



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.

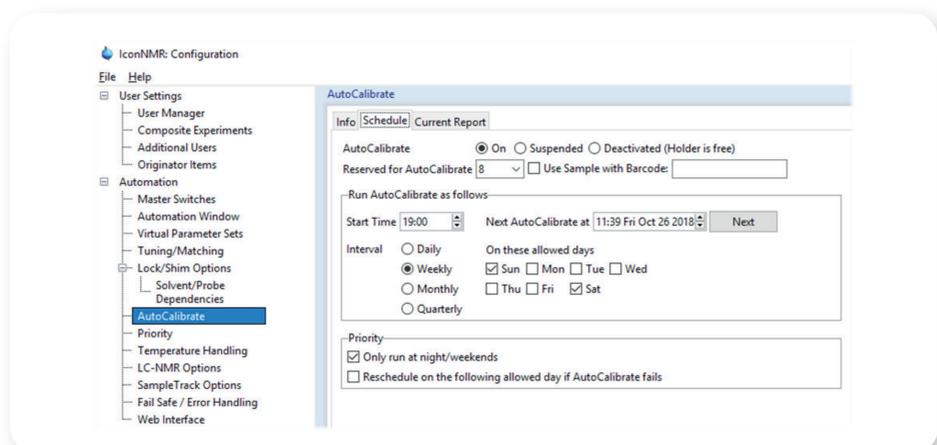


Fig. 2: Implemented since TopSpin 4.0.6/TopSpin 3.6.1 and run through IconNMR, AutoCalibrate is accessible to customers running with AVNeo, AVIIIHD and AVIII hardware as long as the appropriate software is installed.

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 Comparison with AssureSST

- | | |
|--|---|
| <ul style="list-style-type: none"> • AutoCalibrate – sets optimal parameters for data acquisition <ul style="list-style-type: none"> • 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. | <ul style="list-style-type: none"> • AssureSST – measures sensitivity and lineshape results to ensure system is running in specification – Part of GxP PQ tests <ul style="list-style-type: none"> • Proton sensitivity & lineshape • Carbon sensitivity • Water suppression sensitivity & lineshape • Other x-nuclei tests (¹³C, ³¹P, ¹⁹F, ¹⁵N, 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 |
|--|---|

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.

Summary

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

