# Agilent VnmrJ Software for Nuclear Magnetic Resonance Spectroscopy

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## Introduction

Agilent's VnmrJ software makes acquiring high quality NMR data as easy as simply specifying the desired experiments, with tuning, shimming, and parameter setup optimized automatically on the fly for each sample.  VnmrJ includes an entire range of tools for system administration, experimental setup, optimization, acquisition, processing, and analysis, all in a single software environment that provides each user with just the right tools needed to support their goals and level of expertise. Powerful core features make sophisticated solutions reliable and routine, delivering superior spectral quality and expanding the productivity of structural investigations, biomolecular studies, complex mixture analysis, and more.

## Why Upgrade to VnmrJ 4.2?

Users already familiar with VnmrJ 3.2 or earlier Varian/Agilent NMR software will find powerful new features, refinements to familiar Core Features, and a beautifully refactored graphical interface.

VnmrJ 4.2 is a synchronizing release, allowing you to take advantage of VnmrJ's latest features conveniently by using the same software version on recent Agilent NMR systems as well as legacy Agilent/Varian systems. VnmrJ 4.2 supports Direct Drive systems (ProPulse, DD2, 400-MR, 400-MR DD2, VNMRS), and the legacy systems Inova, MercuryPlus, and Mercury-Vx, while VnmrJ 4.2 Datastation version provides off-line use on Windows and Mac OS X systems.

Major new features in VnmrJ 4.2 include:

- o **VeriPulse**: automatically optimizes shimming and RF calibrations from any starting point, generating comprehensive test reports of sensitivity, lineshape, and more. VeriPulse ensures that your system continues meet all of its installation specifications consistently and easily.

- o **CRAFT**: automated reduction of 1D spectra to a spreadsheet of frequencies and amplitudes. CRAFT can effectively analyze even the most complex spectra without supervision, making it possible to quantify an entire series of related spectra with the same amount of effort as a

single spectrum.  And since CRAFT operates in the time-domain, it avoids potentional quantification problems caused by phase and baseline.

- o **Non-Uniform Sampling (NUS):**  to get sharper spectra with less measurement time.  NUS can be used as easily as a conventional acquisition for most every pulse sequence, old or new, without modification.  VnmrJ NUS implementation automates both acquisition setup and processing. Advanced NUS sampling options include Poisson Gap and custom schedules.

- o **BioPack Express:** BioNMR setup and processing with walk-up simplicity.  Queue a complete series of BioNMR experiments in minutes, complete with automated setup of acquisition parameters, checkbox-easy options for Non-Uniform Sampling, and fully automated processing and display by NMRPipe.

- o **Enhancements to the User Experience, Graphical Interface, and Data Visualization:**
    - Help Overlays to introduce the software interface and basic workflow.
    - Context-sensitive help.
    - Attractive refactored User Interface.
    - Enhanced spectral drawing.
    - Enhanced Hard Copy formats.
    - Interactive spectral annotation.

## VnmrJ Core Features

- o Quick Submit: streamlined options for walk-up sample submission. Submit your sample in as little as 20 seconds and get your results by email.

- o Persona Manager: configure the system so that each user sees just the right software features and experiments for their goals and skill level.

- o Study Queue: build and automate collections of experiments and analysis to achieve a desired goal, independently of sample and spectrometer (i.e. once created, a study can be re-used for other samples and on other spectrometers).

- o ProShim: reliable automated shimming with methods adapted for specifically for sample type.

- o Quantitative NMR: calibrate it only once, and then get quantifications precise over six orders of magnitude in concentration for all subsequent measurements.

- o Adaptive NMR: automatic determination of optimal measurement time, so that no unneeded measurement time is used, and every measurement yields a useful result.

- o Industry-leading solutions for acquiring and analyzing Diffusion Spectroscopy (DOSY) data.

- Easy and effective setup of Band-Selective experiments and arrayed spectral series.

- Dynamic Parameter Inheritance: set up new experiments conveniently using previous settings with Sample-Specific Optimization of parameters:

    - Pulse widths and power settings calibrated specifically for the sample.
    - Shaped pulses are calculated on the fly, and recalculated automatically as needed.
    - All future experiments on sample can inherit these optimizations
    - Easily build new experiments by transforming existing ones: 1H 1D to 19F 1D to 19F/13C HSQC to 19F/195Pt HSQC … 1H/31P 2D …

- VnmrJ Secure Environment:   validation features, audit trails, and other tools to facilitate compliance with regulations for electronic record authenticity, such as 21 CFR Part 11.

## Other Features in VnmrJ 4.2:

- 3D Gradient Shimming:
    - Fully automated mapping and optimization of all RT shims with no additional hardware.
    - Compatible with all probe types.
    - Customizable "sample-to-sample" 3D shimming under automation (StudyQ)
    - 3D shimming can be incorporated into sample-centric shim method with Proshim 2

- Select Lock Signal: Select specific 2H signal to lock, useful for mixed solvents.

- New experiments, including Pureshift, AMESPack for solids, Excitation Sculpting.

- Enhanced central logging of accounting information.

- SolidsPack integration: provides VnmrJ's automation or parameter setup, experiment queuing, and Non-Uniform Sampling.

## VnmrJ and NMRPipe

- BioPack integration with NMRPipe: automated generation of NMRPipe spectral processing scripts for experiments in the BioPack sequence library.

- NMRPipe implementation of Iterative Shrinkage Thresholding (IST) for effective NUS processing.

- NMRPipe Applications: specView (1D and 2D Spectral Series Viewing with interactive Principal Component Analysis.

- NMRPipe application: automated local spectral alignment (for CRAFT).

# Spinsights

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