

Electronic Supplementary Information

# The Structural Changes of a Bovine Casein Micelle during Temperature Change; In situ Observation over a Wide Spatial Scale from Nano to Micrometer

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Table S1. Fraction, molecular weight, chemical formula and electron density of casein proteins.

Casein	%	Molecular weight (g/mol)	Chemical formula	Electron density ( $e^-/\text{nm}^3$ )
$\alpha_{s1}$	38.2	23614	$\text{C}_{1035}\text{H}_{1595}\text{N}_{265}\text{O}_{341}\text{S}_5\text{P}_8$	437.3
$\alpha_{s2}$	11	25228	$\text{C}_{1083}\text{H}_{1718}\text{N}_{287}\text{O}_{371}\text{S}_6\text{P}_{11}$	437.5
$\beta$	39.5	23983	$\text{C}_{1080}\text{H}_{1697}\text{N}_{268}\text{O}_{325}\text{S}_6\text{P}_5$	438.6
$\kappa$	11.3	19003	$\text{C}_{850}\text{H}_{1323}\text{N}_{222}\text{O}_{262}\text{S}_4\text{P}_1$	438.2

Table S2. Concentration of lactose,  $\beta$ -Lactoglobulin and  $\alpha$ -Lactalbumin in skim milk used in this study.

	Concentration g/L
Lactose	47.4
$\beta$ -Lactoglobulin	4.61
$\alpha$ -Lactalbumin	1.02

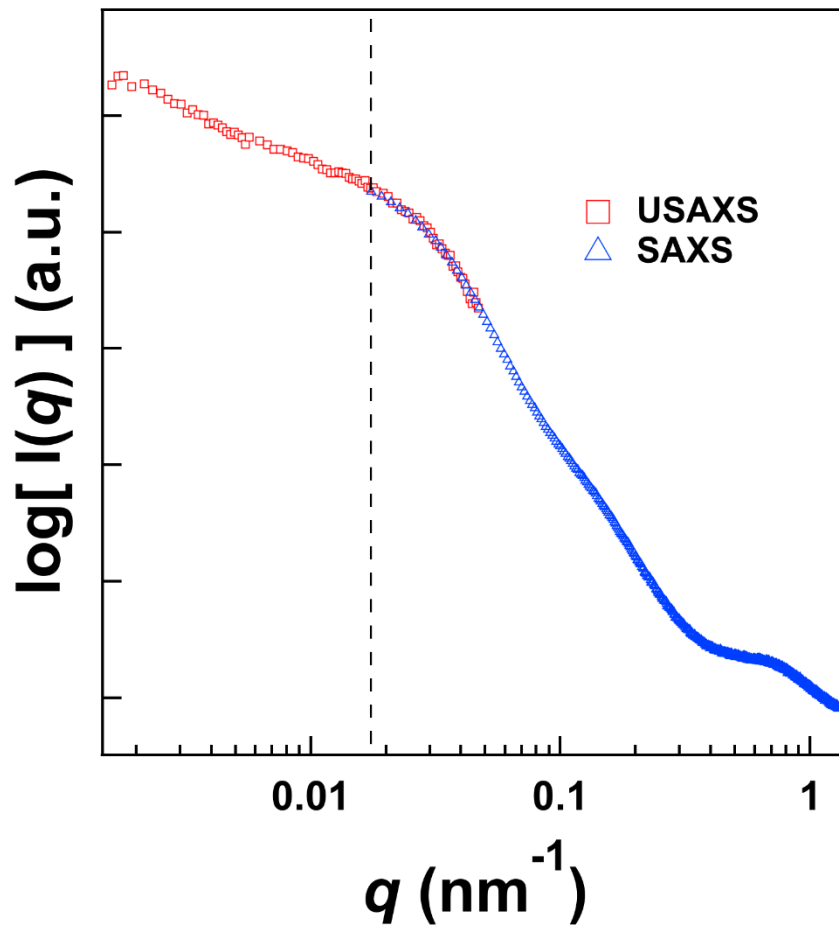


Figure S1. USAXS and SAXS profiles of skim milk obtained at 30 °C. Red squares and blue triangles represent USAXS ( $0.0016 < q < 0.047 \text{ nm}^{-1}$ ) and SAXS ( $0.017 < q < 1.3 \text{ nm}^{-1}$ ) data, respectively. The USAXS data in the range of  $0.017 < q < 0.047 \text{ nm}^{-1}$  overlapped almost completely.

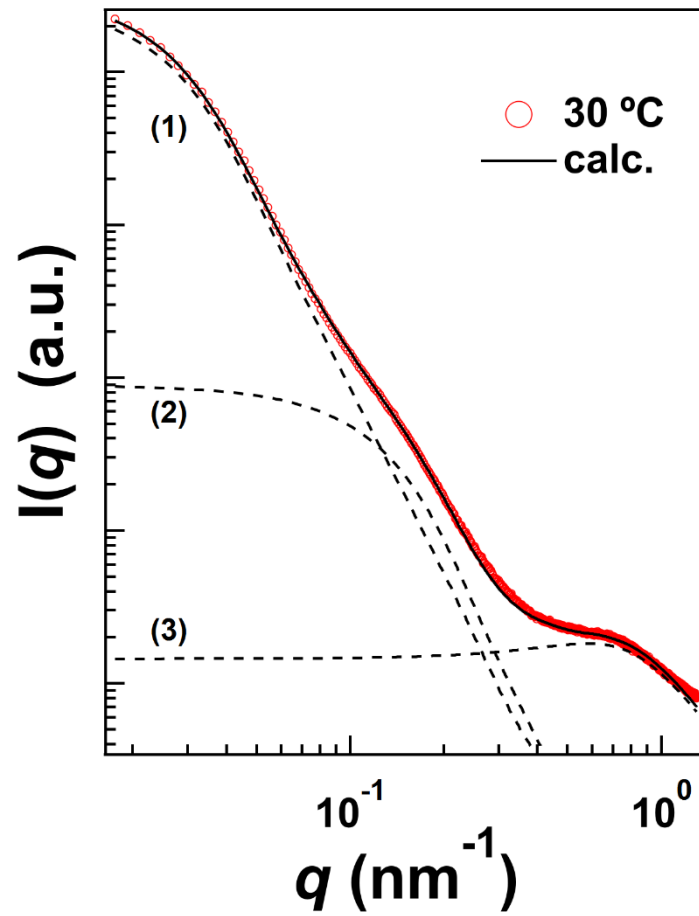


Figure S2. SAXS profile obtained at 30 °C during the heating process. The solid lines represent the curves calculated using eq. (2). The dashed lines (1)–(3) refer to the contribution of the first three terms in eq. (2)