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Impact of solvent pH on buried charge formation and protein quake of photoactive yellow protein AIHUA XIE, SANDIP KALEDHONKAR, LORAND KELEMEN, WOUTER D. HOFF, ANUPAMA THUBAGERE, Oklahoma State University — Embedding a charge group inside a protein in a low dielectric environment is energetically unfavorable. Therefore, most charged groups are solvent exposed. We have developed a hypothesis that a new buried charge transiently formed in a non-polar environment serves as an electrostatic epicenter that drives protein quake (protein conformational changes). Here we report an experimental study on the effects of solvent pH on the protonation states of buried ionizable groups, and their correlation with protein quakes. Time-resolved Fourier transfer infrared (FTIR) difference absorbance spectroscopy is the major experimental technique for simultaneous detection of the proton transfer event (to generate a new buried charge) and the protein quake event. The results are expected to provide insight into the impact of solvent pH on protein structural dynamics in general.

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