

Chem 400 Training Protocol

Fu Chen

University of Maryland, College Park
Department of Chemistry & Biochemistry

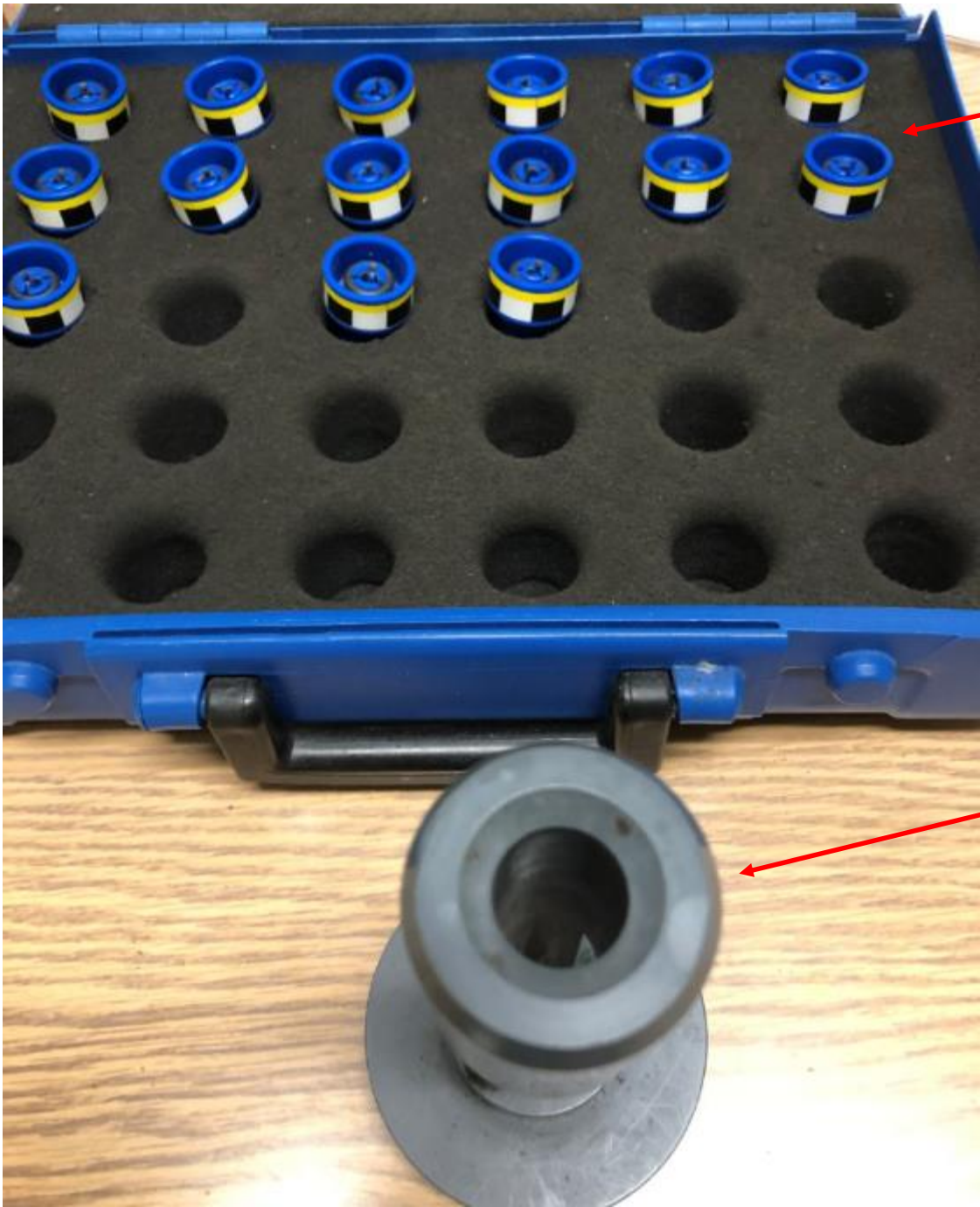


The automated spectrometer only accepts

7 inches NMR tubes



Best volume
~ 1.5"
0.8ml





Research
ALL USERS: DO NOT ADJUST ANY BUTTONS
ALL USERS: DO NOT ADJUST ANY BUTTONS

FEBRUARY 2013 | VOL. 7, NO. 1



BRUKER
B-ACS 60

POSITION No.
(22)

ICON: Automation Sep11-2020-1029-nmr

File Run Holder View Find Parameters Options Tools Help

Holder	Type	Status	Disk	Name	No.	Solvent	Experiment	Par	Title / Orig	Pri	Time	User
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43		Available										
44		Available										
45		Available										
46		Available										
47		Available										
48	1	Available	C:\	48-contract-0929	10			contract				contract
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52		Available										
53		Available										
54		Available										
55		Available										
56		Available										
57		Available										
58	1	Running										XinZhang

Submit Cancel Edit Delete Add 1 Cgpy 1

Change User

Preceding Experiments

#	Date	Holder	Name	No.	Experiment	Load	Rotation	Lock	Shim	Acq	Proc	User	Dis	Title / Orig	Remarks
139	2020-09-29 14:12:46	58	58-XinZhang-0929	10	Aproton_64	✓		✓	✓	✓	✓	contract	C:\	User Name XinZhang Group contract Sample Label 2.2	
138	2020-09-29 14:01:07	10	10-XinZhang-0929	10	Aproton_64	✓		✓	✓	✓	✓	contract	C:\	User Name XinZhang Group contract Sample Label 1.1	
137	2020-09-29 12:28:12	23	D5_3-28_8MQ_Pdnix_h24	10	Aproton_16	✓		✓	✓	✓	✓	soemardi	C:\	User Name soemardi Group vedernikov Sample Label D5_3-28_8MQ_Pdnix_h24 D5_3-28_8MQ_Pdnix_h24	
136	2020-09-29 12:16:51	22	D5_3-28_8MQ_pdaPdMSO_h24	10	Aproton_16	✓		✓	✓	✓	✓	soemardi	C:\	User Name soemardi Group vedernikov Sample Label D5_3-28_8MQ_pdaPdMSO_h24 D5_3-28_8MQ_pdaPdMSO_h24	
135	2020-09-29 11:40:33	41	41-madeline-0929	10	Aproton_16	✓		✓	✓	✓	✓	madeline	C:\	User Name madeline Group gutierrez Sample Label MR11100-1	
134	2020-09-29 11:29:26	40	40-madeline-0929	10	Aproton_16	✓		✓	✓	✓	✓	madeline	C:\	User Name madeline Group gutierrez Sample Label MR11100-1	
133	2020-09-28 15:14:11	25	D5_3-26_glymest	10	Aproton_16	✓		✓	✓	✓	✓	soemardi	C:\	User Name soemardi Group vedernikov Sample Label D5_3-26_glymest D5_3-26_glymest	
132	2020-09-28 15:02:37	24	D5_3-27_pyrimestPd_CDC13	10	Aproton_16	✓		✓	✓	✓	✓	soemardi	C:\	User Name soemardi Group vedernikov Sample Label D5_3-27_pyrimestPd_CDC13 D5_3-27_pyrimestPd_CDC13 some ppt in tube	
131	2020-09-28 12:48:06	23	D5_3-19_8MQ_pdaPdMSO_h0	10	Aproton_16	✓		✓	✓	✓	✓	soemardi	C:\	User Name soemardi Group vedernikov Sample Label D5_3-19_8MQ_pdaPdMSO_h0 D5_3-19_8MQ_pdaPdMSO_h0	
130	2020-09-28 12:38:01	22	D5_3-19_8MQ_Pdnix_h0	10	Aproton_16	✓		✓	✓	✓	✓	soemardi	C:\	User Name soemardi Group vedernikov Sample Label D5_3-19_8MQ_Pdnix_h0 D5_3-19_8MQ_Pdnix_h0	
129	2020-09-25 17:48:17	16	WL2-95-6	10	Aproton_16	✓		✓	✓	✓	✓	lee	C:\	User Name lee Group gutierrez Sample Label WL2-95-6 WL2-95-6	

Search Preceding include previous runs

Busy until: Tue 14:05 Day Experiments: 00:03 Night Experiments: 00:00 User: contract

start TOPSPIN 2.1 Bruker TOPSPIN 2.1... ICON-NMR: spect ICON: Automation Se... untitled - Paint 2:21 PM

zppuhar

CDCl3	Aproton_64	00:07:57	zppuhar
CDCl3	Aproton_64	00:07:57	zppuhar
CDCl3	Aproton_64	00:07:57	zppuhar

ICON-NMR: Identify User

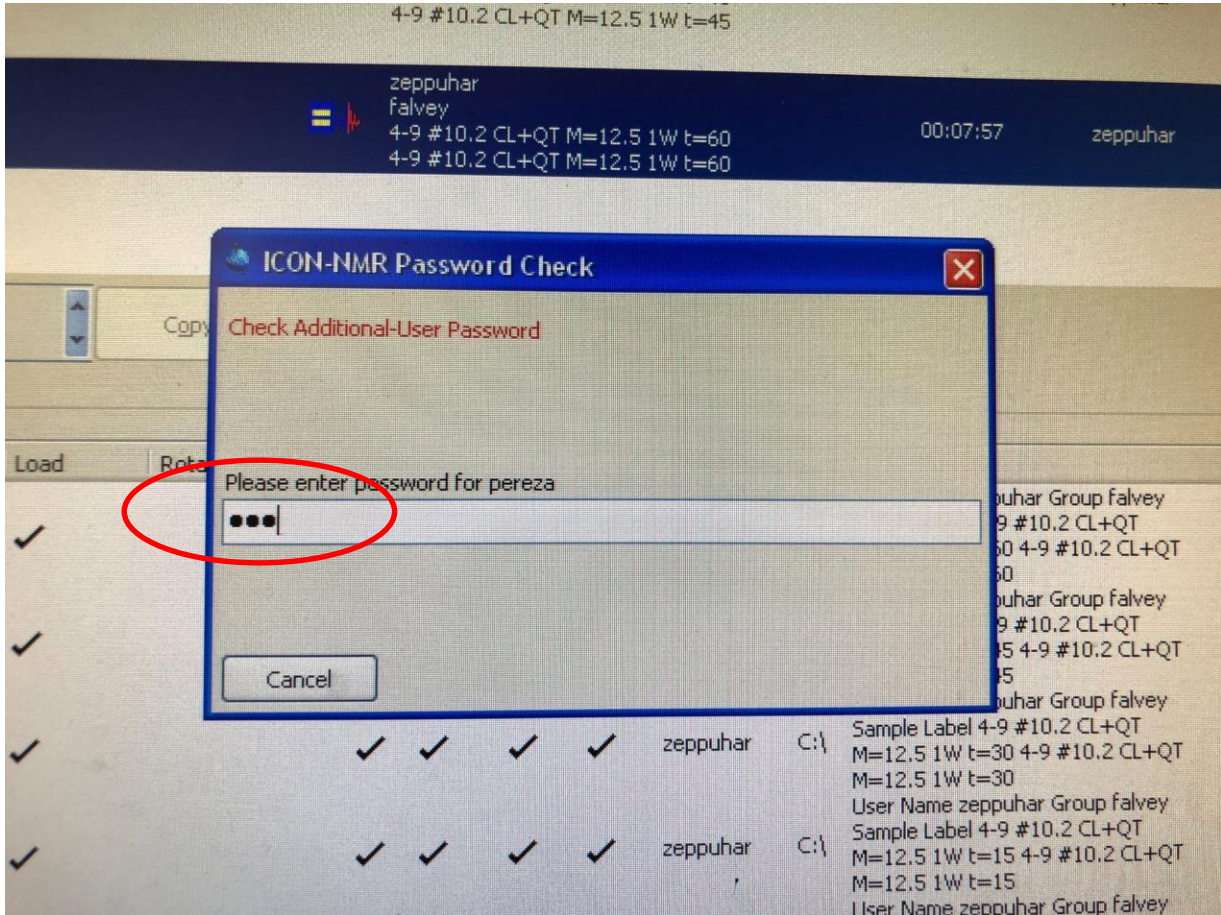
Help on logging in

User ID	User's Full Name
madeline	Madeline Poccia
melton	Michael Melton
murkli	Steve Murkli
New	New Template
nmr	
nmsu	nmsu
oliver	Kyle Oliver
ouchong	cheng ou
patterson	Delaney Patterson
pereza	Suvenika Pereza
ruan	Jiaheng Ruan
sahadeo	Emily Sahadeo
samanta	soumen samanta
shaya	David Shaya
soemardi	Diandra Soemardi
staff	staff
sutyak	Keith Sutyak
syzhang	Zhang Shaoyi
template	template_jan282008
thompson	Rick Thompson
thum	Matthew Thum
toonstra	Christian Toonstra
torres	Leo Torres
tyrlik	michal tyrlik
wallace	Mark Wallace
wang127	Shaochi Wang
watts	david watts
webb	kyla webb
wentz	Charlotte Wentz
wolf	Steven Wolf
xiao	Songjun Xiao
xue	Weijian Xue
zebaze	sandra zebaze
zppuhar	Andrea Zeppuhar
zhou	jun zhou
zong	quanghui zong

User ID: pereza

OK Lock Icon-NMR

No.	Experiment	Load	Orig	Remarks
10	Aproton_64	✓	Name zppuhar Group falvey le Label 4-9 #10.2 CL+QT 2.5 1W t=60 4-9 #10.2 CL+QT 2.5 1W t=60	
10	Aproton_64	✓	Name zppuhar Group falvey le Label 4-9 #10.2 CL+QT 2.5 1W t=45 4-9 #10.2 CL+QT 2.5 1W t=45	
10	Aproton_64	✓	Name zppuhar Group falvey le Label 4-9 #10.2 CL+QT 2.5 1W t=30 4-9 #10.2 CL+QT 2.5 1W t=30	
10	Aproton_64	✓	Name zppuhar Group falvey le Label 4-9 #10.2 CL+QT 2.5 1W t=15 4-9 #10.2 CL+QT 2.5 1W t=15	
10	Aproton_64	✓	Name zppuhar Group falvey le Label 4-9 #10 CL+QT M 5 1W t=60 4-9 #10 CL+QT 2.5 1W t=60	
10	Aproton_64	✓	Name zppuhar Group falvey le Label 4-9 #10 CL+QT M =12.5 1W t=45 4-9 #10 CL+QT M=12.5 1W t=45	
10	Aproton_64	✓	User Name zppuhar Group falvey Sample Label 4-9 #10 CL+QT M	



ICON: Automation Sep11-2020-1029-nmr

File Run Holder View Find Parameters Options Tools Help

Holder	Type	Status	Disk	Name	No.	Solvent	Experiment	Par	Title / Orig	Pri	Time	User
41	Finished	1 Finished		41-madeline-0929	10	CDCl3	Aproton_16		madeline gutierrez MR111100-1		00:05:20	madeline
42	Available											
43	Available											
44	Available											
45	Available											
46	Available											
47	Available											
48	Available	1 Available		3-XinZhang-0929	10	CDCl3	ch0		contract			contract
49	Available											
50	Available											
51	Available											
52	Available											
53	Available											
54	Available											
55	Available											
56	Available											
57	Available											
58	Available	1 Running										

CH3OH-D2O HPLC Solvent (Methanol/D2O)

D2O deuterium oxide

DCL deuterium chloride

DEE diethylether-d10

Dioxane dioxane-d8

DME dimethylether-d6

DME dimethylformamide-d7

DMSO dimethylsulfoxide-d6

EtOH ethanol-d6

H2O-D2O 90%H2O and 10%D2O

MeOD methanol-d4

None no Solvent

Pyr pyridine-d5

TEA trifluoroacetic acid-d

THF tetrahydrofuran-d8

Submit Cancel Edit

Change User

Preceding Experiments

#	Date	Holder	Name	No.	Experiment	Load	Rotation	Lock	Shim	Acq	Proc	User	Disk	Title / Orig	Remarks
139	2020-09-29 14:12:46	58	58-XinZhang-0929	10	Aproton_64	✓		✓	✓			contract	C:\	User Name XinZhang Group contract Sample Label 2 2	
138	2020-09-29 14:01:07	10	10-XinZhang-0929	10	Aproton_64	✓		✓	✓	✓	✓	contract	C:\	User Name XinZhang Group contract Sample Label 1 1	
137	2020-09-29 12:28:12	23	DS_3-28_8MQ_Pdmix_h24	10	Aproton_16	✓		✓	✓	✓	✓	soemardi	C:\	User Name soemardi Group vedernikov Sample Label DS_3-28_8MQ_Pdmix_h24 DS_3-28_8MQ_Pdmix_h24 User Name soemardi Group vedernikov	
136	2020-09-29 12:16:51	22	DS_3-28_8MQ_pdaPdDMSO_h24	10	Aproton_16	✓		✓	✓	✓	✓	soemardi	C:\	Sample Label DS_3-28_8MQ_pdaPdDMSO_h24 DS_3-28_8MQ_pdaPdDMSO_h24 User Name soemardi Group vedernikov	
135	2020-09-29 11:40:33	41	41-madeline-0929	10	Aproton_16	✓		✓	✓	✓	✓	madeline	C:\	User Name madeline Group gutierrez Sample Label MR111100-1	
134	2020-09-29 11:29:26	40	40-madeline-0929	10	Aproton_16	✓		✓	✓	✓	✓	madeline	C:\	User Name madeline Group gutierrez Sample Label MR111100-1	
133	2020-09-28 15:14:11	25	DS_3-26_glymest	10	Aproton_16	✓		✓	✓	✓	✓	soemardi	C:\	User Name soemardi Group vedernikov Sample Label DS_3-26_glymest DS_3-26_glymest User Name soemardi Group vedernikov	
132	2020-09-28 15:02:37	24	DS_3-27_pyrimestPd_CDCl3	10	Aproton_16	✓		✓	✓	✓	✓	soemardi	C:\	Sample Label DS_3-27_pyrimestPd_CDCl3 DS_3-27_pyrimestPd_CDCl3 some ppt in tube User Name soemardi Group vedernikov	
131	2020-09-28 12:48:08	23	DS_3-19_8MQ_pdaPdDMSO_h0	10	Aproton_16	✓		✓	✓	✓	✓	soemardi	C:\	User Name soemardi Group vedernikov Sample Label DS_3-19_8MQ_pdaPdDMSO_h0 DS_3-19_8MQ_pdaPdDMSO_h0	
130	2020-09-28 12:38:01	22	DS_3-19_8MQ_Pdmix_h0	10	Aproton_16	✓		✓	✓	✓	✓	soemardi	C:\	User Name soemardi Group vedernikov Sample Label DS_3-19_8MQ_Pdmix_h0 DS_3-19_8MQ_Pdmix_h0	
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Search Preceding Include previous runs

Busy until: Tue 14:25 Day Experiments: 00:01 Night Experiments: 00:00 User: contract

start TOPSPIN 2.1 Bruker TOPSPIN 2.1 ... ICON-NMR: spect ICON: Automation Se... untitled - Paint 2:23 PM

ICON: Automation Sep11-2020-1029-nmr

File Run Holder View Find Parameters Options Tools Help

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43	Available	Available										
44	Available	Available										
45	Available	Available										
46	Available	Available										
47	Available	Available										
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53	Available	Available										
54	Available	Available										
55	Available	Available										
56	Available	Available										
57	Available	Available										
58	Running	Running										

Submit Cancel Edit Delete

Change User

Preceding Experiments

#	Date	Holder	Name	No.	Experiment	Load	Rotation	Lock	Shim	Acq	Proc	User	Dis	Title / Orig	Remarks
139	2020-09-29 14:12:46	58	58-XinZhang-0929	10	Aproton_64	✓		✓	✓			contract	C:\	User Name XinZhang Group contract Sample Label 2 2	
138	2020-09-29 14:01:07	10	10-XinZhang-0929	10	Aproton_64	✓		✓	✓	✓		contract	C:\	User Name XinZhang Group contract Sample Label 1 1	
137	2020-09-29 12:28:12	23	DS_3-28_8MQ_Pdmix_h24	10	Aproton_16	✓		✓	✓	✓		soemardi	C:\	User Name soemardi Group vedernikov Sample Label DS_3-28_8MQ_Pdmix_h24 DS_3-28_8MQ_Pdmix_h24	
136	2020-09-29 12:16:51	22	DS_3-28_8MQ_pdaPdDMSO_h24	10	Aproton_16	✓		✓	✓	✓		soemardi	C:\	User Name soemardi Group vedernikov Sample Label DS_3-28_8MQ_pdaPdDMSO_h24 DS_3-28_8MQ_pdaPdDMSO_h24	
135	2020-09-29 11:40:33	41	41-madeline-0929	10	Aproton_16	✓		✓	✓	✓		madeline	C:\	User Name madeline Group gutierrez Sample Label MR11100-1	
134	2020-09-29 11:29:26	40	40-madeline-0929	10	Aproton_16	✓		✓	✓	✓		madeline	C:\	User Name madeline Group gutierrez Sample Label MR11100-1	
133	2020-09-28 15:14:11	25	DS_3-26_glyimest	10	Aproton_16	✓		✓	✓	✓		soemardi	C:\	User Name soemardi Group vedernikov Sample Label DS_3-26_glyimest DS_3-26_glyimest	
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131	2020-09-28 12:48:08	23	DS_3-19_8MQ_pdaPdDMSO_h0	10	Aproton_16	✓		✓	✓	✓		soemardi	C:\	User Name soemardi Group vedernikov Sample Label DS_3-19_8MQ_pdaPdDMSO_h0 DS_3-19_8MQ_pdaPdDMSO_h0	
130	2020-09-28 12:38:01	22	DS_3-19_8MQ_Pdmix_h0	10	Aproton_16	✓		✓	✓	✓		soemardi	C:\	User Name soemardi Group vedernikov Sample Label DS_3-19_8MQ_Pdmix_h0 DS_3-19_8MQ_Pdmix_h0	
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Search Preceding Include previous runs

BusY until: Tue 14:25 Day Experiments: 00:01 Night Experiments: 00:00 User: contract

Start TOPSPIN 2.1 Bruker TOPSPIN 2.1 ... ICON-NMR: spect ICON: Automation Se... 2.JPG - Paint 2:24 PM

ICON: Automation Sep11-2020-1029-nmr

File Run Holder View Find Parameters Options Tools Help

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43	Available											
44	Available											
45	Available											
46	Available											
47	Available											
48	Available	1 Available										
49	Available		C:\	3-XinZhang-0929	10	DMSO	dim	N Aproton_64	A proton 64 sans		00:07:57	contract
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51	Available											
52	Available											
53	Available											
54	Available											
55	Available											
56	Available											
57	Available											
58	Running	1 Running										

Click here to edit specific parameters

CPD	18.9521	[ppm]
15W	18.9521	[ppm]
O2P	6.175	[ppm]
DS	8	
1TD	39392	
NS	64	
PULPROG	zg30	
D1	4	[sec]
GPZ1	0	
GPZ2	0	
L30	1	

Submit Cancel Edit Delete Add 1 Cgpy

Change User

Preceding Experiments

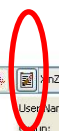
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138	2020-09-29 14:01:07	10	10-XinZhang-0929	10	Aproton_64	✓		contract	C:\	User Name XinZhang Group contract Sample Label 1 1	
137	2020-09-29 12:28:12	23	D5_3-28_8MQ_Pdmix_h24	10	Aproton_16	✓		soemardi	C:\	User Name soemardi Group vedernikov Sample Label D5_3-28_8MQ_Pdmix_h24 D5_3-28_8MQ_Pdmix_h24	
136	2020-09-29 12:16:51	22	D5_3-28_8MQ_pdaPdMSO_h24	10	Aproton_16	✓		soemardi	C:\	User Name soemardi Group vedernikov Sample Label D5_3-28_8MQ_pdaPdMSO_h24 D5_3-28_8MQ_pdaPdMSO_h24	
135	2020-09-29 11:40:33	41	41-madeline-0929	10	Aproton_16	✓		madeline	C:\	User Name madeline Group gutierrez Sample Label MR11100-1	
134	2020-09-29 11:29:26	40	40-madeline-0929	10	Aproton_16	✓		madeline	C:\	User Name madeline Group gutierrez Sample Label MR11199-1	
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132	2020-09-28 15:02:37	24	D5_3-27_pyrimestPd_CDCl3	10	Aproton_16	✓		soemardi	C:\	User Name soemardi Group vedernikov Sample Label D5_3-27_pyrimestPd_CDCl3 D5_3-27_pyrimestPd_CDCl3 some ppt in tube	
131	2020-09-28 12:48:08	23	D5_3-19_8MQ_pdaPdMSO_h0	10	Aproton_16	✓		soemardi	C:\	User Name soemardi Group vedernikov Sample Label D5_3-19_8MQ_pdaPdMSO_h0 D5_3-19_8MQ_pdaPdMSO_h0	
130	2020-09-28 12:38:01	22	D5_3-19_8MQ_Pdmix_h0	10	Aproton_16	✓		soemardi	C:\	User Name soemardi Group vedernikov Sample Label D5_3-19_8MQ_Pdmix_h0 D5_3-19_8MQ_Pdmix_h0	
129	2020-09-25 17:48:17	16	WL2-95-6	10	Aproton_16	✓		lee	C:\	User Name lee Group gutierrez Sample Label WL2-95-6 WL2-95-6	

Search Preceding Include previous runs

Busy until: Tue 14:36 Day Experiments: 00:08 Night Experiments: 00:00 User: contract

start TOPSPIN 2.1 Bruker TOPSPIN 2.1... ICON-NMR: spect ICON: Automation Se... 3.JPG - Paint 2:24 PM

Holder	Type	Status	Disk	Name	No.	Solvent	Experiment	Par	Title / Orig	Pri	Time	User
41	Finished	1 Finished	C:\	41-madeline-0929	10	CDC13	Aproton_16	madeline gutierrez MR11100-1			00:05:20	madeline
42	Available											
43	Available											
44	Available											
45	Available											
46	Available											
47	Available											
48	Available	1 Available	C:\	3-XinZhang-0929	10	DMSO	dim	N Aproton_64	A proton 64 sans		00:07:57	contract



User Name: XinZhang
 Up: contract
 Sample Label: 3
 Title: 3
 Set Title Set & Copy Title

1 1 Cgpy 1

Preceding Experiments

#	Date	Holder	Name	No.	Experiment	Load	Rotation	Lock	Shim	Acq	Proc	User	Dis	Title / Orig	Remarks
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138	2020-09-29 14:01:07	10	10-XinZhang-0929	10	Aproton_64	✓		✓	✓	✓	✓	contract	C:\	User Name XinZhang Group contract Sample Label 1 1	
137	2020-09-29 12:28:12	23	D5_3-28_8MQ_Pdmix_h24	10	Aproton_16	✓		✓	✓	✓	✓	soemardi	C:\	User Name soemardi Group vedernikov Sample Label D5_3-28_8MQ_Pdmix_h24	
136	2020-09-29 12:16:51	22	D5_3-28_8MQ_pdaPdDMSO_h24	10	Aproton_16	✓		✓	✓	✓	✓	soemardi	C:\	User Name soemardi Group vedernikov Sample Label D5_3-28_8MQ_pdaPdDMSO_h24	
135	2020-09-29 11:40:33	41	41-madeline-0929	10	Aproton_16	✓		✓	✓	✓	✓	madeline	C:\	User Name madeline Group gutierrez Sample Label MR11100-1	
134	2020-09-29 11:29:26	40	40-madeline-0929	10	Aproton_16	✓		✓	✓	✓	✓	madeline	C:\	User Name madeline Group gutierrez Sample Label MR11100-1	
133	2020-09-28 15:14:11	25	D5_3-26_glyimest	10	Aproton_16	✓		✓	✓	✓	✓	soemardi	C:\	User Name soemardi Group vedernikov Sample Label D5_3-26_glyimest	
132	2020-09-28 15:02:37	24	D5_3-27_pyrimestPd_CDC13	10	Aproton_16	✓		✓	✓	✓	✓	soemardi	C:\	User Name soemardi Group vedernikov Sample Label D5_3-27_pyrimestPd_CDC13	
131	2020-09-28 12:48:08	23	D5_3-19_8MQ_pdaPdDMSO_h0	10	Aproton_16	✓		✓	✓	✓	✓	soemardi	C:\	User Name soemardi Group vedernikov Sample Label D5_3-19_8MQ_pdaPdDMSO_h0	
130	2020-09-28 12:38:01	22	D5_3-19_8MQ_Pdmix_h0	10	Aproton_16	✓		✓	✓	✓	✓	soemardi	C:\	User Name soemardi Group vedernikov Sample Label D5_3-19_8MQ_Pdmix_h0	
129	2020-09-25 17:48:17	16	WL2-95-6	10	Aproton_16	✓		✓	✓	✓	✓	lee	C:\	User Name lee Group gutierrez Sample Label WL2-95-6	

ICON: Automation Sep11-2020-1029-nmr

File Run Holder View Find Parameters Options Tools Help

Holder	Type	Status	Disk	Name	No.	Solvent	Experiment	Par	Title / Orig	Pri	Time	User
41	Finished	Finished	C:\	41-madeline-0929	10	CDC3	Aproton_16		madeline guterrez MR111100-1		00:05:20	madeline
42	Available	Available										
43	Available	Available										
44	Available	Available										
45	Available	Available										
46	Available	Available										
47	Available	Available										
48	Available	Available	C:\	3-XinZhang-0929	10	DMSO	dim	N Aproton_64	A proton 64 sans		00:07:57	contract
49	Available	Available										
50	Available	Available										
51	Available	Available										
52	Available	Available										
53	Available	Available										
54	Available	Available										
55	Available	Available										
56	Available	Available										
57	Available	Available										
58	Available	Finished										

Submit all selected experiments for run

Submit Cancel Edit Delete Add 1 Copy 1

#	Date	Holder	Name	No.	Experiment	Load	Rotation	Lock	Shim	Acq	Proc	User	Dis	Title / Orig	Remarks
139	2020-09-29 14:12:46	58	58-XinZhang-0929	10	Aproton_64	✓		✓	✓	✓	✓	contract	C:\	User Name XinZhang Group contract Sample Label 2 2	
138	2020-09-29 14:01:07	10	10-XinZhang-0929	10	Aproton_64	✓		✓	✓	✓	✓	contract	C:\	User Name XinZhang Group contract Sample Label 1 1	
137	2020-09-29 12:28:12	23	DS_3-28_8MQ_Pdmix_h24	10	Aproton_16	✓		✓	✓	✓	✓	soemardi	C:\	User Name soemardi Group vedernikov Sample Label DS_3-28_8MQ_Pdmix_h24 DS_3-28_8MQ_Pdmix_h24 User Name soemardi Group vedernikov	
136	2020-09-29 12:16:51	22	DS_3-28_8MQ_pdaPdDMSO_h24	10	Aproton_16	✓		✓	✓	✓	✓	soemardi	C:\	Sample Label DS_3-28_8MQ_pdaPdDMSO_h24 DS_3-28_8MQ_pdaPdDMSO_h24 User Name madeline Group gutierrez	
135	2020-09-29 11:40:33	41	41-madeline-0929	10	Aproton_16	✓		✓	✓	✓	✓	madeline	C:\	User Name madeline Group gutierrez Sample Label MR111100-1	
134	2020-09-29 11:29:26	40	40-madeline-0929	10	Aproton_16	✓		✓	✓	✓	✓	madeline	C:\	User Name madeline Group gutierrez Sample Label MR111199-1	
133	2020-09-28 15:14:11	25	DS_3-26_glyimest	10	Aproton_16	✓		✓	✓	✓	✓	soemardi	C:\	User Name soemardi Group vedernikov Sample Label DS_3-26_glyimest DS_3-26_glyimest User Name soemardi Group vedernikov	
132	2020-09-28 15:02:37	24	DS_3-27_pyrimestPd_CDC3	10	Aproton_16	✓		✓	✓	✓	✓	soemardi	C:\	Sample Label DS_3-27_pyrimestPd_CDC3 DS_3-27_pyrimestPd_CDC3 some ppt in tube User Name soemardi Group vedernikov	
131	2020-09-28 12:48:08	23	DS_3-19_8MQ_pdaPdDMSO_h0	10	Aproton_16	✓		✓	✓	✓	✓	soemardi	C:\	Sample Label DS_3-19_8MQ_pdaPdDMSO_h0 DS_3-19_8MQ_pdaPdDMSO_h0 User Name soemardi Group vedernikov	
130	2020-09-28 12:38:01	22	DS_3-19_8MQ_Pdmix_h0	10	Aproton_16	✓		✓	✓	✓	✓	soemardi	C:\	User Name soemardi Group vedernikov Sample Label DS_3-19_8MQ_Pdmix_h0 DS_3-19_8MQ_Pdmix_h0 User Name lee Group gutierrez	
129	2020-09-25 17:48:17	16	WL2-95-6	10	Aproton_16	✓		✓	✓	✓	✓	lee	C:\	Sample Label WL2-95-6 WL2-95-6 User Name lee Group gutierrez	

Search Preceding Include previous runs

Busy until: No Jobs! Day Experiments: 00:00 Night Experiments: 00:00 User: contract

start TOPSPIN 2.1 Bruker TOPSPIN 2.1... ICON-NMR: spect ICON: Automation Se... 5.JPG - Paint 2:26 PM

ICON: Automation Sep11-2020-1029-nmr

File Run Holder View Find Parameters Options Tools Help

Holder	Type	Status	Disk	Name	No.	Solvent	Experiment	Par	Title / Orig	Pri	Time	User
41	Finished	1 Finished	C:\	41-madeline-0929	10	CDCl3	Aproton_16	madeline gubierrez MR111100-1			00:05:20	madeline
42	Available											
43	Available											
44	Available											
45	Available											
46	Available											
47	Available											
48	Running	2 Running	C:\	3-XinZhang-0929	10	DMSO	Aproton_64	XinZhang contract 3			00:07:57	contract
49	Available		C:\	3-XinZhang-0929	11	DMSO		XinZhang contract 3 3				contract
50	Available											
51	Available											
52	Available											
53	Available											
54	Available											
55	Available											
56	Available											

Submit Cancel Edit Delete Add 1 Cgpy 1

Change User

Preceding Experiments

#	Date	Holder	Name	No.	Experiment	Load	Rotation	Lock	Shim	Acq	Proc	User	Dis	Title / Orig	Remarks
140	2020-09-29 14:26:31	48	3-XinZhang-0929	10	Aproton_64							contract	C:\	User Name XinZhang Group contract Sample Label 3 3	
139	2020-09-29 14:12:46	58	58-XinZhang-0929	10	Aproton_64	✓		✓	✓	✓	✓	contract	C:\	User Name XinZhang Group contract Sample Label 2 2	
138	2020-09-29 14:01:07	10	10-XinZhang-0929	10	Aproton_64	✓		✓	✓	✓	✓	contract	C:\	User Name XinZhang Group contract Sample Label 1 1	
137	2020-09-29 12:28:12	23	DS_3-28_8MQ_Pdmix_h24	10	Aproton_16	✓		✓	✓	✓	✓	soemardi	C:\	User Name soemardi Group vedernikov Sample Label DS_3-28_8MQ_Pdmix_h24	
136	2020-09-29 12:16:51	22	DS_3-28_8MQ_pdaPdDMSO_h24	10	Aproton_16	✓		✓	✓	✓	✓	soemardi	C:\	User Name soemardi Group vedernikov Sample Label DS_3-28_8MQ_pdaPdDMSO_h24	
135	2020-09-29 11:40:33	41	41-madeline-0929	10	Aproton_16	✓		✓	✓	✓	✓	madeline	C:\	User Name madeline Group gutierrez Sample Label MR111100-1	
134	2020-09-29 11:29:26	40	40-madeline-0929	10	Aproton_16	✓		✓	✓	✓	✓	madeline	C:\	User Name madeline Group gutierrez Sample Label MR111100-1	
133	2020-09-28 15:14:11	25	DS_3-26_glyimest	10	Aproton_16	✓		✓	✓	✓	✓	soemardi	C:\	User Name soemardi Group vedernikov Sample Label DS_3-26_glyimest	
132	2020-09-28 15:02:37	24	DS_3-27_pyrimestPd_CDCl3	10	Aproton_16	✓		✓	✓	✓	✓	soemardi	C:\	User Name soemardi Group vedernikov Sample Label DS_3-27_pyrimestPd_CDCl3 some ppt in tube	
131	2020-09-28 12:48:08	23	DS_3-19_8MQ_pdaPdDMSO_h0	10	Aproton_16	✓		✓	✓	✓	✓	soemardi	C:\	User Name soemardi Group vedernikov Sample Label DS_3-19_8MQ_pdaPdDMSO_h0	
130	2020-09-28 12:38:01	22	DS_3-19_8MQ_Pdmix_h0	10	Aproton_16	✓		✓	✓	✓	✓	soemardi	C:\	User Name soemardi Group vedernikov Sample Label DS_3-19_8MQ_Pdmix_h0	

Search Preceding Include previous runs

Busy until: Tue 14:38 Day Experiments: 00:08 Night Experiments: 00:00 User: contract

start TOPSPIN 2.1 Bruker TOPSPIN 2.1 ... ICON-NMR: spect ICON: Automation Se... 6.JPG - Paint 2:26 PM

Holder	Type	Status	Disk	Name	No.	Solvent	Experiment	Par	Title / Orig	Pri	Time	User
41	Finished	1 Finished	C:\	41-madeline-0929	10	CDCl3	Aproton_16	+	madeline gutierrez MR11100-1		00:05:20	madeline
42	Available											
43	Available											
44	Available											
45	Available											
46	Available											
47	Queued	1 Queued	C:\	4-XinZhang-0929	10	DMSO	Aproton_64	+	XinZhang contract 4 4		00:07:31	contract
48	Running	1 Running	C:\	3-XinZhang-0929	10	DMSO	Aproton_64	+	XinZhang contract 3 3		00:07:57	contract
49	Available											
50	Available											
51	Available											
52	Available											
53	Available											
54	Available											

Preceding Experiments

#	Date	Holder	Name	No.	Experiment	Load	Rotation	Lock	Shim	Acq	Proc	User	Disk	Title / Orig	Remarks
140	2020-09-29 14:26:31	48	3-XinZhang-0929	10	Aproton_64							contract	C:\	User Name XinZhang Group contract Sample Label 3 3	
139	2020-09-29 14:12:46	58	58-XinZhang-0929	10	Aproton_64	✓		✓	✓	✓	✓	contract	C:\	User Name XinZhang Group contract Sample Label 2 2	
138	2020-09-29 14:01:07	10	10-XinZhang-0929	10	Aproton_64	✓		✓	✓	✓	✓	contract	C:\	User Name XinZhang Group contract Sample Label 1 1	
137	2020-09-29 12:28:12	23	D5_3-28_8MQ_Pdmix_h24	10	Aproton_16	✓		✓	✓	✓	✓	soemardi	C:\	User Name soemardi Group vedernikov Sample Label D5_3-28_8MQ_Pdmix_h24	
136	2020-09-29 12:16:51	22	D5_3-28_8MQ_pdaPdDMSO_h24	10	Aproton_16	✓		✓	✓	✓	✓	soemardi	C:\	User Name soemardi Group vedernikov Sample Label D5_3-28_8MQ_pdaPdDMSO_h24	
135	2020-09-29 11:40:33	41	41-madeline-0929	10	Aproton_16	✓		✓	✓	✓	✓	madeline	C:\	User Name madeline Group gutierrez Sample Label MR11100-1	
134	2020-09-29 11:29:26	40	40-madeline-0929	10	Aproton_16	✓		✓	✓	✓	✓	madeline	C:\	User Name madeline Group gutierrez Sample Label MR11199-1	
133	2020-09-28 15:14:11	25	D5_3-26_glyimst	10	Aproton_16	✓		✓	✓	✓	✓	soemardi	C:\	User Name soemardi Group vedernikov Sample Label D5_3-26_glyimst	
132	2020-09-28 15:02:37	24	D5_3-27_pyrimstPd_CDCl3	10	Aproton_16	✓		✓	✓	✓	✓	soemardi	C:\	User Name soemardi Group vedernikov Sample Label D5_3-27_pyrimstPd_CDCl3 some ppt in tube	
131	2020-09-28 12:48:08	23	D5_3-19_8MQ_pdaPdDMSO_h0	10	Aproton_16	✓		✓	✓	✓	✓	soemardi	C:\	User Name soemardi Group vedernikov Sample Label D5_3-19_8MQ_pdaPdDMSO_h0	
130	2020-09-28 12:38:01	22	D5_3-19_8MQ_Pdmix_h0	10	Aproton_16	✓		✓	✓	✓	✓	soemardi	C:\	User Name soemardi Group vedernikov Sample Label D5_3-19_8MQ_Pdmix_h0	

ICON: Automation Sep11-2020-1029-nmr

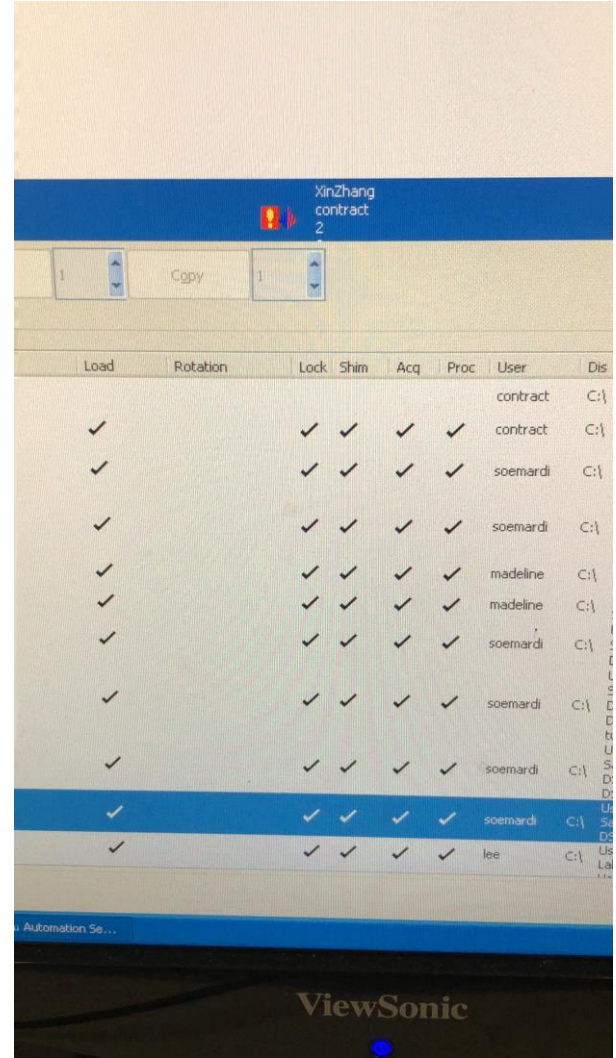
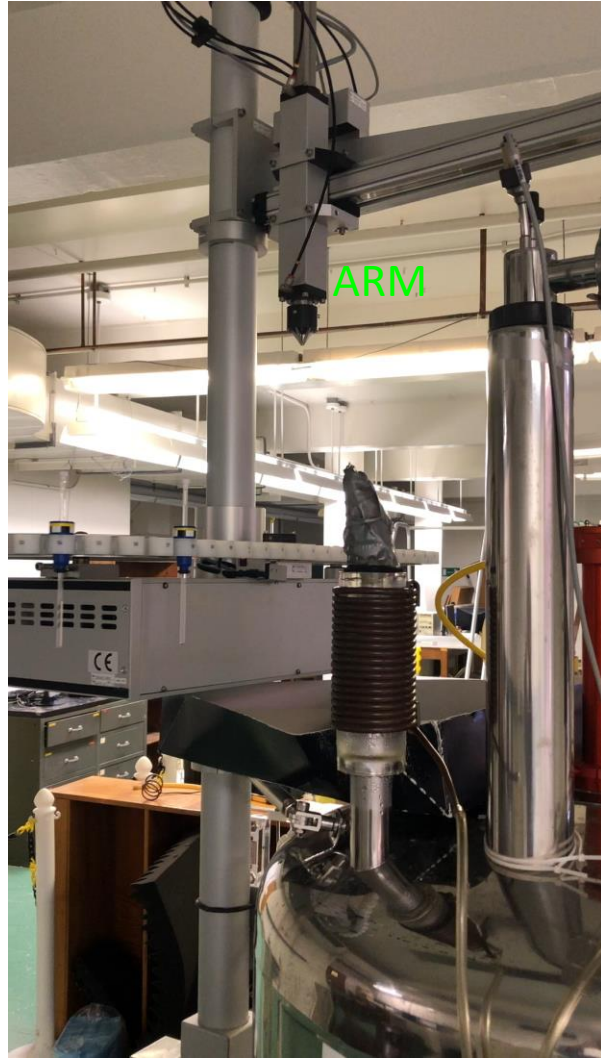
File Run Holder View Find Parameters Options Tools Help

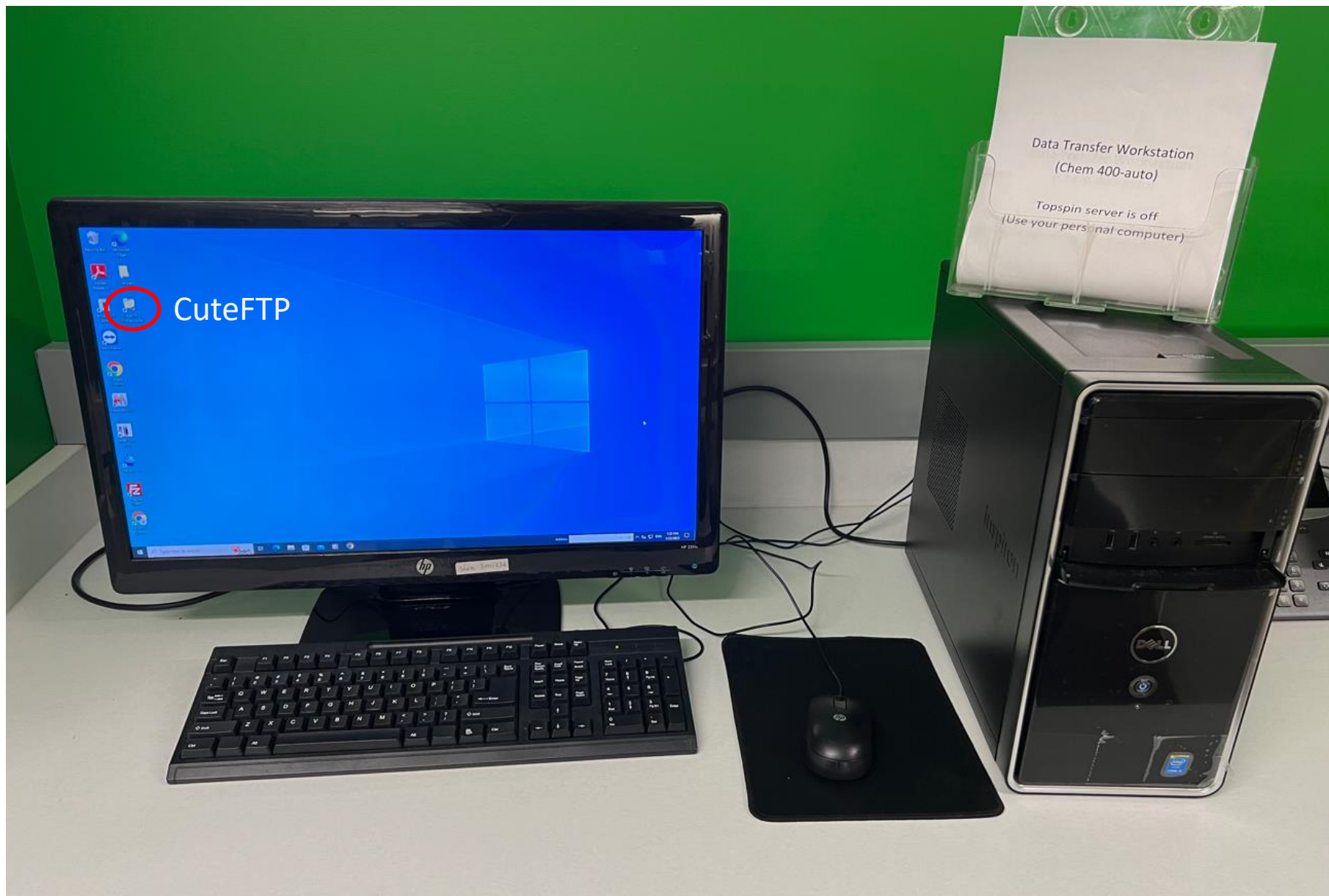
Holder	Type	Status	Disk	Name	No.	Solvent	Experiment	Par	Title / Orig	Pri	Time	User
		Finished	C:\	41-madeline-0929	10	CDCl3	Aproton_16		madeline guterrez MRIIII100-1		00:05:20	madeline
42		Available										
43		Available										
44		Available										
45		1 Queued										
		Queued	C:\	6-XinZhang-0929	10	DMSO	Aproton_64		XinZhang contract 6 6		00:07:31	contract
46		1 Queued										
		Queued	C:\	5-XinZhang-0929	10	DMSO	Aproton_64		XinZhang contract 5 5		00:07:31	contract
47		1 Queued										
		Queued	C:\	4-XinZhang-0929	10	DMSO	Aproton_64		XinZhang contract 4 4		00:07:31	contract
48		1 Running										
		Running	C:\	3-XinZhang-0929	10	DMSO	Aproton_64		XinZhang contract 3 3		00:07:57	contract
49		Available										

Submit Cancel Edit Delete Add 1 Cgpy 1

Preceding Experiments

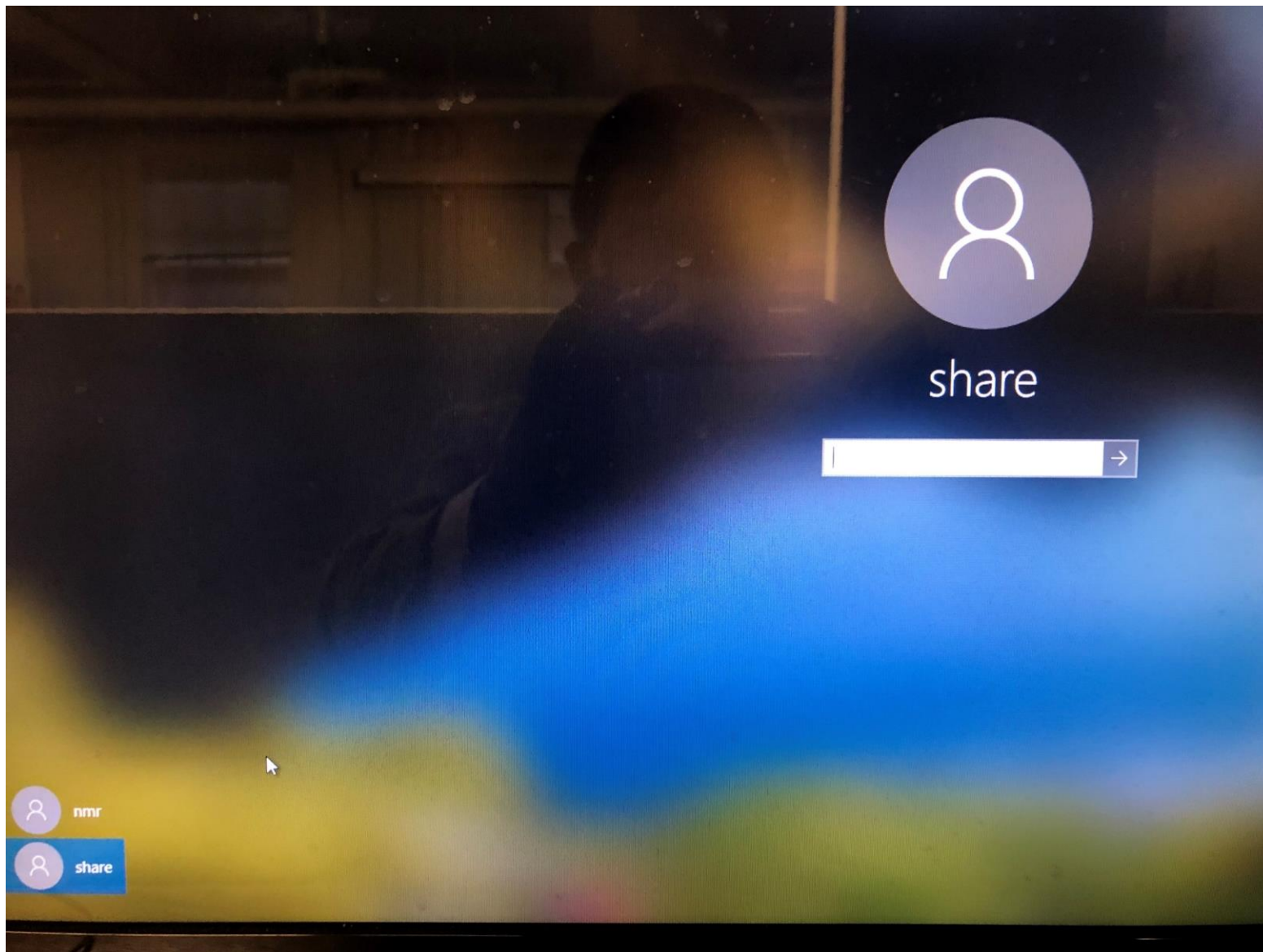
#	Date	Holder	Name	No.	Experiment	Load	Rotation	Lock	Shim	Acq	Proc	User	Dis	Title / Orig	Remarks
140	2020-09-29 14:26:31	48	3-XinZhang-0929	10	Aproton_64	✓		✓	✓	✓	✓	contract	C:\	User Name XinZhang Group contract Sample Label 3 3	
139	2020-09-29 14:12:46	58	58-XinZhang-0929	10	Aproton_64	✓		✓	✓	✓	✓	contract	C:\	User Name XinZhang Group contract Sample Label 2 2	
138	2020-09-29 14:01:07	10	10-XinZhang-0929	10	Aproton_64	✓		✓	✓	✓	✓	contract	C:\	User Name XinZhang Group contract Sample Label 1 1	
137	2020-09-29 12:28:12	23	DS_3-28_8MQ_Pdmix_h24	10	Aproton_16	✓		✓	✓	✓	✓	soemardi	C:\	User Name soemardi Group vedernikov Sample Label DS_3-28_8MQ_Pdmix_h24 DS_3-28_8MQ_Pdmix_h24	
136	2020-09-29 12:16:51	22	DS_3-28_8MQ_pdaPdDMSO_h24	10	Aproton_16	✓		✓	✓	✓	✓	soemardi	C:\	User Name soemardi Group vedernikov Sample Label DS_3-28_8MQ_pdaPdDMSO_h24 DS_3-28_8MQ_pdaPdDMSO_h24	
135	2020-09-29 11:40:33	41	41-madeline-0929	10	Aproton_16	✓		✓	✓	✓	✓	madeline	C:\	User Name madeline Group gutierrez Sample Label MRIIII100-1	
134	2020-09-29 11:29:26	40	40-madeline-0929	10	Aproton_16	✓		✓	✓	✓	✓	madeline	C:\	User Name madeline Group gutierrez Sample Label MRIIII199-1	
133	2020-09-28 15:14:11	25	DS_3-26_glyimest	10	Aproton_16	✓		✓	✓	✓	✓	soemardi	C:\	User Name soemardi Group vedernikov Sample Label DS_3-26_glyimest DS_3-26_glyimest	
132	2020-09-28 15:02:37	24	DS_3-27_pyrimestPd_CDCl3	10	Aproton_16	✓		✓	✓	✓	✓	soemardi	C:\	User Name soemardi Group vedernikov Sample Label DS_3-27_pyrimestPd_CDCl3 DS_3-27_pyrimestPd_CDCl3 some ppt in tube	
131	2020-09-28 12:48:08	23	DS_3-19_8MQ_pdaPdDMSO_h0	10	Aproton_16	✓		✓	✓	✓	✓	soemardi	C:\	User Name soemardi Group vedernikov Sample Label DS_3-19_8MQ_pdaPdDMSO_h0 DS_3-19_8MQ_pdaPdDMSO_h0	
130	2020-09-28 12:38:01	22	DS_3-19_8MQ_Pdmix_h0	10	Aproton_16	✓		✓	✓	✓	✓	soemardi	C:\	User Name soemardi Group vedernikov Sample Label DS_3-19_8MQ_Pdmix_h0 DS_3-19_8MQ_Pdmix_h0	





CuteFTP

Data Transfer Workstation
(Chem 400-auto)
Topspin server is off
(Use your personal computer)



sun1234

chem400.umd.edu

share
sun1234
21

GlobalSCAPE - CuteFTP 8.3 Professional - [chem400.umd.edu, Status: Connected]

Host: chem400.umd.edu Username: share Password: ***** Port: 21

Local Drives: C:\Users\share\Desktop\Us

Site Manager: chem400.umd.edu

Name	Size	Type	Modified	Attributes	Description	Owner
erdi	0 bytes	File Folder	8/20/2019	drwxr-xr-x		ftp
klemm	0 bytes	File Folder	7/24/2019	drwxr-xr-x		ftp
patterson	0 bytes	File Folder	6/24/2019	drwxr-xr-x		ftp
soemardi	0 bytes	File Folder	6/10/2019	drwxr-xr-x		ftp
melton	0 bytes	File Folder	6/7/2019	drwxr-xr-x		ftp
hitt	0 bytes	File Folder	5/3/2019	drwxr-xr-x		ftp
kayla	0 bytes	File Folder	4/23/2019	drwxr-xr-x		ftp
wang127	0 bytes	File Folder	4/19/2019	drwxr-xr-x		ftp
wentz	0 bytes	File Folder	4/16/2019	drwxr-xr-x		ftp
lachmayr	0 bytes	File Folder	4/15/2019	drwxr-xr-x		ftp
bistany	0 bytes	File Folder	4/3/2019	drwxr-xr-x		ftp
sahadeo	0 bytes	File Folder	4/1/2019	drwxr-xr-x		ftp
hong	0 bytes	File Folder	3/12/2019	drwxr-xr-x		ftp
king	0 bytes	File Folder	11/30/2018	drwxr-xr-x		ftp
zeppuhar	0 bytes	File Folder	8/10/2018	drwxr-xr-x		ftp
xiao	0 bytes	File Folder	7/20/2018	drwxr-xr-x		ftp
ruan	0 bytes	File Folder	6/15/2018	drwxr-xr-x		ftp
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john	0 bytes	File Folder	6/5/2018	drwxr-xr-x		ftp
webb	0 bytes	File Folder	4/12/2018	drwxr-xr-x		ftp
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tyrik	0 bytes	File Folder	3/12/2018	drwxr-xr-x		ftp
alejandro	0 bytes	File Folder	1/4/2018	drwxr-xr-x		ftp
xue	0 bytes	File Folder	12/4/2017	drwxr-xr-x		ftp
fchenqc	0 bytes	File Folder	10/4/2017	drwxr-xr-x		ftp
ouchong	0 bytes	File Folder	9/18/2017	drwxr-xr-x		ftp
wallace	0 bytes	File Folder	8/4/2017	drwxr-xr-x		ftp
brady	0 bytes	File Folder	7/19/2017	drwxr-xr-x		ftp
sdamc	0 bytes	File Folder	6/26/2017	drwxr-xr-x		ftp

COMMAND: [9/18/2020 4:06:45 PM] LIST
 STATUS: [9/18/2020 4:06:45 PM] Connecting FTP data socket... 128.8.176.154:58762...
 [9/18/2020 4:06:47 PM] 150 Opening data channel for directory listing of "/"
 STATUS: [9/18/2020 4:06:47 PM] 226 Successfully transferred "/"
 [9/18/2020 4:06:47 PM] Directory listing completed.

#	Item Name	Address	Size	Progress	Local	Remote	Start time	Finish time	Elapsed	Left	Speed	Multi...	Status
P	30-madeline-0...	chem4...	0 bytes	0%	C:\Gutierrez\30-madeline-0915	/madeline/nmr/30-ma...	9/15/2020 4:43:10...		0:00:00	?	?	Normal	Cancelled
E	JCK-01-07 M2 ...	chem4...	0 bytes	0%	F:\NMR Backup\JCK-01-07 M2 0.2mM-L...	/murkii/nmr/JCK-01-0...	3/6/2020 5:56:36 ...		0:00:00	?	?	Normal	Error
E	SM-03-76 Texa...	chem4...	0 bytes	0%	F:\NMR Backup\SM-03-76 Texas Box.M...	/murkii/nmr/SM-03-7...	3/6/2020 5:56:36 ...		0:00:00	?	?	Normal	Error
E	SM-03-76 Spar...	chem4...	0 bytes	0%	F:\NMR Backup\SM-03-76 Spartaine.M2...	/murkii/nmr/SM-03-7...	3/6/2020 5:56:36 ...		0:00:00	?	?	Normal	Error
E	SM-03-M3G3...	chem4...	0 bytes	0%	F:\NMR Backup\SM-03-M3G3 meoh wa...	/murkii/nmr/SM-03-M...	3/6/2020 5:56:36 ...		0:00:00	?	?	Normal	Error
E	SM-03-97 2.1 3...	chem4...	0 bytes	0%	F:\NMR Backup\SM-03-97 2.1 350 hv 1 ...	/murkii/nmr/SM-03-9...	3/6/2020 5:56:36 ...		0:00:00	?	?	Normal	Error
E	SM-03-M3c60 ...	chem4...	0 bytes	0%	F:\NMR Backup\SM-03-M3c60 extractio...	/murkii/nmr/SM-03-M...	3/6/2020 5:56:36 ...		0:00:00	?	?	Normal	Error