

EASY-GOING ON-SPECTROMETER OPTIMISATION OF PHASE MODULATED HOMONUCLEAR DECOUPLING SEQUENCES IN SOLID-STATE NMR

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A global optimisation scheme for phase modulated proton homonuclear decoupling sequences in solid-state NMR is presented. Phase modulations, parameterised by DUMBO Fourier coefficients, were optimized using a Covariance Matrix Adaptation Evolution Strategies algorithm^a. Our method, denoted EASY-GOING homonuclear decoupling, starts with featureless spectra and optimises proton-proton decoupling, during either proton or carbon signal detection. On the one hand, our solutions closely resemble (e)DUMBO^b for moderate sample spinning frequencies and medium radio-frequency (rf) field strengths. On the other hand, the EASY-GOING approach resulted in a superior solution, achieving significantly better resolved proton spectra at very high 680 kHz rf field strength.

^aN. Hansen, and A. Ostermeier. *Evol. Comput.* 9 (2001) 159–195

^bB. Elena, G. de Paëpe, L. Emsley. *Chem. Phys. Lett.* 398 (2004) 532–538