Artifact reduction in pure shift NMR by SAPPHIRE technique

Product used : Nuclear Magnetic Resonance (NMR)

Pure shift NMR spectroscopy, also known as homonuclear broadband decoupling, offers a significant advancement in NMR analysis. While conventional ^{1}H NMR spectra provide valuable information including chemical shift, splitting patterns, coupling constants, and intensity, they often suffer from complexity due to signal overlap. Pure shift NMR techniques effectively suppress homonuclear ^{1}H-^{1}H interactions, collapsing multiplets into singlets and thereby minimizing signal overlap. This makes it particularly advantageous for analyzing complex molecules and mixtures. In pure shift NMR, a series of Free Induction Decay (FID) blocks, typically spanning several tens of milliseconds, are acquired. These blocks are then combined to produce a single FID (as illustrated in Fig. 1) which is subsequently Fourier transformed.
However, it's important to note that in pure shift NMR spectra, periodic sidebands occur due to discontinuities in the FID. These sidebands, with a period inversely proportional to the length of the FID block, can complicate analysis for certain samples (refer to Fig. 2).

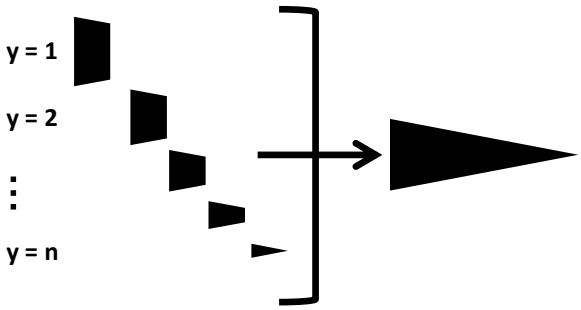

Fig. 1: Acquiring and processing pure shift NMR data

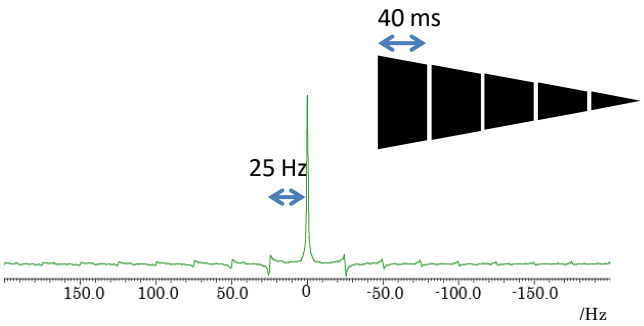

Fig. 2: Sideband in pure shift NMR spectra

SAPPHIRE

The SAPPHIRE (Sideband Averaging by Periodic PHase Incrementation of Residual *J* Evolution) technique[1] reduces the periodic sidebands and yields clean pure shift spectra. The SAPPHIRE method suppresses the sidebands by collecting and averaging FID blocks of slightly different length before they are combined. SAPPHIRE pulse programs and data processing algorithms have been part of Delta NMR software since V.6.1. The SAPPHIRE approach aids in identifying small signals that may be obscured by larger sidebands and enables the observation of ^{1}H-^{19}F couplings that are typically challenging to discern amidst ^{1}H-^{1}H couplings. As illustrated in Fig. 3, the SAPPHIRE method effectively suppresses sidebands and enhances the lineshape of signals.

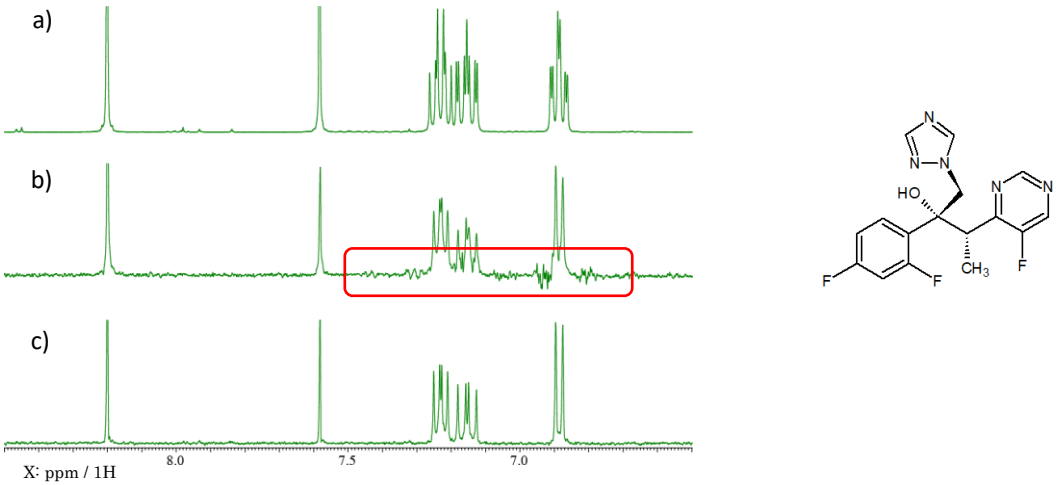

Fig. 3: a) ^{1}H NMR, b) standard PSYCHE, c) PSYCHE SAPPHIRE spectra of Voriconazole.

Reference : [1] *Chem. Commun.* 2017, 53, 10188-10191

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