



NMR BIOPHARMA SOLUTIONS

Enhance your Productivity with Bruker NMR Integrated Solutions

Innovation with Integrity

From early discovery to late development and quality control, Bruker NMR integrated solutions empower laboratories to maximize the productivity of both their existing and new systems. Built on industry-leading, ultra-robust NMR spectrometers, the Bruker software ecosystem provides comprehensive tools to deliver intuitive, automated processes making sophisticated NMR accessible to everyone in the lab. Experts can dedicate their time to innovation and interpretation, while non-specialists achieve robust, reproducible outcomes with minimal training—ensuring productivity gains never come at the expense of data quality.

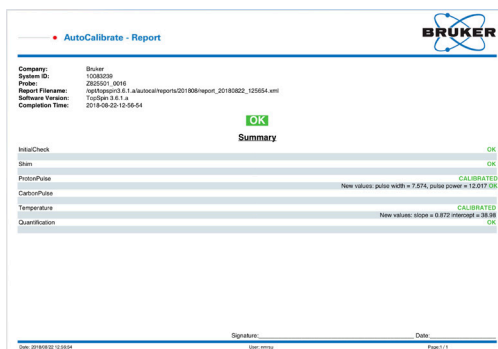


Benefits:

- ✓ Optimal throughput enabled by self-calibrating, intelligent NMR spectrometers
- ✓ Accelerated turnaround time through fully automated workflows for maximum quality
- ✓ Reduced downtime thanks to proven hardware and proactive, automated diagnosis

Effortless optimization for continuous operations

Focus on results, not on maintenance, with Bruker **AutoCalibrate**. NMR spectrometers are continuously monitored for key parameters and optimized under full automation. It ensures continuous quality and confidence in the data without user intervention.



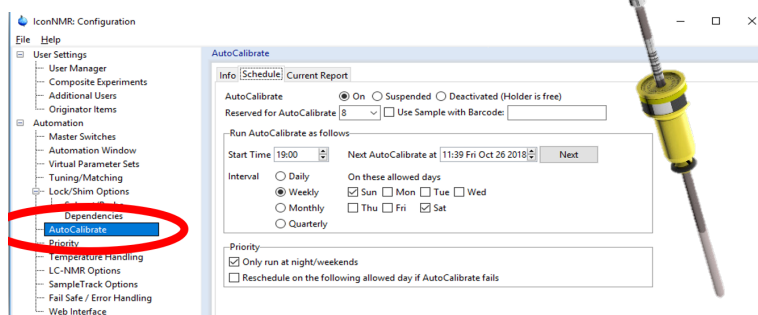
AutoCalibrate 1-page report: direct general pass/fail assessment and detailed information about performed tests.

AutoCalibrate includes the automated **verification and optimization** of:

- **Pulse lengths** for optimal signal with minimal artifacts, including auto-updating of the pulse table and warning in case of strong deviation
- **Temperature** for consistency and stability, eliminating tedious, manual calibration
- **3D Shimming** to optimize resolution and reduce the amount of time spent on routine shimming
- **Quantification** to ensure qNMR integrity and detect trends, so users have confidence in the spectrometer calibration

AutoCalibrate **integrates seamlessly** with IconNMR, offering high customizability for settings such as testing frequency and time, pass/fail behavior, and priority. It can also be started manually from TopSpin whenever needed.

The entire procedure is performed automatically with a **single test tube** delivered with the software.



AutoCalibrate configuration in IconNMR.

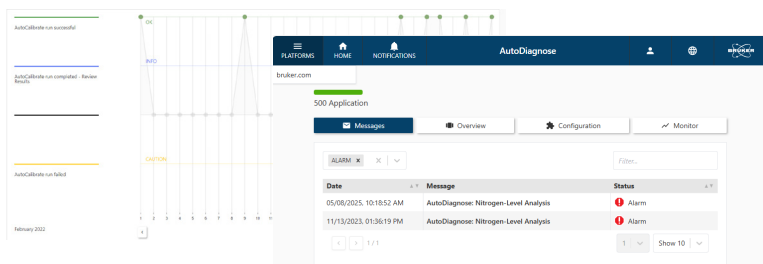
Leimin Wang, Scientist, Roche



Using AutoCalibrate with our open access 400 MHz Neo spectrometer has been a game-changer. It ensures consistent data quality for our users through full automation, saving valuable time for NMR experts who can now focus on more demanding tasks without compromising day-to-day operations.

The automated calibration process is user-friendly to set up and then runs reliably without any intervention. It automatically updates the shims and optimizes the pulses so resolution and sensitivity are optimal. The generated reports provide an easy way to check the spectrometer's health and performance at a glance. AutoCalibrate has also enabled us to catch drifts and proactively anticipate maintenance needs, avoiding downtime and ensuring the quality of our data remains uncompromised.

Overall, AutoCalibrate is a great addition to our laboratory, ensuring reliable operations for our open-access NMR system without the need for regular supervision.



AutoDiagnose dashboard: One-stop overview of all connected NMR spectrometers, including cryogenic status, critical errors, and calibration alerts.

AutoCalibrate can be coupled with **AutoDiagnose** for direct system status and health monitoring of the NMR spectrometers. All critical system parameters are automatically controlled, and results are accessible in a user-friendly graphical interface. It delivers streamlined performance monitoring and enables proactive maintenance, further limiting downtime.

Push-button, on-the-fly optimized data acquisition

Achieve optimal use of instrument time and data quality for routine 1D and 2D experiments. SmartDriveNMR enables acquisition under full automation with on-the-fly optimized settings, ensuring data quality in the minimum amount of time. It enables consistent results in both quality and productivity, without supervision.

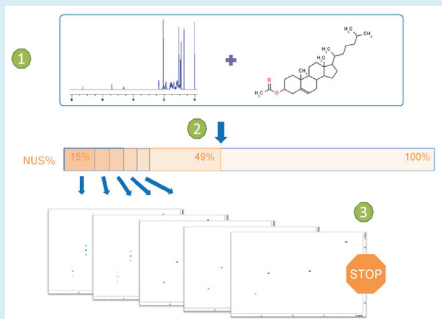
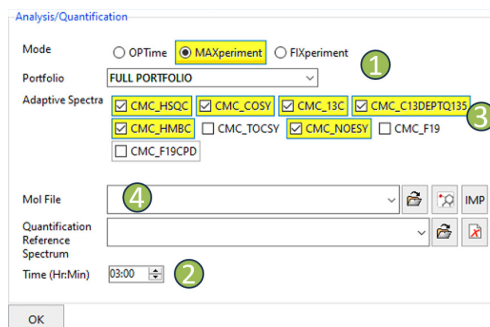
Typical SmartDriveNMR **workflow**:



1. The user creates and submits the acquisition job. The description of the job mainly contains time allocations and might include structural information
2. A fast 1D proton spectrum is collected and analyzed
3. Depending on the analysis results regarding the complexity of the problem and the signal strength, further experiments with optimal parameters can be triggered by the software
4. Follow-up experiments are scheduled and acquired in full automation if sufficient time is available. The software recommends follow-up if the allocated time is too short to deliver high-quality data

SmartDriveNMR operates in the background of IconNMR and provides a high level of **customizability** so the lab manager can define who can start a SmartDriveNMR run and which sets of experiments (portfolio) can be used.

The routine user can then start the run as is, or further customize for each sample, defining the type of run (1) focusing on minimizing acquisition time or maximizing number of spectra, within the maximum time allowed (2). Furthermore, specific experiments can be (de) selected from the portfolio (3) and an optional structure file provided (4).

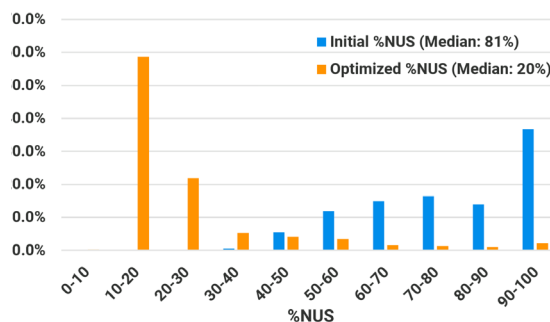


SmartDriveNMR performs **on-the-fly optimization** of 2D acquisition: Using the 1D Proton spectrum and the structure (if available) as the input (1) a conservative upper limit for the amount of sampling (NUS%) is estimated (2) e.g. 49%. Now the acquisition of the 2D experiment is started with a significantly 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 artifacts without passing the conservative estimate (3).

Discover a real **pharmaceutical use-case** where SmartDriveNMR increased the instrumental capacity by a **factor of 2** for routine structural analysis workflows (^1H /HSQC/HMBC/COSY/ ^{13}C) using the automatic settings for the number of scans and the on-the-fly optimized acquisition.

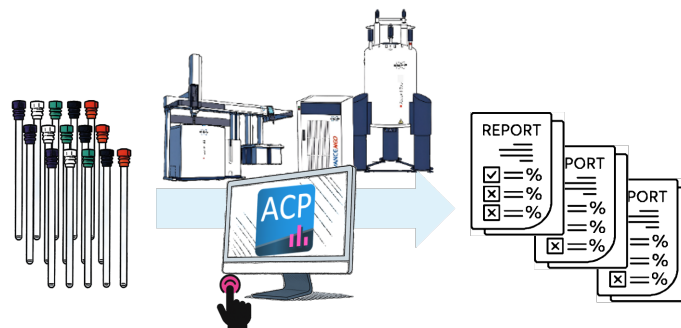


HMBC - Initial vs Optimized %NUS

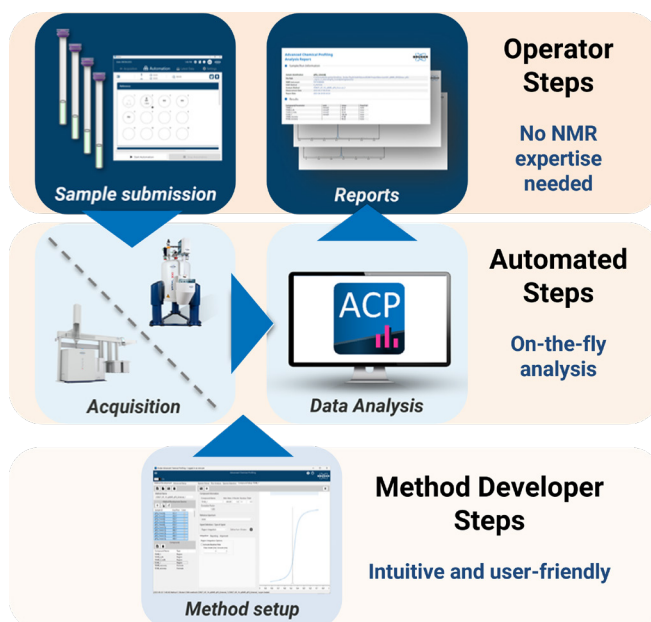


Sample-to-report automation for maximal productivity

Leverage Bruker next-generation **Advanced Chemical Profiling (ACP)** software for hands-off, sample-to-report NMR analysis. ACP enables push-button operations for all routine quantitative NMR workflows. It adapts to tasks ranging from simple routine purity determinations or relative quantifications to very complex matrices with overlapping signals in multicomponent mixtures.



- ✓ Unified solution for all qNMR workflows (internal, external relative)
- ✓ User-friendly interface for method setup - no scripts, no external files
- ✓ User-selectable algorithms for each target to adapt to each product and matrix, including complex baselines and overlapped signals
- ✓ Highly customizable, with direct pass/fail decision capabilities, tailored calculation methods, and flexible reporting options
- ✓ Seamless integration with the Bruker NMR ecosystem (Topspin, IconNMR, GoScan)



Bruker BioSpin is continually improving its products and reserves the right to change specifications without notice. Order No. BS-100117 © 10/2025 Bruker BioSpin.

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