

Optimized Experiment Selection for Routine NMR Tasks

SmartDriveNMR is an intuitive and easy-to-use solution for open access routine NMR. Users submit their structure verification samples within IconNMR, along with the proposed structure, allowed instrument time and the desired level of confidence.

SmartDriveNMR will set up an initial scout experiment and, based on the result, may set up and run further experiments – provided they will significantly improve the confidence in the result and comply with the restrictions set by the user.

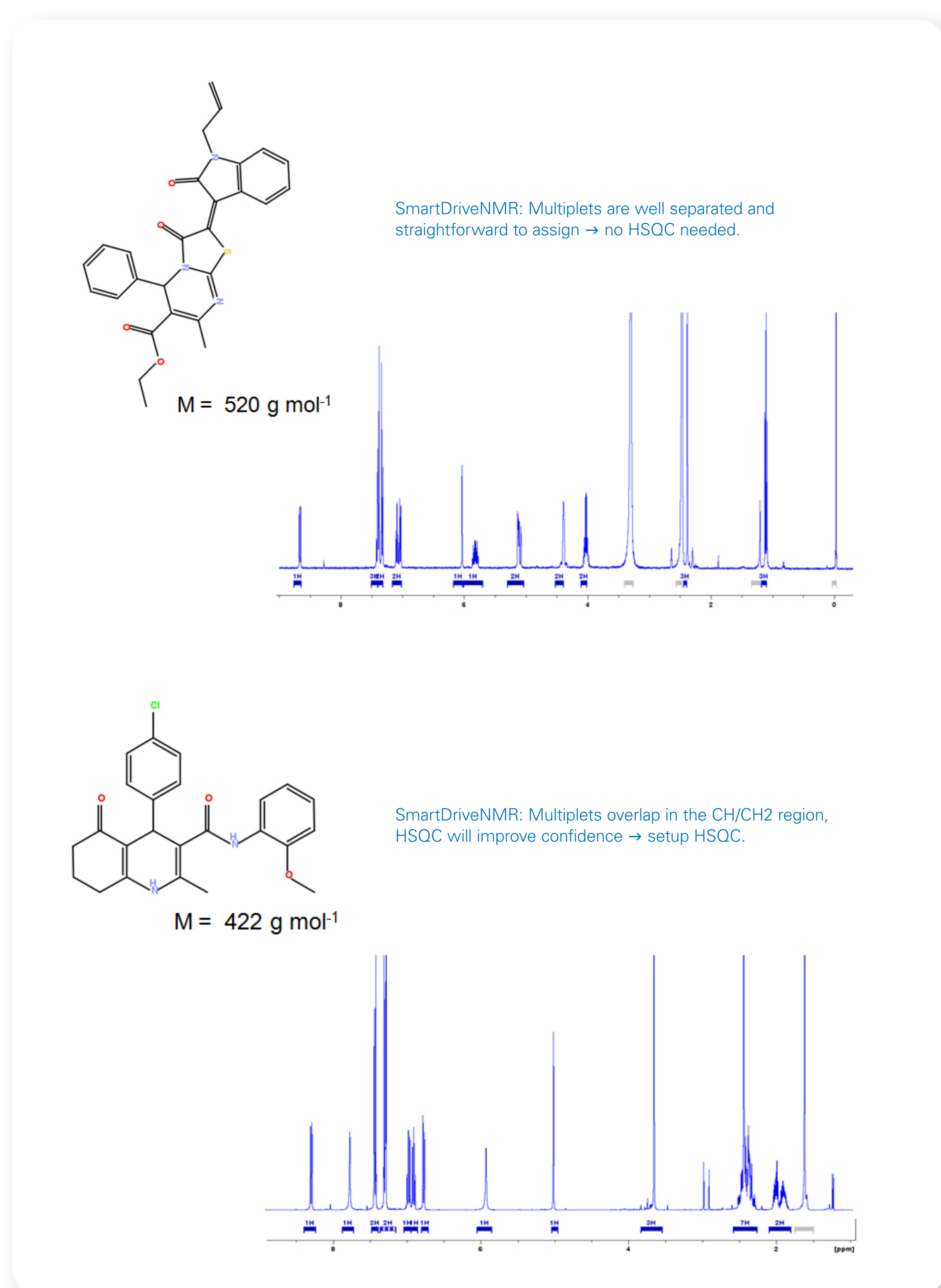


Fig. 1 Active decision making on-the-fly saves experiment time – simply considering the structure alone might have demanded an HSQC in both cases.

SmartDriveNMR in Open Access Labs

SmartDriveNMR gives users in open access NMR environments the autonomy to perform optimized and problem tailored sets of modern experiments on their sample. The automated structure verification indicates the confidence level and is documented in a full, professional report.

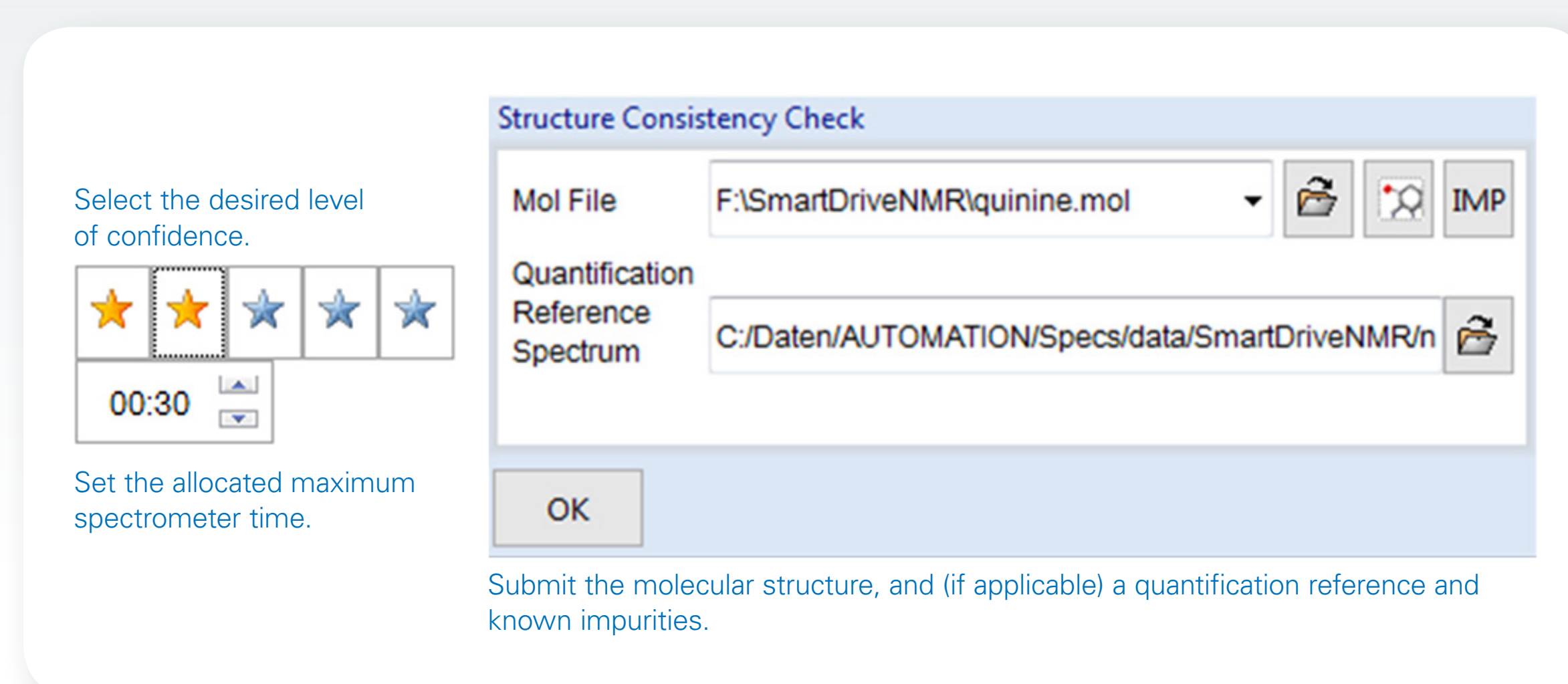


Fig. 2 Setting up a structure verification task in IconNMR with SmartDriveNMR: no spectroscopic input required.

SmartDriveNMR in Supervised Service Labs

SmartDriveNMR automatically optimizes the spectrometer for efficiency, without jeopardizing the quality of results. It's on-the-fly decisions improve the data quality by running additional scans or using solvent suppression when necessary. If time allows, further structure verification experiments are run, provided they add significant value for the solution.

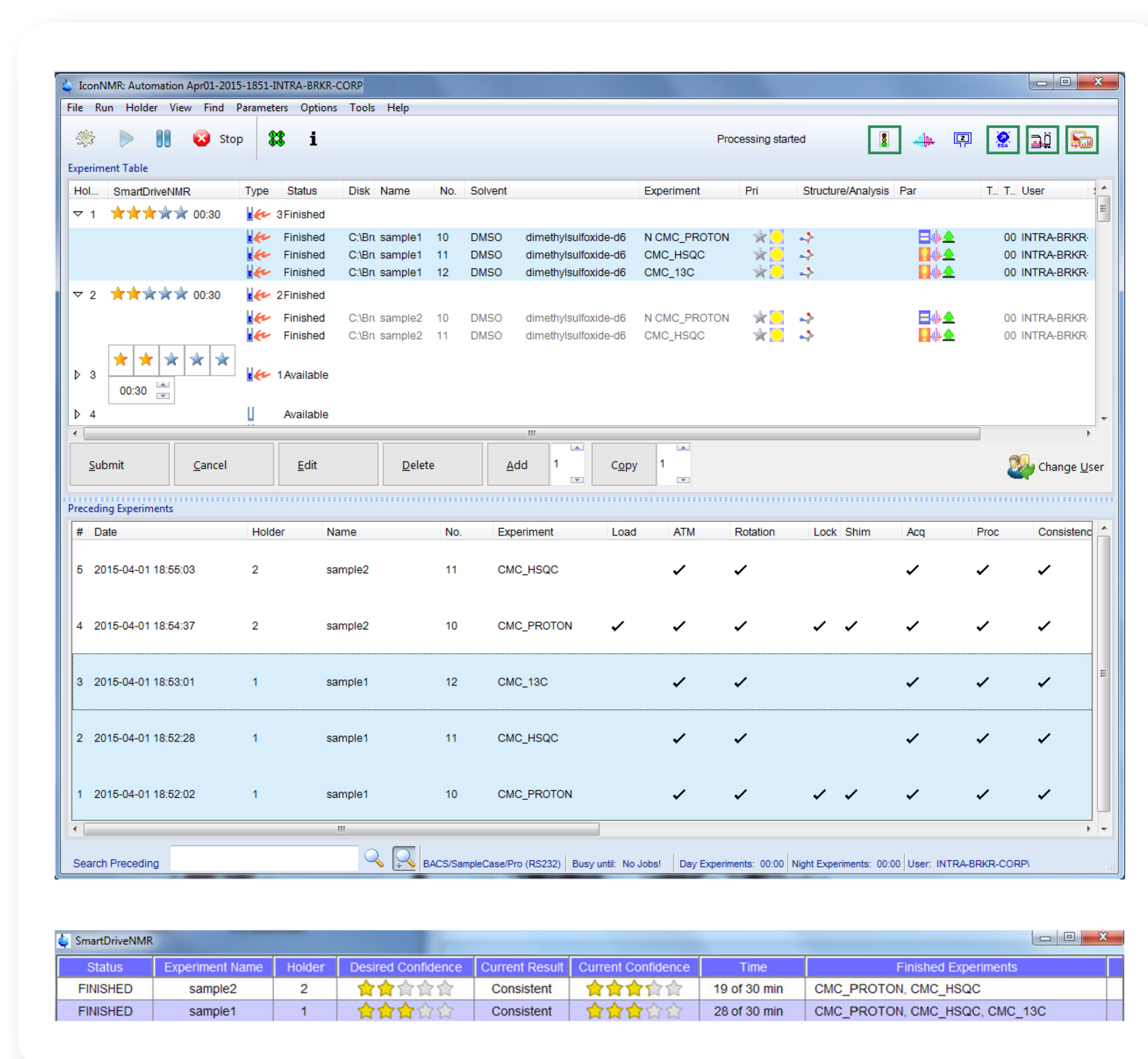


Fig. 3 SmartDriveNMR runs a 1D Proton and then decides whether to acquire further scans, with solvent suppression and/or additional experiments such as multiplicity edited HSQC, 1D¹³C and HMBC.

Summary

- SmartDriveNMR is an easy-to-use solution for open access, routine NMR.
- Submit your allowed instrument time and desired level of confidence and let the software take over.
- SmartDriveNMR's on-the-fly decisions will improve data quality.

