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Selective Covalent Inhibition as a New Strategy in Hepatitis C Virus Therapy: A Detour from Conventional Approaches

Selective covalent inhibition of Hepatitis C virus (HCV) is a highly neglected domain in literature, intensified by the evident lack of efficient structure-based drug design protocols. Herein, we provide an atomistic insight into a novel selective approach to potentially inhibit HCV polymerase. Covalent molecular dynamic analyses revealed the inhibitory mechanism of compound 47 on the polymerase. Inhibitor binding induced unusual internal movements resulting in the disruption of normal physiological interdomain interactions. Compound 47 elicits reorganization of key protein elements required for RNA transcription. The outcomes generated in this study suggest that selective covalent inhibition is promising and will open new avenues for the design of novel selective potent inhibitors against HCV as well as other viral families.

Presenter Biography

My name is Letitia Shunmugam. I obtained a BSc Biomedical Science in 2013 and graduated with Honours and Masters in Medical Biochemistry and Chemical Pathology at the University of KwaZulu-Natal. I am currently a second year PhD student in Prof Mahmoud E. S. Soliman's Molecular Bio-computation and Drug Design Laboratory at the Department of Pharmaceutical Sciences. My current research focuses on the inhibition of Hepatitis C Virus through in silico studies.

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