Electronic Supplementary Material (ESI) for Dalton Transactions. This journal is © The Royal Society of Chemistry 2014

Supporting Information

Axial Bonded Pentads Constructed on Sn(IV) Porphyrin Scaffold

Yogita Pareek, Vellanki Lakshmi and Mangalampalli Ravikanth*

Department of Chemistry, Indian Institute of Technology Bombay, Powai,

Mumbai 400 076, India. E-mail: ravikanth@chem.iitb.ac.in

CONTENTS

Entry		Page No.
1	Figure S1 ES-MS spectrum of dyad 4	3
2	Figure S2 ES-MS spectrum of dyad 5	4
3	Figure S3 ES-MS spectrum of dyad 6	5
4	Figure S4 ¹ H NMR spectrum of dyad 4	6
5	Figure S5 ¹ H NMR spectrum of dyad 5	7
6	Figure S6 ¹ H NMR spectrum of dyad 6	8
7	Figure S7 MALDI-TOF spectrum of pentad 1	9
8	Figure S8 MALDI-TOF spectrum of pentad 2	10

1

9	Figure S9 MALDI-TOF spectrum of pentad 3	11
10	Figure S10 ¹ H NMR spectrum of pentad 1	12
11	Figure S11 ¹ H NMR spectrum of pentad 2	13
12	Figure S12 ¹ H NMR spectrum of pentad 3	14
13	Figure S13 Partial ¹ H- ¹ H COSY NMR spectrum of pentad 1	15
14	Figure S14 Partial ¹ H- ¹ H COSY NMR spectrum of pentad 1	16
15	Figure S15 Comparison of ¹ H NMR spectrum of pentad 1 with dyad 4 and monomers 7 and 11.	17
16	Figure S16 Comparison of ¹ H NMR spectrum of pentad 2 with dyad 5 and monomers 7, 9 and 11	18
17	Figure S17 Comparison of ¹ H NMR spectrum of pentad 3 with dyad 6 and monomers 7, 10 and 11.	19
18	Table S1: Selected ¹ H NMR data for pentads 1, 2 and 3	20
19	Genaral experimental section	21



Figure S1: ES-MS spectrum of dyad 1.



Figure S2: ES-MS spectrum of dyad 2.



Figure S3: ES-MS spectrum of dyad 3.



Figure S4: ¹H NMR spectrum of dyad 1.



Figure S5: ¹H NMR spectrum of dyad **2**.



Figure S6: ¹H NMR spectrum of dyad 3.



Figure S7: MALDI-TOF spectrum of pentad 1



Figure S8: MALDI-TOF spectrum of pentad 2



Figure S9: MALDI-TOF spectrum of pentad 3.



Figure S10: ¹H NMR spectrum of pentad **1**.

12



Figure S11: ¹H NMR spectrum of pentad 2.

13



Figure S12: ¹H NMR spectrum of pentad **3**.



Figure S13: Partial ¹H-¹H COSY NMR spectrum of pentad 1.



Figure S14: Partial ¹H-¹H COSY NMR spectrum of pentad 1.











Figure S17: Comparison of ¹H NMR spectrum of pentad 3 with dyad 6 and monomers 7, 10 and 11.

Table S1: Selected ¹H NMR data for pentads 1, 2 and 3 with monomers axial porphyrin unit 7 and basal Sn(IV) porphyrin unit 11.

Compounds	Basal Sn(IV) porphyrin	Porphyrin unit of axial dyads		Basal Sn(IV) Phenoxo grou porphyrin		o group	
	β-Pyrrole protons	β-Pyrrole protons		β-Pyrrole protons	3,5 protons	2,6 protons	
		type c	type b	type a			
11	9.13 (s)	-	-	-	9.13 (s)	-	-
7	-	8.87 (m) multiplet for a, b and c type		-	8.00 (d)	7.17 (d)	
1	9.40 (m)	8.83 (m)	8.57 (d)	8.14 (m)	9.40 (m)	6.58 (d)	2.44 (d)
2	9.48 (d),	8.93 (m)	8.59 (d)	8.13 (m)	9.48 (d),	6.59 (d)	2.42 (d)
	9.42 (s),				9.42 (s),		
	9.31 (d)				9.31 (d)		
3	9.41 (d)	8.85 (m)	8.58 (m)	8.48 (d)	9.41 (d)	6.59 (d)	2.44 (d)

General Experimental Section:

All general chemicals and solvents were procured from S.D. Fine chemicals, India. Column chromatography was performed using silica gel and basic alumina obtained from Sisco Research Laboratories, India. All the solvents used were of analytical grade and were purified and dried by routine procedures immediately before use.

¹H NMR spectra were recorded with Bruker 400 MHz instrument using trimethylsilane (TMS) as an internal standard. All NMR measurements were carried out at room temperature in deuterochloroform (CDCl₃). Absorption and steady state fluorescence spectra were obtained with Perkin-Elmer Lambda-35 and Varian Cary-Eclipse respectively. The fluorescence quantum yields (ϕ_f) were estimated from the emission and absorption spectra by comparative method.³⁷ ES-MS mass spectra were recorded with a Q-Tof Micromass spectrometer. MALDI-TOF mass spectra were recorded on Bruker MALDI-TOF spectrometer. Cyclic voltammetric (CV) and differential pulse voltammetric (DPV) studies were carried out with BAS electrochemical system utilizing the three electrode configuration consisting of a glassy carbon (working electrode), platinum wire (auxiliary electrode) and saturated calomel (reference electrode) electrodes in dry dichloromethane using 0.1 M tetrabutylammonium perchlorate as supporting electrolyte.