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An In-silico Pharmacophore-Based Anti-Viral Drug Development for Hepatitis C Virus

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Abstract : Millions of people worldwide suffer from Hepatitis C, one of the fatal diseases. Interferon (IFN) and ribavirin are the available treatments for patients with Hepatitis C, but these treatments have their own side-effects. Our research focused on the development of an orally taken small molecule drug targeting the proteins in Hepatitis C Virus (HCV), which has lesser side effects. Our current study aims to the Pharmacophore based drug development of a specific small molecule anti-viral drug for Hepatitis C Virus (HCV). Drug designing using lab experimentation is not only costly but also it takes a lot of time to conduct such experimentation. Instead in this in silico study, we have used computer-aided techniques to propose a Pharmacophore-based anti-viral drug specific for the protein domains of the polyprotein present in the Hepatitis C Virus. This study has used homology modeling and ab initio modeling for protein 3D structure generation followed by pocket identification in the proteins. Drug-able ligands for the pockets were designed using de novo drug design method. For ligand design, pocket geometry is taken into account. Out of several generated ligands, a new Pharmacophore is proposed, specific for each of the protein domains of HCV.

Keywords : pharmacophore-based drug design, anti-viral drug, in-silico drug design, Hepatitis C virus (HCV)
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