

Chem 400 Training Protocol

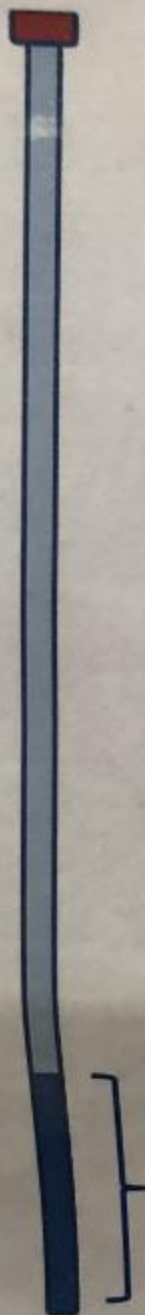
Fu Chen

University of Maryland, College Park
Department of Chemistry & Biochemistry

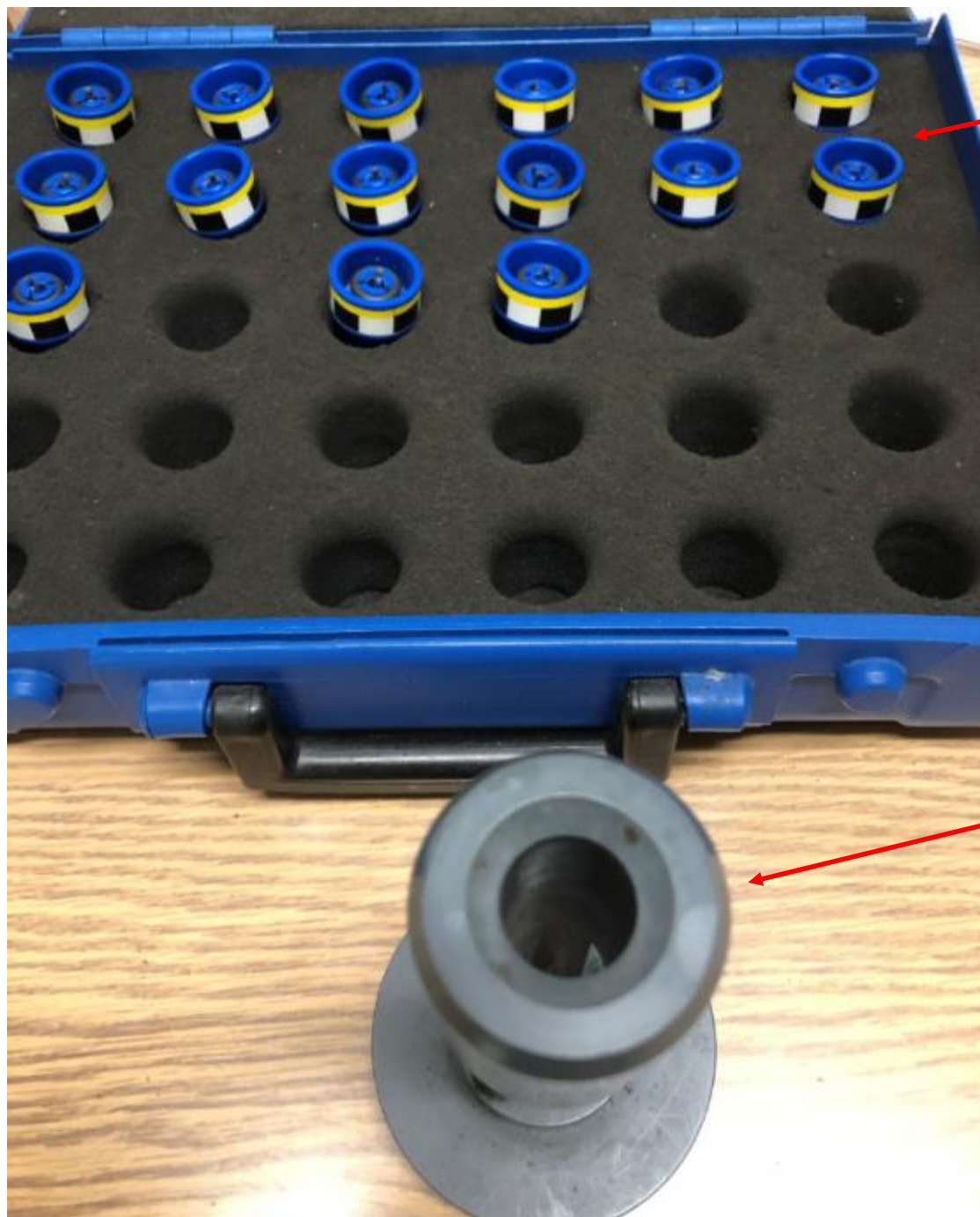


The automated
spectrometer
only accepts

**7 inches NMR
tubes**



Best volume
~ 1.5"
0.8ml





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 guterrez MR111100-1			00:05:20	madeline
42	Available											
43	Available											
44	Available											
45	Available											
46	Available											
47	Available											
48	Available	1 Available	C:\	48-contract-0929	10			contract				contract
49	Available											
50	Available											
51	Available											
52	Available											
53	Available											
54	Available											
55	Available											
56	Available											
57	Available											
58	Running	1 Running										

XinZhang

Submit Cancel Edit Delete Add 1 Cgpy 1

Change User

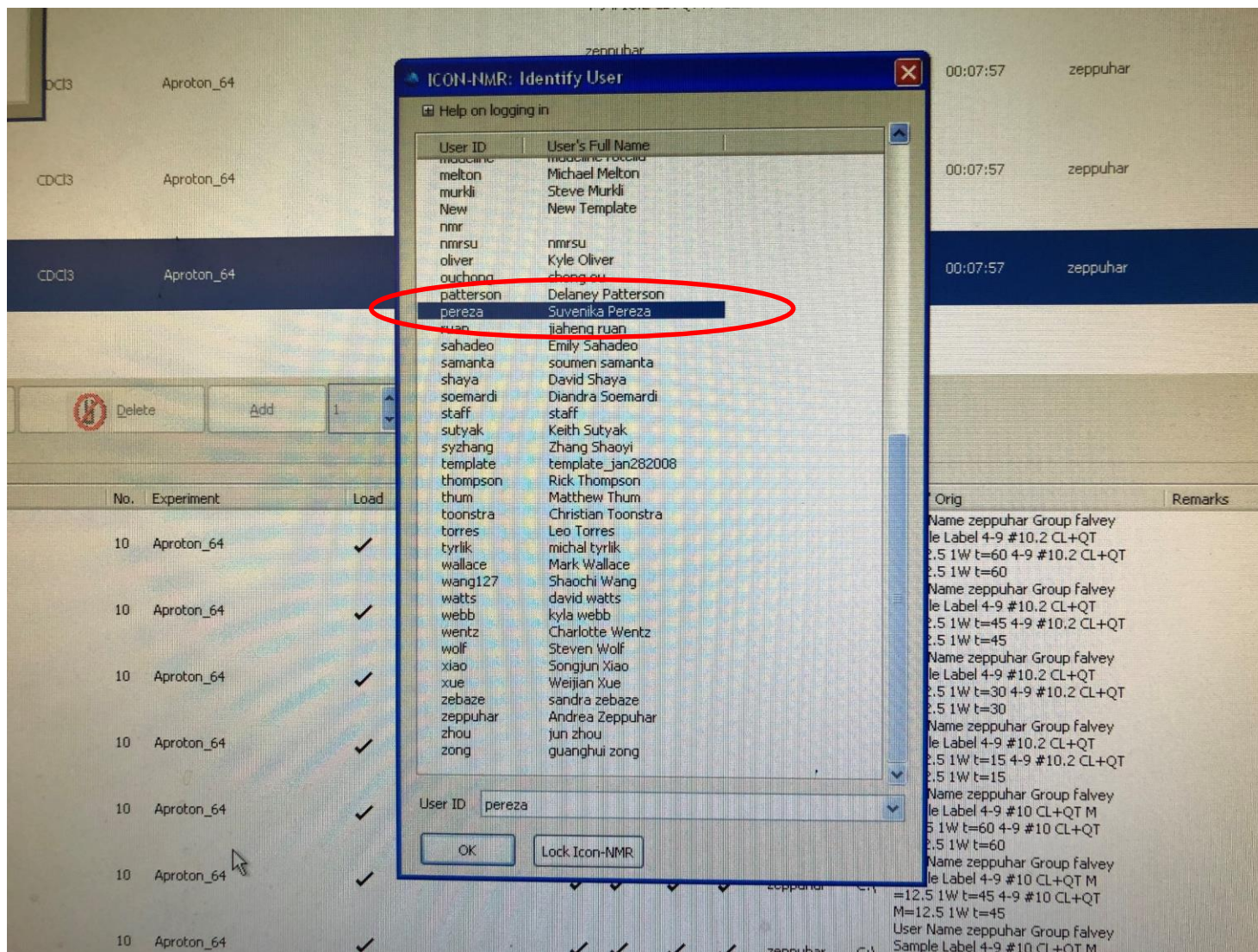
Preceding Experiments

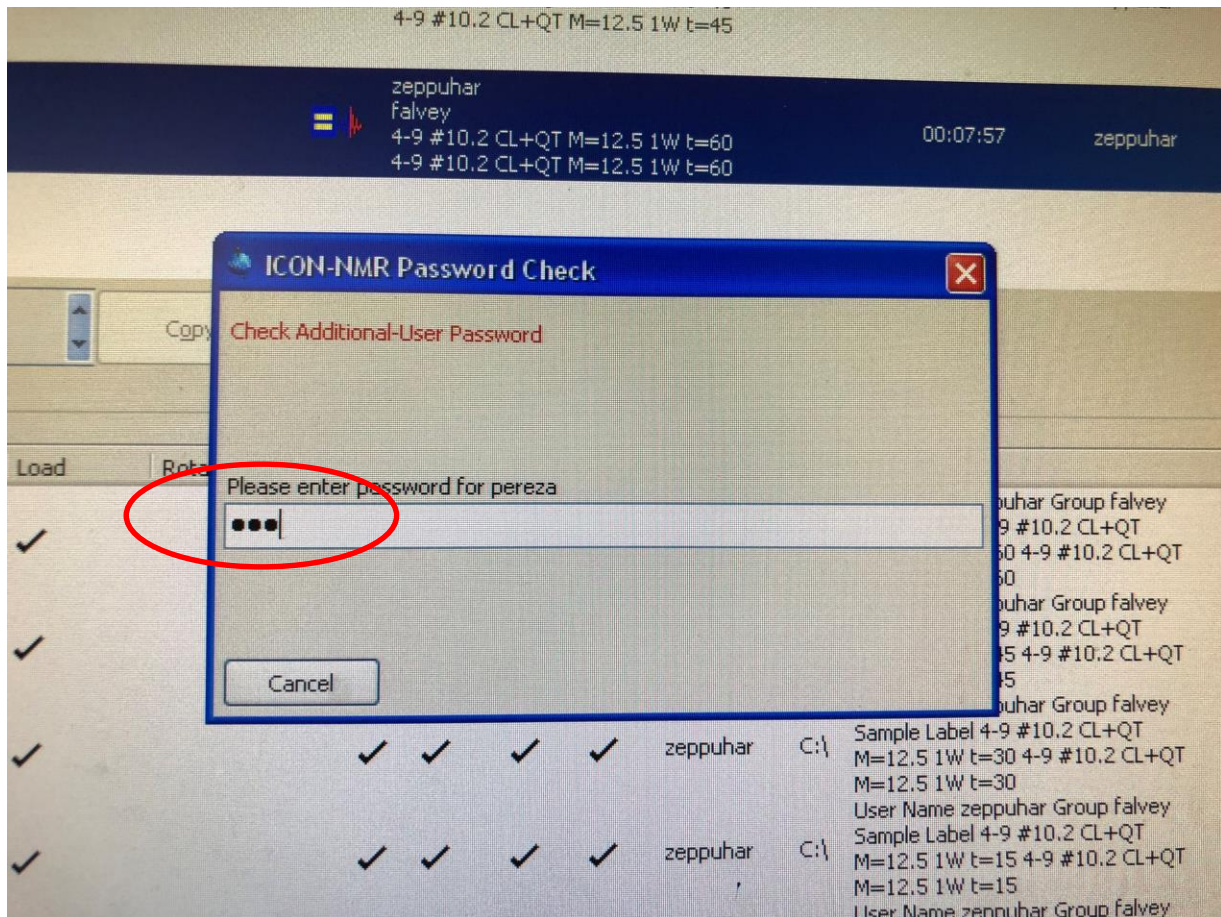
#	Date	Holder	Name	No.	Experiment	Load	Rotation	Lock	Shim	Acq	Proc	User	Dis	Title / Orig	Remarks
139	2020-09-29 14:12:46	58	58-XinZhang-0929	10	Aproton_64	✓		✓	✓			contract	C:\	User Name XinZhang Group contract Sample Label 2.2	
138	2020-09-29 14:01:07	10	10-XinZhang-0929	10	Aproton_64	✓		✓	✓	✓	✓	contract	C:\	User Name XinZhang Group contract Sample Label 1.1	
137	2020-09-29 12:28:12	23	D5_3-28_8MQ_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 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	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 12:48:08	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

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

Busy until: Tue 14:25 Day Experiments: 00:03 Night Experiments: 00:00 User: contract 2:21 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		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			contract			contract
49	Available											
50	Available											
51	Available											
52	Available											
53	Available											
54	Available											
55	Available											
56	Available											
57	Available											
58	1 Running											

Submit Cancel Edit

CH3OH-B2O RPLC Solvent (Methanol/B2O)
B2O deuteriumchloride
DCL diethylether-d10
DEE dioxane-d8
DME dimethylether-d6
DMF dimethylformamide-d7
DMSO dimethylsulfoxide-d6
EtOD ethanol-d6
H2O-B2O 90% H2O and 10% B2O
MeOD methanol-d4
None no solvent
Pyr pyridine-d5
TFA trifluoroacetic acid-d
TME tetrahydrofuran-d8

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 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	
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:\	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:\	Sample Label DS_3-19_8MQ_Pdmix_h0 DS_3-19_8MQ_Pdmix_h0 User Name soemardi Group vedernikov	
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 14:25 Day Experiments: 00:01 Night Experiments: 00:00 Users: 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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54	Available											
55	Available											
56	Available											
57	Available											
58	Running	1 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_pdaPdMSO_h24	10	Aproton_16	✓		✓	✓	✓	✓	soemardi	C:\	User Name soemardi Group vedernikov Sample Label DS_3-28_8MQ_pdaPdMSO_h24 DS_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 MRII100-1	
134	2020-09-29 11:29:26	40	40-madeline-0929	10	Aproton_16	✓		✓	✓	✓	✓	madeline	C:\	User Name madeline Group gutierrez Sample Label MRII100-1	
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	
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_pdaPdMSO_h0	10	Aproton_16	✓		✓	✓	✓	✓	soemardi	C:\	User Name soemardi Group vedernikov Sample Label DS_3-19_8MQ_pdaPdMSO_h0 DS_3-19_8MQ_pdaPdMSO_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	
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 14:25 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	C:\	3-XinZhang-0929	10	DMSO	dim	N Aproton_64	A proton 64 sans		00:07:57	contract
49	Available											
50	Available											
51	Available											
52	Available											
53	Available											
54	Available											
55	Available											
56	Available											
57	Available											
58	Running	1 Running										

Click here to edit specific parameters

Q1	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 Copy

Preceding Experiments

#	Date	Holder	Name	No.	Experiment	Load	Rotation	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_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_pdaPdDMSO_h24	10	Aproton_16	✓	✓	soemardi	C:\	User Name soemardi Group vedernikov Sample Label D5_3-28_8MQ_pdaPdDMSO_h24 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_glyimest	10	Aproton_16	✓	✓	soemardi	C:\	User Name soemardi Group vedernikov Sample Label D5_3-26_glyimest D5_3-26_glyimest	
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_pdaPdDMSO_h0	10	Aproton_16	✓	✓	soemardi	C:\	User Name soemardi Group vedernikov Sample Label D5_3-19_8MQ_pdaPdDMSO_h0 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 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 Users: contract

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

2:24 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	CDCI3	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										
49	Available		C:\	3-XinZhang-0929	10	DMSO	dim	N Aproton_64	A proton 64 sans		00:07:57	contract
50	Available											
51	Available											
52	Available											
53	Available											
54	Available											
55	Available											
56	Available											
57	Available											
58	Available	1 Finished										

User Name: XinZhang
Up: contract
Sample Label: 3
Title: 3
Set Title Set & Copy Title
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	DS_3-28_BMQ_Pdmix_h24	10	Aproton_16	✓		✓	✓	✓	✓	soemardi	C:\	User Name soemardi Group vedernikov Sample Label DS_3-28_BMQ_Pdmix_h24 DS_3-28_BMQ_Pdmix_h24	
136	2020-09-29 12:16:51	22	DS_3-28_BMQ_pdaPdDMSO_h24	10	Aproton_16	✓		✓	✓	✓	✓	soemardi	C:\	User Name soemardi Group vedernikov Sample Label DS_3-28_BMQ_pdaPdDMSO_h24 DS_3-28_BMQ_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	
132	2020-09-28 15:02:37	24	DS_3-27_pyrimestPd_CDCI3	10	Aproton_16	✓		✓	✓	✓	✓	soemardi	C:\	User Name soemardi Group vedernikov Sample Label DS_3-27_pyrimestPd_CDCI3 DS_3-27_pyrimestPd_CDCI3 some ppt in tube	
131	2020-09-28 12:48:08	23	DS_3-19_BMQ_pdaPdDMSO_h0	10	Aproton_16	✓		✓	✓	✓	✓	soemardi	C:\	User Name soemardi Group vedernikov Sample Label DS_3-19_BMQ_pdaPdDMSO_h0 DS_3-19_BMQ_pdaPdDMSO_h0	
130	2020-09-28 12:38:01	22	DS_3-19_BMQ_Pdmix_h0	10	Aproton_16	✓		✓	✓	✓	✓	soemardi	C:\	User Name soemardi Group vedernikov Sample Label DS_3-19_BMQ_Pdmix_h0 DS_3-19_BMQ_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: No Job Day Experiments: 00:00 Night Experiments: 00:00 Users: contract

start TOPSPIN 2.1 Bruker TOPSPIN 2.1 ICON-NMR: spect ICON: Automation Se... 4.JPG - Paint

2:25 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	1	Finished	C:\	41-madeline-0929	10	CDCl3	Aproton_16		madeline guterrez MR111100-1		00:05:20	madeline
42		Available										
43		Available										
44		Available										
45		Available										
46		Available										
47		Available										
48	1	Available	C:\	3-XinZhang-0929	10	DMSO	dm	N Aproton_64	A proton 64 sans		00:07:57	contract
49		Available										
50		Available										
51		Available										
52		Available										
53		Available										
54		Available										
55		Available										
56		Available										
57		Available										
58	1	Finished										

Submit all selected experiments for run!

Submit Cancel Edit Delete Add 1 Cgpy 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	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_pdaPdDMSO_h24	10	Aproton_16	✓		✓	✓	✓	✓	soemardi	C:\	User Name soemardi Group vedernikov Sample Label D5_3-28_8MQ_pdaPdDMSO_h24 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 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	D5_3-26_glyimest	10	Aproton_16	✓		✓	✓	✓	✓	soemardi	C:\	User Name soemardi Group vedernikov Sample Label D5_3-26_glyimest D5_3-26_glyimest	
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_pdaPdDMSO_h0	10	Aproton_16	✓		✓	✓	✓	✓	soemardi	C:\	User Name soemardi Group vedernikov Sample Label D5_3-19_8MQ_pdaPdDMSO_h0 D5_3-19_8MQ_pdaPdDMSO_h0	
130	2020-09-28 12:30:01	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

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

Busy until: No Job! Day Experiments: 00:00 Night Experiments: 00:00 User: contract 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 MRIII100-1			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 3			00:07:57	contract
49	Available			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 gubierrez Sample Label MRIII100-1	
134	2020-09-29 11:29:26	40	40-madeline-0929	10	Aproton_16	✓		✓	✓	✓	✓	madeline	C:\	User Name madeline Group gubierrez Sample Label MRIII100-1	
133	2020-09-28 15:14:11	25	DS_3-26_glytimest	10	Aproton_16	✓		✓	✓	✓	✓	soemardi	C:\	User Name soemardi Group vedernikov Sample Label DS_3-26_glytimest	
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 Users: contract

start TOPSPIN 2.1 Bruker TOPSPIN 2.1 ... ICON-NMR: spect ICON: Automation Se... 6.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	1	Finished	C:\	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	1	Queued	C:\	4-XinZhang-0929	10	DMSO	Aproton_64	XinZhang contract 4 4			00:07:31	contract
48	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										

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	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 User Name soemardi Group vedernikov Sample Label	
136	2020-09-29 12:16:51	22	D5_3-28_8MQ_pdaPdDMSO_h24	10	Aproton_16	✓		✓	✓	✓	✓	soemardi	C:\	D5_3-28_8MQ_pdaPdDMSO_h24 D5_3-28_8MQ_pdaPdDMSO_h24 User Name madeline Group gutierrez Sample Label MR111100-1	
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	D5_3-26_glymest	10	Aproton_16	✓		✓	✓	✓	✓	soemardi	C:\	User Name soemardi Group vedernikov Sample Label D5_3-26_glymest D5_3-26_glymest User Name soemardi Group vedernikov Sample Label	
132	2020-09-28 15:02:37	24	D5_3-27_pyrimestPd_CDC13	10	Aproton_16	✓		✓	✓	✓	✓	soemardi	C:\	D5_3-27_pyrimestPd_CDC13 D5_3-27_pyrimestPd_CDC13 some ppt in tube User Name soemardi Group vedernikov Sample Label	
131	2020-09-28 12:48:08	23	D5_3-19_8MQ_pdaPdDMSO_h0	10	Aproton_16	✓		✓	✓	✓	✓	soemardi	C:\	D5_3-19_8MQ_pdaPdDMSO_h0 D5_3-19_8MQ_pdaPdDMSO_h0 User Name soemardi Group vedernikov Sample Label D5_3-19_8MQ_Pdmix_h0 D5_3-19_8MQ_Pdmix_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	

Search Preceding ☐ include previous runs

Busy until: Tue 14:51 Day Experiments: 00:15 Night Experiments: 00:00 User: contract

start TOPSPIN 2.1 Bruker TOPSPIN 2.1 ... ICON-NMR: spect ICON: Automation Se... 7.JPG - Paint 2:27 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		C:\	41-madeline-0929	10	CDCl3	Aproton_16		madeline gutierrez MRII1100-1		00:05:20	madeline
42	Available											
43	Available											
44	Available											
45	1 Queued											
46	Queued		C:\	6-XinZhang-0929	10	DMSO	Aproton_64		XinZhang contract 6		00:07:31	contract
47	1 Queued		C:\	5-XinZhang-0929	10	DMSO	Aproton_64		XinZhang contract 5		00:07:31	contract
48	1 Queued		C:\	4-XinZhang-0929	10	DMSO	Aproton_64		XinZhang contract 4		00:07:31	contract
49	Running		C:\	3-XinZhang-0929	10	DMSO	Aproton_64		XinZhang contract 3		00:07:57	contract

Subnet Cancel Edit Delete Add 1 Cgpy 1

Change User

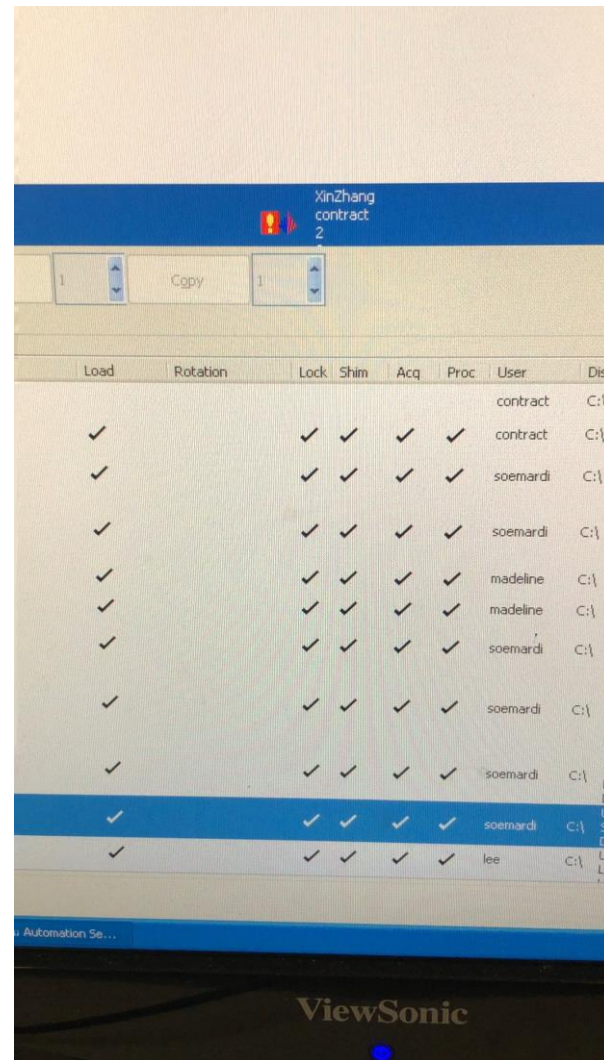
Preceding Experiments

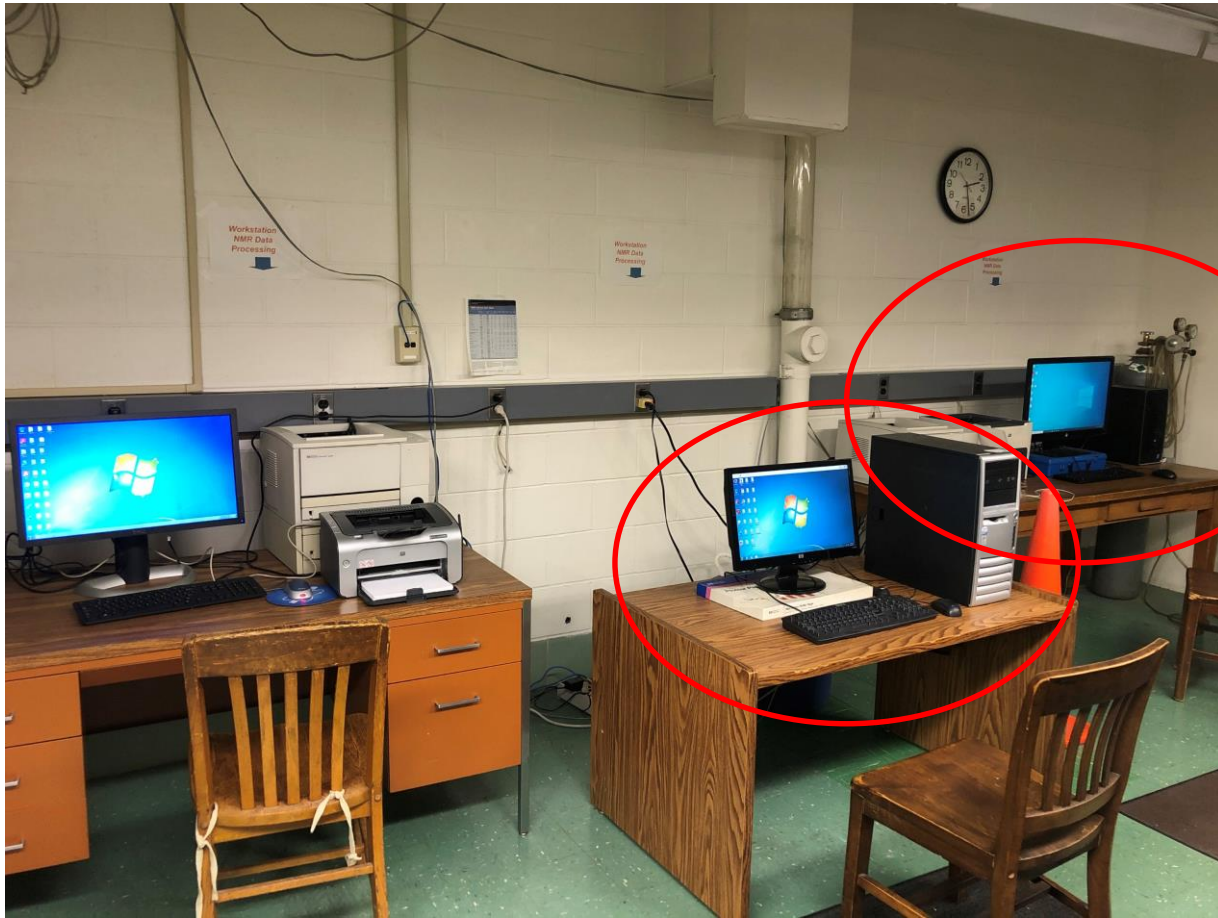
#	Date	Holder	Name	No.	Experiment	Load	Rotation	Lock	Shim	Acq	Proc	User	Dis	Title / Orig	Remarks
140	2020-09-29 14:26:31	48	3-XinZhang-0929	10	Aproton_64	✓						contract	C:\	User Name XinZhang Group contract Sample Label 3 3	
139	2020-09-29 14:12:46	58	58-XinZhang-0929	10	Aproton_64	✓		✓	✓	✓	✓	contract	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	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_pdaPdDMSO_h24	10	Aproton_16	✓		✓	✓	✓	✓	soemardi	C:\	User Name soemardi Group vedernikov Sample Label D5_3-28_8MQ_pdaPdDMSO_h24 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 MRII1100-1	
134	2020-09-29 11:29:26	40	40-madeline-0929	10	Aproton_16	✓		✓	✓	✓	✓	madeline	C:\	User Name madeline Group gutierrez Sample Label MRII1100-1	
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 D5_3-26_glyimest	
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_pdaPdDMSO_h0	10	Aproton_16	✓		✓	✓	✓	✓	soemardi	C:\	User Name soemardi Group vedernikov Sample Label D5_3-19_8MQ_pdaPdDMSO_h0 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 D5_3-19_8MQ_Pdmix_h0	

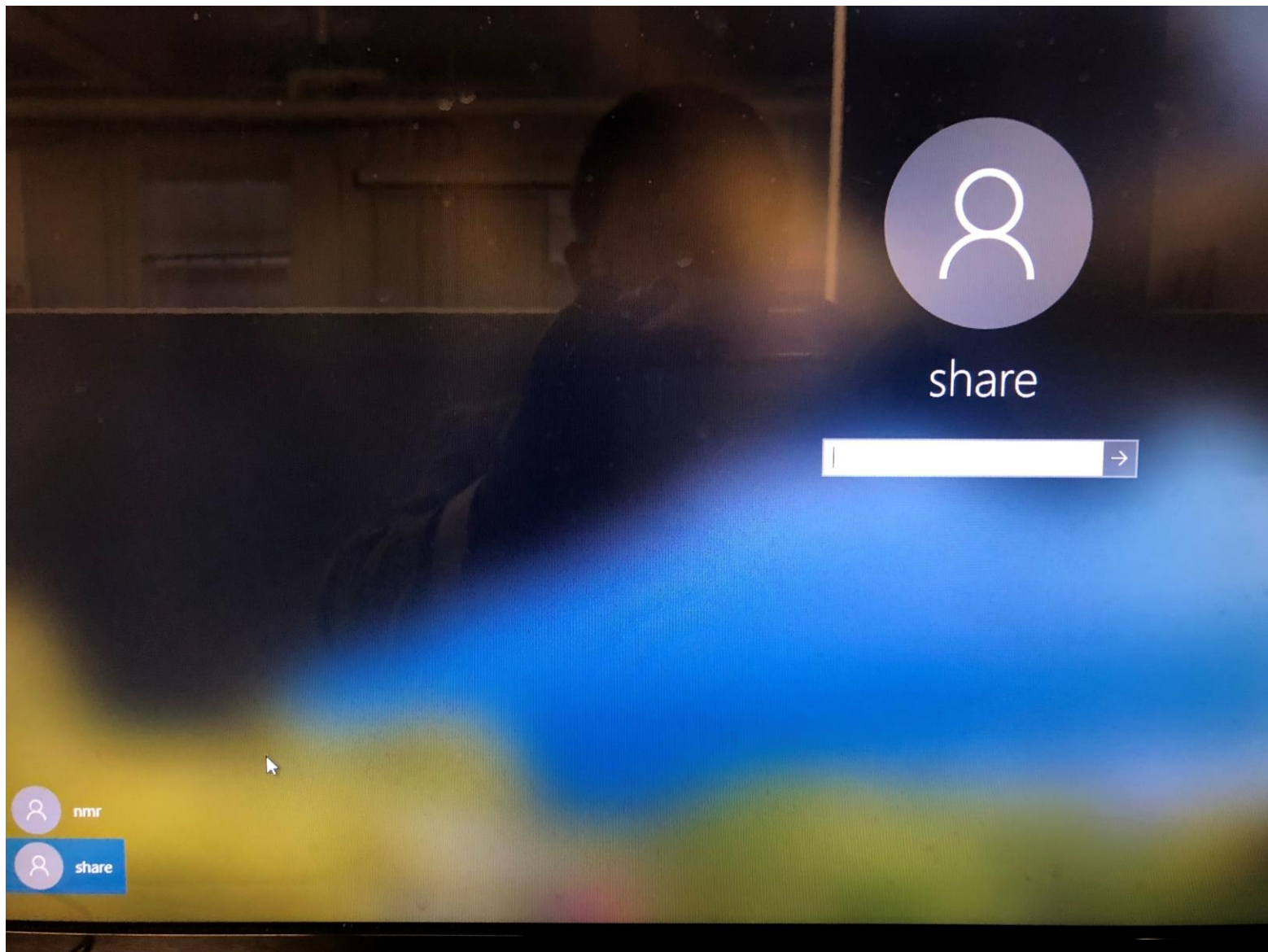
Search Preceding Include previous runs

Busy until: Tue 15:17 Day Experiments: 00:30 Night Experiments: 00:00

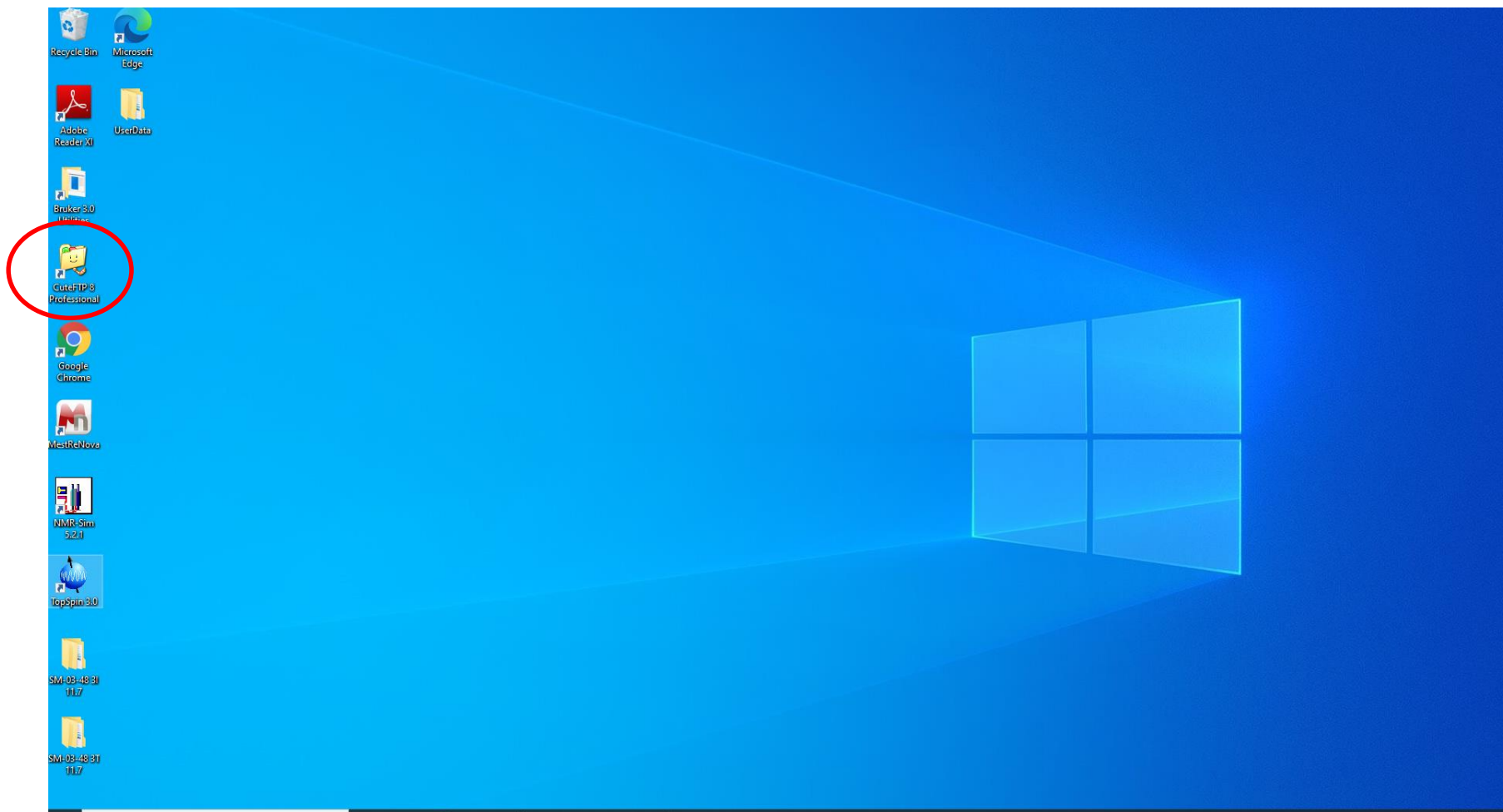
start TOPSPIN 2.1 Bruker TOPSPIN 2.1 ... ICON-NMR: spect. ICON: Automation Se... 8.JPG - Paint







sun1234



CuteFTP

chem400.umd.edu
share
sun1234
21

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

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

Local Drives Site Manager chem400.umd.edu chem400.umd.edu

C:\Users\share\Desktop\Us

WL2-82A
DK-MV_cal40mL
1-tj_1-101_5apr19
1-tj-1-86_20190308

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
zong	0 bytes	File Folder	6/14/2018	drwxr-xr-x		ftp
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tyrilk	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
sidamc	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 "/"
[9/18/2020 4:06:47 PM] 226 Successfully transferred "/"
STATUS:> [9/18/2020 4:06:47 PM] Directory listing completed.

Queue Window Log Window

#	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...	/murkli/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...	/murkli/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...	/murkli/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...	/murkli/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 ...	/murkli/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...	/murkli/nmr/SM-03-M...	3/6/2020 5:56:36 ...		0:00:00	?	?	Normal	Error

For Help, press F1

chem400.umd.edu: 79 clients(0) 0 bytes

NIIM