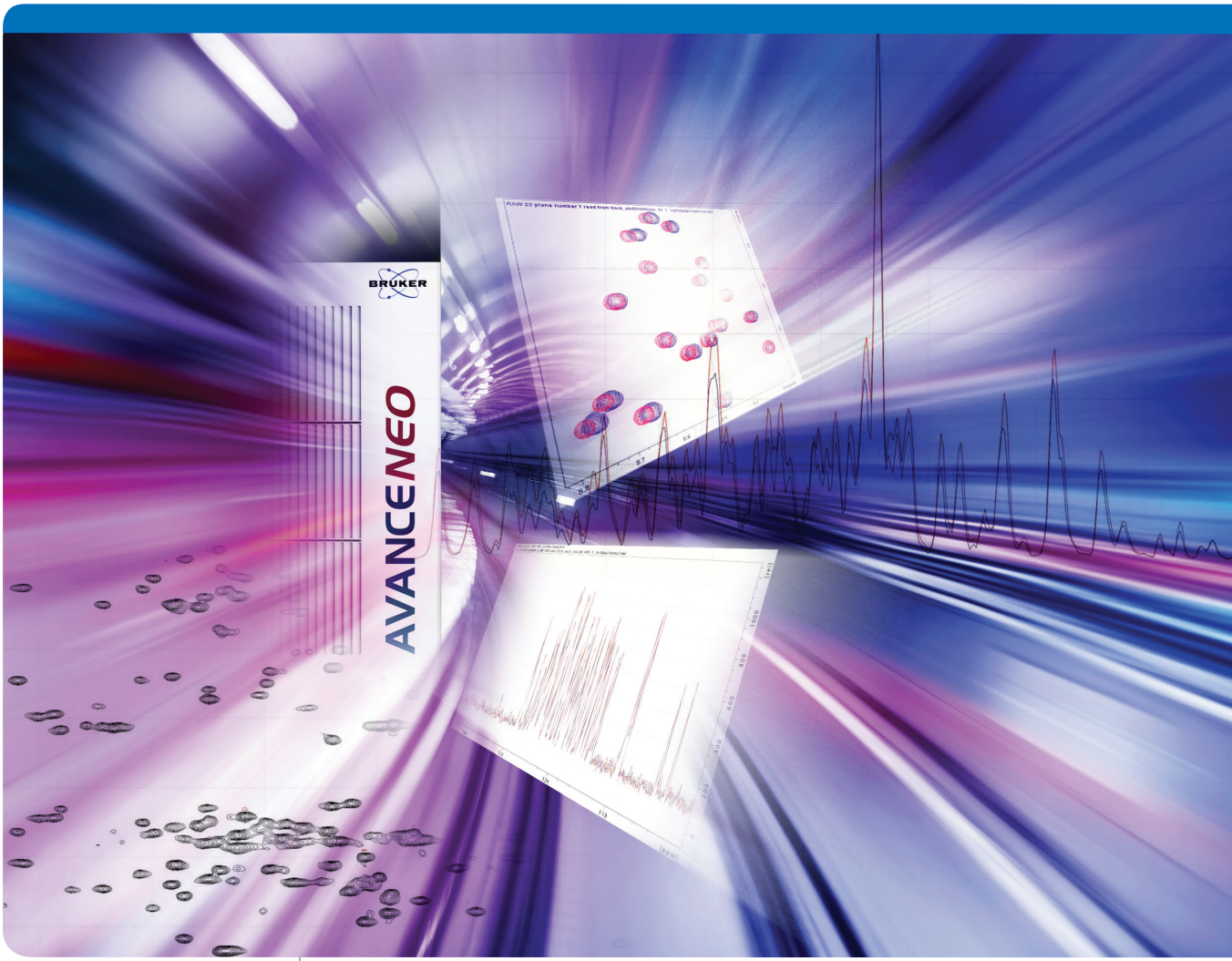

AVANCE NEO

- Takes NMR to a New, Highly Controlled, Ultra-fast Level

Innovation with Integrity

NMR

Ready for the future in NMR research

The AVANCE NEO is the next generation of Bruker's successful AVANCE product line. Offering ultra-fast control, greater dynamic range and enhanced flexibility, the AVANCE NEO takes NMR research to an even higher performance level.

True NMR Channel System

The AVANCE NEO NMR acquisition system is based on a fully modular, highly integrated RF transmit and receive concept. Each NMR channel (a TRX1200 transceiver) consists of a fully autonomous and independent pulse programmer, transmitter and receiver. All transceivers can be synchronized with each other within a 12.5ns timescale at pulse program level, which is 4 times faster than before. RF pulses are generated with the simultaneous amplitude, phase and frequency setting, within 12.5ns.

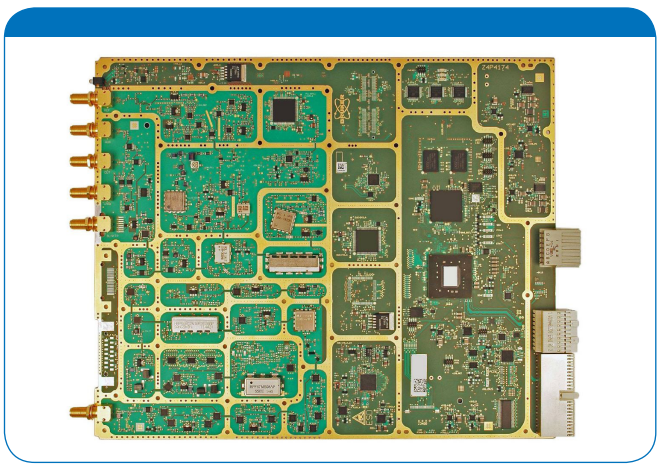

Fig. 1: TRX1200 transceiver.

Each channel has a dedicated pulse program execution engine (system on chip) with an onboard high speed 1GB waveform memory. The highly digital implementation incorporates a 960 MSPS digital up-converter (DUC) for transmit, and a high speed 240 MSPS ADC with a high speed digital down converter (DDC).

This provides ultra stable and precise RF pulse generation, as well as high dynamic, spurious free NMR detection with further enhanced dynamic range. A state-of-the-art and well-designed heterodyne receiver results in approximately 50% less noise than previous technology. This delivers full sensitivity even at very low receiver gains.

Further Enhanced Dynamic Range

State-of-the-art ADC and receiver electronics improve the sensitivity of AVANCE NEO consoles at low receiver gains compared to the AVANCE III HD.

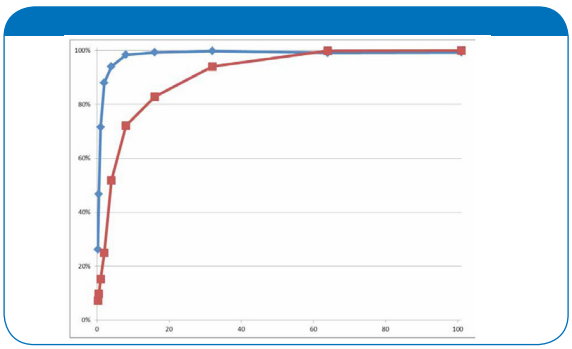

Fig. 2: Increased sensitivity for AVANCE NEO (blue) compared to AVANCE III HD (red) in high dynamic range situations. For receiver gains below 32, the gain is 20% to over 100%.

High IF Technology

The receiver within the TRX1200 uses a very high intermediate frequency (IF) of 1.852 GHz for NMR signal generation and detection. This avoids any compromise with local oscillator (LO) windows, with regards to noise and decoupling leakage.

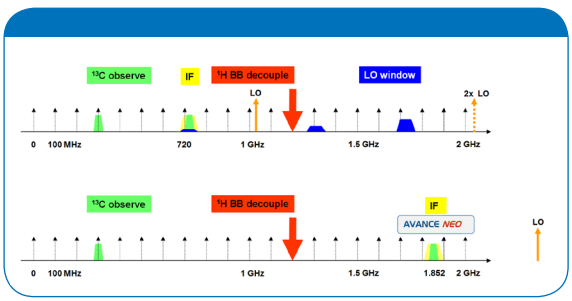

Fig. 3: A high IF avoids unwanted folding of noise and leakage from unintended LO windows (blue, upper) into the IF. With a high IF the unwanted LO window can be avoided by design.

With this architecture, there is no possible conflict between any observed and decoupled nuclei within the full range of NMR at any NMR field (eg 1.2 GHz).

Enhanced Sensitivity for X-Nuclei

GaAs transistor technology has been used with ^{1}H preamplifiers for decades. Its superior performance provides maximum sensitivity on ^{1}H. Preamplifiers for low γ nuclei such as ^{13}C, ^{2}H, ^{15}N, etc are now also using GaAs transistor technology, benefiting from a sensitivity increase of 6 - 8% together with RT probes. This corresponds to about 15% higher throughput, for example with a SmartProbe™.

With the enhanced sensitivity of the ^{2}H preamplifier, field stability can be increased under experimental conditions with a low amount of deuterated solvent and labs exposed to external field perturbations (trams, elevator, etc).

Full Broadband RF Amplifiers

Latest RF power transistor technology used in the new and fully broad-banded RF amplifiers (BLABB) provides high RF power from 15 MHz up to 600 MHz. Together with the ^{1}H RF amplifier this larger bandwidth allows any combination of ^{1}H / ^{19}F or low γ-nucleus. In addition, ^{1}H and ^{19}F experiments run in parallel with independent RF channels even on two channel systems equipped with broad-banded probes (e.g. SmartProbe™).

Ready for the Future

AVANCE NEO is a truly unified NMR electronics platform for all applications from high resolution to solids spectroscopy and micro-imaging. Most additional functionality can be easily added to an existing AVANCE NEO configuration, offering maximum flexibility and possibilities for future evolution. Your AVANCE NEO NMR spectrometer is ready for any routine or high-end NMR experiment. Its improved performance and capabilities allow plenty of headroom for future NMR developments.

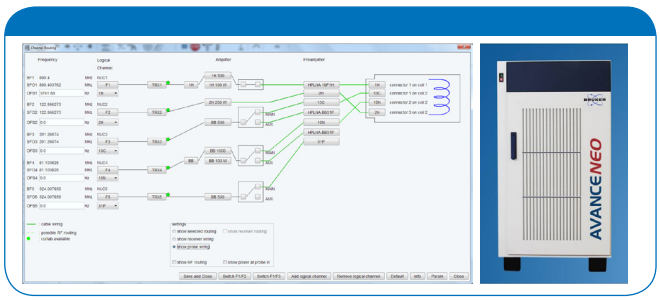

Fig 4: Number of RF channels (transmit) equals number of receivers (RX). AVANCE NEO has lean point-to-point connection for easy, simple RF routing, also for very complex experiments.

More Compact and Always Multi-Receive

AVANCE NEO has an integrated and compact design: Each RF channel contains frequency generation, ADC and receiver in a single transceiver board. This means that every AVANCE NEO console is inherently multi-receive capable with any available nucleus and probe combination.

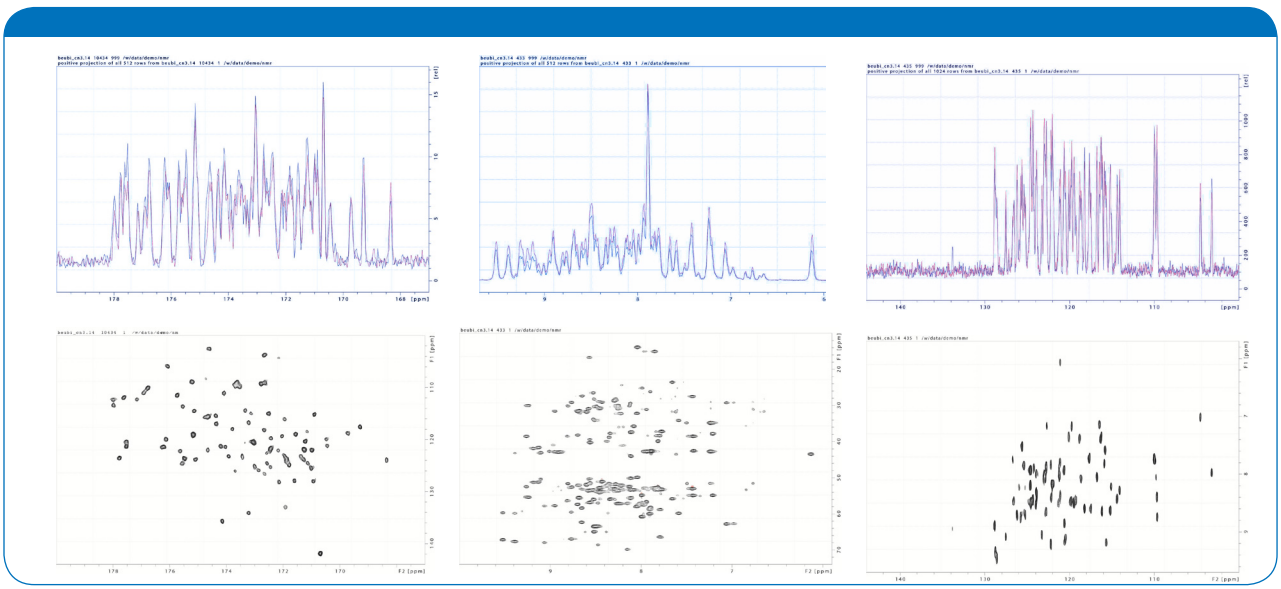

Fig. 5: UTOPIA-NMR*: triple receive experiment with double labeled ubiquitin: 2D CON (left), 2D HCBCA (center) and 2D NH (right) correlation experiment acquired simultaneously. 1D projections on top illustrate the well matched relative sensitivity of individual 2D's. Note virtually equal sensitivity for Multi-receive Utopia experiments as shown in projections (blue) compared to individually optimized single experiments (red).

Network Analyzer Functionality

Factory calibrated preamplifiers and complex tuning data give AVANCE NEO users enhanced 2nd generation automatic tuning and matching (2G ATMA). Routine applications profit from even faster and more reliable tuning and matching. Method developers benefit from the network analyzer functionality built in to the NMR console for spin noise experiments and probe over-coupling.

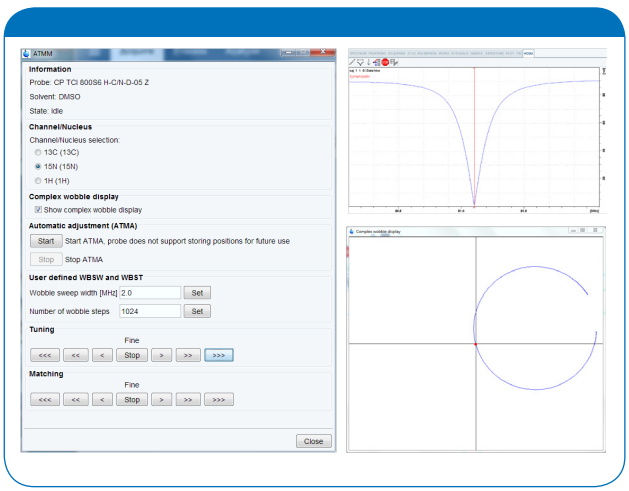

Fig. 6: Automatic tuning and matching (left) with AVANCE NEO electronics using real and cartesian (complex) wobble data representation (right).

NMR Thermometer™

By combining both 2G DigiLock and SmartVT, Bruker's unique NMR Thermometer controls the sample temperature via the temperature dependent ^{2}H chemical shift of NMR signals inside the sample.

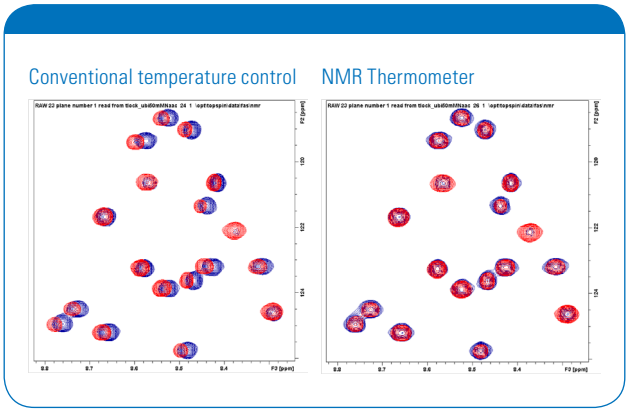

Fig. 7: Overlay of NOESY-HSQC (blue) and TOCSY-HSQC (red) experiments. Conventional temperature control results in peak shifts (left) induced by RF heating, NMR Thermometer control (right) maintains perfect chemical shift match between the spectra.

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Specifications AVANCE™ *NEO*

300 – 600 MHz NMR Systems (Onebay/Twobay)

		Standard	Comment
System	Number RF channels	Min. 2	Max. 8
	Multi-Receive capability	Inherent	Default for all systems
	Number of Receive channels	Min. 2	Equal to number of RF channels
	System Control	Embedded	1 TB Hard Disk Drive included
		Power ON / OFF by Software	Ethernet ROUTER PDU
	Operating System	Embedded	
Timing Controller	Timing Resolution	12.5 ns	
	Channel Synchronicity	12.5 ns	For all channels
	Trigger (Input) Real-time Control (Output)	4 11	12.5 ns synchronized
RF channel	Frequency Range	5 – 1280 MHz	^{3}H @1.2 GHz
	Frequency Resolution	< 0.005 Hz	
	Phase Resolution	< 0.006 °	
	Attenuation Resolution and Range	< 0.1 dB 90 dB	
	Amplitude Modulation	> 90 dB	
	Min. Time for Simultaneous setting of Frequency, Phase and Amplitude	12.5 ns	
	Monotony Amplitude and Phase	< +/- 0.1 dB < +/- 0.5 °	
	Waveform / Pulse Program Memory	1 GB	
	RF Intermediate Frequency	1.852 GHz	
	NMR Signal Generation	960 MSPS	Digital Up Converter (DUC)
	NMR Signal Detection	240 MSPS / 16 Bit ADC	Digital Down Converter (DDC)
	Spectral Width	50 Hz - 7.5 MHz	
	Effective Dynamic Range	> 17 Bit (SW < 7.5 MHz) > 19 Bit (SW < 1 MHz) > 23 Bit (SW < 6 kHz)	

		Standard	Option #1	Option #2
RF amplifier #1 (1st)	Frequency Range and RF power	180 – 600 MHz Min. 100 W (25 CW max.)	180 – 600 MHz Min. 500 / 100 W (50 / 25 CW max.)	180 – 600 MHz Min. 1000 / 100 W (50 / 25 CW max.)
RF amplifier #2 (2nd)	Frequency Range and RF power	15 – 600 MHz Min. 500 W (50 CW max.)		15 – 600 MHz Min. 1000 W (50 CW max.)
Additional RF Amplifiers			Various Options	Various Options
Preamplifier #1 (1st)	Nuclei RF Power and Noise Figure	^{19}F / ^{1}H 4 kW peak ~1 dB / GaAs		
Preamplifier #2 (2nd)	Frequency Range / Power and Noise Figure	^{109}Ag - ^{19}F or ^{13}C 500 W peak ~1.1 .. 1.5 dB / GaAs		
Preamplifier #3 (Lock)*	Frequency Range / Power and Noise Figure	^{2}H 500 W peak ~1.4 dB / GaAs		
Additional Preamplifiers			^{13}C, ^{15}N, ^{31}P 500 W peak ~1.5 dB / GaAs	^{57}Fe – ^{31}P 4 kW peak ~1 dB / GaAs
Console	Mains Power Rating	230 V~ / 16A 50 or 60 Hz Single Phase	230 V~ / 16A 50 or 60 Hz Single Phase	230 V~ / 32A 50 or 60 Hz Single Phase
	Power Dissipation	~1.3 kW	~ 2 kW	~ 3 kW
	Dimensions (w x d x h)	**Onebay** 0.69 x 0.83 x 1.30 m	**Onebay with Heightening** 0.69 x 0.83 x 1.58 m	**Twobay** 1.31 x 0.83 x 1.30 m
	Weight	< 230 kg	< 260 kg	< 340 kg
				

* Only needed for probes requiring 2H lock Technical Specifications subject to change without notice

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Magnet Sales Information

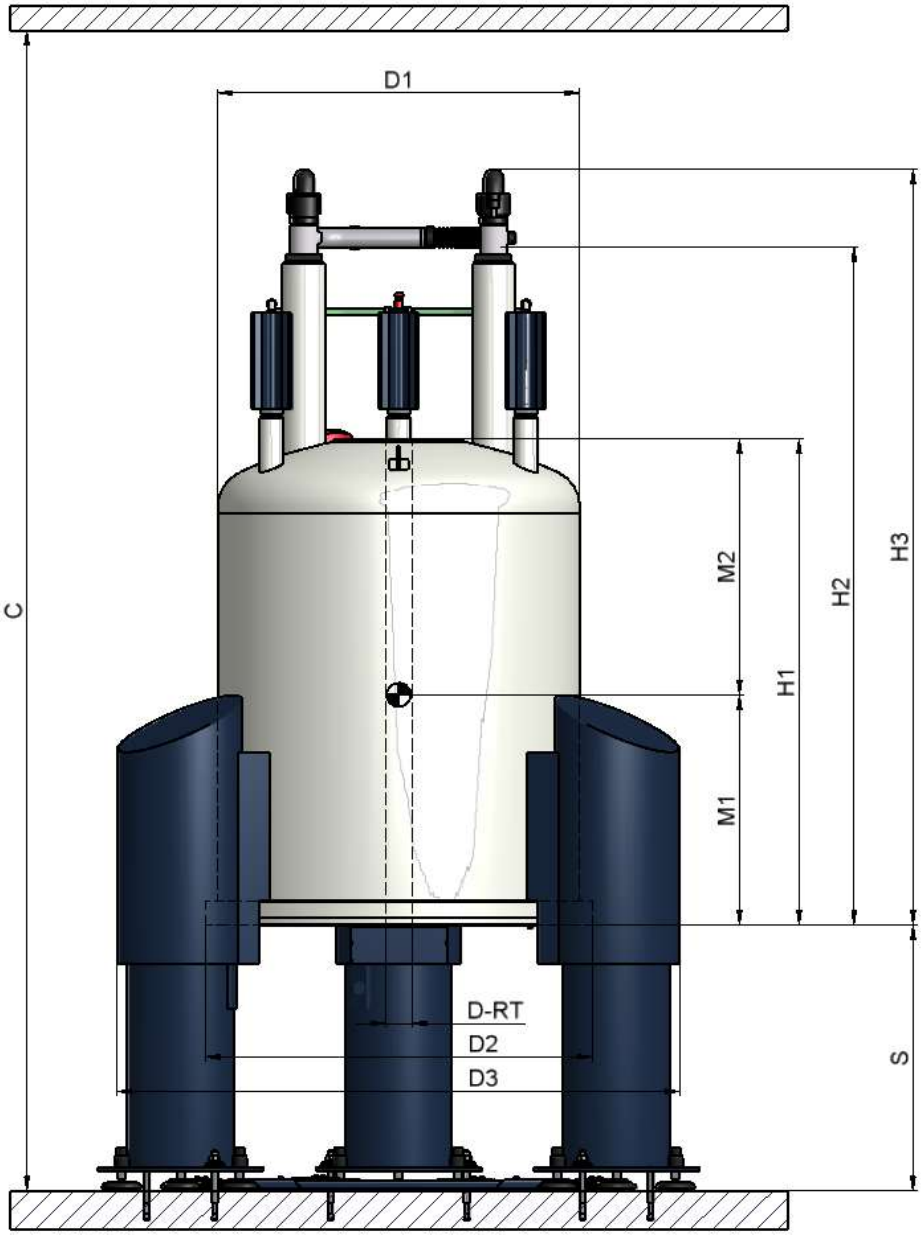
Ascend™

600 MHz / 54 mm

Magnet System Ascend™ 600 MHz / 54 mm

Part Number Z115312

Geometrical Dimensions



Geometrical Dimensions

		Description
C =	2845 mm	Operational ceiling height
D-RT =	54 mm	Diameter room temperature bore tube
D1 =	745 mm	Diameter cryostat upper part
D2 =	795 mm	Diameter cryostat bottom plate
D3 =	1477 mm	Width of magnet stand
H1 =	1205 mm	Height of cryostat from bottom flange to upper flange
H2 =	1604 mm	Height of cryostat from bottom flange to helium tower Minimum height for transportation
H3 =	1763 mm	Height of cryostat from bottom flange to helium manifold
S =	700 mm	Height between floor and magnet bottom flange

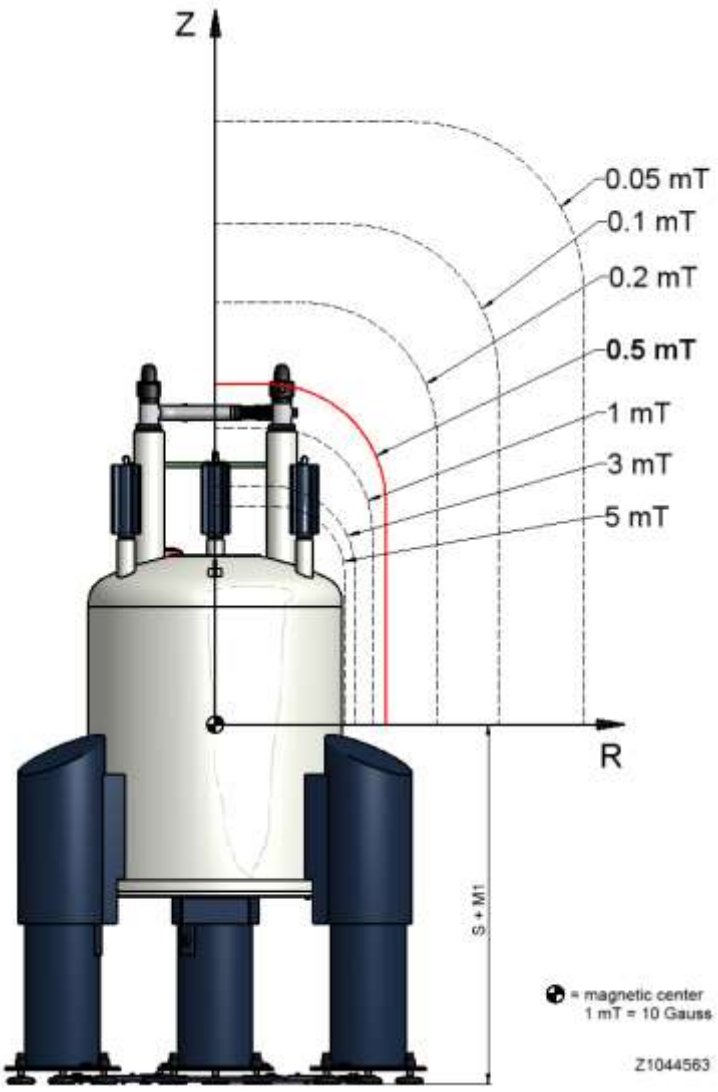
System Data

Minimum operational ceiling height (helium transfer line 29085)	2845 mm
Minimum ceiling height with standard helium transfer line 53962	3135 mm
Required space (footprint, width x depth)	~ 1.4 m^2
System weight (empty, without magnet stand)	609 kg
Magnet stand	111 kg
System weight (filled completely, with magnet stand)	839 kg

NMR Magnet Specifications

Type	BZH 600’70 ASCEND™
NMR-frequency (^{1}H)	600 MHz
Operating field	14.09 Tesla
Field stability (guaranteed value in persistent mode)	< 10 ppb/hr (< 6.0 Hz/hr)
Axial range with homogeneity better than 10 ppm	~ 55 mm
Radial fringe field (horizontal distance of the 0.5 mT (5G line from the magnetic centre)	< 0.70 m
Axial fringe field (vertical distance of the 0.5 mT (5G line from the magnetic centre)	< 1.40 m
Cryo shims	X, Y, Z, Z^2, Z^3, XZ, YZ, XY, X^2-Y^2
Electromagnetic Disturbance Suppression EDS** typical	> 99 %

Fringe Field Plot



Fringe field contour	Radial [R]	Axial [Z]
200 mT (Directive 2013/35/EU)	Inside cryostat	Inside cryostat
5 mT	0.50 m	0.88 m
3 mT	0.54 m	0.97 m
1 mT	0.62 m	1.21 m
0.5 mT (5 Gauss)	**0.70 m**	**1.40 m**
0.2 mT	0.92 m	1.73 m
0.1 mT	1.17 m	2.07 m
0.05 mT (~Earth magnetic field)	1.52 m	2.49 m

Cryostat Specifications

Type	D 325/54 ASCEND™
Room temperature bore	54 mm
Approx. helium evaporation rate under stabilized conditions (T=20°C, p=1030 mbar)	~ 16 ml liquid helium/hour
Maximum liquid helium refill volume/total volume	58/91 litres
Minimum helium hold time	150 days
Approx. nitrogen evaporation rate under stabilized conditions (T=20°C, p=1030 mbar)	~ 240 ml liquid nitrogen/hour
Maximum liquid nitrogen refill volume/total volume	104/134 litres
Minimum nitrogen hold time	18 days

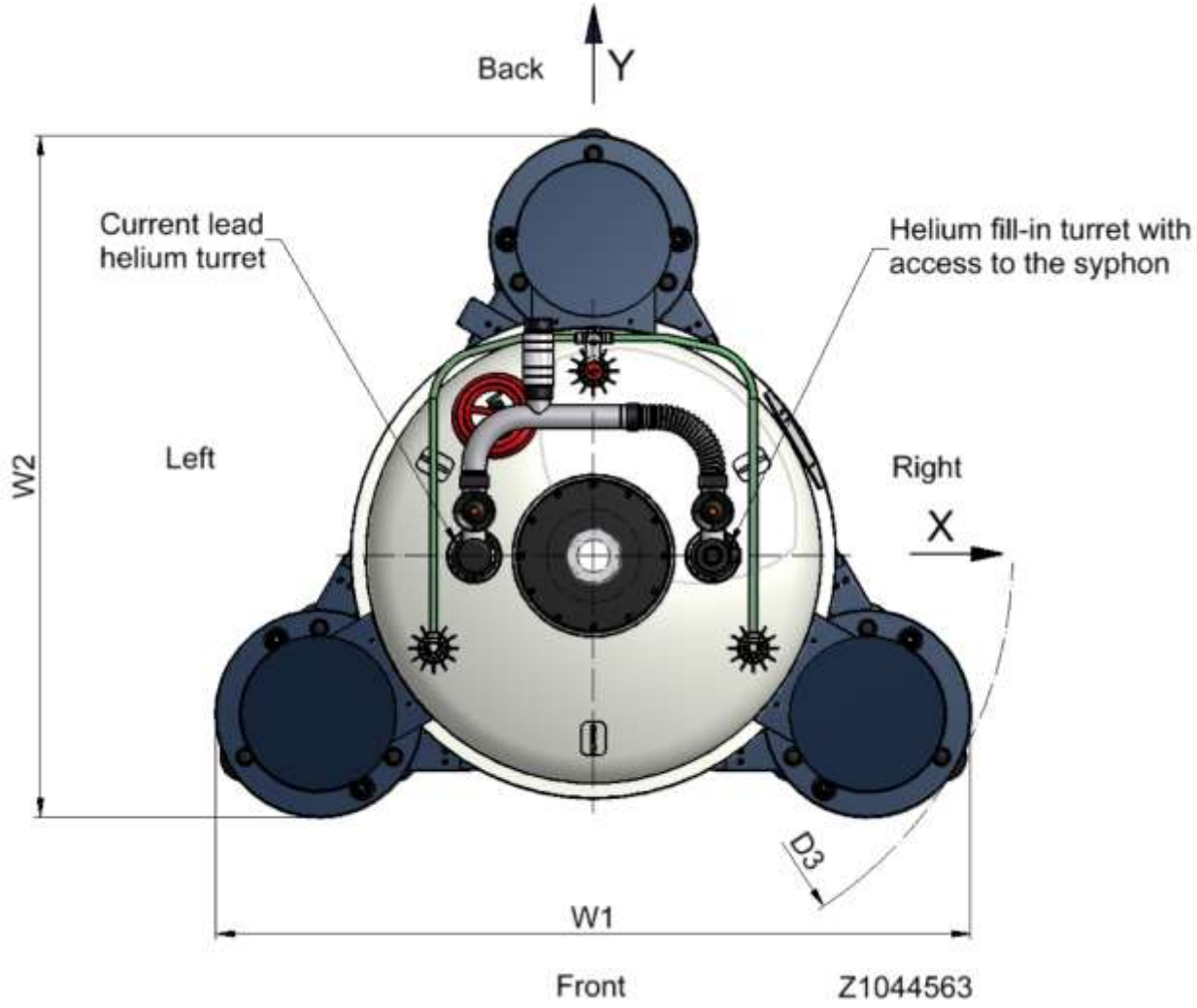
Accessories

Magnet stand F80-700 **ADI** (height 700 mm) **A**ir Spring and **D**amped **I**solator with **vertical** damping Frequencies damped > 3.8 Hz / resonance frequency 2.6 Hz	Included	Z112741
Magnet stand F80-700 **API** (height 700 mm) **A**ir **P**iston and Damped **I**solator with **vertical** and **horizontal** damping Frequencies damped > 3.8 Hz / resonance frequency 2.6 Hz	Optional AH0065	Z117692
Upgrade from **ADI** to **API** cylinders when magnet stand F80 is existing **A**ir **P**iston Damped **I**solators with **vertical** and **horizontal** damping Frequencies damped > 3.8 Hz / resonance frequency = 2.6 Hz		Z114651
Electronic atmospheric pressure device with adjustable set point*	Optional	Z102597
Nitrogen level sensor for BSMSII (SCB3)	Included	Z122404

Equipment for Cryogen Transfer

Helium transfer line* D3xx (1455/2060/655)	AH0070	53962
Helium transfer line* with bendable extensions (1455/2060/380) for minimum operational ceiling height (2850 mm)		29085

Top View



Geometrical Dimensions

Width of magnet stand	W1	1236 mm
Depth of magnet stand	W2	1116 mm
Diameter of magnet stand = 2 x radius	D3	1375 mm

Transport

Overall system dimensions for transportation		
Magnet box	L x D x H	93 x 114 x 199 cm^3
Magnet stand box	L x D x H	75 x 79 x 120 cm^3
Minimum system dimensions of magnet, unpacked (without manifold)		∅ 79.5 cm, H 160 cm
Magnet System weight for transportation		~ 741 kg
Magnet stand box weight for transportation		~ 168 kg

Installation

Liquid nitrogen needed for cool down	600 litres
Liquid helium needed for cool down	300 litres
Liquid helium needed for energizing, cryo shimming and quench reserve	300 litres
Nitrogen gas for flushing, minimum grade 4.6	1 cylinder 50 l/200 bar
Helium gas for flushing, minimum grade 4.6	2 cylinder 50 l/200 bar

* A detailed description of the marked objects can be found in „Magnet Accessories“ ZTKS0041.

Electromagnetic Disturbance Suppression **EDS™:

Ascend™ magnets efficiently suppress external electromagnetic field disturbances using a proprietary Bruker technology **EDS™**. Sources of such disturbances are corridor traffic, elevators, power lines, outside vehicular traffic and railway lines.

Definition:

The **EDS™ factor** for spatially homogeneous disturbances is defined as the fraction of the external disturbance suppressed by the magnet in the magnetic centre at a given disturbance frequency. Thereby, no digital lock system or other field compensation device is used.

Detailed specification for magnet system 600/54 Ascend™:

Disturbance frequency	EDS™ factor
< 0.01 Hz	> 99 %
0.01 - 1 Hz	> 97 %
1 - 5 Hz	> 98 %
> 5 Hz	> 99 %
16.667 Hz (railways)	> 99.9 %
50 Hz (power lines)	> 99.9 %
60 Hz (power lines)	> 99.9 %

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Magnet Sales Information

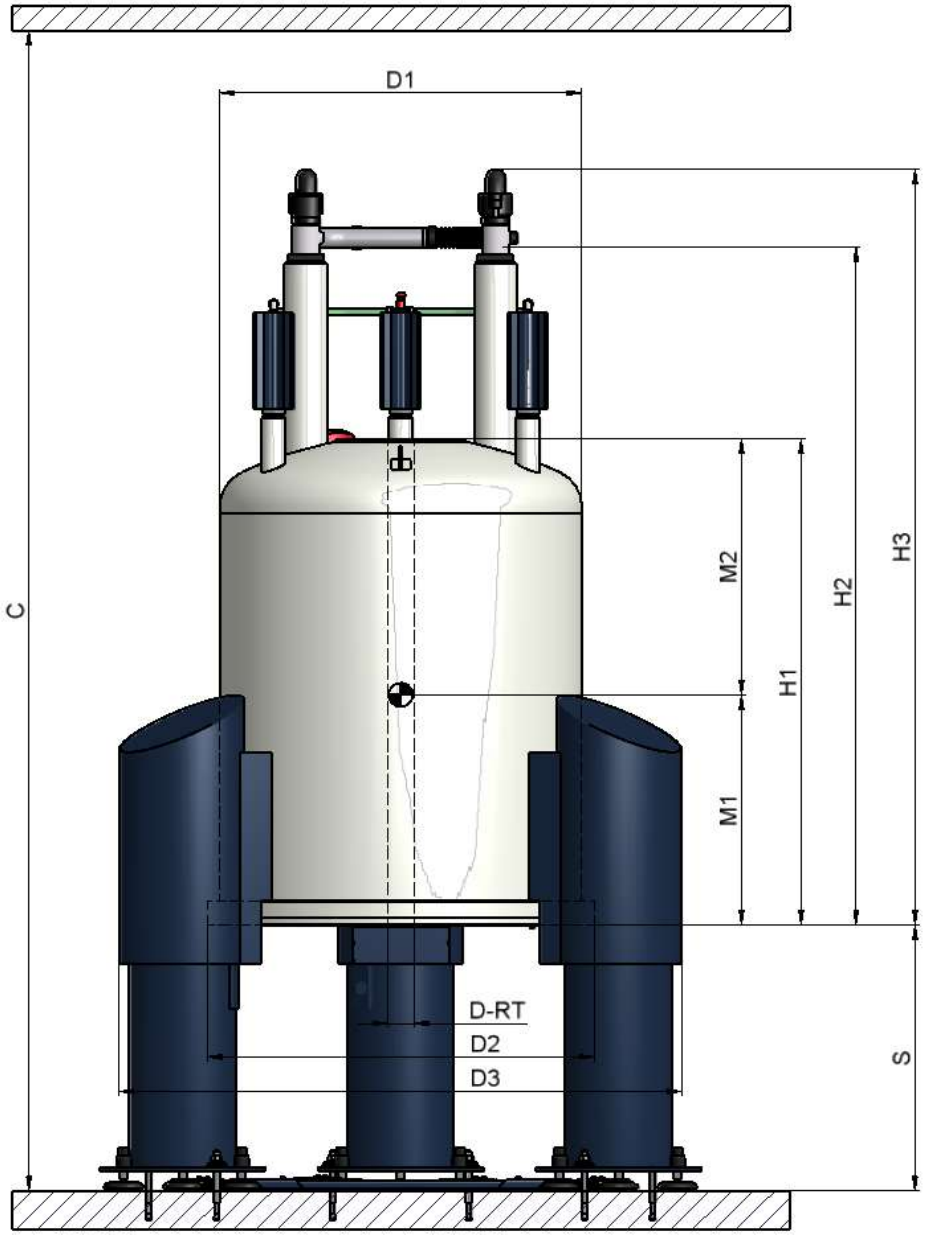
Ascend™

400 MHz / 54 mm

Magnet System Ascend™ 400 MHz / 54 mm

Part Number Z115310

Geometrical Dimensions



Geometrical Dimensions

		Description
C =	2520 mm	Operational ceiling height
D-RT =	54 mm	Diameter room temperature bore tube
D1 =	745 mm	Diameter cryostat upper part
D2 =	795 mm	Diameter cryostat bottom plate
D3 =	1295 mm	Diameter magnet stand
H1 =	1005 mm	Height of cryostat from bottom flange to upper flange
H2 =	1391 mm	Height of cryostat from bottom flange to helium tower Minimum height for transportation
H3 =	1564 mm	Height of cryostat from bottom flange to helium manifold
S =	570 mm	Height between floor and magnet bottom flange

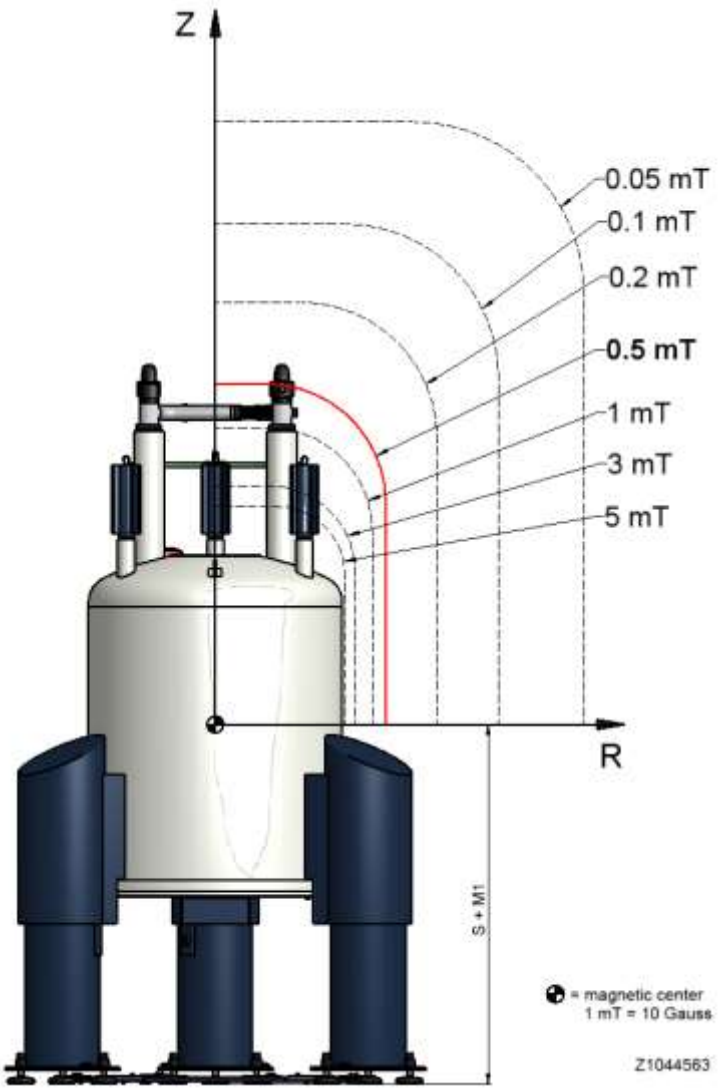
System Data

Minimum operational ceiling height (helium transfer line 29085)	2520 mm
Minimum ceiling height with standard helium transfer line 53962	2805 mm
Required space (footprint)	~ 1.4 m^2
System weight (empty, without magnet stand)	358 kg
Magnet stand	96 kg
System weight (filled completely, with magnet stand)	553 kg

NMR Magnet Specifications

Type	BZH 400'70 ASCEND™
NMR-frequency (^{1}H)	400 MHz
Operating field	9.39 Tesla
Field stability (guaranteed value in persistent mode)	< 10 ppb/hr (< 4.0 Hz/hr)
Axial range with homogeneity better than 10ppm	~ 55 mm
Radial fringe field (horizontal distance of the 0.5mT (5G) line from the magnetic centre)	< 0.50 m
Axial fringe field (vertical distance of the 0.5mT (5G) line from the magnetic centre)	< 1.00 m
Cryo shims	X, Y, Z, Z^2, Z^3, XZ, YZ, XY, X^2-Y^2
Electromagnetic Disturbance Suppression EDS** typical	> 99 %

Fringe Field Plot



Fringe Field Plot	Radial [R]	Vertical [Z]
200 mT (Directive 2013/35/EU)	Inside cryostat	0.35 m
5 mT	0.37 m	0.64 m
3 mT	0.40 m	0.70 m
1 mT	0.46 m	0.87 m
0.5 mT (5 Gauss)	**0.50 m**	**1.00 m**
0.2 mT	0.62 m	1.23 m
0.1 mT	0.78 m	1.46 m
0.05 mT (~Earth magnetic field)	1.00 m	1.75 m

Cryostat Specifications

Type	D 315/54 ASCEND™
Room temperature bore	54 mm
Approx. helium evaporation rate under stabilized conditions (T=20°C, p=1030 mbar)	~ 13 ml liquid helium/hour
Maximum liquid helium refill volume/total volume	94/106 litres
Minimum helium hold time	300 days
Approx. nitrogen evaporation rate under stabilized conditions (T=20°C, p=1030 mbar)	~ 220 ml liquid Nitrogen/hour
Maximum liquid nitrogen refill volume/total volume	85/106 litres
Minimum nitrogen hold time	16 days

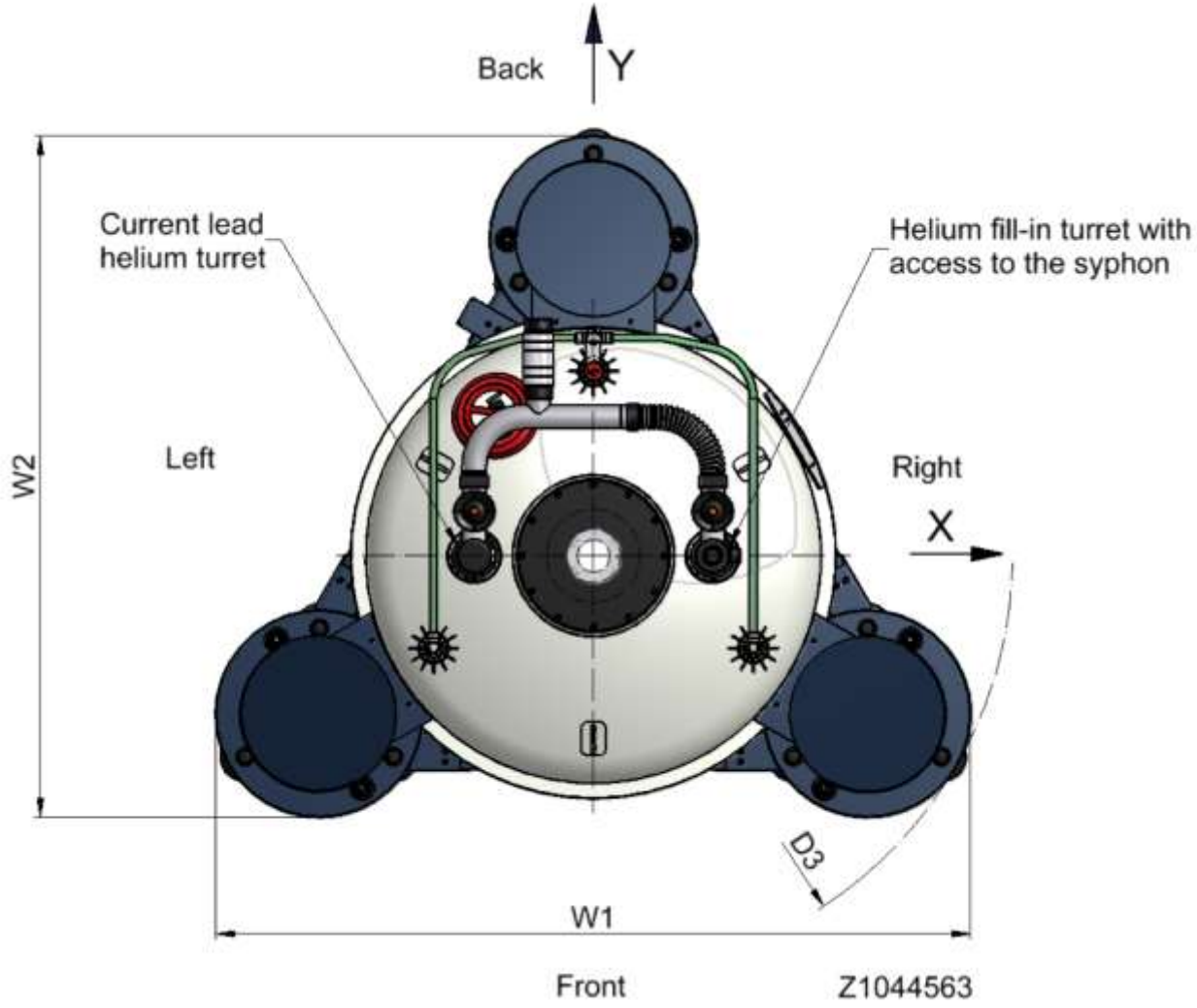
Accessories

Magnet stand F80-570 **EMI** **E**lasto**m**eric **I**solators Frequencies damped > 14 Hz / resonance frequency = 9.5 Hz	Standard	Z130990
Magnet stand F80-700 **EMI** **Easy** installation of magnet system with **E**lasto**m**eric **I**solators Frequencies damped > 14 Hz / resonance frequency = 9.5 Hz	Optional	Z113884
Magnet stand F80-570 **ADI** (height 570 mm) **A**ir Spring **D**amped **I**solators with **vertical** damping Frequencies damped > 3.8 Hz / resonance frequency = 2.6 Hz	Optional AH0063	Z112742
Magnet stand F80-700 **ADI** (height 700 mm) **A**ir Spring **D**amped **I**solators with **vertical** damping Frequencies damped > 3.8 Hz / resonance frequency = 2.6 Hz	Optional	Z112741
Magnet Stand F80-570 **API** (height 570 mm) **A**ir **P**iston Damped **I**solator with **vertical** and **horizontal** damping Frequencies damped > 3.8 Hz / resonance frequency 2.6 Hz	Optional AH0065	Z117691
Magnet Stand F80-700 **API** (height 700 mm) **A**ir **P**iston Damped **I**solator with **vertical** and **horizontal** damping Frequencies damped > 3.8 Hz / resonance frequency 2.6 Hz	Optional	Z117692
Upgrade from **EMI** to **ADI** cylinders when magnet stand F80 is existing **A**ir **P**iston Damped **I**solators with **vertical** damping Frequencies damped > 3.8 Hz / resonance frequency = 2.6 Hz		Z139987
Upgrade from **EMI** to **API** cylinders when magnet stand F80 is existing **A**ir **P**iston Damped **I**solators with **vertical** and **horizontal** damping Frequencies damped > 3.8 Hz / resonance frequency = 2.6 Hz		Z139988
Upgrade from **ADI** to **API** cylinders when magnet stand F80 is existing **A**ir **P**iston Damped **I**solators with **vertical** and **horizontal** damping Frequencies damped > 3.8 Hz / resonance frequency = 2.6 Hz		Z114651
Electronic atmospheric pressure device with adjustable set point*	Optional	Z102597
Nitrogen level sensor for BSMSII (SCB3)	Included	Z122394

Equipment for Cryogen Transfer

Helium transfer line* D3xx (1455/2060/655)	AH0070	53962
Helium transfer line* with bendable extensions (1455/2060/380) for minimum operational ceiling height (2850 mm)		29085

Top View



Geometrical Dimensions

Width of magnet stand	W1	1236 mm
Depth of magnet stand	W2	1116 mm
Diameter of magnet stand = 2 x radius	D3	1375 mm

Transport

Overall system dimensions for transportation		
Magnet box	L x D x H	93 x 114 x 158 cm^3
Magnet stand box (Standard stand)	L x D x H	75 x 79 x 120 cm^3
Minimum system dimensions of magnet, unpacked (without manifold)		∅ 79.5 cm, H 139 cm
System weight for transportation		~ 469 kg
Magnet stand box weight for transportation		~ 153 kg

Installation

Liquid nitrogen needed for cool down	400 litres
Liquid helium needed for cool down	200 litres
Liquid helium needed for energizing, cryo shimming and quench reserve	300 litres
Nitrogen gas for flushing, minimum grade 4.6	1 cylinder 50 l/200 bar
Helium gas for flushing, minimum grade 4.6	1 cylinder 50 l/200 bar

* A detailed description of the marked objects can be found in „ Magnet Accessories“ ZTKS0041.

Electromagnetic Disturbance Suppression **EDS™:

Ascend™ magnets efficiently suppress external electromagnetic field disturbances using a proprietary Bruker technology **EDS™**. Sources of such disturbances are corridor traffic, elevators, power lines, outside vehicular traffic and railway lines.

Definition:

The **EDS™ factor** for spatially homogeneous disturbances is defined as the fraction of the external disturbance suppressed by the magnet in the magnetic centre at a given disturbance frequency. Thereby, no digital lock system or other field compensation device is used.

Detailed specification for magnet system 400/54 Ascend™:

Disturbance frequency	EDS™ factor
< 0.01 Hz	> 98 %
0.01 - 1 Hz	> 96 %
1 - 5 Hz	> 95 %
> 5 Hz	> 98 %
16.667 Hz (railways)	> 99.5 %
50 Hz (power lines)	> 99.9 %
60 Hz (power lines)	> 99.9 %

Ascend 400 MHz / 54 mm

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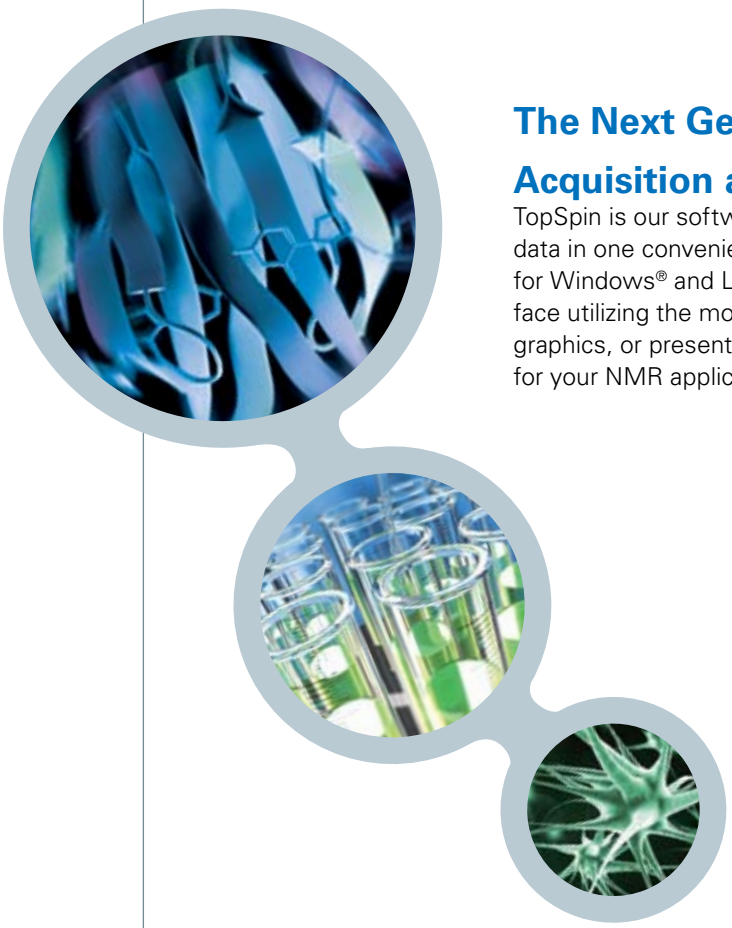
NMR

TopSpin™

Ideal for first-time spectrometer users as well as routine users, TopSpin's different acquisition tools make it easy for both beginner and expert to find their way to an NMR spectrum.

Key Features

- PC-standard user interface offers easy accessibility for Windows® and Linux® users
- Comprehensive functionalities for processing, displaying and analyzing single and multi-dimensional spectra
- Intuitive acquisition
- Non-uniform sampling
- Small molecule characterization
- BioTools™ - Biomolecular NMR made easy
- Method development environment
- Result publishing, predefined and user-defined layouts
- Lineshape analysis for solid-state NMR, including dynamic NMR
- Regulatory compliance support tools (audit trailing, electronic signature, auto-archiving)
- Special licenses for students and universities



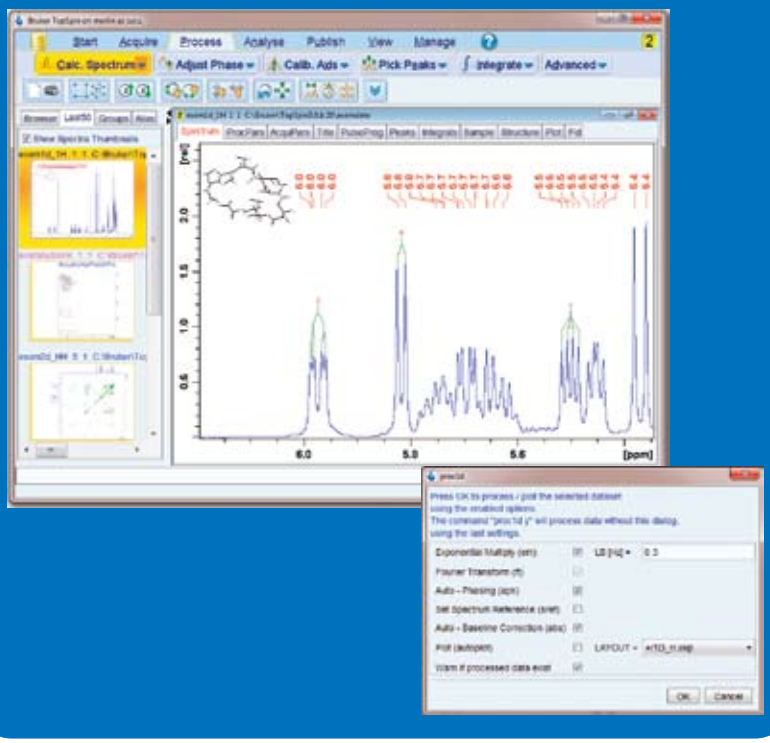
The Next Generation of NMR Data Acquisition and Processing Software

TopSpin is our software for acquiring, processing and analyzing NMR data in one convenient, streamlined package. TopSpin is designed for Windows® and Linux® users, and features a highly intuitive interface utilizing the most widespread standards from word processing, graphics, or presentation programs, providing the same look-and-feel for your NMR applications.

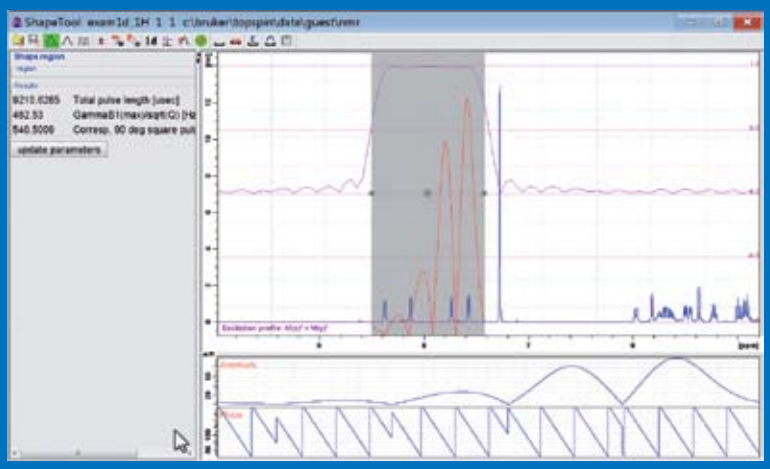
Optimized Workflow

The TopSpin Flow User Interface of menus and icons offers convenient access to the most commonly used tools and commands.

In addition, each TopSpin user can customize their own menus, icons and macros. This makes it possible for the user to optimize the software interface to suit their individual needs.



Each user can define their individual set up for standard 1D processing. This set of commands is then available as a push-button solution.



Simple setup of selective experiments:
Define excitation regions interactively and choose a shape to calculate the excitation profile prior to acquisition.

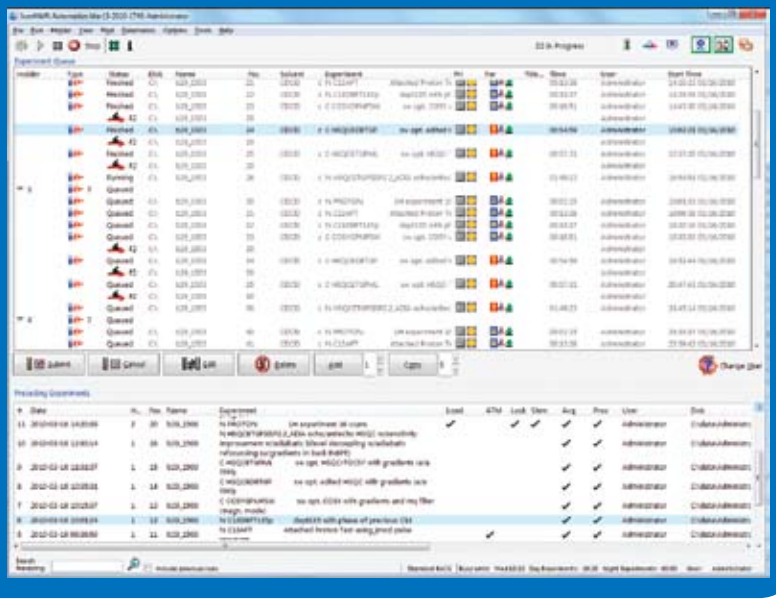
Automation

Maximize your sample throughput

IconNMR is the graphical user interface for fully automated acquisition and processing. This productivity tool excels whenever large numbers of samples accrue, or many users access your spectrometer. IconNMR supports sample changers and sample preparation robots. The user can set up or supervise measurements remotely via WEB browser from your desktop, Smartphone or iPhone.

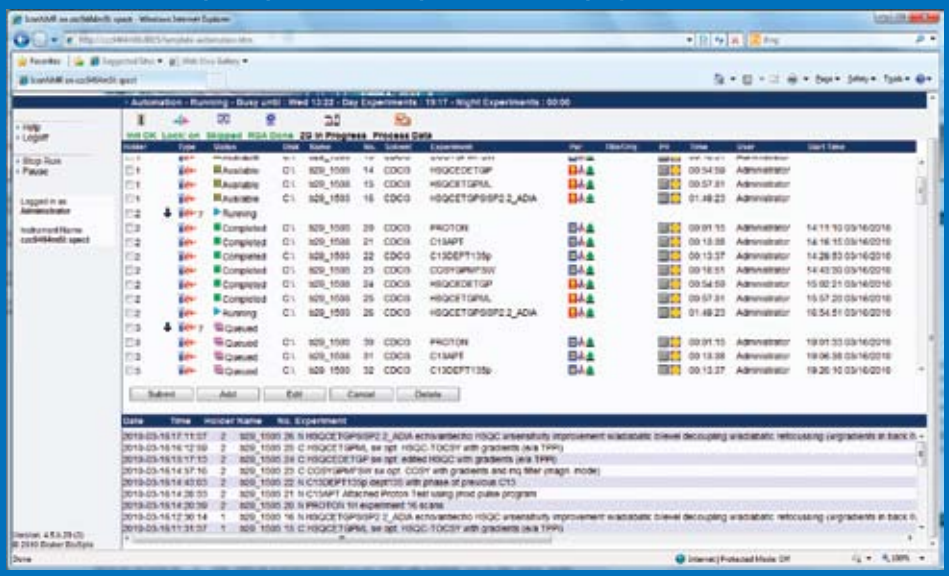
- Multi-user support
- Configurable 1-click experiment setup
- Integrated title selection / collation
- Spreadsheet import
- Experiment duplication / iteration
- Lock, shim tuning / matching control
- Intelligent temperature handling
- Failsafe Watchdog timer
- Comprehensive search tool
- Automate any TopSpin dataset
- Acquire & view spectra via internet
- Multiple user login safeguards
- Regulate access for 'view-only' monitoring
- Secure server SSL mode
- Small screen PDA support

Multi-sample experiment set up and status display



Remote multi-sample experiment set up and status display using a Smartphone or iPhone.

Remote multi-sample experiment set up and status display via WEB browser

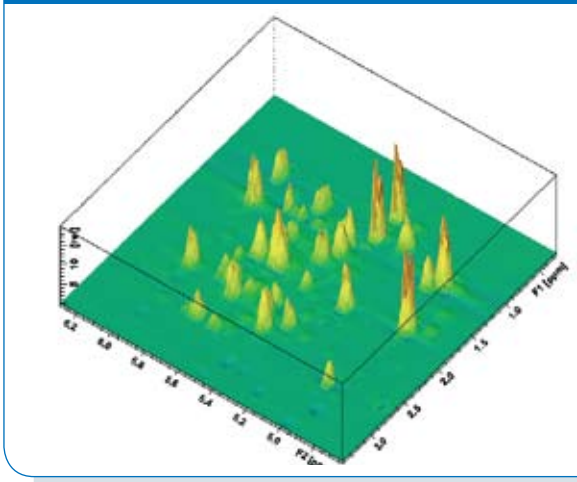


Data Evaluation

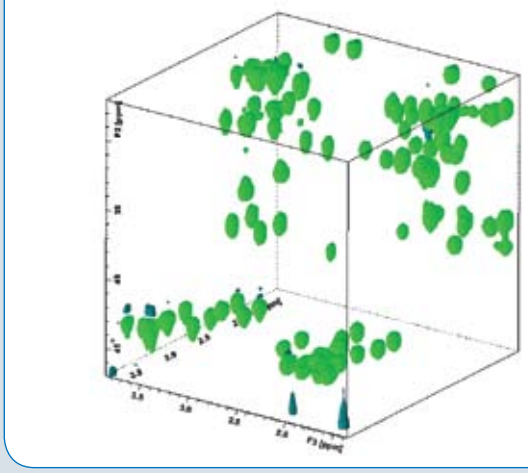
Visualize and process your data in comprehensive detail

TopSpin provides a wealth of data visualization and administration features and a comprehensive set of NMR data processing functionalities from 1D to 5D.

3D-view of a 2D spectrum



3D spectrum

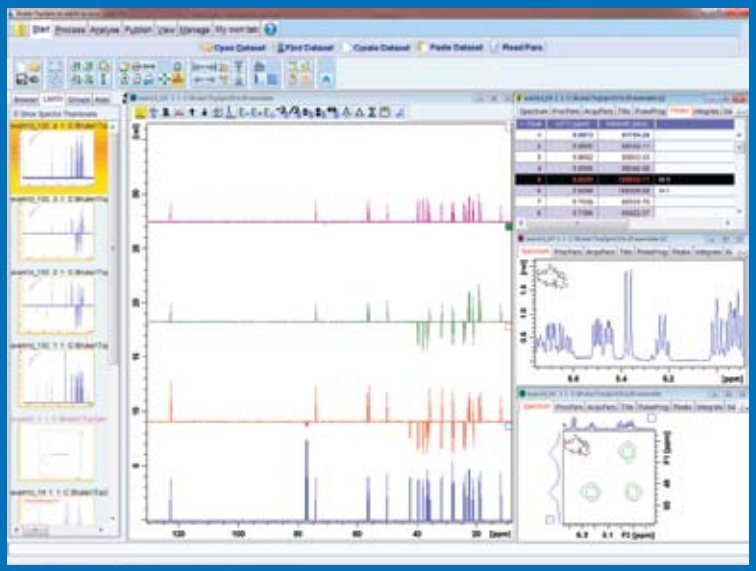


Data Evaluation

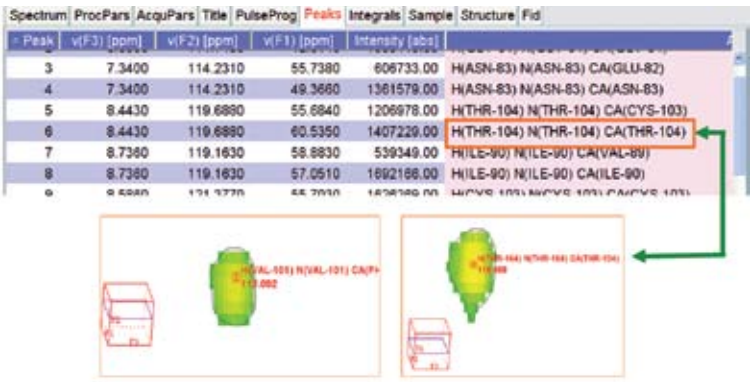
Key Features

- Window multiplication, Fourier transform, phase correction, baseline correction; all interactive or automatic
- Forward/backward and Delayed Linear Prediction
- Inverse Fourier and Hilbert transform
- Processing of rows, columns, planes and subcubes of nD datasets
- Dosy diffusion processing
- Interactive and automatic multi-dimensional peak picking and integration
- Automatically process series of datasets
- Import a variety of NMR data formats
- Administer groups of datasets to manage projects
- Export data displays to png, jpg, emf, bmp formats
- Send data via e-mail or save to a zip archive
- Drag & Drop data from Windows®/Linux® explorer
- Write own TopSpin extensions in C or Python, including graphics
- Search for datasets based on name, data, pulse program, title, dimension
- Print window contents

Multiple window interface



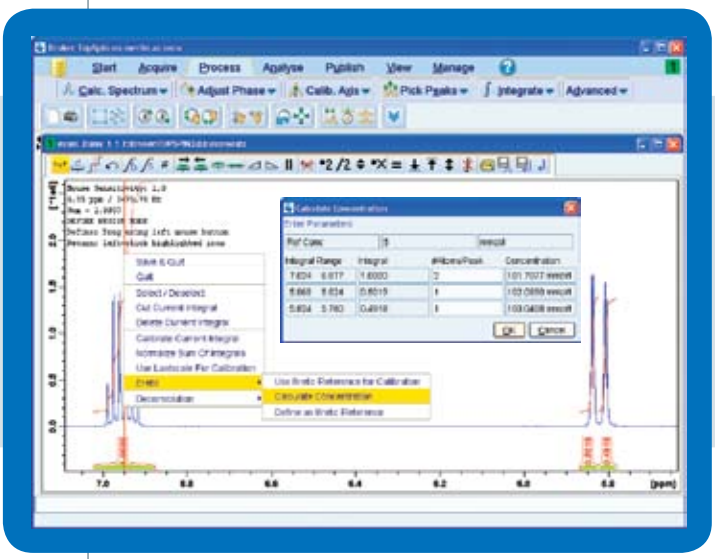
3D peak list of a protein with backbone assignments and direct link (1-click) into spectrum.



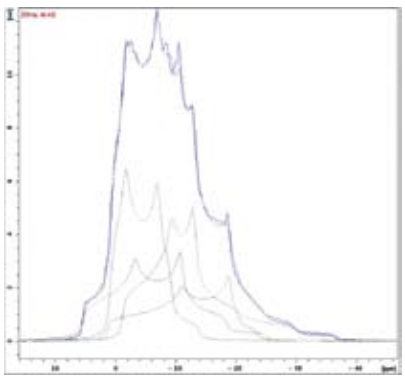
Structure Analysis

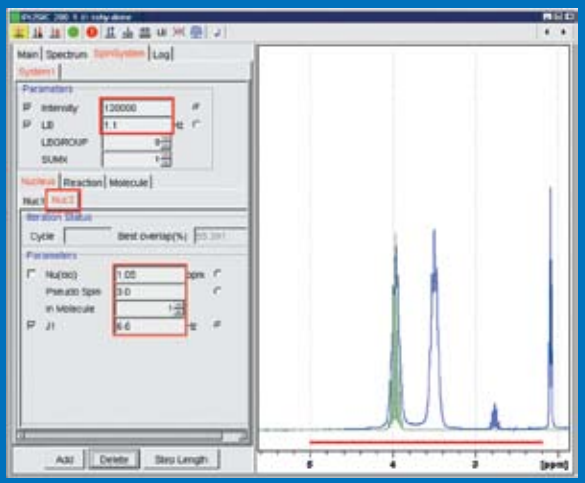
Discover molecular features by exploiting TopSpin Structure Analysis Tools

TopSpin provides a number of valuable tools for interpreting spectra and relating them to a molecular structure.



- Relaxation analysis (T1/T2)
- Gaussian / Lorentzian deconvolution of 1D and 2D spectra
- Maximum Entropy deconvolution
- Dynamic exchange lineshape analysis (DNMR), 7 nuclei, chemical shifts and scalar couplings, mutual / non-mutual exchange
- Solid state lineshape analysis: Computes various line shape models and fits them to spectra
- Interactive and automatic multiplet analysis
- Daisy spectrum simulation / iteration for obtaining accurate chemical shifts, couplings and linewidths. Uses multiplet analysis results or spin system definitions in various formats
- Integrated structure editor (2D) and viewer (3D)
- Prediction of ^{1}H and ^{13}C NMR shifts from chemical structure including a complete molecular modelling system with a 3D structure editor (optional)
- Computation of the fids of 1D/nD experiments from a pulse program using acquisition parameters and a spin system using quantum mechanics
- NMR quantification
- HSQC structure verification aids





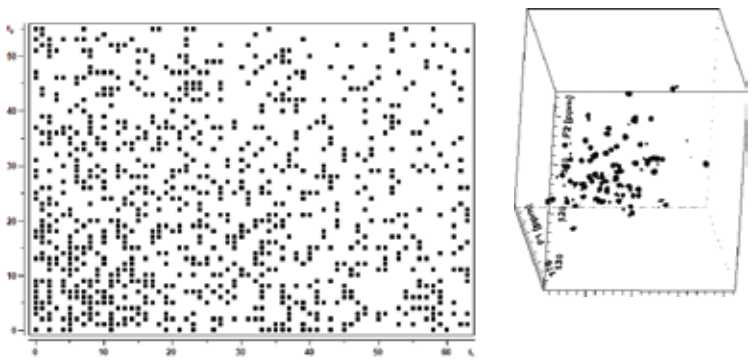
DNMR Analysis: The methine spectrum region of the experimental iPr2SIC spectrum with one fitting curve

Non-Uniform Sampling (NUS)

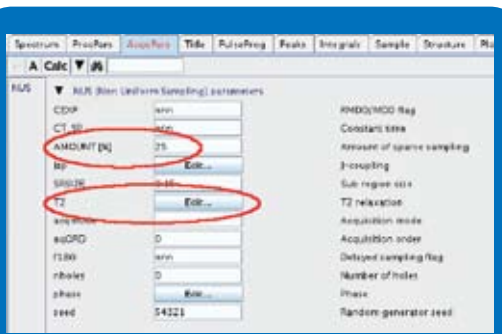
Non Uniform Sampling (NUS) is now a fully integrated acquisition and processing feature of TopSpin 3.0. It enables routine use and is available for all kinds of NMR experiments. An automatically generated and optimized NUS sparse list defines the sampling pattern leading to the fractional data acquisition. TopSpin uses multi-dimensional decomposition to calculate the missing data points, enabling regular Fourier Transform processing of the complete data set automatically.

NUS removes the existing time barrier to high resolution multidimensional NMR spectroscopy, making it especially useful for multi-dimensional experiments in biomolecular NMR where time savings, up to a factor of 4 in 3D experiments, or even 10 or more in 4D and 5D experiments, can be achieved. With NUS, new protein structure determination experiments now become feasible.

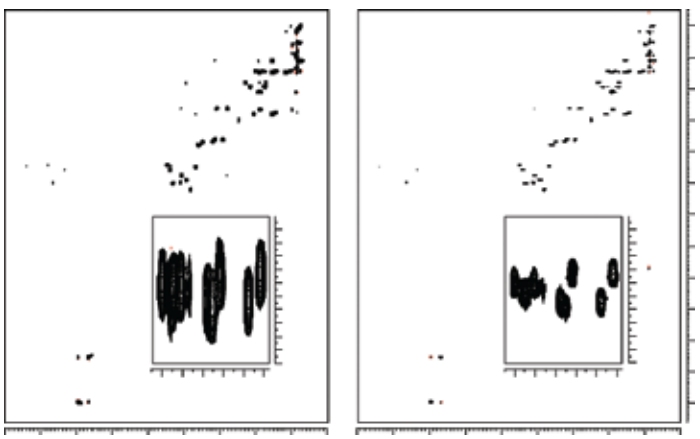
Small molecule applications based on 2D spectra also benefit from an accelerated acquisition of a factor of 2. Of special interest are improvements in spectral resolution and quality delivered by NUS without the need to increase overall acquisition time.



Increased recording speed of multi-dimensional NMR data in a HNCO experiment on ubiquitine. NUS reduces the experiment time by a factor of 4 yet still maintains high quality spectral data.



Routine character of implementation now enables everyone to apply NUS to any experimental protocol. Sparseness and weighting parameters for optimum signal-to-noise can be easily adjusted.



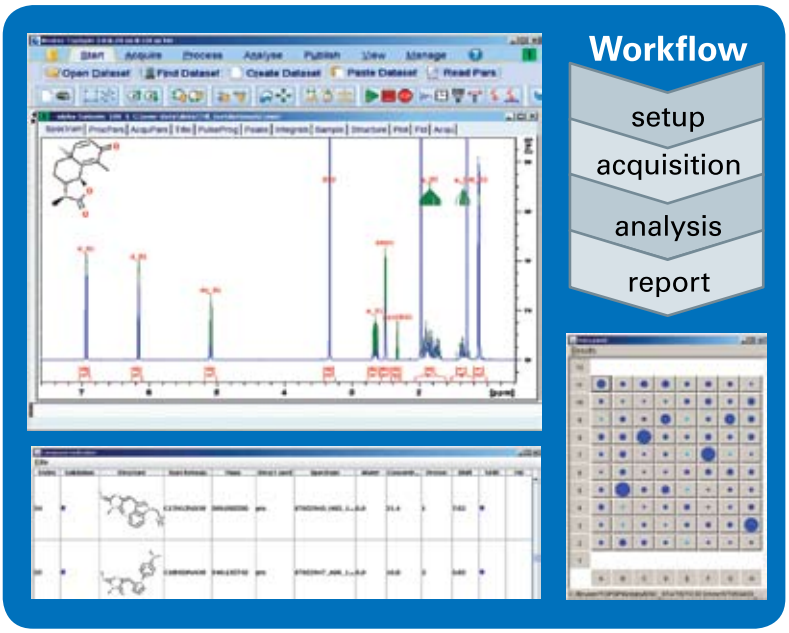
Increased resolution without extended acquisition time using NUS. Fully acquired 256 matrix spectra at lower resolution compared to a NUS experiment of a 1024 matrix, both recorded at identical acquisition times.

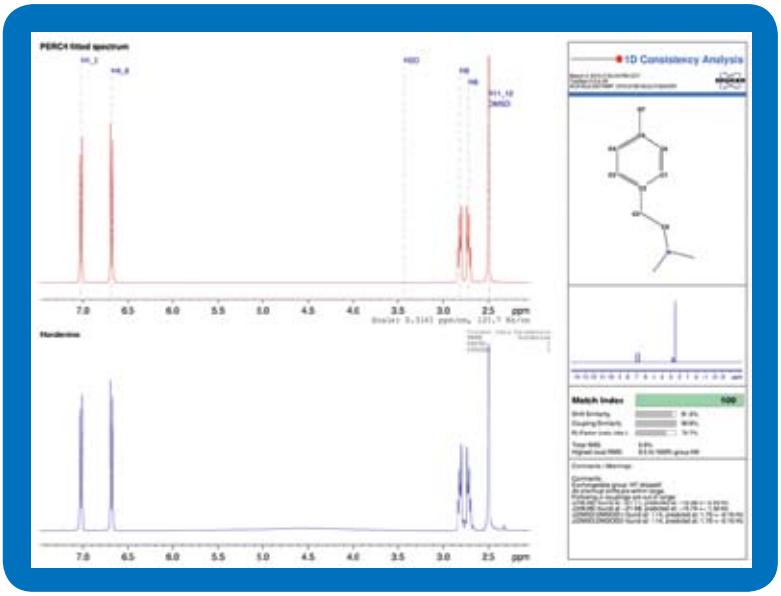
Complete Molecular Confidence™

Small molecule applications greatly benefit from the development of the Complete Molecular Confidence (CMC) concept (optional package). The solutions within this concept aim at two major areas of NMR application: Single sample routine NMR for open access systems and NMR service labs as well as for high throughput NMR batch analysis.

Absolute Quantification - CMC-q

Absolute quantification of a series of samples can be automatically performed including the whole workflow from sample setup, automatic NMR measurements, analysis and spreadsheet reporting. This enables users to determine mass contents, relative amounts of substances and purity. CMC-q delivers fully automated concentration determination for example in drug discovery screening applications—even in non-deuterated solvents.





Structure Consistency Analysis - CMC-i

The automated consistency analysis (ACA) routine provides a safe assessment of the consistency between molecular structure and ^{1}H-spectrum. By performing a complete NMR spectral analysis, the ACA routine returns the fully assigned spectrum and the accurate NMR parameters (chemical shifts & couplings) extracted from the experimental data. The automatically generated report gives a clear answer for the major part of the samples, therefore the specialist only needs to spend time on few unclear results, such releasing him to perform other tasks.

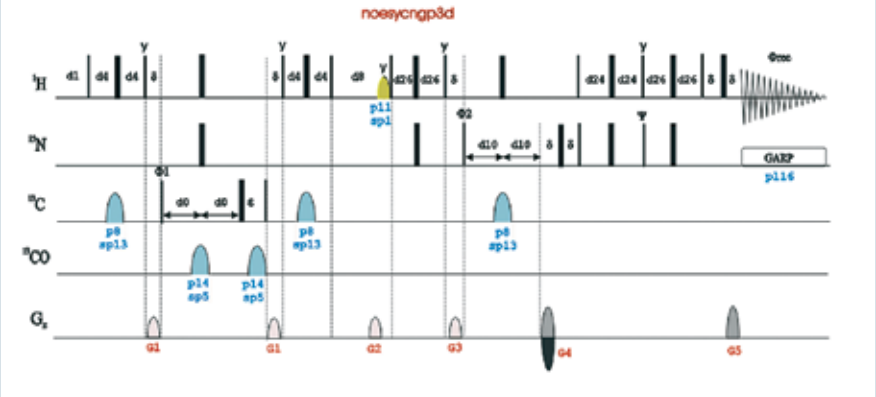
Knowledge Data Base

Utilize the cumulative knowledge stored in the NMR Guide

Through a Web browser, TopSpin provides access to the unique NMR Encyclopedia called NMR Guide, which is an extensive database of pulse program diagrams, experiment descriptions, spectra of 100 representative experiments and more than 4,000 literature references. Browse through the content or perform searches with any keyword.

- Pulse program catalogue
- Experiment descriptions
- Literature references
- Comprehensive search engine
- Examples of spectra

Pulse program diagram

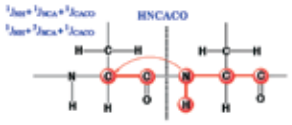


Experiment description (extract)

4D HNCACO

DESCRIPTION

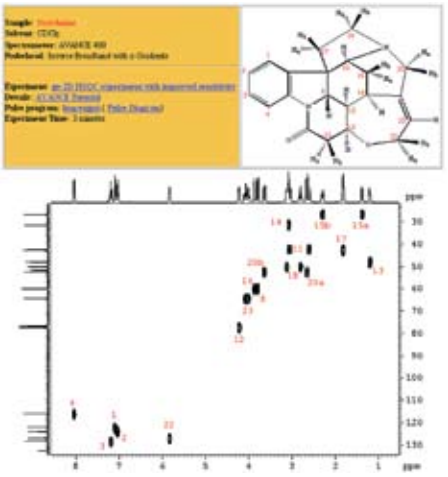
The **4D HNCOCA experiment** has been designed to trace out backbone connectivites in large proteins and protein complexes.



REQUIREMENTS

Sucessful implementation on AVANCE spectrometers equipped with a triple-resonance probehead equipped with PFGs. The experiment is recorded on a $^{13}C,^{15}N$-labeled protein in H_2O.

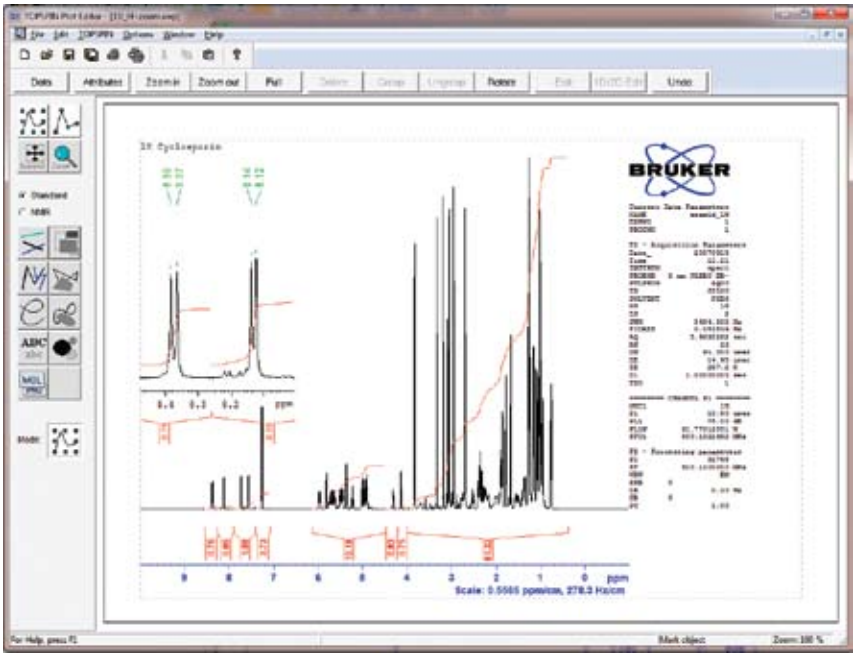
Example from the spectra data base

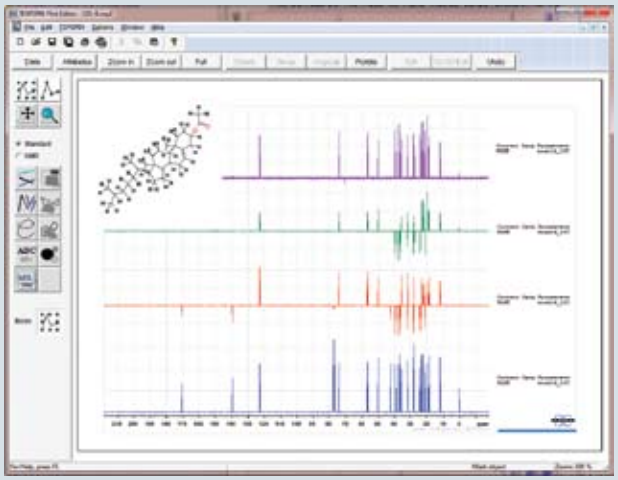


Professionally Print Your Spectra

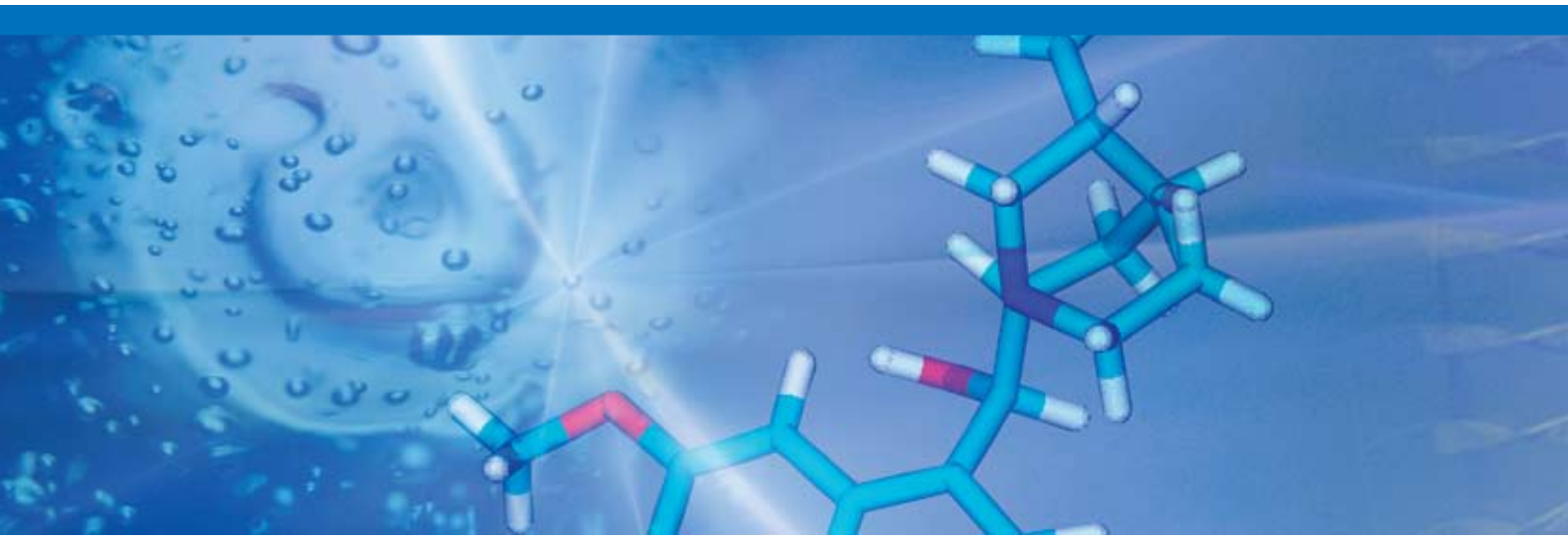
Animate your spectra documentation using intelligent layouts

A rich set of predefined plot layouts enable you to create detailed documentation of your spectra with a few mouse clicks. TopSpin's plot editor also allows you to interactively design and save your desired layouts.





- Tight integration: Rapid access to standard plots
- Predefined plot layouts
- Easy user interface: Comfortable, interactive customization
- Intelligent reusability: Fits your requirements for maintaining standards
- Reliable performance: Fast automation for high data throughput
- Wide inter-operability: Export to many file formats (PostScript, PDF, Windows Metafile, pixel graphics)
- Programmatic access: Flexibility for even the most sophisticated plot solutions



Bruker BioSpin

info@bruker-biospin.com
www.bruker.com/topspin

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SmartDriveNMR
The Intelligent Spectrometer

Advanced Acquisition for Open Access NMR

Collecting the right type of data with the optimal parameters tailored for the problem at hand is crucial for any analytical investigation. With regards to synthesis control by NMR, SmartDriveNMR fully automates the process to deliver high quality results.

First SmartDriveNMR analyzes the situation using a fast scout experiment along with all inputs given by the user, and determines if follow-up experiments would significantly benefit the analysis. These optimal experiments are scheduled and carried out in full automation within the time limits set by the user.

The experiment portfolio includes heteronuclear 2D experiments such as HSQC and HMBC, 1D ^{13}C and a variety of different types of solvent suppression schemes for 1D ^{1}H experiments. The different aspects of data quality include fail-safe Non-Uniform Sampling data acquisition and Signal-to-Noise optimization.

Fig. 1: SmartDriveNMR workflow

SmartDriveNMR Workflow

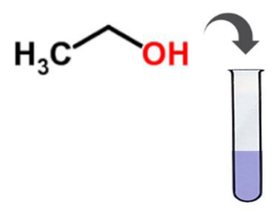
1. The user describes and submits the acquisition job using IconNMR. The description can (but does not have to) include structural information (.mol file).
2. A fast 1D proton spectrum is collected and analyzed.
3. Depending on the analysis results concerning complexity of the problem and the signal strength, further experiments with optimal parameters might be requested.
4. Follow-up experiments are scheduled and acquired in full automation if sufficient time is available. Reasoning triggering the acquisition is made available to the user. An automatic structure verification (ASV) at the end of the run is an integrated part of SmartDriveNMR but not mandatory.

Usage of SmartDriveNMR

SmartDriveNMR is a fully integrated part of IconNMR. The activation is governed by the spectrometer administrator for each user group individually. The user can decide whether SmartDriveNMR should be used for each individual sample; the required inputs are the operating mode and the maximal allowed time per sample. The following table describes the different available modes.

Mode	Behaviour
OPTime	Only the experiments highly beneficial for the given synthesis control task that fit in the given time are carried out, with optimized parameters. → **You get time-optimal spectrometer usage**
MAXperiment	All experiments that are technically possible and fit into the given time will be carried out, with optimized parameters. → **You get the maximum possible number of experiments**
FIXperiment	Experiments are carried out exactly as they are set up by the user WITHOUT parameter optimization. The measurement time depends on these experiments. → **You get what you ordered**

To best highlight the difference between OPTime and MAXperiment modes, an NMR sample with an abundant amount of ethanol is considered. In OPTime the acquisition is terminated directly after the scout experiment, whereas in MAXperiment the complete experiment portfolio is fully utilized:



Settings	Results
OPTime, 60 min	1D ^{1}H in < 3 min
MAXperiment, 60 min	1D ^{1}H, HSQC, 1D ^{13}C, HMBC in ca. 50 min

Fail-Safe Non-Uniform Sampling (NUS)

NUS is an acquisition technique applicable for nD NMR experiments in which a certain amount of increments in the indirect dimension(s) are skipped during acquisition followed by a post-acquisition data reconstruction. When used correctly, this saves time without compromising data quality. The optimal settings depend on the sample under investigation and are set by SmartDriveNMR in automation.

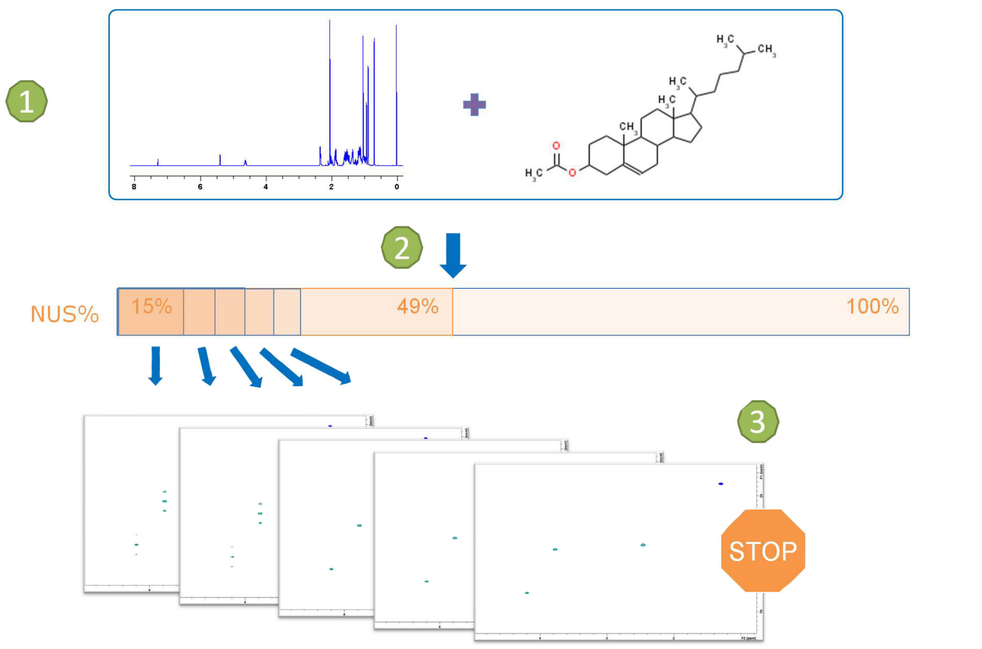


Fig. 2: With the 1D Proton spectrum and the structure (if available) as the input (1) a conservative upper limit for the amount of sampling (NUS%) is estimated (2) e.g. 49%. Now the acquisition of the 2D experiment is started with a significantly lower NUS% than the conservative estimate e.g. 15%. The acquisition continues, increasing the NUS% step by step until the spectrum reaches a high quality and is free of artefacts without passing the conservative estimate (3).

Summary

- Advanced acquisition tool optimizing measurement time and delivering high quality data.
- Fail-Safe NUS and Signal-to-Noise optimization.
- Verification and structure info as input are optional.
- Experts and non-experts can benefit from SmartDriveNMR.

AutoCalibrate

The Well-Tuned Instrument

AutoCalibrate will maintain optimal performance levels of your spectrometer, ensuring your users are generating great data no matter their level of NMR expertise. Designed to run with minimal involvement on the part of the user, AutoCalibrate will free up your time to do more of the science you enjoy instead of the maintenance you avoid.

AutoCalibrate monitors several key parameters including pulse length, temperature and shims, making sure they are always current. Designed to run daily, AutoCalibrate determines the optimal settings for each parameter then logs results, monitors deviations and, when warranted, updates necessary tables with best values.

- ☑ **Pulse lengths measured**
- ☑ **3D shims updated**
- ☑ **Temperature settings optimized**
- ☑ **ERETIC II calibration check**

Fig. 1: These four comprehensive tests evaluate the most common parameters that deviate on an NMR spectrometer. Tracking the history of these test results offer the trained technician a glimpse into the short term and long term health of the spectrometer.

Easy Set-up

AutoCalibrate runs through IconNMR. It needs only to be turned on and scheduled; no other settings are necessary. Log files tracking all tests are stored and can be accessed easily by Bruker's second level support teams when advanced troubleshooting is required.

It is recommended to run AutoCalibrate daily, but with the scheduling available in the GUI (shown below) users have the flexibility to run AutoCalibrate when it fits into their workflow. The testing routine takes approximately an hour, depending on field strength and probe. AutoCalibrate can be run on hardware from AVIII to the most recent AVNeo hardware, on room temperature probes, PRODIGY and Helium CryoProbes. When run daily, AutoCalibrate can address small problems quickly to avoid larger problems later.

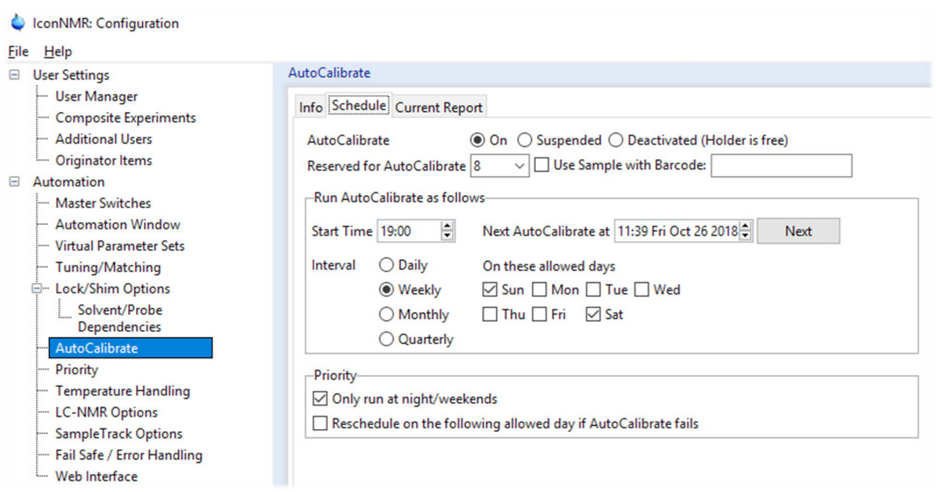


Fig. 2: Implemented since Topspin 4.0.7/TopSpin 3.6.2 and run through IconNMR, AutoCalibrate is accessible to customers running with AVNeo, AVIIIHD and AVIII hardware as long as the appropriate software is installed.

Testing via the Scientific Method

By keeping the sample the same, we are able to isolate problems to hardware. The AutoCalibrate sample is similar to the 2mM sucrose standard, with the exception that it is fixed in the spinner to ensure its position in the probe is the same during each test. TopShim data maps created each time AutoCalibrate runs can then be studied to see changes happening day-to-day as well as over the long term.

Temperature parameters are also optimized each time AutoCalibrate is run, picking up issues like blockages in the variable temperature airflow path or cracked glassware in the probe.

Pulses are calibrated for proton and carbon, ensuring the best sensitivity and overall data quality. Changes to underlying tables are made only when the pulse differs more than nominal drift.

Finally the overall health of the system is checked by determining the concentration of DSS in the sample. Using exactly the same AutoCalibrate sample ensures that any changes in the concentration of DSS are a result of hardware inefficiencies and not differences between samples.

Paired with AssureSST

AutoCalibrate will measure and store basic parameters like pulse lengths, shims, and temperature calibration. However, if users are interested in a comprehensive performance test of the NMR spectrometer, users are directed to use AssureSST. This system suitability test program runs various samples through multiple tests and compares results against specification tables. Using both AutoCalibrate and AssureSST ensures that the NMR spectrometer is running at optimal performance levels and generating data of the highest quality.

AutoCalibrate Comparison with AssureSST

- AutoCalibrate – sets optimal parameters for data acquisition
  - Proton Pulse
  - Carbon Pulse
  - Temperature correction, flow rate measurement, self-tune
  - 3D shims
  - qNMR consistency
- Only 1 sample and no user or manager decisions needed.

- AssureSST – measures sensitivity and lineshape results to ensure system is running in specification – Part of GxP PQ tests
  - Proton sensitivity & lineshape
  - Carbon sensitivity
  - Water suppression sensitivity & lineshape
  - Other x-nuclei tests (^{13}C, ^{31}P, ^{19}F, ^{15}N, etc...)
  - User defined tests
  - qNMR value for AssureNMR qNMR tests (user must set these methods up in advance)
  - 1D shims
  - Temperature correction
- Requires multiple samples as well as some user or manager defined specifications and methods

Summary

AutoCalibrate is key to maintaining a well-tuned NMR spectrometer, tracking changes and monitoring the long-term health of the entire system.

InsightMR

Real-Time Data Analysis and Acquisition Control for Process Monitoring

InsightMR - Process monitoring on-the fly

Designed for the analysis of chemical processes by NMR, InsightMR is the ideal solution for both industrial and academic scientists studying or optimizing organic reactions. The user-friendly interface streamlines process monitoring for the NMR expert while allowing less experienced users, or experts in other disciplines such as synthetic organic chemistry, process chemistry and PAT, to utilize NMR tools for process understanding. InsightMR incorporates functionality from three robust, well established software programs into a single platform: TopSpin for acquisition control, IconNMR for automation, and Dynamics Center for unparalleled data processing and analysis capabilities.

InsightMR's intuitive, flexible interface ensures comprehensive chemical reaction understanding.

Your Key benefits:

- Answers to key chemical questions: reaction yield, reaction kinetics
- Reaction understanding, identification of reaction intermediates and mechanistic information
- Rapid and straightforward generation of data to build kinetic models
- Intuitive - straightforward acquisition and processing workflow – makes NMR an accessible PAT tool for all audiences (no NMR experience required!)
- Enables the facile use of NMR data to make strategic process chemistry decisions, ultimately leading to cost savings

Acquisition Control

Utilization of Bruker's automation software IconNMR, in conjunction with the new features provided by the cutting-edge InsightMR software, provides seamless interaction between experiment set up and spectrometer control for following dynamic processes. These features include the ability to change parameters on-the-fly and propagate these changes to queued experiments with only a couple of mouse clicks. These changes allow the user to be in full control of the data they are acquiring at all times, providing the best data possible when results count!

Data Processing and Analysis

The incorporation of Dynamics Center allows myriad post-acquisition options. In addition to robust, powerful analysis algorithms, InsightMR enables automated processing of data in real time. Once the first data set is processed as desired these parameters are propagated to the remaining spectra, enabling real-time display of kinetic build-up curves. Immediate access to these data allows the scientist to make informed decisions about whether any changes need to be made to the chemistry, acquisition, or data processing to get the best results possible.

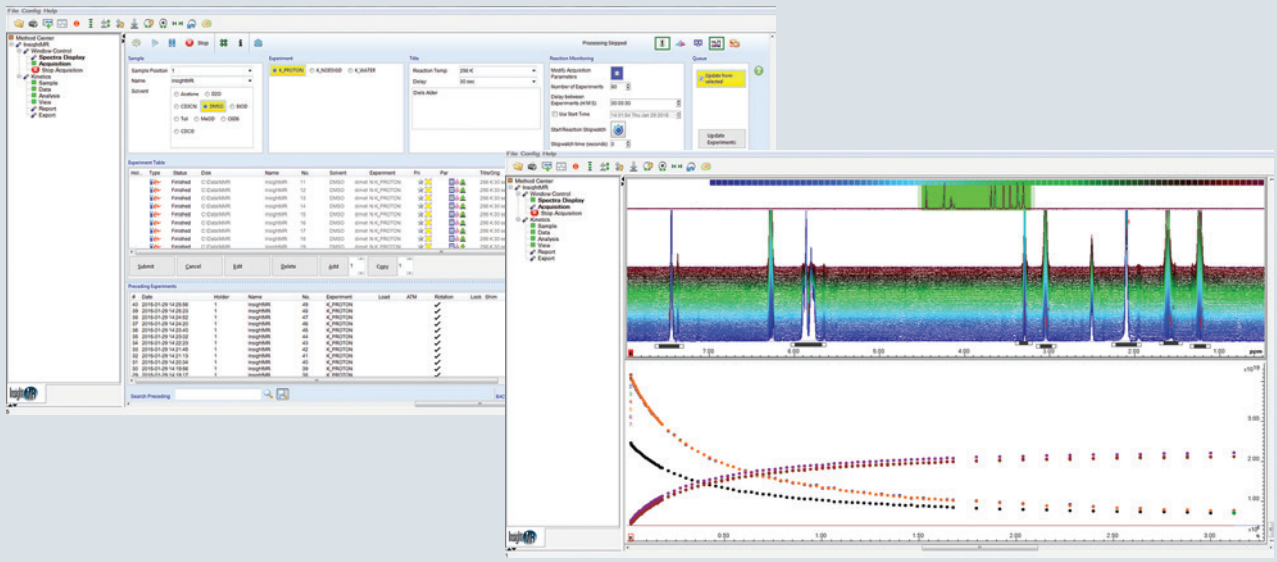
Interaction between Acquisition and Processing – Facile user control

InsightMR provides a single interface to easily toggle between acquisition control and data analysis. The acquisition control and data processing have been seamlessly integrated allowing the user to quickly make strategic decisions about the acquisition and chemistry experimental parameters.

Features

- A single interface for automated acquisition control, interactive processing and analysis, resulting in real-time kinetic profiles
- Complete workflow from data acquisition to project report with ability to export data in other formats for additional processing
- Acquisition and real-time analysis of a series of 1D NMR spectra, using different nuclei and interleaved experiments
- Default kinetic parameter sets provided, enabling facile experiment set up to monitor processes in deuterated and non-deuterated solvents
- Simultaneous monitoring of multiple reactions at the same time using parallel acquisition and analysis capabilities
- On-the-fly acquisition changes as needed based on real-time data processing and kinetic profile calculations
- Seamless integration with Bruker spectrometers for on-the-fly data analysis
- Supports Windows PC configuration running TopSpin 3.5

InsightMR Software



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Product: **5 mm TBO 600 MHz Z-Gradient high resolution probe (Bruker iProbe)**

Description: An observe triple resonance high resolution probe fitted with an actively shielded single axis Z-gradient for 5 mm sample diameters and 600 MHz standard-bore magnets. The inner NMR coil can be tuned to observe ^{19}F or any nucleus in the range from ^{31}P - ^{199}Hg and ^{17}O - ^{109}Ag. The outer NMR coil is double tuned for simultaneous decoupling ^{1}H and ^{19}F. Any nucleus can be fully automatically selected and optimally tuned and matched (ATM).

Specification:

Signal/Noise

^{13}C sensitivity	≥ 330:1	(ASTM; 40ppm noise; LB=3.5 Hz; s=0.23mm) [1]
	≥ 365:1	(ASTM; 5ppm noise; LB=3.7 Hz; s=0.23mm) [1, 2]
^{31}P sensitivity	≥ 250:1	(TPP; 5ppm noise; LB=5 Hz; s=0.38mm) [1]
^{15}N sensitivity	≥ 45:1	(90% Formamide; 2ppm noise; LB=0.3 Hz; s=0.38mm) [1]
^{19}F sensitivity (BB)	≥ 950:1	(TFT; 1ppm noise; LB=0.5 Hz; s=0.38mm) [1]
^{1}H sensitivity	≥ 750:1	(0.1% EB; 200 Hz noise; LB=1 Hz; s=0.23 mm) [1]

Pulse Widths

^{1}H pulse width	≤ 12 µs
^{13}C pulse width	≤ 12 µs
^{31}P pulse width	≤ 12 µs
^{15}N pulse width	≤ 18 µs
^{19}F pulse width (BB)	≤ 12 µs

Lineshape and Spinning Sidebands

^{13}C spinning lineshape	≤ 0.2/3/5 Hz	(50%/0.55%/0.11%, ASTM)
^{1}H spinning lineshape	≤ 0.6/6/12 Hz	(50%/0.55%/0.11%, 1% CHCl3)

Z-Gradient

Gradient strength	≥ 0.5 T/m	(max current 10 A) [2]

Variable Temperature Range

Standard Range	-150°C to +150°C [2, 4]

Model: **Z172446,** PI HR-600-S3-BBF/H/F/D-5.0-Z FB (standard probe)

Performance is specified for an *Avance™ III* spectrometer fitted with a BOSS3-SB shim system.
Technical data and specifications subject to change without notice.
2019-03-18/DSC, Bruker BioSpin AG Probe Department.

1) s = wall thickness of sample tube
2) Specifications verified at production, not at installation
3) With sample 0.1 mg $GdCl_3$ / ml D_2O + 1% H_2O + 0.1% CH_3OH; 5 ms gradient square pulses with strength +/– 37.5 G/cm
4) The shim system temperature must not be allowed to exceed +80°C. At low temperatures, precautions must be taken to prevent the magnet dewar O-rings from freezing.

Product: **Bruker 5 mm TBI 600 MHz Z-Gradient high resolution probe (standard probe)**

Description: An inverse triple resonance high resolution probe fitted with an actively shielded single axis Z-gradient for 5 mm sample diameters and 600 MHz standard-bore spectrometers. The inner NMR coil is double tuned to observe ^{1}H with ^{13}C decoupling. The outer NMR coil can be tuned for decoupling with any nucleus in the range from ^{31}P to ^{15}N. The probe is fitted with a ^{2}H lock channel. It is equiped with automatic tuning and matching accessory (ATM).

Specification:

Signal/Noise		
^{1}H sensitivity	≥ 850:1	(0.1% EB; 200 Hz noise; LB=1 Hz; s=0.23 mm) [1]
Pulse Widths		
^{1}H pulse width	≤ 10 µs	
^{13}C pulse width	≤ 20 µs	
^{13}C pulse width (BB)	≤ 15 µs	
^{31}P pulse width	≤ 25 µs	
^{15}N pulse width	≤ 30 µs	
Lineshape and Spinning Sidebands		
^{1}H spinning lineshape	≤ 0.45/5/10 Hz	(50%/0.55%/0.11%, 1% CHCl3)
^{1}H non-spinning lineshape	≤ 0.7/6/12 Hz	(50%/0.55%/0.11%, 1% CHCl3)
^{1}H spinning sidebands	≤ 2 %	(1% CHCl3 sample)
Z-Gradient		
Gradient strength	≥ 0.5 T/m	(max current 10 A) [2]
Variable Temperature Range		
Standard Range	-150°C to +150°C [2, 4]	

Model: **Z144570,** PA TBI 600S3 H/C-BB-D-05 Z

Performance is specified for an *Avance™ III* spectrometer fitted with a BOSS2-SB shim system (or higher) and 300 Watt X-transmitters.
Technical data and specifications subject to change without notice.
2014-10-27/FRT, Bruker BioSpin AG Probe Department.

1) s = wall thickness of sample tube
2) Specifications verified at production, not at installation
3) With sample 0.1 mg $GdCl_3$ / ml D_2O + 1% H_2O + 0.1% CH_3OH; 5 ms gradient square pulses with strength +/– 37.5 G/cm
4) The shim system temperature must not be allowed to exceed +80°C. At low temperatures, precautions must be taken to prevent the magnet dewar O-rings from freezing.

Product: **Bruker 5mm BBI 400 MHz Z-Gradient high resolution probe**

Description: An inverse broadband high resolution probe fitted with an actively shielded single axis Z-gradient for 5 mm sample diameters and 400 MHz standard bore magnets. The inner NMR coil is tuned to observe ^{1}H. The outer NMR coil can be tuned for decoupling with any nucleus in the range from ^{31}P to ^{109}Ag. The probe is fitted with a ^{2}H lock channel. It is equipped with automatic tuning and matching accessory (ATM).

Specification:

Signal/Noise

^{1}H sensitivity	≥ 600:1	(0.1% EB; 200 Hz noise; LB=1 Hz; s=0.23 mm) [1]

Pulse Widths

^{1}H pulse width	≤ 8 µs
^{31}P pulse width	≤ 25 µs
^{13}C pulse width	≤ 15 µs
^{15}N pulse width	≤ 30 µs

Lineshape and Spinning Sidebands

^{1}H spinning lineshape	≤ 0.45/5/10 Hz	(50%/0.55%/0.11%, 1% CHCl3)
^{1}H non-spinning lineshape	≤ 0.6/6/12 Hz	(50%/0.55%/0.11%, 1% CHCl3)
^{1}H spinning sidebands	≤ 1.5 %	(1% CHCl3 sample)

Z-Gradient

Gradient strength	≥ 0.5 T/m	(max current 10 A) [2]

Variable Temperature Range

Standard Range	-150°C to +150°C [2, 4]

Model: **Z175994,** PA BBI 400S1 H-BB-D-05 Z H-SCR (standard probe)

Specifications with a new *Avance™ III* spectrometer fitted with a BOSS3-SB shim system (or higher) and 300 Watt X-transmitters.
Technical data and specifications subject to change without notice.
2019-07-01/DSC, Bruker BioSpin AG Probe Department.

1) s = wall thickness of sample tube
2) Specifications verified at production, not at installation
3) With sample 0.1 mg $GdCl_3$ / ml D_2O + 1% H_2O + 0.1% CH_3OH; 5 ms gradient square pulses with strength +/– 37.5 G/cm
4) The shim system temperature must not be allowed to exceed +80°C. At low temperatures, precautions must be taken to prevent the magnet dewar O-rings from freezing.

SampleCase NMR Automation Solutions

Easy Access to Every NMR Experiment

- Easy to use.
- Safe and accessibile in labs without needing steps or ladders.
- Ideal for medium and high sample throughput.
- Supports various types of tubes, from 7″ or 8″ to shaped and valved glassware with suitable spinners.

Fig. 1: SampleCase.

SampleCase Standard or PLUS

Choose from 24 to 60 sample room temperature storage for almost any type of NMR sample. It's easy to use with push button operation for sample insert and eject, simple LED indicator lights for operational status, and fully integrated software control to TopSpin and IconNMR. The user-friendly system fits all shielded Bruker standard bore magnets from 300–1GHz (3rd party magnets upon request) and can be added to any modern NMR instrument equipped with AVANCE III, AVANCE III HD or AVANCE NEO technology.

Fig. 2: SampleCase PLUS.

SampleCase Cooled

24-sample storage, setpoint control for entire carousel configurable from 4°C to 40°C, ideally suited for bio NMR labs with temperature sensitive samples like Protein- , RNA- or Biofluid solutions for subsequent automation runs in smaller batches

SampleCase Heated

24-sample storage, setpoint control for carousel configurable from room temperature to 125°C, essential for researchers in polymer research who need to maintain samples at high temperatures in the queue.

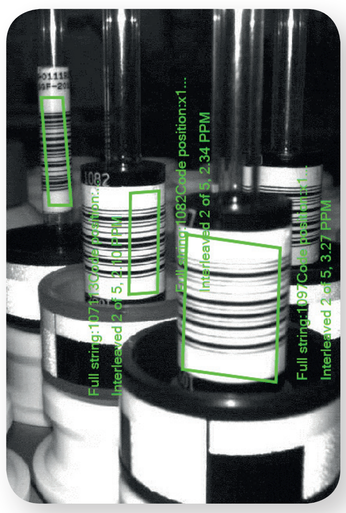

Fig. 3: Vision Kit

Vision Kit

For optimized scanning of 1D sample IDs, while ensuring detection of operator inventions.

The Vision Kit is compatible with existing installations, with easy sample insertion and removal.

AutoCalibrate

For 5 mm probes:

- Set a fixed position for the Auto-Calibrate tube and spinner kit.
- Automatically set proton (1H) pulse length.
- Check carbon (13C) pulse.
- Calibrate and store 3D shims.
- Adjust temperature parameters including flow and heater power.
- Store a quantitation calibration.

Precision Spinners

Designed to work seamlessly with Bruker's NMR instruments:

- Standard bore shim systems
- Shaped sample 5mm tubes
- Shaped Shigemi tubes

Material	Maximum Temperature
Ceramics	-150°C to +150°C
Kel-F	-4°C to +120°C
POM	0°C to + 80°C

Maximize the Use of your NMR Instrument

www.bruker-labscape.store

- NMR lab glass and precision spinners.
- Certified reference samples.
- AutoCalibrate primary level performance monitoring package.