

De Nevo HIV-1 PPT Primer Repressor: Possibility for Molecular Immunity

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The Human Immunodeficiency Virus is a strain of retrovirus that, if left untreated in a human host, leads to the Auto-immune disease AIDS. HIV affects many components of the cellular immune system in order to create a dysfunctional immune system inside the host - rendering even mild infections dangerous to human life. Because of the nature of the prognosis, treating HIV has only lead to a chronic condition for the patient, dependent on daily medications (a situation that is not ideal). With the rise of accessible computing power and protein structure principles, protein design and structure prediction software is now available. Because of the availability to protein design software, and the relative ease to synthesize recombinant proteins on a fit for mass-consumption scale, protein design is now a new avenue for drug development; HIV is particularly vulnerable to this method due to the specific protein structure-PPT primer coupling during the critical step of Reverse Transcription. Using secondary structure first design, this project aims to develop a PPT primer repressor for HIV-1. The project further aims to analyze the potential effectiveness of the pseudo-competitive inhibitor in both affinity and in efficacy of folding into the correct conformation to initiate docking through an examination of the energy landscape using simulations, and docking server orientations.