ELECTRONIC SUPPLEMENTARY INFORMATION (ESI)

Association of iminium and alkanolamine forms of the benzo[c]phenanthridine alkaloid chelerythrine with human serum albumin: Photophysical, thermodynamic and theoretical approach

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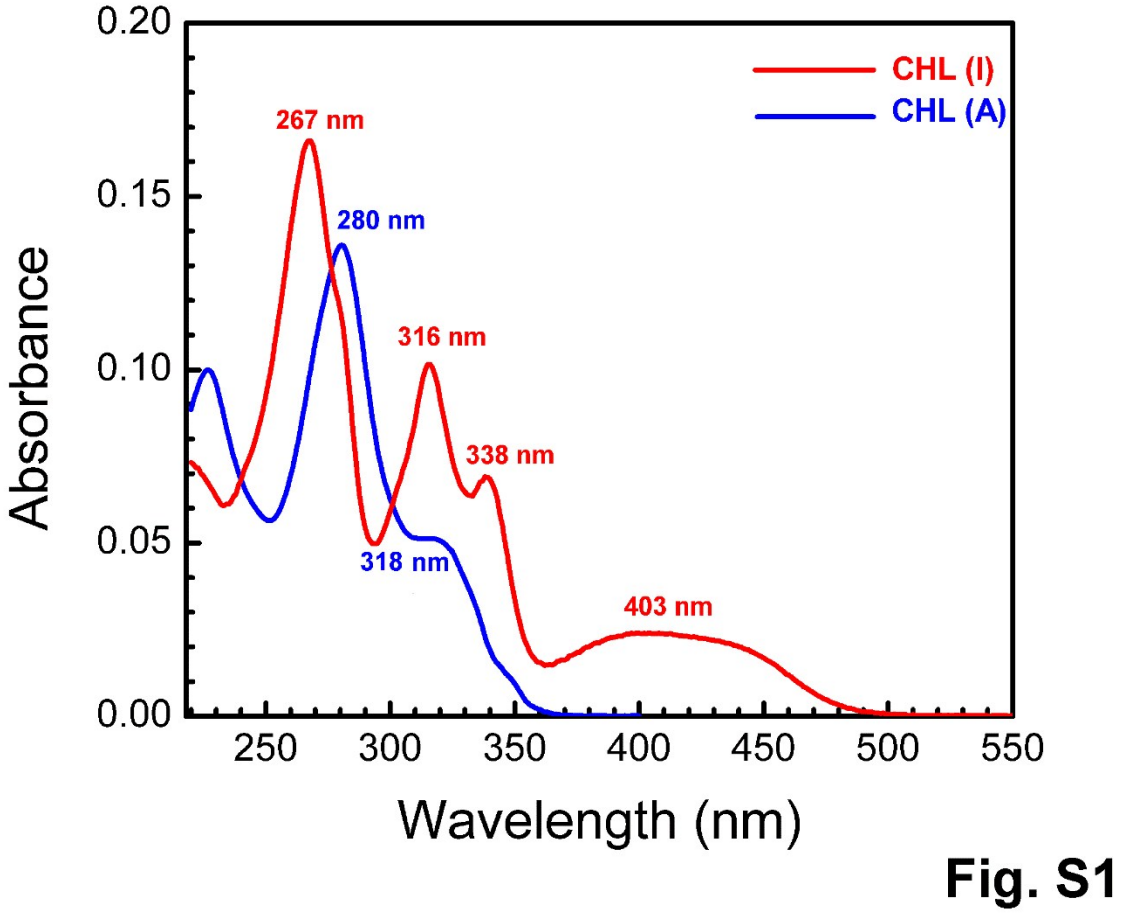

Fig. S1 Absorption spectra of iminium and alkanolamine forms of CHL (2.74 μM) in CP buffer (pH 6.0) and CB buffer (pH 10.2) respectively at 25 °C.

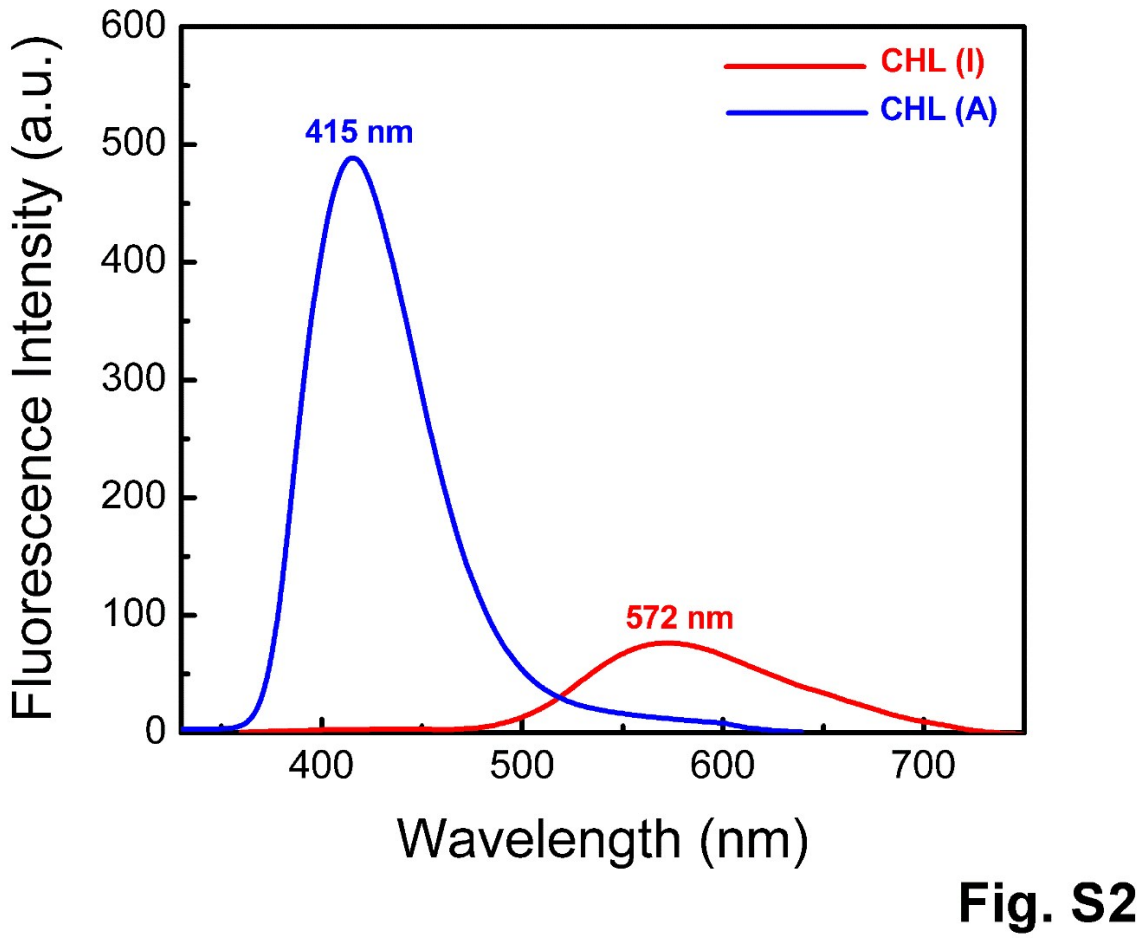

Fig. S2

Fig. S2 Fluorescence emission spectra of iminium and alkanolamine forms of CHL (1.37 μM) in CP buffer (pH 6.0) and CB buffer (pH 10.2) respectively at 25 °C.

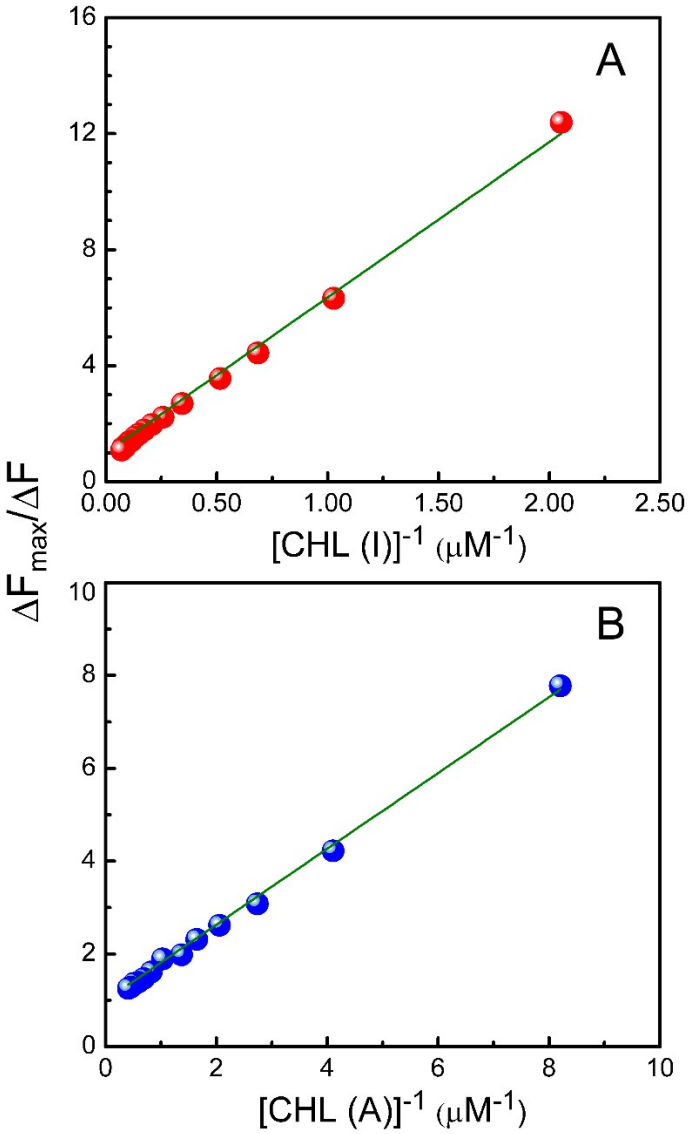

Fig. S3

Fig. S3 Representative Benesi-Hildebrand plot for the complexation of HSA with (A) CHL (I) and (B) CHL (A). The solid line is the linear best fit of the experimental points.

Table S1 Life time data for CHL in absence and in presence of HSA in respective buffers at 25 °C[a]

Drug	[HSA]/[CHL]	τ_1(ns)	$\alpha_1 \times 100$	τ_2 (ns)	$\alpha_2 \times 100$	τ_{avg} (ns)	χ^2
CHL (I)	0.00	0.49	100	-	-	0.49	1.03
	0.49	0.46	95.56	2.80	4.44	0.56	1.03
	0.98	0.46	94.29	2.92	5.71	0.60	1.05
	1.97	0.46	92.29	3.79	7.71	0.72	1.09
	2.95	0.46	91.54	3.80	8.46	0.74	1.01
CHL (A)	0.00	3.19	100	-	-	3.19	1.04
	0.49	3.16	46.68	4.38	53.32	3.81	1.09
	0.98	3.15	43.85	4.54	56.15	3.93	1.09
	1.48	3.13	32.99	4.78	67.01	4.24	1.11
	2.46	3.11	30.49	4.86	69.51	4.33	1.10
	3.44	3.08	29.59	4.91	70.41	4.37	1.11

[a]Average of three determinations.

Table S2 Lifetime data for HSA in absence and in presence of CHL (I) and CHL (A) in respective buffers at 25 °C[a]

Drug	[CHL]/[HSA]	τ_1(ns)	$\alpha_1 \times 100$	τ_2 (ns)	$\alpha_2 \times 100$	τ_{avg} (ns)	χ^2
CHL (I)	0.00	2.17	18.84	6.76	81.16	5.89	1.02
	2.06	2.14	13.27	6.30	86.73	5.75	1.05
	4.11	2.13	11.80	5.99	88.20	5.53	1.04
	6.83	2.08	6.59	5.74	93.41	5.50	1.10
CHL (A)	0.00	2.20	21.66	6.40	78.14	5.48	0.97
	0.69	2.16	22.35	6.27	77.65	5.35	1.02
	1.38	2.10	23.57	6.12	76.43	5.17	1.07
	2.06	2.12	23.99	5.89	76.01	4.99	1.09

[a]Average of three determinations.

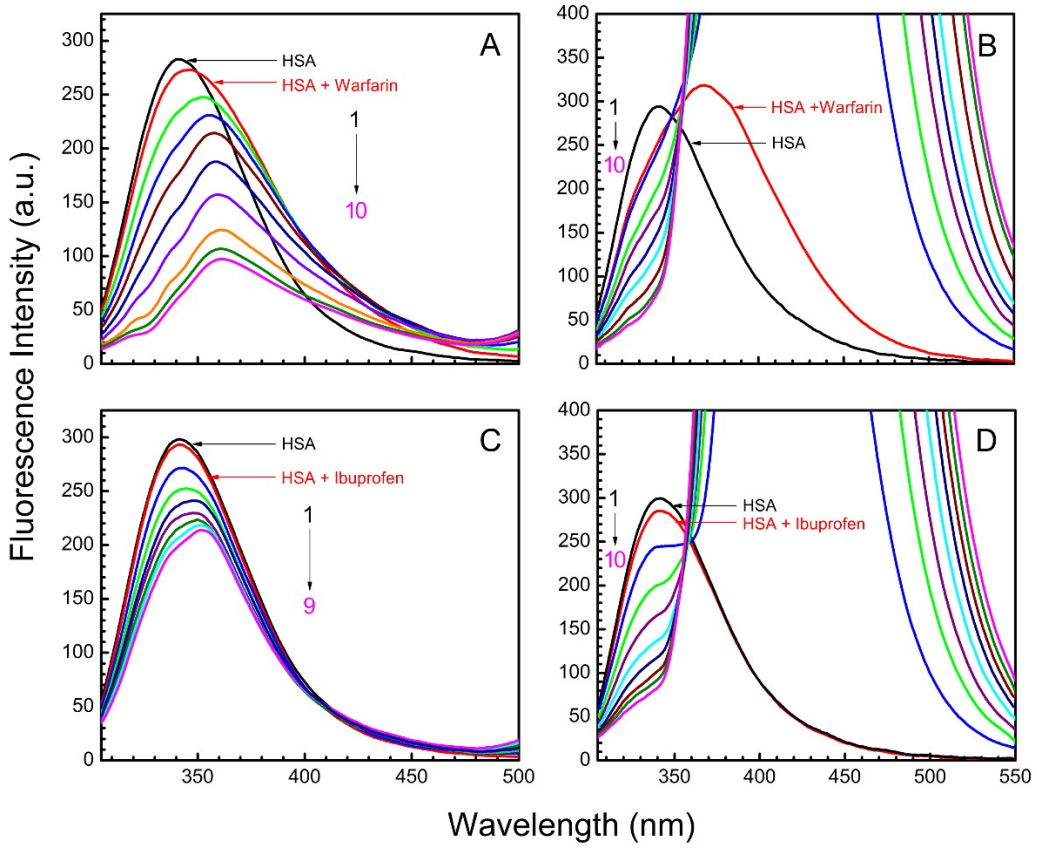

Fig. S4

Fig. S4 Effect of site marker on the CHL-HSA system: [warfarin] = [HSA] = 1 μM with CHL (I) (panel A) and CHL (A) (panel B) respectively. [ibuprofen] = [HSA] = 1 μM with CHL (I) (panel C) and CHL (A) (panel D) respectively. In panel (A) curves 1-10 denote 0, 0, 0.74, 1.48, 2.97, 4.44, 5.92, 7.39, 8.88 and 10.33μM of CHL (I) and in panel (B) curves 1-10 denote 0, 0, 0.37, 0.74, 1.11, 1.86, 2.23, 2.96, 3.71 and 4.44 μM of CHL (A). In panel (C) curves 1-9 denote 0, 0, 0.74, 1.48, 2.97, 4.44, 5.92, 7.39 and 8.88 μM of CHL (I) and in panel (D) curves 1-10 denote 0, 0, 0.37, 0.74, 1.11, 1.86, 2.23, 2.96, 3.71 and 4.44 μM of CHL (A).

Table S3 Binding environment of CHL (I) and CHL (A) at subdomain IIA of HSA

Ligand binding	Neighbouring residues at the binding site		
	Charged polar (basic)	Uncharged polar	Hydrophobic
CHL (I)	Lys 199, His 242, Arg 257	Tyr 148, Tyr 150, Gln 196, Cys 200, Cys 245, Cys 246	Trp 214, Ala 291
CHL (A)	Arg 218, Arg 222, His 242, Arg 257	-	Trp 214, Leu 219, Leu 238, Leu 260, Ile 264, Ala 291