

### Highlights/key benefits

- Streamlined interface sets up complex BioNMR experiments, set up one experiment or queue many with just a few mouse clicks
- Automated non-uniform sampling option for indirect dimensions enables sharper spectra with shorter measurement times
- Automatic setup of spectral processing for both conventional and NUS spectra
- Integrated with NMRPipe, the most widely-used processing solution for BioNMR

### Introduction

Manual setup of a typical BioNMR experiment can be time-consuming, and measuring a useful spectrum requires optimization of dozens of parameters such as pulse widths, frequency offsets, shaped pulses, spectral widths, number of increments, and various power levels.

BioPack is a familiar and robust component of Agilent VnmrJ software, providing a comprehensive collection of BioNMR experiments in a framework with sample-specific optimization of measurement parameters. BioPack provides expert users ultimate control over all experimental parameters. BioPack *Express* is an addition to BioPack that provides a simple and efficient interface to set up commonly-used BioNMR experiments, enabling excellent spectral quality with minimal operator involvement (Figure 1).

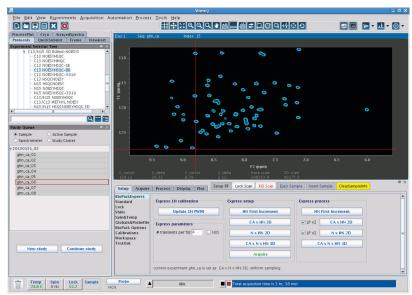


Figure 1. The BioPack Express interface in Agilent's VnmrJ software.



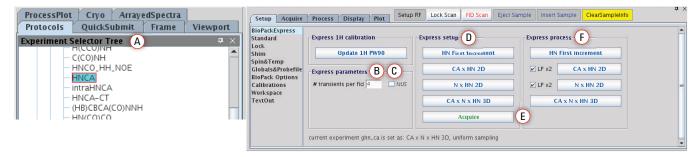


Figure 2. Setting up a single experiment in the BioPack Express interface.

### Setting up a single BioNMR experiment

- 1. Select the desired experiment from the **Experiment Selector Tree** (A).
- 2. Confirm the number of transients in the **Express parameters** frame (B).
- 3. Select the **NUS** check box if optional non-uniform sampling is desired (C).
- 4. Select the measurement type (1D, 2D or full 3D) in the **Express setup** frame (D).
- 5. Click Acquire (E).

# Processing 1D/2D/3D data with the BioPack *Express* interface

Process spectra by clicking a single button in the **Express process** (F) frame. Linear prediction can be selected via check box. If the dataset was acquired in NUS mode, a simple NUS processing panel will appear.

## Setting up a queue of multiple BioNMR experiments

Simply drag an experiment from the **Experiment Selector Tree** (G) into the **Study Queue** (H), and choose the required experiment options from the **BioPack** *Express* interface (Figure 2).

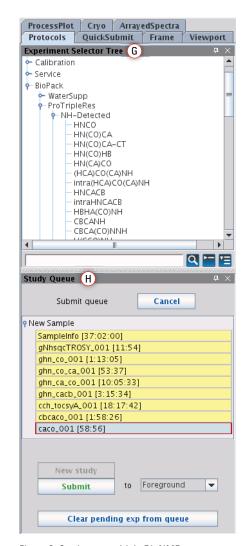


Figure 3. Setting up multiple BioNMR experiments in the queue.

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