Vnmrj 3.1 New and improved features

Automation & Hardware

Printing
USB printers are supported.
Using CUPS, a generic print dialog and JPG, PDF, & other formats have replaced the previous method of sending output to physical and electronic devices.
There is an improved plotter setup interface within VnmrJ - every physical printer can have multiple virtual device names and layouts. A user-friendly print screen interface has been added.

New shim set support
Supports the new Varian 21- and 27-channel shim sets.

Automation Sample Changer Support
New "sample in magnet" pop-up provides additional options.
7600-AS - Supports the three axis SCARA based robot. Supports both the high-throughput (batch) mode and the multi-user (open-access) mode.
7510-AS - Supports the 12-pack plug-and-play autosampler.

Automation ProTune, ProTune-PZT/OneNMR probe support
Improved and unified support of ProTune and ProTune-PZT is provided. This includes automatically setting the RF phase with a reboot of the console. Other enhancements also include increased sensitivity of tuning data averaging; added phase correction for propagation delay in the probe; enhanced status reporting; better handling of exceptional situations when tuning motors.

Support for E5025 Cryogen Monitoring
Integrated interface in VnmrJ for cryogen monitoring of Helium and Nitrogen levels.

Additional support for Remote Operation
Automatic installation of TurboVNC server and viewer with VnmrJ. Integrated VNC server control from within the VnmrJ Admin interface.

Legacy data
Pre-VnmrJ 3.0 data can be converted with a built-in utility to make legacy datasets "sample-centric" aware.
Conversion is not mandatory, legacy data can be read in and interacted with normally, but cannot be made part of a SampleQ without prior conversion.
NMR Experiment Enhancements

Enhanced "Sample-Centric" StudyQ and Workflow

The StudyQ has been re-designed to be "sample-centric", to increase the throughput of samples, and enhance the chemist's 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 "SampleQ" 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 SampleQ 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 SampleQ. 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 SampleQ 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 SampleQ displayed in a StudyQ window.

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.

New for VnmrJ 3.1 - Users can now re-order the Experiment Selector tabs by use of a pop-up accessible from the "Edit" menu.

"Experiments" Menu

Using the "Experiments" menu there is now the ability to start / initialize a new experiment in the current workspace, bringing in default parameters from the disk, overwriting old values if present, and resetting any "Sample Tags" in the process. The experiment is ready for further setup, interaction, customization, and eventual submission to the foreground, background or automation (sample changer required for automation).

From the same menu, converting the current experiment into another is 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 is set to in the current experiment (and all its dimension-specific acquisition parameters and their values). This makes the menu very flexible and extensible, making available far more combinations of possible experiments than that defined by a simple list-count of the experiment library.

**Tray Display**

The Tray Display used to represent the sample tray on systems equipped with robot sample changer has been improved. The display is now interactive allowing a user to right-click any location to perform a number of functions, such as adding new experiments to a location queue, creating a clone of a location queue for reuse later, resubmitting a location queue to acquisition, deleting a location queue from the spectrometer queue, changing the sample for that location, etc.

**Signal Suppression**

In all pulse sequences that support solvent suppression, multi-frequency PRESAT and multi-frequency PURGE methods are available. 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. Control of all of these options is available from a single parameter panel.

**Selective 1D Experiments**

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

**Band-selective 2D Experiments**

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 F1 frequency band interactively, and then run the selective irradiation experiment; or, define the irradiation frequency band explicitly and the experiment will create the band-selective shaped pulse automatically and 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-3 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 X-refocusing. Can select band interactively or explicitly.
• New DEPTQ experiment.

Expanded capability to do 19F/1H experiments

FH_HETCOR, FH_HOESY and 19F/1H observe and/or decouple combination experiments are now available from the Experiment Selector.

Referencing (New for VnmrJ 3.1)

Referencing of spectra has been enhanced in VnmrJ 3.1. 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.

Enhanced Batch Submission

- 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.
- 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.

Study and Experiment "Clones" (new for VnmrJ 3.1)

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.

Enhanced DOSY Package (Optional Add-On)

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

New DOSY processing methods:
- monoexponential fitting with NUG correction
- biexponential fitting, with and without NUG correction (uses a modified SPLMOD)
- multexponential fitting, with and without NUG correction (uses a modified SPLMOD)
- fitting of distributions of diffusion coefficients with CONTIN

Performance enhancements, including
- 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
Absolute Quantification - qNMR

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.

New for VnmrJ 3.1 - 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.

Adaptive NMR (new for VnmrJ 3.1)

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.

Hadamard Experiments Integrated into the StudyQ (new for VnmrJ 3.1)

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 SampleQ.

**ProShim (new for VnmrJ 3.1)**

ProShim is a collection of new 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. Protocols are available in the Experiment Selector that do varying degrees of shimming based on the time available to the user for the task and the requirements for how well shimmed the user wants the sample to be at the end of the process.

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.

**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 the flexibility to choose combinations of shim functions to map and shim. A real time log provides logging as shimming progresses.

**BioPack Enhancements (new for VnmrJ 3.1)**

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 ..." pop-up 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.