APPLICATION OF VIRTUAL SCREENING TO PREDICTION OF BIOLOGICAL TARGETS FOR FULLERENE DERIVATIVES

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Abstract: Fullerene and its derivatives are one of the leading nanomaterials in nanomedicine for pharmaceuticals application. The aim of this study is to find potential biological targets for fullerene derivatives. Using computational chemistry approaches 169 fullerene derivatives have been modeled and then docked against a series of proteins selected from potential drug target database (PDTD). PatchDock package has been utilized to assess millions of docking runs, followed by Schrodinger Suite analysis of selected protein-ligand systems. In preliminary runs 3 ligands (fullerene derivatives) have been found as very selective for 3 proteins. These ligands may act as a Potassium ion channel blocker, Cholesterol lowering drug and Enzyme inhibitor. The details of the present findings will be discussed. The study can assist to list potentially active and/or toxic fullerene derivative that could bind to selected proteins. A database of potential biological targets for fullerene nanoparticles will be generated. The database of pairs (protein - fullerene derivative) with calculated binding affinities will be also created and made available for use by academic and pharmaceutical industry scientists to assist in pharmacological activity or toxicity estimation and drug delivery agents’ development.

Keywords: Nanomedicine, Fullerene, Ligand-Protein, Docking, Drug.