

IconNMR Automation Run Status:

Day Experiments: 00:41

Busy Until: Sat 02:12

Night Experiments: 05:28















History List

HOLDER	TIME	NAME	EXPNO	EXPERIMENT	USER	LOAD	ATMA	SPIN	LOCK	SHIM	ACQ	PROC	TITLE	REMARKS
6	19:07:14	6-25112022- XXXXXXXXXX	11	AA_119Sn_ig	XXXXXXXXXX	-	-	-	-	-	-	-	JU001.3	
8	18:35:21	20221125-CpIIILaI2_Hexan	10	AA_1H	XXXXXXXXXX	-	x	-	-	-	-	-	CpIIILaI2 aus Hexan Extrakt	ATM Failed
60	17:19:59	60-25112022-nmr-abt	23	R-HUMP	XXXXXXXXXX	-	-	-	-	-	-	-		
2	17:00:29	2-25112022- XXXXXXXXXX	10	R-1H-16	XXXXXXXXXX	-	-	-	-	-	-	-	TK_616.mS	
60	15:30:45	60-25112022-nmr-abt	22	AA_1H	XXXXXXXXXX	-	-	-	-	-	-	-		
7	14:53:49	ME99_300	11	AA_31P_dec	XXXXXXXXXX	-	x	-	-	-	-	-	GeHfCl4P + 7 DIBAL-H, Tol-d8 in Kaelte, rotbraun	ATM Failed
7	14:47:28	ME99_300	10	AA_1H	XXXXXXXXXX	-	-	-	-	-	-	-	GeHfCl4P + 7 DIBAL-H, Tol-d8 in Kaelte, rotbraun	
4	13:55:54	MM863_25112022_300	13	AA_1H	XXXXXXXXXX	-	-	-	-	-	-	-	+ 1 eq. tBuNHLI; ueber Nacht bei RT; + 2 Tropfen DFB; + 1 eq. tBuNHLI	
60	13:44:47	60-25112022-nmr-abt	21	AA_1H	XXXXXXXXXX	-	-	-	-	-	-	-		
4	13:37:18	MM863_25112022_300	12	AA_1H	XXXXXXXXXX	-	-	-	-	-	-	-	+ 1 eq. tBuNHLI; ueber Nacht bei RT; + 2 Tropfen DFB; + 2 h	
4	11:31:03	MM863_25112022_300	11	AA_1H	XXXXXXXXXX	-	-	-	-	-	-	-	+ 1 eq. tBuNHLI; ueber Nacht bei RT; + 2 Tropfen DFB	
6	11:13:28	6-25112022- XXXXXXXXXX	10	R-1H-16	XXXXXXXXXX	-	-	-	-	-	-	-	JU001.3	
5	09:56:31	20221125-CpIIILaI2_dept	11	AA_13C_dept135	XXXXXXXXXX	-	-	-	-	-	-	-	CpIIILaI2 nach Waschen mit Hexan	
5	09:49:50	20221125-CpIIILaI2_dept	10	AA_1H	XXXXXXXXXX	-	-	-	-	-	-	-	CpIIILaI2 nach Waschen mit Hexan	
4	09:28:45	MM863_25112022_300	10	AA_1H	XXXXXXXXXX	-	-	-	-	-	-	-	+ 1 eq. tBuNHLI; ueber Nacht bei RT	
3	09:21:59	AE29_251122_300	10	AA_1H	XXXXXXXXXX	-	-	-	-	-	-	-		
1	09:14:02	AE27_251122_300	10	AA_1H	XXXXXXXXXX	-	-	-	-	-	-	-		
60	08:26:39	60-25112022-nmr-abt	20	R-HUMP	nmr-abt	-	-	-	-	-	-	-		
60	08:12:41	60-25112022-nmr-abt	10	R-HUMP	nmr-abt	-	-	-	-	-	-	x		Automation was stopped by user
2	04:33:28	20221124-CpIIILaI2	11	AA_13C_dec	XXXXXXXXXX	-	-	-	-	-	-	-	CpIIILaI2 nach Waschen mit Hexan	
5	04:30:30	5-24112022- XXXXXXXXXX	12	R-13C-UDEFT	XXXXXXXXXX	-	-	-	x	-	-	-	SB128	Lock failed after multiple attempts
1	23:37:13	20221124-CGP108-3	12	AA_29Si_INEPT_ND	XXXXXXXXXX	-	-	-	-	-	-	-	CGP108-3	
1	19:08:07	20221124-CGP108-3	11	AA_13C_dec	XXXXXXXXXX	-	-	-	-	-	-	-	CGP108-3	
6	18:18:46	PMS132	11	AA_1H	XXXXXXXXXX	-	x	-	-	-	-	-	300 Mhz, THF, Kristalle	ATM Failed
6	17:10:02	PMS132	10	AA_31P_dec	XXXXXXXXXX	-	-	-	-	-	-	-	300 Mhz, THFd8, Kristalle	

IconNMR Automation Run Status:

Day Experiments: 00:30
 Busy Until: Wed 22:00
 Night Experiments: 00:00

History List

HOLDER	TIME	NAME	EXPNO	EXPERIMENT	USER	LOAD	ATMA	SPIN	LOCK	SHIM	ACQ	PROC	TITLE	REMARKS
4	21:25:33	4-29112022- 	14	HMBCGP	NA	-	-	-	-	-	-	-	Schwarz, E245_A2_INF1	
4	20:50:32	4-29112022- 	13	HSQCGP	NA	+	+	-	+	+	+	+	Schwarz, E245_A2_INF1	au_getlinv: Reference spectrum does not exist, continuing with default SW.; ro: cannot open reference file 'C:/Bruker/TopSpin3.6.2/prog/curdir/nmrsu/BsmsStatusServer1Shimcntl.ref': No such file or directory
4	19:16:48	4-29112022- 	13	HSQCGP	NA	-	x	-	-	-	-	-	Schwarz, E245_A2_INF1	Failsafe detected hangup, procedure: atm, attempting automation restart...
4	19:08:30	4-29112022- 	12	P31CPD	NA	+	+	-	+	+	+	+	Schwarz, E245_A2_INF1	sref: NUCLEUS '31P' not defined for SOLVENT 'CDCl3' SR is set to 0.0; pp: Cannot find any peak for scaling in E:/NMR-data/NA/data/NA/nmr/4-29112022-  /12/pdata/1/peaks!, sref: NUCLEUS '31P' not defined for SOLVENT 'CDCl3' SR is set to 0.0; pp: Cannot find any peak for scaling in E:/NMR-data/NA/data/NA/nmr/4-29112022-  /12/pdata/1/peaks!
4	17:34:42	4-29112022- 	12	P31CPD	NA	-	x	-	-	-	-	-	Schwarz, E245_A2_INF1	Failsafe detected hangup, procedure: atm, attempting automation restart...
4	16:10:54	4-29112022- 	11	13CUDEFT	NA	-	+	-	-	-	+	+	Schwarz, E245_A2_INF1	
4	16:01:42	3-29112022- 	1	PROTON	NA	+	+	-	+	+	+	+	Schwarz, E245_A2_INF1	
3	15:59:10	3-29112022- 	12	P31CPD	NA	-	+	-	-	-	+	+	Schwarz, E231_Mn_F-H	sref: NUCLEUS '31P' not defined for SOLVENT 'D2O' SR is set to 0.0, sref: NUCLEUS '31P' not defined for SOLVENT 'D2O' SR is set to 0.0
3	15:50:46	3-29112022- 	10	PROTON	NA	+	+	-	+	+	+	+	Schwarz, E231_Mn_F-H	
2	15:47:06	2-30112022- 	11	P31	NA	-	+	-	-	-	+	+	Schwarz, E231Mg_F-H	sref: NUCLEUS '31P' not defined for SOLVENT 'D2O' SR is set to 0.0, sref: NUCLEUS '31P' not defined for SOLVENT 'D2O' SR is set to 0.0
2	15:37:40	2-30112022- 	10	PROTON	NA	+	+	-	+	+	+	+	Schwarz, E231Mg_F-H	
1	14:29:34	1-30112022- 	13	HMBCGP	NA	-	-	-	-	-	-	-	Schwarz, E26_A1_1F1_1PF1	Automation was stopped by user

ICON-NMR on avii400: spect - SeaMonkey

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http://.../template-automation.htm

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ICON-NMR on avii400: spect



Automation - Running - Busy until : No Jobs! - Day Experiments : 00:00 - Night Experiments : 00:00

Instrument Idle

Help
Logoff

Logged in as
mitarbeiter

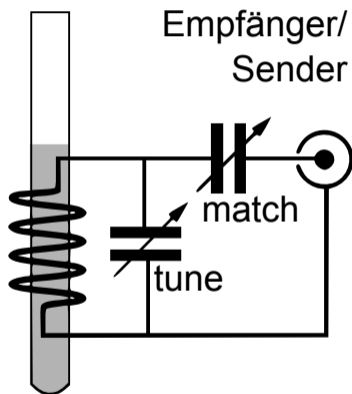
Instrument Name
avii400: spect

Holder	Type	Status	Disk	Name	No.	Solvent	Experiment	Par	Title / Orig	Pri	Time	User
1	6	Completed										
1		Completed	D:\u	Nov30-2022	10	Acetone	AA_1H		TPP in Acetone		00:01:07	nmrguest
1		Completed	D:\u	Nov30-2022	11	Acetone	AA_13C_pg		TPP in Acetone		00:09:40	nmrguest
1		Completed	D:\u	Nov30-2022	12	Acetone	AA_31P_dec		TPP in Acetone		00:00:54	nmrguest
1		Completed	D:\u	Nov30-2022	13	Acetone	AA_1H		TPP in Acetone		00:00:04	nmrguest
1		Completed	D:\u	Nov30-2022	14	Acetone	AA_19F		TPP in Acetone		00:00:53	nmrguest
1		Completed	D:\u	Nov30-2022	15	Acetone	AA_13C_dummy		TPP in Acetone		00:00:01	nmrguest
2												
3												
4												
5	1	Completed										
5		Completed	D:\u	JR117 221130	10	C6D6	AA_1H		nach 18 h		00:02:49	
6	1	Completed										

Date	Time	Holder	Name	No.	Experiment	Load	ATM	Rotation	Lock	Shim	Acq	Proc	User	Title	Remarks
2022-11-30	18:41:57	1	Nov30-2022	15	AA_13C_dummy						✓	✓	nmrguest	TPP in Acetone	Audita.bt file not in data set, AudiTrail update not per acquisition
2022-11-30	18:40:24	1	Nov30-2022	14	AA_19F						✓	✓	nmrguest	TPP in Acetone	QUAD FCA T&M executed. , sref: distance or referen in C:/Bruker/TOPSPIN/conf/instr/spect2/Hlock, line 21 30.0 SR is set to 0.0
2022-11-30	17:38:05	1	Nov30-2022	13	AA_1H	✓			✓	✓	✓	✓	nmrguest	TPP in Acetone	QUAD FCA T&M executed.
2022-11-30	17:15:29	27		10	AA_1H	✓			✓	✓	✓	✓		umkristallisiert	QUAD FCA T&M executed.
2022-11-30	16:31:05	26		11	AA_45Sc_lg						✓	✓			QUAD FCA T&M executed. , sref: distance or referen specified in C:/Bruker/TOPSPIN/conf/instr/spect2/Hlo

Probenkopf-Abstimmung: „Wobble“

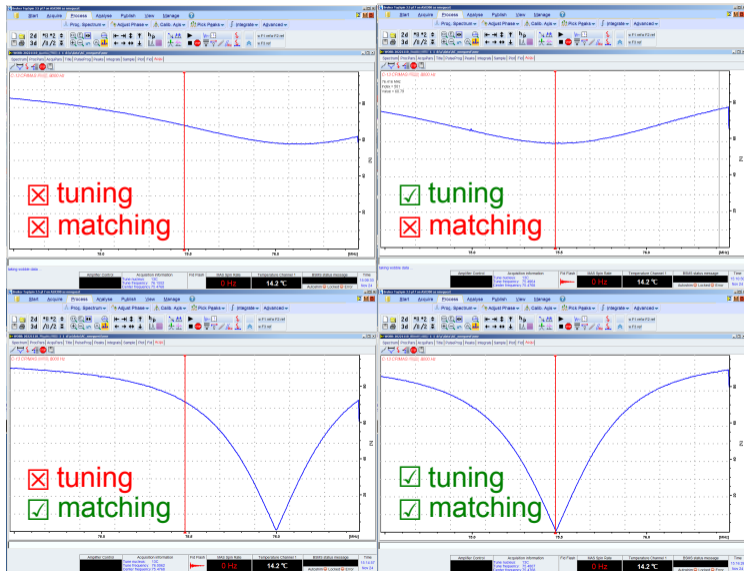
Schema



- Spule parallel zu regelbarem Kondensator („tune“) ergibt Schwingkreis
- Resonanzfrequenz des Schwingkreises muß auf Resonanzfrequenz des beobachteten Kernes abgestimmt werden („tunen“)
- zusätzlich muß reflektierte Leistung minimiert werden durch regelbaren Kondensator „match“
- für beste Ergebnisse für jede Probe zu machen (für jeden beteiligten Kern)

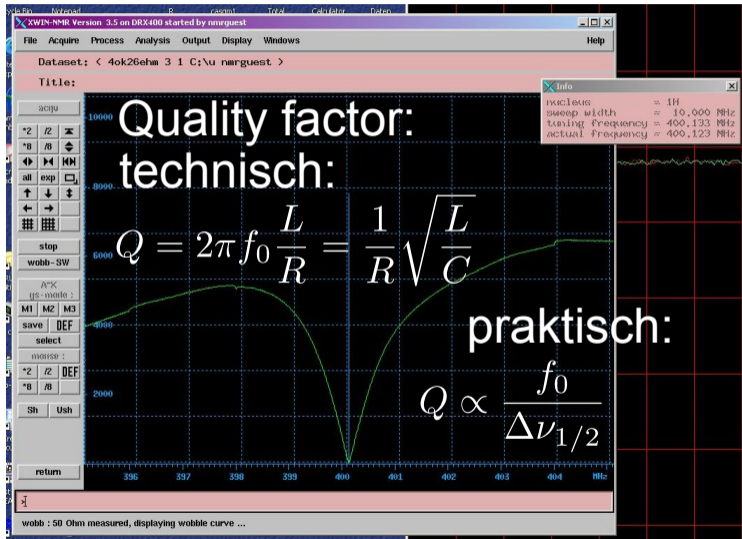
Probenkopf-Abstimmung: „Wobble“

Tuning und Matching



Probenkopf-Abstimmung: „Wobble“

„Wobble“Durchführung



Probenkopf-Abstimmung: „Wobble“

Salzlösungen am AVII+400



- bei H-1: Ende des matching-Bereiches
- bei P-31: Ende des tuning-Bereiches
- **Workaround:**
Lösungsmittel
D2O_salt
THF_salt
- für diese Lösungsmittel wird die Toleranz erhöht, unter Verlust der Empfindlichkeit