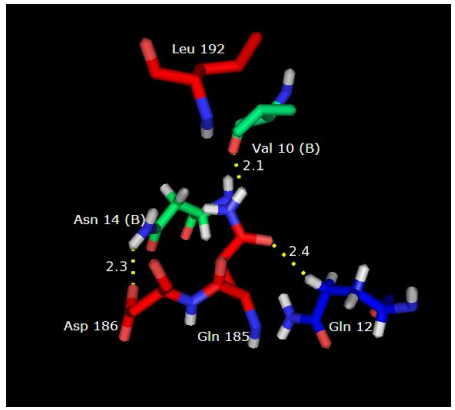
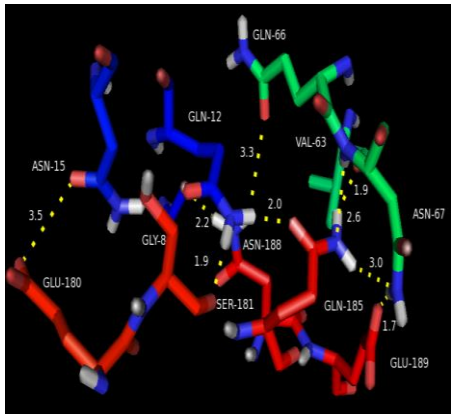
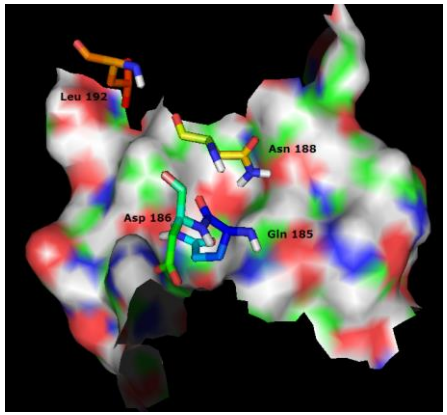
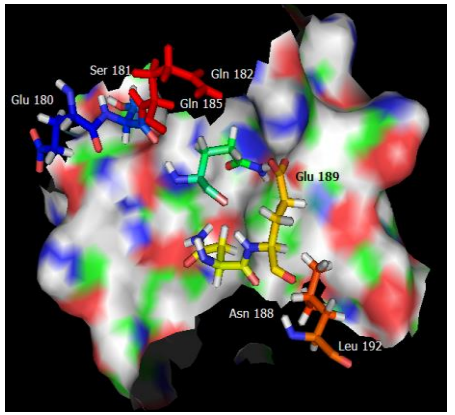
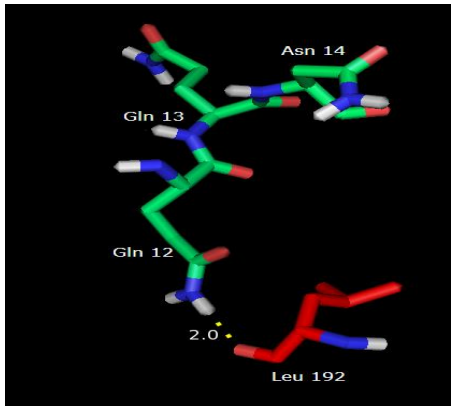
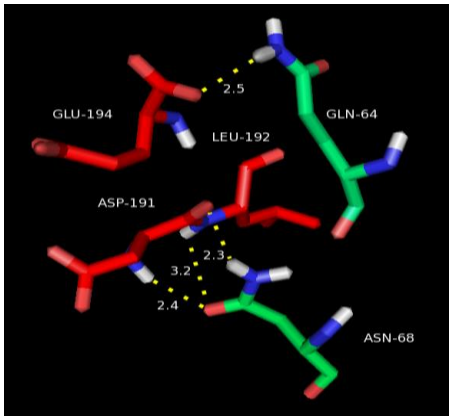
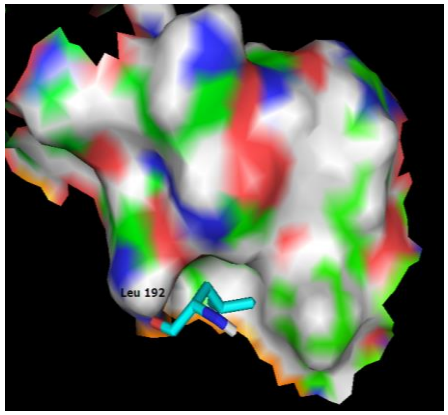
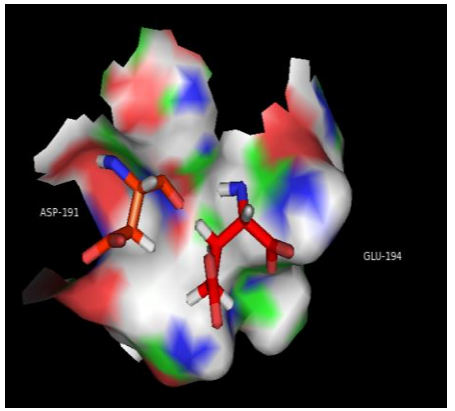
	Docking	MD	Docking	MD
Wild				
	(a)	(b)	(c)	(d)
Mutant				
	(e)	(f)	(g)	(h)

Figure S1: Intermolecular interactions of SFT with the C1 cavity of NHR of gp41 during molecular docking and 50ns MD simulation.

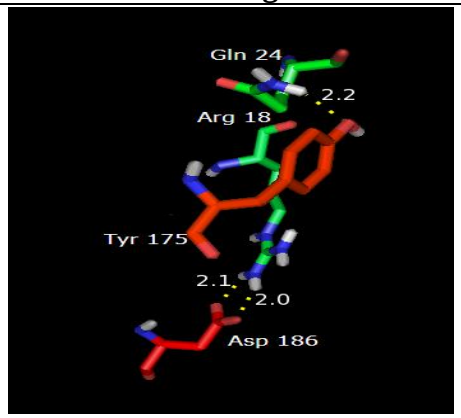
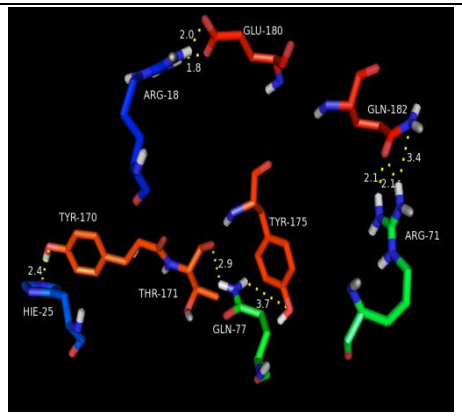
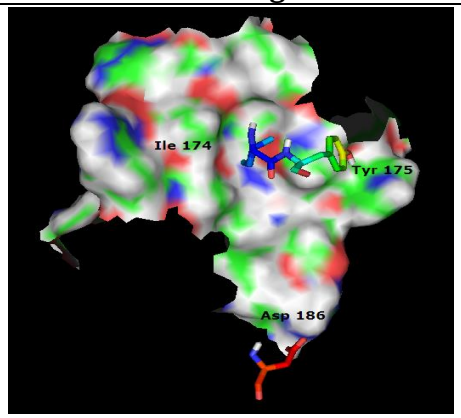
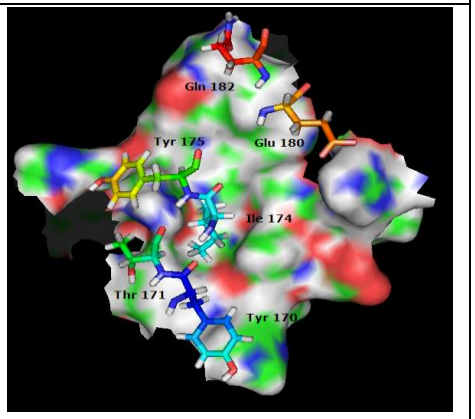
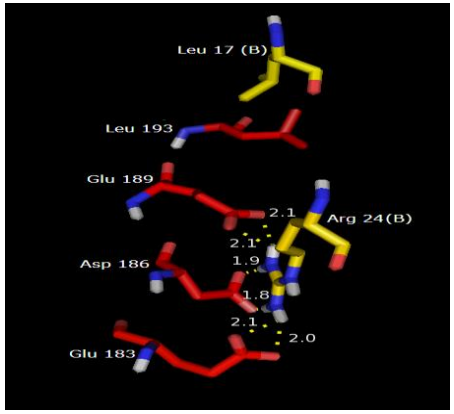
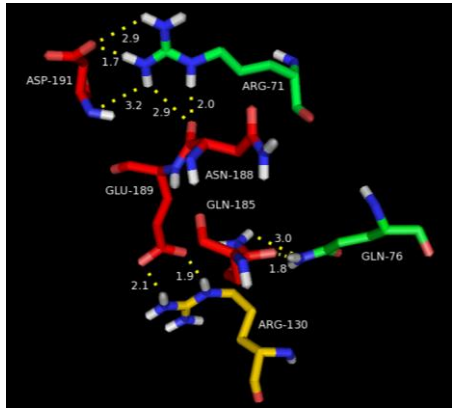
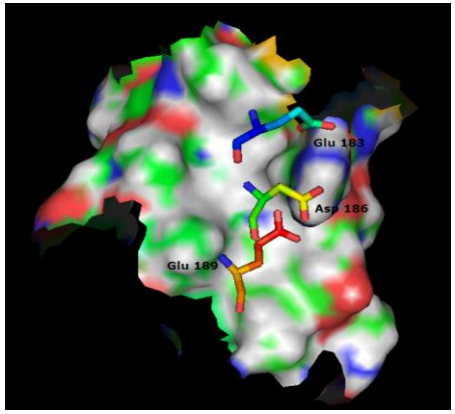
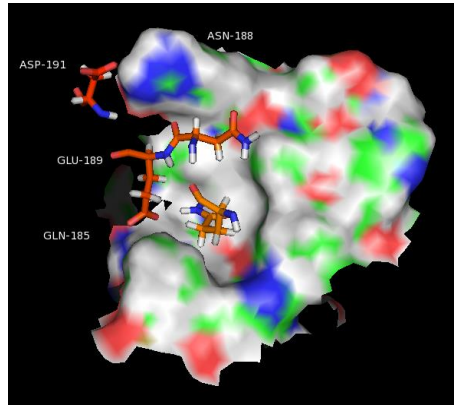
	Doking	MD	Docking	MD
Wild				
	(a)	(b)	(c)	(d)
Mutant				
	(e)	(f)	(g)	(h)

Figure S2: Intermolecular interactions of SFT with the C2 cavity of NHR of gp41 during molecular docking and 50 ns MD simulation.

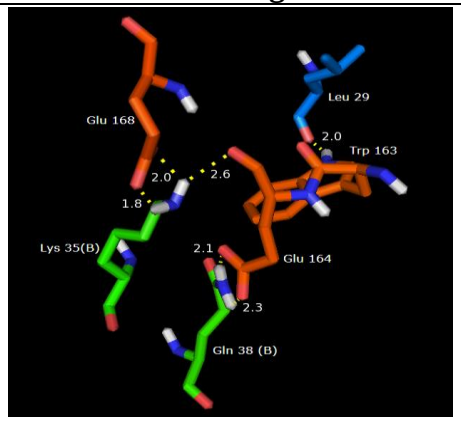
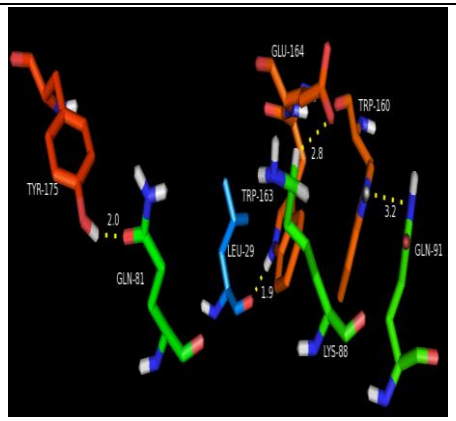
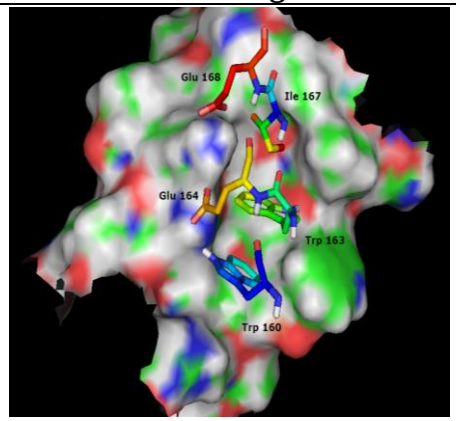
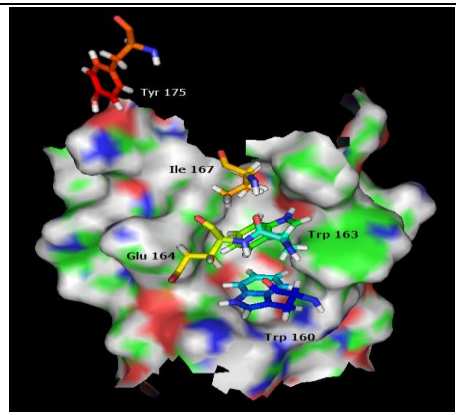
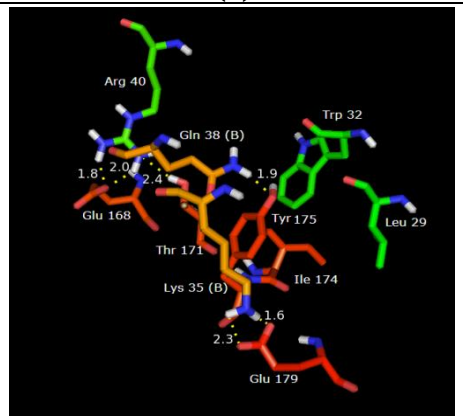
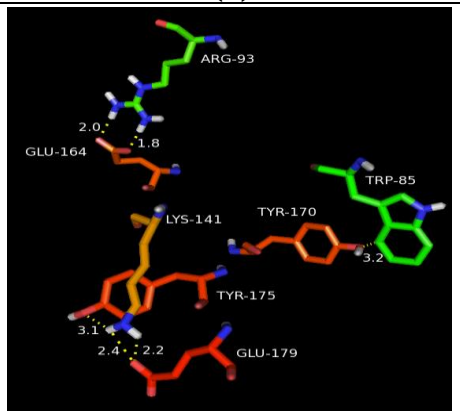
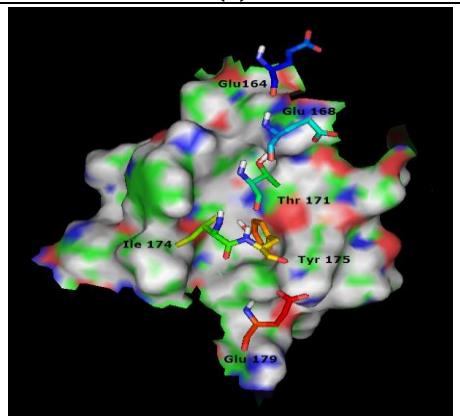
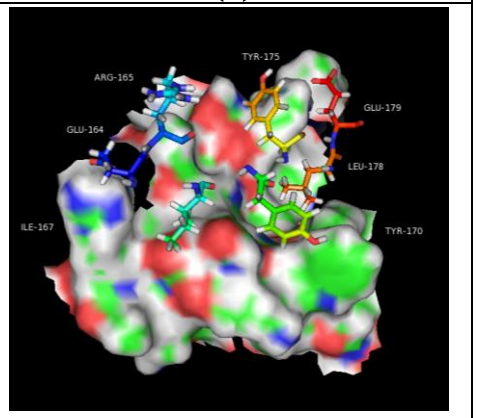
	Docking	MD	Docking	MD
Wild				
	(a)	**(b)**	**(c)**	**(d)**
Mutant				
	(e)	**(f)**	**(g)**	**(h)**

Figure S3: Intermolecular interactions of SFT with the C3 cavity of NHR of gp41 during molecular docking and 50 ns MD simulation.

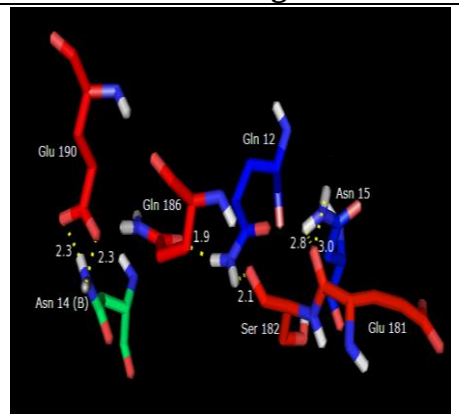
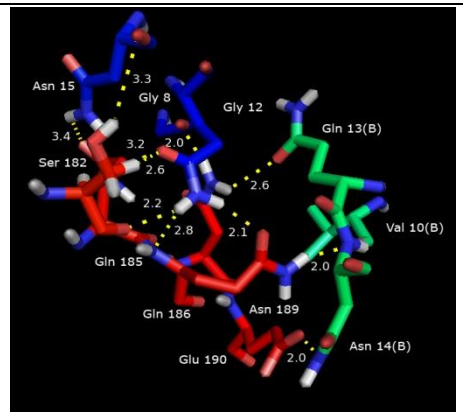
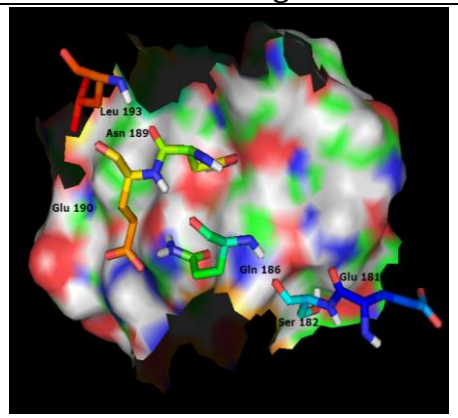
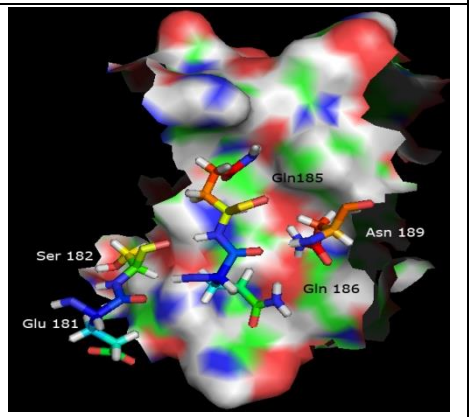
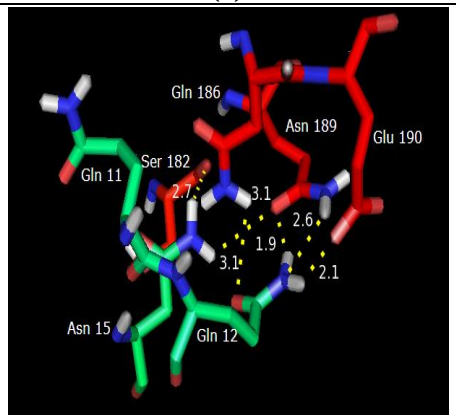
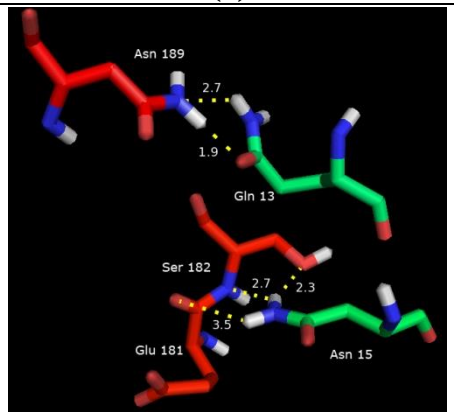
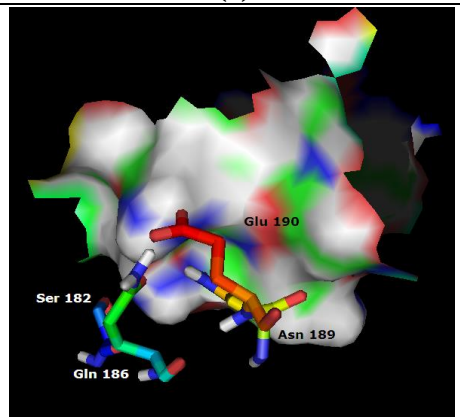
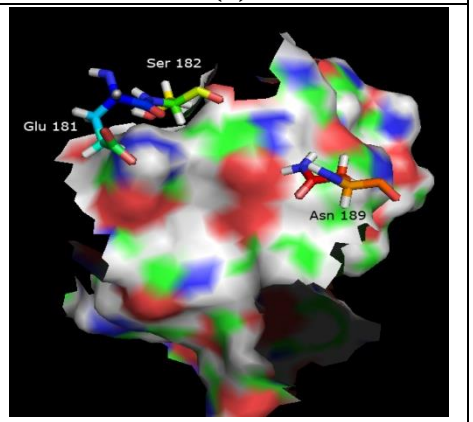
	Docking	MD	Docking	MD
Wild				
	(a)	(b)	(c)	(d)
Mutant				
	(e)	(f)	(g)	(h)

Figure S4: Intermolecular interactions of MTSFT with the C1 cavity of NHR of gp41 during molecular docking and 50 ns MD simulation.

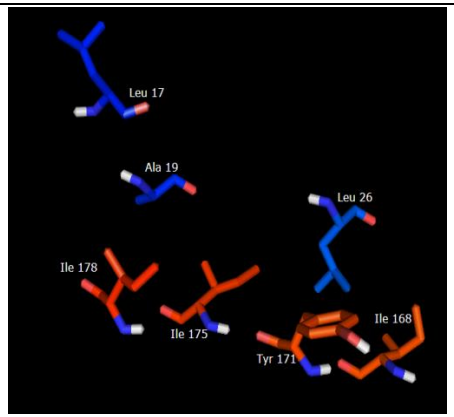
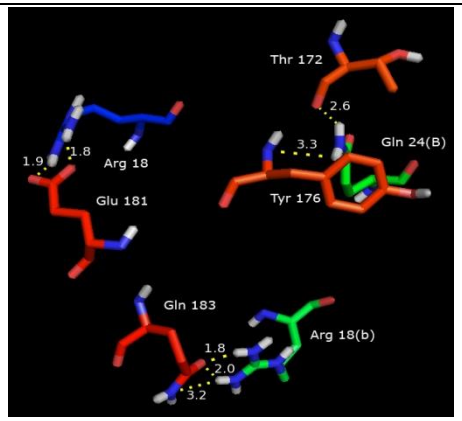
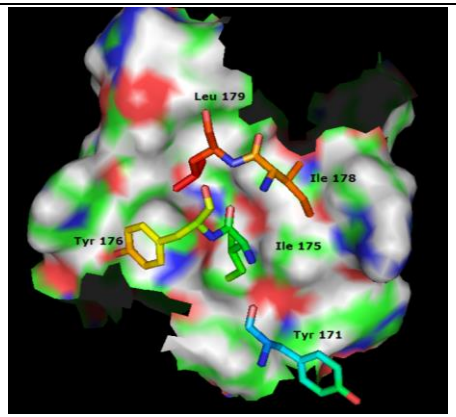
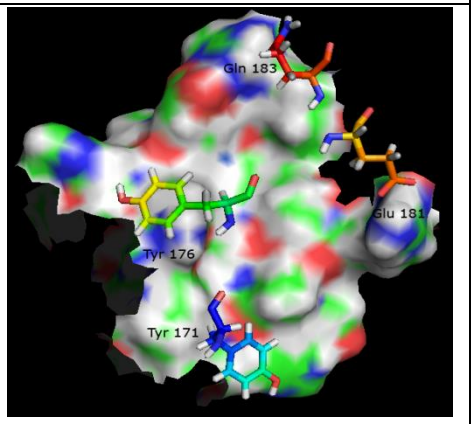
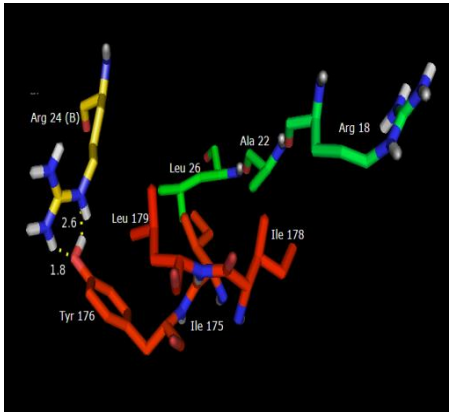
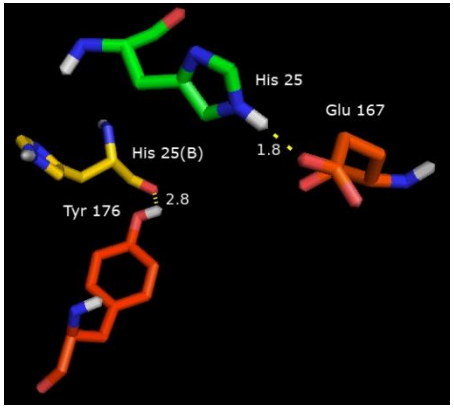
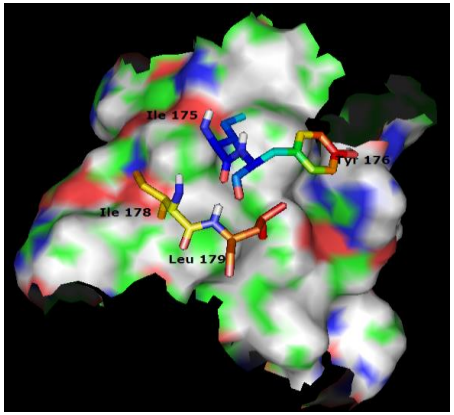
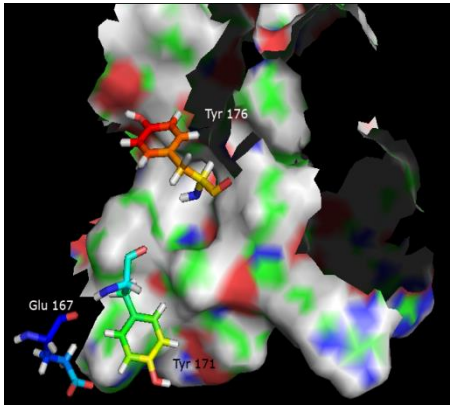
	Docking	MD	Docking	MD
Wild				
	(a)	(b)	(c)	(d)
Mutant				
	(e)	(f)	(g)	(h)

Figure S5: Intermolecular interactions of MTSFT with the C2 cavity of NHR of gp41 during molecular docking and MD simulation.

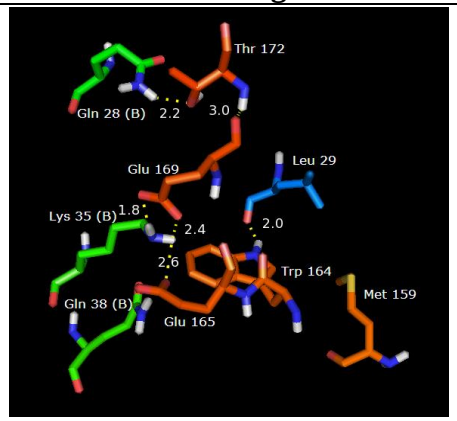
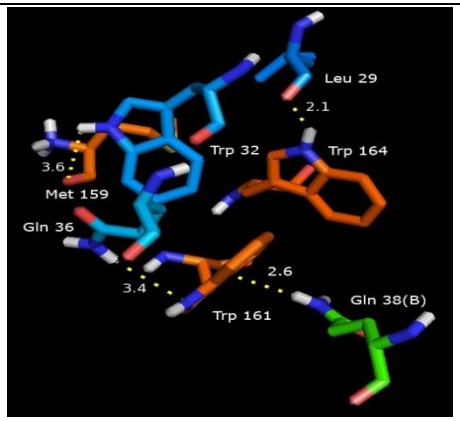
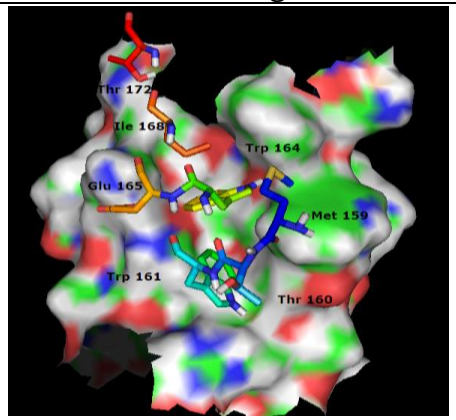
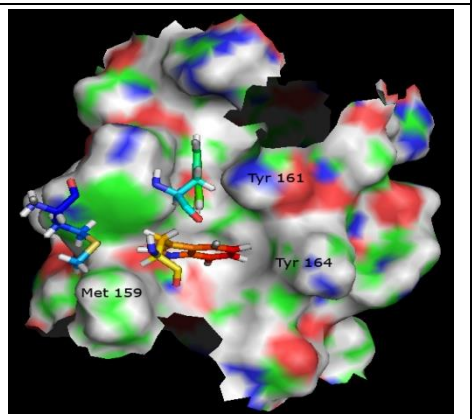
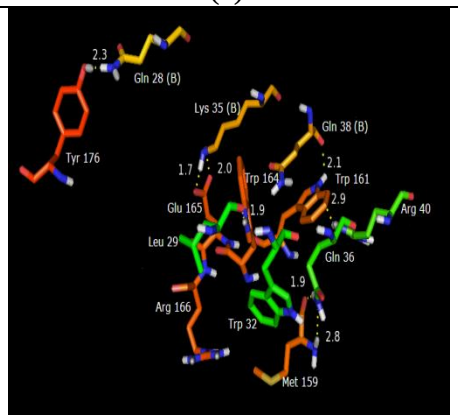
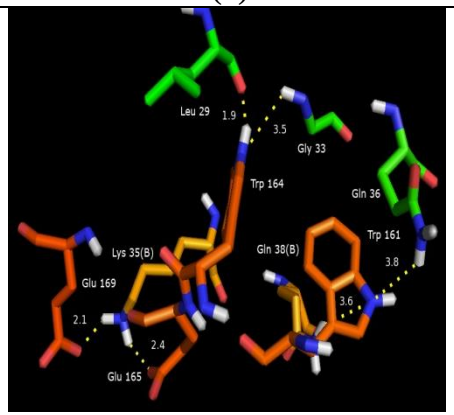
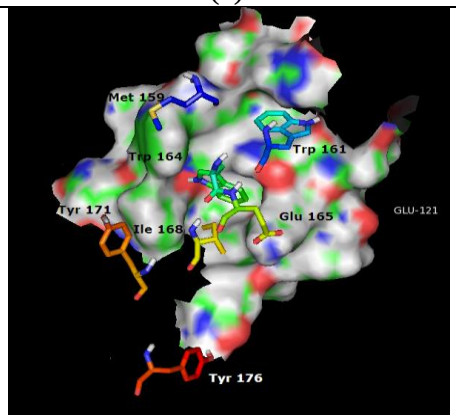
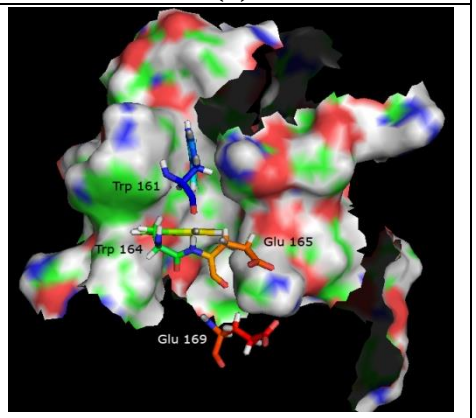
	Docking	MD	Docking	MD
Wild				
	(a)	(b)	(c)	(d)
Mutant				
	(e)	(f)	(g)	(h)

Figure S6: Intermolecular interactions of MTSFT with the C3 cavity of NHR of gp41 during molecular docking and 50 ns MD simulation