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Optimization of Polymer Surfaces for Specific Targeting[1] ELENA DORMIDONTOVA, MATTHEW HAGY, SHIHU WANG, Department of Macromolecular Science and Engineering, Case Western Reserve University — Using Monte Carlo simulations we studied reversible binding between a polymer layer functionalized by ligands and a receptor surface. By analyzing distance-dependent profiles for the average number of ligands bound to receptors, the total free energy of polymer layer-cell surface interaction and the interaction force the influence of different design parameters of a polymer layer on the affinity and specificity of binding were investigated. We show that planar polymer layers with a smaller chain length and grafting density, larger degree of functionalization, and larger absolute binding energy exhibit higher affinity to the cell surfaces with a large density of mobile receptors. A high binding specificity can be achieved by the polymer layers with intermediate ligand-receptor binding energies or an intermediate number of ligands, as a larger binding energy or number of ligands lacks specificity while a smaller binding energy or number of ligands provides inadequate affinity. As a result, the optimal design of the polymer layers can be achieved by using several different strategies, which will be discussed.

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