

G-NMR: Network of German NMR Centers

Treffen Berlin, 2. Oktober 2014



www.g-nmr.de



Program

- 1.) G-NMR Summer School (Bernd Reif, TUM)
- 2.) Pulse Sequence Library (Sam Asami, TUM)
- 3.) Discussion of 2nd funding phase of G-NMR
(Harald Schwalbe, BMRZ)

Ziele im G-NMR-Antrag

- Technologie- bzw. Wissenstransfer und ‘Gute Laborpraxis’ innerhalb der deutschen NMR community
- Erarbeitung gemeinsamer Konzepte zum Betrieb bzw. der Wartung von NMR Infrastrukturen
- Austausch von Software und Pulssequenzen
- Einheitliche Standard-Proben mit “standard operation procedures” für biomolekulare NMR
- NMR Workshops & Schools
- Austausch von Unterrichtsmaterialien und -konzepten



G-NMR web page & intranet Wiki

(Sam Asami)

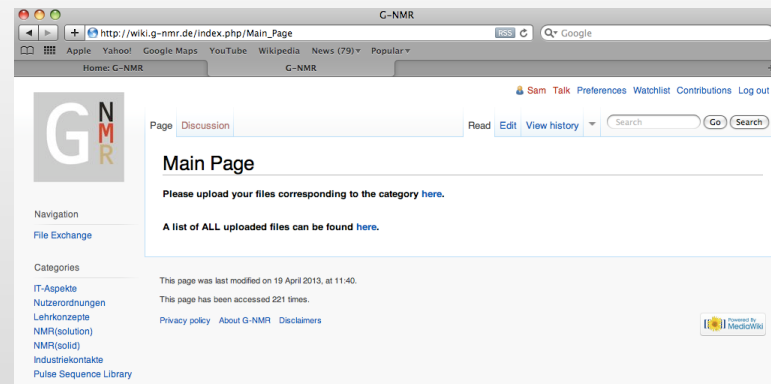
G-NMR web page

- Überblick über G-NMR Projekt
- Aufstellung aller Arbeitsgruppen
- Ankündigung von G-NMR Treffen
- Dokumentierung der Treffen (Präsentationen + Sitzungsprotokolle)
- **Link: G-NMR Mailing Liste**
- Link: Intranet
- Link: Pulse Sequence Library (**NEU**)



Intranet (Wiki)

- User Login
- Datenaustauschplattform
- Ablage von Dokumenten der verschiedenen Arbeitskreise
- Nutzer-Austausch über Pulssequenzen (**NEU**)



Arbeitsgruppen

- G-NMR web page: www.g-nmr.de Sam Asami (TUM)
- DFG-Nutzungsordnungen (Janssen, Schwalbe, Sattler, Graf)
- IT-Aspekte: Betz (BMRZ), Haessner (TUM)
- Spektrometer Maintenance: Richter (BMRZ), Gemmecker (TUM)
- Lehrkonzepte: Richter (BMRZ), Gemmecker (TUM), Sattler (TUM)
- NMR Pulssequenzen:
 - Lösung: Löhr (BMRZ), Gemmecker, Asami (TUM), Bermel (Bruker),
 - Festkörper: Baldus (BMRZ), Reif (TUM)



DFG-Nutzungsordnungen

Hinweise

zu Gerätenutzungskosten und zu Gerätezentren

NMR Service

4 NMR-Spektroskopie

Für die Nutzung von NMR-Spektrometern im automatisierten Routinebetrieb in Gerätezentren können bis max. 10,-- Euro pro Stunde veranschlagt werden. Bei mittleren Feldstärken, bis 400 MHz, erscheinen 5,-- Euro pro Stunde angemessen, der Höchstsatz von 10 Euro bezieht sich auf hohe Feldstärken ab 500 MHz. Bei manuellen Messungen und Hilfe bei der Auswertung erhöht sich der Pauschalsatz um 10,-- Euro (pro Messstunde).

NMR Forschung

Bei komplexen NMR-Experimenten in der Forschung ist die Betreuung bzw. Durchführung des NMR-experimentellen Teils deutlich aufwändiger und erfordert wissenschaftliche Unterstützung bei der Vorbereitung, Durchführung und Datenprozessierung. Dementsprechend können hier Stundensätze von 40,-- Euro (mittlere Feldstärke, 500 MHz) bis 80,-- Euro (sehr hohe Feldstärke, ab 850 MHz) angesetzt werden. Bei mehrtägigen NMR-Messungen sollte sich der Kostensatz reduzieren, da der relative Aufwand für Vor- und Nachbereitung sinkt. Bei einer Gesamtmesszeit von 20 Tagen sollte höchstens der halbe Stundensatz angewendet werden.

Die anrechenbaren Stunden betreffen in allen Fällen die reine NMR-Messzeit.

Ansprechpartner für Fragen zum Thema NMR-Kosten bei der DFG ist Dr. Christian Renner, Gruppe Wissenschaftliche Geräte und Informationstechnik, Tel. 0228/885-2324, E-Mail: Christian.Renner@dfg.de.



Status AG IT-Aspekte

- 28.10.2013 G-NMR Treffen bzgl. IT-Aspekte, Goethe Universität, Frankfurt am Main

- **Teilnehmer:**

M. Betz, C. Richter, J. Wirmer-Bartoschek, M. Hähnke (Uni-Frankfurt), S. Asami & R. Haessner (TU-München), S. Kuhn (Uni-Köln), J. Liermann (Uni Mainz), T. Hackl (Uni-Hamburg), V. Schmidts (Uni Darmstadt), F. Furtado (IPB Halle) O. Ohlenschläger (FLI Leibniz), J. Lopez (Magic-Angle-Solutions)

- Vorstellung der verschiedenen Betriebskonzepte
- Diskussion über Datenbanken
- **Fazit: NMR-Rohdaten speichern und der Allgemeinheit zur Verfügung stellen.**
→ **Kontrolle & Informationsaustausch**

Status AG Spektrometer maintenance

- 26.03.2013, BMRZ, Frankfurt/Main
12.09.2013, FGMR2013, Frauenchiemensee
- Standardexperimente für Festkörper NMR
- Standardexperiment für Lösungs-NMR:
 - Test's basieren auf Experimenten die bei Bio-NMR etabliert sind, angewendet auf Ubiquitin.
 - Ubiquitin Proben kaufen und nach Bedarf an die Institute senden.
 - Preis pro Probe ca. 1500,-€
 - 5000,-€ steht zur Verfügung
 - **Bisher keine endgültige Entscheidung**

Status AG Pulssequenzen liquid/solids

- Liquid state pulse sequences

Diskussion BNMRZ, Garching, 15.01.2014

Monika Beerbaum (FMP Berlin), Wolfgang Bermel (Bruker BioSpin; Rheinstetten), Dirk Bockelmann (MPI Göttingen),

Jörg Fohrer (Uni Hannover), Gerd Gemmecker (TU München), Steffen Glaser (TU München), Donghan Lee (MPI Göttingen), Frank Löhr (Goethe Universität Frankfurt), Tobias Madl (TUM), Senada Nozinovic (Uni Bonn), Bernd Reif (TUM), Christian Richter (BMRZ, Ffm), Michael Sattler (TU München), Peter Schmieder (FMP Berlin)

- Presentation Sam Asami

- Solid-state pulse sequences (Bernd Reif)

Treffen: 26.03.2013, BMRZ, Frankfurt/Main

12.09.2013, FGMR2013, Frauenchiemensee

Status Lehrkonzepte

- G-NMR Workshop: Teaching day , 21.11.2013 Frankfurt

- Teilnehmer:

C. Glaubitz, H. Schwalbe, C. Richter, J. Becker-Baldus, J. Ferner (Uni-Frankfurt), G. Gemmecker & B. Reif (TU-München), C. Räuber (RWTH Aachen), E. Brendler (TU Freiburg), R. Kerssebaum (Bruker BioSpin), L. Hennig (Uni-Leipzig), M. Beerbaum & Peter Schmieder (FMP Berlin), I. Shenderovich (Uni Regensburg), N. Schlörer (Uni Köln), S. Nozinovic (Uni-Bonn), S. Kemper TU Berlin), M. Hartl (Uni-Bayreuth), C. Fares (MPI Kohlenforschung) , D. Bockelmann (MPI Göttingen), E. Haupt (Uni-Hamburg), J. Graf (Uni-Heidelberg)

- Vorstellung der verschiedenen Konzepte für die NMR Lehre

- Ergebnis:

Empfehlung für Lehrinhalte der Kernresonanzspektroskopie im Studiengang Bachelor Chemie (Erstellt von N. Schlörer, J. Graf & J. Ferner); Weiterleitung an C. Thiele, Vorsitzende von FMGR, Letzte

Version:



Status

- DFG-Nutzungsordnungen
 - → etabliert und von der DFG akzeptiert
- IT-Aspekte
 - Arbeitsgruppe
- Lehrkonzepte (Studium, Doktoranden/Postdocs)
 - Konzeptpapier, Studienkommission GDCh ($\Leftrightarrow$ FGMR)
- NMR Pulssequenzen
 - Arbeitsgruppen
- Training courses & workshops
 - 1st G-NMR School Oct 13-15, 2014, Munich
- Industriekontakte
 - Beteiligt an Arbeitsgruppen

1st G-NMR School on Magnetic Resonance in Biological Systems

Helmholtz-Zentrum Neuherberg, October 13-15, 2014

<http://www.helmholtz-muenchen.de/g-nmr-school>



Speakers:

- Johanna Becker, Universität Frankfurt
- Monika Beerbaum, FMP Berlin
- Wolfgang Bermel, Bruker Biospin Rheinstetten
- Teresa Carlomagno, EMBL Heidelberg
- Gerd Gemmecker, TU München
- Steffen Glaser, TU München
- Christian Griesinger, MPI Göttingen
- Adam Lange, FMP Berlin
- Donghan Lee, MPI Göttingen
- Tobias Madl, TU München
- Michael Nilges, Institute Pasteur Paris
- Philipp Neudecker, FZ Jülich / HHU Düsseldorf
- Hartmut Oschkinat, FMP Berlin
- Bernd Reif, TU München
- Christian Richter, Universität Frankfurt
- Michael Sattler, TU München
- Peter Schmieder, FMP Berlin
- Harald Schwalbe, Universität Frankfurt
- Remco Sprangers, MPI Tübingen
- Markus Zweckstetter, MPI Göttingen

Future of G-NMR – 2nd phase

- Information zur Situation bei DFG
- Teaching, Schools
- Fortsetzung AGs: IT, Pulssequenzen, ???
- NMR in drug discovery -->
- Industriekontakte (bis jetzt nicht so viel passiert)

G-NMR

Pulse Sequence Library

Sam Asami

AG Sattler
TU Munich

02.10.2014

Challenges...

User

- Finding correct pulse sequence
 - redundant pulse sequences with similar names
 - not sufficiently commented
 - out-dated syntax
- Relevant input parameters?
 - Shape? Delays? Offsets? Water Suppression? Incrementation?
 - Routing?
- Processing Parameters
 - Correct phases? Forward-prediction? Back-prediction?

NMR Facility

- Implementation of pulse sequences
 - Relying on tested release sequences
 - Specialized, “un-released” sequences?
 - Further optimizations?
- Providing working datasets with correct processing for every sequence
 - “rpar”
 - Making “rpar” more dynamic?
- Adapting datasets to hardware changes?
 - e.g. change of re-routing
- Maintaining pulse sequence library on several spectrometers in large NMR centers?
 - Time-consuming
 - More efficient?

“Mseq”

Python scripts

- Input dialogs for user-optimized hard pulse (^1H , ^{13}C , ^{15}N hard pulse) and ^1H offset
 - Default value taken from prosol
- Calculation and setting all **relevant parameters**
 - Pulse **shape** names, alignments
 - Setting of **spectral widths**
 - Correct choice of **incrementation**
- Setting of **processing parameters**
- Writing setup instructions in “title” file, in case manual setup is desired

Pulse Sequences

- Automatic calculations coded **inside** the **pulse sequence** as far as possible
 - Automatic calculation of decoupling powers
 - Calculation of shaped pulse lengths and powers
 - Flags considering isotopic labeling scheme
 - Flags for maximal incrementation in constant-time experiments, minimum recycle delay

Mseq

Step-by-step

The screenshot shows the Bruker TopSpin 3.2 software interface. The main window displays the configuration for the Mseq pulse program. The left sidebar shows a file browser with folders for 'guest', 'sam', and 'service'. The main panel shows the following configuration:

PP: M.CBCACONH.wgfb

Input Parameters:

- > 1H offset O1
- > 13C offset O2P (middle of carbonyl region, 40.0 ppm)
- > 15N offset O3P (middle of amide region, 117.0 ppm)
- > 1H pi/2 pulse length (p1) at 20.0 W
- > 13C pi/2 pulse length (p3) at 199.5 W
- > 15N pi/2 pulse length (p21) at 199.5 W

Instructions:

optimize the solvent suppression in "gs" mode, using SPd821 (PHCOR21), SPd822 (PHCOR22), SPd823 (PHCOR23)

Comments:

- > make sure that TD1 < TD1MAX and at the same TD1 has to be an even number!
- > make sure that TD2 < TD2MAX and at the same TD2 has to be an even number!

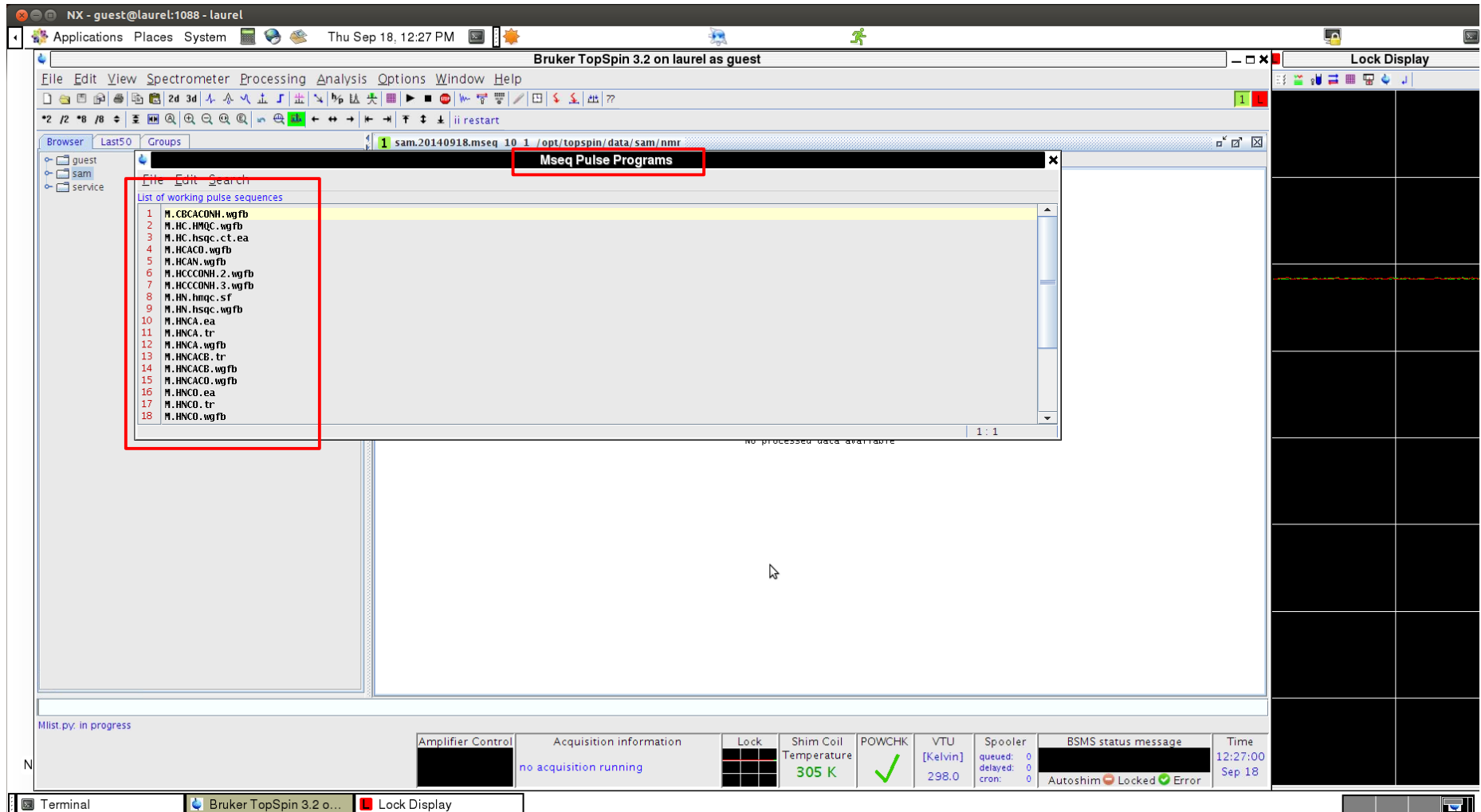
Below the main panel, there is a status bar with various indicators:

- Amplifier Control:** no acquisition running
- Lock:** Lock status indicator (green checkmark)
- Shim Coil Temperature:** 305 K
- POWCHK:** Green checkmark
- VTU [Kelvin]:** 298.0
- Spooler:** queued: 0, delayed: 0, cron: 0
- BSMS status message:** Autoshim Locked Error
- Time:** 12:33:38 Sep 18

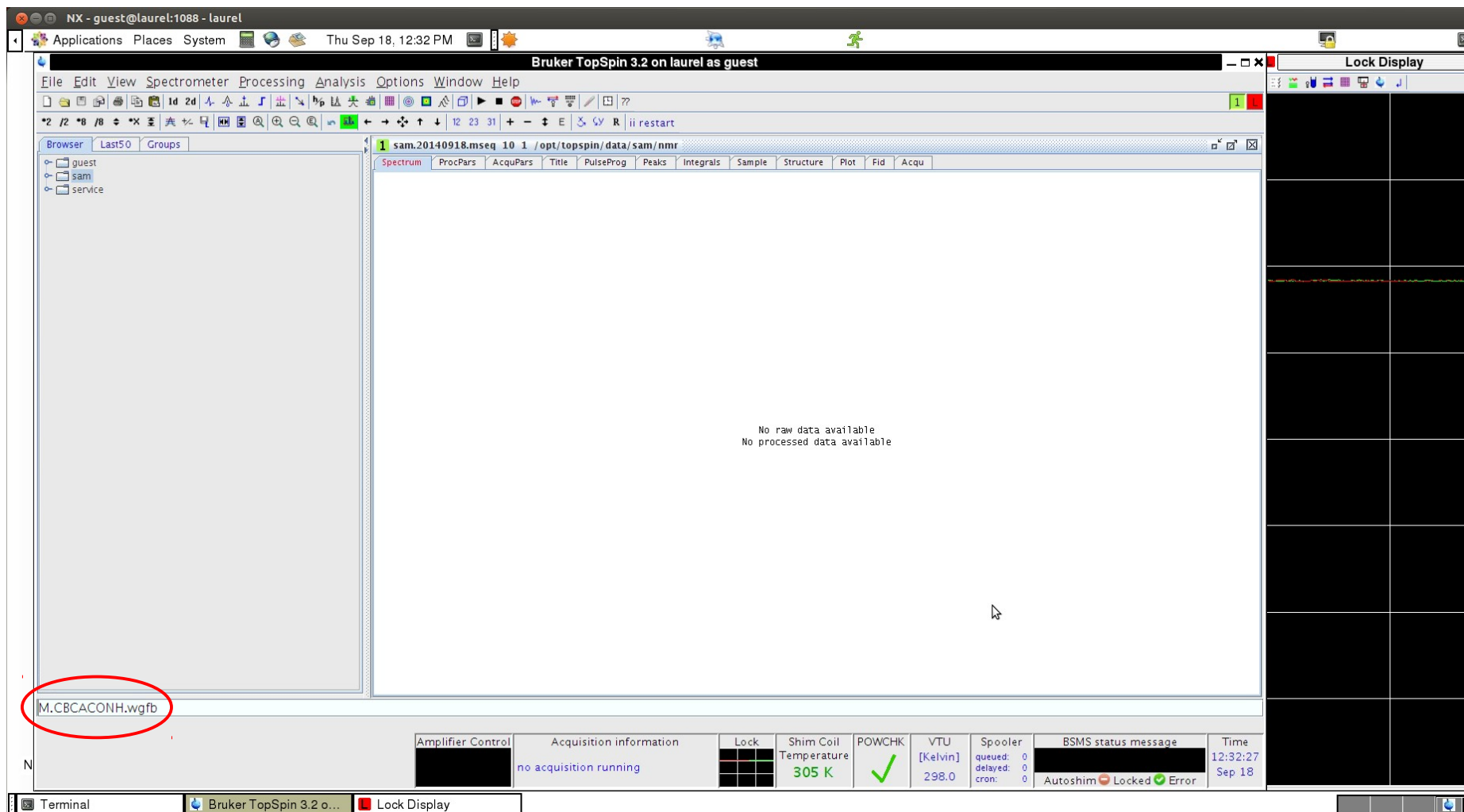
A red circle highlights the 'Mlist' button in the bottom left corner of the interface.

Mseq

Step-by-step

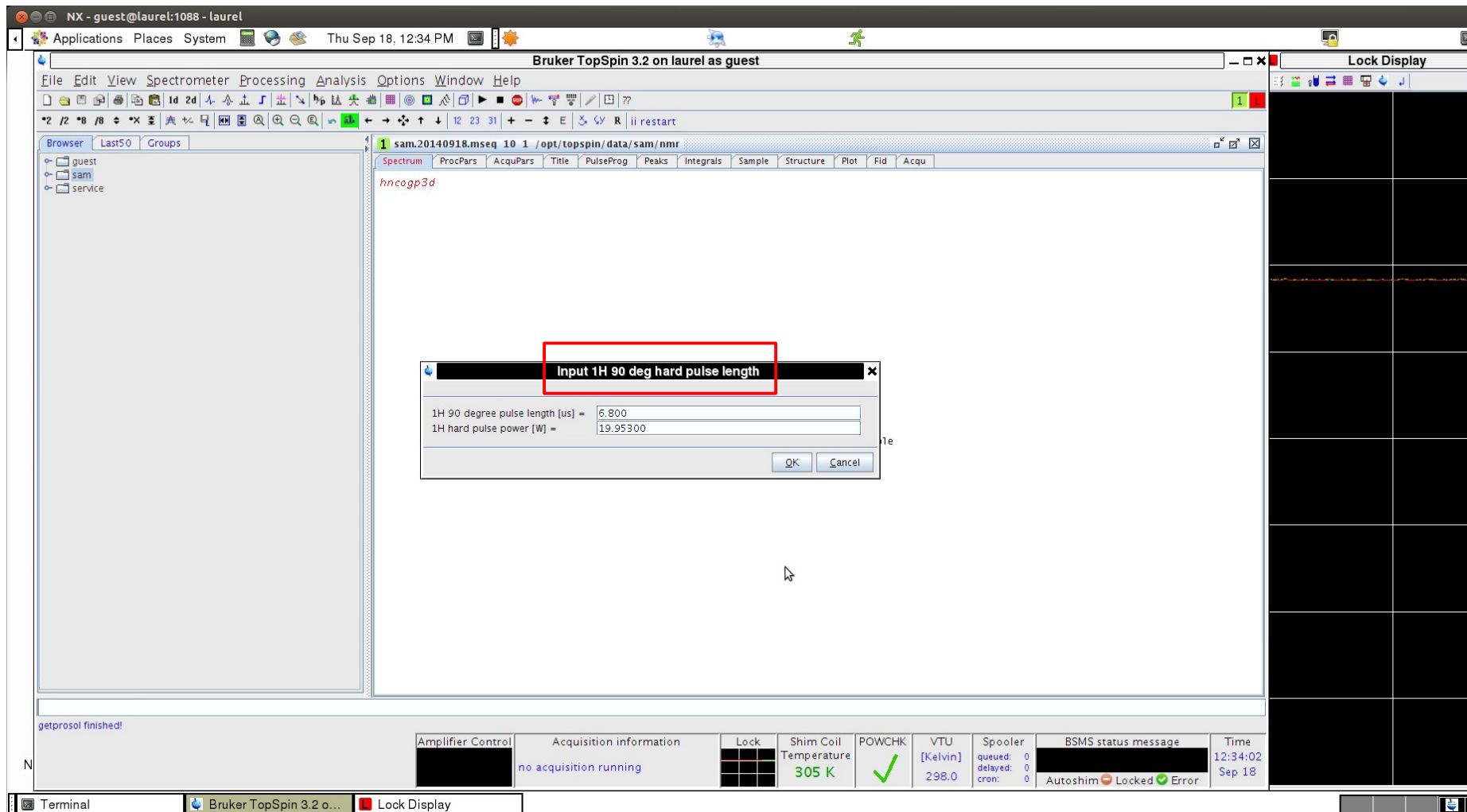


Mseq Step-by-step



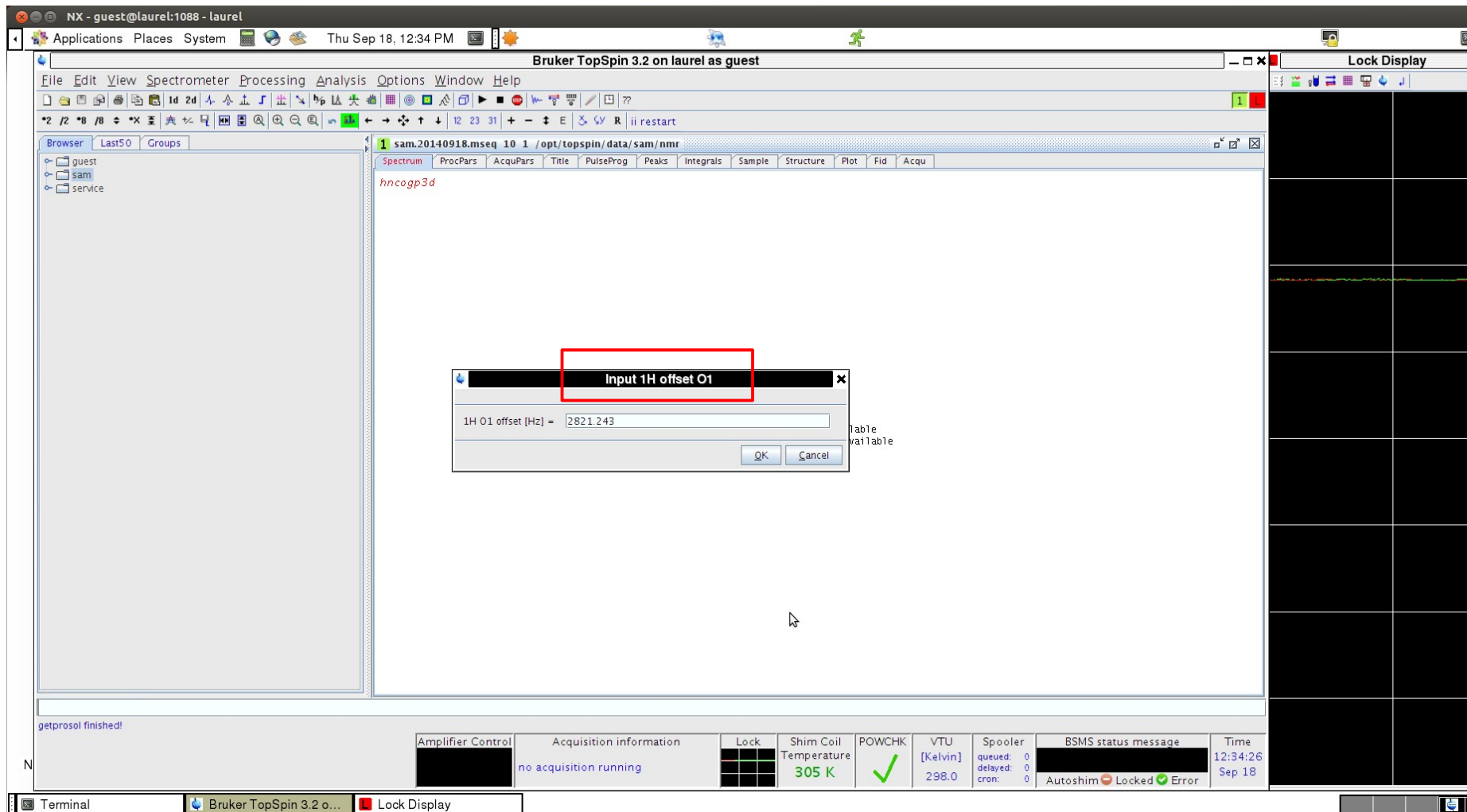
Mseq

Step-by-step



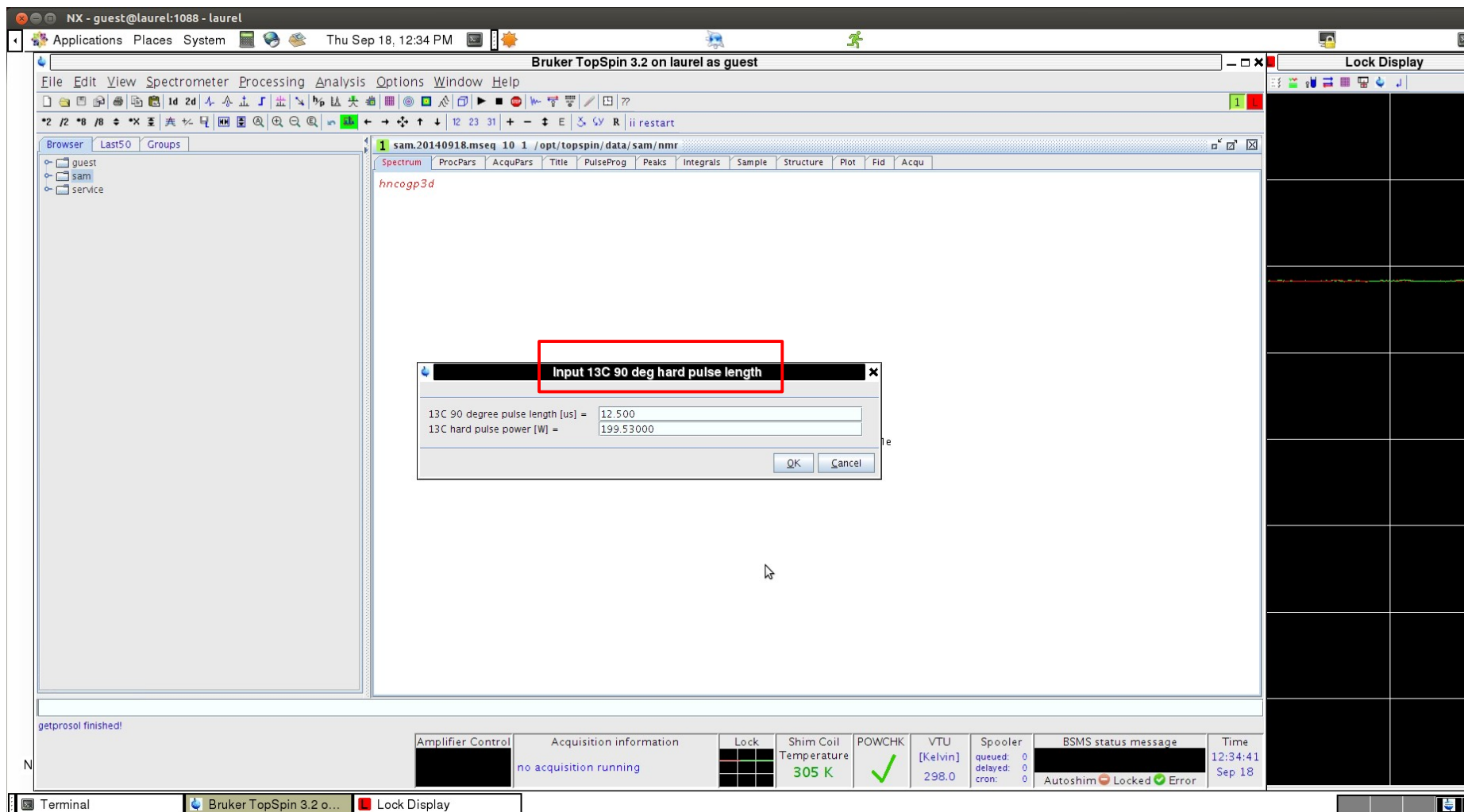
Mseq

Step-by-step



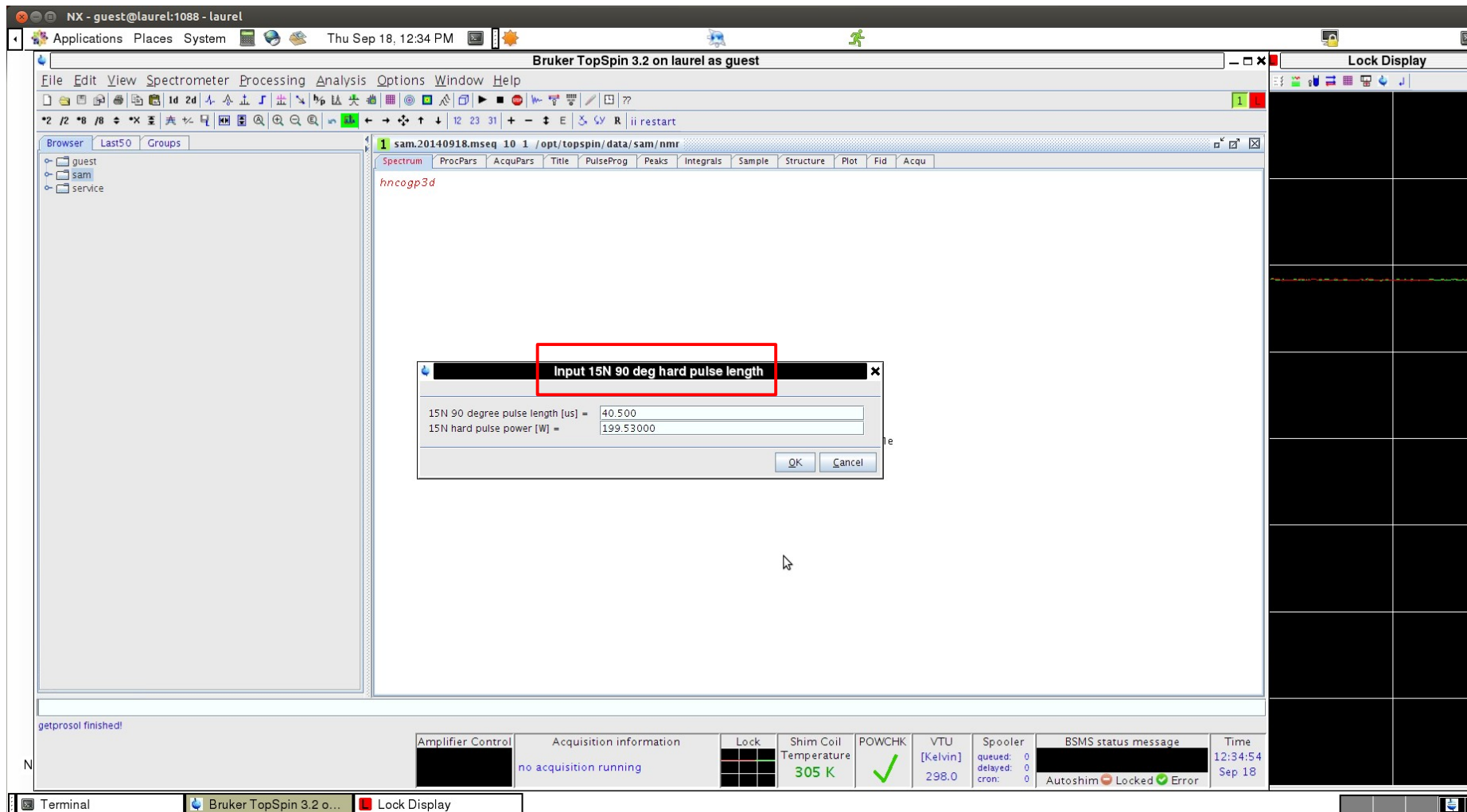
Mseq

Step-by-step



Mseq

Step-by-step



Mseq

Step-by-step

The screenshot displays the Bruker TopSpin 3.2 software interface. The main window shows the configuration for the Mseq pulse program. A red box highlights the 'Input Parameters' and 'Instructions' sections.

Input Parameters:

- > 1H offset O1
- > 13C offset O2P (middle of carbonyl region, 40.0 ppm)
- > 15N offset O3P (middle of amide region, 117.0 ppm)
- > 1H pi/2 pulse length (p1) at 20.0 W
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Comments:

- > make sure that TD1 < TD1MAX and at the same TD1 has to be an even number!
- > make sure that TD2 < TD2MAX and at the same TD2 has to be an even number!

Below the red box, it states: "No raw data available" and "No processed data available".

The bottom status bar shows various system parameters:

Amplifier Control	Acquisition information	Lock	Shim Coil Temperature	POWCHK	VTU [Kelvin]	Spooler	BSMS status message	Time
	no acquisition running		305 K	✓	298.0	queued: 0 delayed: 0 cron: 0	Autoshim Locked Error	12:35:20 Sep 18

Mseq

Step-by-step

The screenshot displays the Bruker TopSpin 3.2 software interface on a Linux system. The main window shows the configuration for the 'Mseq' pulse program. The left sidebar contains a file browser with folders 'guest', 'sam', and 'service'. The main panel displays the following configuration details:

- File:** sam.20140918.mseq 10 1 /opt/topspin/data/sam/nmr
- PP:** M.CBCACONH.wgfb
- Input Parameters:**
 - > 1H offset O1
 - > 13C offset O2P (middle of carbonyl region, 40.0 ppm)
 - > 15N offset O3P (middle of amide region, 117.0 ppm)
 - > 1H pi/2 pulse length (p1) at 20.0 W
 - > 13C pi/2 pulse length (p3) at 199.5 W
 - > 15N pi/2 pulse length (p21) at 199.5 W
- Instructions:**
 - optimize the solvent suppression in "gs" mode, using SPd821 (PHCOR21), SPd822 (PHCOR22), SPd823 (PHCOR23)
- Comments:**
 - > make sure that TD1 < TD1MAX and at the same TD1 has to be an even number!
 - > make sure that TD2 < TD2MAX and at the same TD2 has to be an even number!

Below the main panel, a status bar indicates 'No raw data available' and 'No processed data available'. At the bottom, a control panel shows various system parameters:

Amplifier Control	Acquisition information	Lock	Shim Coil Temperature	POWCHK	VTU [Kelvin]	Spooler	BSMS status message	Time
	no acquisition running		305 K	✓	298.0	queued: 0 delayed: 0 cron: 0	Autoshim Locked Error	12:36:28 Sep 18

A red circle highlights the 'zg' button in the bottom left corner of the interface.

Challenges...

User

- Finding correct pulse sequence
 - redundant pulse sequences with similar names
 - not sufficiently commented
 - out-dated syntax
- Relevant input parameters?
 - Shape? Delays? Offsets? Water Suppression? Incrementation?
 - Routing?
- Processing Parameters
 - Correct phases? Forward-prediction? Back-prediction?

Mlist

Python
Autocalc in PP

Python

NMR Facility

- Implementation of pulse sequences
 - Relying on tested release sequences
 - Specialized, “un-released” sequences?
 - Further optimizations?
- Providing working datasets with correct processing for every sequence
 - “rpar”
 - Making “rpar” more dynamic?
- Adapting datasets to hardware changes?
 - e.g. change of re-routing
- Maintaining pulse sequence library on several spectrometers in large NMR centers?
 - Time-consuming
 - More efficient?

Optimized sequences
will be provided
for G-NMR users

Only ONE parameter
set has to be created

Adapting of this
ONE parameter set

“rsync”

Outlook

- Further optimization of sequences
 - improvement of water suppression
 - using adequate shapes and bandwidths
 - optimal control pulses
 - implement auto-calc functionality
- Simplification of setup of relaxation experiments
 - automatic creation of delay and power lists
 - automatic peak integration?
- Version control software “git”
 - accessible to G-NMR users
 - easily distributable
 - transparent tracking of changes

Tasks from last meeting

(15.01.2014, Garching, TUM):

- Improving pulse sequences
- Platform for distribution?
- Discussion forum for pulse sequences?

Online Pulse Sequence Library for (Specialized) Sequences

G-NMR Pulse Sequence Library - Chromium

G-NMR Pulse Sequence x

wiki.g-nmr.de/pp/

G-NMR

Solution-State Solid-State

Pulse Sequences: Protein

Experiment	Explanation	Reference	Download	Contact(s)
CDCA(NCO)CAHA	E/AE, $2\times^{13}\text{C}$ CT periods with Ca/Cd and Ca selective pulses; for assignment of proline stretches	Bottomley MJ, Macias MJ, Liu Z, Sattler M J Biomol NMR, 13:381-385 (1999) [Link]	PP Download	sattler[at]helmholtz-muenchen[dot]de
TROSY-HA[HB,HN](CACO)NH	TROSY version of an experiment for simultaneous measurement of $3J(\text{Ha,Hb})$ and $3J(\text{HN,Ha})$ coupling constants; requires $^{13}\text{C}/^{15}\text{N}$ -labeled protein in H_2O solution	Lohr F, Schmidt JM, Rüterjans H JACS, 121:11821-11826 (1999) [Link]	PP Download	murph[at]hpc[dot]uni-frankfurt[dot]de

Pulse Sequences: RNA

Experiment	Explanation	Reference	Download	Contact(s)
(lr) HNN-COSY	J(N-N) correlation in isotope-labeled RNA	Dallmann A, Simon B, Duszczek MM, Kooshapur H, Pardi A, Bermel W, Sattler M Angew Chem Int Ed Engl, 52:10487-10490 (2013) [Link]	PP Download	sattler[at]helmholtz-muenchen[dot]de
Py H(CC)NN-COSY	J(N-N) correlation in isotope-labeled RNA	Dallmann A, Simon B, Duszczek MM, Kooshapur H, Pardi A, Bermel W, Sattler M Angew Chem Int Ed Engl, 52:10487-10490 (2013) [Link]	PP Download	sattler[at]helmholtz-muenchen[dot]de
Adenine HCCH-COSY	Adenine HCCH-COSY	Simon B, Zanier K, Sattler M J Biomol NMR, 20:173-176 (2001) [Link]	PP Download	sattler[at]helmholtz-muenchen[dot]de

Miscellaneous

Name	Explanation	Reference	Download	Contact(s)
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Contributions:
Frankfurt ($\Sigma = 2$)
TUM ($\Sigma = 5$)
...hoping for further contributions...

Pulse Sequence Library Wiki

Category:Pulse Sequence Library - G-NMR - Chromium

Category:Pulse Sequen x

wiki.g-nmr.de/index.php/Category:Pulse_Sequence_Library

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Category:Pulse Sequence Library

This category currently contains no pages or media.

This page was last modified on 25 September 2014, at 16:35.

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Navigation

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- Lehrkonzepte
- NMR(solution)
- NMR(solid)
- Industriekontakte
- Pulse Sequence Library

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Acknowledgement

- Michael Sattler (TU Munich)
- Wolfgang Bermel (Bruker BioSpin, Karlsruhe)
- Bernhard Brutscher (IBS Grenoble)

Thanks for your attention!