

Electrostatically-controlled protein adsorption onto lipid bilayer: Modeling adsorbate aggregation behavior

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Abstract

Using adsorption models based on scaled particle (SPT) and double layer theories the electrostatically-controlled protein adsorption onto membrane surface has been simulated for non-associating and self-associating ligands. The binding isotherms of monomeric and oligomeric protein species have been calculated over a range of variable parameters including lipid and protein concentrations, protein and membrane charges, pH and ionic strength. Adsorption behavior of monomers appeared to be the most sensitive to the changes in the protein aggregation state. The hallmarks of the protein oligomerization are identified. The practical guides for optimal design of binding experiments focused on obtaining proofs of protein self-association are suggested.

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