Effect of caffeine and flavonoids on the binding of tigecycline to HSA: A spectroscopic study and molecular docking

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Supplementary material

Content

1.1. UV–Vis spectra of HSA-TGC in the presence of ALK and FLAVs

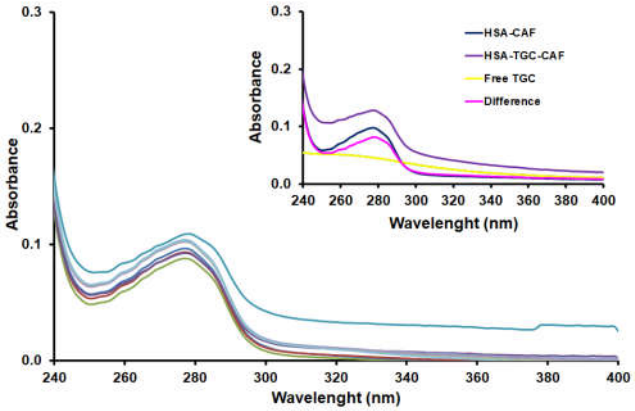


Figure S1. UV–Vis absorption spectra of HSA-CAF (1:1) in the absence and presence of increasing amounts of TGC (T = 298 K, pH = 7.4). [HSA] = 2 μM; [CAF] = 2 μM; [TGC] = 0 to 1 x 10^{-5} M. Inset: absorption spectrum of HSA-CAF; absorption spectrum of TGC only; absorption spectrum of HSA-TGC-CAF (1:2:1) complex; difference between absorption spectrum of HSA-TGC-CAF complex and free TGC.

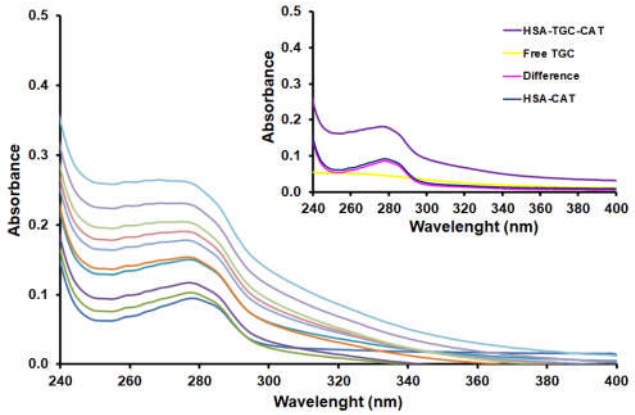


Figure S2. UV–Vis absorption spectra of HSA-CAT (1:1) in the absence and presence of increasing amounts of TGC (T = 298 K, pH = 7.4). [HSA] = 2 μM; [CAT] = 2 μM; [TGC] = 0 to 1 x 10^{-5} M. Inset: absorption spectrum of HSA-CAT; absorption spectrum of TGC only; absorption spectrum of HSA-TGC-CAT (1:2:1) complex; difference between absorption spectrum of HSA-TGC-CAT complex and free TGC.

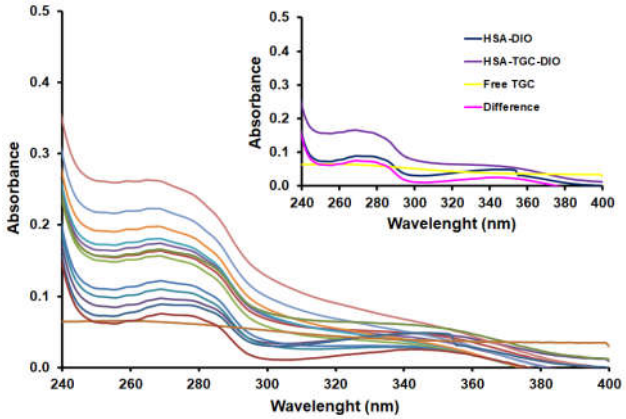


Figure S3. UV–Vis absorption spectra of HSA-DIO (1:1) in the absence and presence of increasing amounts of TGC (T = 298 K, pH = 7.4). [HSA] = 2 μM; [DIO] = 2 μM; [TGC] = 0 to 1 x 10^{-5} M. Inset: absorption spectrum of HSA-DIO; absorption spectrum of TGC only; absorption spectrum of HSA-TGC-DIO (1:2:1) complex; difference between absorption spectrum of HSA-TGC-DIO complex and free TGC.

1.2. Fluorescence emission spectra of HSA-TGC-CAT system

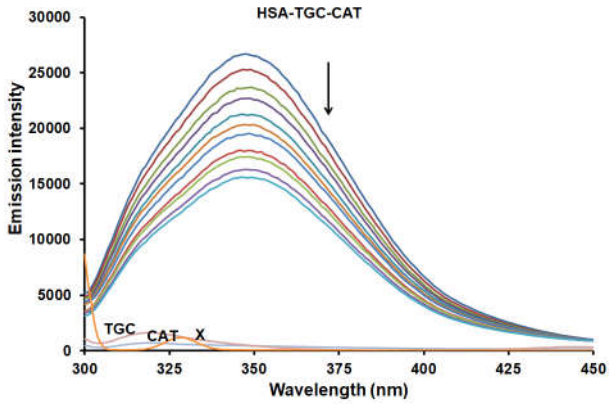


Figure S4. Fluorescence emission spectra of HSA-TGC (T = 298 K, pH = 7.4) in the presence of CAT. [HSA] = 2 μM, [CAT] = 2 μM and [TGC] = 0 to 1 x 10^{-5} M. X represents buffer only.

1.3. Fluorescence emission spectra of HSA-TGC-DIO system

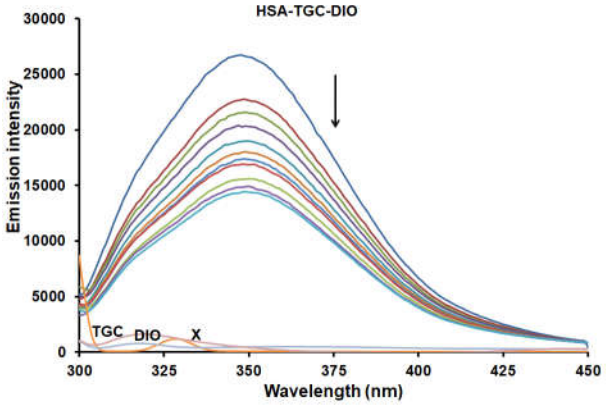


Figure S5. Fluorescence emission spectra of HSA-TGC (T = 298 K, pH = 7.4) in the presence of DIO. [HSA] = 2 μM, [DIO] = 2 μM and [TGC] = 0 to 1 x 10^{-5} M. X represents buffer only.

1.4. Stern-Volmer plots of the fluorescence quenching of HSA-TGC system by ALK and FLAVs

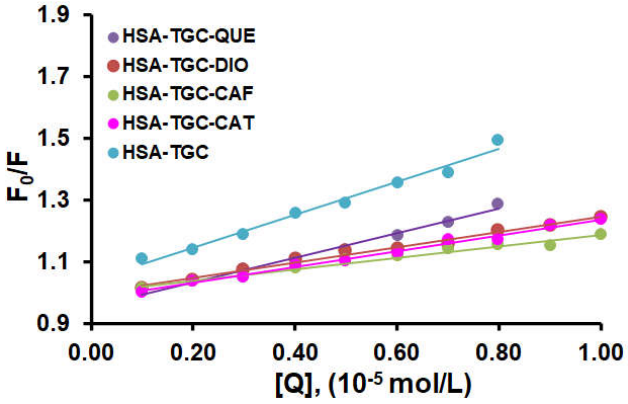
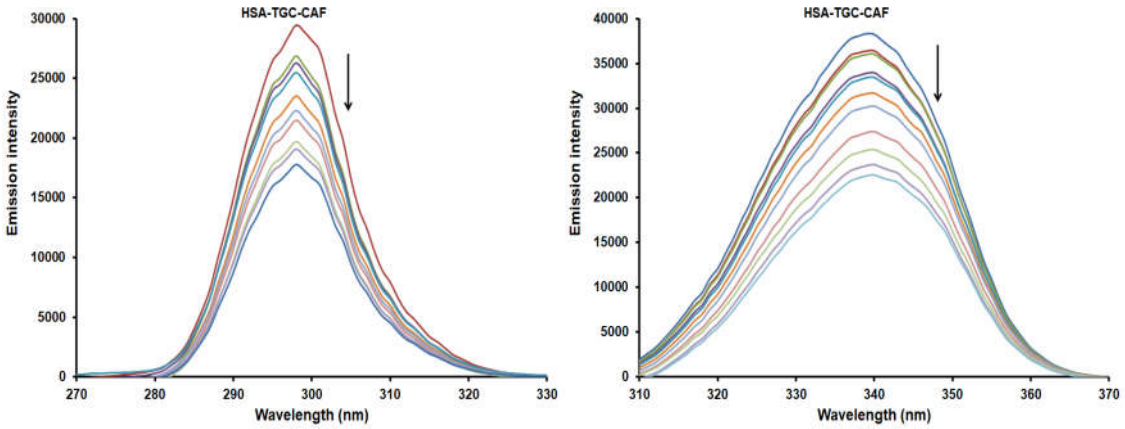


Figure S6. Stern-Volmer plots of the of the fluorescence quenching of HSA by TGC in the presence of CAF/FLAVs (QUE, CAT and DIO) at 298 K

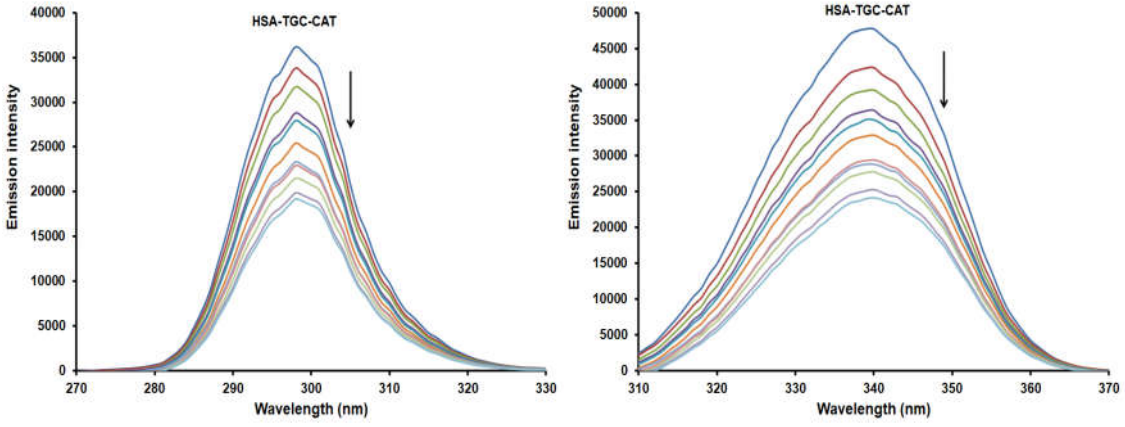
1.5. Synchronous fluorescence emission spectra of HSA-TGC-CAF system



(a) (b)

Figure S7. The effect of CAF on the synchronous fluorescence emission spectra of HSA-TGC system (T = 298 K, pH = 7.4): a) $\Delta\lambda$=15 nm and b) $\Delta\lambda$=60 nm. [HSA] = 2 μM, [CAF] = 2 μM and [TGC] = 0 to 1 x 10^{-5} M.

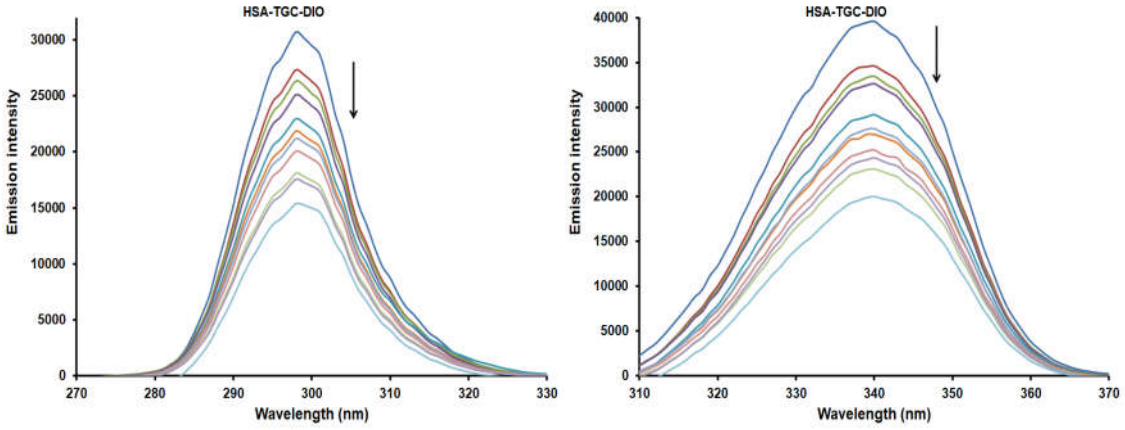
1.6. Synchronous fluorescence emission spectra of HSA-TGC-CAT system



(a) (b)

Figure S8. The effect of CAT on the synchronous fluorescence emission spectra of HSA-TGC system (T = 298 K, pH = 7.4): a) $\Delta\lambda$=15 nm and b) $\Delta\lambda$=60 nm. [HSA] = 2 μM, [CAT] = 2 μM and [TGC] = 0 to 1 x 10^{-5} M.

1.7. Synchronous fluorescence emission spectra of HSA-TGC-DIO system



(a) (b)

Figure S9. The effect of DIO on the synchronous fluorescence emission spectra of HSA-TGC system (T = 298 K, pH = 7.4): a) $\Delta\lambda$=15 nm and b) $\Delta\lambda$=60 nm. [HSA] = 2 μM, [DIO] = 2 μM and [TGC] = 0 to 1 x 10^{-5} M.

1.8. FT–IR spectra of HSA in presence and absence of TGC and CAT

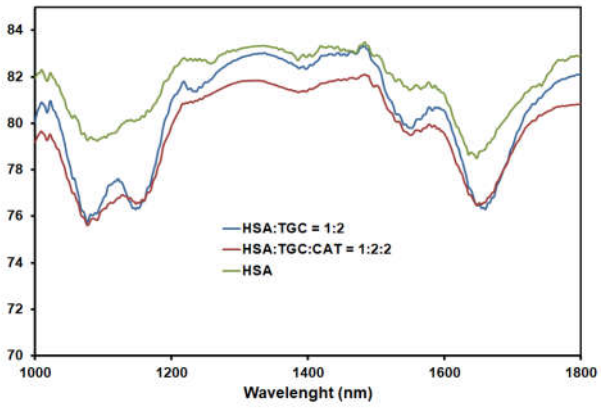


Figure S10. FT-IR spectra (wavenumber = 1000–1800 cm^{-1}) for HSA (2 μM) in presence and absence of TGC and CAT (4 μM)