Supplementary material

Molecular Dynamics and DFT Study on the structure and dynamics of N-Terminal Domain HIV-1 Capsid Inhibitors

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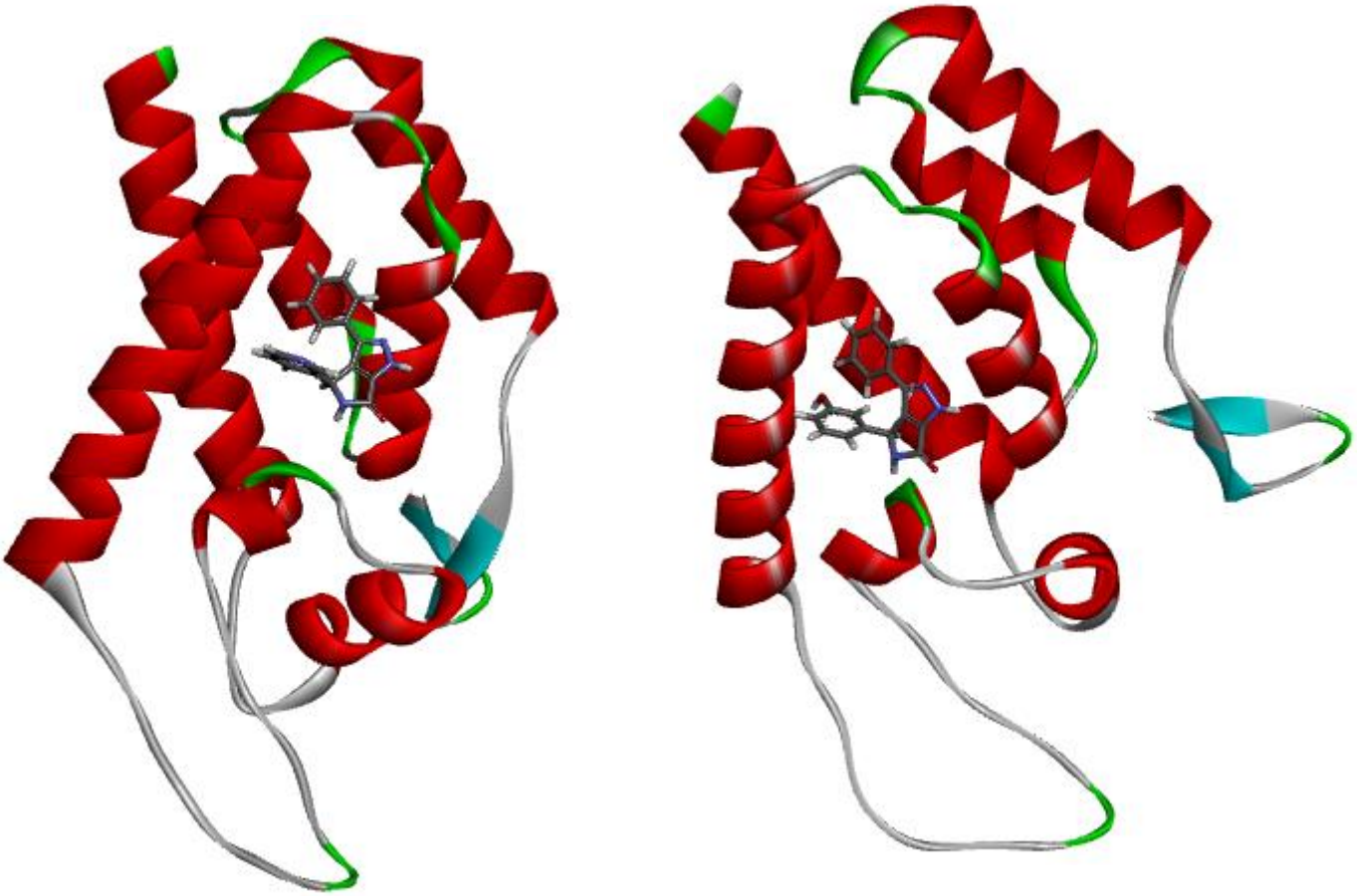
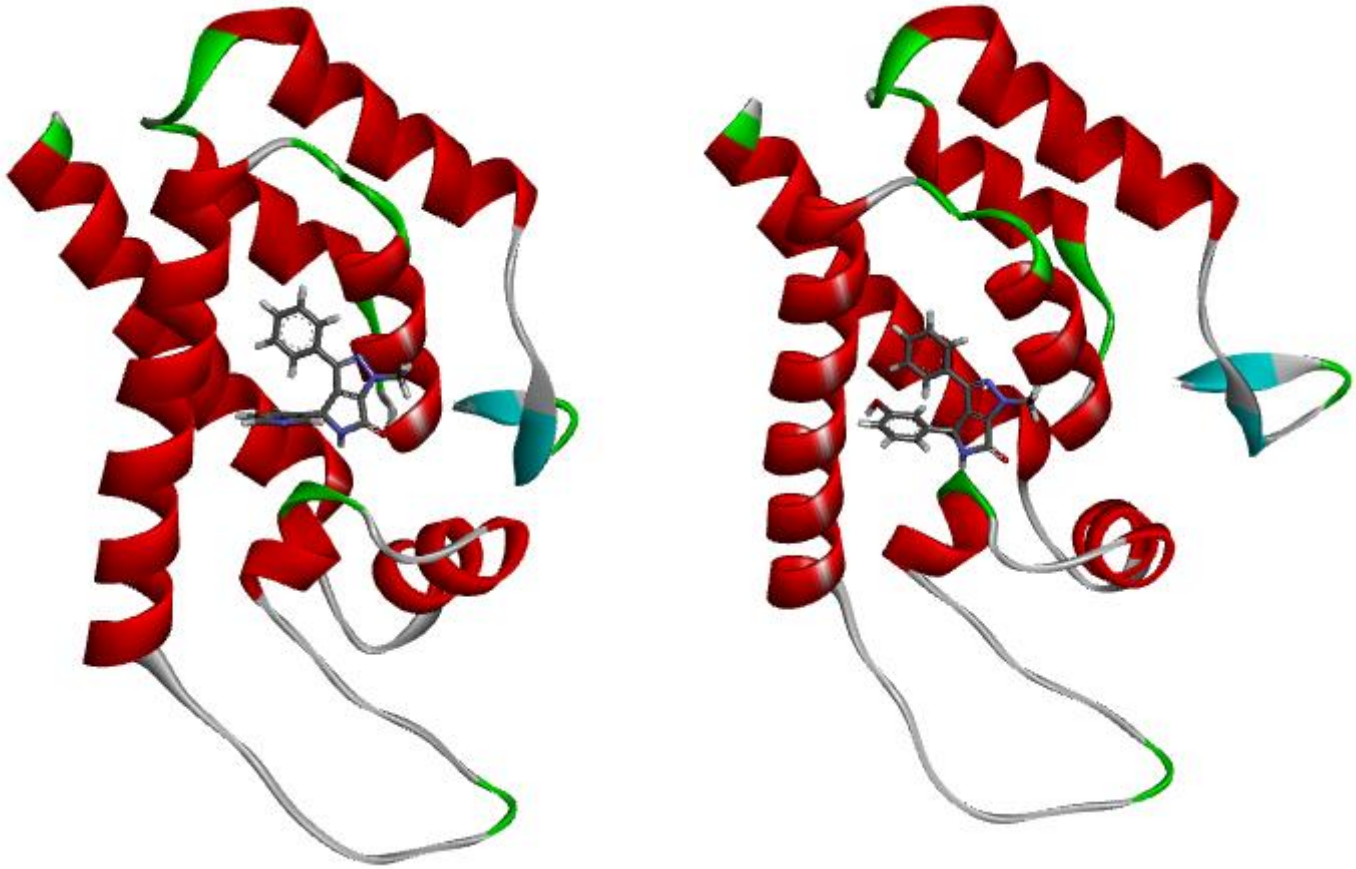


BI-1 BI-2



BI-1_N-methyl BI-2_N-methyl

Figure S1: The 3D minimized structures for BI-1, BI-2, B1-1_N-methyl and B1-2_N-methyl complexed with N-terminal HIV-1 capsid over the 60 ns MD simulations

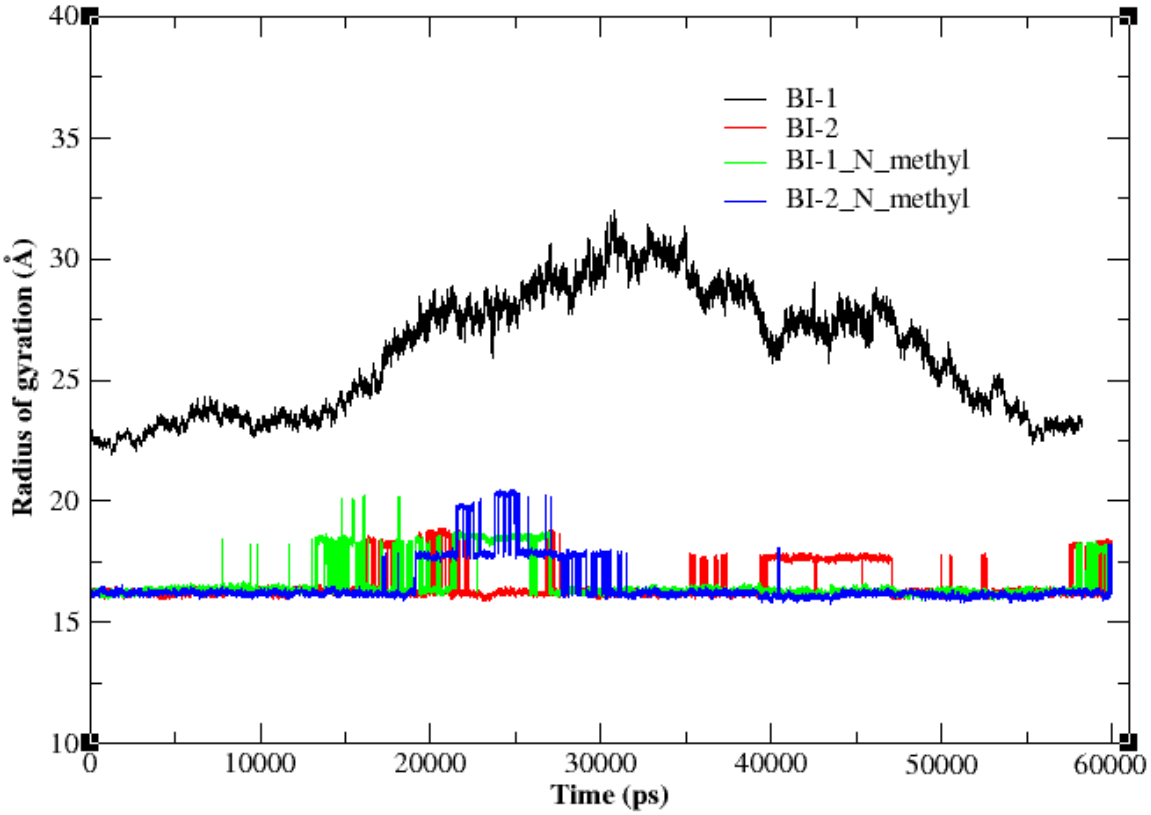


Figure S2. The plot of the radius of gyration (Rg) for BI-1 (black) and BI-2 (red) B1-1_N-methyl (green) B1-2_N-methyl (blue) complexed with N-terminal HIV-1 capsid over the last 60 ns MD simulations