New Features of TopSpin and New Hardware

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TopSpin Versions

TopSpin 2.1.pl6

TopSpin 3.0

- Released Spring 2010
- Status: **TS3.0.pl4**

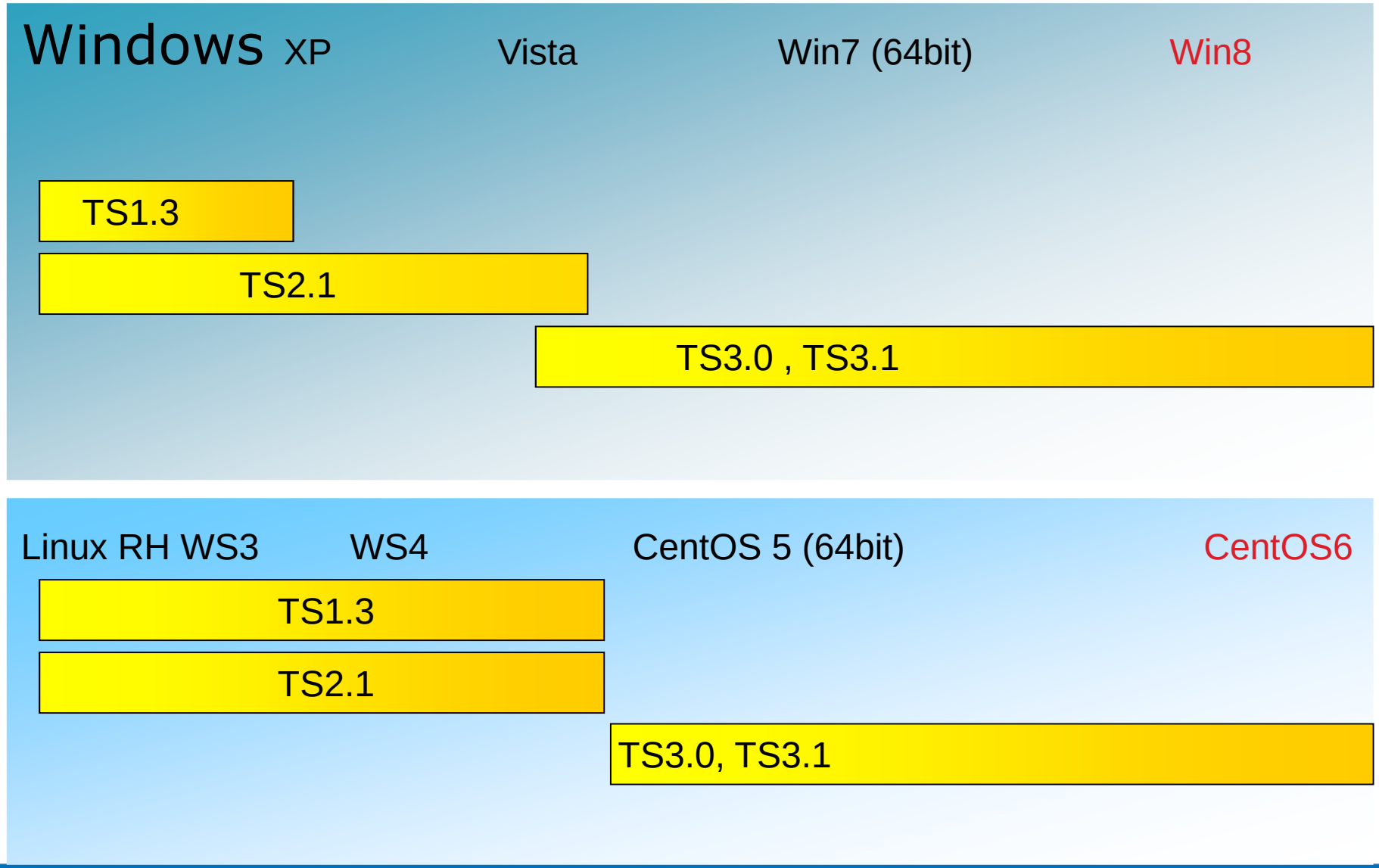
TopSpin 3.1

- Released April 2011 (ENC Conference)
- Status: TS3.1.pl2
- Minor 3.1 pl2 Upgrade

TopSpin 3.1.5

Released April 2012 (ENC Conference)

TopSpin Versions



Student licenses are now available

- For students only (student certificate may be checked)
- inexpensive
- limited for 3 years
- full access to processing, simulation and plotting
- node locked license type
- no license transfer possible
- cannot be upgraded to next major TopSpin version
- can be ordered via Bruker web shop
- has to be bought with a credit card or invoice
- software has to be downloaded

Student Version

Available for

- Macintosh
- Linux RedHat or CentOS
- Windows 7 or XP

contain:

- TopSpin (processing only)
- FlexLM
- NMR-Sim

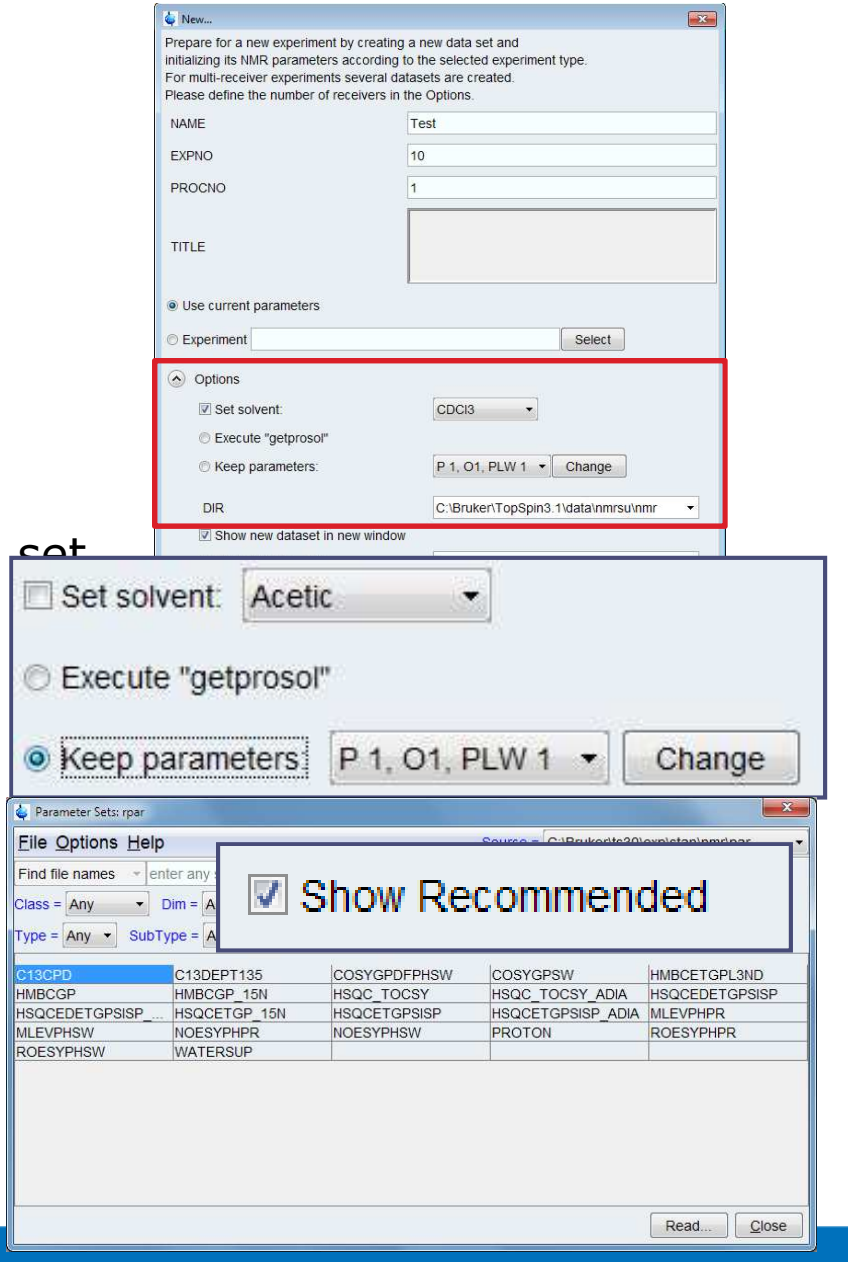
You should have a fast connection to down load these, The Flexlm license will be e-mailed to you

TopSpin 3.1.5 Developments

Preparing data sets:

`edc/rpar`

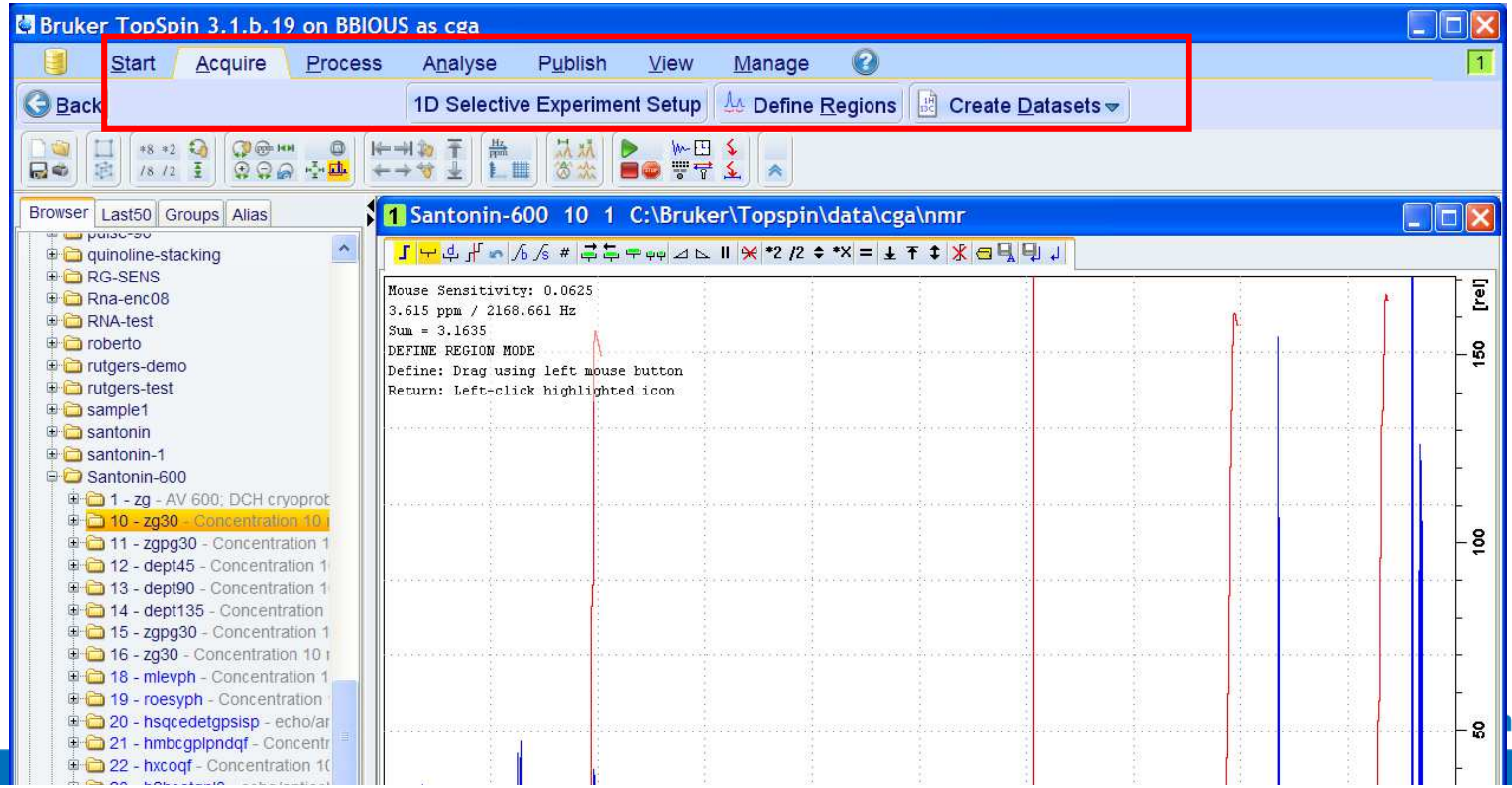
- Solvent selection,
  access to **`getprosol`**
- "Use current parameters"
  to transfer all paramaters to new data set
- "Keep parameters" to transfer a
  personal selection only (configurable)
  - Choose experiment via rpar dialog,
    link to NMRGuide available
  - "Show recommended"
    restricts selection to standards



Selective Experiments are easy to set up and run !

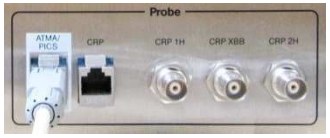
***Selective Acquisition* Experiments:**

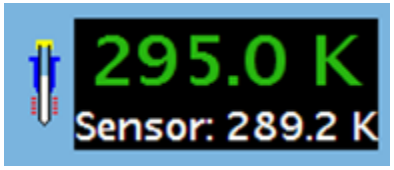
- GUI now provides better help when setting up Selective experiments
- Supports 1D NOESY, COSY, TOCSY, Region selective 2D HMBC

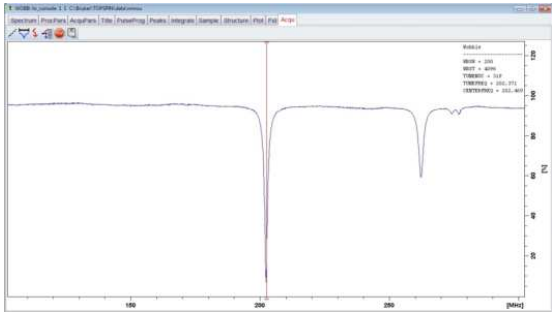


AVANCE III HD
New features

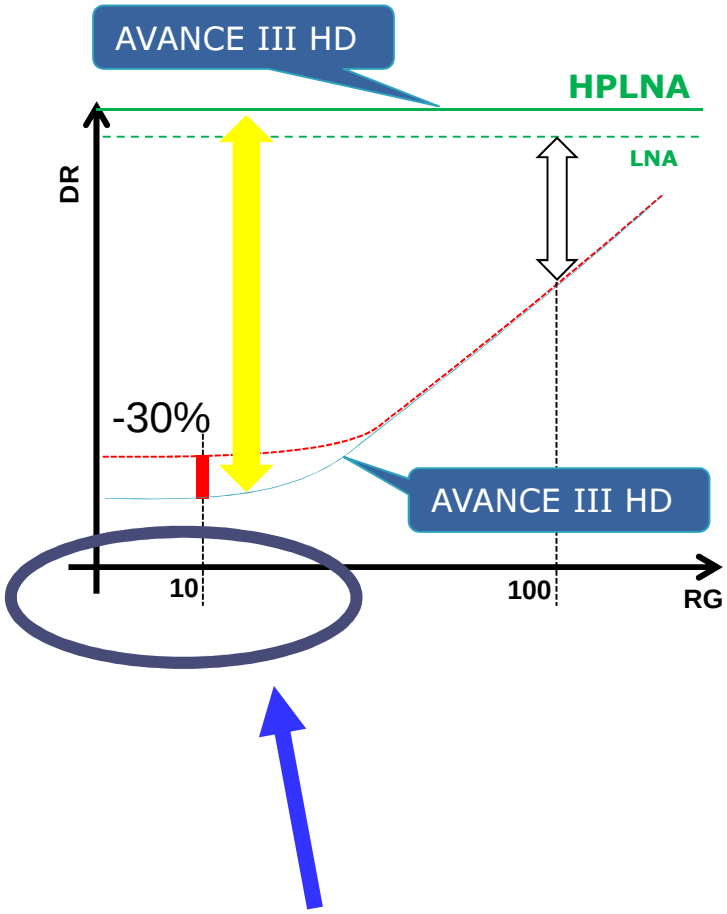
- Digital RF synthesizer **SGU3**
- Enhanced Receiver **RXAD/2**
- Enhanced **HPLNA** ^{1}H with ^{19}F
- **HPLNA XBB** solids preamplifier
- **Enhanced Tune & Match**
- **Preamplifier user interface / Touchscreen**
- **Nanobay 'CryoProbe ready'**
- Support of **NMR Thermometer™**







AVANCE III HD - Enhanced receiver and new synthesizer electronics



Sample with high concentration / protonated buffers

HPLNA ^{1}H Preamplifier

- Enhanced dynamic range
- New ^{19}F capability

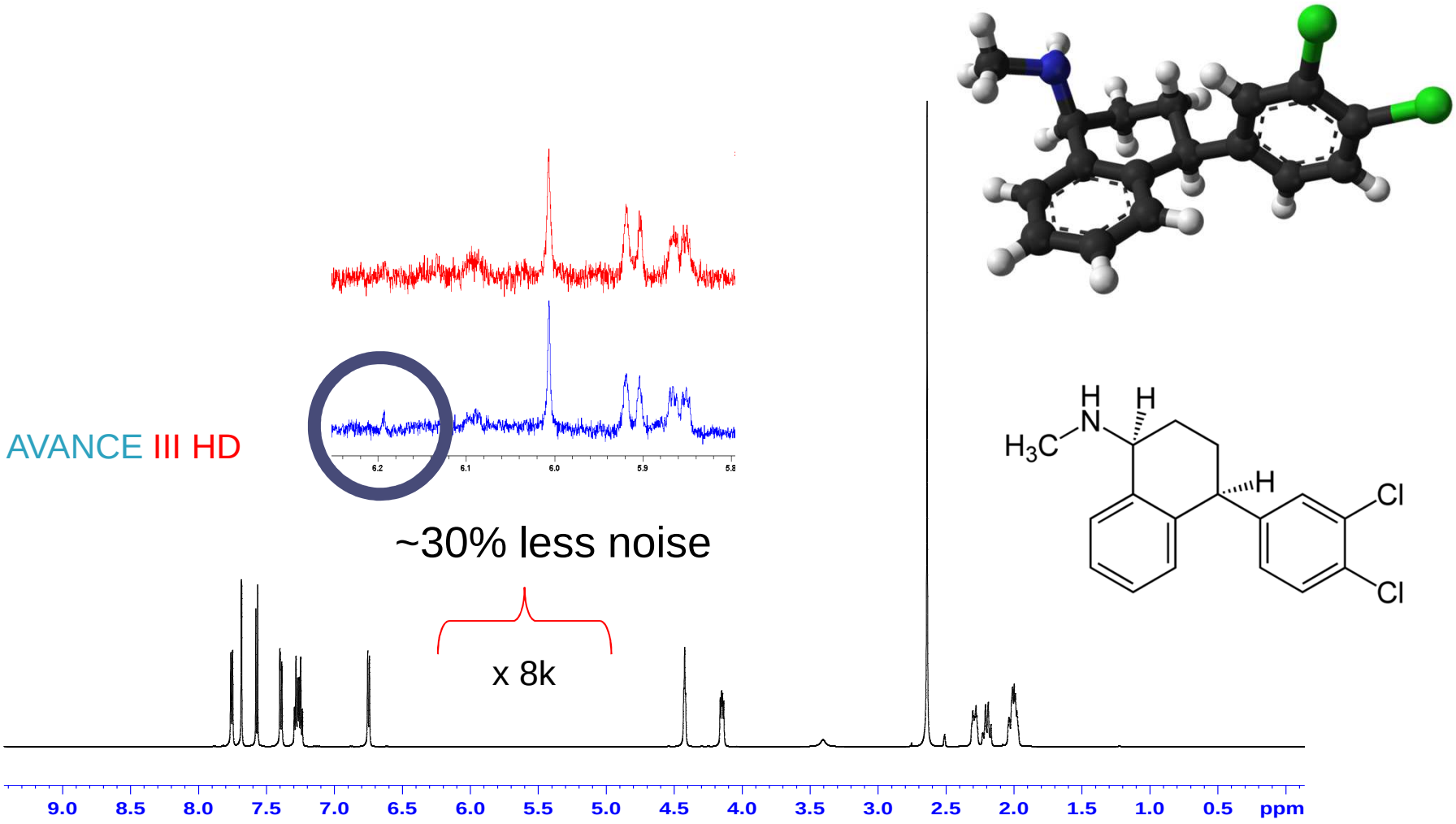
Receiver / Synthesizer

- RXAD2: enhanced electronics
- SGU3: 960 MHz digital up-converter

Benefits:

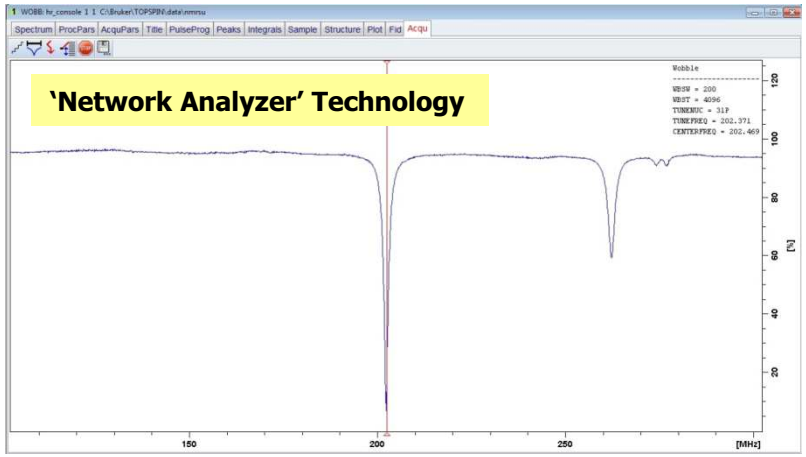
- Higher dynamic range
- Cleaner RF, less phase noise
- Enhanced digital RF and power setting
- Better stability & reproducibility

AVANCE III HD – Receiver electronics
Enhanced Dynamic Range

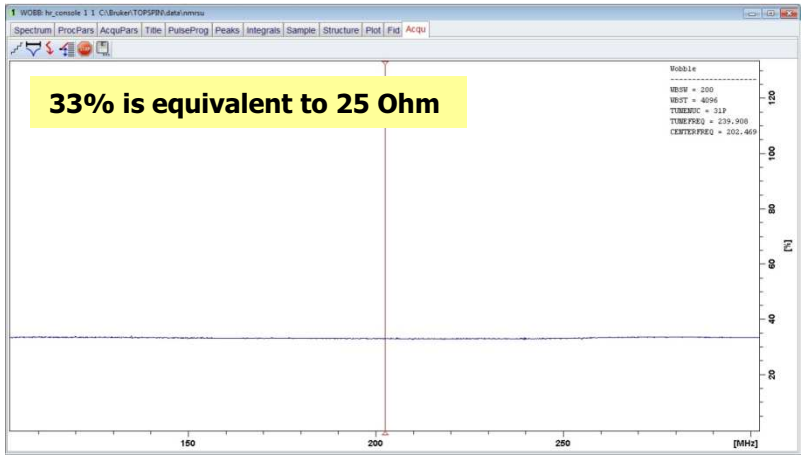


600 MHz ^{1}H of 100mg/ml sertraline (Zoloft) in DMSO-d6

AVANCE III HD – Enhanced ‘wobb’
Accurate Tune & Match



^{31}P @ 500 MHz with 200 MHz span



$$r = \frac{U_r}{U_h} = \frac{Z_a - Z_l}{Z_a + Z_l} \qquad |r| \leq 1$$

Benefits:

- **Precise tuning and matching**
- What you see is what you get
- Easy T&M with probes
- Factory calibrated preamplifiers

Good to know:

- May be used to check instrument

AVANCE III HD – HPPR
Advanced Preamplifier User Interface

- Touch Screen display
- Ready to run
- Hot Plug operation with PICS

Now available

'wobble curve' displayed at the probe

- Easy Tune & Match for solids probes
- Optimal impedance matching for probes without ATM™

AVANCE III HD – NMR Thermometer
Where to measure sample temperature?

High Resolution

H_2O: ~ 0.01ppm / K
@600MHz = 6Hz / K

RF Loading 0 to ~2K

0 – 12 Hz shifts

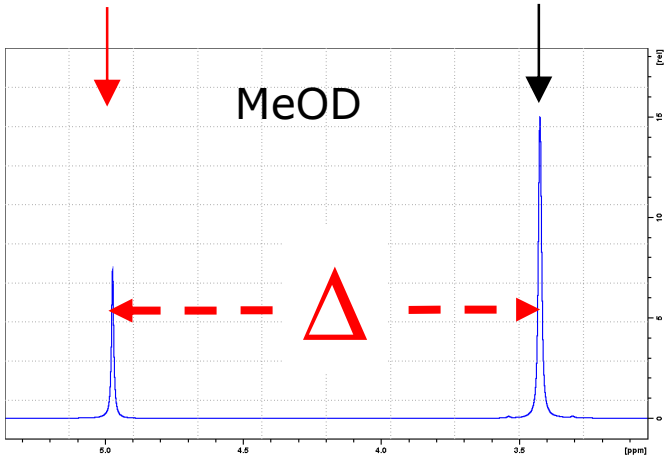
HR-MAS

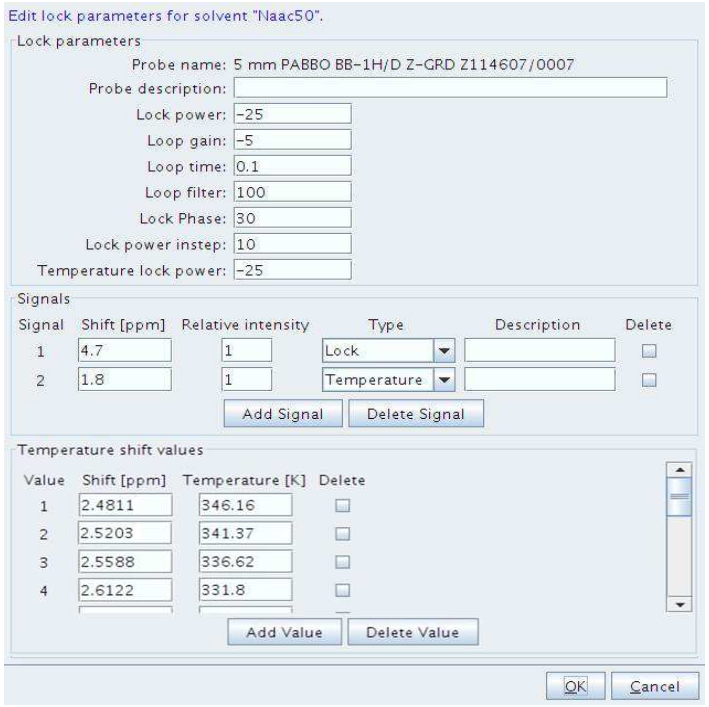
Other heating effects

MAS spinning speed

up to 5 - 20K

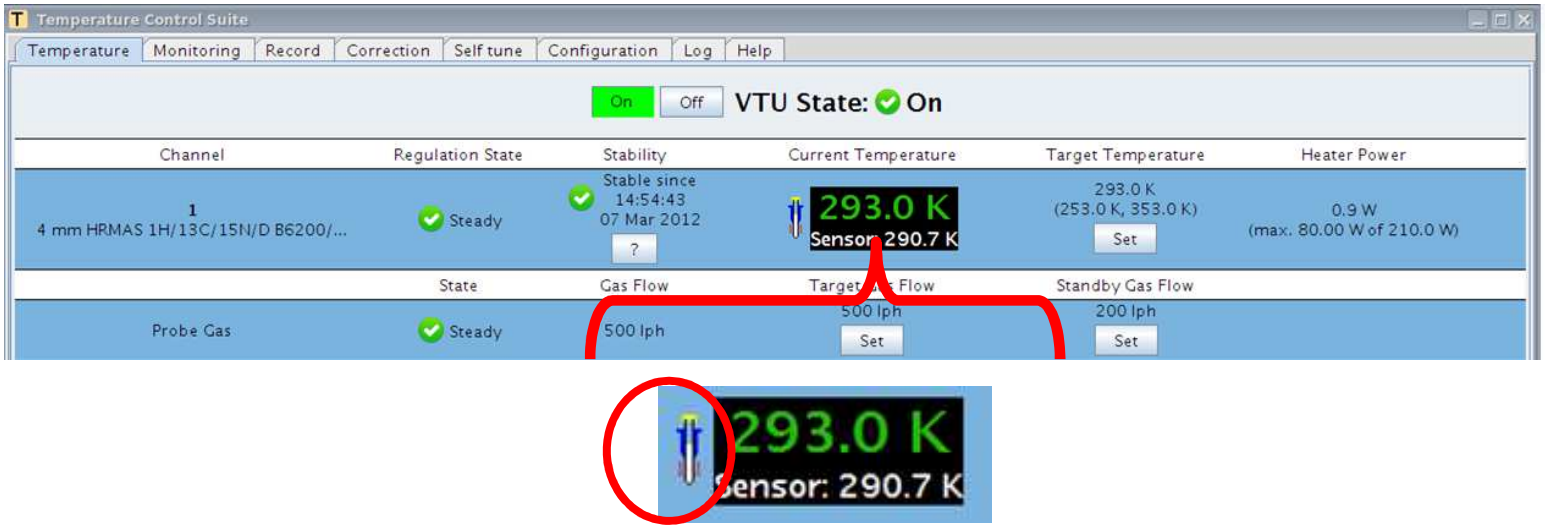
AVANCE III HD – NMR Thermometer
Measure the temperature with the spins





Sample with thermo-sensitive ^{2}H compound

AVANCE III HD – NMR Thermometer
Topspin User Interface



Benefits NMR Thermometer:

- **Measure**
- **Maintain**
- **Monitor**

} **temperature within the sample**

AVANCE III HD - Ultimate NMR Platform for Life Science and Materials Research

Further improved and new electronics:

- ^{1}H Preamplifier, Receiver & Digital RF Synthesizer
- High power Broadband LNA Preamplifier with 50 Ohm
- Touchscreen Tune & Match at the probe

Benefits:

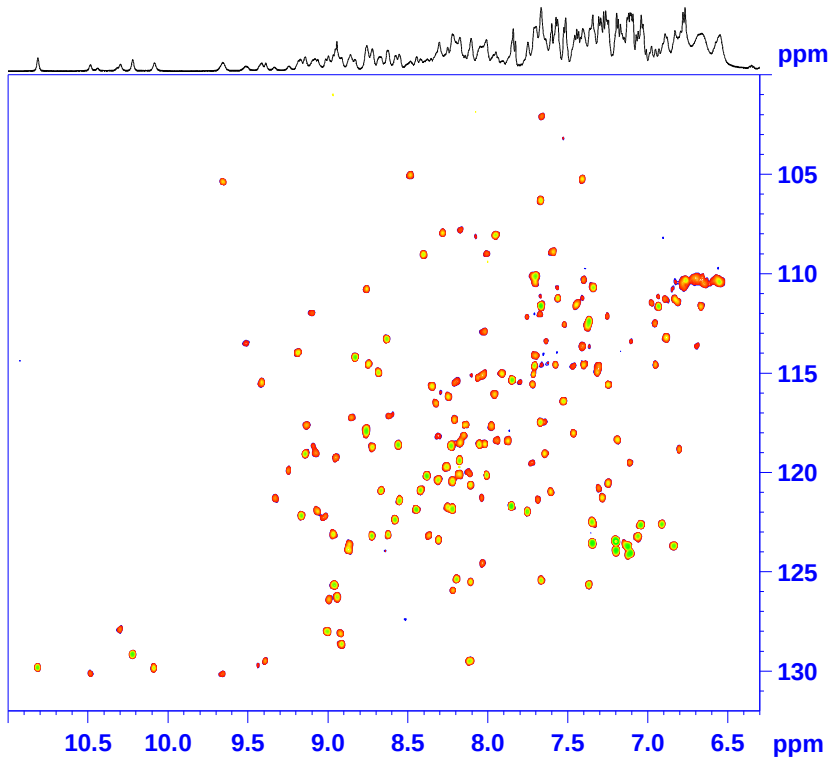
- Higher dynamic range and 30% less noise
- Up to 35% SNR gain with the dynamic sample
- Up to 20% increase in sensitivity for X-nuclei Solid State experiments
- State of the art solids spectra without manual adjustments
- Easy and accurate experiment setup

New NMR Thermometer™:

- Accurate sample temperature
- Perfect chemical shifts match
- Measure the temperature with your spins!

CryoProbe Revolution Continues
➔ over 1,100 CryoProbes installed worldwide
CryoProbe™ Prodigy TCI 600

- 2.5 times proton sensitivity boost at affordable prices (compared to RT probes)
- 2 times carbon sensitivity
- More than 6-fold throughput increase
- Minimum operating and maintenance costs, long service intervals of 2 years
- Requires no additional infrastructure: easy to site within a small footprint
- Avance III HD 600 spectrometer with Prodigy TCI surpasses conventional 950 MHz RT-probe system in proton sensitivity!
- ~35 ultra-high field 900, 950 and 1 GHz systems now installed by Bruker in customer labs worldwide.



^{15}N-HSQC spectrum of a 2mM lysozyme sample with ^{15}N at natural abundance in 50 min

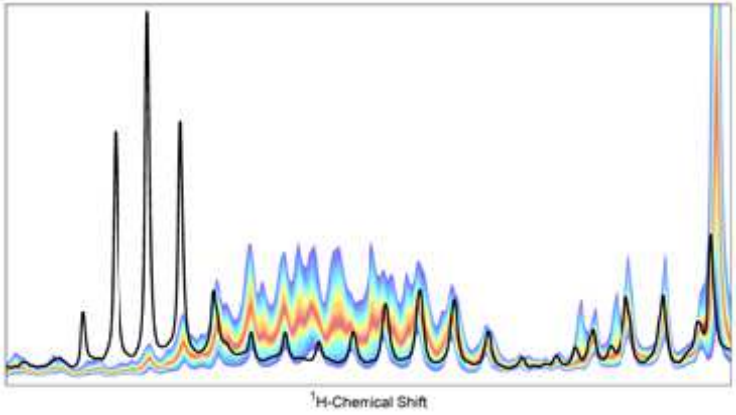
WineScreener™

Cost-Effective, Automated and High Throughput Solution for Wine Quality Control

- Rapid, cost-effective quantitative targeted and non-targeted statistical analyses of wine
- Based on proven NMR ***JuiceScreener™***
- Frequent wine scandals in recent years demonstrated need for new technology that assesses quality and safety within a single experiment
- First product release will offer a targeted analysis applicable to wines produced worldwide
- Non-targeted analysis developed on and applicable to German wines (for now)

Compound	Value	Unit	Official Reference Flag	Official Reference max. Value	Wine-Profiling™ Authentic NMR Database
acetic acid	525	mg/L	○	-	165 … 1007
benzoic acid	<5	mg/L	●	0 mg/L	<5 mg/L in reference set
citric acid	299	mg/L	●	1000 mg/L	<200 … 471
ethanol	91.7	g/L	○	-	56.2 … 108.0
fumaric acid	<5	mg/L	○	-	<5 … 12
glycerol	7.1	g/L	○	-	4.5 … 11.1
malic acid	5.5	g/L	○	-	<0.2 … 8.2
methanol	53	mg/L	●	250 mg/L	6 … 146
shikimic acid	88	mg/L	○	-	<20 … 100
sorbic acid	<5	mg/L	●	200 mg/L	<5 mg/L in reference set

WineScreener sample quantification report.



White wine model: 1,3-Propanediol indicates uncontrolled organic acid decomposition

Nitrogen Liquefier BNL

More Efficient, Sustainable and Economic Magnet Operation

- Essentially zero nitrogen boil-off for Ascend™ standard-bore magnets up to 700/54
- ***BNL*** eliminates nitrogen refills for maximum user convenience
- No interruptions of long-term experiments
- Lower cost of ownership
- Solution to concerns about limited availability or logistics of cryogens in some emerging markets
- Monitoring Unit ensures easy visual monitoring
- Everyone can benefit from nitrogen refrigeration (CryoProbe™ customers could already benefit from BSNL, using extra cooling capacity of latest generation CryoPlatform™)

Ascend 600, equipped with a ***BNL*** nitrogen liquefier

CryoProbe™ BBFO 500 MHz

- The new BBFO CryoProbe offers the highest commercially available sensitivity for the broadest range of nuclei.
- The probe is designed for both observe and inverse detection. This first fully broad banded CryoProbe can be automatically tuned over it‘s entire range from 15N to 19F, as well as of course on the proton channel.
- Allows not only all X-observe 1H decoupled experiments and their inverse detected counterparts, but also 19F{1H}/1H{19F}) in full automation.
- In addition it provides a great solution for research applications on less commonly measured nuclei as well as low natural abundance / low sensitivity nuclei.

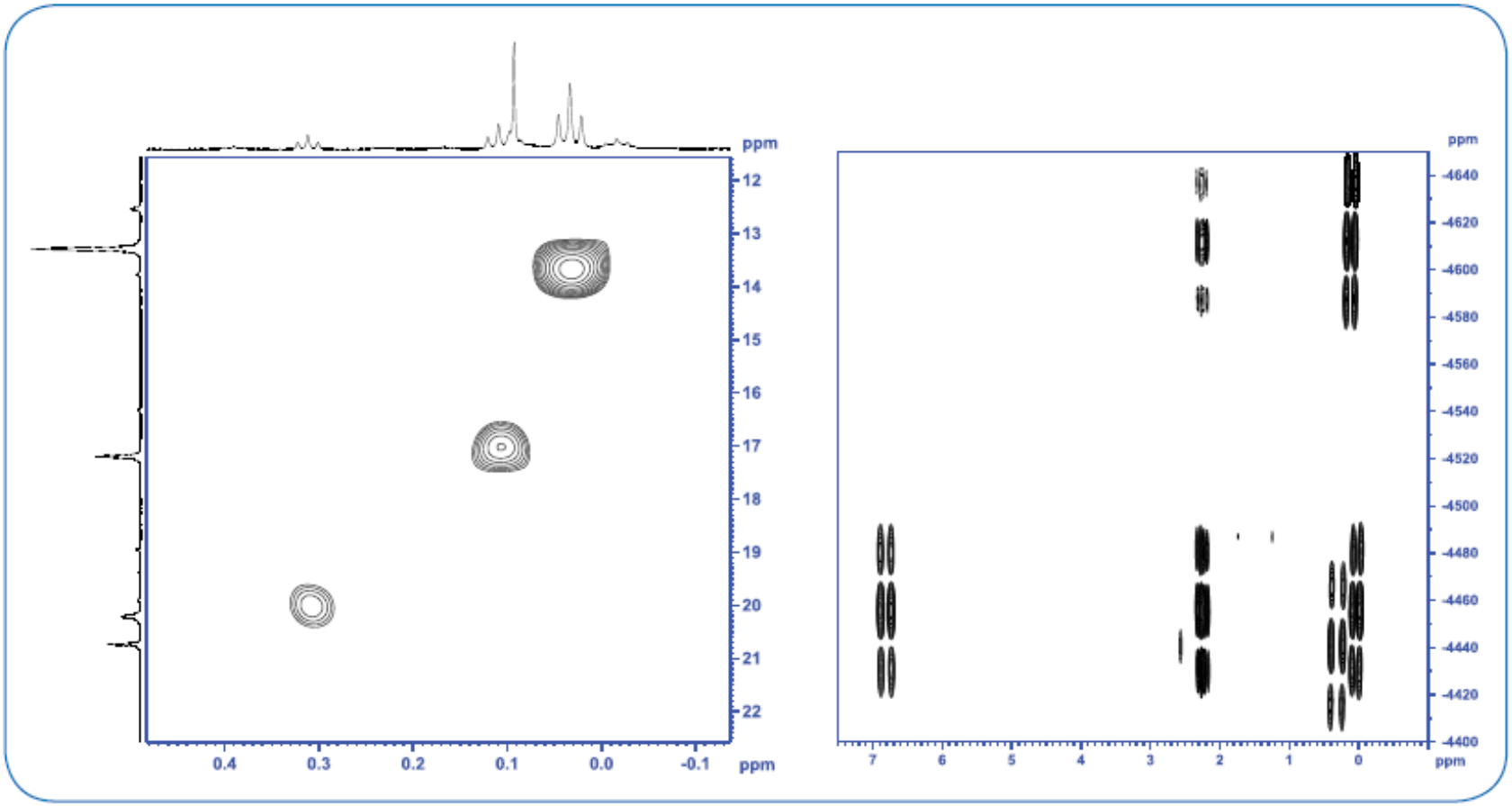
CryoProbe™ BBFO 500 MHz

Features

- BBFO including 19F{1H} and 1H {19F}
- 15N-19F S/N gain: factor ~4*
- 1H S/N gain: factor ~3*
- Cold preamplifiers for all nuclei (BB/19F/1H/2H)
- Z-gradient and ATM™ compatible
- 0° C–> 80° C sample temperature range, other ranges on request
- Available at 500 MHz, other frequencies on request

* Compared to The Smart Probe

CryoProbe™ BBFO 500 MHz

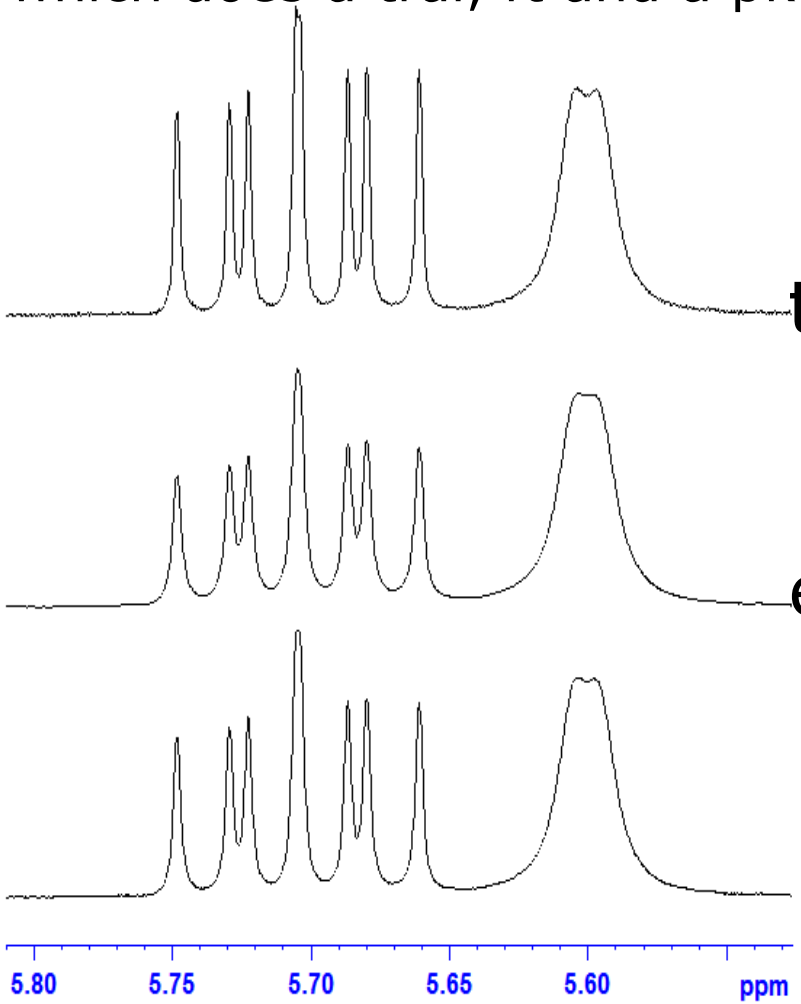


Left: 1H-31P HMQC of MePt(PR3)2(C4F6H).

Right: 1H-195Pt-HMQC of MePt(PR3)2(C4F6H).

A new command has been added: tfp

A new command called tfp has been added which does a traf, ft and a pk on a spectra



tfp with lb set for 0.3 Hertz

efp with lb set for 0.3 Hertz

fp with lb set for 0.3 Hertz

New Manuals for TopSpin 3.1

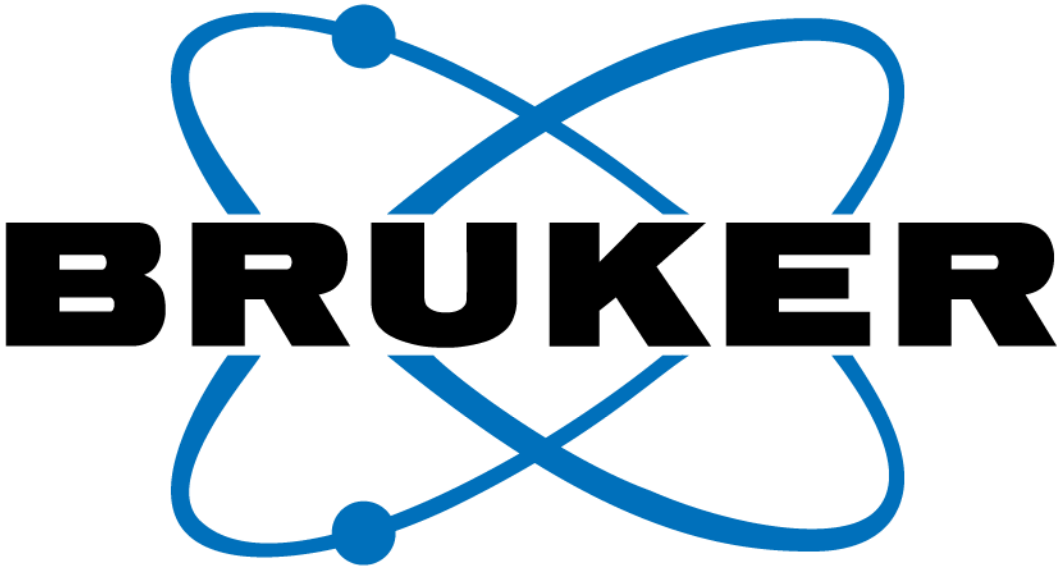
- There is a new manual that explains the edlock panel. It gives a method for updating the Field value, using any solvent. It is called **Edlock Guide**

- There is a new manual for edprosol, which explains the inner workings and how to use it for different solvent, and probes. It is called the **Edprosol Manual**

- There is a new manual for diffusion, called **Diffusion**. It gives new information about how to measure diffusion and the new interface for this.

- The **Shapetool** manual has been updated.

Are there any Questions ?



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