Supporting Information

Characterization of Hydroxycinnamic Acids Derivatives Binding to Bovine Serum Albumin

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 HCAs



Figure S1. (a) ¹H NMR spectrum and (b) STD ¹H NMR spectrum of CFA in the presence of BSA. Spectra were taken at 298 K on a 400 MHz spectrometer with a room temperature probe. NS = 256, TD = 32K, sat pulse = -0.5 ppm for 3.0 sec (see Methods).



Figure S2. (a) ¹H NMR spectrum and (b) STD ¹H NMR spectrum of *m*-CA in the presence of BSA. Spectra were taken at 298 K on a 400 MHz spectrometer with a room temperature probe. NS = 256, TD = 32K, sat pulse = -0.5 ppm for 3.0 sec (see Methods).



Figure S3. (a) ¹H NMR spectrum and (b) STD ¹H NMR spectrum of *p*-CA in the presence of BSA. Spectra were taken at 298 K on a 400 MHz spectrometer with a room temperature probe. NS = 256, TD = 32K, sat pulse = -0.5 ppm for 3.0 sec (see Methods).



Figure S4. (a) ¹H NMR spectrum and (b) STD ¹H NMR spectrum of FA in the presence of BSA. Spectra were taken at 298 K on a 400 MHz spectrometer with a room temperature probe. NS = 256, TD = 32K, sat pulse = -0.5 ppm for 3.0 sec (see Methods).



Figure S5. (a) ¹H NMR spectrum and (b) ¹H STD NMR spectrum of SA in the presence of BSA. Spectra were taken at 298 K on a 400 MHz spectrometer with a room temperature probe. NS = 256, TD = 32K, sat pulse = -0.5 ppm for 3.0 sec (see Methods).



Figure S6. (a) ¹H STD NMR of 50 μ M BSA, 3 mM CHA without the site probe; (b) ¹H STD NMR of 50 μ M BSA, 3 mM CHA in the presence of 4.8 mM WAR; (c) ¹H STD NMR of 50 μ M BSA, 3 mM CHA in the presence of 4.8 mM Trp. The STD effects of H-8, calculated as I_{STD}/I_0 , were shown in the Figure. Spectra were taken at 298 K on a 400 MHz spectrometer with a room temperature probe. NS = 256, TD = 32K, sat pulse = -0.5 ppm for 3.0 sec (see Methods).



Figure S7. (a) ¹H STD NMR of 50 μ M BSA, 3 mM CFA without the site probe; (b) ¹H STD NMR of 50 μ M BSA, 3 mM CFA in the presence of 4.8 mM WAR; (c) ¹H STD NMR of 50 μ M BSA, 3 mM CFA in the presence of 4.8 mM Trp. The STD effects of H-8, calculated as I_{STD}/I_0 , were shown in the Figure. Spectra were taken at 298 K on a 400 MHz spectrometer with a room temperature probe. NS = 256, TD = 32K, sat pulse = -0.5 ppm for 3.0 sec (see Methods).



Figure S8. (a) ¹H STD NMR of 50 μ M BSA, 3 mM *m*-CA without the site probe; (b) ¹H STD NMR of 50 μ M BSA, 3 mM m-CA in the presence of 4.8 mM WAR; (c) ¹H STD NMR of 50 μ M BSA, 3 mM *m*-CA in the presence of 4.8 mM Trp. The STD effects of H-8, calculated as I_{STD}/I_0 , were shown in the Figure. Spectra were taken at 298 K on a 400 MHz spectrometer with a room temperature probe. NS = 256, TD = 32K, sat pulse = -0.5 ppm for 3.0 sec (see Methods).



Figure S9. (a) ¹H STD NMR of 50 μ M BSA, 3 mM 4-CA without the site probe; (b) ¹H STD NMR of 50 μ M BSA, 3 mM *p*-CA in the presence of 4.8 mM WAR; (c) ¹H STD NMR of 50 μ M BSA, 3 mM *p*-CA in the presence of 4.8 mM Trp. The STD effects of H-8, calculated as I_{STD}/I_0 , were shown in the Figure. Spectra were taken at 298 K on a 400 MHz spectrometer with a room temperature probe. NS = 256, TD = 32K, sat pulse = -0.5 ppm for 3.0 sec (see Methods).



Figure S10. (a) ¹H STD NMR of 50 μ M BSA, 3 mM SA without the site probe; (b) ¹H STD NMR of 50 μ M BSA, 3 mM SA in the presence of 4.8 mM WAR; (c) ¹H STD NMR of 50 μ M BSA, 3 mM SA in the presence of 4.8 mM Trp. The STD effects of H-8, calculated as I_{STD}/I_0 , were shown in the Figure. Spectra were taken at 298 K on a 400 MHz spectrometer with a room temperature probe. NS = 256, TD = 32K, sat pulse = -0.5 ppm for 3.0 sec (see Methods).



Figure S11. The Stern-Volmer curves of fluorescence quenching of BSA by CHA(a), CFA(b), m-CA(c), p-CA(d), FA(e), SA(f) at 298 K.



Figure S12. Double-log plot of fluorescence quenching of BSA by CHA(a), CFA(b), m-CA(c), p-CA(d), FA(e), SA(f) at 298 K.