Molecular Dynamics Study of the Inhibition of Monomeric HIV-1 Protease as Alternative to Overcome Drug Resistance by RNA Aptamers

Marzieh Ajamgard[1], Jaber jahanbin sardroodi[1], and Alireza Rastkar Ebrahimzadeh[1]

[1]Azarbaijan Shahid Madani University Faculty of Basic Sciences

May 5, 2020

Abstract

Here the interaction of three aptamers with HIV-1 protease has been investigated with the help of molecular dynamics simulations. These simulations lead to precise structural and energetic results. The sequencing of the considered aptamers is AP1 as the aptamer number 1: (CUUCAUUGUAACUUCUCAUAAUUUCCCGAGGCUUUUACUUUCGGGGUCCU), AP2 as the aptamer number 2: (CCGGGUCGUCCCCUACGGGGACUAAAGACUGUGUCCAACCGCCCUCGCCU) and AP3 as the aptamer number 3: (C, U, A, C, and C nucleotides of AP1 were replaced with A, G, G, A, and C to yield AP3). The results of molecular dynamics simulations show that aptamers 2 and 3 are good alternatives to interact with the protease enzyme and to control this enzyme, but in AP2 has somewhat improved the results. The results of MM-PBSA show that although aptamer three as a mutant aptamer has a good affinity with the protease enzyme compared to aptamer one and by impairing dimerization, it disrupts its structural stability and function. However, the results indicate that aptamer 2 is a better inhibitor because it causes a more severe conformational change in the structure of the enzyme.

Hosted file

`Proteins1.pdf` available at https://authorea.com/users/295766/articles/424632-molecular-dynamics-study-of-the-inhibition-of-monomeric-hiv-1-protease-as-alternative-to-overcome-drug-resistance-by-rna-aptamers