Supplementary Information

Effect of the Single and Double Chain Surfactant–Cobalt(III) Complexes on Their Hydrophobicity, Micelle Formation, Interaction with Serum Albumins and Antibacterial Activities

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Calculation of thermodynamic parameters

The thermodynamic parameters were obtained from the following equations (1–3),

$$\Delta G_m^o = RT(2 - \alpha_{ave}) \ln CMC \quad (1)$$

$$\Delta H_m^o = -RT^2 (2 - \alpha_{ave}) d\ln CMC / dT \quad (2)$$

$$\Delta S_m^o = (\Delta H_m^o - \Delta G_m^o) / T \quad (3)$$

where ΔG^o_m, ΔH^o_m and ΔS^o_m are the respective change in the standard Gibbs free energy, standard enthalpy and standard entropy per mole of monomer at micelle formation. R, T and α_{ave} are gas constant, absolute temperature and average degree of micellar ionization, respectively (α_{ave} is the ratio of slopes between above and below the CMC).

Calculation for interaction between surfactant–cobalt(III) complexes and BSA/HSA

i) Correction of inner filter effect. To eliminate the inner filter effect, absorbance measurements were performed at the excitation and emission wavelength for each concentration of metal complex (including the protein without metal complex), and then multiply the observed fluorescence value using the following equation,

$$F_{cor} = F_{obs} * 10^{(A_1 + A_2)/2}$$

where F_{cor} and F_{obs} are the fluorescence intensities corrected and observed, respectively, and A_1 and A_2 are the sum of the absorbance of protein and ligand at the excitation and emission wavelengths, respectively.

ii) Quenching and Binding parameters. In order to understand the quenching and binding behaviour, data were analyzed using the following equations (4) and (5) at 278, 293 and 308 K,

$$F_0/F = 1 + K_{sv}[Q] = 1 + k_q \tau_0 [Q] \quad (4)$$

$$\log [(F_o - F)/F] = \log K_b + n \log[Q] \quad (5)$$

where, F_0 and F are the steady state fluorescence intensities of protein in the absence and presence of the surfactant–cobalt(III) complex respectively, [Q] is the total concentration of the surfactant–cobalt(III) complex, τ_0 is the average lifetime of protein in the absence of surfactant–cobalt(III) complex, K_{sv} is Stern–Volmer quenching constant, k_q is quenching rate constant, K_b is the binding constant showing the extent of interaction between protein and surfactant–cobalt(III) complex and n is the binding number per albumin molecule. The values of K_{sv} and k_q can be obtained from the slope of plot between (F_0/F) versus [Q] (**Figure S9**and **S10**). Similarly, the values of K_b and n were evaluated from the intercepts and slopes of double logarithm regression curve respectively by plotting log(F_0-F/F) versus log[Q] (**Figure S11** and **S12**).

iii) Thermodynamics of interactions. In order to analyse thermodynamics of protein interaction, Ross and Subramanian have summarised the following equations 6 and 7, which can be used to indicate the type of binding associated with various interactions.

$$\ln K = -\Delta H^{o}/RT + \Delta S^{o}/R \quad (6)$$

$$\Delta G^{o} = -RT\ln K_b \quad (7)$$

where K_b is analogous to the associative binding constant at the corresponding temperature, and R is the gas constant. The enthalpy change (ΔH^{o}) and entropy change (ΔS^{o}) can be calculated from the slope and intercept of the van't Hoff relationship, respectively. The free energy (ΔG^{o}) change was estimated based on the binding constants at three different temperatures (**Figure S13**).

iv) Percentage of α–helix content. The observed ellipticity of CD results (in mill degrees) was expressed in terms of mean residue ellipticity (MRE) in deg cm^2 $dmol^{-1}$ according to the following equation:

$$\mathrm{MRE} = \frac{\mathrm{observed CD\,(mdeg)}}{10 n l C_p} \quad (8)$$

$$\alpha\,\mathrm{helix}\,(\%) = \frac{(-\mathrm{MRE}_{208} - 4000)}{33000 - 4000} \times 100 \quad (9)$$

where n is the number of amino acid residues in the protein, l is the cell path length and C_p is the molar concentration of the protein. The α–helix contents of free and combined BSA/HSA were calculated from mean residue ellipticity (MRE) values at 208 nm using the following equation: MRE_{208} is the observed MRE value at 208 nm, 4000 is the MRE of the β–form and random coil conformation cross at 208 nm, and 33,000 is the MRE value of a pure α-helix at 208 nm.

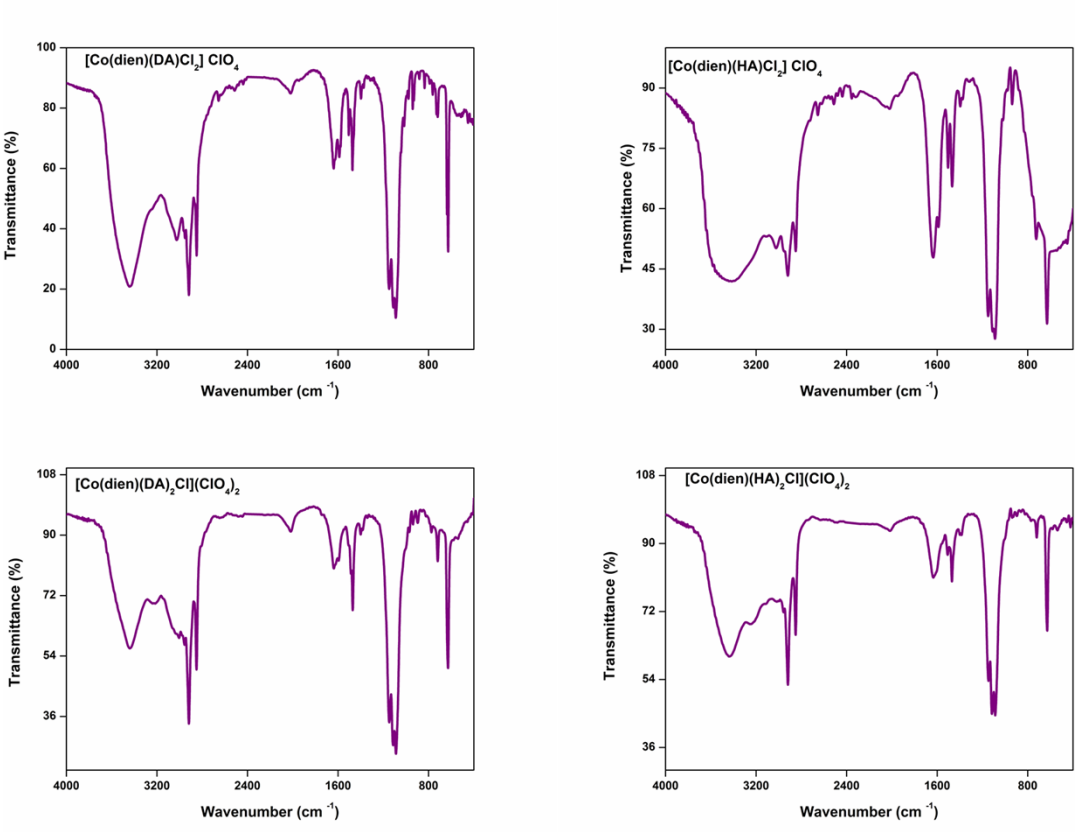

Figure S1. IR spectra of the surfactant–cobalt(III) complexes (**1**–**4**)

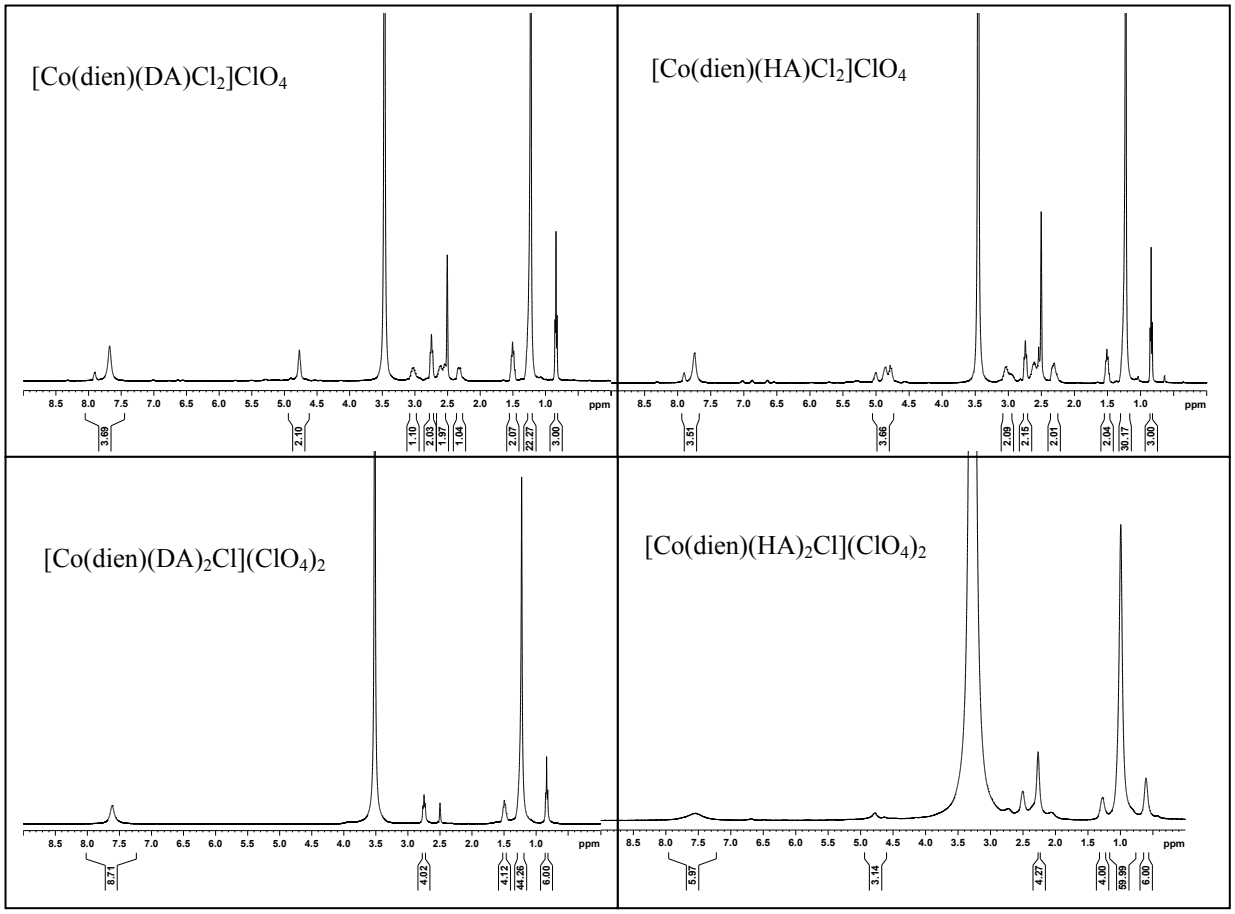

Figure S2. ^{1}H NMR spectrum of the surfactant–cobalt(III) complexes (**1–4**)

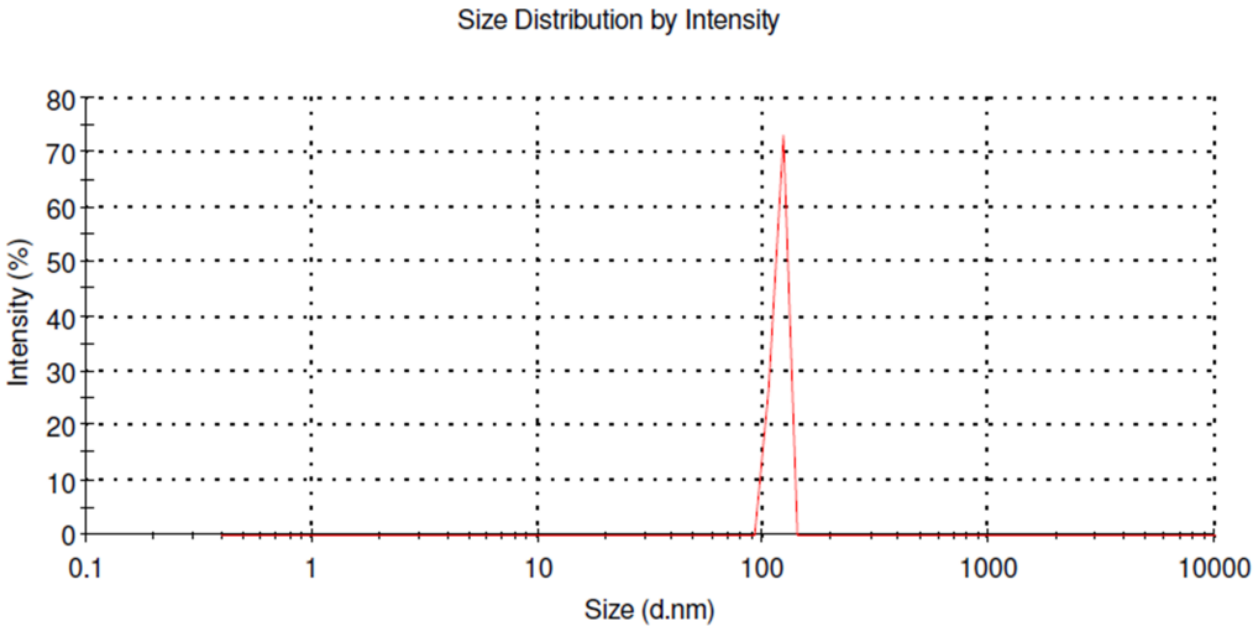

Figure S3(a). DLS measurements for the size distributions of self–assembled surfactant–cobalt(III) complex **1**

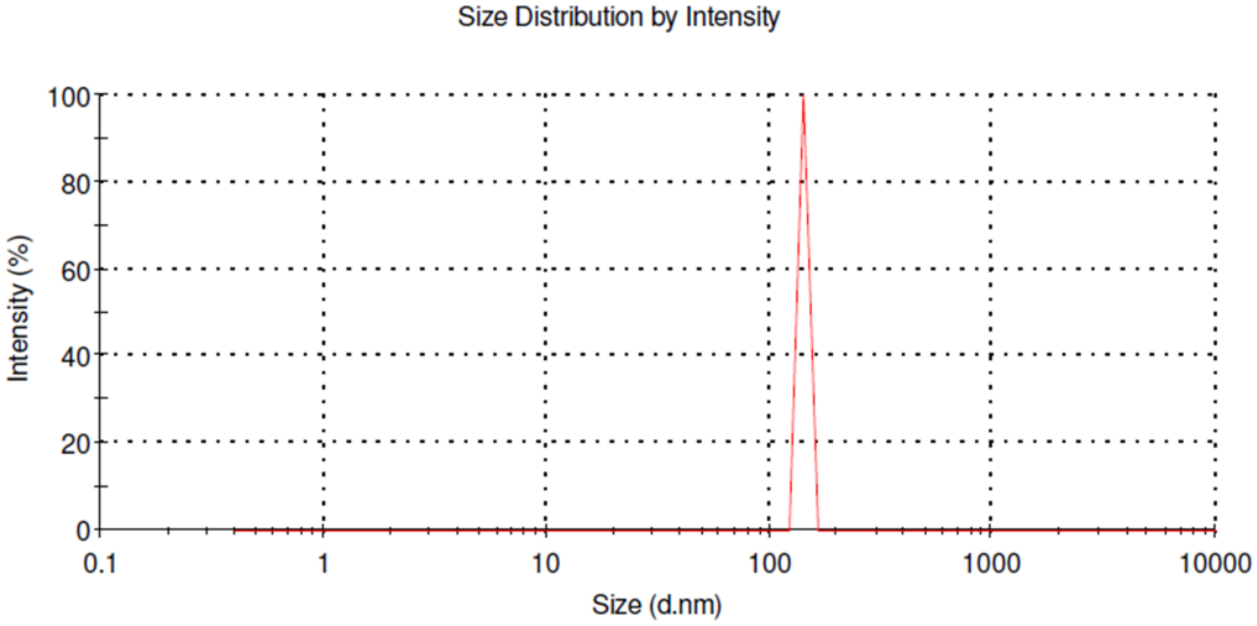

Figure S3(b). DLS measurements for the size distributions of self–assembled surfactant–cobalt(III) complex **2**

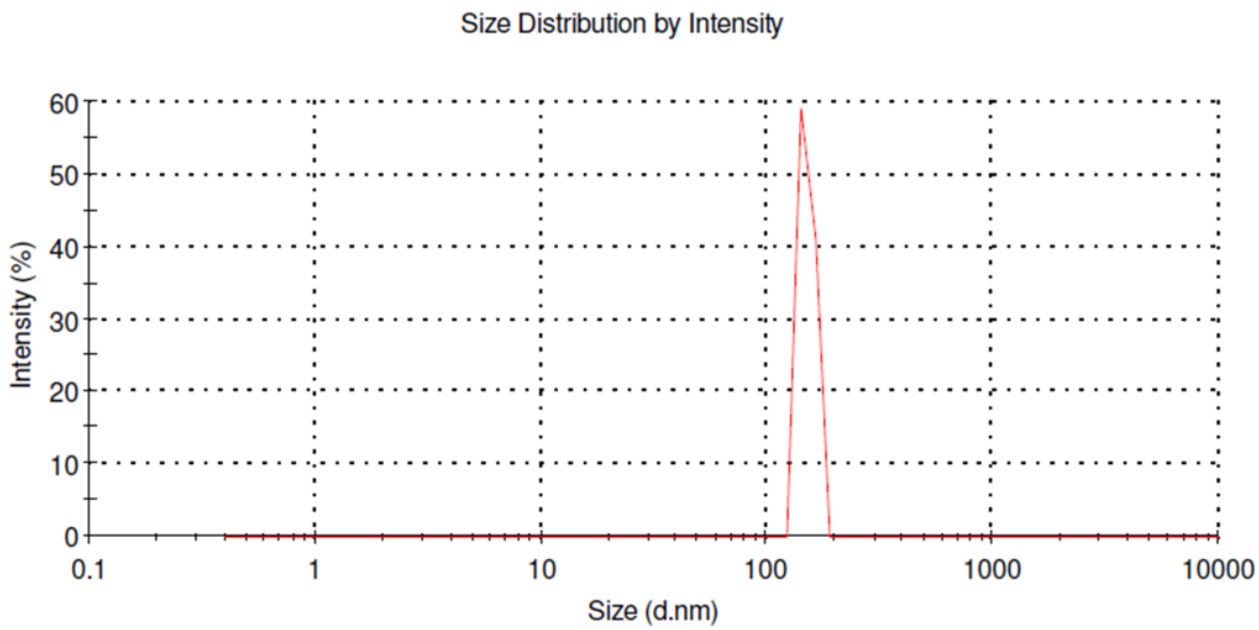

Figure S3(c). DLS measurements for the size distributions of self–assembled surfactant–cobalt(III) complex **3**

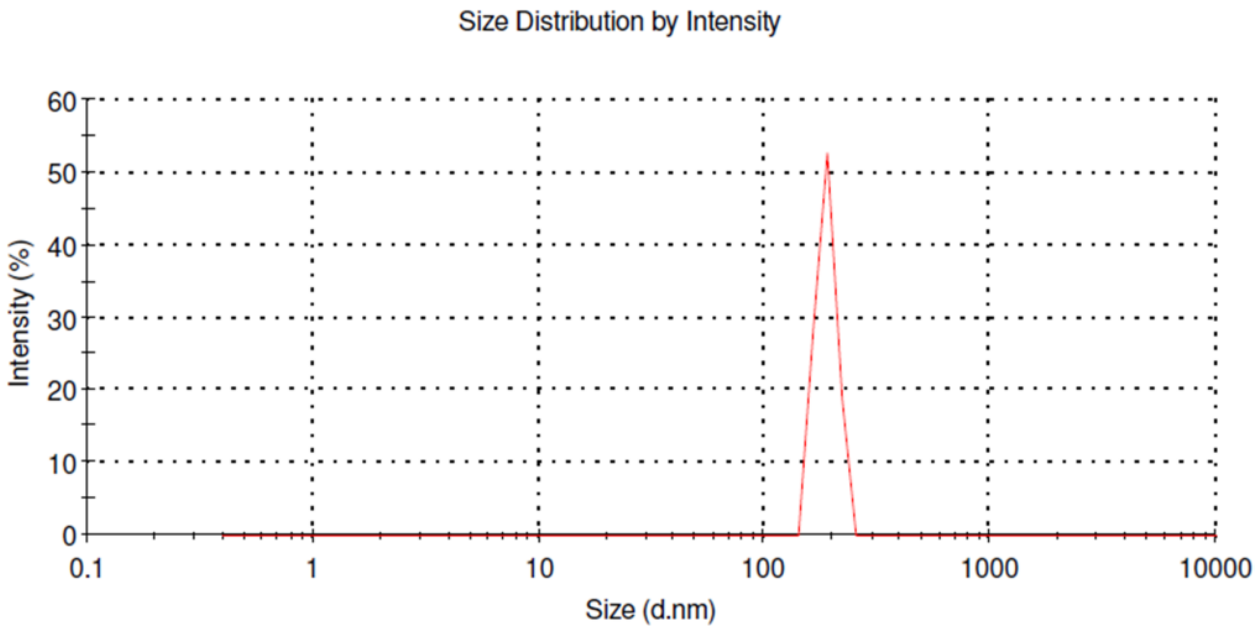

Figure S3(d). DLS measurements for the size distributions of self–assembled surfactant–cobalt(III) complex **4**

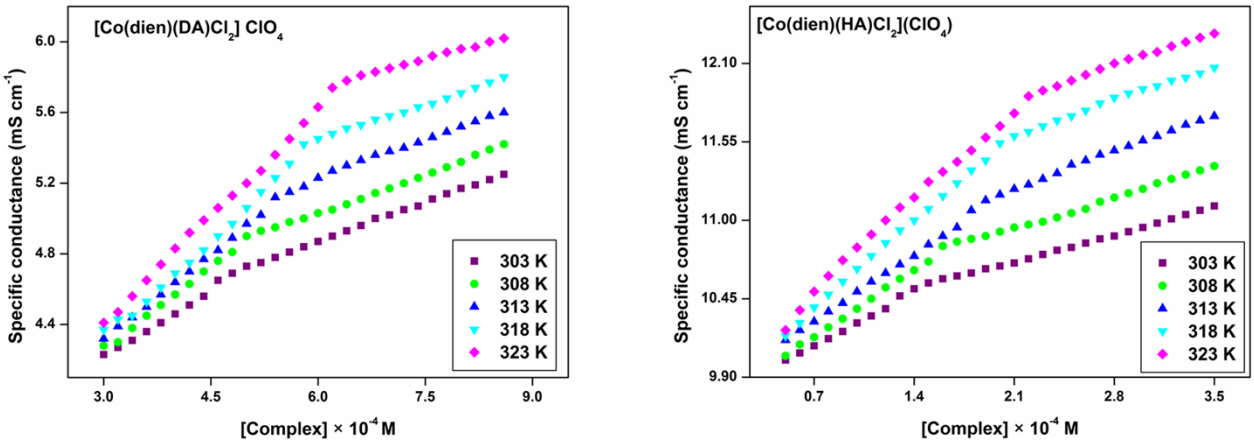

Figure S4. Plots of concentration versus conductance of surfactant–cobalt(III) complexes (**1** and **2**) in aqueous solution.

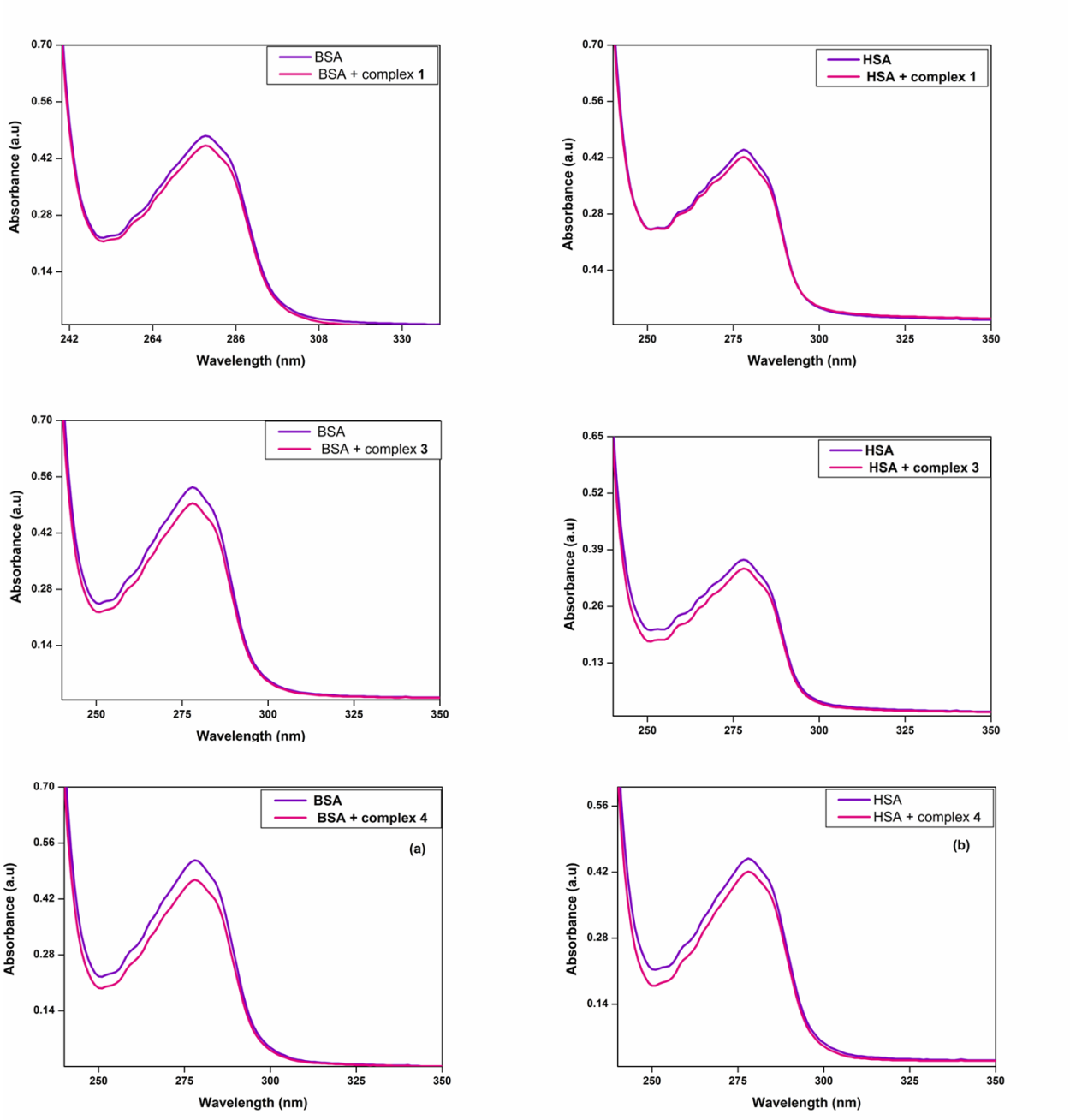

Figure S5. UV–visible absorption spectra of BSA/HSA in the absence and presence of surfactant–cobalt(III) complexes (**1**–**3**). [BSA] = [HSA] = 10 μM and [surfactant–cobalt(III) complexes] = 90 μM

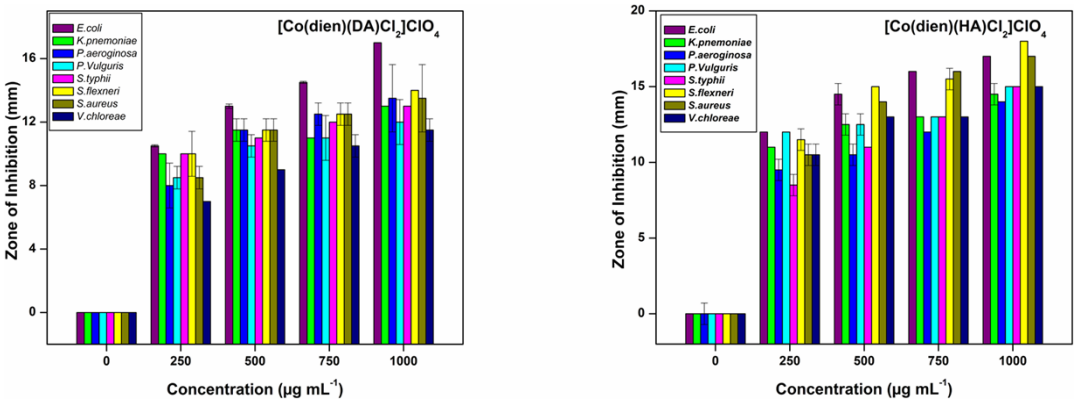

Figure S6. Effects of concentrations on the antibacterial activities of surfactant–cobalt(III) complexes (**1 and 2**) (0, 250, 500, 750, 1000 µg mL^{-1}) against human pathogens.

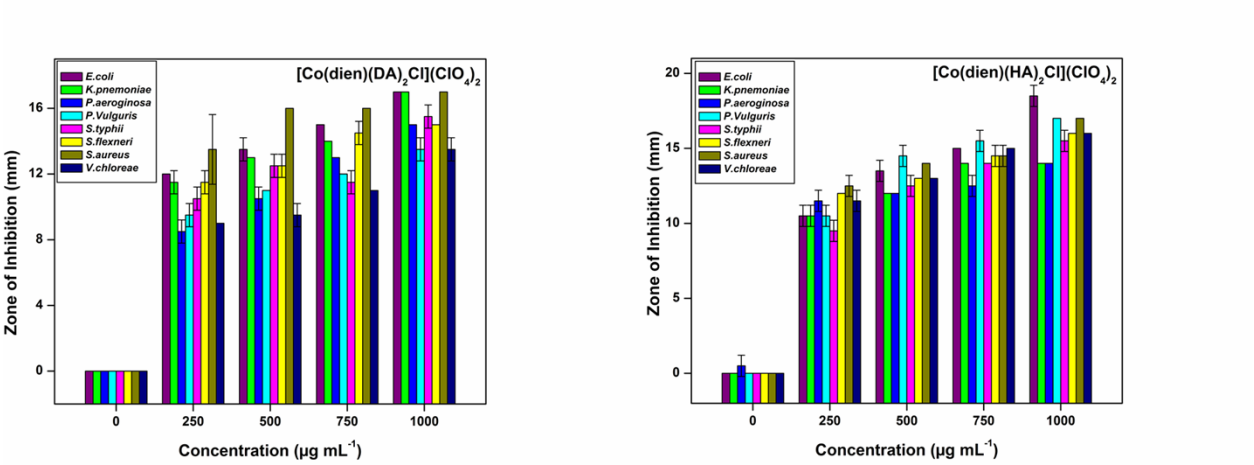

Figure S7. Effects of concentrations on the antibacterial activities of surfactant–cobalt(III) complexes (**3 and 4**) (0, 250, 500, 750, 1000 µg mL^{-1}) against human pathogens.

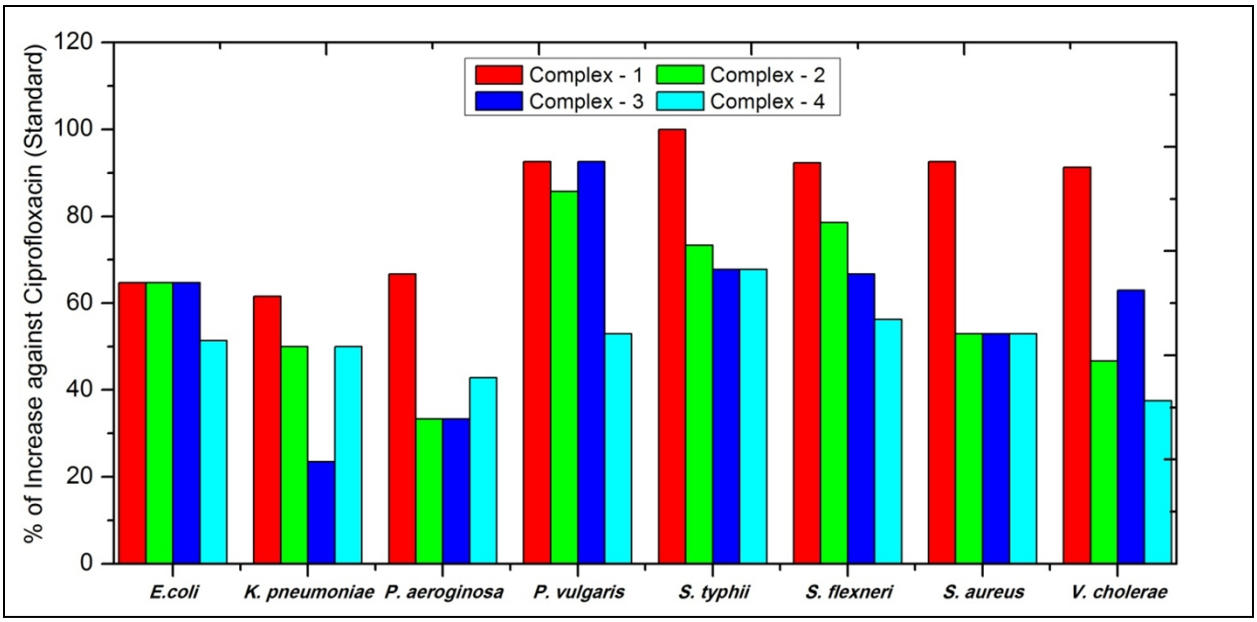

Figure S8. Percentage of Inhibition between Ciprofloxacin (Standard) and Complexes (**1 – 4**)

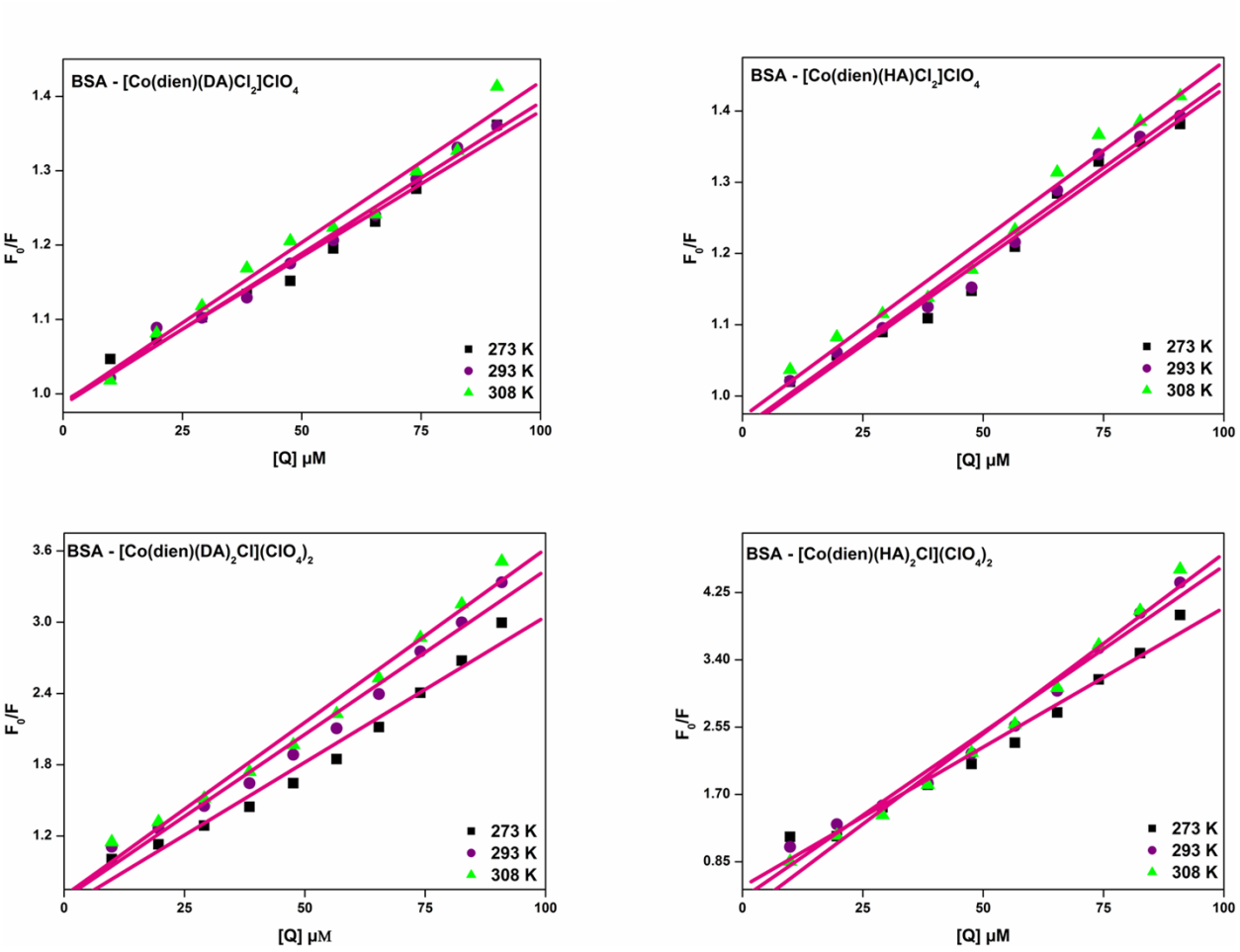

Figure S9. Stern–Volmer plots for quenching of BSA by surfactant–cobalt(III) complexes (**1**–**4**) at three different temperatures (273 K, 293 K, 308 K)

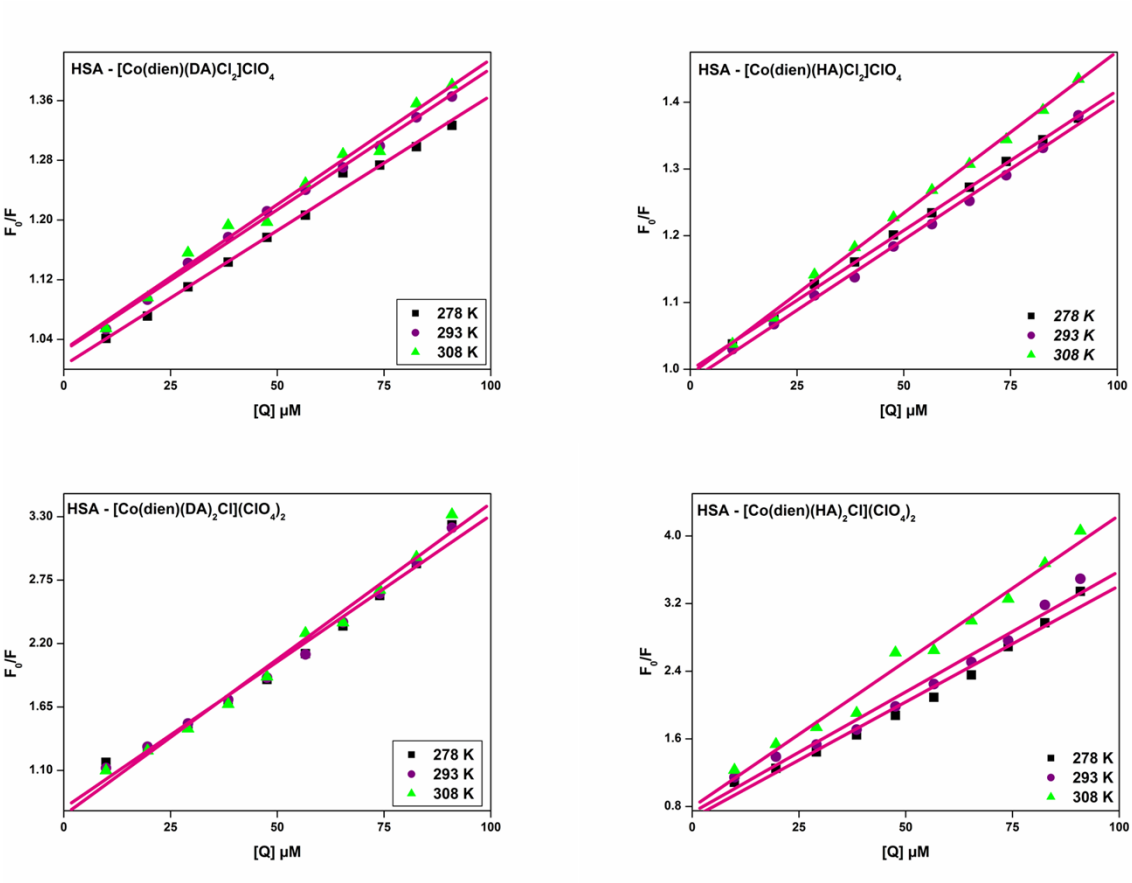

Figure S10. Stern–Volmer plots for quenching of HSA by surfactant–cobalt(III) complexes (**1**–**4**) at three different temperatures (273 K, 293 K, 308 K)

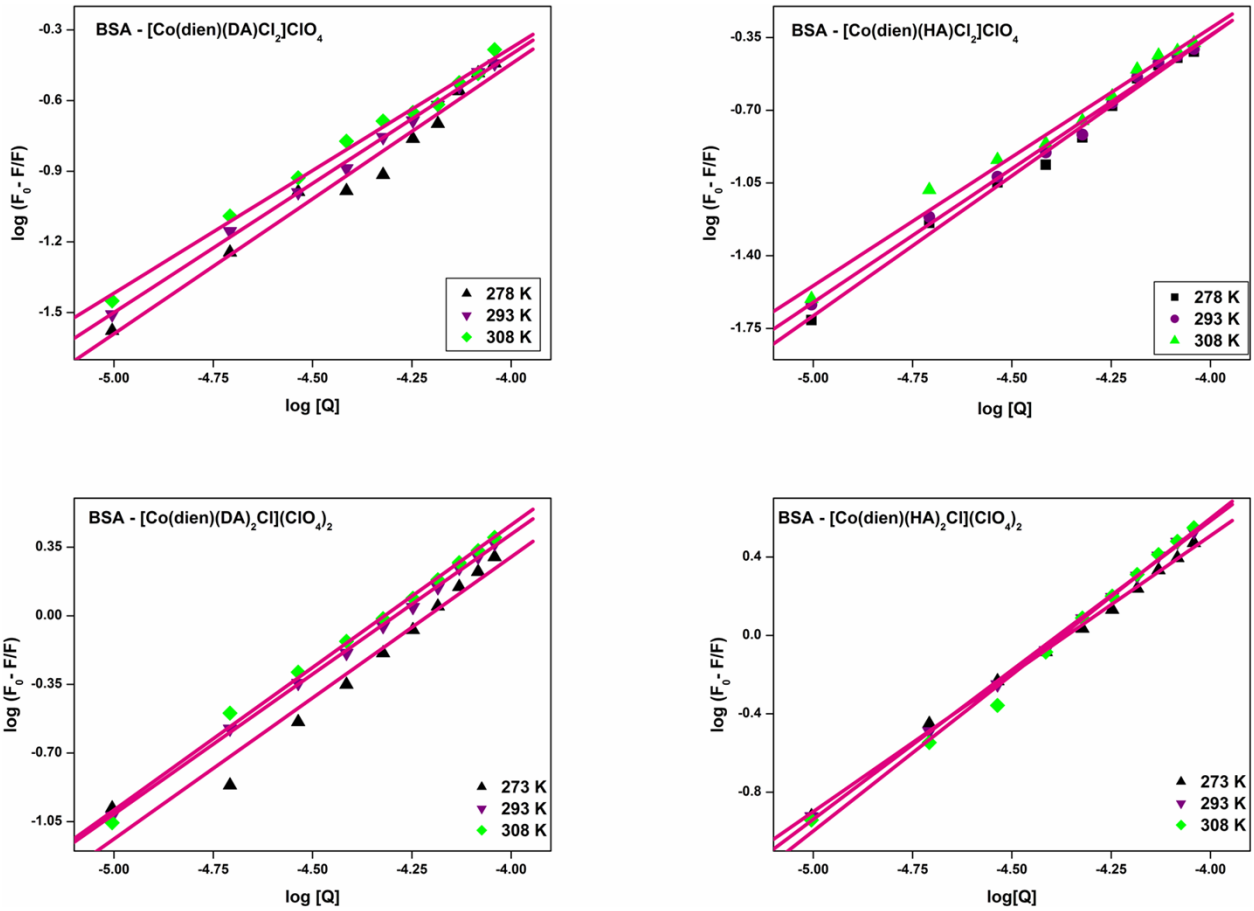

Figure S11. Double–logarithmic plots for the quenching of BSA by surfactant–cobalt(III) complexes (**1**–**4**) at three different temperatures (273 K, 293 K, 308 K)

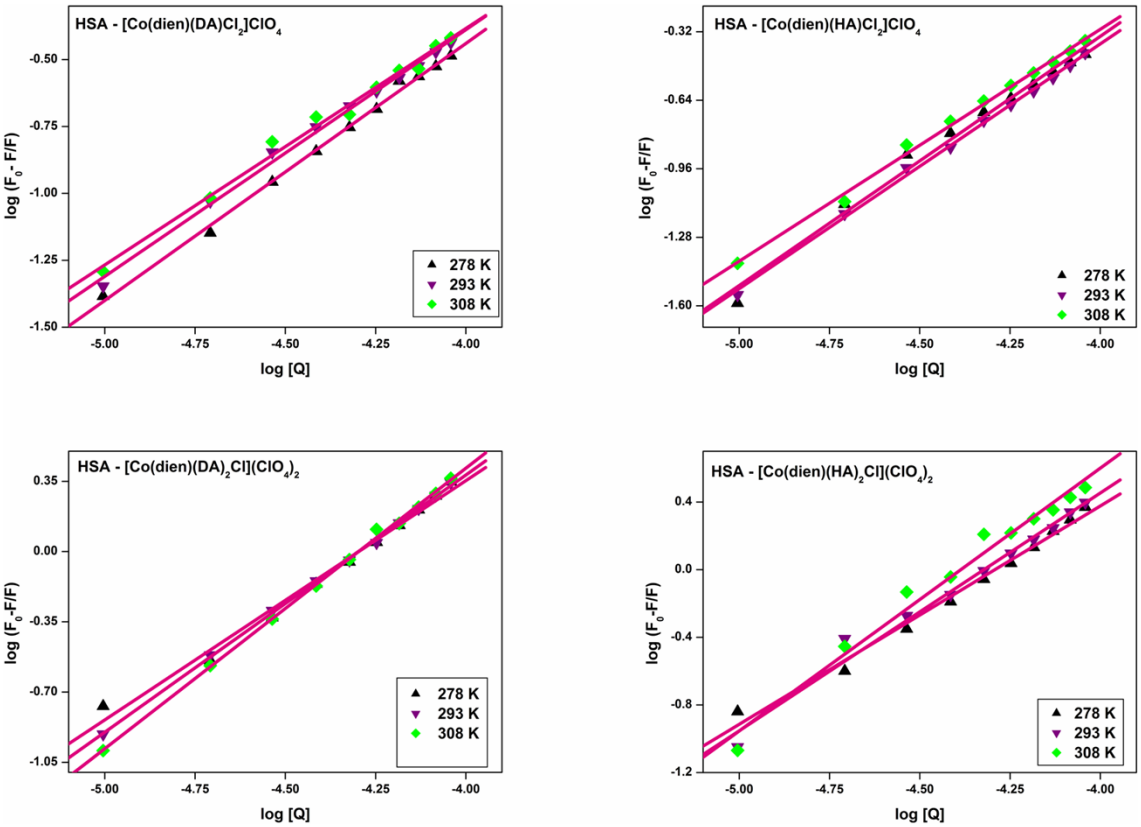

Figure S12. Double–logarithmic plots for the quenching of HSA by surfactant–cobalt(III) complexes (**1**–**4**) at three different temperatures (273 K, 293 K, 308 K)

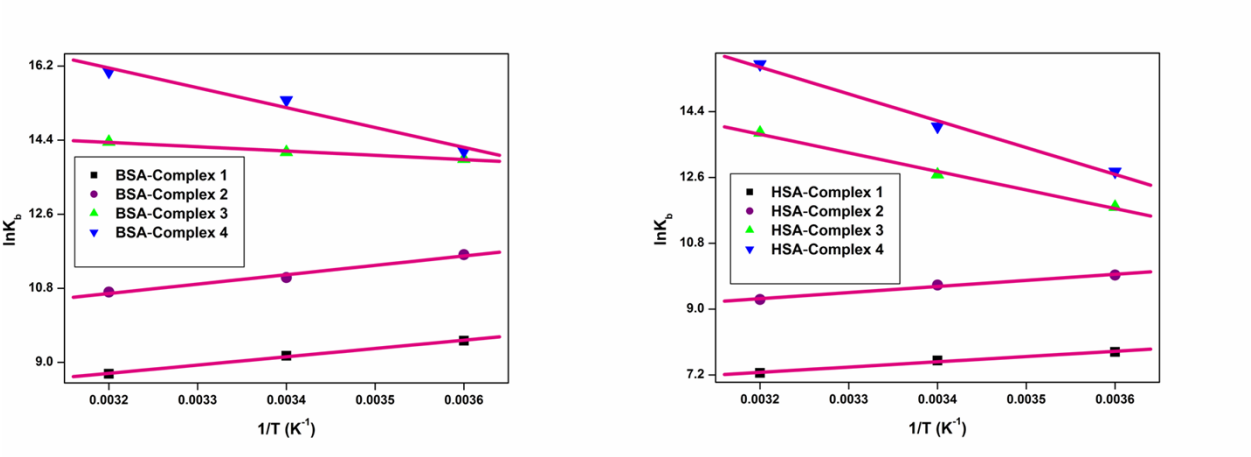

Figure S13. van't Hoff plots for the interaction of surfactant–cobalt(III) complexes (**1**–**4**) with BSA and HAS.

Table S1

Bacterial Strains used	Percentage of Increase against Ciprofloxacin (Standard)			
	Complex – 1	Complex – 2	Complex – 3	Complex - 4
E.coli	64.70	64.70	64.70	51.35
K. pneumoniae	61.53	50.00	23.52	50.00
P. aeroginosa	66.66	33.33	33.33	42.85
P. vulgaris	92.59	85.71	92.59	52.94
S. typhii	100.00	73.33	67.74	67.74
S. flexneri	92.30	78.57	66.66	56.25
S. aureus	92.59	52.94	52.94	52.94
V. cholerae	91.30	46.66	62.96	37.5