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Abstract

Most therapeutic agents suffer from poor solubility, rapid clearance from the blood stream, a lack of targeting, and often poor translocation ability across cell membranes. Drug/gene delivery systems (DDSs) are capable of overcoming some of these barriers to enhance delivery of drugs to their right place of action, e.g. inside cancer cells. In this review, we focus on nanoparticles as DDSs. Complementary experimental and computational studies have enhanced our understanding of the mechanism of action of nanocarriers and their underlying interactions with drugs, biomembranes and other biological molecules. We review key biophysical aspects of DDSs and discuss how computer modeling can assist in rational design of DDSs with improved and optimized properties. We summarize commonly used experimental techniques for the study of DDSs. Then we review computational studies for several major categories of nanocarriers, including dendrimers and dendrons, polymer-, peptide-, nucleic acid-, lipid-, and carbon-based DDSs, and gold nanoparticles.