



Measuring at the Autosampler

F. Traeger / M. John

January 2025



Sample

Standard and Young NMR tubes only

Diameter: 5 mm

Length: 18 – 24 cm (7 – 9 inch)

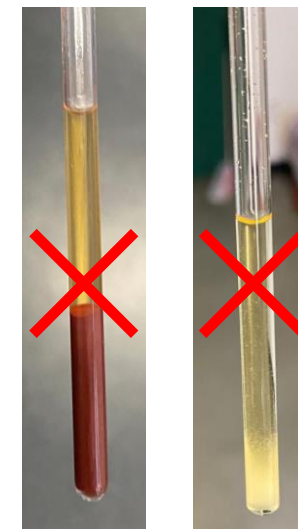
No broken tubes and caps

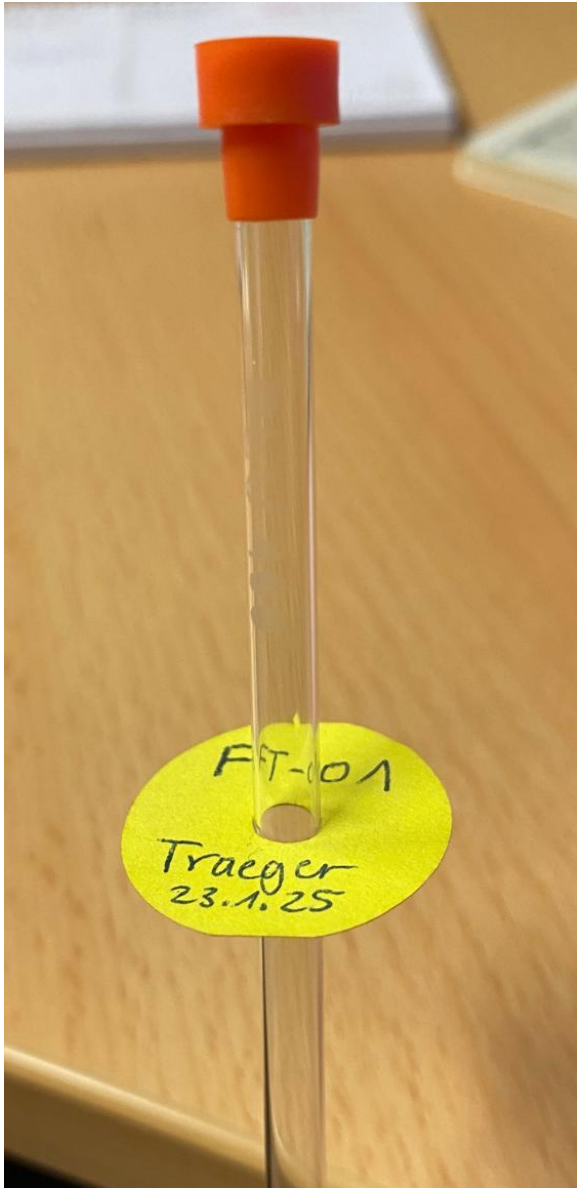
Cap must sit firmly on tube

Minimum filling height: 4 cm

Deuterated solvents only!

Homogeneous solutions only (no solids, no bubbles, no two-phase mixtures)





Label

Color code for each research group

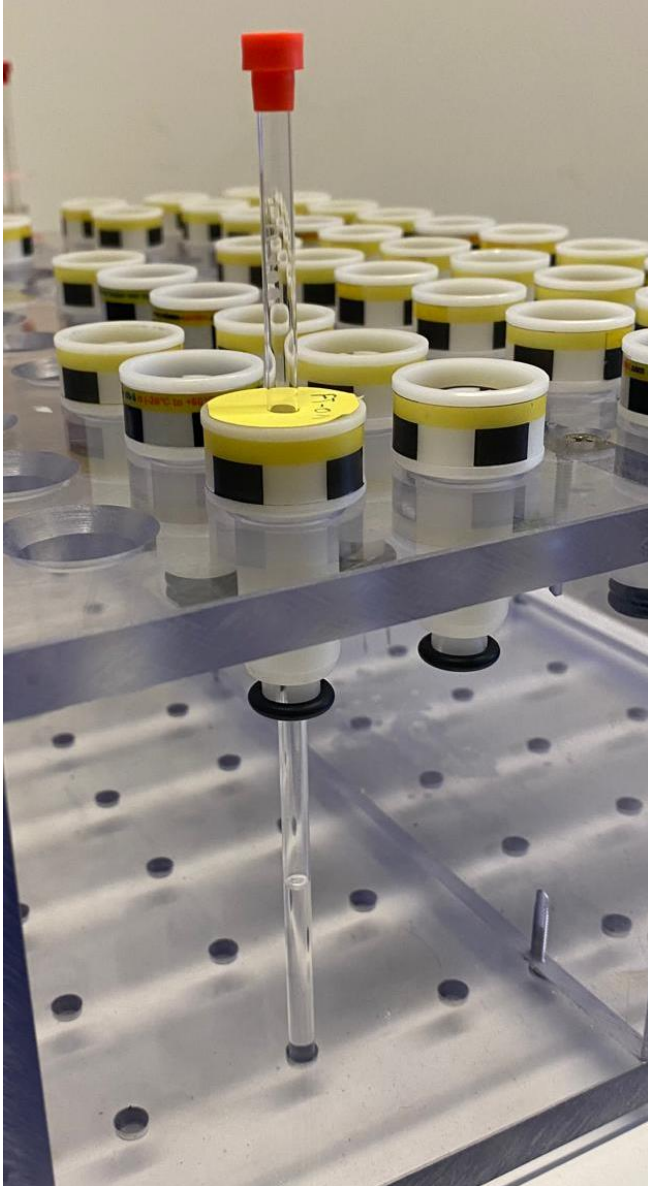
What should be on the label:

- > Name
- > Personal sample number
- > Date

Use paper label only once!

If your group is out of labels, you can pick up new ones at the NMR department

Any unlabelled, damaged or wrong tubes will be removed and discharged without further notice!



Spinner

Clean sample

Push sample all the way down in the spinner rack

Do not change the position of the sample in the spinner afterwards! If the tube is sitting too low in the spinner, the glass can break in the spectrometer!

Label must lie flat and firmly on the spinner

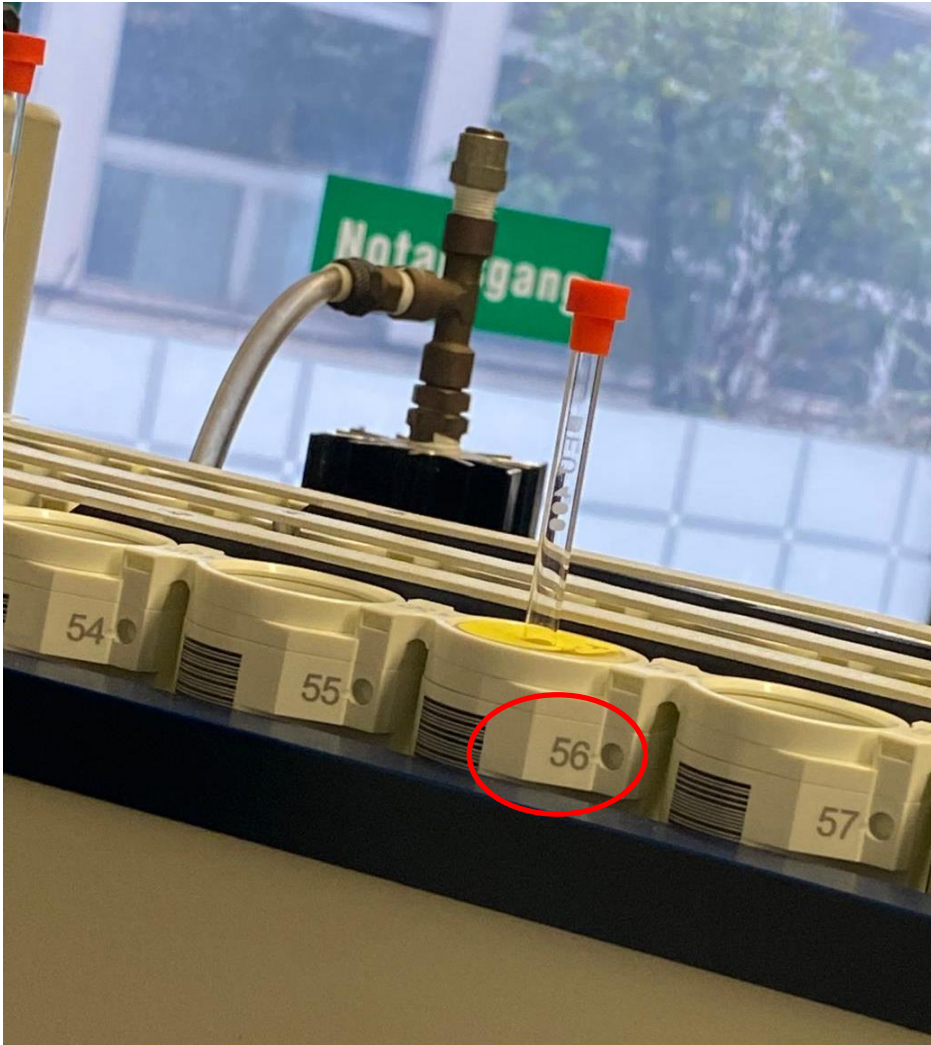
Do not use any other (selfmade) labels, otherwise the sample might get stuck in the spectrometer!

Avoid touching the spinner

Autosampler

Clean tube again!

Use the next free holder on the left side of the magnet



Experiment Table

Holder	Type	Status	Name	No.	Type	Solvent	Experiment	Pri	Par	Title/Orig	Time	User	Start Time
45		Automation Locked				CDCI3	chloroform-d	N 19F					
46						CDCI3	chloroform-d	N 1H					
47	2	Finished	si-ka-VI-113a_80deg_1d	1									
48	2	Finished	si-ka-VI-113b_80deg_1d	1									
49	1	Finished	JDI-91	1									
50	1	Finished	NI-WEN-089-frk70-88	1									
53	2	Running	MA-WEN-041	4						crude	00:00:50	alcarazo	10:53 Thu Jan 23 2025
53	2	Running	MA-WEN-041	5							00:00:52	alcarazo	11:14 Thu Jan 23 2025

Automation Locked

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

IconNMR: Identify User

Help on logging in

User's Full Name	User ID
Ak Ackermann	ackermann
AC-Synthesepraktikum	acs
Ak Alcarazo	alcarazo
OC-Synthesepraktikum	aos
Ak Bismuto	bismuto
Ak Diederichsen	diederichsen
Ak Fischer	fischer
Ak Hell	hell
Ak Janssen-Mueller	janssen-mueller
Katalyse-Praktikum	kat
Ak Koszinowski	koszinowski
Ak Krawczuk	krawczuk
MEMO-Praktikum	memo
Ak Meyer	meyer
MMC Praktikum	mmc
NMR User	nmr
NMR Super User	nmrsu
OC-Grundpraktikum	ocg
Ak Otte	otte
Reaction Monitoring	ReactionMonitoring
Ak Roesky	roesky
Ak Schneider	schneider
Ak Siewert	siewert
Ak Simeth	simeth
Ak Stalke	stalke
Ak Steinem	steinem
Ak Tietze	tietze
Ak Vana	vana
Ak Vondung	vondung
Ak Waitz	waitz
Ak Walker	walker
Ak Zhang	zhang

User ID: nmrsu

OK Lock IconNMR

Jan23-2025-0624-nmrso Status

1	2	3	4	5	6	7	8	9	10
11	12	13	14	15	16	17	18	19	20
21	22	23	24	25	26	27	28	29	30
31	32	33	34	35	36	37	38	39	40
41	42	43	44	45	46	47	48	49	50
51	52	53	54	55	56	57	58	59	60

Log in with your research group ID

Preceding Experiments

#	Holder	Date	No.	Name
25	53	2025-01-23 11:10:04	4	MA-WEN-041
24	50	2025-01-23 11:05:15	1	NI-WEN-089-frk70-88
23	49	2025-01-23 11:00:32	1	JDI-91
22	48	2025-01-23 10:58:42	2	si-ka-VI-113b_80deg_1d
21	48	2025-01-23 10:53:46	1	si-ka-VI-113b_80deg_1d
20	47	2025-01-23 10:51:47	2	si-ka-VI-113a_80deg_1d
19	47	2025-01-23 10:46:40	1	si-ka-VI-113a_80deg_1d
18	44	2025-01-23 10:45:05	2	DA-GAV 205 M1
17	44	2025-01-23 10:40:48	1	DA-GAV 205 M1



Green
Yellow
Red
Light red

position free
measurement completed
currently measuring
queued sample

Experiment Table

Holder	Type	Status	Name	No.	Solvent	Experiment	Pri	Par	Title/Orig	Time	User	Start Time
		Queued	DA-GAV 205 M2	2	CDCI3	chloroform-d	N 19F			00:00:52	alcarazo	11:21 Thu Jan 23 2025
▶ 46		2 Queued	DA-GAV 237-CR	1	C2D2Cl4	tetrachloroethane	N 1H					
		Queued	DA-GAV 237-CR	2	C2D2Cl4	tetrachloroethane	N 19F					
▼ 47		2 Finished	si-ka-VI-113a_80deg_1d	1	CD3CN	acetonitrile-d3	N 1H					
		Finished	si-ka-VI-113a_80deg_1d	2	CD3CN	acetonitrile-d3	N 31P{1H}					
▼ 48		2 Finished	si-ka-VI-113b_80deg_1d	1	CD2Cl2	dichlormethane-d2	N 1H					
		Finished	si-ka-VI-113b_80deg_1d	2	CD2Cl2	dichlormethane-d2	N 31P{1H}					
▼ 49		1 Finished	JDI-91	1	CDCI3	chloroform-d	N 1H					crude
▼ 50		1 Finished	NI-WEN-089-frk70-88	1	CDCI3	chloroform-d	N 1H			00:00:50	alcarazo	11:03 Thu Jan 23 2025
▶ 51		Available										
▶ 52		Available										
▼ 53		Available										
▶ 54		Available										
▶ 55		Available										
▼ 56		1 Available										
▶ 57		Available										
▶ 58		Available										
▶ 59		Available										

Jan23-2025-0624-nmrsu Status

1	2	3	4	5	6	7	8	9	10
11	12	13	14	15	16	17	18	19	20
21	22	23	24	25	26	27	28	29	30
31	32	33	34	35	36	37	38	39	40
41	42	43	44	45	46	47	48	49	50
51	52	53	54	55	56	57	58	59	60

Double-click on available position

Select experiment

Enter title of experiment

FT_3h

1

D2O

deuteriumoxide

N 1H

Citric Acid in D2O

00:00:50

nmrsu

Set Start Time

Name of file
(no spaces and
special characters
like ä, ö, ü)

Number in file
(automatically
continued)

Select solvent

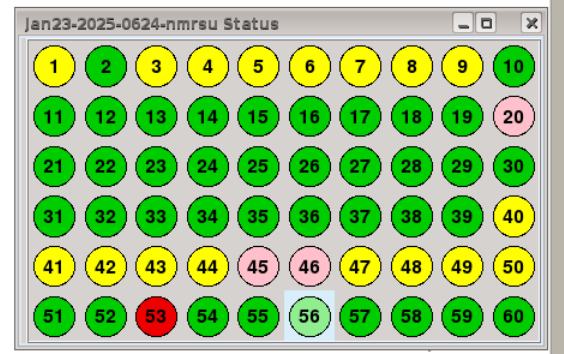
Measurement time
< 5 min -> day
> 5 min -> night

Preceding Experiments

#	Holder	Load	Experiment	ATM	Rotation	Lock	Shim	Acq	Proc	Title/Orig
26	53		19F	✓	✓					
25	53		1H	✓	✓					
24	50		1H	✓	✓	✓	✓	✓	✓	
23	49		1H	✓	✓	✓	✓	✓	✓	
22	48		31P{1H}	✓	✓	✓	✓	✓	✓	/opt/topspin3.5pl7/data/walker/nmr walker
21	48		1H	✓	✓	✓	✓	✓	✓	/opt/topspin3.5pl7/data/alcarazo/nmr alcarazo
20	47	2025-01-23 10:51:47	31P{1H}	✓	✓	✓	✓	✓	✓	/opt/topspin3.5pl7/data/alcarazo/nmr alcarazo
19	47	2025-01-23 10:46:40	1H	✓	✓	✓	✓	✓	✓	/opt/topspin3.5pl7/data/alcarazo/nmr alcarazo
18	44	2025-01-23 10:45:05	1H	✓	✓	✓	✓	✓	✓	/opt/topspin3.5pl7/data/alcarazo/nmr alcarazo
			19F	✓	✓					/opt/topspin3.5pl7/data/alcarazo/nmr alcarazo

Experiment Table

Holder	Type	Status	Name	No.	Solvent	Experiment	Pri	Par	Title/Orig	Time	User	Start Time
46	2	Queued	DA-GAV 205 M2	2	CDCI3	chloroform-d	N 19F			00:00:52	alcarazo	11:21 Thu Jan 23 2025
47	2	Finished	DA-GAV 237-CR	1	C2D2Cl4	tetrachloroethane	N 1H					
47	2	Finished	DA-GAV 237-CR	2	C2D2Cl4	tetrachloroethane	N 19F					
48	2	Finished	si-ka-VI-113a_80deg_1d	1	CD3CN	acetonitrile-d3	N 1H					
48	2	Finished	si-ka-VI-113a_80deg_1d	2	CD3CN	acetonitrile-d3	N 31P{1H}					
49	2	Finished	si-ka-VI-113b_80deg_1d	1	CD2Cl2	dichlormethane-d2	N 1H					
49	2	Finished	si-ka-VI-113b_80deg_1d	2	CD2Cl2	dichlormethane-d2	N 31P{1H}					
50	1	Finished	JDI-91	1	CDCI3	chloroform-d	N 1H		crude			
50	1	Finished	NI-WEN-089-frk70-88	1	CDCI3	chloroform-d	N 1H			00:00:50	alcarazo	11:03 Thu Jan 23 2025
51	1	Available										
52	1	Available										
53	2	Running										
53	2	Running	MA-WEN-041	4	CDCI3	chloroform-d	N 1H			00:00:50	alcarazo	11:09 Thu Jan 23 2025
53	2	Running	MA-WEN-041	5	CDCI3	chloroform-d	N 19F			00:00:52	alcarazo	11:14 Thu Jan 23 2025
54	1	Available										
55	1	Available										
56	2	Available										
56	2	Available	FT_3h	1	D2O	deuteriumoxide	N 1H		Citric Acid in D2O			
56	2	Available	FT_3h	2	D2O	deuteriumoxide			Citric Acid in D2O			



Click on change user after you are done

Submit

Add 1

Change User

Submit experiment(s)

Add another experiment for the same sample

Preceding Experiments

#	Holder	Date	Name	No.	Solvent	Experiment	Pri	Par	Title/Orig	User
26	53	2025-01-23 11:00:52	JDI-91	1	CDCI3	chloroform-d	N 1H			alcarazo
25	53	2025-01-23 11:00:52	JDI-91	1	CDCI3	chloroform-d	N 19F			alcarazo
24	50	2025-01-23 10:58:42	NI-WEN-089-frk70-88	1	CDCI3	chloroform-d	N 1H			alcarazo
23	49	2025-01-23 10:58:42	NI-WEN-089-frk70-88	1	CDCI3	chloroform-d	N 19F			alcarazo
22	48	2025-01-23 10:58:42	si-ka-VI-113b_80deg_1d	2	CD2Cl2	dichlormethane-d2	N 1H			alcarazo
21	48	2025-01-23 10:53:46	si-ka-VI-113b_80deg_1d	1	CD2Cl2	dichlormethane-d2	N 1H		crude	alcarazo
20	47	2025-01-23 10:51:47	si-ka-VI-113a_80deg_1d	2	CD3CN	acetonitrile-d3	N 1H			alcarazo
19	47	2025-01-23 10:51:47	si-ka-VI-113a_80deg_1d	1	CD3CN	acetonitrile-d3	N 31P{1H}			alcarazo
18	44	2025-01-23 10:45:05	DA-GAV 205 M1	2	CDCI3	chloroform-d	N 19F			alcarazo



Automation - Running - Busy until : Thu 17:00 - Day : 00:17 - Night : 01:21

Lock Field Shim Receiver Gain Acquire Data Process Data

- ▶ Help
- ▶ Logoff
- ▶ Stop Run
- ▶ Pause
- Logged in as nmrsu
- Instrument Name av300: spect

Holder	Type	Status	Name	No.	Solvent	Experiment	Par	Title/Orig	Pri	Time	User	Start Time
<input type="checkbox"/> 1												
<input type="checkbox"/> 2			Queued									
<input type="checkbox"/> 2			Queued	2	CDCI3	13C{1H}				00:13:38	aos	16:49 Thu Jan 23 2025
<input type="checkbox"/> 2			Queued	3	CDCI3	13C-APT				00:13:29	aos	17:08 Thu Jan 23 2025

Check the status of your measurement online

Web address for av402: 134.76.66.88

Date	Time	Holder	Name	No.	Experiment	Load	ATM	Rotation	Lock	Shim	Acq	Proc	User	Title	Remarks
2025-01-23	16:23:34	27	DK126_250123_first_cryst	1	1H	✓							fischer	DK126 firt patch rot eher orange Crzst 20 mg c6d6 23.01.25	
2025-01-23	16:18:31	26	Memo-MR	12	1H	✓	✓	✓	✓	✓	✓	✓	walker	1H, BCH nach zweiter Saeule, Fr.2.2, CDCI3	
2025-01-23	16:12:54	25	Memo-MR	11	1H	✓	✓	✓	✓	✓	✓	✓	walker	1H, BCH nach zweiter saeule Fr.2.1, CDCI3	
2025-01-23	16:07:30	38	300-NW282	1	1H	✓	✓	✓	✓	✓	✓	✓	meyer	1H, column, residual fractions	
2025-01-23	16:02:54	37	300-NW291	3	1H	✓	✓	✓	✓	✓	✓	✓	meyer	1H, soxhlet, liquid	
2025-01-23	15:57:51	36	300-NW293	2	1H	✓	✓	✓	✓	✓	✓	✓	meyer	1H, after washing	
2025-01-23	15:52:51	35	300-NW294	1	1H	✓	✓	✓	✓	✓	✓	✓	meyer	1H, crude	
2025-01-23	15:48:08	34	LHN	8	1H	✓	✓	✓	✓	✓	✓	✓	alcarazo	LHN-35 2nd CDCI3 PROTON	
2025-01-23	15:41:25	33	LHN	7	1H	✓	✓	✓	✓	✓	✓	✓	alcarazo	LHN-13-2 CDCI3 PROTON	
2025-01-23	15:37:09	17	SUN_SC_535_Suger_SM	1	1H	✓	✓	✓	✓	✓	✓	✓	janssen-mueller		
2025-01-23	15:32:25	16	SUN_SC_389_Sm_check	1	1H	✓	✓	✓	✓	✓	✓	✓	janssen-mueller		
2025-01-23	15:28:15	15	Schwarz	2	1H	✓	✓	✓	✓	✓	✓	✓	meyer	418-6	
2025-01-23	15:17:24	14	300-AR36.crd-AlkoholChalcone-Zink	1	1H	✓	✓	✓	✓	✓	✓	✓	walker		
2025-01-23	15:09:29	13	WAL_4_ns.F13-17_JS	1	1H	✓	✓	✓	✓	✓	✓	✓	walker		

How to download your data using Bitwise ssh client

Bitwise SSH Client 9.42

Profile: Chemie_Cluster.tlp (changed) [Window behavior](#)

Login Options Terminal RDP SFTP Services C2S S2C SSH Notes About

Load profile Save profile Save profile as New profile Close profile

Server Host: 134.76.66.90 Port: Enable obfuscation Obfuscation keyword:

Authentication Username: nmrsu Initial method: password Initial method dropdown: Store encrypted password in profile Password: Enable password over libdi fallback

Kerberos Request delegation gssapi-keyex authentication

Proxy settings Host key manager Client key manager Help

av402: 134.76.66.88

Enter your research group ID here

Log in Exit

16:26:18.929 Current date: 2025-01-23
16:26:18.929 Bitwise SSH Client 9.42, a fully featured SSH client for Windows. Copyright (C) 2000-2024 by Bitwise Limited.
16:26:18.929 Visit www.bitwise.com for latest information about our SSH software.
16:26:18.929 Run 'BvSsh -help' to learn about supported command-line parameters.
16:26:18.929 Cryptographic provider: Windows CNG (x86) with additions
16:26:19.289 Version status: Unknown
The status of the currently installed version is unknown because there has not been a recent, successful check for updates.
16:26:19.340 Loading last used profile 'C:\Users\Franziska\Desktop\Chemie_Cluster.tlp'.
16:26:19.344 Last used profile loaded successfully.
16:26:20.192 Automatic check for updates completed successfully.
16:26:20.192 Version status: Current
This is the latest release.

Bitwise SSH Client 9.42

Profile: Chemie_Cluster.tlp (changed) [Window behavior](#)

Login Options Terminal RDP SFTP Services C2S S2C SSH Notes About

Load profile Save profile Save profile as New profile Close profile

Local and Upload Settings Initial directory: Treat as home Start in last directory Auto refresh folders Upload Ask if file exists

Remote and Download Settings Initial directory: /opt/topspin3.5pl7/data/nmrsu/nmr Treat as home Start in last directory Auto refresh Cache folders Queue paused Follow download Download mode: Default Pipeline kB: 512 Use SFTP v3-6

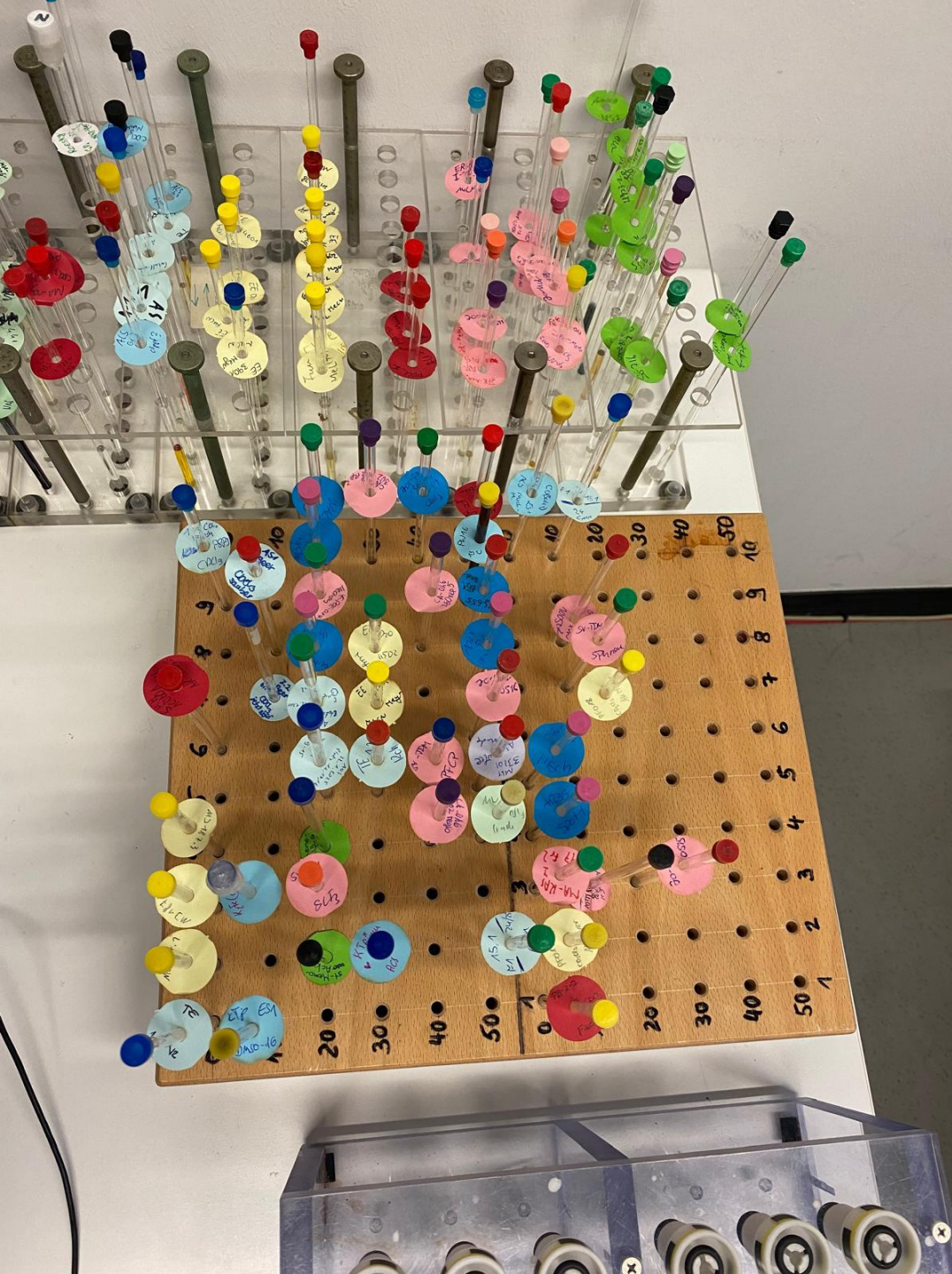
Set Permissions after Upload Files: 660 Directories: 770

av402: topspin4.0.6

Enter your research group ID here

Log in Exit

16:26:20.192 Version status: Current
This is the latest release.
16:27:34.895 Started a new SSH connection.
16:27:34.903 Connecting to SSH server 134.76.66.90:22.
16:27:34.903 Connection established.
16:27:34.919 Server version: SSH-2.0-OpenSSH_6.6.1
16:27:34.919 First key exchange started. Cryptographic provider: Windows CNG (x86) with additions
16:27:34.935 Received host key from the server. Algorithm: Ed25519, size: 255 bits, SHA-256 fingerprint: d5pOosovcw95aXa9jqgSDTugj0Ijbc57Jspi0JTrbQ.
16:27:34.942 First key exchange completed using Curve25519@libssh (lax). Connection encryption and integrity: aes256-gcm, compression: none.
16:27:38.832 Attempting password authentication.
16:27:38.879 Authentication completed.
16:27:42.820 Connection disconnected on user's request.
16:27:42.820 The SSH connection has been terminated.



Pick up

Finished samples will be placed in timber pick up rack under holder no. on the left (morning measurements) and on the right (afternoon measurements) for av300

Samples not picked up will end up in the storage rack behind or the fume hood

Samples from av402 will be placed in timber pick up rack in the sample submission room -1.117 in the IOBC building

When you want to pick up your sample directly after the measurement, wait until the light on top of the magnet is green or the next sample has been inserted!