

Supporting Information

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

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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
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sw 30030.0 pw90 8.500
at 1.993 alfa 20.000
np 119706 FLAGS
fb 16600 ll n
bs 4 in n
d1 1.000 dp y
nt 400 hs nn
ct 184 PROCESSING
TRANSMITTER 1b fn 0.10
tn H1 fn not used
sfrq 399.883 DISPLAY
tfr 200.0 sp -1843.0
tpwr 59 wp 6274.1
pw 4.250 rfl 12773.1
DECOUPLER C13 rfp 0
dn 0 lp 169.7
dof 0 1p -429.6
dm nnn PLOT
dmm c wc 250
dpwr 51 sc 0
dmf 17100 vs 45
th ai 2
ai ph

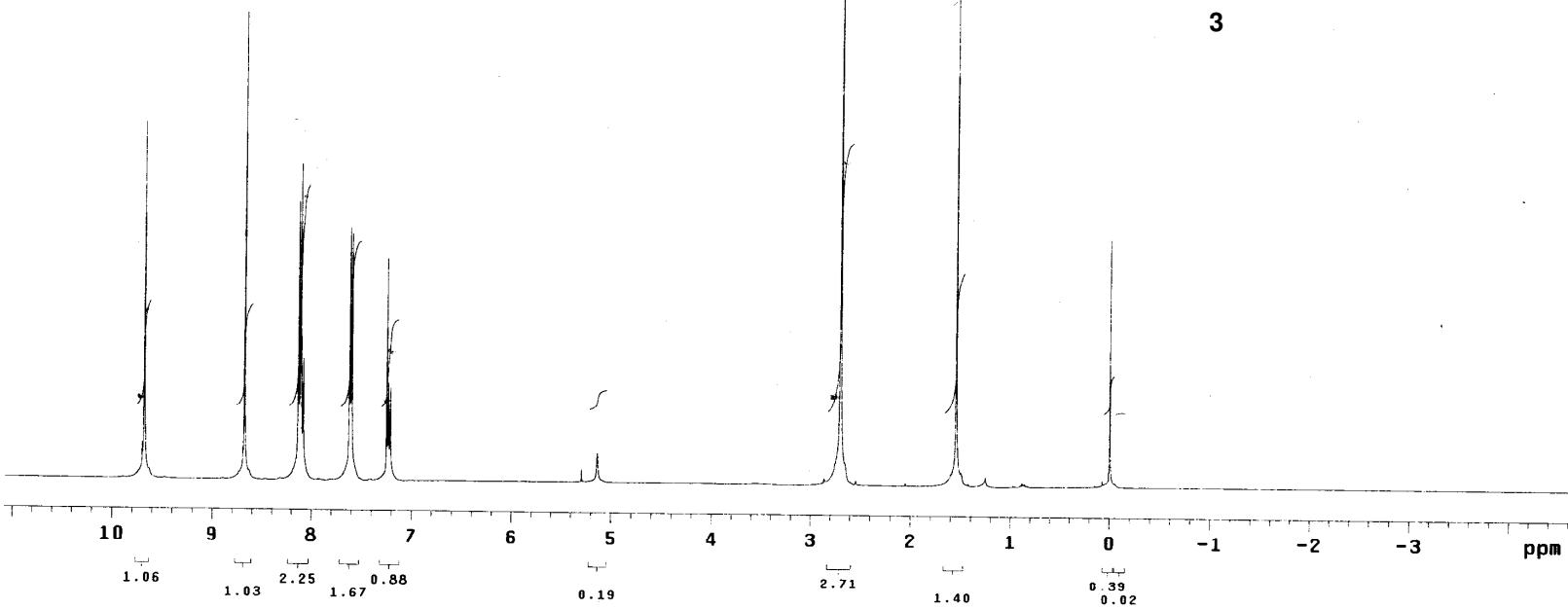
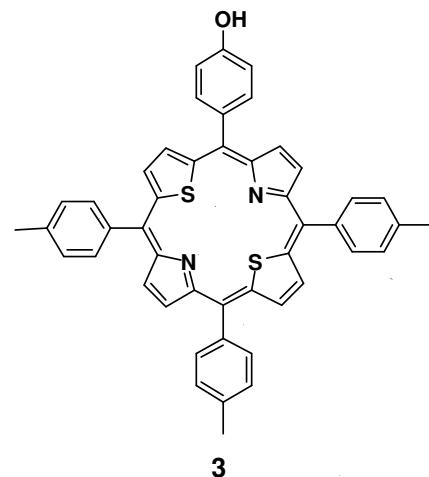
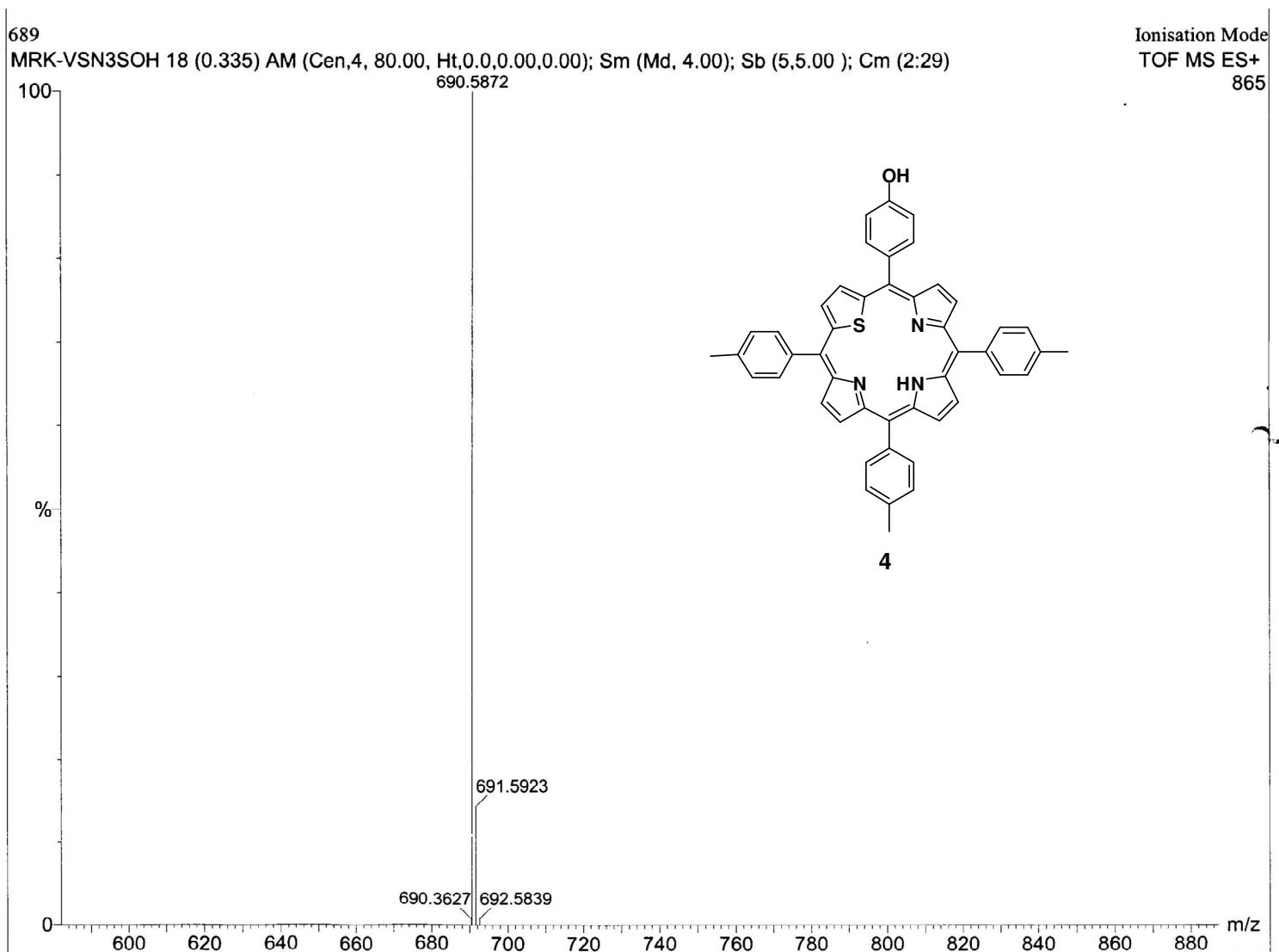


Figure S1. ¹H NMR spectrum of 3



Expected Mol.Wt. = 689.25

M.F = $C_{47}H_{35}N_3OS$

Observed Mol.Wt. = 690.58 $[M + H]^+$

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

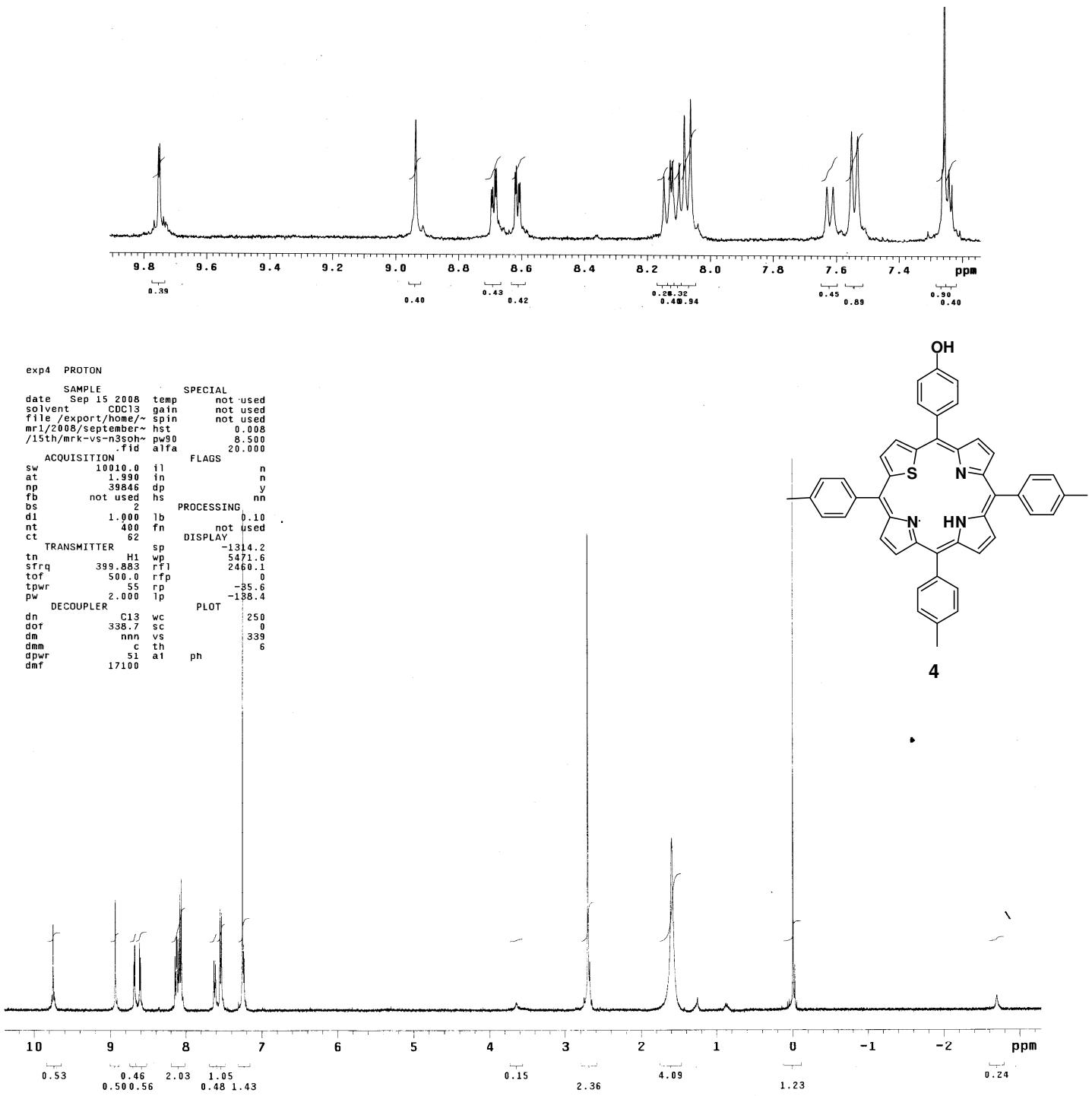


Figure S3. ¹H NMR spectra of **4**

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)

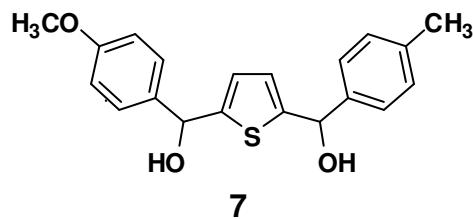
323.1980

100

%

0

79.0458 119.0824 135.0781 244.0746 322.9893 324.2106 363.2090 379.2840 446.1669 462.1428 584.3073 m/z



7

Expected Mol.Wt. = 340.11

M.F = C₂₀H₂₀O₃SObserved Mol.Wt. = 323.19 [M-OH]⁺

Figure S4. ES-MS spectrum of 7

mrk-vs-ome udiol

exp4 PROTON

SAMPLE SPECIAL
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solvent CDCl₃ gain not used
file/export/home/~/spin not used
mri/2009/Apr/9th/mr hst 0.008
rk-vs-omeudiol.fid pw90 8.500
ACQUISITION alfa 20.000
sw 10010.0 FLAGS
at 1.990 ll n
np 39846 in n
fb not used dp y
bs 2 hs nn
di 1.000 PROCESSING
nt 400 lb 0.10
ct 120 tn not used
TRANSMITTER DISPLAY
tn H1 sp -213.2
sfrq 399.883 wp 3354.0
tof 500.0 rfl 2462.3
tpwr 55 rfp 0
pw 2.000 rp 47.5
DECOUPLER C13 PLOT
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dof nnn sc 0
dm c vs 45
dmm s th 6
dpwr 17100 ai ph

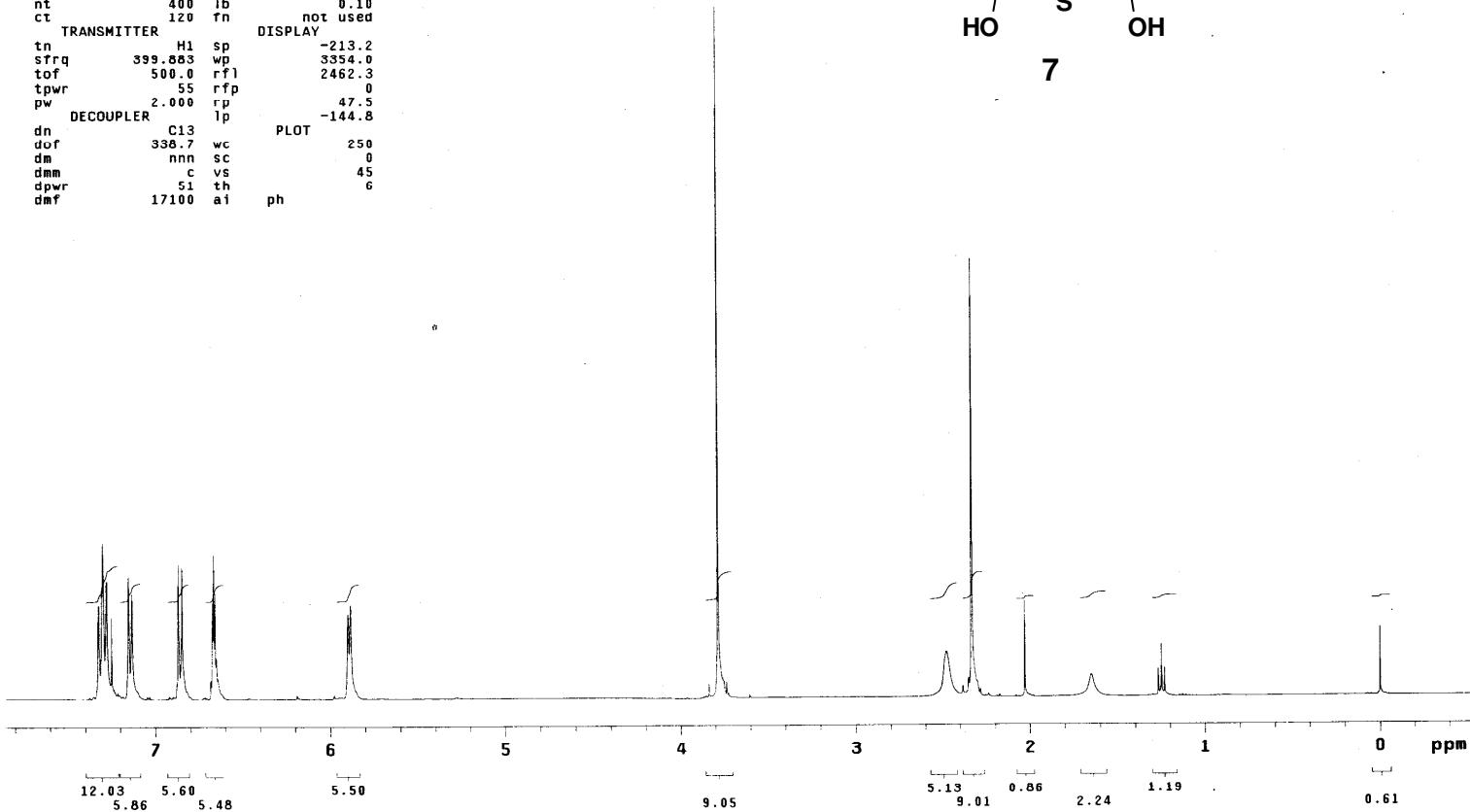
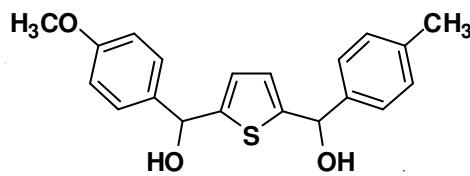


Figure S5. ¹H NMR spectrum of 7

mrk-vs-omeudiol-13c
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Archive directory: /export/home/vnmri/vnmrsys/data
Sample directory:
File: C13
Pulse Sequence: s2pul

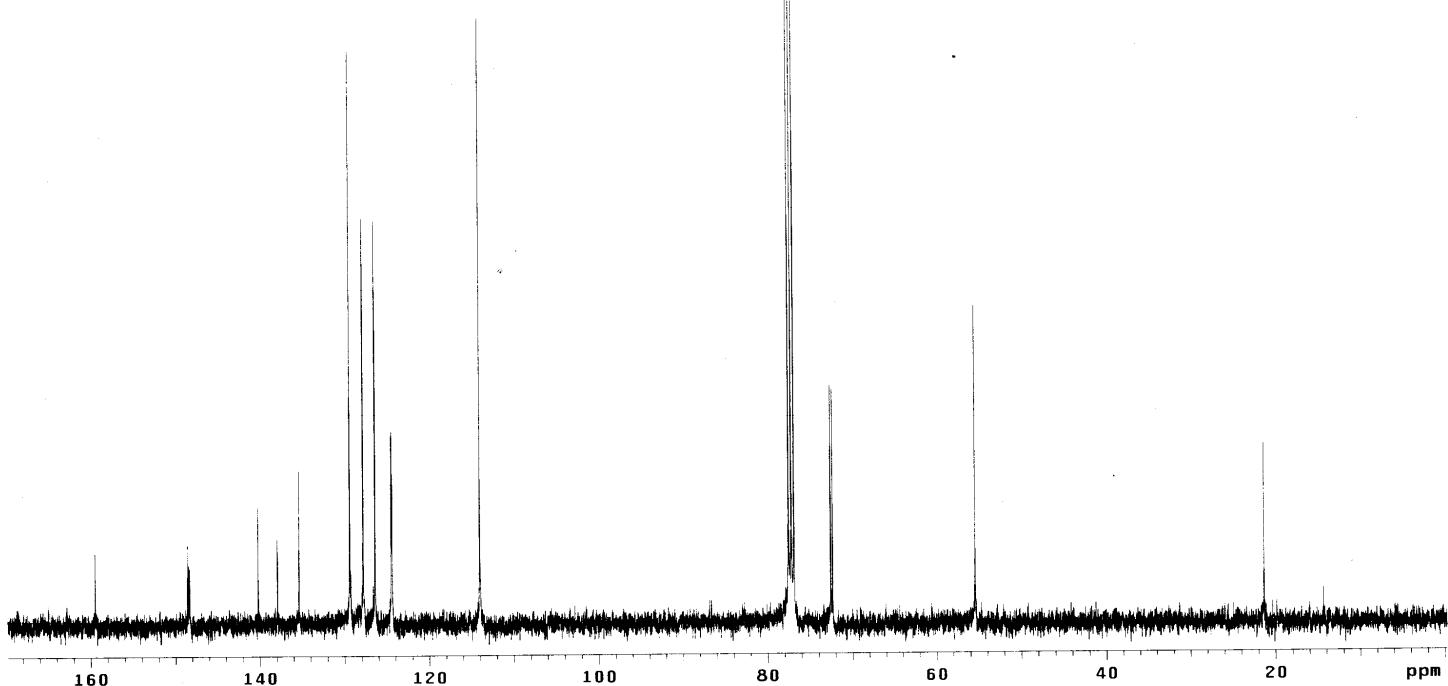
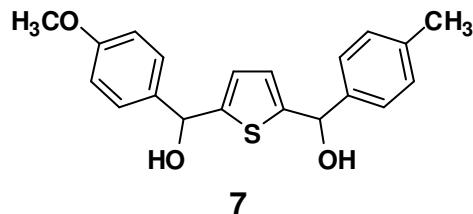
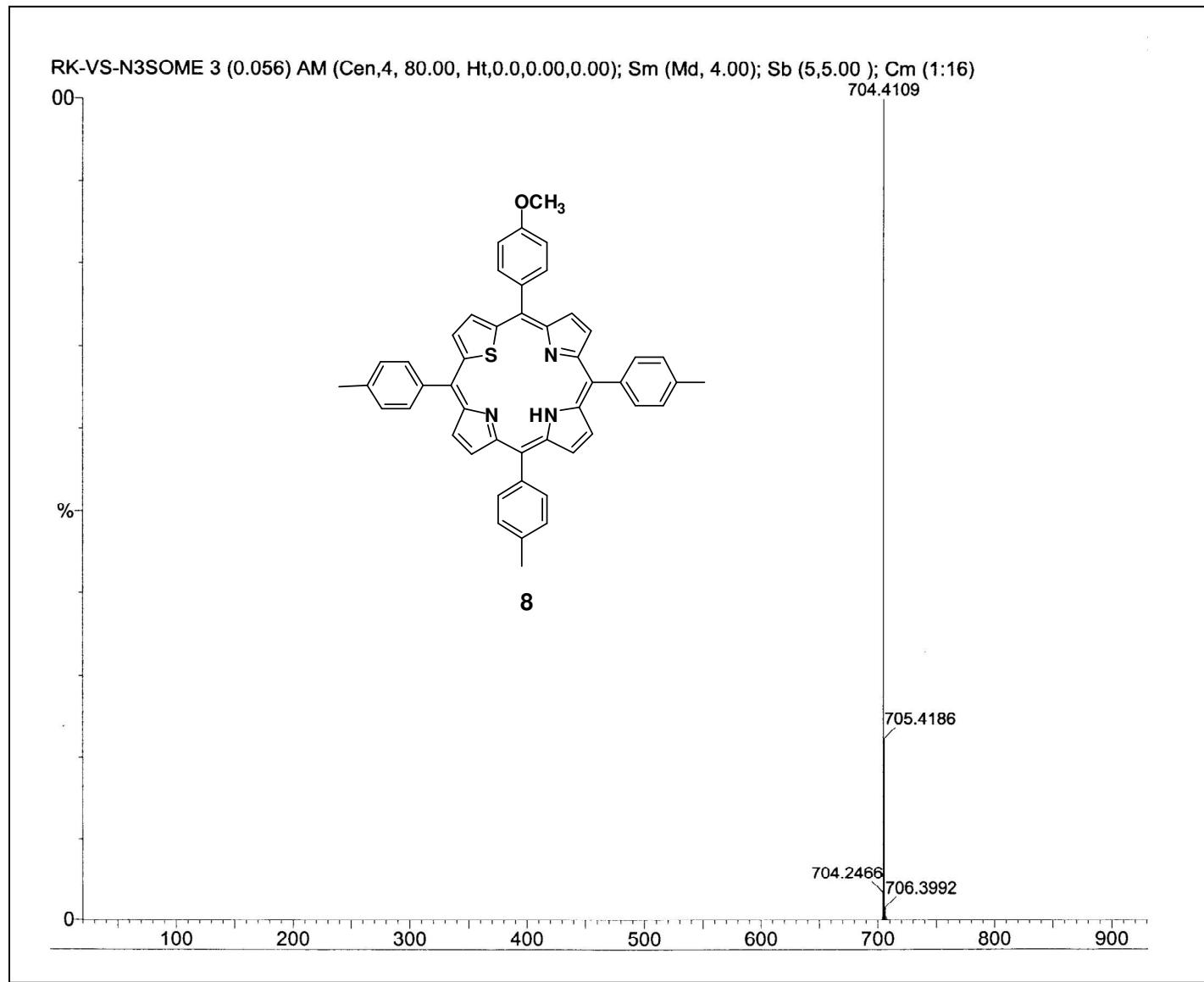


Figure S6. ¹³C NMR spectrum of **7**



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**

mrk-vs-n3s-ome

exp5 PROTON

SAMPLE SPECIAL
date Nov 2 2008 temp not used
solvent CDCl₃ gain not used
file /export/home/~/spin not used
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ACQUISITION alfa 20.000
sw 10010.0 FLAGS
at 1.990 ll n
np 39846 in y
fb not used dp nn
bs 2 hs
di 1.000 PROCESSING
nt 400 lb 0.10
ct 96 fn not used
TRANSMITTER DISPLAY
tn H1 sp -1186.5
sfrq 399.883 wp 5351.6
tof 500.0 rfl 2461.9
tpwr 55 rfp 0
pw 2.000 rp 43.1
DECOUPLER C13 PLOT
dn 338.7 wc 250
dof nnn sc 0
dmn c vs 183
dpwr 51 th 6
dmf 17100 ai ph

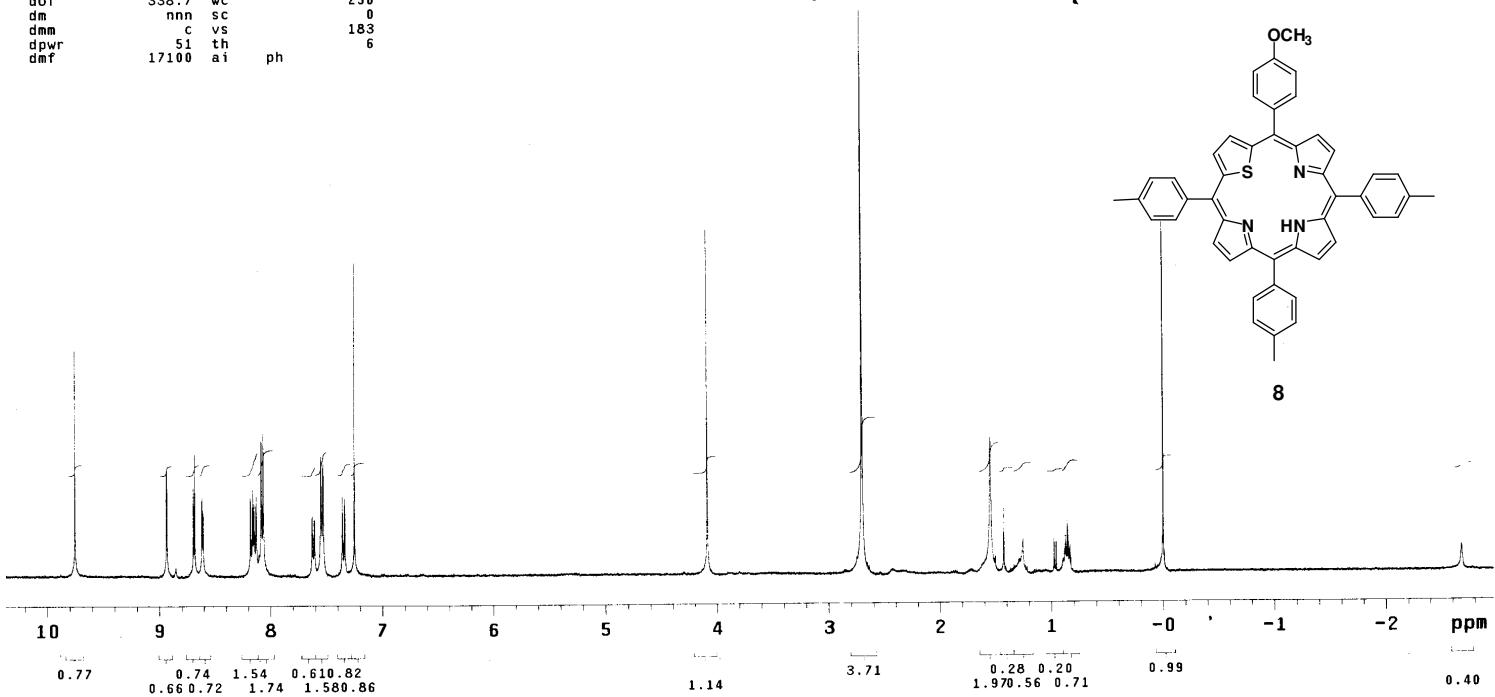
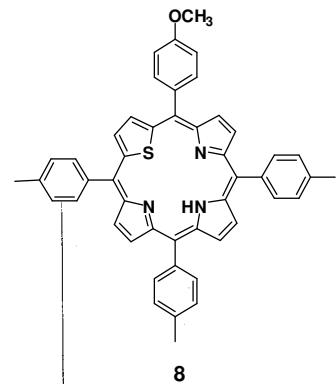
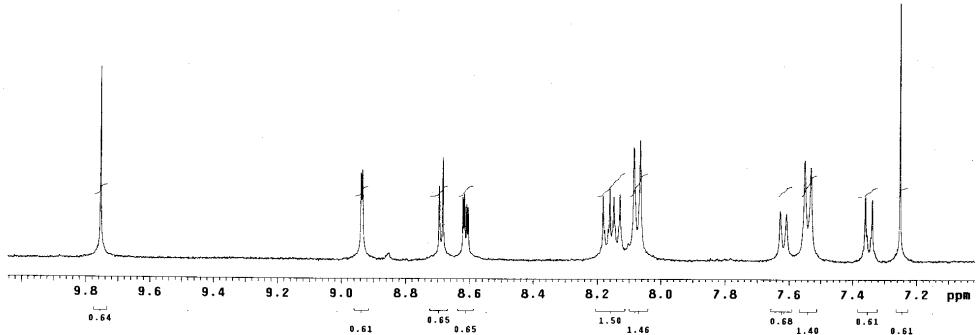
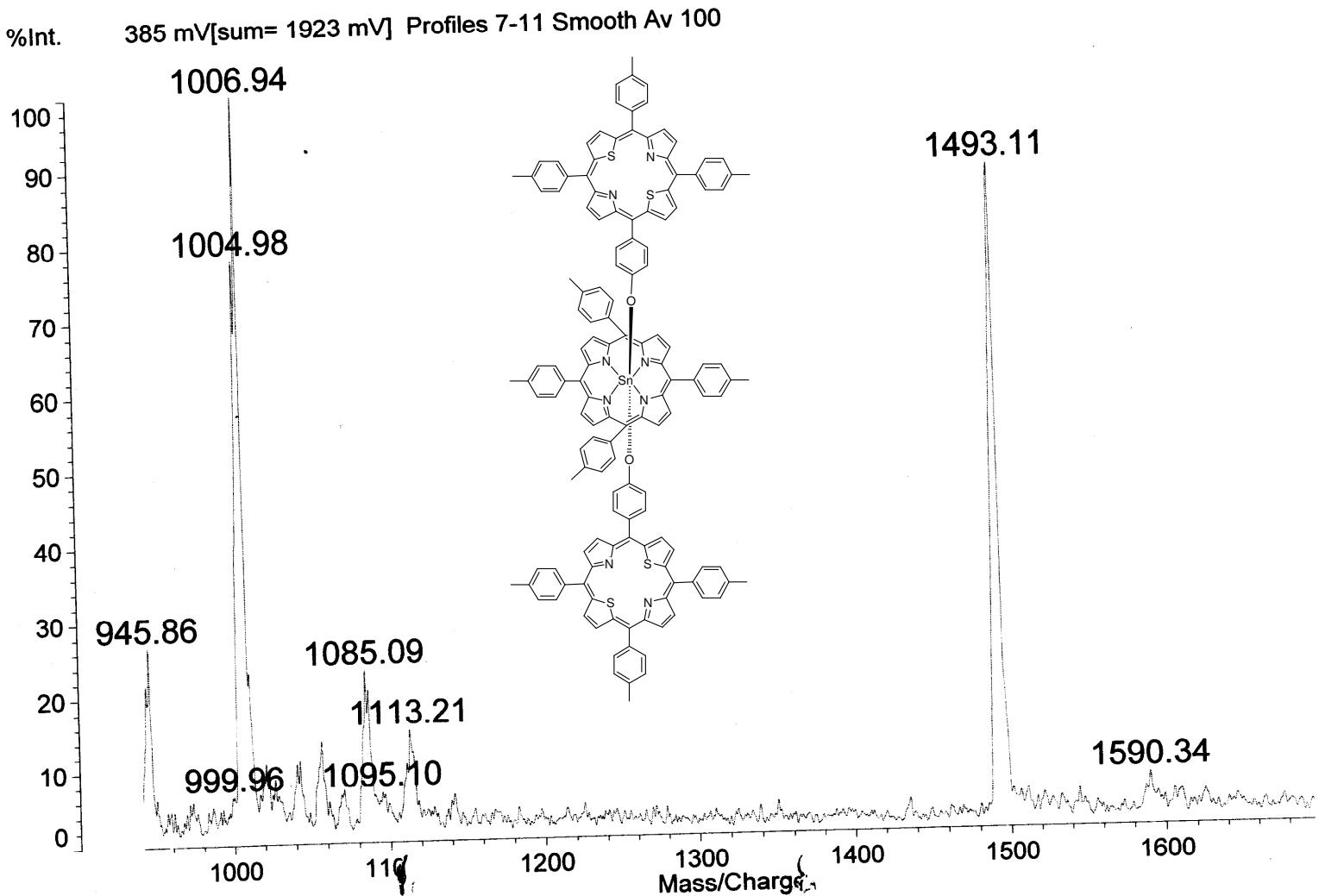


Figure S8. ¹H NMR spectra of **8**



Expected Mol.Wt.=2200.47

M.F = C₁₄₂H₁₀₂N₈O₂S₄Sn

Observed Mol.Wt.= 1493.11 (M-C₄₇H₃₄N₂OS₂)

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

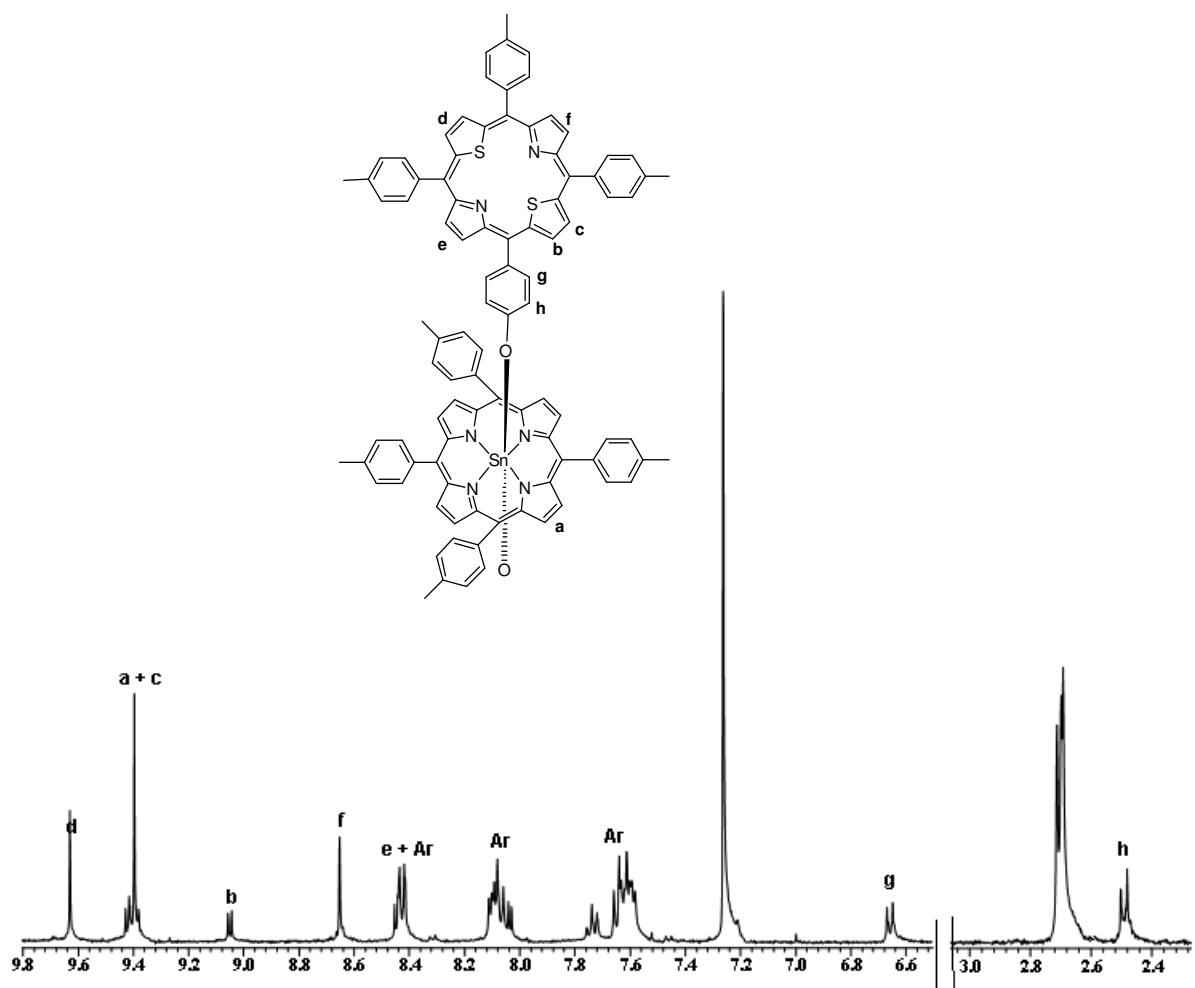
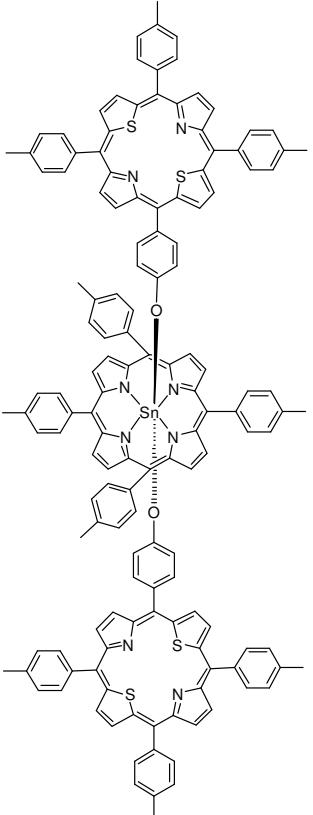
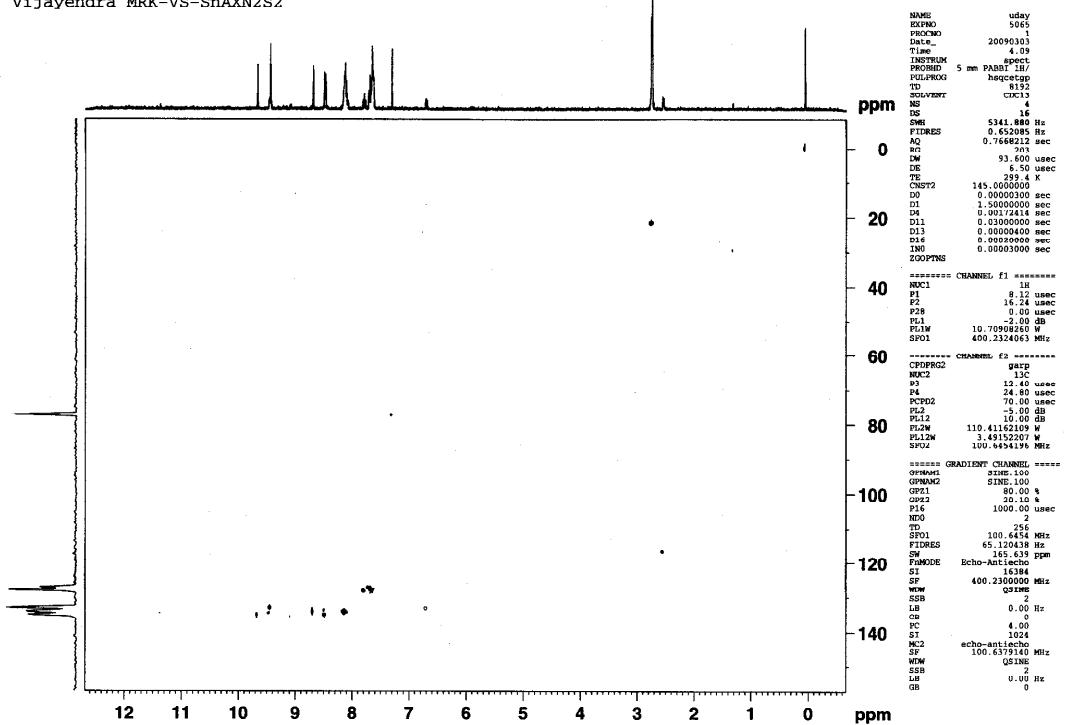


Figure S10. ¹H NMR spectrum of **1**

Vijayendra MRK-VS-SnAXN2S2



Vijayendra MRK-VS-SnAXN2S2

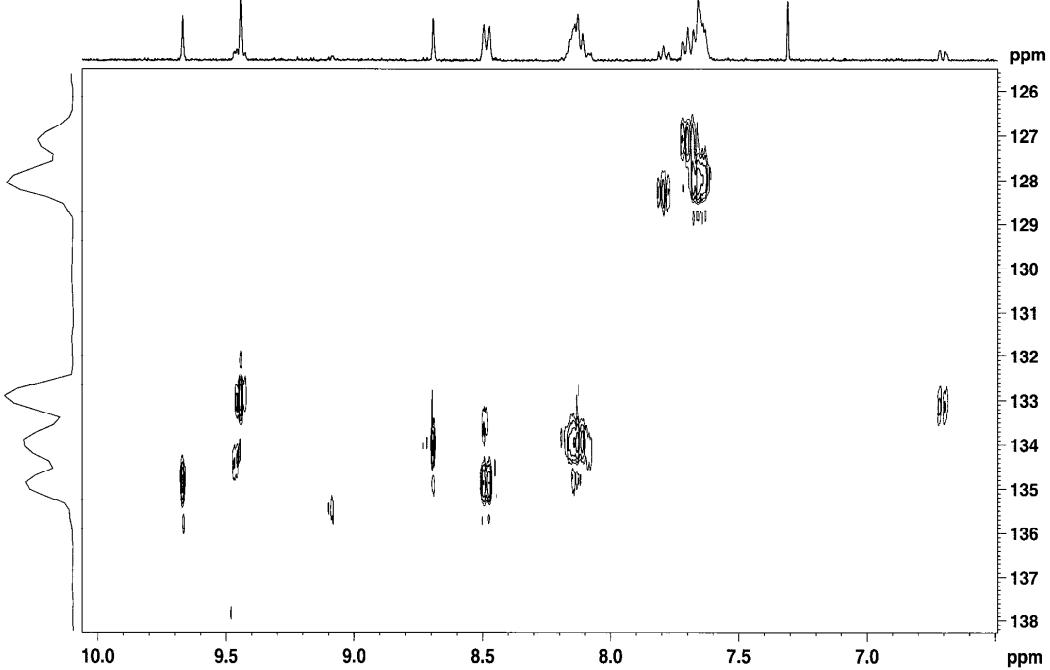


Figure S11. ^1H - ^{13}C HSQC spectra of **1**

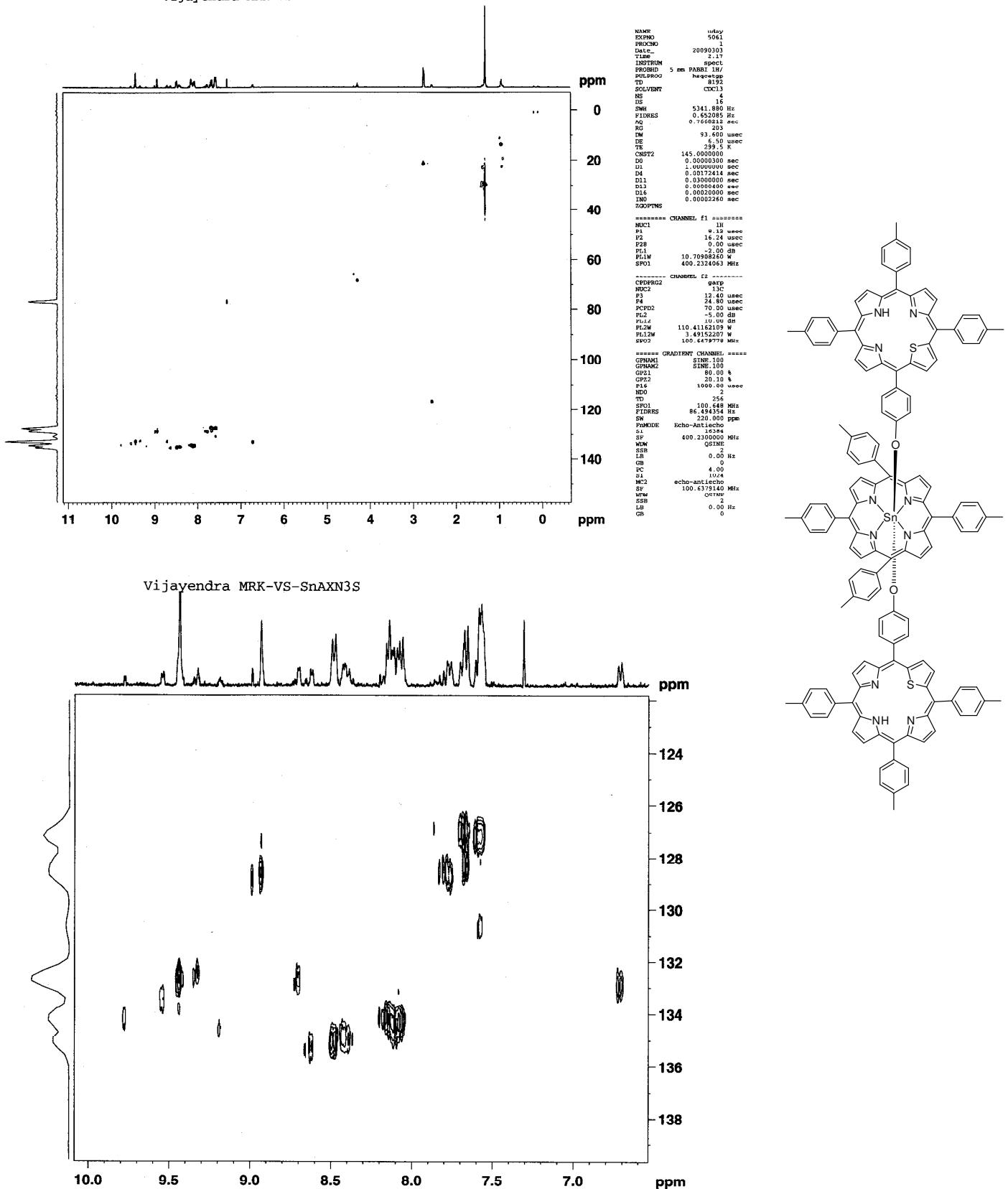
**Figure S12.** ^1H - ^{13}C HSQC spectra of **2**

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)		
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)