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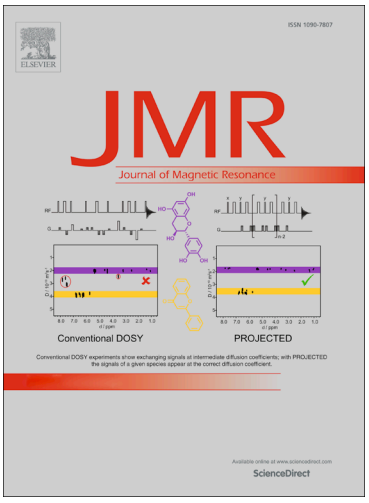

Quick, sensitive serial NMR experiments with Radon transform.

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Quick, sensitive serial NMR experiments with Radon transform.

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Abstract

The Radon transform is a potentially powerful tool for processing the data from serial spectroscopic experiments. It makes it possible to decode the rate at which frequencies of spectral peaks shift under the effect of changing conditions, such as temperature, pH, or solvent. In this paper we show how it also improves speed and sensitivity, especially in multidimensional experiments. This is particularly important in the case of low-sensitivity techniques, such as NMR spectroscopy. As an example, we demonstrate how Radon transform processing allows serial measurements of ^{15}N-HSQC spectra of unlabelled peptides that would otherwise be infeasible.

Keywords: Radon transform , multidimensional spectroscopy, HSQC, variable temperature

1. Introduction

NMR spectroscopy is one of the most powerful tools that exists in analytical chemistry. Several improvements over the decades have contributed to its efficiency. In the 1960s Ernst showed how it was possible to increase speed and sensitivity by performing the acquisition of a free induction decay signal (FID) in time domain, and processing it by Fourier transform (FT) to get the spectrum [1]. This discovery opened the way to multidimensional (ND) spectroscopy, first proposed by Jeener[2] and Ernst[3]. In ND NMR one acquires a signal that is a function of multiple time variables, and which contains information on interactions between

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