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In silico analytico-mathematical interpretation of biomacro-molecular assemblies for biomedical applications: Quantification of energy surfaces and molecular attributes using atomistic simulations

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Static-lattice atomistic simulations, in vacuum and solvent phase, have been used for the first time to quantify the *in silico* performance profile of various drug delivery devices and tissue engineering scaffolds. To date, we have successfully demonstrated the role of molecular mechanics energy relationships (MMER) towards the interpretation and understanding of the mechanisms that control the formation, fabrication, selection, design, complexation, interaction, sterospecificity, and preference of various biomaterial systems for biomedical applications. We hereby present a very basic yet effective computational algorithm employing HyperChem™ 8.0.8 and ChemBio3D Ultra 11.0 programs, MM+ and Amber 3 force fields and Polak-Ribiere conjugate gradient. The representing examples that will be discussed during the presentation involve the molecular tectonics of polyelectrolyte complexes; the catalytic action of enzymes, pectinase and glucosidase on pectin and chitosan, respectively; the crosslinked-polymer morphologies; the protein-polysaccharide complexes; the enzyme-substrate complexes; the miscibility and properties of specific polymer/plasticizer and polymer/mucopeptide complexes; the effect of varying the plasticizer and crosslinking ion concentration on Young's modulus and ultimate strain of the fibers; the justification of using a definite combination of polymers to meet the requirements of a "drug delivery system with desired release profile"; the degree of esterification and the addition of Ca^{2+} resulting in the formation of a mucin-pectin intermacromolecular network; the conformational profiles of the possible interactions involving polyamide-salts complexes; the possible mechanism of zero-order release from respective layers of a multi-layered system; the chelation energetics of EDTA with Cu(II)/Zn(II)-Amyloid-β-protein; and the nanoformation of the solvation properties of the emulsified polymers.

Biography

Pradeep Kumar is a Lecturer of Pharmaceutics at Department of Pharmacy and Pharmacology, University of the Witwatersrand, South Africa, and a SARChI doctoral research candidate at Wits Advanced Drug Delivery Platform. He is working on biomaterial strategies for spinal cord injury interventions along with computational simulations inherent to synthesis and performance of polymer engineered devices. He is a recipient of Elsevier's ISDN 2012 Scholarship, WCNR 2012 Executive Committee award, Elsevier's NanoToday 2011 award, WITS Postgraduate Merit award (2011/12), and WITS Local Merit scholarship (2011/12). He has more than 50 high-impact peer-reviewed publications to his credit that include editorials, book chapters, research papers, and expert reviews.

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The nanocomposite laminate structure in fish scales from *Arapaima Gigas*

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Scales are the skeletal elements that cover and protect the skin of fish. They are laminated composites structures formed by mineralized collagen fibers in a plywood pattern of layers. These fibers are co-aligned within each individual layer that alternately rotates at angles of around 90º. The scales are reinforced with nano-crystals of hydroxyapatite. *Arapaima Gigas* is a fish from the Amazonian region with a rather prehistorical aspect which is known for its large tough scales.

The aim of this paper is to study the underlying structure of these scales using a materials science approach, particularly trying to understand the scales mechanical behavior in the wet state. The structure and composition of the *Arapaima Gigas* scales were assessed by means of X-ray diffraction (XRD) and Fourier transform infrared spectroscopy (FTIR). Morphology studies and fracture analysis of the native scales were carried out using transmission electron microscopy (TEM), light optical microscopy (LOM) and scanning electron microscopy (SEM). The mechanical behavior of dry and wet scales was assessed by tensile tests. The effect of water content on the thermal transitions of scales is also discussed.

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