Supporting Information

Deciphering the binding patterns and conformation changes upon the bovine serum albumin-rosmarinic acid complex

Xin Peng,^{‡ab} Xiangchao Wang, ^{‡b} Wei Qi,^{*bcde}, Renliang Huang,^f Rongxin Su^{bcde} and Zhimin He^{bc}

^aSchool of Life Sciences, Tianjin University, Tianjin 300072, PR China

^bChemical Engineering Research Center, School of Chemical Engineering and Technology, Tianjin University, Tianjin 300072, PR China

^cState Key Laboratory of Chemical Engineering, Tianjin University, Tianjin 300072, PR China

^dCollaborative Innovation Center of Chemistry Science and Engineering (Tianjin), Tianjin 300072, PR China

^eTianjin Key Laboratory of Membrane Science and Desalination Technology, Tianjin, 300072, China

^fSchool of Environmental Science and Engineering, Tianjin University, Tianjin 300072, PR China

[‡] These authors contributed equally to this work.

Tel: +86-22-27407799

E-mail: qiwei@tju.edu.cn (W. Qi)

^{*}Corresponding author: Wei Qi

Address: Chemical Engineering Research Center, School of Chemical Engineering and Technology, Tianjin University, Tianjin 300072, PR China

Fax: +86-22-27407599



Fig. S1. Fluorescence titration curves of BSA-RA system at λ_{ex} = 280 and 295 nm. C_{BSA} = 5.0 × 10⁻⁶ mol L⁻¹, T = 298 K, pH = 7.4.



Fig. S2. UV-vis absorption spectra of BSA in the presence of RA. T = 298 K, pH = 7.4, $C_{BSA} = 5.0 \times 10^{-6}$ mol L⁻¹, $C_{RA}/(\times 10^{-6})$ (a-m): 0, 2.5, 5, 7.5, 10, 15, 20, 25, 30, 35, 40,50, 60, respectively.



Fig. S3. The synchronous fluorescence spectra of BSA-RA at 298 K. (A) $\Delta \lambda = 15$ nm, (B) $\Delta \lambda = 60$ nm. The concentration of BSA was fixed at 5.0 × 10⁻⁶ mol L⁻¹ and the concentration of RA (1-10) were 0, 0.5, 1.0, 1.5, 2.0, 2.5, 3.0, 4.0, 5.0 and 6.0×10^{-5} mol L⁻¹, respectively.



Fig. S4. The three-dimensional fluorescence spectra (A, B) and corresponding contour spectra (A', B') of BSA and BSA-RA system at 298 K. (A and A') $C_{BSA} = 5.0 \times 10^{-6} \text{ mol } L^{-1}$, $C_{RA} = 0$, (B and B') $C_{BSA} = 5.0 \times 10^{-6} \text{ mol } L^{-1}$, $C_{RA} = 10.0 \times 10^{-6} \text{ mol } L^{-1}$.