Figure S1: Ligand interaction diagrams of compound 287 throughout molecular dynamics simulations

Figure S2: Protein ligand interactions graph of compound 287 throughout the simulations.

Figure S3: Ligand interaction diagrams of compound 338 throughout molecular dynamics simulations

Figure S4: Protein ligand interactions graph of compound 338 throughout the simulations.

Figure S5: First MM/GBSA free energy analysis for the studied molecules at the binding pocket of HIV-1 PR throughout the 100 ns MD simulations. (MM/GBSA binding energy values in kcal/mol)

Figure S6: Second MM/GBSA free energy analysis for the studied molecules at the binding pocket of HIV-1 PR throughout the 100 ns MD simulations. (MM/GBSA binding energy values in kcal/mol)

Table S1: 2D structures, average MM/GBSA scores of selected 5 hits and FDA approved drug Amprenavir.

Mol_Number	2D Structure	**MM/GBSA (First MD) (kcal/mol)**	**MM/GBSA (Second MD) (kcal/mol)**
Mol-25		69.459±4.639	68.629±4.771
Mol-287		56.456±7.517	57.725±6.806
Mol-290		57.805±3.870	58.015±3.952
Mol-315		52.609±5.623	50.252±5.950
Mol-338		52.022±4.370	52.650±4.069
Amprenavir		78.642±4.787	79.026±4.637