Protein structural dynamics and interactions modulated by infrared light.

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Motion is an essence of protein biological activity. In order to perform their action proteins undergo certain conformational fluctuations. These collective motions are driven not only by direct interactions between atoms in protein but they are also affected by the solvent.

Our study shows that it is possible to induce fluctuations of protein structure with the use of infrared light (IR) as a remote physical trigger. By exposing proteins in aqueous solution to IR stimuli we can observe reversible conformational changes going from partially disordered and more hydrated to folded and less hydrated state. Whole range of intermediate protein sub states can also be captured by Fourier Transform Infrared Spectroscopy. Those fluctuations can go back and forth in many cycles on protein exposure to pulsed IR light. The two end conformations can be related to Gilbert Ling's active (folded, high entropy) and resting (partially unfolded, low entropy) states. According to Ling, transition from resting to active state can provide the force to drive biological work due to entropy gain on release of water of hydration (bound and polarized by extended unfolded compartments). Going in this direction we tested effect of IR trigger on lysozyme enzymatic activity and our results indicate that IR-induced protein motions can indeed increase kinetics of the enzymatic reaction. Further to this end, we show that effect of IR light on protein-surface interactions (studied by Quartz Crystal Microbalance) is also consistent with the idea of hydration modulation in response to IR.

We can explain effect of IR light on protein structural fluctuations assuming that nanobubbles are the main factor mediating response of biomolecules to IR stimuli. Such assumption is consistent with previous findings showing that weak electromagnetic radiation can trigger oscillations of bubbles in solution and that this phenomena has certain consequences for biological systems [1]. Our spectroscopic studies suggest that IR can promote i) nucleation and/or adsorption of nanobubbles on protein hydrophobic compartments (thus displacement of hydration waters) and transition to folded high entropy state and ii) further coalescence, growth and desorption of nanobubbles (and surface rehydration) thus transition to unfolded, extended, high entropy (due to bound water) state.

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[1] V. M. Shatalov, Biophysics, 2012, 57, 808-813