NMR diffusometry data sampling optimization for mixture analysis

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Résumé en anglais	NMR diffusometry is a powerful but challenging method to analyze complex mixture. Each component diffuses differently, from the faster small species to the slower large species, corresponding to different signal attenuation. However, the method is highly sensitive to the quality of the acquired data and the performance of the processing used to resolve multiexponential signals influences. Adapting the signal decay sampling to the mixture composition is one way to improve the precision of the measure. In this work, we propose a prediction tool, based on the calculation of the Cramér-Rao lower bound to minimize the variance of diffusion coefficient estimation in order to determine the optimal number of diffusion gradient steps, the best diffusion gradient sampling (among linear, exponential, quadratic and sigmoidal ones) and the optimal maximum diffusion factor. The tool was validated experimentally on a unimer/micelle solution of sodium dodecyl sulfate and on Caelyx®, a commercial liposomal preparation containing a mixture of pegylated-liposomes and sucrose.
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Liens

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