

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

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Supporting figure file:

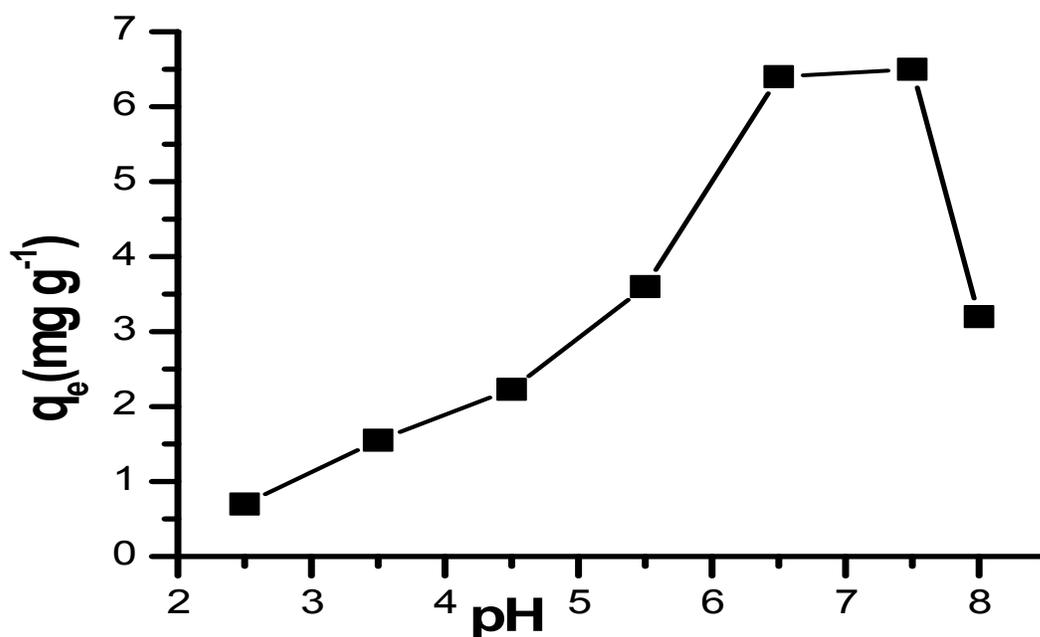
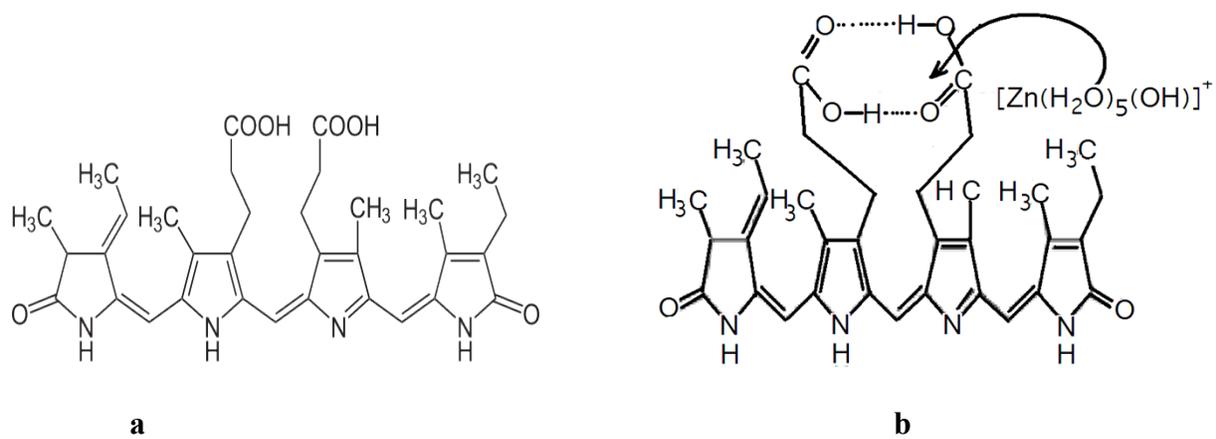
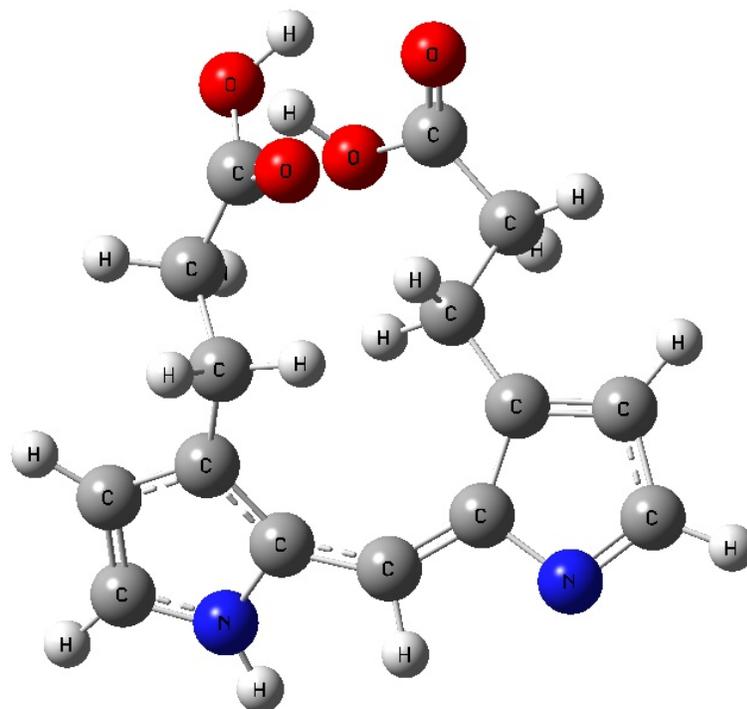


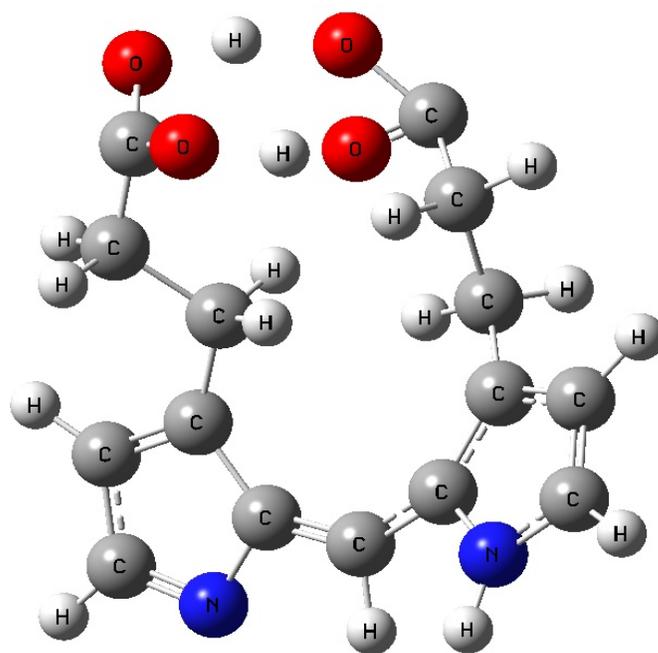
Fig. S1 Plot of pH Vs.  $q_e$



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

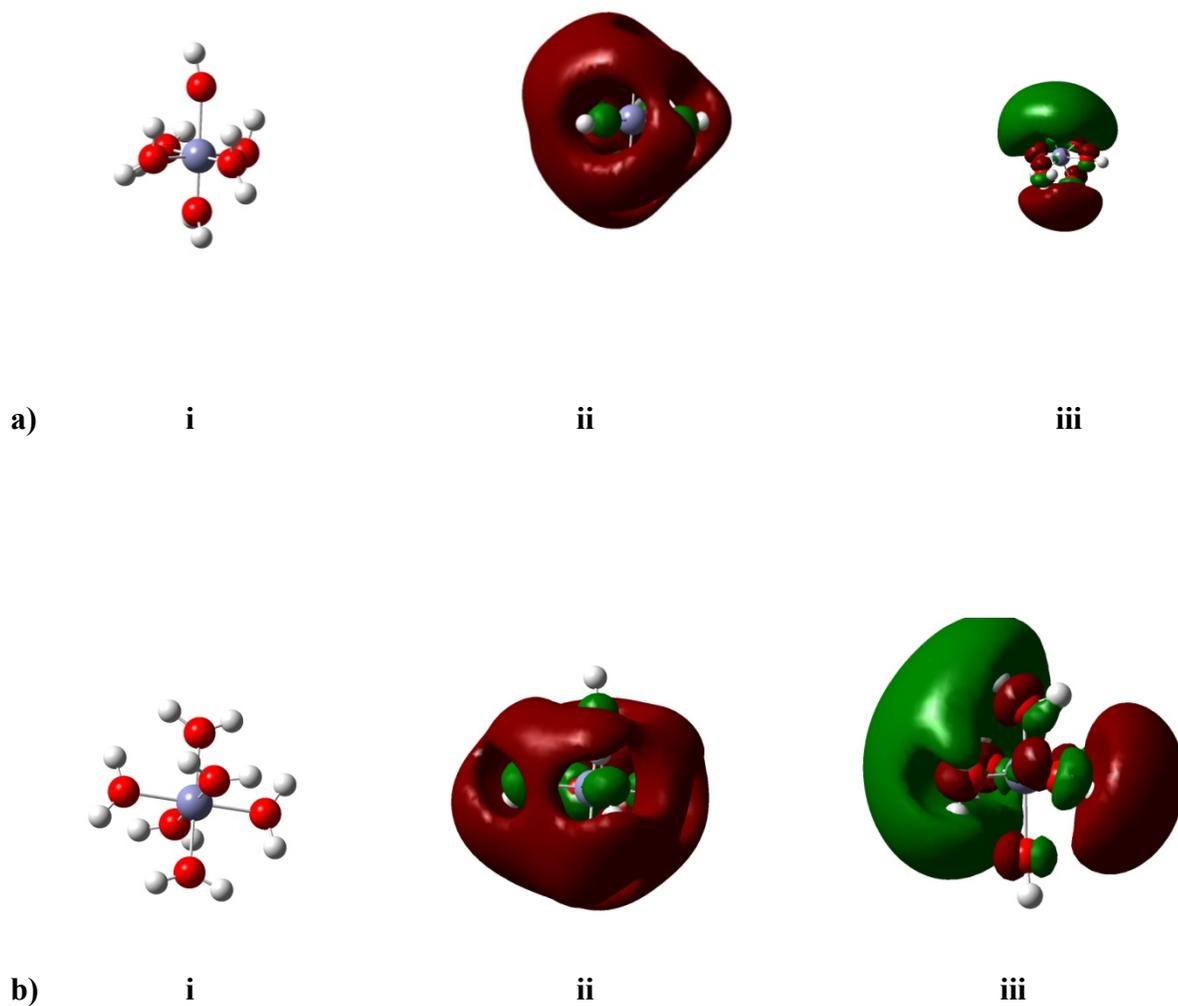


a



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  $[\text{Zn}(\text{H}_2\text{O})_6]^{+2}$