Gears Purity 3.0.1

STARTING GUIDE

Document Number

P/N 263 R1

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Gears Purity is an automation brick for batch or continuous (real-time) analysis of samples for the determination of compound purity/potency. It allows the configuration of analysis methods (SOPs) by experts, streamline analysis by chemists, and generates customizable reports with purity results.

This document is intended to help you configure and run a batch purity analysis from the Mgears platform.

The Workflow

First, launch Mgears from the Mnova **Tools** ribbon. The dialog with the usual six tabs will open.
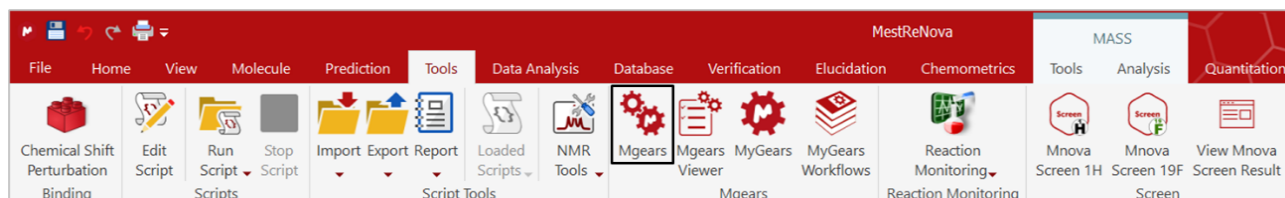
In the **Input** tab, select the data files for analysis by Mgears. Input files can come from **Disk** directories, a database (**DB**), or from **Real-Time** acquisition, and must contain some metadata under the **Comment** field of the **Parameters Table**, which will be used for purity determination.

The minimum required metadata includes **SW**: Sample Weight, **MW**: Sample Molecular Weight, and **CR**: Reference Compound. In some cases, it may also be necessary to define other parameters such as **RW**: Reference Weight.

More parameters can be added and read by the Purity plugin such as **SM**: followed by a molecule in smiles format, or **NS**: for Number of scans, etc. Valid values are listed below.

All metadata must be entered one after another as shown below. A semi-colon delimiter is also acceptable.

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


Use the **Automatic Detection** mode, with which Mgears will use the saved masks to find experiment files. You can manually add file masks to the **Mask manager** under the **Settings** tab, if needed.
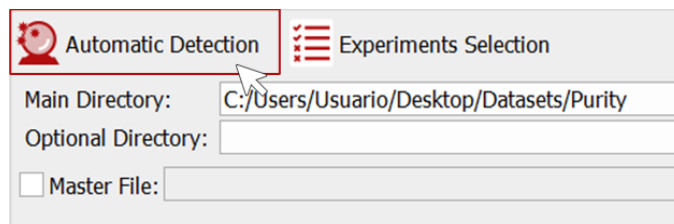
Use the **Automatic inspection** button 🔍 to check whether the experiments detected correspond to your selection criteria.
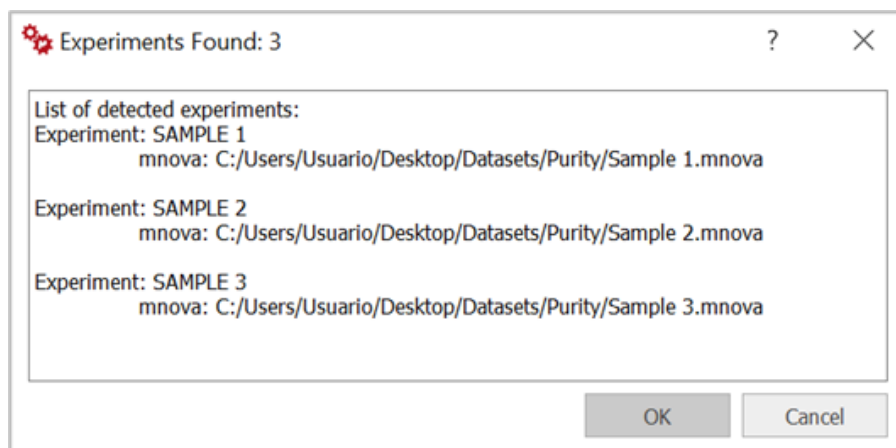

For advanced input selection, you can configure the options in the **Advanced** and **Filtering** sections. You can for instance use the grouping options to allow Mgears recognize and analyze replicate samples together.
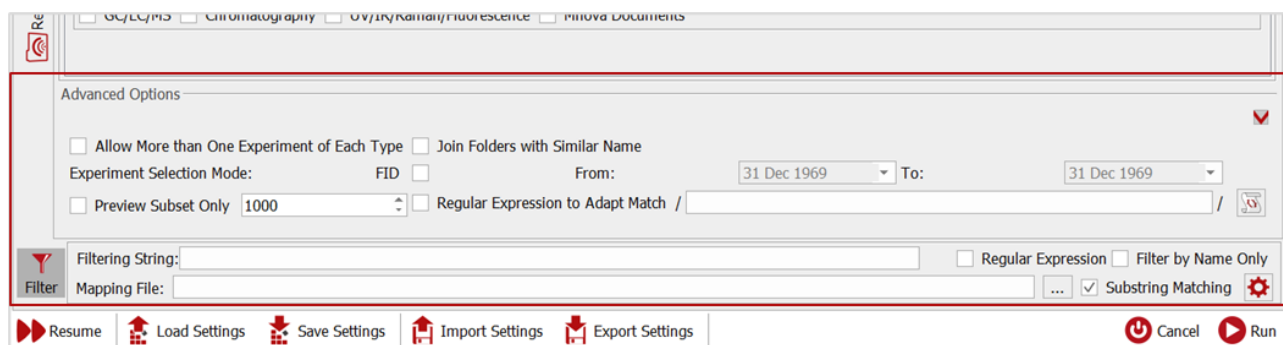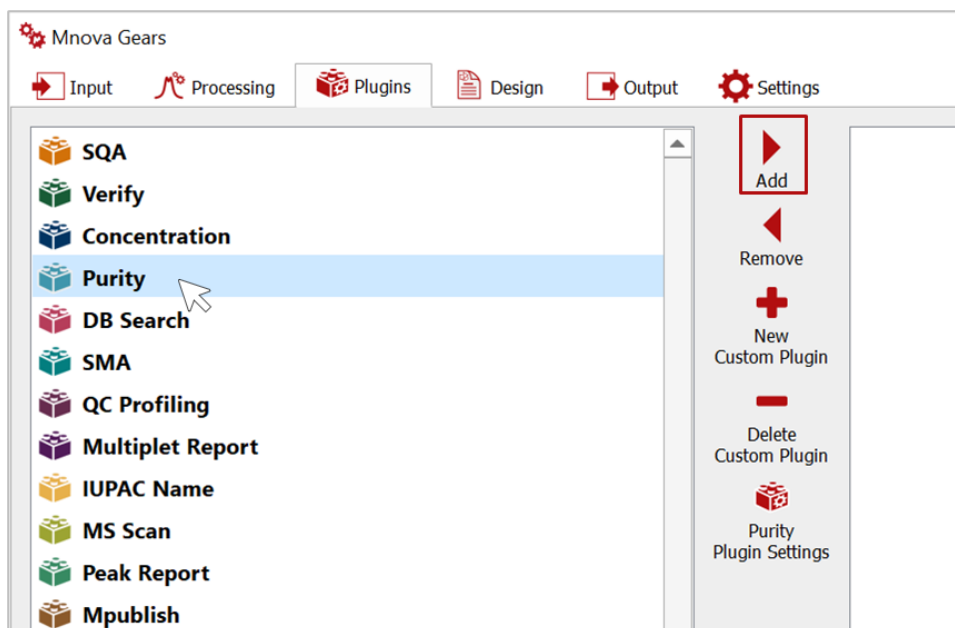
ƒ° Processing

In the **Processing** tab, you can either add a processing template to your analysis, as in this example, enable the **Advised Processing** to automatically apply the best processing options to your spectra, or upload a script to allow for more advanced and customized processing options.
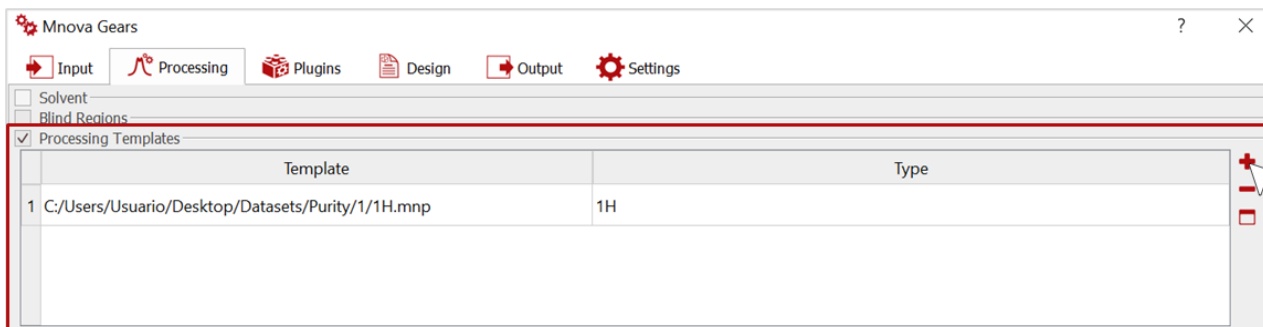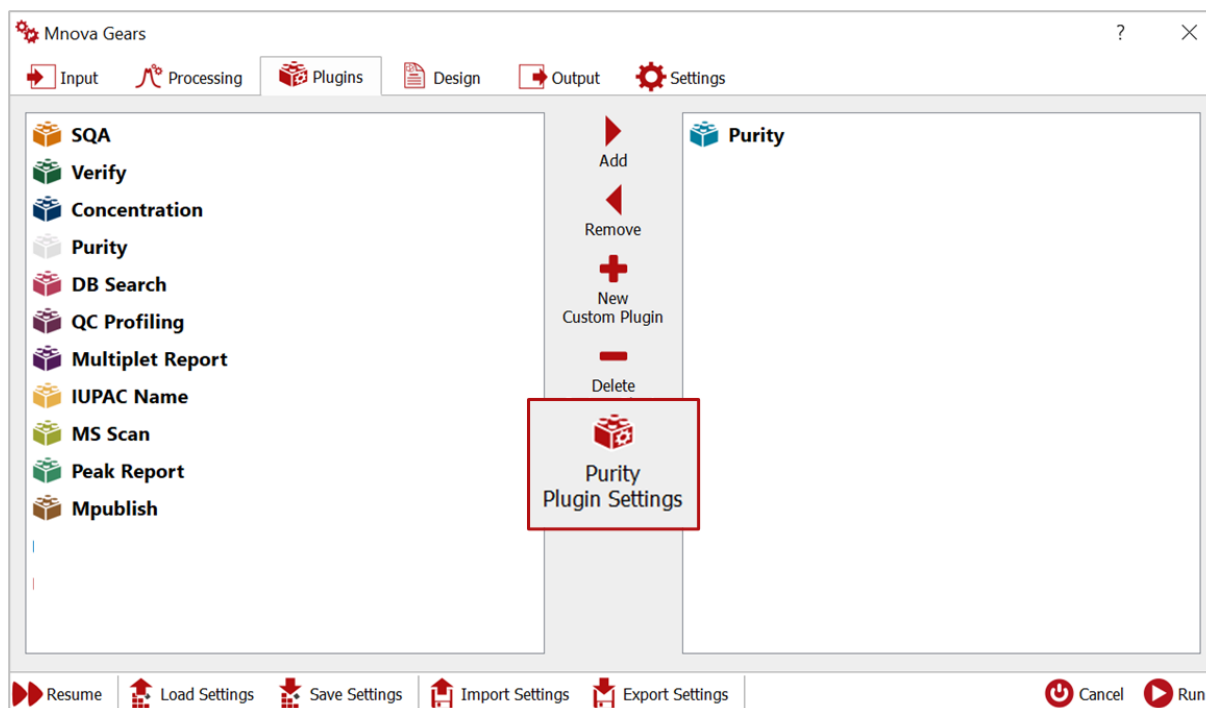

Plugins

In the **Plugins** tab, select and add the **Purity** plugin.

The added plugin will appear on the right-hand side of the dialog. You should now click on **Purity Plugin Settings** to configure the analysis parameters.


In the **Purity Settings** dialog, you can click on ⋯ to add the **Experiment library**. This is useful if you already have one or more saved experiments that you want to invoke and use with your samples. In this case, a string indicating the experiment name must be added to the parameters table of each sample, "EX: *ExperimentName*" or "Experiment: *ExperimentName*".

Then, select and add the **References library** containing all the reference compounds used in your analysis.
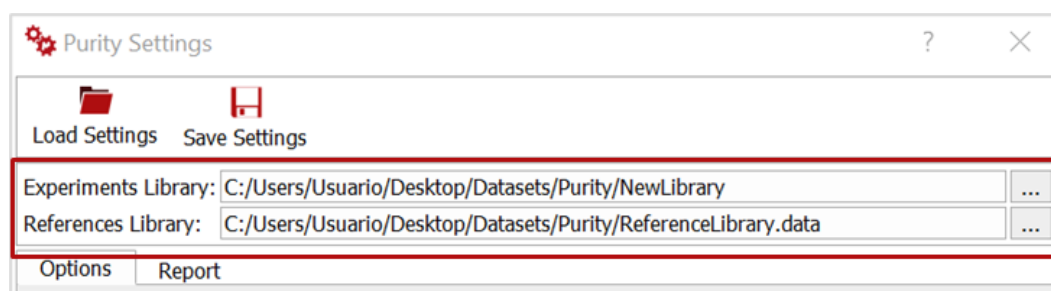
Now, in the **Options** tab, configure the purity calculation parameters. Check the **Autodetect Replicates** option if your analysis data include sample replicates or experiment repetitions. Mgears will then automatically detect and group such samples. In this case, replicate spectra must be grouped in a same Mnova document, otherwise it may be necessary to correctly configure input grouping options. *You can always contact our team to support you in your workflow implementation.*
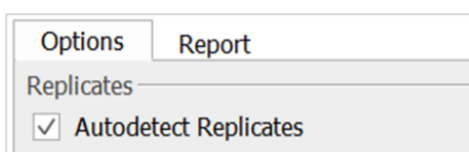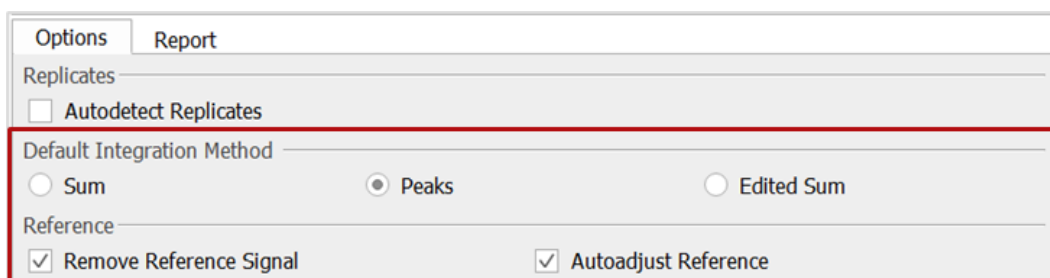
Then, choose the peak integration method you want to apply…

- **Sum**-based integration
- **Peak**-based integration (using global spectra deconvolution, GSD)
- **Edited sum** integration (a combination of sum- and peak-based methods).

…and the desired options for the reference peak:

- **Remove Reference signal**: can be checked to ignore the reference signal in multiplet analysis and auto-assignments when using the default analysis.
- **Autoadjust Reference**: can be checked to automatically detect the highest intensity reference peak and center it within the reference range.

In the **Multiplet Calculation Options** section, you should first decide if you want to base the calculation on all multiplets (check **Use All Multiplets**) or otherwise (manually set the number of multiplets to be used).
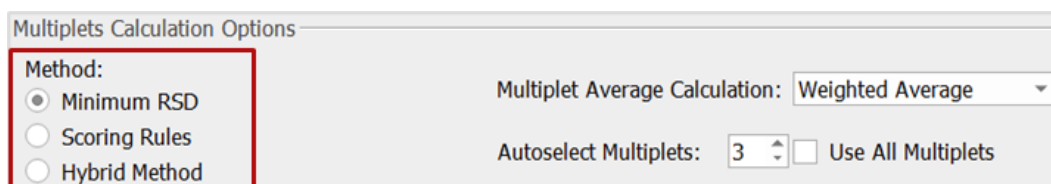

When integrating a number of multiplets (≠ all multiplets) a method for their autoselection should be defined. You can either:

- select multiplets that give the smallest RSD (**Minimum RSD**);
- rank multiplets using the Multiplet Autoselection rules (**Scoring rules**);
- or go for a **Hybrid method** in which multiplets are first ranked by scoring rules and then by the smallest RSD.
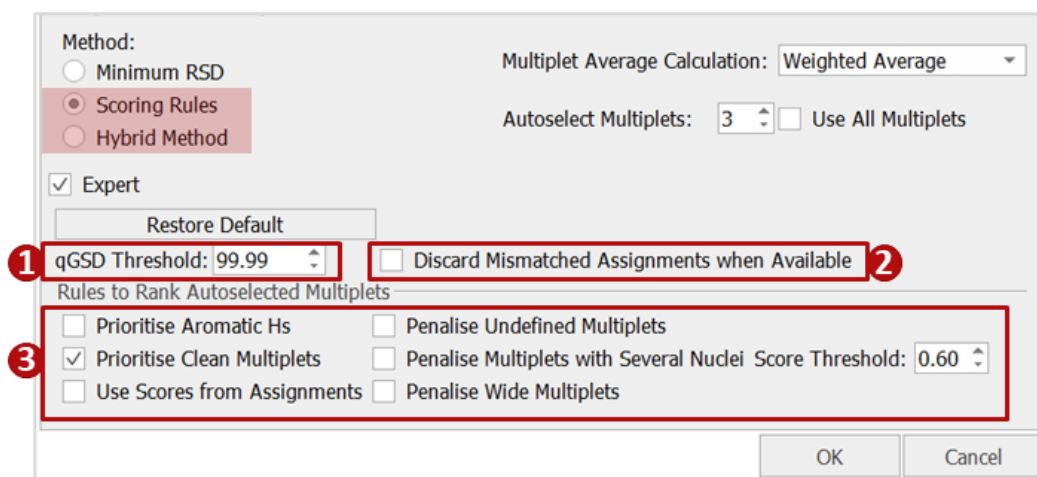
If you choose one of the latter two options, custom scoring rules can be defined in the **Expert** section. Here, it is possible to:

1. Ignore multiplets with a qGSD value that is greater than a fixed threshold
2. Discard mismatched assignments when available
3. Prioritize and penalize multiplets over others

Finally, decide the **Multiplet Average Calculation** method:

- **Simple Average:** the mean average of the concentrations will be calculated.
- **Weighted Average**: the concentration with the sum of the integrals, divided by the sum of the nuclei and multiplied by the scaling factor.
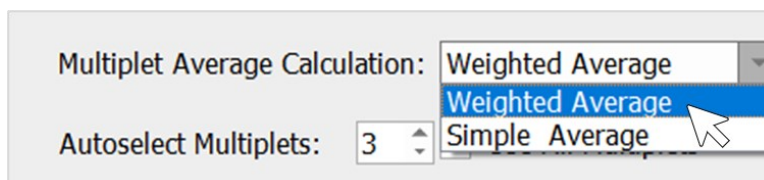

Now go to the **Report** tab to configure the results report. Click on ⋯ and upload a **Custom Layout Template** to apply to your report, or otherwise use the **Default Layout** included with the plugin (you can **Download** and view this default layout, edit it as needed, then save it to use it as a custom layout).

If your layout template has only one page, you can check the **Apply Single Page Template to Each Page** to apply it recursively to all the pages of the results report.
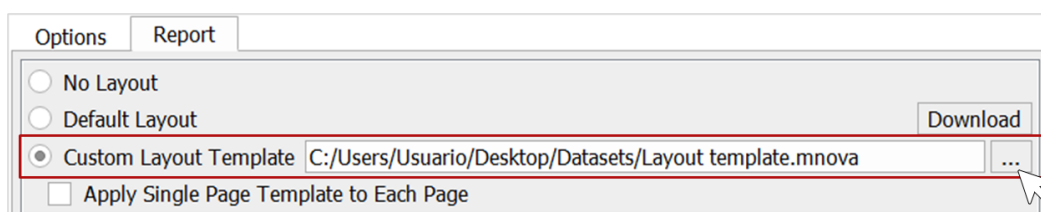
Then, check the sections you want to include in the report: **Title, Main Result, Multiplet Table, Standard Information, Analysis Conditions, Experiment Information, Replicate information, Errors and Hints.**
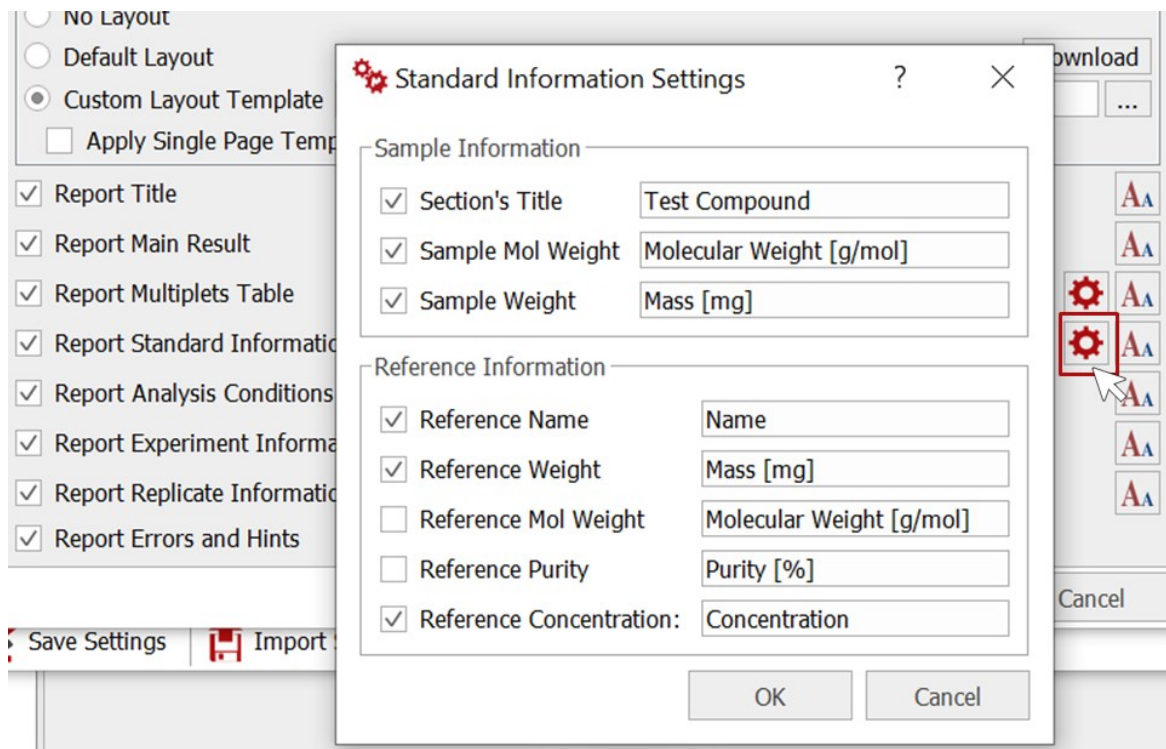
Font style can be customized for each of the report sections. Click on AA, choose your preferred font options, and then click on **OK** to save your choices.
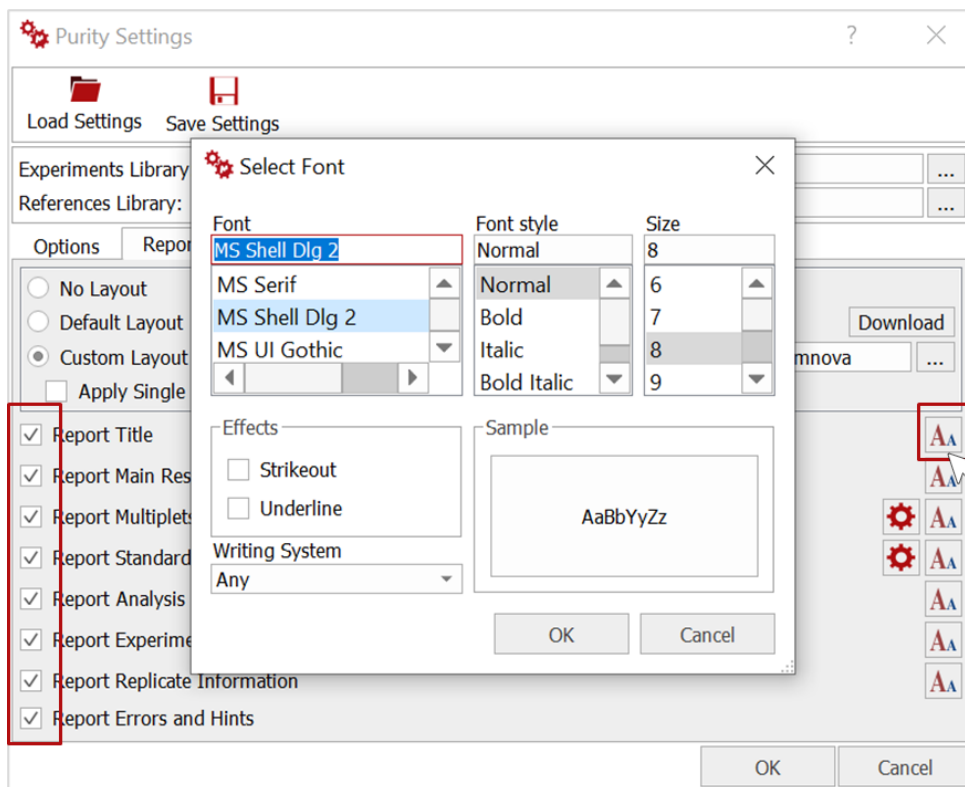

The **Multiplet Table** can be customized by clicking on ⚙, as shown below:
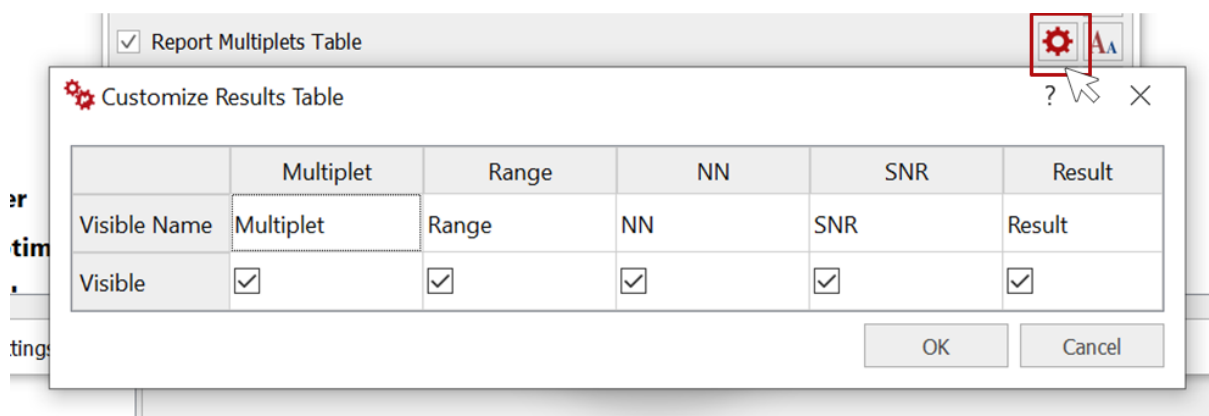
Standard Information can include sample and/or reference compound information. Click on ⚙ to open the settings dialog.


Top Tip! The **Report Errors and Hints** option is an excellent way to get relevant feedback when an analysis fails. An error message and its possible cause will be written in the result files, as seen below:
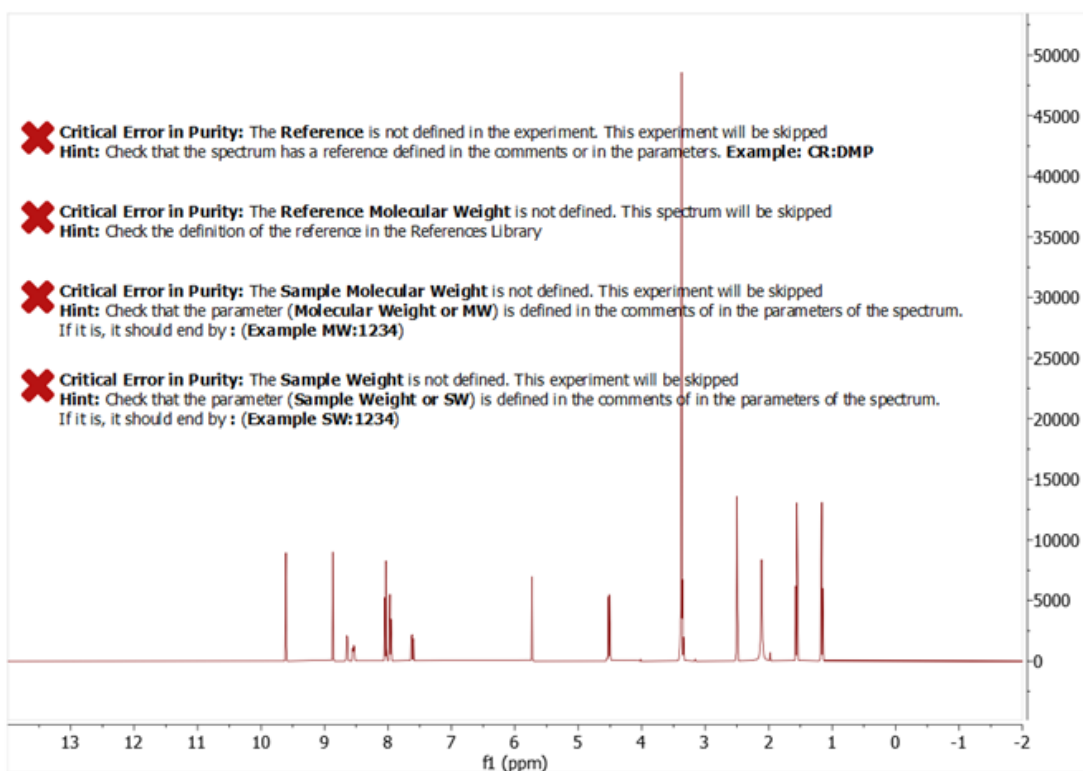
Once all the **Purity Settings** have been completed to your satisfaction, click on **OK**, and proceed to the next Mgears tab.
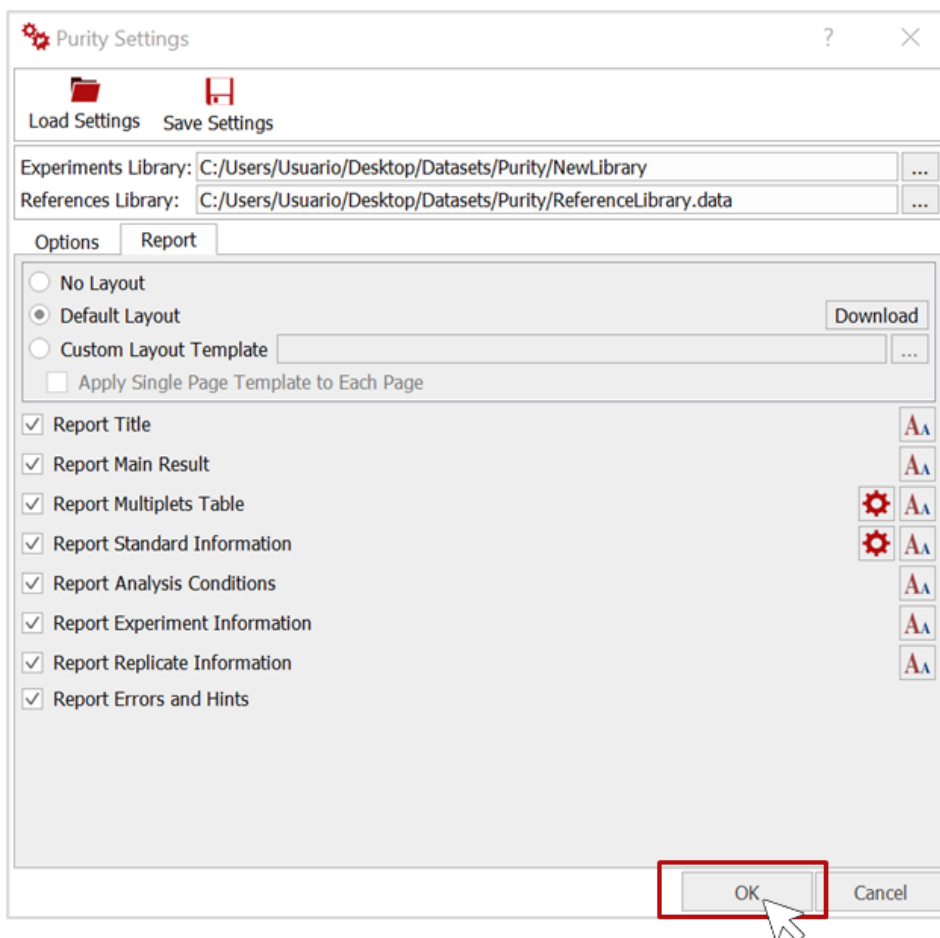
Top Tip! When running routine qNMR analyses with the same configuration settings, you can save these settings once and then load them easily for future analyses. A ".data" file will be created and saved to the directory of your choice.
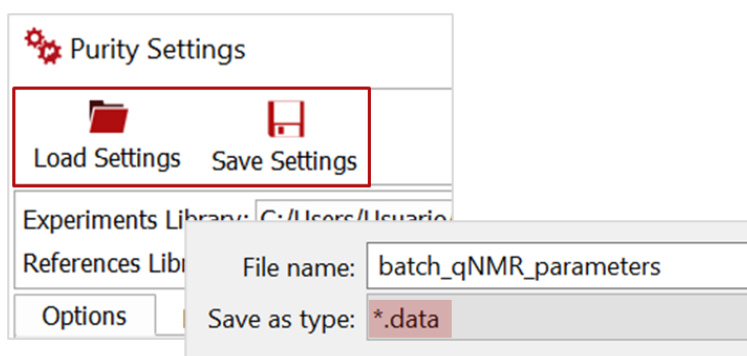
Design

When running various analyses on a given dataset, you may want to upload an **Mnova layout template** or a **Script** in the **Design** tab to produce a final, customized report that combines the results of all the analyses. For the current Purity analysis, this is not needed, so let´s proceed to the next tab.

Output

In the **Output** tab, select a directory in which to save your analysis results, and decide whether to include an Mnova or PDF results file, or save the results to a connected DB *(please refer to the Mgears manual for more details about the output tab).*
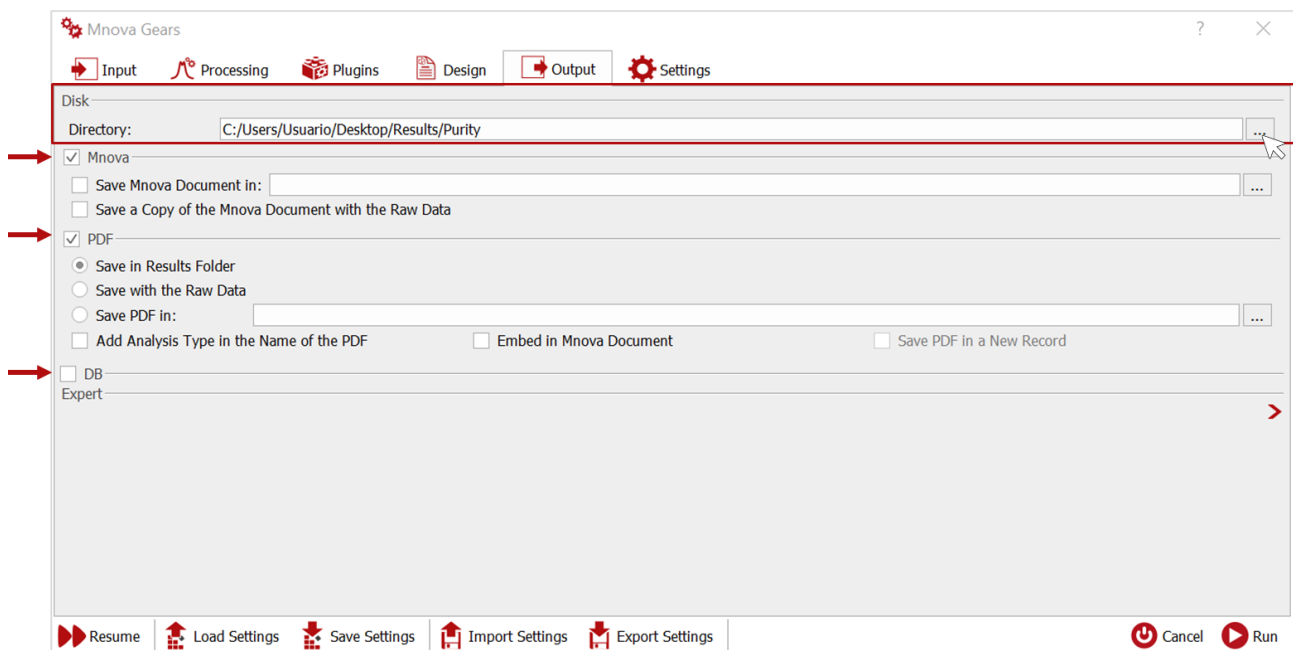
Now click on **Run** to start the analysis.

The output folder

Once the analysis has completed, you can go the directory specified previously to check the results. The output folder is named according to the date and time at which your analysis was conducted and contains all the output generated in the current evaluation.
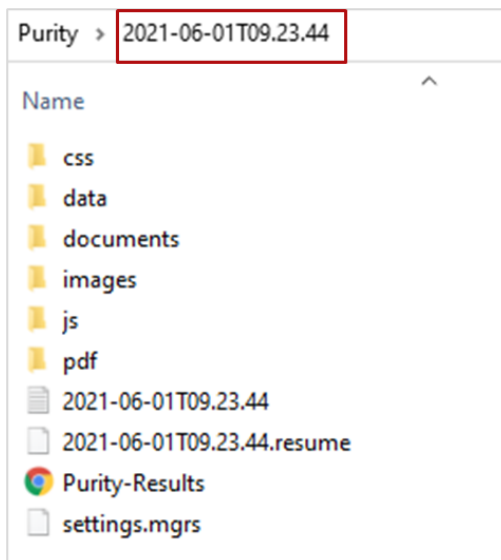
The Mnova and PDF results files are saved under "**documents**" and "**pdf**", respectively.

An HTML report is also created with all the analysis results; each row contains the average **Purity (% ± RSD)** result for a sample and links to the corresponding Mnova and PDF results files.

Mgears Purity Results

Parameters

Parameter	Value
Results Directory	C:/Users/Usuario/Desktop/Results/Purity/2021-06-01T09.23.44
Started On	2021-06-01T09:23:44
Completed On	2021-06-01T09:24:24

Detailed Results

Show 5 entries   Copy CSV Columns PDF Print   Search:

#	Purity	Mnova File	Pdf File
1	99.42%+-0.24	SAMPLE 1.mnova	SAMPLE 1.pdf
2	100.16%+-0.24	SAMPLE 2.mnova	SAMPLE 2.pdf
3	100.38%+-0.25	SAMPLE 3.mnova	SAMPLE 3.pdf

Showing 1 to 3 of 3 entries

Previous 1 Next

You can **Copy**, **Print**, or save these global results into a **CSV** or **PDF** file.

Results review with the Mgears Viewer

Detailed Purity results can be reviewed in the **Mgears Viewer**. Click on ▮ and select the Purity analysis output folder.

Mgears Viewer

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

Purity Results include the global **Purity** value (99.4226 in this example), the absolute **Concentration**, the Standard Deviation **SD**, and the Relative Standard Deviation **RSD**. The **Purity** and **RSD** values are also pasted into the Mnova document.

The autoselected multiplets are highlighted in green and included in the **Multiplet table** in the Mnova report with the corresponding calculated purity.

Other experimental and analysis information is included to the report (as predefined in the settings).

To review the individual results for each sample, it is possible to use the Mnova Standard Purity plugin. Open the **Purity** plugin dialog from the **Quantitation** tab in the Mnova ribbon.
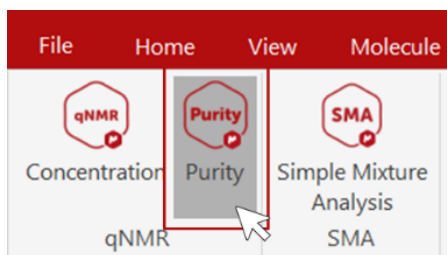
Then, click on to load the purity results from the open Mnova document. Sample and reference details, as well as all spectral multiplets, are loaded into the **Purity** dialog.

You can select/deselect multiplets as preferred. The results will be automatically updated in the Mnova document and in the Mgears Viewer.

Click on to save the new results to the output folder.

For more detailed information about Mgears, please refer to the Mgears Manual or to our Resources section on the web.

You can also read the [MyGears Application Note](#) to see how an Automated Triplicate qNMR analysis can be performed with a single click.