Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting Information

Chelerythrine-lysozyme interaction: spectroscopic studies, thermodynamics and molecular modeling exploration

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Table S1 Summary of the optical properties of chelerythrine [a]

Absorbance		
Parameter	Chelerythrine	
	iminium	alkanolamine
λ_{max} (free)	316	318
ε (at λ_{max})	37,060	16,790
Fluorescence		
λ_{max} (excitation)	338	318
λ_{max} (emission)	550	419

[a] Units of λ, nm, ε (molar extinction coefficient), M^{-1} cm^{-1}.

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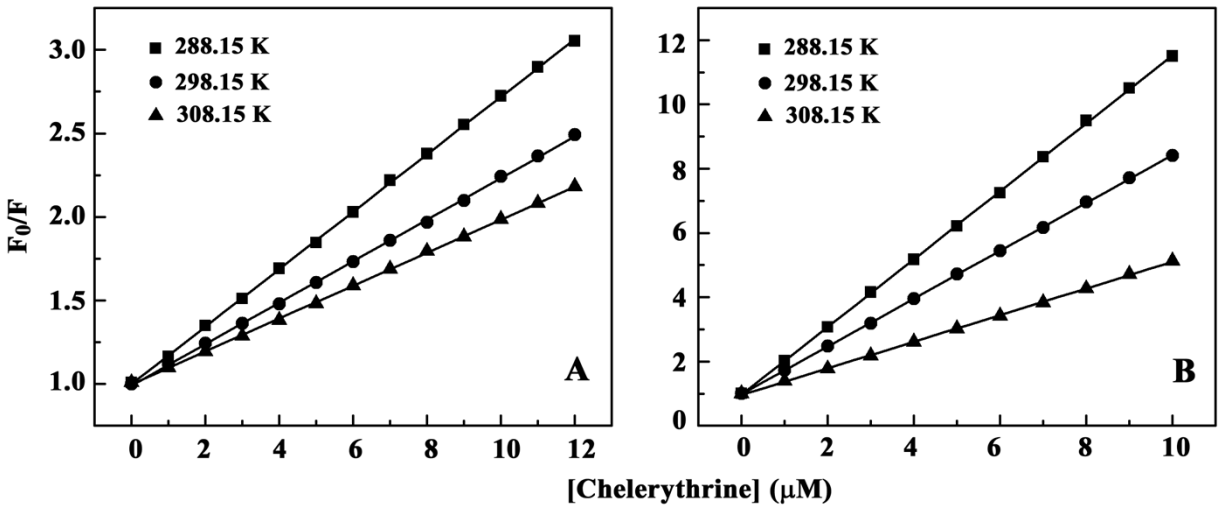

Figure S1. Stern–Volmer plots for the quenching of Lyz fluorescence by (A) iminium and (B) alkanolamine form of chelerythrine at different temperatures.

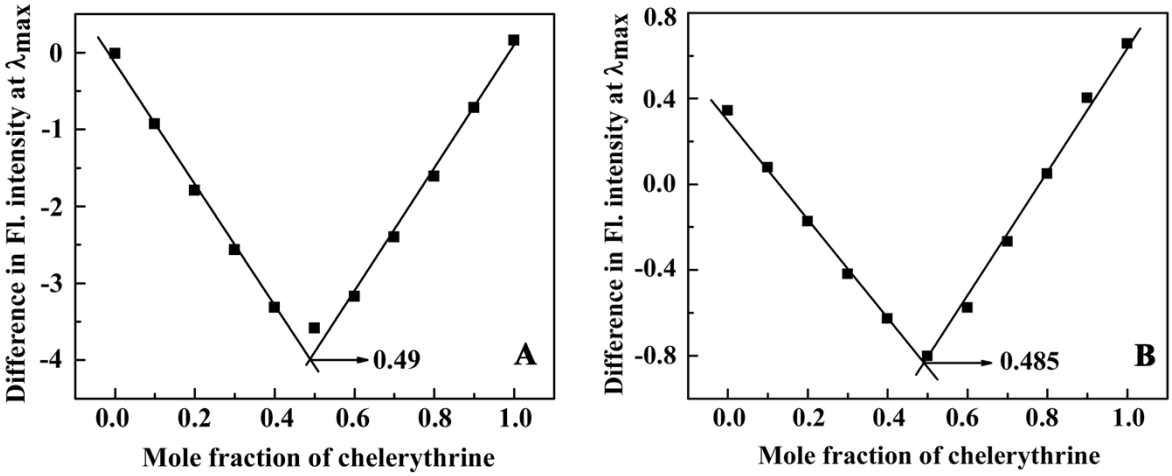

Figure S2. Job plot for the binding of chelerythrine (A) iminium and (B) alkanolamine forms to the Lyz. Fluorescence quenching of Lyz was monitored at 339 nm exciting at 295 nm.

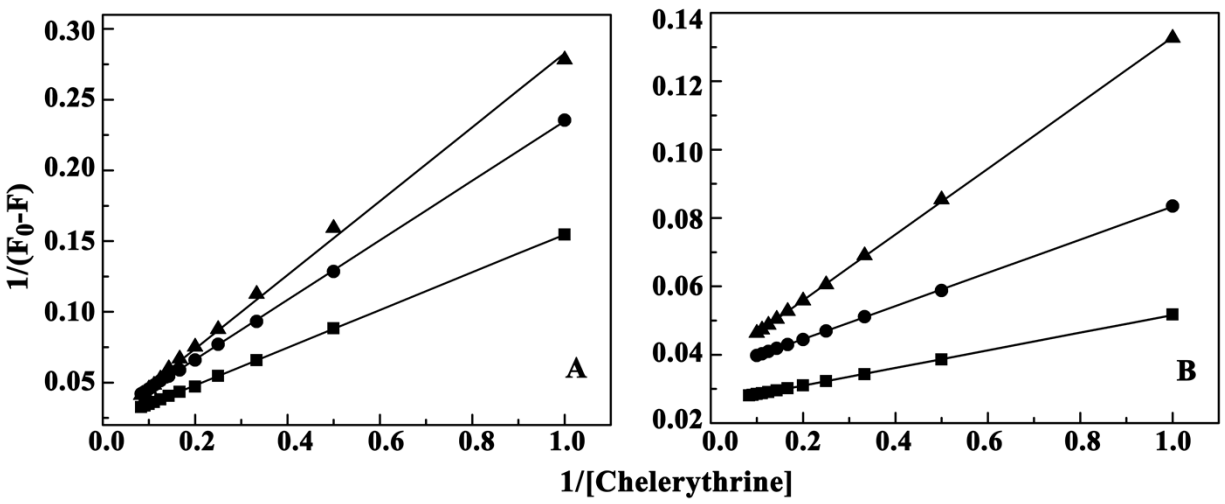

Figure S3. Lineweaver-Burk plots for the quenching of Lyz fluorescence by chelerythrine (A) iminium and (B) alkanolamine at temperatures 288.15 K (filled square), 298.15 K (filled circle) and 308.15 K (filled triangle).

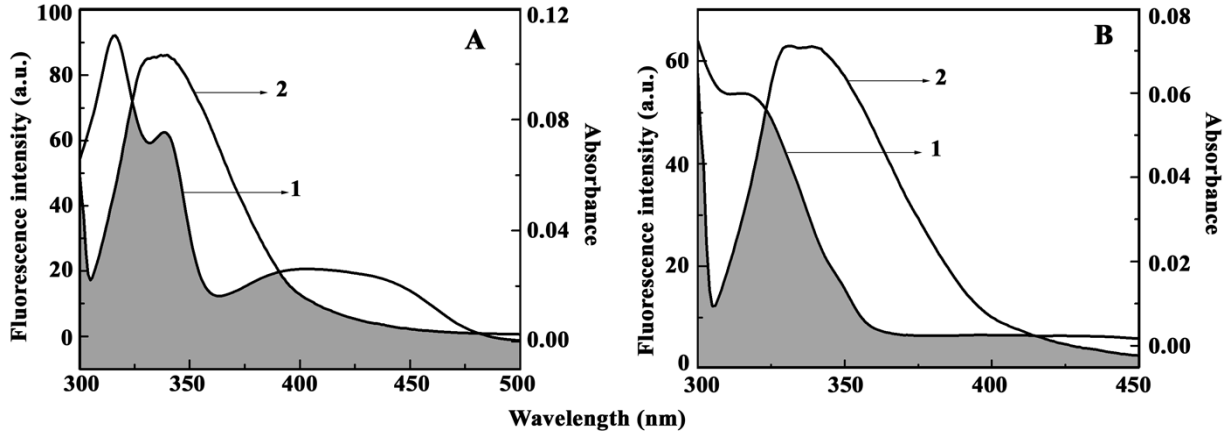

Figure S4. Overlap (shaded portion) of Lyz fluorescence spectrum and absorption spectra of chelerythrine (A) iminium and (B) alkanolamine. In panel (A) and (B) curve 1 represent absorption spectra of (A) iminium and (B) alkanolamine and curve 2 represent the fluorescence spectrum of Lyz. The excitation of Lyz was done at 295 nm. The ratio of the concentration of [Lyz]:[alkaloids] = 1:1.

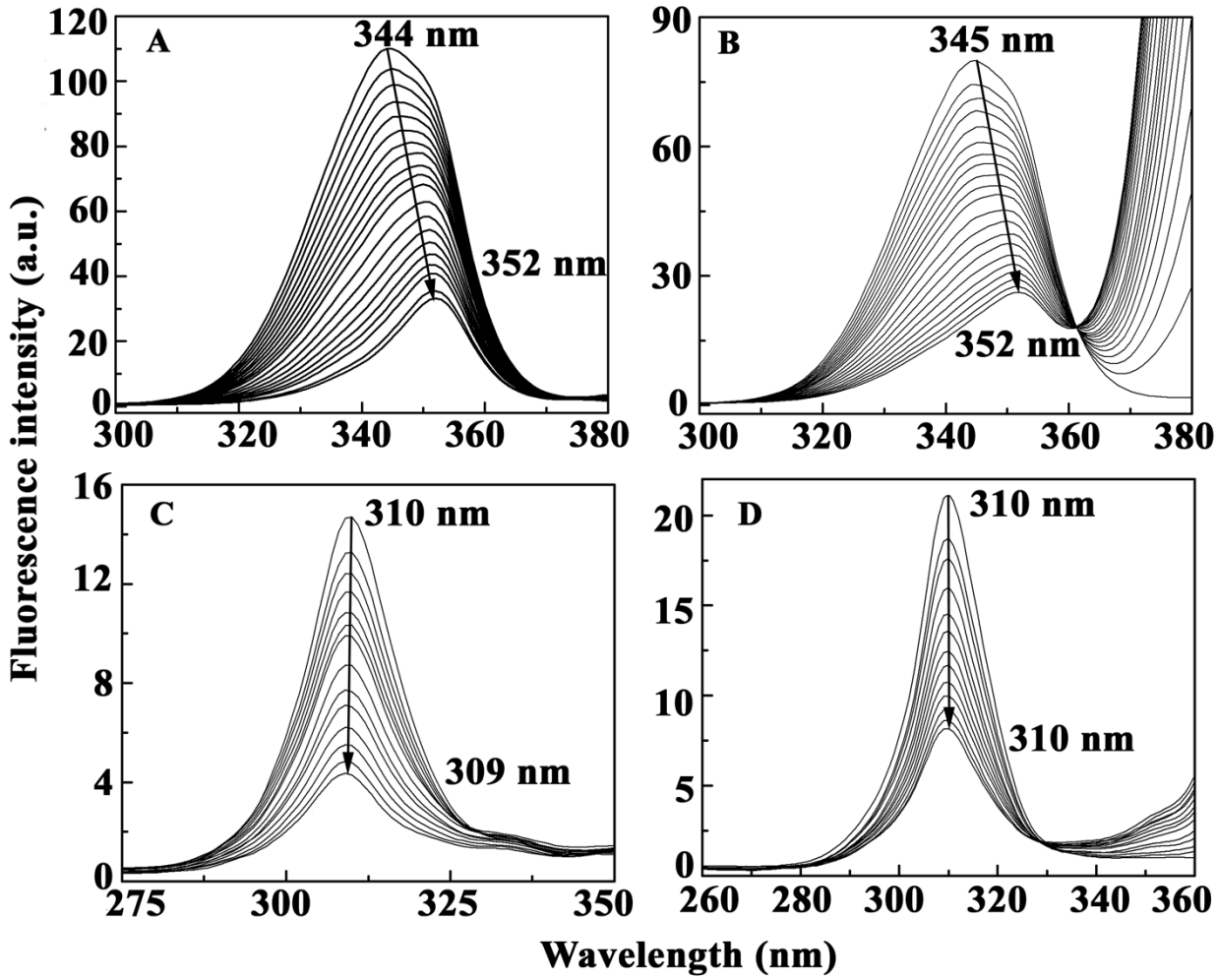

Figure S5. Synchronous fluorescence spectra at $\Delta\lambda$ = 60 nm (A, B) and $\Delta\lambda$ = 15 nm (C, D) of Lyz in the presence of different concentrations of (A,C) iminium and (B,D) alkanolamine form of chelerythrine. [Lyz] = 1μM.

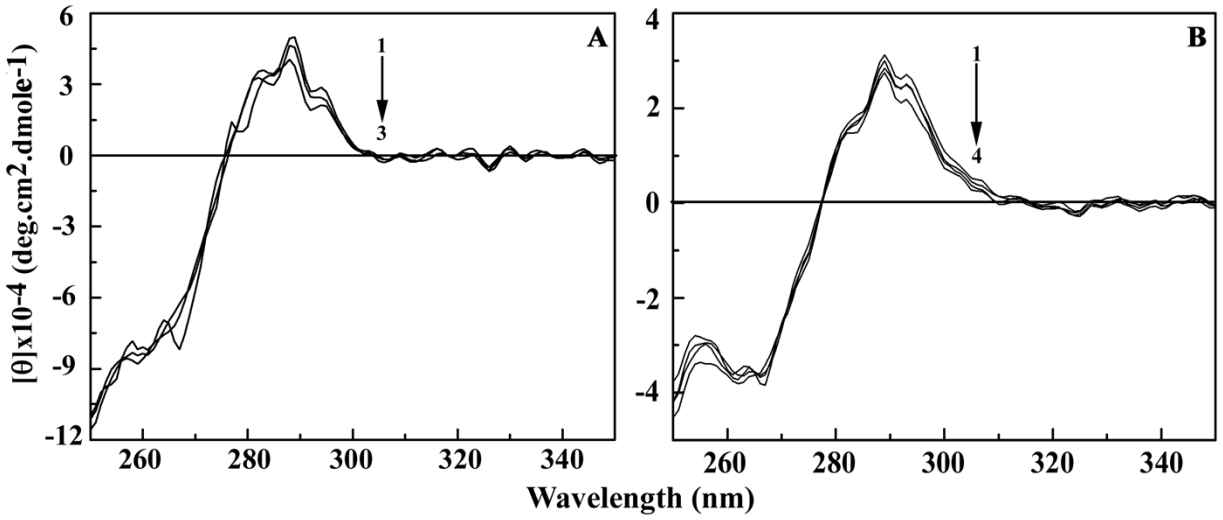

Figure S6. Near UV CD spectra of Lyz (25 μM) treated with various concentrations of chelerythrine (A) iminium and (B) alkanolamine. In panel (A) curves (1–3) denote 0, 20 and 40 μM of iminium and (B) curves (1–4) denote 0, 10, 20 and 40 μM of alkanolamine, respectively.

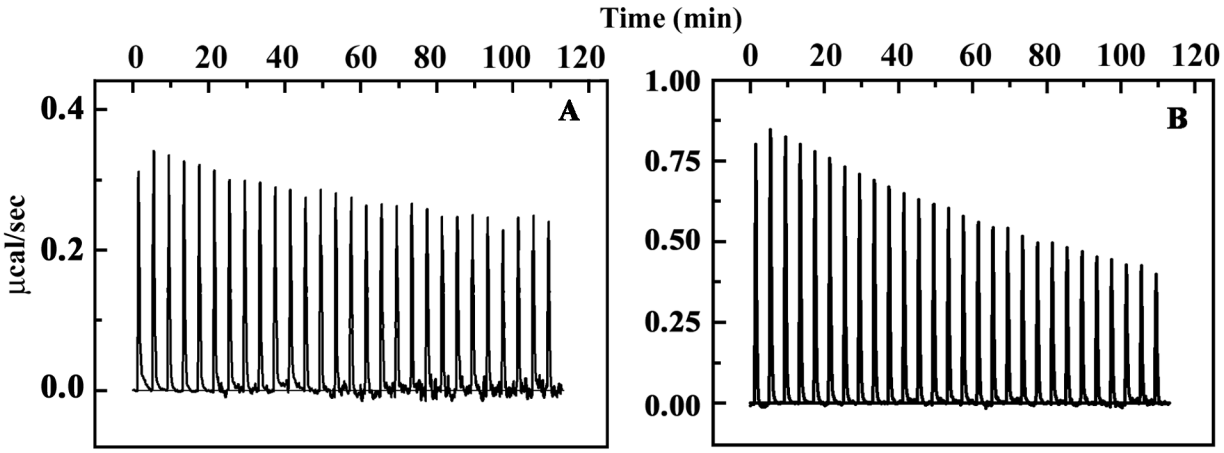

Figure S7. The panels present raw results for the sequential injection of Lyz of 0.5 mM and 0.8 mM into respective buffer of (A) pH 6.4 and (B) pH 9.2.

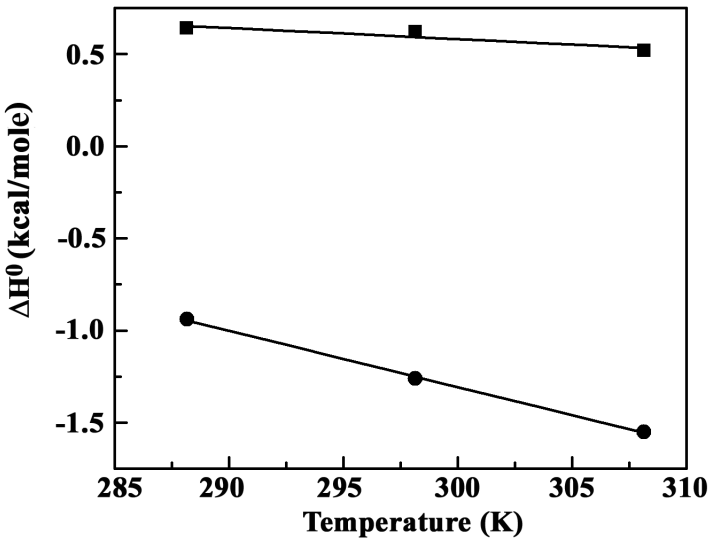

Figure S8. Plot of variation of thermodynamic parameter Δ*H*° for alkaloids–Lyz complex formation. Δ*H*° *versus* Temperature (Kelvin) for the binding of iminium (filled square) and alkanolamine (filled circle) form of chelerythrine with Lyz.