Mestrelab Research

Gears Mpublish 1.0

STARTING GUIDE

MPublish

GEARS

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P/N 227 R1

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The sharing of primary research data is an extremely powerful way to preserve research integrity and replicability and to allow for its reuse by peers. However, preparing research data for publication requires considerable time and effort on the part of the researcher. It can be tedious and error prone.

Mpublish is a plugin for Mnova Gears that solves this problem. It allows easy and automatic preparation of supporting information for publications. Mpublish inputs the primary instrumental data files and generates both human- and machine-readable output files of the research data and metadata.

The current version of Mpublish works with NMR primary datasets (raw data files) and with processed, analyzed, and annotated spectra within the Mnova platform (.mnova files); however, the concept is extensible to many other types of spectroscopic data.

The workflow

Mpublish workflow is both simple and straightforward. So, let's launch Mgears and get started.
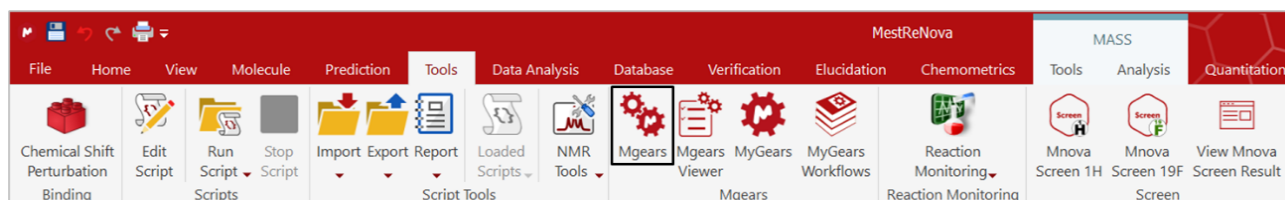

In the **Input** section, you should select the analytical data you want to publish. Data files can be saved on a **Disk** directory or can be retrieved from a connected **database** (**DB**). In this guide we will be using input files from the **Disk**. *(Please refer to the Mgears manual for further details about other input modes).*

Click on ··· and select your data folder. Both 1D and 2D spectra files can be processed by Mpublish.
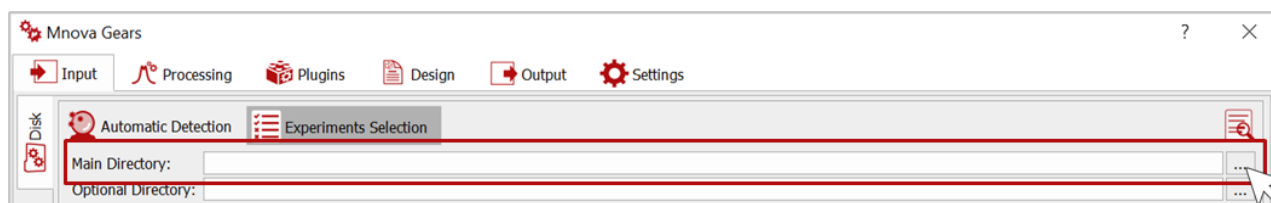
You can then choose and configure your experiment detection mode: you can either use **Manual Detection** and therefore enter **Path Masks** for each type of experiment manually, or you can use the **Automatic Detection** option and select the experiments of interests, as per the image below.
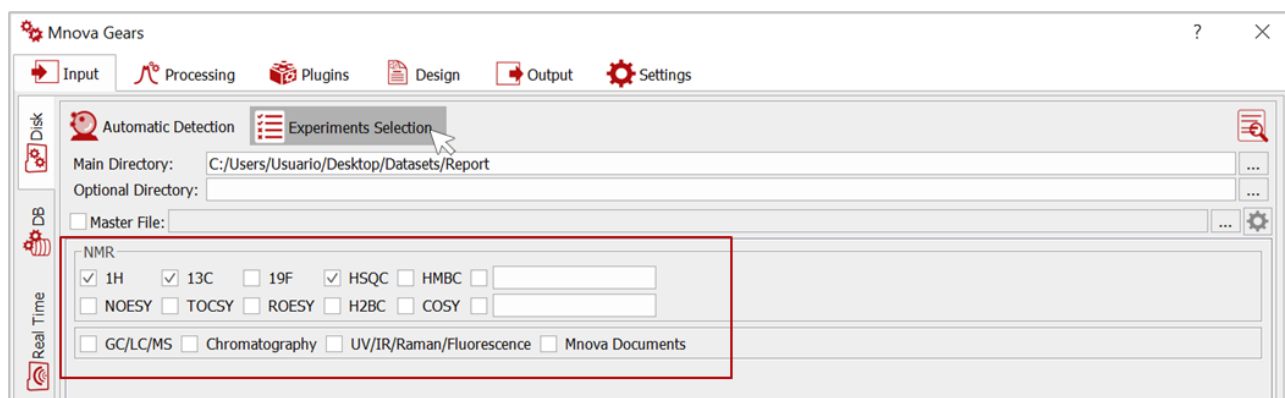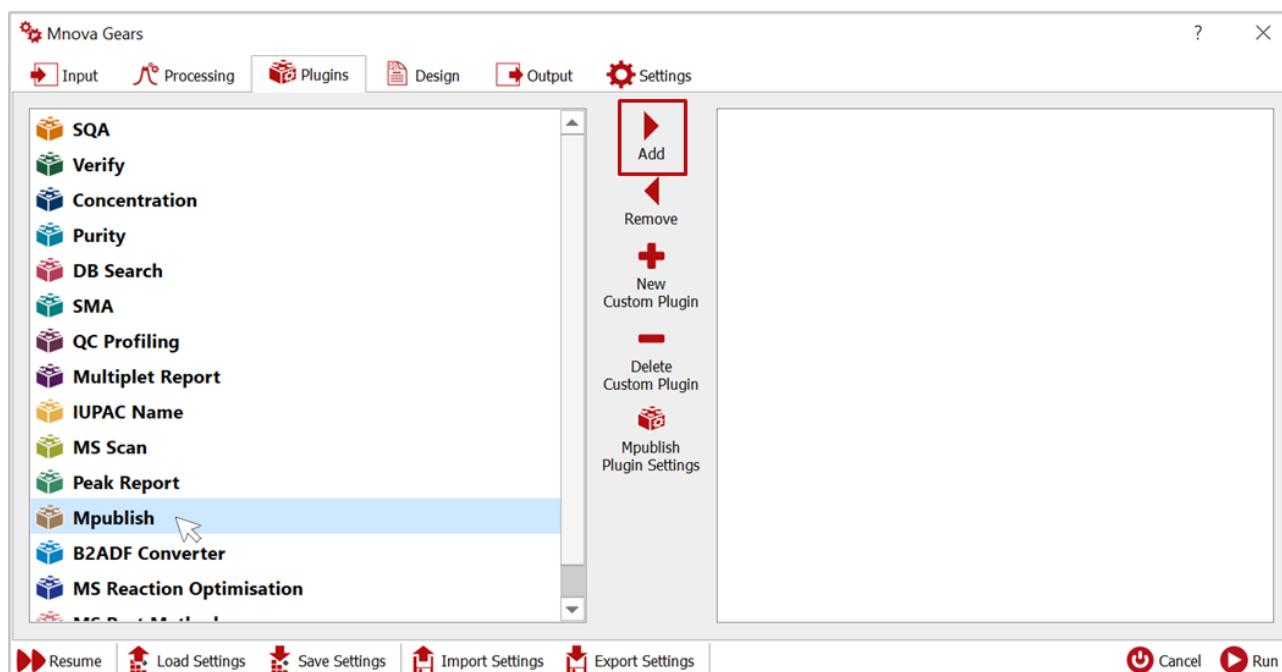
If needed, configure the **Advanced Options** or use the **Filtering Options** to refine the detection of your data files of interest.

Top Tip! Before moving to the next step, use the **Automatic inspection** button to check if the data detected corresponds to your configuration.

![Plugins icon] Plugins

In the **Plugins** section, select and add the Mpublish plugin.

The plugin will appear on the right-hand side of the window. You should now click on **Mpublish Plugin Settings** to configure the format and information to include in the final report.
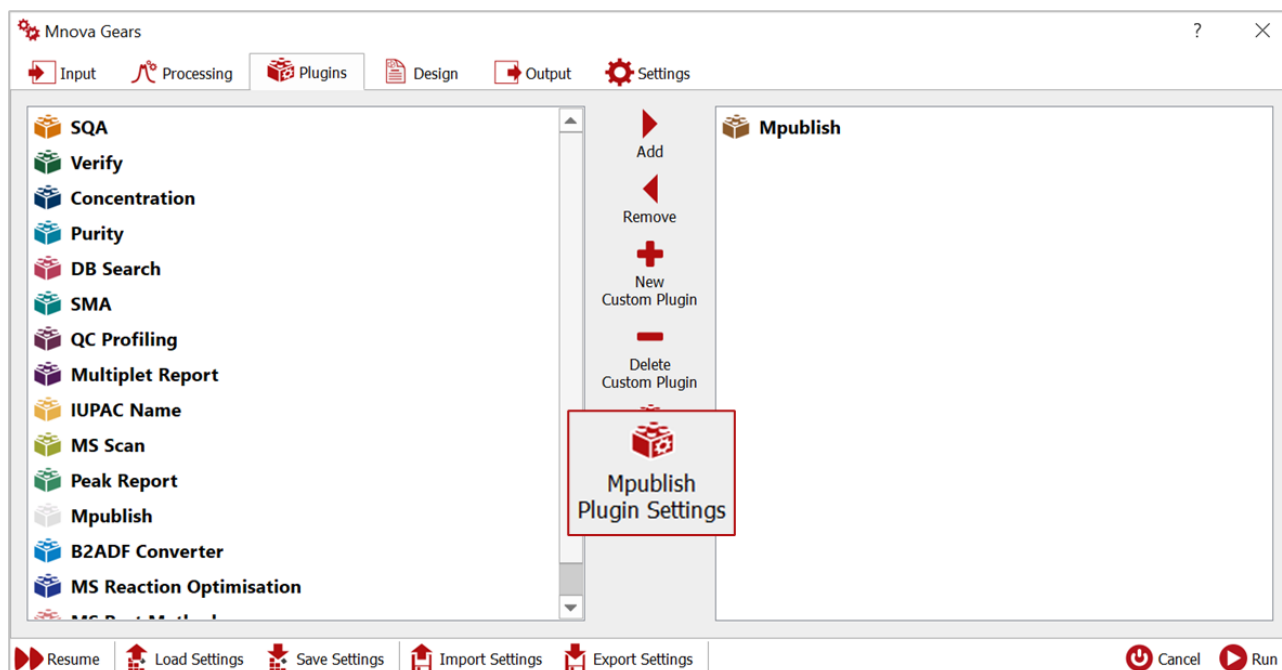

In the **Mnova Publish** Settings dialog, first choose the journal template required for your output document. Two formats are available by default with Mpublish 1.0:

- Organic Letters for Supporting Information
- ACS for Supporting Information
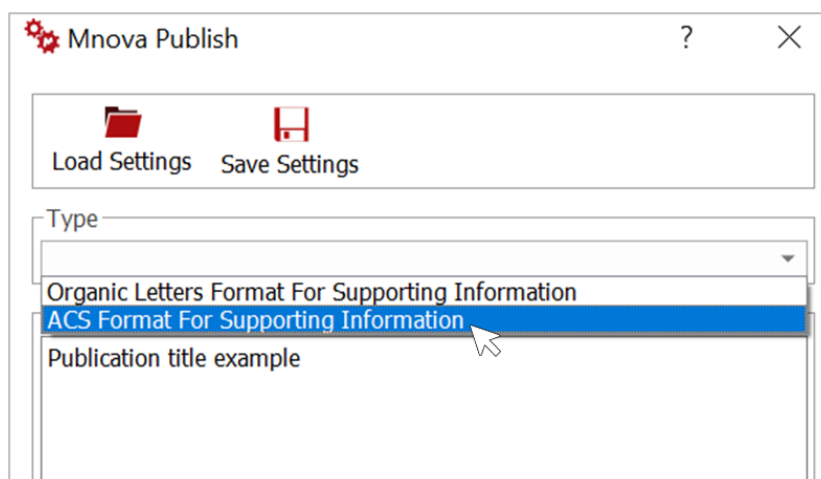
If you need additional customizations, please contact us to discuss your requirements.
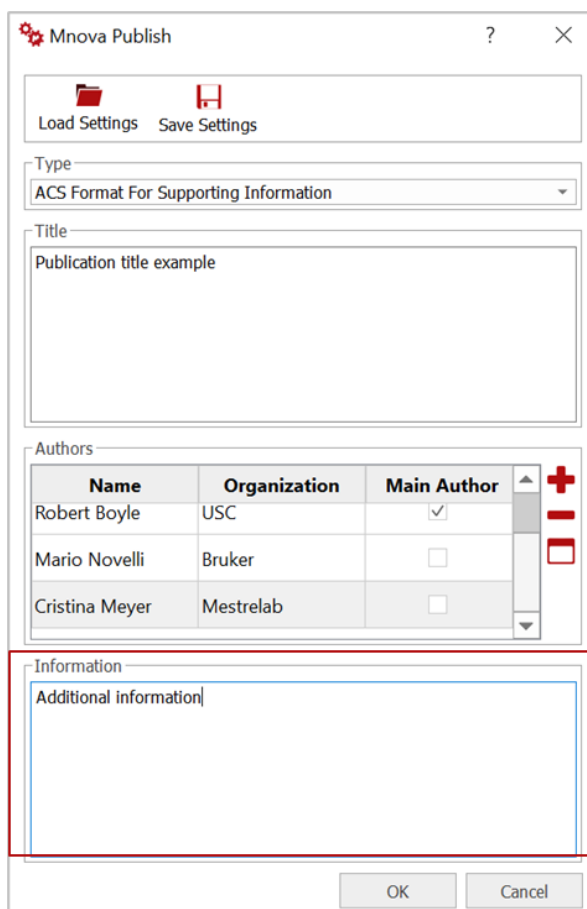
Type the **Title** of your publication, then click on ✚ to add the **Authors** and corresponding **Organization**. You can indicate the publication's **Main Author** simply by ticking the corresponding checkbox.
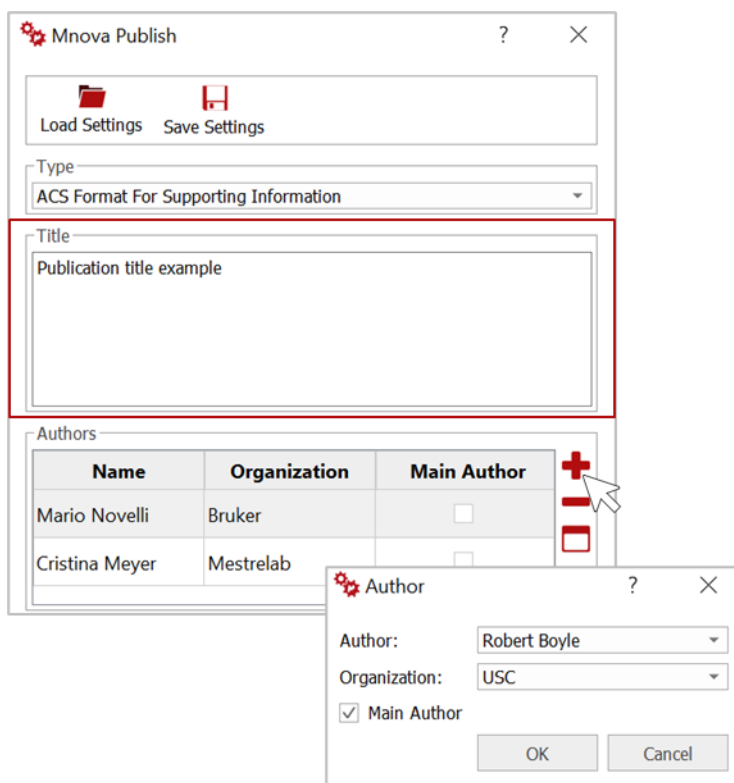
The authors added will be listed in the **Authors** table. You can select any such entry and click on ➖ to delete it. You can also click on ▭ to clear the table content.
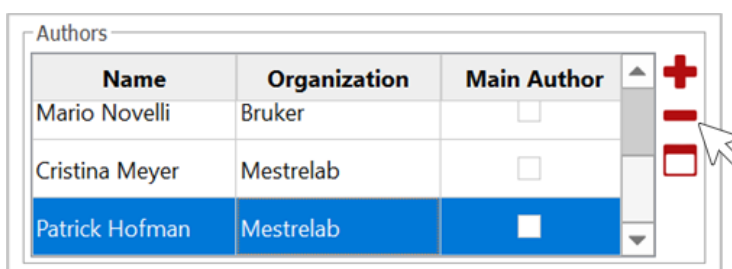
Finally, you can add any relevant information, abstracts, etc., in the **Information** section.
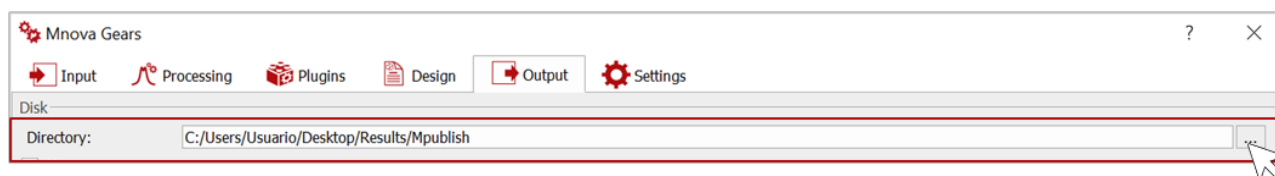

Once all the above has been completed to your satisfaction, click on **OK.**

Output

The last step would be to configure the **Output** section. As with any Mgears plugin, you must choose the location where you would like to save your analysis results.

To save your results on the **Disk**, click on ··· and select the **Directory** folder.

Here you can also choose to create an Mnova document or a PDF by ticking the corresponding checkbox and indicating the desired output location.
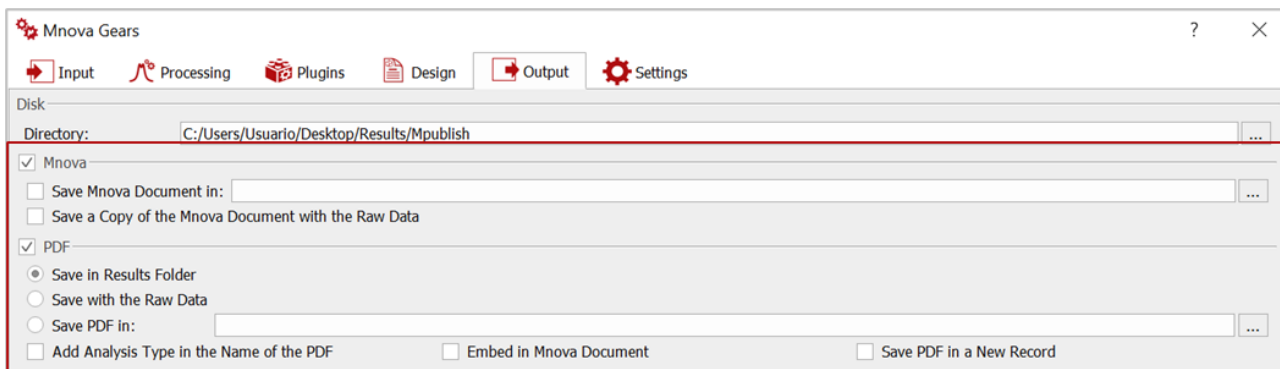

Finally, it is possible to include data in a DB. To do so, you must enter the DB **Server**, **Port**, **User**, and **Password** then click on **Connect**. You will then be able to select the Database.

Now that everything is set, click on to start the analysis. Mgears will run the analysis and save the results in the previously defined location.

The output folder

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.
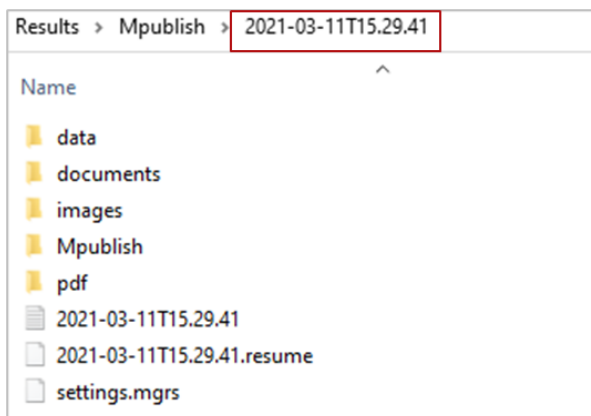
In the Mpublish subfolder you will find:

- your final report saved as an ODT (open document text) file including the pre-defined title and author information, and where all the processed data has been templated according to the journal format selected.

- a folder containing the primary raw data used to generate these processed and analyzed data. The subfolders and files are renamed and reorganized so they match the titles included in the automatically generated report.

The other output subfolders include the Mnova and PDF documents, and Mgears execution files, including the log file and a copy of the mgears settings.

Pro-Tip! The log file is a great way to trouble shoot any issues with the workflow.

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