Interaction of human immune-deficiency virus (HIV) aspartic protease with spherical gold nanoparticles: Computer simulations.

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The interaction of gold nanoparticles (AuNP) with human immune-deficiency virus aspartic protease (HIVPR) is modelled using a regime of molecular dynamics simulations. The simulations of the 'docking', first as a rigid-body complex, and eventually through flexible-fit analysis, creates 36 different complexes from four initial orientations of the nanoparticle strategically positioned around the surface of the enzyme. The structural deviations of the enzymes from the initial x-ray crystal structure during each docking simulation are assessed by comparative analysis of secondary structural elements, root mean square deviations (RMSD), B-factors, interactive bonding energies, dihedral angles, radius of gyration (Rg), circular dichroism (CD), volume occupied by Cα, electrostatic potentials, solvation energies and hydrophobicities. Normalisation of the data narrows the selection from the initial 36 to one 'final' probable structure. It is concluded that, after computer simulations on each of the 36 initial complexes incorporating the 12 different biophysical techniques, the top five complexes are the same no matter which technique is explored. The significance of the present work is an expansion of an earlier study on the molecular dynamic simulation for the interaction of HIVPR with silver nanoparticles. This work is supported by experimental evidence since the initial 'orientation' of the AgNP with the enzyme is the same as the 'final' AuNP-HIVPR complex generated in the present study. The findings will provide insight into the forces of the binding of the HIVPR to AuNP. It is anticipated that the protocol developed in this study will act as a standard process for the interaction of any nanoparticle with any biomedical target.

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