

Supporting Information

In silico mutation and binding studies of human FVIIa GLA-domain to endothelial protein C receptor: A molecular dynamics simulation approach

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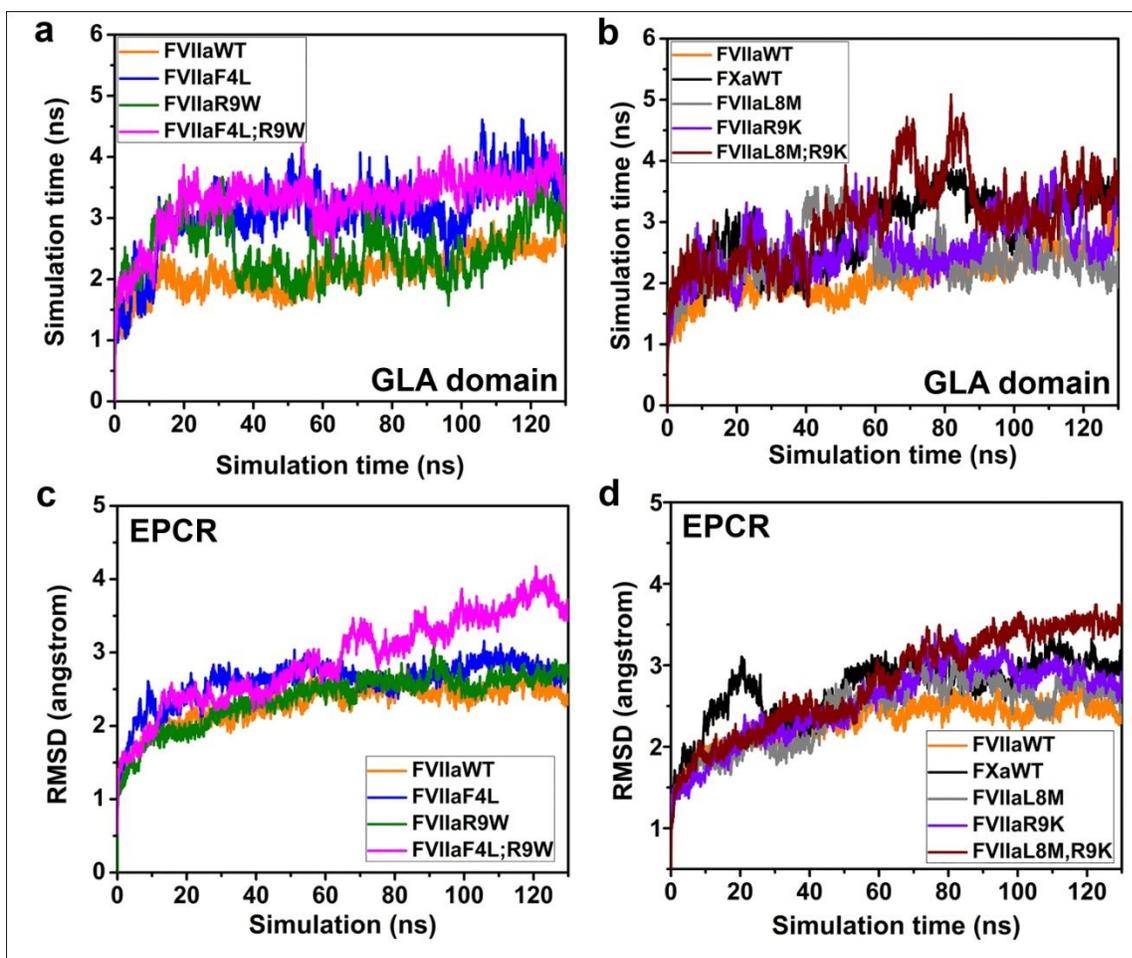


Figure S1. Root mean square deviation (RMSDs) of the backbone of (a) GLA domain of FVIIa_{WT}, FVIIa_{F4L}, FVIIa_{R9W} and FVIIa_{F4L;R9W} in complex system, (b) GLA domain of FXa_{WT}, FVIIa_{L8M}, FVIIa_{R9K} and FVIIa_{L8M;R9K} in complex system, (c) EPCR of FVIIa_{WT}, FVIIa_{F4L}, FVIIa_{R9W} and FVIIa_{F4L;R9W} in complex systems, (d) EPCR of FXa_{WT}, FVIIa_{L8M}, FVIIa_{R9K} and FVIIa_{L8M;R9K} in complex system, obtained from 130 ns unbiased MD simulation trajectories of EPCR-GLA complex for all the systems.

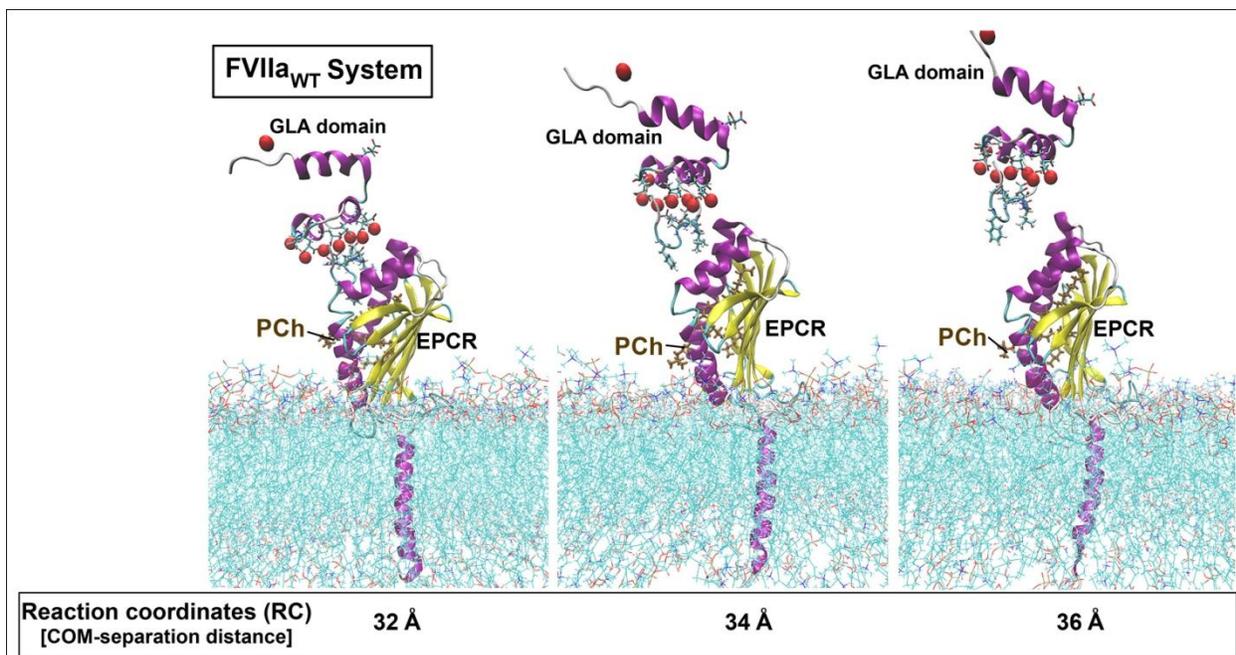


Figure S2. The conformational changes of EPCR-GLA domain for FVIIa_{WT} system in presence of PCh-containing lipid within EPCR groove at center-of-mass (COM) distance of 32 Å, 34 Å and 36 Å, obtained from the ABF simulation trajectories. For the calculation of free energies, COM-separation distance between GLA domain and EPCR were chosen as the reaction coordinates. Antigenic PCh-containing lipid within EPCR groove is represented by brown licorice color.

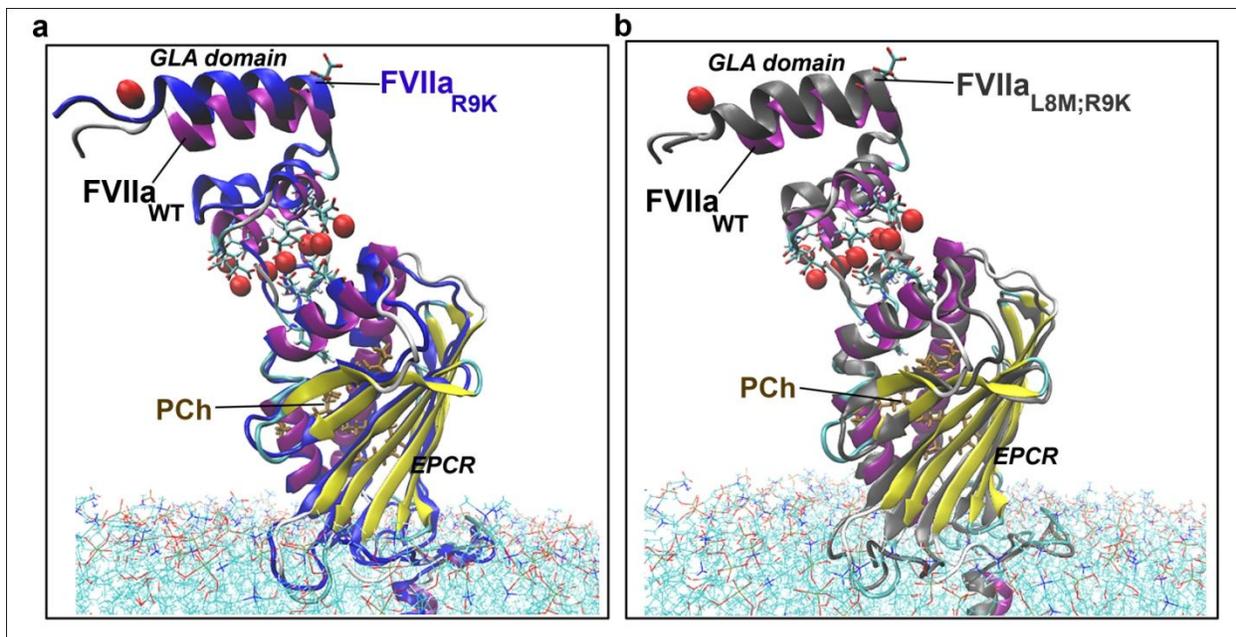


Figure S3. Cartoon representation of superimposed structure of (a) energy minima structure between FVIIa_{WT} and FVIIa_{R9K} complex system and, (b) between FVIIa_{WT} and FVIIa_{L8M;R9K} complex system. FVIIa_{WT} minimized complex structure is shown by secondary structure color representation. FVIIa_{R9K} and FVIIa_{L8M;R9K} system are shown by blue and gray color representation, respectively. Antigenic PCh-containing lipid within EPCR groove is represented by brown licorice color.