

How to recover your data

Your data acquired on any of the NMR Service spectrometers are available at all times and from anywhere through our data server. To recover 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 [W \] protocol FTPS/FTPES](#). This data transfer protocol uses [W 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 [W 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 Avance III 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 Avance III+ 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. |

| Folder name | Former spectrometers |
|-------------|--|
| av2-400-wb | Spectrometer Avancell 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 recover 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

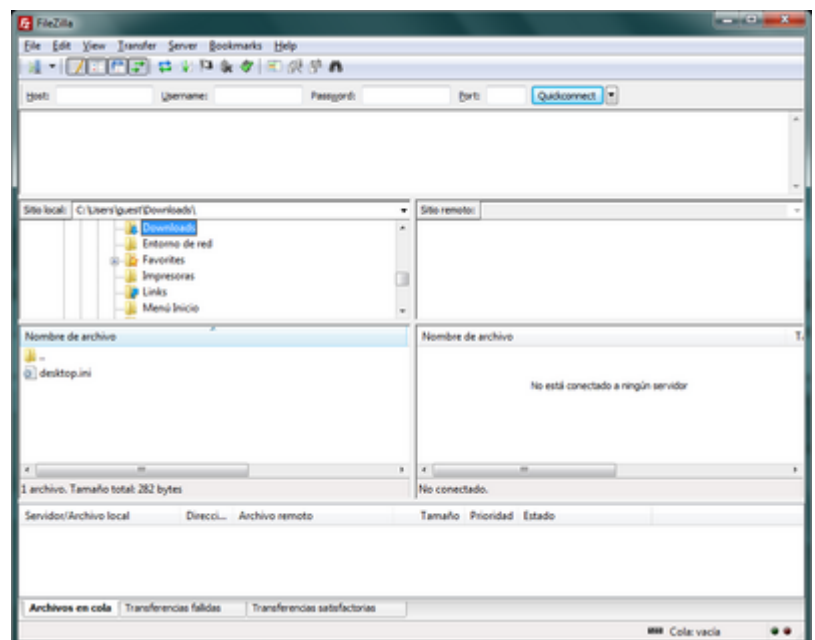
so that you can connect to our FTPS-TLS server via **FTPS-Passive** from inside the firewall.

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.



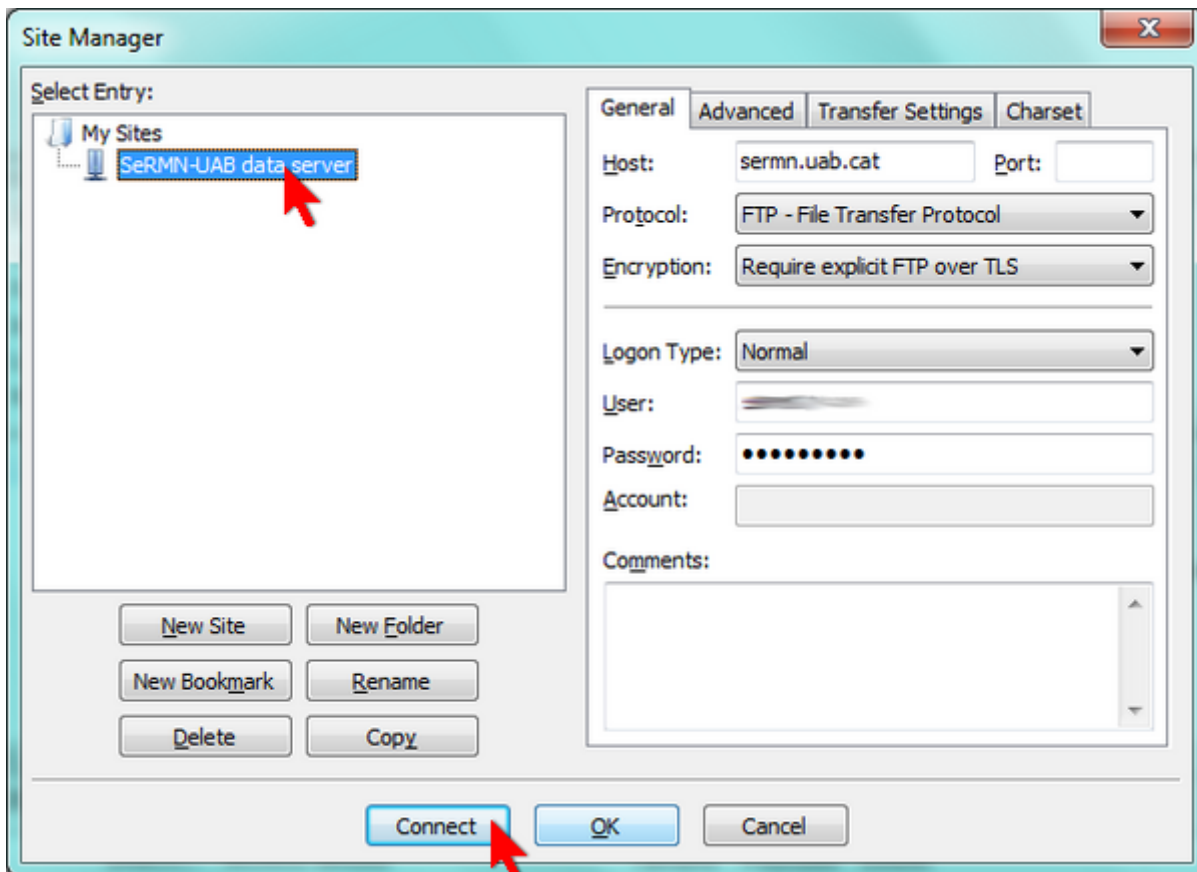
Remember that each research group **only has access to its data folders**. When you acquire spectra, **make sure you save the data in your group folder**. Otherwise you won't be able to retrieve it over the network.



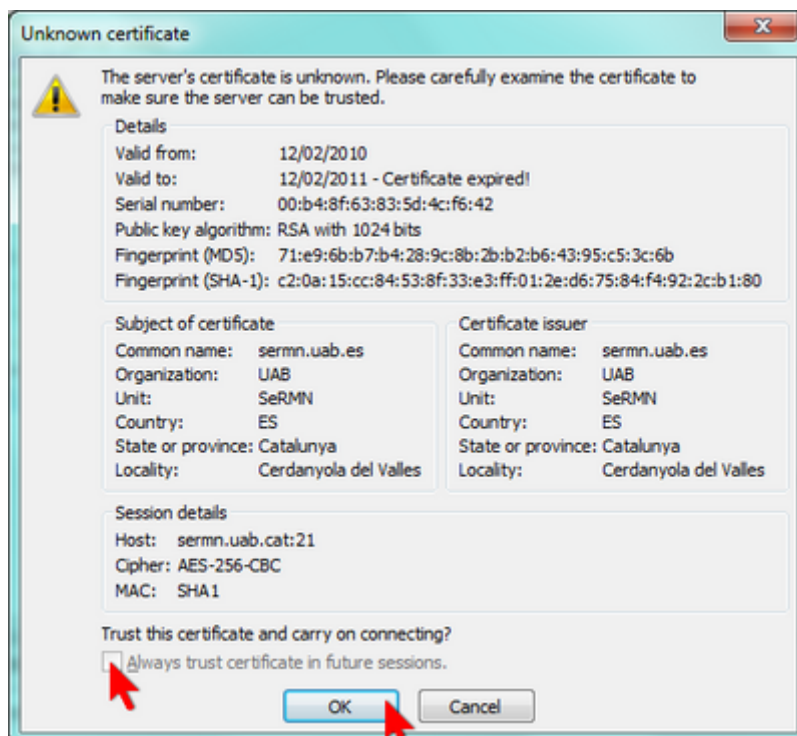
If you have any problems retrieving your data through the server, please contact the service staff and we will try to resolve the issue.

Exemple de sessió per transferir dades


Les imatges següents mostren com descarregar-se dades des del servidor de dades. El primer que hauràs de fer és obrir el *Site Manager*, seleccionar el compte on has definit la connexió al nostre servidor de dades, i prémer el botó **Connect** per iniciar una sessió,



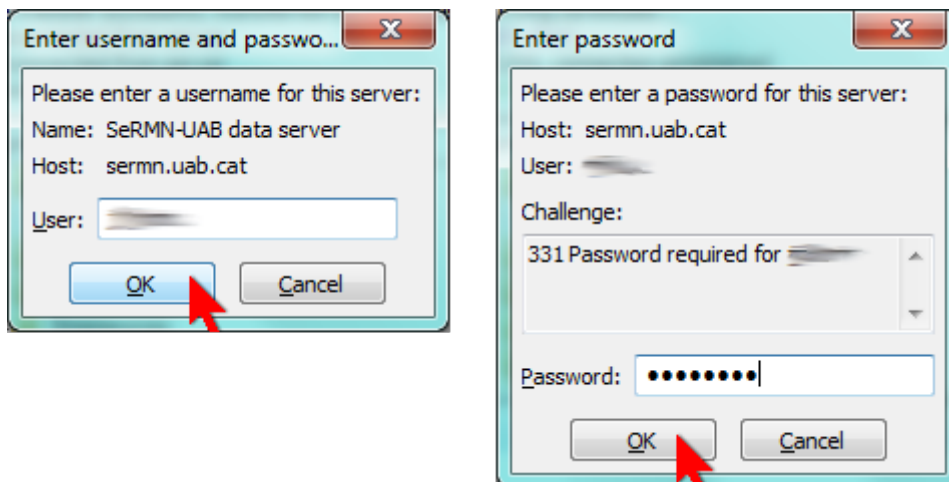
Si has configurat correctament els paràmetres de la connexió, i si no hi ha cap problema a la xarxa, de seguida s'obrirà una pantalla amb el certificat digital que identifica el nostre servidor de dades. Per connectar-te has d'acceptar-lo prement el botó OK.



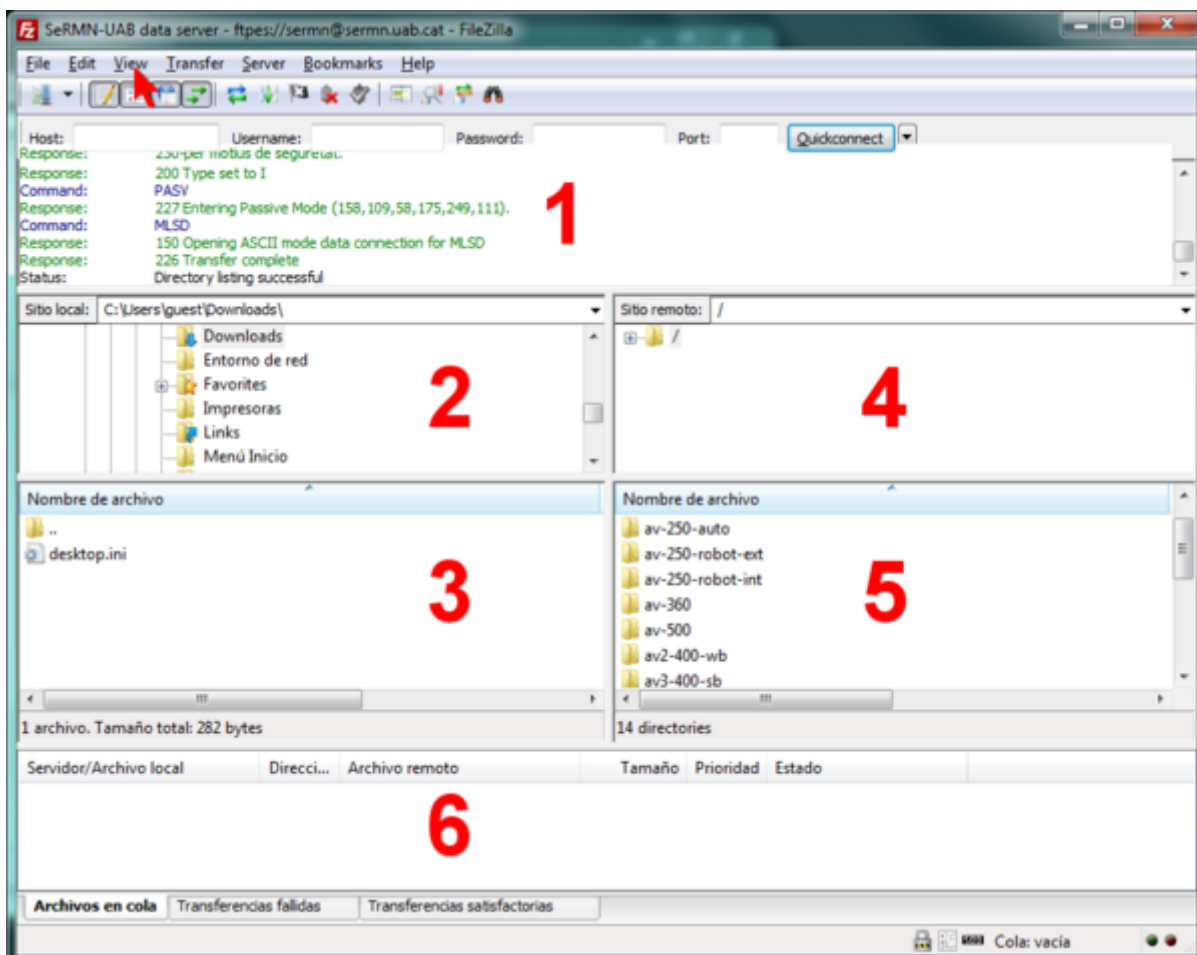
El servidor de dades fa servir un certificat oficial de la UAB generat per GEANT Vereniging que es renova anualment.

 Si no vols haver d'acceptar el certificat cada cop que et connectis, marca l'opció *Always trust certificate in future sessions*.

Si el nom d'usuari i la contrasenya d'accés ja estan definits al compte (veure més amunt, *Logon type* definit com a *Normal*) el client procedirà directament a iniciar una sessió. En canvi, si has definit un compte de tipus interactiu (veure més amunt, *Logon type* definit com a *Interactive*), el programa et demanarà primer el nom d'usuari i després la contrasenya abans d'iniciar una sessió,



En tots dos casos el programa et mostrarà les comandes que executi i el contingut de la carpeta remota al servidor de dades,

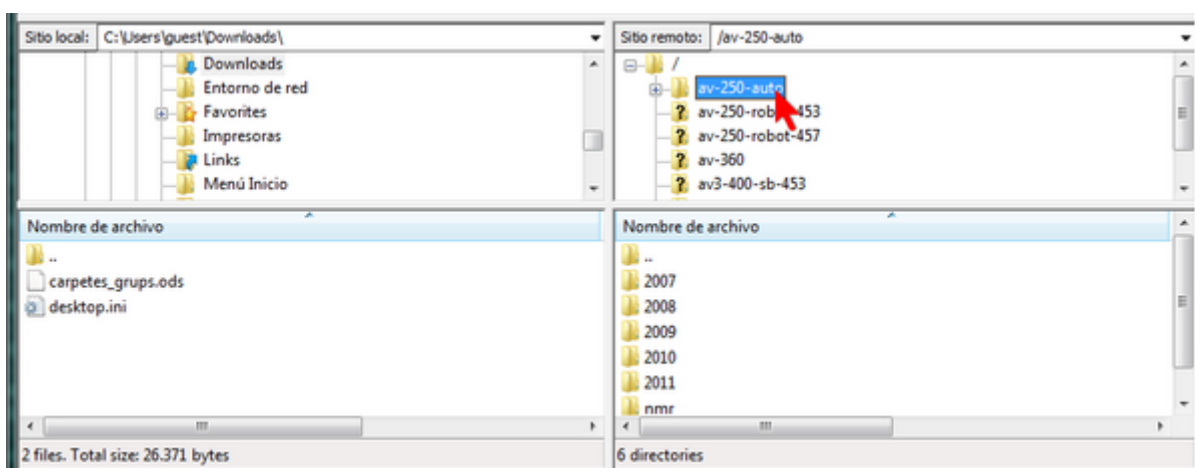


La figura anterior mostra la pantalla del FileZilla amb la configuració gràfica per defecte,

- Al **panel 1** es poden veure els missatges bescanviats entre el client i el servidor. En cas de problemes, aquesta informació pot ajudar a identificar la causa del problema i a resoldre'l.
- Al **panel 2** es mostra l'arbre de directoris local, i al **panel 3** el llistat de fitxers continguts a la carpeta actualment oberta
- De forma semblant, al **panel 4** es mostra l'arbre de directoris al servidor de dades, i al **panel 5** el llistat de fitxers continguts a la carpeta del servidor actualment oberta.
- Finalment, en funció de la pestanya triada, al **panel 6** es pot consultar l'estat de la transferència de fitxers: fitxers en cua, fitxers transferits, i errors a la transferència de fitxers.

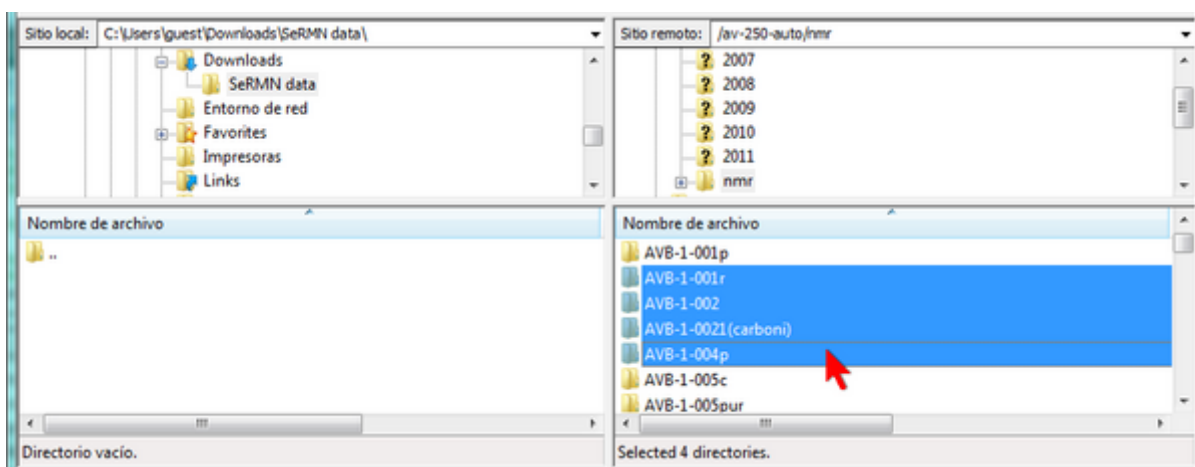
La configuració de la interfície gràfica es pot modificar a través del menú *View*.

Per transferir dades hauràs de triar primer l'espectròmetre o ordinador al qual vols accedir,

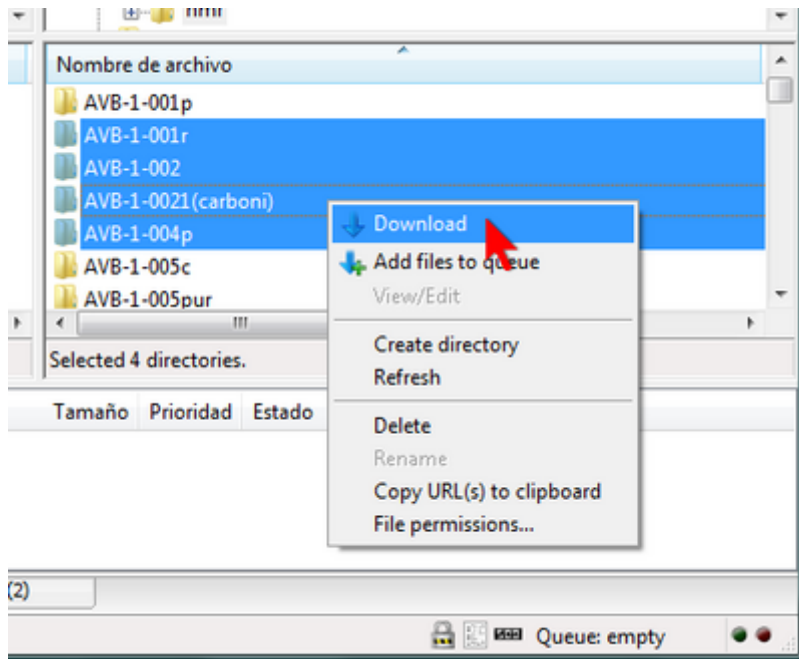


dins de la carpeta de cada espectròmetre trobaràs com a mínim una carpeta de nom *nmr* que conté les dades més actuals, tot i que també poden haver-hi altres carpetes corresponents a anys anteriors.

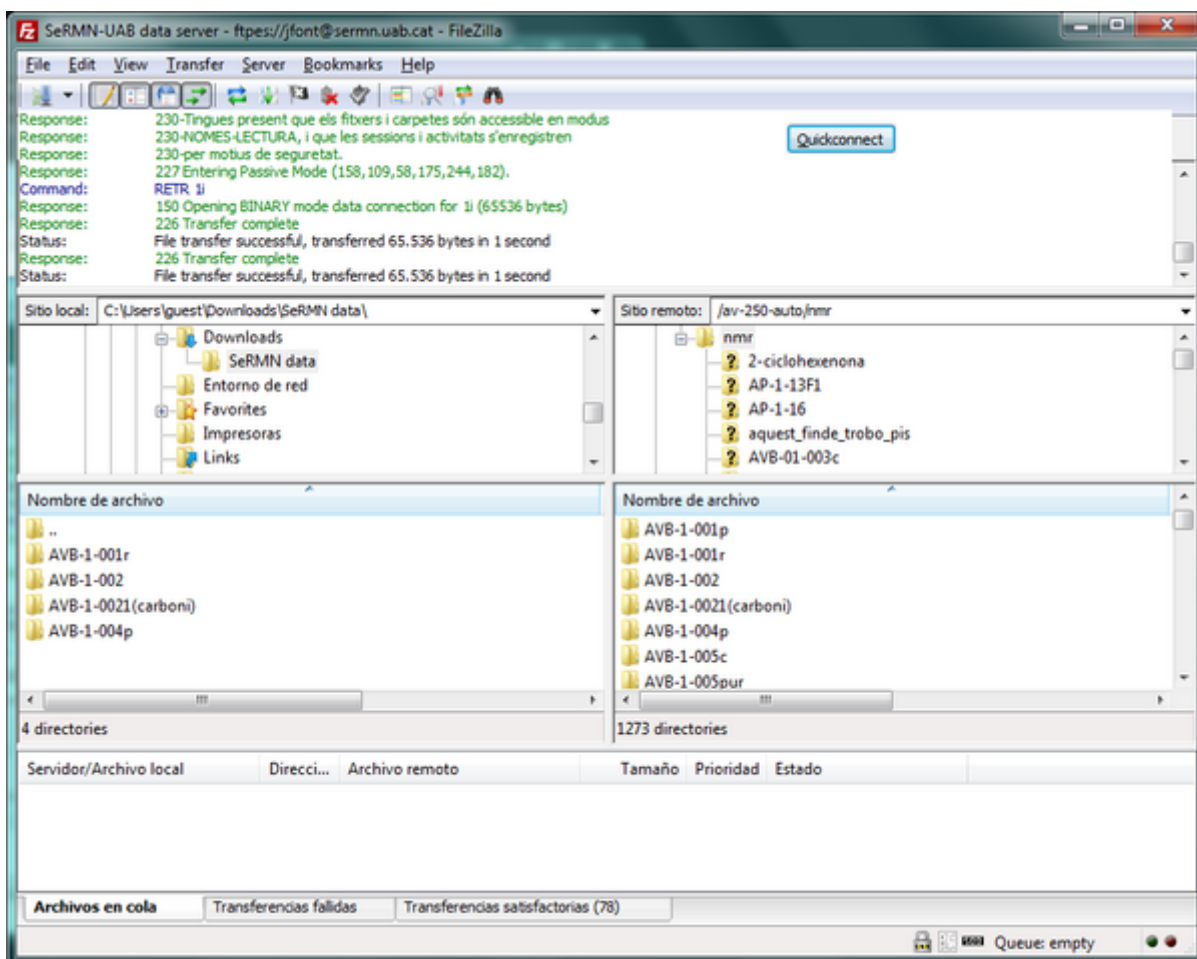
Per transferir les dades d'un experiment has de seleccionar la carpeta corresponent



i, amb el botó dret del ratolí, desplegar el menú i triar l'opció *Download*



Un cop completada la transferència de fitxers, les carpetes de dades apareixeran al panel corresponent a la carpeta local del teu ordinador.



Alternativament, pots arrossegar les carpetes seleccionades al panel on es mostra el directori local, o fins i tot pots arrossegar-les a una finestra de l'explorador de Windows o a l'escriptori.

Quan hakis acabat de transferir dades, només cal que tanquis el FileZilla per desconnectar-te del servidor de dades i finalitzar la sessió.

Per més informació sobre l'ús del FileZilla pots consultar l'ajuda del programa o la [documentació](#) disponible a la seva pàgina web.

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