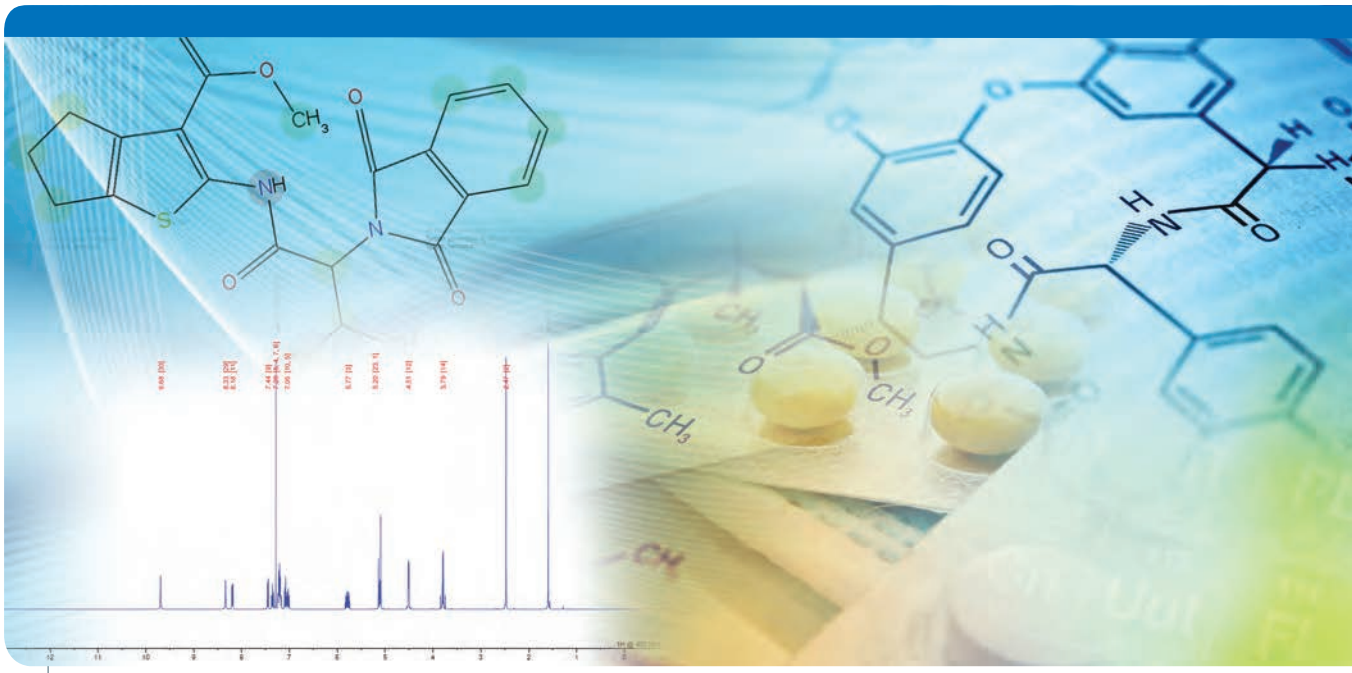

SmartDriveNMR

The Smart Spectrometer for Verification

SmartDriveNMR is the software application 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 determine and carry out the ideal combination of NMR experiments in a predetermined amount of time.

SmartDriveNMR offers flexible fully automated structure verification conducted at measurement time connecting instrument and analysis seamlessly

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.

Key features:

- Flexible on-the-fly structure verification
- Powered by CMC-assist
- Seamless connection between instrument and analysis
- Optimized spectrometer use
- No NMR expertise required

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
- Solvent

SmartDriveNMR at work

A scout 1D ^{1}H experiment is launched followed by an automatic structure verification powered by modern human logic emulation algorithms. 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 is the ideal tool to review and report the verification results. Features of CMC-assist are:

- State-of-the-art analysis engine
- Powerful structure editor
- Automatic data analysis includes:
  - Consistency statement
  - Fully automated ^{13}C analysis
  - Multiplet and integration determination
  - Visualized predicted chemical shifts
  - Structural assignment
  - Concentration and purity assessment
- Comprehensive reporting including detailed PDF document and multiplet string in different journal formats
- Streamlined user interface

Bruker BioSpin
info@bruker.com
www.bruker.com/SmartDriveNMR