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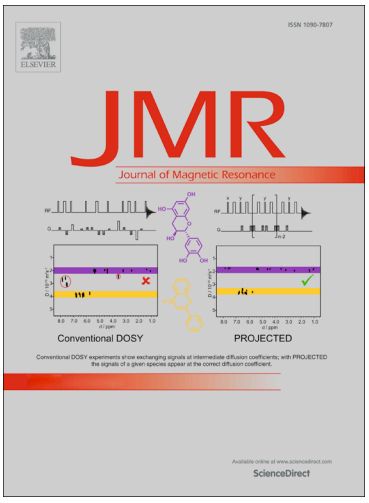

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A pure shift experiment with increased sensitivity and superior performance for strongly coupled systems

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1 Abstract

Motivated by the persisting need for enhanced resolution in solution state NMR spectra, pure shift techniques such as Zangger-Sterk decoupling have recently attracted widespread interest. These techniques for homonuclear decoupling offer enhanced resolution in one- and multidimensional proton detected experiments by simplifying multiplet structures.

In this work, a modification to the popular Zangger-Sterk technique PEPSIE (**P**erfect **E**cho **P**ure **S**hift **I**mproved **E**xperiment) is presented, which decouples pairs of spins even if they share the same volume element. This in turn can drastically improve the sensitivity, as compared to classical Zangger-Sterk decoupling, as larger volume elements can be used to collect the detected signal. Most interestingly, even in the presence of moderate strong coupling, the PEPSIE experiment produces clean and widely artifact free spectra. In order to better understand this – to us initially – surprising behaviour we performed analyses using numerical simulations and derived an (approximate) analytical solution from density matrix formalism.

We show that this experiment is particularly suitable to study samples with strong signal clustering, a situation which can render classic Zangger-Sterk decoupling inefficient.

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