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Supplementary information

Interaction of Plant Alkaloid Berberine with β-Lactoglobulin: An Account from Spectroscopic, Thermodynamic and Small-angle X-ray Scattering Studies Aided by Theoretical Calculations

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Figure S1: Scatchard plot: Variation of [PL]/[L] as a function of [PL] for the binding of BER with β -LG.



Figure S2: Benesi-Hildebrand (B–H) plot of 1/[F0 – F] as a function of 1/[BER]. Inset shows the modified B-H plot of 1/[F0 – F] vs $1/[BER]^2$ for the binding interaction between β -LG and BER.



Figure S3: Variation of [(F0 - F)/F] as a function of [BER] for the binding of BER with β -LG.



Figure S4. MRE value of β -LG [5 μ M] in absence (Black) and in the presence of 15 μ M (Red) and 30 μ M (Blue) BER.

Table S1. Percentages of the secondary structural components of β -LG in absence and in the presence of BER of varied concentrations

BER Concentration (µM)	% of α–helix	% of β–sheet	% of random coil
0 (pure β-LG)	14.4	45.5	40.1
15	15.4	43.8	40.8
30	15.8	42.7	41.5