SmartDriveNMR

The Smart Spectrometer for Structure Verification

SmartDriveNMR is custom-built for use in open access NMR environments often found in medicinal chemistry and organic synthesis. This intuitive and easy-to-use software allows users to input basic experimental parameters and then turn the controls over to the software to identify and carry out the ideal combination of NMR experiments in a predetermined amount of time.

The software will decide on-the-fly if further experiments can significantly improve the verification confidence while complying with the user's demands concerning allocatable spectrometer time and confidence.

Starting SmartDriveNMR

SmartDriveNMR is fully integrated in Bruker's acquisition software IconNMR and TopSpin. The relevant inputs are intuitive and NMR independent - only relating to the structure verification task:

- Desired verification confidence
- Maximum measurement time
- Molecular structure and solvent

SmartDriveNMR at work

A scout 1D 1H experiment is launched followed by an automatic structure verification powered by modern human logic emulation algorithms.

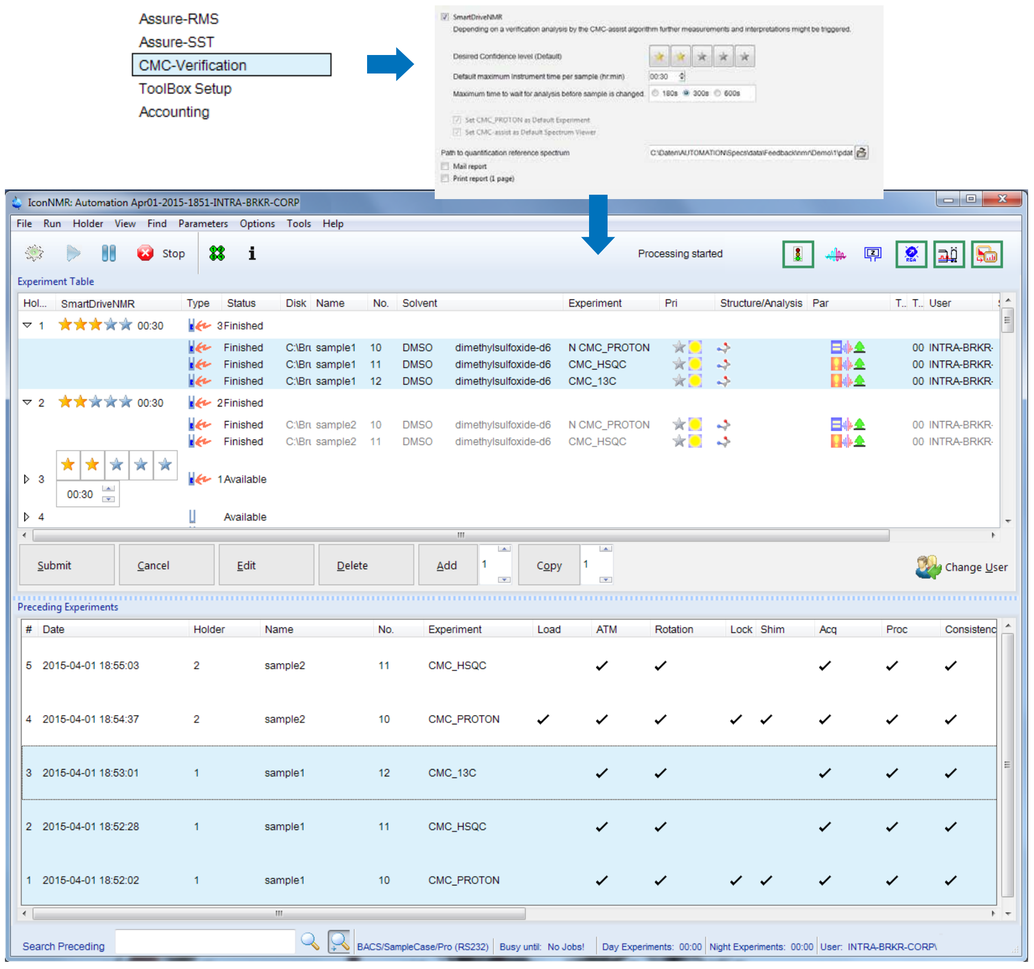

Fig. 1 Setting up SmartDriveNMR: Activation via one click in the configuration of IconNMR. Each sample can get individual settings for the desired confidence and the measurement time. SmartDriveNMR running: Additional experiments are suggested and acquired depending on the achieved verification confidence and the limits on the measurement time.

The result is analyzed and optional experiments are triggered according to the desired confidence and the assessed measurement time given by the user as well as the complexity of the problem. Options are:

- Solvent suppression
- 1D ^{13}C spectroscopy
- 2D ^{1}H-^{13}C correlation spectroscopy
- Signal-to-Noise optimization

Finalizing with CMC-assist

CMC-assist version 2.3 is the ideal tool to review and report the verification results.

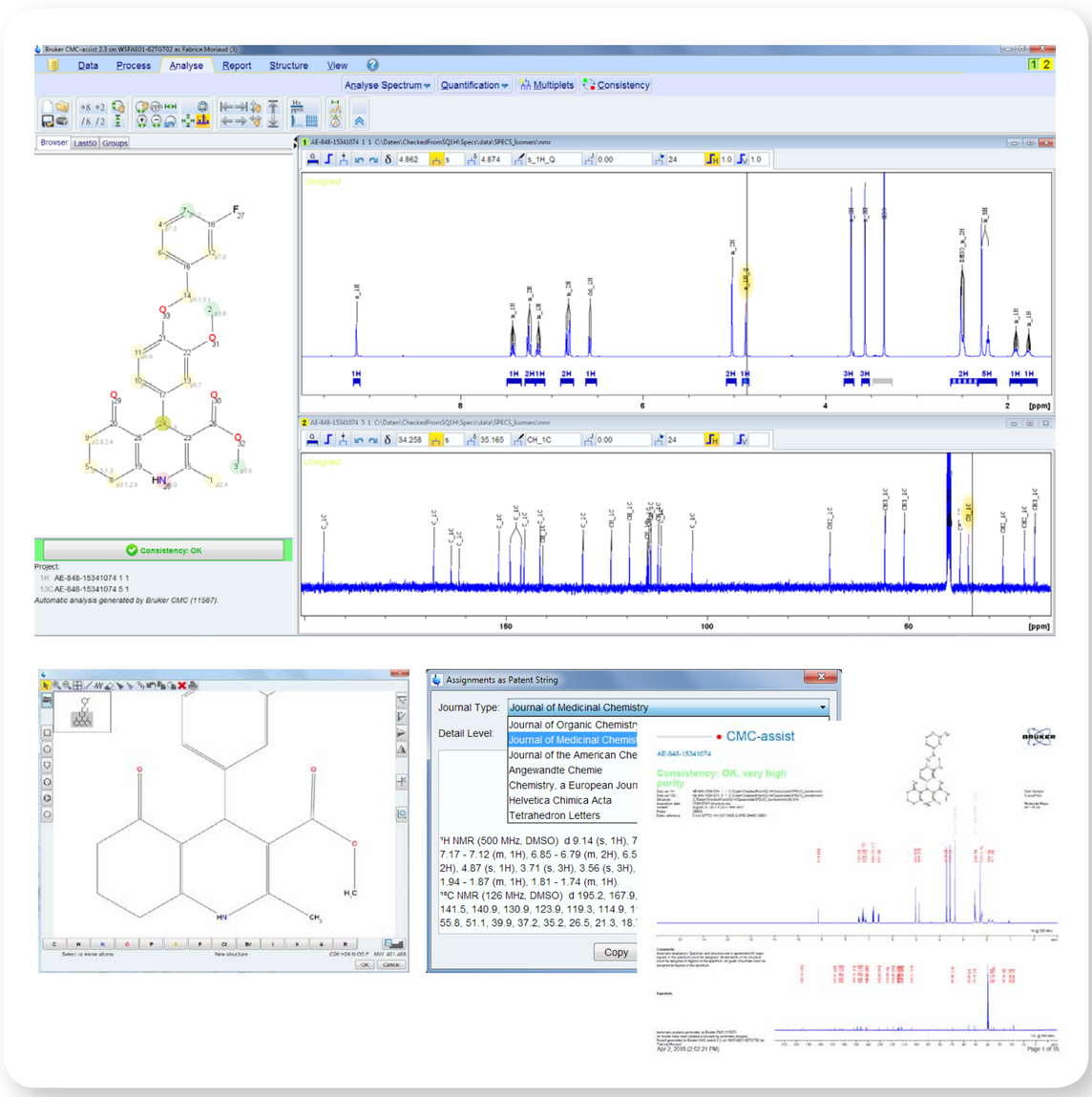

Fig. 2 Reviewing and reporting SmartDriveNMR results with CMC-assist.

New Features of CMC-assist 2.3

- Powerful structure editor
- Automatic data analysis includes:
  - Fully automated ^{13}C analysis
  - Visualized predicted chemical shifts
- Streamlined user interface

Summary

- SmartDriveNMR – Seamless connection between instrument and analysis
- Problem driven on-the-fly structure verification
- Powered by CMC-assist version 2.3
- No NMR expertise required
- Optimized spectrometer use