Generating the charge transfer spectral profile of entire proteins

Apoorva Badaya, Ravindra Venkatramani

Proteins absorb light in the ultraviolet (UV) portion of the electromagnetic spectrum (185-320 nm). It is anticipated that proteins lacking aromatic amino acids, disulphide linkages, and active-site chromophores will remain optically silent at wavelengths greater than 250 nm. Recent experimental and computational studies have shown that the spectra of monomeric proteins rich in charged amino acids span the entire UV-Visible spectral band (from 200-800 nm). This novel label-free spectral band is termed Protein Charge Transfer Spectra (ProCharTS). These investigations have demonstrated that such broad absorption profiles of the proteins arise from photoexcited charge transfer (CT) transitions in spatially proximal charged amino acids such as lysine (Lys) and glutamate (Glu). Our objective is to examine ProCharTS, to generate the spectral profile of the entire protein using molecular dynamics simulations and electronic structure calculations. We assume that the absorption of ProCharTS should be responsive to events that neutralize or modify the charged state of protein residues. Such events comprise biologically significant processes such as a) post-translational modifications, b) interactions between protein subunits c) protein-protein interactions, d) interactions between protein and DNA interactions, and e) protein folding. The model proteins we investigated to validate this hypothesis are Human serum albumin, Bovine serum albumin and histone proteins. We aim to include all potential charge residue clusters that may be present in the protein and may influence its spectral profile in order to construct the ProCharTS profile of the entire protein. ProCharTS is a newly developed spectroscopic technique, and these investigations will greatly broaden its application to explore many significant biological events in vitro.