AMMRL Meeting

Bottlenecks and Pitfalls in NMR Practice: Working Toward Collective Solutions

Access to Working Published Pulse Program Code

Eldon L. Ulrich
BMRB

49th ENC, Asilomar, CA

Biological Magnetic Resonance Data Bank

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BMRB

BioMagResBank

A Repository for Data from NMR Spectroscopy on Proteins, Peptides, and Nucleic Acids

Department of Biochemistry
University of Wisconsin–Madison

BMRB Data Listed By:

- Macromolecular types
- NMR spectral parameters
- Kinetics
- Thermodynamics
- Restraints
- Structure
- Time-domain sets
- Solid-state NMR
- Unfolded proteins

Search BMRB

Data Browser, FASTA Search of BMRB, NMR Restraints, Time-domain Data Sets

Deposit Data

ADIT NMR

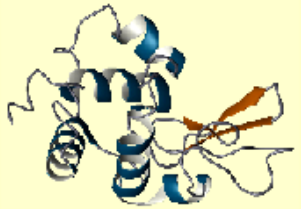
BMRB Mirrors

Madison USA, Osaka Japan, Florence Italy

About BMRB

Mission Statement, Aims and Policies, Data Accepted, Distribution

Biomolecular Highlight:
Lysozyme



New Entries

NMR Browser

FASTA

FTP Access

Relational Tables

Entries on Hold

NMR Time-domain Data

NMR Restraints from PDB MR Files

Time Domain Data for BMRB Entries

Available pulse programs

4678	Solution Structure of the RNA Polymerase Subunit RPB5 from Methanobacterium thermoautotrophicum
5106	An NMR Approach to Structural Proteomics
5166	Solution structure of hemolysin expression modulating protein Hha
5307	Basic Pancreatic Trypsin Inhibitor
5329	Backbone and Side Chain 1H, 13C, and 15N chemical shift assignments for conserved eukaryotic protein ZK652.3 from C. elegans
5335	Backbone and side chain 1H, 13C, and 15N chemical shift assignments for E.coli protein YacG
5589	Backbone and side chain 1H, 13C, and 15N chemical shift assignments for V. cholerae VC0424
5596	Solution Structure of the hypothetical protein yggU from E. coli. Northeast Structural Genomics Consortium Target ER14.
5597	Structure and dynamics of reduced Bacillus pasteurii cytochrome c: oxidation state dependent properties and implications for electron transfer processes
5656	Resonance Assignments for the Z Domain of Staphylococcal Protein A using a 2H, 13C, 15N enriched, selective methyl protonated sample
5691	Solution Structure of the 30S ribosomal protein S28E from Pyrococcus horikoshii. Northeast Structural Genomics Consortium target JR19
5842	Backbone and side chain 1H, 13C, and 15N chemical shift assignments for Haemophilus influenza protein IR24
5843	Solution Structure of At3g17210
5844	ZR18 Structure determination
5845	Backbone 1H, 13C, and 15N chemical shift assignments for S. aureus protein MW2441
5859	Structure of Antibacterial Peptide Microcin J25: A 21-Residue Lariat Protoknot
6011	Solution structure of a homodimeric hypothetical protein, At5g22580, a structural genomics target from Arabidopsis Thaliana
6052	Backbone and side chain 1H, 13C, and 15N chemical shift assignments for Haemophilus human protein HR969
6128	Structure of At3g01050.1, a ubiquitin-fold protein from Arabidopsis thaliana
6138	Hypothetical protein At2g24940.1 from Arabidopsis thaliana has a cytochrome b5 like fold
6173	PfR48 final project

NMR Pulse Programs from BMRB Time Domain Data Sets

BMRB entry 5597	Bruker	500	Avance
	Bruker	800	Avance

- 15Nhsqc
- 2Dnoesy
- 2DnoesyT286
- 2Dtocsy
- 2DtocsyT286
- 3Dhnha
- 3Dhnhb
- 3Dnoesy15Nhsqc

BMRB entry 15339	Bruker	600	Avance
	Bruker	800	Avance

- c13noesy_aliph
- c13noesy_aromatic
- cbcaconh
- ccconh
- cch-tocsy
- chsqc
- chsqc_NC5
- hbhaconh
- hcch-tocsy
- n15noesy
- nhcacb
- nhco
- nhsqc

Mozilla Firefox

File Edit View History Bookmarks Tools Help

http://www.bmrb.wisc.edu/data_library/timedomain/1/bmr15339/timedomain_data/Fiddeposit/c13noesy_aromatic_VpR5

CCPN timedomain

```
# 1 "/opt/topspin/exp/stan/nmr/lists/pp/noesyhsqcetgp3d_arom"
;noesyhsqcetgp3d
;avance-version (04/03/08)
;NOESY-HSQC
;3D sequence with
;   homonuclear correlation via dipolar coupling
;   dipolar coupling may be due to noe or chemical exchange.
;   H-1/X correlation via double inept transfer
;phase sensitive (t1)
;phase sensitive using Echo/Antiecho-TPPI gradient selection (t2)
;using trim pulses in inept transfer
;with decoupling during acquisition
;using shaped pulses for inversion on f2 - channel
;(use parameterset NOESYHSQCETGP3D)
;
;A.L. Davis, J. Keeler, E.D. Laue & D. Moskau, J. Magn. Reson. 98,
;   207-216 (1992)
;A.G. Palmer III, J. Cavanagh, P.E. Wright & M. Rance, J. Magn.
;   Reson. 93, 151-170 (1991)
;L.E. Kay, P. Keifer & T. Saarinen, J. Am. Chem. Soc. 114,
;   10663-5 (1992)
;J. Schleucher et al., Angew. Chem. 114(10), 1518 (1993)


# 1 "/opt/topspin/exp/stan/nmr/lists/pp/Avance.incl" 1
;Avance2.incl
;   for 1
;
;avance-version (03/02/17)
```

Library of Pulse Sequences

Please understand the **Disclaimer** before using these pulse sequences.

Pulse Sequences Listed by their Accession Numbers

Limit Pulse Sequence Files to:

(leaving a column blank ignores restrictions)

Manufacturer

- ☐ Bruker
- ☐ Varian

Experiment Type

- ☐ Homonuclear Chemical Shift
- ☐ Heteronuclear Chemical Shift
- ☐ Homonuclear Exchange Spectroscopy
- ☐ Heteronuclear Exchange Spectroscopy
- ☐ T1 Relaxation
- ☐ T1rho Relaxation
- ☐ T2 Relaxation
- ☐ Homonuclear J-coupling
- ☐ Heteronuclear J-coupling
- ☐ Calibration - Test

Dimension

- ☐ One-dimensional
- ☐ Two-dimensional
- ☐ Three-dimensional
- ☐ Four-dimensional

Find Pulse File

---

88 entries match this query

Acc. Num	Pulse Sequence File
1	TOCSY-HSQC 3D experiment
2	NOESY-HSQC 3D experiment
3	Bruker DMX 15N-1H 2D HSQC with Sensitivity-enhanced

The pulse sequences found in this library are provided "as is" for your information. They have NOT been tested, and no guarantee as to the accuracy of the pulse sequence or its functionality is given or implied. NO support for the use of these pulse sequences is provided by BMRB or those who submit a sequence. Please DO NOT contact BMRB or authors concerning the implementation of pulse sequences.

Submission Procedure

ASCII text files containing pulse sequences, text files describing the experiments, and other ancillary files can be submitted by anonymous ftp to "ftp.bmrb.wisc.edu". Please place the files in the incoming/pulse_sequence directory and notify Eldon Ulrich by e-mail (elu@bmrb.wisc.edu) that a pulse sequence has been deposited. Please indicate in the e-mail to Eldon Ulrich the names of all the files included in the submission.

Required:

- Brief title for the pulse sequence.
- Suggested location for the pulse sequence in the library.
- Concise description of what the pulse sequence is intended to provide.
- Spectrometer manufacturer and model(s) on which the pulse sequence is known to operate.
- Pulse sequence with phase cycling as an ASCII text file.
- Literature reference, if appropriate.
- Name(s) of author(s)

This information can be included as comments in the file containing the pulse sequence.

Optional:

- File containing a figure describing the pulse sequence. Please indicate the format of the file (postscript, GIF, MPEG, etc.).
- Files containing parameter lists used to execute the pulse sequence (shaped pulses, gradient programs, frequency lists, delay lists, etc.)

Sample Minimal Submission

```
nnhb.bv
Bruker DMX Avance, XwinNMR version
for correlation of 15N with hb
use hnhbref.bv as reference for quantitation
use with hn(co)hb to get hb stereoassignments
and chi-1 angles in proteins
for use with 15N-only-labeled proteins
Ref Archer et al., (1991) JMR 95,636-641
STATES-Tppi with presat
for gradient version, see hnhbgr.bv
implemented by Brian Volkman,
volkman@nmrfam.wisc.edu
last modified 10/5/95
BMRB Pulse Sequence Accession Number: 29


p1 1H 90
p2 15N 90 Hipower
p31 15N low power
d0 hb  t1
d10 15N t2
d2=1/4JNH
d3=27ms

d26=p2-p1"
d2=2.3m"
p21=0.5m"
p22=2m"
d11=50m"
d12=11m"
d3=27m"
d25=(p1*2)+(d10*2)"

 ze
 d11 do:f2
 d12
  d12
 d12
  d12*2
 d12
  d12
 d12 pl2:f2
 d12 pl9:f1
 p18 ph0    ;presat
 d15 pl1:f1
```

- AQUA Validation Server
- Wattos
  A software package consisting of programs for analyzing, annotating, parsing, archiving, and disseminating experimental NMR data deposited by authors world wide into the PDB

NMR Software Hosted at BMRB but Maintained by Other Users

- BBReader is a program to speed the search for information in NMR-STAR files.
- calc_cs - The program calculates random coil chemical shifts for a protein sequence
- calc - A program to calculate pulse lengths for NMR experiments.

Libraries

- Library of NMR Software
  Listing of the macros available
- Academic and Commercial Software is a collection of analytical tools hosted by members of the NMR community.

NMR Experiments and Pulse Programs

- Ad Bax Group
  Pulse Sequence Library
- BMRB Library of NMR Pulse Sequences
  Listing of the pulse sequences available
- GFT NMR Package G-matrix Fourier Transform Package
- Lewis Kay Lab Pulse Sequence Request Form
- Art Palmer Group Bruker AMX Pulse Programs
- Pulse Sequence Library hosted by NMRFAM
- Michael Sattler Triple resonance pulse programs for 13C, 15N labeled proteins
- Solid State Pulse Programs from ENS Lyon
- Michael Summers Group NMR Toolkit at the Howard Hughes Medical Institute
- NMR Pulse Sequence Library of Carlsberg Laboratory
- CABM NMR Pulse Sequence Library at the Center for Advanced Biotechnology and Medicine - Rutgers
- Eric Zuiderweg Group University of Michigan - see bottom of page

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Source References

Pulse program deposition issues

- Ease of deposition
- Deposition content
- Deposition validation (submitted versus complete)
- Pulse program version updates
- Preference for publication on local lab web site
- Liability

Submission requirements

UCL/LICR Joint NMR Laboratory

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bout these pages

low to use the files

Getting Started NEW

Select an archive:

TRIPLE RESONANCE
Containing:
2D ^{15}N HSQC
3D HNCA
3D HN(CO)CA
3D HNCO
3D HN(CA)CO
3D HNCACB
3D HN(COCA)CB

SIDE CHAIN
Containing:
2D ^{13}C HSQC
2D HCCH-TOCSY
3D HCCH-TOCSY (18ms)
3D HCCH-TOCSY (7ms)

NOE
Containing:
2D ^{15}N HSQC
3D^{15}N NOESY-HSQC
3D^{15}N TOCSY-HSQC
2D ^{13}C CT-HSQC
2D ^{13}C CT-HSQC (folded)
3D^{13}C NOESY-HSQC

The Ubiquitin NMR Resource Page

By Richard Harris, BBSRC Bloomsbury Centre for Structural Biology, UCL

About this Resource Page

The purpose of these pages is to give access to the NMR data that has been acquired on ubiquitin here at UCL.

The experiments have run on a ubiquitin sample from VLI Research, dissolved in ~250uL phosphate buffer, pH 5.8, in a Shigemi tube on either a Varian Unity^{+} 500 or 600MHz spectrometer.

The data has been used, here at UCL, to provide a sample data set for teaching the basics of assigning proteins.

The data has been split into three archives for ease of downloading:

- Triple resonance experiments to assign the backbone nuclei
- Side-chain experiments to assign all the side-chain protons and carbons
- NOE experiments to obtain restraints for structure calculations

There are two files to download; one contains the raw Varian fid data including the nmrPipe script for processing; and the other contains the ANSIG session files (with contours and peak lists) with which to analyse the data. So that you can either reprocess the raw data and use your own preferred analysis software, or you can download pre-processed spectra to use in ANSIG.

The ANSIG sessions are not a "how to use ANSIG", although it may provide a good starting point. The ANSIG session works for SGI machines and linux with one amendment to the control file (see the 'how to use the files' section) - if anyone tests them on ANSIG for windows then can you let me know if they work.

NEW A general guide to using the triple resonance data within ANSIG - see 'Getting Started'

Please feel free to contact me with any questions.

NMR data-sets Bank:

A repository for raw NMR data-sets

NMRb.

The development of NMR in structural genomics requires the availability of automatic structure determination methods. An initial group gathered and decided it would be very helpful to have access to complete data-sets easily on the WEB. We believe that this availability will help the development of new NMR analysis methods by alllowing complete testing procedures on raw data.

This site is operated by people working in the field of NMR and molecular modeling methods for NMR at the Centre de Biochimie Structurale (Montpellier; France) and Institut de Biologie Physico-Chimique (Paris, France).

According to the will of the depositors, datasets found here can be either in free access or confidential. In case of confidential access, the datasets are distributed through a login/password procedure (which should be asked directly to the depositor). Naturally, the free access is preferable for the NMR methodologists community.

NMRb offers both dowloadable raw NMR data and spectra information organized in a relational data-base.

Available data-set: ***Sorted by data-set*** *or* ***by spectra.***

The data-sets are provided « as it » to users, without guarantee on their contents.

Spectra Repository or Entry Update