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Anisotropic Motion of Lipids in Hydrophobic Core of DPPC Bilayers. Simulation of ESR spectra

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Abstract: Planar samples prepared by drying phospholipid dispersions on glass slides provide a convenient model to examine motion and orientation in lipid bilayer structures. In the present work, hydrophobic cores of DPPC multibilayers were studied using a 16-DSA spin label consisting of a nitroxide free radical bonded to the 16 position of stearic acid. This spin label is in great demand for investigation of phase transitions occurring in the hydrophobic cores of lipid multibilayers. Thus, its room temperature motional and orientational features in phospholipid bilayers must be known accurately to avoid any misinterpretation in using it in these types of studies. The aim of the present work was to reinvestigate the orientation distribution and motion characteristics of 16-DSA spin label in DPPC multibilayers. The orientation of the sample with respect to external magnetic field direction was monitored by a goniometer and ESR spectra in a plane perpendicular to the plane of glass slide were recorded with an angular increment of 5°. These spectra were used to study the variations of line separations, g factor, line widths and line amplitudes with orientation angle. Assuming a Gaussian distribution of the labels in the bilayers and attributing a restricted random walk motion to labels, we have simulated experimental spectra recorded for parallel and perpendicular orientations and have calculated the values of the distribution width (σ), tilt angle (δ) and random walk half amplitude (γ) of 16-DSA spin label in DPPC multibilayers.

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