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Docking of HIV aspartic protease to gold nanoparticles: Molecular dynamics simulations

Statement of the Problem: There is an increasing need for the development of new drug protocols against human immunodeficiency virus (HIV) and HIV protease (HIVPR) is identified as a promising biomedical target in this regard.

Methodology: The interaction of gold nanoparticles (AuNP) with HIVPR is modelled using a molecular dynamics simulation computer programme (Colores) from the Situs suite package.

Findings: The simulation of the 'docking', first as a rigid-body docked 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 [Fig A]. The rigid-body docked complex is conformationally flexible to accommodate the AuNP that orientates itself within the 'docking' site until a more stable structure is formed at convergence. Normalization of the data, for these AuNP-HIVPR complexes, is obtained from changes to interactive binding energy profiles, RMSD, B-factors, dihedral angles [ϕ , $\Delta\phi$; ψ , $\Delta\psi$; χ , $\Delta\chi$], size, volume occupied by $C\alpha$ [$\Delta V_{C\alpha}$], secondary structural elements (α -helix, β -strands, random coil), number of contact residues, their hydrophobicities and surface electrostatic potentials.

Conclusion & Significance: From a molecular dynamic simulation perspective it is possible to provide insights into the 'best' most probable AuNP-HIVPR complex formed no matter which biophysical technique is monitored.

Biography

Chris Whiteley is an Emeritus Professor of Biochemistry at Rhodes University, Grahamstown, South Africa and distinguished Research Professor at National Taiwan University Science & Technology, Visiting International Professor in Enzymology at School of Bioscience & BioEngineering of South China University Technology, Guangzhou, PRC. He served as Visiting Research Scientist at the Department of Chemical Engineering, National Taiwan University, Taipei, Taiwan in 2004 and as Visiting Professor of Biochemistry at Institute of Biomedical Technology, Veterans General Hospital, Yang Ming University, Taipei, Taiwan. He also worked as Visiting Professor of Enzymology & Organic Synthesis at Oregon State University, Corvallis, Oregon, USA and Visiting Professor of Organic Synthesis at University British Columbia, Vancouver, Canada. He is the Executive Member of Royal Chemical Society (London), MRSC (C. Chem), South African Chemical Institute (SACI). He has published 6 chapters in books and has 110 peer-reviewed papers on Biomedical Enzymology and Nanomaterials.

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