Electronic Supplementary Material (ESI) for Integrative Biology.

Binding Free Energy Based Structural Dynamics Analysis of HIV-1 RT RNase H-Inhibitor Complexes †

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Fig. 1: Right: Binding mode of BHMP07 (green stick) in RNH compared to the X-ray crystal bound ligand (pink stick). The active and allosteric sites are indicated by yellow and green surface, respectively. Left: Overall topology of reverse transcriptase is shown and important structural domains are labeled.

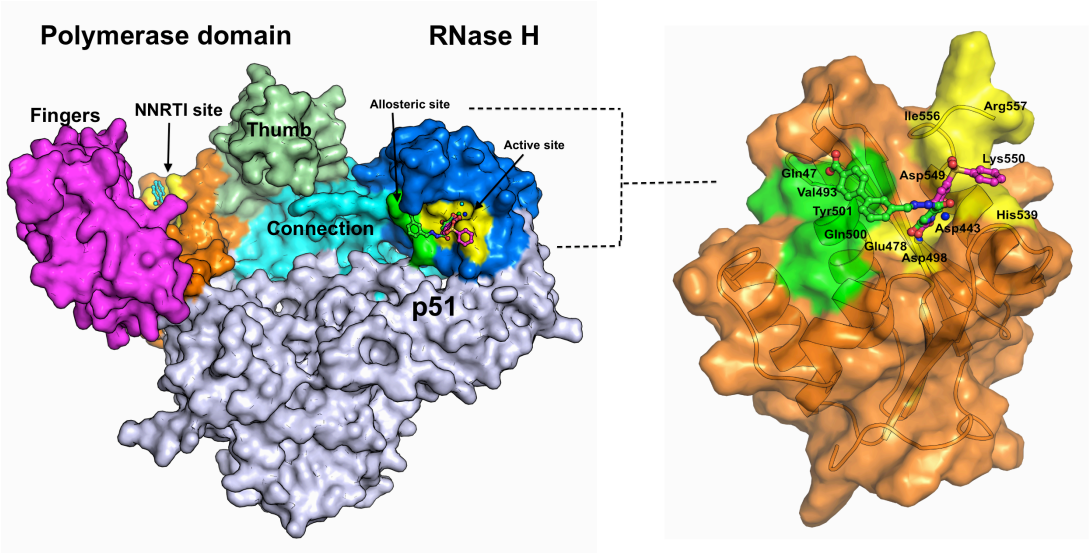

Fig. 2: Energy convergence check for protein-ligand complexes.

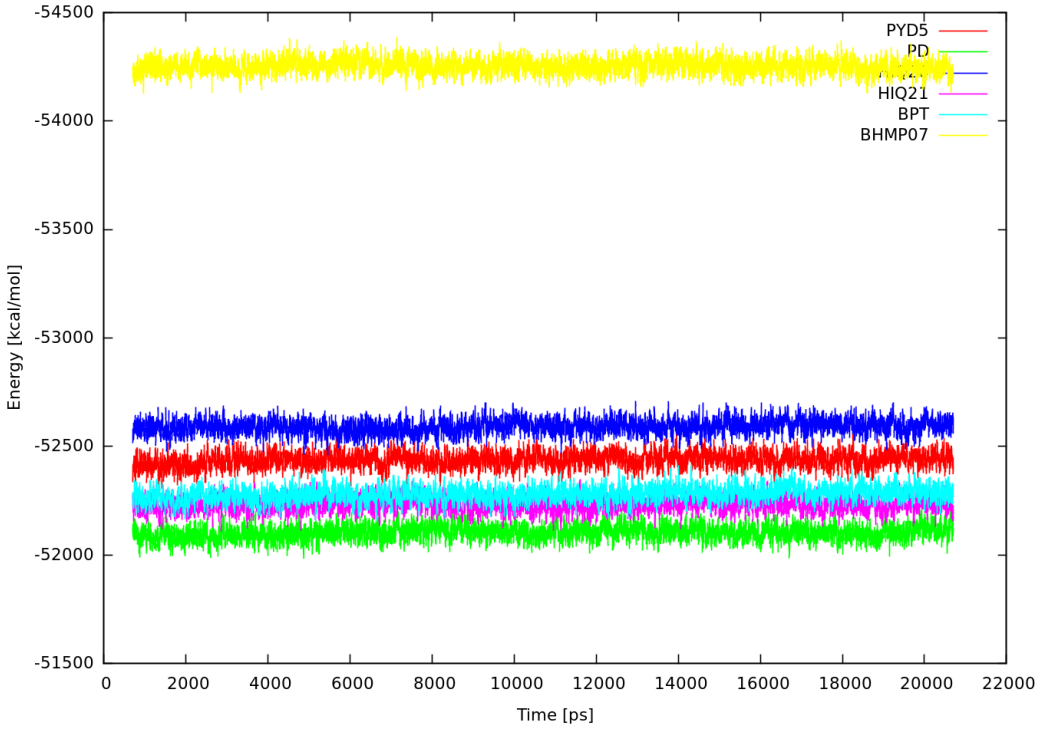

Fig. 3 RMSD of backbone heavy atoms relative to their initial structure.

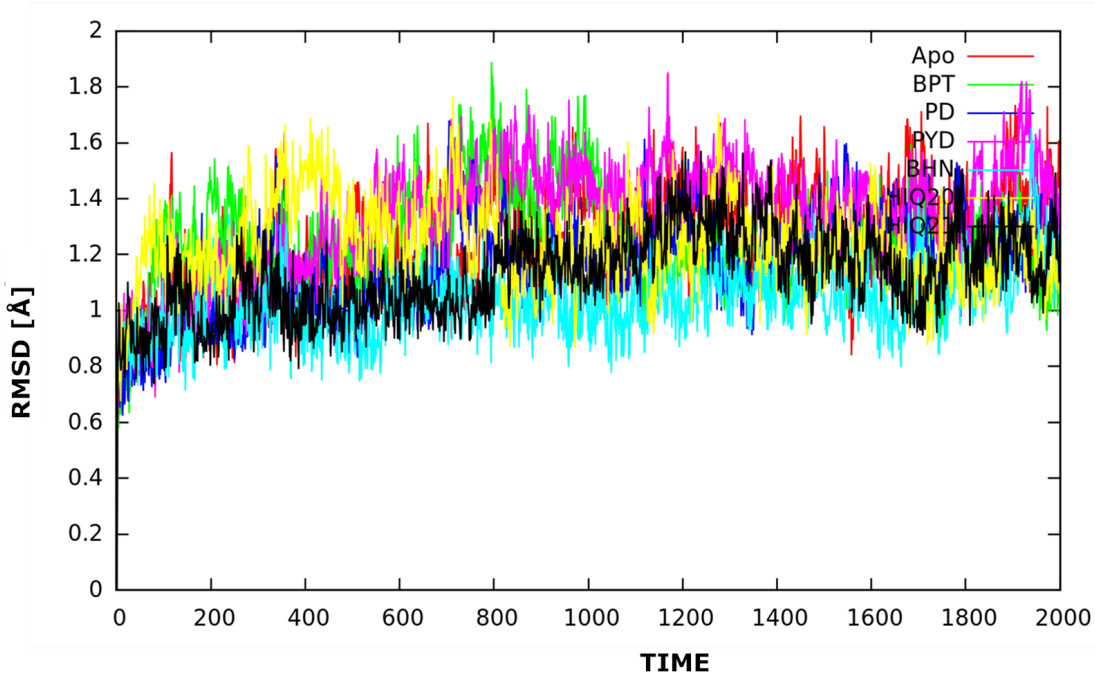

Fig. 4: Correlation between the observed activity (pIC50) and energy contribution of different components to overall binding affinity based on the MM-GB/SA model