Supporting Information

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Theoretical investigation of interactions between

HIV-1 Tat and p53 proteins

Sinem Koseoglu¹, Cansu M. Yenici¹, Sena Celikbas¹, Serra Aygun¹,

Dicle Altun¹, Sefer Baday² and Onur Alpturk¹

¹ Department of Chemistry, Faculty of Science and Letters, Istanbul Technical University, Istanbul, 34467, Türkiye

² Applied Informatics Department, Informatics Institute, Istanbul Technical University, Istanbul, 34467, Türkiye

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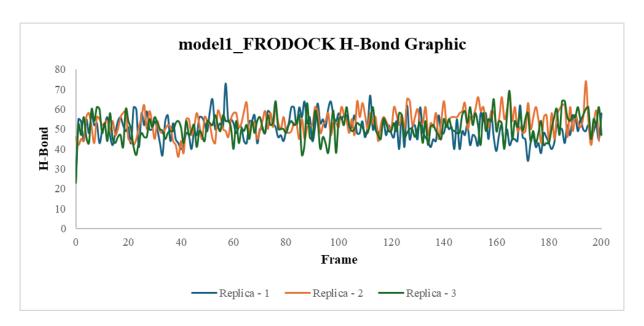


Figure S1: The number of hydrogen bonds between p53 and Tat in model1_FRODOCK for three replicas in the last 200 ns.

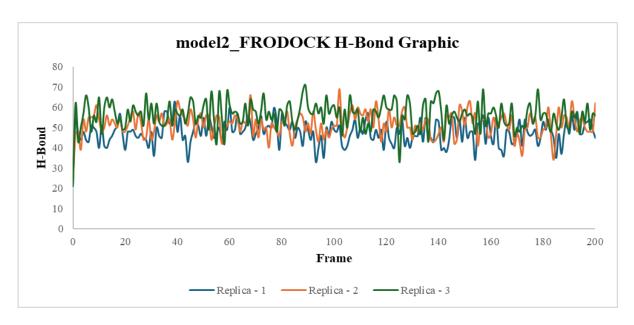


Figure S2. The number of hydrogen bonds between p53 and Tat in model2_FRODOCK for three replicas in the last 200 ns.

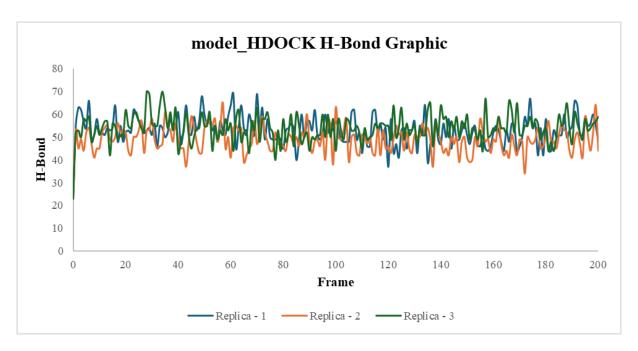


Figure S3: The number of hydrogen bonds between p53 and Tat in model_HDOCK for three replicas in the last 200 ns.

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

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