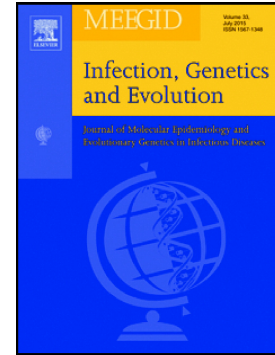


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Chemical system biology based molecular interactions to identify inhibitors against Q151M mutant of HIV-1 reverse transcriptase

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Abstract

The emergence of mutations leading to drug resistance is the main cause of therapeutic failure in the human HIV infection. Chemical system biology approach has drawn great attention to discover new antiretroviral hits with high efficacy and negligible toxicity, which can be used as a prerequisite for HIV drug resistance global action plan 2017-21. To discover potential hits, we docked 49 antiretroviral analogs (n=6,294) against HIV-1 reverse transcriptase Q151M mutant & its wild-type form and narrow down their number in three sequential modes of docking using Schrödinger suite. Later on, 80 ligands having better docking score than reference ligands (tenofovir and lamivudine) were screened for ADME, toxicity prediction, and binding energy estimation. Simultaneously, the area under the curve (AUC) was estimated using receiver operating characteristics (ROC) curve analysis to validate docking protocols. Finally, single point energy and molecular dynamics simulation approaches were performed for best two

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