Ultrafast diffusion-based unmixing of 1H-NMR spectra

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Résumé

Usage of the spatial-parallelization concept in diffusion-ordered NMR spectroscopy (DOSY), which is known for separation-free identification of mixtures and molecules, reduces the acquisition-time of the experiment from few minutes to few hundreds of milliseconds. Recent years have witnessed the use of this spatially encoded-DOSY (SPEN-DOSY) method in mixture analysis via univariate processing methods, where each peak is fitted individually to extract its diffusion constant. However, such analysis on overlapping-peaks of complex mixtures restricts the identification / separation of molecules and leads to wrong values of diffusion constants. This work addresses this problem by using Direct Exponential Curve Resolution Algorithm (DECRA);a fast multivariate processing algorithm, which separates components of a mixture. Applying DECRA to SPEN data required the design of a radio-frequency (rf) pulse that provides a quadratic spacing of the spatially parallelized gradient area. In addition, clean unmixing of components required additional pre-processing step, to account for the effect of chemical shifts during spatial encoding and during acquisition. Once designed, these new tools are straightforward to implement and use. Combining existing SPEN-DOSY pulse sequence with this newly designed rf pulse, 2D data was acquired for model mixtures, with experiment durations of less than 500 ms. All processing steps are then completed in less than 2 s, out of which only 100 ms required for DECRA.Together these tools provide an "ultrafast" unmixing of 1H NMR spectra, which should be useful for the analysis of reaction mixtures and hyperpolarized substrates.

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