ESI: Using open data to rapidly benchmark biomolecular simulations: Phospholipid internal dynamics

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1 Experimental setup and analysis of R_1, $R_{1\rho}$ and τ_e

All experiments were conducted on a standard bore E-free CP-MAS 4mm probe, using a Bruker AVANCE II-500 NMR spectrometer, operating at a ^{13}C Larmor frequency of 125.78 MHz. The magic angle spinning (MAS) rate used was 5 kHz and the effective temperature was 298 K. Sample preparation and the R_1 and $R_{1\rho}$ experiments were as described in reference.[?]

The following pages show the fits performed to determine the relaxation rates shown in figures x and y of the main manuscript. The error estimates for R_1 and $R_{1\rho}$ were defined as the highest deviation between the 95% confidence bounds and the fitted values of R_1 and $R_{1\rho}$ using MATLAB 2018b and the curve fitting toolbox package to fit single exponential decays of the form $a\exp(-R_1 t)$ (figures x-y). Each point of the relaxation decays for each individual ^{13}C peak was calculated by analytical integration of a fitted gaussian lineshape to the ^{13}C peak.