

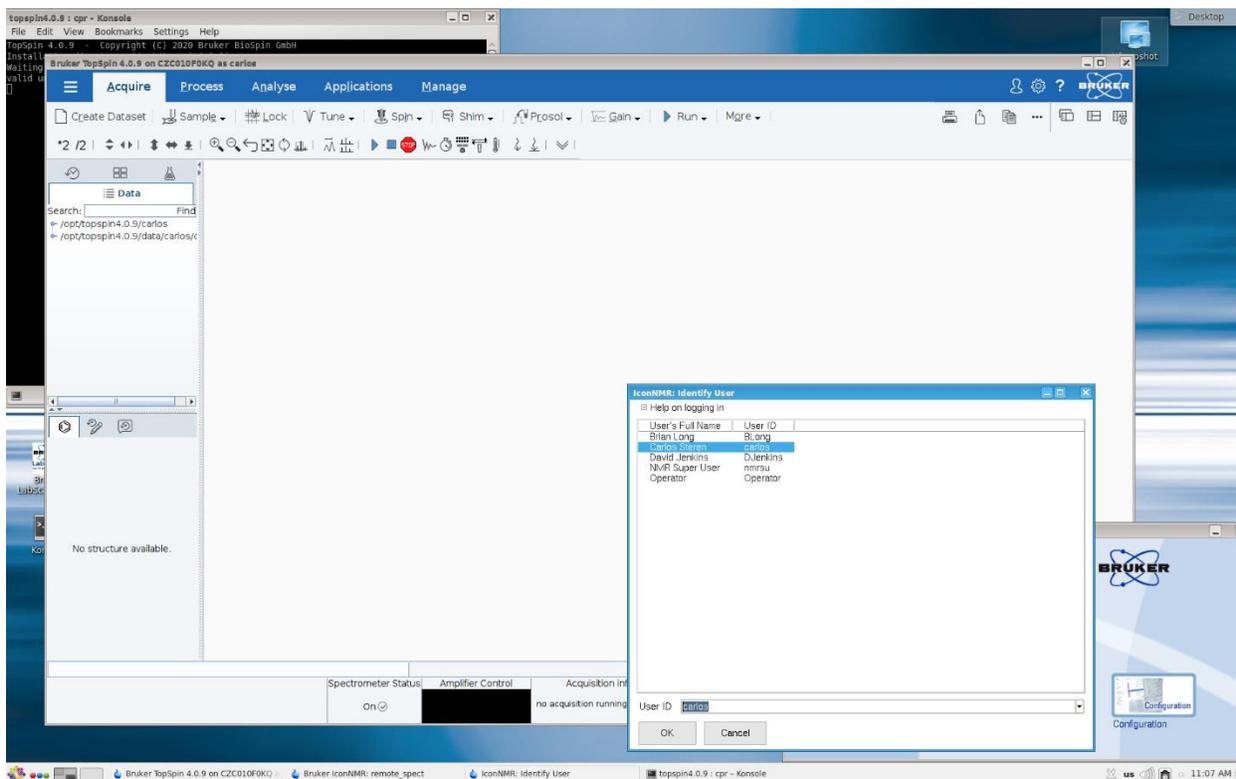


Department of Chemistry

NMR Facilities

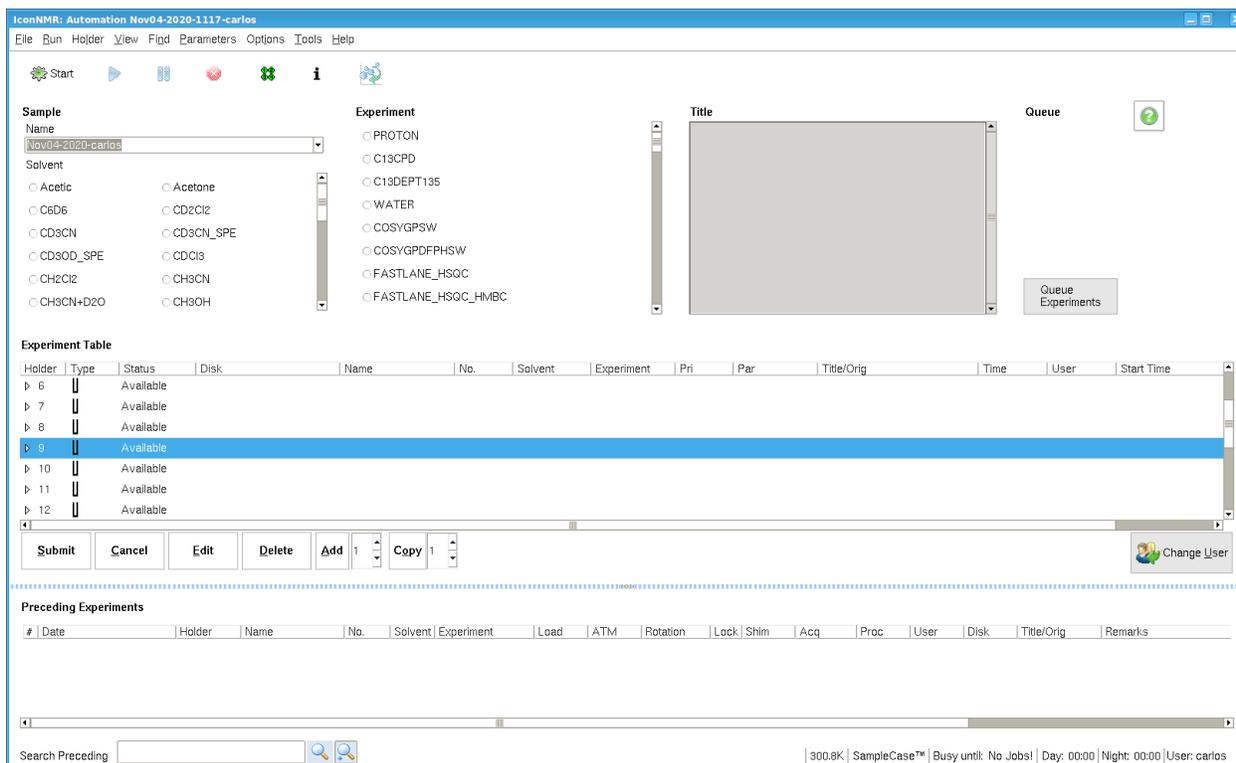
Bruker 500 - ICON-NMR automation Tutorial.

- 1.- Log into the group's account.
- 2.- Double click on the TOPSPIN icon to start the program.
- 3.- Type "icona" in the command line.
- 4.- A window with the list of groups pops up as shown in the picture. Select your group and click <ok>.



- 5.- Another window pops up requesting the password of the group's account.
- 6.- Once the password is entered, the ICON-NMR window is displayed.

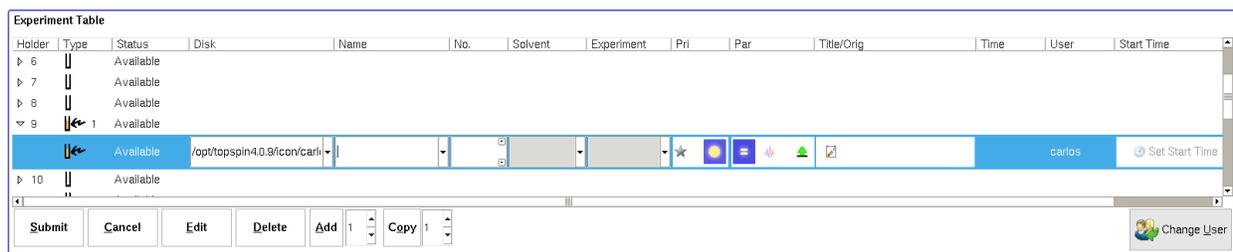
ICON-NMR window.



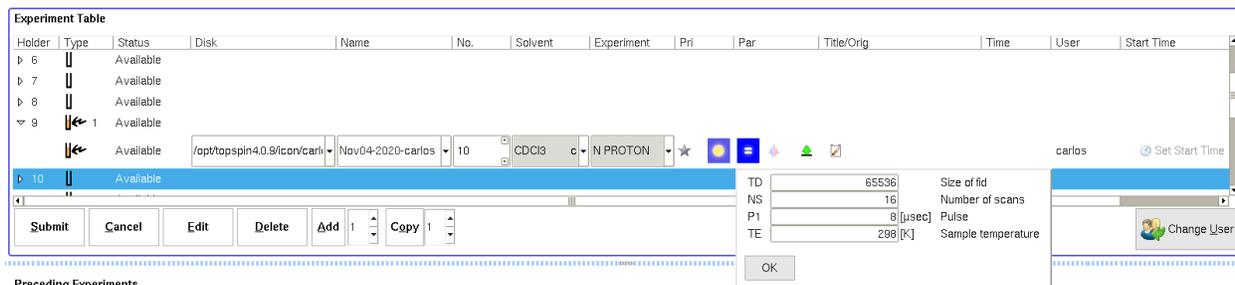
The numbers in the “Experiment Table” correspond to the position of the tubes in the autosampler.

7.- Double click on the number corresponding to the position of the NMR tube in the autosampler. Another line appears, where the information on the experiment is entered.

8.- Select the information for the experiment, from left to right: Disk, Name (make sure to choose an option that includes the date), Solvent, Experiment, and Title.



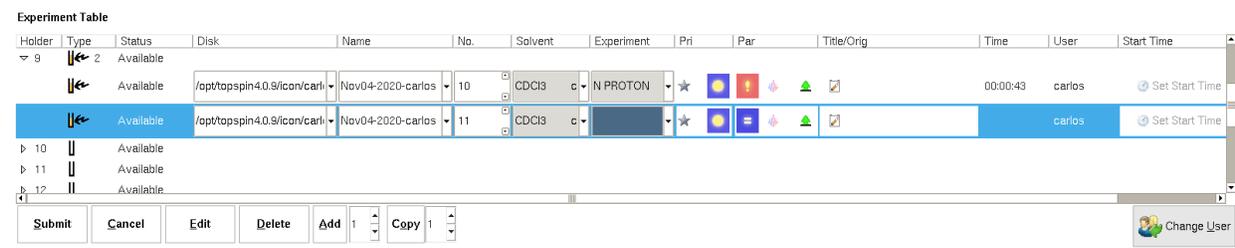
9.- Click on . A window with the experimental parameters is displayed. Check and change the parameters as needed.



The screenshot shows the 'Experiment Table' window with a table of experiments. The table has columns: Holder, Type, Status, Disk, Name, No., Solvent, Experiment, Pri, Par, Title/Orig, Time, User, Start Time. Row 10 is selected. A parameters dialog box is open, showing fields for TD (65536), NS (16), P1 (8 [usec]), and TE (298 [K]). The dialog also includes fields for 'Size of fid', 'Number of scans', 'Pulse', and 'Sample temperature'. Buttons for 'Submit', 'Cancel', 'Edit', 'Delete', 'Add', and 'Copy' are visible at the bottom of the table.

10.- To add another experiment for the same sample, click on <Add>.

11.- Complete the information for the new experiment; Experiment, Parameters, and Title(if needed).



The screenshot shows the 'Experiment Table' window with two experiments added. The table now has three rows. Row 10 is highlighted in blue. The parameters dialog box is still open, showing the same parameters as in the previous screenshot. The 'Add' button is visible at the bottom of the table.

Continue **adding** experiments, or setting the experiments for another sample in your batch.

Same experiments for multiples samples; a) highlight the lines with the experiments. b) set the number of samples in the batch. c) click <Copy>.

12.- **Running the experiments.**

a) On the Experiment Table, highlight all the lines including the samples and experiments to run and click on <Submit>.

b) The experiments will show as “Queued” instead of “Available”.

c) Click on <Start> , at the top left of the window.

d) Click <Start> on the windows that pops up. The queued experiments will start running.



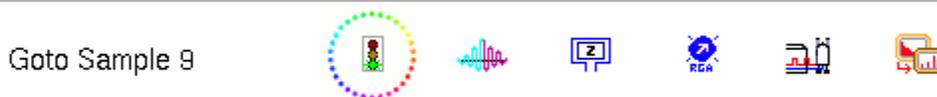
The screenshot shows the software interface with a menu bar (File, Run, Holder, View, Find, Parameters, Options, Tools, Help) and a toolbar. The 'Start' button is highlighted in blue. A tooltip is visible below the 'Start' button, containing the text: ".|Set Automation mode and start the run|".

What happens next.

First, the dummy (yellow) sample inside the magnet is ejected.

Second, the first sample of the batch is inserted. All the calibrations and experiment are performed automatically one after the other and the experiments are ran for all the samples in the batch.

The process can be followed from the icons shown at the top right of the window.



The sample and experiment running are indicated on the Experiment Table.

Holder	Type	Status	Disk	Name	No.	Solvent	Experiment	Pri	Par	Title/Orig	Time	User	Start Time
8		Available											
9	2	Running	/opt/topspin4.0.9/icon/carlos	Nov04-2020-carlos	10	CDCI3	ch1c N PROTON	★		Sample 1	00:00:43	carlos	11:36 Wed Nov 04 20

In “Preceding experiment”, at the bottom of the window, the processes, once completed, are checked.

#	Date	Holder	Name	No.	Solvent	Experiment	Load	ATM	Rotation	Lock	Shim	Acq	Proc	User	Disk	Title/Orig	Remarks
1	2020-11-04 11:28:20	9	Nov04-2020-carlos	11	CDCI3	C13CPD	✓							carlos	/opt/topspin4.0.9/icon/carlos		

Experiment finished.

Once an experiment is finished, all the processes are shown finished.



In the Experiment Table, the experiment is showed as Finished. If all the experiments for the sample are finished, that is indicated as “Finished” next to the sample number.

Holder	Type	Status	Disk	Name	No.	Solvent	Experiment	Pri	Par	Title/Orig	Time	User	Start Time
8		Available											
9	2	Finished	/opt/topspin4.0.9/icon/carlos	Nov04-2020-carlos	10	CDCI3	ch1c N PROTON	★		Sample 1	00:00:43	carlos	11:36 Wed Nov 04 20
		Finished	/opt/topspin4.0.9/icon/carlos	Nov04-2020-carlos	11	CDCI3	ch1c N C13CPD	★			00:00:37	carlos	11:28 Wed Nov 04 20
10		Available											

