Title:	Resolving overlaps in diffusion encoded spectra using band-selective pulses in a 3D BEST-DOSY experiment
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Abstract:	A novel diffusion-edited 3D NMR experiment that incorporates a BEST-HMQC pulse sequence in its implementation is presented. Heteronuclear 3D DOSY NMR experiments are useful in elucidating the diffusion coefficients of individual constituents of a mixture, especially in cases where the proton NMR 2D DOSY spectra show considerable overlap. The present 3D BEST-DOSY pulse sequence provides a more sensitive and less time-consuming alternative to standard 3D HMQC-DOSY experiments. Cleanly separated subspectra of individual mixture components are obtained, leading to the determination of diffusion coefficients with better accuracy. The feasibility of the technique is demonstrated on a mixture of amino acids, on a mixture of small molecules with similar diffusion coefficients, and on a complex mixture with large dynamic range (commercial gasoline). The implications of using adiabatic decoupling schemes and band-selective shaped pulses for selective BEST-DOSY experiments on proteins are also discussed.
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