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Investigation of the Key Parameters Impacting the Receptor Dependent Clathrin-mediated Endocytosis through Stochastic Modeling and Simulations[1] MD MUHTASIM BILLAH, HUA DENG, PRASHANTA DUTTA, JIN LIU, School of Mechanical and Materials Engineering, Washington State University, Pullman WA USA — Receptor dependent clathrin-mediated endocytosis (CME) is one of the most important endocytic pathways taken by bioparticles, such as viruses and drug carriers, to enter the cells. During CME, the ligand-receptor interactions, assembly/disassembly of clathrin-coated pit (CCP) and membrane deformation all act together to drive the internalization of bioparticles. Study of CME through experiments is significantly challenging because of the number of parameters impacting this complex biological process. In this work, we develop a stochastic computational model for the CME based on the Metropolis Monte Carlo simulations. After validation, we implement the model to systematically investigate effects of a wide range of biochemical and geometrical parameters on the overall internalization efficiency of particles. Specifically, results from our simulations demonstrate that the particle size and shape play critical roles during internalization. In addition, the ligand-receptor parameters, such as the receptor flexural rigidity/size and ligand-receptor reaction cutoff/energy, also significantly impact the internalization efficiency. Our model and simulations yield critical insights into CME and may provide guidelines for intra/transcellular drug delivery design.

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