

Table S4 – MM/PBSA Results.

Receptor	Ligand	Binding Free Energy (ΔG , kJ/mol)			
		0 – 25 ns	25 – 50 ns	50 – 75 ns	75 – 100 ns
NRP-1	tLyp1	-109.64 +/-101.47	-104.56 +/- 93.00	-86.60 +/- 71.98	-43.23 +/- 78.39
	CP-tLyp1	-3.80 +/- 83.15	-74.11 +/- 85.42	-86.97 +/- 91.77	-91.07 +/- 74.47
FABP3	CooP	-118.27 +/- 25.75	-118.20 +/-22.96	-128.41 +/-18.41	-129.30 +/- 21.66
	CP-CooP	-502.9 +/- 68.07	-457.36 +/-108.67	-391.34 +/-101.20	-377.07 +/- 131.58

Note: Binding Free Energy (ΔG) of the binding sites of receptors in complex with the free peptides and the peptides fused to the CP of TBSV, as predicted by MM/PBSA calculations. The values clearly show that CooP peptide fused to the viral CP recognize with almost 3-fold higher binding affinity the FABP3 receptor ($\Delta G = -377.07$ kJ/mol vs $\Delta G = -129.30$ kJ/mol).