Supplementary File

Compounds	Docking Score
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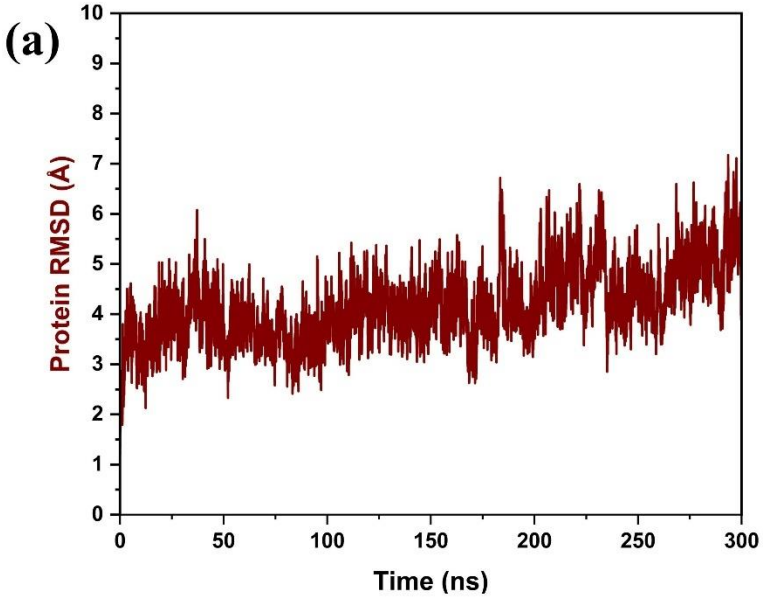
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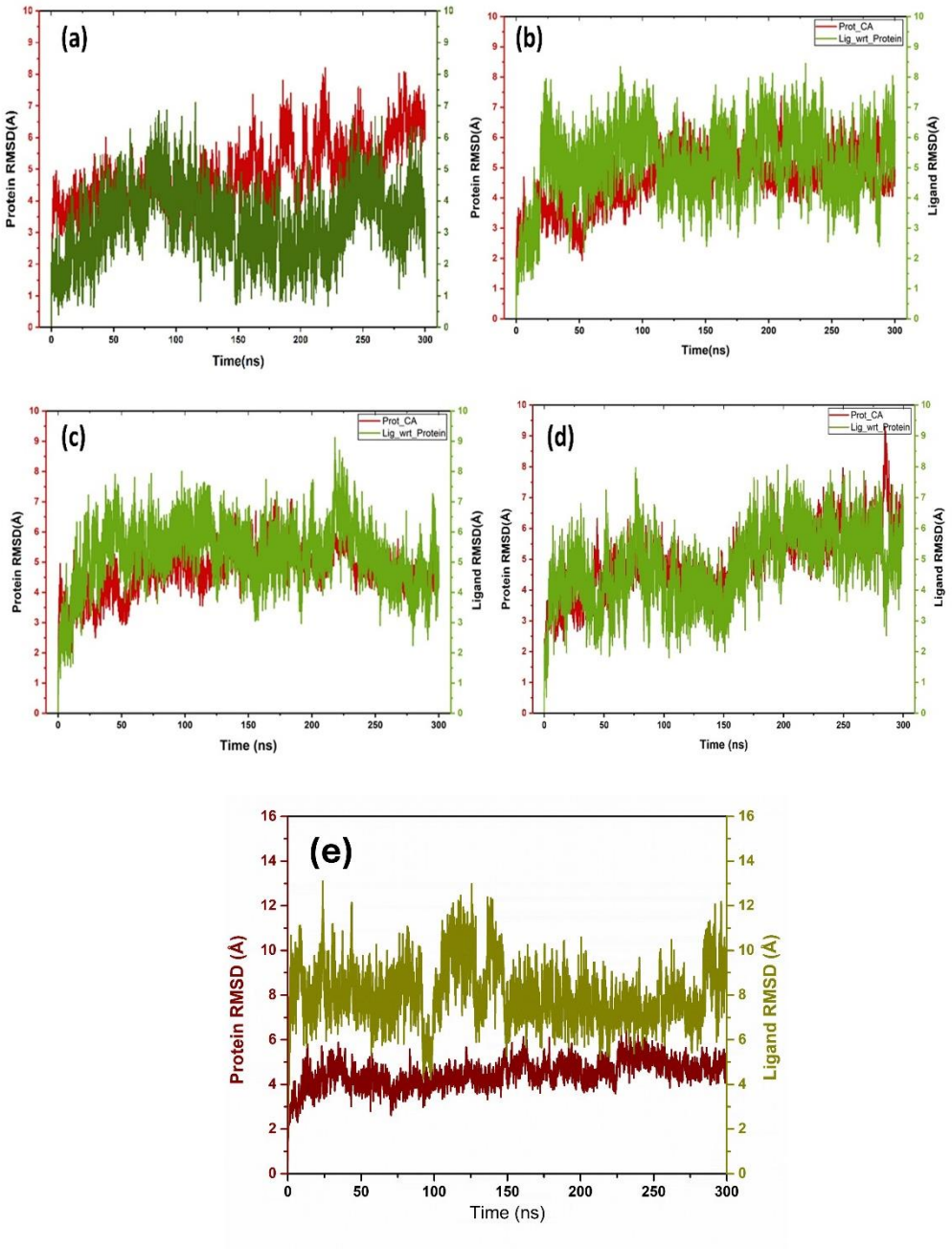
Supplementary Table S1. The list compounds along with docking score after virtual screening.

Name	Leverage	Leverage_AD	Distance_Cutoff_95th	Distance_AD	Final_Applicability_Domain
IMPHY007084	-64242362563	Inside AD	26.82	Inside AD	Inside AD
IMPHY012021	-7.08206E+11	Inside AD	26.82	Inside AD	Inside AD
IMPHY000687	3.53321E+11	Outside AD	26.82	Inside AD	Outside AD
Reference	-1.53152E+12	Inside AD	26.82	Inside AD	Inside AD
IMPHY004619	1.52687E+12	Outside AD	26.82	Inside AD	Outside AD

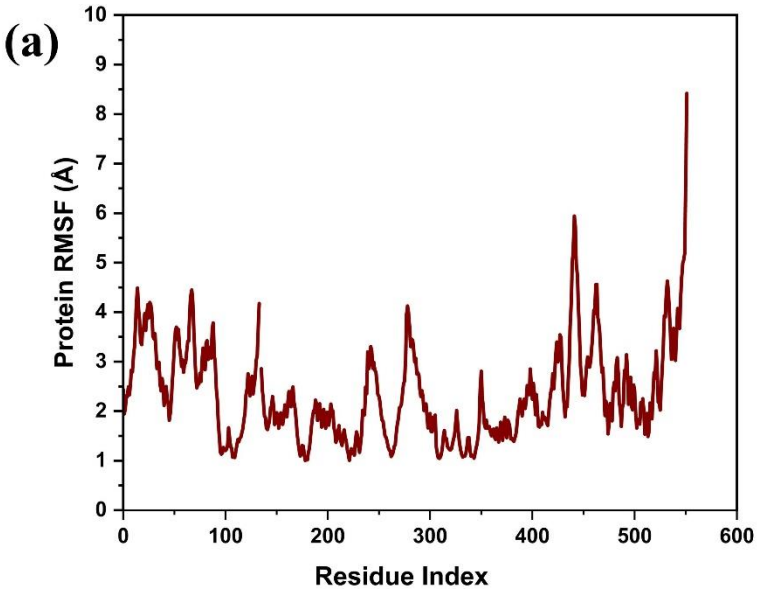
Supplementary Table S2. Leverage- and distance-based applicability domain (AD) analysis indicating the prediction reliability of the shortlisted phytochemicals and the reference inhibitor.



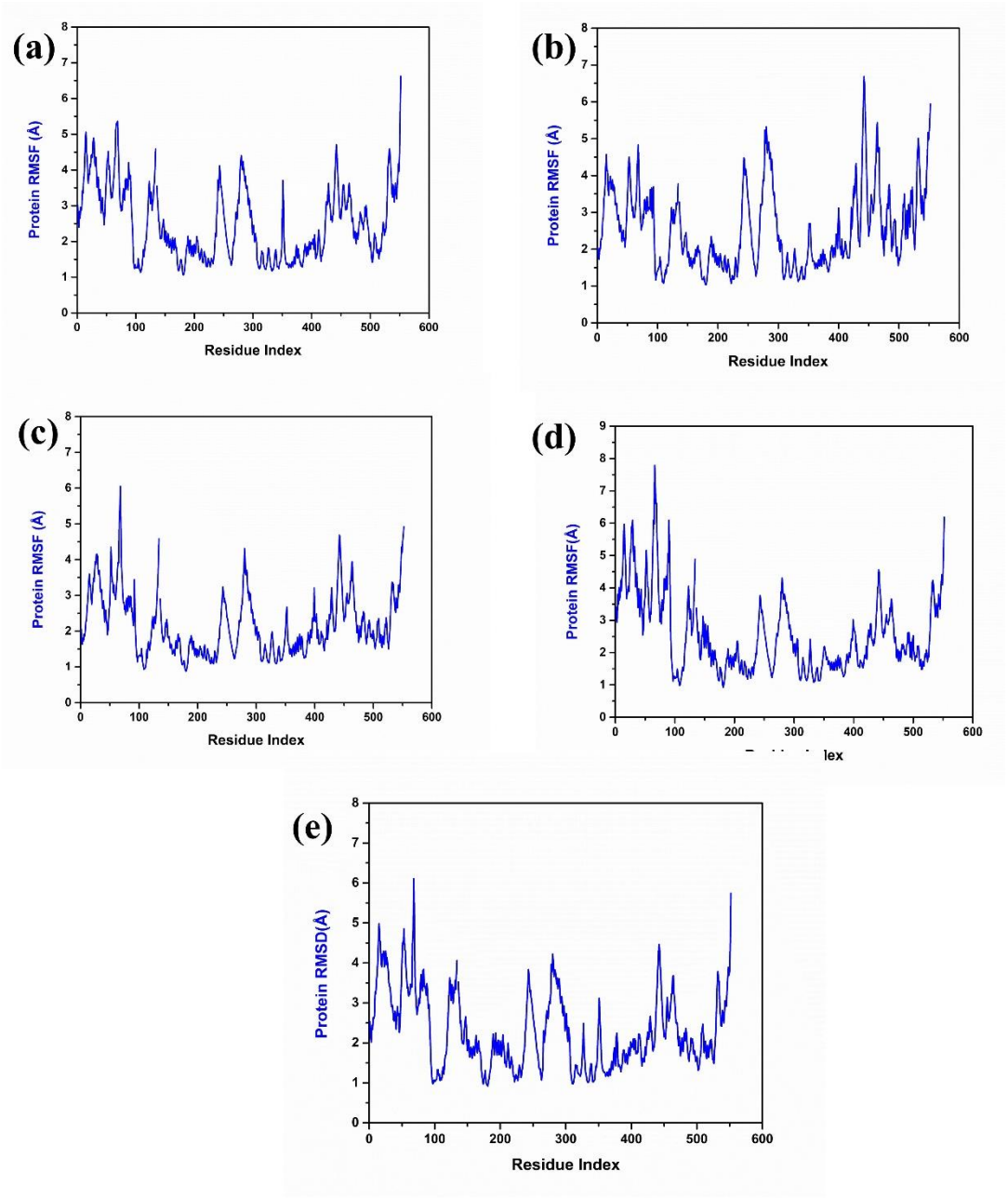
Supplementary Figure S1. RMSD of Apo-protein



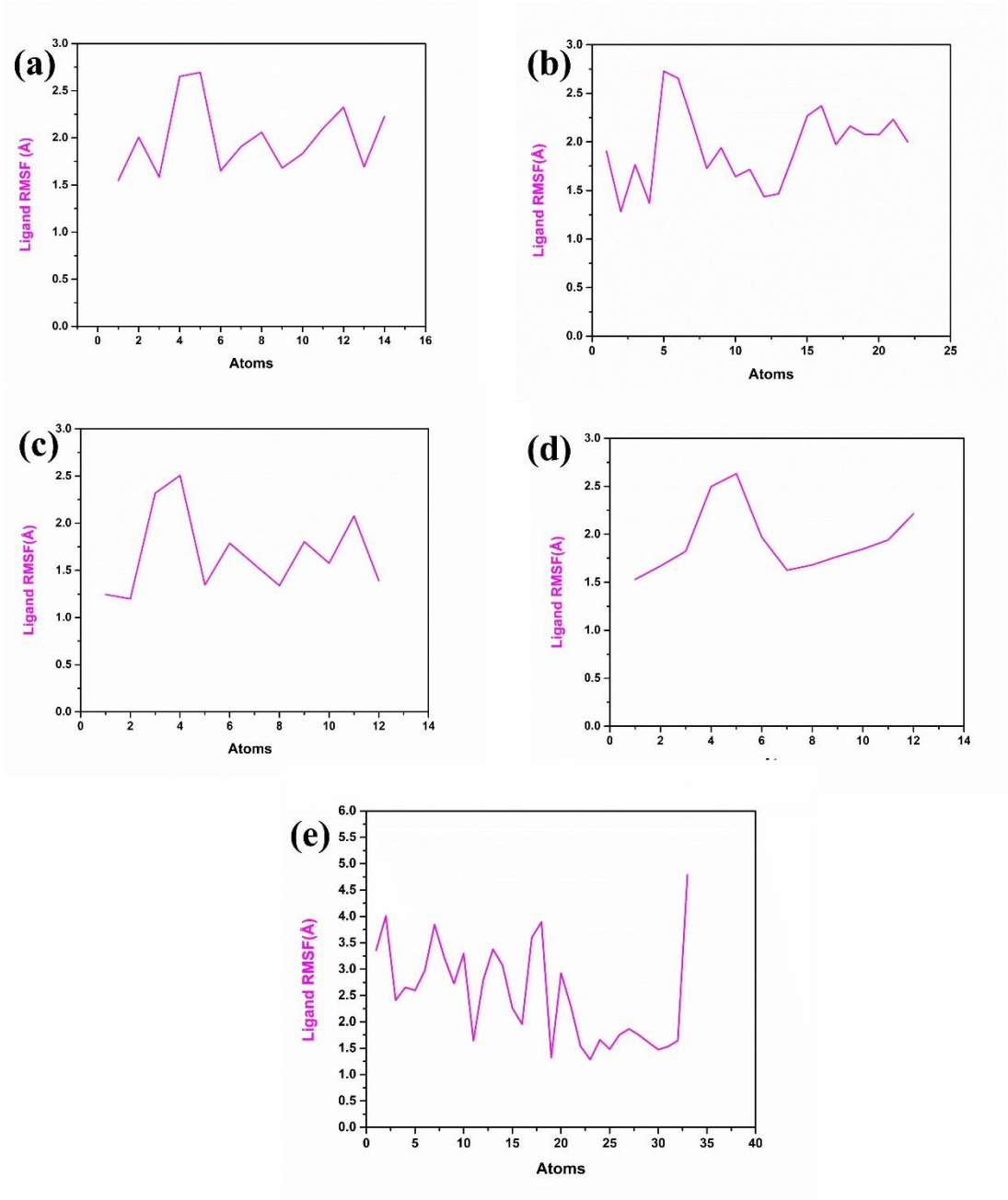
Supplementary Figure S2: RMSD analysis of replica simulation (a) IMPHY000687, (b) IMPHY004619, (c) IMPHY007084, (d) IMPHY012021, (e) Reference inhibitor



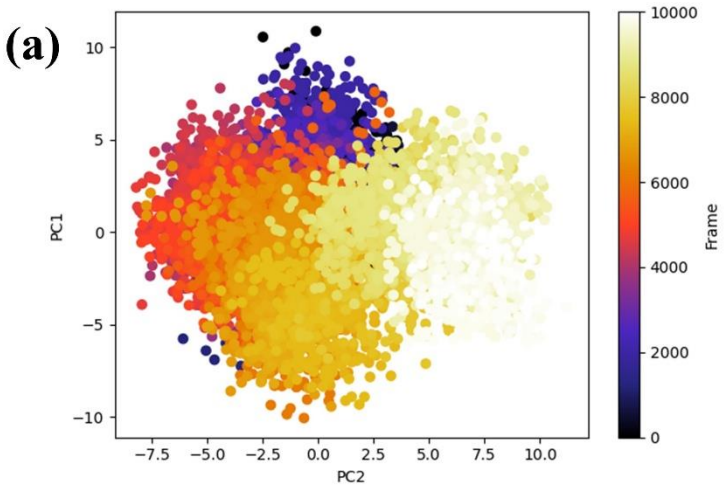
Supplementary Figure S3. RMSF of Apo-protein



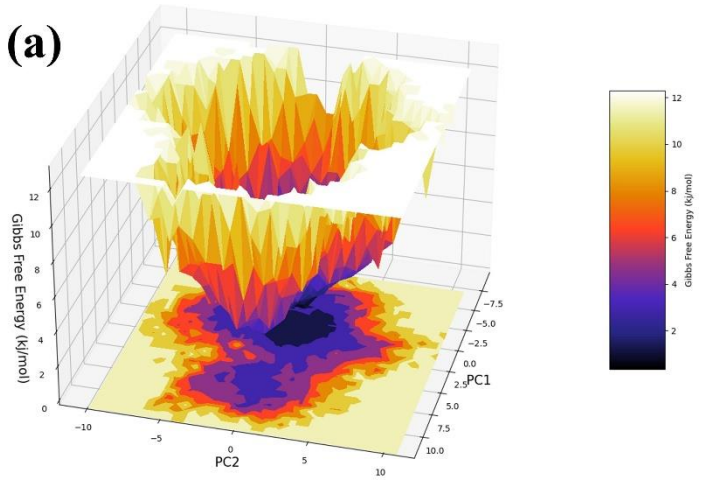
Supplementary Figure S4: RMSF analysis of protein replica simulation (a) IMPHY000687, (b) IMPHY004619, (c), IMPHY007084, (d) IMPHY012021 (e) Reference inhibitor



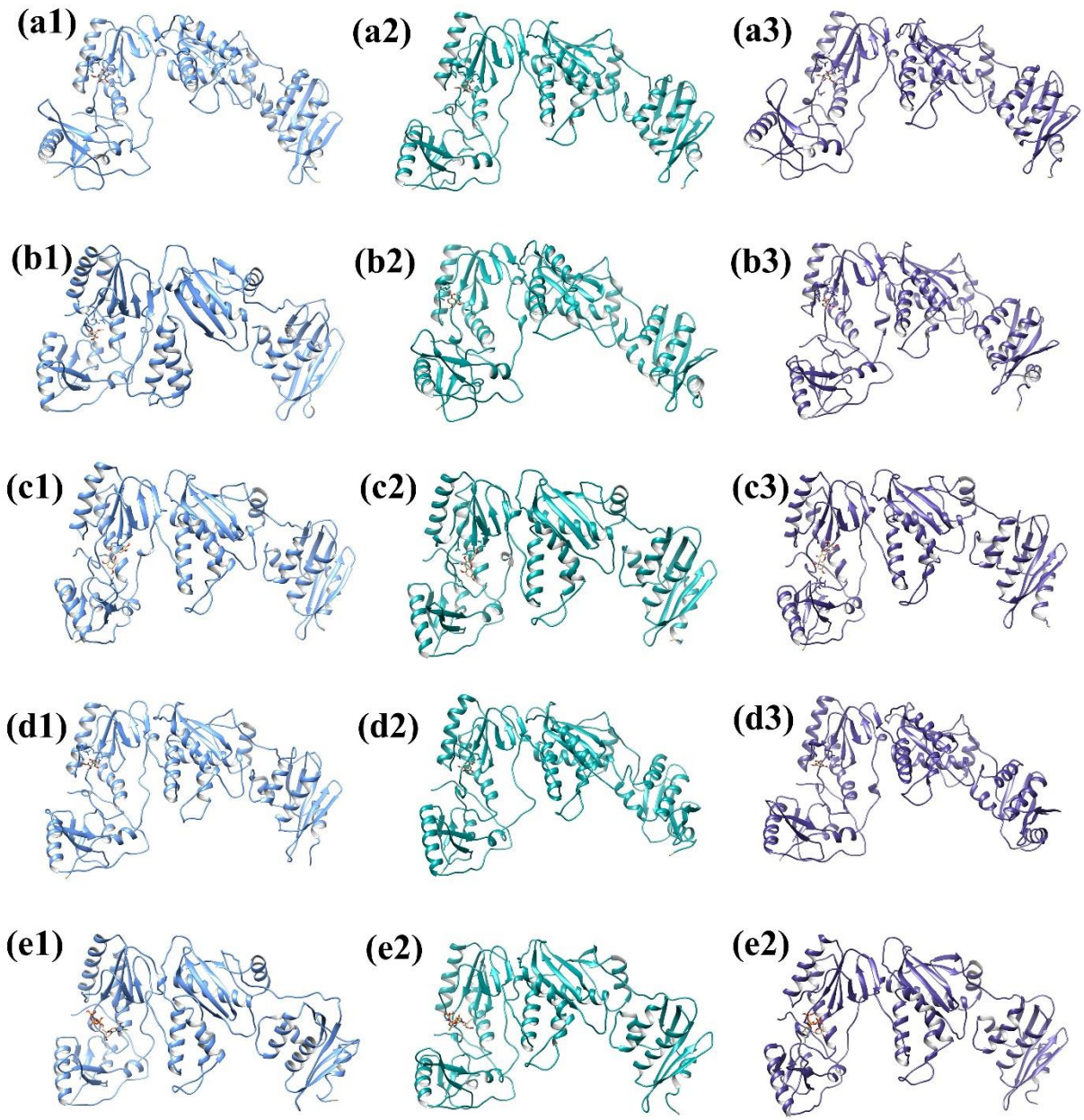
Supplementary Figure S5: RMSF analysis of Ligand replica simulation (a) IMPHY000687, (b) IMPHY004619, (c), IMPHY007084, (d) IMPHY012021 (e) Reference inhibitor



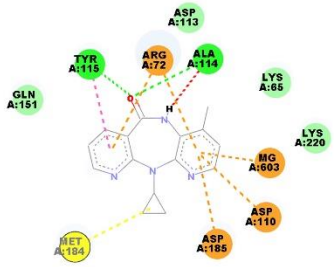
Supplementary Figure S6. PCA of Apo-protein



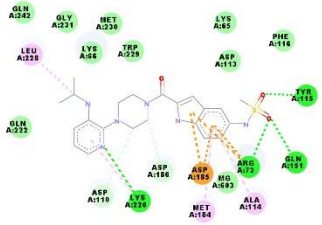
Supplementary Figure S7. FEL of apo-protein



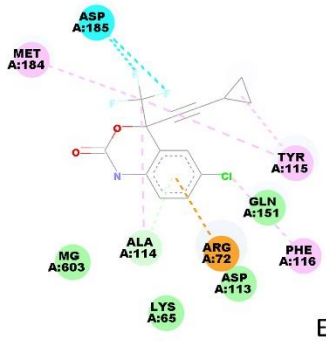
Supplementary Figure S8. Global minimum conformations extracted from FEL analysis for HIV-RT complexes and used for structural superimposition. Panels (a1–a3) IMPHY000687, (b1–b3) IMPHY007084, (c1–c3) IMPHY004619, (d1–d3) IMPHY012021, and (e1–e3) reference inhibitor, showing representative low-energy binding poses adopted during the MD simulations



Nevirapine

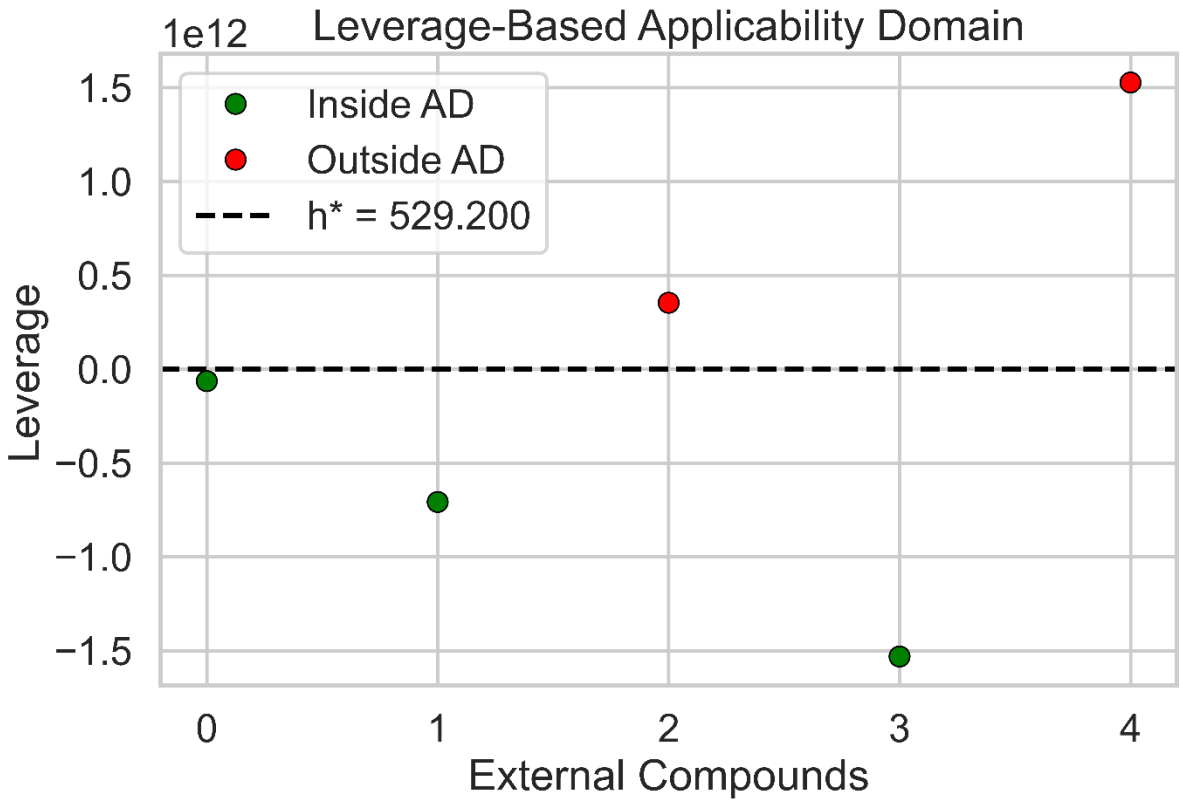


Delavirdine



Efavirenz

Supplementary Figure S9: detailed 2D interaction profiles of the selected reference inhibitors delavirdine, efavirenz, and nevirapine.



Supplementary Figure S10 – Applicability domain Analysis