```
##########################################
#                                        #
#           TopSpin 2.0 pl2              #
#                                        #
#                 for                    #
#                                        #
#   Acquisition, Processing, Automation  #
#   Plotting, Simulation, and NMR-GUIDE  #
##########################################
```

In our last mailing from October 26, 2006, we informed you about the upcoming TopSpin 2.0 release.

The new TopSpin version 2.0 pl2 is now available for

- Windows XP
- Red Hat Enterprise Linux WS 3
- Red Hat Enterprise Linux WS 4

The TopSpin 2.0 pl2 DVD contains the following program versions:

TOPSPIN	2.0 pl2
TOPSPIN Plot Editor	4.4 pl2
ICON-NMR	4.1.1 build 1
NMR-SIM	4.6
NMR-GUIDE	4.1
GLP	5.0

TopSpin 2.0 pl2 comes as a full program version on a DVD. It can not be downloaded as a separate patch file.

To order TopSpin 2.0 pl2 DVD please contact your local Bruker office. Bruker BioSpin addresses can be found on our Web site:

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

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New features in TopSpin 2.0

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1) *New method for gradient shimming*

The new command 'topshim' has been introduced with TopSpin 2.0. It executes a new method for automatic shimming based on gradient shimming.

The tool is easy to use, fast, and gives very good results. For more

details please open the topshim manual with the TopSpin command:

help topshim

2) *New digital filter*

A new digital software filter is available. This filter method can be used on any type of spectrometer which is supported by TopSpin 2.0. This new filter has several advantages:

- No first order phase distortion, so first order phase correction is not necessary.
- No so-called smilies (distortions of the spectrum at the left and right edges of the spectrum).
- The baseline of the resulting spectrum will be exactly zero provided that no other effects distort the FID and that a correct zero order phase correction has been done.
- Signals at the very edge of the spectrum are not attenuated or distorted nor are they folded in.

The filter is activated with the two parameters DSPFIRM (set to rectangle) and DIGMOD (set to baseopt). For more details see the description of these parameters in the Acquisition Reference manual, which can be opened with the TopSpin command:

help acqref

In this manual search for the keyword "DSPFIRM".

3) *Electronic signatures*

Internal user management introduced by TopSpin 2.0 allows TopSpin internal users to add electronic signatures to raw and/or processed data.
The command 'audit' allows to view/check all electronic signatures on a dataset.
Plot layouts can be set up to show the last signature and/or display warnings if a signature is missing (cf. TopSpin User manual and Plot Editor manual).

4) *New acquisition tool*

A new acquisition tool (command 'topguide') has been implemented together with a database of experiments. This tool intelligently guides a beginner through data acquisition and processing. Based on some general information about the sample and the detected hardware it only shows the relevant experiments and parameters to be set, requiring a minimum of user input (cf. Acquisition Commands and Parameters manual).

5) *Command spooling*

Command spooling has been implemented. Acquisition commands like 'zg', 'rga', 'atma', and 'go' can be automatically queued if this feature has been turned on
(defaults to off but can be set with the command 'set'). All other commands can be

queued with the command 'qu', e.g., 'qu xfb'. The acquisition status bar contains
a "Spooler" field where you can view and cancel queued commands.
(cf. TopSpin User manual).

6) *User-defined plot layouts*

Plotting in automation supports user-defined layouts with the same names as Bruker layouts stored in a different directory. 'plot' and 'autoplot' use a configurable search path for locating the layout file defined by the parameter LAYOUT (cf. Plot Editor manual).

7) *Selection of acquisition and processing parameters to be plotted*

The command 'parplot' has been implemented to select the acquisition and processing parameters that should be listed on the plot.
(cf. Processing Commands and Parameters manual).

8) *Daisy package*

The Daisy package for simulating spectra based on chemical shifts and coupling constants has been implemented. A preliminary manual is available under Help -> Manuals -> Simulation -> Daisy.

9) *Interactive 2D peak integration*

Interactive 2D peak integration has been implemented (cf. TopSpin User manual).

10) *2D molecule structure drawing program*

A 2D molecule structure drawing program (command 'edstruc') has been implemented
as a complement to the 3D structure viewer (command 'jmol'). The 2D structure can
be displayed along with the spectrum. Right-click in the spectrum window, select "Display Properties", and enable the entry "Molecular Structure"
(cf. TopSpin User manual).

11) *Printout suppression*

Printouts (plots) from Processing may be eliminated via one configuration setting (cf. ICON-NMR Complete manual).

12) *New temperature handling*

Temperature handling now on a per experiment basis instead of per sample
(cf. ICON-NMR Complete manual).

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Bug fixes compared to TopSpin 2.0 patchlevel 0 / 1

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The following topics describe some of the fixes which come with TopSpin 2.0 pl2. Details can be found in the description of the item in the Bruker Knowledge Base.

- item 6395
  On AVII+ systems, the pulse program statements ze, zd, st, and st0 are ignored if written in one line with a write statement, e.g., d11 wr #0 if #0 zd st0

- item 6391
  zg sometimes does not finish. The acquisition counts into infinite, despite the fact that no go process is running anymore. It is not possible to start a new acquisition (aborts with error message). Only after an ii was performed a new zg is possible again.

- item 6371
  ATMA fails on X-nuclei not in the PIC System List

- item 6367
  On AVII+ systems the pulse program statement wr #x with x>0 does not work as desired. Instead, x is always interpreted as '0'.

- item 6357
  Switching the wobble channels leads to an error because the pulse program can not be compiled.

- item 6343
  atma fails on 19F on a AV400 with RXAD400 and some other ATMA problems

- item 6318
  edhead appends 19F to some probe's names

- item 6305
  wrong calculation of SW in f1/ND_010 in pulse program HSQCETGPSIWT

- item 6285
  spin rate calibration in bsmsdisp not possible

- item 6280
  atma does not start 2nd time on QNP probes

- item 6258
  Homodecoupling doesn't work with default routing

- item 6249
  Status parameter solvent is None after 'gradshim'

- item 6230
  getprosol fails with permission problem in /tmp

- item 6208

On RCU machines the real-time FT shows an ill-phased spectrum compared to the actual spectrum stored on disk; shimming on this spectrum during gs therefore becomes impossible.

- item 6200
  On an RCU system the FID-area parameter displayed shows incorrect values. Additionally, this parameter varies heavily even if the fid only marginally changes its shape and therefore renders shimming impossible.

The Bruker Knowledge Base can be found on our Web server:

www.bruker-biospin.com/shell/bkb/index.cgi

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Work in progress

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Some bugs in TopSpin 2.0 pl2 are already known, e.g.,

- item 6256
  On some systems, atmm/atma don't work, but a corrected atmaserver program (vs. 3.64) is available from ftp.bruker.ch.

- item 6336 and 6530.
  'gs' under certain circumstances doesn't work.

We have a patch for these, and possibly other, bugs in preparation. This patch will be made available in early 2007.

For more details see the updated Release Letter for TopSpin 2.0 pl2. It is available on the Bruker BioSpin Web server:

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

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