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Tethered Ligand-Receptor Binding in Confined Environments G. LONGO, Purdue University, I. SZLEIFER, Purdue University — The binding of small proteins with ligands that are attached to polymers tethered to a surface is studied using a molecular theory. The effects of changing the intrinsic binding equilibrium constant, the polymer surface coverage, the polymer molecular weight, and protein size are studied. The results are compared with the case where the ligands are directly attached to the surface without a polymer acting as a spacer. Within biological range of binding constants the protein adsorption is enhanced by the presence of the polymer spacers. There is always an optimal surface coverage for which ligand-receptor binding is a maximum. This maximum increases as the binding energy or the polymer molecular weight increases. The presence of the maximum is due to the ability of the polymer bound proteins to form a thick layer by dispersing the ligand in space to optimize binding and minimize lateral repulsions. The binding of proteins is reduced as the size of the protein increases. The orientation of bound proteins can be manipulated by proper choice of the grafted layer conditions. A surface modified with a mixture of long ligand-conjugated polymers in low surface density and short polymers in high surface coverage will present optimal binding properties at the same time as nonspecific adsorption of proteins onto the surface is suppressed. The results of the theoretical calculations can be used in the design of experimental systems, providing the kind of polymer and the surface coverage required to optimize ligand-receptor binding.

Igal Szleifer
Purdue University

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