#### **ELECTRONIC SUPPLEMENTARY INFORMATION**

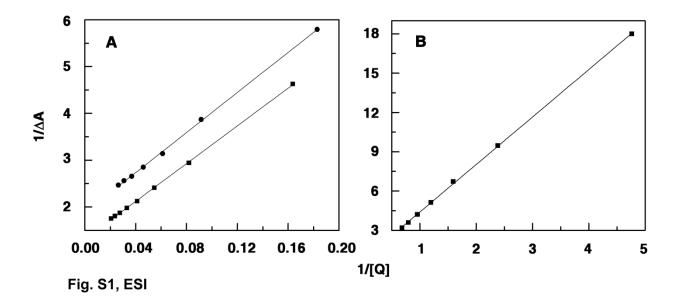
# Binding of isoquinoline alkaloids berberine, palmatine and coralyne to hemoglobin: Structural and thermodynamic characterization studies

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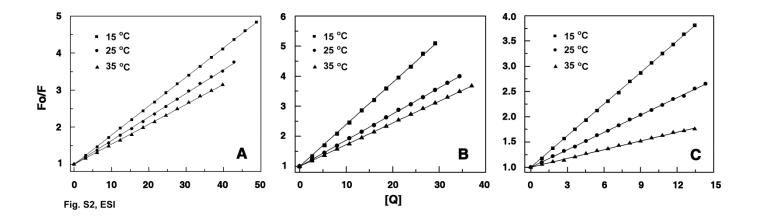
Biophysical Chemistry Laboratory

CSIR- Indian Institute of Chemical Biology

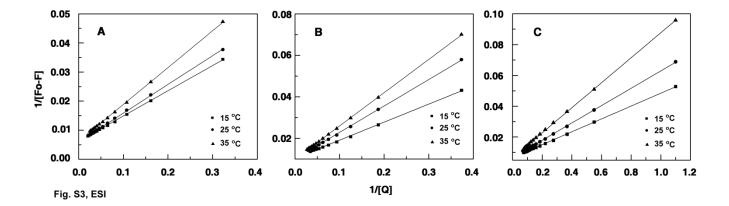
Kolkata 700 032, India



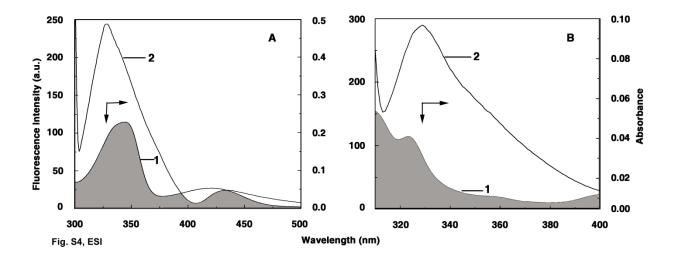
**Fig. S1** Representative Benesi-Hildebrand plots for binding of Hb with (A) berberine (■), palmatine (●) and (B) coralyne.



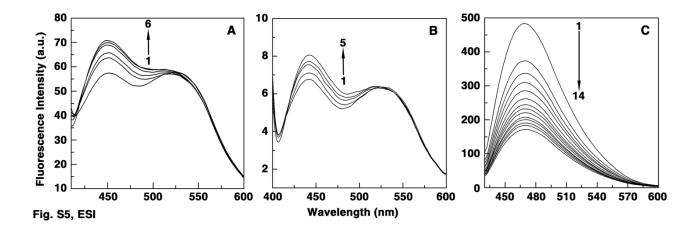
**Fig. S2** Stern-Volmer plots for the quenching of Hb fluorescence by (A) Berberine, (B) palmatine and (C) coralyne at different temperatures.



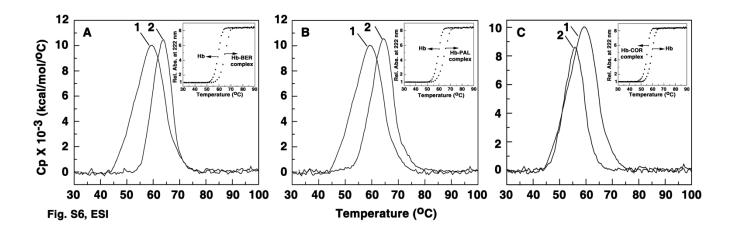
**Fig. S3** Lineweaver-Burk plots for the quenching of Hb fluorescence by (A) Berberine, (B) palmatine and (C) coralyne at different temperatures.



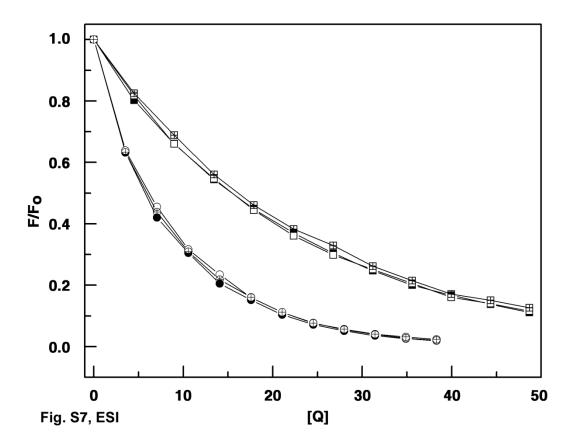
**Fig. S4** Overlap (shaded portion) of Hb fluorescence spectrum and absorption spectra of (A) berberine and (B) coralyne. In panel (A) and (B) curve 1 represent absorption spectra of (A) berberine and (B) coralyne and curve 2 represent the fluorescence spectrum of Hb. The excitation of Hb was done at 295 nm. The ratio of the concentration of [Hb]:[alkaloids] = 1:1.



**Fig. S5** DSC thermograms of Hb and Hb-alkaloids complex. In panel (A), (B) and (C) curve 1 and curve 2 represents for Hb and Hb-alkaloids complex. Inset thermal melting profiles for Hb and Hb-alkaloid complexes.



**Fig. S6** Representative fluorescence spectra of (A) berberine (10  $\mu$ M, curve 1-6) with 0, 0.98, 1.96, 2.94, 3.92 ,4.90  $\mu$ M of Hb, (B) palmatine (5  $\mu$ M, curve 1-5) with 0, 0.98, 1.96, 2.94, 3.92  $\mu$ M of Hb and (C) coralyne (0.1  $\mu$ M, curve 1-15) with 0, 0.15, 0.30, 0.44, 0.59, 0.74, 0.89, 1.03, 1.18, 1.32, 1.47, 1.61, 1.76, 1.90  $\mu$ M of Hb.



**Fig. S7** Displacement study of hydrophobic probe ANS bound to Hb by the alkaloids. Plots of F/Fo versus [Q] of palmatine and coralyne with Hb ( $\blacksquare$ , $\bullet$ ), Hb-ANS (1:1) complex ( $\square$ , $\circ$ ) and Hb-ANS (1:5) (cross symbol) complex.