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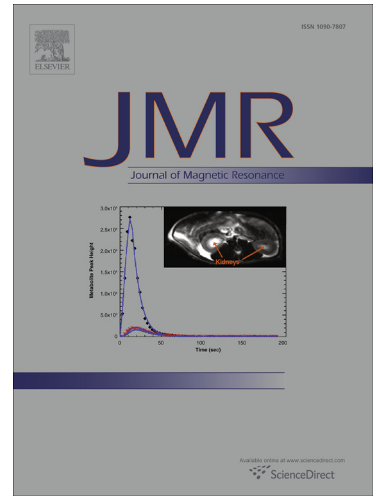

Diagonal free homonuclear correlation using heteronuclei at natural abundance

Bikash Baishya

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Diagonal free homonuclear correlation using heteronuclei at natural abundance

Bikash Baishya[a]*

[a]*Center of Biomedical Research (Formerly Centre of Biomedical Magnetic Resonance), SGPGIMS Campus, Raebareli Road, Lucknow, 226014, India*

Abstract

Homonuclear correlated spectroscopy such as COSY and TOCSY provides crucial structural information. In all homonuclear correlation, the most intense peaks are represented by the diagonal. As a result, the useful cross peaks close to the diagonal gets obscured by the huge tails of diagonal peaks. Herein, we show that by editing the proton magnetization by a C-13 nucleus in natural abundance, it is possible to eliminate the inphase coherence or untransferred magnetization that leads to the diagonal peak while retaining the antiphase coherence or transferred magnetization required for creation of cross peak. After the coherence transfer step, the untransferred magnetization directly attached to C-13 evolves under one bond heteronuclear coupling while the transferred transeverse magnetization directly attached to remote C-12 does not. As a result, the untransferred magnetization directly attached to C-13 can be converted to an unobservable heteronuclear multiple quantum coherence leading to a diagonal free correlated spectrum with a sensitivity penalty of two order of magnitude but comparable to HSQC kind of experiments at natural abundance. The method demonstrated for COSY and TOCSY allows all proton-proton correlations to be observed except the geminal proton-proton correlations. Further, protons directly attached to heteronuclei other than C-13 must be scalar coupled to protons directly attached to C-13 to have a detectable cross peak.

Key words: diagonal free COSY; TOCSY, INEPT, Multiple Quantum Coherence (MQC);

Introduction:

The intense diagonal peaks in typical 2D homonuclear correlation spectra represent a drawback when assignment of cross peaks close to the diagonal is essential. While all the valuable information can be retrieved from the cross peaks, the intense diagonal peaks can obscure nearby cross peaks, lead to t_1 noise along the indirect dimension, and reduce the dynamic range of the spectrometer resulting in a lower sensitivity of low intensity cross peaks. In fact the problems associated with the detection of cross peaks close to the diagonal are strongly related to the ratio of diagonal to cross peak intensity.

Several schemes have been proposed and demonstrated in the literature to suppress diagonal peaks. The 1st such approach achieves diagonal suppression by subtracting two spectra-one conventional 2D spectrum, and another containing only the diagonal obtained

** Corresponding author Fax: 91-522-2668215, E-mail address: bikashbaishya@gmail.com*