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SCoT: Swept Coherence Transfer for Quantitative Heteronuclear 2D NMR

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Abstract

Nuclear magnetic resonance (NMR) spectroscopy is frequently applied in quantitative chemical analysis (qNMR). It is easy to measure one-dimensional (1D) NMR spectra in a quantitative regime (with appropriately long relaxation delays and acquisition times); however, their applicability is limited in the case of complex samples with severe peak overlap. Two-dimensional (2D) NMR solves the overlap problem, but at the cost of biasing peak intensities and hence quantitativeness. This is partly due to the uneven coherence transfer between excited/detected ^{1}H nuclei and the heteronuclei coupled to them (typically ^{13}C). In the traditional approach, the transfer occurs via the evolution of a spin system state under the J-coupling Hamiltonian during a delay of a fixed length. The delay length is set on the basis of the predicted average coupling constant in the sample. This leads to disturbances for pairs of nuclei with coupling constants deviating from this average. Here, we present a novel approach based on non-standard processing of the data acquired in experiments, where the coherence transfer delay is co-incremented with non-uniformly sampled evolution time. This method allows us to obtain the optimal transfer for all resonances, which improves quantitativeness. We demonstrate the concept for the coherence transfer and multiplicity-edit delays in a heteronuclear single-quantum correlation experiment (HSQC).

Keywords: Swept coherence transfer, Non-uniform sampling, HSQC, Quantitative NMR