

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 ^1H experiments. The different aspects of data quality include fail-safe Non-Uniform Sampling data acquisition and Signal-to-Noise optimization.

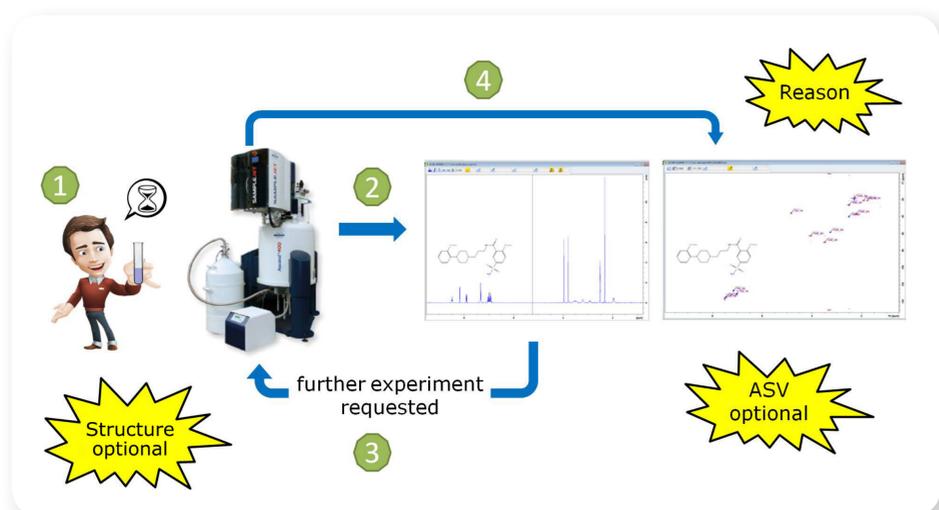


Fig. 1: SmartDriveNMR workflow

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 ^1H in < 3 min
MAXperiment, 60 min	1D ^1H , 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.

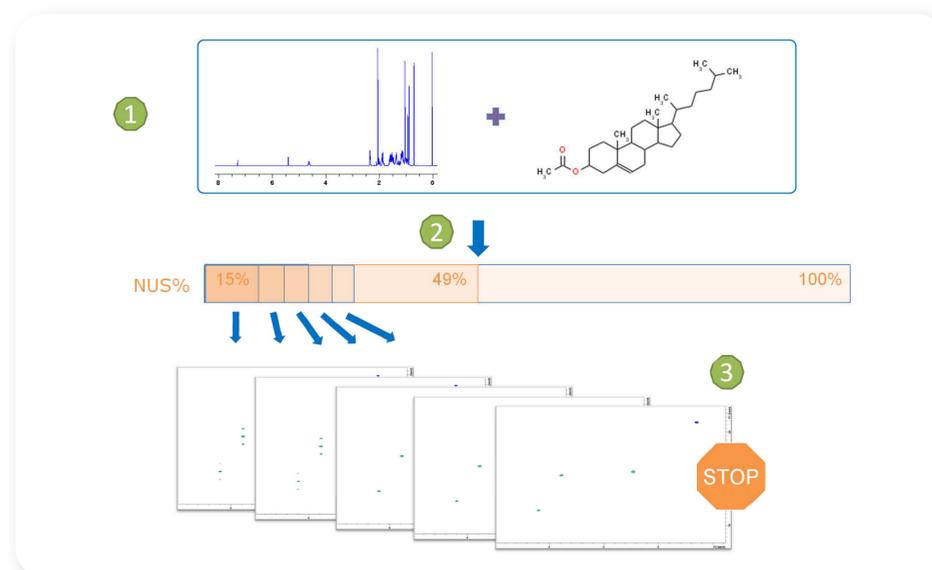


Fig. 2: With the 1D Proton spectrum and the structure (if available) as the input (1) a conservative upper limit for the amount of sampling (NUS%) is estimated (2) e.g. 49%. Now the acquisition of the 2D experiment is started with a significantly lower NUS% than the conservative estimate e.g. 15%. The 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.