

A theoretical and experimental investigation on the effect of sodium dodecyl sulfate on the structural and conformational properties of bovine β -casein

Meng Zhou ^{a1}, Yuanyuan Xiao ^{a1}, Feng Cao ^{a1}, Na Li ^c, Yacine Hemar ^d, Shangwen Tang^{a*}, Yang Sun ^{a,b*}

^a School of Food Science and Technology & School of Chemical Engineering, Hubei University of Arts and Science, Xiangyang, Hubei 441053, China

^b School of Life Sciences, Tsinghua University, Beijing 100084, China

^c Shanghai Science Research Center, Chinese Academy of Sciences, Shanghai, 201204, China

^d The Riddet Institute, Palmerston North, New Zealand.

¹ These authors are equal to this work

* Corresponding authors: tsw830629@163.com, sunyang@hbuas.edu.cn

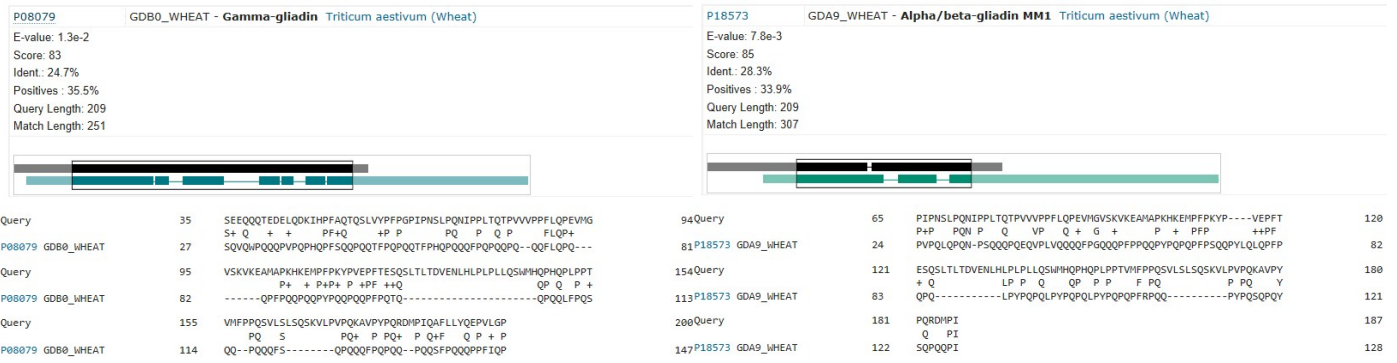


Figure. S1. The Protein sequence alignment of bovine β -casein with γ -Gliadin (PDB ID: 5KSA) and α/β -gliadin MM1 (PDB ID: 2NNA) using BLAST against Protein Data Bank (PDB).

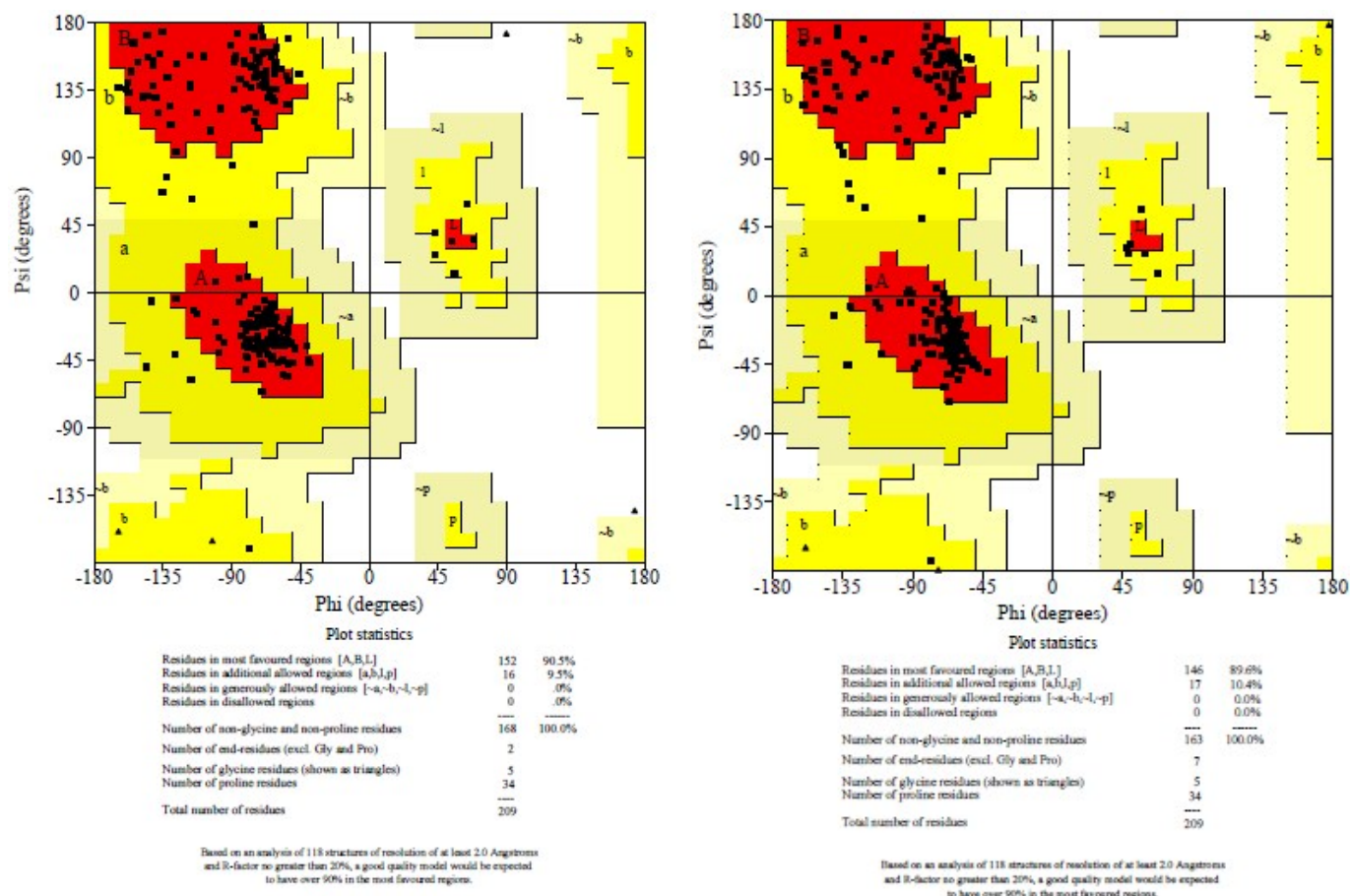


Figure S2. Stereochemical analysis of MODELLER (left) and I-TASSER (right) modelling structure obtained from Ramachandran plots. Red color in the plots represents the most favorable region, yellow indicates additionally allowed, light yellow suggests generously allowed and white field indicates disallowed region.

Table S1 Details of MD simulations

System	Number of SDS/Na ⁺	Volume of box (nm ³)	Temperature (K) pressure (Bar)	Simulation time (ns)
β -Casein-water	0	502.25	300 / 1	300
β -Casein-1 mM SDS	132	1402.72	300 / 1	300
β -Casein-10 mM SDS	504	1273.79	300 / 1	300

Table S2 Calculated energy components of bovine β -casein with different concentrations of SDS

Energy component (kJ mol ⁻¹)	β -casein-1 mM SDS	β -casein-10 mM SDS
ΔE_{elec}	-383.90 \pm 16.89	-1765.24 \pm 17.47
ΔE_{vdw}	-767.79 \pm 33.78	-882.62 \pm 34.29
ΔE_{MM}^*	-1151.69 \pm 10.21	-2647.87 \pm 20.23
$\Delta G_{\text{nonpolar,sol}}$	-881.84 \pm 30.63	-2076.39 \pm 28.83
$\Delta G_{\text{polar,sol}}$	-105.08 \pm 3.02	-206.00 \pm 2.317
$\Delta E_{\text{vdw}} + \Delta G_{\text{nonpolar,sol}}$	-1649.63 \pm 17.35	-2959.01 \pm 31.36
$\Delta E_{\text{elec}} + \Delta G_{\text{polar,sol}}$	-488.97 \pm 22.32	-1971.25 \pm 24.31
ΔG_{total}	-2138.60 \pm 33.10	-4930.26 \pm 27.53