

Photoinduced Charge Transfer Transitions in Charged Amino Acids: New Label Free Spectroscopic Markers to Probe Protein Structure and Dynamics

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The absorption of light by proteins can induce electronic charge transfer (CT) transitions in the UV-visible wavelength range of the electromagnetic spectrum. Well known examples of chromophores which exhibit CT transitions include metal-ligand complexes in enzymes and the protein backbone. In this talk, I will present recently discovered [1, 2] optical CT transitions in proteins arising from amino acids with charged side-chains (Lys, Glu, Arg, Asp, and doubly protonated His) and post translationally phosphorylated amino acids (Ser, Thr and Tyr). Electronic structure calculations coupled with classical molecular dynamics sampling of molecular conformations show that all charged amino acids are directed electronic donor-bridge-acceptor chromophores exhibiting facile photoinduced charge separations [2]. The new protein charge transfer spectra (ProCharTS) is highly sensitive to the interactions among charged sidechains imposed by protein tertiary fold and to the dynamics and solvation of the chromophore. In fact, the environment of the charged chromophores can modulate the spectral range of ProCharTS to produce protein UV-Visible absorption between 200-800 nm [1]. These results open up a new optical window to study prominent proteins of biomedical relevance which are rich in charged amino acids.

References:

- (1) S. Prasad, I. Mandal, S. Singh, A. Paul, B. Mandal, R. Venkatramani, R. Swaminathan, Chem. Sci. **8**, 5416 (2017).
- (2) I. Mandal, S. Paul, R. Venkatramani, Faraday Discuss., DOI: 10.1039/C7FD00203C. (2017)