

Abstract Submitted  
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**A Molecular Framework for Tunable Functional Response of Programmable Polyesters**<sup>1</sup> KSHITIJ C. JHA, ABRAHAM JOY, MESFIN TSIGE, Department of Polymer Science, The University of Akron — All-atom molecular dynamics (MD) simulations, using the OPLS force field, were carried out on a library of multifunctional polyesters with peptide-like functional pendant groups. The polyesters are structural peptidomimetics and can be utilized for applications in sensing, and separation, and as biomedical scaffolds. The modular design of the polyesters affords a range of hydrophilic and hydrophobic behavior. We used MD to quantify the hydrogen bond dynamics, end-to-end distance, and radii of gyration with changes in side group functionality, concentration, and temperature. We discerned trends for the physical behavior of polyesters with change in nature and ratio of the side groups. We also observed functional assembly for dissimilar polyesters, and correlated the assembly to the affinity of side groups. The trends in physical behavior and dissimilar assembly can be mined for iterative design towards programmatic assembly of the modular multifunctional polyesters under study.

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