Biomolecular NMR Experiments Using Agilent BioPack in VnmrJ 3.2

Data Sheet

Key Features

- Menu-based automatic experiment setup
- Automatic calibration using your own mono or di-labeled samples
- Efficient experiment planning: perform the most productive experiments first
- Access to the latest fast NMR methods simplifies multidimensional data analysis

Agilent BioPack is a standard part of VnmrJ 3.2 software which provides a full set of Biomolecular NMR experiments for use with water-based solutions of proteins, peptides, and mono or polynucleotides.

A combination of highly flexible C pulse sequence and MAGICAL macro languages makes it possible to fully automate the setup and execution of the most sophisticated multidimensional, multinuclear experiments. As a result, BioPack allows the user to concentrate only on the total time of the experiment without compromising performance.

Recent methods such as nonuniform sampling (NUS) compressive sensing, automatic spectral compression (ASCOM), and automated projection reconstruction (APR) are standard in BioPack, including CLEAN processing software for NUS data. In addition, NMRPipe can be accessed directly from BioPack using an optimized NMRPipe interface.

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Using BioPack

BioPack simplifies complex Biomolecular NMR experiments, facilitating the automatic setup, sample calibration, planning, and multidimensional data analysis. All parameter settings are stored in the **probefile** and are automatically calibrated using the sample to be studied. Table 2 details the ^{1}H and ^{13}C experiments available using BioPack in VnmrJ 3.2. The key features of BioPack are shown below:

Automatic experiment setup, including 3D and 4D

- Experiments are selected from a menu
- All parameters are set automatically based on experiment selected
- Only the number of transients per fid and evolution time increments need to be set

Automatic sample calibration

- Accommodates mono- and di-labeled proteins
- Complex parameters are set using a single mouse click
    - PW90s for each channel
    - Decoupling and spinlock waveforms
    - Coherence transfer gradients
    - Bloch-Seigert phase corrections
    - Probefile calibration table updates

Efficient experimental planning and execution

- Automatic 1D survey of multiresonance nD experiments
- Automated 2D survey series of 37 experiments
- Select the most productive 2D/3D experiments based on the actual data produced

The latest fast NMR methods

- All nD sequences can be run using NUS with the click of a mouse and processed within VnmrJ 3.2
- Projection-reconstruction experiments can be used for running 3D or 4D experiments as a series of 2D experiments

Data collected using BioPack is shown in Figures 1 and 2. Figure 1 shows a display of 2D-^{15}N HSQC data comparing a contour and stacked display along with the Pulse Sequence panel displaying experimental options available within the pulse sequence.

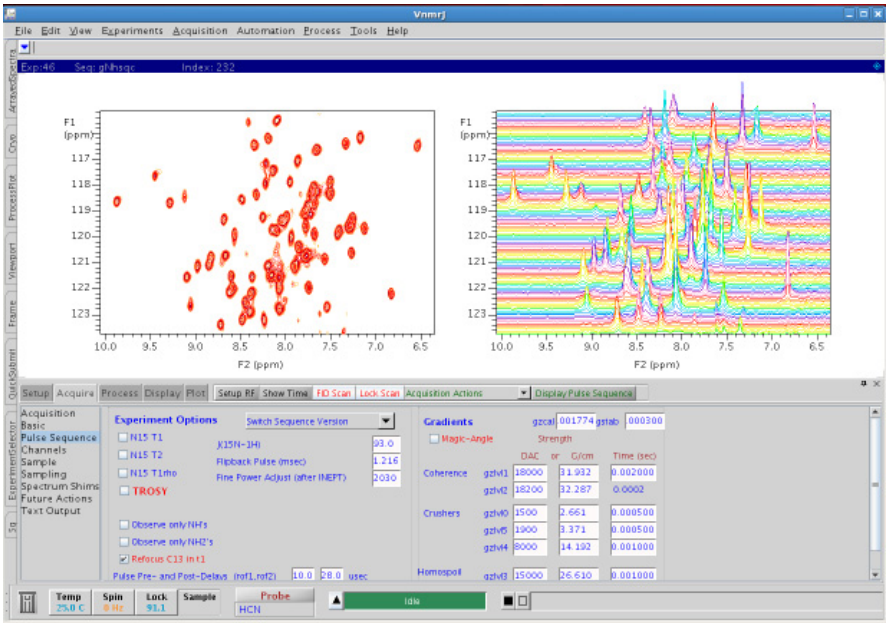

Figure 1. BioPack display of 2D-^{15}N HSQC data comparing a contour and stacked display, along with the Pulse Sequence panel showing experimental options available within the pulse sequence.

A comparison of linear and non-linearly sampled ^{15}N HSQC 700 MHz DD2 data is shown in Figure 2, based on the conditions described in Table 1. The results vary only in the number of t1 increments, yielding comparable resolution in a shorter time span with NUS.

Table 1. Comparison of NUS and conventional data acquisition.

Sample	A	B	C
Sampling/ processing	Linear	NUS with CLEAN	Linear
t1 increments	32	32*	128
Acquisition time	4 min 43 s	4 min 43 s	19 min 13 s
Processing time	~1 s	~ 2 s	~ 1 s
Resolution	Low	High	High

*randomly spaced over a 0-128 point grid (25 % sampling density).

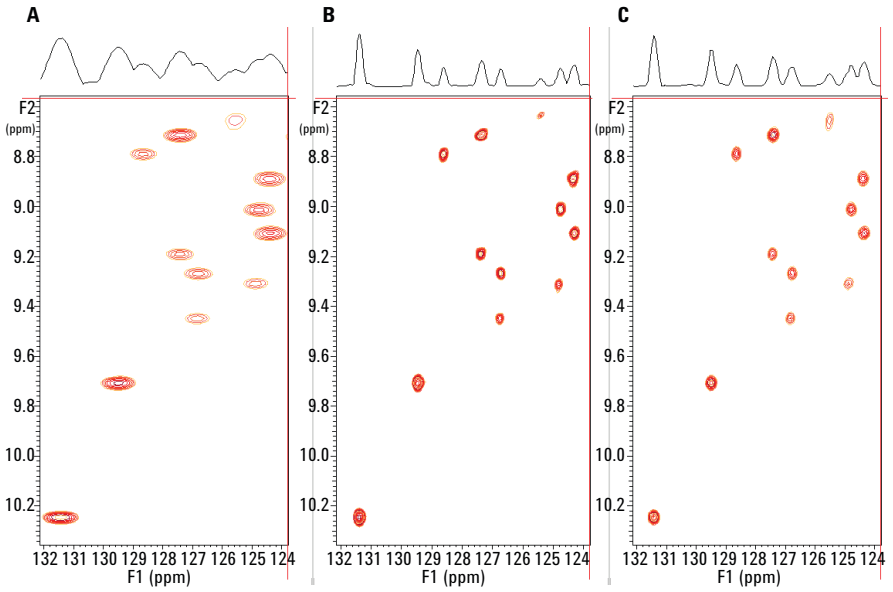

Figure 2. A comparison of linearly and nonlinearly sampled ^{15}N HSQC 700 MHz DD2 data demonstrates that higher resolution can be achieved in a shorter time period using NUS with CLEAN processing. Conditions used for A, B, and C are shown in Table 1.

Table 2. BioPack experiments*

^{1}H Observe experiments in 1, 2, 3, and 4 dimensions

1D

PRESAT, WET, WATERGATE, JUMP-RETURN, PURGE, SWET, SOGGY, FLIPSY
NOE-DIFFERENCE, NOE-PUMPING
EXCIATION-SCULPTING (DPFGSE)
WATERLOGSY
SATURATION-TRANSFER
CLEANEX-PM
NH-DIFFUSION

2D

DPFGSE	SATURATION TRANSFER NOESY/TOCSY, ROESY
COSY	MAGIC-ANGLE, WATERGATE, DQCOSY, DQFCOSY
NOESY	SS, PRESAT, WATERGATE, WET, 1-1, QUIET
TOCSY	PRESAT, DIPSI, WET, WATERGATE

^{13}C-^{1}H 2D

HSQC	TROSY, WATERGATE HSQC, CT-JCH
HMBC	CLEAN, GRADIENT
HMQC	HMQC, CT-HMQC, SOFAST METHYL

*All nD experiments can be run with nonuniform sampling and processed using CLEAN within VnmrJ. Experiments beginning with PR can be run using automatic projection angle determination and queued using the PR Manager.

^{15}N-^{1}H 2D

HMQC	HMQC, HMQCJ, HAADAMARD SOFAST, SOFAST
HSQC	HSQC, CPMGHSQC, TROSY, WATERGATE HSQC, IPAP HSQC, HAADAMARD, HADAMAC, seq-HADAMAC, CCLS, CCLS-TROSY, TROSY-CH2, ^{13}C/^{15}N METHYL HSQC/TROSY, BEST-HSQC, HOMODECOUPLED HSQC: HSQCHD, IPAP HSQCHD, IPAP HSQC for gels, WATERGATE, WATERGATE IPAPHD
CPMGNOESY	
CRINEPT	
^{15}N RELAXATION	T1, T1, T2, NOE, RELAXATION DISPERSION
SOLVENT-EXPOSED AMIDES	HSQC, TROSY, CLEAN-HSQC, CLEAN-TROSY
RNA	HNNCOSY

^{13}C-^{1}H 3D

METHYLNOESY
HSQC-NOESY, HSQC-TOCSY, HMQC-TOCSY
^{13}C/^{15}N FILTERED NOESY/TOCSY
HCCHCOSY, HCCHTOCSY, DE-HCCHTOCSY,
METHYL HCCHTOCSY
HACAHB
CCHTOCSY
HMCMCBCA, HMCMCGCBCA, HMCMCGCBCACO,
HBCBCACOCCAHA, HBCBCACONNH, CB(CGCDCE) HE, CB(CGC)DHD
NOESYHMQC, NOESYHSQC, CN-FILTERED NOESYHSQC,
CN-EDITED NOESYHSQC
TOCSYHSQC
LRCC, LRCH

Table 2. BioPack experiments (continued)*

^{15}N-^{1}H 3D

HNHA, HNHB
HSQCNOESY, ROESYHSQC, TOCSYHSQC

^{1}H-^{13}C-^{31}P 3D

RNA HCP, HPCOSYHCP

^{13}C-^{15}N-^{1}H 3D

CACB-TOCSY_CMHM
CBCA(CO)NNH, PR-CBCA(CO)NNH
CBCANH, PR_CBCANH
HBHACONH
HCACOCANH
HCACON
HCAN
CCONH
H(CCO)NNH, PR-H(CCO)NNH
HNCA CT, BEST, BEST-TROSY, PR
Intra-residue BEST-TROSY HNCA, BEST-TROSY HNCACB, HCACONCA, (HCA)CON(CA)H, H(CA)CO(NCA)H, (HCA)CON(CA)H, (HCACO)NCAH
HNCACB CT, BEST, BEST-TROSY, PR
HNCO BEST, BEST-TROSY, PR
HNCONOE
HN(CO)CA BEST, BEST-TROSY, PR, JCH
HNCOCACB BEST, BEST-TROSY
BEST-TROSY-(HN)CO(CA)NH
BEST-TROSY-(H)N(COCA)NH
HNCOCO
HNCOHB
HNCO JCOCA, JNCA, JNCO, JCC, JCOH, JNHA
HNCN, HNN, (H)N(CA)NH, (H)NCA(N)H
NOESY-^{13}CHSQC, CN-Filtered NOESY-^{13}CHSQC
NOESY-^{15}NHSQC, CN/N-FILTERED NOESY-^{15}NHSQC
CCTOCSYNCH
H2CN
RNA AHNCTOCSYCH, CUHNCCCH, CUHNCCCH-CCdec, GHNCTOCSYCH, HCN, MQHCN, BEST-TROSY HBONDS

^{13}C-^{15}N 4D

^{13}C/15N-NOESYTROSY
^{13}C-HMQCNOESY-^{15}N-HSQC
NN4DNOESYTROSY
^{15}N-HSQCNOESY-^{15}N-HSQC, ^{15}N-HMQCNOESY-^{15}N-HSQC
^{15}N-HSQCTOCSYNOESY-^{15}N-HSQC
^{15}N-TOCSYNOESY-^{15}N-HSQC
CNHSQC_NOE_CNHSQC4D
Projection-Reconstruction DIAG-^{13}C-HSQCNOESY-^{13}C-HSQC
^{13}C-HMQCNOESY-^{15}N-HSQC
^{13}C-HSQCNOESY-^{13}C-HSQC
HACOCANH
HACANH
HNCACB
HNCACO
HNCOCACB
HNCOCA
INTRA-HNCACB
SIM-HNCOCA
HCCONH
INTRA-CCN

^{13}C Observe experiments

^{13}C OBSERVE 1D
COSY, DQCOSY
CACO_SQ
COCACO_SQ/MQ
CBCACO
CCTOCSY

*All nD experiments can be run with nonuniform sampling and processed using CLEAN within VnmrJ. Experiments beginning with PR can be run using automatic projection angle determination and queued using the PR Manager.

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