Electron paramagnetic resonance (EPR) spectra are simulated by solving the stochastic Liouville equation (SLE) of motion with the incorporation of a hindering potential that restricts the Brownian rotational diffusion of the spin-label. Such a potential has been expanded in spherical harmonic functions in the past, under the assumptions of cylindrical and inversion symmetries appropriate for the description of liquid crystals and other ordered systems. In this work, the theory is formulated to allow for a general potential with no symmetry restrictions. This extends the utility of EPR as a structural tool, by facilitating its connection with molecular dynamics (MD) since the spectral simulation incorporates a more realistic representation of the complicated topology around the spin-label that is found in labeled biomolecules.

Interaction of Antimalarial Drugs with DMPC Model Membranes

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Primaiquine Dihosphosphate (PQD) and Chloroquine Dihosphosphate (CQD) are potent therapeutic agents used in the treatment of malaria. The investigation of drug-lipid interactions is pivotal for understanding their biological activity. Electron Spin Resonance (ESR) and Differential Scanning Calorimetry (DSC) were used to investigate the effects of drug binding on the lipid phase transition and acyl chain dynamics of model membranes made up of 1,2-Dimyristoyl-sn-Glycero-3-Phosphocholine (DMPC) phospholipids. Labels located at different positions along the lipid chain were used to monitor different membrane regions. Results indicated that PQD is more effective in changing the membrane structure than CQD. PQD is effective in perturbing the whole chain of DMPC vesicles, whereas the effect of CQD is more pronounced near the polar headgroup region. Furthermore, the results showed a slight decrease of the membrane packing in DMPC gel phase for both drugs. However, PQD causes a slight increase of the lipid packing close to the membrane center, suggesting a deeper insertion of this molecule into DMPC bilayers. DSC thermograms presented that indicate conformational changes in the DNA structure that are evidenced through changes in its Raman spectrum, upon stretching. The typically low Raman scattering cross section of DNA is countered with the incorporation of silver colloids that enhance the scattered fields. The utilization of surface-enhanced Raman scattering (SERS) allows fast acquisition of spectra during the DNA intermediate stretched states which helps in elucidating its conformational change pathways.

Pressure-induced Conformational Changes in Poly-peptides and Protein Solutions Probed with Micro-Raman Spectroscopy

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Functional properties of proteins and cells are affected by an elevated pressure environment. Combining Raman microscopy with a micro-capillary high pressure cell enables structural sensitive studies of small amounts of biological material using vibrational signatures. The cell contains less than 50 nano-liter of sample, and Raman spectra can be acquired from atmospheric pressure to 4 kBar. The resolution of the setup is evaluated by measuring the Raman spectrum of standard solutions. We investigate pressure effects of the Raman spectrum on poly(L-glutamic acid) and proteins in solution. Spontaneous Raman spectra of poly(L-glutamic acid) in D2O buffer (pH5.4) solution were measured at variable pressure. A shift of the amide I band in poly(L-glutamic acid) to lower frequency with pressure may suggest significant change in secondary structure towards a-helical conformation.