Agilent NMR System

Receiver response for quantitative NMR

Technical Overview

Introduction

Advantage Statement

The Agilent NMR System provides an unprecedented level of precision in the response of the receiver through the performance characteristics of the digital filters employed. This contributes significantly to an improvement in the accuracy of quantitation of NMR spectra, particularly when spectra are referenced based on an internal standard at one edge of the NMR spectrum.

NMR spectroscopy is used for many purposes including quantitative analysis of mixtures. NMR is ideal for quantitation in that all protons across the spectrum are theoretically equally sensitive, therefore, understanding quantitative results does not require the need for compound-specific extinction coefficients or calibrations. Implicit in the above statement is that all frequencies in a spectrum are detected with the same absolute sensitivity, for example, the amplitude of any NMR peak is independent of its frequency or position in the spectrum.

However this frequency-independent uniformity of amplitude has often not been realized in practice. While there are many factors that can influence NMR peak intensities, for example, uniform excitation by the observe pulse, a significant factor on many NMR hardware systems has been non-uniformity of the receive chain as a function of frequency, including amplitude distortions in the analog components and digital filters.

The Agilent NMR System has essentially eliminated non-uniformity in the receiver chain as a source of amplitude errors for NMR peaks. Shown in Figure 1 is data from an arrayed experiment on a standard sample (2 Hz doped water) in which the transmitter off set is shifted in 40 steps of 250 Hz each so that the doped water peak moves from outside the spectra on the left, through the 5 kHz spectral width in spectra 12 to 31, and then again outside of the spectral window on the right. While the extremely sharp transition of the standard Brickwall filter is impressive, even
more important to quantitative NMR is the flat response within the spectral window. Statistical analysis of the peak heights in array elements 12 to 31 show a standard deviation of only 0.02%, essentially the same standard deviation as one obtains by simply repeating the same 1 µsec pulse at a fixed offset.

This impressive level of precision in the receiver response has been achieved in the Agilent NMR System through:

1. Direct sampling of the NMR data at the 20 MHz intermediate frequency, and
2. The use of time-corrected Brickwall filters

![Figure 1. Data from an arrayed experiment.](image)

This flat frequency-independent response of the NMR receiver can greatly improve the accuracy of quantitation of NMR spectra, particularly in the common instances when spectra are referenced based on an internal calibration standard which appears at one edge of the NMR spectrum, for example, DSS.