

## Data access and account management for GUEST users (external users)

For confidentiality reasons, we do not store nor backup any external user data. We therefore ask GUESTS users to directly retrieve their data after acquisition and to erase them from the spectrometer (see paragraph 4).

Dedicated folders are specifically not backed-up.

NMR service can not be considered as responsible in case of loss or diffusion of data that have not been correctly removed from the spectrometer by external/guests users.

The two dedicated machines for external users are nmr1504l and nmr1504r.

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### 1 NMR time booking

On the website [isic-reservation.epfl.ch/](http://isic-reservation.epfl.ch/),

Login: mail address associated to the guest account

Pass: password associated to the guest account

You can book spectrometer time in Routine NMR : ISIC-EPFL-EXT or High Field NMR ISIC-EPFL-EXT

### 2 Login to the NMR spectrometer

Login: Guest name USER (e.g. G13000, *G has to be capital*)

Pass: password associated to the guest account

### 3 Data generation

Follow the "Procedure and Topspin commands for manual machines"  
(in front of all machines or on next page)

Only difference: Use the command **newnmrG** to generate a 1D  $^1\text{H}$  dataset (and not newnmr)

Your data will be generated in the following folder : /opt/data/guests/data/USER/nmr/...  
this folder is in mode 770, root : 500000

### 4 Data recovery on the spectrometer

Connect your USB stick to the machine (a folder should popup)

To find your data:

- open "home" folder
- go up to "root"
- go to /opt/data/guests/Gxxxxx/nmr/yourdata (1504L) or /opt/data/guests/data/Gxxxxx/nmr/yourdata (1504R)




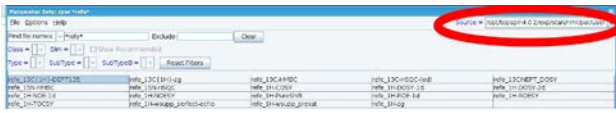

→ drag and drop your data to your USB stick (use the option "move")

Before disconnecting be sure the transfer is over (can take time for 2D especially)


### 4' Data recovery using FileZilla

A dedicated machine is available in the BCH 1504 room. This machine is equipped with FileZilla  
Follow the procedure (next page, or in front of the machine) to recover your data.

## Commands for routine experiment on TOPSPIN 2, 3 & 4

Command	Options / Remarks	Action
	- on the computer desktop	Start topspin program
<b>ej/ij</b>	To start the lift (or eject the sample): <b>ej</b> To stop the lift (or inject the sample): <b>ij</b>  Before starting the lift, remove the black cap on the magnet!	Insert and eject the sample
<b>newnmr</b> <i>(for guests)</i> <b>newnmrG</b>	Enter your sample name If asked : enter you user (Gaspar) name (acknowledge error message)  If you don't want to do a $^1\text{H}$ spectrum → Command : <b>rpar ref*</b> → select the experiment you want to do (  source: .../user)	Generate a new $^1\text{H}$ experiment  Generate preset experiment (ask us if other exp. are needed)
		
<b>Rsh</b>	Choose the most recent file with the name " <b>LS_1H_xx.xx.xxxx</b> " and "read"	Read reference shim file
<b>lock</b>	Select the solvent in the list	Lock the sample
<b>atma</b>	 if another nucleus is set <u>later</u> this step should be done again	Tune and Match the probe
<b>topshim</b>		Shim automatically
<b>rga</b>		Set the receiver gain
<b>ns</b>	- you can estimate the exp time with the command <b>expt</b>	Define the number of scans
<b>zg</b>	- if multiple exp need to be started : <b>multizg</b> (from the 1 <sup>st</sup> one)	Start the acquisition
<b>efp</b>		Fourier transform
<b>apk</b>		Correct phase

### More useful commands...

Command	Action
<b>edc</b>	Create a new dataset or a second experiment in the same dataset Tick "Use current parameters" to keep the parameters of the dataset
<b>rpar ref*</b>	Choose a new method in the list (atma needed if the observed/decoupled nucleus is changed)
<b>tr</b>	Save the FID during an experiment (you need to do "efp" to check the spectrum) ! It is automatically overwrite at the end of the experiment by the final FID!
<b>halt</b>	Stop the experiment before the end and save the FID  If you use the command "stop", your data will be lost!
<b>xfb</b>	Fourier transform for 2D data
<b>expt</b>	Give the duration of the experiment

# NMR Data recovery for external users

Login → user : Gxxxxxx (password : #your password (Swiss qwertz keyboard))

Insert USB stick before starting FileZilla



1) Connect yourself to the server using FileZilla

- Host nmr.epfl.ch
- User : Gxxxxx (or email)
- Pass: your password
- Port 22

2) Find your data (right window, remote machine)

- Spectro (1504 -L, -R, ..)
- Guests/Gxxxxx/nmr/your-data

3) Find your USB stick (left window, local machine)  
/run/media/your-email/your-key

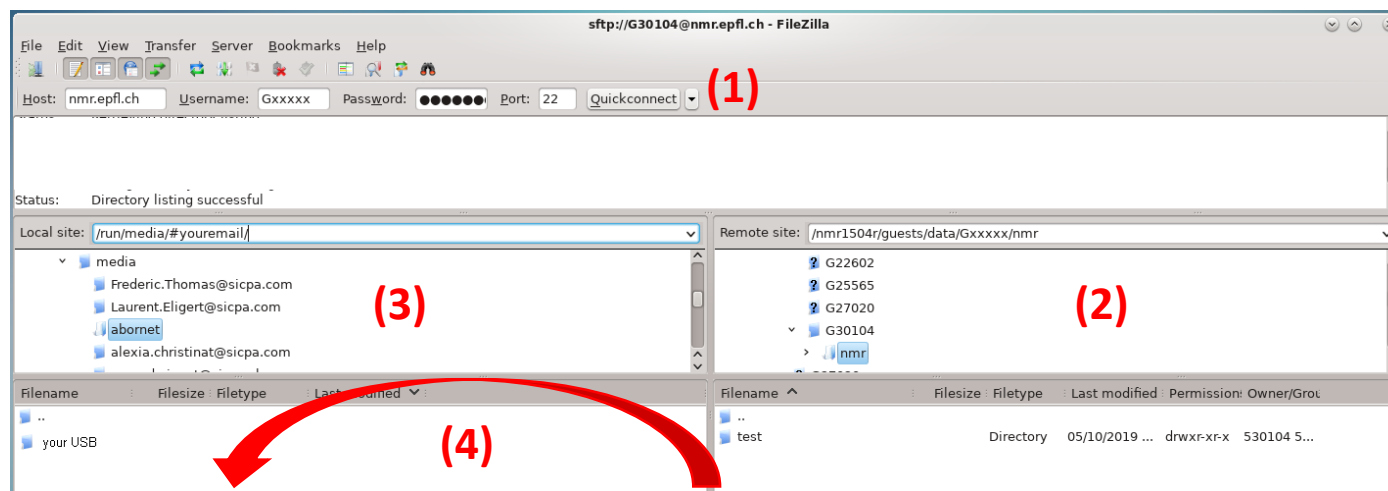
5) Erase your data from the server



Definitive step, make sure transfer is finished  
(data transfer can take time, esp. for 2D)

6) Erase your connection data

- right click “Quickconnect”,
- “Clear history”



4) Transfer your data to your USB stick  
By drag and drop to your USB stick

\*If you don't find your USB stick you can  
as well transfer it to the desktop and then  
to your stick (in folder “home”)

