

☞ When you arrive at the spectrometer, you should have this display on the screen. Select your login and click OK.

ICON-NMR: Automation Nov09-2005-1530-universite

Menu Disabled

Holder Type Status Disk Name No. Solvent Experiment Par Title / Orig Pri Time User

1 Available

Automation Locked

To unlock the automation window click on the change user button at the right hand side of the Automation Setup window.

ICON-NMR Password Check

Check Additional-User Password

Please enter password for OtherUser

Cancel

Submit Cancel Edit Delete Add Copy

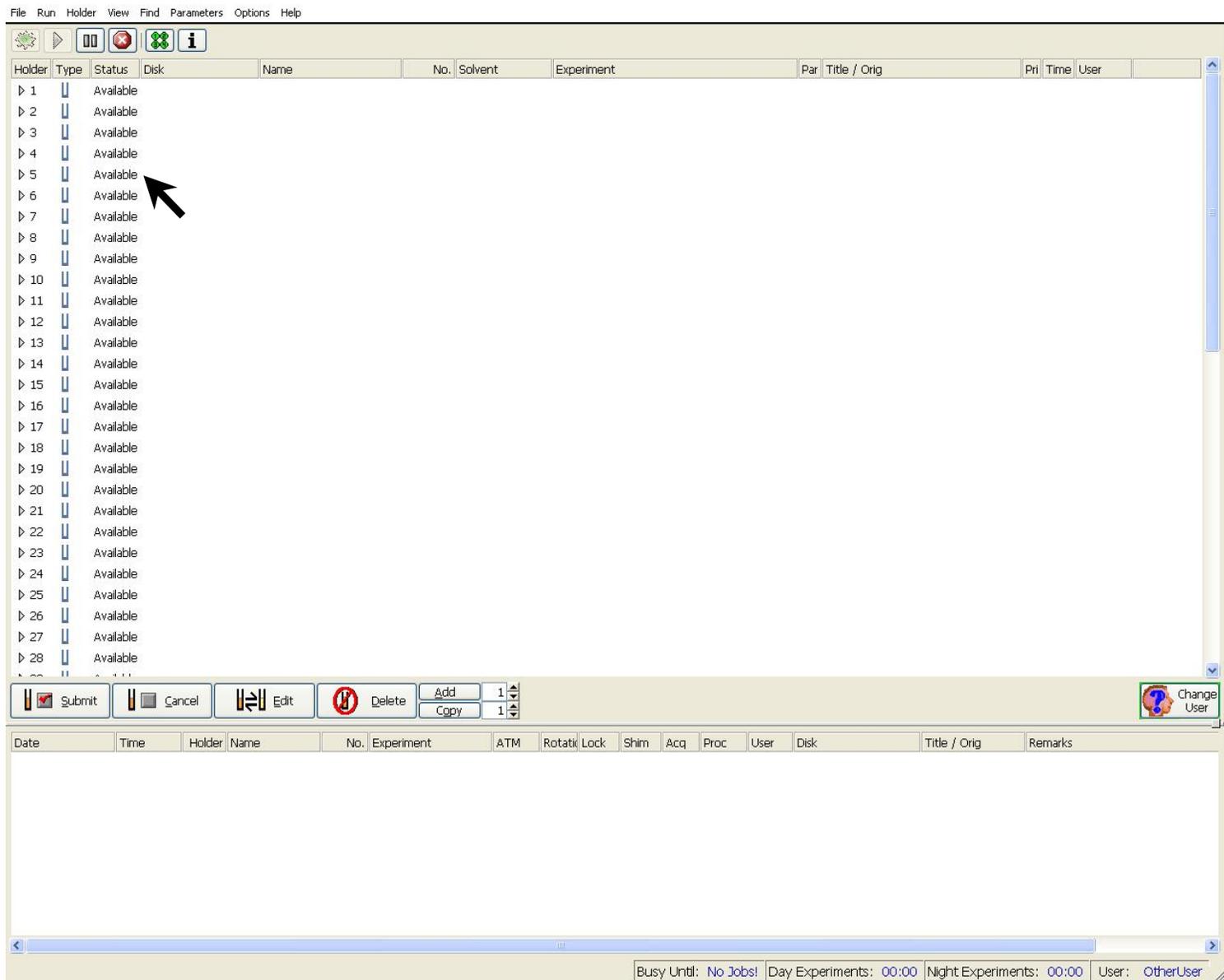
Change User

Date	Time	Holder	Name	No.	Experiment	ATM	Rotati	Lock	Shim	Acq	Proc	User	Disk	Title / Orig	Remarks
2005-11-09	15:45:54	1	example	2	std_13C	✓	✓					universite	D:\Bruker\TOPSPIN	Example 1	
2005-11-09	15:38:23	1	example	1	std_1H	✓	✓	✓	✓	✓		universite	D:\Bruker\TOPSPIN	Example 1	

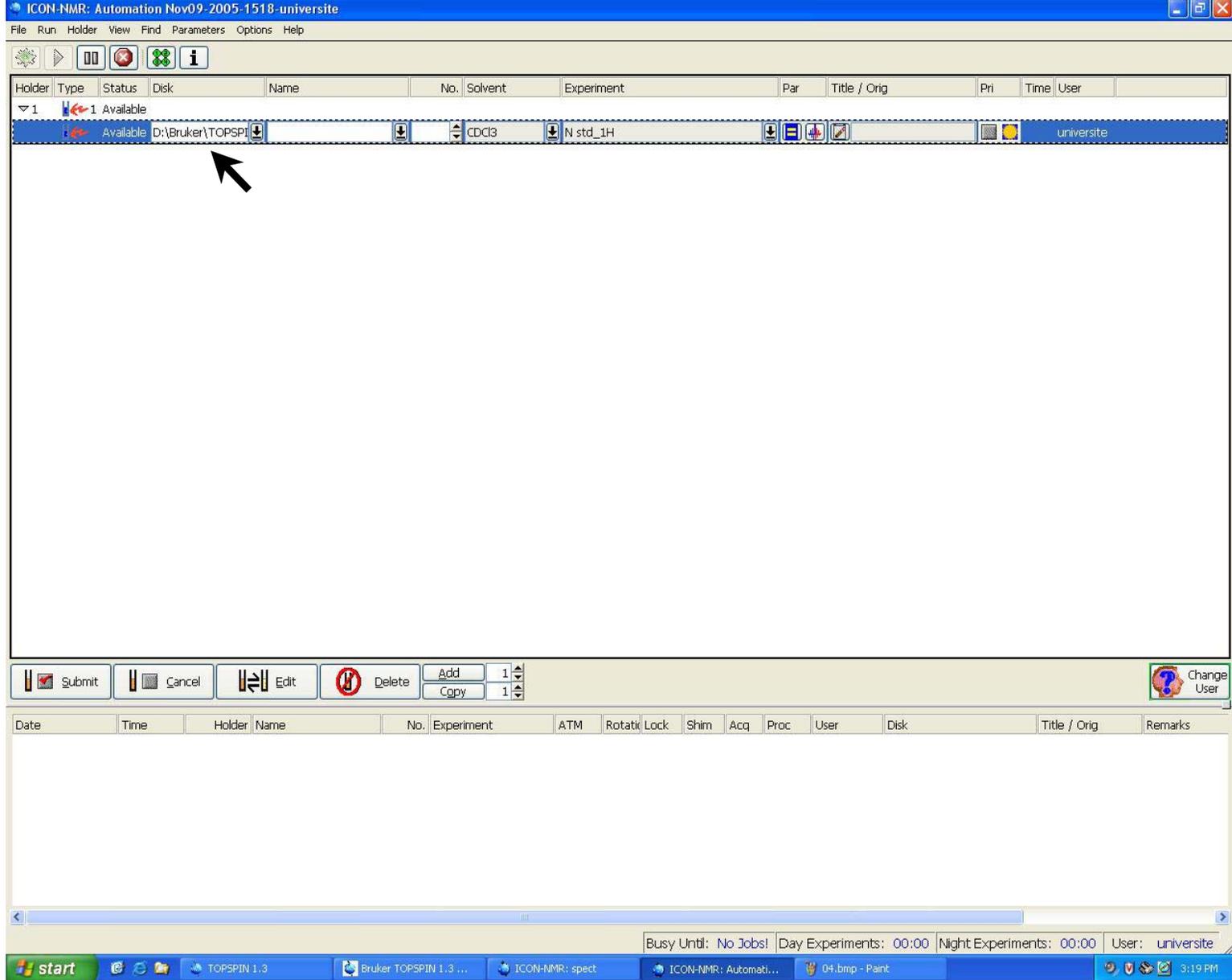
Busy Until: No Jobs! Day Experiments: 00:00 Night Experiments: 00:00 User: universite

start 52.bmp - Paint TOPSPIN 1.3 Bruker TOPSPIN 1.3 ... ICON-NMR: spect ICON-NMR: Automati... 3:53 PM

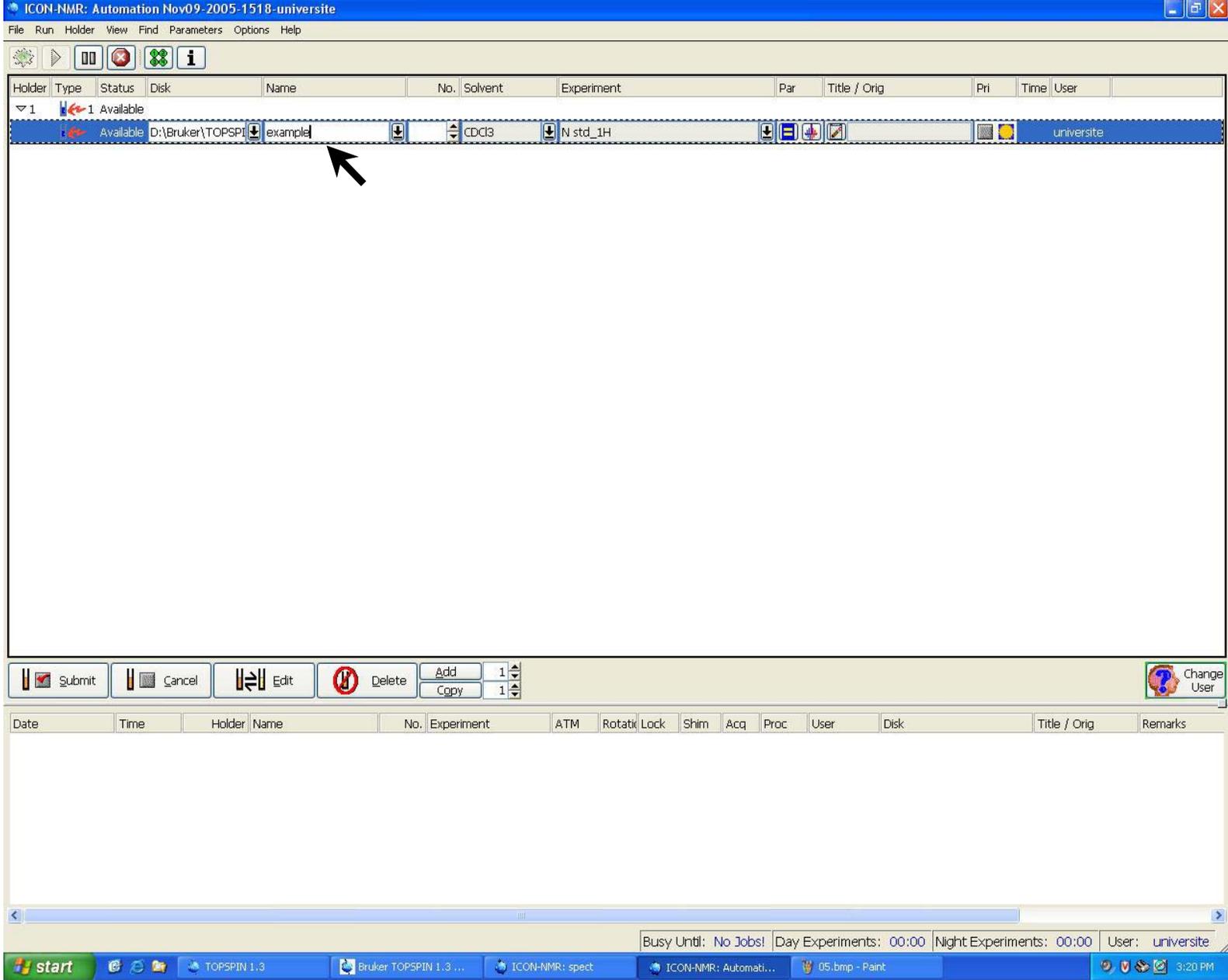
Enter your 'password' and type 'Enter ↵'



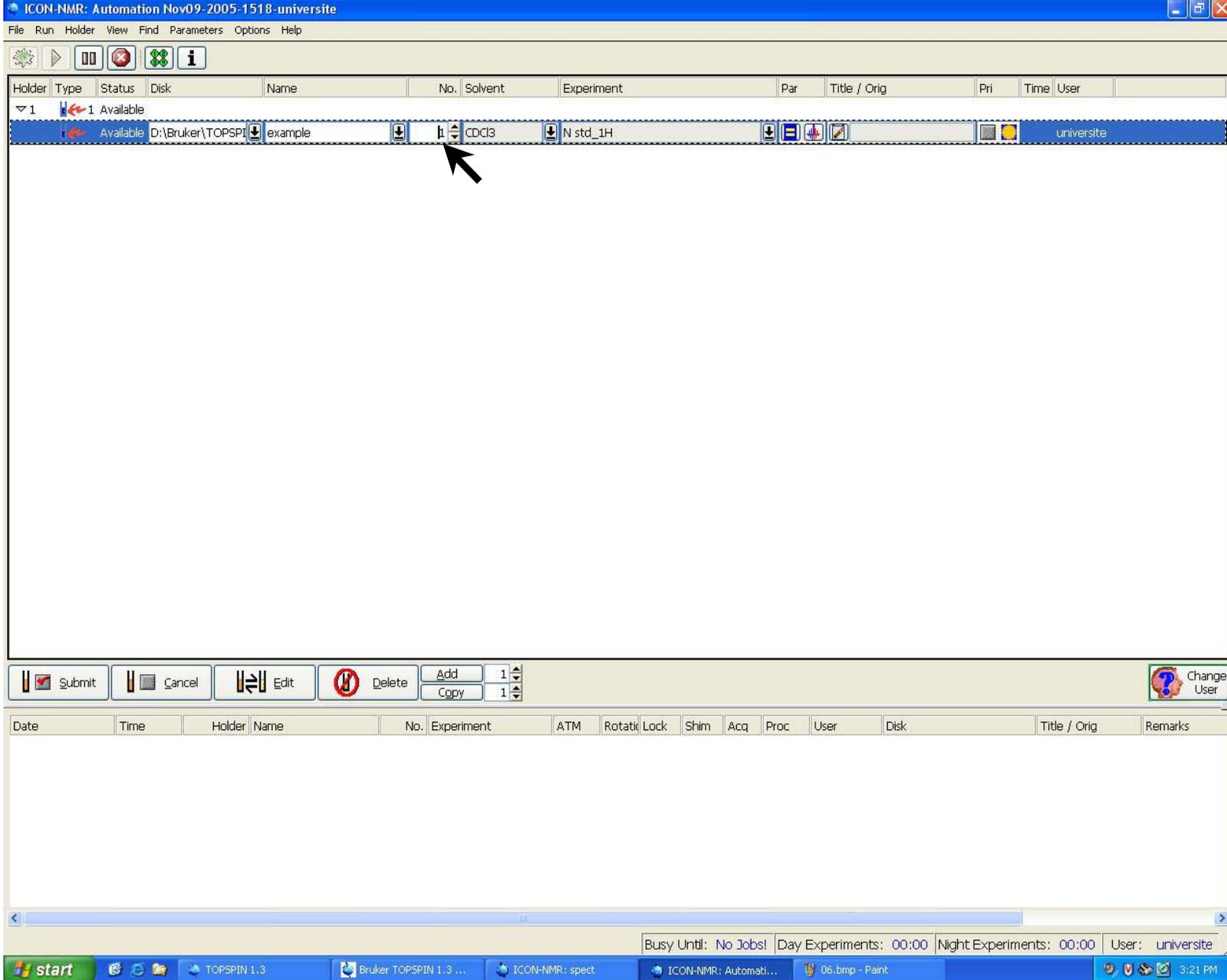
☞ Click on the line corresponding to the holder where you are going to put your sample (choose preferably the holder in chronological order after the last experiment submitted before your experiment)



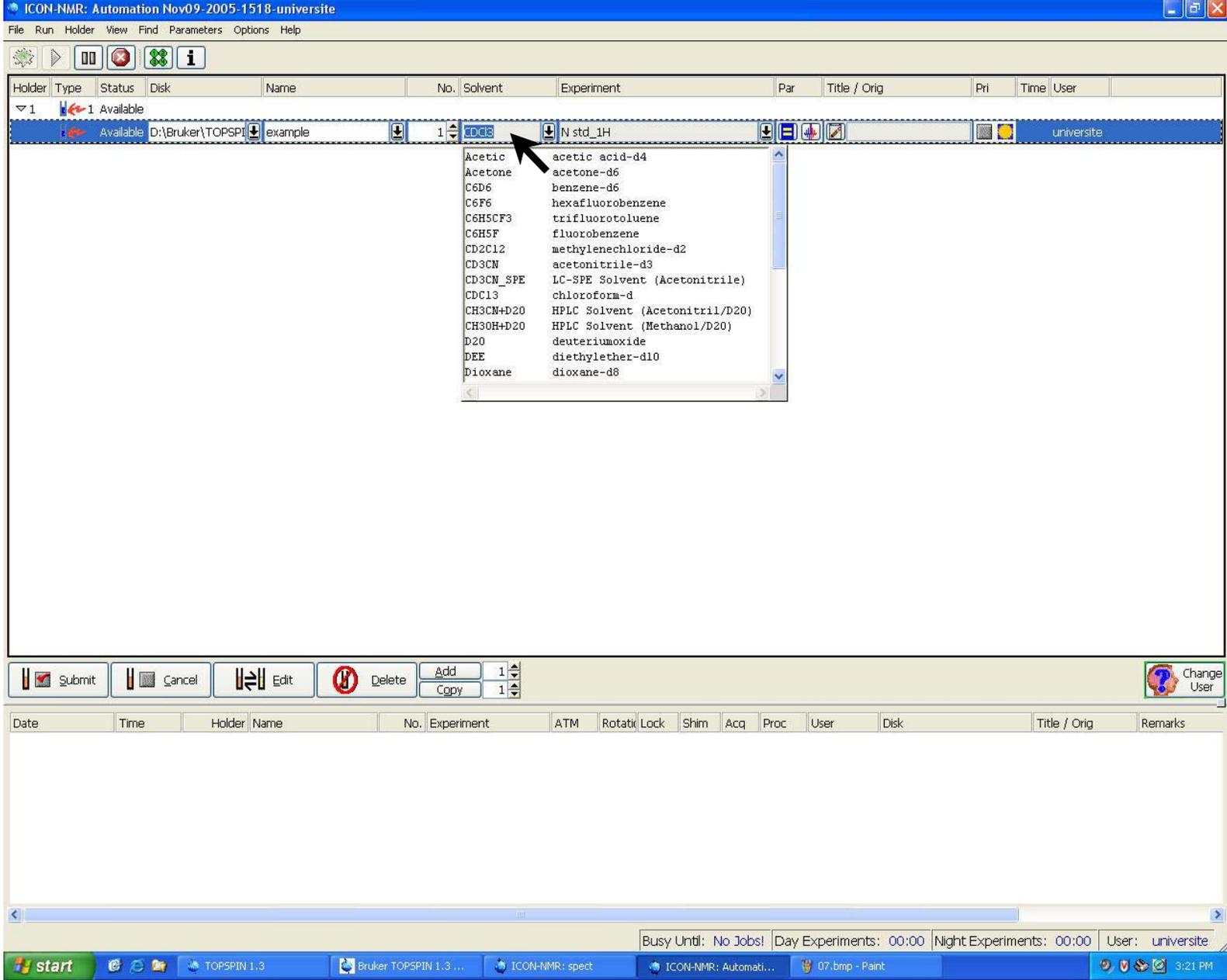
☞ Disk Unit is the partition where your data are saved, don't change it.



☞ Insert a name to your experiment (14 characters max.)



☞ You can select the experiment number ($1 < n^{\circ} \text{exp.} < 999$)



☞ Select your solvent.

File Run Holder View Find Parameters Options Help

Holder	Type	Status	Disk	Name	No.	Solvent	Experiment	Par	Title / Orig	Pri	Time	User
1	Available			test	14	CDCl3	N std_1H					OtherUser
2	Available						N std_1H		1H Standard			
3	Available						N std_13C_15mn		13C Standard (15 mn)			
4	Available						N std_APT_15mn		APT Standard (15 mn)			
5	Available						N std_DEPT135_15mn		DEPT 135 Standard (15 mn)			
6	Available						N std_19F_15mn		19F Standard (15 mn)			
7	Available						n std_13C_1_heure		13C Standard (1 hour)			
8	Available						n std_APT_1_heure		APT Standard (1 hour)			
9	Available						n std_DEPT135_1_heure		DEPT 135 Standard (1 hour)			
10	Available						n std_19F_1_heure		19F Standard (1 hour)			
11	Available						n std_31P_1_heure		31P Standard (1 hour)			
12	Available						n std_gCOSY_1_heure		COSY Gradients (1 hour)			
13	Available						n std_gHMOC_1_heure		1H-13C correlation inverse mode (1 hour)			
14	Available						n std_gHMBC_1_heure		1H-13C multiple bond correlation (1 hour)			
15	Available						n std_gNOESY_1_heure		hour			

Submit Cancel Edit Delete Add 1 Cgpy 1 Change User

Date	Time	Holder	Name	No.	Experiment	ATM	Rotat	Lock	Shim	Acq	Proc	User	Disk	Title / Orig	Remarks

Busy Until: No Jobs! Day Experiments: 00:00 Night Experiments: 00:00 User: OtherUser

- ☞ Select your experiment :
- Day experiment (N) : ~15 mn, between 8:00 AM and 20:00 PM
 - Night experiment (n) : ~1 hour, between 20:00 PM and 8:00 AM

File Run Holder View Find Parameters Options Help

Holder	Type	Status	Disk	Name	No.	Solvent	Experiment	Par	Title / Orig	Pri	Time	User
1	Available	D:\Bruker\TOPSPIN	test	14	CDCl3	N std_1H						OtherUser
2	Available											
3	Available											
4	Available											
5	Available											
6	Available											
7	Available											
8	Available											
9	Available											
10	Available											
11	Available											
12	Available											
13	Available											
14	Available											
15	Available											
16	Available											
17	Available											
18	Available											
19	Available											
20	Available											
21	Available											
22	Available											
23	Available											
24	Available											
25	Available											
26	Available											
27	Available											

SW 15.9952 [ppm]
 O1P 6.000
 D8 0
 OK

Submit Cancel Edit Delete Add 1 Cgpy 1 Change User

Date	Time	Holder	Name	No.	Experiment	ATM	Rotat	Lock	Shim	Acq	Proc	User	Disk	Title / Orig	Remarks

Busy Until: No Jobs! Day Experiments: 00:00 Night Experiments: 00:00 User: OtherUser

☞ Change the default parameters if you want (see next page)

Parameters

SW	<input type="text" value="15.9952"/>	[ppm]
O1P	<input type="text" value="6.000"/>	
D8	<input type="text" value="0"/>	

- SW : Spectral Window (in ppm)
- O1P : Middle of the Spectral Window (in ppm)
- D8 : mixing time (Noesy) (in sec, default = 0.05 sec.)

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File Run Holder View Find Parameters Options Help

Holder Type Status Disk Name No. Solvent Experiment Par Title / Orig Pri Time User

1	Available	D:\Bruker\TOPSPIN	example	1	CDCl3	N std_1H				00:00:24	universite
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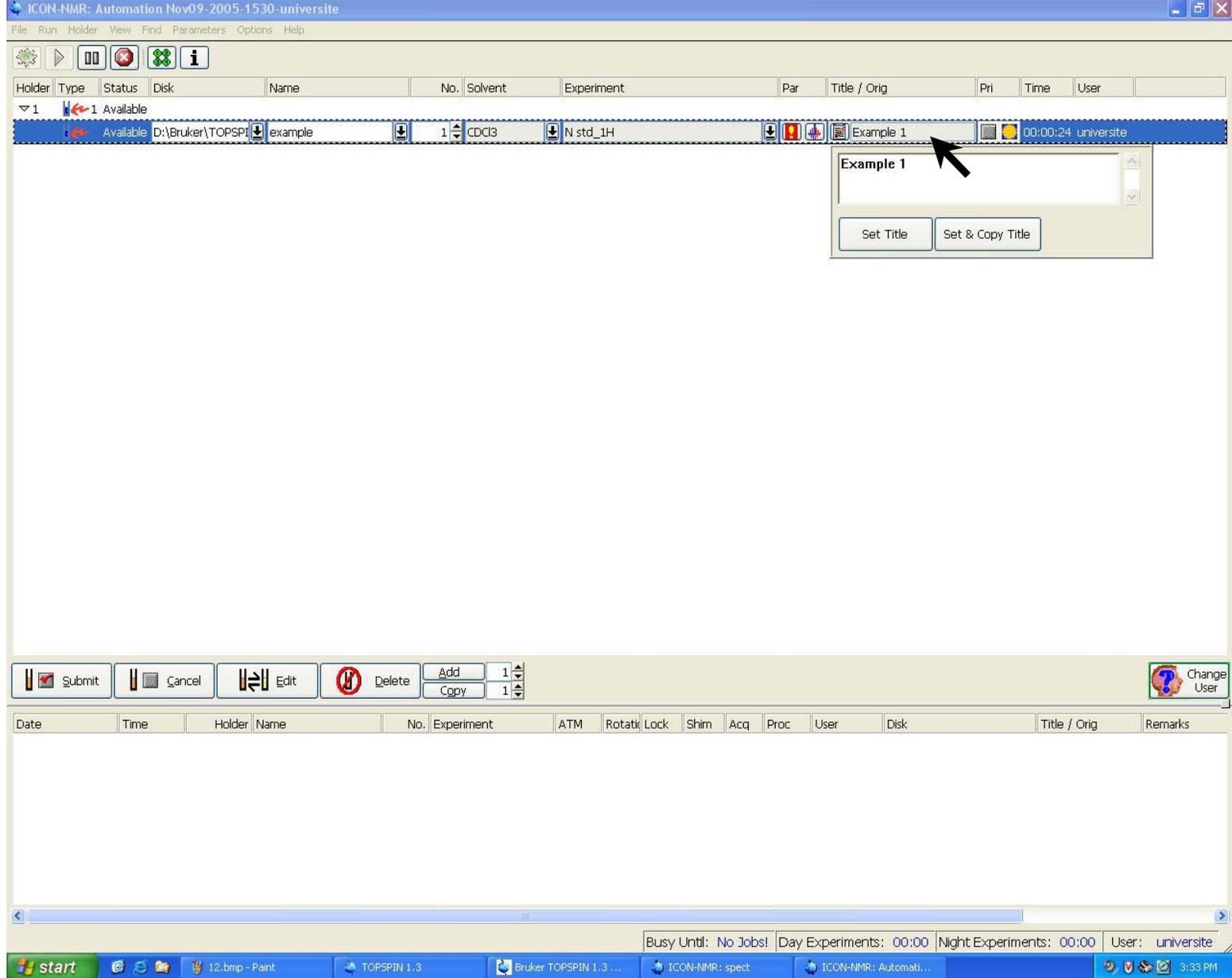
Submit Cancel Edit Delete Add Copy Change User

Date	Time	Holder	Name	No.	Experiment	ATM	Rotati	Lock	Shim	Acq	Proc	User	Disk	Title / Orig	Remarks

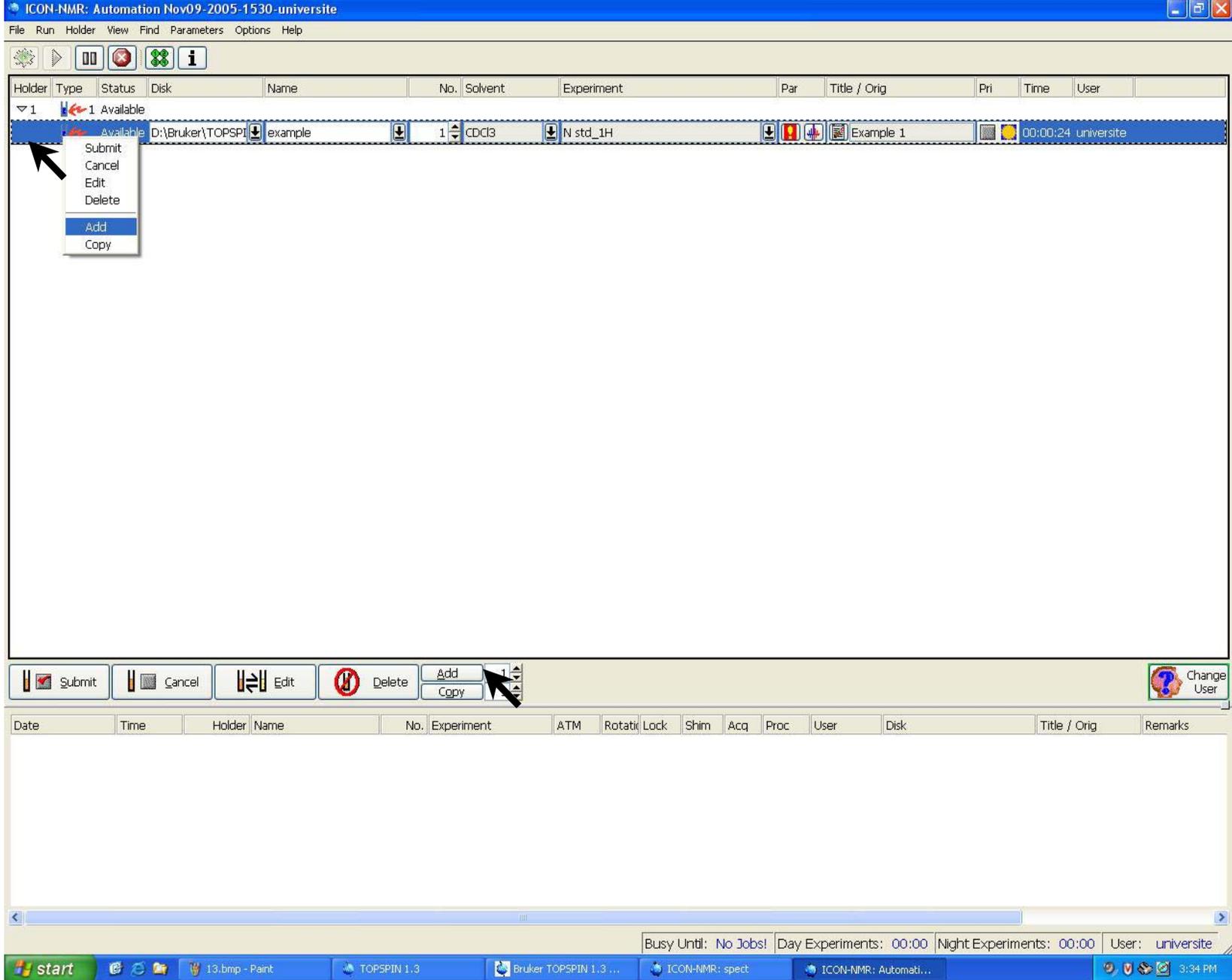
Busy Until: No Jobs! Day Experiments: 00:00 Night Experiments: 00:00 User: universite

start 11.bmp - Paint TOPSPIN 1.3 Bruker TOPSPIN 1.3 ... ICON-NMR: spect ICON-NMR: A ... 3:32 PM

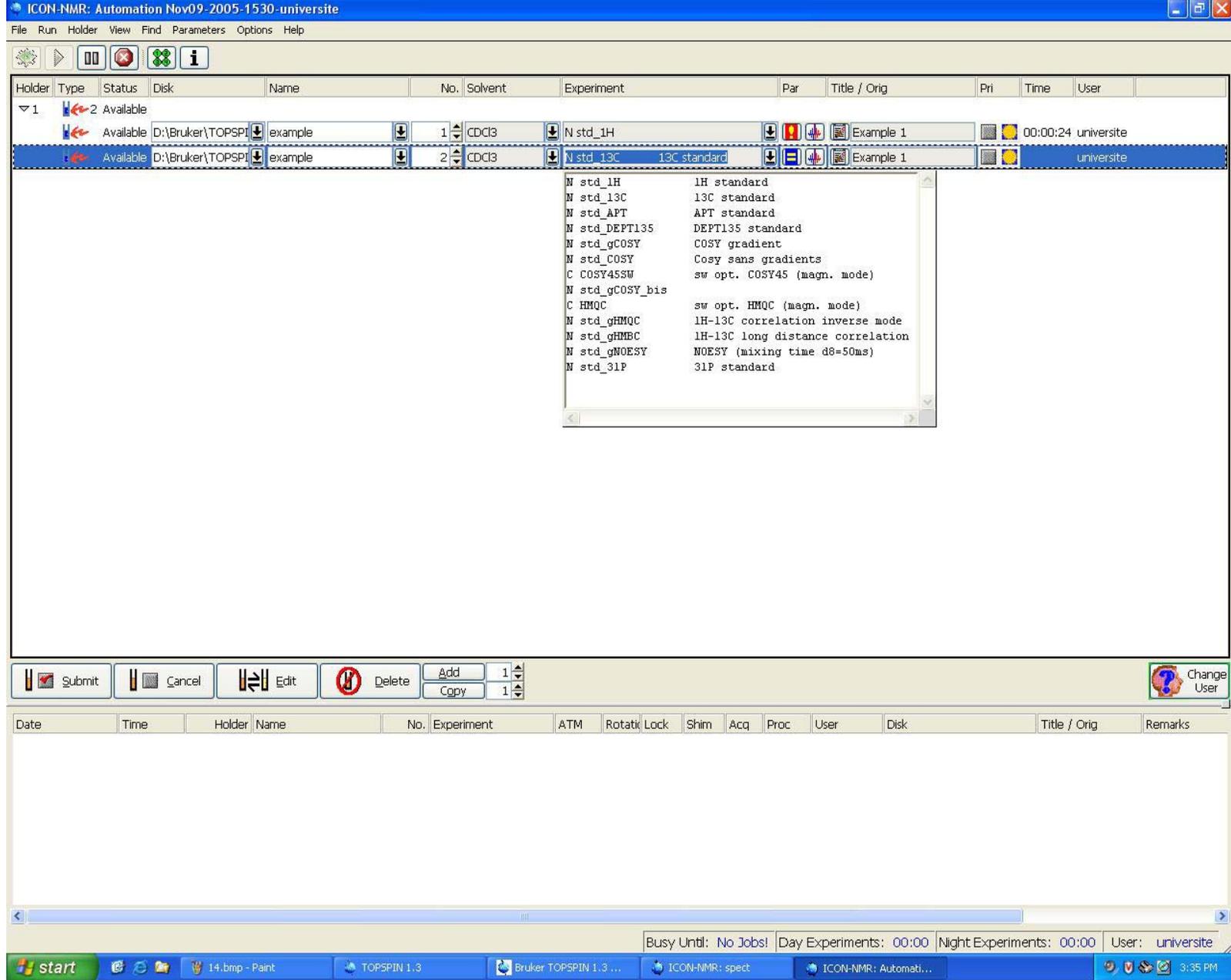
☞ You can see your experiment time on the line selected, and the total of the day and night experiment time at the bottom of the page. 11



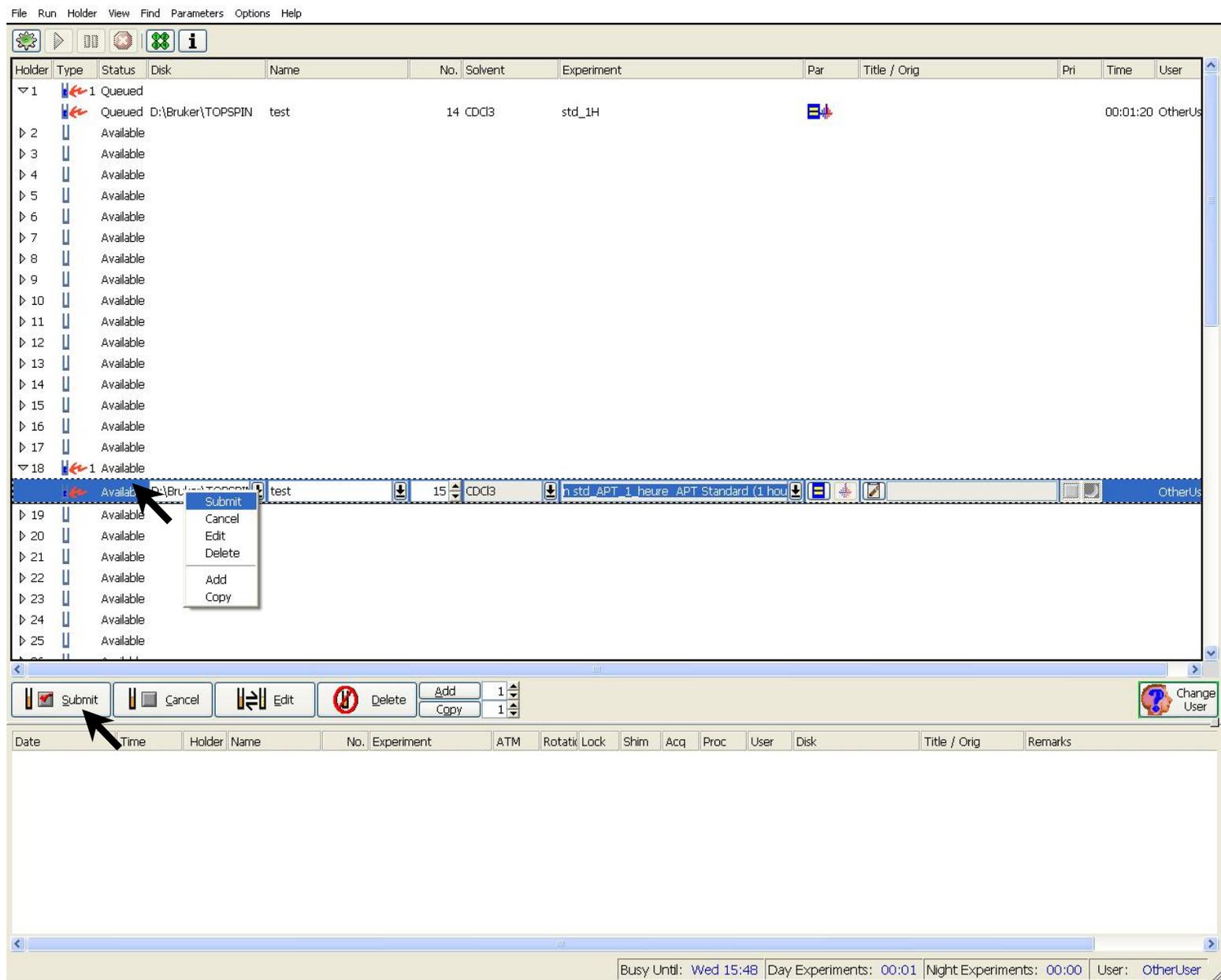
☞ You can put a title and click on ‘Set Title’



☞ You can acquire another experiment on the same sample by a right click on the selected line and select 'Add' (or click on the Icon 'Add' at the bottom of the page)



☞ Select the second experiment and its parameters (and the title if you want) as before. 14



☞ Put your sample in the corresponding holder (after having calibrated it in the adequate gauge). Click on 'Submit' on the line of this holder (right click on the line or Submit icon at the bottom of the page).

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File Run Holder View Find Parameters Options Help

ATM Running

Holder	Type	Status	Disk	Name	No.	Solvent	Experiment	Par	Title / Orig	Pri	Time	User
1	2	Running										
		Running	D:\Bruker\TOPSPIN	example	1	CDCl3	std_1H		Example 1		00:00:24	universite
		Queued	D:\Bruker\TOPSPIN	example	2	CDCl3	std_13C		Example 1		00:49:40	universite

Submit Cancel Edit Delete Add Cgpy 1 1

Change User

Date	Time	Holder	Name	No.	Experiment	ATM	Rotati	Lock	Shim	Acq	Proc	User	Disk	Title / Orig	Remarks
2005-11-09	15:38:23	1	example	1	std_1H							universite	D:\Bruker\TOPSPIN	Example 1	

Busy Until: Wed 16:33 Day Experiments: 00:50 Night Experiments: 00:00 User: universite

start 19.bmp - Paint TOPSPIN 1.3 Bruker TOPSPIN 1.3 ... ICON-NMR: spect ICON-NMR: Automati... 3:40 PM

☞ Your experiment will be done after the experiments submitted before in the other holders.

ICON-NMR: Automation Nov09-2005-1530-universite

File Run Holder View Find Parameters Options Help

ZG In Progress

Holder	Type	Status	Disk	Name	No.	Solvent	Experiment	Par	Title / Orig	Pri	Time	User
1	2	Running										
		Finished	D:\Bruker\TOPSPIN	example	1	CDCB3	std_1H		Example 1		00:00:24	universite
		Running	D:\Bruker\TOPSPIN	example	2	CDCB3	std_13C		Example 1		00:49:40	universite

Submit Cancel Edit Delete Add 1 Cgpy 1 Change User

Date	Time	Holder	Name	No.	Experiment	ATM	Rotati	Lock	Shim	Acq	Proc	User	Disk	Title / Orig	Remarks
2005-11-09	15:45:54	1	example	2	std_13C	✓	✓					universite	D:\Bruker\TOPSPIN	Example 1	
2005-11-09	15:38:23	1	example	1	std_1H	✓	✓	✓	✓	✓		universite	D:\Bruker\TOPSPIN	Example 1	

Busy until : takes into account only day experiments

Busy Until: Wed 16:37 Day Experiments: 00:49 Night Experiments: 00:00 User: universite

start 21.bmp - Paint TOPSPIN 1.3 Bruker TOPSPIN 1.3 ... ICON-NMR: spect ICON-NMR: Autom 3:48 PM

☞ You can see the progress of all the experiments at the bottom of the window.

☞ You can see the end of your experiment by a remote connexion on the NMR booking Web Site.

ICON-NMR: Automation Nov09-2005-1530-universite

Menu Disabled

Holder	Type	Status	Disk	Name	No.	Solvent	Experiment	Par	Title / Orig	Pri	Time	User
1		Available										

Automation Locked

To unlock the automation window click on the change user button at the right hand side of the Automation Setup window.

ICON-NMR: Set User

Identify User

Choose a user and click "OK" to continue. The currently defined user determines which experiments are on the experiment list.

+ -

CMAT	: CMAT Group
ORGJ	: J.Marchand Group
ORGM	: I.Marko Group
ORGR	: O.Riant Group
<u>OtherUser</u>	: <u>Other User</u>
Schanck	: NMR
universite	: bruker

User ID: OtherUser

OK Lock ICON-NMR

Set Selected User & Exit

Date	Time	Holder	Name	No.	User	Disk	Title / Orig	Remarks
2005-11-09	15:45:54	1	example	2	universite	D:\Bruker\TOPSPIN	Example 1	
2005-11-09	15:38:23	1	example	1	universite	D:\Bruker\TOPSPIN	Example 1	

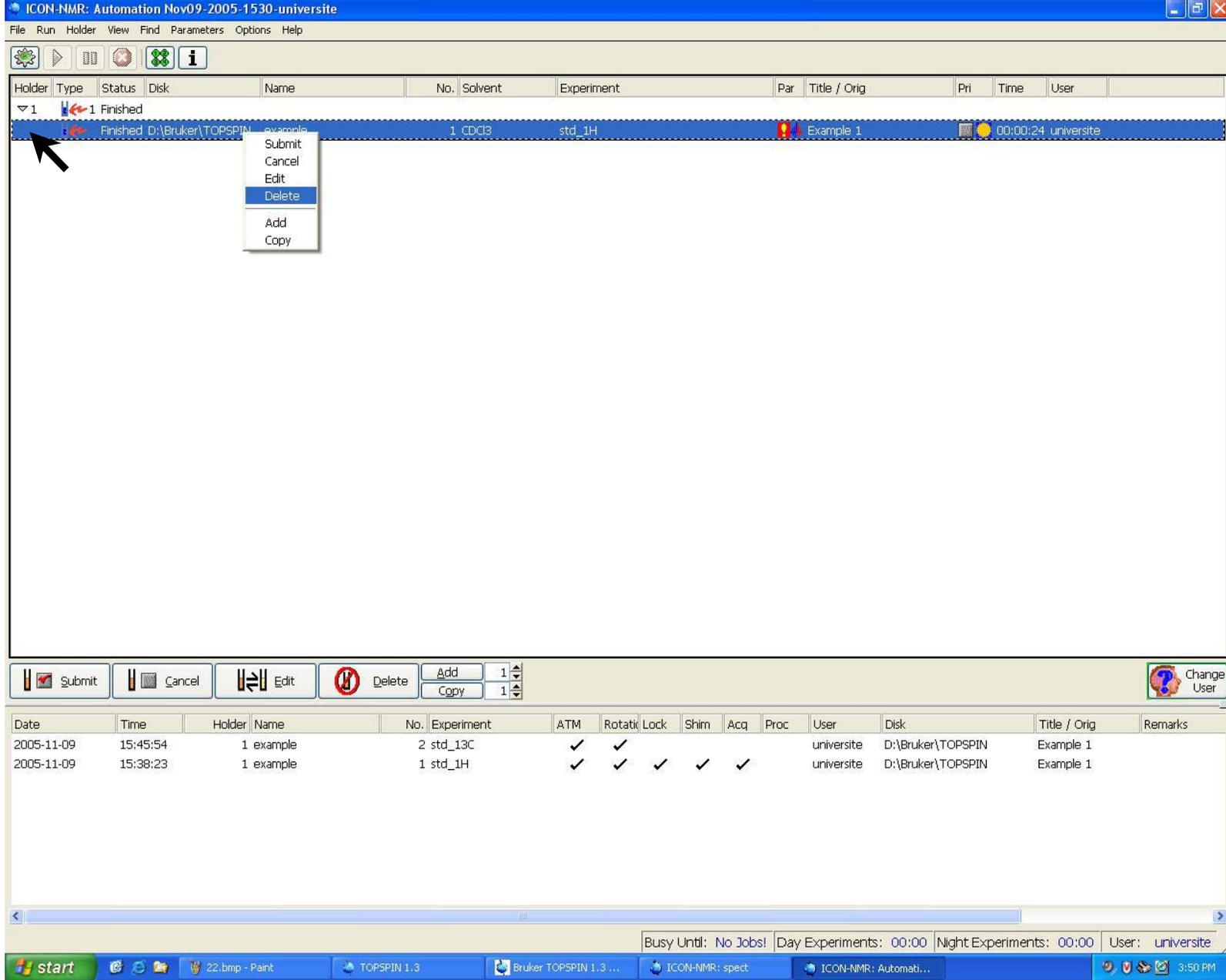
Submit Cancel Edit Delete

Change User

Busy Until: No Jobs! Day Experiments: 00:00 Night Experiments: 00:00 User: universite

start 51.bmp - Paint TOPSPIN 1.3 Bruker TOPSPIN 1.3... ICON-NMR: spect ICON-NMR: Automat... ICON-NMR: Set User 3:52 PM

☞ Before leaving the spectrometer, click on 'Change User' icon to log off



☞ When you come back to pick up your sample, right click with the mouse on your holder line to delete your experiment finished (or delete Icon at the bottom of the page).