Supplemental material

An *in silico* molecular modeling approach of halolactone derivatives as potential inhibitors for human immunodeficiency virus type-1 reverse transcriptase enzyme

Ana Paula Lima da Costa[a], Fábio José Bonfim Cardoso[a], and Fábio Alberto de Molfetta[a]*

[a]Laboratório de Modelagem Molecular, Instituto de Ciências Exatas e Naturais, Universidade Federal do Pará, 60075-110, Belém, Pará, Brazil.

* Current Address: Instituto de Ciências Exatas e Naturais, Universidade Federal do Pará, CP 11101, 60075-110, Belém-PA, Brazil

* Corresponding author

E-mail: fabioam@ufpa.br

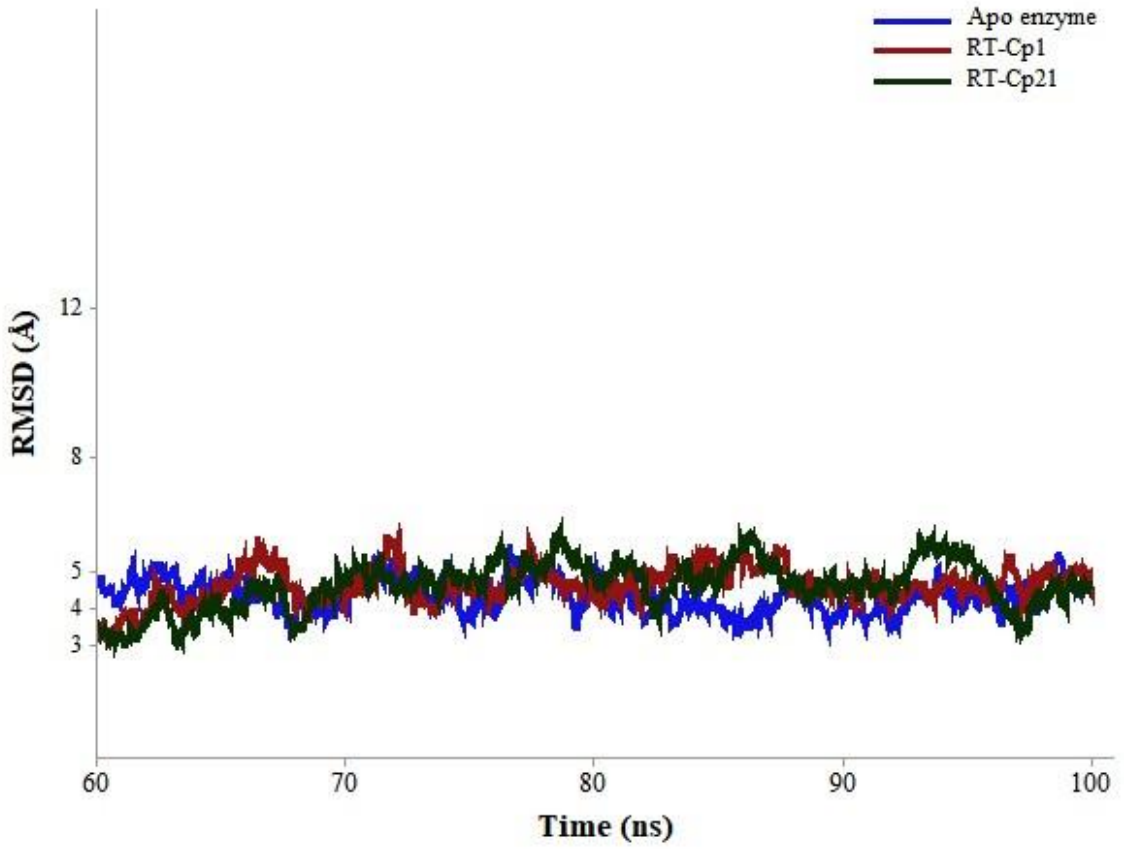
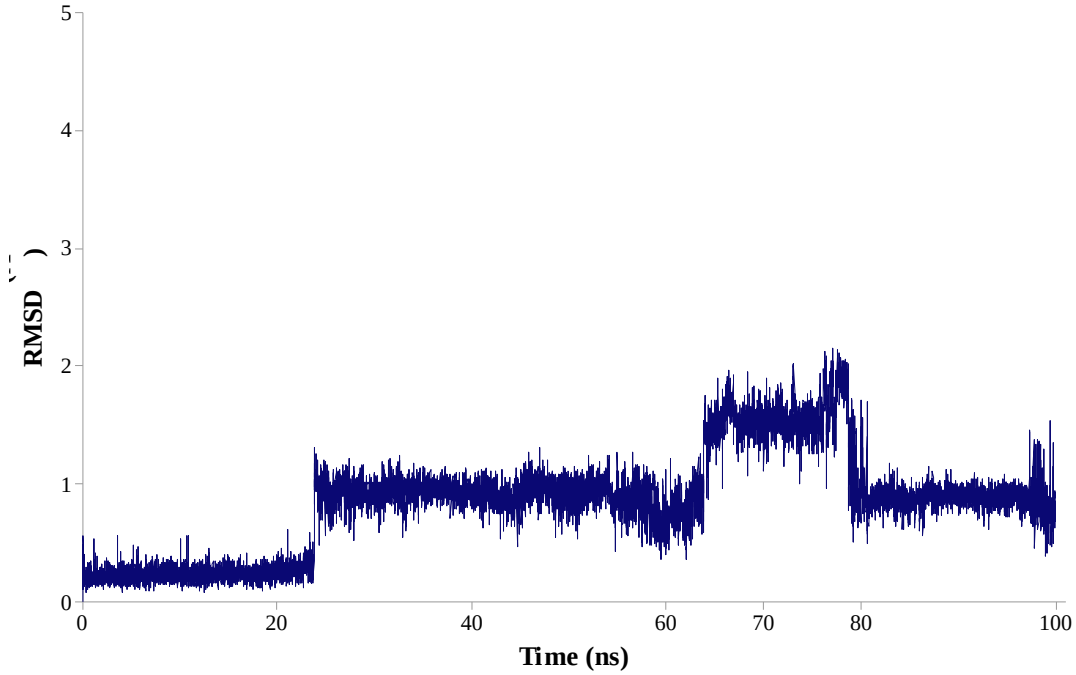
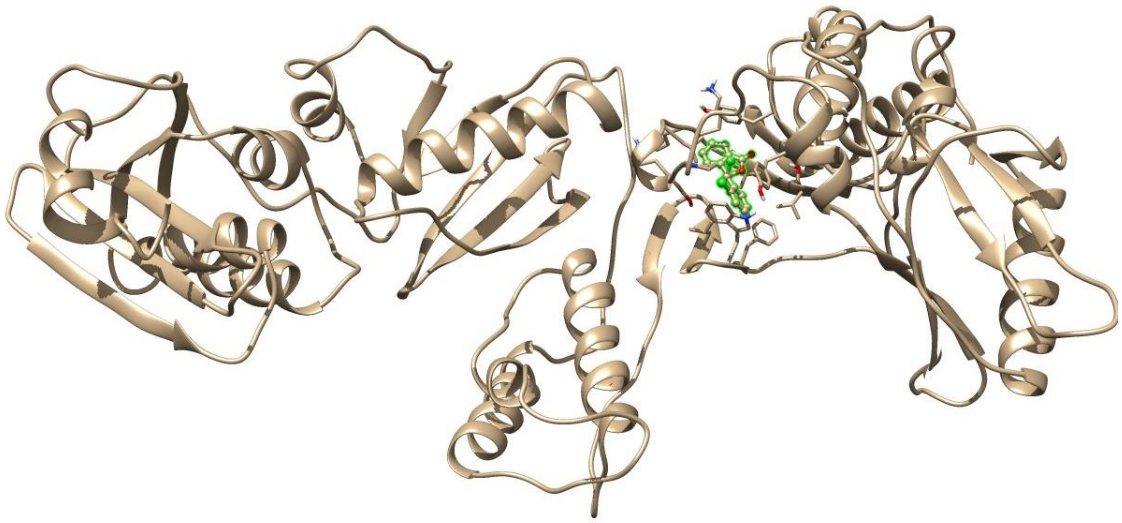


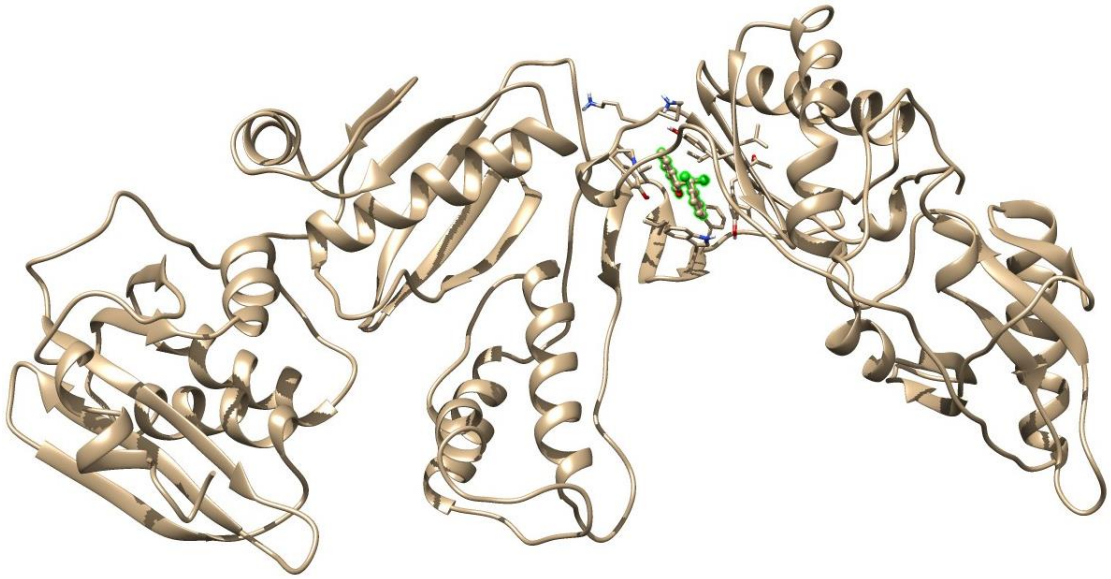
Figure S1. Graphical representation of the RMSD values (Å) in the last 40 ns of MD simulation time: *Apo* enzyme (blue line), RT-Cp1 (blue line) and RT-Cp21 (red line).



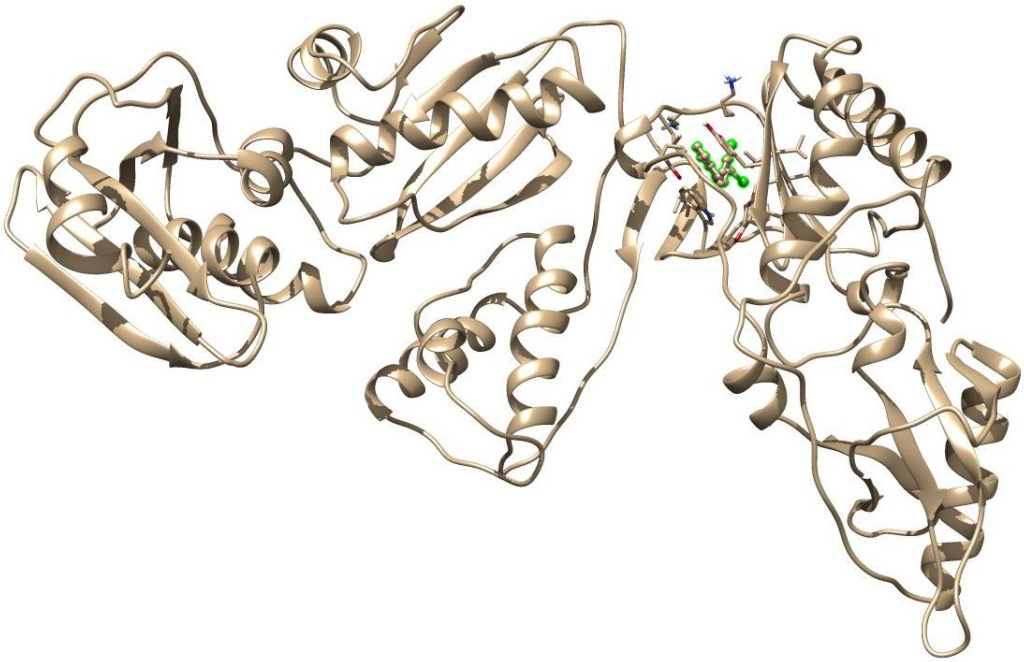
(A)



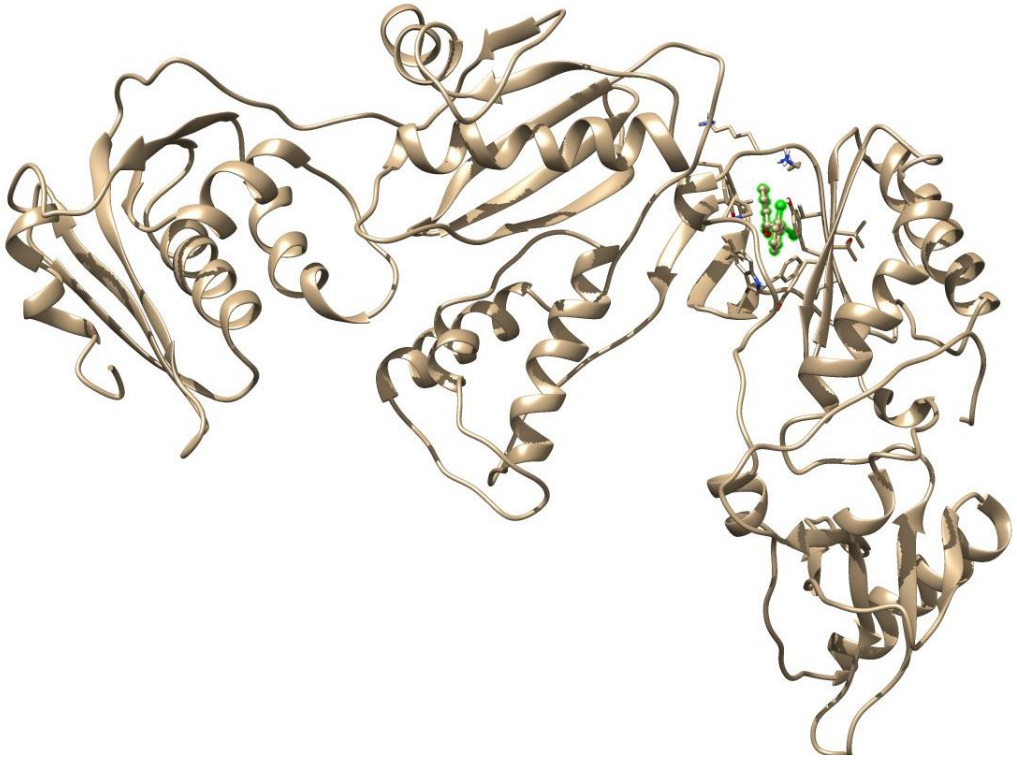
(B)



(C)



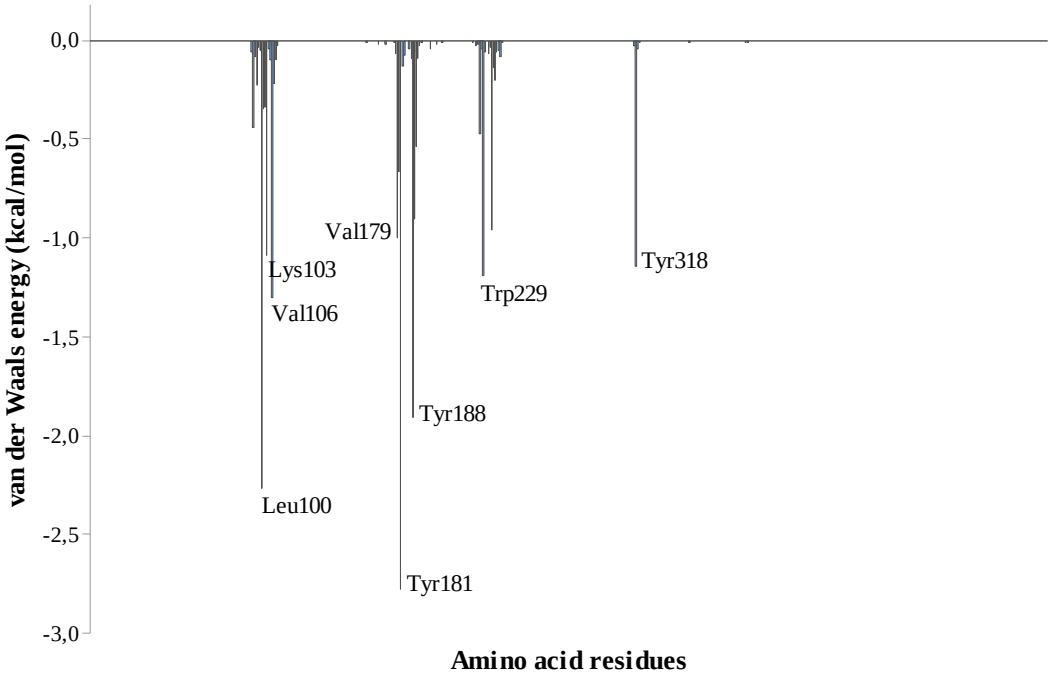
(D)



(E)

Figure S2. (**A**) RMSD plot as a function of the simulation time during 100 ns of MD simulations of CP1 (0.85 ± 0.43 Å) system (highlighted in green); (**B**) 20 ns of simulation; (**C**) 40 ns of simulation; (D) 70 ns of simulation; (**E**) 100 ns of simulation.

(A)



(B)

Figure S3. Per-residue decomposition analysis of the van der Waals interaction decomposition with the MMBGSA method. (**A**) RT-Cp1 and (**B**) RT-Cp21.