Supplementary Materials

Assessment of the interaction between sodium dodecyl sulfate and trypsin enzyme through micellization and thermodynamic analysis

Md Al Amin Hossain[a], Ripa Akter [a], Md. Nasir Uddin[a], Md. Tuhinur R. Joy[a], Bulbul Ahmed[b], Dileep Kumar[*c,d], Md Abdul Goni[e], K. M. Anis-Ul-Haque[a], Md. Anamul Hoque[b] and Ajamaluddin Malik[f]

[a]*Department of Chemistry, Jashore University of Science and Technology, Jashore 7408, Bangladesh*

[b]*Department of Chemistry, Jahangirnagar University, Savar, Dhaka 1342, Bangladesh*

[c]*Laboratory for Chemical Computation and Modeling, Institute for Computational Science and Artificial Intelligence, Van Lang University, Ho Chi Minh City, Vietnam*

[d]*Faculty of Applied Technology, School of Technology, Van Lang University, Ho Chi Minh City, Vietnam*

[e]*Department of Biological and Physical Sciences, South Carolina State University, Orangeburg, SC 29117, USA*

[f]*Department of Biochemistry, Collage of Science, King Saud University, Riyadh, Saudi Arabia University, P.O. Box 2460, Riyadh 11451, Saudi Arabia*

[*]Corresponding author.

E-mail addresses: kumar.dileep@vlu.edu.vn; dileepkmr271@gmail.com (D. Kumar).

Table S1. Magnitudes of $\Delta G_{m,tr}^{0}$, $\Delta H_{m,tr}^{0}$, and $\Delta S_{m,tr}^{0}$ for mixture of SDS and 0.5 % (w/w) trypsin in aq. sodium salt media at certain range of temperature.

Medium	I_{Salt}	T	$\Delta G_{m,tr}^{0}$	$\Delta H_{m,tr}^{0}$	$\Delta S_{m,tr}^{0}$
	(mmol kg^{-1})	(K)	(kJ mol^{-1})	(kJ mol^{-1})	(J mol^{-1} K^{-1})
H_2O + NaBr	0.05	310.55	-0.552		
	0.1	310.55	-0.353		
	1.0	310.55	-0.040		
	3.0	310.55	0.011		
	5.0	310.55	-0.589		
	8.0	310.55	-1.012		
H_2O + NaBr	1.0	290.55	-1.379	5.907	25.08
		295.55	-0.356	5.376	19.40
		300.55	0.033	5.188	17.15
		305.55	-0.601	4.959	18.20
		310.55	-0.720	4.784	17.73
		315.55	-0.507	4.632	16.28
		320.55	-0.019	4.668	14.62
H_2O + Na_2SO_4	0.05	310.55	-0.573		
	0.1	310.55	-0.143		
	1.0	310.55	-0.083		
	3.0	310.55	-0.040		
	5.0	310.55	-0.180		
	8.0	310.55	0.085		
H_2O + Na_2SO_4	1.0	290.55	-1.007	4.808	20.01
		295.55	-1.071	4.668	19.42
		300.55	-1.155	4.508	18.84
		305.55	-0.657	4.287	16.18
		310.55	-0.764	4.212	16.02
		315.55	-0.324	4.257	14.52
		320.55	0.158	4.449	13.39
H_2O + Na_3PO_4	0.05	310.55	-0.584		
	0.1	310.55	-0.395		
	1.0	310.55	-1.063		
	3.0	310.55	-0.787		
	5.0	310.55	-0.474		
	8.0	310.55	-0.456		
H_2O + Na_3PO_4	1.0	290.55	-0.836	5.131	20.54
		295.55	-0.903	5.146	20.47
		300.55	-0.988	5.151	20.42
		305.55	-1.405	5.030	21.06
		310.55	-1.743	4.944	21.53
		315.55	-1.561	4.891	20.45
		320.55	-1.353	4.900	19.51

H_2O + NaOAc	0.05	310.55	-0.531		
	0.1	310.55	-0.342		
	1.0	310.55	-0.868		
	3.0	310.55	-0.570		
	5.0	310.55	-0.239		
	8.0	310.55	-0.162		
H_2O + NaOAc	1.0	290.55	-0.042	2.224	7.799
		295.55	0.160	2.285	7.188
		300.55	0.106	2.410	7.666
		305.55	-0.288	2.459	8.993
		310.55	-1.087	2.414	11.27
		315.55	-0.872	2.505	10.70
		320.55	-0.898	2.532	10.70

Table S2. Top 5 binding site properties.

Bovine trypsin (PDB ID)	SDS (Pubchem ID)	Binding Energy (kcal/mol)	Cavity volume ($Å^3$)	Contact residues
1HJ9	3423265	-5.0	64	HIS57 SER96 ASN97 THR98 LEU99 GLN175 ASP189 SER190 CYS191 GLN192 GLY193 ASP194 SER195 VAL213 SER214 TRP215 GLY216 SER217 GLY219 CYS220 GLY226 VAL227 TYR228
1HJ9	3423265	-4.5	149	TYR39 HIS40 PHE41 CYS42 HIS57 LYS60 ILE73 SER96 ASN97 THR98 LEU99 TRP141 TYR151 PRO152 TYR172 GLY174 GLN175 SER190 CYS191 GLN192 GLY193 ASP194 SER195 VAL213 SER214 TRP215 GLY216 SER217 GLY219 CYS220 VAL227
1HJ9	3423265	-4.4	109	SER32 ASN34 GLY38 TYR39 HIS40 PHE41 CYS42 ARG66 ILE73 ASN74 VAL75 TRP141 TYR151 PRO152 GLN192 GLY193 ASP194 SER195
1HJ9	3423265	-3.9	87	HIS91 PRO92 SER93 ASN100 ASN101 CYS128 ALA129 SER130 ALA132 GLY133 THR134 GLN135 CYS136 LEU137 LYS159 ILE162 LEU163 SER164 ASP165 SER166 THR177 SER178 ASN179 PHE181 VAL200 CYS201 SER202 GLY203 GLN210 LYS230 CYS232 ASN233 TYR234 VAL235 SER236 TRP237
1HJ9	3423265	-3.9	69	PRO28 TYR29 ILE47 ASN48 SER49 GLN50 TRP51 LYS107 ALA119 SER120 ILE121 SER122 LEU123 GLY203 ILE238 LYS239 GLN240 ILE242 ALA243 ASN245

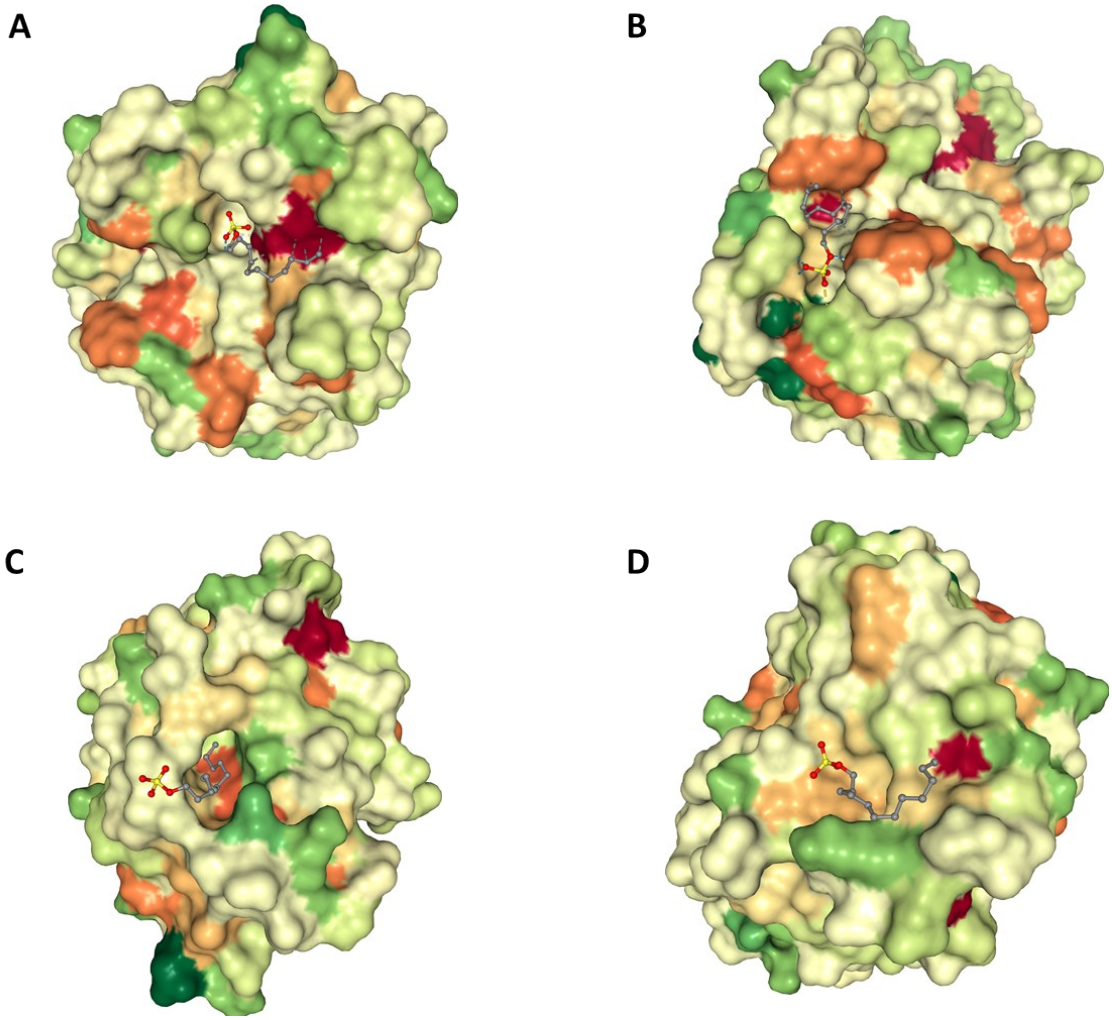

Fig. S1. Molecular docking interactions of trypsin and SDS using CB-dock at different sites revealed binding affinities of (A) -4.5, (B) -4.4, (C) -3.9, and (D) -3.9 kcal/mol.