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In silico Modelling and Docking Studies of Camptothecin Derivatives

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Abstract: The availability of experimental (X-ray, NMR) structures is very less. To overcome this problem the structures have been determined theoretically, especially those determined by homology modeling techniques. Protein-Ligand docking is increasingly used in Drug Discovery. The present study explains computational methods to design Polio virus related protein 2, alpha isoform of human enzyme using the crystal structure available from Protein Data Bank (PDB ID: 4FMK). Model was generated by using Modeler9.16. After designing the model, functional effect was confirmed in terms of protein ligand binding by molecular docking using Autodock4.2. The docking investigation of modelled Q9UEI6 protein with camptothecin derivatives using Autodock4.2 software was performed. Out of 30 compounds nine compounds are involved in interacting with ARG72, SER77 and THR86 with good binding energy. Rest of the compounds shows two interactions with good binding energy. More importantly, it provides insight into understanding and properly interpreting the data produced by these methods.
Key words: Homology modeling, Camptothecin derivatives, Molecular Docking.

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