

# **MnServer Manual**

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# **MnServer 2.0**

by MESTRELAB RESEARCH

This is the manual for MnServer 2.0

## **MnServer Manual**

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# 1 Introduction

Mnova's Database plugin was born as a new concept for the shared storage of molecules, Mnova objects (texts, drawings, images, etc...), NMR, MS and other analytical analysis.

You will need an MnServer to store your databases. There are three different flavours of MnServer:

	Needs extra license?	Connects	DB Backend
MyData	No	Local computer only	SQLite
MnDB Group	Yes	Any computer running Mnova	SQLite
MnDB Enterprise	Yes	Any computer running Mnova	Any (Oracle, MySQL, SQLite or PostgreSQL)



## 2 Quick Start Guide

This is a quick start Guide to install *MyData* and *MnDB Group* on your computer or on a server machine. To install *MnDB Enterprise*, please go to this <u>chapter</u>

1. Install the MnServer (MyData or MnDB Group) from here:

http://mestrelab.com/resources/requirements-db/

Please note that your computer will need a working Java runtime environment (version 1.6 or onwards). Install it from <u>here</u> if necessary. For MnDB Group, you will need to get a license. See this <u>chapter</u> for further information.

2. Run Mnova, follow the menu 'Database/Connection' and enter the details below:

Server:	localhost			
Port:	5504			
User:	Test	Test		
Password:	database			
	Save Pass	word V Show	w Password	

If you have installed *MnDB Group* in a server computer, you will need to type the IP address (or hostname) of the server and make sure that the Port (5504 by default) is enabled.

The default User will be 'Test' and the password will be 'database'. Of course, it will be possible to <u>add</u> <u>further users</u> by running the MnServerAdmin.



# 3 System Requirements and instructions to install the MnServer

Please read this chapter before installation. In this section you will find information on which hardware and software requirements must be met before you can install the MnServer. In any case, it is worth noting that Mnova is a **multiplatform** software which can run on Windows, Mac OS X, Linux and Unix-like systems.

From now on, multiplatform laboratories will be able to allow each researcher to work on their Operating System of choice, and to seamlessly share data and processing capabilities with other researchers working on different platforms.

There is no longer a need to have three different software packages, and three different file formats, for different Operating Systems.

#### 3.1 System Requirements for Server

The minimum requirements for the **server** will depend on the usage patterns (number of concurrent users, amount of data stored, etc.).

Any medium-ranged desktop or server that can be bought nowadays should do just fine. The limiting factor to performance tends to be the available network bandwidth between server and clients.

#### Hardware requirements:

- Processor: Pentium 166 MHz or higher (The server will take advantage of multiple cores if available)
- RAM Memory: 256MB, 1Gb or more recommended (1Gb would allow the data for 100 simultaneous requests to all fit into memory)
- Hard disk space: 20 MB (for installation), plus database. The amount of disk space needed on the server is similar to the space required to save the same data in Mnova documents. For our test data the average storage needs are: ~55K for a molecule, ~1 MB for a 1D NMR Spectrum, and~20 MB for a 2D NMR Spectrum.

#### **OS requirements:**

• You can use any OS which runs Java (Windows 7 or higher, Red Hat 8.0 or Suse Enterprise Linux Server 9 or higher, Mac OS X 10.5.2 or higher). Server components can be virtualized (VMware ESX).

You will also need:

- ✓ A working Java runtime environment. Minimum version for all OS 1.8. Recommended 1.11. We strongly recommend using the Java packages from Sun. Click <u>here</u> to download and install it if necessary.
- ✓ Access to a database server (for *MnDB Enterprise* only): *MnDB Group* and *MyData* can only be used with SQLite. *MnDB Enterprise* can be used with any DB backend (Oracle, MySQL, SQLite or PostgreSQL).

All tests have been conducted with MySQL version 5.6.40 and 8.0.16 and Oracle version 19.0c. If you don't have Oracle, MySQL or PostgreSQL, you will need to install one of them first.

You will need an empty database and table space; plus we recommend a dedicated database user to be used by MnServer to connect to the database server. MnServer and MnServerAdmin will create tables in this table space as needed

The following steps are highly recommended on a database server before having MnDB trying to connect to it:

1. Create a new database user (Good examples are e.g. "mndb" or "mnova")

2. Create some database space for MnDB to store its data in.

a) Oracle/Postgres: All Mnova databases are stored in one database. This database needs to be created and, in the case of Oracle, storage space assigned.

b) MySQL: Each mnova database gets stored in its own mySQL database. Therefore, the database user created in 1) needs database creation rights.

3. Give full access rights (read, write, create tables, create indexes, etc.) to the new user for the new database(s): GRANT ALL ON (<database> or \*.\*) TO <user>

The following is an example of installing MySQL under Windows:

a. Register on this link to install mysql-essential-5.1.48-win32.msi (or later version).

b. Run the .msi file to install MySQL Server by double clicking on it. Follow the Server Instance configuration Wizard. Leave the default options, except in the MySQL Server Instance Configuration Page, where you will need to check 'Include Bin Directory in Windows PATH'. In this process you will also create a user (such as "root") and a password for it.

c. Once this is done, you should be able to see that the MySQL service is running (you can check this by Start > Control Panel > Administrative Tools > Services, and verify that the Status of MySQL is 'Started'). You can run MySQL by Start>Programs>MySQL>MySQL Server 5.1>MySQL Command Line Client.

d. Now you can choose to create an account on MySQL for running Mnova DB Server (unless you want to use root). Use the following MySQL command to create a user account and its password:

mysql> CREATE USER 'Sample'@'localhost' IDENTIFIED BY 'some\_pass'; mysql> GRANT ALL PRIVILEGES ON \*.\* TO 'Sample'@'localhost';

e. A good startup tutorial for MySQL can be found <u>here</u>

For further information about how to run MnDB Enterprise with MySQL backend check this tutorial.

<u>MySQL Notes</u>: Depending on your spectral data, you might have to increase the **max\_allowed\_packet** setting for the MySQL server. A too low max\_allowed\_packet setting will result in the server throwing a com.mysql.jdbc.PacketTooBigException on trying to store complex spectra. You can change this value for the MySql Server by changing the max\_allowed\_packet server variable, usually in the my.cnf or my.ini configuration file.

<u>Java Notes:</u> (Linux/Mac) The supplied startup scripts for MnServer and MnServerAdmin expect the java executable to be found in the current command path. On systems where the java executable is not found in the command search path by default, you can either modify the PATH system variable, or adapt the startup scripts to point to the location of your java executable.

#### 3.2 System Requirements for Clients

The minimum requirements for the client are the same as for the standard Mnova client. The main limitation could be the RAM memory; as a 32 bit application, only makes use of ~1.5Gb of RAM memory, which limits the number of items that can be displayed simultaneously in the compound browser (about 200 and 300).

The minimum recommended configuration for Mnova installation is at least Pentium 300 MHz, 128Mb RAM, a VGA color monitor with 800 x 600 pixels resolution, a compatible mouse and Windows Vista as operating system. However, ideal system requirements for optimum operation of the software are Pentium 1,6 GHz or higher CPU with 2Gb or more of RAM memory and Windows 7 or 10.

Windows: Mnova will not install under Windows XP or lower. The default installation requires about 100 Mb of disk space.

Mac: Mnova requires at least Mac OS X 10.13, with Intel architecture.

Linux: Mnova requires at least Pentium 300 MHz, 128Mb RAM, Video Adapter Super VGA (800 x 600) with X Library (Xlib). Please, make sure to choose the correct setup file for your Operating System (Debian Lenny, Debian Squeeze, OpenSUSE 10.1 and 11, Fedora 10 and 11, Ubuntu 8.04 and 9.04, Red Hat Enterprise 4 or 5 and Mandriva 2007 and 2009).



# 4 Installation

In this chapter, you will find the instructions for installing MnServer.

#### 4.1 Installation of the MnServer (Windows)

Download the applicable installer (MyData, MnDB Group or MnDB Enterprise) from this link.

The complete installation instructions for the installation of Database Server will be displayed on screen and copied to hard disk after having double clicked on the executable (C:\MnDB\Readme.html by default).

The MnServer for *MnDB Enterprise* may reside either on the same or on a different machine from the Oracle/MySQL/PostgreSQL server. All that you will need is a network connection between them (server and client).

Note on Installation Location: During its operation, MnServer needs to write files into the users subdirectory. Some windows operating systems restrict writing access for programs to subdirectories of the Program Files directory. Therefore, on these systems, MnServer should either be run with elevated privileges, or installed into a location outside of the Program Files directory structure.

Uninstallation: To uninstall the Database Server just run the uninstaller after having closed all the programs and removed all of Mnova Server existing services. Please bear in mind that the content of the database will not be removed after having uninstalled the software.

## 4.2 Installation of the MnServer (Mac/Linux)

Download the applicable installer (MyData, MnDB Group or MnDB Enterprise) from this link.

The complete installation instructions for the installation of Mnova DB Server will be displayed on screen and copied to hard disk after having installed the software.

The MnServer for *MnDB Enterprise* may reside either on the same or on a different machine from the Oracle/MySQL/SQLite server. All that you will need is a network connection between them (server and client).

You can install MnServer by double clicking on the .sh file or by typing the following command from the console:

java -jar MnDB-Install-version.jar

The installer can also be run in a full headless mode, i.e., without needing a graphical user interface.

This is useful, e.g., in the case of remotely accessed servers through SSH or similar. To launch an interactive console installation, just type in a console: *java -jar MnDB-Install-version.jar -console* 

Uninstallation: To uninstall Mnova DB just delete the installation directories.Deleting the installation directory will delete the content of SQLite databases (MyData and MnDB Group) which are stored within a subdirectory of the installation folder. It will not delete the contents of databases which are stored on a database server (MySQL, Oracle etc., MnDB Enterprise only).



# 5 Configuring the Server

In this chapter, you will find information about how to configure the server and the Mnova users.

#### 5.1 Activating Licenses

With *MyData*, the user will not need to activate a license. However, if you have acquired *MnDB Group* or *MnDB Enterprise*, you will need to have a license file in the MnDB installation folder (at C: \MnDB\MnServer).

To get that license, please send us the HOST ID of your server to support@mestrelab.com

To find the HOST ID of your server, just open the MnServer.log file (which should be in the 'MnDB\MnServer\log' installation folder):

🗄 M	nServer.log				
12	INFO	[2014-05-27	14:06:06,824]	[main]	root - user.dir=C:\MnDB\MnServer
13	INFO	[2014-05-27	14:06:06,824]	[main]	root - user.home=C:\
14	INFO	[2014-05-27	14:06:06,824]	[main]	root - user.name=UWS7427EA5CA419\$
13	DEBUG	[2014-05-27	14:06:06,825]	[main]	root - NumArgs=1
10	DEBUG	[2014-05-27	14:06:06,825]	[main]	root - 0: logfile.txt
1	INFO	[2014-05-27	14:06:06,958]	[main]	root - licence path=C:\MnDB\MnServer
18	ERROR	[2014-05-27	14:06:06,963]	[main]	com.mestrelab.license.TLicenseValidator - C:\Windo
19	INFO	[2014-05-27	14:06:06,971]	[main]	com.mestrelab licence TLicenceWalidator Leaded 1
20	INFO	[2014-05-27	14:06:06,999]	[main]	root - host id=JHR3M-LMS1PSSZ-FXF63-9TYA7V1P
2:	ERROR	[2014-05-27	14:06:06,999]	[main]	com.mestrerap.ricense.ricensevaridator - License
22	INFO	[2014-05-27	14:06:09,133]	[main]	root - ==================================
23	INFO	[2014-05-27	14:06:09,134]	[main]	root - MnDB Server, Vsn 1.5.0
24	INFO	[2014-05-27	14:06:09,134]	[main]	root - java.version=1.7.0_55
2:	DEBUG	[2014-05-27	14:06:09,134]	[main]	root - java.specification.version=1.7

You can also find it by running StartServer.bat from the installation folder:

🚾 Seleccionar C:\Windows\system32\cmd.exe	
DEBUG [2014-05-27 13:25:49,348] [main] root - os.name=Windows 7	•
INF0 [2014-05-27 13:25:49,348] [main] root - user.dir=C:\MnDB\MnServer	
INF0 [2014-05-27 13:25:49,349] [main] root - user.home=C:\Users\Usuario	
INF0 [2014-05-27 13:25:49,349] [main] root - user.name=Usuario	
DEBUG [2014-05-27 13:25:49,350] [main] root - NumArgs=0	
INF0 [2014-05-27 13:25:49,535] [main] root - product id=d8b0a95e-e052-4e04-86b0	
-a8db8fd143e8	
INF0 [2014-05-27 13:25:49,537] [main] root - product version=1.6.0	
INF0 [2014-05-27 13:25:49,538] [main] root - product date=2014-04-25	
INF0 [2014-05-27 13:25:49,538] [main] root - licence path=C:\MnDB\MnServer	
INFO [2014-05-27 13:25:49,560] [main] com.mestrelab.license.TLicenseValidator -	
Loaded public key	
ERROR [2014-05-27 13:25:49,561] [main] com.mestrelab.license.TLicenseValidator -	
C:\MnDB\MnServer\license.properties (El sistema no puede encontrar el archivo e	
specificado)	
INFO [2014-05-27 13:25:49,561] [main] com.mestrelab.license.TLicenseValidator -	
Host Type not loaded. Assumed default host type	
INFO [2014-05-27 13:25:49,562] [main] com.mestrelab.license.TLicenseValidator -	
Host Type value: 0	
INF0 [2014-05-27 13:25:49,631] [main] root - host id=JBE32-3PX8B05L-F4WJJ-XF7VC	
8A2	
ERROR [2014-05-27 13:25:49,632] [main] com.mestrelab.license.TLicenseValidator -	
License checking fatal error. Please, contact support@mestrelab.com	
Launch4j: An error occurred while starting the application.	
Presione una tecla para continuar	Ŧ

You can also find the HOST ID by running the application below:

Windows: <u>http://www.mestrelab.com/mnova/MHostId.zip</u> Linux: <u>http://www.mestrelab.com/mnova/mhostid\_linux.zip</u> Mac: http://www.mestrelab.com/mnova/MHostID.dmg

Once you have received the license file, please copy it into the MnDB installation folder (under the \MnServer subfolder).

Next, go to Windows Control panel (Local services) and restart the Mestrelab MnDB service:

<ul> <li>Servicios</li> <li>Archivo Acción ⊻er</li> <li>← ➡   □□ □□ □</li> </ul>	Ay <u>u</u> da ≩   <mark>[] □</mark> □   ▶ ■     ▶					×
Servicios (locales)	Servicios (locales)	-				
	Mestrelab MnDB-Enterprise	Nombre	Descripción	Estado	Tipo de inicio	^
	MnServer	Mestrelab MnDB-Enterprise MnSe	erver MnDB Server	En ejecución	Automático	
	Detener el servicio	Q K				>
8	∫ \ Extendido \ Estándar /					

## 5.2 Connection to DB

(Only for MnDB Enterprise) Before starting the server, you will need to install a database engine and use the supplied server admin tool to create a server configuration file (named MnServer.conf).

To create the server configuration file, you will need to:

- 1. Start the admin tool via MnServerAdmin.exe (MnServerAdmin.jar for Linux and Mac).
- 2. Enter the connection data for the database connection.
- 3. Press Save to write the file MnServer.conf.

Double click on the MnServerAdmin.exe (MnServerAdmin.jar in Linux/Mac) to set up the DB Server.

In the example below, we have used SQLite (included with MyData, MnDB Group and MnDB Enterprise):

Database Mnova Users		Database Mnova Users	
Database settings for Mn Serv	er	MnServer settings for Mnova	
Database Engine	SQLite -	Server Port	5504
Database Host Database Port	localhost	Server Timeout (Minutes)	300
Database Name Database User	db1	Max. Clients	0
User Password		Log Sync Interval (Seconds)	60

The entered database connection data can be tested by clicking on the "Test DB Connection" button.

INFOR	MATION	×
i	SUCCEDED: SQLite 3.23 User	=null
	Aceptar	

Only for *MnDB Enterprise*: In the example below, we have used the MySQL account created in the server requirements chapter

Database Engine	MySQL (MyISAM)	-
Database Host	localhost	
Database Port	3306	
Database Name	db1	
Database User	Sample	
Jser Password	•••••	

The entered database connection data can be tested by clicking on the "Test DB Connection" button.

INFOR	MATION
<b>i</b>	SUCCEDED: MySQL 5.1 User=Sample@localhost
	ОК

Please bear in mind that the connection data are not written to disk until you click on the "Save" button. Clicking on "Cancel" without a previous "Store" will discard any change. Make sure that you have the Server Port enabled to allow the Mnova client to connect to the MnDB Group (in the example above the port number is 5504).

If the connection was not successful, please double check that you entered the right password and other information. Sometimes "localhost" may not be recognized on your computer, then you can try to type "127.0.0.1" on the 'Database Host' edit box:

Database Engine	MySQL (MyISAM)	-
Database Host	127.0.0.1	
Database Port	3306	
Database Name	db1	
Database User	Sample	
User Password		

**NOTE:** If the computer you are installing the server on does not have a graphical desktop environment, you can execute the MnServerAdmin Tool on another computer (which does have a desktop environment) and then copy the generated configuration file Mnserver.conf to the remote server, into the same directory as MnServer.

The databases in SQLite are stored by default in this folder: \MnDB\MnServer\db1. You can easily backup the full content of your Databases by just copying the entire db1 folder. For MySQL/Oracle/Postgres, see the documentation for the RDBMS. For example, this link

<u>Oracle Notes</u>: In the case of Oracle backend, the db field in MnServeradmin can take the following forms:

1) /SID if the database field starts with a / it will be interpreted as service name

2) :SID if the database field starts with a / it will be interpreted as SID

3) <SID> if neither colon nor / are used, the field content will be interpreted as SID (same as before)

## 5.3 Mnova Users

Once you have tested that the DB Connection works, select the 'Users' tab. From here, you can select 'Database or Active Directory Mode (only available on MnDB Enterprise)' from the scroll down menu:

atabase Mnova Users		~
lode	Database	-
Database		
	Manage Users	
Active Directory		
Server		
Domain		_
Default Role	No Permissions	-
Referrals	throw	-
Log level	0	
Active Directory Groups:		
No Permissions		
Searcher	MnDB Searcher	_
Reader	MnDB Reader	_
Editor	MnDB Editor	_
∆dministrator	MnDB Administrator	
Autor		

#### 5.3.1 Managing users internally

Clicking on the on the 'Manage Users' button will allow you to set up the Mnova DB users:

user	password	role	max. login	description
Test	database	Administrator	0	
Guest	guest123	Reader	0	
Add User				Delete Selected Users

Click on 'Add User' button to add any user and password. From here you can select the privileges of the user (No Permissions, Searcher, Reader, Creator, Author, Editor and Administrator) or the maximum number of simultaneous logins.

	Searcher	Reader	Creator	Contributor	Author	Editor	Administrator
Search and view hits	yes √	yes √	yes √	yes √	yes √	yes √	yes √

Retrieve existing records	no X	yes √					
Create new record	no X	no X	yes √				
Add new item to existing own record	no X	no X	no X	yes √	yes √	yes √	yes √
Add new item to existing others record	no X	no X	no X	yes √	yes √	yes √	yes √
Modify existing own item	no X	no X	no X	no X	yes √	yes √	yes √
Modify existing others item	no X	no X	no X	no X	no X	yes √	yes √
Delete own item	no X	no X	no X	no X	yes √	yes √	yes √
Delete others item	no X	no X	no X	no X	no X	yes √	yes √
Create databases	no X	no X	no X	no X	no X	no X	yes √
Delete databases	no x	no x	no X	no X	no X	no X	yes √

It will be possible to delete users from here just by clicking on the applicable button.

Once you have added the new user, click on the 'Update User Databases' button and finally Save and Close the MnServerAdmin dialog.

#### 5.3.2 Using Active Directory to manage users

If you are in the **Active Directory mode** (only available in MnDB Enterprise); you would need to select the server, domain and the Default Role:

ode	Active Directory	
Database		
Database		
	Manage Users	
Active Directory		
Server	54 172 181 178	
Domain	mestrelab.localtest	
Default Role	Administrator	-
Referrals	follow	-
Log level	0	
Active Directory Groups:		
No Permissions	MnDB No Permissions	
Searcher	MnDB Searcher	
Reader	MnDB Reader	
Editor	MnDB Editor	

Users authentication can be delegated to Active Directory (AD). Once a user is successfully authenticated, his access rights are determined by membership in Active Directory groups, for example

"MnDB No permissions", "MnDB Normal User", "MnDB Power User" and "MnDB Administrator". Groups, and group's names, can be configured to better suit your team's needs. If the user is not a member of any of these groups, access level will be the one specified in MnAdmin as Default role.

Referrals: we recommend to select '*follow*' from the scroll down menu. For further information about it, please check this documentation.

#### Active Directory Usage scenarios:

Very Small: No Active directory groups, Default role is "Administrator".

#### Small:

- 1. Active Directory group "MnDB Administrator".
- 2. Default role set to "Power User".
- 3. Create an active directory group "MnDB Administrator" in the AD server.
- 4. Assign to the AD group the users and groups which you want to be able to manage databases.
- 5. Using MnAdmin, change the default access role to "Power user".

**Result:** Everybody who can authenticate against AD can read and write records but only the people in the "MnDB Administrator" AD group can create or delete databases.

#### Large:

- 1. Create three active groups "MnDB Administrator", "MnDB Power User", "MnDB Normal User".
- 2. Assign to the AD groups the users and groups.
- Change default access role in MnAdmin depending on your desires access level for people which are not in any of the AD groups. Choose between "MnDB Power User" (can read and write but not create/delete/manage databases), "MnDB Normal User" (can only read but not write), or "MnDB No permissions".

#### Very large:

We recommend several MnServer installations, with access rights determined by distinct AD groups, like options 2 and 3. This setup will involve several groups for each MnDB server: group postfixes in MnDB server setting e.g. "Server1", "Server2", ... Corresponding Active directory groups "MnDB Administrator Server1", "MnDB Power User server2" etc.



# 6 Running

In this chapter, you will find information about running tests and the server. On Windows, the MnServer service is installed by default. If it is needed, the services can also be run by following the instructions described on this <u>chapter</u>.

## 6.1 Starting/Stopping the server

Windows: Now you are ready to start MnServer. To do that, just double click on C:\MnDB\MnServer\startMnServer.bat to display this MS-DOS window:

C:\Windows\system32\cmd.exe	-		×
INF0 [2019-03-15 12:41:48,004] [main] root (MnServer.java:232) - ================			~
INFO [2019-03-15 12:41:48,008] [main] root (MnServer.java:233) - MnDB-Enterprise - M	nServer,	Vsn 1.	8.3
_BETA_461			
	191		
DEBUG [2019-03-15 12:41:48,009] [main] root (MnServer.java:235) - java.specification.	version=	1.8	
DEBUG [2019-03-15 12:41:48,009] [main] root (MnServer.java:236) - java.vm.version=25.	191-b12		
DEBUG [2019-03-15 12:41:48,010] [main] root (MnServer.java:237) - java.vm.info=mixed	mode		
DEBUG [2019-03-15 12:41:48,010] [main] root (MnServer.java:238)  - java.class.path=C:\/	MnDB-Ent	erprise	e∖Mn
Server\MnServer.exe;.;lib\.;lib\;lib\apiguardian-api-1.0.0.jar;lib\commons-codec-1.9	.jar;lib	\gnu-cr	ypt
o.jar;lib\jackson-annotations-2.9.4.jar;lib\jackson-core-2.9.4.jar;lib\jackson-databin	d-2.9.4.	jar;lib	b∖ju
nit-jupiter-api-5.3.1.jar;lib\junit-platform-console-standalone-1.3.1.jar;lib $\log$ 4j-1.	2.16.jar	;lib\my	ysql
-connector-java-5.1.25-bin.jar;lib\ojdbc6.jar;lib\postgresql-9.4.1211.jre6.jar;lib\Saa	SLicense	-1.0.ja	ar;l
ib\sqlite-jdbc-3.23.1.jar;lib\sqlite-jdbc-3.8.11.1.jar			
DEBUG [2019-03-15 12:41:48,010] [main] root (MnServer.java:239) - java.library.path=C	:\Progra	m Files	s∖Ja
va\jre1.8.0_191\bin;C:\Windows\Sun\Java\bin;C:\Windows\system32;C:\Windows;C:\Program	Files (x	86)\Cor	nmon
Files \uracle \Java \Javapach;c: \windows \System52;c: \windows;c: \windows \System52 \web;c: \lindowsPowerShell\v1 @\.c.\Windows\System32\OnenSSH\.c.\Users\Pahlo\AnnData\Local\Micr	\windows	\Syster ndowsAr	152\
C.\Program Files\lava\ire1 & 0 191\bin.	05010 (112		(P-)
DERUG (2019-03-15 12:41:48.013] [main] root (MnServer.iava:240) - java.io.tmpdir=C:\U	sers\Pab		Data
local/Temp	521 5 (i G5	70 (r. P.P.	
<pre>\</pre>	m Files∖	Java\i	re1.
8.0 191			
DEBUG [2019-03-15 12:41:48,014] [main] root (MnServer.java:242) - os.name=Windows 10			
DEBUG [2019-03-15 12:41:48,014] [main] root (MnServer.java:243) - user.dir=C:\MnDB-Em	terprise	MnSer	ver
)\DEBUG [2019-03-15 12:41:48,014] [main] root (MnServer.java:244) - user.home=C:\Users	Pablo		
DEBUG [2019-03-15 12:41:48,014] [main] root (MnServer.java:245) - user.name=Pablo			
DEBUG [2019-03-15 12:41:48,015] [main] root (MnServer.java:246) <u>- Default Locale=es E</u>	5		
DEBUG [2019-03-15 12:41:48,015] [main] root (MnServer.java:247) - NumArgs=0			
INFO [2019-03-15 12:41:48,025] [main] root (MnServer.java:131) - product id=2600f98d	-0dc4-45	3c-ae9t	0-25
74df5e9be0			~

There is a service folder (C:\MnDB\Services) which contains bat files for installing and uninstalling the Windows services:

rchivo $\rightarrow$	Inicio Compartir Vista *		✓ O Buscar en Serv	vices p
*	Nombre	Fecha de modificación	Тіро	Tamaño
	🖀 nssm.exe	26/02/2019 13:20	Aplicación	74 KB
4	service_install_mnserver.bat	28/02/2019 13:38	Archivo por lotes de	1 KB
5	service_uninstall_mnserver.bat	28/02/2019 13:38	Archivo por lotes de	1 KB
<b>E</b>				

In some Windows systems the access to the services manager is disabled. In those cases, you will need to modify the security settings from 'Control Panel/Change user accounts settings/Never notify'

You can also start/stop the service from the 'Control Panel/Local Services':

Servicios						·- 🗆	×
Arc <u>hivo Ac</u> ción	<u>V</u> er Ay <u>u</u> da						
	à 🗟 📲 🖬 🕨 🔳 🕪 🕨						
🧠 Servicios (locale	Servicios (locales)						
	Mestrelab MnDB-Enterprise	Nombre	Descripción	Estado	Tipo de inicio	Iniciar sesión como	^
	MnServer	Mestrelab License Server	The license server for Mestrelab products	En ejecución	Automático	Sistema local	
		Mestrelab MnDB-Enterprise MnServer	MnDB Server	En ejecución	Automático	Sistema local	
	Detener el servicio	Mestrelab MnDB-MyData MnServer	MnDB Server	En ejecución	Automático	Sistema local	
	Reiniciar el servicio	Microsoft App-V Client	Manages App-V users and virtual applicati		Deshabilitado	Sistema local	~
< >	Extendido Estándar						

**Mac/Linux:** You will only need to open a session in a terminal window, go to the installation directory (e.g.: \$> cd ~/Applications/MnDB-MyData) and start the server: \$~Applications/MnDB-MyData> ./startServer.sh

• • •					📄 Mn	Ser	erver — -bash — 80×24
Last	login:	Wed	Aug	21 11	:00:06	on	n ttys000
MEST	REMACTES	ST:~	mest	relab	\$ cd /	App	olications/MnDB-MyData/MnServer
MEST	REMACTES	ST:Mr	nServ	er me	strela	b\$	./startServer.sh

We recommend running the MnServer within a screen session if is installed on a remote server.

## 6.2 Using the TestClient

**Windows:** This is not mandatory, but you can test the installation of the server just by: 1. Using the MnServer Admin tool (startAdmin.bat), create a user called ´test' for example. You can see this <u>chapter</u> about how to do it.

🛃 Manage MnServer Users X										
user	password	role	max. login	description						
Test	database	Administrator	0							
Guest	guest123	Reader	0							
Add User	Add User Delete Selected Users									
	Update User Datab	ase	Ca	ncel						

Please make sure that the username and password are the same that appear in the .conf file

2. Starting up the server (with startServer.bat or startserver.sh)

Organizar 👻 📑 Abrii	r	Imprimir Grabar Nueva carpeta		===	• 🔳 (
Favoritos	-	Nombre	Fecha de modifica	Tipo	Tamaño
🧮 Escritorio		길 lib	11/08/2010 11:05	Carpeta de archivos	
퉳 Descargas		📔 log	09/03/2011 13:18	Carpeta de archivos	
🖳 Sitios recientes		resources 11/08/2010 11:05 Carpeta d		Carpeta de archivos	
	-	🎒 users	01/02/2011 9:47	Carpeta de archivos	
😹 Bibliotecas	-	log4j.properties	23/08/2010 11:00	Archivo PROPERTI	1 KB
Documentos		MnServer.conf	01/02/2011 9:47	Archivo CONF	1 KB
📔 Imágenes		🎼 MnServer.exe	08/02/2011 16:35	Aplicación	509 KB
J Música		🂕 MnServerAdmin.exe	08/02/2011 16:35	Aplicación	204 KB
Vídeos		🚳 startAdmin.bat	09/08/2010 18:32	Archivo por lotes	1 KB
		startServer.bat	09/08/2010 18:32	Archivo por lotes	1 KB
📮 Pablo					
Lisco local (C:)	Ŧ				

3. Starting up the test client (with startClient.bat or startclient.sh)

Organizar 🔻 🛅 Ab	orir	Imprimir Grabar	Nueva carpeta						
🧮 Escritorio	•	Nombre	Fecha de modifica	Тіро	Tamaño				
Descargas		🔒 log	01/02/2011 9:45	Carpeta de archivos					
Sitios recientes		Requests	13/01/2011 13:33	Carpeta de archivos					
		🖟 testcase	08/02/2011 17:06	Carpeta de archivos					
Bibliotecas		🌗 testdata	11/08/2010 11:05	Carpeta de archivos					
Documentos	=	client.plog	02/03/2011 13:08	Archivo PLOG	1 KB				
Imagenes					clientRef.plog	09/08/2010 18:32	Archivo PLOG	6 KB	
		log4j.properties	05/11/2010 12:38	Archivo PROPERTI	1 KB				
Videos		📓 log4j-1.2.16.jar	09/08/2010 18:45	Executable Jar File	471 KB				
		MnClient.conf	26/10/2010 13:45	Archivo CONF	1 KB				
		istartClient.bat	27/10/2010 12:35	Archivo por lotes	1 KB				
Disco local (C:)		TestClient.exe	08/02/2011 16:35	Aplicación	180 KB				

4. Executing the command a)"Test all" will display a "Test result OK" message

C:\Windows\system32\cmd.exe	
ServerThread 4	
1.0.b1	
mn_server_usn=10000	
sendLine: '20101010 TEXT 0 0'	E
sendLine: 'LOGIN'	
sendLine: 'MAIN'	
sendLine: 'MNCLIENT'	
sendLine: 'test'	
sendLine: 'test'	
sendLine: '•'	
receiveLine: 20101010 TEXT 0 0	
HEHDER: 20101010 IEXI 0 0	
PecelveLine HCCEPTED	
receiveline: 'user test accepted'	
Pecerveline: 4	
maccage (9 licen tast lagged in)	
INFO: User test logged in	
Info- Oser test 10gged In	
a) Test all [will delete no testcase1 and no testcase2*]	
x) Evenue file	
r> repeat last x> command	
a) Quit	
Enter a command: _	-
	and the second sec

Linux/Mac: To test the client just:

 Open a session in a terminal window.
 Change to the installation directory. e.g.: \$> cd ~/mndb/MnClient
 Start the testclient: \$~mndb/testclient> ./startClient.sh and follow the steps 3 and 4 described above (for Windows).



## 7 Audit Trail

MnServer keeps two logs in the log/ subdirectory:

- 1. 1) MnServer log. Some basic information is stored by default. This can be changed by editing the log4j.properties file and changing the logging levels, i.e. from INFO to DEBUG.
- 2. 2) Audit.log: All executed SQL statements which modify the database in any way, together with timestamp and user who did the change.

For tracking database changes, the audit log is the better place to use because it is smaller.

Each item (Molecule, Spectrum) in the database is uniquely identified by 3 numbers:

Record ID (cid)

Item Type (1= Molecule, 2= NMR Spectrum, 3 = Mass Spectrum, ...)

Spectrum number (snr): Always 0 for molecules, numbered from 1 for anything else.

The item type is automatically given by what we are looking for and also determines which tables we want to look at: Molecules =  $m1_{fields}$ , NMR Spectrum =  $m2_{fields}$ , Mass spectrum =  $m3_{fields}$  etc.

If the item in question comes from the DBBrowser, the other two numbers Record Id (cid) and Item number (snr) can be easily identified. Otherwise, the first step needs to be to figure out what these are from some unique property (Spectrum title, UUID, Filename, etc. of the item in question. Doing a text search on the Audit log for such a unique search term will reveal at a minimum the line where the item was created as the first occurrence:



CID and SNR are the first two columns in the table, in this case RecordID = 8 and Item number (snr) = 1.

The next step is then to find in the Audit.log all operation on table m2\_fields (NMR spectrum) with Item number 1 of Record 8. This can be done using the search terms

'VALUES ( 8, 1,' for inserts
'cid = 8 AND snr = 1' for updates
'cid BETWEEN 8 AND 8 AND snr BETWEEN 1 AND 1' for deletes (without the quotes).

## 7.1 Configuration of the Audit Trail

1. Install Python 3.8 or newer from their website: <u>https://www.python.org/downloads/</u>

2. Download get-pip.py from the link below (by saving as): <a href="https://bootstrap.pypa.io/get-pip.py">https://bootstrap.pypa.io/get-pip.py</a>

3. Open a command prompt and navigate to the folder containing get-pip.py.

4. Run the following command: python get-pip.py



5. Double click on the 'Audit.py' file from the MnDbServer installation folder:

📙 🛛 🔁 📜 🗧 🛛 MnServer				- 0	I X
Archivo Inicio Compartir	Vista				~ ?
Anclar al Acceso rápido	Mover a V Eliminar	▪ Inombre Nueva carpeta	▼ V Propiedades	Seleccionar too	do <sup>r</sup> nada ón
Portapapeles	Organizar	Nuevo	Abrir	Seleccionar	
$\leftarrow \rightarrow \lor \uparrow$ ] > Este ec	µuipo → OS (C:) → MnDB-N	MyData → MnServei	r	マ ひ Buscar	en 🔎
Nombre	^	Fecha de modifica	Тіро	Tamaño	^
📕 🦲 db1		20/04/2020 14:10	Carpeta de archivo	S	
💄 📜 lib		20/04/2020 14:09	Carpeta de archivo	S	
🖡 📜 log		25/03/2020 11:30	Carpeta de archivo	s	
l resources		02/05/2019 11:03	Carpeta de archivo	S	
📔 📃 users		20/04/2020 14:11	Carpeta de archivo	S	
🖌 🔽 🔤 audit.py		16/04/2020 10:50	Archivo PY	45 KB	
license.prope	erties	15/09/2017 12:42	Archivo PROPERTI.	. 1 KB	
Ville Iog4j.propert	ties	20/09/2019 11:23	Archivo PROPERTI	. 2 KB	
MnServer.exe	<u>}</u>	20/04/2020 12:26	Aplicación	677 KB	
🗸 🗸 🔬 MnServer.I4j.	ini	02/01/2020 10:16	Opciones de confi.	1 KB	~
15 elementos 1 elemento se	eccionado 44,1 KB				

6. The Audit Trail dialog box will be displayed:

🖉 Audit Trail		_		$\times$	
Input					
Input directory:	C:\MnDB-MyData\MnServer\log			<b>-</b>	
Input file mask:	Audit\.log.*				
Input files found:	Audit.log 1 files found			0	
Output					
Output file:	C:\Users\Pablo\Audit.html			=	
Launch browser w	ith results				
Search					
Database:	Drugs				
Record:	1				
Operation:	All				
User:	Test				
Search pattern:					
			🖌 Ok  🗙	Cance	

From here you will be allowed to search in your audit trail, filtering the results by different fields (Like, Record IDs, Users, Databases).

## Thank you!

Thank you for reading this manual. We will be very keen to read your feedback on the application, to hear about any bugs you may find and to also listen to any additional ideas or suggestions you may have.

Please remember that you can send all those, and any queries about the software, or requests for help, to:

support@mestrelab.com

Keep checking our web site (www.mestrelab.com) for additional information on our range of software packages, and for news on our company.