

Supporting Information

Sn(IV) Porphyrin Based Axial-Bonding Type Porphyrin Triads Containing Heteroporphyrins as Axial Ligands

Vijayendra S. Shetti and Mangalampalli Ravikanth*

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

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

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exp5 PROTON

SAMPLE		SPECIAL	
date	Jun 11 2007	temp	not used
solvent	CDCl3	gain	not used
file	exp	spin	not used
ACQUISITION		hst	0.008
sw	30030.0	pw90	8.500
at	1.993	alfa	20.000
np	119706	FLAGS	
fb	16600	il	n
bs	4	in	n
dl	1.000	dp	y
nt	400	hs	nn
ct	184	PROCESSING	
tn	H1	lb	0.10
sfrq	399.883	fn	not used
tof	200.0	DISPLAY	
tpwr	59	sp	-1843.0
pw	4.250	wp	6274.1
DECOUPLER		rfl	12773.1
dn	C13	rfl	0
dof	0	rp	169.7
dm	nnn	lp	-429.6
dmm	c	PLOT	
dpwr	51	wc	250
dmt	17100	sc	0
		vs	45
		th	2
		ai	ph

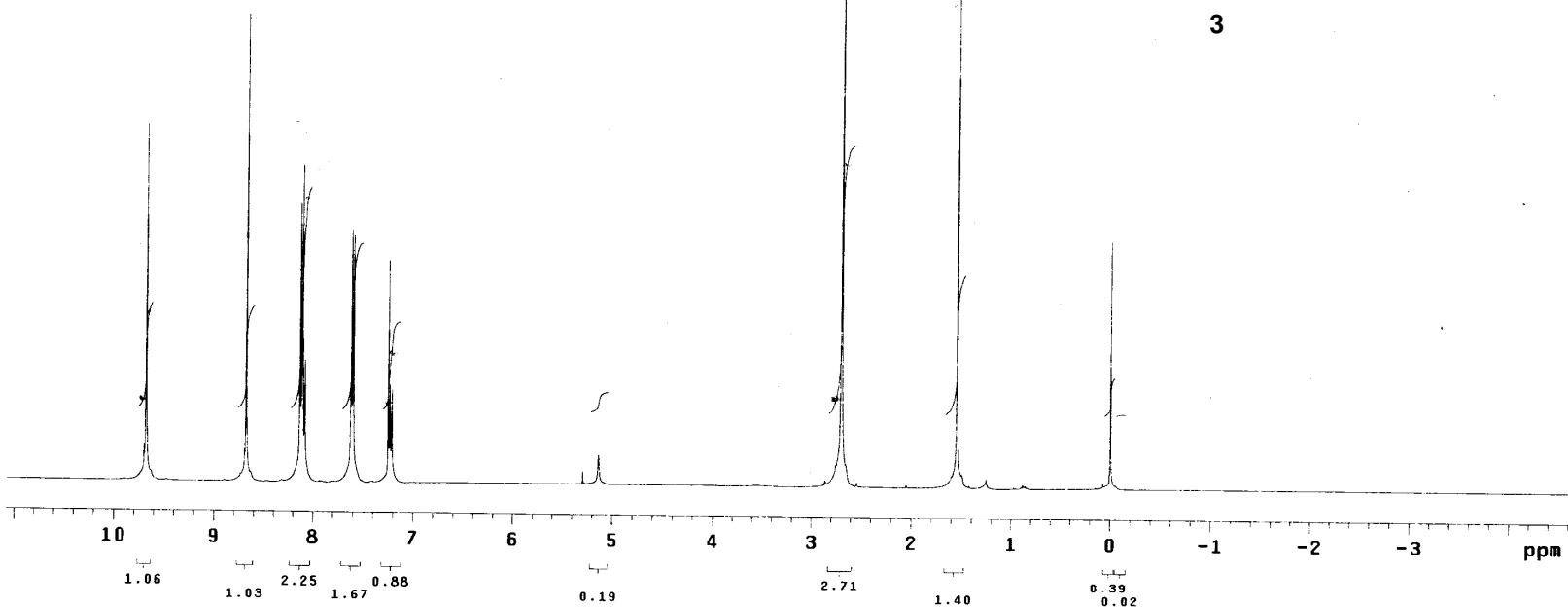
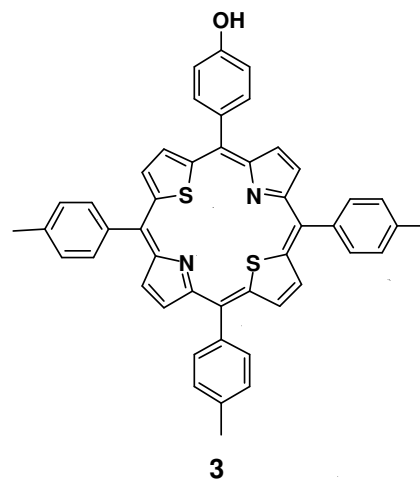
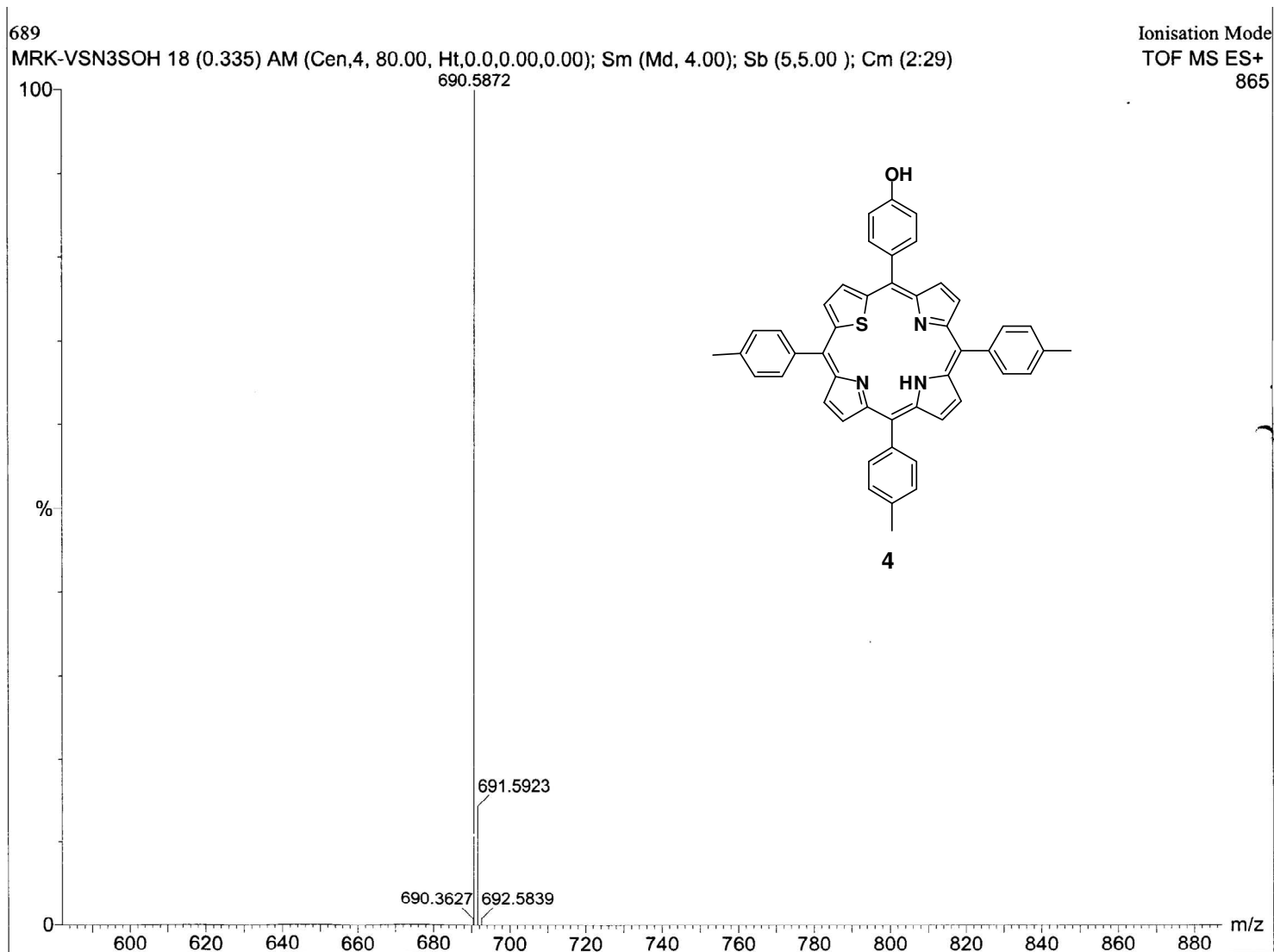


Figure S1. ¹H NMR spectrum of **3**



Expected Mol.Wt. = 689.25

M.F = C₄₇H₃₅N₃OS

Observed Mol.Wt. = 690.58 [M + H]⁺

Figure S2. ES-MS spectrum of **4**

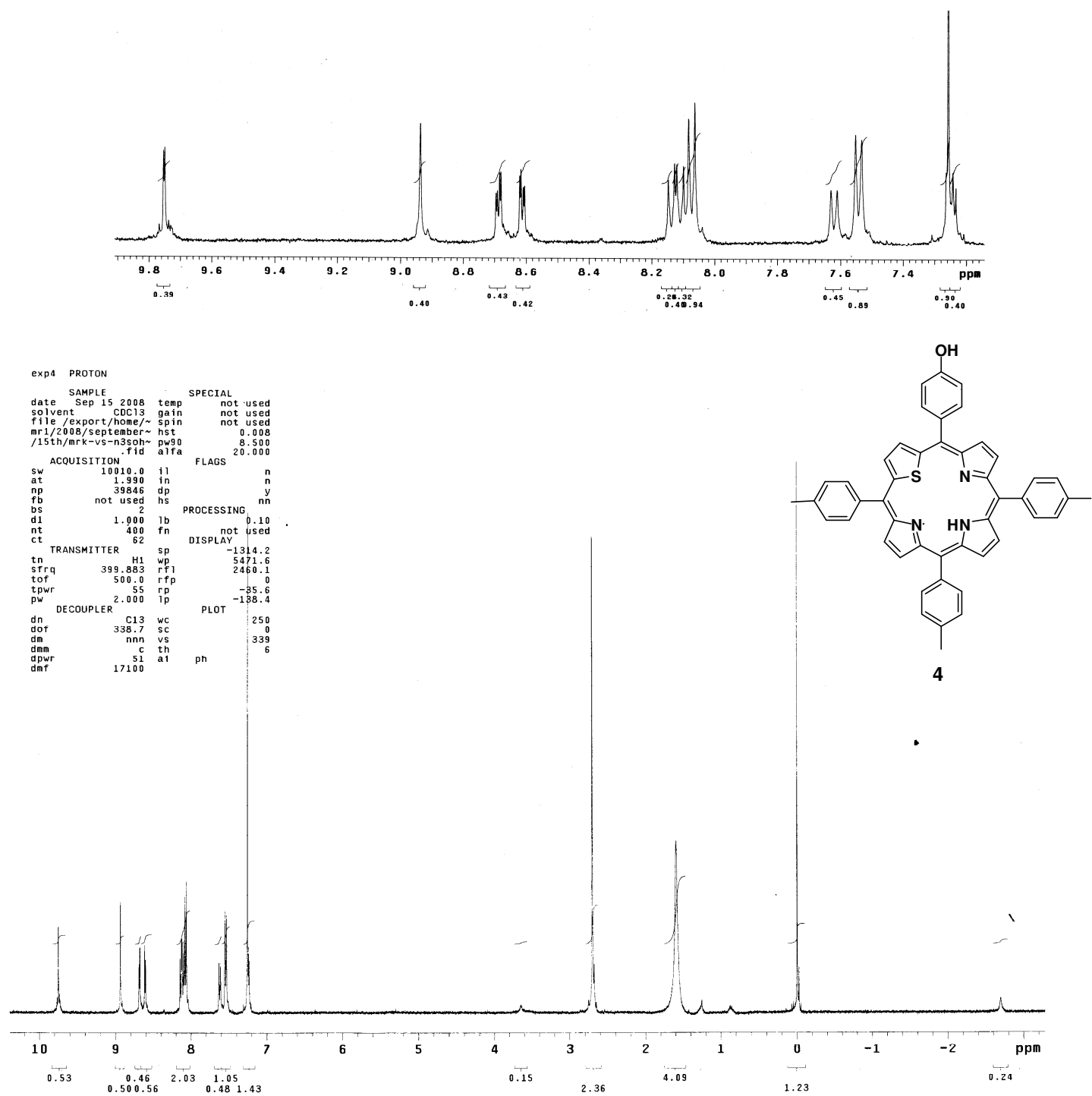
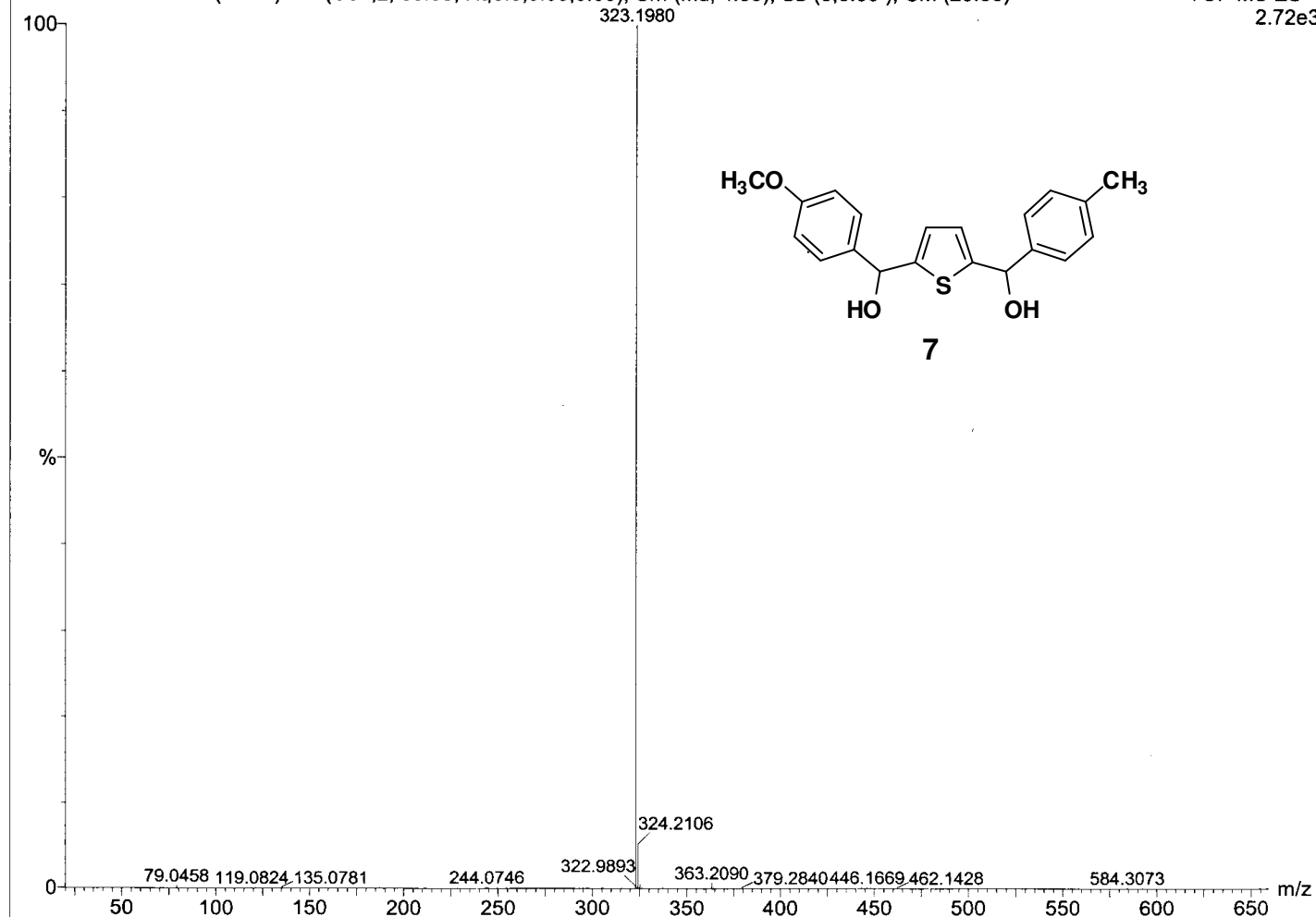


Figure S3. ^1H NMR spectra of **4**

MRK-VS-OCH3D 20 (0.372) AM (Cen,2, 80.00, Ht,0.0,0.00,0.00); Sm (Md, 4.00); Sb (5,5.00); Cm (20:36)

Ionisation Mode
TOF MS ES+
2.72e3

Expected Mol.Wt. = 340.11

M.F = C₂₀H₂₀O₃SObserved Mol.Wt. = 323.19 [M-OH]⁺**Figure S4.** ES-MS spectrum of **7**

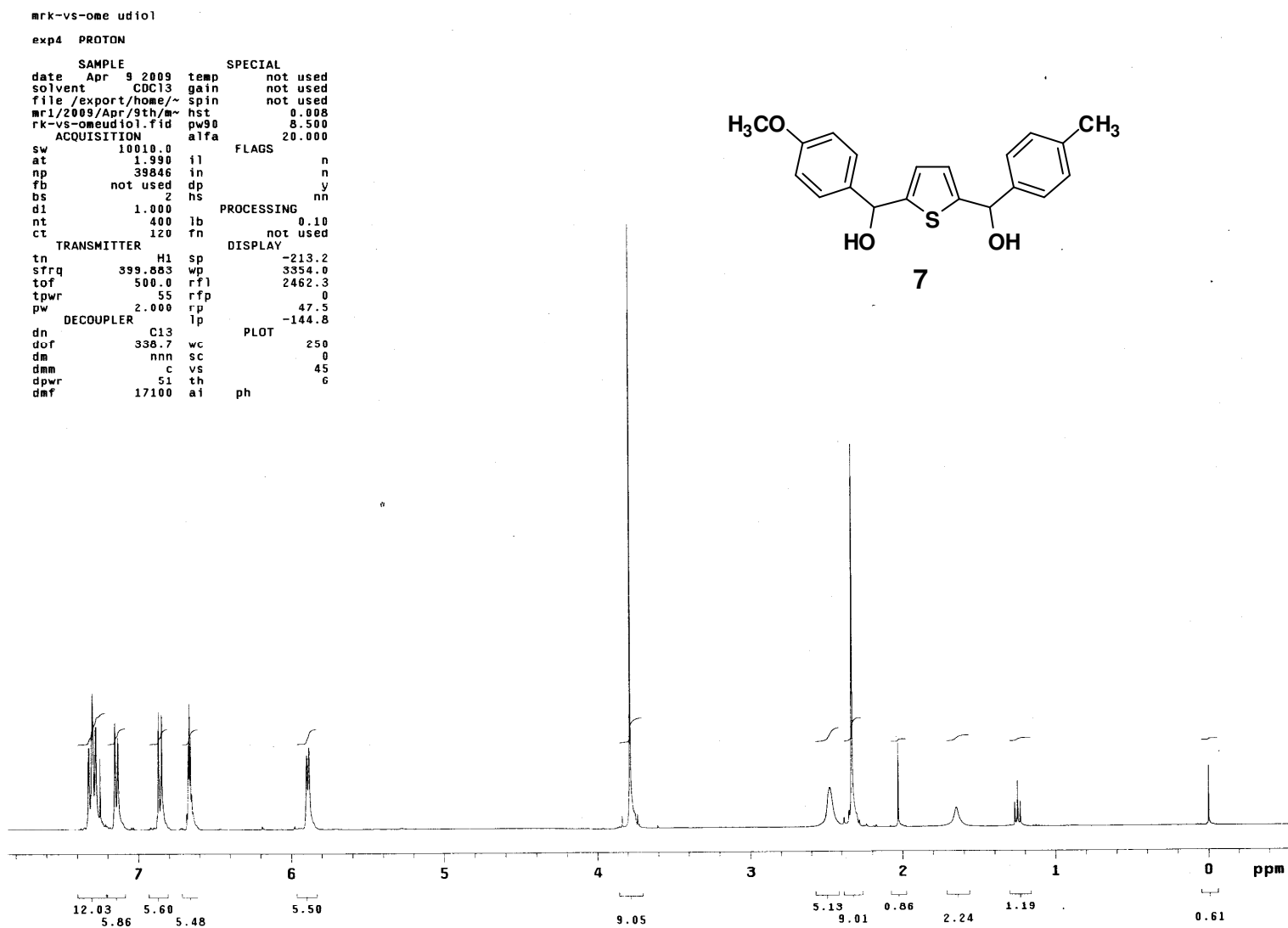


Figure S5. ^1H NMR spectrum of **7**

mrk-vs-omeudiol-13c

Data Collected on: fitbchem-mercuryhifreq
Archive directory: /export/home/vnmr1/vnmrsys/data
Sample directory:
File: C13

Pulse Sequence: s2pul

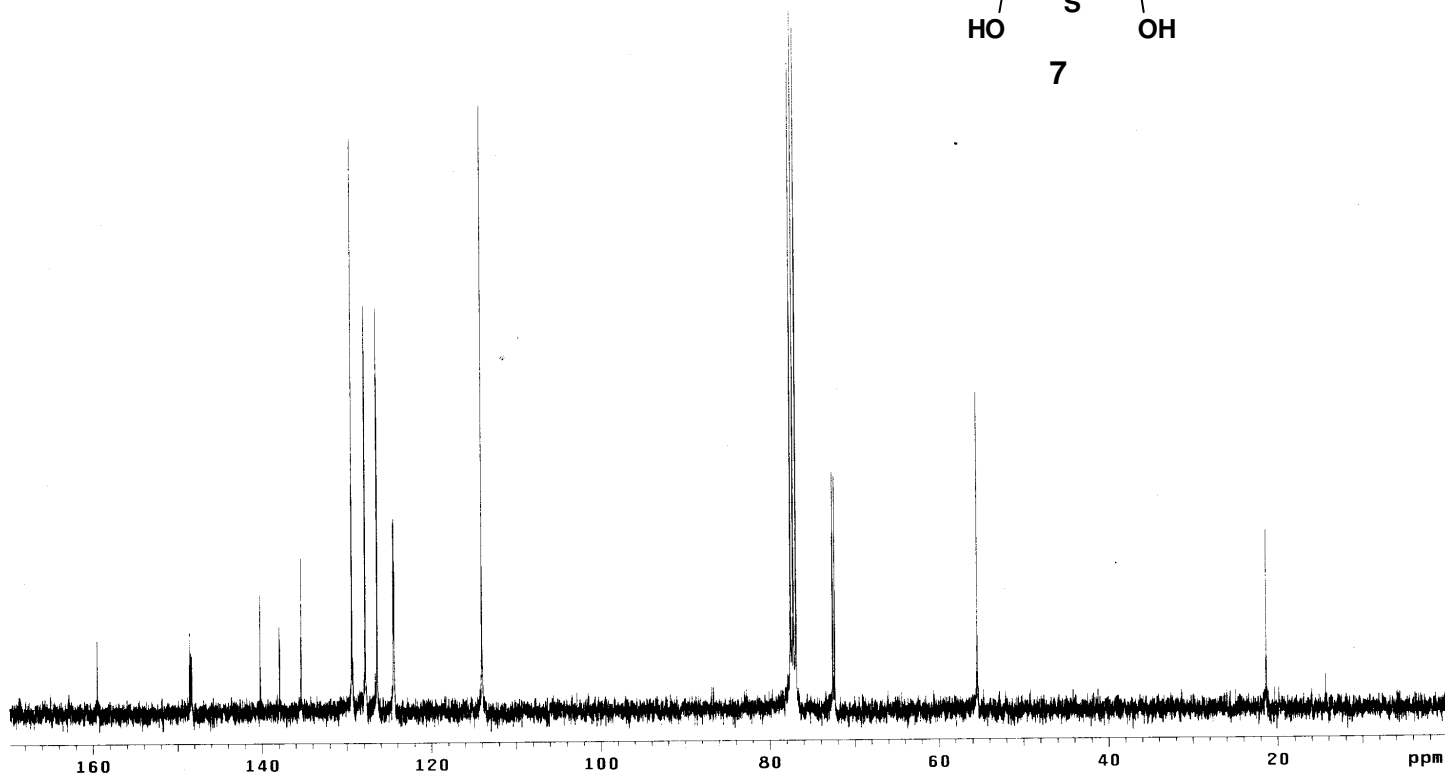
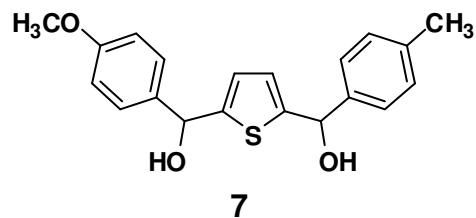
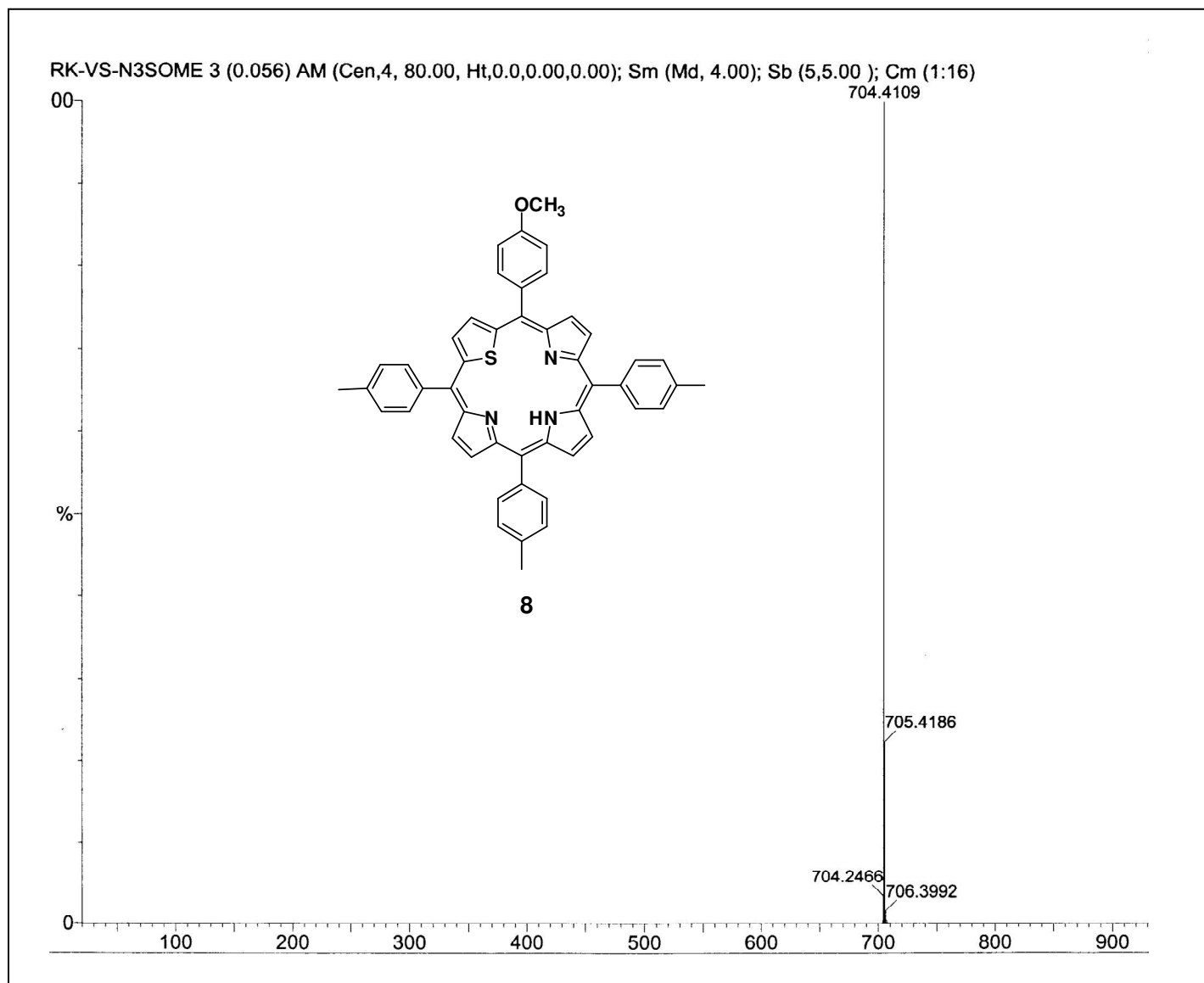


Figure S6. ¹³C NMR spectrum of **7**



Expected Mol.Wt. = 703.27

M.F = $C_{48}H_{37}N_3OS$

Observed Mol.Wt. = 704.41 $[M + H]^+$

Figure S7. ES-MS spectrum of **8**

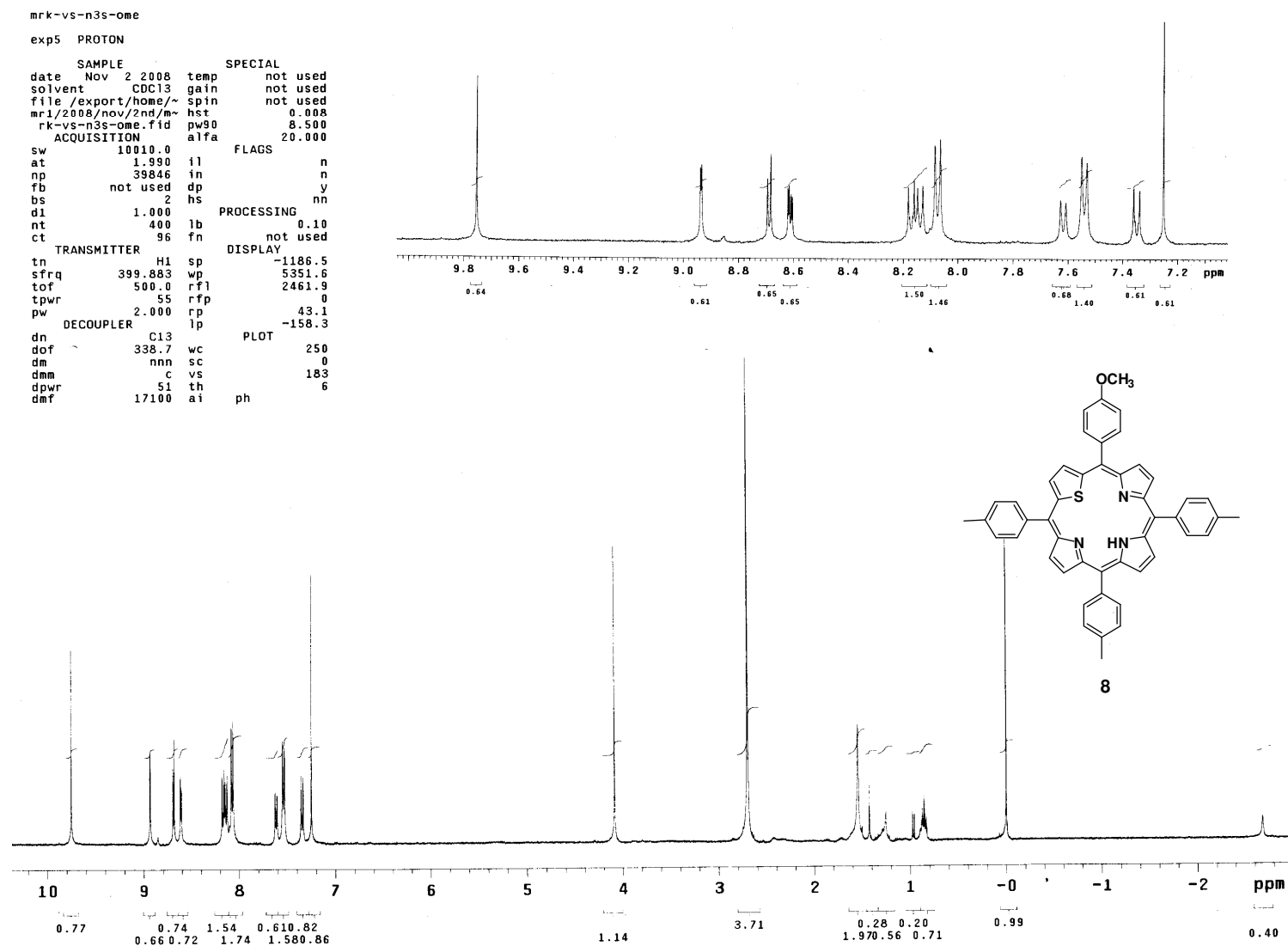
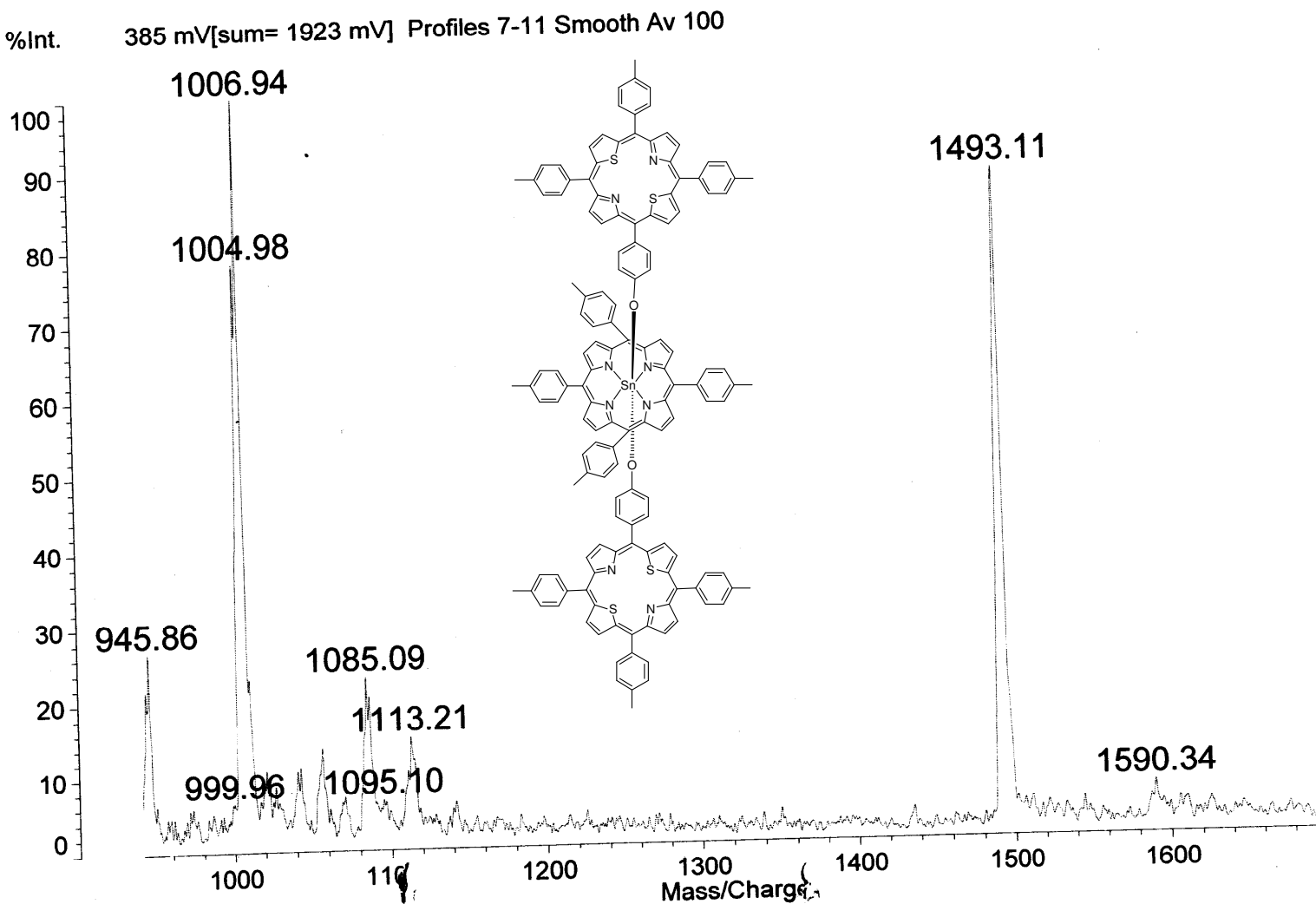


Figure S8. ¹H NMR spectra of **8**



Expected Mol.Wt.=2200.47

M.F = $C_{142}H_{102}N_8O_2S_4Sn$

Observed Mol.Wt.= 1493.11 (M- $C_{47}H_{34}N_2OS_2$)

Figure S9. MALDI-TOF spectrum of **1**

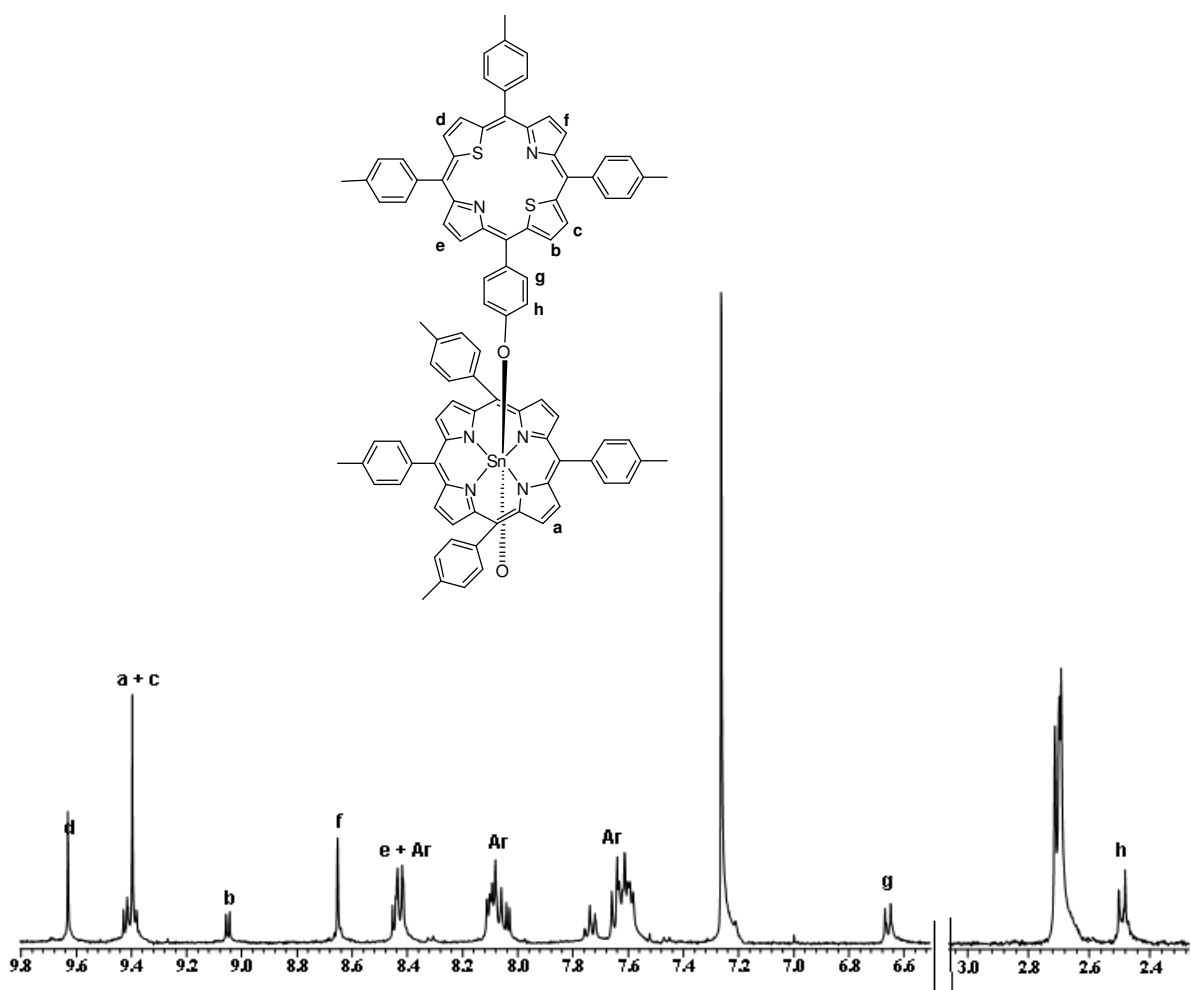
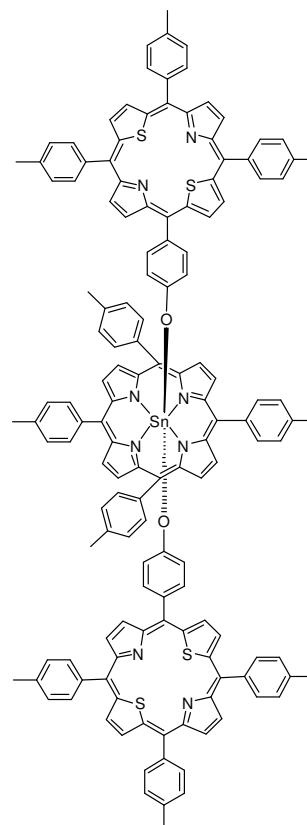
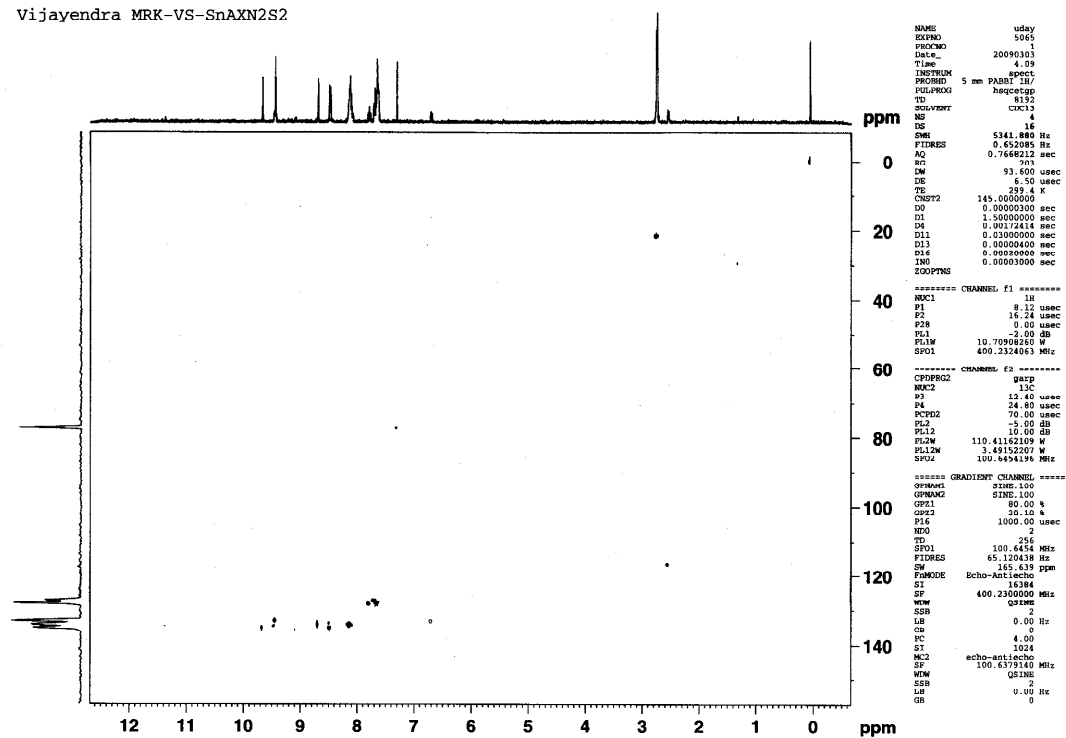


Figure S10. ^1H NMR spectrum of **1**

Vijayendra MRK-VS-SnAXN2S2



Vijayendra MRK-VS-SnAXN2S2

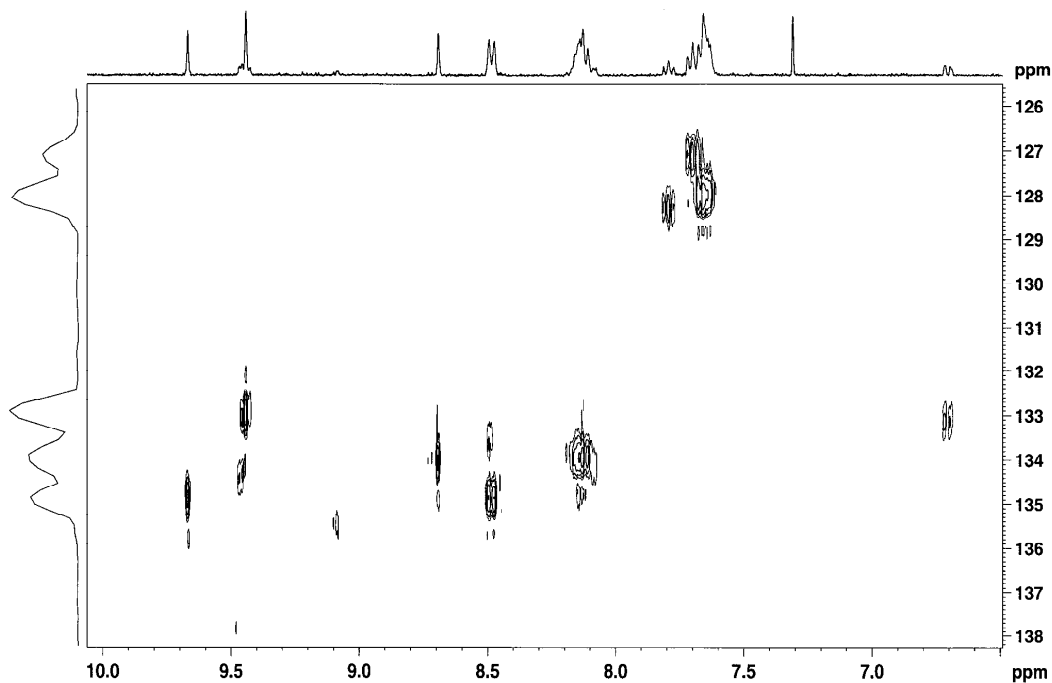
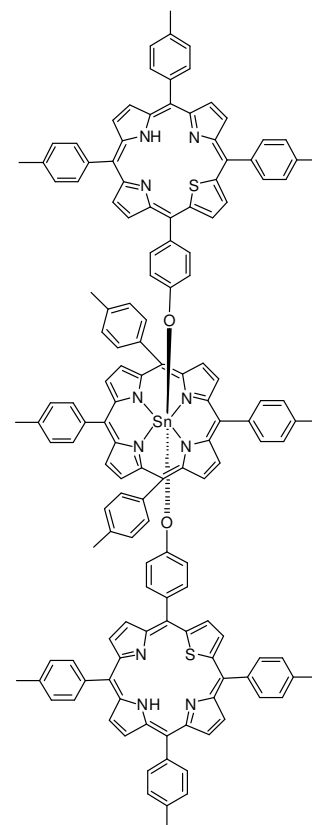
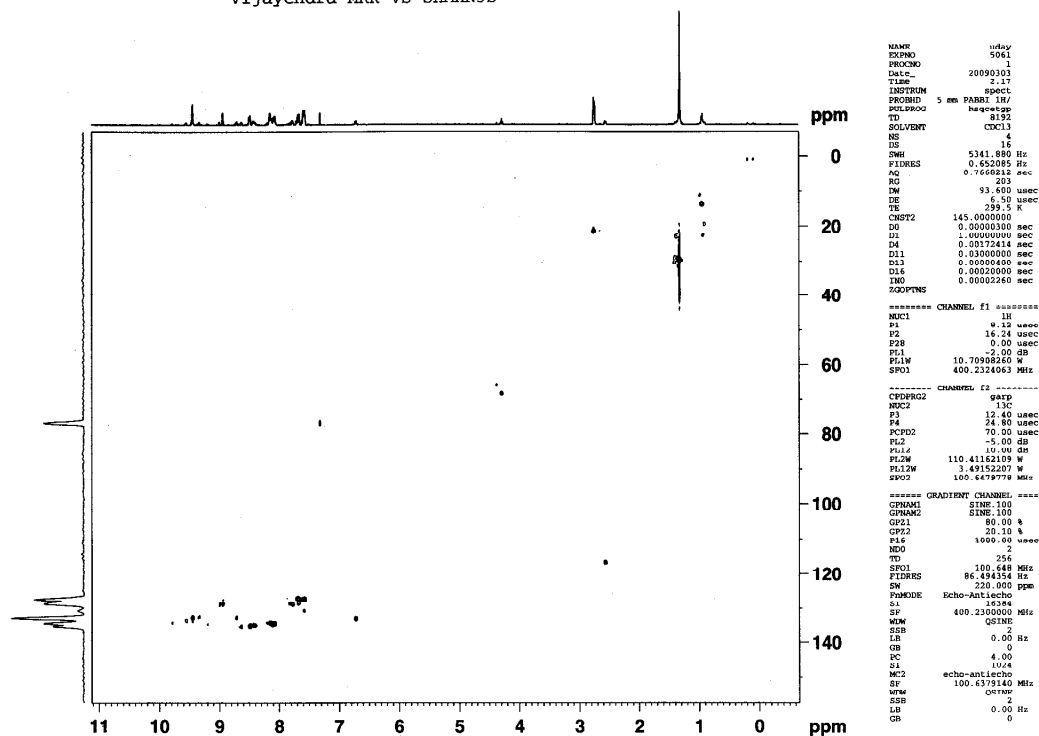


Figure S11. ^1H - ^{13}C HSQC spectra of **1**

Vijayendra MRK-VS-SnAXN3S



Vijayendra MRK-VS-SnAXN3S

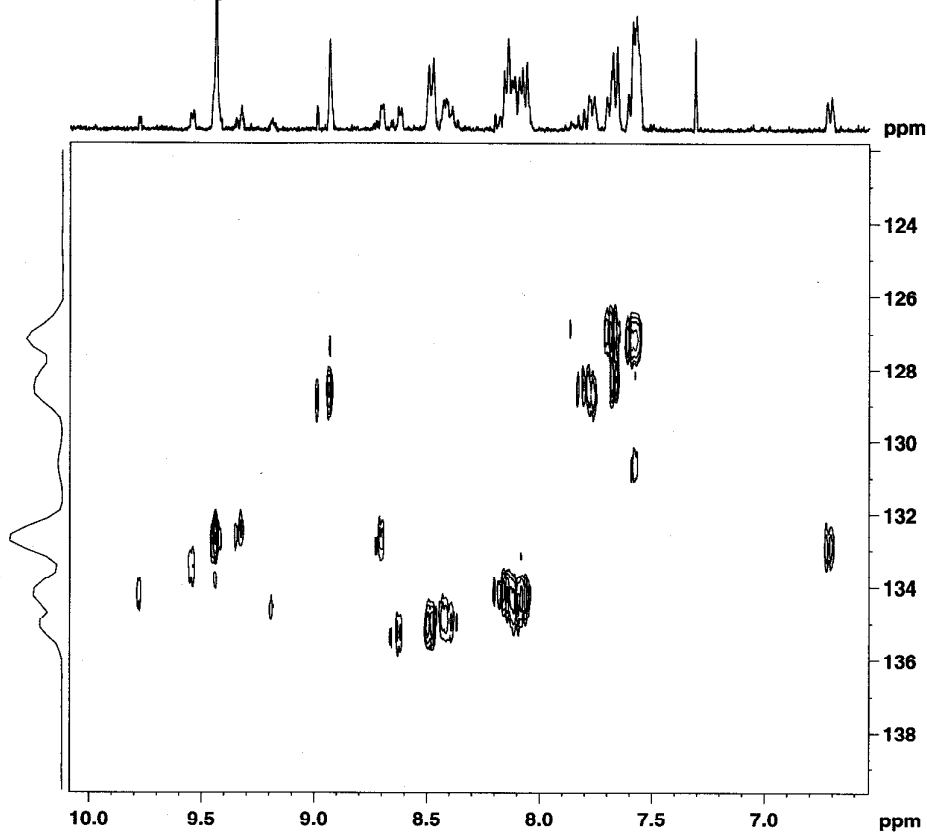


Figure S12. ^1H - ^{13}C HSQC spectra of **2**

Table S1. Selected ^1H NMR data for **1** and **2**

Compound	Axial $\text{N}_2\text{S}_2/\text{N}_3\text{S}$ porphyrins		Basal Sn(IV)porphyrin	Inner NH (ppm)
	β -thiophene (ppm)	β -pyrrole (ppm)	β -pyrrole Sn (ppm)	
SnTTP(OH)₂	-	-	9.13 (s)	-
3	9.68 (s)	8.68 (s)	-	-
1	9.62 (s) 9.41 (s) 9.41 (s))	8.65 (s) 8.05 (m)	9.39 (s)	-
4	9.75 (m)	8.93 (s) 8.68 (d) 8.69(d) 8.60 (d) 8.61(d)	-	-2.70 (s)
2	9.14 (d) 9.50 (d)	8.88 (s) 8.65 (d) 8.57(d) 8.41 (m)	9.38 (s)	-2.78 (s)