Simulation of Magnetization Pathways and Peak Inference in the new NMR Resonance Assignment Program Package CARA

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The analysis of NMR spectra is both a critical step and today the most time consuming task in the process of protein structure determination. All relevant signals of a spectrum must be identified and the chemical shifts uniquely assigned to the atoms of the protein by logical inference. All NMR software packages known to the author base their information management on peak- and atomlists. Each spectrum is associated with a dedicated peaklist consisting of individual peaks. The synchronization of peaks among different peaklists is one of the major causes of the complexity related to resonance assignment. We present a novel approach implemented in CARA which infers the position of expected cross-peaks dynamically from a spectrum-independent signal repository, eliminating the need to synchronize peaklists.

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