^{1}H-^{19}F Analyses on the Agilent 400-MR

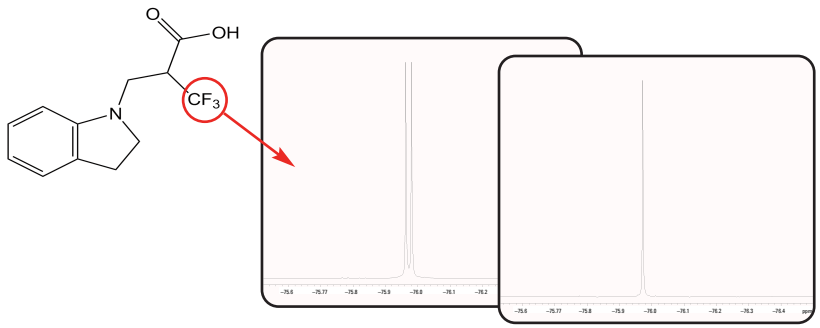
Data Sheet

Introduction

Agilent's 400-MR, when equipped with an Automated Triple Broadband (ATB) or AutoSwitchable (ASW) probe, is ideal for analyses of compounds containing ^{19}F, such as drug precursors. The following experiments are available: 1-dimensional (1-D) fluorine decoupled proton spectra, 1-D proton decoupled fluorine spectra, and 2-D protonfluorine through-bond and through-space correlation.

Key Benefits

- **Simplified spectra**–Reduced complexity ^{19}F and ^{1}H NMR data analyses give you faster fluorine moiety confirmation.
- **Easy to configure**–These applications are included on a standard 400-MR when equipped with a standard ATB or ASW probe. No special hardware or cabling required.
- **Easy to use**–All calibrations and experimental parameters are included in the standard Agilent MR Workstation software available with the 400-MR.
- **Robust and reliable**–The ATB and ASW probes have dual tuned H/F coils and require minimal mechanical operation.



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Studying Compounds Containing ^{19}F

The use of ^{19}F in place of ^{1}H nuclei can radically alter the ADME properties of a drug and is widely used in the drug discovery process [1]. NMR is a valuable tool to ensure that a fluorine moiety remains intact and in the correct position through a synthetic procedure. The standard Agilent 400-MR is capable of analyzing compounds containing ^{19}F constituents, when equipped with an ATB or ASW probe.

Simplified Spectra

In NMR data acquisition, ^{1}H and ^{19}F couple to each other, often creating complex splitting patterns. Using the 400-MR, spectra can be simplified by decoupling techniques resulting in clearer assignments, more visible impurites and more reliable confirmations.

Information Rich Data

The 400-MR is also capable of performing experiments that define the position of a ^{19}F within a molecule by correlating through-space and through-bond H-F information.

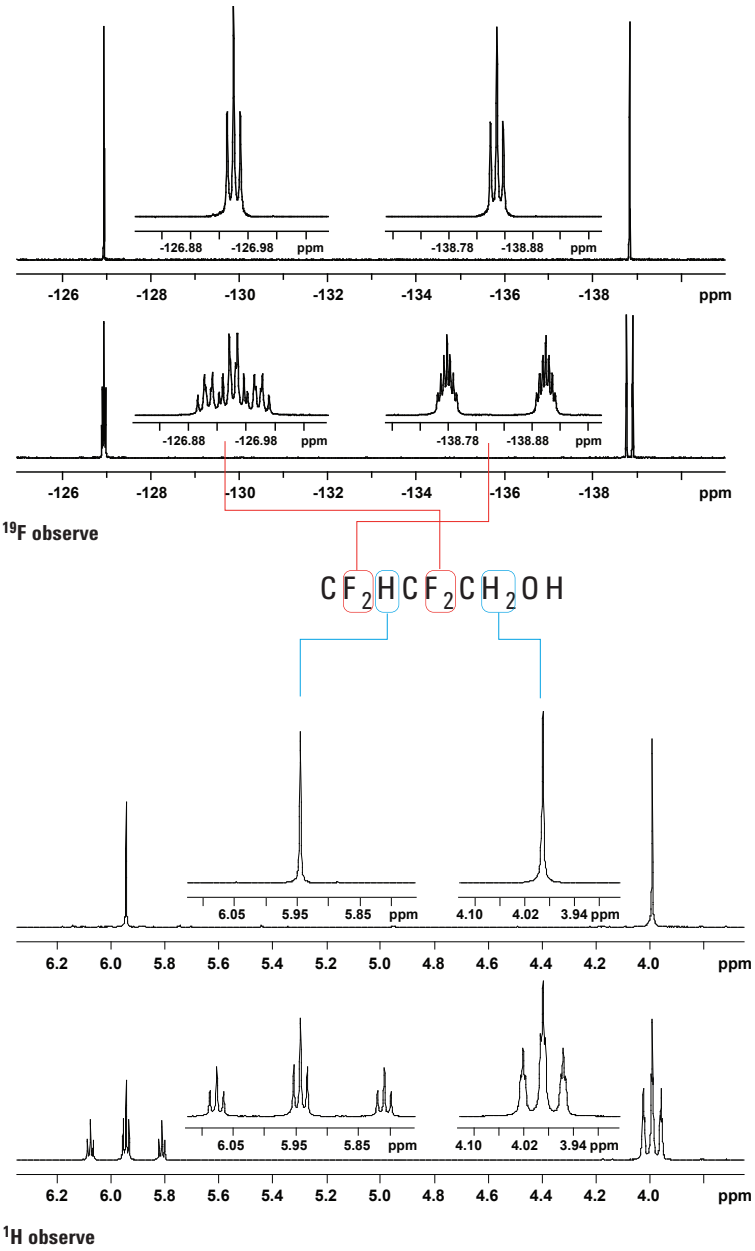
Applications Include

- Drug discovery, organic synthesis confirmation
- Drug development, purity analyses
- Metabolite identification and quantitation

The Agilent 400-MR can be used to provide useful structural information on compounds containing ^{19}F moieties. For the molecule shown, the vertical lines indicate the spectral elements attributed to each nucleus. The bottom spectrum in each group of four shows the coupled data; the top spectrum shows the simplification obtained through decoupled data.

Reference

1. For example, see Kitteringham et al, Annu. Rev. Pharmacol. Toxicol., 2001, 41, 443



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