



- **AutoCalibrate 003**
Quick Start Guide

Safety First

The AutoCalibrate program requires the **AutoCalibrate Test-Sample Z171901**.

This sample has been prepared in accordance with strict SOP's. The AutoCalibrate sample has a validated lifetime of 4 years from the date of certification. Further information about the sample can be found on the Certificate of Conformity delivered with this sample. The sample SDS is available upon request.

The AutoCalibrate sample consists of a colorless solution of sucrose in a 9:1 mixture of H₂O:D₂O. The solution is sealed in a 5mm NMR tube pre-fitted in the AutoCalibrate spinner. The spinner is glued to the tube and cannot be shifted or removed without causing damage to the sample.

Care should be taken when handling the AutoCalibrate sample assembly so as not to break the glass sample tube. It is recommended to keep the sample in the AutoCalibrate sample case when it is not on the Sample Changer.

AutoCalibrate Program Information

The AutoCalibrate program requires both the AutoCalibrate sample as well as a license. The license is valid for a period of 3 years, after which a new license and sample set must be ordered.

AutoCalibrate must be run through IconNMR, and the user must complete the configuration before the program can be started. Brief instructions can be found on the following pages. For more detailed information, please refer to the AutoCalibrate Manual available in TopSpin help under Automation and Data Publishing manuals.

Though it is recommended to run with the latest version of TopSpin software, the minimum required versions are TopSpin 3.6.1 or TopSpin 4.0.6.

AutoCalibrate Setup

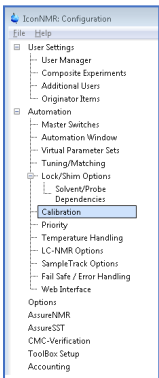
Start TopSpin



Start IconNMR with the TopSpin command: **iconnmr** and open the Configuration window. This will require the NMR Super User password.

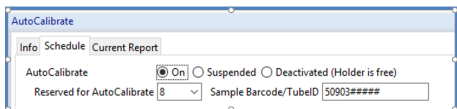


Find the AutoCalibrate setup in the Automation section.



AutoCalibrate Setup

All setup will be done in the Schedule tab.



AutoCalibrate must be turned on to start. Once started, the AutoCalibrate experiments will automatically queue at the scheduled start time. If suspended, the reserved AutoCalibrate sample position will remain unavailable to users, but the program will not run. If deactivated, the reserved holder is released for use by all users.

The user must enter the sample position that is to be reserved for the AutoCalibrate sample as well as the Sample Barcode/Tube ID. This 10-digit number can be found on the cap of the sample. It is a combination of the unique AutoCalibrate number 50903 plus the sample 5-digit serial number found on the certificate. If one looks at the number on the cap, there is an additional checksum number at the end that should be ignored.

AutoCalibrate Scheduling

It is recommended to run AutoCalibrate daily. The program will take approximately 1 hour to complete and can be scheduled to run at a time that will most likely not interfere with daily work on the instrument. The program will not interrupt an experiment already in progress.

Run AutoCalibrate as follows

Start Time Next AutoCalibrate at

Interval Daily Weekly Monthly Quarterly

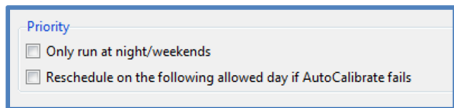
On these allowed days Sun Mon Tue Wed Thu Fri Sat

AutoCalibrate Scheduling

To set the AutoCalibrate program to run each day, select the option Daily and check the days of the week to run. If the program is to be run once a week, on only 1 day, select the weekly option. If multiple days are selected with the weekly option, the AutoCalibrate program will run only on the first day available. The same is true for running monthly (run on the first selected day available) and quarterly. It is possible to see the date and time of the next AutoCalibrate run in the field Next AutoCalibrate at, which is updated whenever the selections are changed.

AutoCalibrate Priority Settings

AutoCalibrate can be set with a few priority settings.

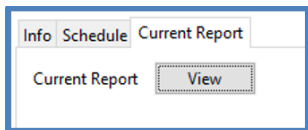
A screenshot of a software dialog box titled "Priority". The dialog box has a light gray background and a blue border. It contains two unchecked checkboxes. The first checkbox is labeled "Only run at night/weekends". The second checkbox is labeled "Reschedule on the following allowed day if AutoCalibrate fails".

Priority	
<input type="checkbox"/>	Only run at night/weekends
<input type="checkbox"/>	Reschedule on the following allowed day if AutoCalibrate fails

AutoCalibrate can be set to run only during night/weekend hours (as set in Priority section of IconNMR Configuration). This ensures that day hours are never used to run AutoCalibrate. With this option selected, it is possible that AutoCalibrate is not run for the day. This is the case if the currently running sample has an experiment running for the entire night. In this case, the program will run at its next scheduled start time.

AutoCalibrate Priority Settings

If AutoCalibrate has a failure or error of any kind, it will be reported to the user in the AutoCalibrate report that can be viewed at any time by clicking on View of the Current Report Tab.



● AutoCalibrate

For information on additional packages or replacement samples, please contact us at:

<https://www.bruker.com/products/mr/contact-forms/contact-us.html>

In case the AutoCalibrate sample breaks or in any way needs replacement, please contact your local sales team. The product can be sold as sample only (in case there is significant time left on the license) or the full product (recommended if there is less than 1 year left on the 3-year license.).

- AH1510: AutoCalibrate sample plus 3-year license
 - Academic discount available
- Z171901: AutoCalibrate sample assembly in case

