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Binding dynamics and conformational stability of graphene-based nanomaterials with Mutant LOX-1: Insights from molecular docking and dynamics simulations in atherosclerosis

Abstract

Oxidized low-density lipoprotein (oxLDL) is a critical factor in endothelial dysfunction and serves as an important biomarker for oxidative stress. Recent research has focused on lectin-like oxidized low-density lipoprotein receptor-1 (LOX-1), a receptor for oxLDL that plays a significant role in atherosclerosis progression. Mutant LOX-1 may show changes in its binding affinity for oxLDL, potentially leading to variations in oxLDL uptake and foam cell formation. Our previous investigation into graphene-based nanomaterials and their interactions with atherosclerosis-related proteins, including LOX-1, provided important insights into their binding characteristics. In this study, we delve deeper into the binding dynamics between graphene-based nanomaterials and mutant LOX-1, aiming to clarify their implications for atherosclerotic development. Using molecular docking techniques with AutodockVina and active site predictions from P2Rank, we evaluated the binding affinities of graphene, graphene oxide (GO), and reduced graphene oxide (rGO) to mutant LOX-1. Notably, all docking scores were below -5 kcal/mol, indicating strong interactions with the receptor. To investigate the dynamics of these interactions further, we performed molecular dynamics (MD) simulations using the CHARMM force field. Our simulations revealed significant conformational changes within the first 100 ns, particularly in the mutant LOX-1 and GO complex, which suggested improved binding stability. These results enhance our understanding of how graphene-based nanomaterials interact with mutant forms of LOX-1, offering potential avenues for targeted therapies in atherosclerosis management related to LOX-1 dysregulation.

Keywords

Graphene; Graphene oxide; Molecular docking; Molecular dynamics simulation; Mutant lectin-like oxidized low-density lipoprotein receptor-1; Oxidized low-density lipoprotein; Reduced graphene oxide