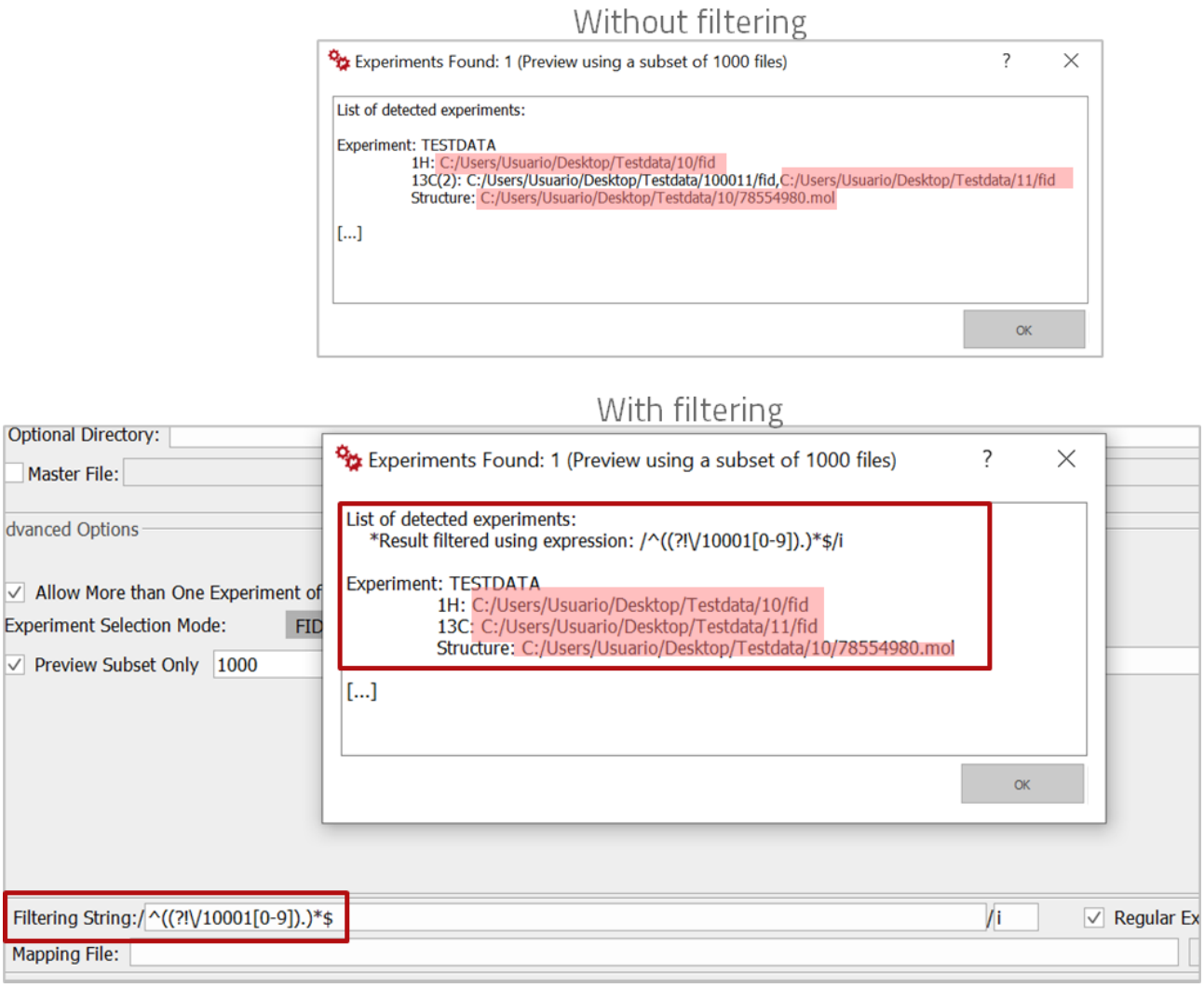
3.1.4. Filtering options

Filtering options are available for all three sources of input data (from Disk, DB, or Real Time), which allows you to refine your data detection and better adapt it to your data configuration.

3.1.4.1. Filtering string

The Filtering string can be used to filter the detected files from Disk or Real time acquisition using a string with common wildcards (* and ?) or a regular expression.

Type your filtering string in the corresponding box. The **Automatic inspection** button is used to preview the detected data before and after filtering.



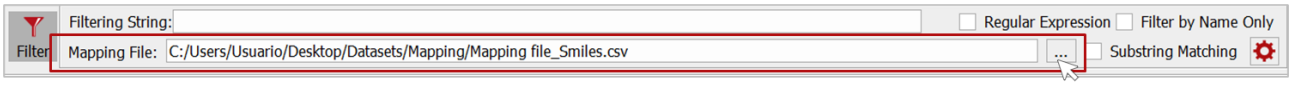
You can check the **Regular expression** option to force the use of a regular expression over the normal filtering string.

Check the option **Filter by name only** to only filter the name and not the full paths of the spectra.

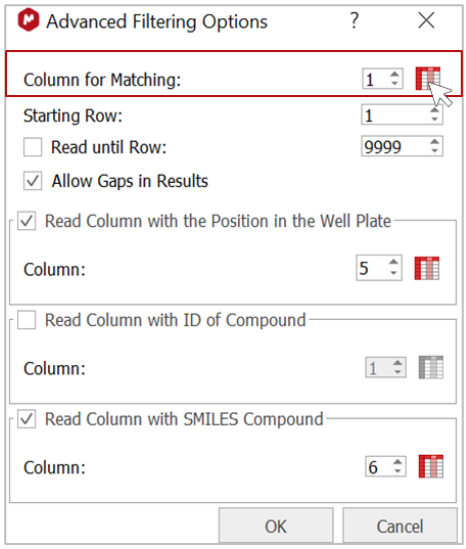
3.1.4.2. Mapping file

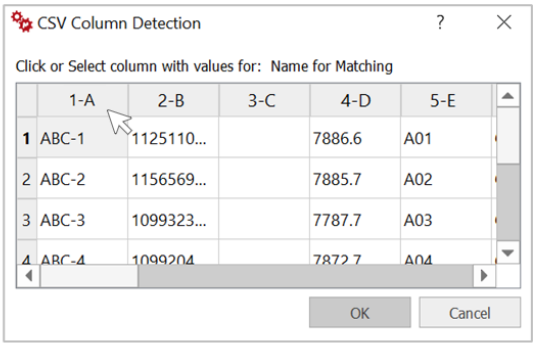
Using a Mapping file is convenient when input files are listed in an .txt or .csv document along with other metadata. Mgears will map the information found in the file provided with the information found in the selected input directory (on Disk, DB, or RT folder).

Click on ... to choose your mapping file from your directory.

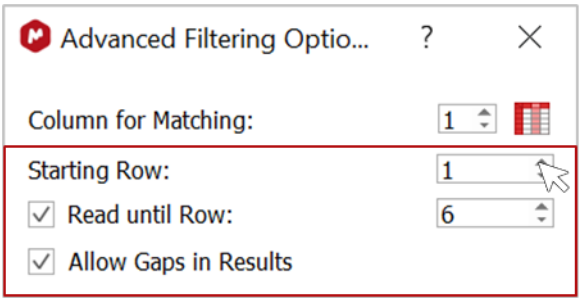


More filtering options are available when the input data is retrieved from Disk or through Real time acquisition. To configure these **Advanced Filtering Options,** click on . In the dialog that appears, indicate which column of the mapping file will be used to match information in your data directory. You can either type the column number or click and open the assistant to visualize the .csv and select the desired column. In the assistant, only the first 10 rows of the filtering file will be loaded.





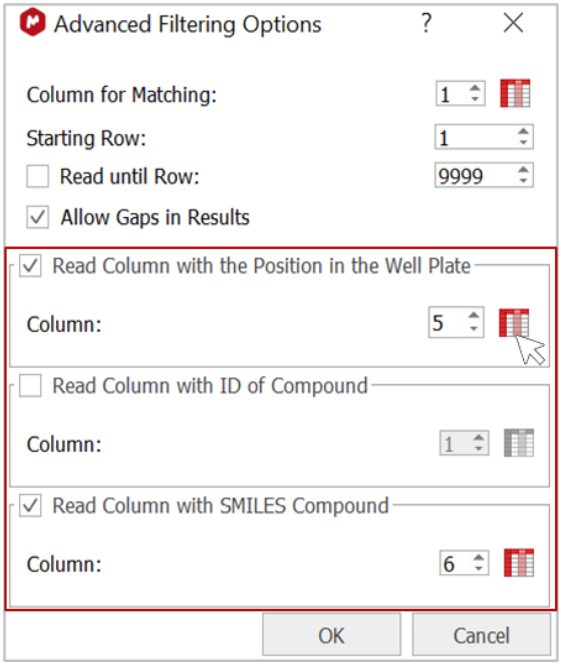
Choose the **Starting row** you want to read your .csv from and, optionally, enter the last row you want to read.

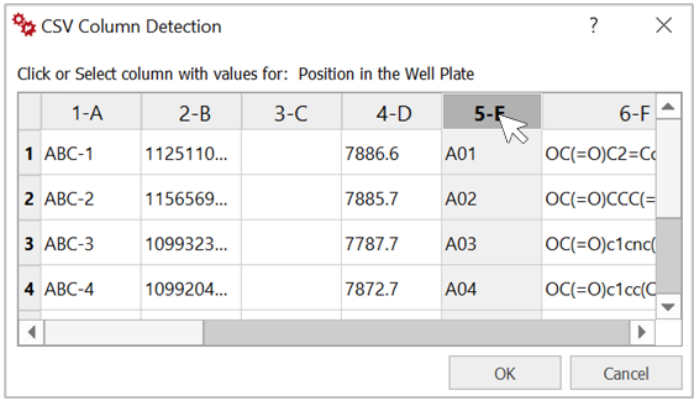


Enable the **Allow Gaps in Results** option if you want to include void results for the empty cells in the plate with the lines in the filtering files.

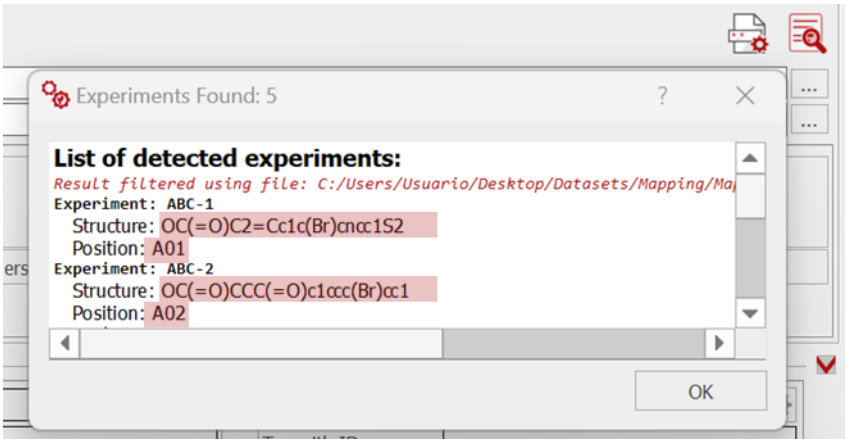
In addition to the mapping of data files, it is possible to read other metadata, such as:

- sample **Position in the well plate** (only available when the Allow Gaps in Results option is enabled)
- compound **ID**
- compounds **SMILES** string.





With this configuration, SMILES strings and well positions are read and recognized by Mgears, as you can see when using the **Automatic inspection** button  .



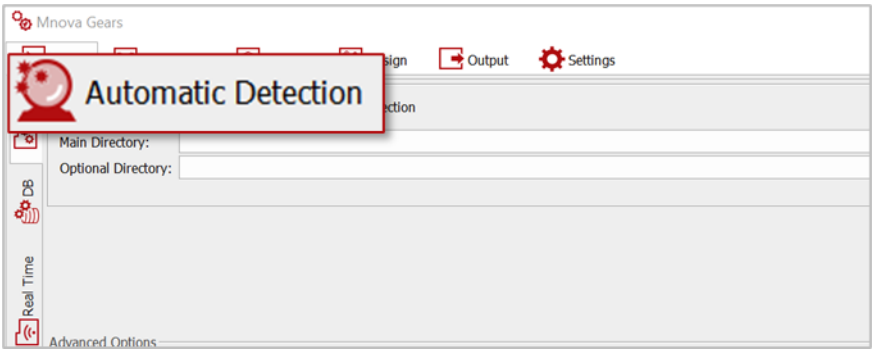
Substring Matching: If this option is checked, the clustering algorithm will include spectra with small differences at the ends of their names. For example, if the requested group is “ABC”, detected files “ABC_1” and “ABC_raw” will be included in the group ABC. If not checked, spectra that do not match the exact name in the file will be discarded.

Top tip! Sometimes the Mapping file can be used to generate final reports with input and output data. In these cases, a configuration of the columns reserved for output can be set in the plugin-specific settings dialog.

3.1.5. Experiment detection modes

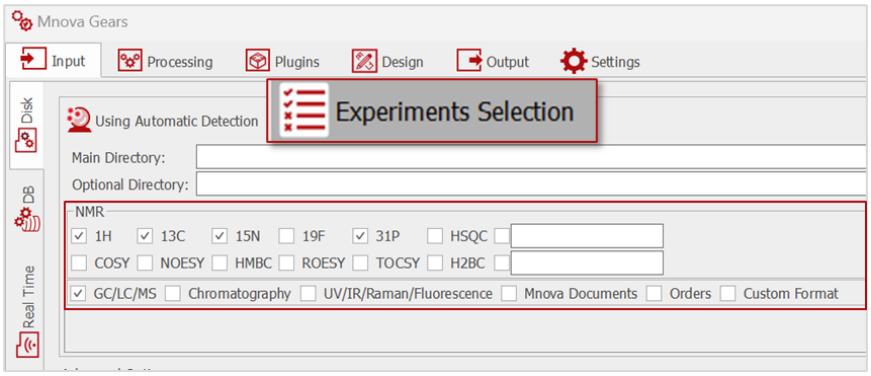
Detection of the experiment files to be used for the analysis can be achieved either automatically or manually. This can be selected at the top left-hand side of the **Input** tab when data files are retrieved from **Disk** or in **Real Time**.

In the **Automatic detection** mode, experiment files will be automatically recognized by the system.



Given that Mgears can support various types of analyses (NMR (1H, 13C, 19F, HSQC…), LC/GC/MS, chromatography, UV/IR/Raman/Fluorescence) as well as any Mnova documents, it is possible to select the type of data files you wish to analyze, and restrict detection by Mgears to those.

To do so, click on **Experiment Selection**. A new section with all available experiment types will appear on your screen. Check the boxes of the experiments of interest.

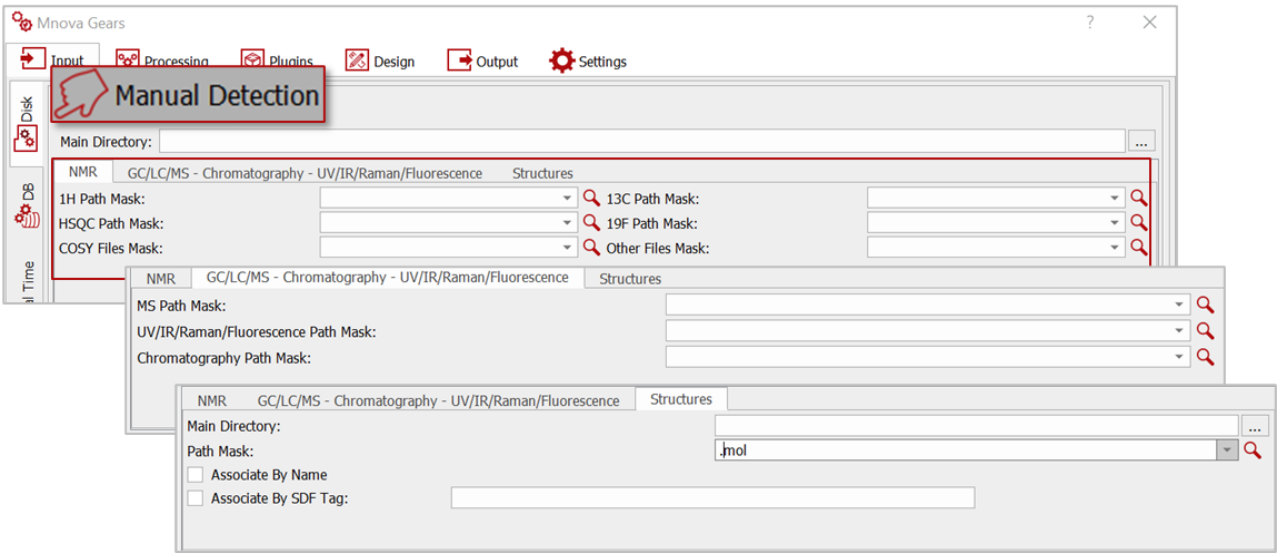


Watch out! You may need to configure the file masks to ensure the correct automatic detection of experiment files.

In the **Manual detection** mode, a **Path Mask** must be provided to define the experiments that should be considered in the analysis. All Operating System standard conventions apply (*, ?, !, etc.).

To do so, enter the **Path mask** for the experiments of interest. Use the **Inspection** option  to inspect the detected files.

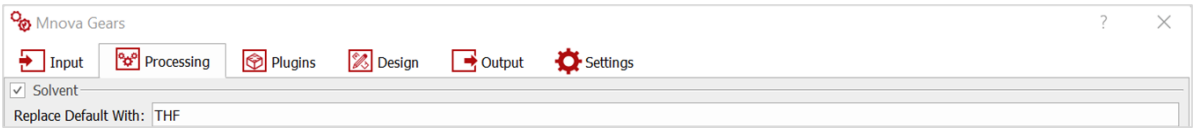
In Disk mode



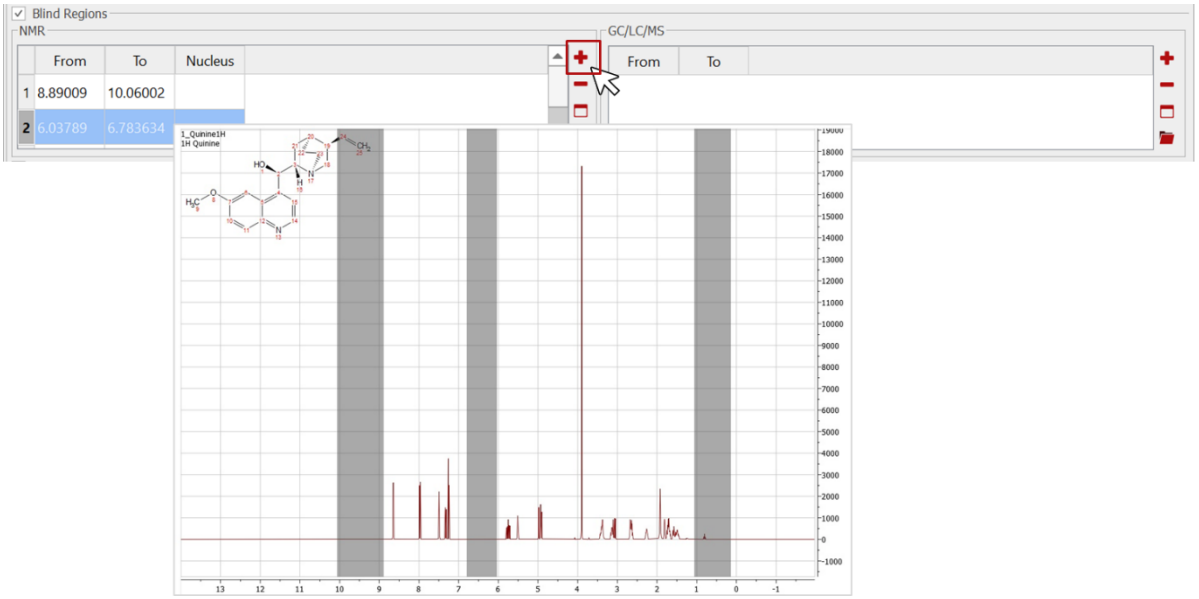
3.2. Processing

The processing tab allows you customize data processing:

- **Solvent:** Tick this option to replace the default solvent with another one by simply typing your new solvent name.

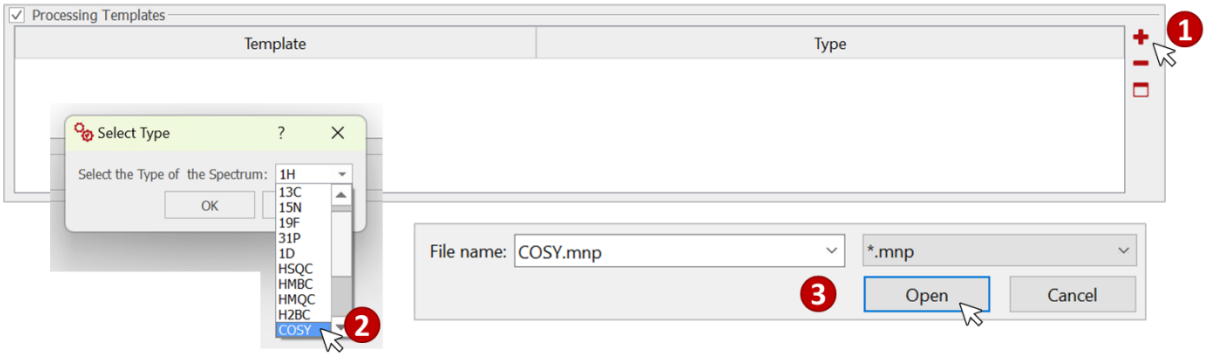


- **Blind regions:** can be added to NMR or LC/GC-MS spectra. You can either:
  - Manually add blind regions
  - Import a "blind regions" file

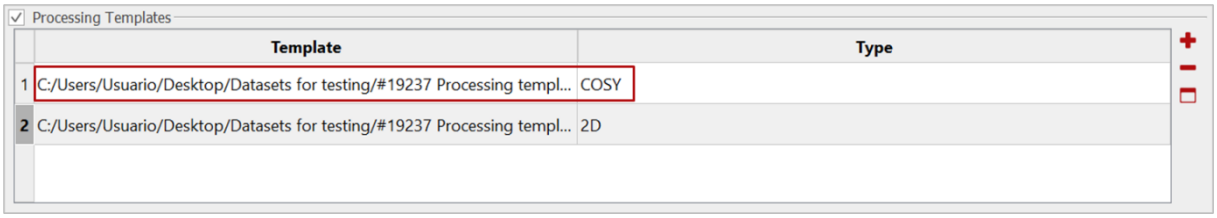


Click on or to **Delete** a row or **Clear** the whole table, respectively.

- **Processing Templates:** To add templates, click on , specify the type of spectra this template should apply to, then add the template path.



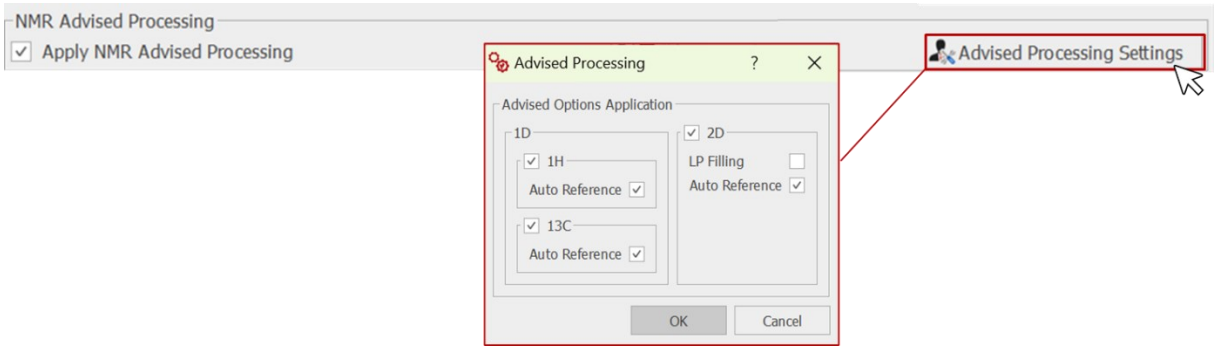
Your added template will be displayed in the table as seen below:



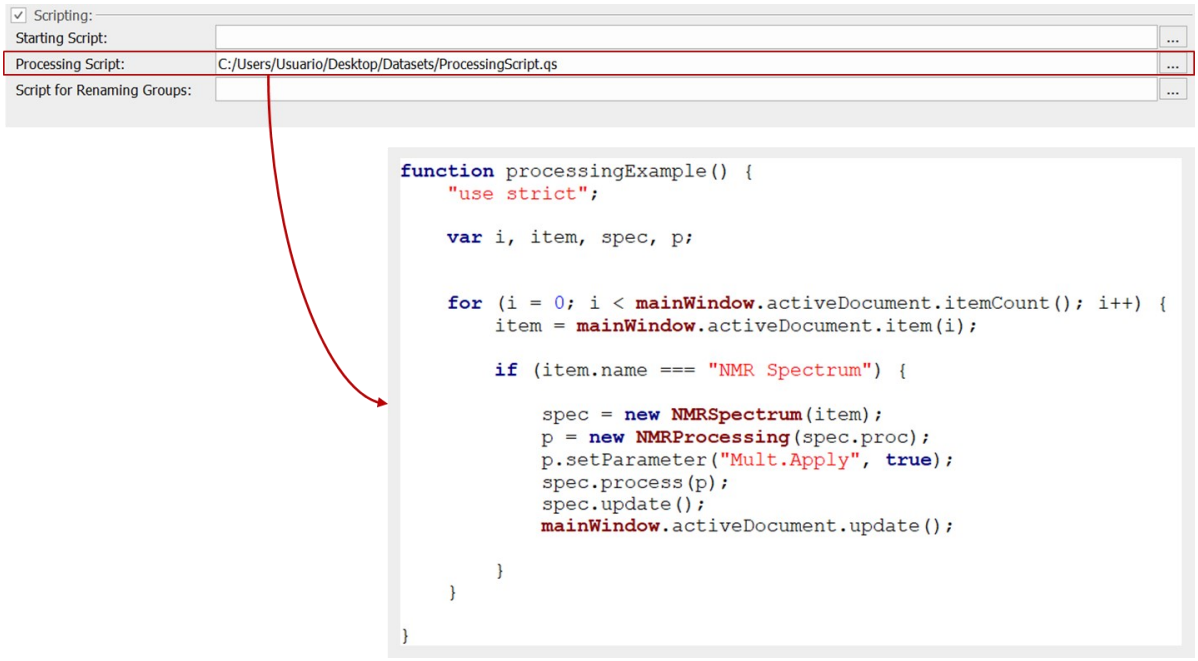
You can add one more template and each will be applied to the corresponding spectra. When simultaneously applying a template for COSY and another for 2D, then the most specific template (in this case the COSY template) will be applied to the COSY spectra, whilst the 2D template will be applied to the 2D spectra in your analysis.

Click on or  to **Delete** a row or **Clear** the whole table, respectively.

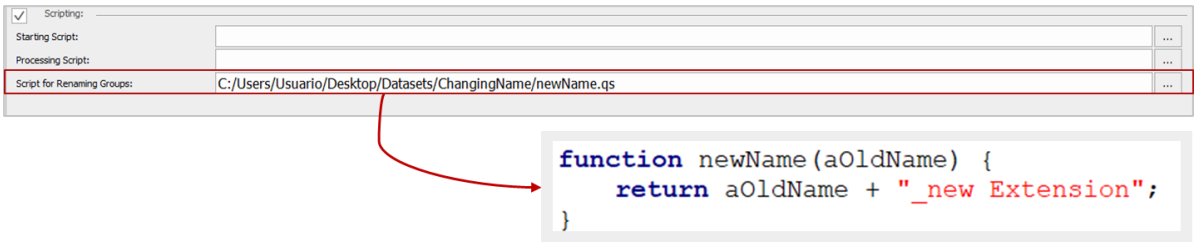
- **Apply NMR Advised Processing**: If you enable this feature, the best processing options will be automatically applied to the data in hand. This includes automatic referencing by solvent and linear prediction for your spectra. You can check/uncheck the type of processing you want to apply in the advised processing setting dialog.



- **Script:** Various custom Mnova scripts can be applied for processing. You can run a single script at the beginning of automation (**Starting script**), a separate script for each sample (**Processing script**), and a third script to automatically rename groups assigned by Mgears (**Script for renaming groups**). Click on ... and upload a script to use. Below is an example of a processing script that will run a multiplet analysis on each spectrum of a document:



In this other example, we will use a script to rename input data groups. The script used will add "_new extension" to our data groups.



After running the Mgears analysis, data files will be renamed as indicated in the script.

Without script for renaming groups

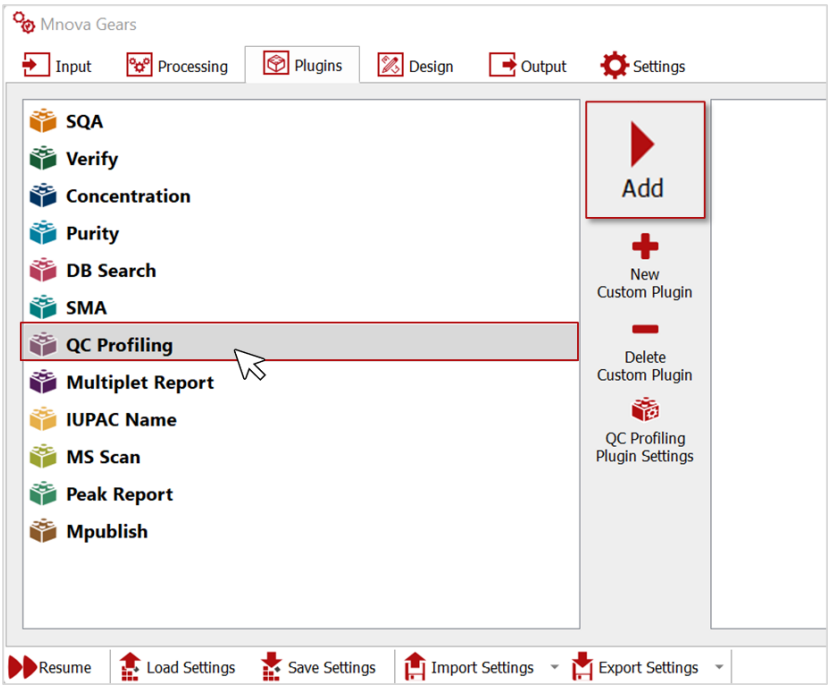
#	Title	Document
1	CATECHIN	CATECHIN.mnova
2	ETHYLBENZENE	ETHYLBENZENE.mnova
3	FELODIPINE	FELODIPINE.mnova
4	QUININE	QUININE.mnova

With script for renaming groups

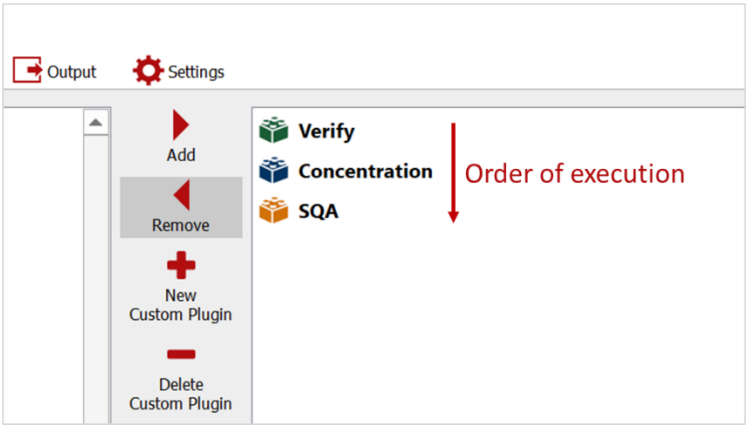
#	Title	Document
1	CATECHIN_new Extension	CATECHIN_new Extension.mnova
2	ETHYLBENZENE_new Extension	ETHYLBENZENE_new Extension.mnova
3	FELODIPINE_new Extension	FELODIPINE_new Extension.mnova
4	QUININE_new Extension	QUININE_new Extension.mnova

3.3. Plugins

The plugins tab is where you select and configure the analysis plugins you want to run. To include a brick in your workflow, select it and click the **Add** button.



You can add one or multiple plugins to run one after the other on the same dataset. The plugins are displayed in the order they will be executed.

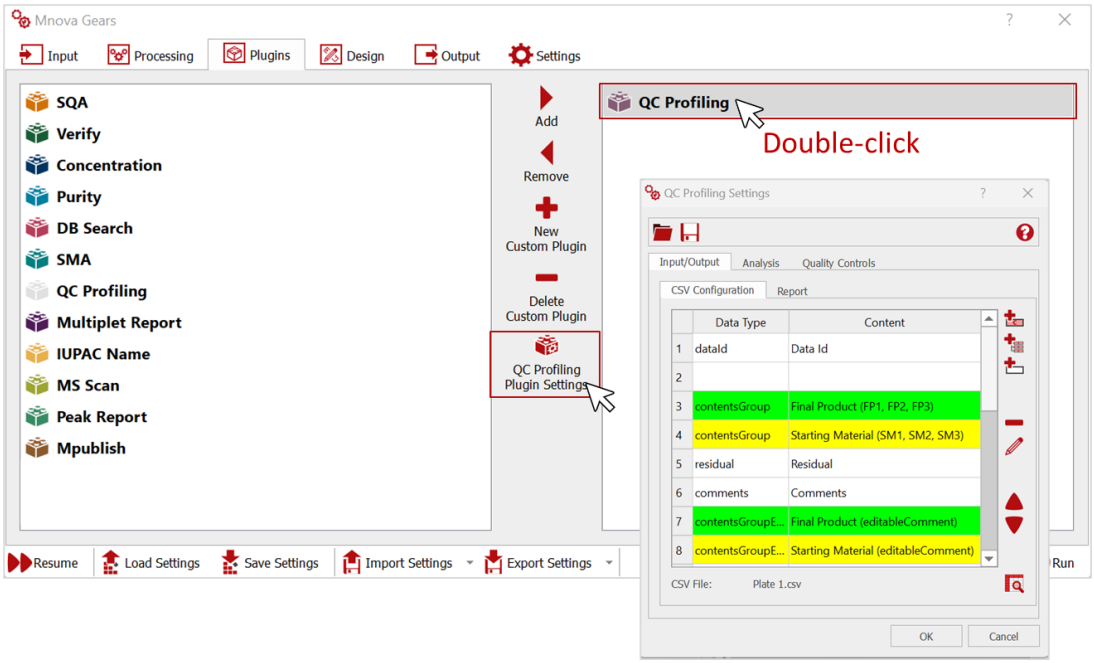


A number of plugins are available with Mgears 2.5:

Plugin	Technique	Analysis
SQA	NMR	Spectral quality assessment
Verify	NMR, LC/GC-MS	Automatic structure verification on NMR and LC/GC-MS data
Purity	NMR	Purity determination by quantitative NMR analysis
Concentration	NMR	Concentration determination by quantitative NMR analysis
Peak Report	NMR	Automated peak reporting
Multiplet Report	NMR	Automated multiplet reporting
MPublish	NMR	Automated preparation of supporting information for publications
IUPAC Name	NMR	Automated and batch IUPAC naming of molecular structures
DB Search	NMR	Automated search of spectral data in one or more databases
SMA	NMR	Targeted mixture analyses by NMR for batch and real time workflows
MANIQ	NMR	Automated identification and quantification of compounds in a mixture
QC profiling	LC/GC-MS	Purity assessment of DNA encoded library compounds
MS Scan	LC/GC-MS	Automated extraction of mass spectra and mass chromatograms for total ion chromatograms
Chrom Reaction Optimization	LC/GC-MS	Automated analysis to determine the optimal chemical reaction conditions
Chrom Cal	LC/GC-MS	Automated evaluation and generation of calibration curves for many compounds at the same time
Affinity Screen	LC/GC-MS	Automated solution for affinity selection mass spectrometry data processing, interpretation, and hit identification
Fraction Analysis	LC/GC-MS	Automated evaluation of fractions collected with preparative chromatography
Chrom Best Method	LC/GC-MS	Automatic scoring tool for selection of chromatographic methods with optimal separation conditions

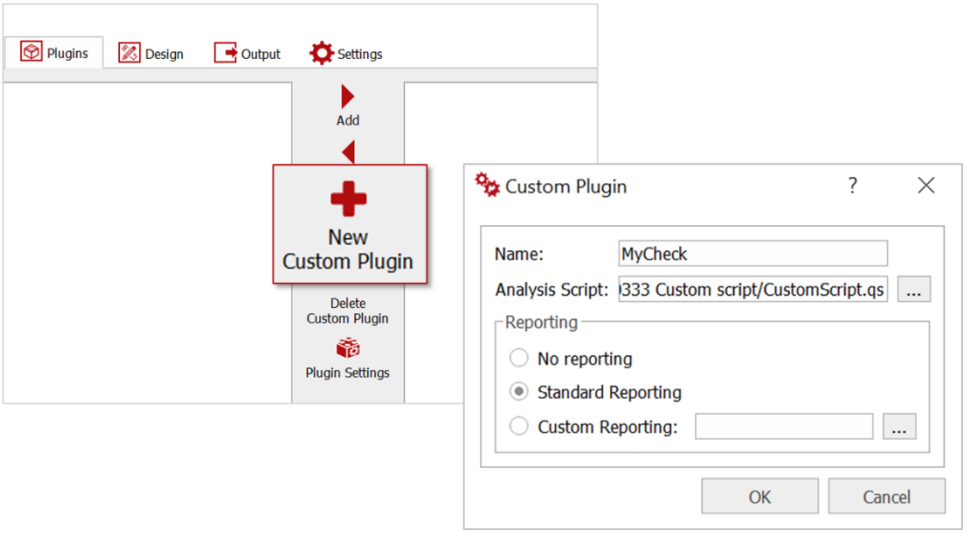
Each brick has its own settings that can be configured in just a few clicks (details about plugin configuration are provided in a separate starting guide for each application).

To open the plugin-specific settings, select the plugin and then click on the settings button, or simply double-click on the plugin.

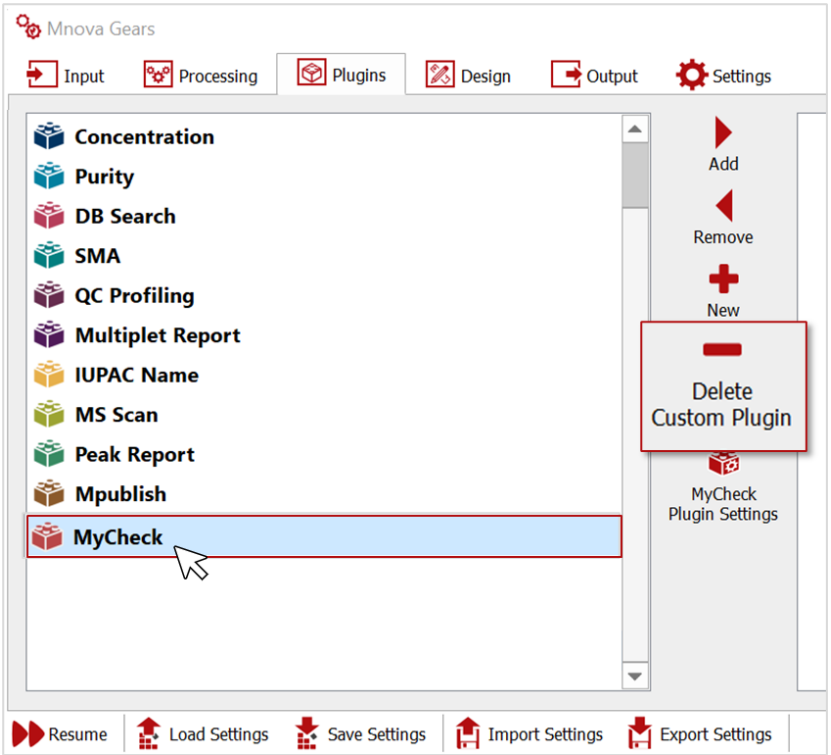


The workflow configuration can be easily saved and shared by clicking on **Save Settings** . A ".data" file will be generated with the saved settings and can be quickly loaded in the future or on another computer with Mgears, by clicking on **Load Settings** .

If the analysis you want to perform is not covered by our plugins, it is possible to create a custom plugin by uploading your own script. To do so, click on the **New Custom Plugin** icon, **Name** your plugin, then upload the **Analysis Script** (which could be developed outside the automation on individual samples). Then, choose the **Reporting** preferences (optionally also using your own reporting script), and click on **OK**.

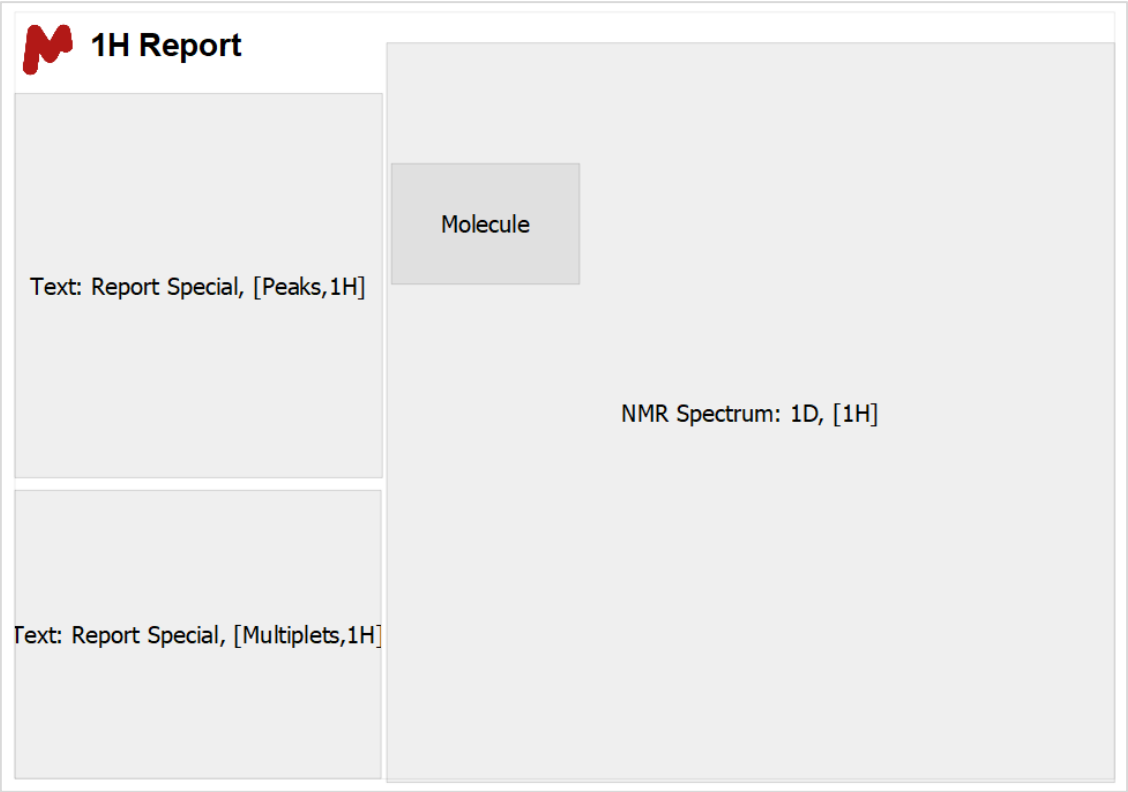


The new custom plugin will appear in the list of available plugins. You can delete a previously added custom plugin by selecting it and clicking on **Delete Custom plugin**.

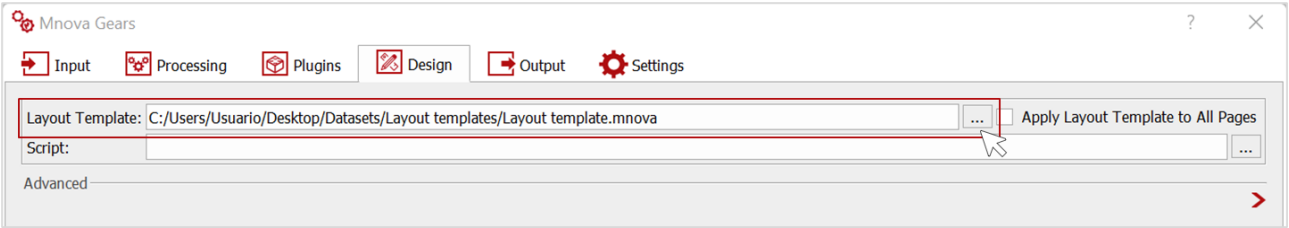


3.4. Design

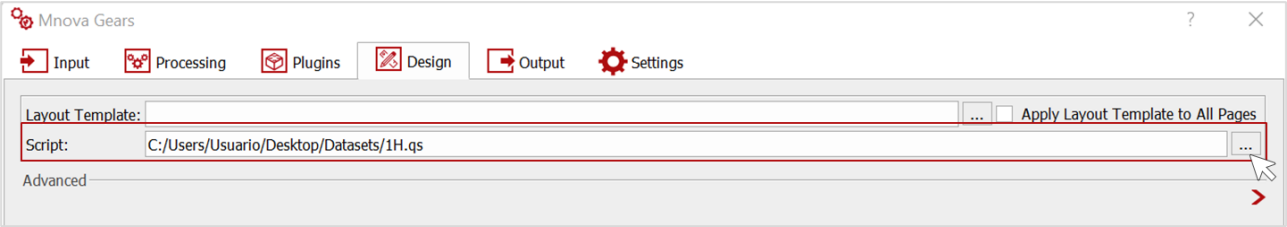
In the design tab, Mnova layout templates can be applied to the output documents resulting from the analysis performed. You can easily create your own template with Mnova, laying out the pages as per your requirement and including any custom graphics or images, then save that document as a template that can be used with Mgears.



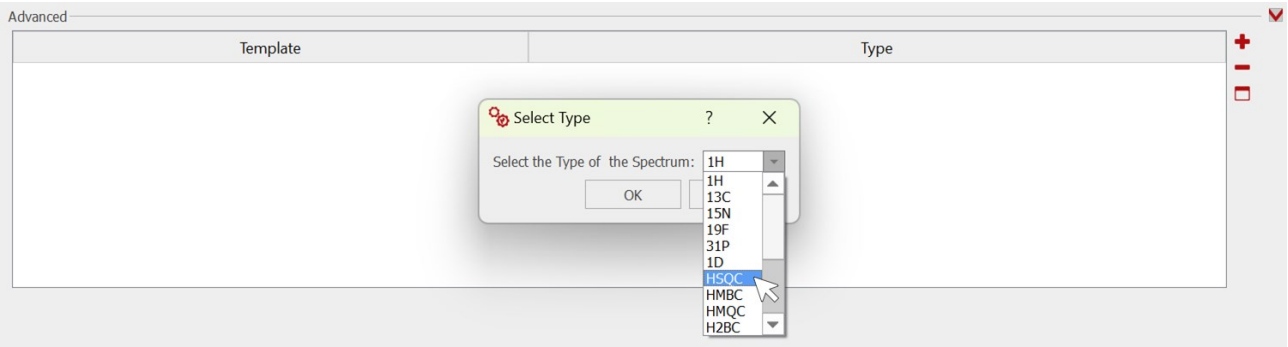
Click on ... and select the template file you want to apply. You can check the **Apply Layout Template to All Pages** option to apply the layout on every page of the output document.



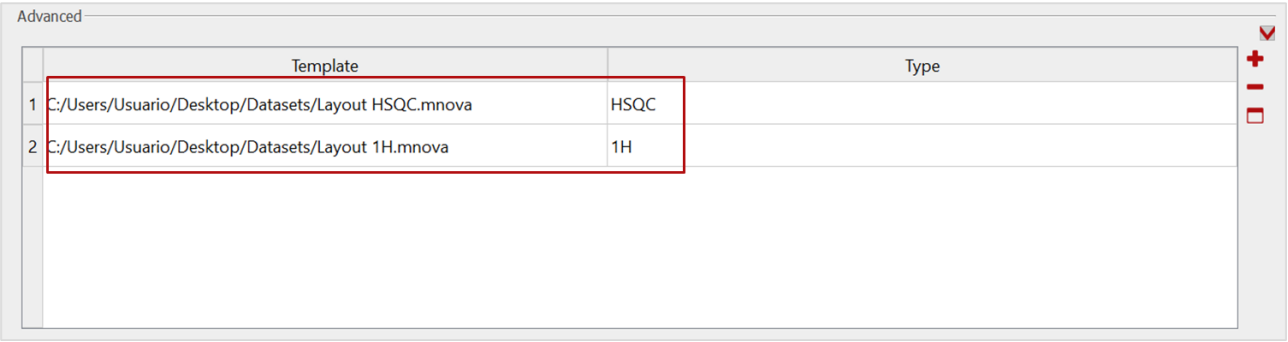
A **Script** can also be applied to achieve highly complex layout needs.



If you have different templates to be applied for different types of analyses, then you can expand the **Advanced** design section and click on to add your different templates. A dialog will open to allow you to choose the analysis type. You can then select the template path from the directory.



Your added templates will be displayed in the table as seen below. You can click on to delete a previously added template, or on to clear the entire table.



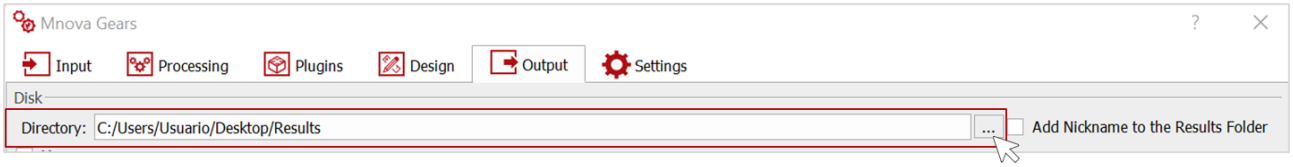
When different templates can be applied to the same dataset, the most specific one will be used. For instance, if a template for COSY and another for 2D spectra are added, then the COSY template will be applied to COSY spectra.

3.5. Output

The output tab is where options for saving reports are configured. There are two main options: saving data in Disk directories and saving data in a Database. In addition, several advanced switches allow you to customize how the output is saved.

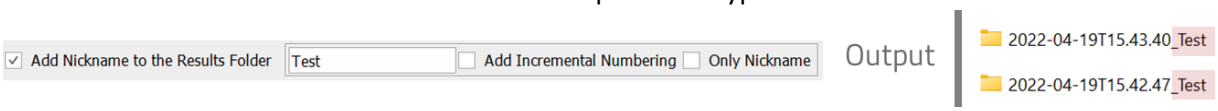
3.5.1. Saving output on Disk

To save output data on disk, click on ... and choose a directory in which to save your analysis results.

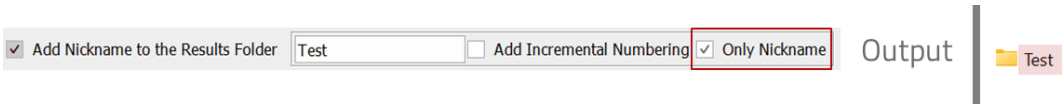


The result folder is by default named according to the date and time of your analysis, e.g., 2021-01-08T08.06.58. However, it is possible to either add a nickname to the result folder name or completely replace the result folder default name with a nickname of your choice.

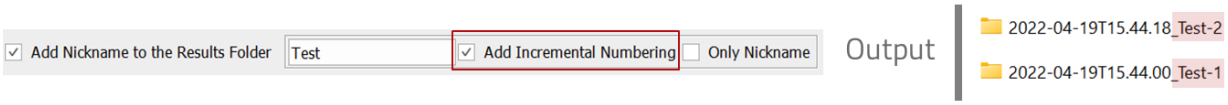
Enable the **Add Nickname to the Results Folder** option and type the desired nickname.

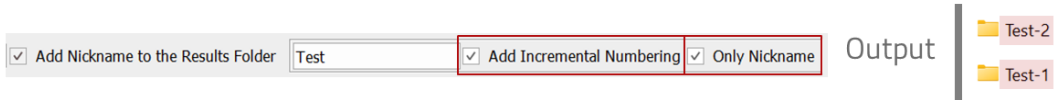


Enable the **Only Nickname** option to remove the timestamp from the folder name and only use the indicated nickname.

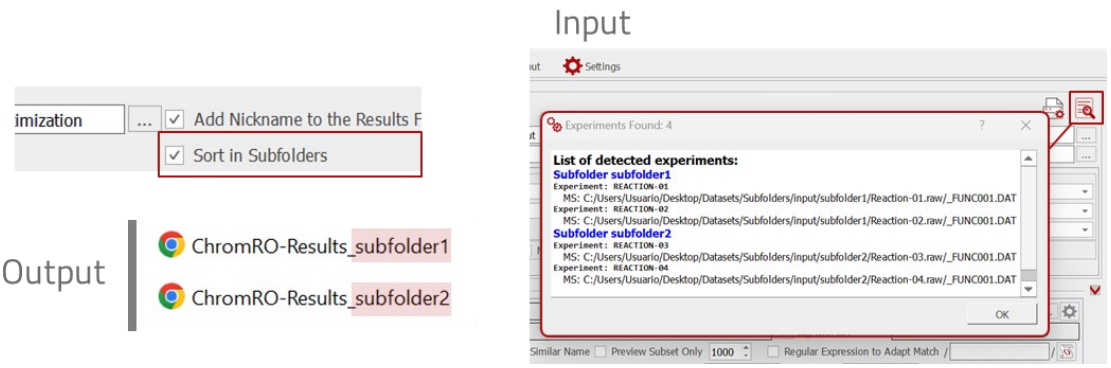


Enable the **Add Incremental Numbering** option to add a number to the folder's name when another folder with the same nickname is detected in the output directory.





If your input data is organized within sub-folders and you want to analyze them individually, you can enable the **Sort in Subfolders** option. Enabling this option will prompt the system to detect and separate the data within each subfolder. A distinct report will be generated for each subfolder. See below an example with an HTML report for each subfolder.



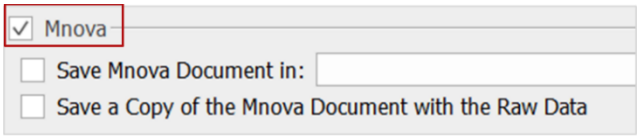
When you activate the **Sort in Subfolders** option, you can also utilize the **Split Results in Subfolders** feature. Enabling this option allows you to save the Mnova and PDF outputs in subfolders named after the corresponding input subfolders.

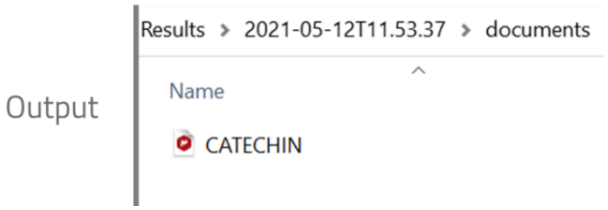
Both an interactive Mnova file and a human readable PDF can be generated and saved along with your analysis results.

3.5.1.1. Saving an Mnova document

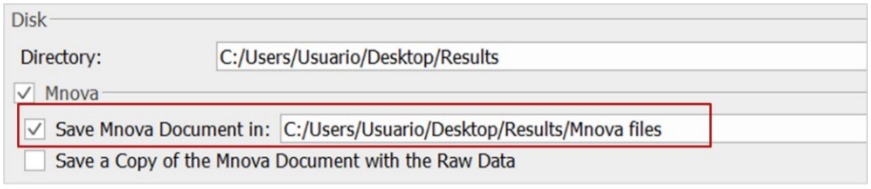
Check the **Mnova** options and configure the saving settings as needed:

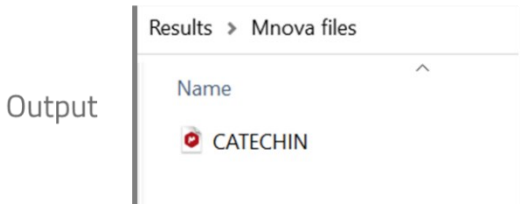
- The Mnova document is saved by default in the output folder in a sub-folder named “documents”.



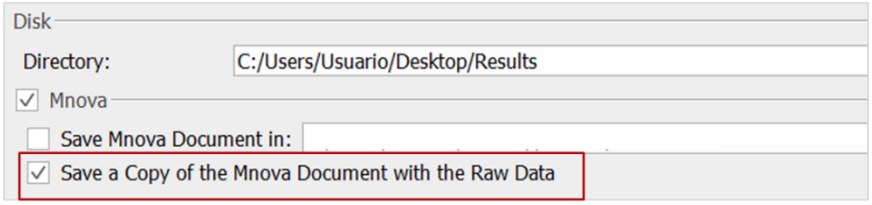


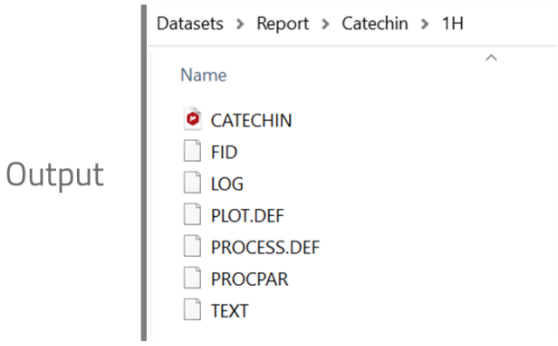
- You can save the Mnova document in the folder of your choice by ticking the option **Save Mnova Document in** and selecting the desired destination folder.





- You can also **Save a copy of the Mnova document with the input data** by ticking the corresponding option.

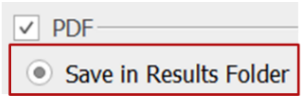


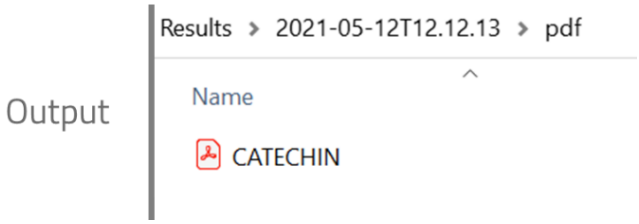


3.5.1.2. Saving a PDF document

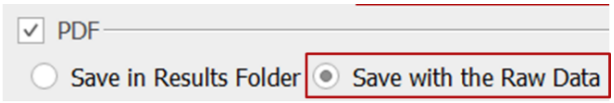
Check the **PDF** options and configure the saving settings as needed:

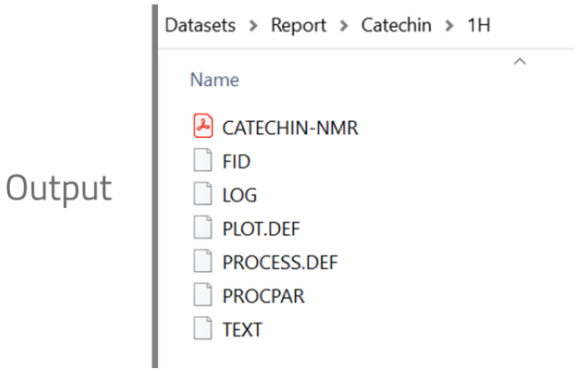
- You can save the PDF document in the **Results folder** (configured above as the Directory). It will be saved in a sub-folder named 'pdf'.



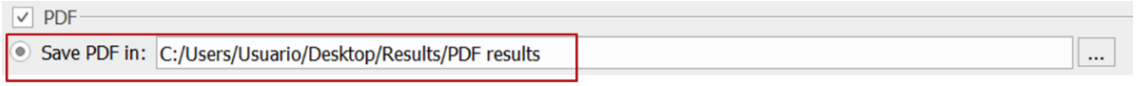


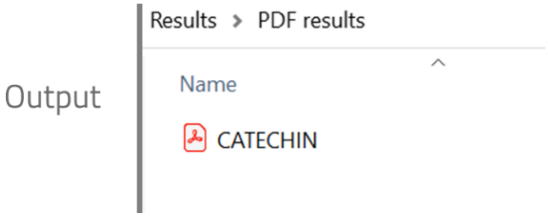
- The PDF can also be saved along **with the input raw data.**



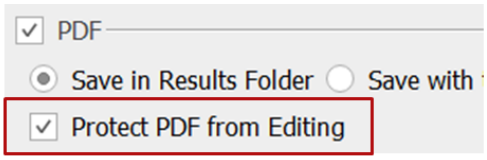


- The PDF can alternatively be saved in a separate folder by ticking the **Save PDF in** option and selecting the desired destination folder.



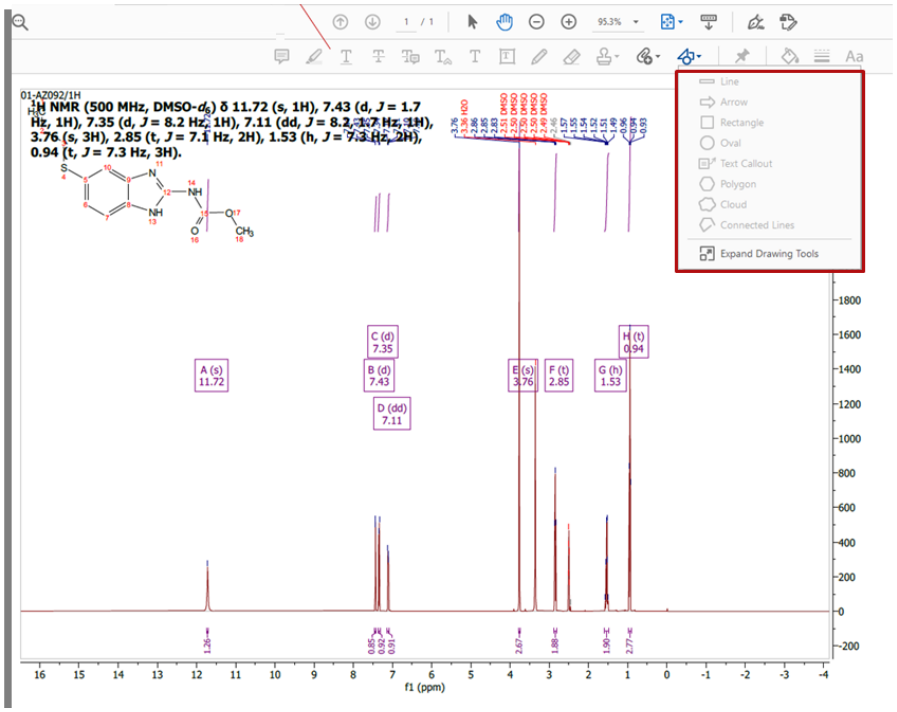


- You can **Protect PDF from Editing** by enabling the corresponding option:

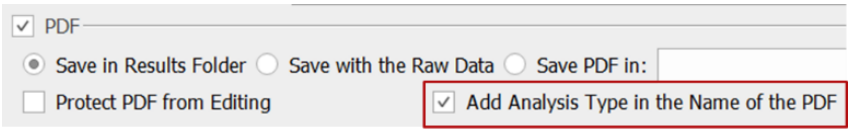


Not editable

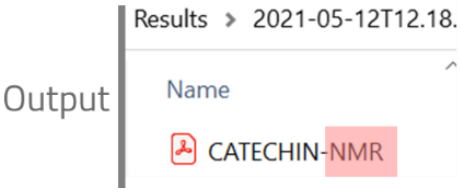
Output



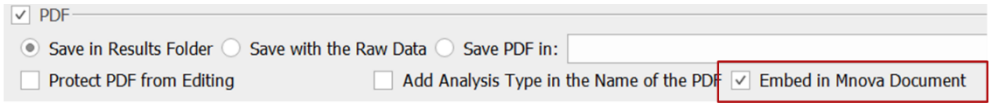
- You can also **Add Analysis type in the Name of the PDF**;



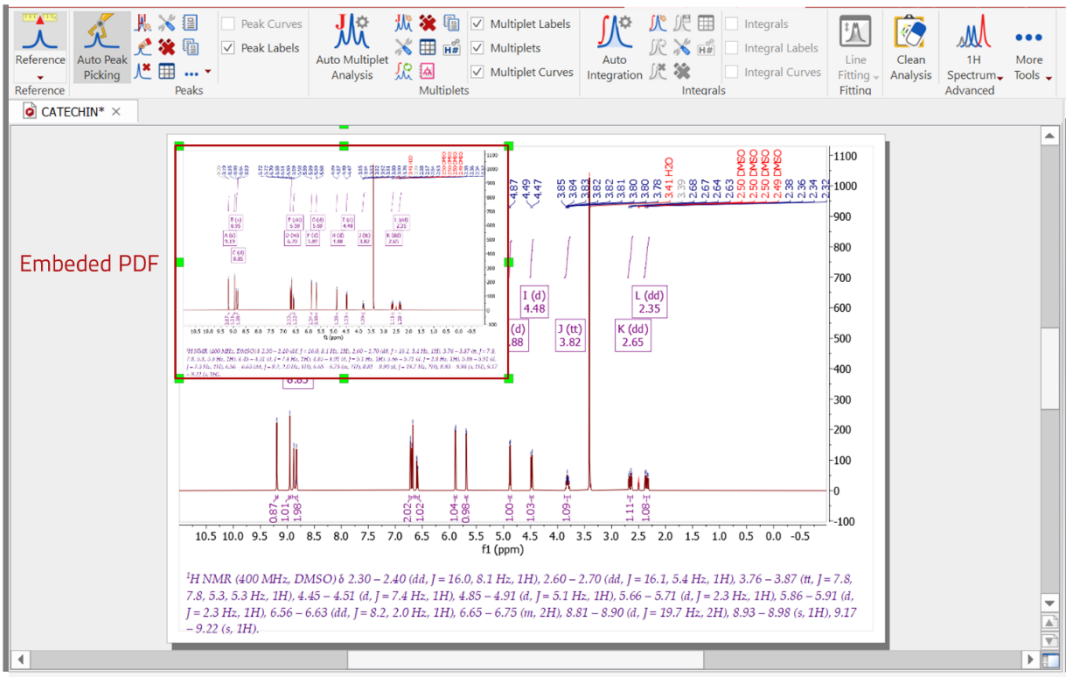
Output



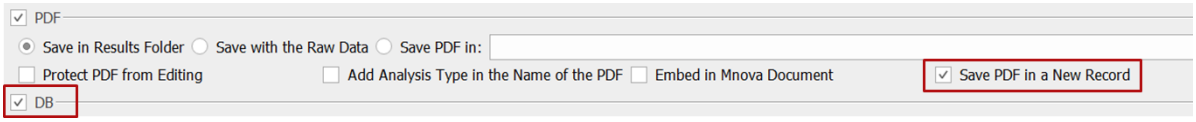
- or **Embed PDF in Mnova document.**



Output

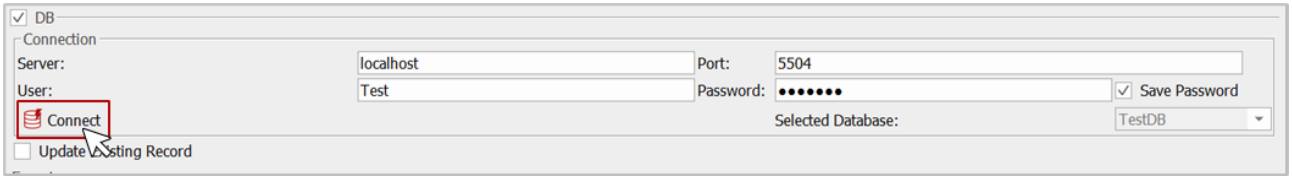


- When results are saved to a database, it is also possible to **Save PDF in a New record**. If this option is unchecked, the PDF will be saved in the record along with the processed data.

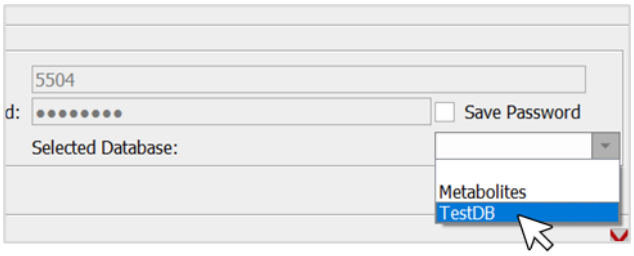


3.5.2. Saving output in a Database

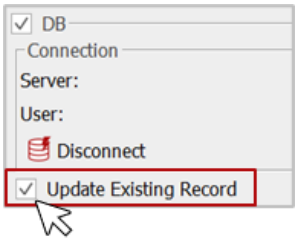
Mgears results can be saved to an Mnova spectral database. To do so, you will need to check the **DB** option, indicate your **Server** address, **Port**, and your credentials (**User** and **Password**), then click on **Connect**.



Once connected to the server, you can select the database you want to save the results to.



Check the **Update Existing Record** option if you want Mgears to search for and attempt to update an existing record in the DB before saving your results to a new one:



- When the input comes from Disk directories, Mgears will search for the name of the experiment in the DB. If the ID is found in one record, it will be updated, otherwise a new record will be created. If the ID is detected in more than one record, the log will show an error, and nothing will be saved to the DB.
- When the input comes from the DB, it will update the registry associated with the input.

Watch out! This feature will only work with DBs created with Mnova 14.0.0 or higher, and the Mnova DB Server version 1.8.3 or higher (with a field custom ID on each item).

3.5.3. Saving output in an ELN

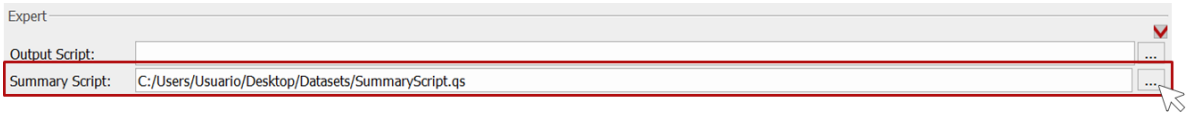
Mgears can detect your ELN plugin and save the analysis output directly to it. Contact us for assistance.

3.5.4. Expert settings

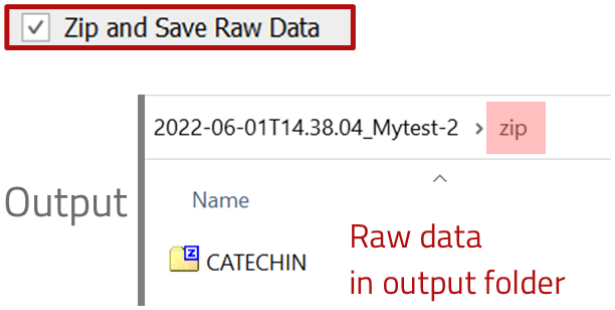
Additional settings can be configured for analysis output under the **Expert** section:

- An **Output Script** that gives complete control over the output generation and saving can be used, for example, to send details of the report to a web service and update an external database, or to write results in a custom data folder structure, etc. Click on ... to select your **Output Script**.

- A **Summary Script** that runs at the end of a batch analysis (in disk or DB modes) to evaluate all the results of the different bricks together and provide a global result (e.g. statistical estimators for all the results). Click on ... to select your **Summary Script**. of running a Summary script to

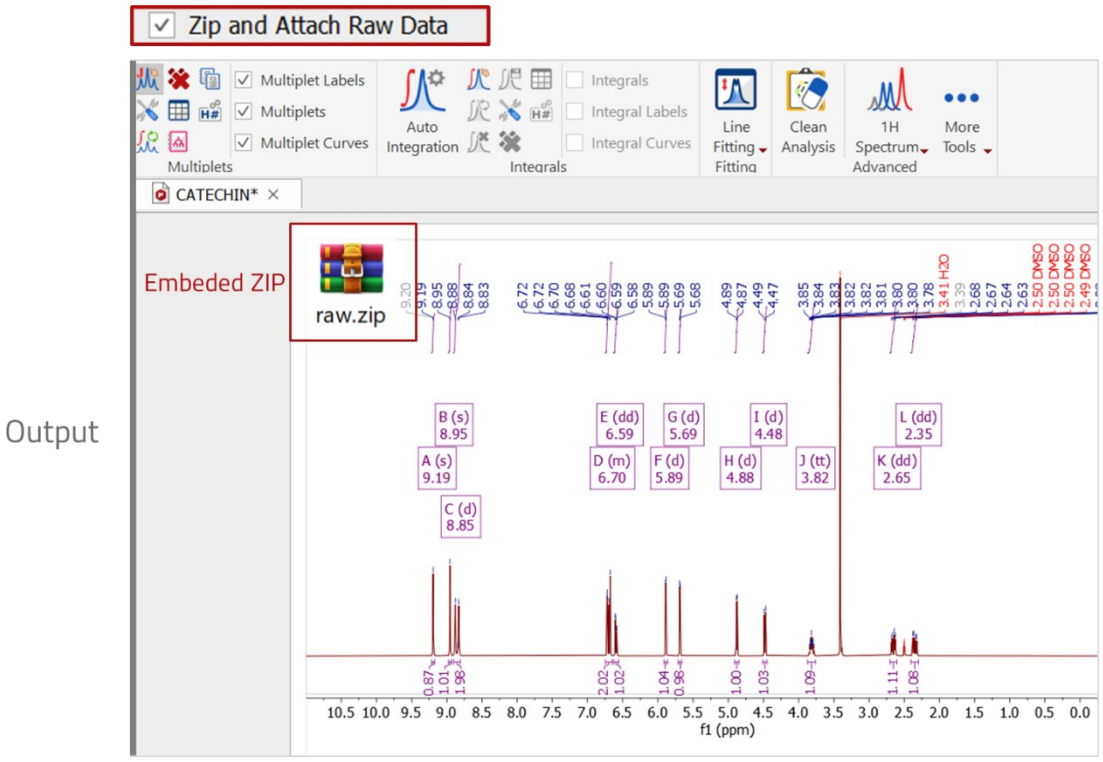


- **Zip and Save Raw Data:** If checked, Mgears will create a zip file with the raw data from the processed directory and save it in the output folder**.**



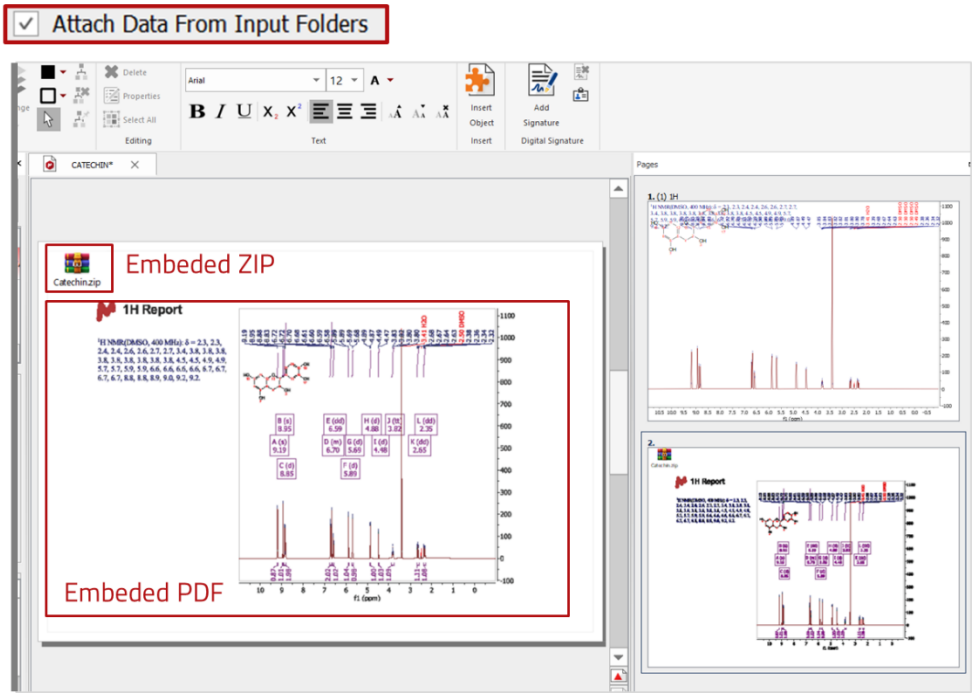
- **Zip and Attach Raw Data:** If checked, Mgears will create a zip file with the raw data from the processed directory and embed it in the resulting Mnova document**.**

Output



- **Attach Data from Input Folders:** Enable this feature if you want to attach all Zip and PDF files from each processed input directory to the Mnova document.

Output

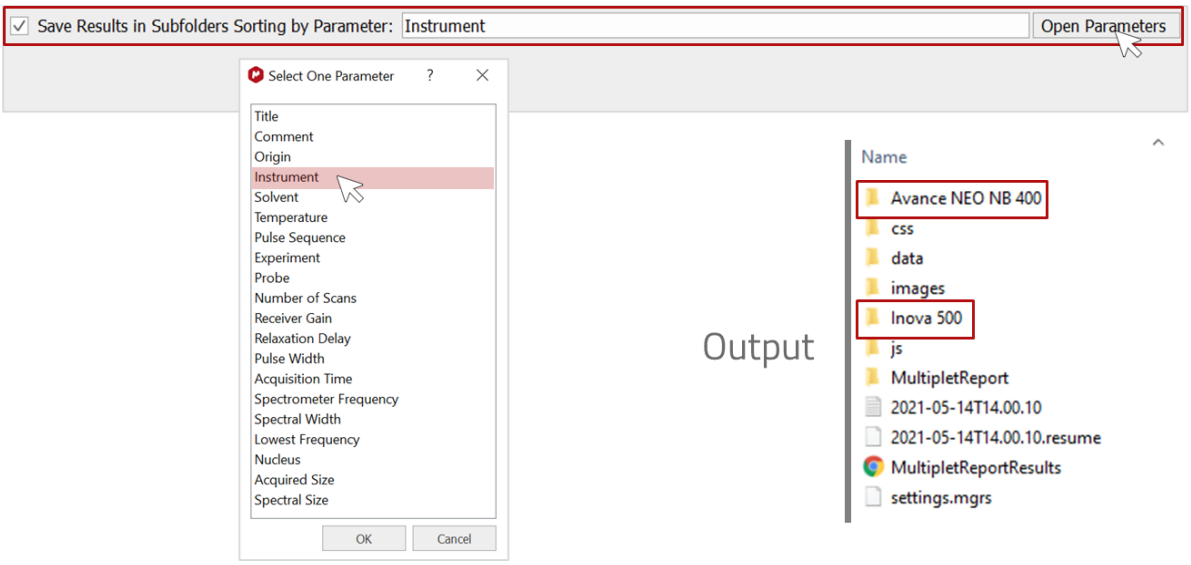


- **Save Structure in a New Record:** This option is available when output is saved into a database. If checked, the structure will be saved in a new separate record, otherwise it will be saved together with the processed spectra.

- **Avoid Saving Images:** You can enable this option to avoid saving images of the molecules and spectra in the output folder. Images will not be displayed in the html report either.

- **Create Reports on-the-fly:** If this option is checked, Mgears will create all reports after processing each experiment instead of waiting until the end of the whole task.

- **Save Results in Subfolders Sorting by Parameter:** With this option enabled, it is possible to distribute the results into different folders according to any of the available spectral parameters. Open an input spectrum by clicking on **Open Parameters.** Mgears will read the available parameters in your input data and list them so you can select one to sort your results. Click on **OK**.



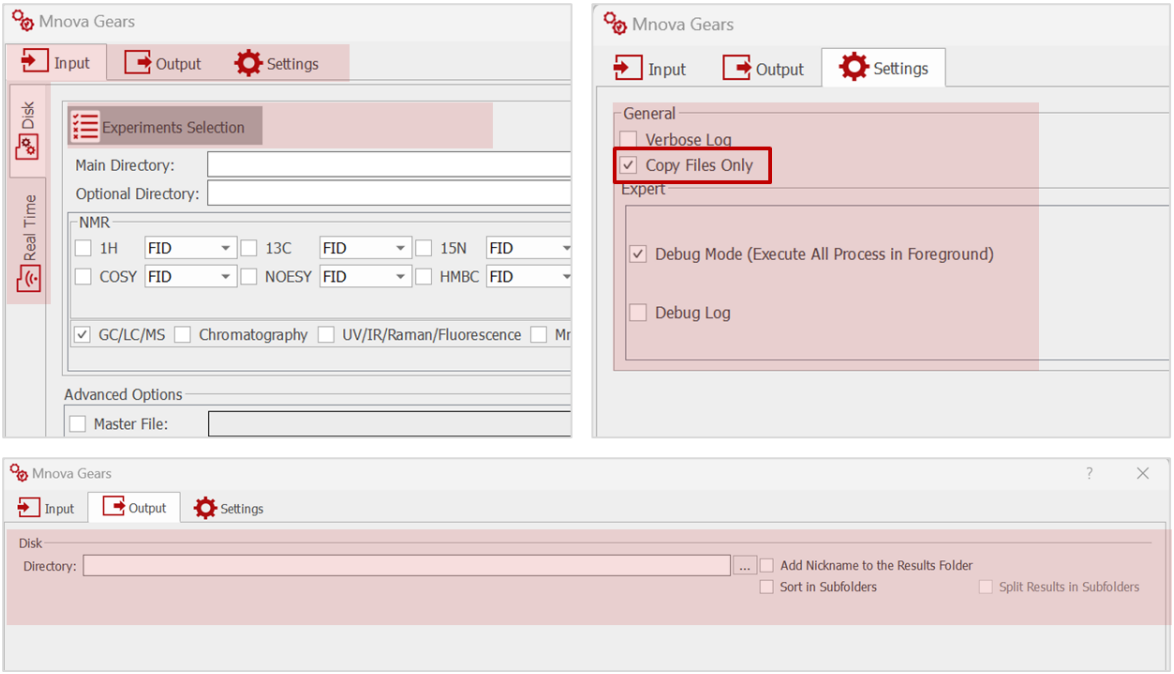
3.6. The Settings tab

The settings tab does not form part of Mgears workflow but allows the specification of various aspects of automation, and the configuration of the **Notifications** system for receiving automatic emails related to your Mgears analyses.

3.6.1. General settings

The general settings include the following:

- **Verbose log:** Check this option to include detailed information in the log.
- **Autoload Results in the Viewer when Finished:** If enabled, the Mgears Result Viewer will automatically load the results of a batch analysis once completed.
- **Autoload Results in the Viewer on-the-fly:** If enabled, the Mgears Result Viewer will automatically load the results in real time, as soon as they are obtained.
- **Copy Files Only:** If enabled, Mgears will exclusively copy data to the output folder without opening, processing, or analyzing it. This option hides processing and analysis related tabs and options and is functional only with automatic data detection in Batch and Real-time modes.



3.6.2. Expert settings

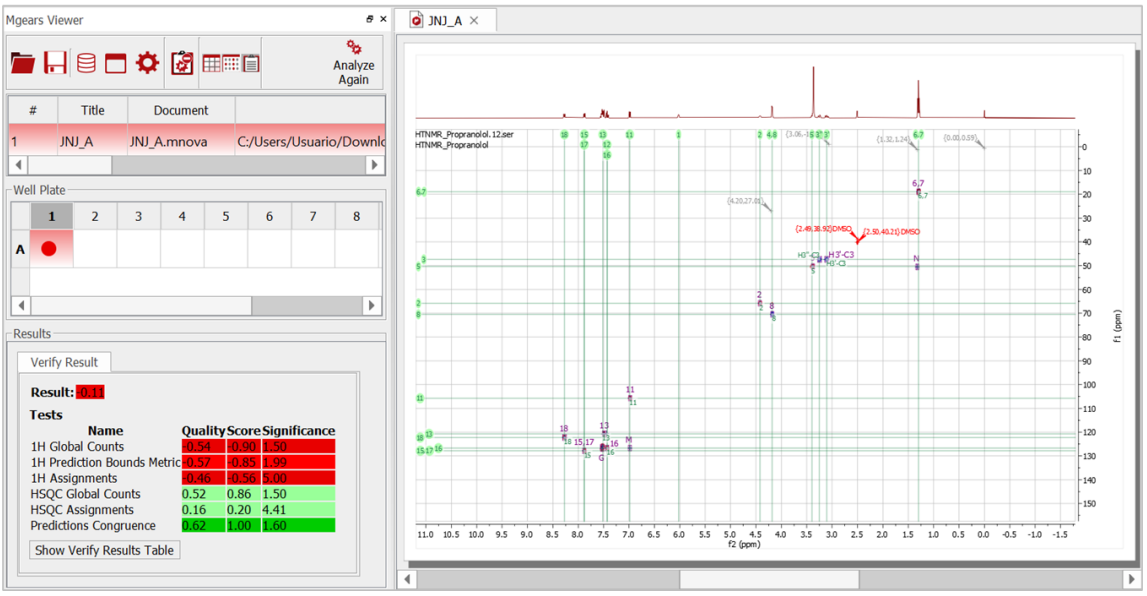
More settings options are included in the **Expert** section:

- **Debug Mode (Execute all processes in Foreground):** If enabled, the log will contain information about the internal state of the objects inside Mgears. This option is mainly used for debugging and development purposes.

- **Debug Log:** If checked, the Mgears log file will give information about Mgears, the available plugins, and the current analysis, and will be saved in the results folder.

```
[2021-03-12T14.34.56] Running Mgears 2.2.0.7037
[2021-03-12T14.34.38] Plugins available:
[2021-03-12T14.34.38] SQA 14.2.0-26256
[2021-03-12T14.34.38] Verify 3.0.0.6085
[2021-03-12T14.34.38] Concentration 3.0.0.6161
[2021-03-12T14.34.38] Purity 3.0.0.6161
[2021-03-12T14.34.38] DB Search 1.0.0.6640
[2021-03-12T14.34.38] SMA 3.0.0.7013
[2021-03-12T14.34.38] QC Profiling 1.1.0.6088
[2021-03-12T14.34.38] Multiplet Report 1.0.0.6703
[2021-03-12T14.34.38] IUPAC Name  1.0.0.6908
[2021-03-12T14.34.38] MS Scan 1.0.0.6933
[2021-03-12T14.34.38] Peak Report 1.0.0.7139
[2021-03-12T14.34.38] Mpublish 1.0.0.6695
[2021-03-12T14.34.38] B2ADF Converter 1.0.0.6496
[2021-03-12T14.34.38] MS Reaction Optimisation 1.0.0.7110
[2021-03-12T14.34.38] MS Best Method 1.0.0.6539
[2021-03-12T14.34.57] Starting MS Scan Engine
[2021-03-12T14.34.57] MS Scan succesfully done in SMPL1
[2021-03-12T14.34.57] Dataset SMPL1 processed
[2021-03-12T14.34.58] Total elapsed time: 1.31 s
```

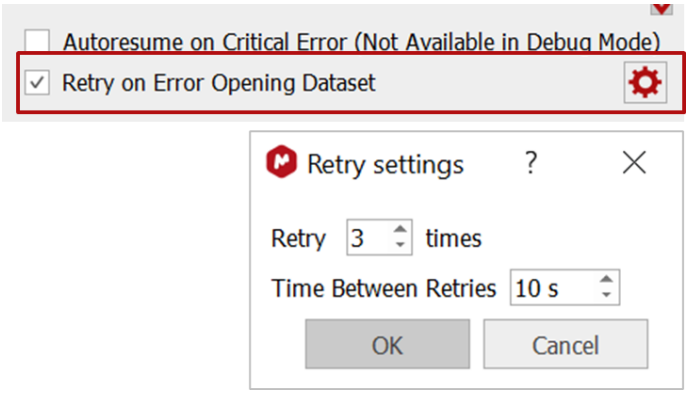
- **Auto Attach traces:** Check this option to automatically attach 1D spectra as horizontal and vertical traces in 2D spectra. With this option selected, the HSQC with the 1H spectrum can be correctly added as the horizontal trace in an HSQC spectrum.



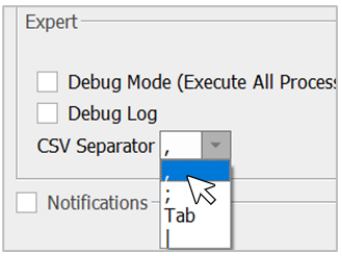
- **Allow events:** If checked, Mgears will not block programmed events (Preferences > Scripting > Events).

- **Autoresume on Critical Error (Not available in Debug Mode):** When enabled, Mgears will resume analysis automatically should a critical error occur.

- **Retry on Error Opening Dataset:** Check this option if you want to force Mgears to retry opening a file after an error occurs (Errors can occur if the file is not in the expected location, or the opening operation fails). Click on the **Retry Settings** icon to set the number of retries and the time the system must wait between each.



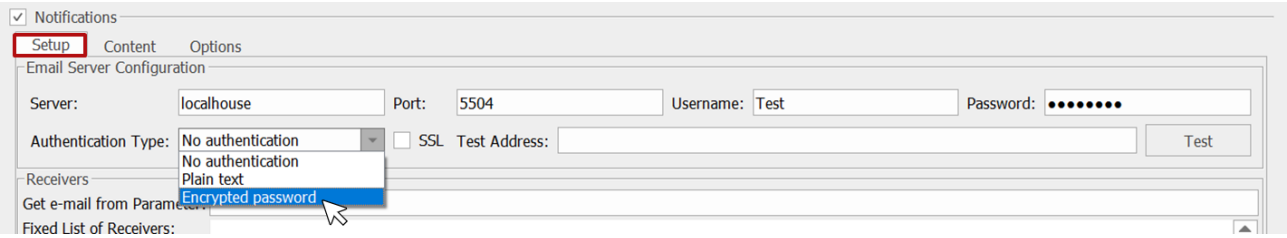
- **CSV Separator:** Select the CSV separator used in your csv input file in order to be read correctly by Mgears.



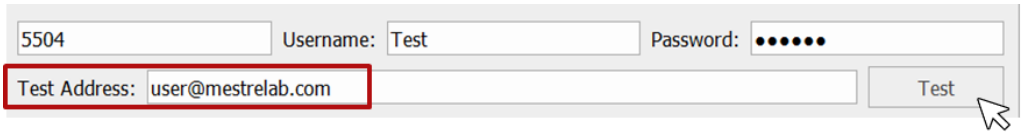
3.6.3. Notifications

Mgears can send automatic email notifications to users to inform them about processing status. To set up email notifications, tick the **Notifications** option and fill in the required information.

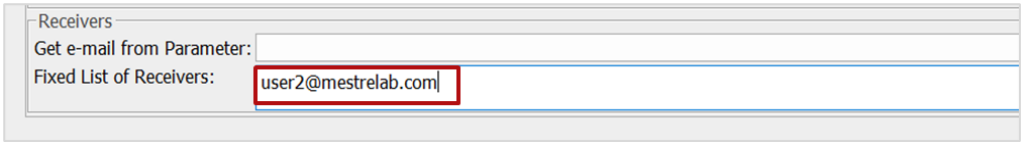
In the **Setup** tab, configure the email server from which the email will be sent by completing the information about your email server (**Server**, **Port**, **Username**, **Password**, etc).



Once all fields are configured, you can test the notification by adding a **Test Address** and clicking on **Test**.

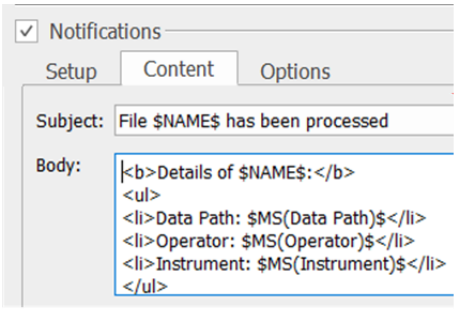


In the **Receivers** section, you can either add a **Fixed List of Receivers** or get the recipients' emails from a **Parameter** in your spectrum**.**

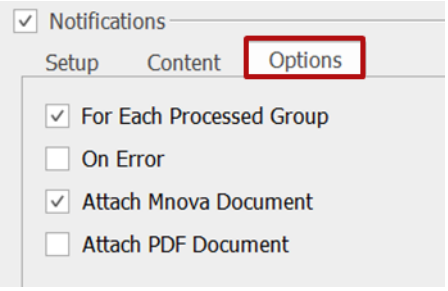


In the **Content** tab, write the notification **Subject** and **Body text**. You can use "$NAME$", "$NMR(Parameter name)$", "$MS(Operator)$", etc., to get analysis-specific information in the subject line and body text. For instance, if you use $NAME$, the name of the dataset in hand will be used, whilst if you use $NMR (parameter name)$, the actual value of the parameter will be displayed.

The **Body** text field also admits HTML formatting.



Finally, in the **Options** tab, choose if you want notifications to be sent when a dataset is processed and/or when an error occurs, and choose if you want to attach an Mnova and/or PDF document to the notification.



Top Tip! All of the configuration settings entered in the various Mgears tabs can be saved and recalled in the future. This is particularly useful when you run many different analyses, as it allows a consistent and quick setup when switching between tasks. The Settings files so created (.mgrs) can therefore be thought of as the way to save a complete automation setup.

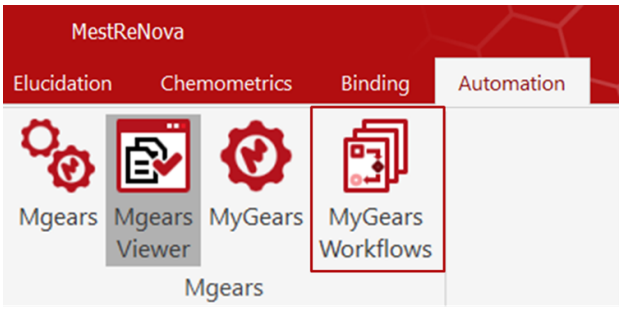
This file can also be used to set up the MyGears workflows, as discussed below.

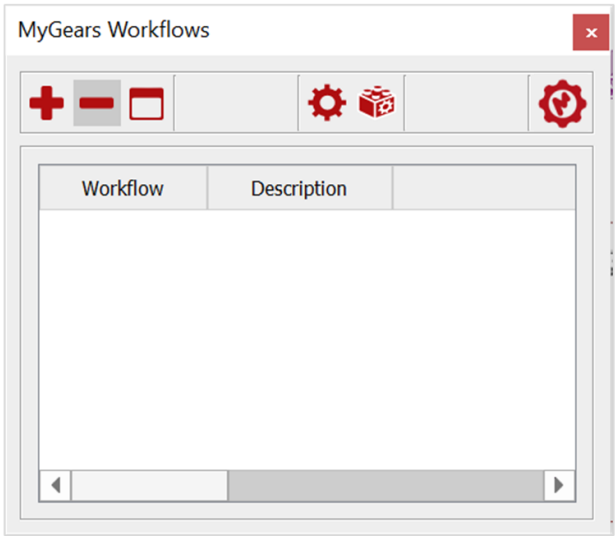
4. MyGears dialog

MyGears' workflow setup is very similar to Mgears´, the main difference being that MyGears will run the automated analysis on a single dataset open in Mnova, and therefore there is no need to configure the **Input** tab.

To create a MyGears workflow from scratch, open the Mgears dialog from the **Automation** section in the Mnova ribbon and proceed as described in sections 3.2, 3.3, 3.4, 3.5, and 3.6 to configure the **Processing**, **Plugins**, **Design**, **Output**, and **Settings** of your analysis. Then, save the settings to a directory of your choice.

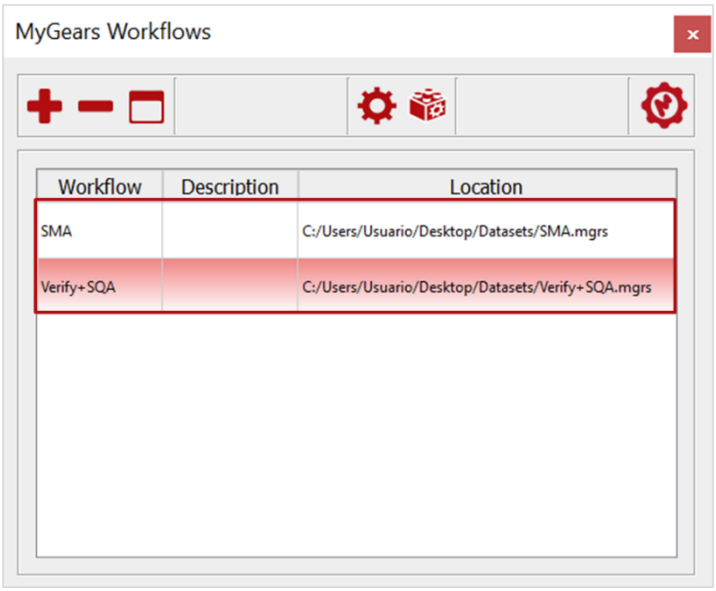
To run a MyGears analysis, first open your dataset in Mnova, then open the **MyGears Workflows** from the **Automation** section in Mnova. A dialog with the following buttons opens:





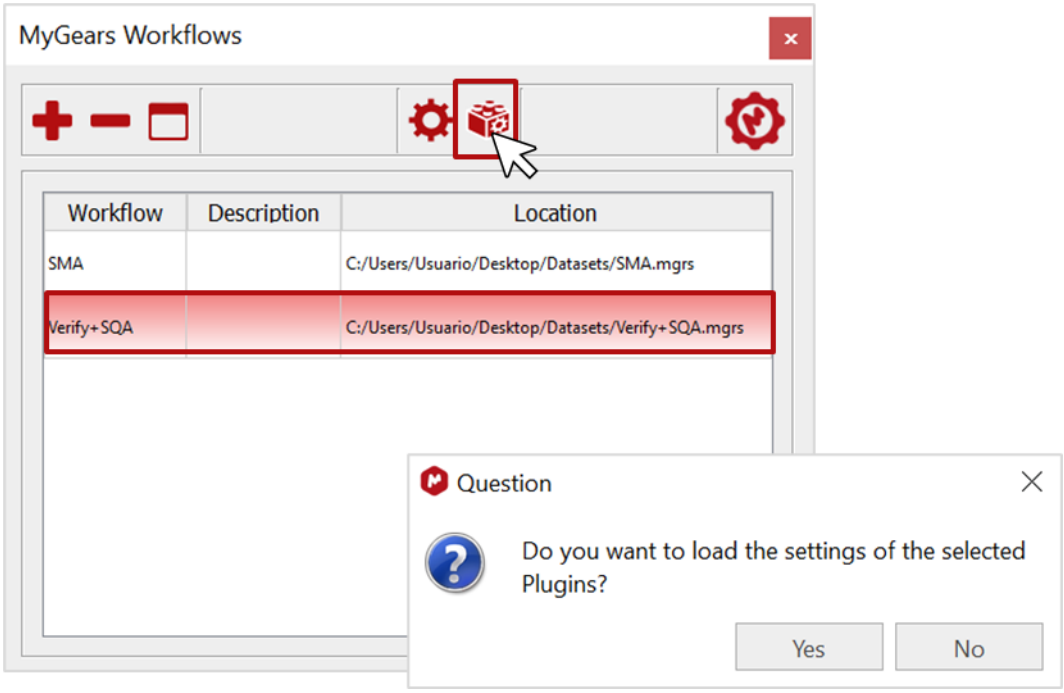
Button	Description
	Add Mgears workflow
	Remove selected workflow
	Clear all
	Options
	Open MGears with the settings of the selected workflow
	Run MyGears

Click on and select the Mgears workflow (.mgrs settings file) you want to run. You can add one or more workflows, delete a selected workflow, or clear the whole table as needed. The workflows added will be displayed as shown below.

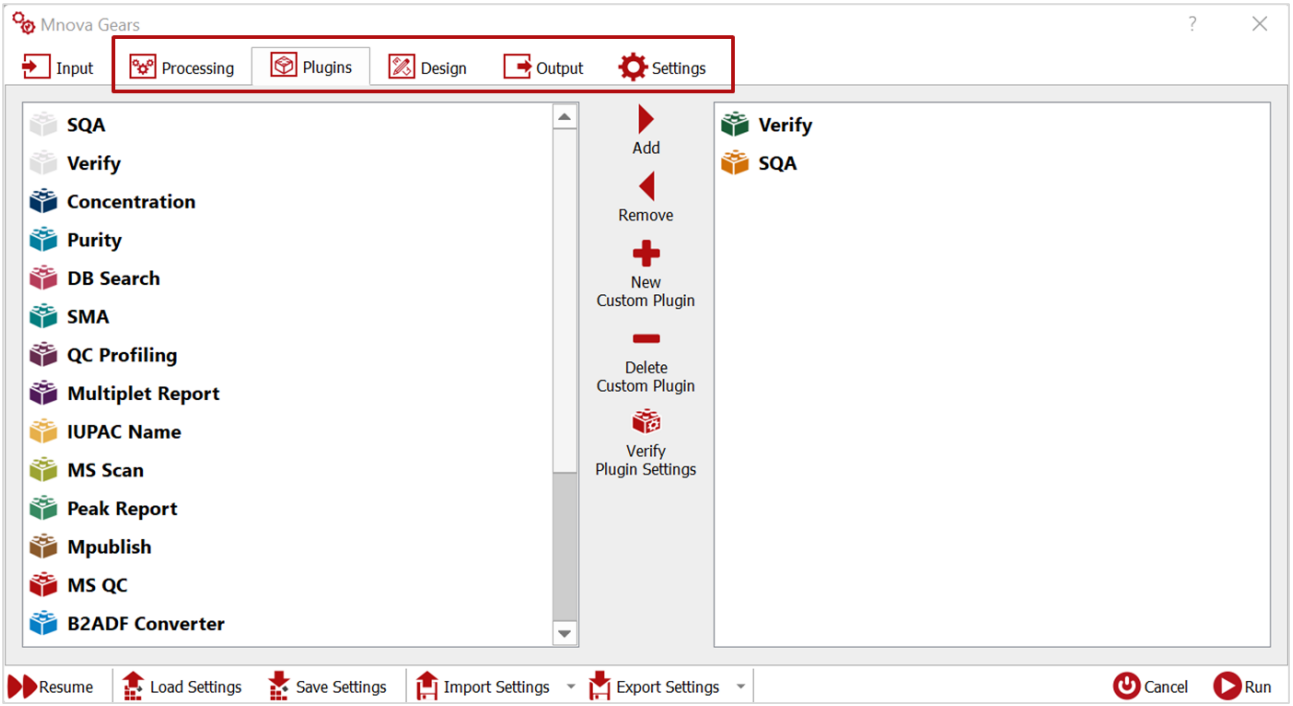


Click on this button to launch the analysis. The data in the open document will be processed and the results laid out and saved as specified in the workflow parameters.

If you wish to review the analysis settings before launching the analysis, you can select the workflow you want to review and click on . A dialog asking if you want to load the settings of the selected plugin will appear. Click **Yes**.



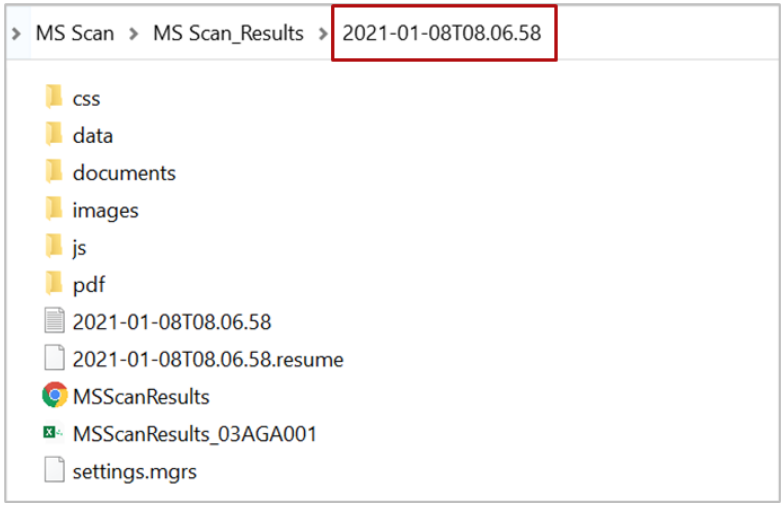
The Mnova Gears dialog will open so you can revise and adjust your analysis configuration as needed, then save the new settings.



Note. It is also possible to run a MyGears workflow by pressing the **MyGears** button in the **Automation** tab. In this case, MyGears will run with the configuration stored in the registry.

5. Output folder

The result folder is saved under the directory previously specified in the **Output** section. This folder contains all the output generated for the current evaluation.



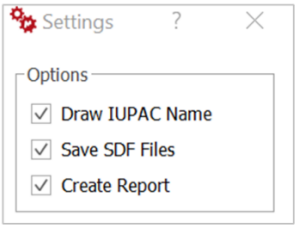
Output folders and files may include:

Type	Name	Description
	Css	Part of the html reporting
	Data	Folder with .result files
	Documents	Folder with Mnova documents
	Images	Part of the html reporting
	Js	Part of the html reporting
	PDF	Folder with PDF report
	Plugin specific	With Plugin specific result files (csv, word, mnova, etc)
	.log	General log of Mgears (information that you see while Mgears is running)
	.resume	File to restart the processing where it was (automatically if there is a crash or manually if the user stops Mgears on purpose)
	.html	Html Dynamic report
	Settings.mgrs	Mgears settings file

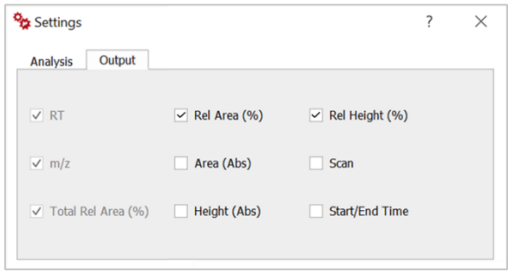
Folder File

Plugin-specific results files (.csv, .odt, .mnova files, etc) are generally customizable in the **Plugin Settings** section. For instance, the IUPAC Name plugin can be configured to generate SDF files for each molecule, and MS Scan to lay out results in a CSV document; HTML reports can be set to include specific parameters and exclude others with Purity; and Peak Reports can be formatted as needed, etc.

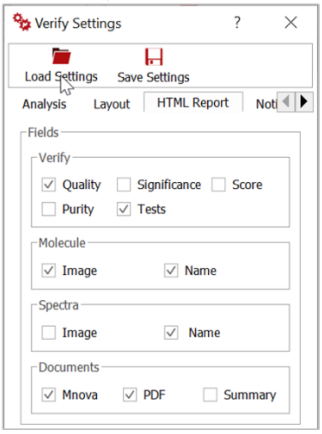
Other outputs



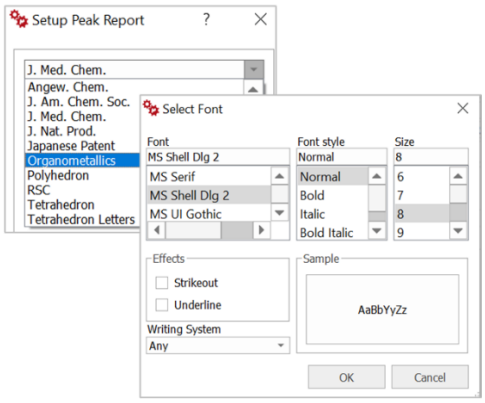
Result file content



HTML report



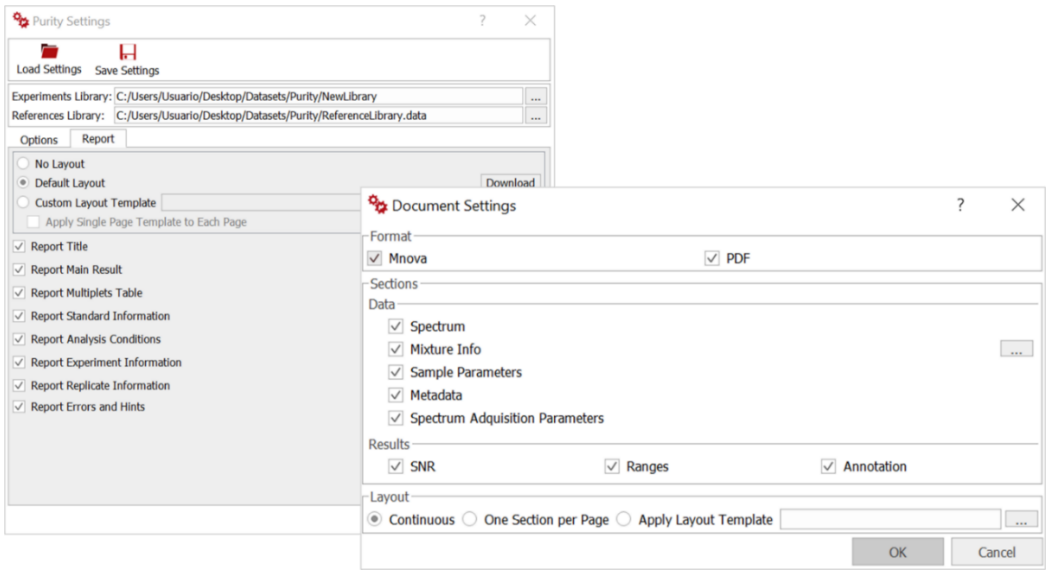
Format and font



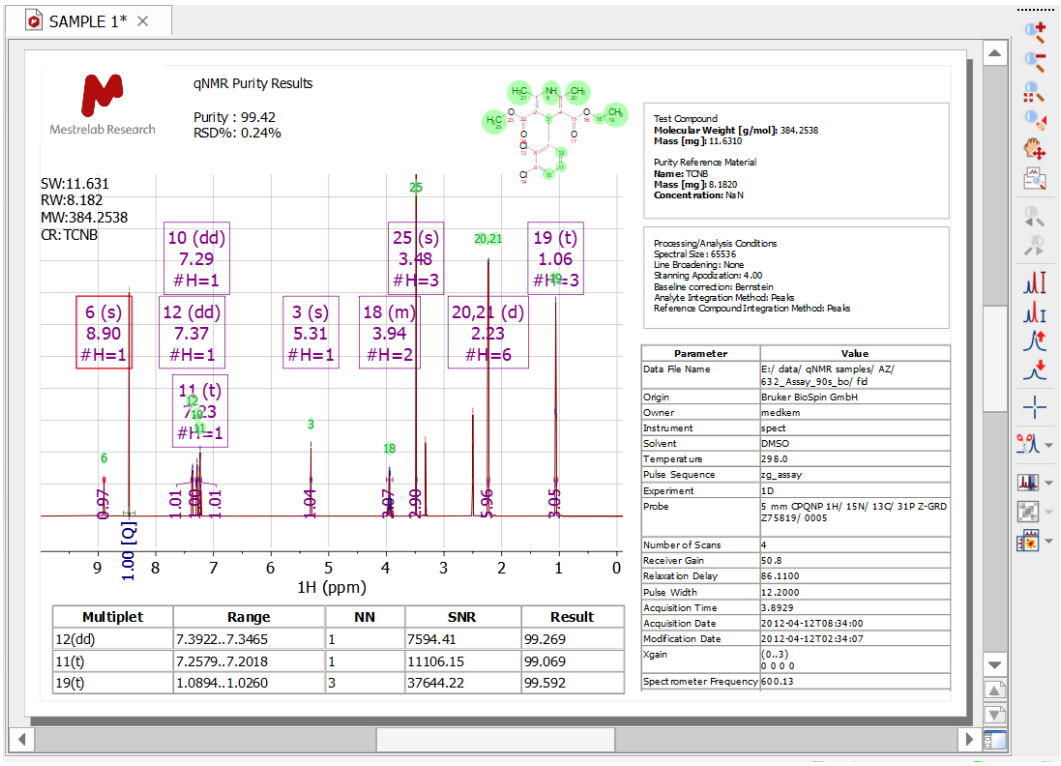
5.1. Mnova Reports

Mnova output files are typically saved under **Documents**. However, it is possible to change the desired destination folder during the setup in the **Output** tab, as explained in the section 3.5.1.1. Other advanced reporting settings are detailed in section 3.5.4.

Mnova reports can be customized to fit a display layout of your choice in the **Design** tab (Section 3.4), and to include the specific information (data, metadata, results, etc.) selected in the **Plugin settings**, as shown below.



Here is an example of an Mnova report obtained with the Purity plugin.

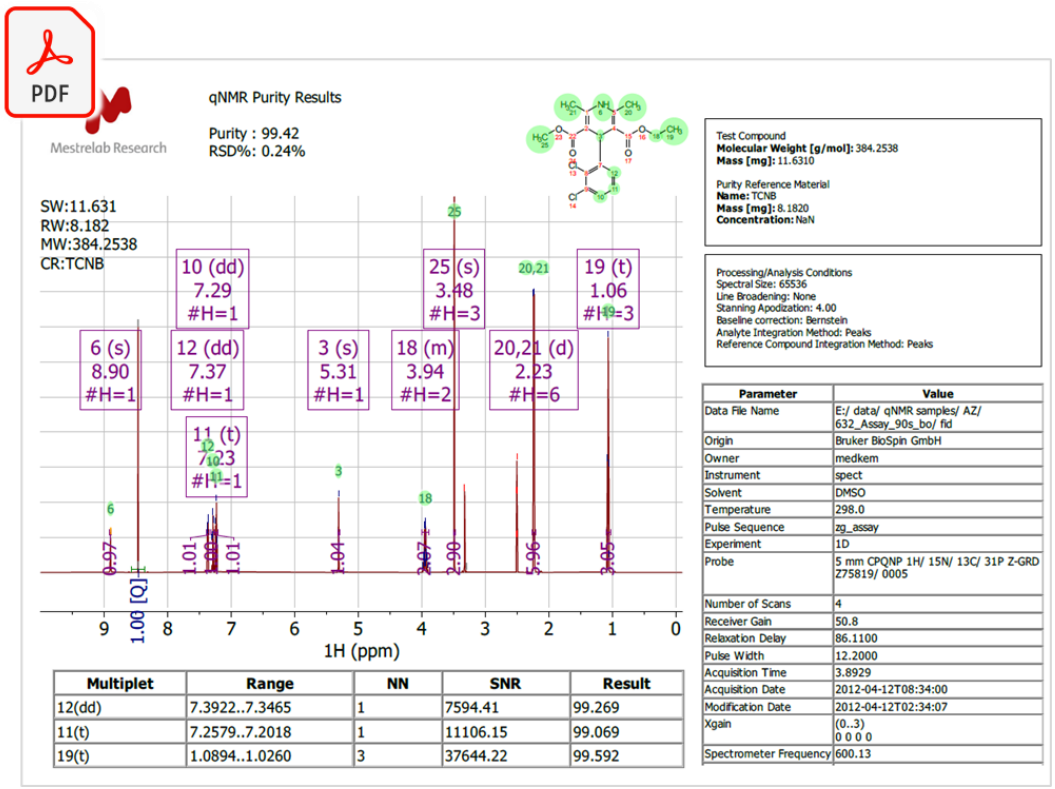


5.2. PDF Reports

PDF reports are typically saved under the **PDF** folder. However, it is possible to change the desired destination folder during the setup in the **Output** tab as explained in the section 3.5.1.2. Other advanced reporting settings are detailed in section 3.5.4.

As with the Mnova reports, PDF reports can be customized to fit a display layout of your choice in the **Design** tab (Section 3.4), and to include the specific information (data, metadata, results, etc.) selected in the **Plugin settings**. PDFs are basically a static version of the Mnova reports generated by Mgears.

Below is an example of a PDF report obtained using the Purity plugin.

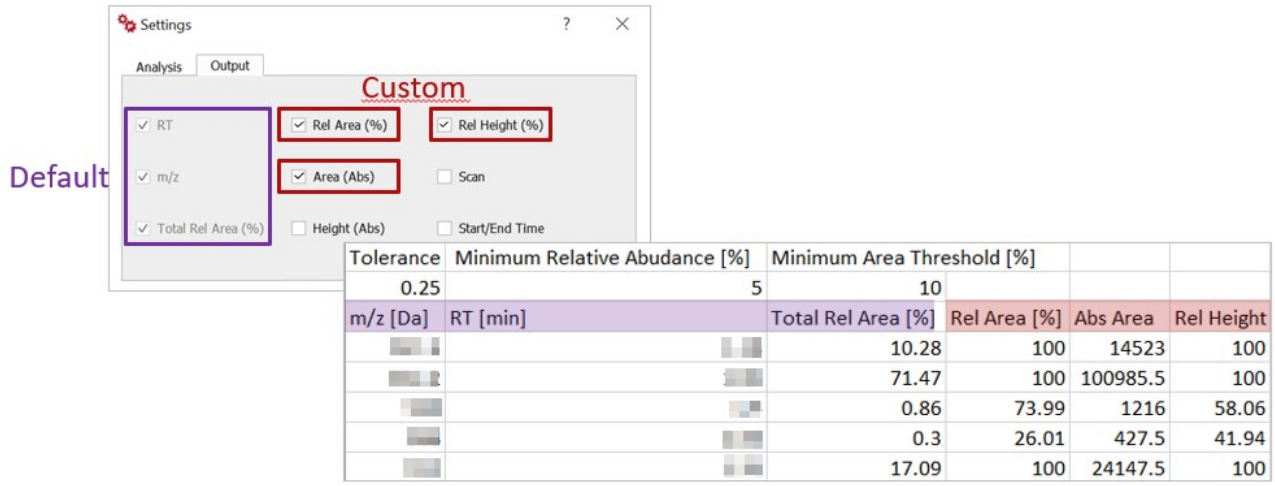


Multiplet	Range	NN	SNR	Result
12(dd)	7.3922..7.3465	1	7594.41	99.269
11(t)	7.2579..7.2018	1	11106.15	99.069
19(t)	1.0894..1.0260	3	37644.22	99.592

Parameter	Value
Data File Name	E:/ data/ qNMR samples/ AZ/ 632_Assay_90s_bo/ fid
Origin	Bruker BioSpin GmbH
Owner	medkem
Instrument	spect
Solvent	DMSO
Temperature	298.0
Pulse Sequence	zg_assay
Experiment	1D
Probe	5 mm CPQNP 1H/ 15N/ 13C/ 31P Z-GRD Z75819/ 0005
Number of Scans	4
Receiver Gain	50.8
Relaxation Delay	86.1100
Pulse Width	12.2000
Acquisition Time	3.8929
Acquisition Date	2012-04-12T08:34:00
Modification Date	2012-04-12T02:34:07
Xgain	(0..3) 0 0 0 0
Spectrometer Frequency	600.13

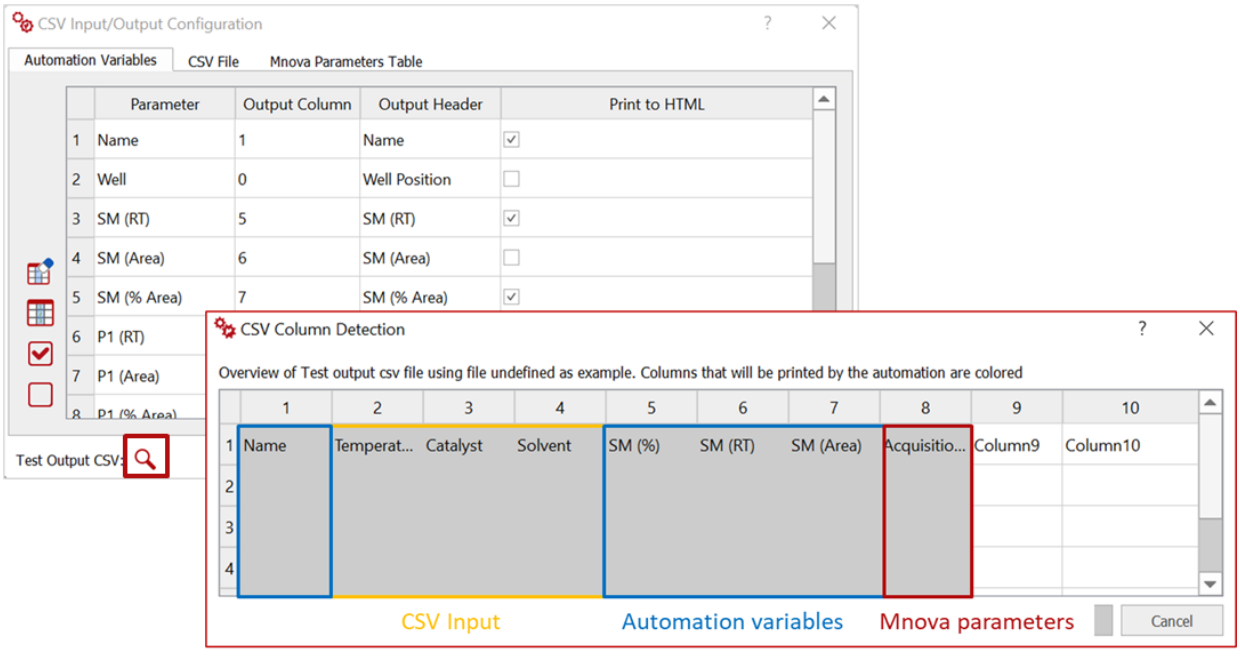
5.3. CSV Reports

Many Mnova Gears Plugins will generate a CSV file with their results. The content of this CSV file is usually customizable in the **Plugin specific settings,** as with the MS Scan plugin.



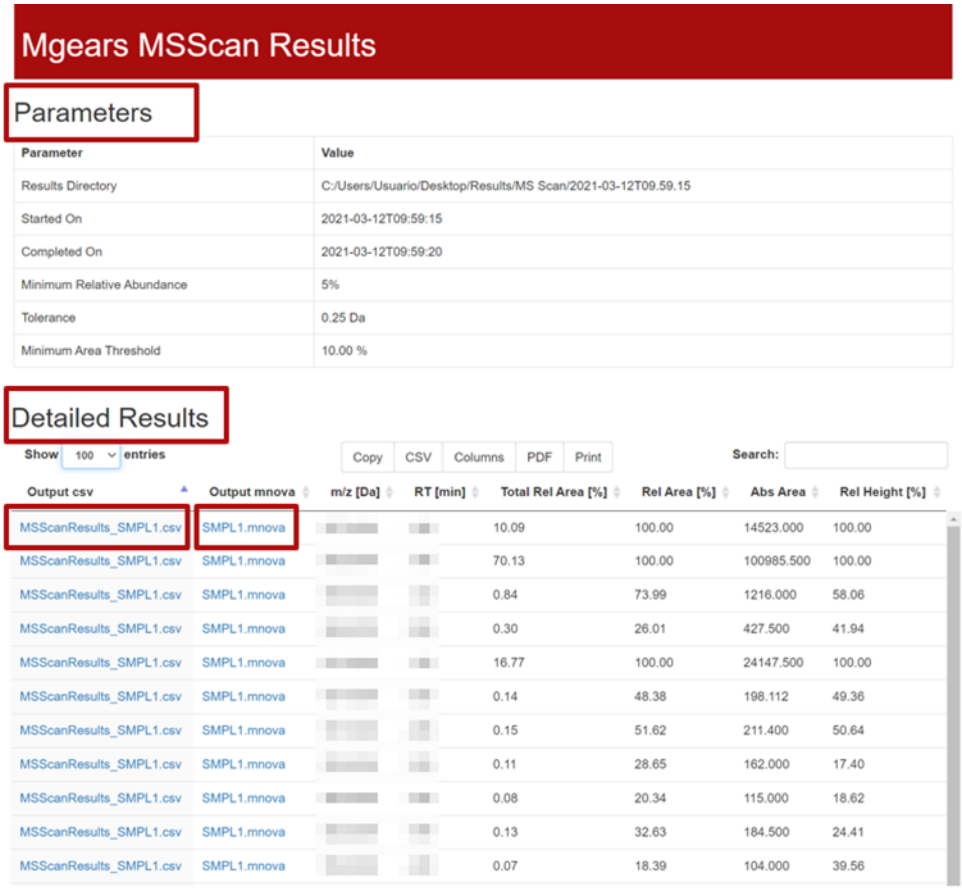
Tolerance	Minimum Relative Abudance [%]	Minimum Area Threshold [%]			
0.25	5	10			
m/z [Da]	RT [min]	Total Rel Area [%]	Rel Area [%]	Abs Area	Rel Height
		10.28	100	14523	100
		71.47	100	100985.5	100
		0.86	73.99	1216	58.06
		0.3	26.01	427.5	41.94
		17.09	100	24147.5	100

Sometimes the **Mapping file** used in the **Input** tab can be used to generate final reports including input and output data. In these cases, a configuration of the columns reserved for outputs is possible in the plugin-specific settings dialog, as shown below for the Chrom Reaction Optimization plugin.



5.4. HTML Reports

HTML reports are commonly generated by Mgears analyses. These global reports include the analysis parameters and allow a dynamic visualization of the analysis results. Direct links to other output files are also embedded in these reports.



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			10.09	100.00	14523.000	100.00
MSScanResults_SMPL1.csv	SMPL1.mnova			70.13	100.00	100985.500	100.00
MSScanResults_SMPL1.csv	SMPL1.mnova			0.84	73.99	1216.000	58.06
MSScanResults_SMPL1.csv	SMPL1.mnova			0.30	26.01	427.500	41.94
MSScanResults_SMPL1.csv	SMPL1.mnova			16.77	100.00	24147.500	100.00
MSScanResults_SMPL1.csv	SMPL1.mnova			0.14	48.38	198.112	49.36
MSScanResults_SMPL1.csv	SMPL1.mnova			0.15	51.62	211.400	50.64
MSScanResults_SMPL1.csv	SMPL1.mnova			0.11	28.65	162.000	17.40
MSScanResults_SMPL1.csv	SMPL1.mnova			0.08	20.34	115.000	18.62
MSScanResults_SMPL1.csv	SMPL1.mnova			0.13	32.63	184.500	24.41
MSScanResults_SMPL1.csv	SMPL1.mnova			0.07	18.39	104.000	39.56

In some cases, HTML reports can include graphics to better represent the results.

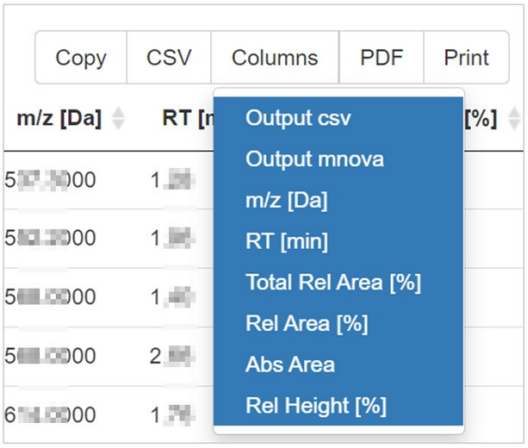
Detailed Results

Show 5 entries — Copy | CSV | Columns | PDF | Print — Search:

#	Name	Cpd X	Cpd Y	EDTA	d-glucose	glycerin	hippuric_acid	quinic_acid	taurin	Trig_HCl	xylitol
1	Sample 1	0.0000	0.0000	1.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
2	Sample 2	0.0000	0.0000	0.0000	0.6150	0.0000	0.0000	0.2492	0.1358	0.0000	0.0000
3	Sample 3	0.0000	0.2665	0.0000	0.4327	0.0000	0.0000	0.0000	0.0898	0.2109	0.0000
4	Sample 4	0.1108									
5	Sample 5	0.0000									

Showing 1 to 5 of 5 entries

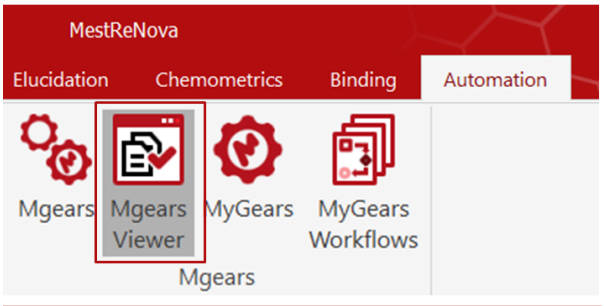
It is possible to change the display of the **Columns** and adapt them to your preferences, then **Copy**, **Print**, or save your results into **CSV** or **PDF** format.



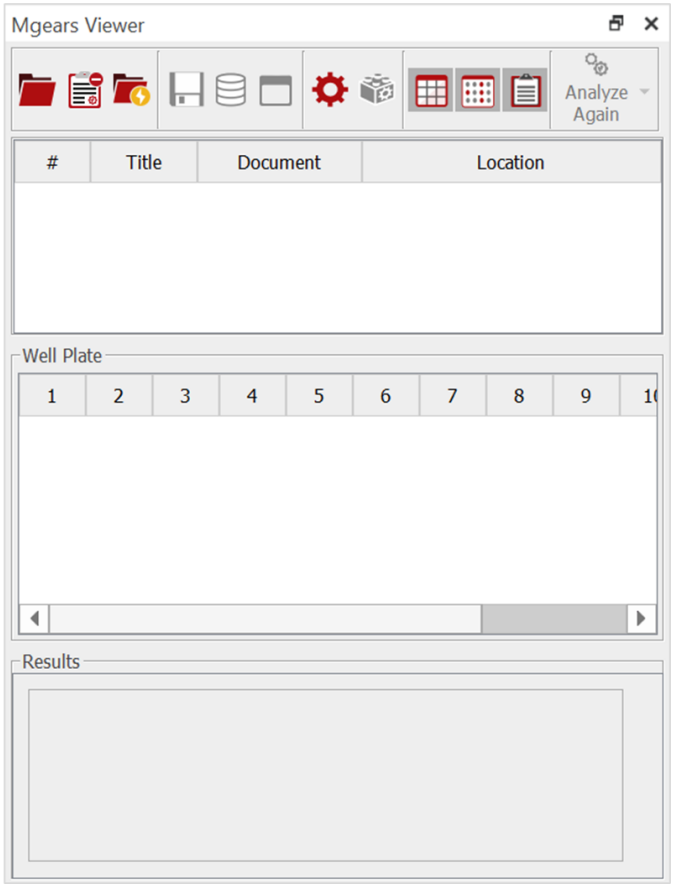
6. Mnova Gears Results Viewer

One of the most interesting features of Mnova Gears is its results viewer, which allows live interaction, reviewing, and rapid update of analysis results once an Mgears analysis has been completed.

The **Mgears Viewer** is accessible from the Mnova **Automation** section. When open, the dialog presents several action buttons described in the table below.

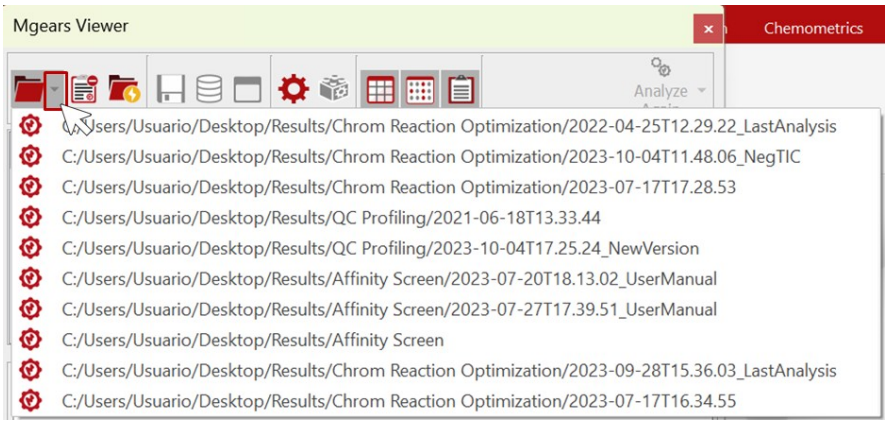


Button	Description
	Load data
	Get latest results from MyGears
	Connect the Viewer to a results folder to get the results on-the-fly
	Save data
	Save and database the current result
	Clear results
	Settings
	Open the Mgears dialog with the current settings
	Show/Hide the samples table
	Show/Hide the wellplate
	Show/Hide the details of the results
Analyze Again	Run analysis again for the active document



6.1. Loading results

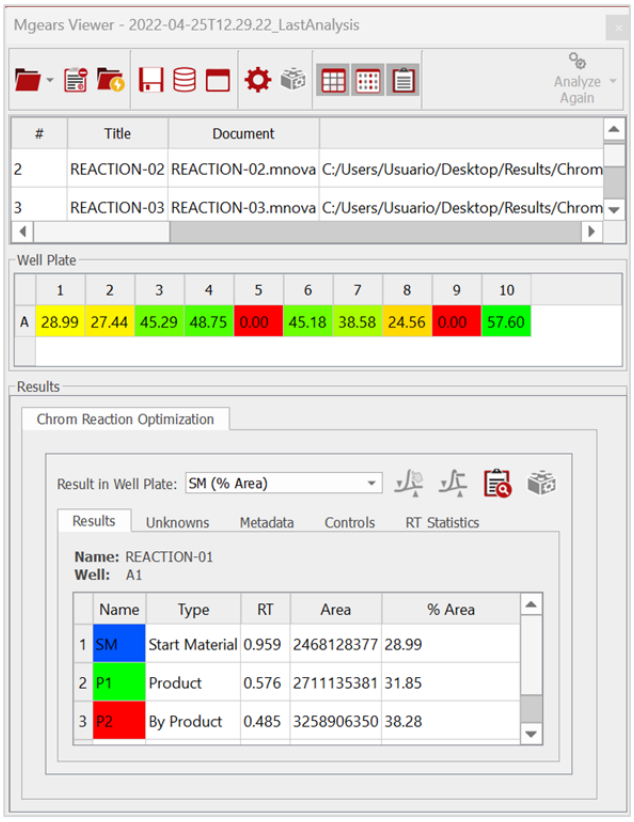
To load analysis results, click on the load button and select the data folder in the predefined output location. Alternatively, click the small arrow next to the **Load** button to see a list of the 10 most recent results for easy access.



All samples processed in the selected analysis are loaded into the Mgears viewer's main list and well plate overview. Detailed results are visible at the bottom section.

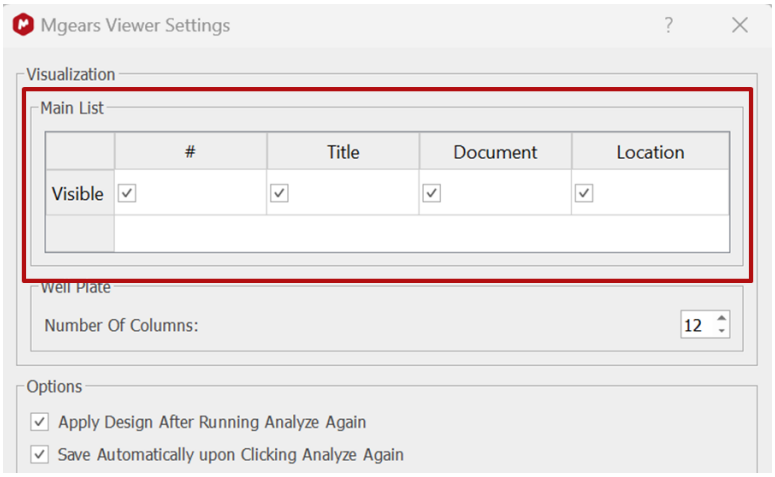
When the viewer is connected to a folder , the results saved to that folder are automatically loaded (on-the-fly) once the analysis is completed.

Note that the Mgears viewer shows the results of one automation run at a time. When using MyGears, it will show the latest results.

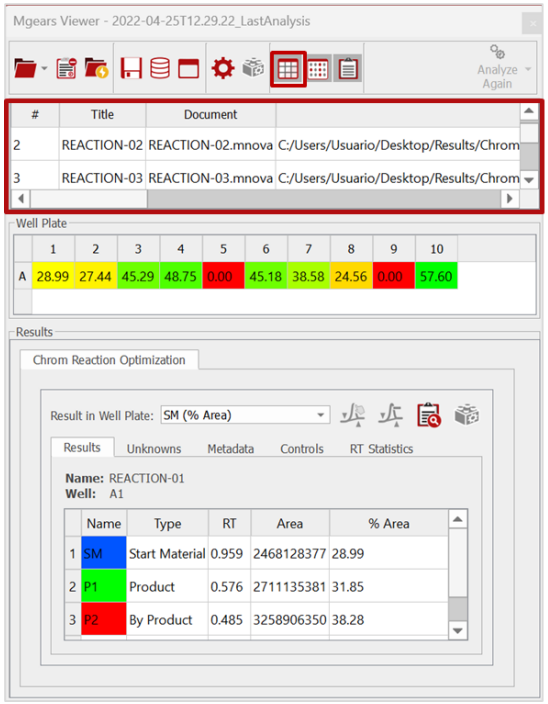


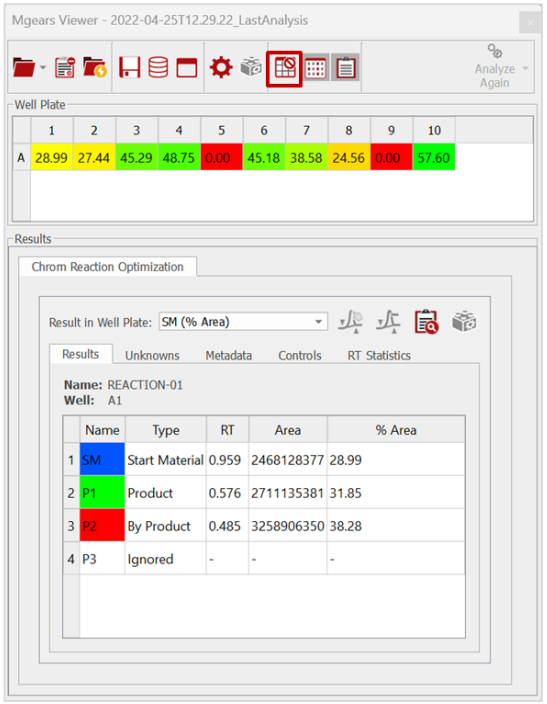
6.1.1. Main list section

In the upper part of the Mgears Viewer, analysis samples are listed and numbered with certain details such as **Title**, **Document**, and **Location**. It is possible to change the configuration of this table. To do so, click on the **Settings** button  and customize the **Main List** visualization by checking/unchecking the available items.



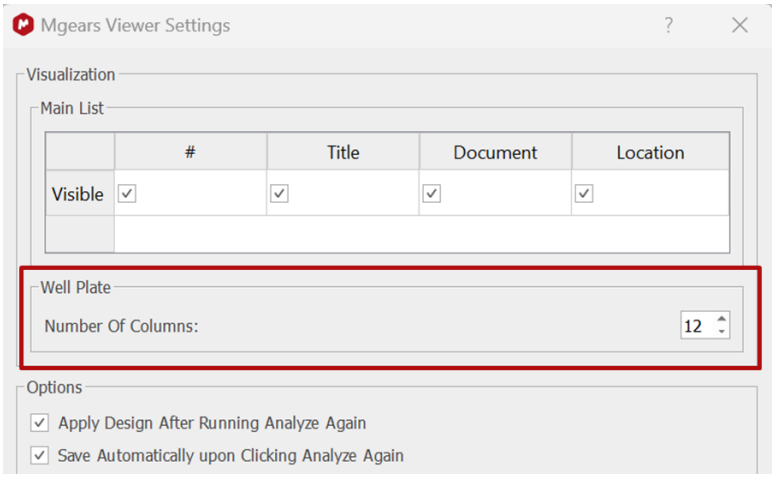
The **Main list** can be completely hidden from the Mgears Viewer by clicking on this button  .



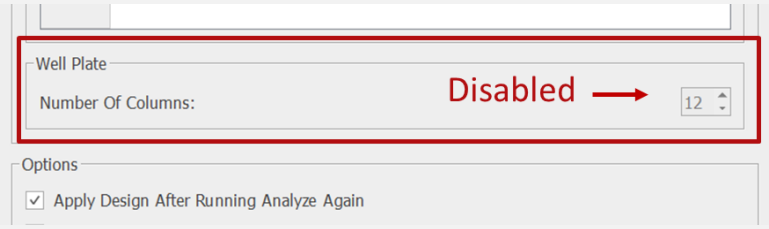


6.1.2. Well plate section

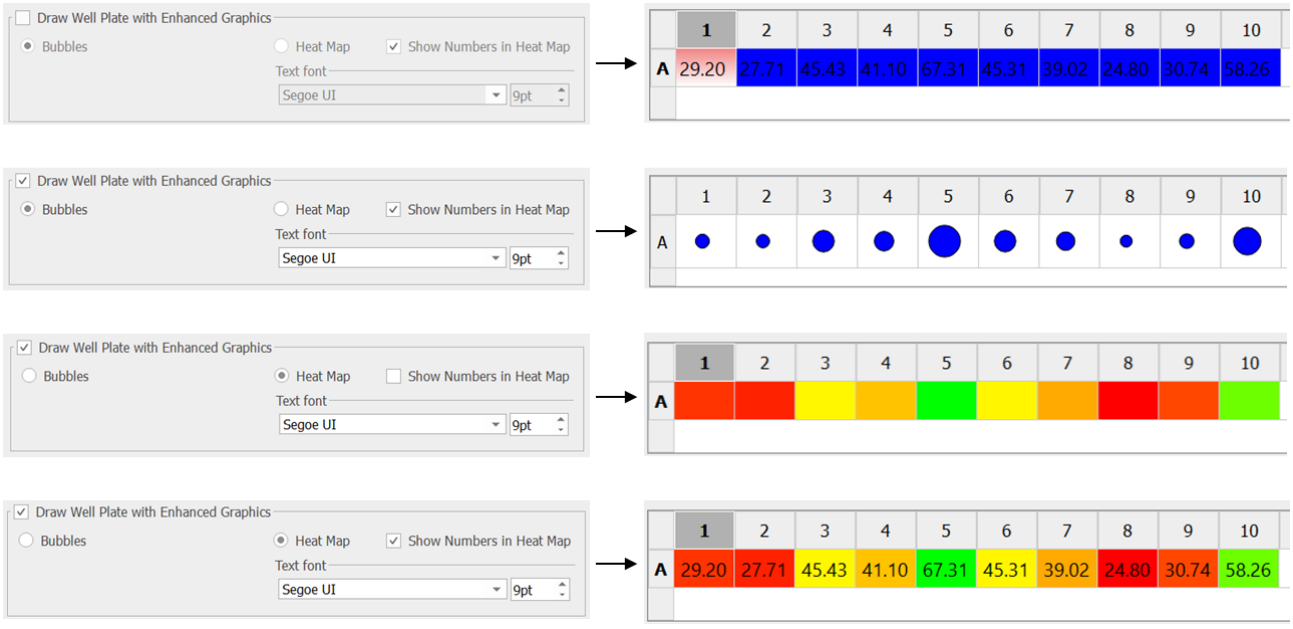
A **Well Plate** overview is available and can be particularly useful when analysis samples are loaded in a well plate. The dimensions of the well plate can be defined in the **Mgears Viewer Settings** dialog.



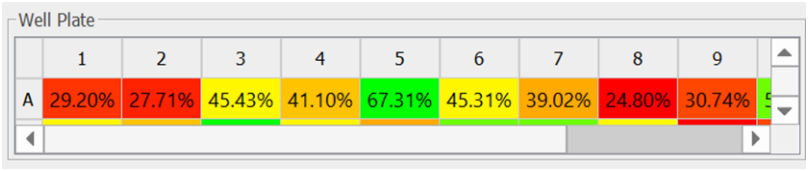
Watch out! If a Mapping file is used in an analysis, and the option for reading position in the well plate is selected in the advanced filtering options, then the dimensions of the well plate will be automatically set and will not be editable in the **Mgears Viewer Settings** dialog.



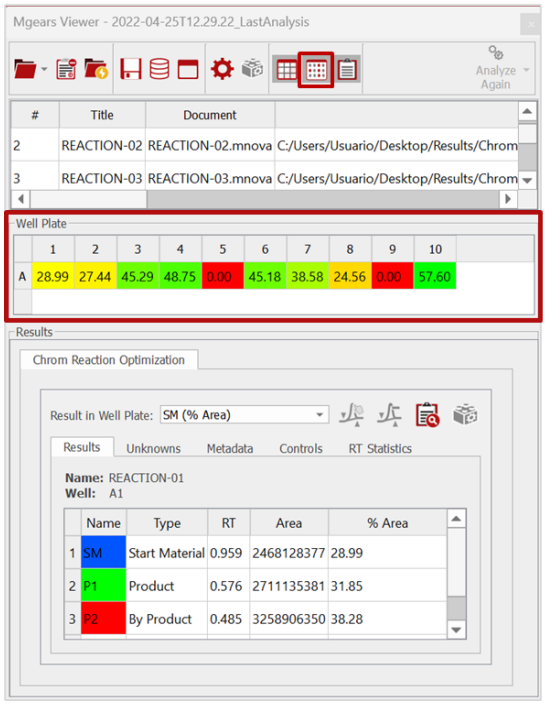
An option to **Draw Well Plate with Enhanced Graphics** is available in the **Mgears Viewer Settings** too. This feature allows you to choose between displaying **Bubble** plots or a **Heat Map** within the well plate, instead of presenting numerical results. The **Text font** and **size** can be customized. See the example below.

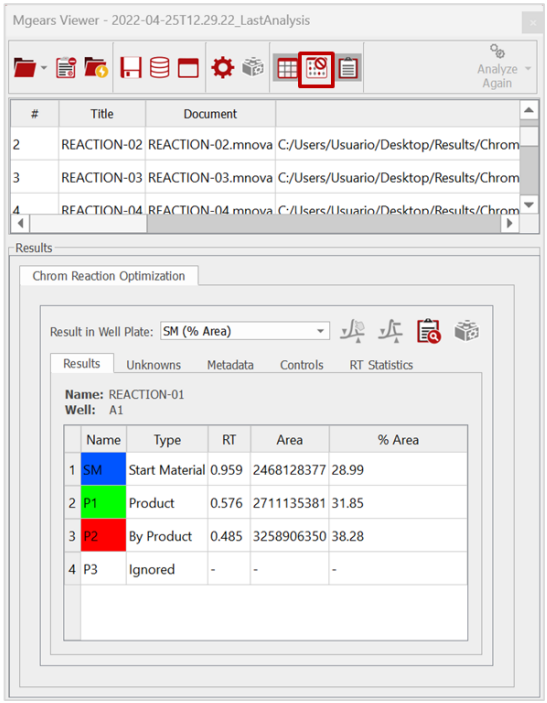


To add a suffix to the results that are displayed in the well plate, enable **Add Suffix to Values in the Well Plate** and type your desired suffix.



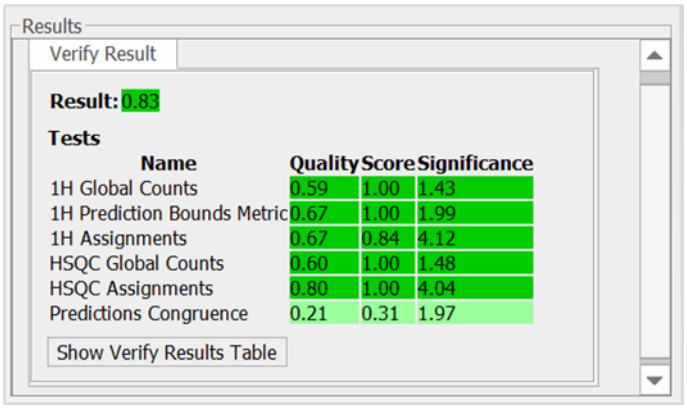
The **Well plate** overview can be completely hidden from the Mgears Viewer by clicking on this button .



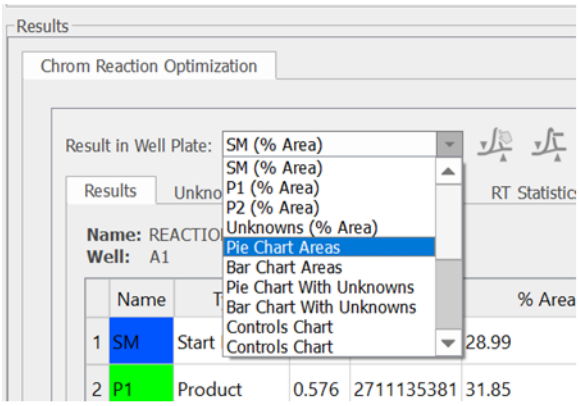


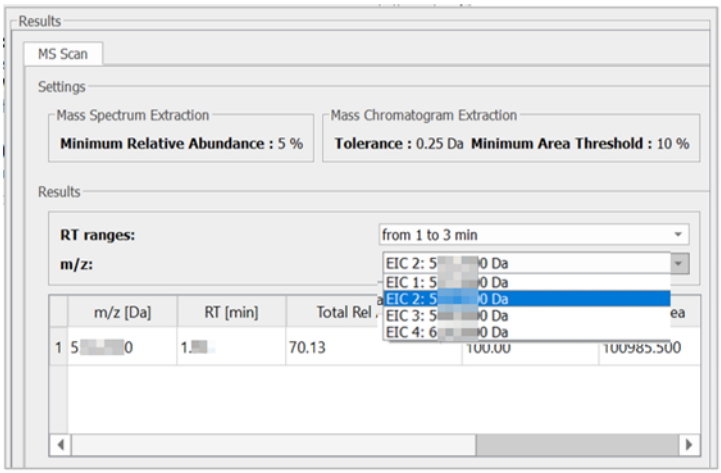
6.1.3. Results section

In the **Results** section, detailed analysis results are displayed.

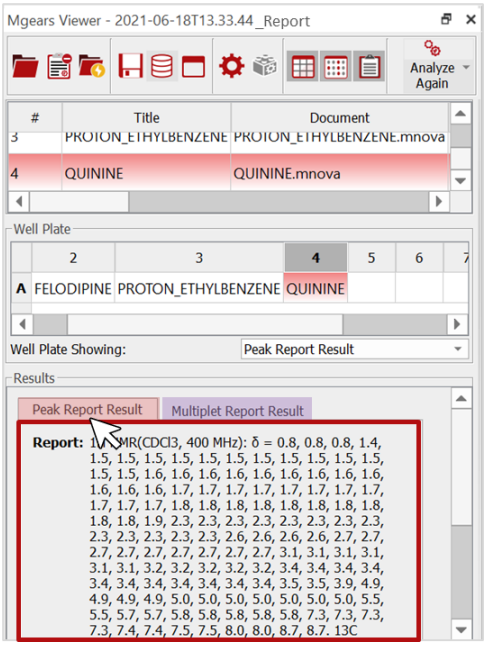


If the analysis performed generates multiple results per sample, the Mgears viewer provides flexibility to display those results.

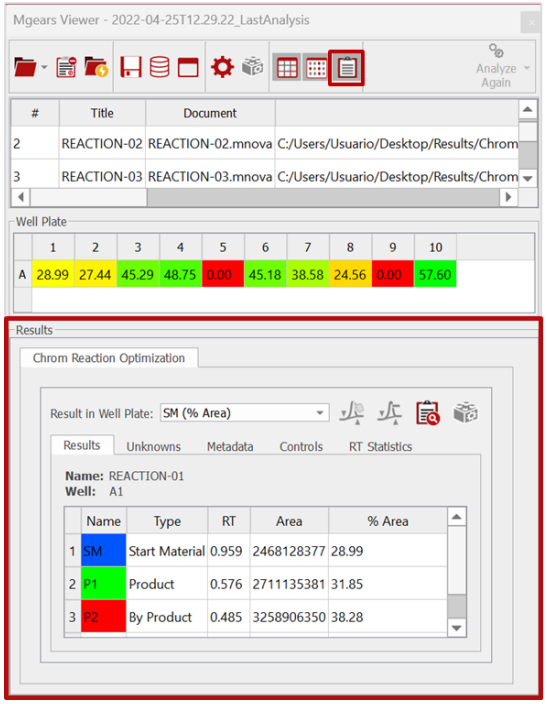


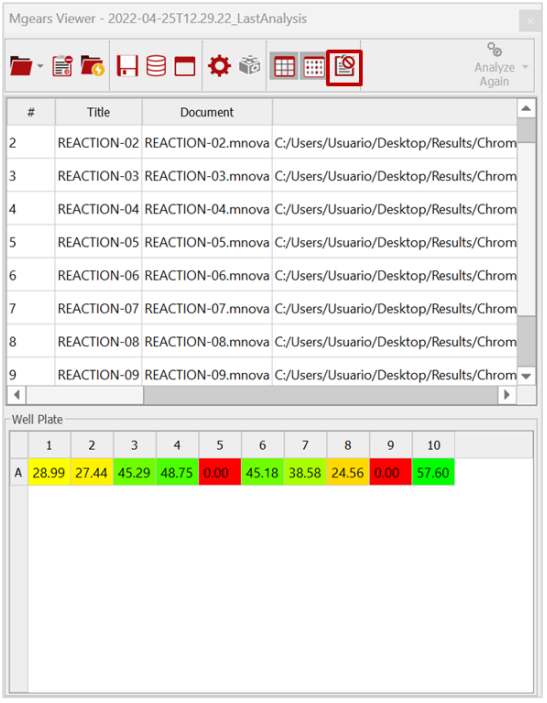


Also, when running multiple analyses (plugins) on the same samples, multiple results tabs will be available to view all the associated results.



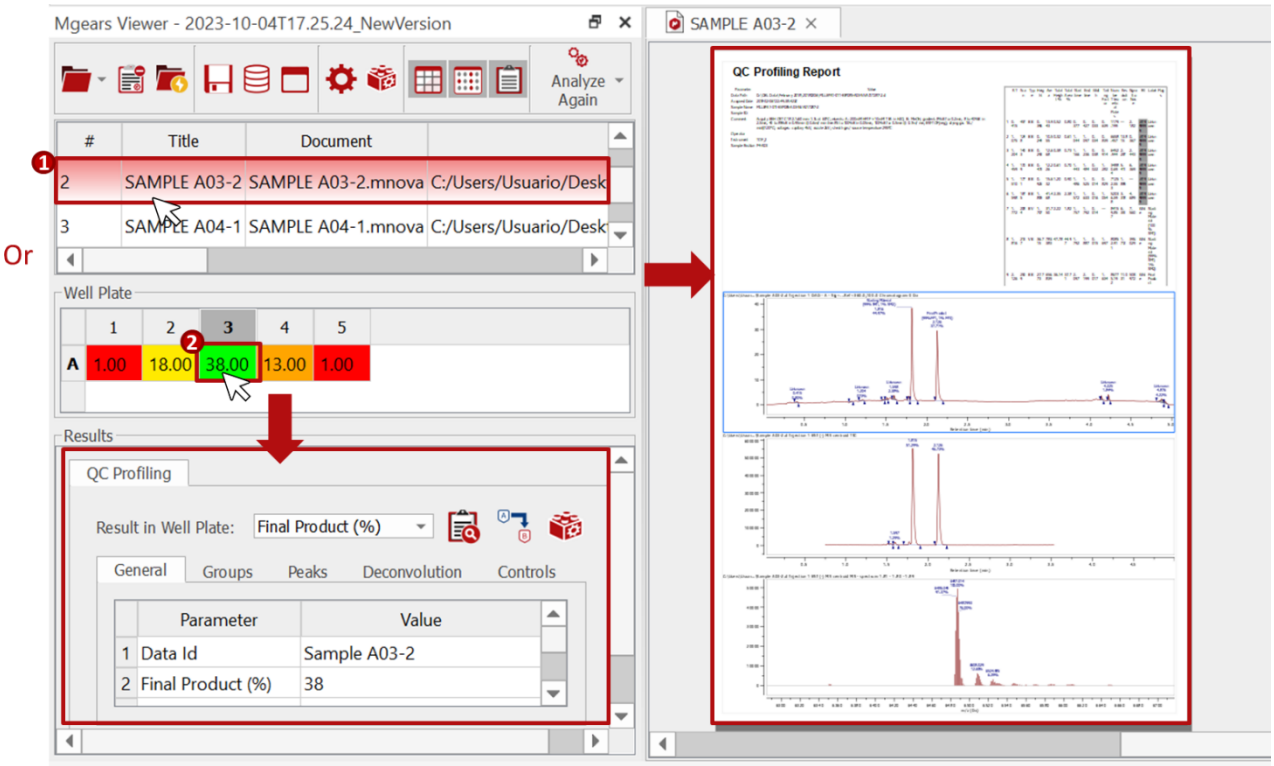
The **Results** section can also be completely hidden from the Mgears Viewer by clicking on this button  .





6.2. Reviewing results

Reviewing analysis results is available for most plugins and can be done on a sample-by-sample basis. Click on a sample (table row or well from the plate overview) to load the corresponding Mnova result document and detailed results.

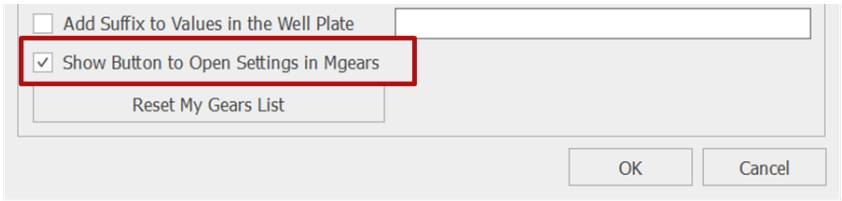


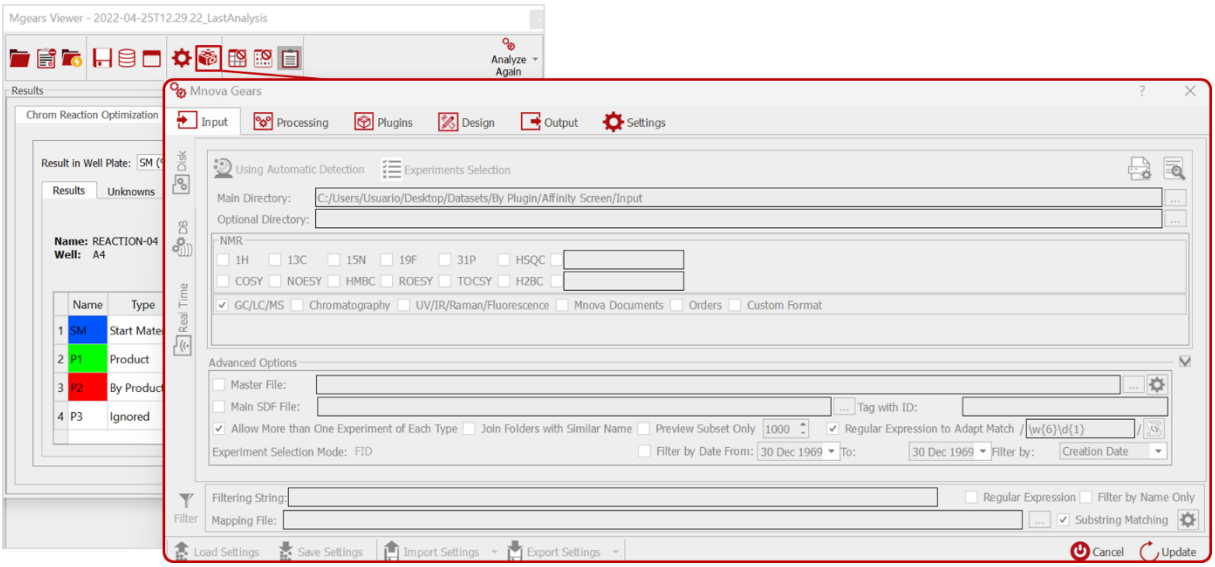
You can review and edit your results using the standard tools from Mnova.

6.2.1. Changing analysis settings

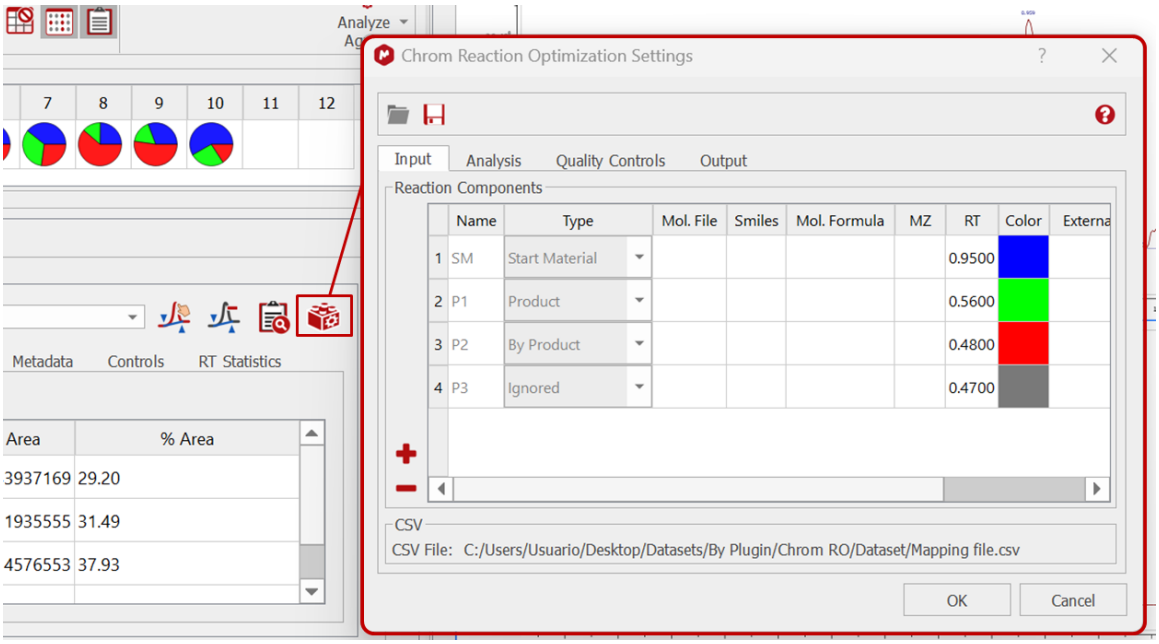
Mgears allows you to modify your current settings and re-run calculations on your data. Depending on what you wish to modify you can either:

a. Click the brick icon in the top bar of the Mgears Viewer. This opens the Mgears dialog with the current settings. The **Input**, **Processing**, **Output**, and **Setting** tabs are not editable, but you can make changes in the **Design** and **Plugins** tab. After making desired adjustments, click **Update**, and then **Analyze Again** to relaunch the analysis with the updated settings.

> **Note.** To access these Mgears settings from the Mgears Viewer, make sure to enable the option **Show Button to Open Setting in Mgears** in the Mgears Viewer Settings . Without this option enabled, the brick icon won't appear in the top bar of the Mgears viewer.
>
> 
>

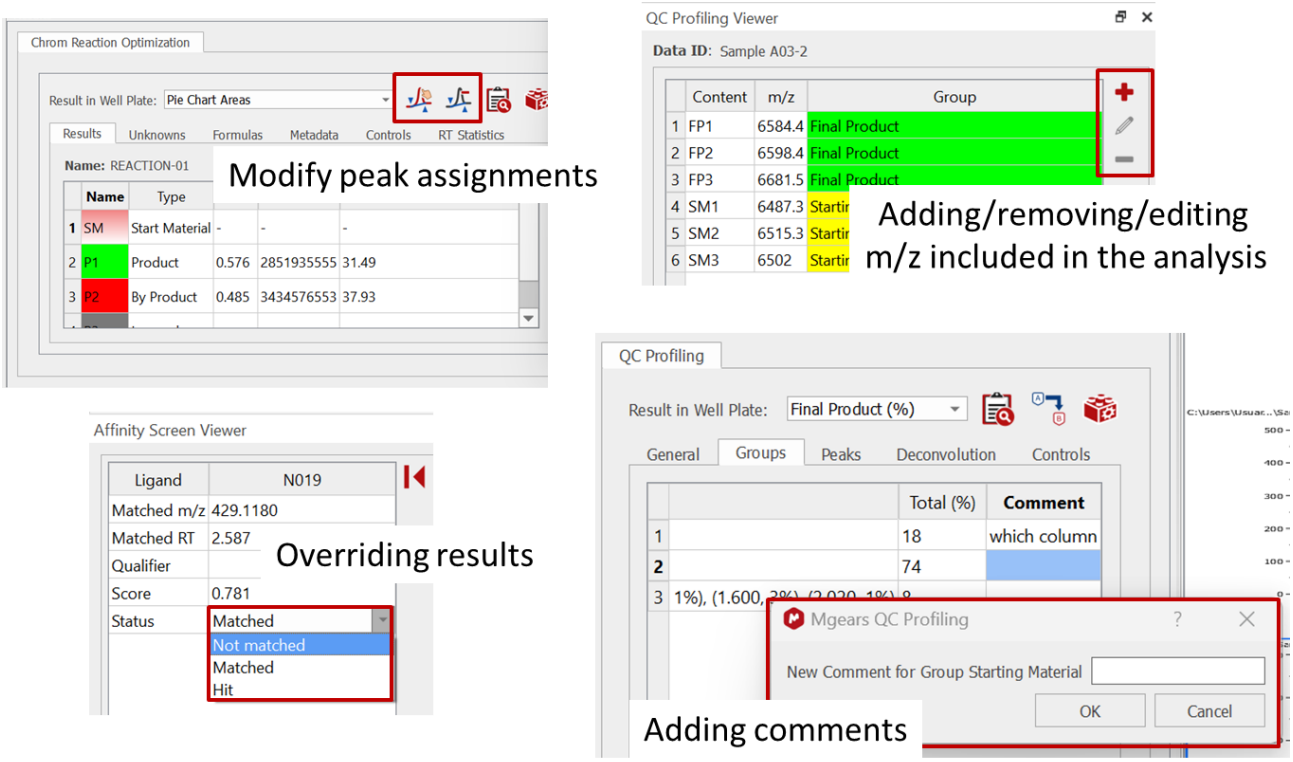


b. For some bricks, you can access specific settings directly by clicking the brick icon in the Results section of the Mgears Viewer. This provides access to brick-specific settings, bypassing the Mgears tabs.



6.2.2. Result reviewing tools

In the **Results** section, you will discover a range of tools to enhance and update your analysis results. These tools may include manual peak assignment, adding comments, overriding results, and more. The specific options available depend on the Mgears brick in use. See some examples in the image below.



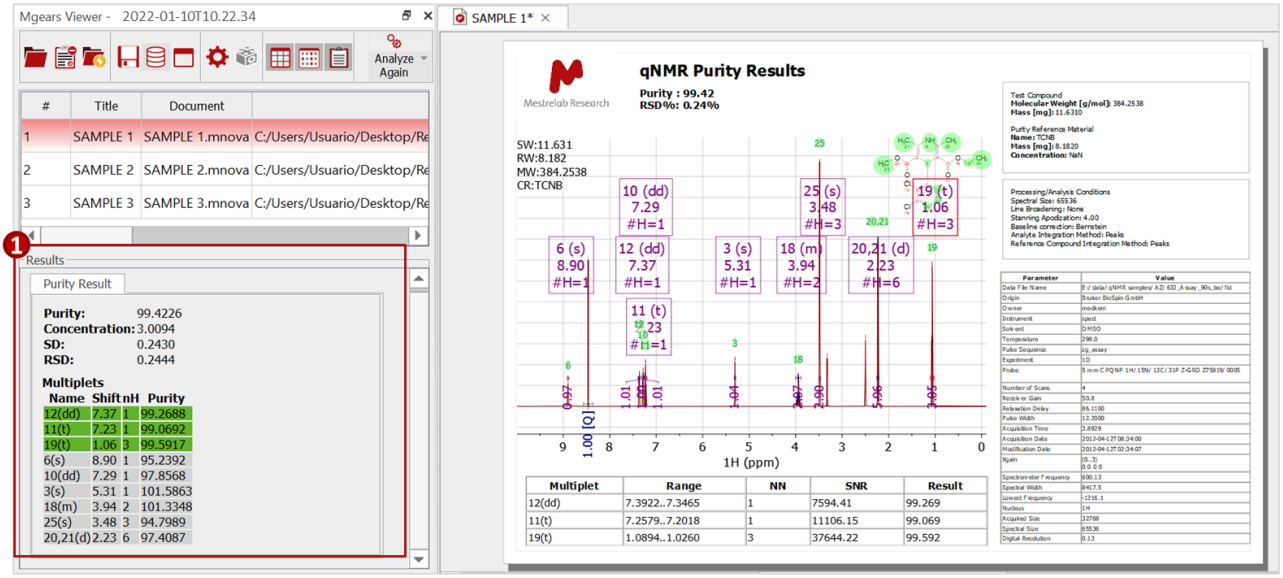
6.2.3. Advanced result reviewing with Mnova plugins

An advanced review of the sample results can sometimes be achieved with the Mnova Standard plugins, as is the case with Purity and SMA, for example.

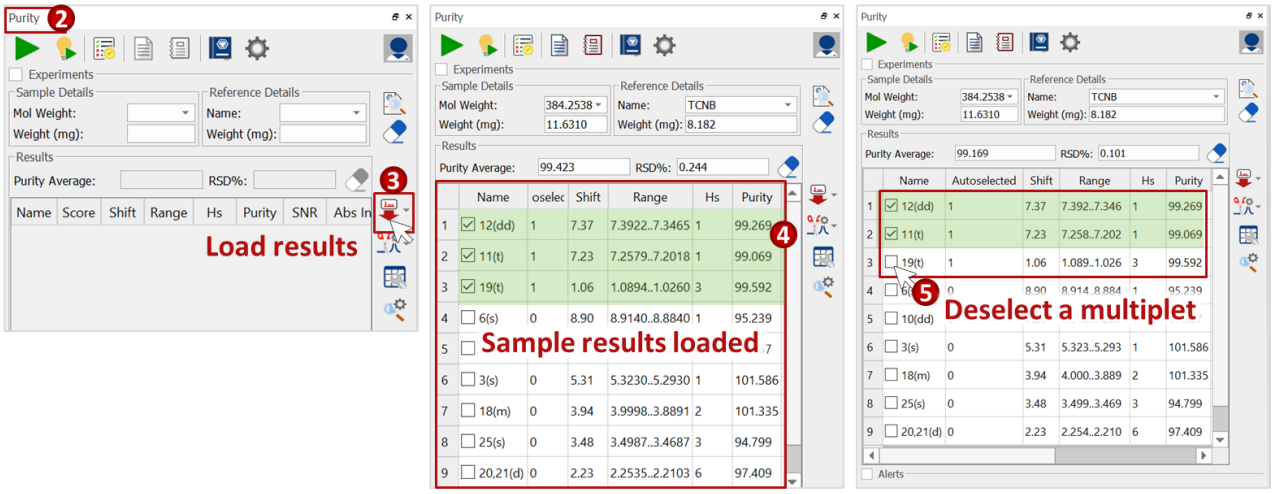
In the example below, an open Mgears results document is loaded into the Mnova Purity dialog:

1- Click on sample to view results in Mgears viewer.
2- Open Purity plugin in the Mnova **Quantitation** ribbon.
3- Then, click on  to load the Purity results from the open Mnova document.
4- Sample and reference details, as well as all spectral multiplets, are loaded in the **Purity** dialog.
5- Revise and edit sample results.
6- Edited results will be automatically updated in the Mgears Viewer and Mnova document.

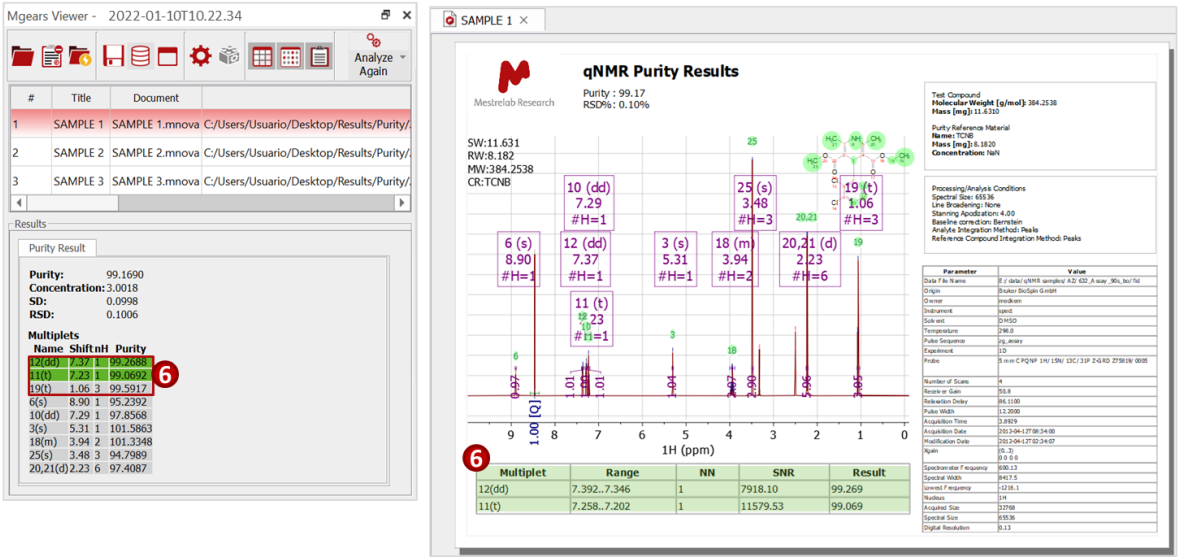
Open a sample result in the Mgears Viewer



Open Mnova Purity plugin

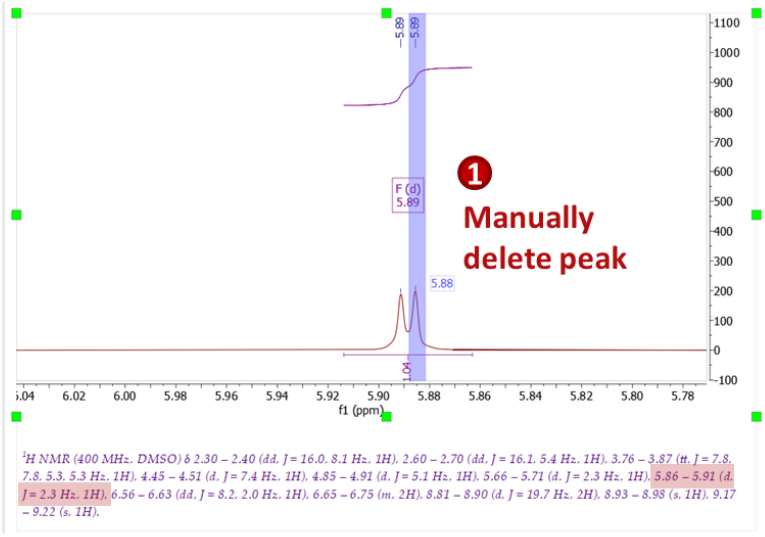


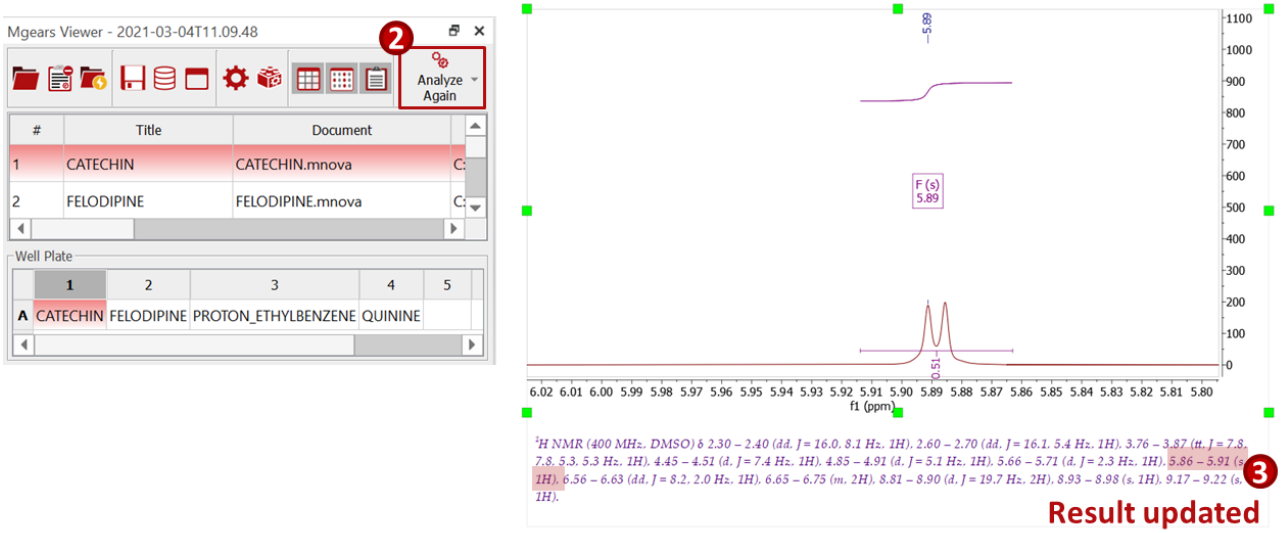
Results automatically updated in the Mgears Viewer



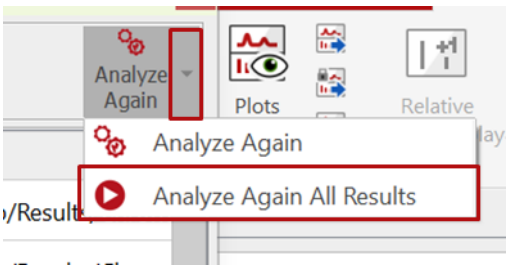
6.3. Saving results

When revising your results, you may want to reanalyze your dataset with the changes you made. To do so, click on the **Analyze Again** button at the top-right side of the **Mgears Viewer**. The analysis results will be automatically updated in the open document, as seen in the example below for the Multiplet report plugin.



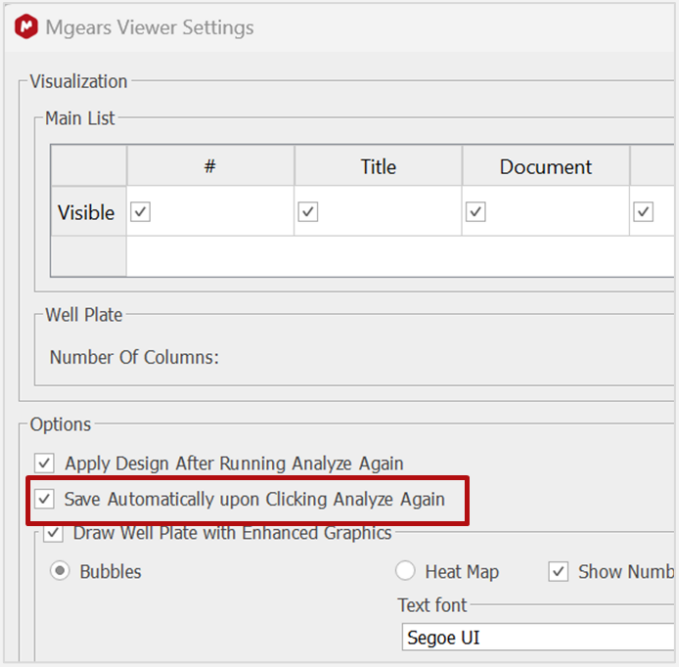


If you wish to reanalyze the whole batch, click on the little arrow next the the **Analyze Again** button and choose **Analyse Again All Results**. Mgears will recalculate and update the results for the whole well plate.



If you are happy with these new results, you can click on  to save them to the output folder.

Top Tip! Enable the option **Save Automatically upon Clicking Analyze Again** in the **Mgears Viewer Settings**. The results will then be automatically saved to the output folder without the need to hit **Save** every time you reanalyze a sample.



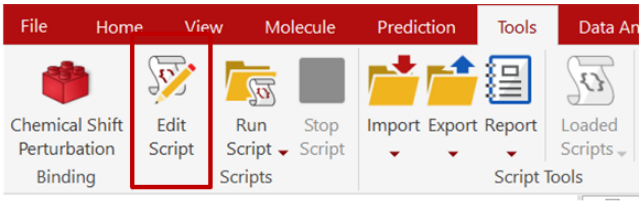
7. Scripting and customization

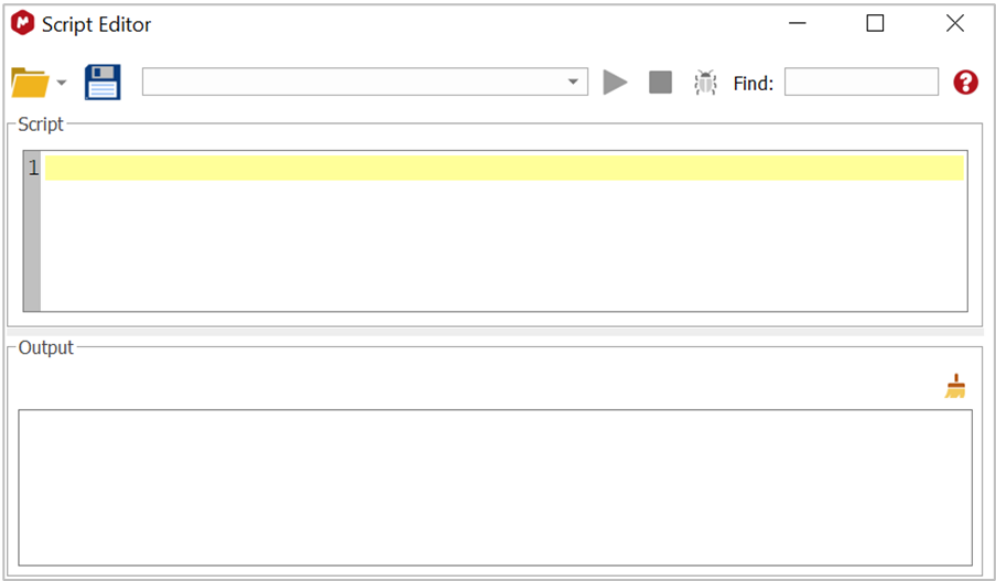
Mgears provides options for customization using scripts at various points in the process, as seen throughout this User Manual. For example:

- On the input tab, a custom script can be provided to read a structured input file (a csv or xml) from another system and use it to drive Mgears input, or to retrieve an identifier from within a parameter file and use that for grouping. It is even possible to change the whole algorithm of detection in batch mode.
- A processing script can be invoked on the processing tab, where there is even the possibility of being able to run a 'pre'-script before individual file processing starts.
- A custom design script can be used to meet complex layout requirements that would not otherwise be easily achieved in a template.
- A custom script can also be used to create a new plugin for running your own analyses.
- Finally, a custom output script and/or a summary scipt can be used to allow a highly complex and specific output to be generated, as is sometimes required by some downstream system in the workflow.

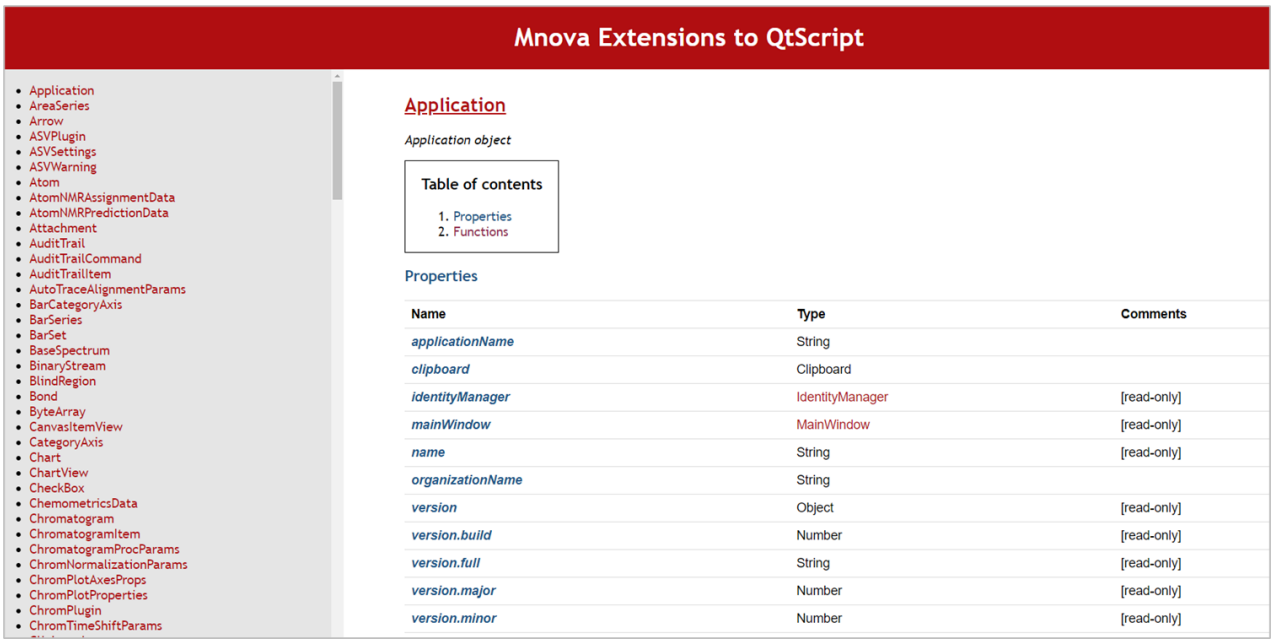
The possibilities are only limited by programming ingenuity.

You can create and save your own scripts in the **Script Editor** accessible form the **Tools** section in Mnova.





An Mnova scripting document is available to help you with Mnova's extensions. Click on  to access this documentation.



8. Conclusion

Mnova Gears provides a robust platform for automation of workflows, and limitless possibilities for customization. Please contact us with your inquiries at info@mestrelab.com and let us help to set up your powerful automation system.