

Release Notes

VNMR 6.1C

VNMR Version 6.1, Release C, adds new features to VNMR software and fixes problems from previous versions of VNMR.

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Information about commands, macros, and parameters printed in a typewriter-like font (e.g., `acqi`, `loc`) can be found in the manual *VNMR Command and Parameter Reference*.

This software also supports a new acquisition computer. Consequently, the VT cable, which used to be plugged into the serial port (of the CPU board) MUST be moved to the serial port of the MSR board no matter which acquisition processor is used.

Everything required to use SpinCAD is included on the CD. JAVA 1.2.5-05 is required. Solaris 2.6 or a later version is required.

Preserving A Previous Version of VNMR

When you install VNMR 6.1C, you can preserve a previous version of VNMR by entering the name of VNMR 6.1C in the destination directory as
`/export/home/vnmr.6.1C`

Specifying the 6.1C version in the name prevents the version of VNMR installed on your system from being overwritten and enables you to save macros that you might have created and linked to the previous version.

SpinCAD

SpinCAD™ is a graphical pulse sequence programming environment. It enables you to create a pulse sequence by dragging and dropping familiar NMR elements such as a pulse, gradient, and delay. At another level, it provides a mechanism to directly set the spectrometer hardware, such as turning on a TTL gate. SpinCAD also enables you to build your own collections of elements for reuse in different pulse sequences. For example, you might build a watergate segment, which can then be dragged out and connected to any sequence.

SpinCAD provides a convenient mechanism for specifying events on different RF channels. These can be constructed as a serial class of events or as events that occur in

parallel. SpinCAD also uses a completely new model for representing the pulse sequence. As a result, the amount of disk space needed to hold the sequence has been reduced for 2D, 3D, and 4D experiments from tens of megabytes to tens of kilobytes. The starting time for these experiments has been reduced to seconds.

The `dps` program can display SpinCAD sequences. A new option to `dps` enables you to view the fine details of a SpinCAD pulse sequence. In this mode, all the primitive hardware events are shown. This mode is selected with `dps ('-fine')`.

A version of `exptime` for SpinCAD produces accurate time estimated by stimulating the sequence.

For more information about SpinCAD, see the *SpinCAD* manual.

Pbox

The same Pbox is now used for UNITY and MERCURY systems.

Pbox has also been directly integrated into SpinCAD and has the following improvements:

- Bloch-Siegert shift compensation for multiple excitation (Ref.: C. Yannoni, M. Steffen, L. Vanderseypen, M. Sherwood, G. Breyta and I. Chuang, *Abstracts of the 41st ENC*, p. 268, Asilomar, 2000). The syntax is `bscor=y`.
- A new directory, `wavelib/flipback`, contains excitation pulses configured to act on xy-magnetization. The pulses are mainly for convenience when used from SpinCAD.
- BIR-4 pulses are easier to generate for an arbitrary flip angle. Syntax: `bir4-45r` generates a plane rotation pulse with 45° flip angle.
- Shape arrays and pulse shaping from within a pulse program. Any of the Pbox parameters can be used as an argument to the command `Pbox` when used from a shell. A new option, `-u userdir`, has been added to support use during automation.
- The `.Pbox_defaults` file has been discontinued. All defaults can be changed via the `.Pbox_globals` file.
- The `cpx` macro accepts the calibration parameters, for instance:
`cpx(pw90*compH, tpwr)`
- A new parameter, `stepsize (-s option)`, enables you to define the length of a single time slice in a shaped pulse.

LC-NMR and VAST

There have been changes in both the acquisition and processing of VAST and LC-NMR data. For both techniques, acquisition now supports automated WET suppression of up to seven solvents, and the Sequence Tcl-dg panel has a new powerful layout to support checkbox selection of searching, suppression, and `ssfilter` capabilities. In LC-NMR processing, when Ethernet to the PC is activated, the LC data is shown with the NMR data in an integrated display. The Spare Tcl-dg panel now supports push-button plotting and optimization of the LC-NMR data. In VAST processing, a number of new and improved routines exist for customized VAST plotting, including matrix plots and contour plots. A new `plateglue.tcl` routine (in `/vnmr/bin`) enables you to rearrange the display order of glued VAST data.

DOSY

3D DOSY is now implemented.

A new family of pulse sequences (whose names begin with a capital D) automates the calculation of the pulse sequence parameters needed to calculate diffusion coefficients, making it unnecessary to modify the `dosy` macro when new pulse sequences are implemented.

The new sequences all use the delay `gt1` to define the total width of gradient pulse used for one diffusion-encoding episode, i.e., the actual gradient pulses in a bipolar sequence are of width `gt1/2`. Similarly, the diffusion delay `del` is the actual time over which diffusion is measured, i.e., the time between the mid-points of the two diffusion-encoding episodes.

The `dosy` command now synthesizes the dosy spectrum in the current experiment, making `showdosy` unnecessary. The `undosy` and `redosy` macros allow easy conversion between 1D and 2D display.

The `fiddle` command has been substantially upgraded.

The `ddif` command has been upgraded to ensure that projections are fully quantitative and sharp diffusion peaks are not missed.

FDM

FDM (Filter Diagonalization Method) is a non-Fourier data processing method that extracts spectral parameters (peak positions, linewidths, amplitudes and phases) directly from time-domain signal by fitting sums of exponentially decaying sinusoids to the FID data.

The `fdm1` macro processes 1D data. The FDM package is available as a separate package.

Solaris

Solaris patches required for Solaris 2.6 and Solaris 7 are also included on the VNMR CD. Although Solaris 8 is compatible with VNMR 6.1C, it has large disk space requirements and is not generally recommended for older systems.

Although VNMR runs with older versions of Solaris, certain features such as `Tcl-dg`, `SpinCAD`, and `jplot` will not work.

Other New Commands and Features

Imaging

Some changes have been made on imaging systems. A complete set of imaging `Tcl-dg` parameter templates has been added. These are selected when `appmode='imaging'`. Interactive image planning tools have also been added. This is initiated by the `iplan` macro. Changes have been made to the `draw` and `box` commands, the `tbox` command has been added, and the `trfunc`, `trfuncd`, `rsliceplan` macros are used to implement image planning.

Support for PowerPC Acquisition Computer

Support for a PowerPC acquisition computer has been added. This new computer supports 10BaseT and 100BaseT Ethernet standards.

Note: As a consequence of this support, the VT cable **MUST** be moved from serial port 3 on the CPU board to serial port 2 on the MSR board for all acquisition computers.

load.nmr Takes a User Name

The command `load.nmr` takes a user name as system administrator. For example, `load.nmr sandy` makes *sandy* the owner of the files in the newly installed VNMR. The default user name is still `vnmr1`. If the default is not used, the user name must already exist as a UNIX account.

Magical Capability Enhanced

Several features have been added to enhance the macro capability. A new parameter (`$##`) is now available to Magical. The value of this parameter is set to the number of return arguments expected by the caller of the macro. So, if a macro has a line

```
mymacro: $val, $type
```

then the value of `$##` in `mymacro` is 2. This feature might be used to decide if a message should be printed or a value should be returned.

The `lookup` command has also been improved. It has an `'mfile'` option to keep track of the search position in multiple files.

The `substr` command can now be used to substitute characters in a string variable.

The new `mt` macro moves text to another experiment.

The rule for determining whether a return value is a string or number has been improved. A return value is interpreted as a real number if it is a proper numeric string. Leading blanks are permitted but extra nonnumeric characters are not permitted. The characters `e` or `E` are permitted as part of a number (e.g., `1.2e4`).

Note: This improvement might affect existing user macros. Potential commands that return strings and numbers are the `shell` command and the `lookup` command.

The `format` command has an `isreal` option that can be used to test a string to determine if it represents a real number.

The `unlock` command has a `force` option that forces the removal of an experiment lock file.

The `au` macro has a `'silent'` option that suppresses the following messages:

- `experiment started`
- `block size complete`
- `exp complete messages`

Error messages are still displayed.

phasef, New n and y Parameters

The global `phasef` parameter controls sensitivity of the right mouse button during phasing. It ranges from 0.01 to 100. The value 8.0 is the default. Global parameters `n` and

y have been added, with values 'n' and 'y'. Therefore, you can use n or y in places that you used to use 'n' or 'y', for example, gain=n or gain='n'.

Waveform Generator

The waveform generator can now set phase to 0.25°.

Shaped pulses that do not use a waveform generator are now scaled by the appropriate pwr parameter.

Adobe Acrobat Reader

Adobe Acrobat Reader version 4 is used for online manuals. The manuals are on a separate CD, which can be used as the manual source (giving access to the complete VNMR documentation) or they can be loaded onto disk, in which case, the generic parts and the manuals that are specific for the selected hardware can be loaded.

Bugs Fixed

+acqaddr.6101 ++	Data station changes acqaddr to troi 33154 2037.
+acqinfo.6101 ++	An extra file causes error messages on data stations.
+acqi.6106 ++	Might set spin=102
+acqi.6120 ++	No lock display.
+acqi.6121	Shim thermometer temporarily loses all signal.
+acqstat.6104	Does not work with pad array.
+acquisition.6102 M	ADC overflow flag is not reset in arrayed acquisitions.
+acquisition.6113 ++	su/go/ga might become very slow.
+acquisition.6115	On MERCURY systems, the console does not boot.
+acquisition.6119	Stops after first bs.
+alock.6101 I	Does not work with methanol under automation.
+apdelay.6101 M	File/definition table is missing on MERCURY.
+apt.6101	Data cannot be phased.
+array.6101 M	Arrays with ss=1 or ss=-1 might not complete.
+autocalibrate.6101	tn='H1' dn='C13' incorrectly sets decoupling parameters.
+autocalibration.6101 ++	Fails if variable "probe" is not set.
+autocalibration.6102 ++	H1 autocalibration fails on H/C GEMINI.
+autocalibration.6104 ++	dpwr is incorrect if solvent is unknown.
+automation.6109 ++	Does not do gradient shimming with custom experiments.
+automation.6110	Customized parameters are not activated.
+automation.6108	Gradient shimming does not work.
+automation.6113 ++	Parameter customization might be inactive.
+autoname.6102	Might extract undesirable characters into file name.
+autosetgpar.6101 ++	Fails for C13 or P31.
+autotest.6101 ++	Unable to remotely run autotest.
+autotest.6102	13° test reports wrong value.
+autotest.6103 ++	Gradient calibration fails with Performa I.
+autotest.6104 ++	Channel 1 amplitude stability tests fails.

+bootup.6101 ++	login macro is not executed if located in maclibpath.
+bp3d.6101 ++	The bp3d.c pulse sequence file is incorrect.
+compressfid.6101	Does not work when in exp>9.
+config.6105	Ejects/inserts sample after "Exit an Save."
+config.6106	Does not include AutoTest for UNITYplus.
+cosy.6102 ++	Does not set window functions.
+dcon.6101 ++	Might crash VNMR when graphics window is iconified.
+dept.5101	Sets the solvent to cdc13.
+dg.6101	Not updated with change of seqfil.
+dg.6114	As supplied, Tcl-dg does not work with LC-NMR.
+dg.6116 ++	Gradual increase in CPU usage when dg not in text mode.
+diffusion.6101 ++	pge_process produces incorrect values for D.
+disp3d.6101	Seems dysfunctional; core dump on launch.
+dotlogin.6103	Value for variable GCC_EXEC_PREFIX is incorrect.
+dps.6101	Problem with multiple settable calls and arrays.
+enter.6107	Erroneous display with automatic user identification.
+enter.6108	Customizing for automatic sample numbering fails.
+enter.6109 ++	Does not allow for customized F19 or P31 acquisitions.
+enter.6110	Customized parameters are not used.
+files_edit.6101 ++	Nonfunctional.
+files.6102	Can cause VNMR core dump when asked for more elements.
+fixpar.6101 ++	Unnecessary compatibility warnings on data stations.
+ft2d.6101	Crashes VNMR if fn is too large.
+ft3d.6102	Fails with experiments above 15.
+gettext.6101 ++	Fails if first character of text is a digit.
+ghmqc.5301 ++,M	Incorrectly sets power levels on MERCURY.
+gilson.6102	Does not retain vast alignment info.
+glide.6101	Queued experiments do not proceed after aph failure.
+glide.6102	P31 Autocalibration gives an error.
+glide.6103	Does not support numeric filenames.
+glide.6104	Text lost from chained 1D experiments.
+glide.6105	Customization in chained 1D experiments is ignored.
+glide.6106	Colors do not properly map to Exceed.
+glide.6107	Autocalibration generates an error.
+glide.6108 ++	Autocalibration options might fail.
+glide.6109	Indirect detection macros all set dn='C13'.
+gmapsys.6102 ++	Button for PFG H2 shimming gives unrecoverable error.
+gradshim.6109	Parameter values gmap_findtof and gmap_z1z4 are not retrieved.
+gradshim.6110	Cannot create shimmap with nt>4.
+hmqc.6101 ++	Produces an error message.
+il.6103	Arraying shims with il='y' fails.
+jdesign.6103	Usable character set might be extremely limited.
+lc-nmr.6101	sw1 is not properly set during gluing.
+lc-nmr.6102 ++	Time axis calculations are incorrect for isocratic runs.

+lcld.6101 ++,U	Sequence does not compile on UNITYplus.
+noedif.6101	Fails with ctrl='y'.
+noedif.6102	Fails on MERCURY.
+nuctab7d.6101 ++	nuctab7d has incorrect frequency values.
+nuctables.6101 ++	Values for H2 and H3 are mostly incorrect.
+pad.6101	Parameter has no effect.
+pacosy.6101	Does not plot correlations.
+patchinstall.6106	Error message: "Is not suitable for this system."
+pbox.6102	Might fail in automation or LC-NMR.
+pbox.6103	Corrupt menu Pbox180b.
+pbox.6104 ++,M	SLP pulse frequency offsets wrong on MERCURY.
+plc.6101 ++	pltmod='user' is no longer defined.
+pwxlvl.6101 ++	Has improper parameter limits.
+qtune.6101	Might use too much power by default.
+qtune.6105	Does not work on MERCURY-Vx.
+qtune.6106	Gives error upon startup.
+qtune.6107	Does not reset oversamp parameter for dsp='r'.
+qtune.6108 ++	FIFO and np errors
+qtune.6109 ++	Does not properly exit.
+return.6101	Disables exit in VNMR.
+rtcmx.6101	Phase-sensitive 2D data is not recalled.
+setacq.6102 ++	Might fail on comment lines.
+setacq.6106 ++	Alternative local IP address is wrong.
+setgcoil.6101	setgcoil does not update compar.
+setup.6101 ++	Always retrieves dpwr and dmf from probe file.
+setref.6103 ++	N14/N15 referencing uses old standard.
+sh2pul.6101 ++	Should support independent powers for the two pulses.
+shaped_pulse.6101	Modulator based shaped pulses do not properly scale.
+su.6101 ++	Causes FIFO underflow with RRI Ultrashims.
+time.6102	Fails to set experiment time (nt) properly.
+time.6103	Fails to set experiment time (nt) properly.
+tmsref.6101 ++	Fails if sw starts above TMS search range.
+unit.6101	intercept argument does not have any effect.
+unlock.6101 ++	Might remove lock file in current experiment.
+userlib.6102	Autocalibration failure on CH3I sample.
+vast.6108	Might fail if Expproc is started by root.
+vastld.6101 ++	Pulse sequence cannot find phase table lcld.
+vnmr.6115	Often crashes on remote X servers.
+vnmr.6117 ++	Might crash when trying cd into a long path.
+wfg.6102	Might skip last pattern element.
+wft2da.6101 ++	Full 2D FT might give corrupt phase file.
+xpolar1.6101 ++	PDP and TOSS are nonfunctional with xpol='n' and nt>2.
+xpolar1.6102 ++	TOSS does not work with dipolar dephasing.
+xpolar1.6103 ++	CP signals disappear when dmm='ccp'.
