Supporting Information

Brave New Surfactant World Revisited by Thermoalkalophilic Lipases: Computational Insights into the Role of SDS as a Substrate Analog

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Table S1 Details of MD systems

System	Protein	SDS	Water	Ca^{2+}	Zn^{2+}	*x,y,z* (Å)
Water (monomer)	388	0	19000	1	1	87,87,112
20 SDS (monomer)	388	20	10000	1	1	105,97,75
180 SDS (monomer)	388	180	10000	1	1	94,94,98
20 SDS (dimer)	773	20	25000	2	2	130,89,116

Number of residues/molecules were listed.
Dimensions of the systems were measured after equilibration.
Dimer system was simulated for 0.5 μs while the rest for 2 μs.

Table S2 Tunnel analysis of the closed lipase systems at 298 K

	Snapshot	n	Radius	Length	Curvature	T.
open	2W22	3	2.5	1.9	1.2	0.94
			2.0	5.3	1.1	0.87
			2.1	11.3	1.5	0.80
closed	1KU0	0				
water	0 μs	0				
	1 μs	1	1.9	3.5	1.0	0.9
	2 μs	0				
20-SDS	0 μs	0				
	1 μs	0				
	2 μs	1	2.2	2.4	1.2	0.92
180-SDS	0 μs	0				
	1 μs	1	2.5	2.5	1.1	0.93
	2 μs	3	2.7	3	1.0	0.93
			2.6	1.5	1.0	0.92
			1.8	7.4	1.1	0.81

Radius and length are in Åunits.
n shows the number of tunnels predicted by CAVER 3.0.
n=0 marks the structures that did not show any tunnels.
T. stands for throughput score.

Figures

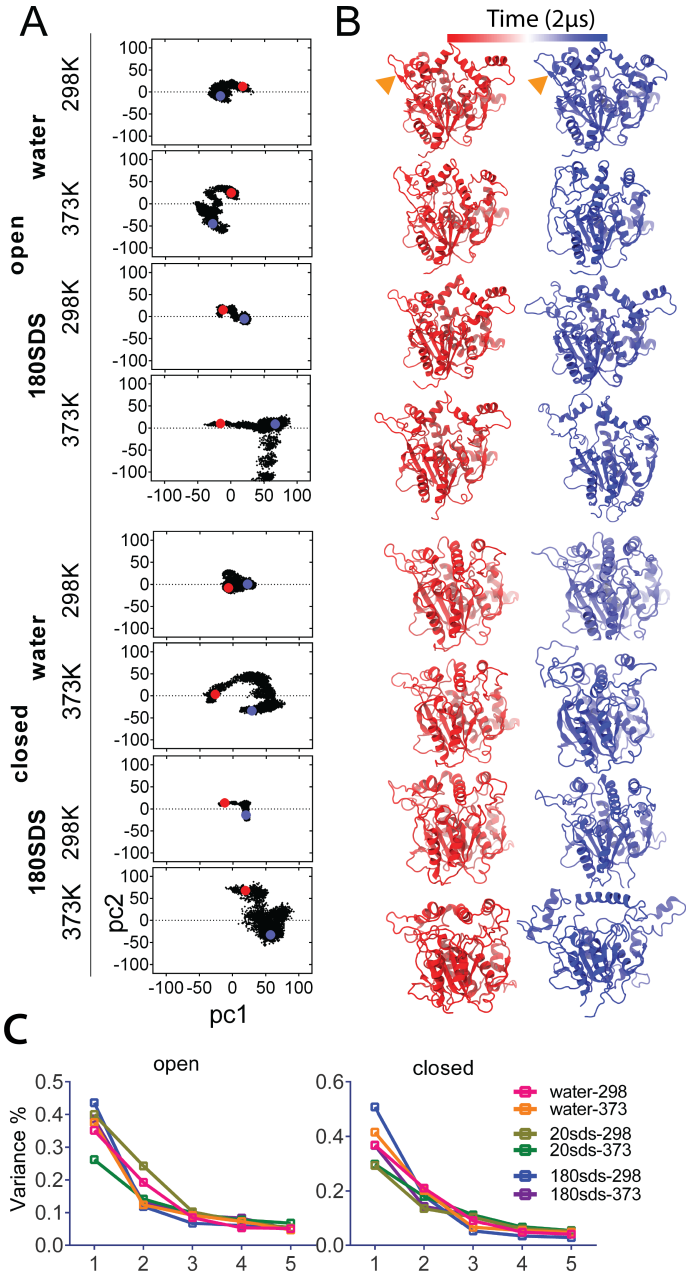

Figure S1 (A) Scatter plots of the first two pcs (x, y; pc1, pc2), (B) Representative conformations showing the start and end configurations that were obtained from the respective dots in (A). Red: start, blue: end. Orange arrow marks the flap structure. (C) Scree plots showing the variance explained by the first 5 pcs.

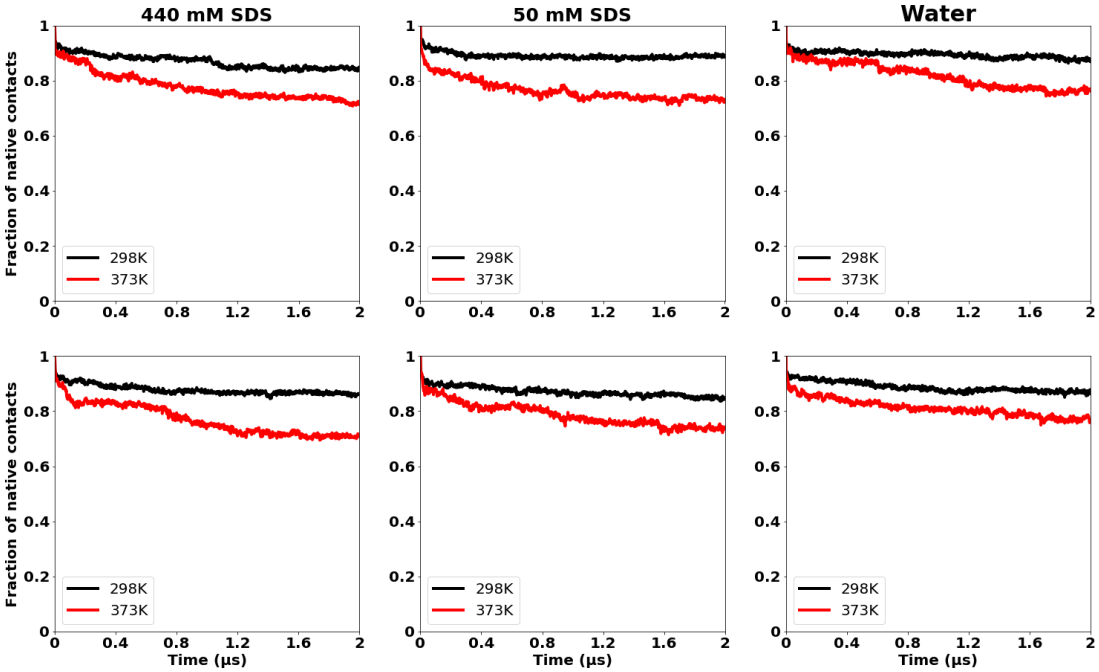

Figure S2 Fraction of native contacts was computed for the closed lipase (top row) and open lipase simulations (bottom row). The first and second columns indicate 180- and 20-SDS containing systems, respectively and the last column shows control/water simulations. For all, black lines show 298 K and red lines show 373 K simulations.

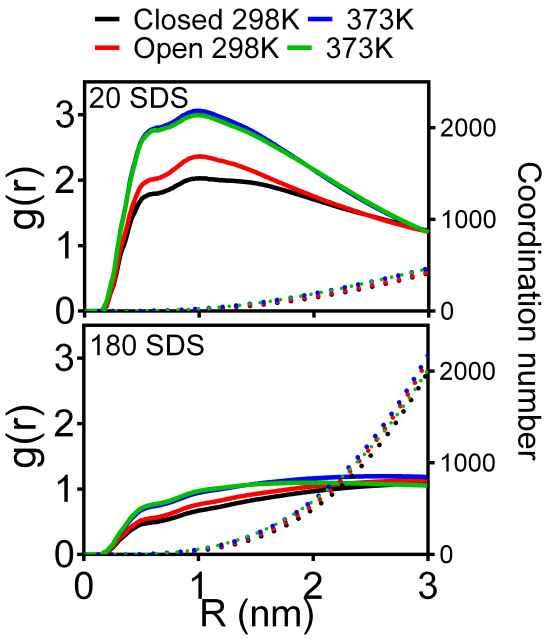

Figure S3 COM-COM RDF analysis of lipase-SDS. Dotted lines show coordination number on the right axes.

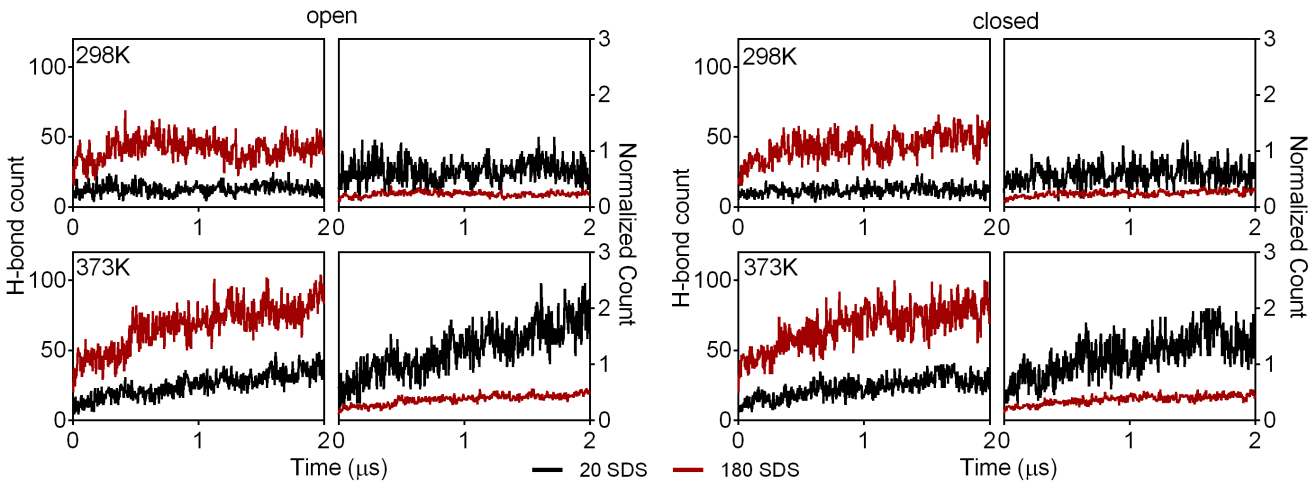

Figure S4 Intermolecular H-bonds formed between (left) SDS-open lipase and (right) SDS-closed lipase. For each panel, left plots show raw counts and the right plots show normalized counts.

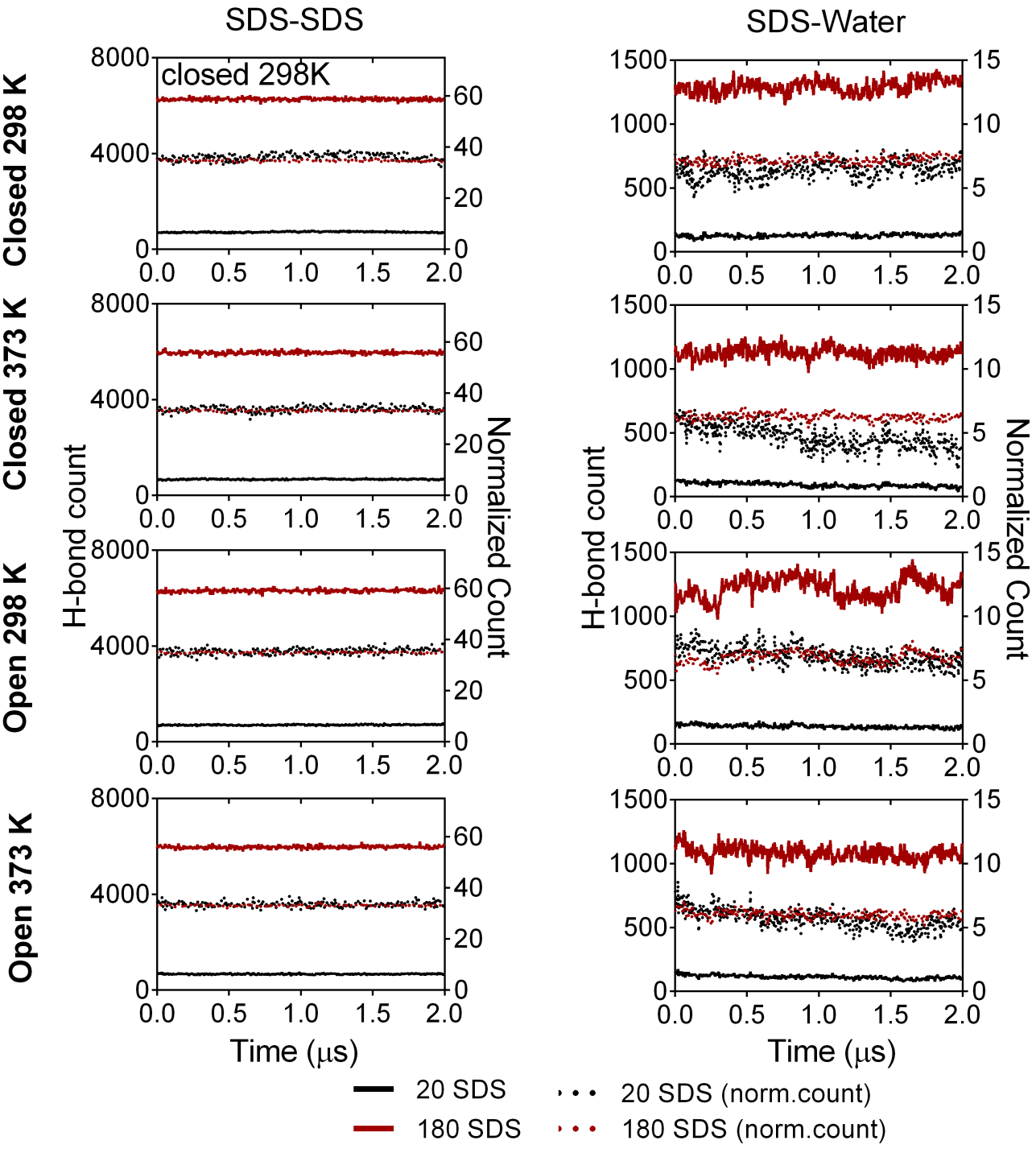

Figure S5 Intermolecular H-bonds between SDS-SDS and SDS-water. Raw counts were shown by solid lines at the left y-axis and normalized counts were shown by dotted lines at the right axis. Normalization constant was 20 and 180 for the 20- and 180-SDS containing systems respectively.

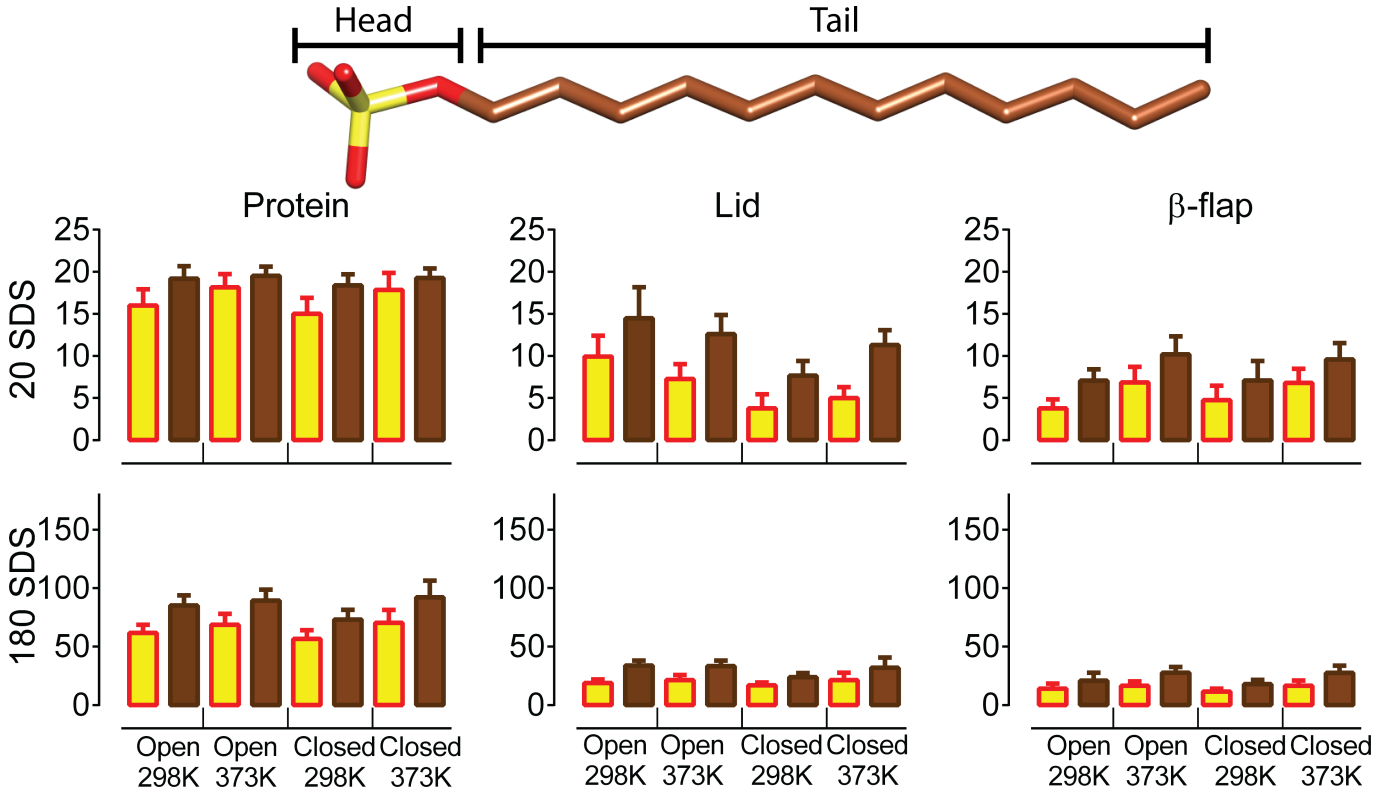

Figure S6 Distributions of lipase-SDS contacts formed by the ionic head group (yellow) or hydrophobic tail (brown).

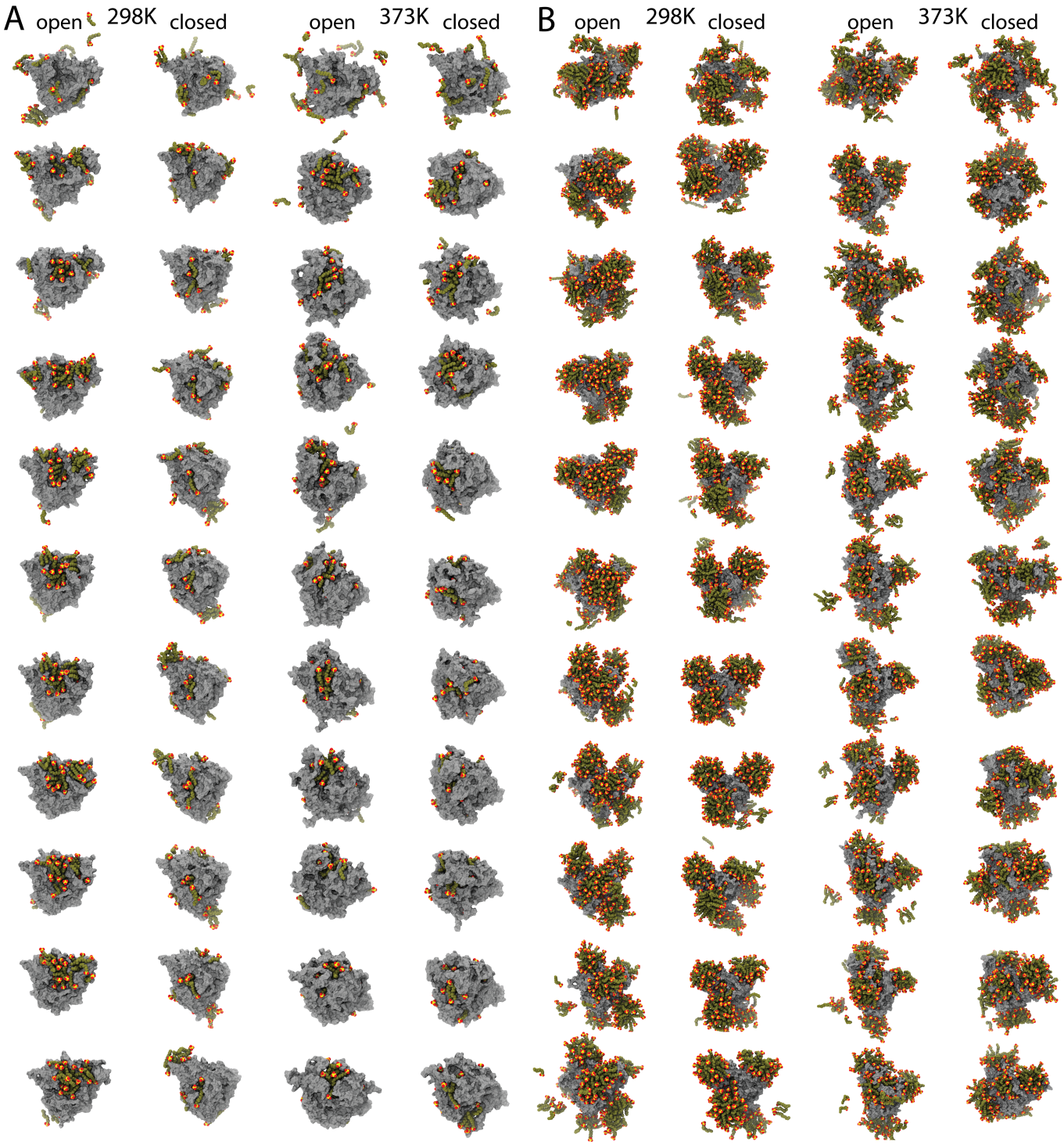

Figure S7 Snapshots were extracted from every 200 ns of (A) 20-SDS and (B) 180-SDS containing simulations. For clarity waters and ions were not shown.

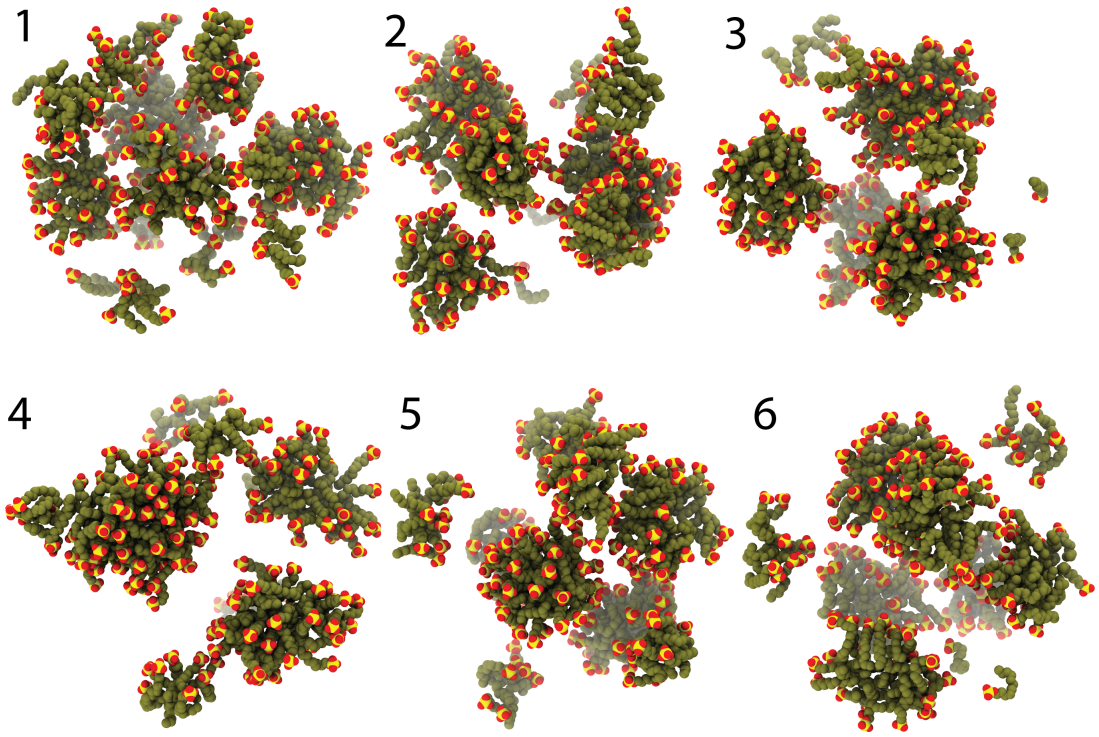

Figure S8 SDS assemblies were visualized from lipase free simulations performed in the presence of 180 SDS for 500 ns at 373 K.

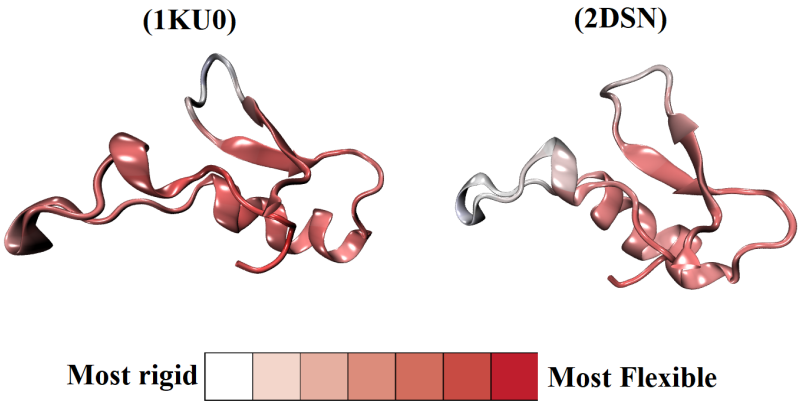

Figure S9 Normalized temperature factor were color-scaled on the structures of the β-flap domains of the 1KU0 and 2DSN structures.

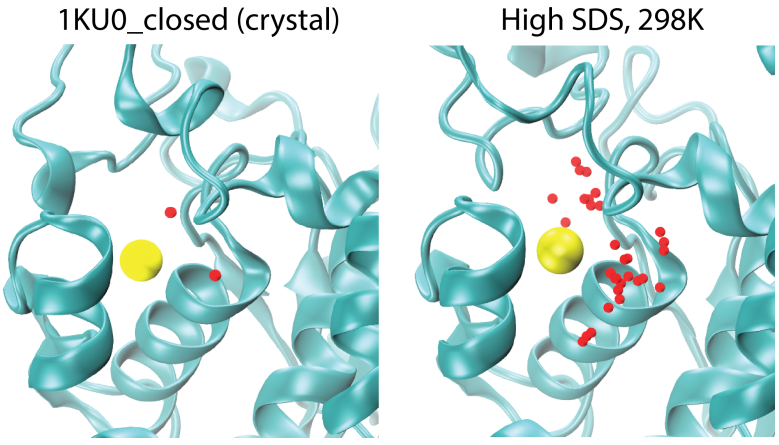

Figure S10 (left) Two crystal waters attached to zinc and (right) the shortened trajectory of waters in close proximity to zinc.