Electronic Supplementary Information for

Binding behaviors and structural characteristics of ternary complexes of β-lactoglobulin, curcumin, and fatty acids

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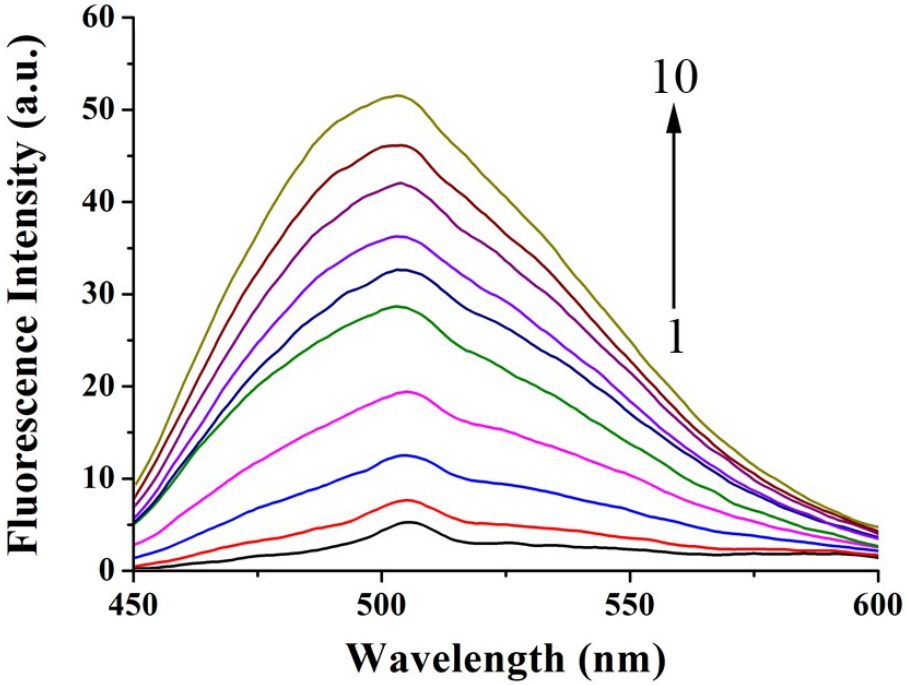

Fig. S1 Fluorescence emission spectra of curcumin (2 μM) in buffer solution in the presence of β-lg at different concentrations. $C_{β\text{-lg}}$ = 0, 3, 9, 12, 15, 18, 21, 24, 27, 30 μM (labeled as 1 to 10). The emission spectra were recorded from 450 nm to 600 nm with an excitation wavelength of 425 nm.

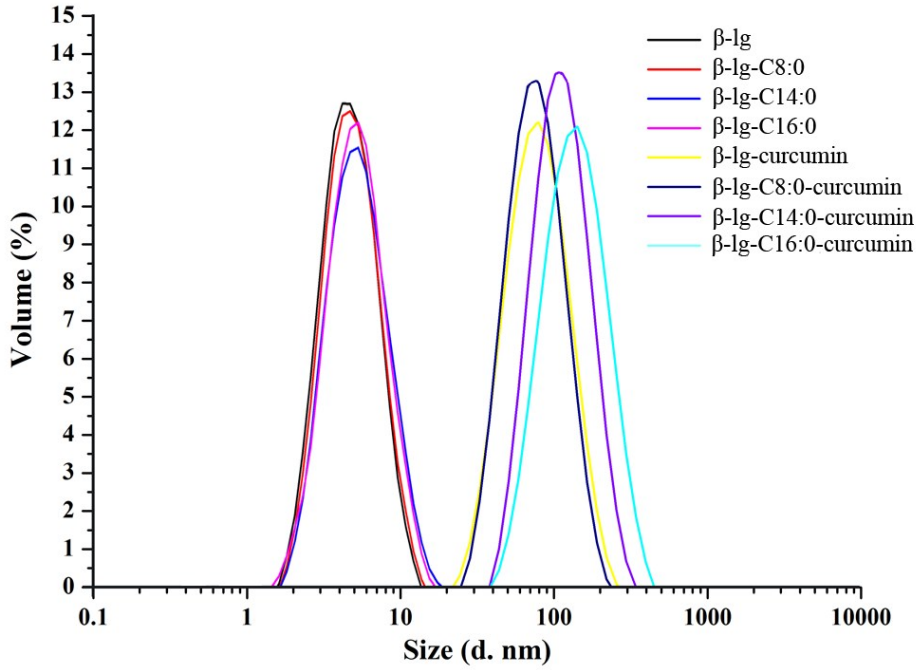

Fig. S2 Particle size distribution curves for the samples determined based on dynamic light scattering data.

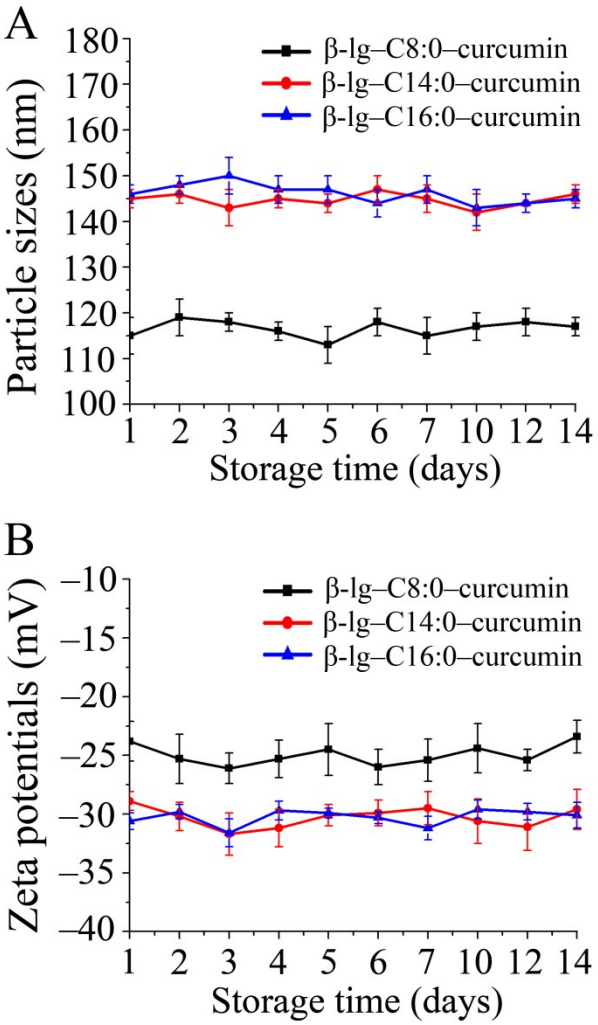

Fig. S3 The mean sizes (A) and zeta potentials (B) of the samples at 4°C during 14 days storage.

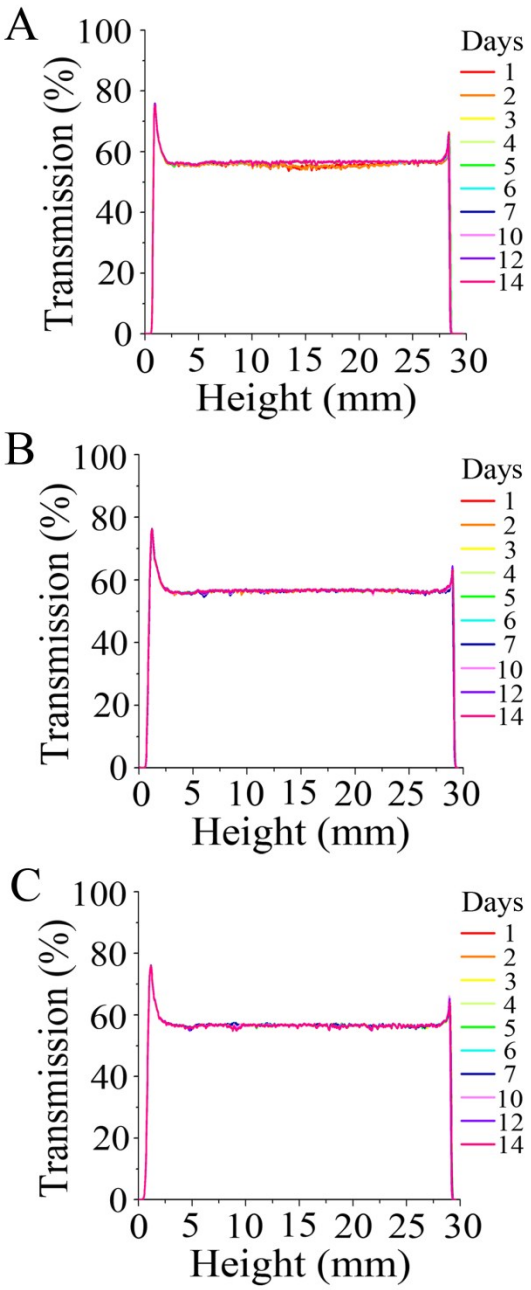

Fig. S4 Transmission profiles of the samples at 4°C during 14 days storage using Turbiscan analysis. (A), (B) and (C) show the profiles of β-lg–C8:0–curcumin, β-lg–C14:0–curcumin, and β-lg–C16:0–curcumin ternary complexes, respectively.

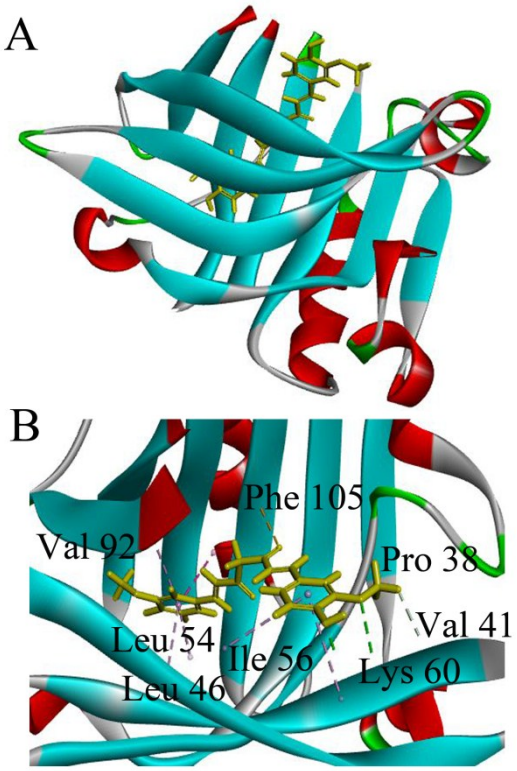

Fig. S5 Docked structure corresponding to the minimum energy conformation for the β-lg–curcumin complex. (A) Overview of binding behaviors of β-lg with curcumin. (B) Detailed illustration of the amino acids near curcumin. In the complex, the yellow ligand represents curcumin.

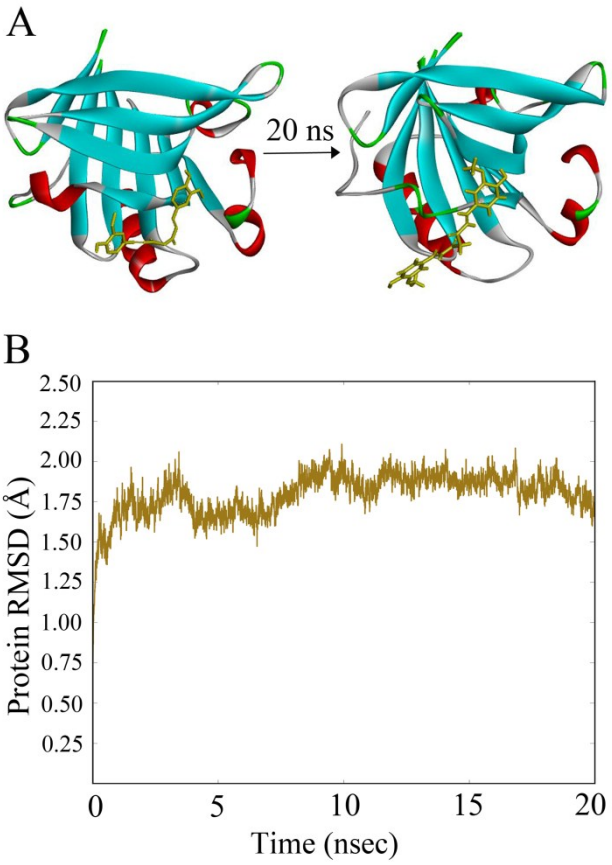

Fig. S6 The conformation changes (A) and the root mean square deviation (RMSD) values (B) of complex during molecular dynamics simulation. In the complex, the yellow ligand represents curcumin.