Supporting Information

β-Substituted Ferrocenyl Porphyrins: Synthesis, Structure, and Properties

Rekha Sharma, Prabhat Gautam, Shaikh M. Mobin, and Rajneesh Misra*

Department of Chemistry, Indian Institute of Technology Indore, Indore- 452017, India.

Table of Contents

I.	Crystallographic data·····S1
II.	Copies of ¹ H NMR, and HRMS Spectra of the Compounds (4a-4c)······S3-S8
III	. Electrochemical Data for 4a, 4c·····S9
IV	. UV-Vis spectra of protonated ferrocennyl-porphyrins (4a- 4c)



Figure S1. The supramolecular structure of compound 3b along *b* axis. The secondary interactions are shown by dashed lines.

¹H NMR Spectra of 4a





HRMS mass spectrum of compound 4a.

¹H NMR Spectra of 4b



HRMS mass spectrum of compound 4b.



¹H NMR Spectra of 4c





HRMS mass spectrum of compound **4c**.

Electrochemical Characterizations:



a) Cyclic voltammogram of 3aH and 4a

Figure 3: Cyclic voltammograms of $(1.0X10^{-4} \text{ M})$ solutions of (a) **3aH**, (b) **4a** Oxidation (c) **4a** reduction, in CH₂Cl₂ containing 0.1 M Bu₄NPF₆ as supporting electrolyte, recorded at a scan speed of 100 mVs⁻¹.

b) Cyclic voltammogram of 3cH and 4c



Figure 3: Cyclic voltammograms of $(1.0X10^{-4} \text{ M})$ solutions of (a) **3cH**, (b) **4c** Oxidation (c) **4c** reduction, in CH₂Cl₂ containing 0.1 M Bu₄NPF₆ as supporting electrolyte, recorded at a scan speed of 100 mVs⁻¹.



Fig. S3.: UV-Vis spectra of protonated ferrocennyl-porphyrins (4a-4c), recorded in toluene.