Computational Modeling and Simulations of Bioparticle Internalization Through Clathrin-mediated Endocytosis[1] HUA DENG, PRASHANTA DUTTA, JIN LIU, Washington State University — Clathrin-mediated endocytosis (CME) is one of the most important endocytic pathways for the internalization of bioparticles at lipid membrane of cells, which plays crucial roles in fundamental understanding of viral infections and interacellular/transcelluar targeted drug delivery. During CME, highly dynamic clathrin-coated pit (CCP), formed by the growth of ordered clathrin lattices, is the key scaffolding component that drives the deformation of plasma membrane. Experimental studies have shown that CCP alone can provide sufficient membrane curvature for facilitating membrane invagination. However, currently there is no computational model that could couple cargo receptor binding with membrane invagination process, nor simulations of the dynamic growing process of CCP. We develop a stochastic computational model for the clathrin-mediated endocytosis based on Metropolis Monte Carlo simulations. In our model, the energetic costs of bending membrane and CCP are linked with antigen-antibody interactions. The assembly of clathrin lattices is a dynamic process that correlates with antigen-antibody bond formation. This model helps study the membrane deformation and the effects of CCP during functionalized bioparticles internalization through CME.

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