Polymer Brush Architecture for Thermal Stabilization of Proteins

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In this experimental project, the polymer brush architecture was used to improve thermal stability of enzymes. The strategy utilizes polyethylene oxide cylindrical molecular brushes for self-assembling of the polymer brush-enzyme conjugates. The molecular brush is bound to the surface of the enzyme globule, promoting the formation of stiff and crowded cages around the enzymes and preventing the water molecules access to the enzyme and enzyme agglomeration. The structure of the moderately stiff polymer ligand results in a significant improvement of biocatalytic activity and thermal stability of example enzymes lysozyme and trypsin that retain their activity even upon heating to 100 ^{o}C and above. The polymer ligand creates a single polymer molecule cocoon-like structure by engulfing about 15 enzyme molecules into the crowded stabilizing polymeric brush environment. The thermal stability of the conjugates can be understood based on our simulation studies, spectroscopic analysis, and kinetic parameters. The molecular dynamic simulations show that the high concentration of polyethylene oxide in the vicinity of the enzyme is critical for their thermal stability at high temperatures, a number of hydrogen bonds remains high and corresponding conformational changes in the protein remains low, indicating a high degree of resilience of the secondary structure and thereby contributing to the high rates of the residual activity.