How to retrieve your data

Cóm recuperar les teves dades (en Català) | Other languages using Google Translate

Your data acquired on any of the NMR Service spectrometers are available at all times and from anywhere through our data server. To retrieve them, you will have to download and install the program FileZilla, and configure it to connect to our server securely.

In order to preserve the privacy of the groups' research data, each research group and company has a virtual account for its exclusive use, that allows it to access only its data folders on the SeRMN spectrometers and computers.

The data server uses ProFTPD to manage the secure connection and transfer of data using the protocol FTPS/FTPES. This data transfer protocol uses TLS to encrypt communications between the client and the server. This is the same encryption protocol that browsers use to access secure web servers via HTTPS.

To access the data server you will need a FTP client that allows TLS encrypted connections. We recommend the program FileZilla although you can use others that support the FTPS/FTPES (FTP over TLS) protocol.

The folders on the data server

When you log in, you will see several folders that link directly to data folders on currently available spectrometers as well as former spectrometers. The name of the folder indicates which spectrometer it corresponds to.

Current spectrometers

These folders correspond to the spectrometers currently installed in the service:

Folder name	Current spectrometers
av-dpx-250-auto	Spectrometer Avance DPX 250 MHz, with sample changer.
av-neo-300	Spectrometer Avance Neo 300 MHz for self-service.
av3-400-sb	Spectrometer AvanceIII 400 MHz, with an HR-MAS accessory.
av-neo-400	Spectrometer Avance Neo 400 MHz for self-service.
av-neo-500	Spectrometer Avance Neo 500 MHz, with cryoprobe.
av3-600	Spectrometer AvanceII+ 600 MHz, with sample changer.
biospec-7T	Spectrometer BioSpec 70/30USR with an horizontal magnet.

Former spectrometers

These folders correspond to spectrometers previously installed in our facility that no longer exist:

Folder name	Former spectrometers
av-dpx-250-robot	Spectrometer Avance DPX-250 MHz, with sample changer.
av-dpx-360	Spectrometer Avance DPX-360 MHz for self-service.
av2-400-wb	Spectrometer AvanceII 400 MHz, wide-bore magnet, with CP/MAS accessory.
av-drx-500	Spectrometer Avance DRX-500 MHz, with cryoprobe and LC-DAD-(SPE)-NMR/MS.

You will probably never see all of these instruments, as each group only sees the spectrometers that at least one member of the group has access to.

Each research group and company only has access to their data folders.

Thus, when acquiring spectra **make sure you save the data in your group folder.** If you save it in the wrong folder, you will not be able to retrieve it through the data server.

Use only unaccented letters, numbers, and dashes (uppercase and lowercase) for experiment names,

It is highly recommended that you only use:

- lowercase and uppercase letters without accents: a-z A-Z
- numbers: 0-9
- hyphens: - _

for experiment names, because other characters (accents, asterisk, quotes, parentheses, etc.) could cause problems when retrieving your data.

Open the firewall of your institute or company

The FTPS/FTPES client and server communicate via ports 990 (FTPS) and 60000-65534 (IANA Ephemeral ports), thus you will have to make sure they are not blocked by any firewalls.

In mid-2022 **we changed the FTPS server port number from 21 to 990** in order to use the official port number for this protocol:

Port 990 Details
Service: ftps
Details: FTPS Protocol, FTP over TLS/SSL (IANA official) uses ports 989 and 990.
https://www.speedguide.net/port.php?port=990

If you access our server from within the UAB, or from a research institute or company on campus that has its network integrated into the UAB network, you should have no problems connecting and

downloading your data.

Conversely, if you connect from an off-campus computer, and your institute or company has a firewall to protect its network, you will have to ask the people responsible for the firewall to configure it so that you can retrieve your data .

The configuration is very simple and does not entail an unacceptable security risk, the steps required are :

- open outbound **port 990 (FTPS)** for the **TCP** protocol; and
- open inbound the **range of ports 60000-65534** (IANA Ephemeral ports for FTPS) for the **TCP protocol** to computers on your network

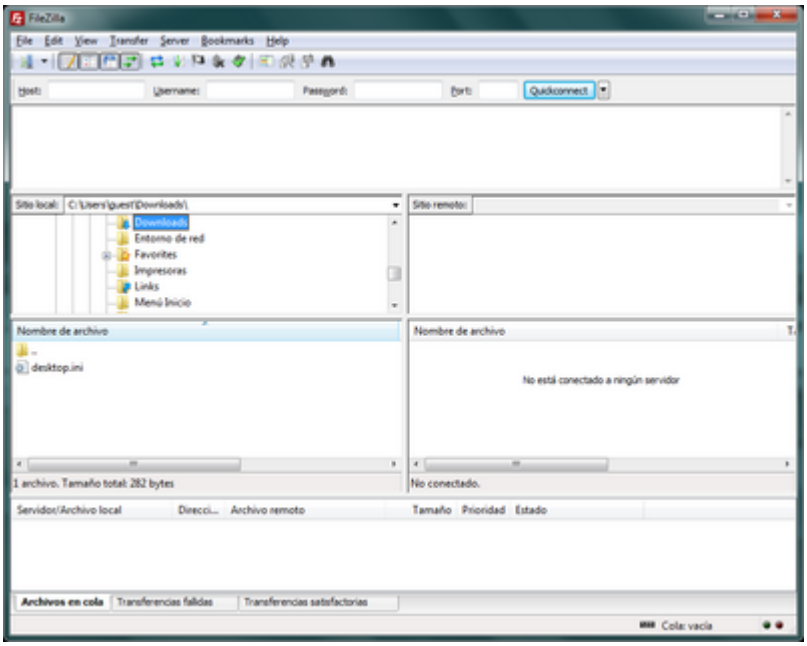
so that you can connect to our FTPS-TLS server via **FTPS-Passive** from inside the firewall.

If they want to further restrict open ports only to our IP address, tell them it's **IP: 158.109.58.175** with **hostname: sermn.uab.cat**

Don't worry if you don't understand this technical information, it is meant for your firewall administrators.

Access your data with FileZilla

The program we recommend to access our data server is FileZilla, an FTP client with a graphical interface, available for Windows, Mac OS X and Linux.



At the time of writing these instructions, the most current version is 3.66.4, but since new versions come out quite often, you will probably find a newer version to download and install. On the other hand, it is highly recommended that you pay attention to the program when it informs you that there is a new version and suggests that you download and install it. Doing so is only takes a moment, and requires no software reconfiguration.

Installation

On the website of the FileZilla program you will find complete, detailed and up-to-date installation

instructions on how to install FileZilla Client on MS-Windows, Mac OS X, and GNU/Linux.

You can download the program directly from the FileZilla website.

Detailed configuration

If you are not familiar with FileZilla configuration follow these detailed instructions. There we explain step by step how to configure the program to access our data server, in addition, the multiple screenshots will help you to successfully complete the configuration process.

Otherwise, use the quick setup instructions in the next section.

Quick setup

If you are familiar with FileZilla use these short instructions to set it up:

1. Go to *Edit* → *Settings*
    1. In *Transfers* → *File Types* set the configuration to,
        - Default transfer type: Binary
        - Uncheck the options *Treat files without extension...* i *Treat dotfiles as...*
    2. In *Language*
        - Choose the interface language
    3. Press Ok to save the changes and to exit the *Settings* window.
2. Go to *File* → *Site Manager*
    1. Press New Site to create a new site. Call it something like *SeRMN-UAB Data Server*.
    2. In the *General* tab enter the following values:
        - Host: sermn.uab.cat
        - Port: **990**
        - Protocol: FTP - File Transfer Protocol
        - Encryption: Require explicit FTP over TLS
    3. Define the account type and access credentials,
        - If this is a computer for exclusive use by members of the research group, set it up with:
            - Logon Type: *Normal*
            - **User: type the *username* of your group (ask your Group Leader or a senior member)**
            - **Password: optionally type the *password* of your group (ask your Group Leader or a senior member for it)**
        - If this is a computer shared with other groups or individuals, set
            - Logon Type: Interactive, and
            - let FileZilla to prompt you for the user name and password everytime that someone wants to log in.
    4. Press Ok to save the configuration and to exit the *Site Manager* window.

Now you can try to connect to our data server:

1. Select the site *SeRMN-UAB Data Server* (or the name you have entered) at *File* → *Site Manager*
    1. If you have configured your account as *Logon Type: Normal* the program will only ask for your group's *password* if you did not save it.

    2. If you have configured your account as *Interactive* the program will only ask for your group's *username* and *password*.
2. In both cases press the Ok button to start the connection.
3. If you have not yet accepted our server certificate, or if we have renewed it, the program will show you the certificate data and ask you if you accept it. Press the Ok button to accept the certificate and continue with the connection.
4. If everything went well, you should now see the list of instruments that your research group has access to.

You must ask the head of your research group or company for access credentials.

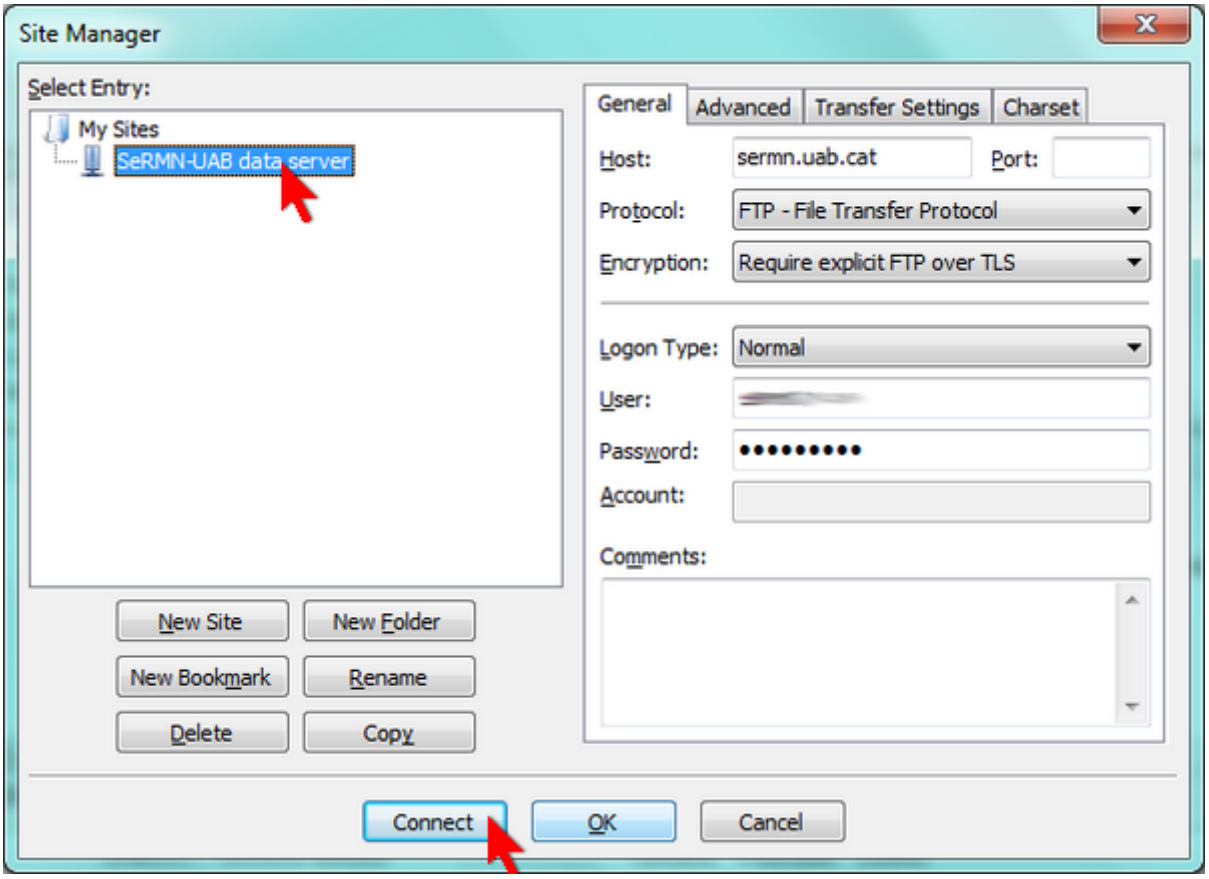
The SeRMN only provides the access credentials (*username* and *password*) to those responsible at each research group or company, and the distribution of this information within the research group or company is their responsibility.

Remember that each research group **only has access to its data folders**. When you acquire spectra, **make sure you save the data in your group folder.** Otherwise you won't be able to retrieve it over the network.

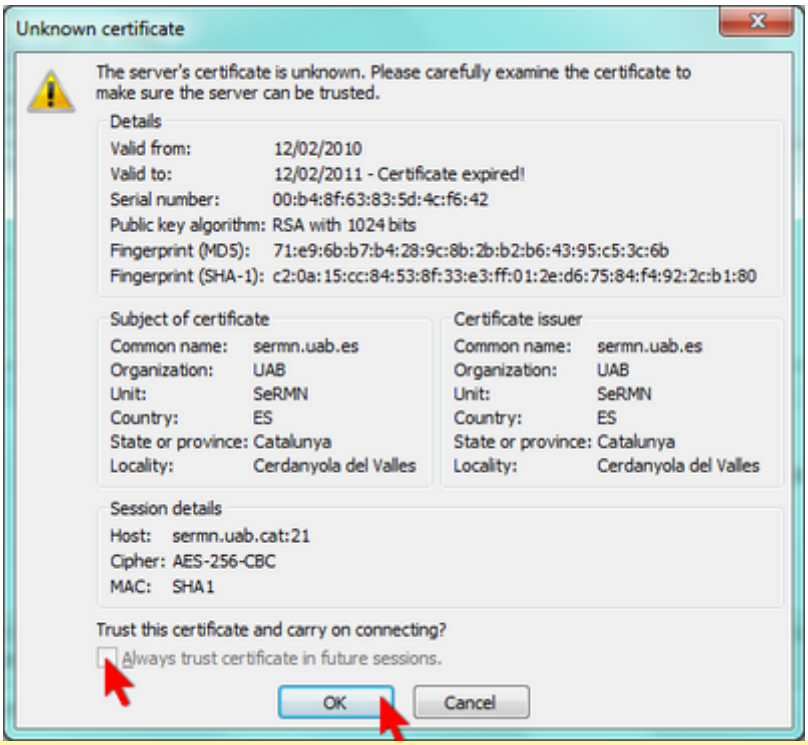
If you have any problems retrieving your data through the server, please contact the service staff and we will try to resolve the issue.

Example of data transfer session

The following images show how to download data from the data server. The first thing you will have to do is open the *Site Manager*, select the account where you have defined the connection to our data server, and press the Connect button to start a session,



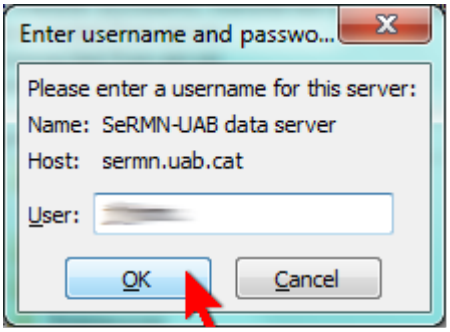
If you have configured the connection parameters correctly, and if there are no problems with the network, a screen will immediately open with the digital certificate that identifies our data server. To continue you must accept it by pressing the OK button.

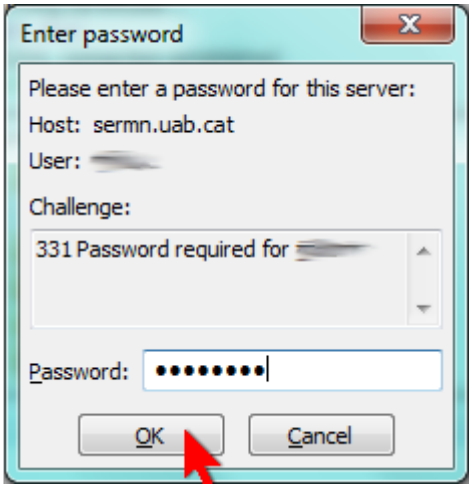


The data server uses an official UAB certificate generated by GEANT Vereniging that is renewed annually.

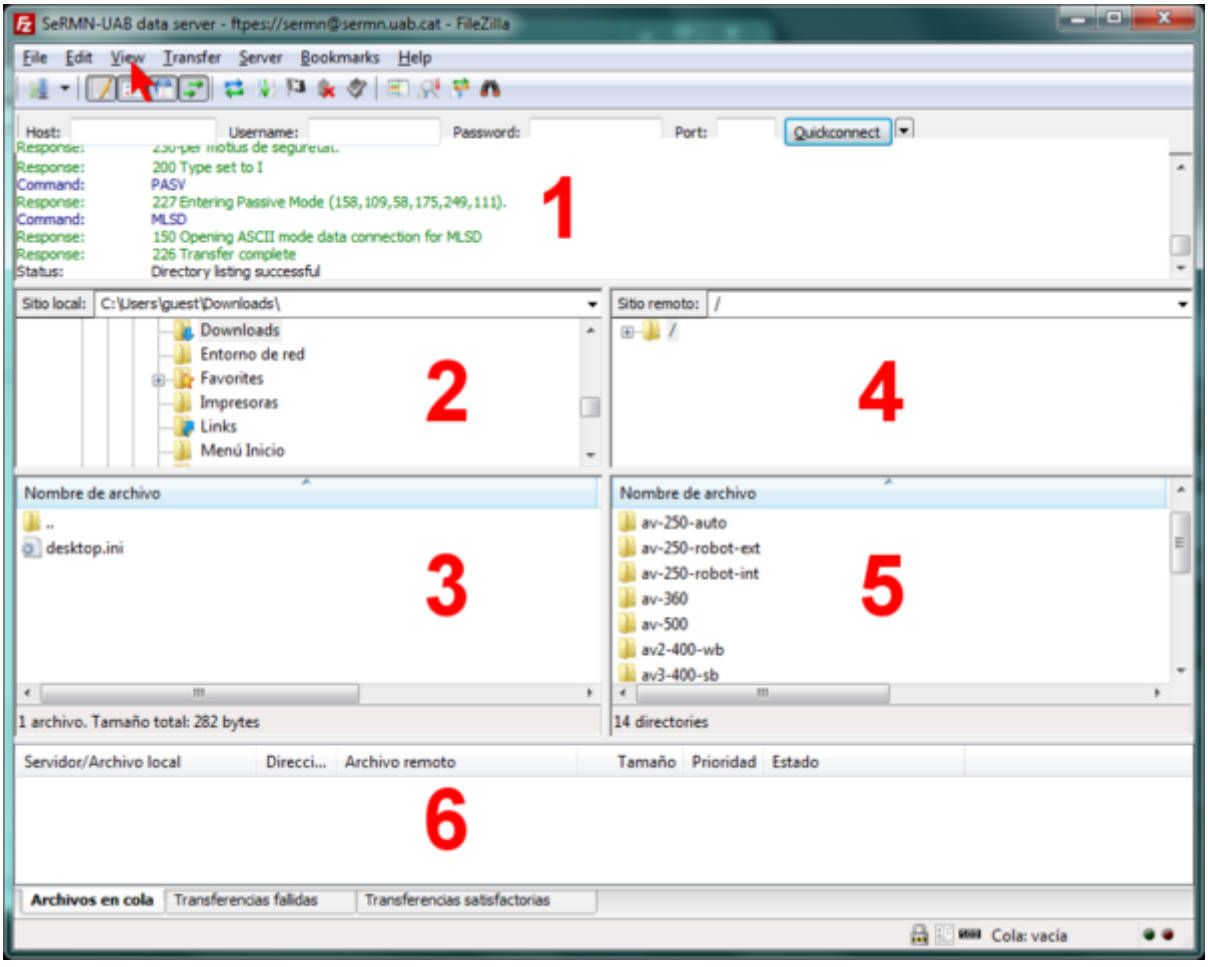
If you don't want to have to accept the certificate every time you connect, check the option *Always trust certificate in future sessions.*

If the login username and password are already defined in the account (see above, *Logon type* set to *Normal*) the FTP client will proceed directly to start a session. On the other hand, if you have defined an interactive type account (see above, *Logon type* set to *Interactive*), the program will first ask for your username and then your password before starting a session,





In both cases the program will show you the commands it executes and the contents of the remote folder on the data server,

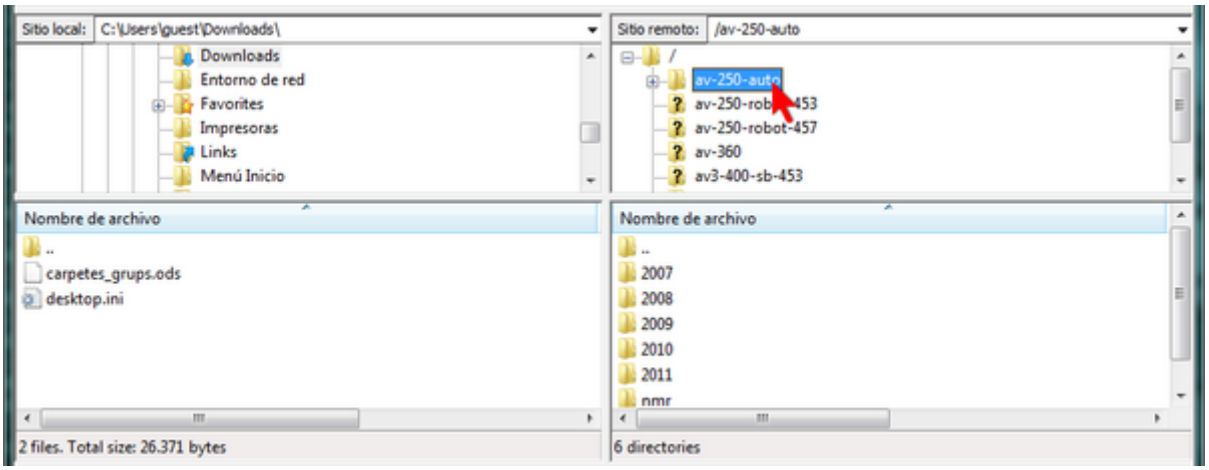


The figure above shows the FileZilla screen with default graphics settings,

- In **panel 1** you can see the messages exchanged between the client and the server. In the event of problems, this information can help us to identify the cause of the problem and to resolve it.
- **Panel 2** displays the local directory tree, and **panel 3** shows the listing of folders and files contained in the currently open local folder.
- Similarly, **panel 4** shows the directory tree on the remote data server, and **panel 5** shows the list of folders and files contained in the currently open remote server folder.
- Finally, depending on the selected tab, in **panel 6** you can check the status of the file transfer: files in queue, files transferred, and errors in the file transfer.

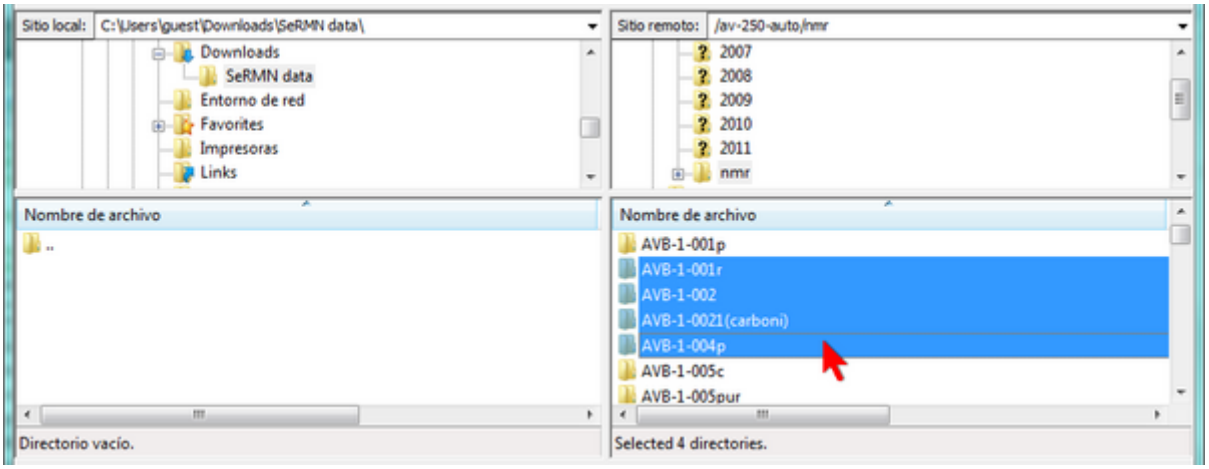
The configuration of the graphical interface can be modified through the *View* menu.

To transfer data you must first choose the spectrometer or computer you want to access,

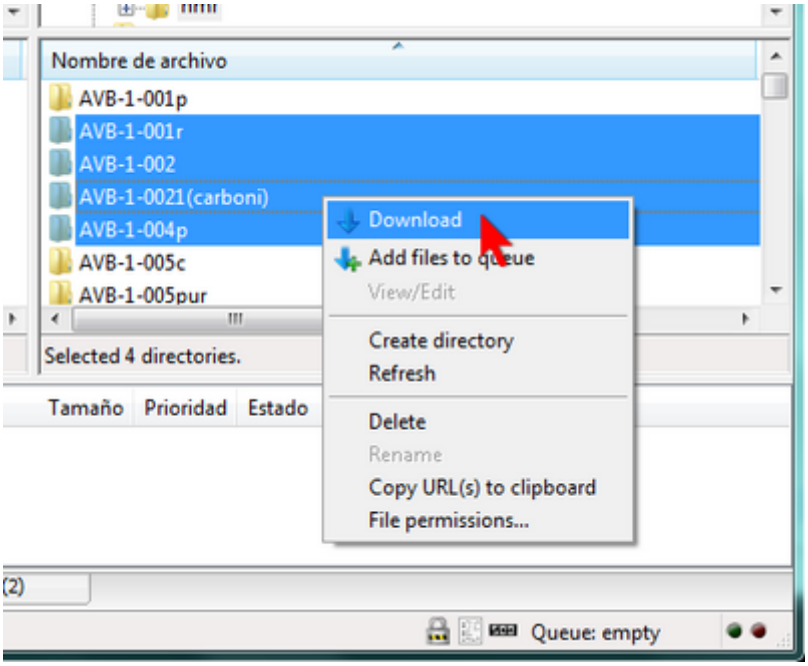


inside each spectrometer folder you will find at least one folder named *nmr* containing the most current data, although there may also be other folders corresponding to previous years.

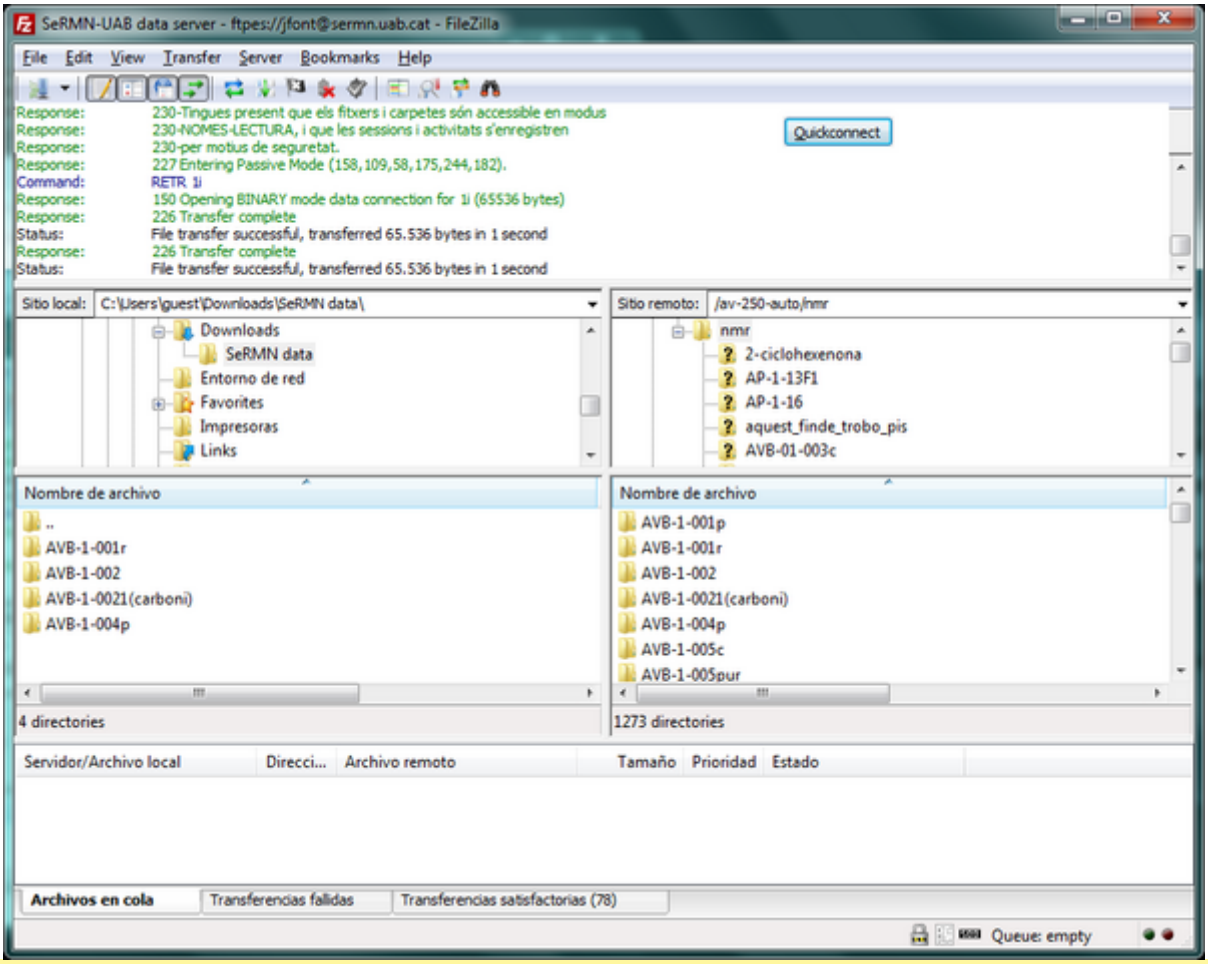
To transfer the data of an experiment you must select the corresponding folder



and, with the right mouse button, expand the menu and choose the option *Download*



After the file transfer is complete, the data folders will appear in the panel corresponding to the local folder on your computer.



Alternatively, you can drag the selected folders to the panel where the local directory is displayed, or you can even drag them to a Windows Explorer window or to the desktop.

When you're done transferring data, just close FileZilla to disconnect from the data server and log out.

For more information on using FileZilla you can consult the program's help or the documentation available on their website.

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