Mestrelab Research

Gears DB Search 1.1

STARTING GUIDE

Document Number

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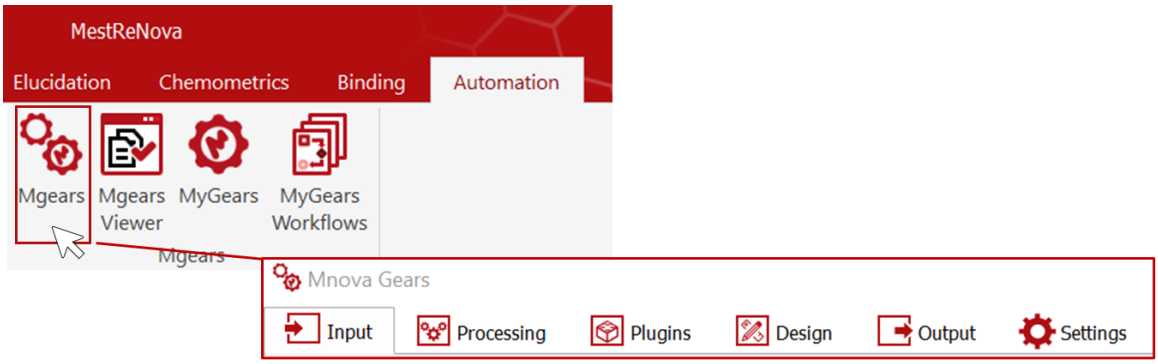
DB Search is an Mgears plugin that will allow you connect to one or more Mnova databases and search input datasets to identify structures that have already been analyzed and saved to them, or to otherwise find potentially similar structures (with similar 1H, 13C, or HSQC spectra) that can be used as references.

Follow the steps detailed below to run your very first analysis.

Remember: In order to run a DB Search analysis, you must have an active Mnova DB license and a connection to the DB server, in addition to the Mnova Gears and DB Search licenses.

1. The workflow

Launch Mgears from the Mnova **Automation** ribbon. A dialog with six tabs will open.



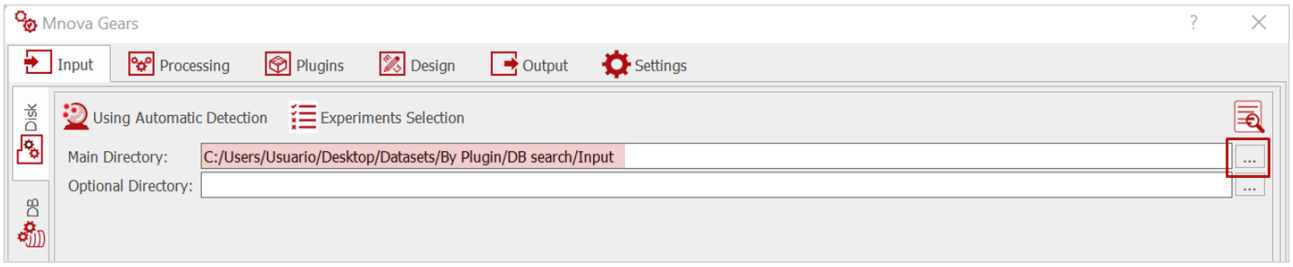
A DB Search analysis will require you to set up the **Input** data, the **Plugin** settings, and the **Output** options.

1.1. The Input tab

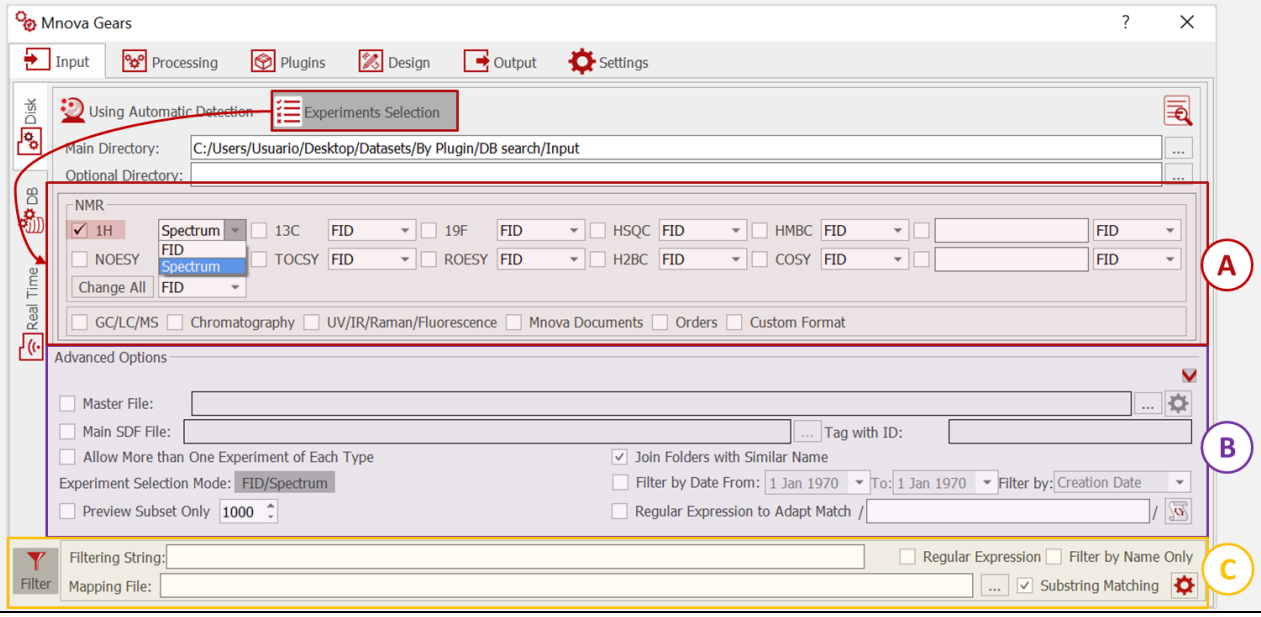
The input spectra to be searched can be retrieved from **Disk** directories, a **DB**, or from **Real-Time** acquisition. The configuration of the input for each of these cases is detailed in the Mnova Gears user manual.

In this example, we are going to analyze data saved in a **Disk** directory.

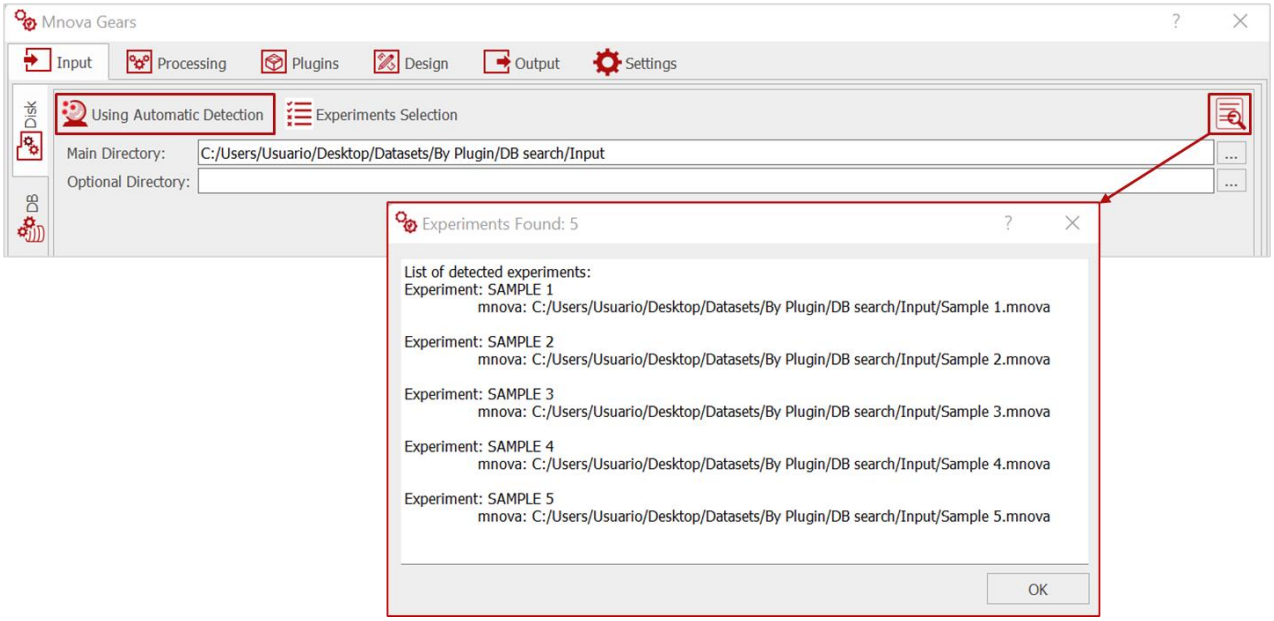
Click on ... and select the data folder from your disk.



Optional. In some cases, you may need an additional layer of configuration to correctly retrieve the data you want to analyze and exclude any other data files saved in the same location. To do so, you can (A) enable the **Experiment Selection** option and manually select the experiment type and data you want to analyze; you can also configure (B) the **Advanced** and (C) **Filtering options** according to your input options – as detailed in the Mgears manual – which gives you huge flexibility and allows you to adapt Mgears to your instrument data organization and formats.



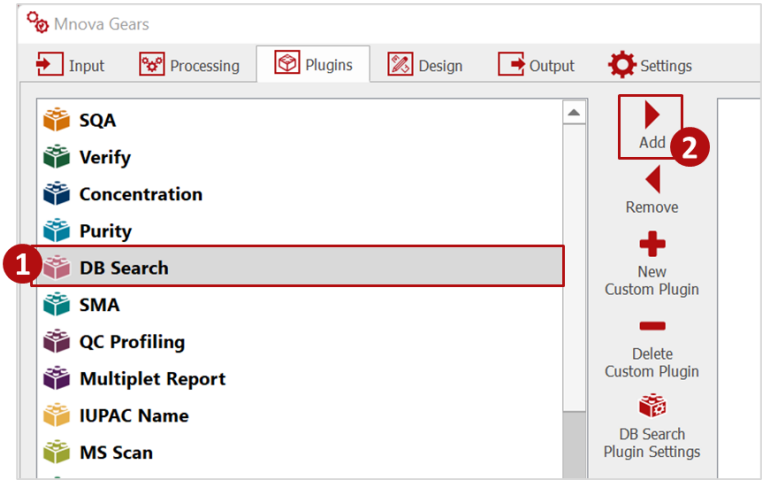
Enable the **Automatic Detection** feature (unless you opt for a manual **Experiment Selection**), then use the **Automatic inspection** button to verify that Mgears has detected the data according to your configuration. The experiments found will be listed as shown in the image below:



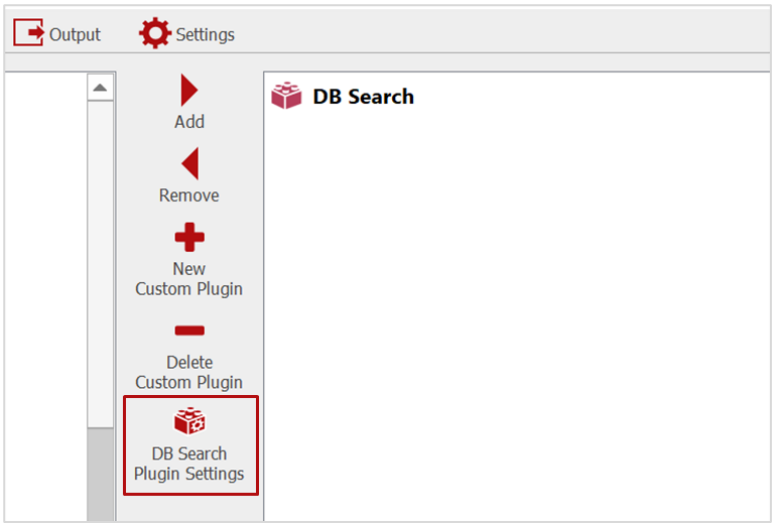
If the experiment detection result is satisfactory you can move to the next step.

1.2. The Plugins tab

In the **Plugins** tab, select and add the DB Search plugin.



Then, click on **DB Search Plugin Settings** to configure your analysis preferences.



The **DB Search Settings** dialog will appear, which has four tabs.

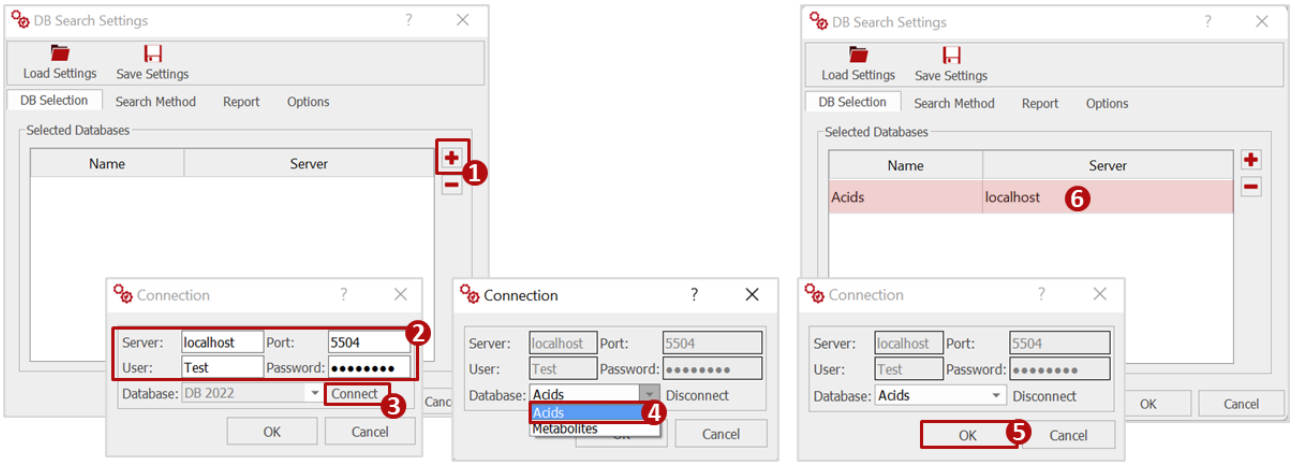
1.2.1. The DB Selection tab

In the **DB selection** tab, you must select the databases to be searched.

Click on + to add a database. In the **Connection** dialog that appears, enter the server connection details and credentials, then press **Connect**.

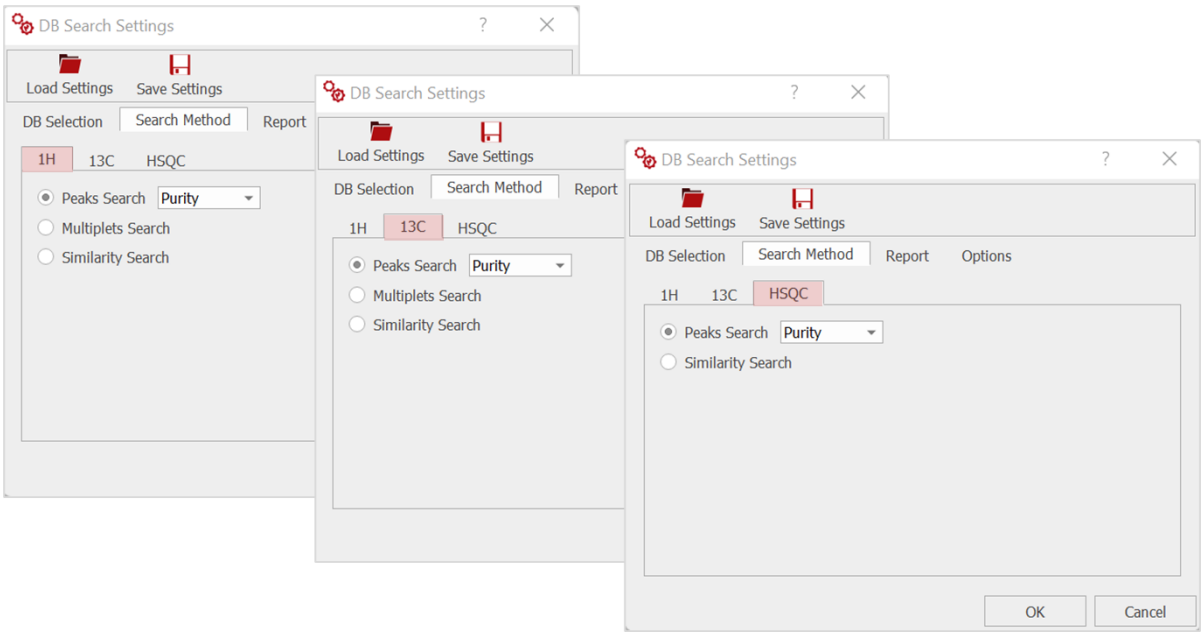
Once the connection is established, select the **Database** you wish to use in your search, then press **OK**. The selected database will appear in the **Selected Databases** table, as shown in the example below.

Click on + a second time to add another database if needed, or on − to delete a previously added database.



1.2.2. The Search method tab

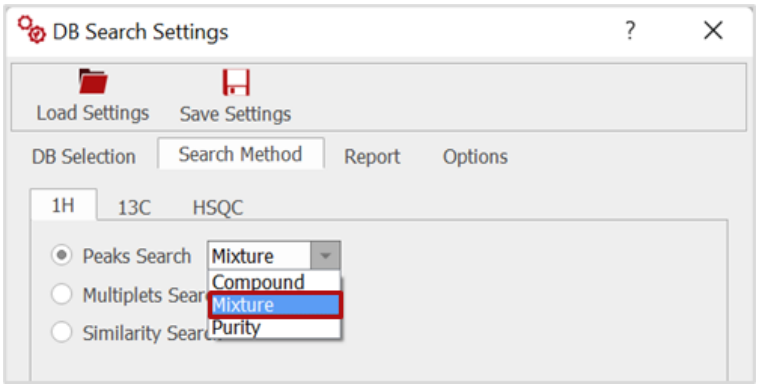
In the **Search Method** tab, choose the method you want to apply to search the database(s). DB Search can use **Peaks**, **Multiplets**, or peak **Similarity** to search 1H or 13C NMR spectra, and **Peaks** and **Similarity** search for HSQC spectra.



Within the **Peak search** option, you can choose one of the three proposed search modes, **Compound**, **Mixture**, or **Purity**, depending on your experiment. Each mode will apply a different scoring algorithm to find the best matches to your query in the searched database(s):

- The **Compound** mode is useful when your query data includes pure compounds, and the searched database(s) contains mixtures and/or compounds with impurities.
- The **Mixture** mode is useful when searching for the components of a mixture within a database of pure compounds.
- The **Purity** mode allows you to search directly for the best match to the query spectrum in the database(s).

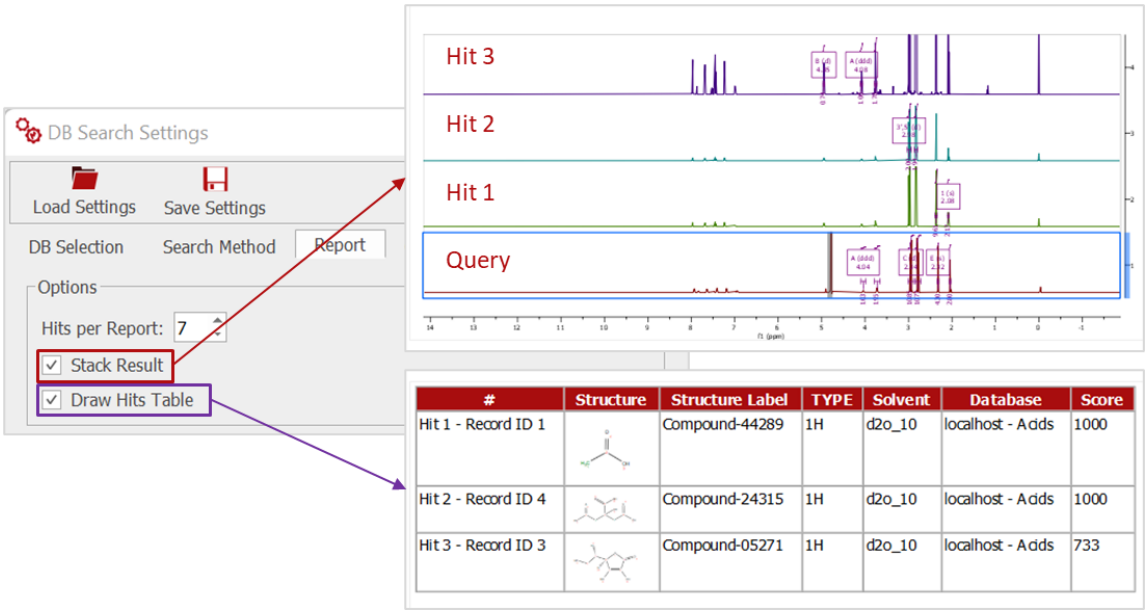
For this example, we will use **Peak search** in the **Mixture** mode.



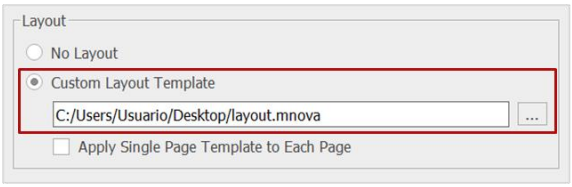
1.2.3. The Report tab

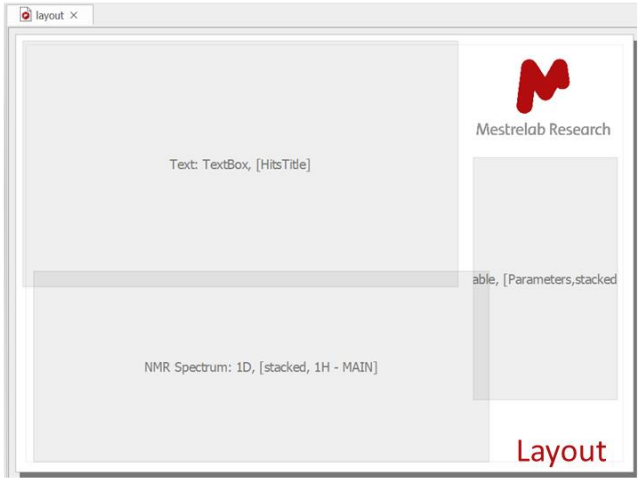
In the **Report** tab, you must decide the maximum number of hits you want to show in each results report.

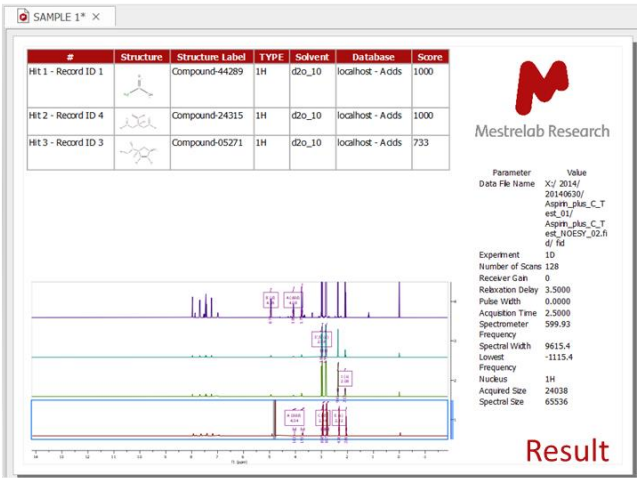
You can also decide whether to include a **Stack** with the analyzed spectrum and the hits found or whether to **Draw a Hits Table**.



If you wish to apply a **Custom Layout Template** to your result reports, you can upload it here. Otherwise, the default layout will be applied.







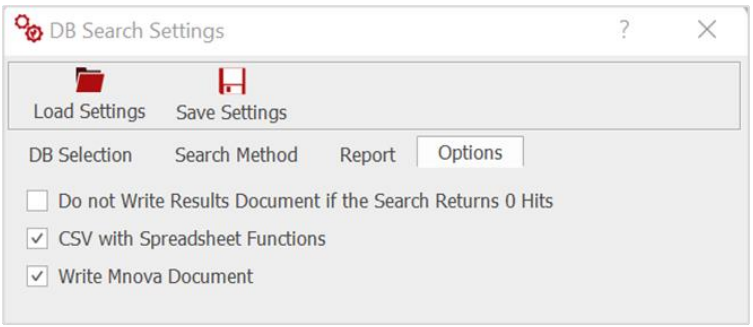
If you enable the **Apply Single page template to each page**, the layout will be applied recursively on every page of your report.

1.2.4. The Options tab

Finally, in the **Options** tab, you can check the **Do not Write Results Document if the Search Returns 0 Hits.** This way, Mgears will not produce Mnova nor PDF documents if the search does not return any hits.

You can choose to include **Spreadsheet Functions** in the CSV results file to easily access the corresponding Mnova and PDF files.

You can also decide whether to **Write Mnova Document** with your search results.

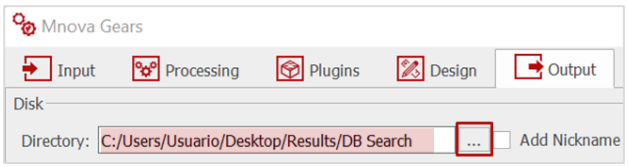


Top tip! Note that you can save the settings of your current analysis for future use by clicking on Save Settings. DB Search settings will be saved as a ".data" file. When you start a new analysis, you will then be able to directly load these settings by clicking on Load Settings and opening the saved settings file.

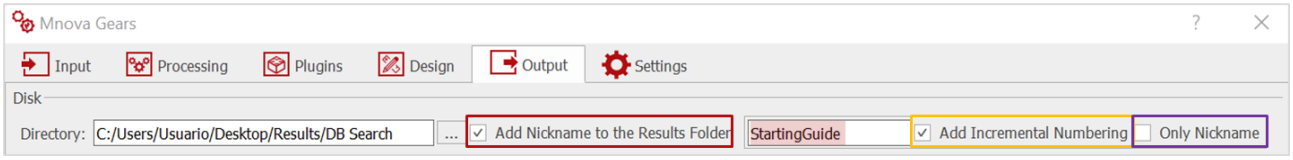
Once you are done choosing you DB Search settings, you must click on **OK** to save them, then proceed to the Mgears output tab.

1.3. The Output tab

Here, you must choose a directory in which to save your analysis results. Click on ... and select a results folder on your disk.



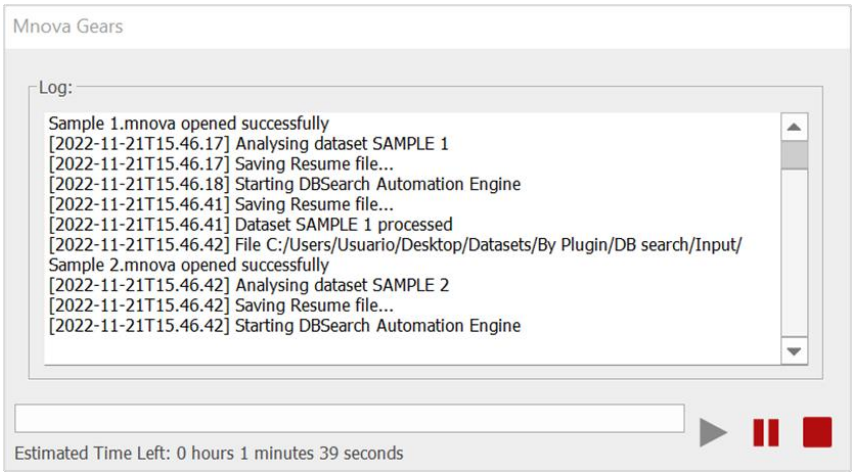
Optionally, enable the **Add Nickname to the Results Folder** and type the nickname of your choice, **Add Incremental Numbering** to your results folder, and/or decide to use **Only the Nickname** in the folder's name.



You can also choose to create an Mnova document, a PDF, or to save your results to a DB.

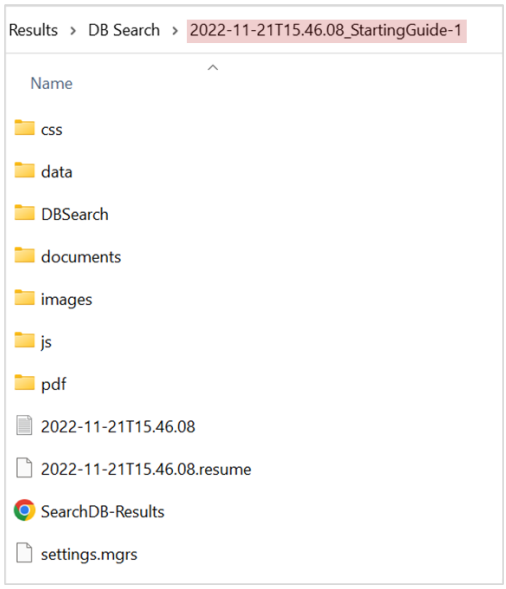
Note. If you wish to view/review the spectra along with the results in the Mgears Result Viewer, you must enable Mnova document creation. Otherwise, when loading the results in the Mgears Result Viewer, only the data will be visible, with no spectra.

Once the configuration has been completed to your satisfaction, click on **Run**  to launch the analysis. Each query file will be opened and run against all the selected DBs.



2. The output folder

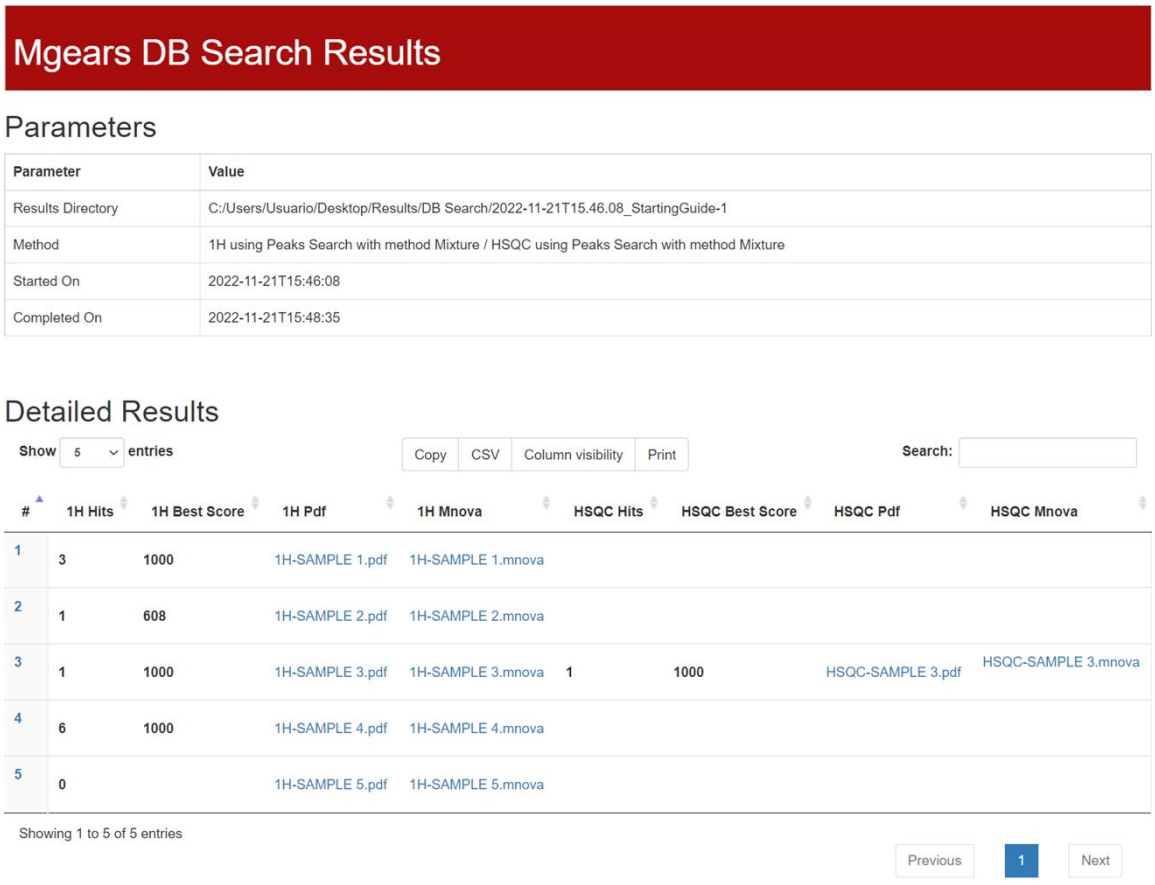
The results folder is saved under the previously specified directory, as described above.



This folder contains all the output generated in the current evaluation, which includes:

2.1. An HTML file

The HTML report gives an overview of the results. Each query spectrum will be displayed on a line with the **Number of Hits**, the **Best score,** and links to the appropriate **PDF** and **Mnova** result files.



Mgears DB Search Results

Parameters

Parameter	Value
Results Directory	C:/Users/Usuario/Desktop/Results/DB Search/2022-11-21T15.46.08_StartingGuide-1
Method	1H using Peaks Search with method Mixture / HSQC using Peaks Search with method Mixture
Started On	2022-11-21T15:46:08
Completed On	2022-11-21T15:48:35

Detailed Results

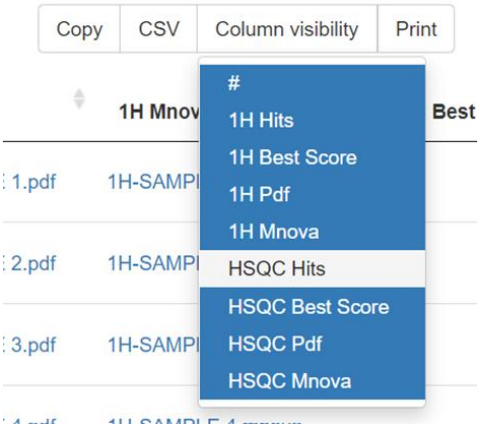
Show 5 entries | Copy | CSV | Column visibility | Print | Search:

#	1H Hits	1H Best Score	1H Pdf	1H Mnova	HSQC Hits	HSQC Best Score	HSQC Pdf	HSQC Mnova
1	3	1000	1H-SAMPLE 1.pdf	1H-SAMPLE 1.mnova				
2	1	608	1H-SAMPLE 2.pdf	1H-SAMPLE 2.mnova				
3	1	1000	1H-SAMPLE 3.pdf	1H-SAMPLE 3.mnova	1	1000	HSQC-SAMPLE 3.pdf	HSQC-SAMPLE 3.mnova
4	6	1000	1H-SAMPLE 4.pdf	1H-SAMPLE 4.mnova				
5	0		1H-SAMPLE 5.pdf	1H-SAMPLE 5.mnova				

Showing 1 to 5 of 5 entries

Previous | 1 | Next

The HTML format allows you to change the display of the columns and adapt them to your preferences. You can then **Copy**, **Print**, or download a **CSV** file with the results.



2.2. A CSV file

The CSV file saved under the "DBSearch" subfolder, contains input and output information data, including the **Dataset** and **Spectrum** names, the **Hit** number, the **Record** ID, the **Type** of hit spectrum, the **Solvent**, the **Server**, the **Database**, the **Score**, and the path to the **Mnova** and **PDF** result files.

If the option to include hyperlinks in the **Mnova** and **PDF** result files is enabled in the plugin settings, those hyperlinks are included in the CSV instead of the location path.

	A	B	C	D	E	F	G	H	I	J	K	L
1	Dataset	Spectrum Title	Structure	Hit	Record	Type	Solvent	Server	Database	Score	Mnova	PDF
2	SAMPLE 1	_NOESY_01	Compound-44289	1	1	1H	d2o_10	localhost	Acids	1000	1H-SAMPLE 1.mnova	1H-SAMPLE 1.pdf
3	SAMPLE 1	_NOESY_01	Compound-24315	2	4	1H	d2o_10	localhost	Acids	1000	1H-SAMPLE 1.mnova	1H-SAMPLE 1.pdf
4	SAMPLE 1	_NOESY_01	Compound-05271	3	3	1H	d2o_10	localhost	Acids	733	1H-SAMPLE 1.mnova	1H-SAMPLE 1.pdf
5	SAMPLE 2	est_NOESY_0	Compound-33456	1	8	1H	d2o_10	localhost	Acids	608	1H-SAMPLE 2.mnova	1H-SAMPLE 2.pdf
6	SAMPLE 3	W_1DP_noe	HMDB00142#0	1	6	1H	D2O	localhost	Acids	1000	1H-SAMPLE 3.mnova	1H-SAMPLE 3.pdf
7	SAMPLE 3	1_HW_2DHS	HMDB00142#0	1	6	HSQC	H2O+D2O_met	localhost	Acids	1000	HSQC-SAMPLE 3.mnova	HSQC-SAMPLE 3.pdf
8	SAMPLE 4	_NOESY_01	Compound-44289	1	1	1H	d2o_10	localhost	Acids	1000	1H-SAMPLE 4.mnova	1H-SAMPLE 4.pdf
9	SAMPLE 4	_NOESY_01	Compound-24315	2	4	1H	d2o_10	localhost	Acids	1000	1H-SAMPLE 4.mnova	1H-SAMPLE 4.pdf
10	SAMPLE 4	_NOESY_01	Compound-33456	3	8	1H	d2o_10	localhost	Acids	956	1H-SAMPLE 4.mnova	1H-SAMPLE 4.pdf
11	SAMPLE 4	_NOESY_01	Compound-05271	4	3	1H	d2o_10	localhost	Acids	933	1H-SAMPLE 4.mnova	1H-SAMPLE 4.pdf
12	SAMPLE 4	_NOESY_01	Compound-87200	5	2	1H	d2o_10	localhost	Acids	913	1H-SAMPLE 4.mnova	1H-SAMPLE 4.pdf
13	SAMPLE 4	_NOESY_01	Compound-26549	6	5	1H	DMSO	localhost	Acids	733	1H-SAMPLE 4.mnova	1H-SAMPLE 4.pdf

Path to location or hyperlink

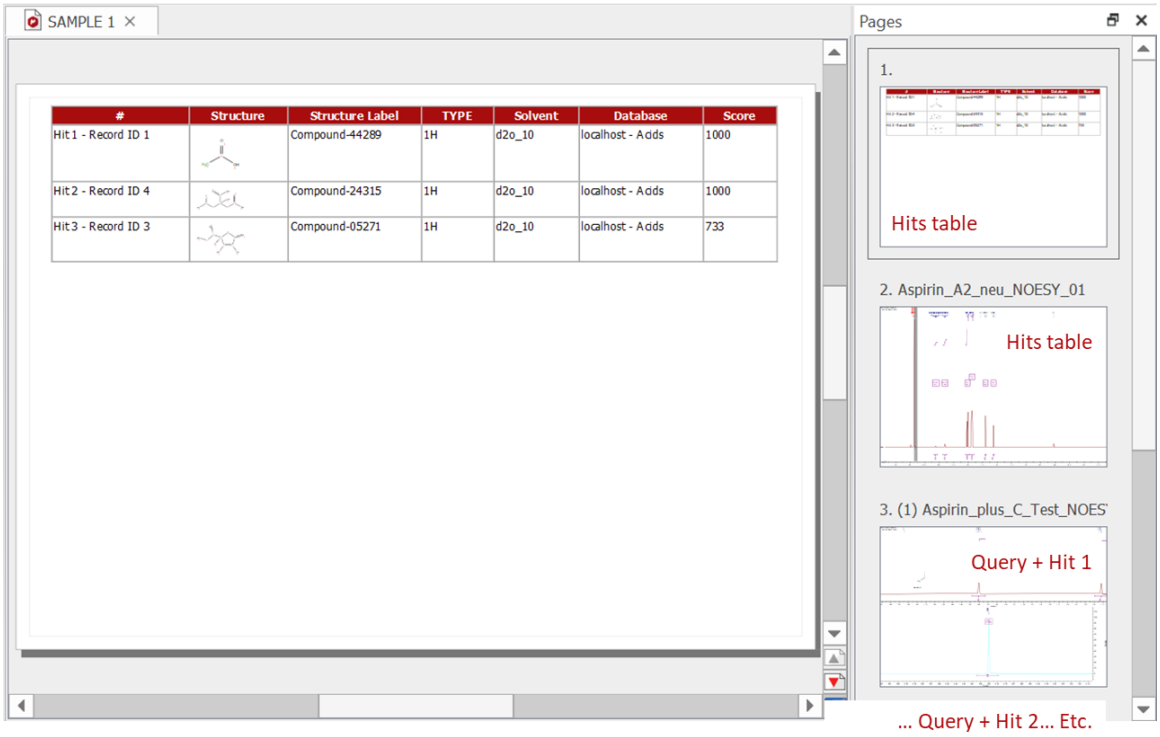
2.3. An Mnova and PDF file

The **PDF** and **Mnova** documents, saved under the "DBSearch" subfolder, have similar structures and follow the applied layout template (default or custom one).

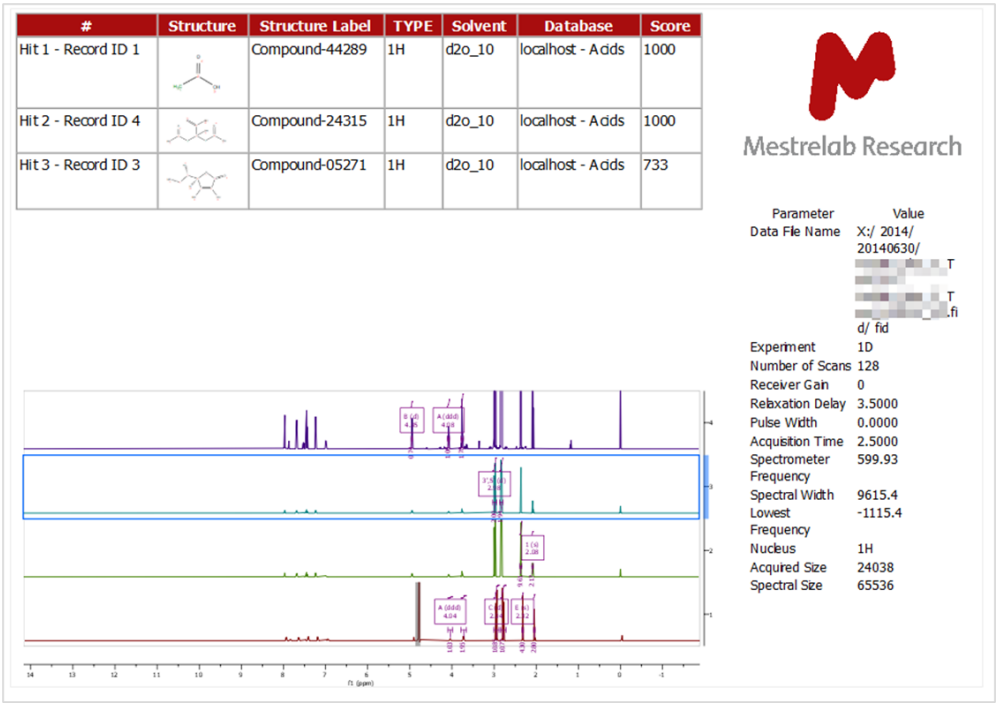
The default layout shows:

- The Hits table on the first page (if the appropriate option is enabled).
- The Query spectrum on the second page.

– Each Hit spectrum displayed with the Query spectrum on a separate page or - if stack option is enabled - the Query and Hit spectra are stacked on the same page.



Below is an example of an Mnova or PDF report using a custom template with the Hit table and Stack options enabled.



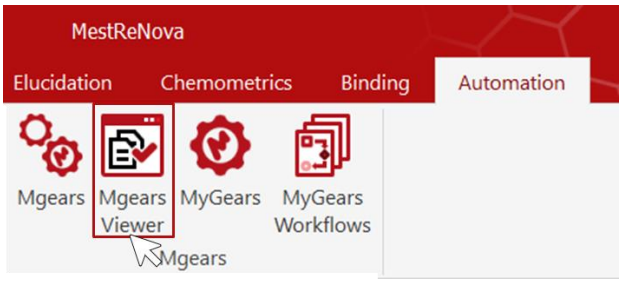
#	Structure	Structure Label	TYPE	Solvent	Database	Score
Hit 1 - Record ID 1		Compound-44289	1H	d2o_10	localhost - Acids	1000
Hit 2 - Record ID 4		Compound-24315	1H	d2o_10	localhost - Acids	1000
Hit 3 - Record ID 3		Compound-05271	1H	d2o_10	localhost - Acids	733

2.4. Other output

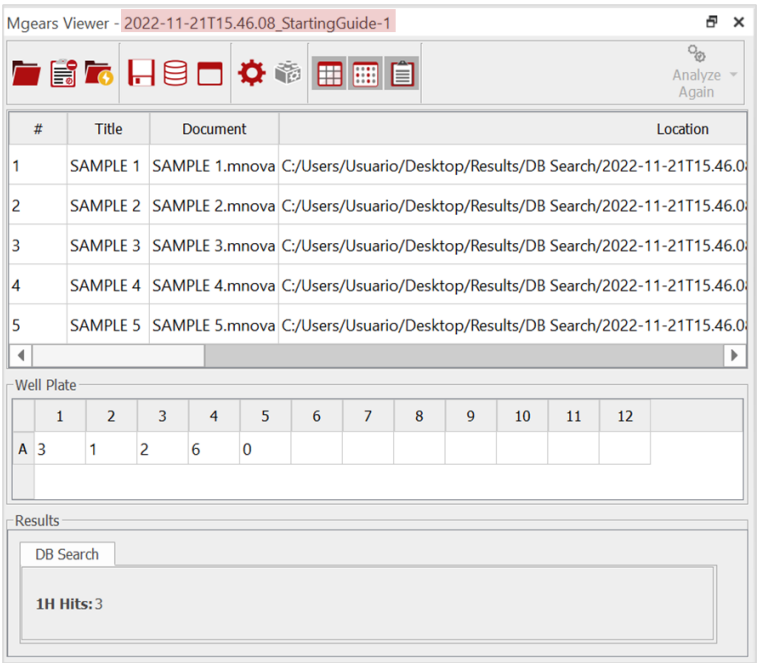
- A “documents” directory, containing the output Mnova files (unless Mgears is configured to save Mnova files in another location).
- A “pdf” directory, containing the output PDF files (unless Mgears is configured to save PDF files in another location).
- A log file of the execution.
- A copy of the settings used in the current evaluation.
- A resume file of the steps followed in the execution.
- A CSS folder, a data folder, an JS folder, and an images folder.

3. Mnova Gears Results Viewer

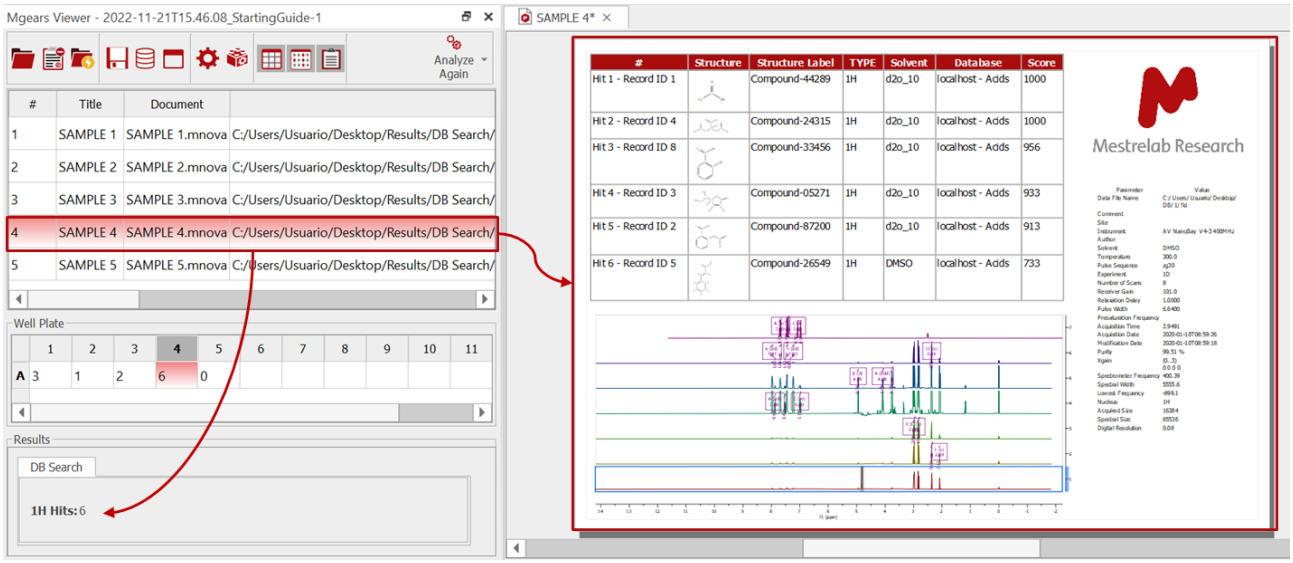
DB Search is compatible with the Mnova Gears Results Viewer. Open the **Mgears Viewer** from the Mnova **Automation** tab.



Click on  and select the DB Search output folder to open. The experiment results will be loaded into the **Mgears Viewer** dialog.



Select a sample in the table or well plate to view the detailed results. The Mgears Viewer dialog will display the **Number of hits** in the **Results** section, and the Mnova results file will be opened to show the hit and query spectra details.



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