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VnmrJ BioPack:
The Easiest Path to High Quality BioNMR Data

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VnmrJ 4.0 and NMRPipe

The NMRPipe engine extends to Bio, Solids, and Small-molecule applications

TALOS+: protein backbone phi,psi torsions from chemical shifts.

SPARTA+: protein backbone chemical shifts from structure.

DYNAMO/PDBUTIL: structure analysis and manipulation, add protons, create extended structures, etc.

DC: manipulation of Dipolar Couplings, NMR Homology Search (MFR).

IST: 2D and 3D NUS processing.

Spectral Alignment for CRAFT.

SpecView: 1D and 2D spectral series analysis with Interactive Principal Component Analysis Navigation.
TALOS+ predicts protein backbone torsions from chemical shifts using a combination of database mining and an artificial neural network (ANN). It can form predictions for 88% of residues on average, with an RMS of better than 15 degrees. A No-Proton mode tuned for Solid State applications is included.
- Create Extended Structure
- Add Protons
- Transformations of PDB Coordinates
- List Secondary Structure, H-Bonds
- Mass, Volume, Surface Area
- Simple simulated annealing
Analyze Titration Curve to Estimate $K_d$
VnmrJ 4.0 – NMRPipe SpecView

1D Series Display with Interactive Principal Component Analysis
VnmrJ 4.0 – NMRPipe SpecView

2D Series Display with Interactive Principal Component Analysis
VnmrJ 4.0 BioPack and NMRPipe

NMRPipe – The Old Way

```
x/bin/csh
var2pipe -in /dev/fd/C/space/delalgo/vj5/pipe_data_sets/AMGA_3D.fid/fid \
   -noeswap -acqRD 1 \ 
   -xN 2048 -yM 64 -zW 64 \ 
   -xc 1024 -yc 32 -zc 32 \ 
   -MODE Complex -yMODE Rance-Key -zMODE Complex \ 
   -xSW 13020.800 -ySW 5031.720 -zSW 2106.600 \ 
   -xOB 799.597 -yOB 201.08S -zOB 61.032 \ 
   -star 4.773 -ySTAR 56.117 -zSTAR 120.144 \ 
   -xLAB 013 -yLAB 013 -zLAB N15 \ 
   -ndim 3 -acq2D states \ 
   -out /dev/fd/C/space/delalgo/vj5/pipe_data_sets/AMGA_3D.fid/data/test%03d.fid -verb -ov
sleep 5
```
Manually Select Acquisition Mode
Manually Select Nucleus
VnmrJ 4.0 BioPack and NMRPipe

NMRPipe – The Old Way

Manually Select Axis Label
Traditionally, NMRPipe scripts are manually edited to set parameter values.
VnmrJ 4.0 BioPack and NMRPipe

BioPack and NMRPipe – Automated Construction of Processing Schemes

**Automatically Create and Run NMRPipe Scripts**
VnmrJ 4.0 BioPack and NMRPipe

BioPack and NMRPipe – Automated Construction of Processing Schemes

The VnmrJ “Do it All” Button
VnmrJ 4.0 BioPack and BioPack Express

BioNMR Setup and Processing with Just a Few Clicks
VnmrJ 4.0 and Non-Uniform Sampling

Background: the Fourier Transform and Non-Uniform Sampling

\[ x( f ) = \sum x( t ) [ \cos( 2\pi ft / N ) - i \sin( 2\pi ft / N ) ] \]
Time Domain Data to Transform
Time Domain (Real Part)

Fourier Term

Multiplied with Time Domain Data

Forms the Product
Time Domain (Real Part)

Fourier Term

Multiplied with Time Domain Data

Forms the Product

\[ \Sigma^+ \quad \Sigma^- \]
Time Domain (Real Part)

Fourier Term

Multiplied with Time Domain Data

Forms the Product

∑+ ∑-

Sum Over Product to Form a Frequency Point:

Frequency Domain (Real Part)
Truncated Time Domain Data to Transform
Time Domain (Real Part)

Fourier Term

Multiplied with Truncated Time Domain Data

Forms the Product

\[ \sum^+ \sum^- \]

Sum Over Product to Form a Frequency Point:

Frequency Domain (Real Part)
Non-Uniform Sampling on a Uniform Grid
Time Domain

NUS Time Domain Data

Non-Uniform Sampling: Skip a Fraction of the Points
Time Domain

NUS Time Domain Data

Non-Uniform Sampling
Non-Uniform Sampling:
for Fourier Transform, Replace Missing Points with Zeros
NUS Time Domain Data to Transform
Time Domain (Real Part)

Fourier Term

Multiplied with NUS Time Domain Data

Forms the Product

Σ+  Σ-

Sum Over Product to Form a Frequency Point:

Frequency Domain (Real Part)
Linear versus Non Uniform Sampling

Linear Sampling: Broad Line and Periodic Truncation Wiggles
Non Uniform Sampling: Narrow Line and Random Noise-Like Artifacts

Time Domain (Real Part)
- Time Domain Data
- Truncated Time Domain Data
- NUS Time Domain Data

Frequency Domain (Real Part)
Non Uniform Sampling
Threshold Methods

Time Domain

NUS Time Domain Data

Discrete Fourier Transform

Frequency Domain

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Non Uniform Sampling

Threshold Methods

Time Domain

Frequency Domain

NUS Time Domain Data

Discrete Fourier Transform

Clipped Fourier Transform
Non Uniform Sampling

Threshold Methods

Time Domain

NUS Time Domain Data

Inverse Transform of Clipped Data

Discrete Fourier Transform

Clipped Fourier Transform

Frequency Domain

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Non Uniform Sampling

IST – Iterative Soft Thresholding

Fourier Spectrum

IST Spectrum

Threshold: 70.07
VnmrJ 4.0 allows Routine Users to apply Non-Uniform Sampling (NUS) to most any experiment.
Pulse sequence-independent data acquisition:

- Works seamlessly with every experiment, automatically.
- Effortless - just set check a NUS checkbox in the graphical interface.
- Comprehensive set of options for sampling schedules, including any user-supplied schedule.
- NMRPipe Users - No need to figure out data acquisition order, reshuffling dimensions etc… No hassle, just press the processing button.
- NUS Reconstruction is handled automatically – no need to download and learn complicated signal processing software packages from academic labs, no need to construct NMRPipe scripts by hand.
BioPack *Express – Introduced at ENC 2013*
BioPack **Express**

An overview

**BioPack:**

An comprehensive software framework for automated, optimized bioNMR measurement setup, with fully-automated, supplemented with the most extensive library of pulse sequences. BioPack provides expert users with ultimate control over all experimental parameters.

**BioPack Express:**

A streamlined enhancement to BioPack that allows a user to acquire the most commonly used bioNMR experiments with near optimum performance and minimum operator involvement.
A vast majority of bioNMR experiments require very few “input parameters” in order to get decent results:

- What experiments to run (i.e. HNCA, HSQC, etc.)
- Spectrometer time available (i.e. nt, NUS or not)
- One or two “specials” per experiment (ex. mixing time in TOCSY/NOESY, max T2 in CPMGs, etc.)

Everything else can be predicted based on knowledge about the nature of a particular experiment and spectrometer calibrations.
BioPack *Express*

A single panel is sufficient to acquire, and process the most widely-used experiments.
BioPack Express

BioPackExpress Features

- Intuitive high-level user interface that allows a user to set up and run a bioNMR experiment or a queued set of experiments with a few clicks of a button.
- NUS made easy: automatic experiment-specific and pulse-sequence independent set-up for Non-Uniform data acquisition and processing.
- Automatic set-up of data processing parameters.
- Top-level acquisition and processing algorithms are experiment-specific and can be easily customized, while a unified graphical interface is used for all experiment types.
BioPack *Express*

In most cases one would need only one panel

*Quick calibration of 1H pw90 (needed once per sample)*
BioPack *Express*

In most cases one would need only one panel

*Key experiment parameters*
BioPack Express
In most cases one would need only one panel

Non-Uniform Sampling
BioPack Express

In most cases one would need only one panel

*Human-readable choices of experiment modes (experiment-specific!)*
BioPack *Express*

In most cases one would need only one panel

*Human-readable options for data processing (dataset-specific!)*
BioPack Express

In most cases one would need only one panel

**Hint/info line**

```
current experiment gnoesyNhsqc is set as: Hnoe x N x HN 3D, uniform sampling
```
How to setup a single experiment
How to setup a queue of experiments
How to process a multidimensional dataset
How to process a multidimensional dataset
How to process a multidimensional dataset acquired using Non-Uniform Sampling (NUS)
Agilent VnmrJ BioPack Express
The Most Widely-Used BioNMR Experiments in Just a Few Mouse Clicks

Shown here:
- NUS HNCO
- NUS HNCACB
- NUS HNCA
- NUS HC(CO)HN
- N15NOE
Agilent Spinsights NMR Community
https://spinsights.chem.agilent.com

More Questions?
Join the Spinsights NMR Community and Help Yourself, Help Each Other, or Ask Agilent

Note: registration is required to access the Spinsights online community.