

# **Nanoparticle drug vectors in a bloodstream, theoretical study of competition between carbon nanotubes and testosterone for interactions with serum albumin**

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Recent advances in nanotechnologies have led to a wide use of nanoparticles in biomedical applications. In some cases, interaction of nanoscale objects with biomolecules such as proteins could lead to hazardous consequences like abnormal conformational changes or unusual cooperative effects such as self-assembling of macromolecules onto nanoparticles serving as a template (the so-called “protein corona”). It is obvious that better understanding of the molecular mechanisms of nano-bio interactions is crucial for further advances in all nanotechnological applications. In this work, molecular dynamics simulations are used to study the affinity of testosterone molecules and single-walled carbon nanotubes to human serum albumin (HSA). We find that testosterone binds weakly to the protein but in numerous sites. At least, 8 binding sites were elucidated with associated energies ranging [1-5] kcal/mol. By contrast, single-walled nanotubes bind strongly to HSA in a non-specific manner. Binding energies ranging between 10 and 30 kcal/mol were found. As a consequence, the secondary structure of the protein is almost lost and its tertiary structure is strongly affected. Finally, the competition between steroid molecule and the carbon nanoparticles is investigated. The strong modification of the protein structure induced by the carbon nanotubes prevents testosterone molecule to bind to HSA, these ones having a stronger affinity to the nanotubes than for HSA. These results show that the carbon nanotubes significantly might alter the pharmacodynamics profiles molecules like steroids or drugs that bind weakly to HSA protein.

**Keywords:** Human Serine Albumin; Carbon Nanotubes; Testosterone; Molecular Dynamics;