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Docking guided QSAR study on a series of *N*-Acetamideindolecarboxylic acid derivatives acting as HCV NS 5B polymerase inhibitors

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Abstract

Recently, a series of *N*-acetamideindolecarboxylic acids were studied for their HCV NS5B polymerase inhibition activity. We report here a QSAR and docking study on them to investigate the physicochemical and structural properties of the molecules that govern their activity in order to rationalize the structural modification to have more potent drugs. A multiple regression analysis reveals a significant correlation of NS5B inhibition activity of compounds with their hydrophobicity, Kier's first order valence molecular connectivity index of a substituent and an indicator parameter, suggesting that the hydrophobicity and a particular substituent of the compounds containing atoms with low valence and high saturation will be conducive to the activity. Also the binding of compounds to Site 1 concluded that conformations of HCV NS5B polymerase could be an important regulatory step in RNA synthesis and can be further exploited by designing non-nucleoside inhibitors.

Biography:

Vaishali M. Patil is an assistant professor of pharmaceutical chemistry at Bharat Institute of Technology, Meerut. She has submitted her PhD at Birla Institute of Technology (Mesra), completed B Pharm from North Maharashtra University and M. Pharm from Uttar Pradesh Technical University. Mrs. Vaishali has some of reviews to her credit in highly esteemed journal Current Medicinal Chemistry, dozens of excellent original research publications in various internationally reputed journals and in addition to few chapters in Birkhauser Verlog, Basel published books. Her research interests are computer aided drug design, synthetic chemistry and development of antiviral agents.