



Mestrelab Research

Mnova Hub 1.0

USER MANUAL



Document Number
P/N 489 R1

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Table of Contents

1. INTRODUCTION	3
2. INSTALLATION	3
3. MNOVA HUB DIALOG	4
4. CONNECTING MNOVA HUB TO YOUR DATA SOURCE	5
4.1. SQL SERVER.....	6
4.1.1. <i>The Database tab</i>	6
4.1.2. <i>The Query tab</i>	7
4.2. FILE SYSTEM	9
4.3. MNDB.....	11
4.4. TOPSPIN.....	12
4.5. ZONTAL.....	14
5. EXPLORING AND ANALYZING THE DATA	15
5.1. DATA DISPLAY.....	15
5.2. OPENING DATA IN MNOVA.....	17
5.3. SEARCH FILTERS FOR DATA.....	18
5.3.1. <i>Search filters for ZONTAL</i>	19
5.3. SAVING THE DATA.....	22
5.3.1. <i>Saving data with SQL</i>	22

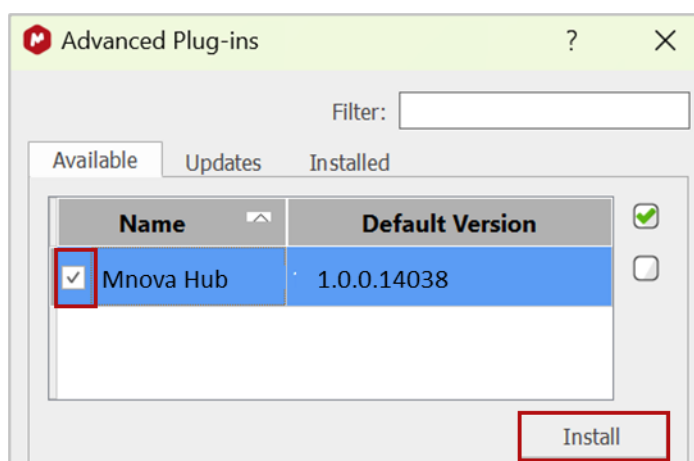
1. Introduction

Mnova Hub is a plugin for Mnova which connects to various data sources and presents users with a comprehensive list of documents (raw and processed Mnova files), allowing them to effortlessly search, browse, filter, preview, open, and save documents directly from Mnova into the source system.

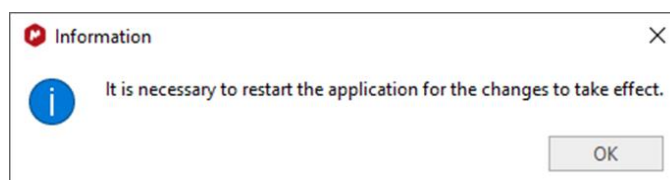
2. Installation

Before installing Mnova Hub, make sure you already have Mnova version 15.0.1 or greater installed and running with valid licenses.

Go to **Files > Advanced Plug-ins > Available**. Tick the **Mnova Hub** plugin, then press **Install**.



Restart Mnova.

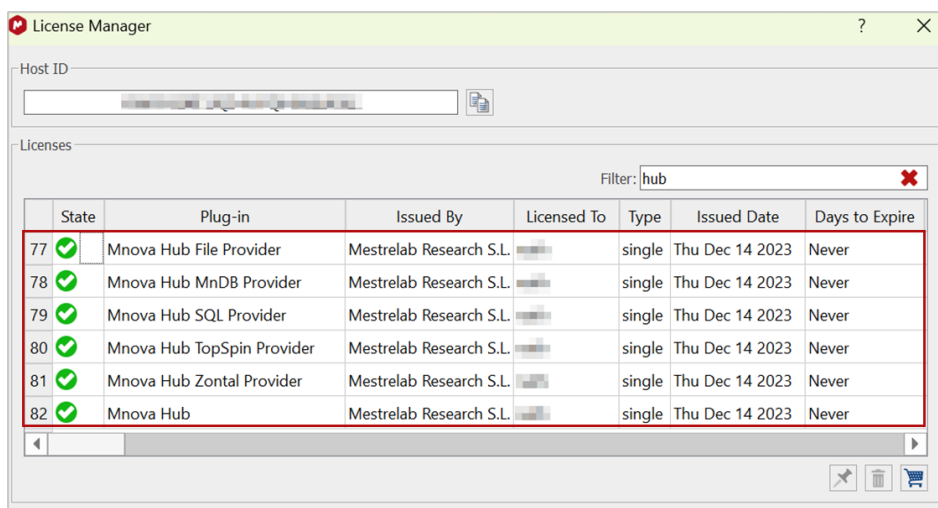


Mnova Hub supports the following data providers:

- SQL Server*
- File system – free for Mnova users
- Mnova Database – free for Mnova DB users
- TopSpin – provided with the Bruker Chemist Suite
- ZONTAL datahub*

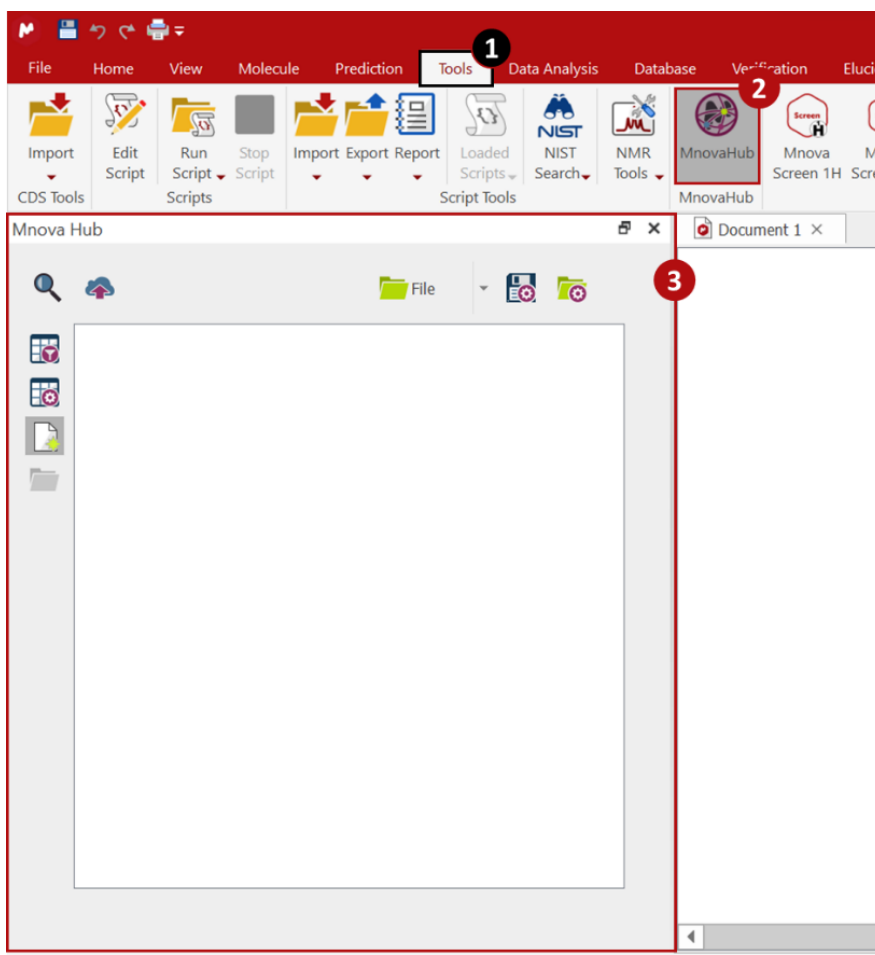
* Please visit our [Store](#) to purchase the required licenses.

You can check your license status by going to **Files > Help > License Manager**; a green check should appear in the plugin's status column.














3. Mnova Hub dialog

Once the plugin is installed and the license activated, you can click on the Mnova **Tools** tab and press the Mnova Hub icon group. The Mnova Hub window will then open. This window can be docked like any other widget, and its visibility and docking position will be retained even after closing and restarting Mnova.



The Mnova Hub dialog features a simple and straightforward design with tooltips that provide information about the buttons/commands.

Command	Description
	Refresh search
 *	Configure search filters
 +	Save file to provider
 File ▾	Configure/change data provider
	Save the configuration of all the providers
	Load the configuration of all the providers
	Show/hide table filters
	Setup results table
 / 	Open in current document or in a new document
	Open the selected files

* Only available with Zontal provider.

+ Not available with TopSpin provider

4. Connecting Mnova Hub to your data source

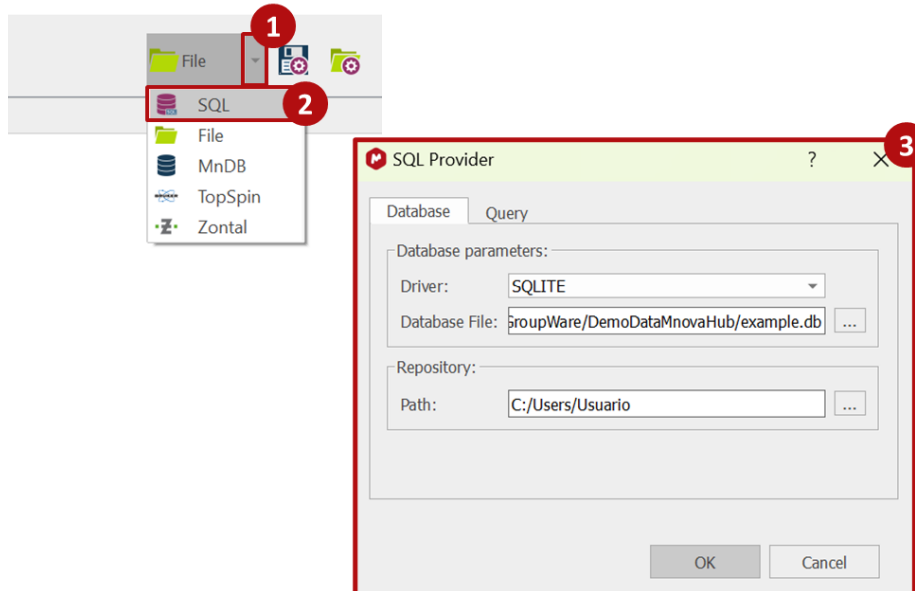
This version of Mnova Hub 1.0 supports the following data providers:

- SQL Server
- File system
- Mnova Database
- TopSpin
- ZONTAL datahub

In the following sections, we will explain how to connect to each of these providers.


4.1. SQL Server

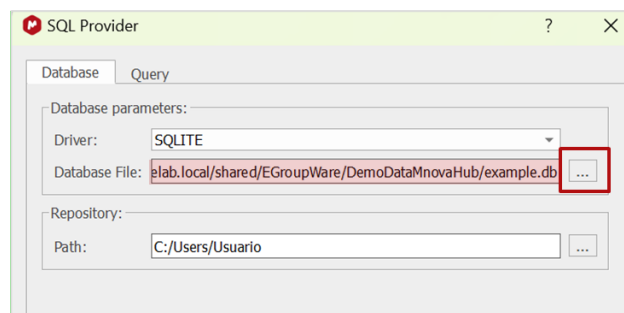
To establish an SQL server as a data provider, initiate the process by clicking on the small arrow adjacent to the dedicated button located at the upper part of the dialog box. By default, this button displays the "File" option, or the name of the most recent provider used. In the dropdown list that appears, select the "SQL" option to proceed with the setup. A dialog box with two tabs will appear: the **Database** tab, and the **Query** tab.



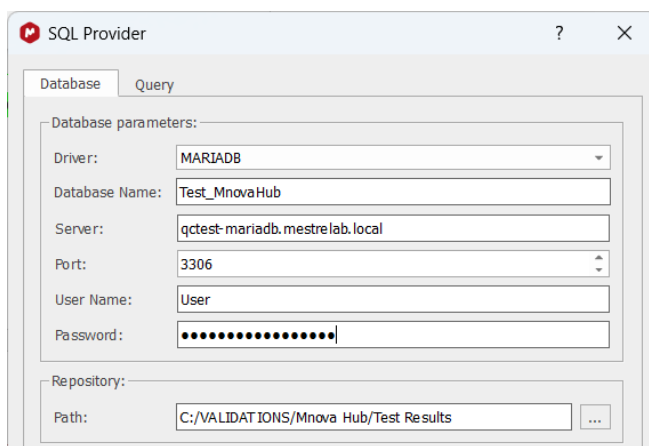
4.1.1. The Database tab

In the **Database** tab, you can configure appropriate database parameters. Depending on the driver used, the required information will vary.

For instance, for the SQLITE driver, you must configure the path to your database file. Click on this button, , and navigate through your files to choose the desired SQL database you want to set as a data source. Select the file and click on **Open**. The chosen database path will be displayed in the dialog, as illustrated in the image below.



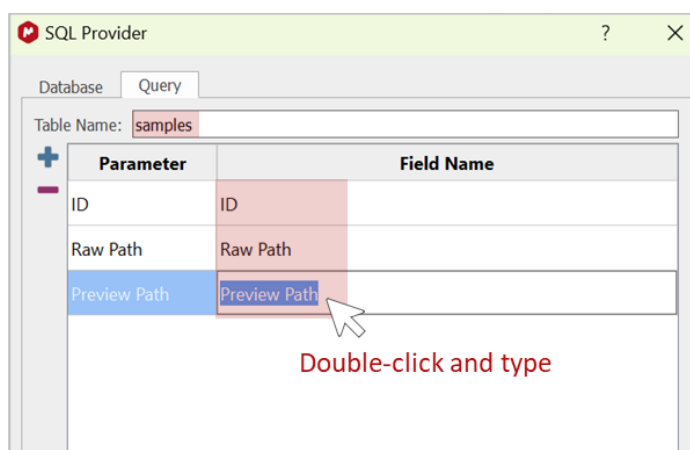
For all other drivers (MariaDB, MySQL, Oracle, and Postgres) you must enter the following parameters: **Database Name**, **Server Name**, **Port**, **Username**, and **Password**.



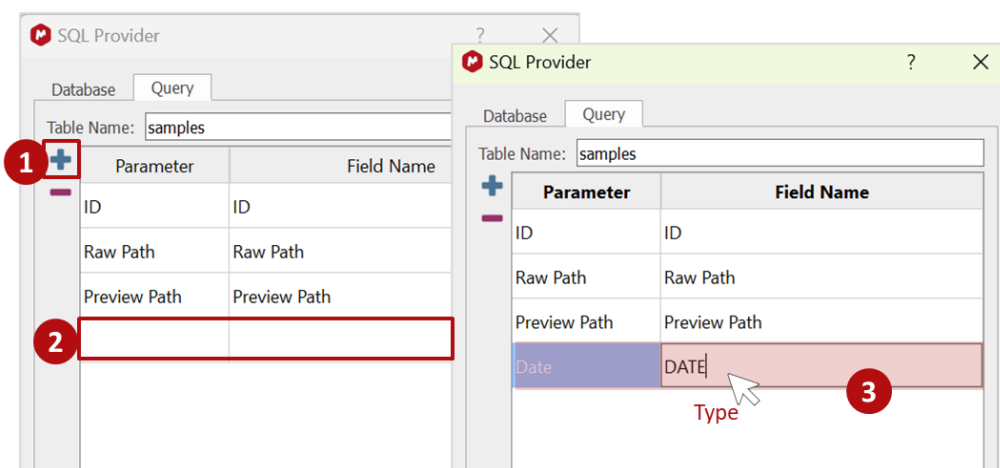
Select the repository path where you wish to save new data files. When saving a record, both .png and .mnova files will be saved at that location.

4.1.2. The Query tab

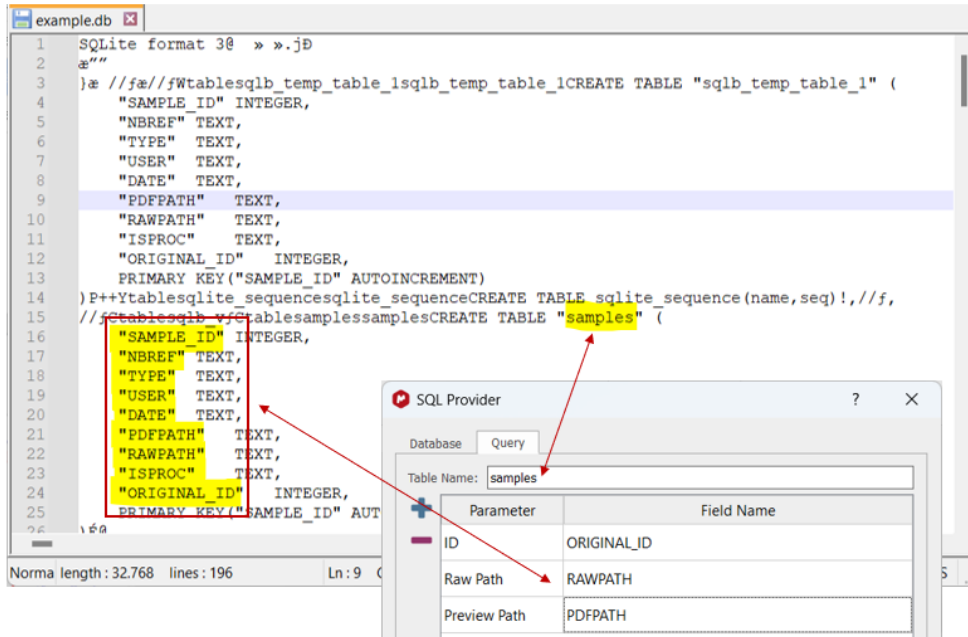
In the **Query** tab, you must identify the SQL table and columns you want to view in Mnova Hub. To do so, you must indicate the **Table Name** and the **(Field) Names** of the parameters **ID**, **Raw Path**, and **Preview Path** of your SQL database.



In addition to the three mandatory fields mentioned above, it is possible to import any other columns you wish to visualize within the Mnova Hub browser. To do so, press the **add** button, . A new line will be added to the table. Type the parameter's name and the database column's header. You can remove a previously added parameter by selecting it and then pressing this button, .

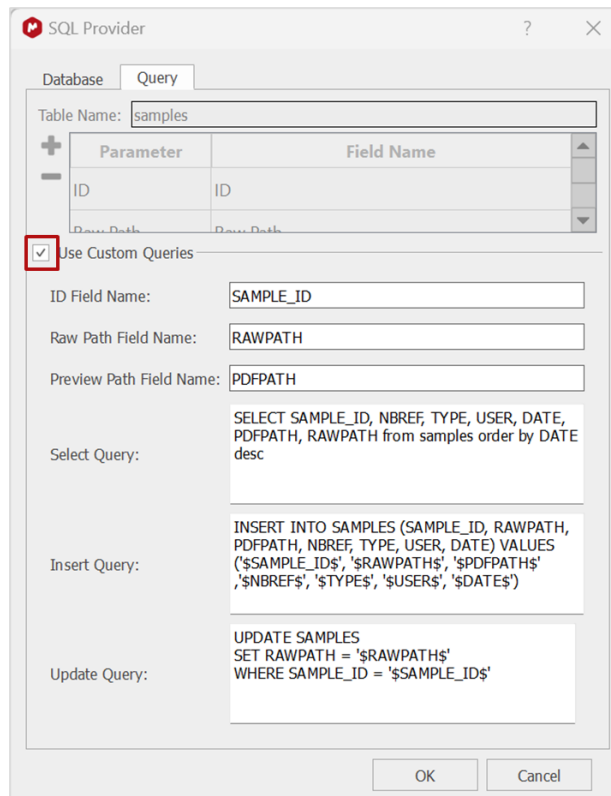



Since these parameters are specific to each database, we advise you to carefully check your database and input the headers of the columns you wish to import into Mnova Hub.



For advanced use, you can set up custom queries to view database columns in a defined order or manner, and to save or update information in your table. To do so, you must enable the **Use Custom Query** option and fill in the available fields for **ID**, **Raw Path**, and **Preview Path**, then enter the **SELECT**, **INSERT**, and **UPDATE** statements. See an example in the image below.

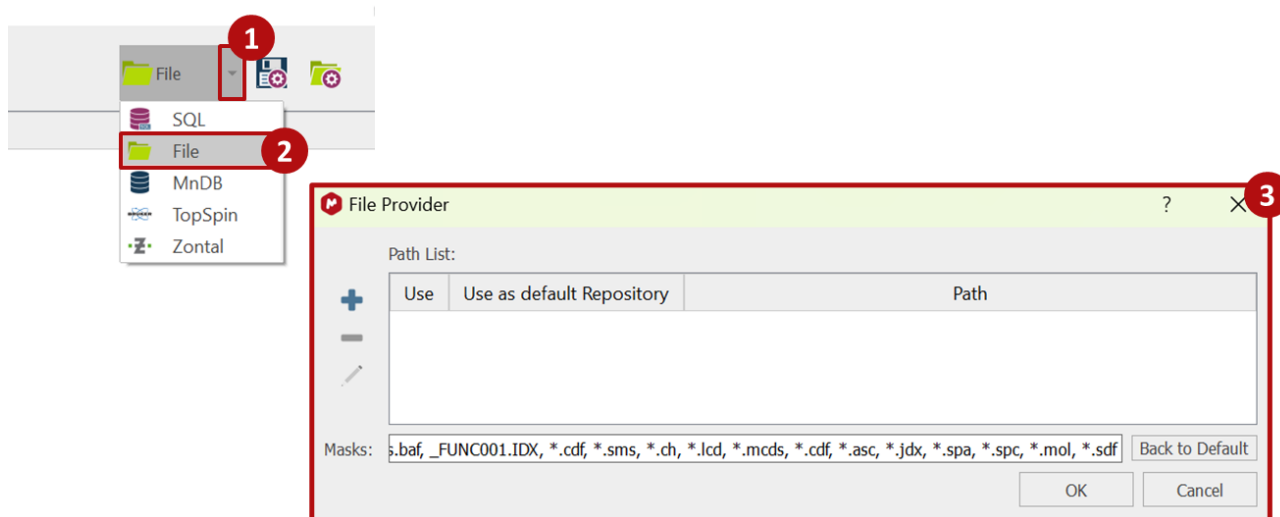
Note. To enable Mnova Hub to save changes to your database, both the database and work fields must be unprotected.




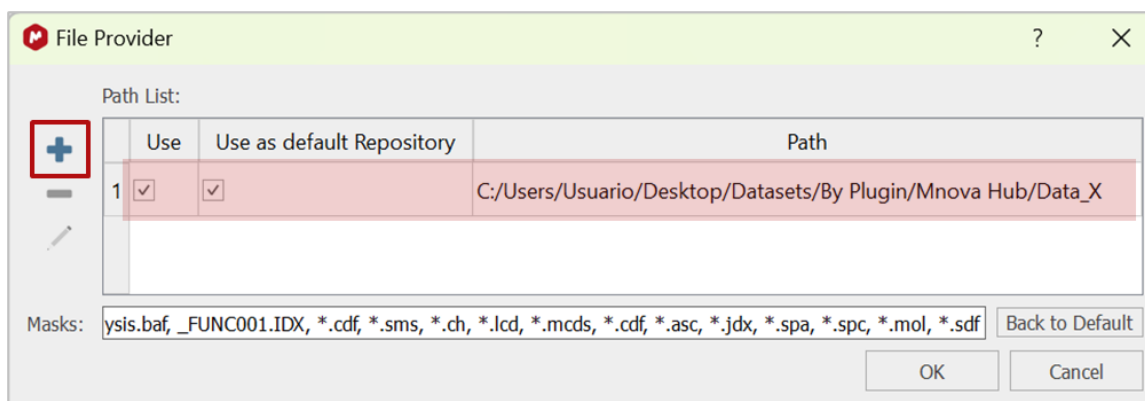
Once you have completed the setup, click **OK** to save the configuration. Press this button, , to refresh and display the datasets found in the specified database. The table setup can be customized as explained in [section 5.1](#).



4.2. File system

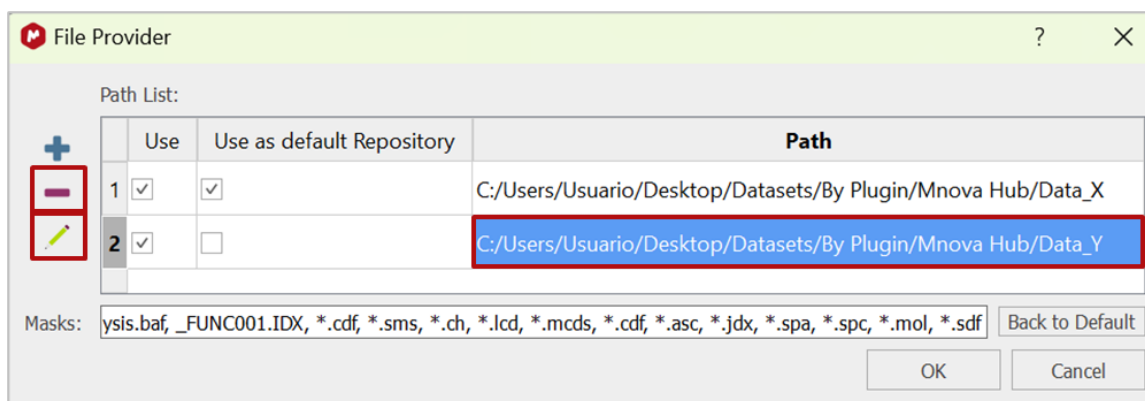
To establish a file system as a data provider, initiate the process by clicking on the small arrow adjacent to the dedicated button located in the upper part of the dialog box. By default, this button displays the "File" option, or the name of the most recent provider used. In the ensuing dropdown list, select the "File" option to proceed with the setup.



A dialog box will appear, allowing you to configure the path to your files. Click on **Add**  and navigate through your folders to choose the one you want to set as the data source. Select the folder. The chosen folder's path will be displayed in the table, as illustrated in the image below.

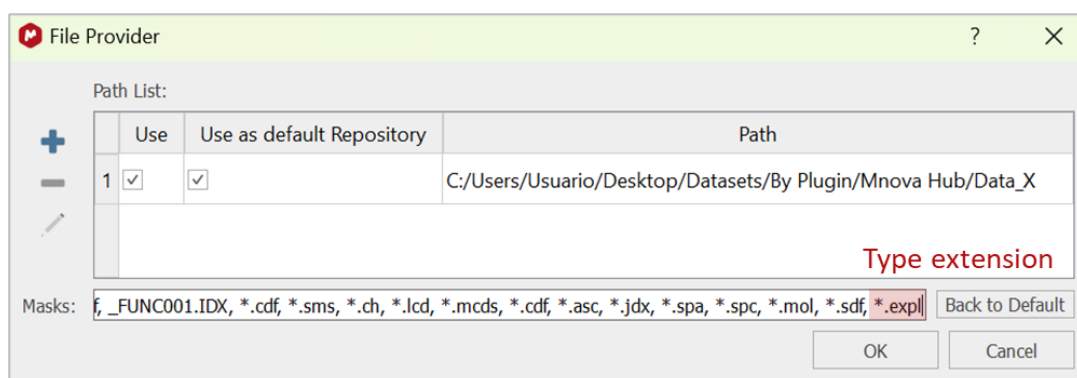



You can add multiple folders by repeating the same process. You can also remove or edit a previously added folder by selecting the desired folder and then pressing this button, , to remove it, or this button, , to edit it.



All added files are automatically set to be used by Mnova Hub by default. To control whether these files should be utilized, you can select or deselect the corresponding checkbox. Also, the first added file is automatically set as the default repository, but you can manually change this setting if required.

Mnova Hub supports various file formats, and a default list of extensions is available. If your file's extension is not in the provided list, simply type it in the corresponding box, and click **OK** to save your changes.



Once you have completed the setup of your data provider, click **OK** to save the configuration. Press this button, , to refresh and display the datasets found in the specified file. The table setup can be customized as explained in [section 5.1](#).

Default view

	Path	Type	ID
1	C:/Users/Usuario/Desktop/...	mnova	AMLODIPINE
2	C:/Users/Usuario/Desktop/...	mnova	ANASTROZOLE
3	C:/Users/Usuario/Desktop/...	mnova	CELEBREX
4	C:/Users/Usuario/Desktop/...	mnova	CLARITHROMYCIN
5	C:/Users/Usuario/Desktop/...	mnova	LAMICTAL
6	C:/Users/Usuario/Desktop/...	mnova	LEVOFLOXACIN
7	C:/Users/Usuario/Desktop/...	mnova	LEVOTHYROXINE
8	C:/Users/Usuario/Desktop/...	mnova	LORATADINE
9	C:/Users/Usuario/Desktop/...	mnova	MOXIFLOXACIN
10	C:/Users/Usuario/Desktop/...	mnova	NASONEX
11	C:/Users/Usuario/Desktop/...	mnova	OLANZAPINE
12	C:/Users/Usuario/Desktop/...	mnova	OLMESARTAN
13	C:/Users/Usuario/Desktop/...	mnova	ONDANSETRON

29 results

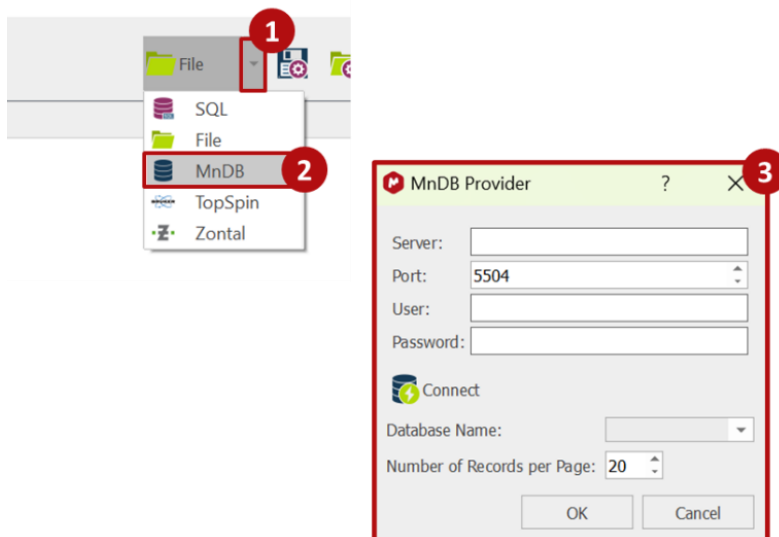
Table view setup

	Show	Column
1	<input checked="" type="checkbox"/>	Path
2	<input checked="" type="checkbox"/>	Type
3	<input checked="" type="checkbox"/>	ID
4	<input type="checkbox"/>	Date
5	<input type="checkbox"/>	Preview Path

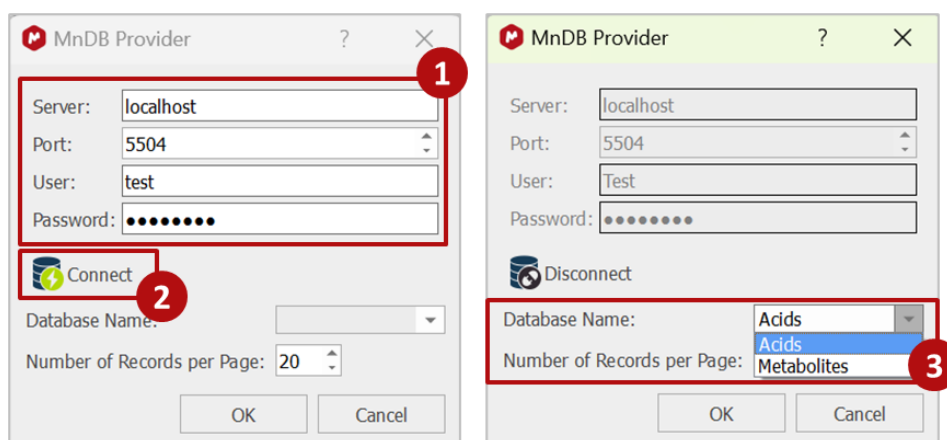
29 results

4.3. MnDB


To establish an Mnova Database as a data provider, initiate the process by clicking on the small arrow adjacent to the dedicated button located in the upper part of the dialog box. By default, this button displays the "File" option or the name of the most recent provider used. In the dropdown list that appears, select the "MnDB" option to proceed with the setup.



A dialog box will appear, enabling you to connect to a DB server and choose the desired database. Enter the connection information and click **Connect**. Once connected, select the desired database from the available options in the dropdown list.

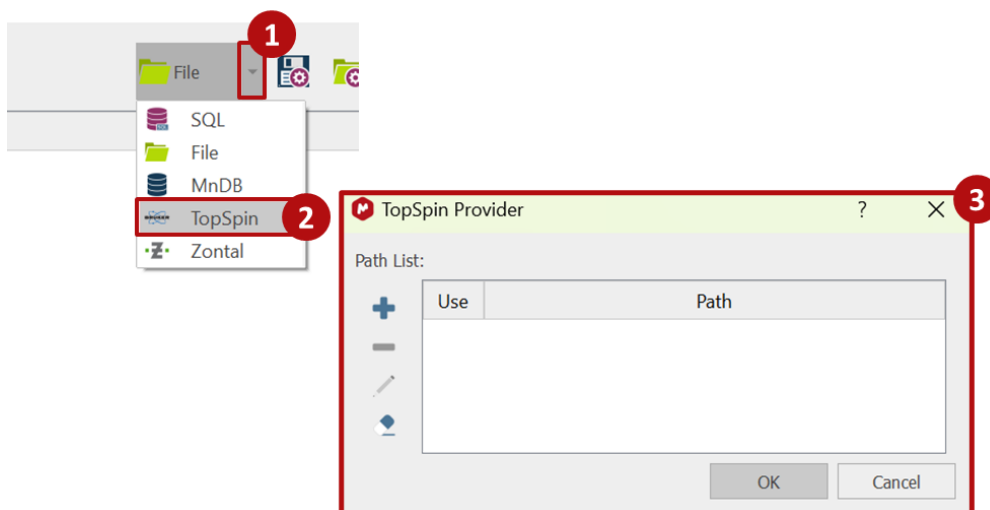


Additionally, you can define the number of records you wish to display per page. Use the text box to enter the value, or the selector to set the page number.

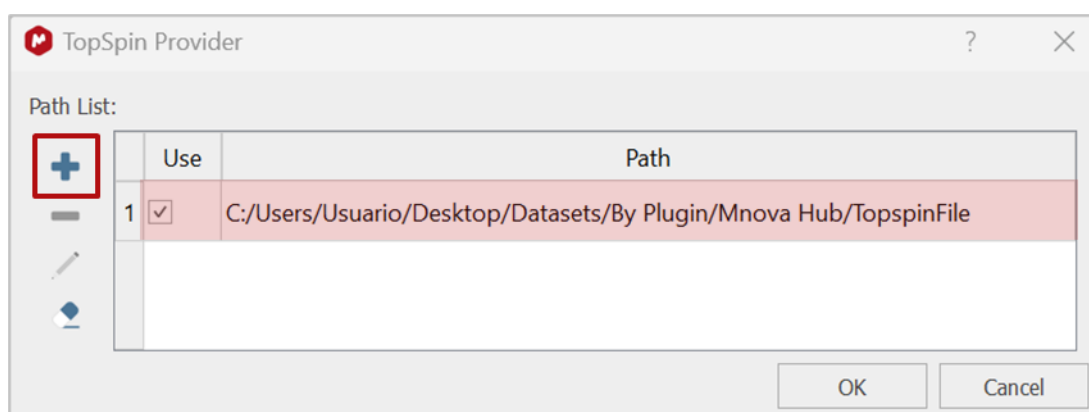
Once you have completed the setup of your data provider, click **OK** to save the configuration. Press this button, , to refresh and display the datasets found in the specified database. The table setup can be customized as explained in [section 5.1](#).



4.4. TopSpin

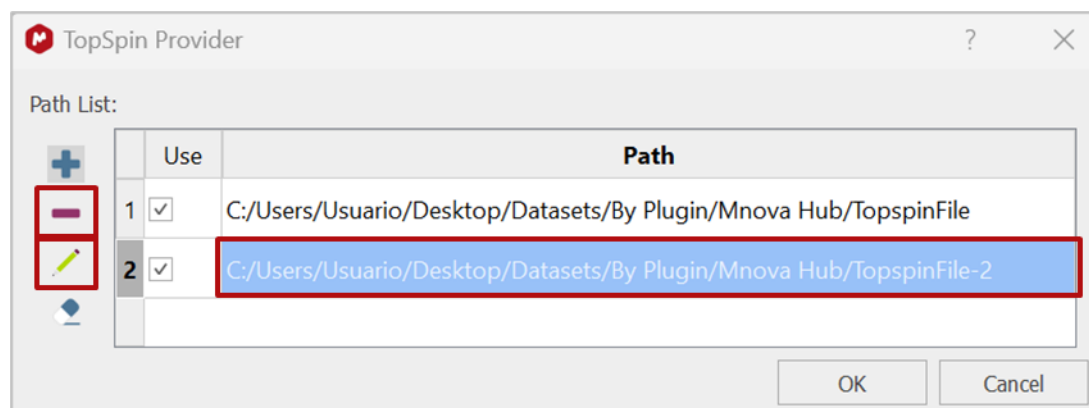
To establish TopSpin as a data provider, initiate the process by clicking on the small arrow adjacent to the dedicated button located in the upper part of the dialog box. By default, this button displays the "File" option or the name of the most recent provider used. In the ensuing dropdown list, select the "TopSpin" option to proceed with the setup.



A dialog box will appear, allowing you to configure the path to your files. Click on **Add +** and navigate through your folders to choose the Topspin folder you want to set as a data source. Select the folder. The chosen folder's path will be displayed in the table, as illustrated in the image below.





You can add multiple folders by repeating the same process. You can also remove or edit a previously added folder by pressing this button, , to remove it, or this button, , to edit it.



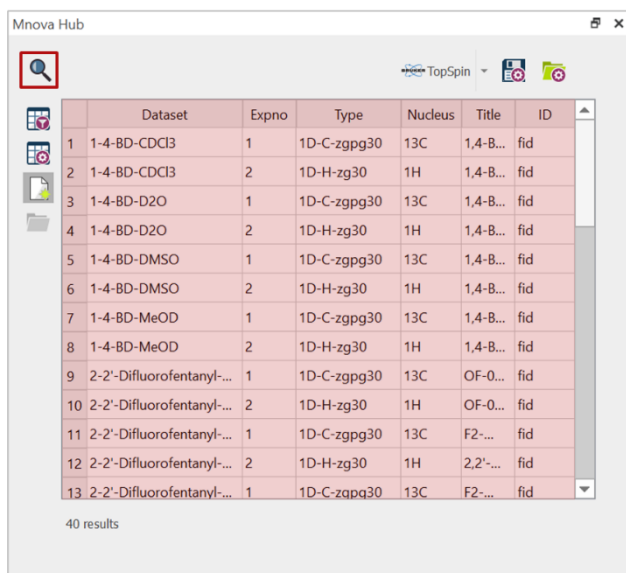
To control whether these folders will be utilized, you can select or deselect the corresponding checkbox.

	Use	
1	<input checked="" type="checkbox"/>	C:/Users/Usuario/Des
2	<input type="checkbox"/>	C:/Users/Usuario/Des

You can press this button, , to clear cached metadata from TopSpin.

Once you have completed the setup of your data provider, click **OK** to save the configuration. Press this button, , to refresh and display the datasets found in the specified folder. The table setup can be customized as explained in [section 5.1](#).

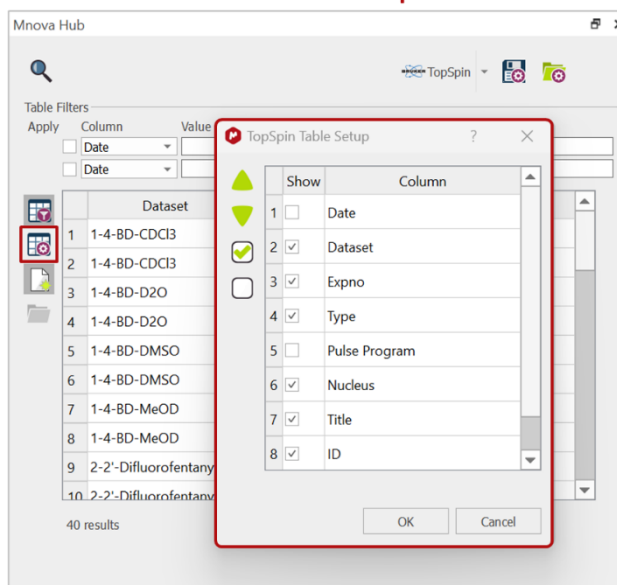
Default view



	Dataset	Expno	Type	Nucleus	Title	ID
1	1-4-BD-CDCI3	1	1D-C-zgpg30	13C	1,4-B...	fid
2	1-4-BD-CDCI3	2	1D-H-zg30	1H	1,4-B...	fid
3	1-4-BD-D2O	1	1D-C-zgpg30	13C	1,4-B...	fid
4	1-4-BD-D2O	2	1D-H-zg30	1H	1,4-B...	fid
5	1-4-BD-DMSO	1	1D-C-zgpg30	13C	1,4-B...	fid
6	1-4-BD-DMSO	2	1D-H-zg30	1H	1,4-B...	fid
7	1-4-BD-MeOD	1	1D-C-zgpg30	13C	1,4-B...	fid
8	1-4-BD-MeOD	2	1D-H-zg30	1H	1,4-B...	fid
9	2-2'-Difluorofentanyl-...	1	1D-C-zgpg30	13C	OF-0...	fid
10	2-2'-Difluorofentanyl-...	2	1D-H-zg30	1H	OF-0...	fid
11	2-2'-Difluorofentanyl-...	1	1D-C-zgpg30	13C	F2-...	fid
12	2-2'-Difluorofentanyl-...	2	1D-H-zg30	1H	2,2'-...	fid
13	2-2'-Difluorofentanyl-...	1	1D-C-zgpg30	13C	F2-...	fid

40 results

Table view setup

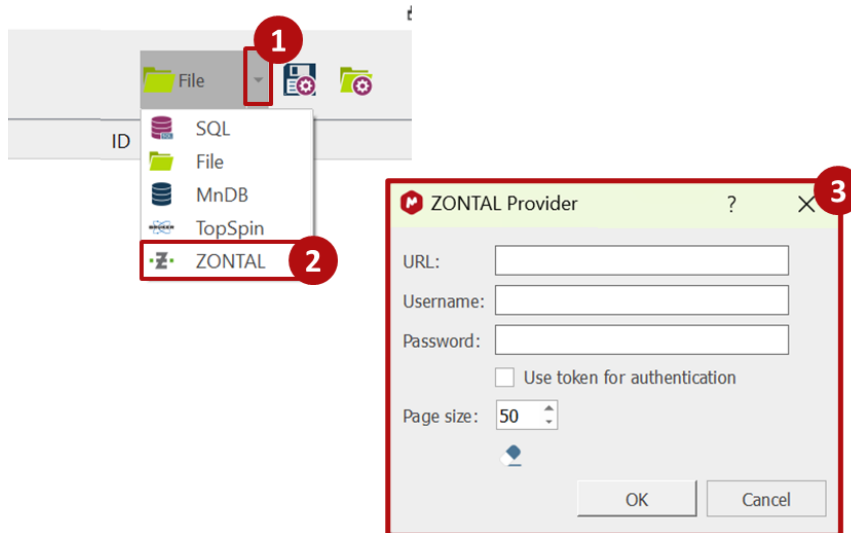


	Show	Column
1	<input type="checkbox"/>	Date
2	<input checked="" type="checkbox"/>	Dataset
3	<input checked="" type="checkbox"/>	Expno
4	<input checked="" type="checkbox"/>	Type
5	<input type="checkbox"/>	Pulse Program
6	<input checked="" type="checkbox"/>	Nucleus
7	<input checked="" type="checkbox"/>	Title
8	<input checked="" type="checkbox"/>	ID

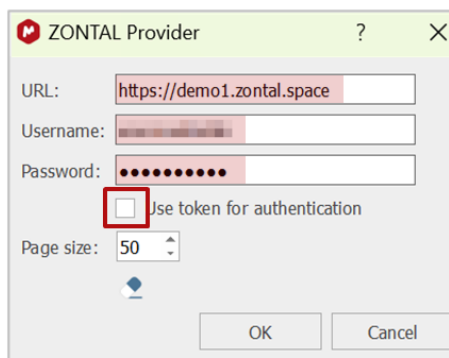
OK Cancel

4.5. ZONTAL

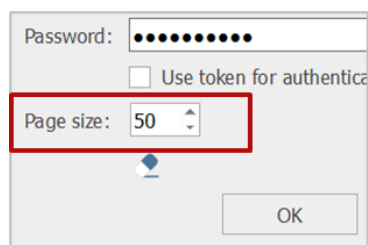
To establish a ZONTAL Space as a data provider, initiate the process by clicking on the small arrow adjacent to the dedicated button located in the upper part of the dialog box. By default, this button displays the "File" option or the name of the most recent provider used. In the ensuing dropdown list, select the "ZONTAL" option to proceed with the setup. A dialog box will appear.




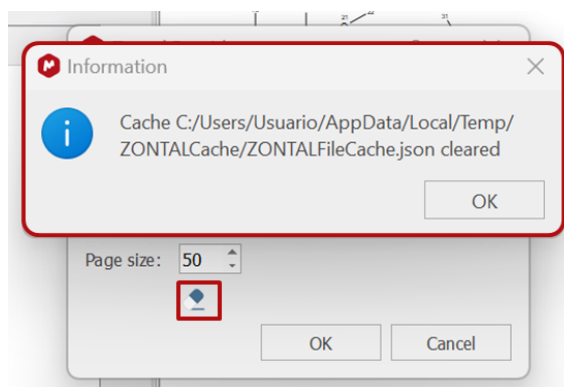
Fill in the required connection information: **URL**, **Username**, and **Password**. When necessary, enable the **Use Token for authentication** option.




The ZONTAL provider allows you to define a page size to display in Mnova Hub. Use the text box to type in, or the selector to set the number of results, per page.



You can press this button, , to clear cached metadata from ZONTAL.



Once you have completed the setup of your data provider, click **OK** to save the configuration. Press this button, , to refresh and display the datasets found in the specified location. The table setup can be customized as explained in [section 5.1](#).

Default view

ID	Type
1 CSAA676860_S02A481142...	MNova Demo
2 acquis	TopSpin Raw MVP
3 Columbo-PM-22-291-...	XCalibur Raw MVP
4 JR_20211013_Dimitri_mixe...	XCalibur MDM
5 STARK_210426_PM-20-315...	XCalibur MDM
6 acquis	TopSpin Raw MVP
7 NewTest.mnova	MNova Demo
8 Test.mnova	MNova Demo
9 CSAA676860_S02A481142...	MNova Demo
10 Test_2D.mnova	MNova Demo
11 testUpload.mnova	MNova Demo
12 Document 14.mnova	MNova Demo
13 Document 13.mnova	MNova Demo

Table view setup

Show	Column
<input type="checkbox"/>	Date
<input checked="" type="checkbox"/>	ID
<input type="checkbox"/>	Type


Note. Deleted or purged datafiles from the ZONTAL Space cannot be previewed or opened with Mnova Hub. If you attempt to open a deleted or purged document, a warning message will appear.

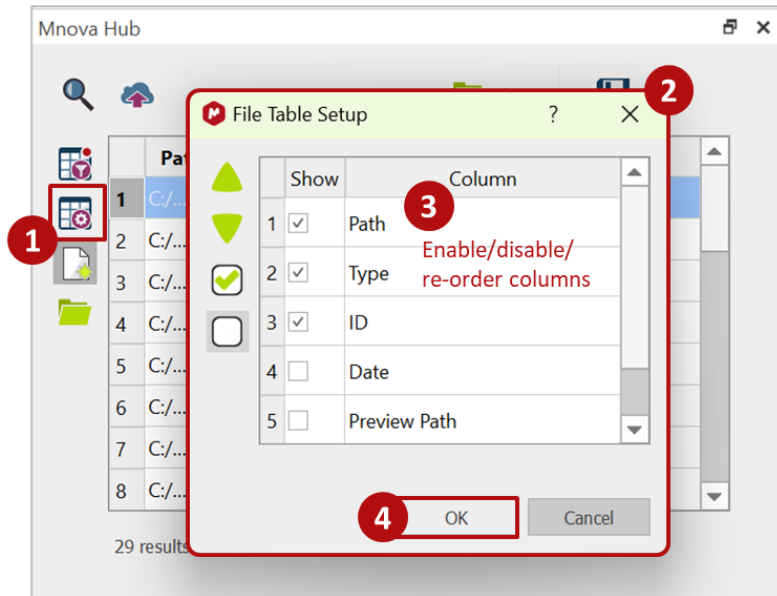
5. Exploring and analyzing the data

The usage of Mnova Hub is independent of the data source, although certain data providers may offer additional functionality such as a filter dialog or saving back to the host system. In this section, we will describe the general Mnova Hub functionalities that enable you to view, open, and save data.

5.1. Data display

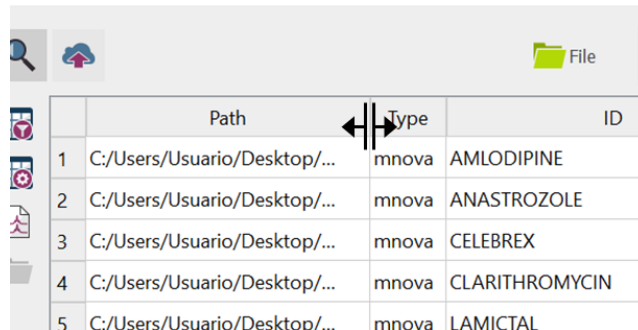
The available data is presented in a table within the Mnova Hub main window, featuring columns displaying information such as dataset path, Type, ID, and other details. The specifics of this information depend on your chosen data provider and your data.

To customize the dataset results table, click on this button, , to open the table setup. Here, you can choose to display or hide specific columns and use the green arrows to arrange columns in your preferred order. Options to select all or deselect all columns are available. Press **OK** to save the setup.

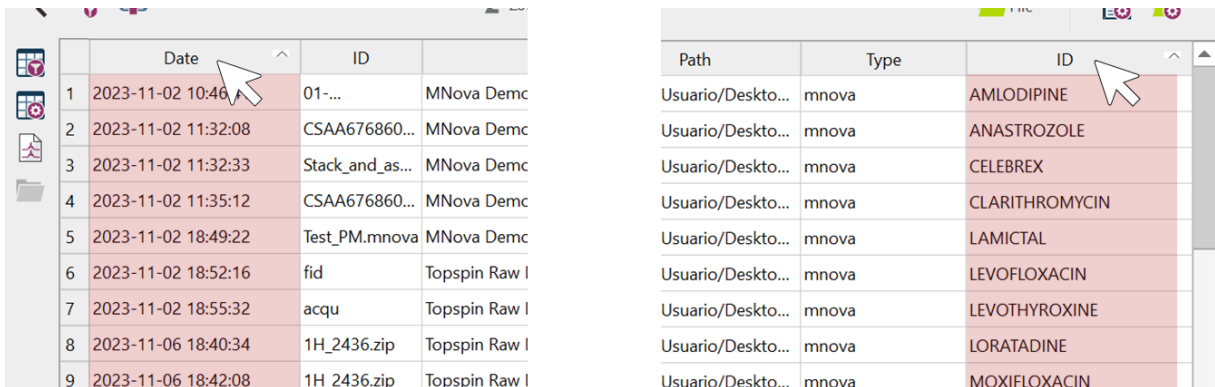


Note. The available fields depend on the provider. For instance, when a provider, such as SQL Server, allows additional fields to be imported into Mnova Hub, these will automatically be updated and become visible in the **Table Setup** dialog box.

You can manually adjust the width of the columns to enhance visualization.

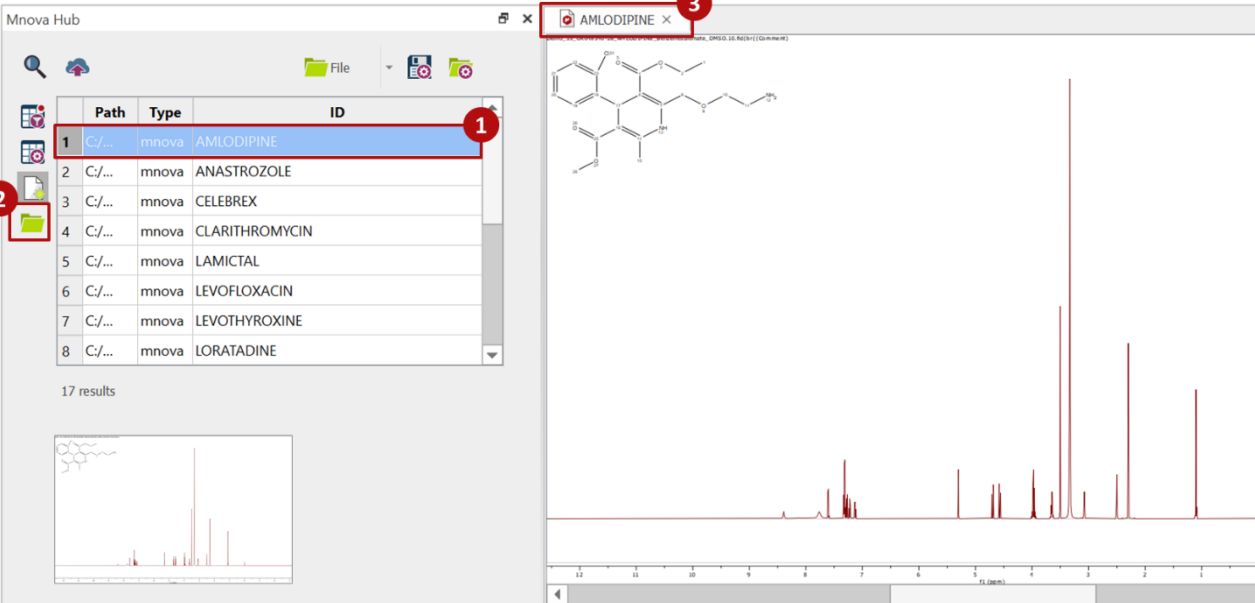


Clicking a column header will sort the data based on that header. For example:



5.2. Opening data in Mnova


To open a dataset in Mnova, you can either select the dataset and press the open button, or simply double-click on the dataset. A single click will display a preview of the dataset if the files (.png) are available from the provider.

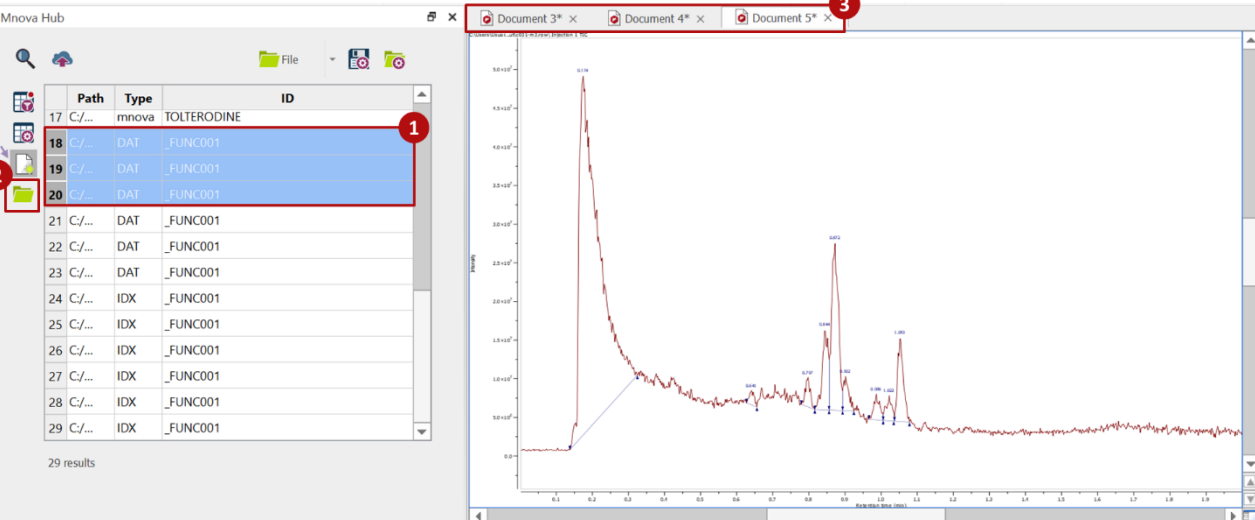


The screenshot displays the Mnova Hub interface. On the left, a file list table is visible with columns for Path, Type, and ID. The first row is highlighted in blue. A red box with the number 1 points to the 'AMLODIPINE' entry. A red box with the number 2 points to the open button icon in the toolbar. A red box with the number 3 points to the 'AMLODIPINE' document tab at the top. The main area shows the chemical structure of Amlodipine and its corresponding NMR spectrum with peaks labeled.

Path	Type	ID
C:/...	mnova	AMLODIPINE
C:/...	mnova	ANASTROZOLE
C:/...	mnova	CELEBREX
C:/...	mnova	CLARITHROMYCIN
C:/...	mnova	LAMICTAL
C:/...	mnova	LEVOFLOXACIN
C:/...	mnova	LEVOTHYROXINE
C:/...	mnova	LORATADINE


It is possible to open multiple datasets at once. To do so, select the datasets of interest by holding the “Ctrl” key. Then press the open button. The selected spectra will be opened in separate Mnova documents or on the same page depending on the selection of the toggle **Open in current Document/Open in a new Document**.

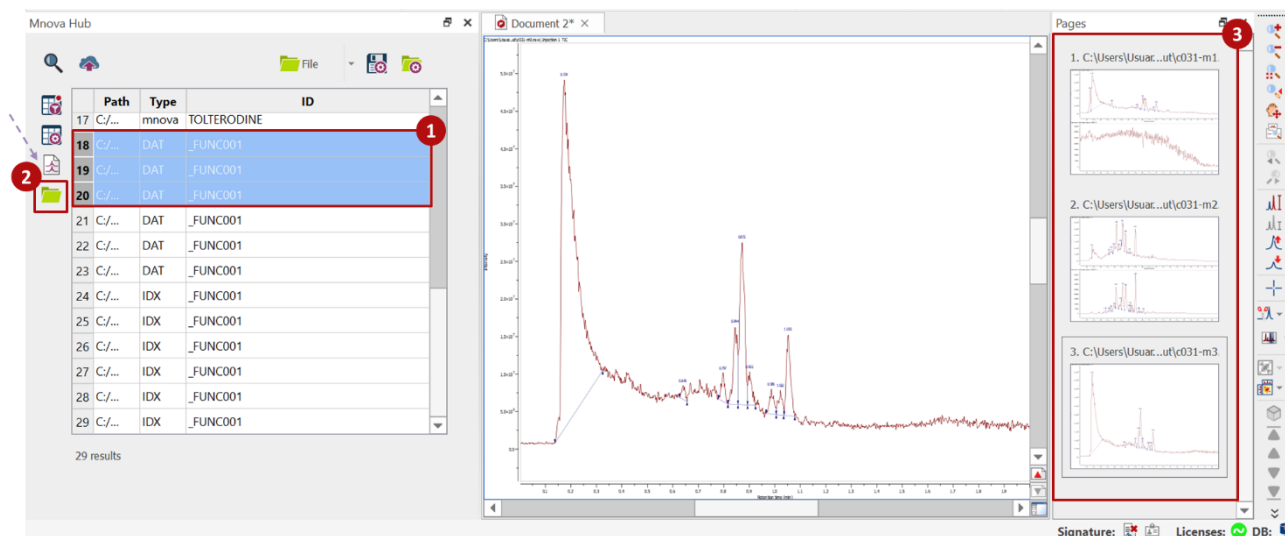
Using the **Open in a New document** () option will generate three documents with the selected three datasets, as per the image below.




The screenshot shows the Mnova Hub interface with multiple datasets selected. The file list table on the left has rows 18, 19, and 20 highlighted in blue. A red box with the number 1 points to the 'TOLTERODINE' entry. A red box with the number 2 points to the open button icon. A red box with the number 3 points to the three document tabs at the top: 'Document 3*', 'Document 4*', and 'Document 5*'. The main area shows the NMR spectrum of Tolterodine with peaks labeled.

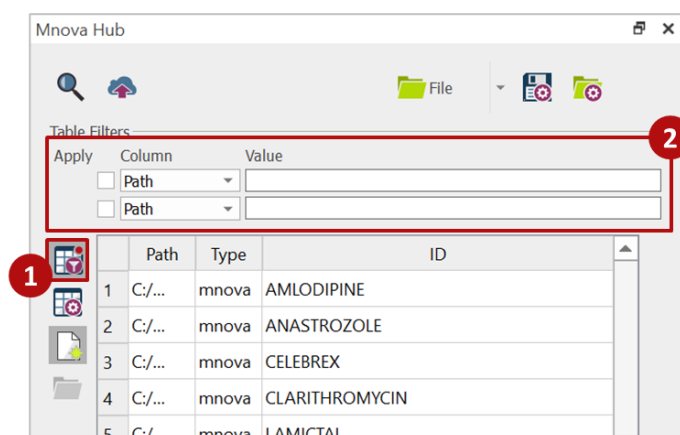
Path	Type	ID
C:/...	mnova	TOLTERODINE
C:/...	DAT	_FUNC001
C:/...	DAT	_FUNC001
C:/...	DAT	_FUNC001
C:/...	DAT	_FUNC001
C:/...	DAT	_FUNC001
C:/...	DAT	_FUNC001
C:/...	IDX	_FUNC001
C:/...	IDX	_FUNC001
C:/...	IDX	_FUNC001
C:/...	IDX	_FUNC001
C:/...	IDX	_FUNC001
C:/...	IDX	_FUNC001
C:/...	IDX	_FUNC001
C:/...	IDX	_FUNC001

Using the **Open in current document** () option will generate one document with one page per dataset, as shown in the image below. **NOTE:** this option is only available for non-Mnova documents (raw data).

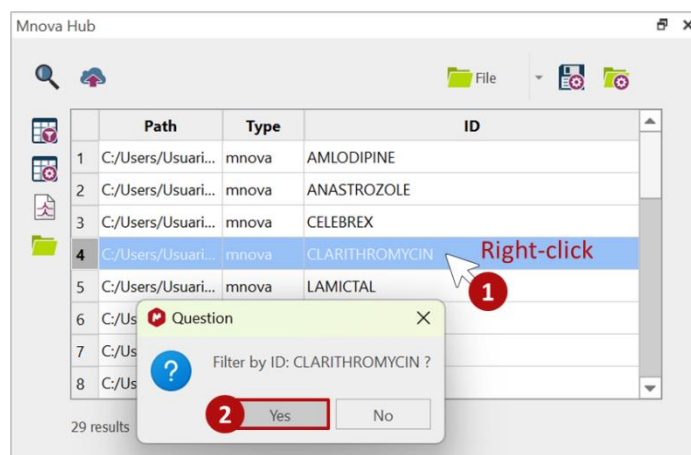


5.3. Search filters for data


Mnova Hub enables you to easily fine-tune your search results using column-specific filters. You can either click on this button, , to expand the table filters menu, where you can select the column from the drop-down list and enter the substring for your desired filter, as per the image below:

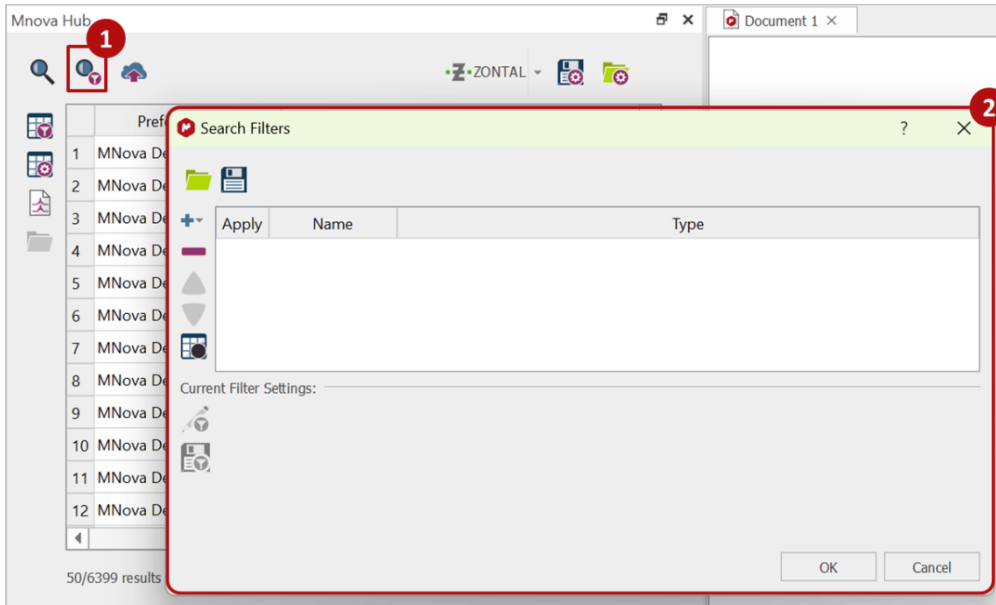


or alternatively, you can right-click on any table result, and the filter will be automatically generated with the corresponding column and value.




5.3.1. Search filters for ZONTAL

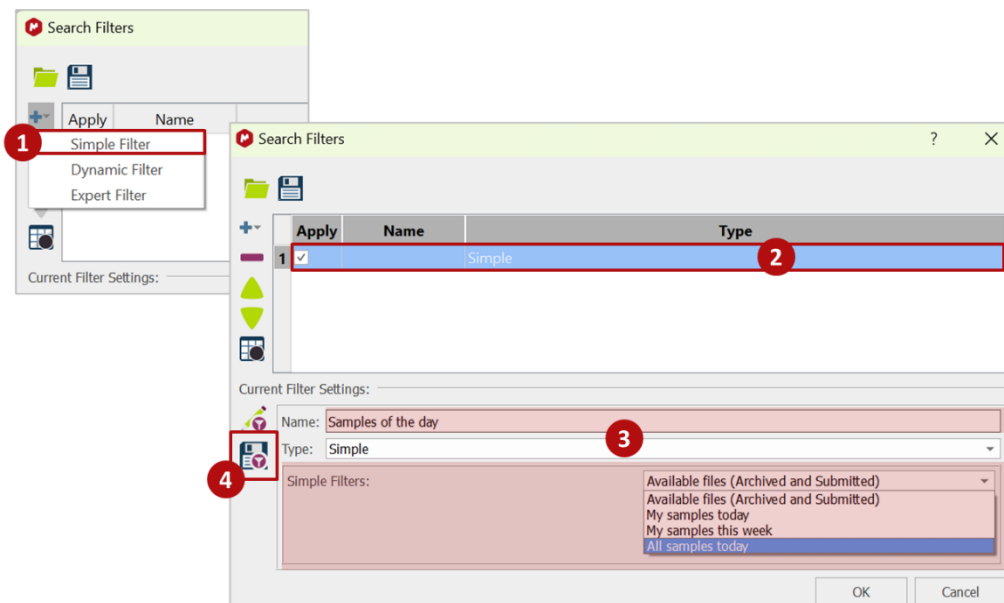
ZONTAL provides advanced options to optimize search efficiency. After configuring the ZONTAL provider, an additional button, , appears in the upper part of the Mnova Hub main dialog. Click this button to open the **Search Filters** dialog.




To add a search filter, press the **Add** button and choose one of the following filter options: **Simple Filter**, **Advanced Filter**, or **Expert Filter**. The tool is designed to work seamlessly with single or multiple filters, offering high adaptability and flexibility.

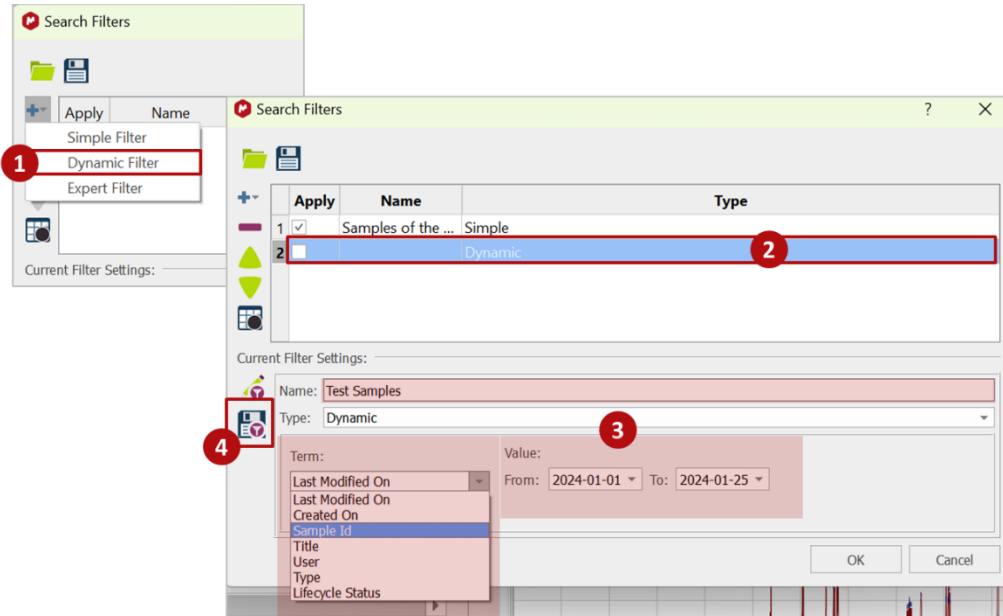
5.3.1.1. Simple Filters

Simple filters are pre-built and easy to configure. Upon selecting this option, provide a name for your filter and choose the desired filter option (e.g., **Available files (Archived and Submitted)**, **My samples today**, **My samples this week**, or **All samples today**). Press this button, , to save your configuration.




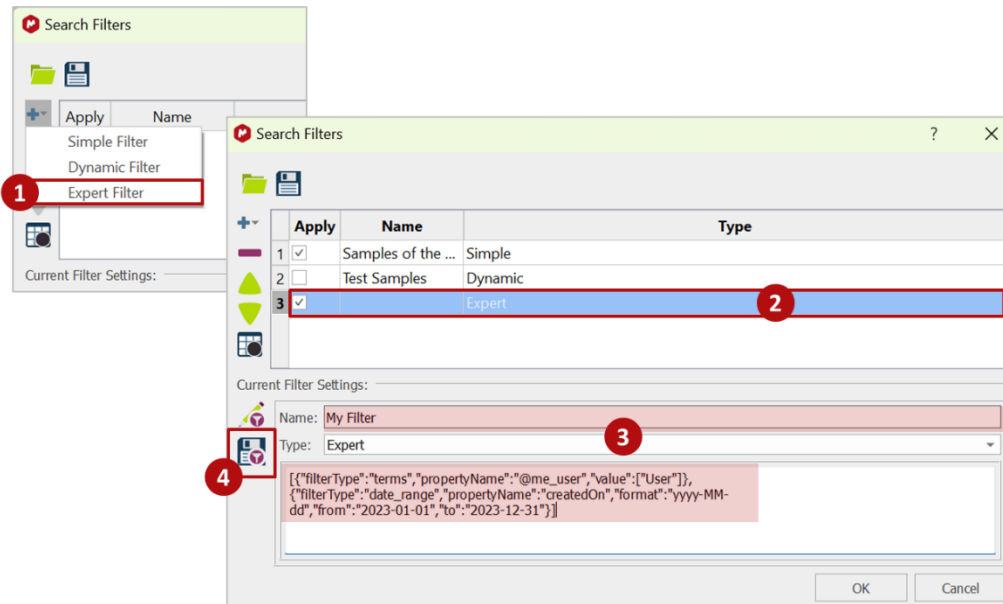
5.3.1.2. Dynamic Filters

Dynamic filters allow you to build queries using available search fields such as **Last Modified On**, **Created On**, **Sample ID**, **Title**, **User**, **Type**, and **Lifecycle Status**. Upon selecting this option, provide a name for your filter and choose the desired filter option then press this button, , to save your configuration.

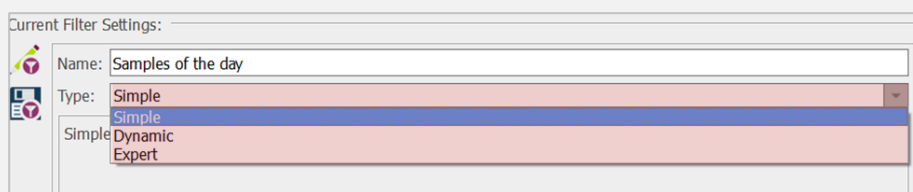


5.3.1.3. Expert Filters

Expert filters offer expert-level flexibility for complete customization. When choosing this option, the text box already displays an arrayed filter in JSON format to serve as an example. You can either edit this text or enter your own filter in the [native language](#) of the provider. Press this button, , to save the configuration.



Note. You can modify the type of filter after adding it to the table by selecting the desired type from the dropdown menu.



5.3.1.4. Managing ZONTAL filters

Managing filters is made easy through an intuitive set of features:

Simultaneous Filter Application: Apply multiple filters simultaneously by checking or unchecking the desired filters using the checkboxes in the first column of the table.

Editing and Removing Filters: It is possible to edit or remove a filter at any time, providing flexibility in adjusting your search criteria.

Filter Order: Filters are applied in the same order as they appear in the table. You can modify the order to prioritize them by using the green arrows on the left side of the table.

Saving and Loading Filters: Save and load filters using the indicated buttons. The filters are stored in *.data format, ensuring easy retrieval and reuse.

Command	Description
	Load filters (*.data)
	Save filters (*.data)
	Add a filter
	Remove filter
	Move filter (up/down)
	Show/Hide filter settings column
	Edit filter
	Save current filter

5.3.1.5. Displaying search results

Once you have completed your filter setup, press **OK** to apply the filters. In the main Mnova Hub dialog, press **Refresh** to display the filtered results.

Note. If a filter is being applied, the **Search Filters** button in the main Mnova Hub dialog displays a red indicator to alert the user, .

In the example below, a search using **Expert Filters** by user “*Usuario*” within the date range “*from 01.03.2021 to 10.04.2021*” displays three results in Mnova Hub, identical to the results obtained in the ZONTAL space.

In ZONTAL Space

In Mnova Hub

Current Filter Settings:

Name:

Type: Expert

```

[{"filterType": "terms", "propertyName": "@me_user", "value": ["Usuario"]},
{"filterType": "date_range", "propertyName": "createdOn", "format": "yyyy-MM-dd", "from": "2023-03-01", "to": "2023-04-10"}

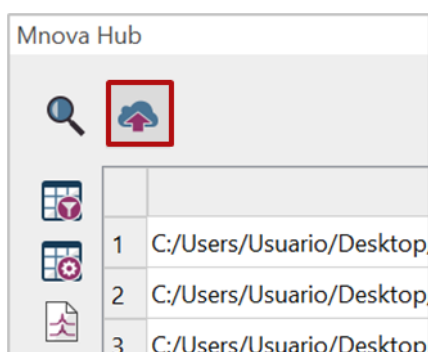
```

Note. When performing searches using any kind of search filter, all kinds of documents (archived, submitted, deleted, and purged) are displayed. However, only archived/submitted documents can be loaded onto the canvas. Attempting to open deleted/purged documents triggers a warning message.

5.3. Saving the data

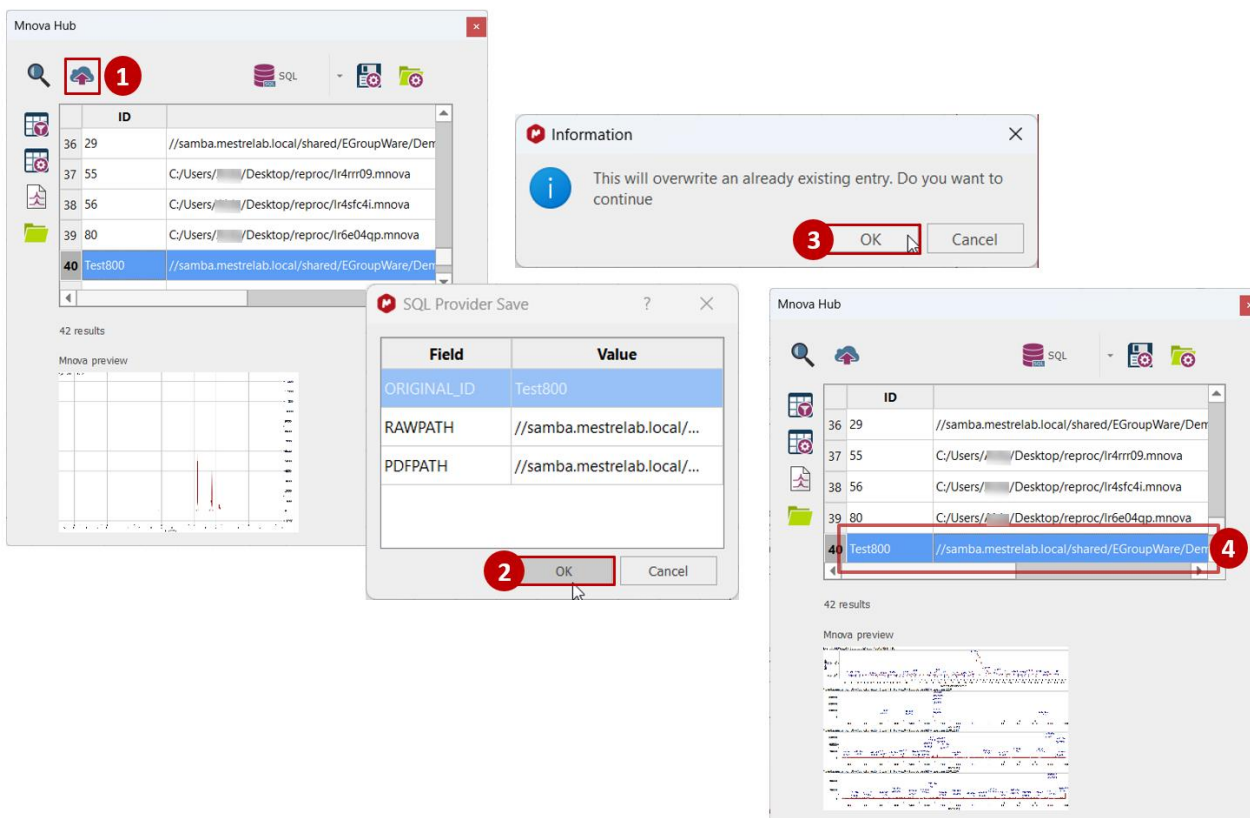
Some providers present a **Save** option to send data back to the remote system once you have processed it in Mnova:

- When dealing with data from a **file provider**, users can upload new documents or overwrite existing ones.
- When using the **MnDB** as a data provider, Mnova documents can be uploaded to the database as new entries. Please note that all objects present in the document (mol file, NMR spectra, MS spectra, etc.) will be saved as different items in a new record in the database.
- For the **ZONTAL** provider, Mnova documents are uploaded as new entries. When clicking Save, a dialog will open asking the user for the title of the new entry.



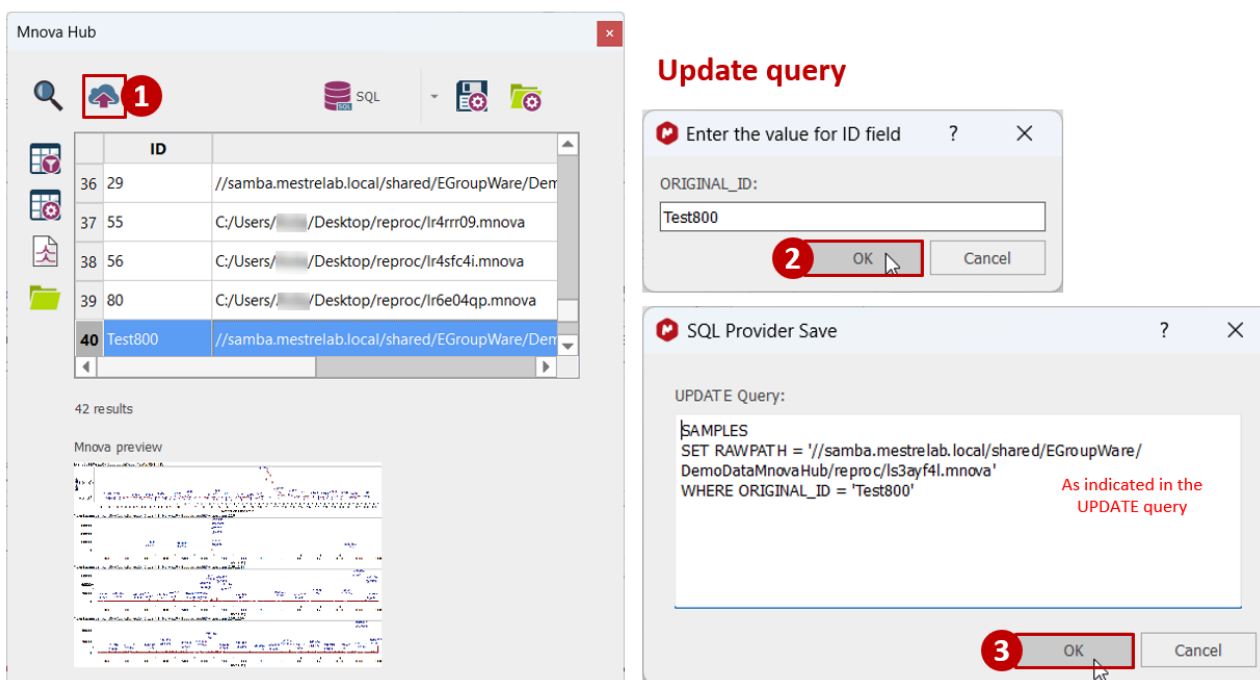
5.3.1. Saving data with SQL

When saving a document using basic queries with the **SQL** provider, Mnova Hub opens a dialog allowing you to choose the document ID. If you input an ID that is already in use, the system will prompt you for confirmation to overwrite the existing document.



In the case of custom queries, Mnova Hub displays a message with a predesigned query and prompts you to modify/complete it before executing it:

- When overwriting an existing entry, it employs the “UPDATE” query, automatically populating the columns it can, and providing a manual editing option for the remaining columns before saving.



- If creating a new entry, Mnova Hub uses the “INSERT” query to pre-fill known fields and allows manual input for the others.

The screenshot illustrates the process of creating a new entry in Mnova Hub. It shows the main application window with a table of existing entries. A dialog box prompts for the 'ORIGINAL_ID' value, which is entered as 'Test801'. Two subsequent 'SQL Provider Save' dialog boxes show the generated SQL INSERT query, with the 'OK' button highlighted in each.

Mnova Hub Table:

ID	RAWPATH
36	29 //samba.mestrelab.local/shared/EGroupWare/Dem
37	55 C:/Users/ /Desktop/reproc/lr4rr09.mnova
38	56 C:/Users/ /Desktop/reproc/lr4sf4i.mnova
39	80 C:/Users/ /Desktop/reproc/lr6e04qp.mnova
40	Test800 //samba.mestrelab.local/shared/EGroupWare/Dem

Dialog 1: Enter the value for ID field

ORIGINAL_ID:

Dialog 2: SQL Provider Save

INSERT Query:

```
INSERT INTO SAMPLES (ORIGINAL_ID, RAWPATH, PDFPATH, NBREF, TYPE, USER, DATE) VALUES ('Test801', '//samba.mestrelab.local/share/EGroupWare/DemoDataMnovaHub/reproc/lr3b68lu.mnova', '//samba.mestrelab.local/share/EGroupWare/DemoDataMnovaHub/previews/lr3b68lu.png', '$NBREF$', '$TYPES$', '$USERS$', '$DATES$')
```

Type to complete the information

Dialog 3: SQL Provider Save

INSERT Query:

```
INSERT INTO SAMPLES (ORIGINAL_ID, RAWPATH, PDFPATH, NBREF, TYPE, USER, DATE) VALUES ('Test801', '//samba.mestrelab.local/share/EGroupWare/DemoDataMnovaHub/reproc/lr3b68lu.mnova', '//samba.mestrelab.local/share/EGroupWare/DemoDataMnovaHub/previews/lr3b68lu.png', 'nbref_test', 'Mnova', 'Usuario', '01-01-2001')
```