β-Casein, Revealed by using Spin Probe EPR Spectroscopy

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Solvent Dynamics and Confinement Effects around an Intrinsically Disordered Protein, [1] ERIN NEELY, WEI LI, KURT WARNCKE, Emory University — Electron paramagnetic resonance (EPR) spectroscopy with the spin probe TEMPOL, a paramagnetic nitroxide with detectable rotational motion, is used to study the temperature-dependent structure and dynamics of the solvent phases surrounding the protein β-casein in solution at temperatures from 195-265 K. We have previously studied ordered globular proteins; by contrast, β-casein is an *intrinsically disordered* protein (IDP), i.e. it has no fixed, well-defined structure. The goal of this project is to determine whether and how the EPR spectra of the TEMPOL-β-casein systems differ from those of systems with more ordered proteins. Experimental spectra have already been collected for these systems with and without added DMSO cosolvent over the temperature range. By simulating these experiments using Matlab and finding the parameters for best fit of the experimental spectra, we can determine the physical parameters of these systems such as TEMPOL rotational correlation time, linewidth and component amplitudes. Comparing β-casein's EPR spectra and parameters with those of globular proteins will offer insight into how IDP's interact with and structure their solvent environment. Insights into the solvent-protein structures and dynamics that control aggregation and reactivity will be gained.

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