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Axial Rotation of Lipids in Membranes

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This study was motivated by Mary Roberts and Al Redfield, who proposed that the observed 10 ns decay time in their phosphorous NMR measurements of DPPC in bilayers originated from axial rotation of the lipid. Analyses of correlation functions and average first passage times from 50 ns molecular dynamics of DPPC bilayers strongly support their interpretation. The rotational anisotropy of a lipid in a bilayer is close to 1.0, in contrast to the 2.5 expected for a hydrodynamic cylinder with lipid dimensions. This implies that axial rotation is dominated by headgroup, not tail, interactions.