In silico modeling and experimental evidence of coagulant protein interaction with precursors for nanoparticle functionalization

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Table S1. MMPBS and MM GBSA calculations of binding free energy components of the monomer protein with one citrate molecule from separate trajectories.

	Method	VDWAALS			EEL			EGB			ESURF			TOTAL		
		TSC	TEOS	APTE S	TSC	TEOS	APTES	TSC	TEOS	APTES	TSC	TEOS	APTE S	TSC	TEOS	APTES
Protein	Genaeralized Born	-373.0	-367.1	-368.5	-2586.1	-2578.6	-2565.1	-1178.3	-1173.9	-1180.5	40.5	41.0	41.3	-4096.9	-4078.7	-4072.7
	Poisson Boltzmann	-372.9	-367.1	-368.5	-2586.1	-2578.6	-2565.1	-1166.3	-1155.6	-1169.6	28.4	28.2	29.1	-4097.0	-4073.1	-4073.1
Ligand	Genaeralized Born	-1.2	-2.3	-2.4	248.1	247.8	67.0	-466.8	-4.0	-12.9	2.4	2.4	2.4	-217.5	244.0	54.2
	Poisson Boltzmann	-1.2	-2.3	-2.4	248.1	247.8	67.0	-455.1	-5.4	-14.0	0.8	1.5	1.7	-207.3	241.7	52.3
Complex	Genaeralized Born	-377.1	-388.5	-393.7	-2970.9	-2331.3	-2500.4	-1024.1	-1171.3	-1181.5	41.2	40.9	40.7	-4330.7	-3850.1	-4034.9
	Poisson Boltzmann	-377.1	-388.5	-393.7	-2970.9	-2331.3	-2500.4	-1002.5	-1154.5	-1171.8	28.8	27.9	28.4	-4321.6	-3846.4	-4037.5
Difference (complex-ligand)	Genaeralized Born	-2.9	-19.1	-22.8	-632.9	-0.5	-2.3	621.1	6.6	11.9	-1.6	-2.5	-3.1	-16.3 (ΔG binding)	-15.4 4(ΔG binding)	-16.4 (ΔG binding)
	Poisson Boltzmann	-2.9	-19.1	-22.8	-632.9	-0.5	-2.3	618.9	6.5	11.8	-0.4	-1.9	-2.4	-17.3 (ΔG binding)	-14.9 (ΔG binding)	-15.8 (ΔG binding)

VDW - Van der Waals energy; ELE - Electrostatic energy; INT – Internal energy; G gas = VDW + ELE + INT; EGB, EPB - Polar solvation energy; ESURF, ECAVITY - Non polar solvation energy, G sol = Polar solvation energy + non polar solvation energy; GB - Generalized Born; PB - Poisson Boltzmann

Table S2. MM PBSA and MM GBSA calculations of binding free energy components of the homodimer with one and two citrate molecules from separate trajectories.

		Homodimer with one citrate molecule								Homodimer with two citrate molecules							
Contributions (kcal/mol)	Method	Complex		Protein		Citrate		Delta		Complex		Protein		Citrate		Delta	
		Mean	σ	Mean	σ	Mean	σ	Mean	σ	Mean	σ	Mean	σ	Mean	σ	Mean	σ
VDW	MM GBSA	-874.8	2.0	-868.1	2.0	1.0	0.3	-7.6	0.8	-870.7	2.3	-864.1	2.3	1.0	0.4	-7.5	0.5
	MM PBSA	-874.78	2.0	-868.1	2.0	1.0	0.3	-7.6	0.8	-870.7	2.3	-864.1	2.3	1.0	0.4	-7.5	0.5
ELE	MM GBSA	-6040.5	9.4	-5360.5	9.4	233.7	2.2	-913.7	2.1	-6406.5	13.6	-6019.6	10.6	201.7	1.8	-588.6	5.0
	MM PBSA	-6040.5	9.4	-5360.5	9.4	233.7	2.2	-913.7	2.1	-6406.5	13.6	-6019.6	10.5	201.7	1.8	-588.6	5.0
G gas	MM GBSA	-6915.2	9.6	-6228.6	9.5	234.6	2.2	-921.2	1.9	-7277.2	13.0	-6883.7	10.1	202.7	1.9	-596.1	4.7
	MM PBSA	-6915.2	9.6	-6228.6	9.5	234.6	2.2	-921.2	1.9	-7277.2	13.0	-6883.7	10.1	202.7	1.9	-596.1	4.7
EGB/EPB	MM GBSA	-2256.9	8.1	-2663.7	7.8	-483.4	0.9	890.3	1.7	-2139.8	9.7	-2257.6	9.2	-470.1	1.2	588.0	4.1
	MM PBSA	-2149.3	7.8	-2572.1	7.3	-471.2	0.9	894.1	1.7	-2010.9	10.1	-2142.1	9.7	-458.1	1.2	589.3	3.6
ESURF/ ECAVITY	MM GBSA	60.3	0.2	60.8	0.2	2.3	0.0	-2.8	0.1	61.5	0.2	61.1	0.2	2.3	0.0	-1.8	0.0
	MM PBSA	42.1	0.1	42.5	1.0	0.7	0.0	-1.1	0.0	42.7	0.1	42.7	0.1	0.7	0.0	-0.8	0.0
G sol	MM GBSA	-2196.5	8.0	-2602.9	7.8	-481.1	0.9	887.5	1.7	-2078.3	9.7	-2196.6	9.2	-467.8	1.2	586.1	4.0
	MM PBSA	-2107.1	7.8	-2529.6	7.3	-470.5	1.0	893.0	1.7	-1968.2	10.1	-2099.4	9.7	-457.4	1.2	588.6	3.6
G gas+sol	MM GBSA	-9111.8	7.3	-8831.5	6.8	-246.5	2.0	-33.8	0.7	-9355.4	6.0	-9080.3	5.8	-265.1	2.5	-10.02	3.8
	MM PBSA	-9022.3	7.3	-8758.2	6.69	-235.9	2.0	-28.3	0.8	-9245.3	6.8	-8983.1	6.2	-254.7	2.4	-7.5	1.6

VDW - Van der Waals energy; ELE - Electrostatic energy; INT – Internal energy; G gas = VDW + ELE + INT; EGB, EPB - Polar solvation energy; ESURF, ECAVITY - Non polar solvation energy, G sol = Polar solvation energy + non polar solvation energy; GB - Generalized Born; PB - Poisson Boltzmann