



### NMR

### **AvanceCore**

High resolution, streamlined. More affordable than ever.

Innovation with Integrity

# The AvanceCore offers high-resolution NMR with an impressive price/performance ratio, making NMR more accessible than ever before.

Created with Bruker's extensive NMR expertise and streamlined production processes, the AvanceCore offers a cost-effective solution for NMR users who value resource efficiency.

- Select from 3 different standard configurations to match your specific needs.
- Enjoy flexible features which are enabled and disabled using software subscriptions.
- Only pay for what you need, when you need it.

"A standard liquid chromatography mass spec instrument costs approximately \$200,000. The AvanceCore solution offers NMR at a similar price point."



### Time to Get an NMR

NMR is an extremely powerful analytical method. In combination with the affordability of the AvanceCore, this makes NMR the ideal tool to address a large range of analytical questions.

#### **Structure Elucidation, Verification and Molecular Interaction**

- Examine functional groups and how atoms are connected within a molecule.
- Study molecules at atomic resolution
- Uncover molecular interactions at the atomic level, for example:
  - Examine substrate-catalyst interaction
  - Discriminate monomers and polymers
  - Explore aggregation, micelle formation and emulsification

#### **Never Miss a Signal**

- With NMR, what you see is what is present.
  Chromatographic analysis requires process steps such as liquid injection or sample evaporation. Potential sample degradation or unwanted reactions complicate the assignment of signals.
- NMR selectively detects nuclei such as <sup>1</sup>H, <sup>13</sup>C, <sup>19</sup>F and <sup>31</sup>P which are present in organic molecules.

This is not apparent with other analytical techniques. For example, UV detectors for chromatography miss many substances without a chromophore. IR and mass detectors have similar limitations.





Increase Productivity

NMR experiments can be run without dedicated method development and in full automation, benefiting large groups of users and boosting productivity. The AvanceCore and technological advancements make it easier and cost-effective to equip a laboratory with long-lasting NMR hardware, requiring minimal maintenance, chemicals, and space. The system can measure up to 70 samples in 8 hours, meeting growing analytical demands without additional investments.



### **Three AvanceCore Configurations**

In order to keep costs low, Bruker has streamlined the AvanceCore into three pre-configured packages.

**AvanceCore Foundation:** In the most fundamental version, the AvanceCore provides high-resolution <sup>1</sup>H NMR spectroscopy. The bundle includes a 400 MHz NMR magnet, a console and a 5 mm probe.

**AvanceCore Select:** The AvanceCore Select includes all the hardware and software for <sup>1</sup>H and heteronuclear (<sup>13</sup>C, <sup>31</sup>P...) state-of-the-art experiments. The software subscription for the first year of broad-band operation is included.

**AvanceCore Convenience:** The AvanceCore Convenience includes a 24-position sample changer. The IconNMR software enables open access use and automated routine measurements. The IconNMR subscription for the first year is included.

Your instrument can grow with your needs: An existing AvanceCore can easily be upgraded from Foundation to Select and from Select to Convenience.

		Foundation	Select	Convenience
		<sup>1</sup> H NMR H H	<sup>1</sup> H & Broadband B C P S C Ar C G G C Ar	Multi-User/ Open Access
Yearly Subscription Hardware	400 MHz NMR magnet <sup>1</sup>	Ø	Ś	Ś
	AvanceCore console	Ø	Ś	Ś
	RT shim system	Ø	Ø	Ø
	5 mm NMR probe <sup>2</sup>	Ø	Ø	Ø
	Windows workstation (incl. screen)	Ø	Ø	Ø
	Sample cooling unit <sup>3</sup>		Ø	Ø
	Vibration isolators		Ø	Ø
	Sample changer with 24-positions			Ø
	Nitrogen level gauge and heat exchanger			Ø
	Installation included <sup>4</sup>	Ø	Ø	Ø
	TopSpin Foundation for AvanceCore⁵	Nessesary	Nessesary	Nessesary
	Broadband subscription⁵	Optional	Recomended	Recomended
	lconNMR⁵		Optional	Recomended
	Method Development for AvanceCore⁵			Optional
	AutoCalibrate			
	GoScan⁵			
	TopSpin for data processing			

<sup>1</sup>Foundation, Convenience and Select are also available as a console and probe replacement if a 400 MHz NMR magnet is already in place. The mechanical interfaces of the AvanceCore magnet are compatible with the Avance NEO hardware. Future upgrades to a full Avance NEO are thus possible by exchanging the console and the probe. <sup>2</sup>The AvanceCore probe supports automatic tuning and matching and is ready for broadband capability depending on the "Broadband subscription". <sup>3</sup>To stabilize and regulate the temperature between 0 and 80° C. Increases temperature stability. <sup>4</sup>Including installation, excluding cryogens. <sup>5</sup>To operate the spectrometer, a yearly subscription of TopSpin for AvanceCore is necessary and depending on the hardware configuration, the broadband subscription and the IconNMR subscription are recommended to operate the sample changer.

Software subscriptions can be subscribed/unsubscribed on an annual basis and will be invoiced annually. Alternatively, a software subscription package can be ordered for an arbitrary number of years together with the system hardware. In the latter case, no yearly payments for software will be required for the selected number of years.

### **Example Spectra**

The AvanceCore is highly cost effective and facilitates uncompromized performance in high-resolution NMR. Outstanding dispersion and signal-to-noise ratio enable mixture analysis down to ppm concentrations. With the Method Development subscription, the AvanceCore supports all 2D NMR experiments that are included in the TopSpin software.



Identification and quantitation: The above <sup>1</sup>H spectrum was acquired with the AvanceCore Foundation from a 20 mg sample in less than 5 minutes. The sample contains 100 ppm (0.002 mg) of the following impurities: acetonitrile, acetone, ethyl acetate and acetic acid in DMSO-d<sub>s</sub>.



The AvanceCore Foundation also supports state-of-the-art <sup>1</sup>H-<sup>1</sup>H 2D experiments such as TOCSY, COSY, ROESY and NOESY. The above spectrum shows TOCSY-correlations of the anti-inflammatory drug lbuprofen.

The TOCSY can be used for structure assignment.



With the AvanceCore Foundation, the <sup>1</sup>H DOSY NMR experiment for mixture analysis can be performed. DOSY is often referred to as "chromatographic NMR". Just like LC-MS, it resolves the different mass and diffusion properties of indivual mixture components.



The AvanceCore Select supports heteronuclear experiments (HSQC, HMBC...) which are essential for molecular structure elucidation. The above spectrum shows a 2D <sup>1</sup>H/<sup>13</sup>C HSQC-TOCSY experiment recorded from a 20 mg lbuprofen sample.

## **TopSpin Subscriptions**

Software enables powerful features on the AvanceCore. With our yearly subscription model, you only pay for what you need, when you need it. This makes your AvanceCore NMR spectrometer more affordable than ever before. The AvanceCore software blends perfectly into the existing Bruker ecosystem utilitzing the same pulse programs and parameter sets.

Software subscriptions can be subscribed/unsubscribed on an annual basis and will be invoiced annually. Alternatively, a software subscription package can be ordered for an arbitrary number of years together with the system hardware. In the latter case, no yearly payments for software will be required for the selected number of years.



#### **TopSpin for AvanceCore**

A streamlined software for the acquisition and processing of NMR data.

- Fixed lock solvents: acetone-d<sub>6</sub>, benzene-d<sub>6</sub>, acetonitrile-d<sub>3</sub>, methanol-d<sub>4</sub>, CDCl<sub>3</sub>, D<sub>2</sub>O, 9:1 H2O:D2O, DMSO-d<sub>6</sub>
- Fixed pulse programs (Foundation): 1D <sup>1</sup>H, 1D pre-saturation, 1D decoupled, COSY, TOCSY, NOESY, ROESY, DOSY
- Fixed pulse programs (Select and Convenience): 1D <sup>1</sup>H, 1D pre-saturation, 1D decoupled, COSY, TOCSY, NOESY, ROESY, DOSY, HSQC, HMBC, HSQC-TOCSY, INADEQUATE
- Pulse programming, AU and Python programming not supported
- Command and experiment queue (spooler) not supported
- Auto lock/shim. Manually accessible shims: Z, Z2, Z3, X, Y, XZ, YZ
- Updates to the current release version are mandatory throughout the product lifecycle.
- An internet connection is necessary.
- The following applications are not supported: CMC-Assist, SmartDrive NMR, AssureSST, NUS, nmrsim, 2D/3D structure drawing/viewing, simulation of 1D spectra, identification of <sup>13</sup>C spectra with CSEARCH, Amix viewer and fragment based screening.
- Only Microsoft Windows supported

#### **TopSpin Method Development for AvanceCore**

Bruker's industry standard TopSpin for acquisition and method development with the AvanceCore.

- All lock solvents
- All Bruker pulse programs
- Pulse programming, AU and Python programming supported
- Command and experiment queue (spooler) included
- Auto lock/shim. All shims manually accessible
- Updates to the current release version are mandatory throughout the product lifecycle. An internet connection is necessary

# ifdef CALC\_SP "p41=(bwfac25/(cnst55\*cnst51\*bf1))\*1000000"

"spoal25=1" "spoal27=0"

"p42=(bwfac26/(cnst55\*cnst52\*bf1))\*1000000" "spw26=plw1/((p42\*90.0)/(p1\*totrot26))\*((p42\*90.0) "spoal26=0.5"

"spw28=plw1/((p43\*90.0)/(p1\*totrot28))\*((p43\*90.0)

### **Additional Software Subscriptions**



#### **TopSpin for Data Processing and Evaluation**

Additional TopSpin subscriptions are available for data processing away from the spectrometer.

- Yearly subscription
- Can be easily moved between client PCs
- Can be used as a pool-license on a server
- Expert solution for data processing away from the spectrometer
- NMR data can be accessed by a folder tree or by drag and drop from the Windows explorer



#### **Broadband Subscription**

In combination with the Select hardware package, the broadband subscription enables the following:

- Broadband channel: <sup>19</sup>F and <sup>31</sup>P <sup>109</sup>Ag without <sup>171</sup>Yb to <sup>9</sup>Be
- Experiments with hetero nuclei such as <sup>13</sup>C, <sup>31</sup>P, etc.
- Heteronuclear 2D correlation experiments such as HSQC, HMBC etc.

#### **IconNMR**

In combination with the Convenience hardware package, IconNMR enables open access NMR (non-expert mode) for automated and routine measurements.

- Controls the 24-position sample changer
- Turns the system into an open access platform by providing an intuitive user interface for the easy setup of NMR measurements
- Provides automation and routine functionality for the measurement of multiple samples





#### GoScan

GoScan for AvanceCore facilitates easy and intuitive, push-button acquisition of NMR spectra combined with automated data processing.

- Straightforward entry-level software for the acquisition of NMR spectra
- Push-button operation of the AvanceCore NMR spectrometer
- Facilitates open access capabilities
- Controls the sample changer (if available)
- Based on industry-standard TopSpin. Parameter sets and pulse programs are compatible.

#### **AutoCalibrate**

AutoCalibrate facilitates the evaluation and calibration of the most important NMR system parameters.

- Optimizes the 3-dimensional shim
- Monitors the pulse length
- Generates a pdf report with the most important calibration results
- With an AvanceCore Convenience, AutoCalibrate runs can be started at pre-set times during the night



### **AvanceCore**

High resolution, streamlined. More affordable than ever.



BrukerBioSpin info.brkr@bruker.com

bruker.com

Worldwide offices bruker.com/



Online information bruker.com

