Title:	Numerically optimized band-selective pulses in SOFAST-HMQC experiments for biomolecular NMR
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Abstract:	This work demonstrates the efficacy of numerically optimized band-selective pulses in 2D fast-pulsing NMR pulse sequences of the SOFAST-HMQC variety. In order to achieve robust band selectivity the amplitude and phase of the shaped RF pulses are modulated according to a numerically optimized function. During the pulse duration, the spin trajectories evolve along complex and often unexpected pathways. The pulses have been designed using the GRAPE algorithm and are experimentally implemented on a model protein ubiquitin (13C, 15N labeled). Signal to noise ratios of peaks have been computed and compared for the different experiments performed using both numerically optimized band-selective pulses and standard pulse shapes. The numerically optimized pulses perform better in terms of signal enhancement and phase, as compared to standard pulse shapes.
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