Novel Methods in Small Molecule NMR Spectroscopy

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Novel basic methods will be presented that concern the acquisition of fast experiments on small molecules at natural abundance. The Clean InPhase or CLIP-COSY as a homonuclear correlation experiment with excellent sensitivity can be applied with intermediate resolution in $\omega_1$ in about 5 minutes, and can be further reduced if non-uniform sampling is applied [1]. The experiment can be extended to relayed transfer and finally TOCSY-type correlations with approximate planar mixing Hamiltonian and considerable bandwidth.

A second class of experiments will concern heteronuclear correlations based on the ASAP-HSQC approach [2]. An improved, symmetrized version is introduced as well as several extensions (e.g. [3]). As the experiment has a high duty cycle, we also looked into multiple pulse sequences for heteronuclear decoupling. Here we introduced cooperative decoupling sequences optimized using optimal control theory. The resulting sequences called BROCODE allow the broadband decoupling of carbon spins over a bandwidth of 40 kHz with an effective rf-amplitude of 2 kHz, corresponding to a 90° pulse length of 125 $\mu$s.

References