Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting Information for:

Computational Approach to Identify Differential Behaviours of Soluble Tissue Factor and Full-length Tissue Factor towards Factor VIIa

Ramesh Prasad and Prosenjit Sen*

Department of Biological Chemistry, Indian Association for the Cultivation of Science, Jadavpur, Kolkata- 700032, India.

*Corresponding author email: bcps@iacs.res.in

Supplementary Figures:

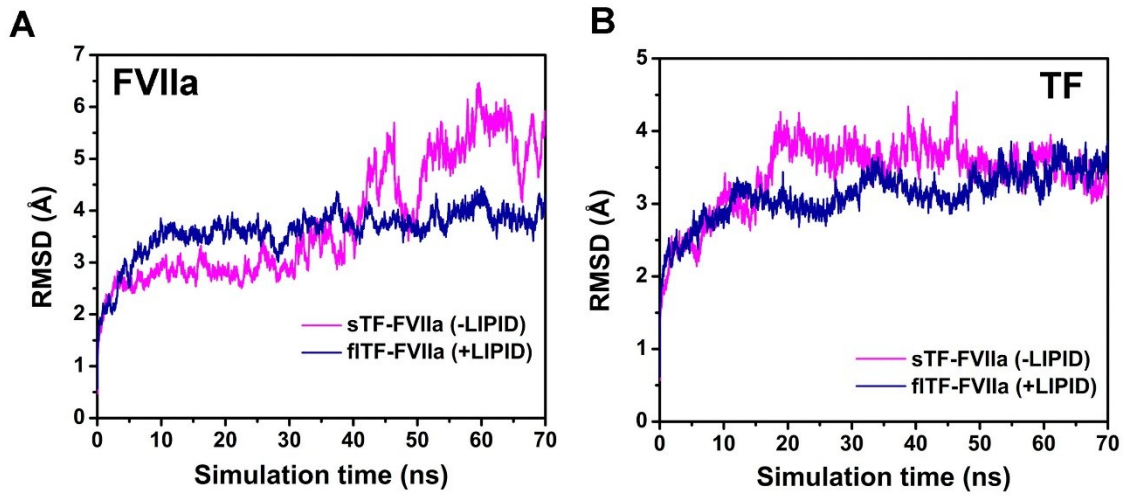

Figure S1: RMSDs of the backbone Cα-atoms of (A) factor VIIa (FVIIa) and (B) tissue factor ($TF_{1\text{-}219}$) obtained from 70 ns unbiased MD simulation trajectory of sTF-FVIIa (-LIPID) and flTF-FVIIa (+LIPID) system.

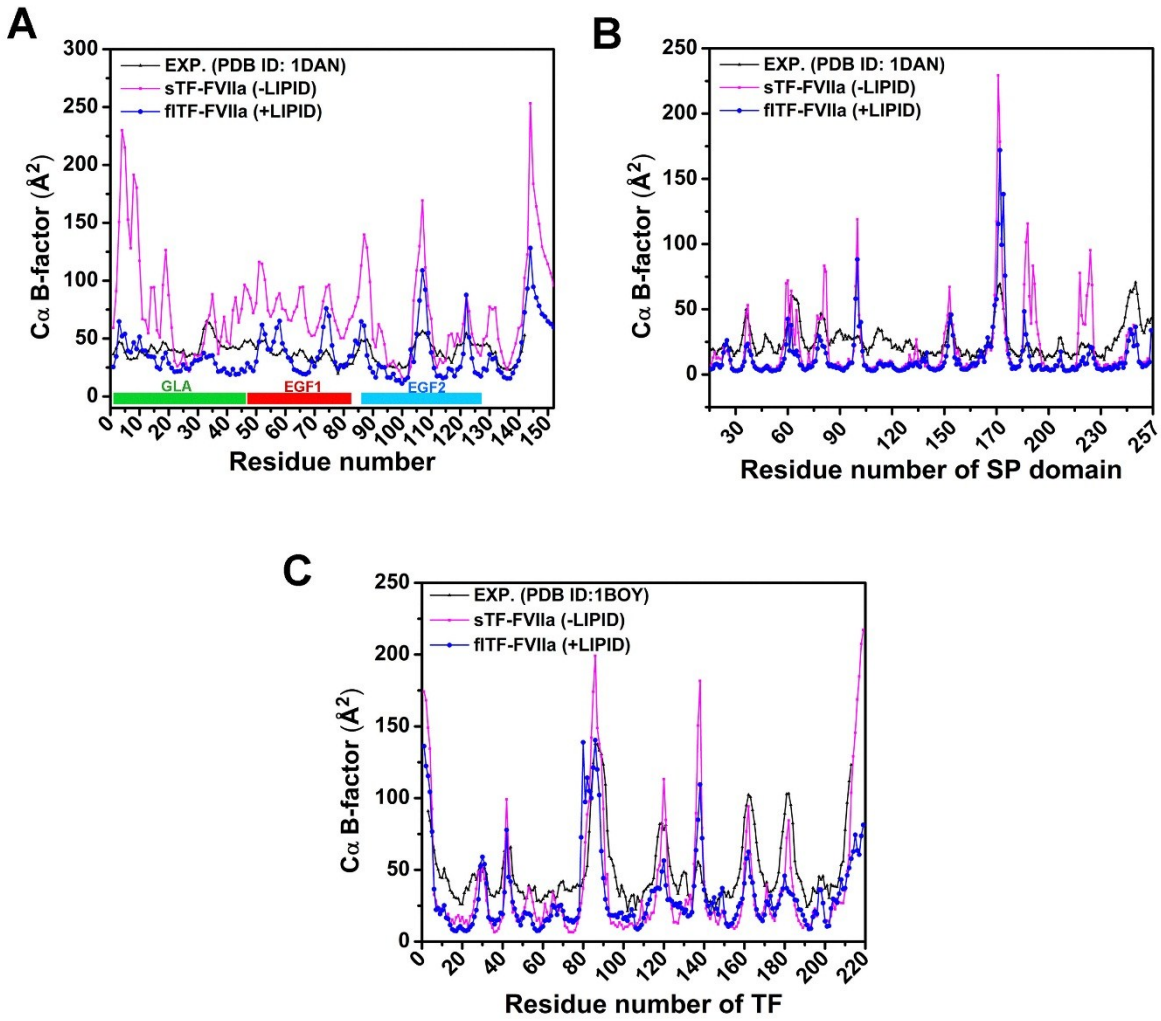

Figure S2: Comparison of computed atomic B-factors obtained over the course of last 20 ns simulation trajectory from simulations of sTF-FVIIa and flTF-FVIIa to experimental data (crystal structure) for FVIIa and TF. Experimental (PDBID:1DAN) and calculated B-factors of (A) FVIIa-light chain residue (domainwise: GLA, EGF1 and EGF2), (B) FVIIa-heavy chain residue (SP domain), obtained from last 20 ns simulation of sTF-FVIIa (-LIPID) and flTF-FVIIa (+LIPID). (C) Experimental (PDBID:1BOY) and calculated B-factors of TF residue obtained from last 20 ns simulation trajectory.

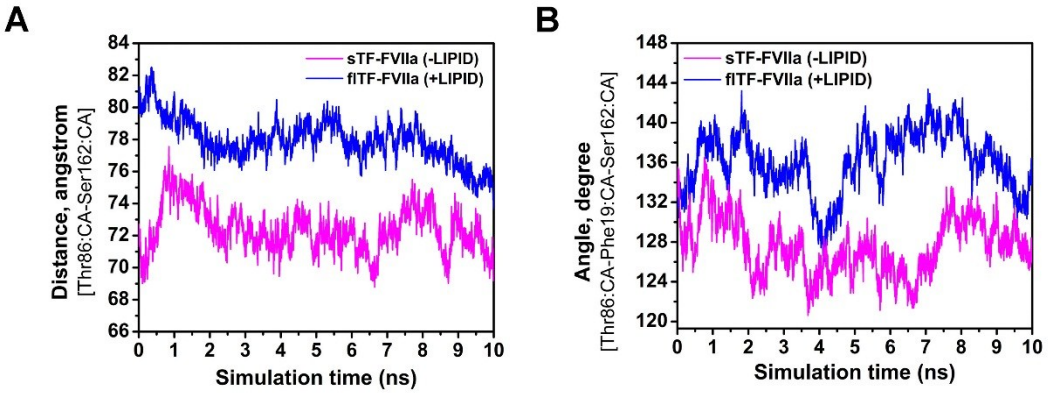

Figure S3: (A) Distance plot between Cα-atom of residues Thr86 and Ser162 of TF. (B) Angle formed among Cα-atom of residues Thr86, Phe19 and Ser162. Last 10 ns of 110 ns simulation trajectory is shown in the plots.

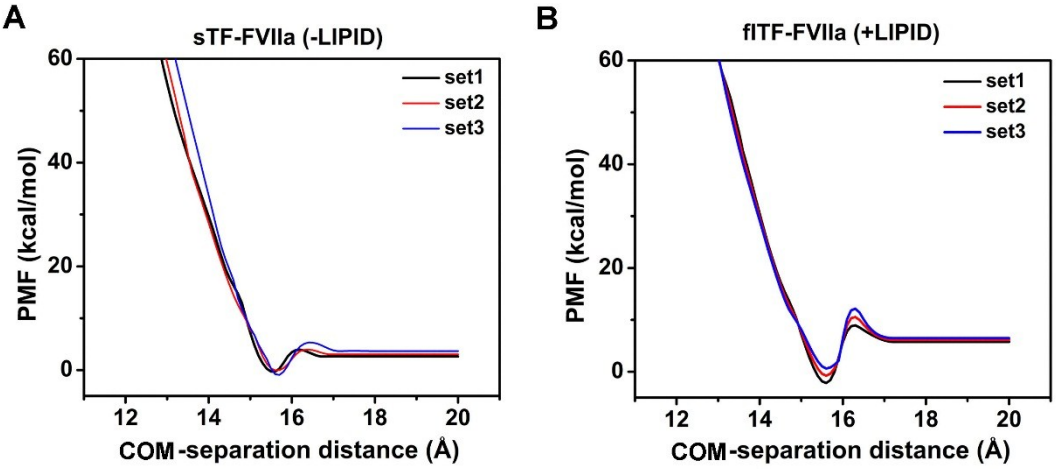

Figure S4: Individual PMF profiles three each for (A) sTF-FVIIa and (B) flTF-FVIIa) for the estimation of free energy binding between FVIIa (light chain) and TF, obtained from 2.5 ns simulation for each set using ABF method.