Discovery of Novel Proteins Binding to HIV Reverse Transcriptase

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Abstract

HIV (human immunodeficiency virus) is a retrovirus that affects 38.4 million people across the globe. It targets and disrupts the immune system that helps the body fight infections and diseases. HIV uses reverse transcriptase (RT) to convert its RNA into viral DNA, a process called reverse transcription. Blocking reverse transcriptase and reverse transcription prevents HIV from replicating. For this reason, an algorithm software was used to prognosticate human proteins that can bind with different types of inhibitors of HIV reverse transcriptase. HIV Rev 1 (RT) was imputed into Python and MGL software tools to visualize, analyze molecular structures and predict protein intercalation properties. The results illustrated proteins such as ACTB, KIF14, Prostatic Acid Phosphatase/ACPP, Aminopeptidase B/RNPEP, VPS23 (TSG101), RPL37A, RPL27A, HSP90AB1, HSPA8, HSPB1, SH3GL1, CD53, SLC38A2, CBL, SLA2, DIP2 showed signs of binding to HIV Rev 1 at the allosteric site. Other proteins such as ACTN1, ACTN4, KIF23, RACGAP1, and VPS28 did not show signs of binding at the active nor allosteric site. Binding at the allosteric site or active may enhance RT activity, or it may inhibit it. Therefore, further testing in the lab will aid in the reasoning and efficacy behind the binding properties of these novel protein inhibitors, which can potentially lead towards the discovery of innovative therapeutic drugs and initiatives against HIV transmission and infection.