# Agilent VnmrJ 3.2 for INOVA and MERCURY*plus* Release Notes

Agilent Technologies

## Associated Products and Part Numbers

G9291AA: VnmrJ 3.2 for INOVA and MERCURY*plus* Media Kit
G9291-90001: *VnmrJ 3.2 Installation and Administration User Guide for INOVA and MERCURYplus*
91000170C*:* *VnmrJ 3 .2 User Programming Guide for INOVA and MERCURYplus*
91001988B: *VnmrJ 3.2 Spectroscopy User Guide*
91001987B: *VnmrJ 3.2 Automation User Guide*
91000167A: *VnmrJ 3.2 Imaging User Guide*

## System Applicability

The VnmrJ 3.2 for INOVA and MERCURY*plus* software is available only for INOVA, MERCURY*plus*, and MercuryVx spectrometer systems.

**NOTE** All references to MERCURY*plus* are applicable to MercuryVx as well.

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## System Requirements

### *Host computers with Linux OS*

- Hewlett-Packard Z400 (Red Hat Enterprise Linux 6.1)
- Dell Precision T3500 (Red Hat Enterprise Linux 5.3)
- Dell Precision T3400 (Red Hat Enterprise Linux 5.1, 5.3)
- Dell Precision 390N (Red Hat Enterprise Linux 5.1,5.3)
- Dell Optiplex 755N (Red Hat Enterprise Linux 5.1,5.3)
- No Sun/Solaris support

## System Compatibility

This software supports the following accessories and modalities.

| Accessories and modalities | INOVA | MERCURY*plus* |
|---|---|---|
| Liquids | yes | yes |
| Imaging/microimaging | no | no |
| Solids | yes | no |
| Cold Probe | yes | no |
| H/F experiments | no | no |
| Parallel PSG | no | no |
| LC-NMR/MS | no | no |
| VAST | no | no |
| SpinCAD | no | no |
| Secure Environments | yes | yes |
| AutoTest | yes | no |
| BioPack | yes | no |
| Nanoprobe | yes | yes |
| Agilent 21, 27 shimsets | no | no |
| Probe ID | no | no |

| **Automatic sample changers:** | | |
|---|---|---|
| 7600-AS | no | no |
| 7510-AS | no | no |
| AS-768 | no | no |
| SMS | yes | yes |
| Carousel | yes | yes |
| NMS | no | no |

| **Automatic probe tuning:** | | |
|---|---|---|
| ProTune | yes | yes |
| ProTune H/F | no | no |

## VnmrJ Password-Protected Options

There are several VnmrJ password-protected options that can be installed during or after installation. After VnmrJ 3.2 has been installed, these password-protected options can subsequently be installed using the VnmrJ command 'vnmrjOptions'. See the *VnmrJ 3.2 Command and Parameter Reference Guide* for details of the 'vnmrjOptions' command.

## New or Improved Features

### *Printing*

USB printers are supported.

### *Improved printing features*

Using CUPS (Common Unix Printing System) - a generic print dialog, JPG, PDF, and other formats are supported. Through the improved plotter setup interface, every physical printer can have multiple virtual device names and layouts.
A user-friendly, print-screen interface has been added.

### *International support*

Chinese and Japanese GUI versions have been updated.

### *Automation ProTune, ProTune-PZT/OneNMR probe support*

Improved and unified support of ProTune and ProTune-PZT. This includes automatically setting the RF phase with a console reboot.

Other enhancements include: increased sensitivity of tuning data averaging, added phase correction for propagation delay in the probe, enhanced status reporting, and better handling of exceptional situations when tuning motors.

**NOTE** VnmrJ 3.2 for INOVA and MERCURY*plus* does not support ProTune H/F.

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### *3D Gradient shimming*

Fully automated 3D gradient shimming is now integrated into the standard software. The automated features include: use of multiple samples, calibration, creation of 3D maps, and one-click-shim. There are additional options available

for interactive operation, such as flexibility to choose combinations of shim functions to map and shim. A real-time log provides logging as shimming progresses.

### *ProShim*

ProShim is a collection of routines that enables users to very rapidly and automatically shim a system. These routines are new in nature and complement all the other shimming methods available in VnmrJ. ProShim was introduced in VnmrJ 3.1 and enhanced in VnmrJ 3.2. It can use simplex optimization for multiple shims or third-order polynomial fitting for optimizing a single shim. The ProShim methods are implemented as a "prescan" for data acquisitions. It can be used for foreground data acquisition as well as for background automation. Shimming using the ProShim tools can take several minutes. Running the VnmrJ command killpshim will abort the currently executing ProShim method.

One of the main uses of ProShim will be to take the lineshape sample and automatically shim it to within specification in a much shorter time than it would take to do the same task manually. The resultant shims can then be stored for future use as reference or as a starting point for user's samples.

A further feature is the ability to schedule maintenance shimming on a regular basis. For this application, there is a requirement for a sample handling device so as to be able to insert the sample tube into the magnet at the scheduled time.

User's samples can be used in place of the lineshape sample with some restrictions.

These shimming tools are available in the "Tools" => "Standard Calibration Experiments".

### *qNMR: Absolute quantification*

This feature provides tools for facile display of integrals with 1H spectrum in absolute concentration, and for automatic creation of reports for quantification for purity analysis of known compounds.

An interactive analysis tool has been added to the interface allowing a user to individually select each integral in a processed data set, assign the number of nuclei represented by each integral, and then select the desired integral regions for inclusion in the calculation of absolute sample concentration.

After a one-time calibration of the system using a known concentration of calibrant in its own discrete sample tube, any further spectra recorded on samples of unknown concentration with the same pulse sequence can be

quantified absolutely. The calibration information is stored in the probe file for subsequent use. The software takes into account differences in pulse widths, gain settings, number of scans etc. to arrive at an estimated concentration for signals in the unknown sample.

There is no need for any internal or external chemical additive or any synthetic electronic substitute signal. It is the intrinsic stability and robustness of the console that provides the ability to quantify any sample based on information from another known quantity.

Additionally, an 'Application Directory' is provided that enables automatic creation of reports when doing quantification experiments, for purity analysis of known compounds.

### *Adaptive NMR*

Based on the same calibration done in qNMR using an external sample, further experiments submitted for acquisition on a user's sample can have the number of scans, or scans per row, adjusted automatically to ensure good quality data in terms of S/N. All that is needed is for the user to enter the sample concentration at submission time.

This new feature avoids a common situation where considerable amounts of time can be wasted gathering inadequate/noisy data. This is especially applicable to those experiments with low sensitivity whether it is because of intrinsically lower nuclear gyromagnetic ratio(s) and/or inefficiencies in coherence transfer during a pulse sequence. Users tend to guess high to avoid this situation, and that can waste valuable magnet time when the sample is actually of sufficient concentration. User experiments can be incorporated by editing a simple text file.

The user can view the estimated time the adjusted experiment would take before committing the experiment to the queue for acquisition. If it is decided that the experiment will take too long then the user can preemptively choose to add more sample if available, or possibly move to a spectrometer with more sensitivity, or choose not to do the experiment at all, all the while avoiding wasting valuable magnet time that other experiments or users can make good use of.

In the majority of cases when an experiment fails due to an unacceptably high noise level the sample is usually re-submitted anyway with corrected parameters,

therefore this valuable feature can actually save total time taken on a per sample basis.

### *Additional support for remote operation*

Automatic installation of TurboVNC server and viewer with VnmrJ 3.2.
Integrated VNC server control from within the VnmrJ 3.2 Admin interface.

### *Enhanced batch submission*

1. 'csvimport' has been replaced with 'csv2cpQ'. The new utility still parses incoming spreadsheet files in comma separated value format, but allows for more flexibility in the contents and formatting of the file. For example, if a column header is not recognized as an NMR parameter it is skipped. This allows one file to be created that contains sample information for more than just the NMR technique, e.g. MS or HPLC, yet still be used as direct input for submission to the NMR instrument.
2. It is now possible to run VnmrJ on an offline datastation in a way that mimics experimental submission to a spectrometer. The information submitted is saved in a convenient form, whereupon at a later time it can be digitally transferred to a real spectrometer host along with the sample tubes for batch acquisition, automatic processing, analysis, and delivery of results.

### *System-Specific Parameter Retention*

While upgrading to VnmrJ 3.2, the installation copies system-specific parameters from the previous "/vnmr/conpar" file to the VnmrJ 3.2 "/vnmr/conpar.prev" file. System Configuration, **Edit > System Settings > System config**, loads VnmrJ 3.2 'conpar' parameters then reads and loads parameters from "conpar.prev".

### *Study and experiment 'Clones'*

Using standard tools found in the menus, it is now possible for the user to create new entries in the Experiment Selector that can execute individual or a collection of customized experiments. At the time of creation, these new entries can be placed in any tab in the Experiment Selector.

The mechanism used to clone studies allows a user to create a palette of customized experiments without the need to edit any system files. Clones can be created to perform a highly detailed investigation such as a customized experiment to analyze a specific molecule, or they can be used to create a

general set of experiments containing all the user-specific customizations one wants.

## *NMR Experiment enhancements*

### Enhanced sample-centric Study Queue and workflow

The Study Queue has been re-designed to be sample-centric and to increase the throughput of samples and enhance the workflow.

Up until VnmrJ 3.0 one had to decide up front whether the experiment for the sample of interest was going to be acquired in the foreground ( using the 'go'/'ga'/'au' commands directly or buttons that executed these commands ) or in the background ( via the StudyQ window ). This required the user to learn two different workflows by pressing different buttons or typing commands in an unrelated manner. Now in VnmrJ 3.x, the user can set up all desired experiments in a generic Study using the familiar Experiment Selector and StudyQ interface without having to commit how the acquisition will take place, and at the end the user can decide whether to send the list to the foreground or background. If a sample changer is present then there will be a further choice to send the list to automation.

After the experiments have finished, regardless of whether they were acquired in the foreground or background, the Study can be used to drag & drop data into any Viewport for interactive analysis, or it can be used to 'Continue Study' if more experiments are desired for this Study. All 'Continue Study' operations have the same flexibility to choose whether to send any new experiments to the foreground, background or automation, so it is possible to mix & match at the user's discretion.

This 'sample-centric' approach is partly achieved using a new concept : 'Sample Tags', which are simply a persisted group of values of user-defined NMR parameters within individual datasets that connect related data together wherever they may be filed and/or whenever they were acquired. Each Study maintains its own mini-database of file and content information such that, when located on a shared network disk, it can contain data from multiple spectrometers and/or dates all in one Study displayed in a StudyQ window.

The Study Queue also sports an improved and user-friendly interface. The new Study Queue is integrated to work with automatic sample changers.

Pre-VnmrJ 3.2 data can be converted with a built-in utility to make legacy datasets "sample-centric" aware.

## Experiment Selector

The Experiment Selector has been re-laid out to accommodate a whole slew of new and improved pulse sequences. They are all still grouped into "families" of related functionality but there are new tab names and many more members in each tab than found previously.

Users can now re-order the Experiment Selector tabs by use of a popup accessible from the 'Edit' menu.

## Experiment menu

Using the Experiments menu there is now the ability to: start / initialize a new experiment in the current workspace, bring in default parameters from the disk, overwrite old values if present, and reset any Sample Tags in the process. The experiment is ready to be further setup / interaction / eventual submission to the Study Queue or to be acquired in the foreground. Morphing / converting the current experiment into another is now sensitive to the observe nucleus, thereby preserving a subset of relevant parameters from the old experiment, whilst bringing in required parameters and their values from disk for the new experiment. This means that the same menu selection may morph into different experiments depending on what the observe nucleus, and all its dimension-specific acquisition parameters and their values, are set to. This makes the menu very flexible and extensible, allowing far more combinations than defined by a simple list-count of the menu itself.

Now available are multi-frequency PRESAT and multi-frequency PURGE methods in all pulse sequences that support solvent suppression. WET suppression has been enhanced to ease the selection of signals that need to be removed from the spectrum. The software can now be directed to: pick the biggest N peaks, use explicit values input by the user in a table, pick as many peaks as it finds above a certain vertical threshold. All of this is now available from one parameter panel.

Selective 1D experiments have been greatly enhanced. From the same set of parameter panels it is possible to: set up the experiment, run a trial spectrum, display it on screen in a 'wait' state, let the user define the irradiation frequencies interactively using the mouse, and run the selective irradiation experiment or define the irradiation frequencies explicitly. The experiment will create the shaped pulses automatically and then run the experiment.

Several band-selective 2D experiments are now available. In a similar manner to the selective 1D experiments, the user can set up the experiment to: run a trial

spectrum, display it on screen in a 'wait' state, define the frequency band interactively, and run the selective irradiation experiment or define the irradiation frequency band explicitly. The experiment will create the band-selective shaped pulse automatically and then run the experiment.

### *Specific experiment improvements:*

- NOESY experiment now has a zero-quantum suppression option. Solvent suppression is now available during the relaxation delay and/or the mixing period.
- TOCSY experiment now has a choice of MLEV17, MLEV17c, DISPSI-2, and DIPSI-3 mixing schemes. An optional z-filter with or without an H2O flipback pulse is now available.
- ROESY experiment now has an optional z-filter with or without an H2O flipback pulse.
- TOCSY1D experiment now has independent control of power/shape/gradient strength for both of the PFG echo pulse trains. There is a choice of MLEV17, MLEV17c, DISPSI-2, and DIPSI-mixing schemes.
- ROESY1D experiment now has independent control of power/shape/gradient strength for both of the PFG echo pulse trains.
- NOESY1D experiment now has independent control of power/shape/gradient strength for both of the PFG echo pulse trains. Zero-quantum suppression is now an option.
- HSQCAD and gHSQCAD experiments use adiabatic pulses for inversion and CRISIS adiabatic pulses for X-refocusing.
- HMBC, HMBCAD, gHMBC, and gHMBCAD experiments are now phase-sensitive for narrower line shapes. Uses adiabatic pulses for inversion.
- New gH2BCAD experiment. Uses adiabatic pulses for inversion.
- New gHMBCme experiment. Allows for multiplicity editing to simplify spectra and categorize signals by the number of attached protons. Uses adiabatic pulses for inversion and CRISIS adiabatic pulses for X-refocusing.
- New bsHSQCAD and bsgHSQCAD experiments. These select the band in F1 using the DPFGSE method. Uses adiabatic pulses for inversion and CRISIS adiabatic pulses for X-refocusing. Can select band interactively or explicitly.
- New bsgHMBC experiment. Band-selective in F1 using DPFGSE. Uses adiabatic pulses for inversion and CRISIS adiabatic pulses for Xrefocusing. Can select band interactively or explicitly.
- New DEPTQ experiment.

## *Updated DOSY package (optional add-on)*

A new calibration and correction for non-uniformity of the pulsed field gradients (NUG) in 2D and 3D DOSY is implemented.

**New DOSY processing methods:**

- monoexponential fitting with NUG correction
- biexponential fitting, with and without NUG correction (using a modified SPLMOD)
- multiexponential fitting, with and without NUG correction (using a modified SPLMOD)
- fitting of distributions of diffusion coefficients with CONTIN

**Performance enhancements:**

- improved support for 3D DOSY, including P- and N-type absolute value and phase-sensitive processing
- display of residuals
- optional point-by-point instead of peak-segmented 2D DOSY fitting and display
- removal of peak number limitations in 2D DOSY

## *Referencing*

Referencing of spectra has been enhanced in VnmrJ 3.2. There is a new default method, 'auto referencing', that pre-calculates referencing parameters when any the 'go/ga/au' commands are given, in foreground or background. By default, 'auto referencing' will use a scheme based on IUPAC recommended nuclear frequency ratios, which we call 'standard referencing'. Users can override 'standard referencing' and apply 'user referencing', which will also be respected by the 'auto referencing' calculation just prior to acquisition.

- Reference standard can be selected using "Select Reference Standard..." dialog from the Tools menu. User may select 'Standard' or 'Bio', or select reference compound for individual nucleus.
- If reference is manually set by the user using rl (or rl1, rl2), the difference between 'user referencing' and 'standard referencing' is stored in refpos (or refpos1, refpos2 etc.). User referencing will be respected by 'auto referencing' in the 'go/ga/au' commands.
- The command to restore 'standard referencing' as the default method is 'setref' (or setref1, setref2). The command to clear 'user referencing' (so that 'auto referencing' will be the same as 'standard referencing') is setrefpos(0). The command to clear any referencing (so that the upfield edge of the spectrum starts from zero) is crl.

- When lock is not used (enabled by creating and setting global parameter uselockref='n'), a pre-calculated H1reffrq will be used to calculate reference frequencies for all nuclei. H1reffrq can be set using a known peak with setBaseref(freq) command.

## *Hadamard experiments integrated into the StudyQ*

**NOTE** This feature is only available for INOVA systems.

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It is now possible to submit an expanded suite of Hadamard experiments for acquisition in the background by choosing them from the 'Hadamard' tab in the Experiment Selector. Previously they were only available from the 'Experiments' menu and could only be run in foreground.
It is now possible to manually pre-define any line lists that subsequent Hadamard experiments need by generating them from previously acquired data present in the Study.

## *BioPack enhancements*

**NOTE** BioPack is only available for INOVA systems.

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BioPack is now an 'Application Directory' that is directly installable using the generic VnmrJ installation utility. When installed all files reside in '/vnmr/biopack' and can be turned on or off via the 'Edit Applications ...' popup found in the 'Edit' menu.

Projection Reconstruction experiments are supplied separately as a password protected installation option. Please contact your local sales representative for more information on how to obtain the password.

BioPack integrates access to NMRPipe (optional add-on) for data processing and display. One can access the standard NMRPipe tools from within VnmrJ 3.2. One can also bring NMRPipe processed data back into VnmrJ for display and plotting. Support for non-linearly sampled (NLS) data is included. One can acquire the data and process it using the CLEAN technique or the MDD technique. See the BioPack documentation for details of these additions.

### *Persona Manager*

VnmrJ allows customization of access to interface panels and tools using a "rights" mechanism. VnmrJ 3.2 introduces a tool to simplify administration of these rights by defining a persona with rights. Users and operators are then associated with a persona. For example, VnmrJ 3.2 provides default rights for Chemist, Owner, Spectroscopist, and Student personae. The "Persona Manager" is available from the Tools menu.

### *Secure Environments*

VnmrJ has had a "Secure Environment" product. In VnmrJ 3.2, this has been made into a freely available option. To use this option, you must select the "Secure Environments" option from the VnmrJ installer. This option is not available for the Mac and Windows versions of VnmrJ. See the Secure Environments manual for details.

### *Study Queue*

New features for the VnmrJ Study Queue include an "express submit" mechanism. An enhanced event log tracks many events during the execution of a study. There is also a new tool to mimic the operation of the study queue. Experiments can be swapped between the day queue and night queue. Autocalibration is supported, in background automation and in foreground operation. Using the tray display, one can copy and paste a study from one location (from any tray) to another location in the current tray. Probe files can be maintained in any valid appdir, not only userdir and systemdir. All scout experiment results are accessible from the study queue. Adaptive NMR, introduced in VnmrJ 3.1, is enhanced to allow optional manual entry of the concentration at the time a study is submitted. This allows the adaptive NMR feature to set the number of scans for each experiment in a study, based on user estimated/entered concentration.

### *Alternating gradients*

The parameter gradalt is introduced to facilitate implementation of alternative gradients in a pulse sequence. This can help minimize gradient recovery. See the User Programming manual for details.

### *Miscellaneous enhancements*

VnmrJ 3.2 introduces several enhancements to commands. Details will be found in the Command and Parameter Reference manual and the manual page in /vnmr/manual.

### *Added functionalities for existing commands*

- Data acquisition allows parallel arrays for nD experiments.
- Autogain allowed for arrayed experiments.
- ‘array’ parameter can disable arrayed experiments.
- ‘change’ command modified to remove sample if ‘loc’ parameter is set to 0.
- ‘seqgen’ updated to handle ‘appdirs’. ‘seqgenupdate’ added for appdir support.
- ‘ft1d’, ‘ft2d’, ‘ft3d’ commands now have ‘noft’ option.
- ‘substr’ has additional options and return values.
- New arguments for ‘create’ command.
- ‘autoname’ allows embedding of the ‘Rn’ specification.
- Additional options for ‘appdir’, ‘debug’, ‘spadd’, ‘setprotect’, ‘readparam’, ‘atcmd’, ‘readhw’, ‘au’, ‘su’, ‘diffparams’, ‘procmd’, and ‘go_Options’ commands.
- ‘vnmrjcmd’ opens a browser panel in a specific directory with ‘LOC browserPanel’ argument.
- ‘destroy’ command handles multiples arguments.
- ‘aph’ can select or ignore regions of the spectrum during optimization.
- arrayed spectra displays (dssh, dss, etc) support vertical scale adjustment by using the mouse wheel.
- ‘getvalue’ supports the ‘size’ option.
- ‘atcmd’ supports the ‘active’ option.
- ‘sqLog’ allows multiple arguments.
- ‘setallshims’ can set subsets of shims.
- ‘unixtime’ and ‘systemtime’ will return formatted time stamps and interconvert formatted time stamps and elapsed time.
- ‘chkname’ allows the dash character (-) in filenames. It also supports local macro “$ variables” (e.g., $val) as template variables.
- ‘sethw’ can set the ‘status’ value of the console.
- ‘go’ supports the ‘checkarray’ option to check all elements of an arrayed experiment.
- ‘write’ can write warning messages (typically in yellow, but the color is selectable with the “Display options” popup).
- ‘debug’ supports a ‘c0’ option.
- An interactive baseline correction tool is available from the Process menu.
- An interactive “Sample in Magnet” tool is available from the Tools menu for systems with a sample changer.

## Fixed Defects

Bugs that have been fixed since the release of VnmrJ 2.2D can be found on this web page :

http://www.chem.agilent.com/en-US/Support/Pages/NMRBugLists.aspx

## Technical Support

Online technical support, including a bug reporting form is available at:

http://www.chem.agilent.com/en-US/Support/Pages/NMRSoftwareCorner.aspx

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