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Virtual screening of natural compounds that can inhibit HCV

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Hepatitis C virus (HCV) is highly prevalent in Pakistan, and its infection can lead to chronic liver disease and hepatocellular carcinoma. The currently available treatment for treating HCV infection is not effective in all patients, has adverse side effects, and is not easily affordable. The aim of this study was to explore for the natural compounds that can inhibit the replication of Hepatitis C virus (HCV). Fluoroquinolones are the chemicals known as potent-active compounds that inhibit the replication of HCV genome by targeting its helicase protein NS3. Using 40 fluoroquinolones as reference molecules, a data set of 4000 natural products was screened that bore structural similarities with fluoroquinolone. From this data set, Random Forest classifier was used to predict active natural compounds that may have an inhibitory effect against HCV NS3 activity. This Random Forest classifier builds a set of decision trees by using a set of 0D, 1D, 2D, 3D and others, total 2080 molecular descriptors, of the two data sets i.e., the training and testing set. Compounds with RF score >0.5 are classified as an active compound against HCV. Using this approach, out of 4000 test molecules, 147 molecules were predicted to be active against HCV NS3 helicase. These predicted active compounds can be analyzed further using *in silico* and *in vitro* experimental models to discover an effective drug against HCV. The above-described approach is useful in discovering new, more portent and affordable drugs for treating HCV infection.

Biography

Saima Kashif has completed Master's in Biomedical Engineering from NED University of Engineering and Technology, Karachi, Pakistan. Currently, she is working as a Lecturer and Research Supervisor at Department of Biomedical Engineering, NED University of Engineering and Technology Karachi, Pakistan.

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