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NMR Suite 3.5 for SGI, Red Hat Linux 7.1/7.3 and Windows 2000/XP

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The new NMR Suite version 3.5 is now available for SGI IRIX, Red Hat Linux 7.1, Windows 2000

and now also for

Red Hat 7.3 and Windows XP systems.

All programs of the NMR Suite offer the same functionality on all operating systems. So it's your choice what platform you want to use.

The major changes which have been made compared to the last program versions can be found in the subsequent sections. For the full information on all changes and bug fixes, please refer to the Release Letter that comes on the CD or get the Release Letter from our Web server. It can be downloaded via

http://www.bruker-biospin.com/software_nmr.html

There you can also find several updated documents containing important details about working with NMR Suite up to version 3.5:

- Installation Guide for Windows 2000
- Installation Guide for Red Hat Linux 7.1
- Acquisition Reference
- Processing Reference
- Pulse Program Reference
- Basic Experiments

and a short description with important installation notes:

http://www.bruker-biospin.com/software_nmr.html

New Features

Peak Power Limitation

Probes with PICS firmware usually contain information about the maximum peak power level that must not be exceeded for a given nucleus. In order to avoid probe damage caused by peak power levels above those values one can activate the POWCHK flag during the 'cf' procedure.

(more information in the Release Letter, chapter 2.1)

Pulse Programming

XWIN-NMR 3.5 offers several new features for pulse programming:

1. Subroutines
2. Phase Programs
3. Pulse Train Alignment
4. Frequency Setting
5. Conditional Pulse Program Execution
6. BILEV Decoupling

(more information in the Release Letter, chapter 2.2)

A detailed description is given in the new Pulse Program Reference Manual that is available in the Help menu of XWIN-NMR or on the Bruker Web server:

http://www.bruker-biospin.com/software_nmr.html

Pulse Programs

All Bruker 1D pulse programs now use the 'mc' syntax. The total number of scans is the product of ns (number of scans) * tdo (number of loops).

After every loop the pulse program will store the so far acquired scans on harddisk.

Automation

- Processing AU programs can create a PDF file of the plot
- New AU program 'disconv' for converting DISNMR datasets

(more information in the Release Letter, chapter 2.5)

License

- NMR Suite for Linux can be used with floating licenses

(more information in the Release Letter, chapter 2.7)

Configuration

- New option in the backup script 'xwinnmr.save'

(more information in the Release Letter, chapter 2.8)

ICON-NMR

- Automation can e-mail the print-out file of the

experiment optional in PostScript or in PDF format.

- New Priority mode: "First come, first served" mode.
- BEST-NMR Automation: Support for probe preparation and measurement on one(!) Gilson Liquid Handler
- BEST-NMR Automation: Implementation of 384 wellplate
- BEST-NMR Automation: Implementation of the wash switch and the WDP procedure
- ToolBox: New Experiment Definition Browser window
- ToolBox: New one-click submit: Submit all experiments under branch in one swoop
- ToolBox: Experiment definitions spanning multiple samples now supported
- ToolBox: Special features included for handling kinetic experiments

(more information in the Release Letter, chapter 3)

XWIN-PLOT

- Two new Automation Actions ("Reset Actions") for 1D objects have been added:
 - a) 'Keep zero line fixed on ___ %' of box size'
 - b) 'Keep integrals fixed on ___ %' of box size'
- XWIN-PLOT now supports more file formats for graphics export:
 - o Portable Network Graphics (*.png)
 - o JPEG
 - o PCX monochrome (*.pcx)
 - o PCX 24-bit color (*.pcx)
 - o TIFF uncompressed
 - o TIFF packed
- XWIN-PLOT is now able to export plot graphics directly to PDF files.

(more information in the Release Letter, chapter 4)

NMR-GUIDE 3.5

- Increased search functionality
- Updated in accordance with XWIN-NMR 3.5

- New tutorial "Titration controlled NMR Spectroscopy" by Prof. Dr. G. Haegele
- Using the search function of NMR-GUIDE in XWIN-NMR: 'ghelp'

(more information in the Release Letter, chapter 5)

NMR-SIM 3.5

- New pulse program syntax
The new alignment commands for pulse trains are fully implemented.
The pulse program display shows correct alignment of pulse train branches.

(more information in the Release Letter, chapter 6)

Spectrometer hardware requirements

XWIN-NMR 3.5 is released for datastations and Avance spectrometers.

Systems that are working well with XWIN-NMR 3.0 or 3.1 do not need any hardware upgrade.

Systems that are upgraded from XWIN-NMR \leq 2.6 must have at least the EC levels that are shown in the Release Letter.

(more information in the Release Letter, chapter 1.2)

Software requirements for Windows

- Visual C++ is not necessary anymore

(more information in the Release Letter chapter 1.3.1 and in the Installation Guide for Windows, chapter 9)

- NT Toolkit 2 is available, it contains the programs:
 - o Hummingbird Exceed X Server 7.1.1 and
 - o Hummingbird NFS Server 7.1

Whether you need those new versions or whether you can work with the older versions can be checked in the Release Letter, chapter 1.3.2 or in the Installation Guide for Windows, chapter 10.

Special requirements for Linux

A new graphics card for Linux has been tested and is supported by
Bruker BioSpin:

- o NVIDIA Quadro4 380/550/580/700/750/780/900/980 XGL1

(NVIDIA graphics cards are working properly only with the original
driver of NVIDIA. More information in the Release Letter, chapter 1.4.)

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mail with the word UNSUBSCRIBE in the subject line.
