

**Chromatographic method of pre-concentration and separation of Zn (II) with  
microalgae; Density Functional optimization of extracted species**

Bhabatosh Mandal\*, Monalisha Mondal, Bhavya Srivastava, Milan K. Barman Chandan

Ghosh & Mousami Chatterjee

Analytical Laboratory, Department of Chemistry,

Visva-Bharati, Santiniketan 731235, India-731235

Author to whom correspondence to be addressed. E-mail: [bhabatosh\\_mandal@yahoo.co.in](mailto:bhabatosh_mandal@yahoo.co.in)

Supporting figure file:

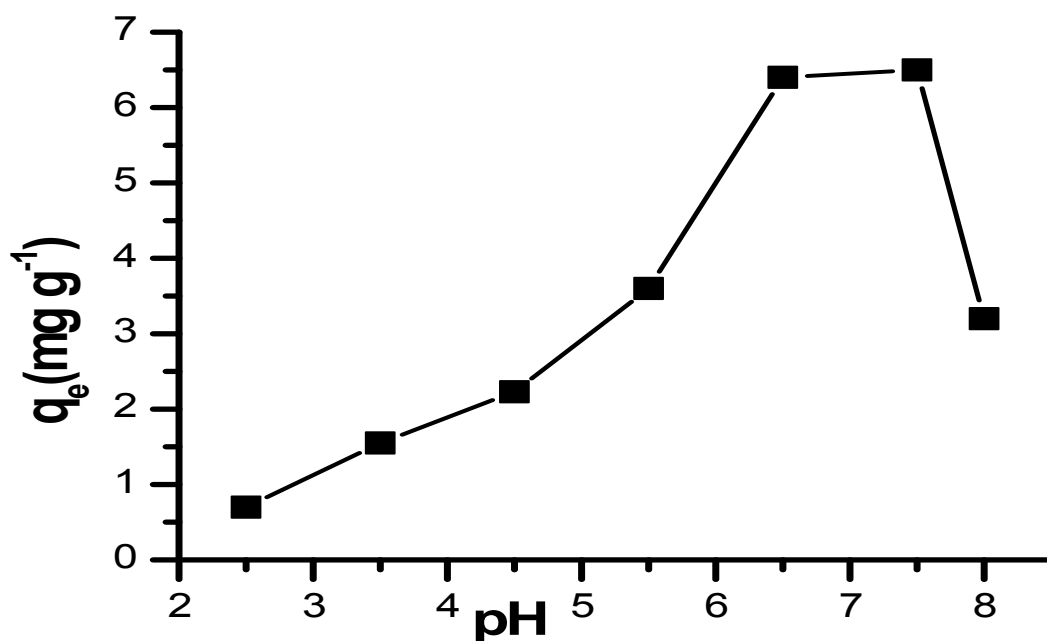
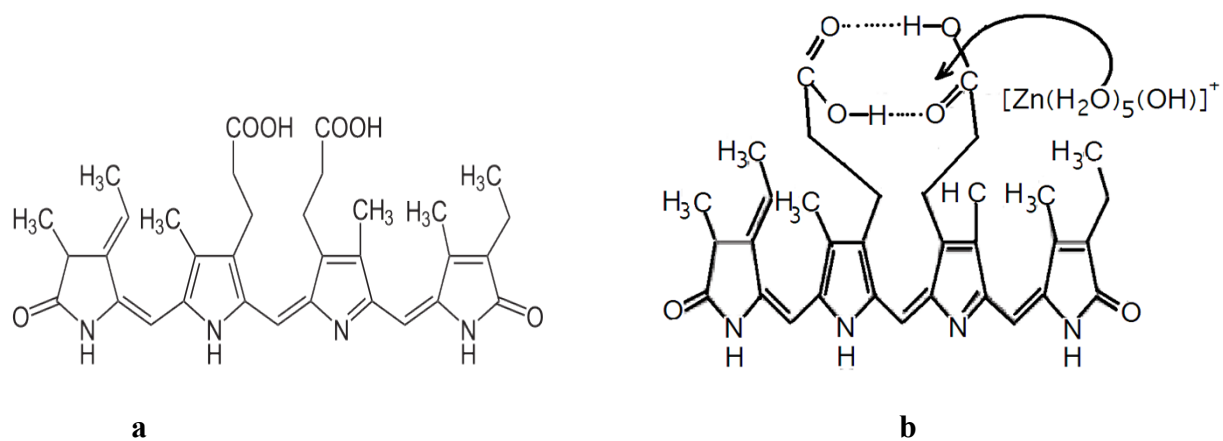
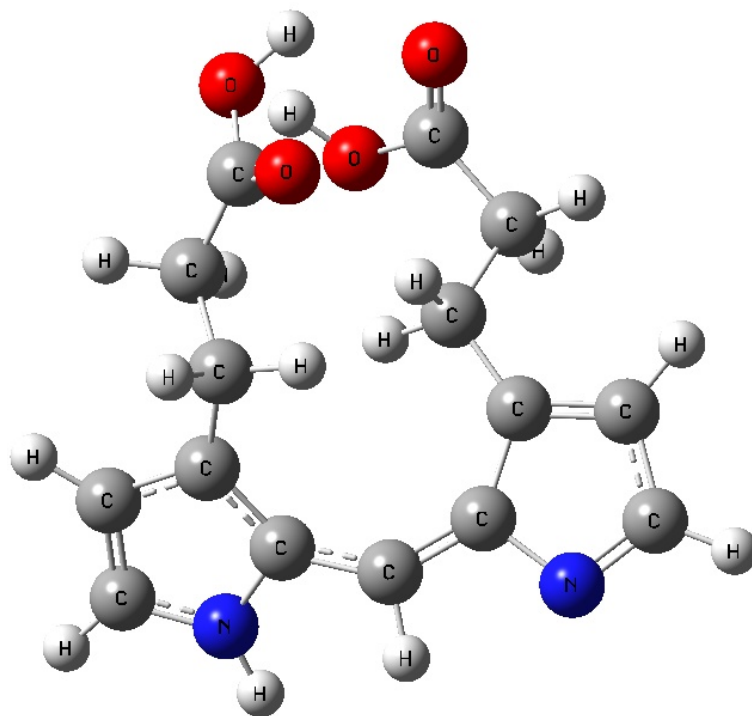


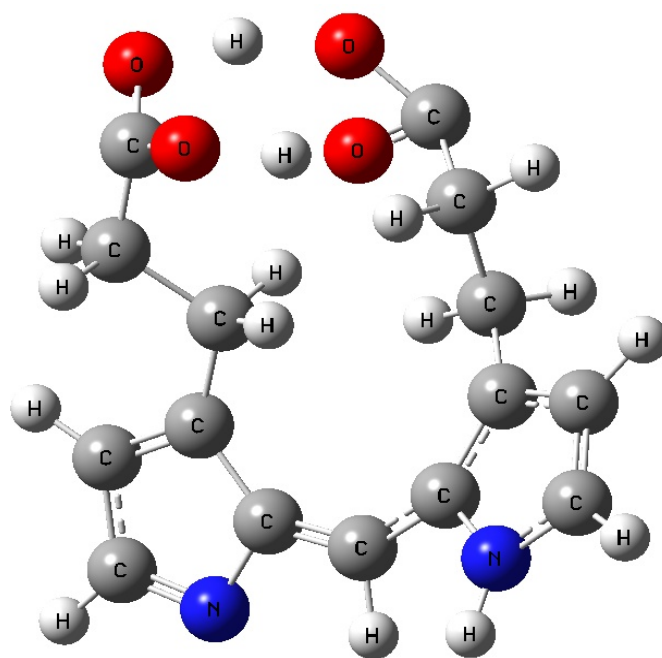
Fig. S1 Plot of pH Vs.  $q_e$



**Fig. S2: (a) Phycocyanobilin2; (b) insertion of Zn(II) into the proposed dimeric core**

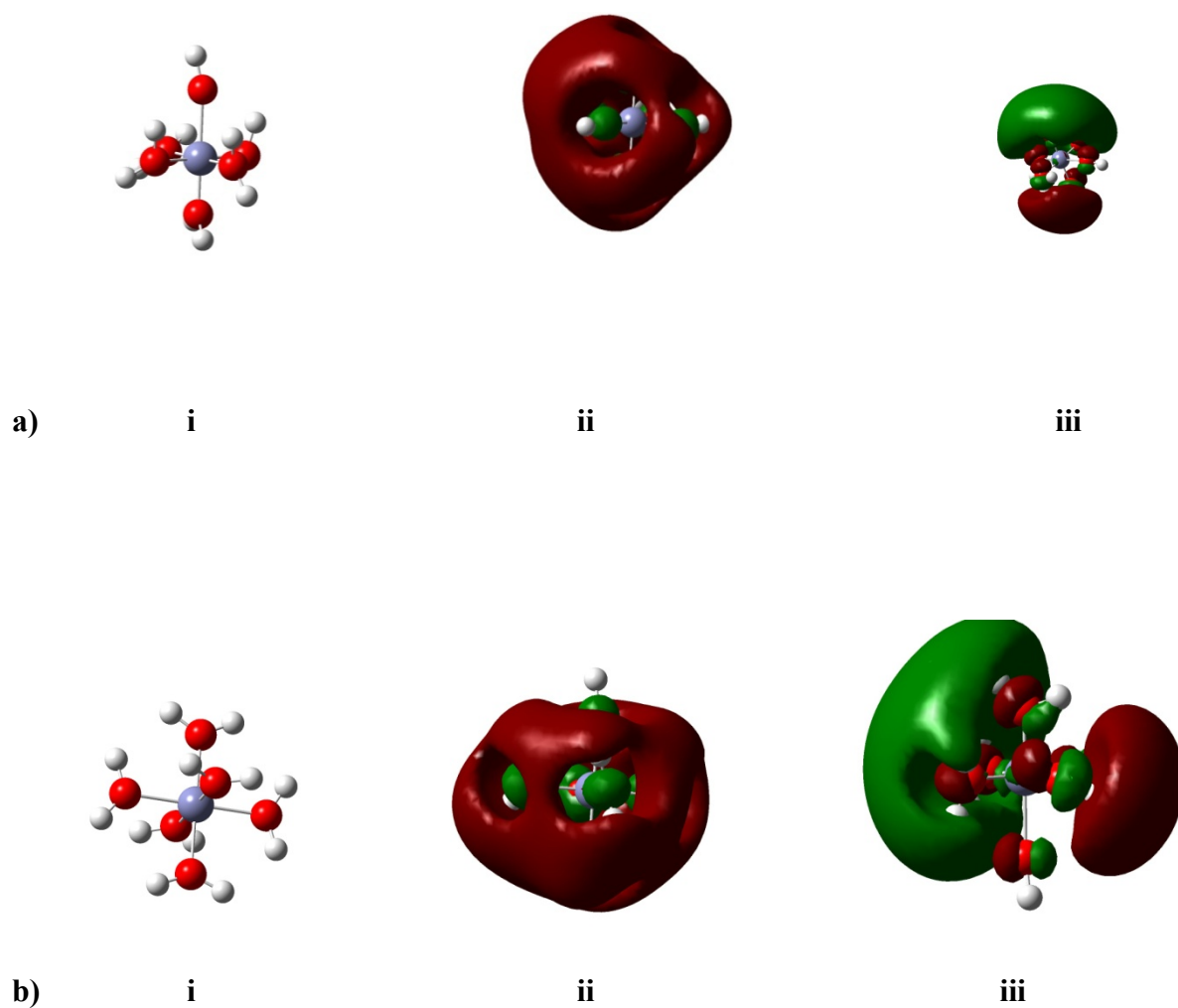


**a**



**b**

**Fig. S3: The DFT optimized structure of a) the protein fragment and b) its hydrogen bonded dimeric core**



**Fig. S4: The DFT optimized structure of (a) i)  $[\text{Zn}(\text{H}_2\text{O})_5\text{OH}]^+$ ; ii) HOMO of  $[\text{Zn}(\text{H}_2\text{O})_5\text{OH}]^+$  ; iii) LUMO of  $[\text{Zn}(\text{H}_2\text{O})_5\text{OH}]^+$  and (b) i)  $[\text{Zn}(\text{H}_2\text{O})_6]^{+2}$  ; ii) HOMO of  $[\text{Zn}(\text{H}_2\text{O})_6]^{+2}$  ; iii) LUMO of  $[\text{Zn}(\text{H}_2\text{O})_6]^{+2}$**