Bayesian DOSY: A New Approach To Diffusion Data Processing

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In this work we present a newly developed Bayesian approach to the processing of NMR diffusion experiments which is computationally very efficient and physically eminently meaningful. It treats all data points in the same way, and gives very satisfactory and artifact-free results. Applied specifically to DOSY data sets, it leads to what we call the **BDT** algorithm (standing for *Bayesian DOSY Transform*). It is also an excellent example of the broad class of Bayesian approaches to the evaluation of NMR data.

The BDT algorithm is the core of the BayDOSY evaluation and presentation method implemented in Mnova, which is now beta-tested in practice on real experimental data. Apart from BDT, BayDOSY includes also a novel algorithm for a substantial improvement of the resolution in the diffusion-constant dimension and a contextual improvement in the alignment of peaks belonging to the same molecular species. Ongoing work aims at Bayesian handling of overlapping spectral peaks belonging to different sample components..