

# Mnova Hub 1.0

# **USER MANUAL**



Document Number P/N 489 R1

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### **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.

Advanced	Plug-ins		?	×
		Filter:		
Available	Updates	Installed		
Nam	ie 🗠	Default Ve	ersion	<b></b>
🗹 Mnov	a Hub	1.0.0.14038		
			Insta	II

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\*

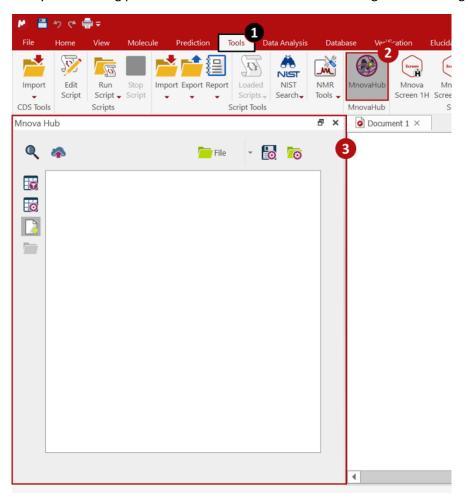
\* Please visit our <u>Store</u> to purchase the required licenses.

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

	SC IVI	anager					?
ost ID							
censes							
				Fil	ter: hub		×
St	tate	Plug-in	Issued By	Licensed To	Туре	Issued Date	Days to Expire
77 🝼		Mnova Hub File Provider	Mestrelab Research S.L.	-	single	Thu Dec 14 2023	Never
78 🝼		Mnova Hub MnDB Provider	Mestrelab Research S.L.	100	single	Thu Dec 14 2023	Never
79 🝼		Mnova Hub SQL Provider	Mestrelab Research S.L.	-	single	Thu Dec 14 2023	Never
80 🝼		Mnova Hub TopSpin Provider	Mestrelab Research S.L.	-	single	Thu Dec 14 2023	Never
81 🔮		Mnova Hub Zontal Provider	Mestrelab Research S.L.	100	single	Thu Dec 14 2023	Never
82 🝼		Mnova Hub	Mestrelab Research S.L.		single	Thu Dec 14 2023	Never
•							•

## 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
Q	Refresh search
•	Configure search filters
*	Save file to provider
File 👻	Configure/change data provider
	Save the configuration of all the providers
<b>6</b>	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.

File SQL File MnDB	2 SQL Provider	? ×3
TopSpin • <b>Z</b> • Zontal	Database       Query         Database parameters:	v ub/example.db

#### 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.

SQL Provider		?	2
Database Qu	iery		
Database paran	neters:		
Driver:	SQLITE	-	
Database File:	elab.local/shared/EGroupWare/DemoDataMnovaHub/examp	le.db	
Repository:			
Path:	C:/Users/Usuario		

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



		_	
SQL Provider		?	×
Database Query	1		
Database paramet	ers:		
Driver:	MARIADB		-
Database Name:	Test_MnovaHub		51
Server:	qctest- mariadb. mestrelab. local		51
Port:	3306		•
User Name:	User		5
Password:			
Repository:			
	Г		_1
Path:	C:/VALIDAT IONS/Mnova Hub/Test Results		

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.

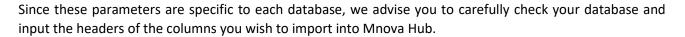
#### 4.1.2. The Query tab

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.

. Provider			?	×
Dase Query				
Name: samples				
Parameter		Field Name		
D	ID			
Raw Path	Raw Path			
	Preview Path	>		
	$\vee$	5		
	Dou	ble-click and type		
	vaase Query Name: samples Parameter D Raw Path	Aase Query Name: samples Parameter D ID Raw Path Raw Path Preview Path	Aaae Query Name: samples Parameter ID ID Raw Path Raw Path	Aase Query Name: samples Parameter Field Name D ID Raw Path Raw Path Preview Path

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, **•**.

SQL Provider		?	X		_
atabase Query	G		. Provider		?
ole Name: samples		Datab	oase Query		
Parameter	Field Name		Name: samples		
D ID		+	Parameter	Field Name	
Raw Path Raw Path			D	ID	
Preview Path Preview		F	Raw Path	Raw Path	
		F	Preview Path	Preview Path	
		C	Date	DATE	
				Туре	



🔚 exam	ple.db 🗵	
1	SQLite format 30 » ».jĐ	
2	æ""	- 11
3	<pre>}æ //fæ//fWtablesqlb_temp_table_1sqlb_temp_table_1CREATE TABLE "sqlb_temp_table_1" (</pre>	- 11
4	"SAMPLE_ID" INTEGER,	
5	"NBREF" TEXT,	
6	"TYPE" TEXT,	
7	"USER" TEXT,	
8	"DATE" TEXT,	_
9	"PDFPATH" TEXT,	
10	"RAWPATH" TEXT,	
11	"ISPROC" TEXT,	
12	"ORIGINAL_ID" INTEGER,	
13	PRIMARY KEY("SAMPLE_ID" AUTOINCREMENT)	
14	)P++Ytablesqlite_sequencesqlite_sequenceCREATE TABLE_sqlite_sequence(name,seq)!,//f,	
15	// <del>jCtablesqlb_v/C</del> tablesamplessamplesCREATE_TABLE " <mark>samples</mark> " (	
16	"SAMPLE_ID" INTEGER,	
17 18	"NBREF" TEXT,	
18	"TYPE" TEXT, "USER" TEXT, OSOL Provider 2 X	
20	"USER" TEXT, "DATE" TEXT,	
20	"PDFPATH" TEXT,	
21	"RAWPATH" TEXT, Database Query	
22		
24	"ISPROC" TEXT, Table Name: samples"	
25	PRIMARY KEY ("SAMPLE_ID" AUT  Parameter Field Name	
25	Leadence Participante The Addition Participante Participa	
_	ID ORIGINAL_ID	
Norma le	ength : 32.768 lines : 196 Ln : 9 ( Raw Path RAWPATH	S
	Preview Path PDFPATH	

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.

Table Name: Samples           Parameter         Field Name           ID         ID	Database Query	
Parameter       Field Name         ID       ID         Daw Datk       Daw Datk         Vse Custom Queries       ID         ID Field Name:       SAMPLE_ID         Raw Path Field Name:       RAWPATH         Preview Path Field Name:       PDFPATH         Select Query:       SELECT SAMPLE_ID, NBREF, TYPE, USER, DATE, PDFPATH, RAWPATH from samples order by DATE desc         Insert Query:       INSERT INTO SAMPLES (SAMPLE_ID, RAWPATH, PDFPATH, NBREF, TYPE, USER, DATE) VALUES (\$SAMPLE_ID5, `\$RAWPATH\$', `\$PDFPATH\$', `\$NBREF\$', `\$TYPE\$', `\$USER\$, DATE\$')         UPDATE SAMPLES       UPDATE SAMPLES         UPDATE SAMPLES       SET RAWPATH = `\$RAWPATH\$'		
Daw Dath       Daw Dath         Daw Dath       Daw Dath         Use Custom Queries       ID Field Name:         ID Field Name:       SAMPLE_ID         Raw Path Field Name:       RAWPATH         Preview Path Field Name:       PDFPATH         Select Query:       SELECT SAMPLE_ID, NBREF, TYPE, USER, DATE, PDFPATH, RAWPATH from samples order by DATE desc         Insert Query:       INSERT INTO SAMPLES (SAMPLE_ID, RAWPATH, PDFPATH, NBREF, TYPE, USER, DATE) VALUES ('\$SAMPLE_ID5,' \$RAWPATH\$,' \$PDFPATH\$,' \$NBREF\$', \$TYPE\$', \$USER\$,' \$DATE\$')         UPDATE SAMPLES       UPDATE SAMPLES         UPDATE SAMPLES       SET RAWPATH\$'		Field Name
Use Custom Queries ID Field Name: RAWPATH Preview Path Field Name: PDFPATH Select Query: Select Query: Insert Query: Insert Query: Query	- ID	ID —
ID Field Name: SAMPLE_ID Raw Path Field Name: RAWPATH Preview Path Field Name: PDFPATH Select Query: Select SAMPLE_ID, NBREF, TYPE, USER, DATE, PDFPATH, RAWPATH from samples order by DATE desc INSERT INTO SAMPLES (SAMPLE_ID, RAWPATH, PDFPATH, NBREF, TYPE, USER, DATE) VALUES (\$SAMPLE_ID5, '\$RAWPATH5', '\$PDFPATH5' '\$NBREF\$', '\$TYPE\$', '\$USER\$', '\$DATE\$') UPDATE SAMPLES SET RAWPATH = '\$RAWPATH5'	Daw Dath	Daw Dath
Raw Path Field Name:       RAWPATH         Preview Path Field Name:       PDFPATH         Select Query:       SELECT SAMPLE_ID, NBREF, TYPE, USER, DATE, PDFPATH, RAWPATH from samples order by DATE desc         Insert Query:       INSERT INTO SAMPLES (SAMPLE_ID, RAWPATH, PDFPATH, NBREF, TYPE, USER, DATE) VALUES (\$SAMPLE_ID5, '\$RAWPATH\$,' \$PDFPATH\$,' \$NBREF\$', '\$TYPE\$,' \$USER\$,' \$DATE\$')         UPDATE SAMPLES       UPDATE SAMPLES SET RAWPATH\$,' \$PDFPATH\$,' \$P	✓ Use Custom Queries –	
Preview Path Field Name:       PDFPATH         Select Query:       SELECT SAMPLE_ID, NBREF, TYPE, USER, DATE, PDFPATH, RAWPATH from samples order by DATE desc         Insert Query:       INSERT INTO SAMPLES (SAMPLE_ID, RAWPATH, PDFPATH, NBREF, TYPE, USER, DATE) VALUES (\$SAMPLE_ID5, '\$RAWPATH\$', '\$PDFPATH\$', '\$NBREF\$', '\$TYPE\$', '\$USER\$, '\$DATE\$')         UPDATE SAMPLES       UPDATE SAMPLES         SET RAWPATH = '\$RAWPATH\$'       '\$RAWPATH\$'	ID Field Name:	SAMPLE_ID
Select Query:       SELECT SAMPLE_ID, NBREF, TYPE, USER, DATE, PDFPATH, RAWPATH from samples order by DATE desc         Insert Query:       INSERT INTO SAMPLES (SAMPLE_ID, RAWPATH, PDFPATH, NBREF, TYPE, USER, DATE) VALUES (\$SAMPLE_ID5', '\$RAWPATH\$', '\$PDFPATH\$', '\$NBREF\$', '\$TYPE\$', '\$USER\$', '\$DATE\$')         UPDATE SAMPLES       UPDATE SAMPLES SET RAWPATH\$'	Raw Path Field Name:	RAWPATH
Select Query:       PDFPATH, RAWPATH from samples order by DATE desc         Insert Query:       INSERT INTO SAMPLES (SAMPLE_ID, RAWPATH, PDFPATH, NBREF, TYPE, USER, DATE) VALUES (\$SAMPLE_ID5, '\$RAWPATH\$', '\$PDFPATH\$', '\$NBREF\$', '\$TYPE\$', '\$USER\$', '\$DATE\$')         UPDATE SAMPLES       UPDATE SAMPLES         SET RAWPATH = '\$RAWPATH\$'       '\$RAWPATH\$'	Preview Path Field Nam	e: PDFPATH
Insert Query: (\$SAMPLE_ID5; '\$RAWPATH\$', '\$PDFPATH\$' ,'\$NBREF\$', '\$TYPE\$', '\$USER\$', '\$DATE\$') UPDATE SAMPLES SET RAWPATH = '\$RAWPATH\$'	Select Query:	PDFPATH, RAWPATH from samples order by DATE
SET RAWPATH = '\$RAWPATH\$'	Insert Query:	PDFPATH, NBREF, TYPE, USER, DATE) VALUES ('\$SAMPLE_ID\$', '\$RAWPATH\$', '\$PDFPATH\$'
	Update Query:	SET RAWPATH = '\$RAWPATH\$'



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 <u>section</u> <u>5.1</u>.

#### 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.

SQL				
	2			
MnDB	File Provide	r		?
😁 TopSpin	File Provide	I		:
• <b>Z</b> • Zontal	Path Lis	t:		
	🔶 Use	Use as default Repository	Path	
	—			
	1			
	Masks: s.baf, _f		*.lcd, *.mcds, *.cdf, *.asc, *.jdx, *.spa, *.sp	oc, *.mol, *.sdf Back to D

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.

💙 File	Provider			?	$\times$
	Path List:				
+	Use	Use as default Repository	Path		
	1 🗸	$\checkmark$	C:/Users/Usuario/Desktop/Datasets/By Plugin/Mnova H	ub/Data_X	c
/					
Masks:	ysis.baf, _F	UNC001.IDX, *.cdf, *.sms, *.ch,	*.lcd, *.mcds, *.cdf, *.asc, *.jdx, *.spa, *.spc, *.mol, *.sdf	Back to De	fault
			ОК	Cance	!

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.

Pa	th List:			
	Use	Use as default Repository	Path	
1	$\checkmark$	$\checkmark$	C:/Users/Usuario/Desktop/Datasets/By Plugin/Mnova Hub/Dat	ta_X
2	~		C:/Users/Usuario/Desktop/Datasets/By Plugin/Mnova Hub/Dat	ta_Y

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.

😮 File f	Pro	vider			?	×
	Pat	th List:				
+		Use	Use as default Repository	Path		
-	1	$\checkmark$	$\checkmark$	C:/Users/Usuario/Desktop/Datasets/By Plugin/Mnova Hu	b/Data_X	
/				Туре ех	tensio	n
Masks:	f, _	FUNCO	)1.IDX, *.cdf, *.sms, *.ch, *.lcd,	*.mcds, *.cdf, *.asc, *.jdx, *.spa, *.spc, *.mol, *.sdf, *.expl	ack to Defa	ault
				ОК	Cancel	

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 <u>section 5.1</u>.

	Default view							Table view setup								
Mnova I	Hub	)			đΧ	Mnova	Hub	)								đΧ
٩	4	4		🧮 File 👻 🛃 🐻		٩	4	8	_			<u>/</u>	File	· 👩	Ō	
		Path	Туре	ID	<b>A</b>			Path	🕑 Fil	e Tab	le Set	up ?	$\times$		4	<b>^</b>
	1	C:/Users/Usuario/Desktop/ r	mnova	AMLODIPINE		0	1	C:/Users/Usuario/De			how	Column				
	2	C:/Users/Usuario/Desktop/ r	mnova	ANASTROZOLE			2	C:/Users/Usuario/De								
	3	C:/Users/Usuario/Desktop/ r	mnova	CELEBREX			3	C:/Users/Usuario/De		1		Path	_		_	
	4	C:/Users/Usuario/Desktop/ r	mnova	CLARITHROMYCIN			4	C:/Users/Usuario/De	$\checkmark$	2	1	Туре	_			
	5	C:/Users/Usuario/Desktop/ r	mnova	LAMICTAL			5	C:/Users/Usuario/De	$\cap$	3	1	ID				
	6	C:/Users/Usuario/Desktop/ r	mnova	LEVOFLOXACIN			6	C:/Users/Usuario/De	0	4		Date				
	7	C:/Users/Usuario/Desktop/ r	mnova	LEVOTHYROXINE			7	C:/Users/Usuario/De		5	1	Preview Path				
	8	C:/Users/Usuario/Desktop/ r	mnova	LORATADINE			8	C:/Users/Usuario/De			_					
	9	C:/Users/Usuario/Desktop/ r	mnova	MOXIFLOXACIN			9	C:/Users/Usuario/De								
	10	C:/Users/Usuario/Desktop/ r	mnova	NASONEX			10	C:/Users/Usuario/De								
	11	C:/Users/Usuario/Desktop/ r	mnova	OLANZAPINE			11	C:/Users/Usuario/De								
	12	C:/Users/Usuario/Desktop/ r	mnova	OLMESARTAN			12	C:/Users/Usuario/De			OK	Cano	el .			
	13	C:/Users/Usuario/Desktop/ r	mnova	ONDANSETRON	-		13	C:/Users/Usuario/De			OR	Curre			•	-
	29	results					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.

· · · · ·	ile 🔽 🗓 🖊		
9	SQL		
<u> </u>	File		
9	MnDB 2	MnDB Provider ?	×
-88-	TopSpin		
·₹·	Zontal	Server:	
		Port: 5504	1
		User:	_
		Password:	
		Connect	
		Database Name:	•
		Number of Records per Page: 20 🗘	

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.

MnDB	Provider ? X	MnDB F	Provider	?	×
Server:	localhost	Server:	localhost		
Port:	5504	Port:	5504		*
User:	test	User:	Test		
Password:	•••••	Password:	••••		
<b>T</b> Conne	ect 2	Discon	nect		
Database N		Database Na	ame:	Acids	-
Number of	Records per Page: 20 🌻	Number of F	Records per Page:	Acids Metabolites	3
	OK Cancel		ОК	Car	icel

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.

File				
SQL File				
	oSpin 2 Co Top	Spin Provider		? X
	+ /	Use	Path	
	•		OK	Cancel

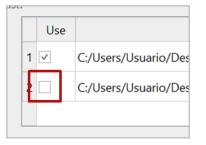
A dialog box will appear, allowing you to configure the path to your files. Click on **Add** + and navigate through your folders to choose the Topspin folder you want to set as a data source. Select the folder. The chosen folder's path will be displayed in the table, as illustrated in the image below.

🕑 TopS	pin Provi	der	? >	<
Path List	:			
+	Use	Path		
_	1 🗹	C:/Users/Usuario/Desktop/Datasets/By Plugin/Mnova Hub/TopspinFile	•	
1				
•				
		ОК	Cancel	_

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.

🕑 TopS	pin Provid	der ? X
Path List	:	
+	Use	Path
-	1 🗹	C:/Users/Usuario/Desktop/Datasets/By Plugin/Mnova Hub/TopspinFile
	2 🗸	C:/Users/Usuario/Desktop/Datasets/By Plugin/Mnova Hub/TopspinFile-2
•		
		OK Cancel

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



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 <u>section 5.1</u>.

ova H	lub							5
R					- 🗺 TopSp	in 👻 🖁	0 0	
8		Dataset	Expno	Туре	Nucleus	Title	ID	
	1	1-4-BD-CDCl3	1	1D-C-zgpg30	13C	1,4-B	fid	
_	2	1-4-BD-CDCl3	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	H
	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-zqpq30	13C	F2	fid	-

Anova Q	Hut	2				TopSpin 👻 📘	5
Table F Apply		Column Value Date •	🗘 То	pSp	oin Tabl	e Setup ? >	×]
		Date 👻			Show	Column	<b></b>
		Dataset	-	1		Date	<b>^</b>
	1	1-4-BD-CDCl3		2	~	Dataset	
	2	1-4-BD-CDCl3		⊢			
	3	1-4-BD-D2O	$\bigcirc$	3	~	Expno	
	4	1-4-BD-D2O		4	<ul> <li>Image: A start of the start of</li></ul>	Туре	
	5	1-4-BD-DMSO		5		Pulse Program	
	6	1-4-BD-DMSO		6	<b>v</b>	Nucleus	
	7	1-4-BD-MeOD		7	~	Title	
	8	1-4-BD-MeOD		⊢			
	9	2-2'-Difluorofentany		8	~	ID	▼
	10	2-2'-Difluorofentany					-
	40	results				OK Cancel	

#### Table view setup



#### 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.

				ť				
<u>/</u>	Fi	ile 🔽 🚺	o					
ID		SQL						
		File						
		MnDB		🕑 ZONTA	L Provider		?	×3
	8	TopSpin					·	T
	٠Z·	ZONTAL 2	3	URL:				]
				Username:				]
				Password:				1
					Use tol	ken for auther	itication	, 
				Page size:	50 🗘			
					Ξ.			
						ОК	Cance	9

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

🕲 ZONTA	?	×	
URL:	https://demo1.zontal.space	2	
Username:			
Password:	•••••		
	Jse token for authentic	ation	
Page size:	50 ‡		
	<b>•</b>		
	ОК	Cano	el

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.

Password:	•••	••••	•••	,
		Use to	ken	for authentica
Page size:	50	*		
	1			
				ОК

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



C Inf	formation	×
i	Cache C:/Users/Usuario/AppD ZONTALCache/ZONTALFileCach	
		ОК
	Page size: 50 ‡	
	OK	Cancel

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 <u>section 5.1</u>.

		De	fault view					Ta	ble	vie	w se	tup		
ova H	lub				8 ×	× Mnova H	ub							ė
Q	Q	•		-Z-ZONTAL -	0	٩	O <sub>c</sub>	, 🐴				-Z-ZONTAL -	0	3
0		ID		Туре	<b>^</b>			ID		🗘 Zo	ntal Table	Setup ? >	<	-
0	1	CSAA676860_S02A481142	MNova Demo				1	CSAA676860_S02A481142	M		Show	Column		_
	2	acqus	TopSpin Raw MVP				-	acqus	Тор		1	Date		_
	3	Columbo-PM-22-291	XCalibur Raw MVP				3	Columbo-PM-22-291	XC		2 2			-
	4	JR_20211013_Dimitri_mixe	XCalibur MDM				4.	JR_20211013_Dimitri_mixe	XC	$\checkmark$	2 🗸	ID		
	5	STARK_210426_PM-20-315	XCalibur MDM				5	STARK_210426_PM-20-315	XC	$\Box$	3 🗸	Туре		
	6	acqus	TopSpin Raw MVP				6	acqus	Тор					
	7	NewTest.mnova	MNova Demo				7	NewTest.mnova	M					
	8	Test.mnova	MNova Demo				8	Test.mnova	M					
	9	CSAA676860_S02A481142	MNova Demo				9	CSAA676860_S02A481142	M					
	10	Test_2D.mnova	MNova Demo				10	Test_2D.mnova	M					
	11	testUpload.mnova	MNova Demo				11	testUpload.mnova	M					
	12	Document 14.mnova	MNova Demo				12	Document 14.mnova	M		O	Cancel		
	13	Document 13.mnova	MNova Demo		-		13	Document 13.mnova	MI			Curreer		-
		Document 13.mnova	MNova Demo		Ţ			Document 13.mnova 745 results 💙	MN					

**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.



~			🕑 File	e Ta	ble Set	rup ? × 2	
	1	Pat			Show	Column	
0	2	C:/		1	<b>v</b>	Path <b>3</b>	
	3	C:/	$\checkmark$	2	<b>~</b>	Type Enable/disable/ re-order columns	
	4	C:/		3	$\checkmark$	ID	
	5	C:/	)	4		Date	
	6	C:/		5		Preview Path	
	7	C:/				<b>\</b>	
	8	C:/					-

**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.

٩	4	8		<b>File</b>
		Path 🗲	Type	ID
0	1	C:/Users/Usuario/Desktop/	mnova	AMLODIPINE
No.	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

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

		Date	ID	
0	1	2023-11-02 10:46	01	MNova Demc
	2	2023-11-02 11:32:08	CSAA676860	MNova Demc
	3	2023-11-02 11:32:33	Stack_and_as	MNova Demc
	4	2023-11-02 11:35:12	CSAA676860	MNova Demc
	5	2023-11-02 18:49:22	Test_PM.mnova	MNova Demc
	6	2023-11-02 18:52:16	fid	Topspin Raw I
	7	2023-11-02 18:55:32	acqu	Topspin Raw I
	8	2023-11-06 18:40:34	1H_2436.zip	Topspin Raw I
	9	2023-11-06 18:42:08	1H_2436.zip	Topspin Raw I

Path	Туре	
Usuario/Deskto	mnova	
Usuario/Deskto	mnova	ANASTROZOLE
Usuario/Deskto	mnova	CELEBREX
Usuario/Deskto	mnova	CLARITHROMYCIN
Usuario/Deskto	mnova	LAMICTAL
Usuario/Deskto	mnova	LEVOFLOXACIN
Usuario/Deskto	mnova	LEVOTHYROXINE
Usuario/Deskto	mnova	LORATADINE
Usuario/Deskto	mnova	MOXIFLOXACIN



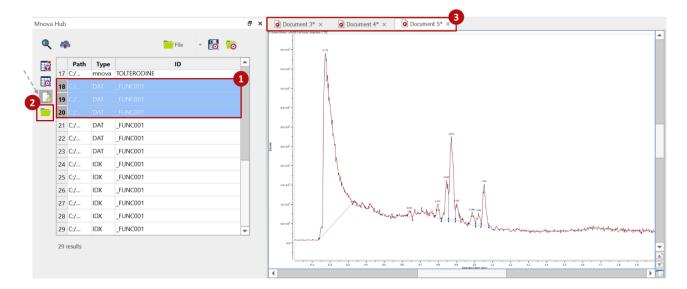
#### 5.2. Opening data in Mnova

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

iova H	lub					8 ×	
Q	4			🦰 File 👻 🛃	o		
6		Path	Туре	ID			
8	1	C:/	mnova	AMLODIPINE	Ψ		
	2	C:/	mnova	ANASTROZOLE			a de la companya de
4	3	C:/	mnova	CELEBREX			
	4	C:/	mnova	CLARITHROMYCIN			
	5	C:/	mnova	LAMICTAL			
	6	C:/	mnova	LEVOFLOXACIN			
	7	C:/	mnova	LEVOTHYROXINE			
	8	C:/	mnova	LORATADINE			
R	17	results					
	1		.   ii 1				

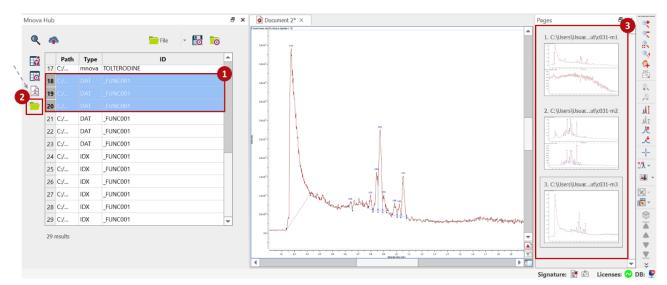
It is possible to open multiple datasets at once. To do so, select the datasets of interest by holding the "Ctrl" key. Then press the open button. The selected spectra will be opened in separate Mnova documents or on the same page depending on the selection of the toggle **Open in current Document/Open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

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





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).

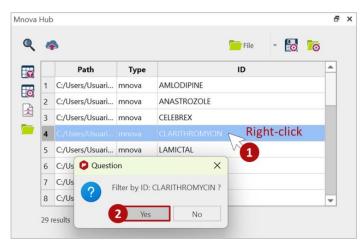


#### 5.3. Search filters for data

Mnova Hub enables you to easily fine-tune your search results using column-specific filters. You can either click on this button,  $\square$ , 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:

Mnova	Hub	)				é
٩	4	-		File	•	0
Table Apply		s Column Path Path	Va •	alue		
		Path	Туре	ID		<b></b>
	1	C:/	mnova	AMLODIPINE		
	2	C:/	mnova	ANASTROZOLE		
	3	C:/	mnova	CELEBREX		
	4	C:/	mnova	CLARITHROMYCIN		

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.

Mnova	Hub		🗗 🗙 🙆 Docu	ment 1 ×
٩	0		•Z•ZONTAL - 🛃 📷	6
		Pref	Search Filters	? ×
0	1	MNova De		
	2	MNova De		
	3	MNova De	+- Apply Name Type	
	4	MNova De	-	
	5	MNova De		
	6	MNova De		
	7	MNova De		
	8	MNova De	Current Filter Settings:	
	9	MNova De	.0	
	10	MNova De		
	11	MNova De		
	12	MNova De		
	4			
	50/6	399 results		OK Cancel

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.

Search Filters			
Apply Name	Search Filters		? ×
Dynamic Filter Expert Filter			
Current Filter Settings:	+ Apply Name 1  ✓ S	Type 2	
	Current Filter Settings:		
	Name: Samples of the day		
	Type: Simple	3	*
4	Simple Filters:	Available files (Archived and Submitted) Available files (Archived and Submitted) My samples today My samples this week All samples today	
		OK	Cancel



#### 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.

Search Filters		
<b>=</b>		
Apply Name     Simple Filter	Search Filters	? ×
1 Dynamic Filter		
Expert Filter	+·· Apply Name Type	
	Image: Samples of the     Simple       Image: Dynamic     2	
Current Filter Settings:	Current Filter Settings:	
	Name: Test Samples	
	Type: Dynamic	
	Term: Value: Last Modified On Value: Last Modified On Created On	Cancel

#### 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 <u>native language</u> of the provider. Press this button, 🔀, to save the configuration.

Search Filters							
Apply Name Simple Filter Dynamic Filter 1 Expert Filter		ch Filter	S			?	×
+-		Apply	Name	Туре			
	1	$\checkmark$	Samples of the	Simple			
Current Filter Settings:	2		Test Samples	Dynamic			_
	3	✓		Expert 2			
				-			
	L						
Curre	ent	Filter Sett	ings:				
	Ν	ame: M	y Filter				
	Т	ype: E	kpert	3			•
4	1	{"filterTy	ype":"terms","propert 'pe":"date_range","pri n":"2023-01-01","to"	tyName":"@me_user","value":["User"]}, opertyName":"createdOn","format":"yyyy-MM- :"2023-12-31"}]			
	Ľ				ОК	Cano	el



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

1	Name:	Samples of the day	
<b>-</b>	Type:	Simple	
EV.		Simple	
	Simple	Dynamic Expert	

#### 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.

Searc	ch Filter	5		Command	Description
					Load filters (*.data)
	Apply	Name			Save filters (*.data)
1 2	_	Samples of the Test Samples	Simple Dynamic	+-	Add a filter
3	~		Expert	-	Remove filter
	Filter Sett	ings:			Move filter (up/down)
N	lame: Sa	mples of the day			Show/Hide filter settings colum
<u>ا</u> ا		mple			Edit filter
	Simple Fi	Iters:			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 ZO	NT	AL Space	2				
🗘 Se	arch Filter	S			• <del>۲</del> •	0	S Lifecycle Sta	tus • S User • M Usuario	Created On - Som From: 2023/Mar/01 - To: 2023/Apr/10	ch	٩	Ad
+-	Apply	Name		Туре	6		bout 3 results	<b>D</b> ( 1111				
-	1	Samples of the	Simple					Preferred Label	Created On		ormation Pack	age Prof
	2	Test Samples	Dynamic				Submitted	felodipinePhaseBase	lineC 2023/Apr/04 12:47:29 (+0)	2:00) MN	lova Demo	
	3 🗸		Expert				Submitted	felodipinePhaseBase	lineC 2023/Apr/04 13:58:03 (+0)	2:00) MN	lova Demo	
							Submitted	felodipinePhaseBase	lineC 2023/Apr/04 12:47:14 (+0)	2:00) MN	lova Demo	
Curre		kpert	yName":"@me_user" <mark>,"value":("Usuario")),</mark>		In Mr Mnova		/a Hub					ē ×
	{"filterTy	/pe":"date_range","pr n":"2023-03-01","to"	opertyName":"createdOn","format":"yyyy-M	M-	Q	(	<b>);</b> 🍙		• <b>Z</b> •2	ONTAL -	0 0	
							Preferre	ed Label	Title	Ту	pe	
				Ok		1	MNova De	mo felod	ipinePhaseBaselineCor.mnova	1D		
						2	MNova De	mo felod	ipinePhaseBaselineCor.mnova	1D		
					×	3	MNova De	mo felod	ipinePhaseBaselineCor.mnova	1D		

**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.

Mnova I	Hub	
Q	4	•
o	1	C:/Users/Usuario/Desktop
	2	C:/Users/Usuario/Desktop
소	3	C:/Users/Usuario/Desktop

#### 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.

36 29 37 55	//samba.mestrelab.local/sha	<u> </u>	Information		×			
37         55         C./Users/         /Desktop/reproc/ir4rrr09.mnova           38         56         C./Users/         /Desktop/reproc/ir4sfc4i.mnova           39         80         C./Users/         /Desktop/reproc/ir6e04qp.mnova			This will overwrite an already existing entry. Do you want to continue					
4		SQL Provider	Save ? X	Mnova Hub				
42 results								
Mnova preview		Field	Value	Q 🐢	🜉 SQL 🛛 👻 📘			
		ORIGINAL_ID	Test800	ID ID				
	Ę	RAWPATH	//samba.mestrelab.local/	36 29	//samba.mestrelab.local/shared/EGroupWare/Den			
		PDFPATH	//samba.mestrelab.local/	37 55	C:/Users// /Desktop/reproc/lr4rrr09.mnova			
	E State			38 56	C:/Users///Desktop/reproc/lr4sfc4i.mnova			
er				39 80	C:/Users////Desktop/reproc/ir6e04qp.mnova			
				40 Test800	//samba.mestrelab.local/shared/EGroupWare/Dem			
			2 OK Cancel					
				42 results				
				Mnova preview				
				المراجع المراجع المراجع المراجع	Constant Constant Constant Constant			

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.

Mnova	Hub		×	
Q	4	1	🜉 SQL 👻 📙 🐻	Update query
				C Enter the value for ID field ? X
	36 2	29	//samba.mestrelab.local/shared/EGroupWare/Den	ORIGINAL_ID:
0	37 5	55	C:/Users/ /Desktop/reproc/lr4rrr09.mnova	Test800
Å	38 5	56	C:/Users/ /Desktop/reproc/lr4sfc4i.mnova	2 OK Cancel
	39 8	30	C:/Users/. /Desktop/reproc/Ir6e04qp.mnova	
	40 T	Test800	//samba.mestrelab.local/shared/EGroupWare/Den	SQL Provider Save ? X
	er dan er de da	<u>preview</u> ۲۰۰۰ ۲۰۰۰ ۲۰۰۰ ۲۰۰۰ ۲۰۰۰ ۲۰۰۰ ۲۰۰۰ ۲۰		UPDATE Query: SAMPLES SET RAWPATH = '//samba.mestrelab.local/shared/EGroupWare/ DemoDataMnovaHub/reproc/Is3ayf4I.mnova' WHERE ORIGINAL_ID = 'Test800' As indicated in the UPDATE query
	74	<u>a</u>	n an	3 OK Cancel



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

Mnova I	Hub		×	Enter the value for ID field ? X				
٩	4	1	sql - 🛃 🏹	ORIGINAL_ID: Test801				
	36 2	<b>ID</b>	//samba.mestrelab.local/shared/EGroupWare/Dem	2 Of Cancel				
0	37 5		C:/Users/ /Desktop/reproc/lr4rrr09.mnova					
×	38 5	56	C:/Users/ /Desktop/reproc/Ir4sfc4i.mnova	SQL Provider Save ?	×			
	39 8	30	C:/Users/ /Desktop/reproc/Ir6e04qp.mnova	INSERT Query:				
	42 res Mnova	<b>preview</b>		INSERT INTO SAMPLES (ORIGINAL_ID, RAWPATH, PDFPATH, NBREF, TYPE, USER, DATE) VALUES ('Test801', '//samba.mestrelab.local/shared/ EGroupWare/DemoDataMnovaHub/reproc/Is3b68lu.mnova', '// samba.mestrelab.local/shared/EGroupWare/DemoDataMnovaHub/previews/ Is3b68lu.png', 'SNBREF\$', '\$TYPE\$', '\$USER\$', '\$DATE\$') Type to complete the information Cancel				
		<u>ar na ar ar ar ar</u>	and and an and an and an and an and an and an	SQL Provider Save ?	×			
				INSERT INTO SAMPLES (ORIGINAL_ID, RAWPATH, PDFPATH, NBREF, TYPE USER, DATE) VALUES ('Test801', '//samba.mestrelab.local/shared/ EGroupWare/DemoDataMnovaHub/reproc/ls3b68lu.mnova', '// samba.mestrelab.local/shared/EGroupWare/DemoDataMnovaHub/preview Is3b68lu.png' ,'Inbref_test', 'Mnova', 'Usuario', '01-01-2001')				

4

ок 📐

Cancel