

UKMRM June 2025 Tips & Tricks

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University of Liverpool



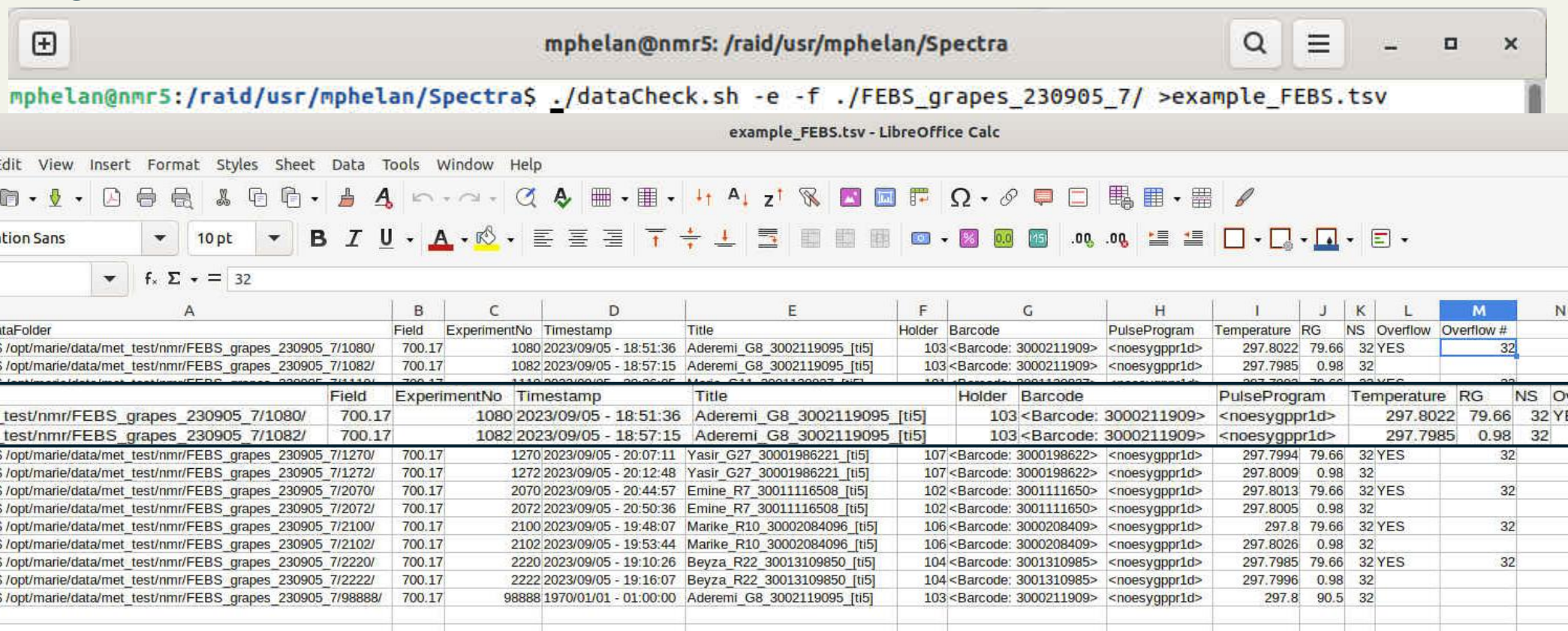
Tips & tricks
Resources

<https://sites.google.com/view/ukmrm2025ttresources/home>

- Cataloguing experiments - simple shell script
 - Pulse sequence libraries - Grenoble & Bruker Users
 - Simulated spectra - from mol file to (somewhat) useful peak predictions
 - Reference databases - 1D 2D experimental datasets
 - NMRbox - virtual machine for NMR software
 - Teaching theory to biologists - reson8 NMR week approach
 - Favourite au programs - Bruker automations
 - Practical things - recycling caps, multi-tube washing, helium recapture
-
- **Most Importantly all this acquired knowledge is thanks to the openness and expertise of the NMR community!**

Cataloguing experiments

- Simple shell script for scraping experiments
 - Caveats – works for linux (probably mac too) looking for info per dataset (so lots of experiments in one file)
- Usage



The screenshot shows a terminal window with the command `./dataCheck.sh -e -f ./FEBS_grapes_230905_7/ >example_FEBS.tsv` being executed. Below the terminal is a LibreOffice Calc spreadsheet titled `example_FEBS.tsv - LibreOffice Calc`. The spreadsheet contains a table with 14 columns: A, B, C, D, E, F, G, H, I, J, K, L, M, N. The data is organized into rows, with the first row being a header and subsequent rows containing experimental data. The table is as follows:

	A	B	C	D	E	F	G	H	I	J	K	L	M	N
1	dataFolder	Field	ExperimentNo	Timestamp	Title	Holder	Barcode	PulseProgram	Temperature	RG	NS	Overflow	Overflow #	
2	\$\$ /opt/marie/data/met_test/nmr/FEBS_grapes_230905_7/1080/	700.17	1080	2023/09/05 - 18:51:36	Aderemi_G8_3002119095 [ti5]	103	<Barcode: 3000211909>	<noesygppr1d>	297.8022	79.66	32	YES	32	
3	\$\$ /opt/marie/data/met_test/nmr/FEBS_grapes_230905_7/1082/	700.17	1082	2023/09/05 - 18:57:15	Aderemi_G8_3002119095 [ti5]	103	<Barcode: 3000211909>	<noesygppr1d>	297.7985	0.98	32			
4	\$\$ /opt/marie/data/met_test/nmr/FEBS_grapes_230905_7/1270/	700.17	1270	2023/09/05 - 20:07:11	Yasir_G27_30001986221 [ti5]	107	<Barcode: 3000198622>	<noesygppr1d>	297.7994	79.66	32	YES	32	
5	\$\$ /opt/marie/data/met_test/nmr/FEBS_grapes_230905_7/1272/	700.17	1272	2023/09/05 - 20:12:48	Yasir_G27_30001986221 [ti5]	107	<Barcode: 3000198622>	<noesygppr1d>	297.8009	0.98	32			
6	\$\$ /opt/marie/data/met_test/nmr/FEBS_grapes_230905_7/2070/	700.17	2070	2023/09/05 - 20:44:57	Emine_R7_30011116508 [ti5]	102	<Barcode: 3001111650>	<noesygppr1d>	297.8013	79.66	32	YES	32	
7	\$\$ /opt/marie/data/met_test/nmr/FEBS_grapes_230905_7/2072/	700.17	2072	2023/09/05 - 20:50:36	Emine_R7_30011116508 [ti5]	102	<Barcode: 3001111650>	<noesygppr1d>	297.8005	0.98	32			
8	\$\$ /opt/marie/data/met_test/nmr/FEBS_grapes_230905_7/2100/	700.17	2100	2023/09/05 - 19:48:07	Marika_R10_30002084096 [ti5]	106	<Barcode: 3000208409>	<noesygppr1d>	297.8	79.66	32	YES	32	
9	\$\$ /opt/marie/data/met_test/nmr/FEBS_grapes_230905_7/2102/	700.17	2102	2023/09/05 - 19:53:44	Marika_R10_30002084096 [ti5]	106	<Barcode: 3000208409>	<noesygppr1d>	297.8026	0.98	32			
10	\$\$ /opt/marie/data/met_test/nmr/FEBS_grapes_230905_7/2220/	700.17	2220	2023/09/05 - 19:10:26	Beyza_R22_30013109850 [ti5]	104	<Barcode: 3001310985>	<noesygppr1d>	297.7985	79.66	32	YES	32	
11	\$\$ /opt/marie/data/met_test/nmr/FEBS_grapes_230905_7/2222/	700.17	2222	2023/09/05 - 19:16:07	Beyza_R22_30013109850 [ti5]	104	<Barcode: 3001310985>	<noesygppr1d>	297.7996	0.98	32			
12	\$\$ /opt/marie/data/met_test/nmr/FEBS_grapes_230905_7/98888/	700.17	98888	1970/01/01 - 01:00:00	Aderemi_G8_3002119095 [ti5]	103	<Barcode: 3000211909>	<noesygppr1d>	297.8	90.5	32			
13														
14														
15														
16														
17														
18														

- Github: <https://github.com/LivUniNMR/NMRdataManagement> (Rudi Grosman)

Pulse Sequence libraries and Optimisations (1)

IBS Grenoble Protein/RNA suite



- <https://www.ibs.fr/en/communication-outreach/scientific-output/software/>
- Fully documented

SOFTWARE

Several software developed by the IBS are available to the international scientific community. Click on the name of the software you are interested in to get information about downloading and copyrights.

Last update 8 November 2022

Software Name	Date	Category	Description
Landmark patterns	18 March 2009	Software	
Non linear Fourier transform of NMR data acquired on a non-cartesian sampling grid	18 March 2009	Software	
SculptorCNS	18 March 2009	Software	Structure Calculation Using Long-range, Paramagnetic, Tensorial and Orientational Restraints
eeFit	4 December 2018	Software	A Microsoft Excel-embedded program for interactive analysis and fitting of experimental dose-response data
Flexible-meccano	10 April 2012	Software	
Module	17 March 2011	Software	Module Version 1.0
Module 2	17 March 2011	Software	Residual dipolar coupling and residual chemical shift analysis software
NMRlib 2.0: IBS pulse sequence tools for Bruker spectrometers	8 November 2022	Software	NMR experiment and processing tool catalog for liquids Presentation A detailed description of the general philosophy of NMRlib and its implementation for solution-state NMR can be found here; (...)
Tensor	17 March 2011	Software	Program for treating solution state ¹⁵ N relaxation for the study of molecular dynamics

- Works on linux
- Free to academia
- Works on Ts3.5 and above (some probe compatibility checks required for Ts4 but fully documented)

Pulse Sequence libraries and Optimisations (1)

IBS Grenoble Protein/RNA suite



- Some useful scripts for optimising pulse lengths / variables per protein / macromolecule

- Quality Control

- Example experiments

15N TRACT 1D

Estimation of tumbling

Sel 1H DOSY

1H region selected with
selective pulse, e.g. methyls

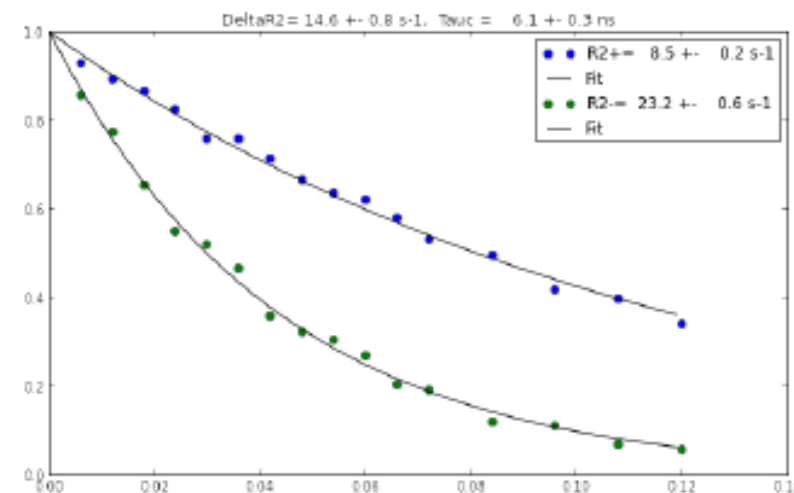
13C 1H DOSY

13C filter for methyl 1H

1 Ubiquitin

```
1 libLoc = '/hosts/ibs1380/nmrdata/nmr-lib/'
2 filename1 = '/hosts/ibs700/ibslrmn/afavier/nmr/2019-02-04_ubi-543/15/pdata/1'
3 filename2 = '/hosts/ibs700/ibslrmn/afavier/nmr/2019-02-04_ubi-543/16/pdata/1'
4 vclist_file_n1 = '/hosts/ibs700/ibslrmn/afavier/nmr/2019-02-04_ubi-543/15/vclist'
5 vclist_file_n2 = '/hosts/ibs700/ibslrmn/afavier/nmr/2019-02-04_ubi-543/16/vclist'
6 d21 = 0.003
7 min_val = 9.5
8 max_val = 8.6
9
```

```
1 tractAna(filename1, filename2, vclist_file_n1, vclist_file_n2, d21, min_val, max_val)
```



Analysis tool provided

- Python (modular if you wish)
- Authors: Vallet, A., Favier, A., Brutscher, B., and Schanda, P <https://doi.org/10.5194/mr-1-331-2020>

- Some useful scripts for optimising pulse lengths / variables per protein / macromolecule

- Example experiments
 - Optimisations through popt
 - Fits and calibrations saved

15N-filt 1H DOSY

15N filter for amide 1H

1D HETSOFAST

Global structural compactness

2D HETSOFAST

Local structural compactness

- Python (modular if you wish)
- Authors: Vallet, A., Favier, A., Brutscher, B., and Schanda, P <https://doi.org/10.5194/mr-1-331-2020>

2 Ubiquitin

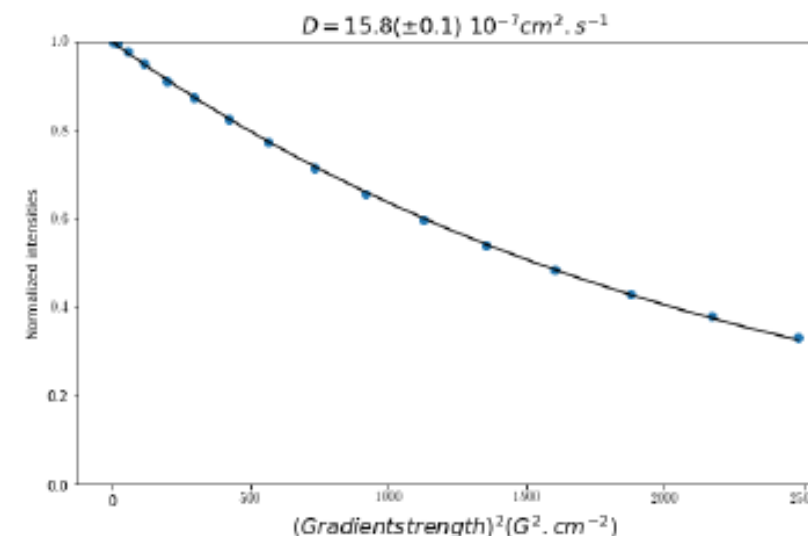
```
1 libLoc = '/hosts/ibs1300/nmrdata/nmr/lib/'
2 filename1 = '/hosts/950neo/ibslrmn/afavier/nmr/2019-12-11_S21-LSFubi/2/pdata/1'
3 difflist_file = '/hosts/950neo/ibslrmn/afavier/nmr/2019-12-11_S21-LSFubi/2/difflist'
4 min_val = 2
5 max_val = -1.0
```

```
1 dosyAna(libLoc, filename1, difflist_file, min_val, max_val)
```

Max: 10581648.267089844

Diffusion fitting values saved in: /hosts/950neo/ibslrmn/afavier/nmr/2019-12-11_S21-LSFubi/2/pdata/1/DOSY.fit

Normalized intensities saved in: /hosts/950neo/ibslrmn/afavier/nmr/2019-12-11_S21-LSFubi/2/pdata/1/DOSY.int



Pulse Sequence libraries and Optimisations (1)

IBS Grenoble Protein/RNA suite



NMRLib

PROTEINS Protein experiment library

RNA RNA experiment library (under construction)

Select your probe for NEOs only, automatic for AVIII

My library put you own experiments here !

Macros Acquisition, display and processing tools

Set pulse lengths Set 90deg pulse widths

Wavemaker Execute wavemaker

Spectro tests LSF test experiments

Library tools Delete or export experiments

Set the path to a python executable including numpy and matplotlib modules.

If you use the host computer OS native python:
set /bin/python

For sbgrid users:
set /programs/i386-linux/python/2.7/bin/python

To change this path later on, edit the following file:
/home/mphelan/topspin1/pythonPath.txt

NMRLib Proteins

SPECTROMETER SETUP Tools for automatic locking, tuning, shimming ...

CALIBRATION TOOLS 1H, 13C and 15N pulse length calibration

SAMPLE QUALITY CONTROL NMR experiments for sample check

PROTON 1D/2D NMR Basic 1D and 2D 1H NMR

HETERO 1Ds 13C, 19F

HETERO 2D NMR 2D 1H-13C (aliphatics, aromatics, methyls), 1H-15N (amides)

BACKBONE ASSIGN 3D HCN and HNN triple-res experiments

ALIPHATIC SC ASSIGN 3D TOCSY HCCH and HCCCONH

AROMATIC SC ASSIGN Aromatic 2D 1H-13C and 1H-15N experiments

13C/15N EDITED NOESY 3D edited NOESY experiments

DIPOLAR COUPLINGS Experiments for up to 6 backbone couplings

H-BONDING trans-H-bond HNCO correlation expts

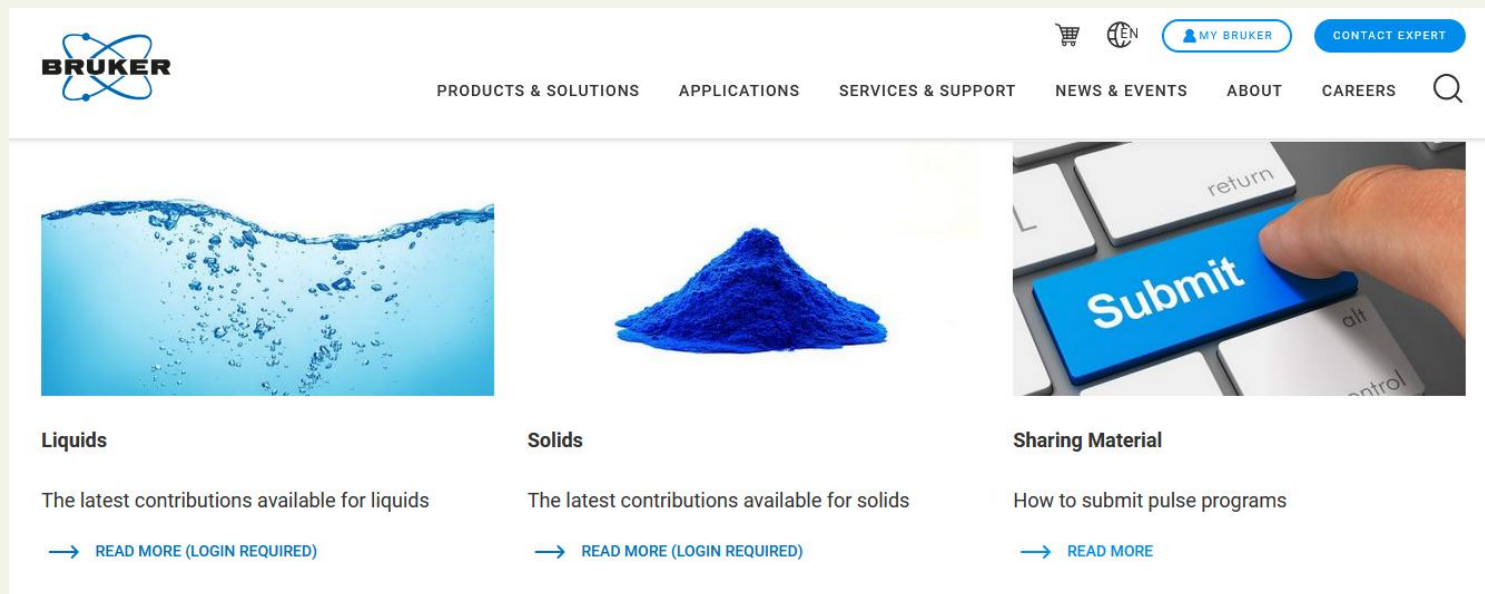
SPIN RELAXATION 15N and 13C spin relaxation experiments

KINETICS SOFAST, CPMG

<https://www.bruker.com/protected/en/services/bruker-user-library/liquids.html>

- Suitability for consoles and topspin versions indicated
- With example data
- Links to publication
- Ordered into Biomolecules and Small molecules
- Search on name or author
 - Zipped repositories so subdirectories not visible
 - Caveat: I have only used this for DREAMTIME so other datasets may be less complete

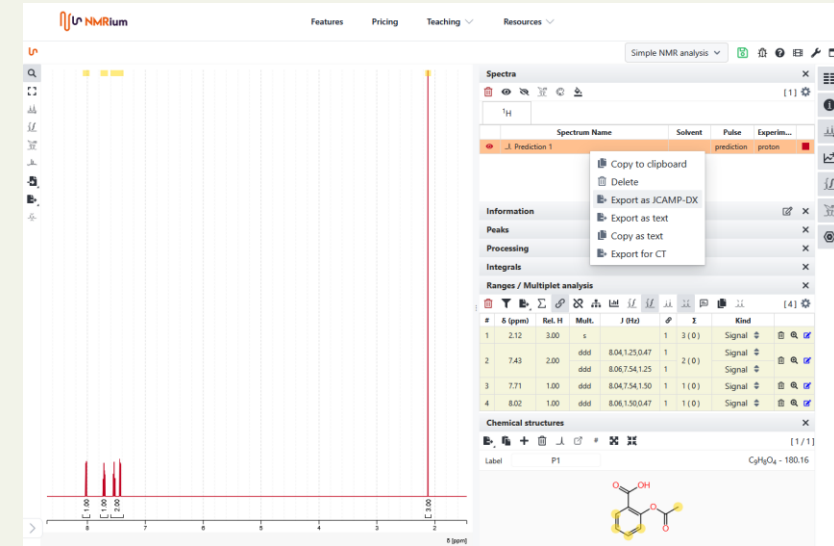


The screenshot displays the Bruker User Library website. The header features the Bruker logo, navigation links (PRODUCTS & SOLUTIONS, APPLICATIONS, SERVICES & SUPPORT, NEWS & EVENTS, ABOUT, CAREERS), and user options (MY BRUKER, CONTACT EXPERT). The main content area is divided into three columns:

- Liquids**: Accompanied by an image of water splashing. Text: "The latest contributions available for liquids". Link: "→ READ MORE (LOGIN REQUIRED)".
- Solids**: Accompanied by an image of a blue powder pile. Text: "The latest contributions available for solids". Link: "→ READ MORE (LOGIN REQUIRED)".
- Sharing Material**: Accompanied by an image of a hand pressing a "Submit" button on a keyboard. Text: "How to submit pulse programs". Link: "→ READ MORE".

Simulated Data

- Nmrium.org
Online
Overlay experimental data
Export jdx tsv etc.



- Gissmo
 - from mol file to (somewhat) useful peak predictions

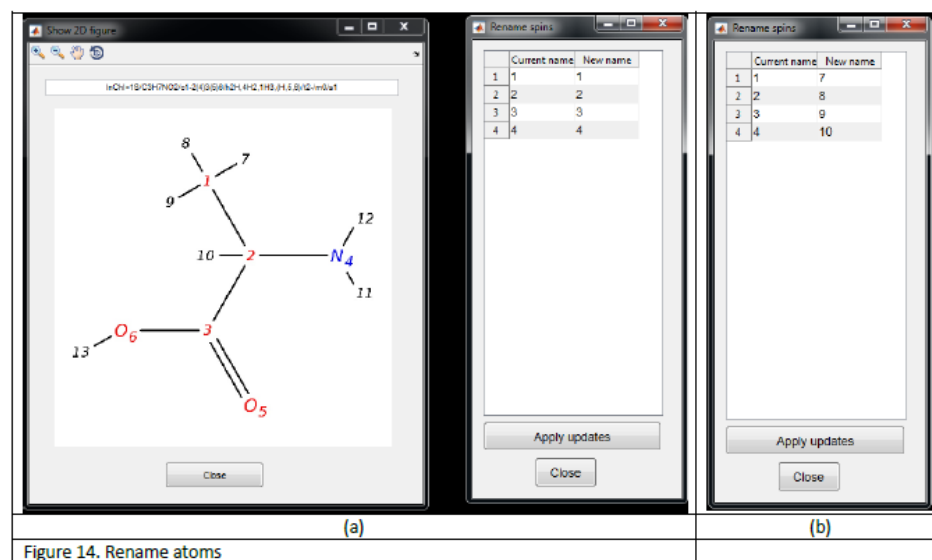


Figure 14. Rename atoms

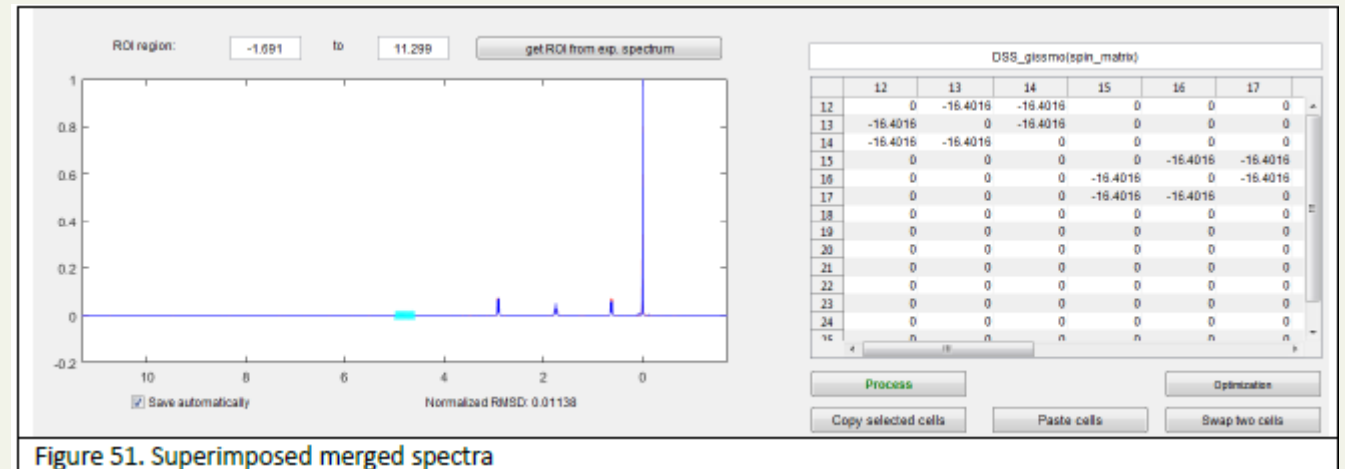


Figure 51. Superimposed merged spectra

- Helpful for teaching and mixture analysis / annotation

Reference Databases (metabolites / natural products)

- Reference databases:
 - Chemspider** can view spectra but not download?
 - BMRB 1D & 2D data available for download
 - HMDB 1D data available for download
 - BML data available for download (registration required)
 - MetaboLights
 - CASMDB / CCPN

ChemSpider
Search and share chemistry

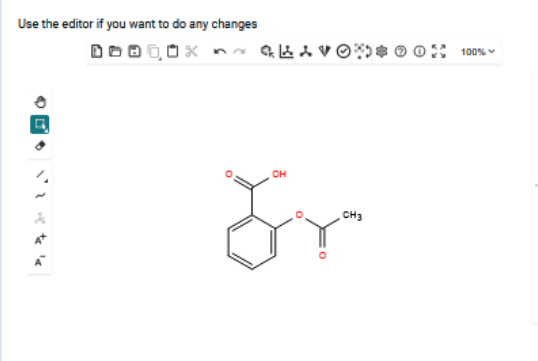
Simple Structure Advanced

Structure search

How would you like to create your search?
Draw or select one of these options

☐ Convert a name into a structure
☐ Load a structure file

Use the editor if you want to do any changes



Exact match
☐ Same skeleton
☐ Substructure Coming soon
☐ Similarity Coming soon

Filter

Clear Search

Search results

Found 1 result

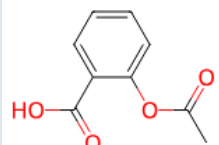
Synonym	Structure	Mol formula	Average Mass	# of Data Sources
Aspirin		C ₉ H ₈ O ₄	180.159	109

ChemSpider
Search and share chemistry

Simple Structure Advanced

Found 1 result
(Found by Structure search Exact Match)

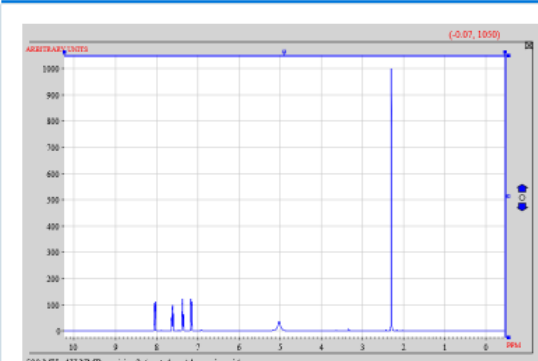
Aspirin



Molecular formula: C₉H₈O₄
Average mass: 180.159
Monoisotopic mass: 180.042259
ChemSpider ID: 2157

Download .mol
Cite this record

Structural identifiers

Names	Properties	Spectra	Vendors	More
¹H NMR				
				
HNMR spectrum of Aspirin				
Close spectrum Associated hyperlink				

Reference Databases (metabolites / natural products)

- Reference databases:

- Chemspider can view spectra but not download?
- BMRB** 1D & 2D data available for download
- HMDB 1D data available for download
- BML data available for download (registration required)
- MetaboLights

The screenshot displays the BMRB (Biological Magnetic Resonance Data Bank) website. The top navigation bar includes links for BMRB, ABOUT, DEPOSIT, SEARCH, VISUALIZE, ANALYZE, DATA, and LEARN. Below this is the BMRB logo and a search bar with the placeholder text 'Searches all entries'. A central grid of icons provides quick access to various features: CONTACT US, DATA ARCHIVES, ENTRIES, CORONAVIRUS, SHIFTS, BMRB Small Molecules (highlighted), DEPOSIT, LITERATURE CITATIONS, NEW RELEASES, PDB LINKS, SMALL MOLECULES, GROWTH, and GEOGRAPHIC DISTRIBUTION. To the right, a 'Search BMRB Metabolomics' section offers a 'General search' with a dropdown menu set to 'Synonym' and a search input field. It also includes options for 'Experimental entries' (selected) and 'Theoretical entries', a 'Select the top 10 matches' option, and a file upload section for batch files. Below these are sections for 'Search by mass', 'Search by structure', 'Search 1D peak lists', 'Search 2D HSQC lists', and 'Solvent and field strength'. A 'Help' link is also present. On the far right, a sidebar lists 'Metabolomics data hosted at BMRB' with links to various datasets and 'Other Metabolomics resources at BMRB' including NMR peaks query, molecular mass calculator, and formula/molecule by mass.

- CASMDB / CCPN bmrbl.io/metabolomics/ Hoch 2023 doi.org/10.1093/nar/gkac1050

2716 Entries

Reference Databases (metabolites / natural products)

- Reference databases:

- Chemspider can view spectra but not download?
- BMRB 1D & 2D data available for download
- HMDB 1D data available for download**
- BML data available for download (registration required)
- MetaboLights

HMDB

Browse Search Downloads About Contact Us

Wishart Node TMIC

Specializing in ready to use metabolomics kits.

Browsing metabolites

Filter by metabolite status (default all):

☐ Detected and quantified ☐ Detected but not quantified ☐ Predicted

Filter by biospecimen:

☐ Blood ☐ Urine ☐ Saliva ☐ Cerebrospinal Fluid ☐ Feces ☐ Sweat ☐ Breast Milk ☐ Bile ☐ Amniotic Fluid ☐ Other Biospecimens

Filter by origin:

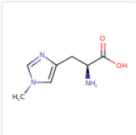
☐ Exogenous ☐ Endogenous ☐ Food ☐ Plant ☐ Microbial ☐ Toxin/Pollutant ☐ Cosmetic ☐ Drug ☐ Drug Metabolite

Filter by cellular location:

☐ Cell Membrane ☐ Cytoplasm ☐ Nucleus ☐ Mitochondria

Displaying metabolites 1 - 25 of 248137 in total

Export

HMDB ID	CAS Number	Name	Structure	Formula	Average Mass	Monoisotopic Mass	Biospecimen Location
HMDB0000001	332-80-9	1-Methylhistidine		C ₇ H ₁₁ N ₃ O ₂	169.1811	169.085126611	Blood Cerebrospinal Fluid (CSF) Feces Urine

- CASMDB / CCPN

hmdb.ca/metabolites

Wishart 2022 DOI:10.1093/nar/gkab1062

220945 Entries

Reference Databases (metabolites / natural products)

- Reference databases:
 - Chemspider can view spectra but not download?
 - BMRB 1D & 2D data available for download
 - HMDB 1D data available for download
 - BML-NMR 1D & JRES data available for download (registration required)**
 - MetaboLights

WWW.BML-NMR.ORG

User: [Click to enter your username](#) Password: [Login](#)

Metabolite Library

- Search Library
- Forgotten Your Password?
- Register
- Contact Us

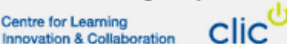
Search The Library By Chemical Name

To search the library, first select your desired experimental conditions using the checkboxes below (minimum of 1 per category). Next, enter a few letters from the chemical's name in the search field, make a selection from the list that appears and push search.

Experiment	Water Suppression	Post-buffer pH	Excitation Angle	Pre-acquisition Delay
☐ 1D ¹ H	☒ Excitation Sculpting	☐ 6.6	☒ 30 Degrees	☒ 1 Second
☒ 2D ¹ H J-resolved	☐ NOESY-Prsat	☒ 7.0	☒ 60 Degrees	☒ 3 Seconds
		☐ 7.4	☒ 90 Degrees	☒ 4 Seconds
				☒ 10 Seconds
				☐ Other

Chemical name contains:

Library Records For Current Selection		
Analysis ID	Chemical Common Name	Experiment Summary

Site designed by:  Project funded by: 

Reference Databases (metabolites / natural products)

- Reference databases:
 - Chemspider can view spectra but not download?
 - BMRB 1D & 2D data available for download
 - HMDB 1D data available for download
 - BML 1D & 2D data available for download (registration required)
 - MetaboLights**

The image displays the MetaboLights website interface. The top header features the MetaboLights logo and a search bar with the text "Examples: Alanine, Homo sapiens, Urine, MTBLS1". Below the header is a navigation menu with links: Home, Browse Studies, Browse Compounds, Browse Species, Download, Help, Give us feedback, About, Submit Study, and Login.

The main content area shows search results for "alpha-D-glucosyl-(1->4)-alpha-D-mannose". It indicates 407 results, showing 1 to 10. The first result is displayed with a "Currently No Image" placeholder. To the right of the placeholder, the compound accession is listed as MTBLC47937, and the CHEBI ID is CHEBI:47937.

The second result is for "(2-aminoethyl)phosphonic acid". It shows a chemical structure diagram of the compound. To the right of the structure, the compound accession is listed as MTBLC15573, and the CHEBI ID is CHEBI:15573. Below the CHEBI ID, it states "Identified in Homo sapiens, Mus musculus".

Biological Study datasets:

1539

MS : 1379

NMR : 177

Compound library:

33253 entries

407 NMR

Reference Databases (metabolites / natural products)

- Reference databases:
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 - BMRB 1D & 2D data available for download
 - HMDB 1D data available for download
 - BML 1D & 2D data available for download (registration required)
 - MetaboLights
 - CASMDB / CCPN

CCPN

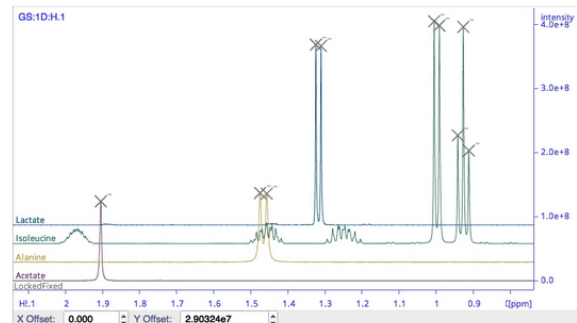
Software ▾

Support ▾

Outreach ▾

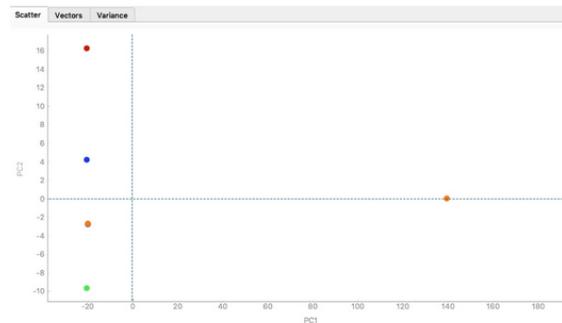
About ▾

AnalysisMetabolomics is designed for the analysis of NMR Metabolomics data. Currently still at the beta-release stage, this part of our program is being actively developed by a PhD student in our group and benefits from our collaborations with academics involved in this field.



Excellent handling of 1D spectra

Load, zoom, pan and peak pick large numbers of 1Ds quickly and easily. Create stacked plots with bespoke X and Y offsets.



Principle Component Analysis

Analyse your results using PCA tools with direct links between graphs and spectra.

Software

Our Approach

Downloads

AnalysisAssign

AnalysisScreen

AnalysisMetabolomics

AnalysisStructure

ChemBuild

NMR Exchange Format

Related Software

Version 2

Licensing

<https://ccpn.ac.uk/software/analysismetabolomics/>

- Virtual machine using VNC viewer (free)
- nmrbox : virtual machine for virtually every nmr software (old, new, and helpful for those with high computational demands)

What is
NMRbox 

NMRbox is a resource for biomolecular NMR (Nuclear Magnetic Resonance) software. It provides tools for finding the software you need, documentation and tutorials for getting the most out of the software, and cloud-based virtual machines for executing the software.

[User benefits](#) | [Developer benefits](#) | [Center overview](#) | [Getting started](#)

- University of Liverpool & ResoN8 training - Getting started:
 - <https://www.youtube.com/playlist?list=PLCfsv-WgdV7KGiPxMGMMjsLAKRnBFQ7F6>

Virtual Machine – NMRbox / NMRhub

- Virtual machine using VNC viewer (free)
- nmrbox : virtual machine for virtually every nmr software (old, new, and helpful for those with high computational demands)
- 274 software packages

nmrglue A module for working with NMR data in Python	NmrLineGuru A graphical user interface (GUI) based user-friendly tool to simulate and fit NMR line shapes with multi-state equilibrium models	NMRmix A Tool for the Optimization of Compound Mixtures in 1D 1H NMR Ligand Affinity Screens
nmrpeaklists A Python library for handling NMR peak lists.	NMRPipe Multidimensional spectral processing and analysis of NMR data	NMRPy A Python module for processing NMR spectra
NMR-scripts A collection of small scripts of various functions	nmrstarlib A Python library that facilitates reading and writing NMR-STAR formatted files used by BMRB for archival of NMR data	NMRViewJ The Application for Visualization and Analysis of Macromolecular NMR Software
nmr_wash Suppression of artifacts in NMR spectra obtained from sparsely sampled data	NUScon Workflow tool for running NUS reconstructions on challenge data in support of NUScon evaluation	nus-tool Utility for generating and analyzing NUS sample schedules
OmegaFold High-resolution de novo structure prediction from primary sequence.	Open Babel A chemical toolbox designed to search, convert, modify, or analyze chemical files	OpenMM A high performance toolkit for molecular simulation
OpenVnmrJ Open source version of Varian's/Agilent's VnmrJ software	OSPREY Suite of programs for computational structure-based protein design	PALES Prediction of sterically induced alignment in a dilute liquid crystalline phase

MotionCor2 Corrects electron beam-induced sample motion	mTM-align Efficient protein structure comparisons	MVAPACK Tools for processing and analyzing chemometric data
MZmine3 User-friendly package for data processing of mass-spectrometry data	NAMD NAMD is computer software for molecular dynamics simulation, written using the Charm++ parallel programming model	NEF-PIPELINES NEF-Pipelines is a set of command line (currently... there maybe a gui later!) tools for manipulating [NEF] or NMR Exchange Format files which can be u
NESSY Analyse NMR relaxation dispersion data of either CPMG or R1p (R1rho) dispersion experiments	NESTA-NMR Fast and accurate reconstruction of NUS data	nightshift Python command line utility and library for plotting simulated 2D and 3D NMR spectra from assigned chemical shifts in the BMRB
NMRDraw NMRDraw is the companion graphical interface for NMRPipe and its processing tools	NMRFAM-SPARKY A graphical NMR assignment and integration program for proteins, nucleic acids, and other polymers	nmrfit Quantitative NMR analysis through least-squares fit of spectroscopy data
NMRfx Analyst Data processing program utilizing Python for scripts and a full Java based GUI	NMRfx Processor Data processing program utilizing Python for scripts and a full Java based GUI	NMRfx Structure Features for structure calculation and chemical shift prediction

MDTraj Read, write and analyze MD trajectories with only a few lines of Python code	MESMER Analyzes the experimentally averaged data obtained from any number of experimental techniques such as SAXS and NMR	MestReNova (Mnova) A top class software suite to process your analytical chemistry data
MetaboAnalystR An R package for comprehensive analysis of metabolomics data	Metabolomics toolbox Metabolomics toolbox	MetScape A bioinformatics framework for the visualization and interpretation of metabolomic and expression profiling data
MGLtools Visualization and analysis of molecular structures.	MINOTAUR Analyzes high-field accurate NMR relaxation rates together with relaxometry intensity decays.	MMMx Matlab package for integrative ensemble modeling of protein structures and complexes
MMTSB Toolset A collection of perl-based utilities and libraries for multiscale protein structure modeling	Modelfree Optimizing "Lipari-Szabo model free" parameters to heteronuclear relaxation data	MODELLER Homology or comparative modeling of protein three-dimensional structures
Module2 Analyzes residual dipolar couplings and residual chemical shifts measured in partially aligned proteins and nucleic acids	mol2sphere Convert a molecule into a set of spheres of variable radii for visualization and modeling	Mollib Program and Python library for the validation, quality analysis and manipulation of molecular structures
MOLMOL Molecular graphics program for displaying, analyzing, and manipulating biological	MolProbity All-atom structure validation for macromolecules	MoSART To provide an easily extensible application for computing biomolecular structure from

The screenshot displays a virtual machine environment with several open applications:

- Terminal (manganese.nmrbox.org):** Shows the command `molmol` and the output of the MOLMOL 2K.2 version information.
- MOLMOL - MOLEcule analysis and MOLEcule display:** The main window showing a 3D molecular model. A 'Property' dialog box is open, listing atoms and their properties.
- GISSMO (Guided Ideographic Spin System Model Optimization):** A window for spin system optimization, showing parameters like 'Num points' and 'Line width'.
- NMR:** A window for NMR analysis and assignments, showing a list of atoms and their properties.

The screenshot displays a virtual machine environment with several windows open:

- NMRbox Software Explorer:** A window titled "manganese.nmrbox.org (manganese:3) - RealVNC Viewer" showing the NMRbox Software interface. It features a search bar, a list of programs (VMD, VMD-XPLOR, Voronota, VTX, Wattos, WHAT IF, XDrawChem, XEASY, Xipp, Xplor-NIH, XSSP, xyza2pipe), and a list of programs to run in the terminal (add2pipe, addazara2pipe, addnv2pipe, adducsf2pipe, addvnmr2pipe, addxeasy2pipe, addxnmr2pipe, addxyza2pipe, azara2pipe, defl2pipe, nv2pipe). The "xyza2pipe" program is selected, and its details are shown below, including its name, synopsis, description, NMRbox web link, developer web link, version (1.0.4), and installed directory (/usr/software/xyza2pipe).
- MestReNova:** A window titled "MestReNova" showing an NMR spectrum plot. The x-axis is labeled "F1 (ppm)" and ranges from 19 to -6. The y-axis is labeled "Intensity" and ranges from -2.0x10^6 to 3.2x10^7. The plot shows a large peak at approximately 7.2 ppm and several smaller peaks between 1 and 4 ppm. The window includes a menu bar (File, Home, View, Molecule, Prediction, Tools, Data Analysis, Processing, Analysis, Assignments, Options) and a toolbar with various analysis tools.
- Terminal:** A window titled "Terminal - mphelan@manganese: ~/Desktop" showing the command prompt "Desktop\$ mnova".
- Web Browser:** A window titled "Web Browser" with the address bar showing "Browse the web".

The screenshot shows a virtual machine environment with the following components:

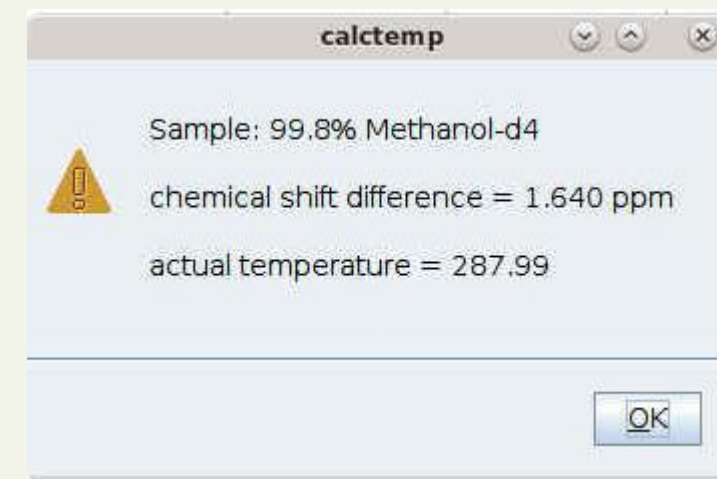
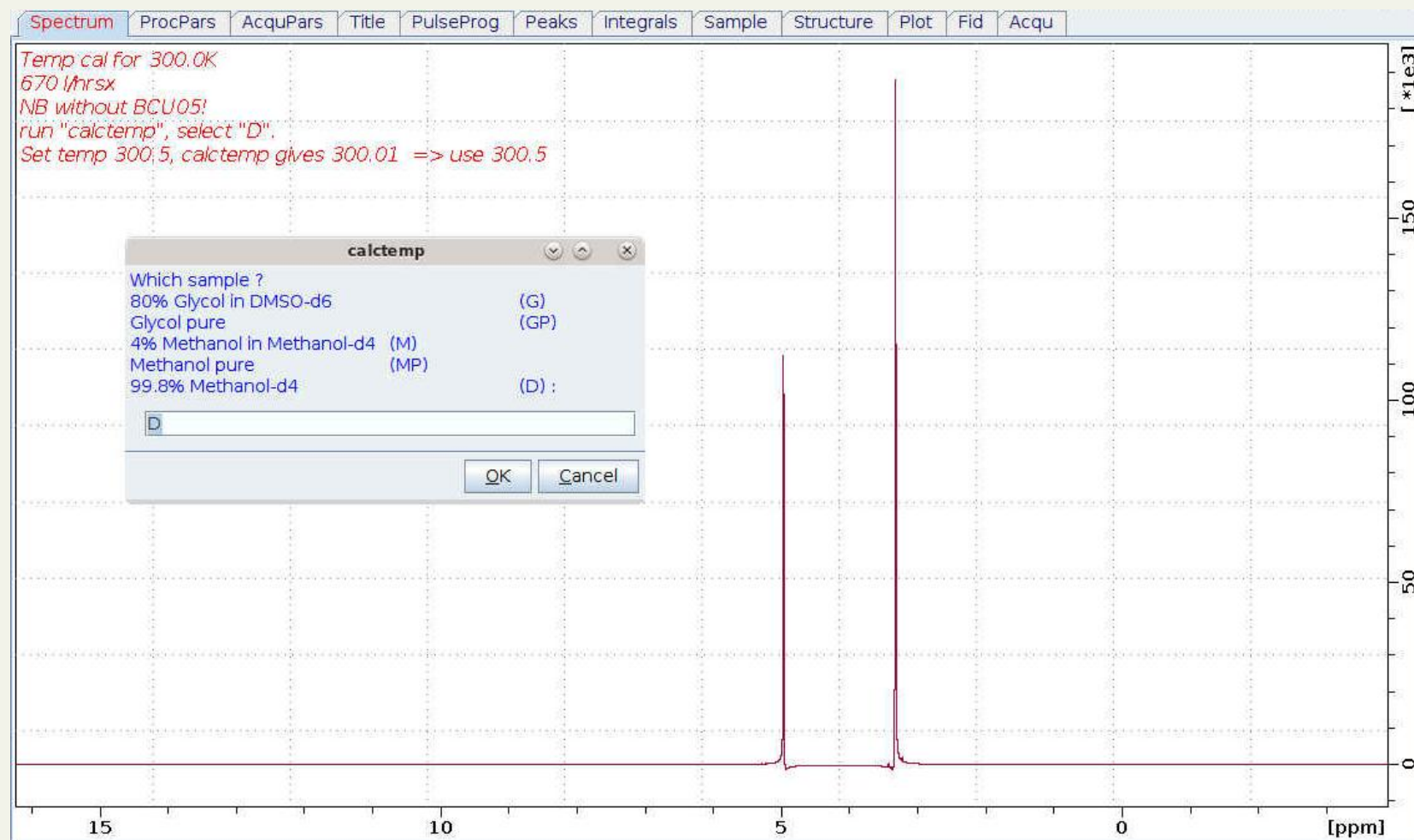
- NMRbox Software Explorer:** A window titled "NMRbox Software Explorer" with the NMRbox logo and the text "It's simple! Let's help you get started." It lists software installed in NMRbox, including ssNake, SSP, STARXML, STRIDE, TALOS+, TALOS-N, tameNMR, Tensor2, TensorView, tiger, TITAN, Topaz, and TnnSnin. A search bar is present. A list of programs to run in the terminal is shown: add2pipe, addazara2pipe, addnv2pipe, adducsf2pipe, addvnmr2pipe, addxeasy2pipe, addxwnmr2pipe, addxyza2pipe, azara2pipe, defl2pipe, and nv2pipe. A button "copy program name to clipboard" is at the bottom.
- Terminal:** A terminal window titled "Terminal - mphelan@manganese: ~/Desktop" showing the command "mnova" being executed.
- PyMOL:** A PyMOL window showing a protein structure (green ribbon) and a list of objects (all, 1LKJ, 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). The PyMOL command line shows "PyMOL>".
- Software Discovery Tool:** A small window at the bottom left showing the NMRbox logo and the text "Software Discovery Tool host: manganese.nmrbox.org version: 2025.19.00".

- Teaching theory to biologists: reson8
 - Reson8 NMR week – annual 2 day residential (Northern 8 universities)
 - **Core NMR Concepts** (spin, nuclei (and their frequency ranges), pulses, coupling)
 - **HSQC** (^1H sensitivity, spin echos, 2D acquisition, energy level, vectors and product operators)
 - **Relaxation** (effect of rel'n on experiments, T1 & T2 manifestations in pulse sequences, typical T1 T2 values for ^1H ^{13}C ^{15}N proteins, T1 & T2 relationship to protein size)
 - **Processing /data analysis** (window functions to improve spectral quality, role of TD, SI, FT and phasing).
 - Local set-up, acquisition, processing practicals

<https://sites.google.com/view/reson8nmr>

- Linux bootcamp
 - Useful commandline operations
 - Local file organisation (including accessing via VLAN local network)
 - Awk, perl and Python basic scripting

- calctemp



Methanol standard
(99.8% MeOD)
Bruker Z10627

- au_lc1d



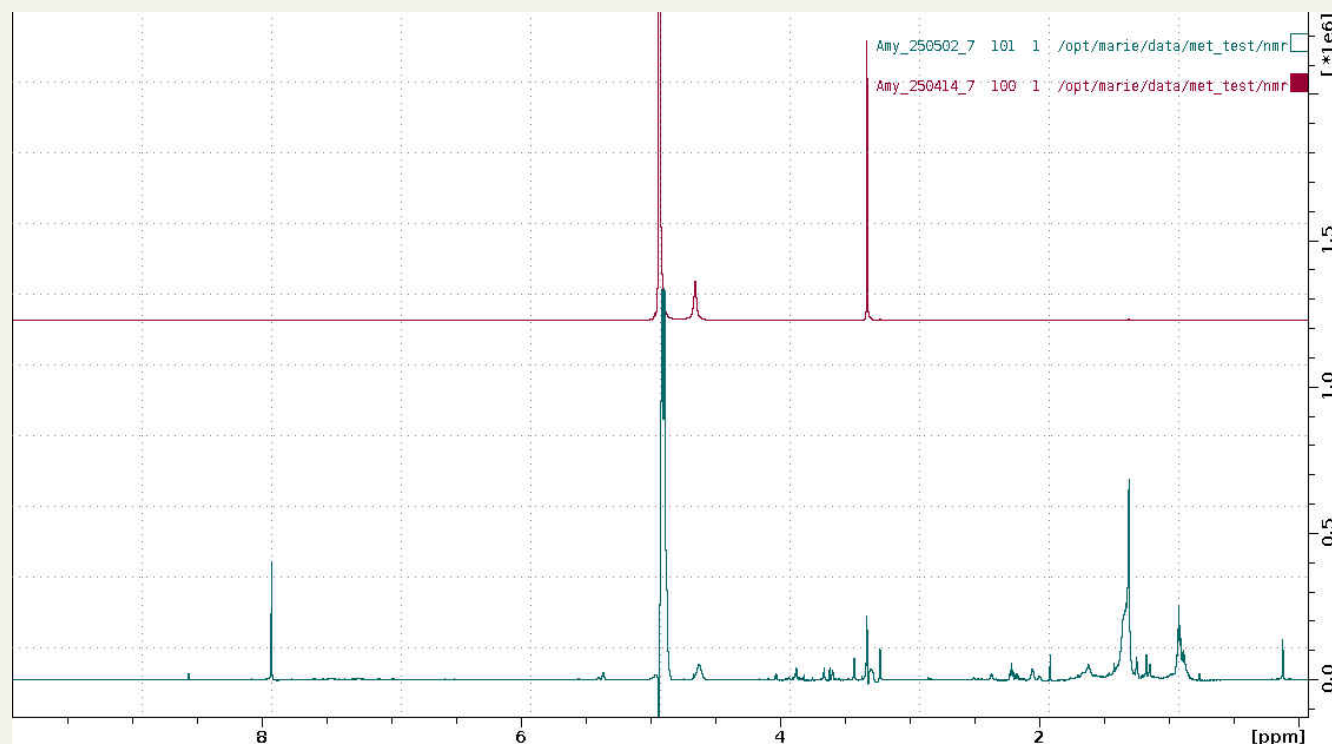
TOPSPIN 3.5 & LC-NMR

Software Manual

Version 140903

LCNMR

Written by
Dr. Ulrich Braumann
ulrich.braumann@bruker-biospin.de



5.6 AU-Program au_lc1d: 1D spectra with solvent suppression

The AU program **au_lc1d** controls the acquisition of 1D spectra with all kinds of solvent suppression techniques. The acquisition can be carried out step wise with signal to noise control.

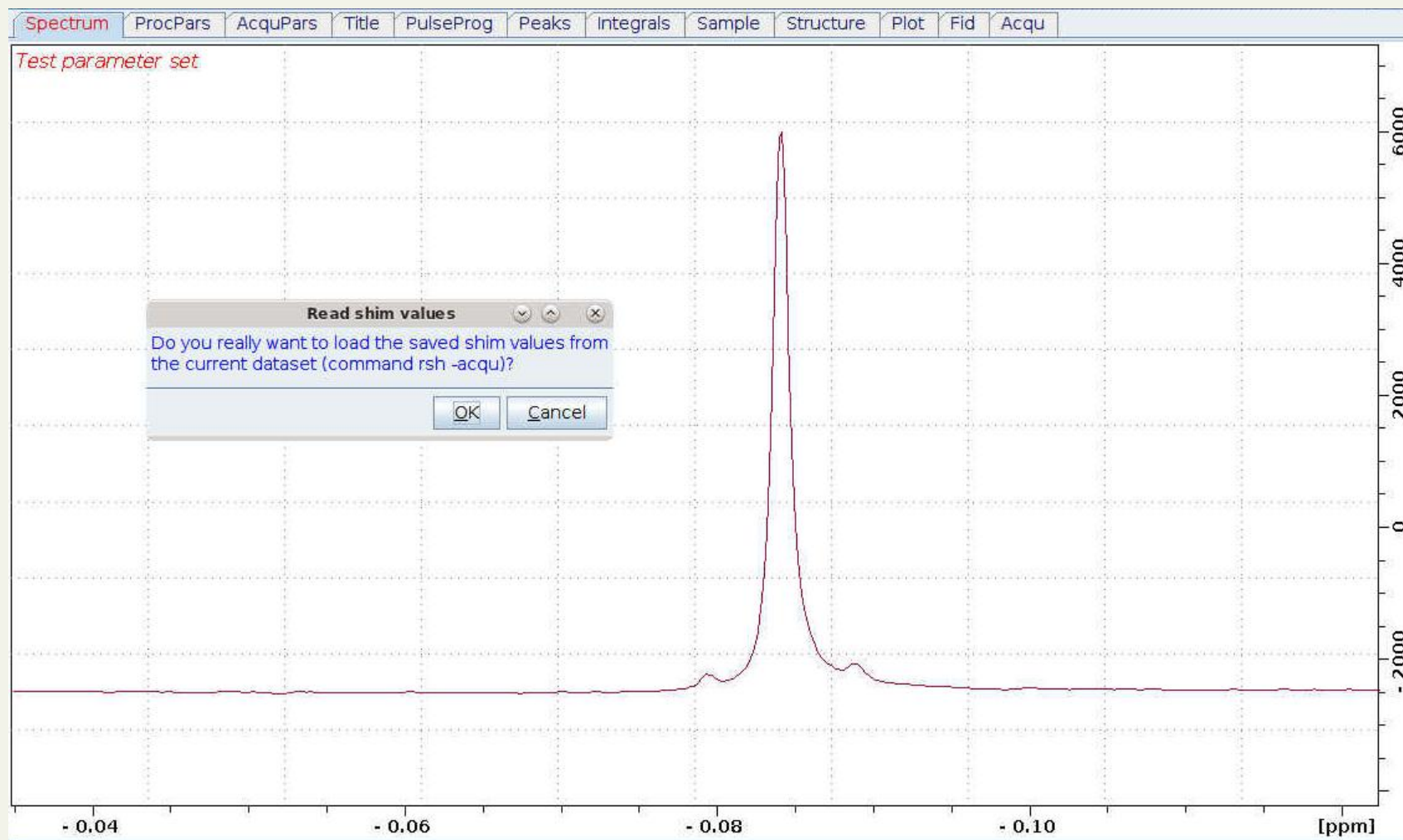
In fact **au_lc1d** use the AU-programs **lcprep** to run a preparation experiment and prepares all parameters for the solvent suppression using the AU-program **lcsetsup**.

The program can be started on any 1D data set with xau au lc1d or normally with xaua.

Actions carried out by au_lc1d

- Run the AU-program **lcprep** to acquire a 1D solvent search spectrum.
- Run the AU-program **lcsetsup** to find the desired number of solvents and adjust all parameters for solvent suppression on the current data set.
- Determine the RG for the experiment. Either a fixed **RG** can be used, or **RGa** is executed and the result is correct by **CNST29**.
- The acquisition is always started with the maximum number of scans, determined by **NS** and **TD0**.
- If the signal to noise control is activated the SINO is first checked after **L31** scans and further in iterations of **NS** scans until **TD0** loops or the requested SINO is reached.
- A basic processing is executed after each increment, the signal to noise is determined with AU program **lcsino**.

- rsh -acqu

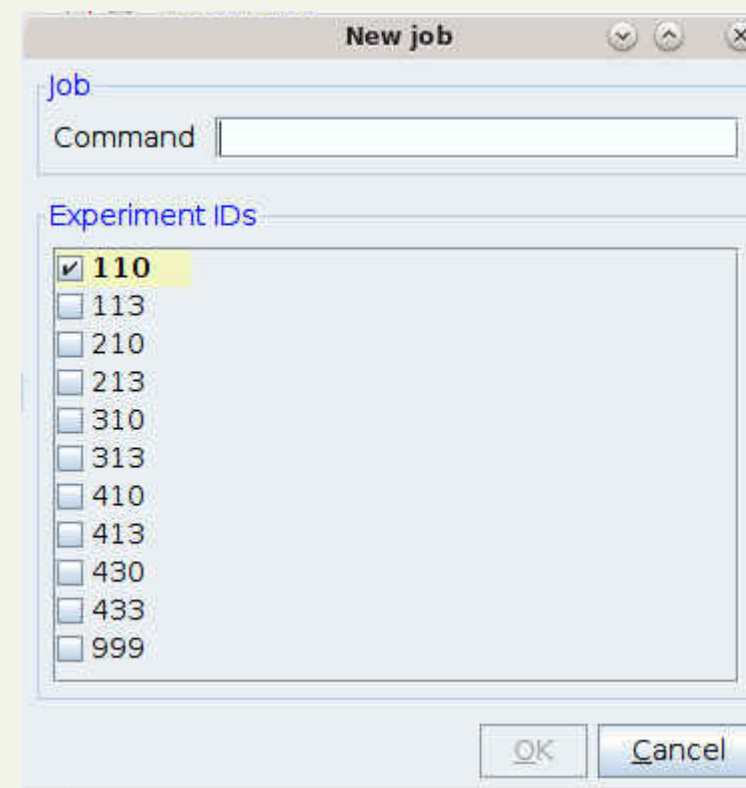
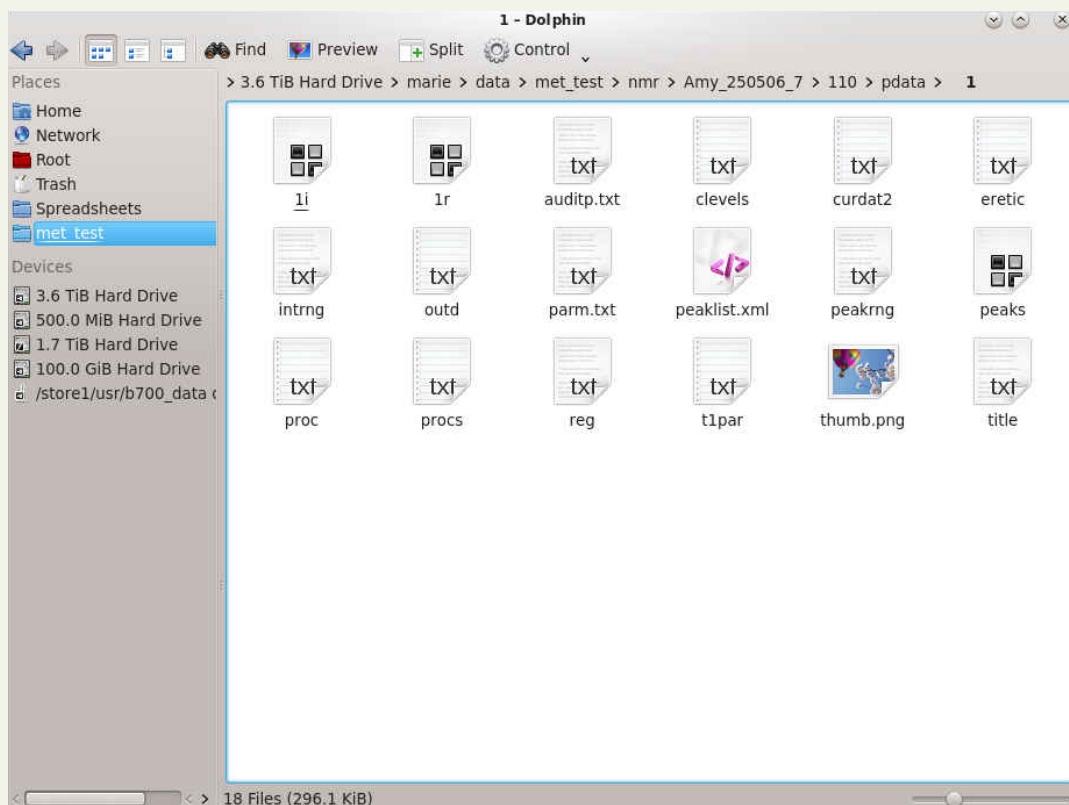


Good reference material for 3D shimming (topshim gui and select 3D)



Sucrose & DSS standard
(10% D₂O 90% H₂O)
Bruker Z10902

- expl & qumulti (thanks Nikita!)



Some manuals here: <https://www.bruker.com/protected/en/services/user-manuals/nmr/general.html>

More supplied with Bruker Topspin install

Practical Things

- SampleJet / high throughput tube usage
 - Use Bruker caps (we recycle caps)
 - Use of 108mm and 178mm tubes
 - Soak in decon90 over night and wash
 - Home made multi-tube (10) washing station
 - <https://rgmetab.github.io/NMRmetab/Miscellaneous/Tube%20washing/>



Practical Things

- SampleJet
 - Training to prevent incorrect operation
 - Recalibrate periodically (every 6 months)
 - Replace gripper periodically (1-2 years)



- User operation
 - <https://www.youtube.com/watch?v=MnFWzC7FDtE>
- Maintenance & Calibration etc:
 - <https://www.youtube.com/playlist?list=PLCfsv-WgdV7JcOa89KUNC-rzHiF-1kVlk>

- Helium recapture –
 - UoL-specific written manual available

He Recovery System SOP

Overview

Helium Recovery system aims to collect the He boiloff from the magnets during the normal operation and fills and compress them into cylinders to be collected by BOC for liquification. Liquified He will then be purchased by the facility to be used during helium fills. This scheme ensures the facility required 500 L allocation from BOC during shortage periods.

High level system architecture

The recovery system comprises of 6 collection points into a balloon that acts as intermediate reservoir which is then transferred into two manifold cylinder pallet (MCP) banks using a compressor. The switching between the MCP banks is performed by an automatic manifold. The overall schematic of the system is shown below with white arrow representing the flow direction of the He gas.

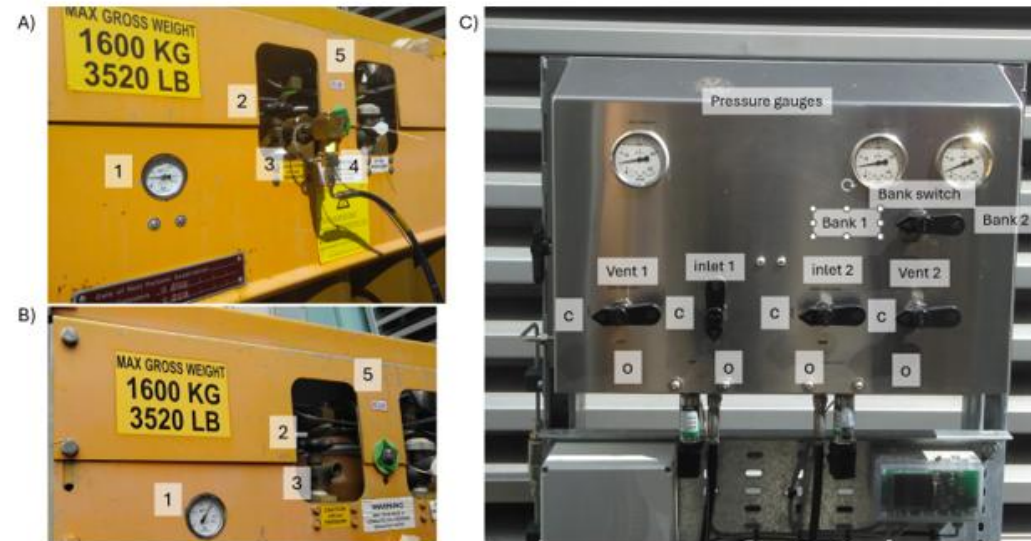
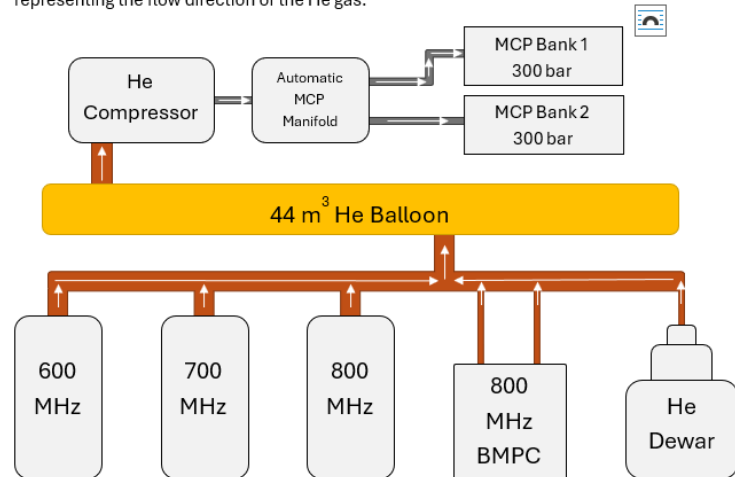
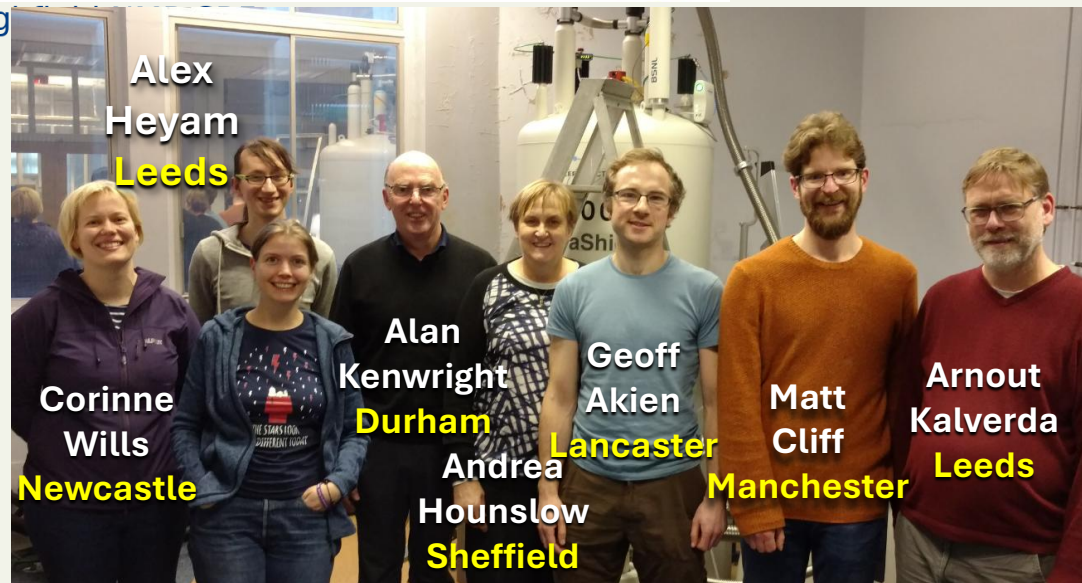


Figure MCP A) bank connected and not ready for collection, B) bank disconnected and read for collection C) external control panel –valve configuration shown for collection in bank 1.



Acknowledgments



Tips & tricks
Resources / links



Peter Gierth
(then Bruker)



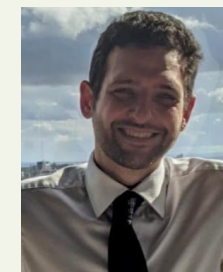
Mark Howard
(now Bruker)



Robin Stein
(Bruker)



Juraj Bella
Edinburgh



Rudi Grosman
(now Bruker)

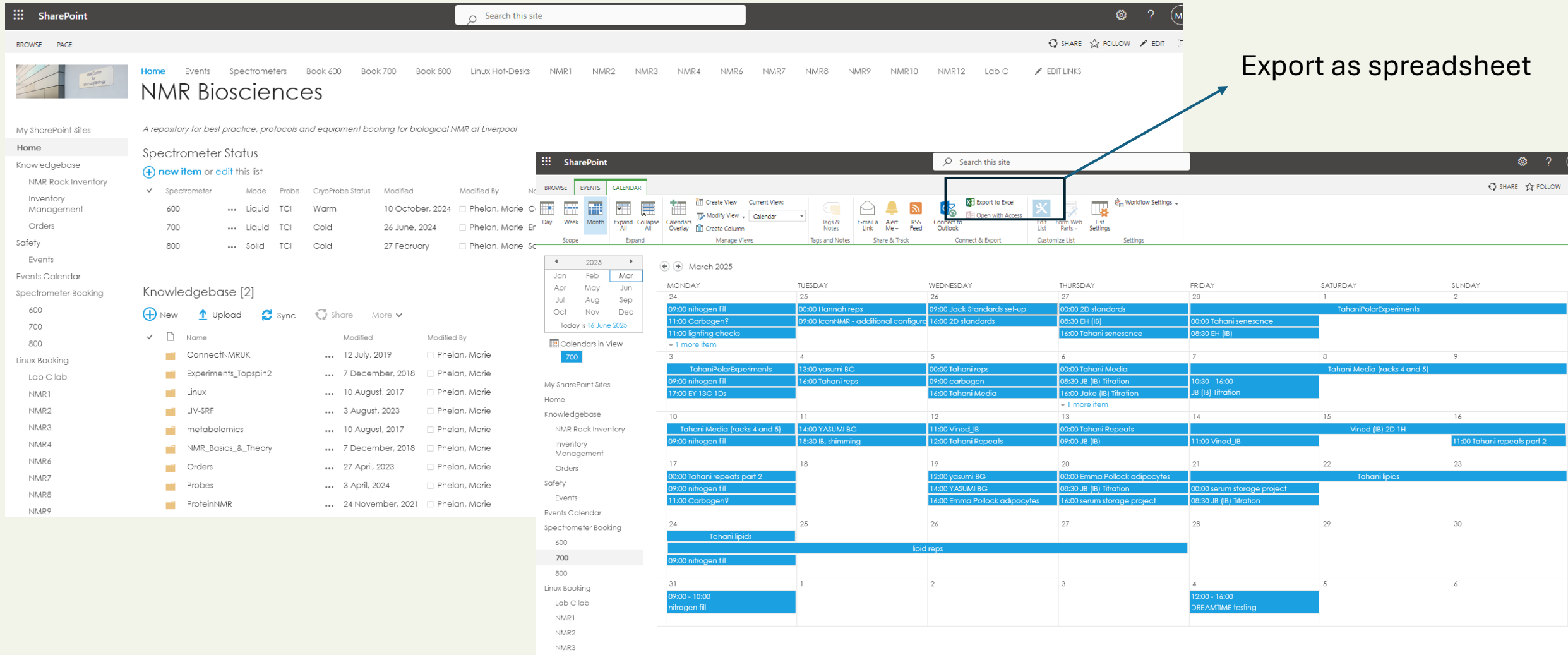


UKMRM
RSC
UCL
thanks Nikita Harvey

Most Importantly all this acquired knowledge is thanks to
the openness and expertise of the NMR community!

Practical Things

- Booking / managing
 - Sharepoint



SharePoint Search this site

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Inventory Management

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Events Calendar

Spectrometer Booking

600

700

800

Linux Booking

Lab C lab

NMR1

NMR2

NMR3

NMR4

NMR6

NMR7

NMR8

NMR9

Spectrometer Status

+ new item or edit this list

✓	Spectrometer	Mode	Probe	CryoProbe Status	Modified	Modified By	NC
	600	...	Liquid	TCI	Warm	10 October, 2024	Phelan, Marie C
	700	...	Liquid	TCI	Cold	26 June, 2024	Phelan, Marie Er
	800	...	Solid	TCI	Cold	27 February	Phelan, Marie Sc

Knowledgebase [2]

+ New Upload Sync Share More

✓	Name	Modified	Modified By
	ConnectNMRUK	12 July, 2019	Phelan, Marie
	Experiments_Topspin2	7 December, 2018	Phelan, Marie
	Linux	10 August, 2017	Phelan, Marie
	LIV-SRF	3 August, 2023	Phelan, Marie
	metabolomics	10 August, 2017	Phelan, Marie
	NMR_Basics_&_Theory	7 December, 2018	Phelan, Marie
	Orders	27 April, 2023	Phelan, Marie
	Probes	3 April, 2024	Phelan, Marie
	ProteinNMR	24 November, 2021	Phelan, Marie

SharePoint Search this site

BROWSE EVENTS CALENDAR

Export to Excel

Export as spreadsheet

March 2025

MONDAY	TUESDAY	WEDNESDAY	THURSDAY	FRIDAY	SATURDAY	SUNDAY
24 09:00 nitrogen fill 11:00 Carbogen? 11:00 lighting checks → 1 more item	25 00:00 Hannah reps 09:00 IconNMR - additional configura 16:00 Tahani senescence	26 09:00 Jack Standards set-up 16:00 2D standards	27 00:00 2D standards 08:30 EH (IB) 16:00 Tahani senescence	28 00:00 Tahani senescence 08:30 EH (IB)	1 TahaniPolarExperiments	2
3 TahaniPolarExperiments 09:00 nitrogen fill 17:00 EY 13C 1Ds	4 13:00 yasumi BG 16:00 Tahani reps	5 00:00 Tahani reps 09:00 carbogen 16:00 Tahani Media → 1 more item	6 00:00 Tahani Media 08:30 JB (IB) Titration 16:00 Jake (IB) Titration → 1 more item	7 10:30 - 16:00 JB (IB) Titration	8 Tahani Media (racks 4 and 5)	9
10 Tahani Media (racks 4 and 5) 09:00 nitrogen fill 15:30 IB, shimmmg	11 14:00 YASUMI BG 15:30 IB, shimmmg	12 11:00 Vinod_IB 12:00 Tahani Repeats	13 00:00 Tahani Repeats 09:00 JB (IB)	14 11:00 Vinod_IB	15 Vinod (IB) 2D 1H	16 11:00 Tahani repeats part 2
17 00:00 Tahani repeats part 2 09:00 nitrogen fill 11:00 Carbogen?	18	19 12:00 yasumi BG 14:00 YASUMI BG 16:00 Emma Pollock adipocytes	20 00:00 Emma Pollock adipocytes 08:30 JB (IB) Titration 16:00 serum storage project	21 00:00 serum storage project 08:30 JB (IB) Titration	22 Tahani lipids	23
24 Tahani lipids 09:00 nitrogen fill	25 lipid reps	26	27	28	29	30
31 09:00 - 10:00 nitrogen fill	1	2	3	4 12:00 - 16:00 DREAMTIME testing	5	6

My SharePoint Sites

Home

Knowledgebase

NMR Rack Inventory

Inventory Management

Orders

Safety

Events

Events Calendar

Spectrometer Booking

600

700

800

Linux Booking

Lab C lab

NMR1

NMR2

NMR3

Practical Things

- Booking / managing
 - BookitLab (Prog4Biz)

bookitlab

+ Reservation

Dashboard

Cores

Instruments

Location Maps

Reservations

Training

Consumables

Request Services

Work Orders

Projects

Billing

Messages

Users

Reports

UNIVERSITY OF LIVERPOOL

*SRF - Hig... Enter an asset name or asset attribute

+ Reservation

+ Request Requests

+ Work Order List

Timeline

Jun 16 - 22

Mon, 1

600AvancelIII

700AvancelIIHD

800Neo

Spectrometer Supervision

Price Sheet

CORE *SRF - High-field NMR Facility PERIOD 28/05/2025 METHOD Resource categories and Project categories

ID	RESOURCE PRICE CATEGORY	PROJECT CATEGORY	PI GROUP NAME	ORGANIZATION TYPE	FEE TYPE	TIME SLOT TYPE	THRESHOLD/ FACTOR	RATE	UNIT	
☐ 856	800NMR	TRAC 24/25			Reservation (time)	Off Peak	N/A	19.4893	Hours	Edit
☐ 855	800NMR	Charity 24/25			Reservation (time)	Off Peak	N/A	21.3242	Hours	Edit
☐ 854	800NMR	University 24/25			Reservation (time)	Off Peak	N/A	4.69	Hours	Edit
☐ 853	800NMR	External Academic 24/25			Reservation (time)	Off Peak	N/A	5.63	Hours	Edit
☐ 852	800NMR	Industry 24/25			Reservation (time)	Off Peak	N/A	20.15	Hours	Edit
☐ 851	800NMR	TRAC 24/25			Reservation (time)	Peak	N/A	19.4893	Hours	Edit
☐ 850	800NMR									
☐ 849	800NMR									
☐ 848	800NMR									
☐ 847	800NMR									

10 25

Return to list

* Invoices p

Billing Preview

Recalculate + Generate Invoices

Columns Export

Dates Period: Last Month Show zero amount invoices: No

#	Date	Project	PI Group Name	Resource Name	Core Name	User Display Name	Fee Type	Quantity	Units
14685	29/05/2025 16:00	[NMR]SP_SPushpakrom	Sudeep Pushpakrom	700AvancelIIHD - without_supervision	*SRF - High-field NMR Facility	Emma Pollock (hlepollo@liverpool.ac.uk)	Reservation (time)	17	Hours
14684	29/05/2025 16:00	[NMR]SP_SPushpakrom	Sudeep Pushpakrom	700AvancelIIHD - without_supervision	*SRF - High-field NMR Facility	Emma Pollock (hlepollo@liverpool.ac.uk)	Reservation (time)	7	Hours

Rows per Page 100

1-2 of 2

Practical Things

- Safetynet.liv.ac.uk
 - Safety Induction, training etc..



Navigation bar: Home, Risk Assessment, Substances, Documents, Training, Equipment, Reporting (selected), Search..., Help, Profile.

Reporting

(IIB Legacy - do not use) authorised users only +1 more Lab C +1 more Document Authoriser Document Maintainer

Reporting home

Your reports

Feedback

Statistics

Sign offs

Documents

Groups

Training

Equipment

Out of Hours

Users

Individual users

View per user what items they have signed off as an author/read plus any training they have completed.

Marie Phelan sign offs

Sign offs

1/1 MANDATORY FOR ALL GENERAL RA

1/2 MANDATORY FOR LAB GENERAL RA

14 SOP

Authored

2 PROJECT RA'S

0 SUPPORTING DOCUMENTS

1 COSHH FORMS

10 TRAINING RECORDS

Export Data

General RAs read Training CoSHH form Projects Supporting documents SOPs read

Title	Sign off date
NMR COVID-19 Temporary Policy	16 Mar 2022
NMR Centre Parking & Etiquette	20 Dec 2023
NMR Centre Induction	2 Jan 2024
Safetynet training	24 Jan 2024
NMR pasteur pipette discard	1 Jul 2024
ISMIB Sherrington Complex Safety Code of Practice	1 Nov 2024

Section A. Details of Standard Operating Procedure

Version Number	4
Author Name	Marie Phelan
Status	Staff
Supervisor	Marie Phelan
Category	Local Rules
Organisational area(s)	Liverpool Shared Research Facilities Institute of Systems, Molecular, and Integrative Biology (ISMIB)
Physical locations(s) this applies to	Lab C NMR (214)
Date Approved	2 Jan 2024
Title	NMR Centre Induction
Document reference	NMRC_Induction

Section B. SOP Documents

Document Name	
NMR_Local_Rules_2024.pdf	View

Section C. Signed off by

✓ Author	I can confirm this document is accurate and the contents within can be followed to ensure repetition of the procedure described.	Marie Phelan 02/01/2024
✓ Supervisor	I can confirm to the best of my knowledge that the document created constitutes to a standard operating procedure.	Marie Phelan 02/01/2024

✓ You have read and signed off on this standard operating procedure.