Designing Highly Thermally Stable Lysozyme-copolymer Conjugates — Effect of Polymer Concentration

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Abstract: Designing efficient enzymes that can work at high temperatures can be used for several industrial applications, such as detergent manufacturing, food and starch processing, production of high fructose corn syrup, polymerase chain reactions and enhanced oil recovery (EOR). Herein, using all atomistic molecular dynamics simulations, we demonstrate that by conjugating enzymes with copolymers at high polymer concentrations one can dramatically improve their thermal stability well beyond that of native enzymes. We conjugated the lysine residues of lysozyme with OEGMA-GMA-OEGMA oligomer (triads) forming lysozyme polymer-conjugated (LPC) and probed its thermal stability with varying polymer concentration. The system also contains free-floating triads which effectively allow us to more closely mimic the conditions in our experiments. Our studies show that LPC, unlike the native lysozyme, largely preserves its secondary structure under the same high temperature. At 50% water concentration, triads phase separate and lysozyme is pushed to the water phase, which onsets the unfolding of lysozyme. The access of water molecules to the lysozyme surface disrupts its 3-D structure at high temperature. We show that increasing copolymer concentration results in stabilization. We characterized the system by analyzing the time evolution of (a) the root mean square deviation (RMSD) of each structure with respect to its initial structure, (b) the number of intra H-bonds of the enzyme, (c) evolution of secondary structures, and (d) number of contacts within lysozyme or with triads or water. Our simulation results are in a good agreement with our experimental observations.