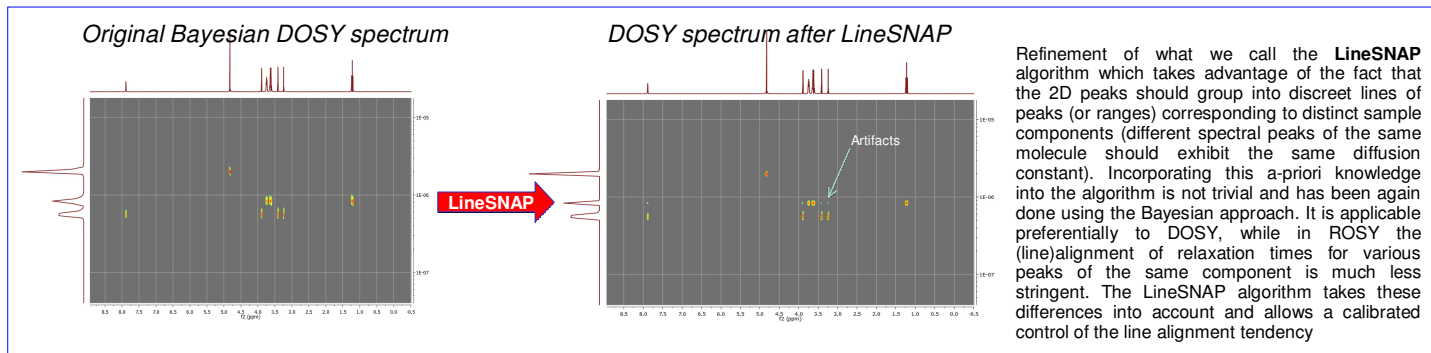


Progress in Bayesian DOSY and ROSY Transforms

Introduction

An efficient Bayesian approach (nicknamed BDT or **Bayesian Data Transform**) to the evaluation and graphic representation of multi-array NMR data sets characteristic of the diffusion (**DOSY**) and relaxation (**ROSY**) spectroscopies was first presented at ENC in 2008. Since then, it was beta tested and a considerable progress has been made which includes (a) a refinement of the LineSNAP section of the algorithm, (b) spectral alignment of the arrayed spectra using the novel **Global Spectrum Deconvolution (GSD)** algorithm and (c) combination of the BDT algorithm with a Bayesian handling of bi-exponentiality of overlapping spectral peaks. We will be happy to discuss with you the details of these developments.

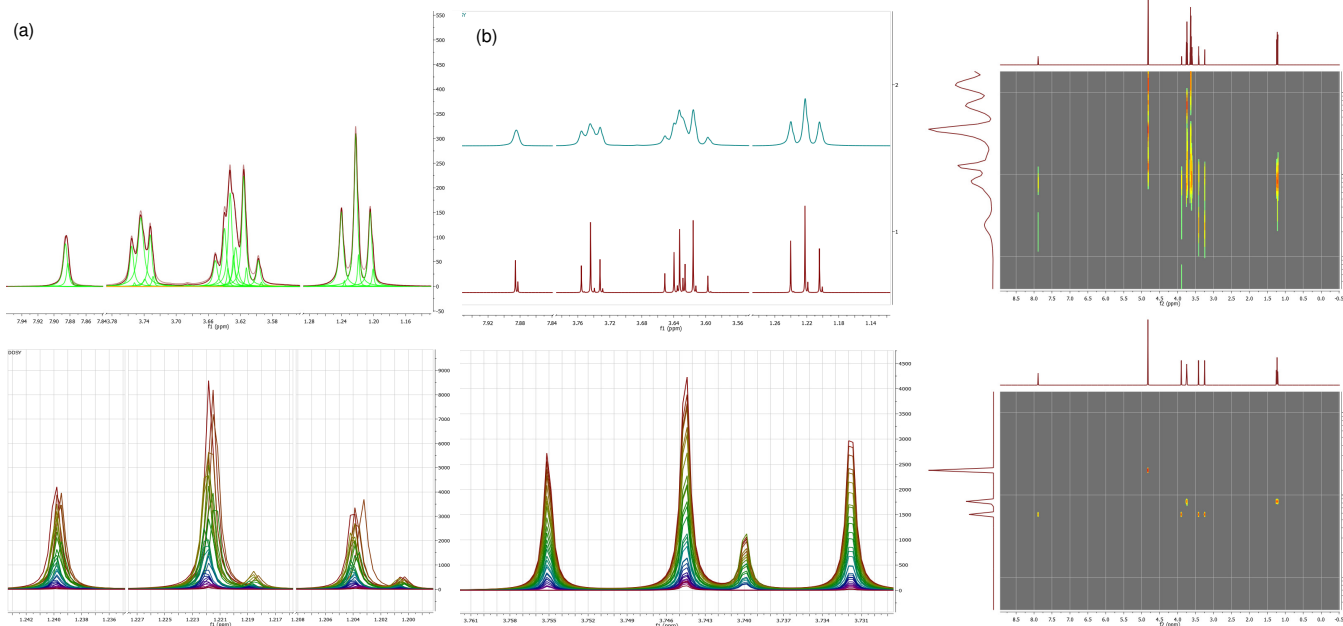
(a) LineSNAP



(b) Spectral Alignment

Spectral overlap is an important problem in any DOSY processing: where peaks overlap, a monoexponential hypothesis yields compromise apparent diffusion coefficient. Overlapping can be minimized by exploiting the resolution power of GSD, as illustrated in the two figures below: (a) shows deconvolved peaks corresponding to the first trace of an PFG experiment whilst (b) shows the result of creating a synthetic GSD spectrum with a uniform line with of 0.2 Hz compared to the original, untreated spectrum

However, when BDT is applied to the GSD resolution enhanced spectra, it yields a DOSY map with long vertical strips



(c) handling of bi-exponentiality

The Bayesian algorithm has been now combined with a Bayesian handling of bi-exponentiality. Considering the very limited number of spectra available in typical arrayed data sets (anything beyond 32 is considered impractical and 16 is a very popular choice), a full multi-exponential analysis is hardly ever feasible, but a separation of two decay components in cases of overlapping spectral peaks can be done with profit. However, since it affects negatively the final z-resolution, it must be applied only to those spectral regions where it is really needed and this, in addition to the incorporation of the bi-exponential hypothesis into the BDT algorithm, implies the need for an automatic procedure capable of selecting the non-exponential regions automatically on the basis of objective statistical criteria.

References

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- 2 C.Cobas, S.Sykora, *Bayesian DOSY and ROSY transforms*, J.Magn.Reson., submitted