Supporting Information

***Org. Commun.* 18:4 (2025) 321-330**

Theoretical investigation of interactions between HIV-1 Tat and p53 proteins

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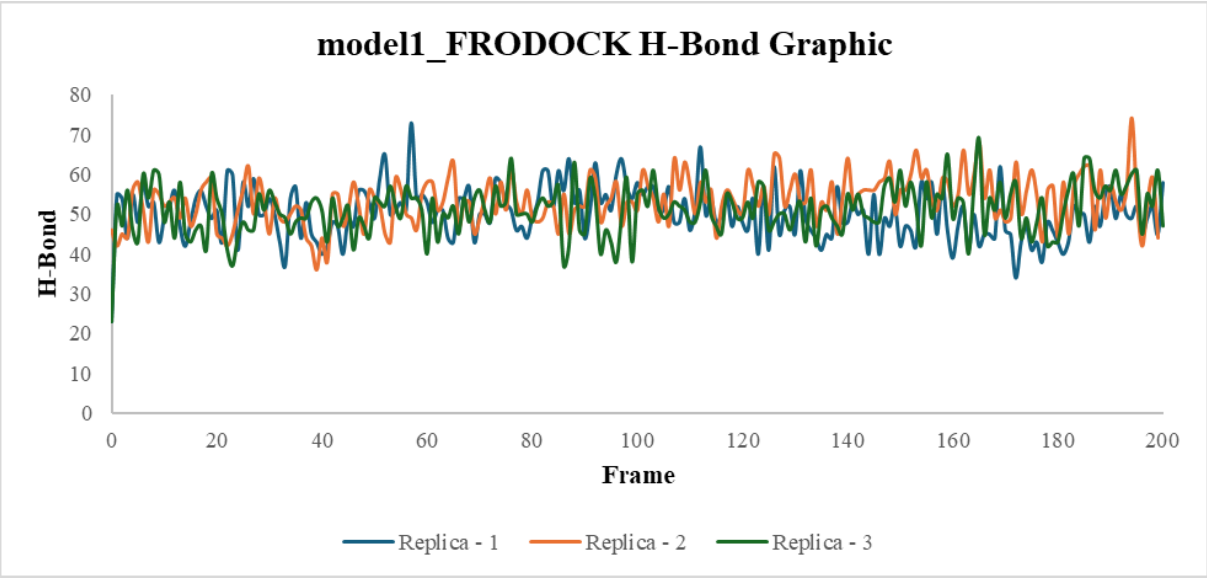

Figure S1: The number of hydrogen bonds between p53 and Tat in model1_FRODOCK for three replicas in the last 200 ns.

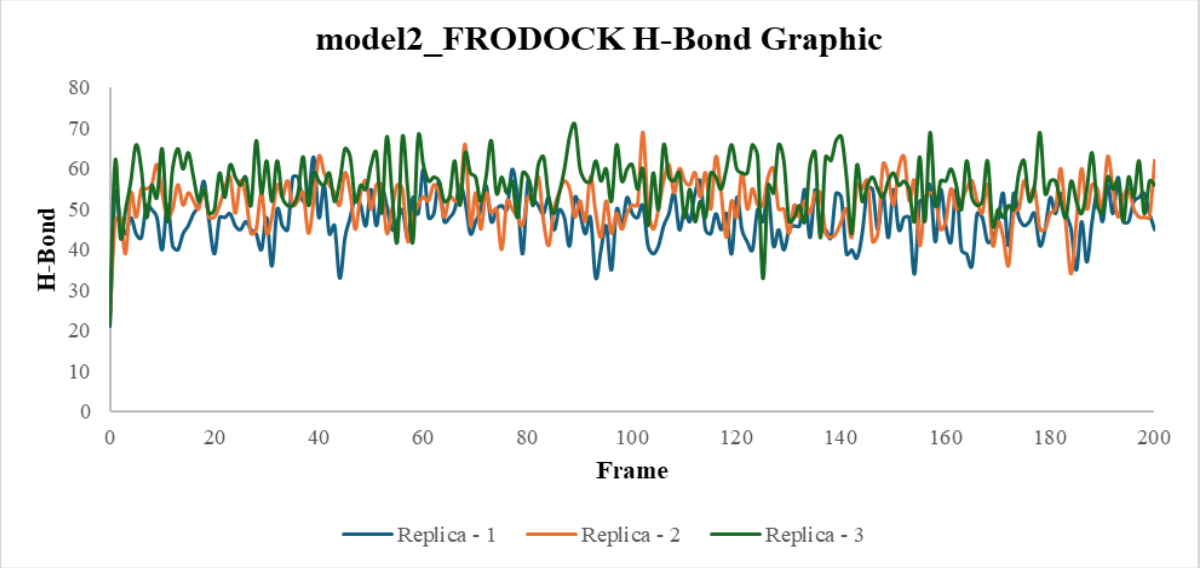

Figure S2. The number of hydrogen bonds between p53 and Tat in model2_FRODOCK for three replicas in the last 200 ns.

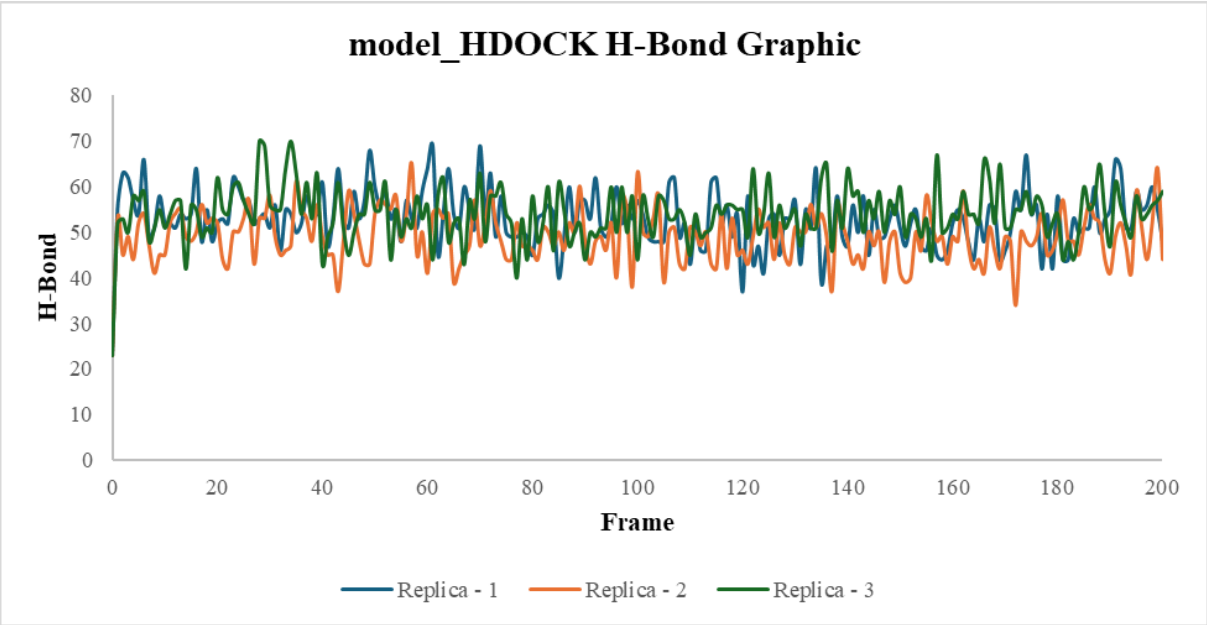

Figure S3: The number of hydrogen bonds between p53 and Tat in model_HDOCK for three replicas in the last 200 ns.

Table S1: PyContact analysis from the model_ZDOCK's replica 2 in the last 200 ns.

p53	Resid	Tat	Resid	interaction_type	mean_score	median_score	percentage
Glu	326	Asp	67	hbond	6.824	7.718	82.025
Arg	333	Asp	67	saltbr	4.241	4.943	62.911
Gly	356	Lys	50	hbond	3.202	3.882	56.733
Asp	352	Gln	63	hbond	2.244	2.282	49.792
Glu	326	Glu	71	hbond	2.695	1.094	45.728
Glu	339	Arg	57	saltbr	1.478	0.000	20.257
Glu	326	Asp	67	hbond	6.824	7.718	82.025
Arg	333	Asp	67	saltbr	4.241	4.943	62.911
Gly	356	Lys	50	hbond	3.202	3.882	56.733