

Supporting Information

2-Formyl Boron-Dipyrromethene as Key Synthon to Prepare Functionalized *Meso*-Boron Dipyrromethenyl Porphyrin Building Blocks

Sunit Kumar and Mangalampalli Ravikanth*

Indian Institute of Technology, Powai, Mumbai, 400076 India. Fax: 91-22-5723480

Tel: 91-22-5767176; E-mail: ravikanth@chem.iitb.ac.in

Entry	Contents	Page no
1	Figure S1. HR mass spectrum of compound 1	4
2	Figure S2. ¹ H NMR spectrum of compound 1 in CDCl ₃	5
3	Figure S3. ¹³ C NMR spectrum of compound 1 in CDCl ₃	6
4	Figure S4. ¹⁹ F NMR spectrum of compound 1 in CDCl ₃	7
5	Figure S5. ¹¹ B NMR spectrum of compound 1 in CDCl ₃	8
6	Figure S6. ¹ H- ¹ H COSY spectrum of compound 1 in CDCl ₃	9
7	Figure S7. ¹ H- ¹ H NOESY spectrum of compound 1 in CDCl ₃	10
8	Figure S8. HR mass spectrum of compound 2	11
9	Figure S9. ¹ H NMR spectrum of compound 2 in CDCl ₃	12
10	Figure S10. ¹³ C NMR spectrum of compound 2 in CDCl ₃	13
11	Figure S11. ¹⁹ F NMR spectrum of compound 2 in CDCl ₃	14
12	Figure S12. ¹¹ B NMR spectrum of compound 2 in CDCl ₃	15
13	Figure S13. HR mass spectrum of compound 3	16
14	Figure S14. ¹ H NMR spectrum of compound 3 in CDCl ₃	17
15	Figure S15. ¹³ C NMR spectrum of compound 3 in CDCl ₃	18
16	Figure S16. ¹⁹ F NMR spectrum of compound 3 in CDCl ₃	19
17	Figure S17. ¹¹ B NMR spectrum of compound 3 in CDCl ₃	20
18	Figure S18. HR mass spectrum of compound 4	21

19	Figure S19. ^1H NMR spectrum of compound 4 in CDCl_3	22
20	Figure S20. ^{13}C NMR spectrum of compound 4 in CDCl_3	23
21	Figure S21. ^{19}F NMR spectrum of compound 4 in CDCl_3	24
22	Figure S22. ^{11}B NMR spectrum of compound 4 in CDCl_3	25
23	Figure S23. HR mass spectrum of compound 5	26
24	Figure S24. ^1H NMR spectrum of compound 5 in CDCl_3	27
25	Figure S25. ^{13}C NMR spectrum of compound 5 in CDCl_3	28
26	Figure S26. ^{19}F NMR spectrum of compound 5 in CDCl_3	29
27	Figure S27. ^{11}B NMR spectrum of compound 5 in CDCl_3	30
28	Figure S28. HR mass spectrum of compound 6	31
29	Figure S29. ^1H NMR spectrum of compound 6 in CDCl_3	32
30	Figure S30. ^{13}C NMR spectrum of compound 6 in CDCl_3	33
31	Figure S31. ^{19}F NMR spectrum of compound 6 in CDCl_3	34
32	Figure S32. ^{11}B NMR spectrum of compound 6 in CDCl_3	35
33	Figure S33. HR mass spectrum of compound 7	36
34	Figure S34. ^1H NMR spectrum of compound 7 in CDCl_3	37
35	Figure S35. ^{19}F NMR spectrum of compound 7 in CDCl_3	38
36	Figure S36. ^{11}B NMR spectrum of compound 7 in CDCl_3	39
37	Figure S37. HR mass spectrum of compound Zn1	40
38	Figure S38. ^1H NMR spectrum of compound Zn1 in CDCl_3	41
39	Figure S39. ^{19}F NMR spectrum of compound Zn1 in CDCl_3	42
40	Figure S40. ^{11}B NMR spectrum of compound Zn1 in CDCl_3	43
41	Figure S41. ^1H NMR spectrum of compound Ni1 in CDCl_3	44
42	Figure S42. ^{19}F NMR spectrum of compound Ni1 in CDCl_3	45
43	Figure S43. ^{11}B NMR spectrum of compound Ni1 in CDCl_3	46
44	Figure S44. LR mass spectrum of compound 8	47
45	Figure S45. ^1H NMR spectrum of compound 8 in CDCl_3	48

46	Figure S46. ^{19}F NMR spectrum of compound 8 in CDCl_3	49
47	Figure S47. ^{11}B NMR spectrum of compound 8 in CDCl_3	50
48	Figure S48. Comparison of Emission spectrum of compound 8 and compound 9 ($5\ \mu\text{M}$) recorded in CHCl_3 solvents. Excitation wavelength used was 488 nm.	51

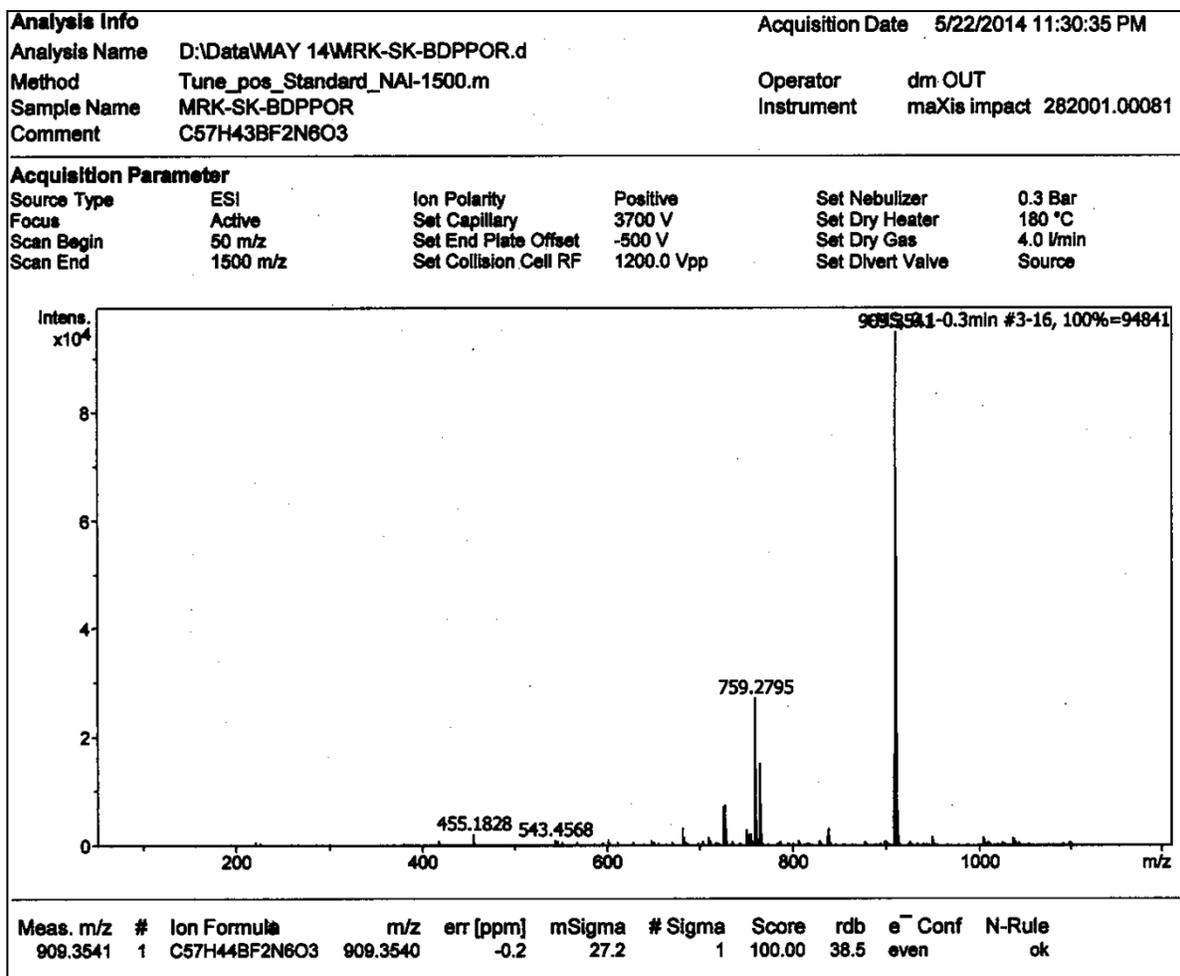
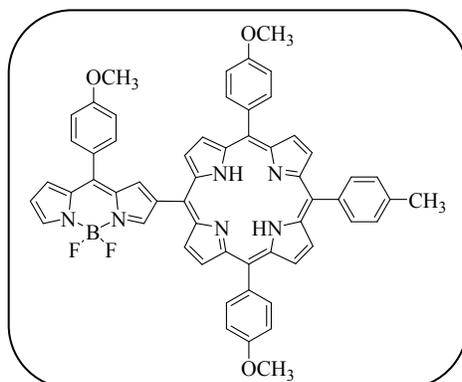
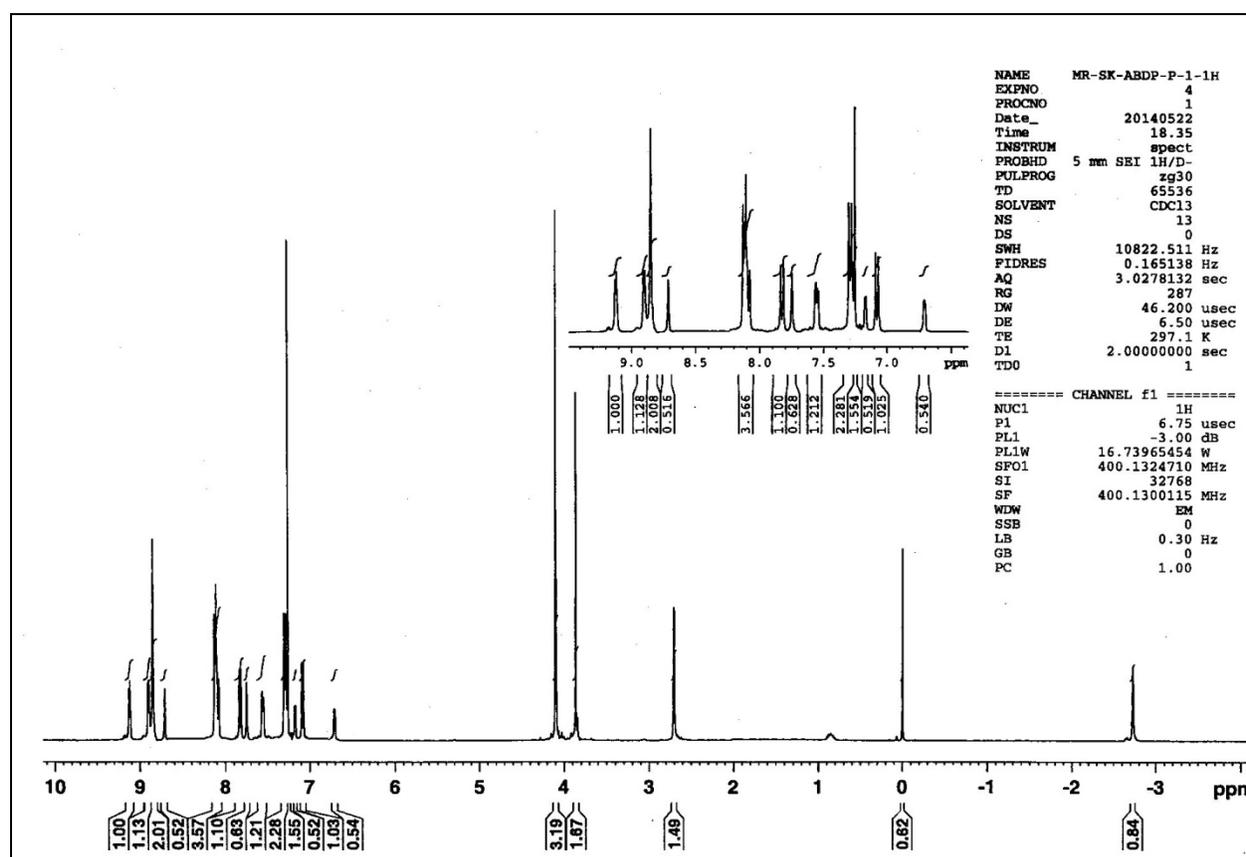
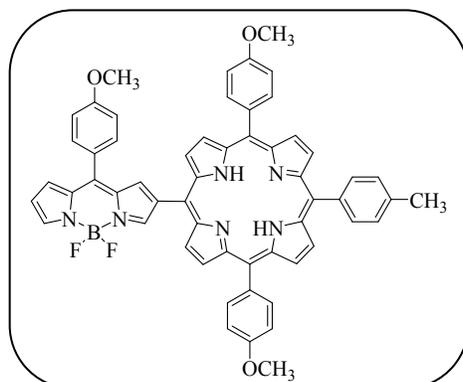


Figure S1: HR mass spectrum of compound 1

Figure S2: ^1H NMR spectrum of compound 1 recorded in CDCl_3

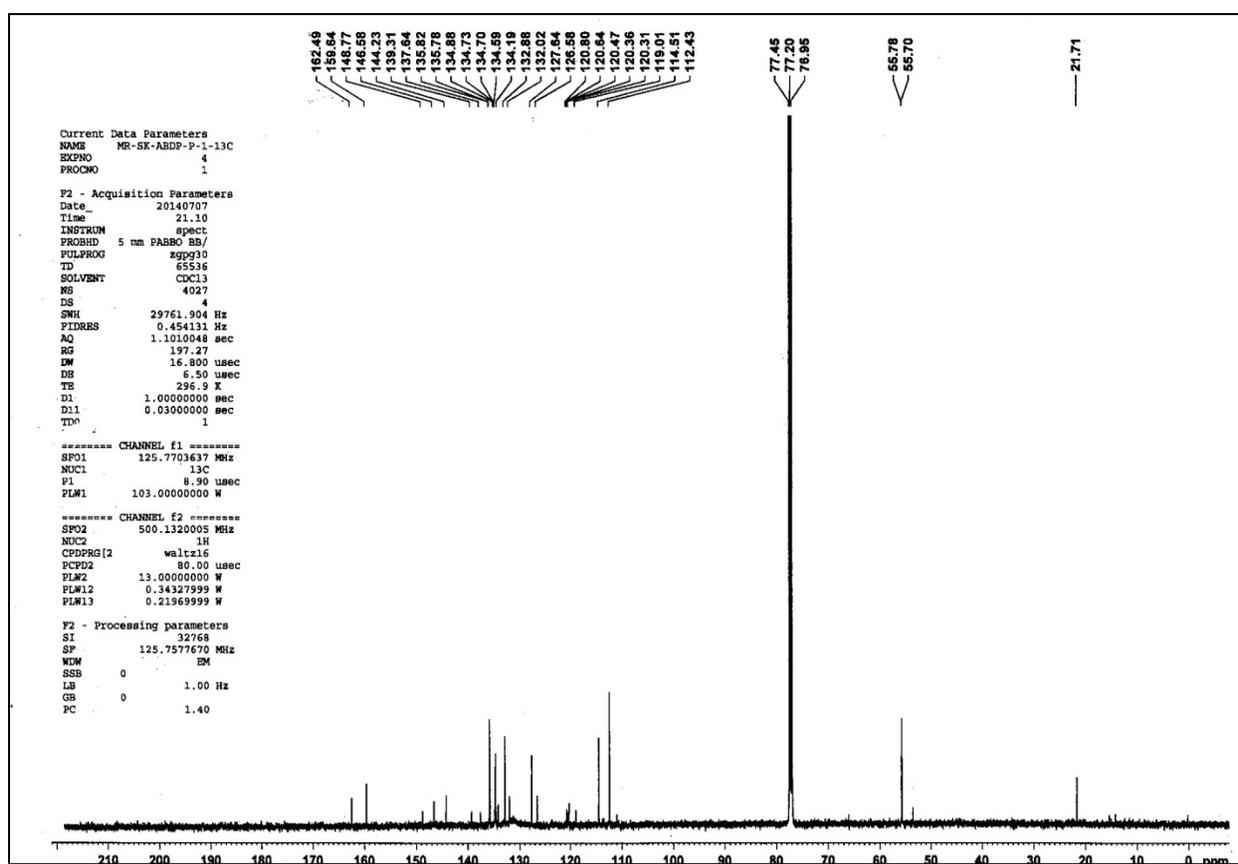
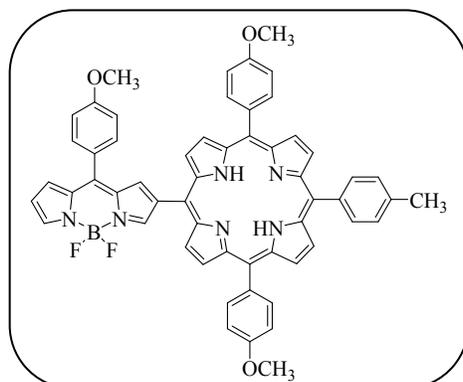


Figure S3: ^{13}C NMR spectrum of compound 1 recorded in CDCl_3

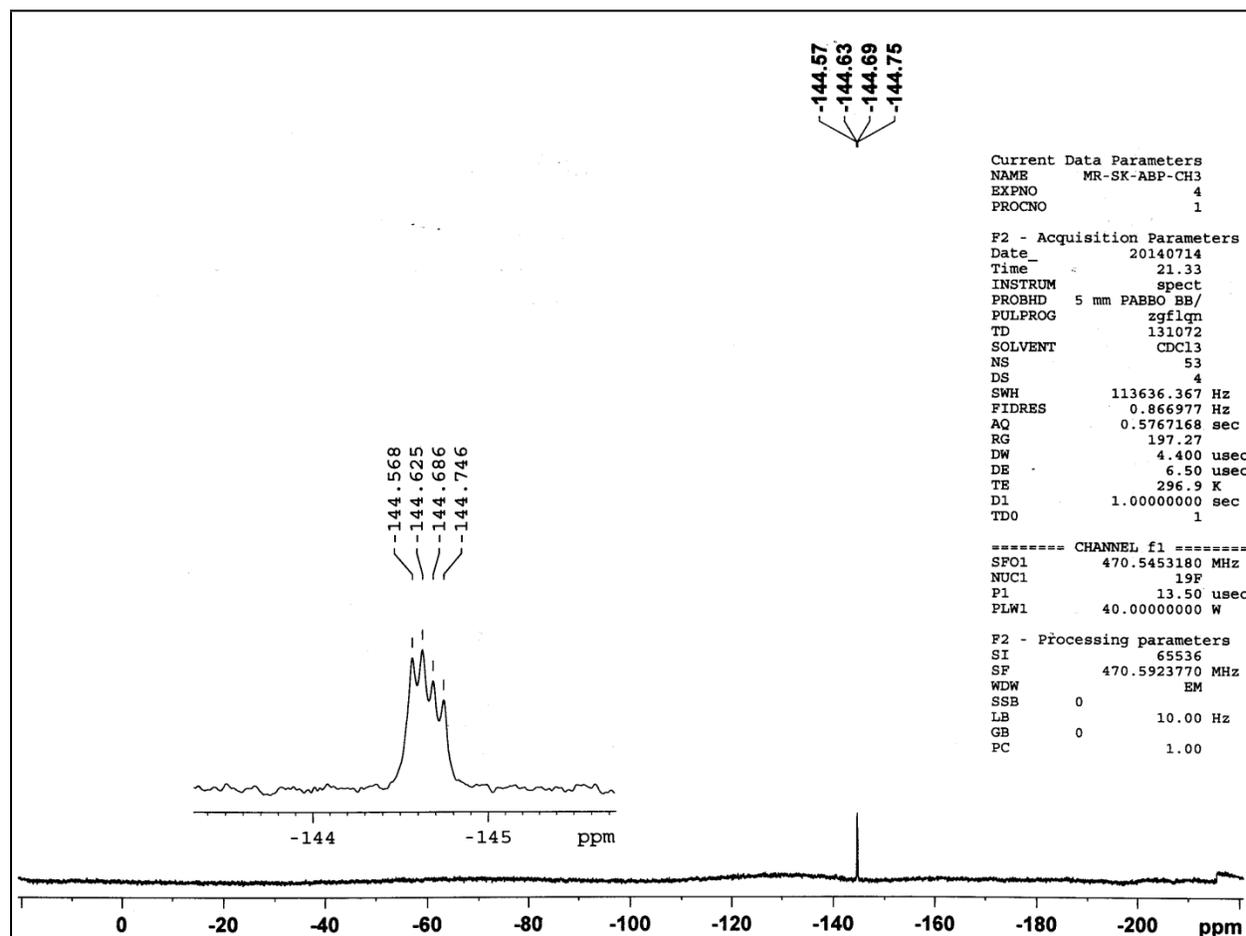
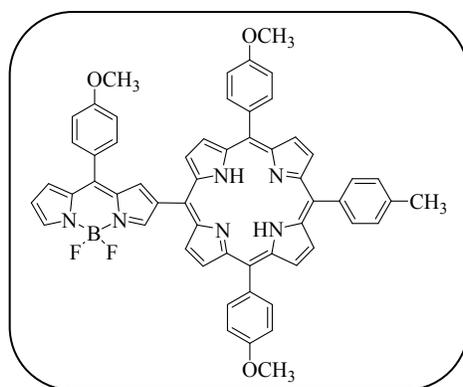


Figure S4: ¹⁹F NMR spectrum of compound 1 recorded in CDCl₃. Inset shows the expansion

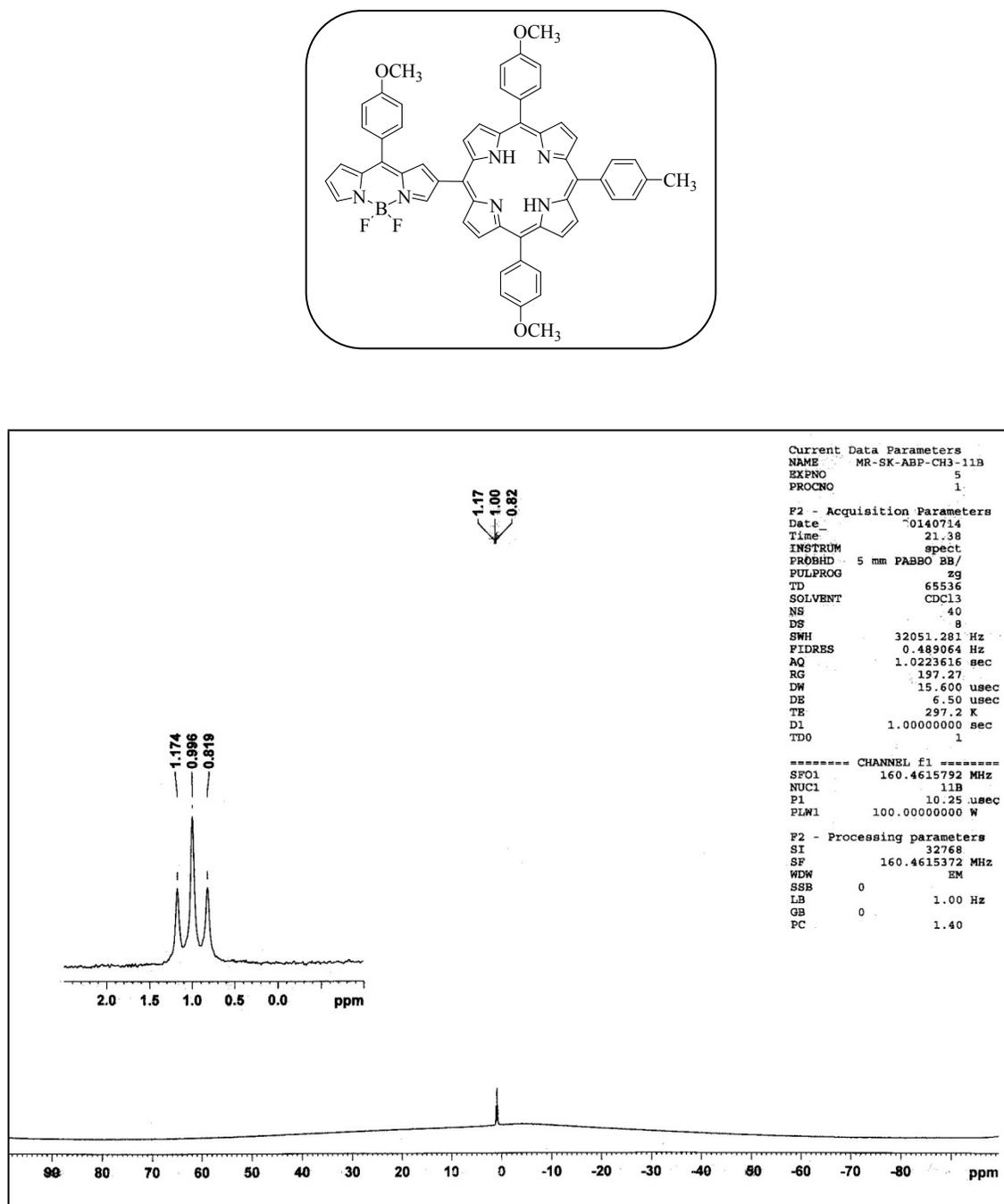


Figure S5: ^{11}B NMR spectrum of compound **1** recorded in CDCl_3 . Inset shows the expansion

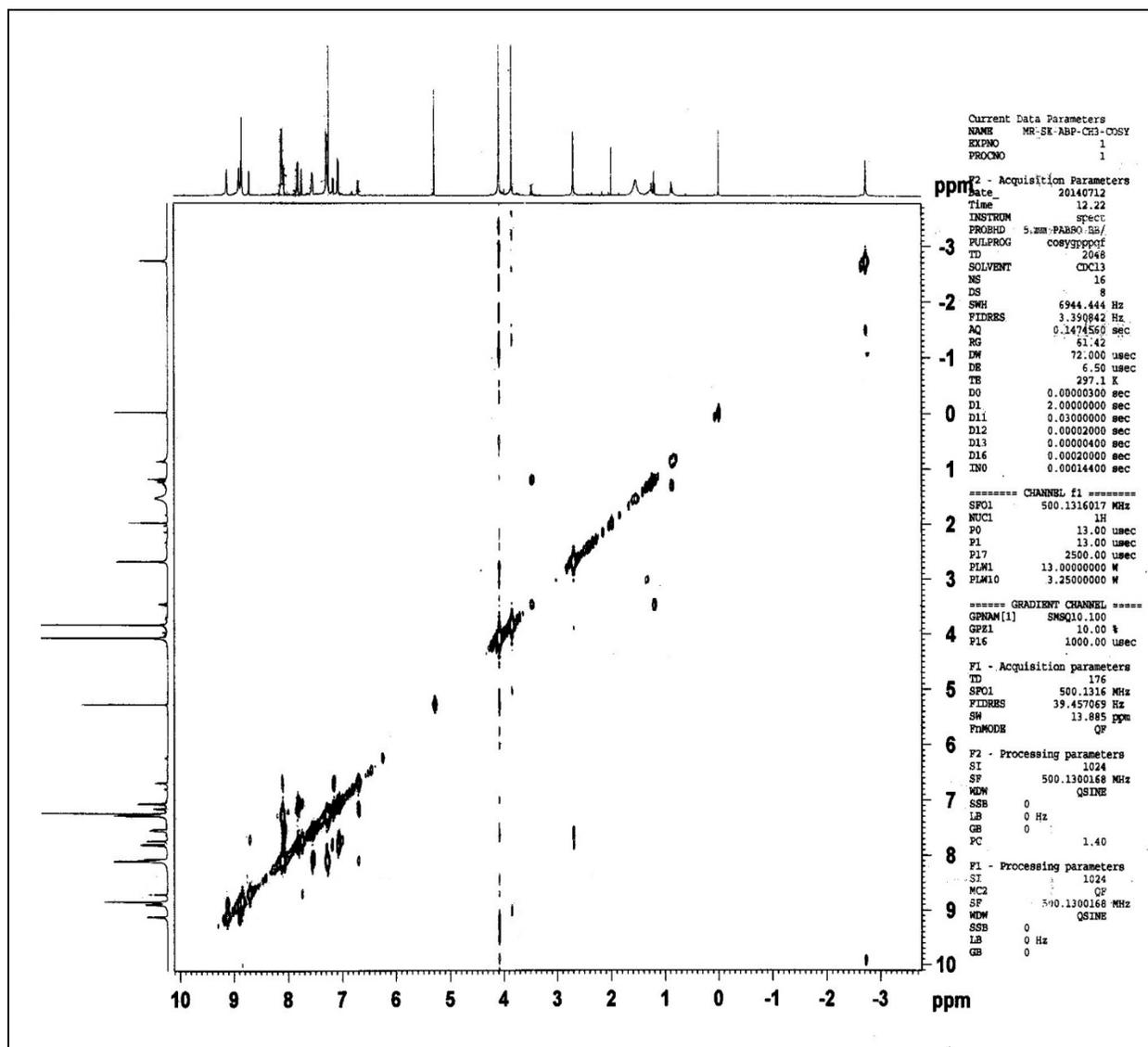
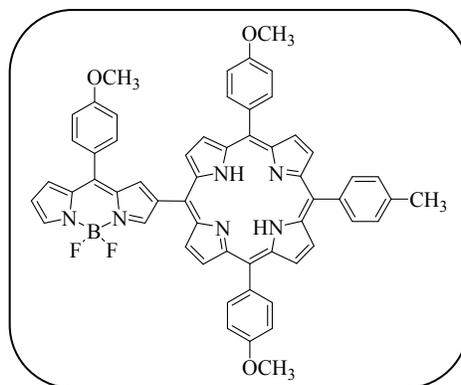


Figure S6: ^1H - ^1H COSY spectrum of compound **1** recorded in CDCl_3 .

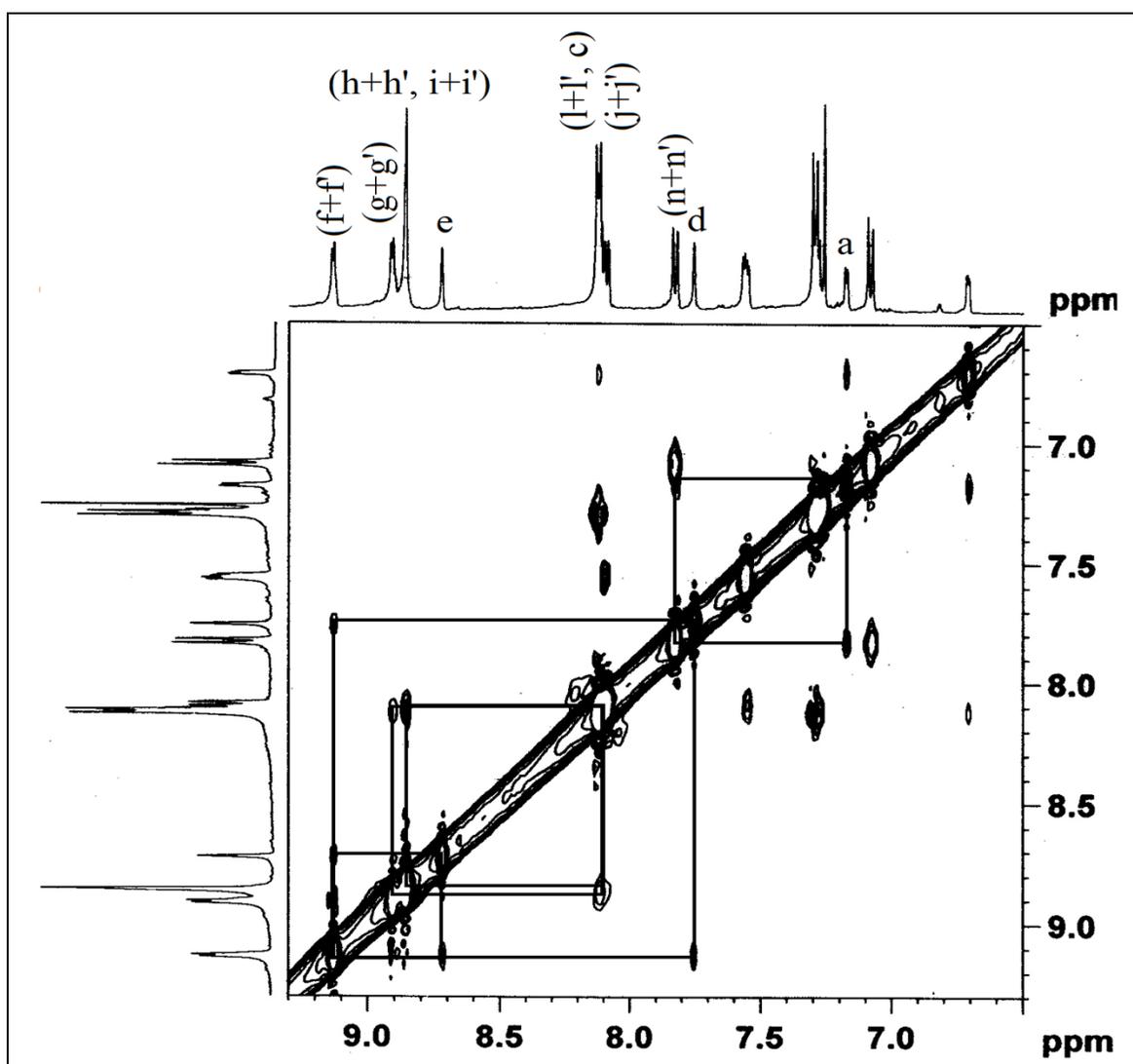
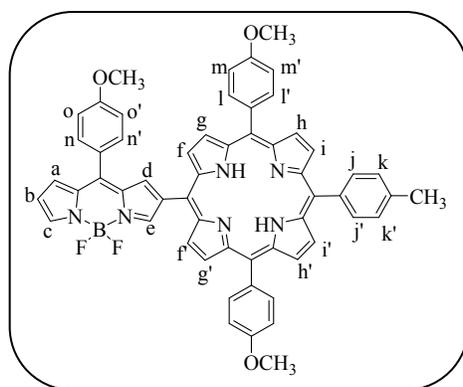


Figure S7: Partial ¹H-¹H NOESY spectrum of compound 1 recorded in CDCl₃.

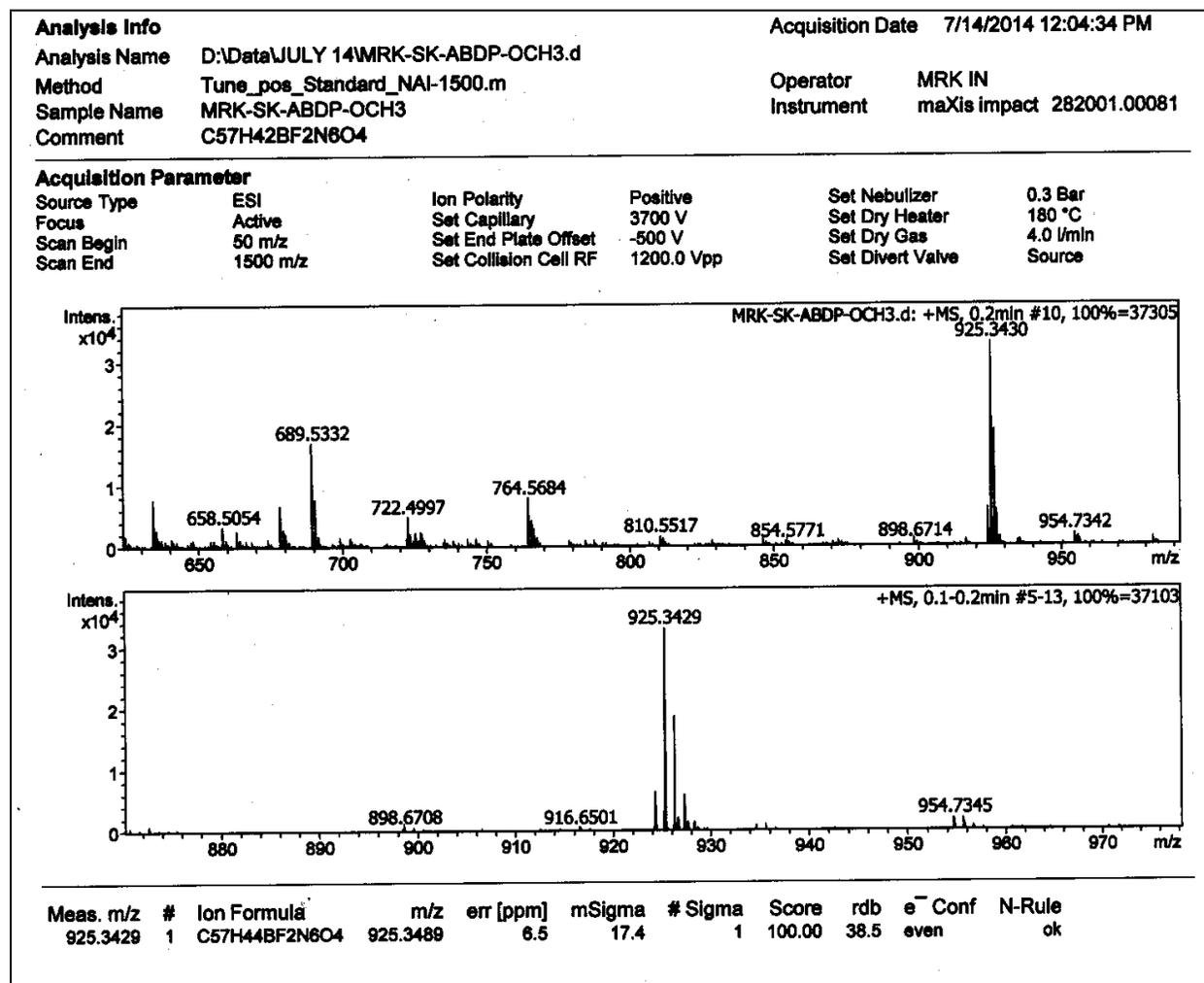
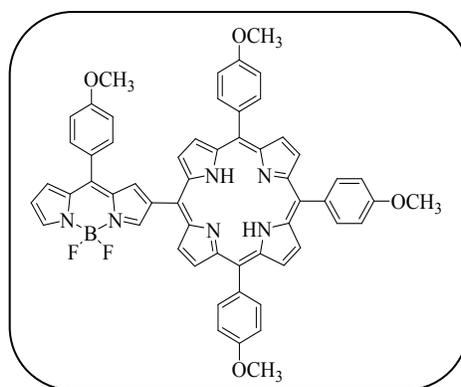


Figure S8: HR mass spectrum of compound 2

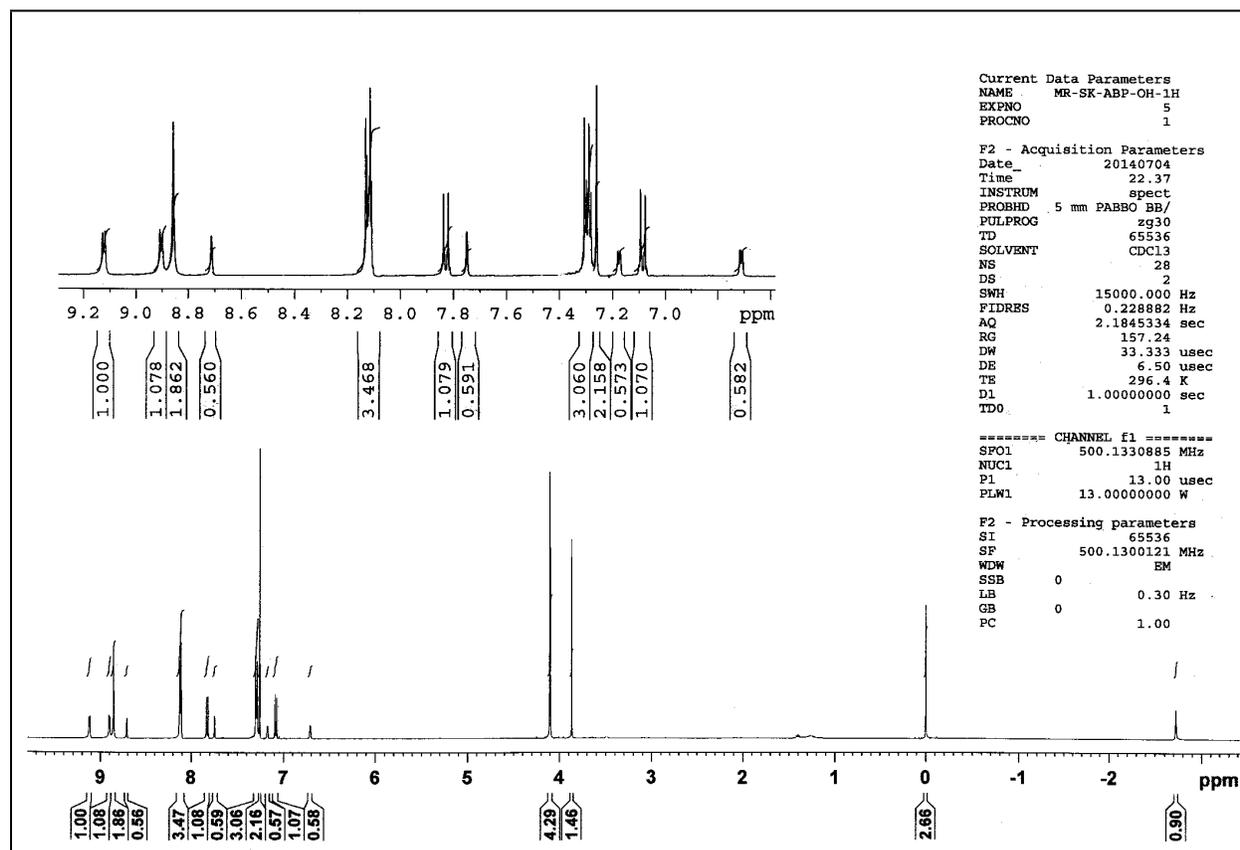
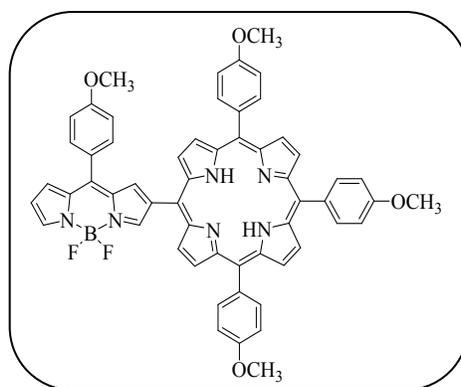


Figure S9: ^1H NMR spectrum of compound **2** recorded in CDCl_3

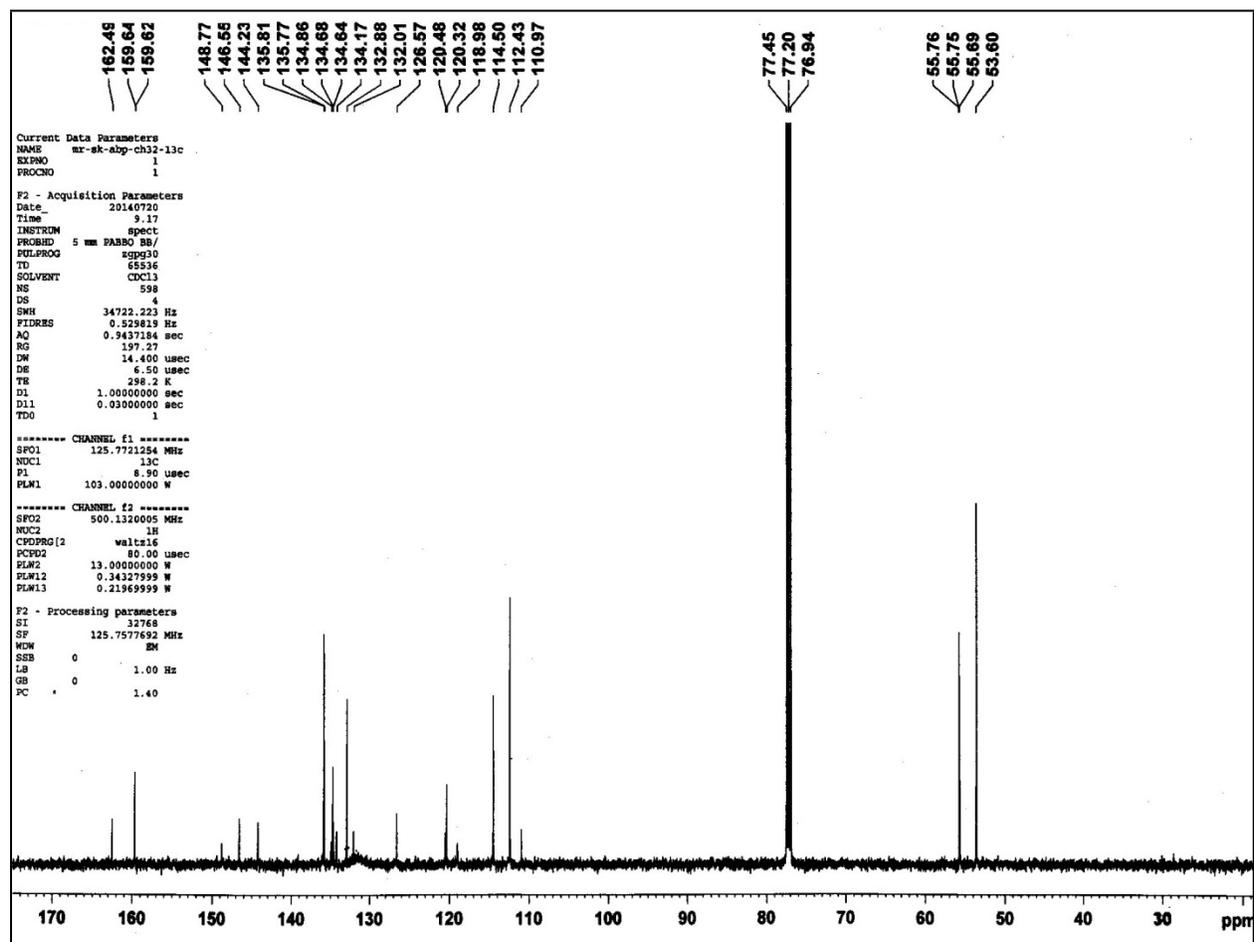
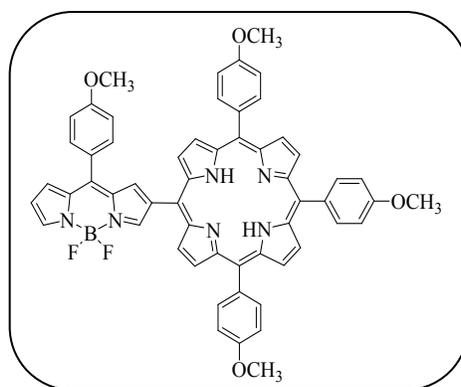


Figure S10: ^{13}C NMR spectrum of compound 2 recorded in CDCl_3

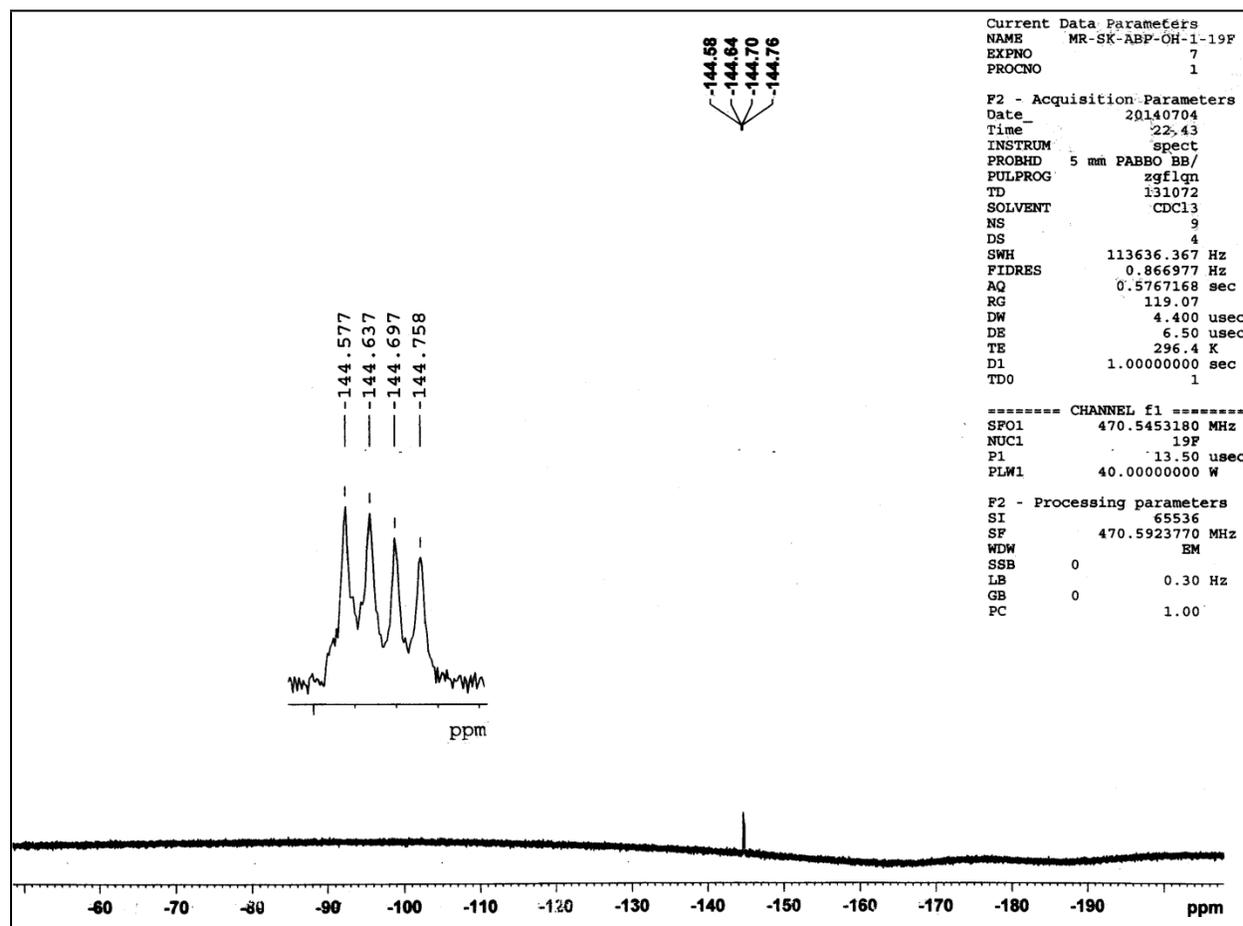
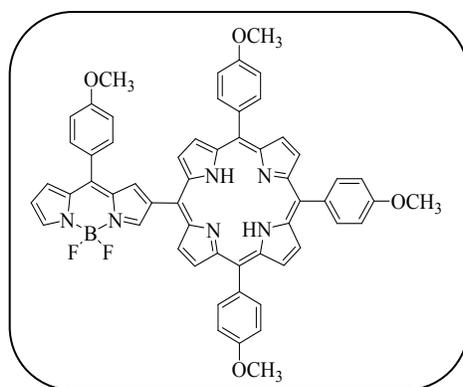


Figure S11: ¹⁹F NMR spectrum of compound 2 recorded in CDCl₃. Inset shows the expansion

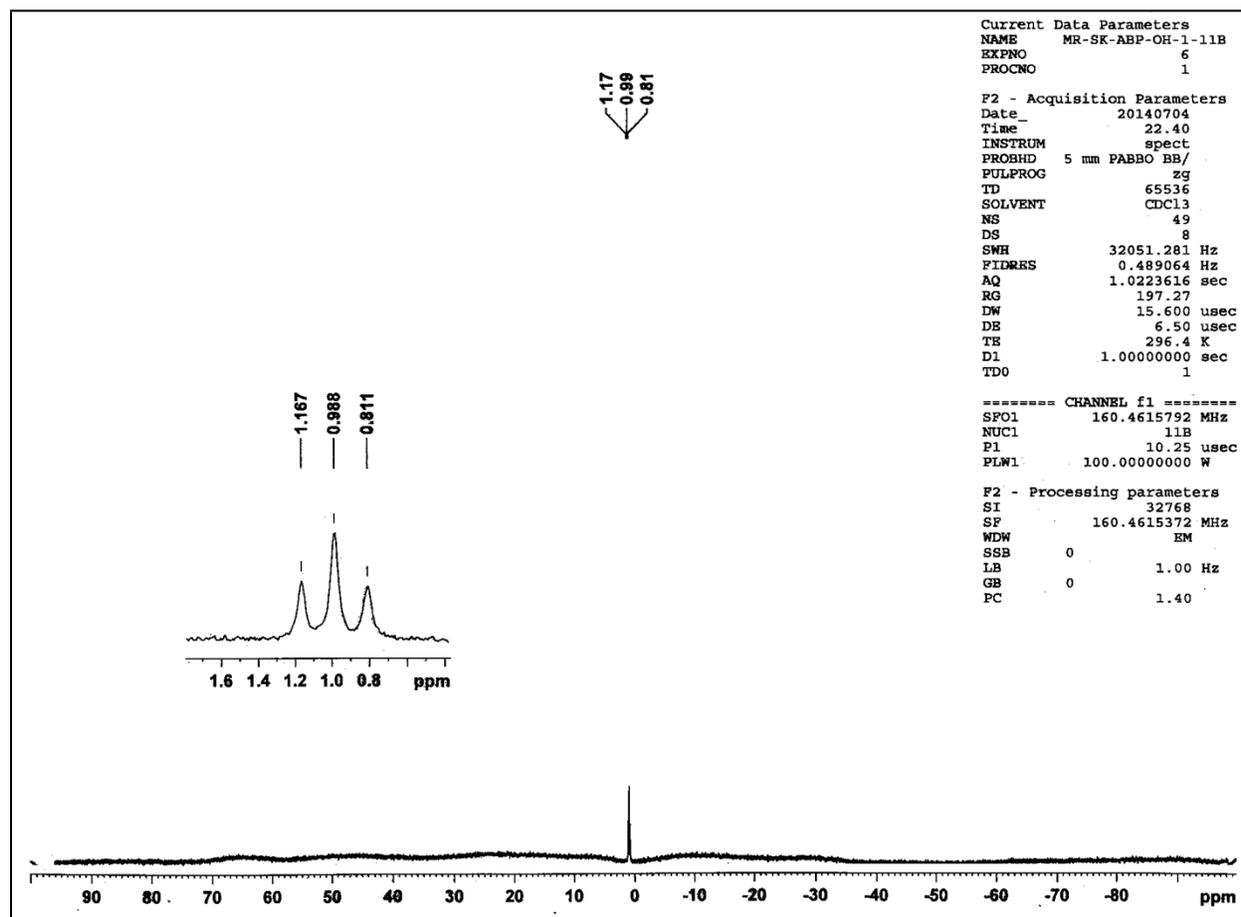
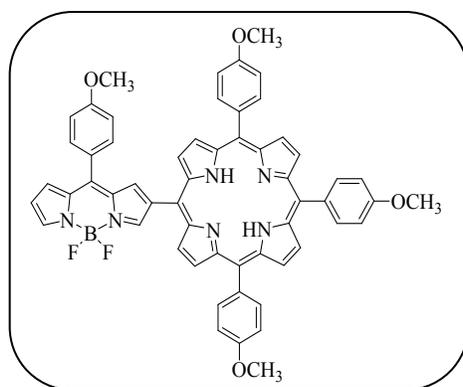


Figure S12: ^{11}B NMR spectrum of compound **2** recorded in CDCl_3 . Inset shows the expansion

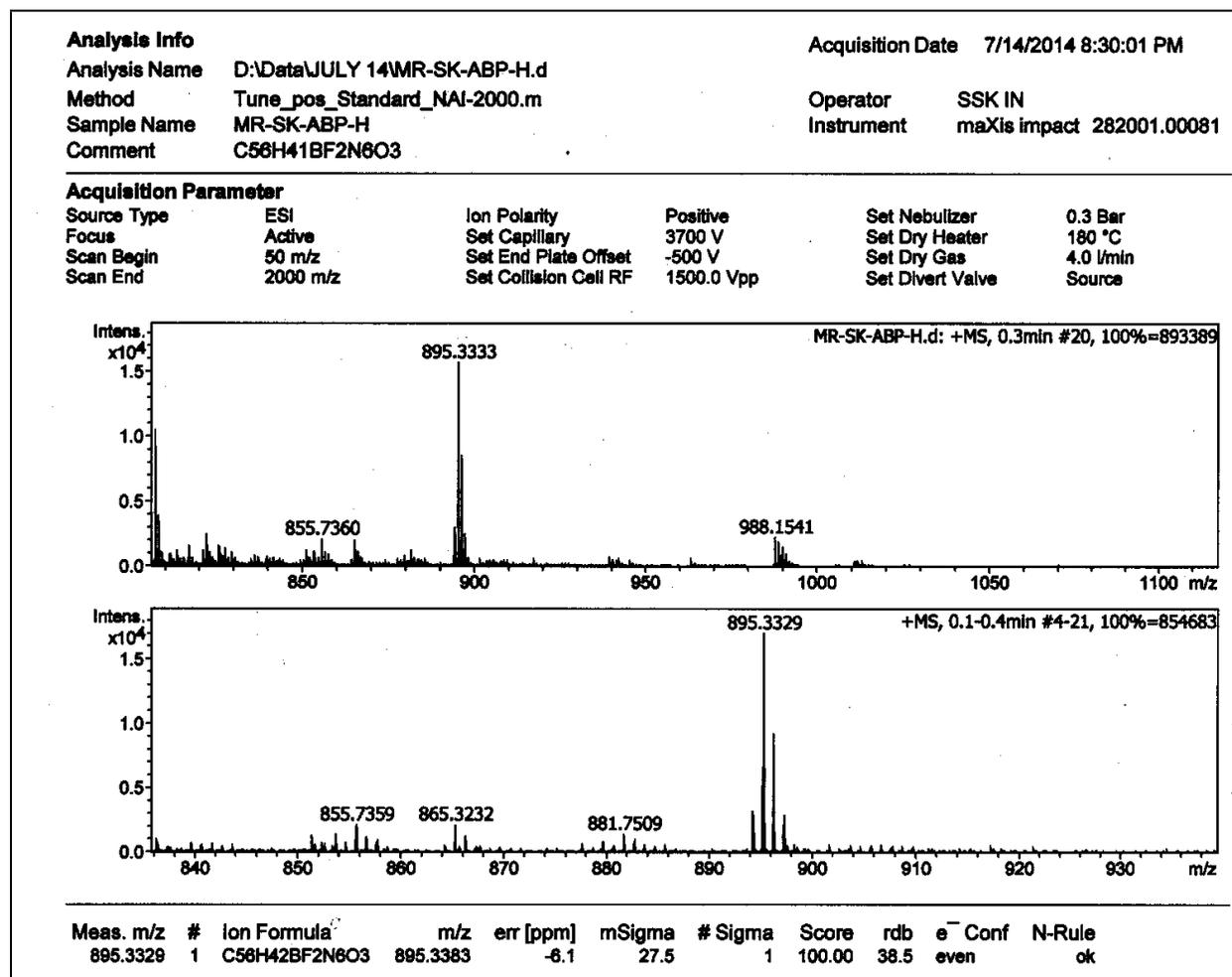
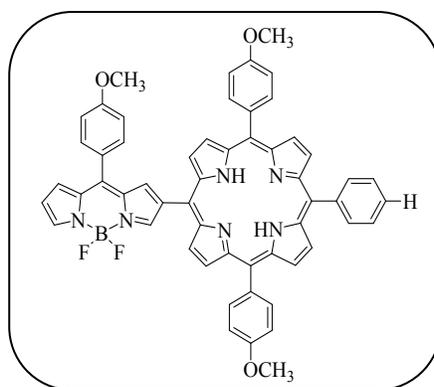


Figure S13: HR mass spectrum of compound 3

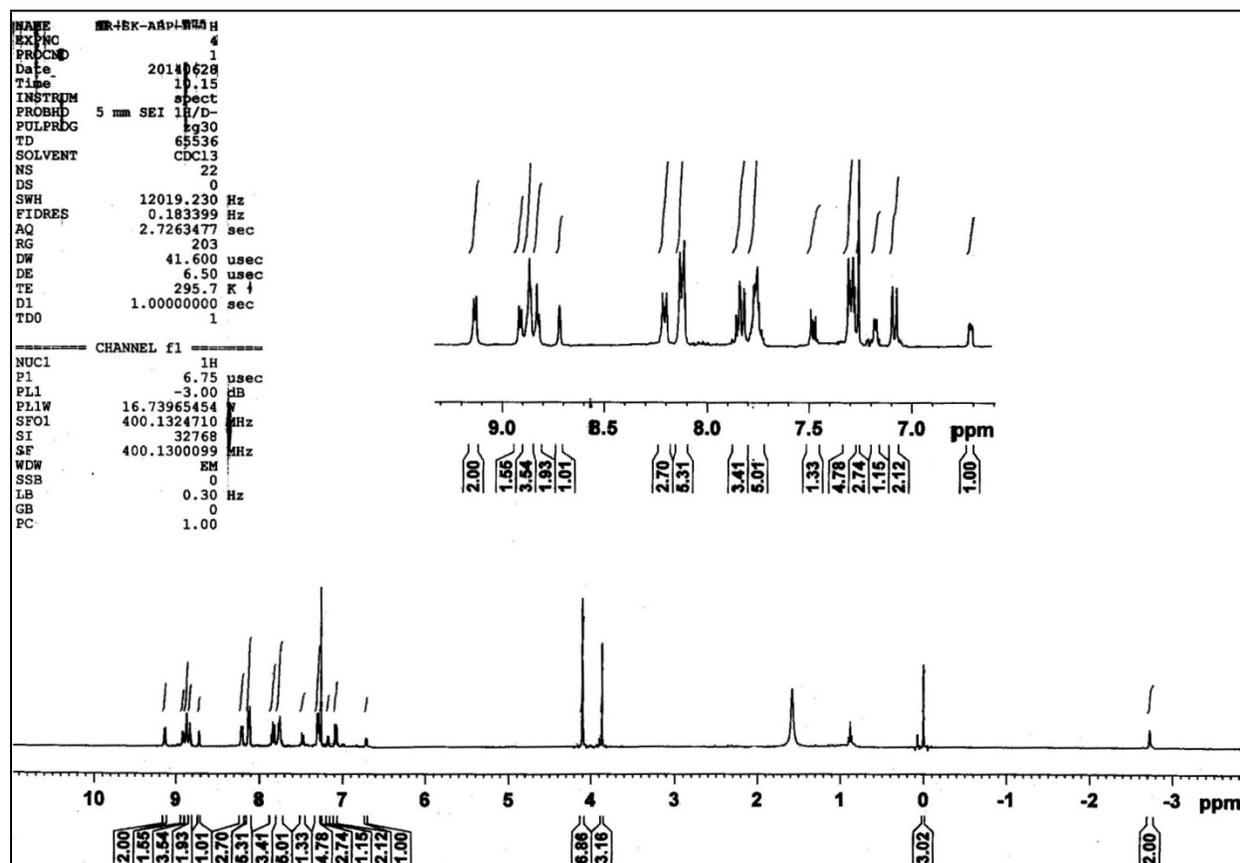
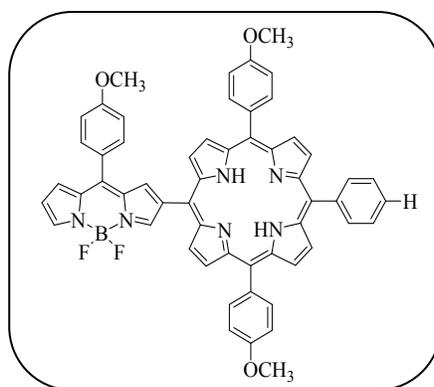


Figure S14: ^1H NMR spectrum of compound **3** recorded in CDCl_3

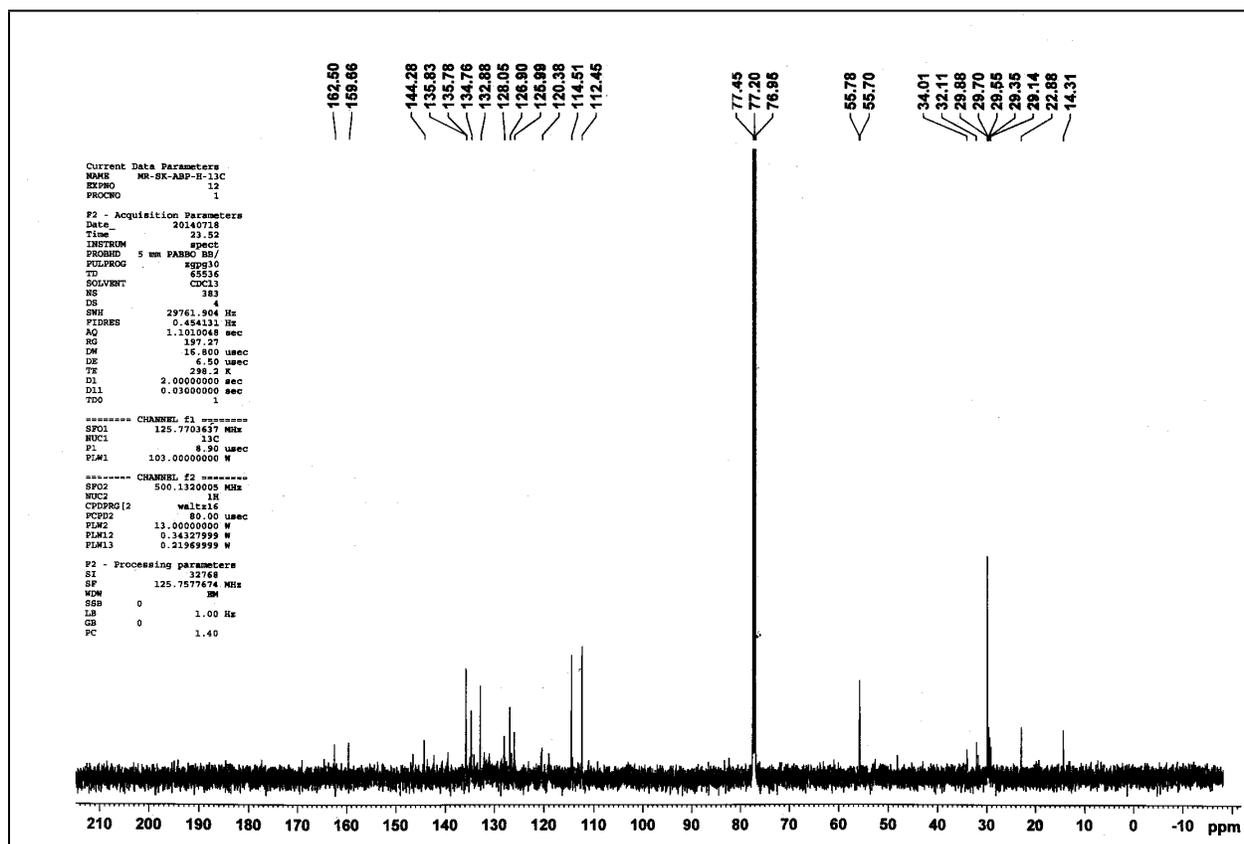
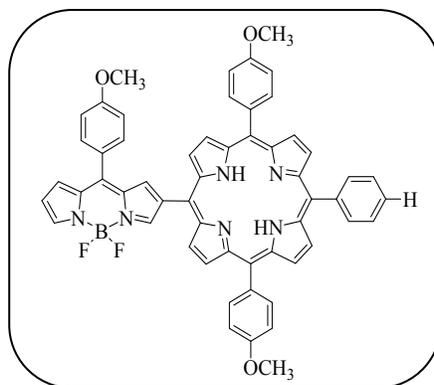


Figure S15: ^{13}C NMR spectrum of compound **3** recorded in CDCl_3

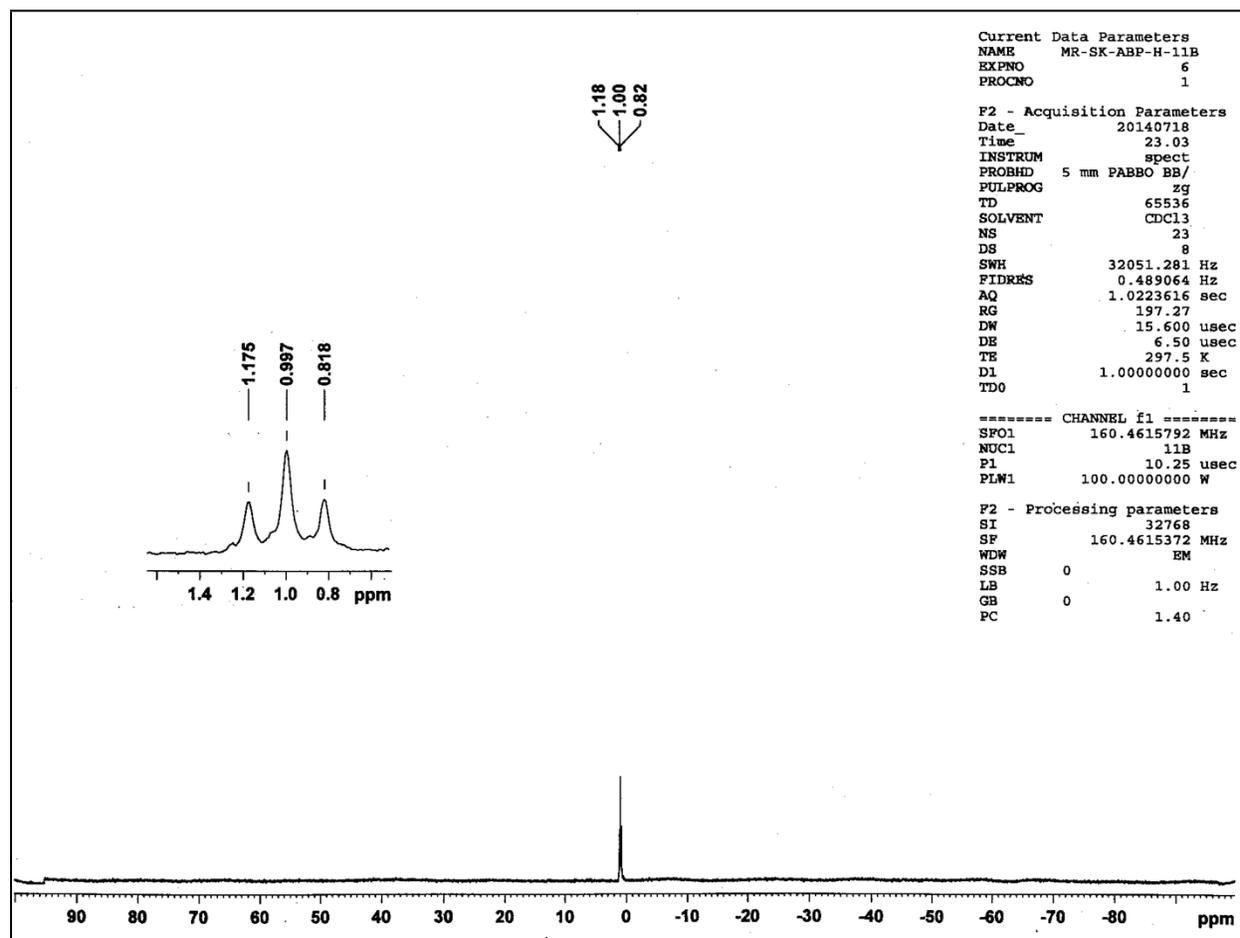
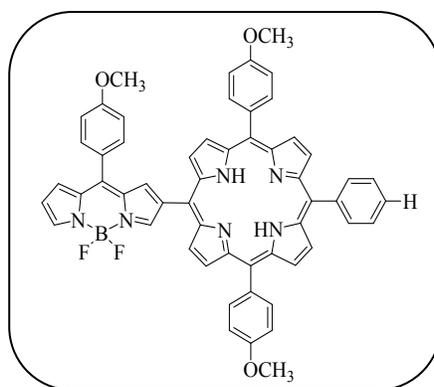


Figure S16: ^{11}B NMR spectrum of compound **3** recorded in CDCl_3 . Inset shows the expansion

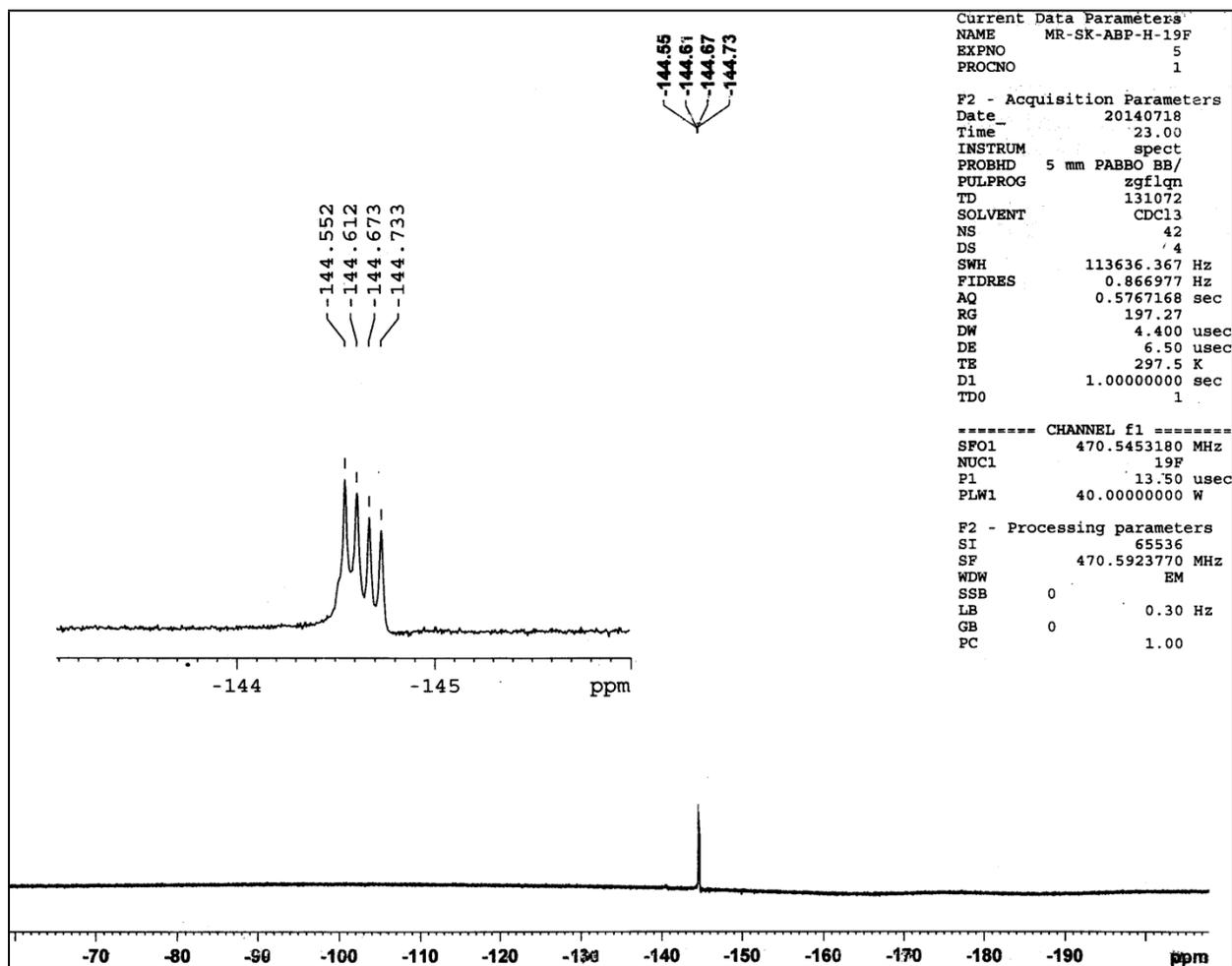
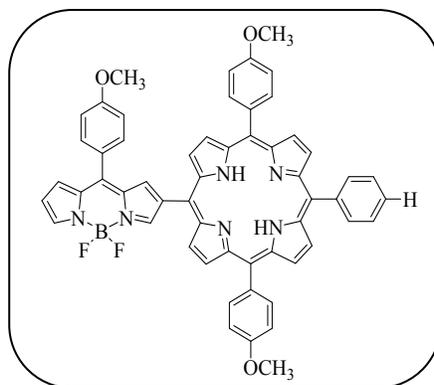


Figure S17: ^{19}F NMR spectrum of compound **3** recorded in CDCl_3 . Inset shows the expansion

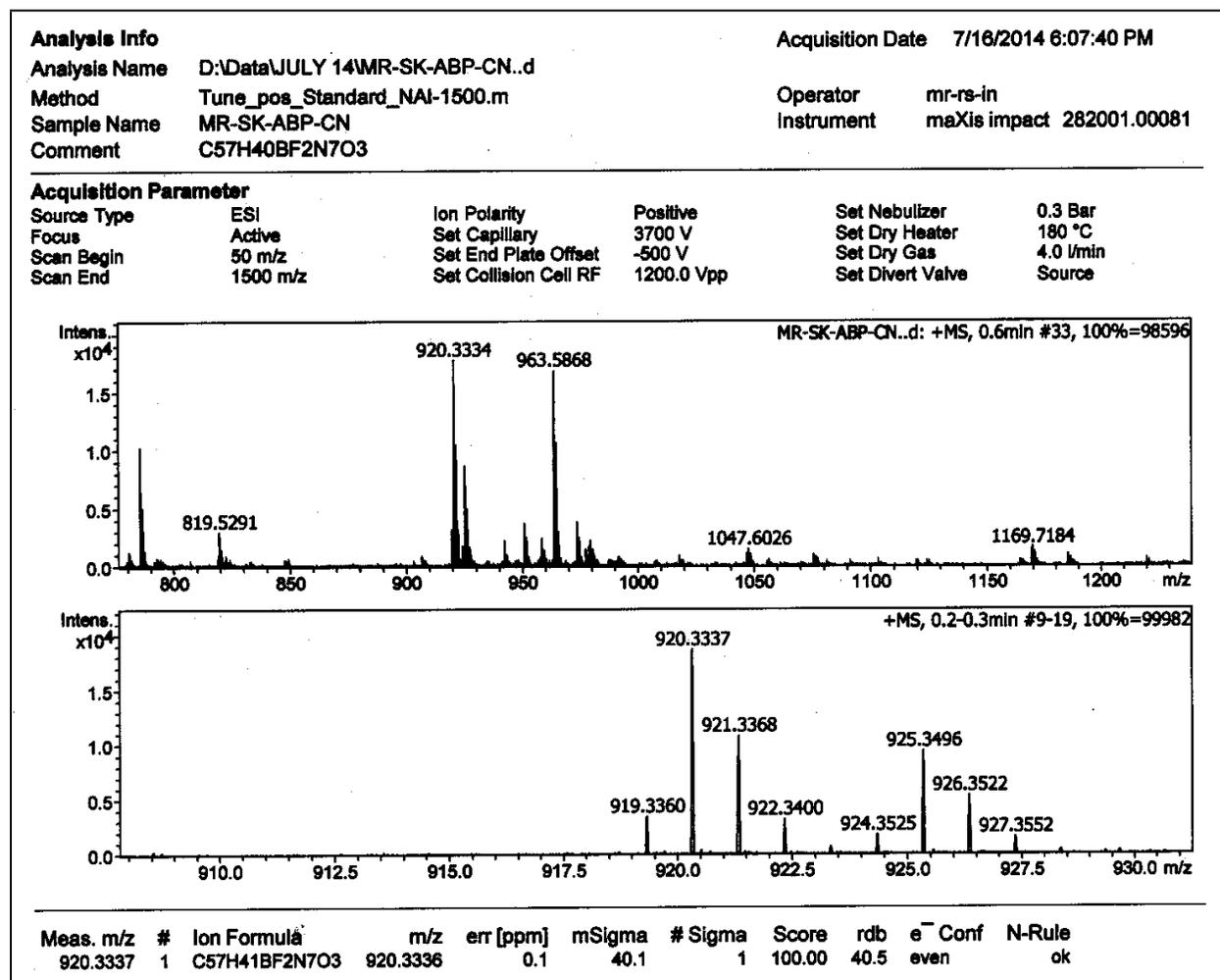
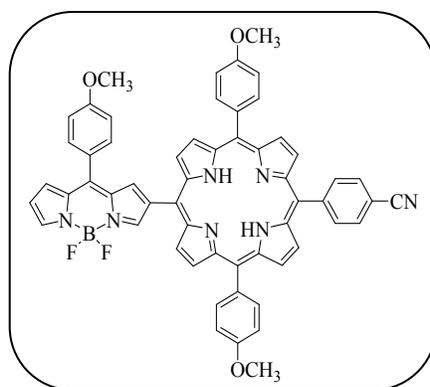


Figure S18: HR mass spectrum of compound 4

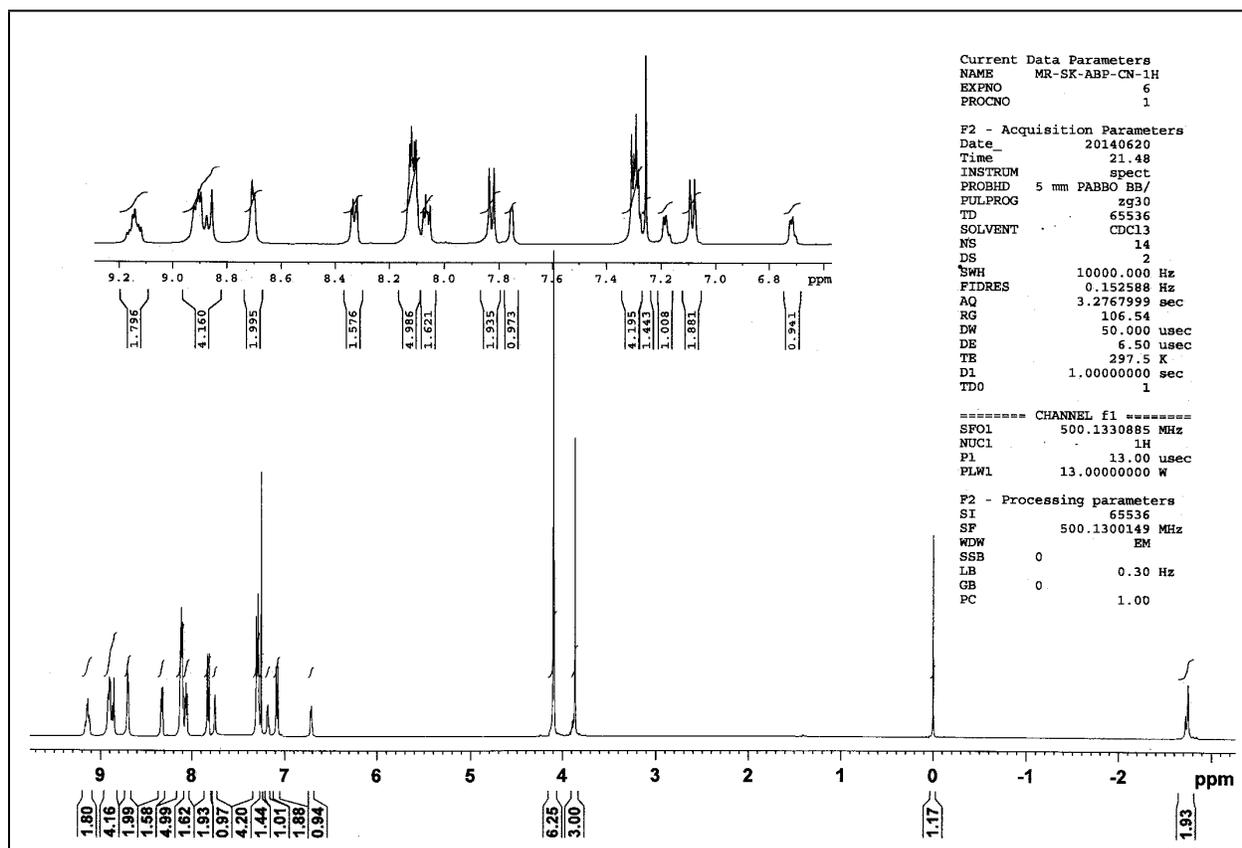
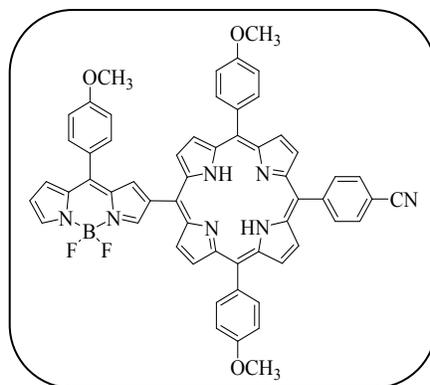


Figure S19: ^1H NMR spectrum of compound **4** recorded in CDCl_3

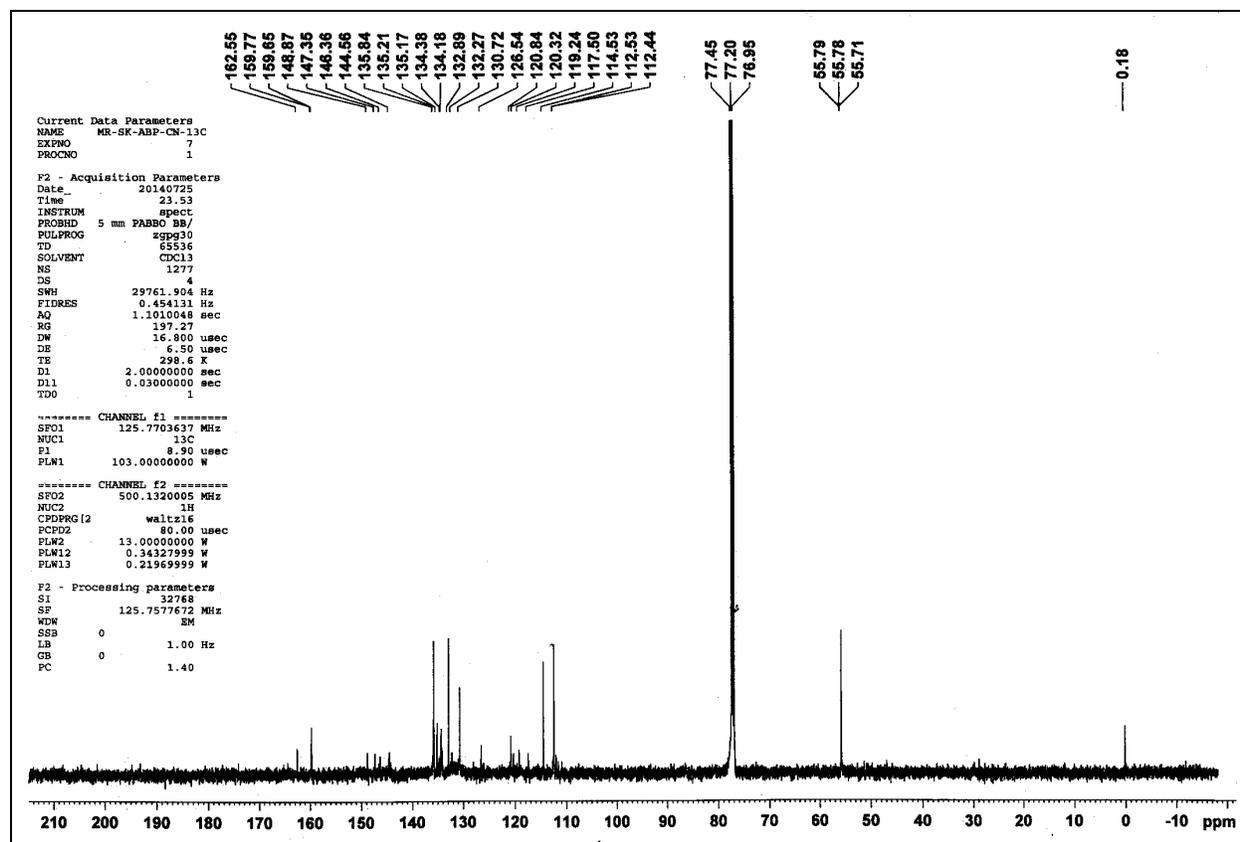
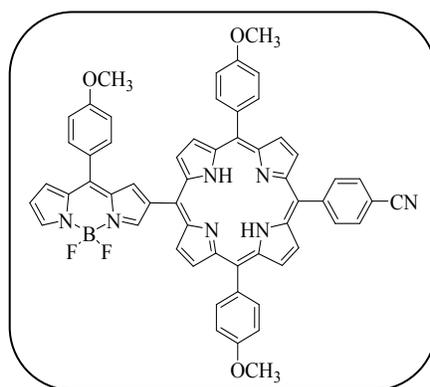


Figure S20: ^{13}C NMR spectrum of compound 4 recorded in CDCl_3

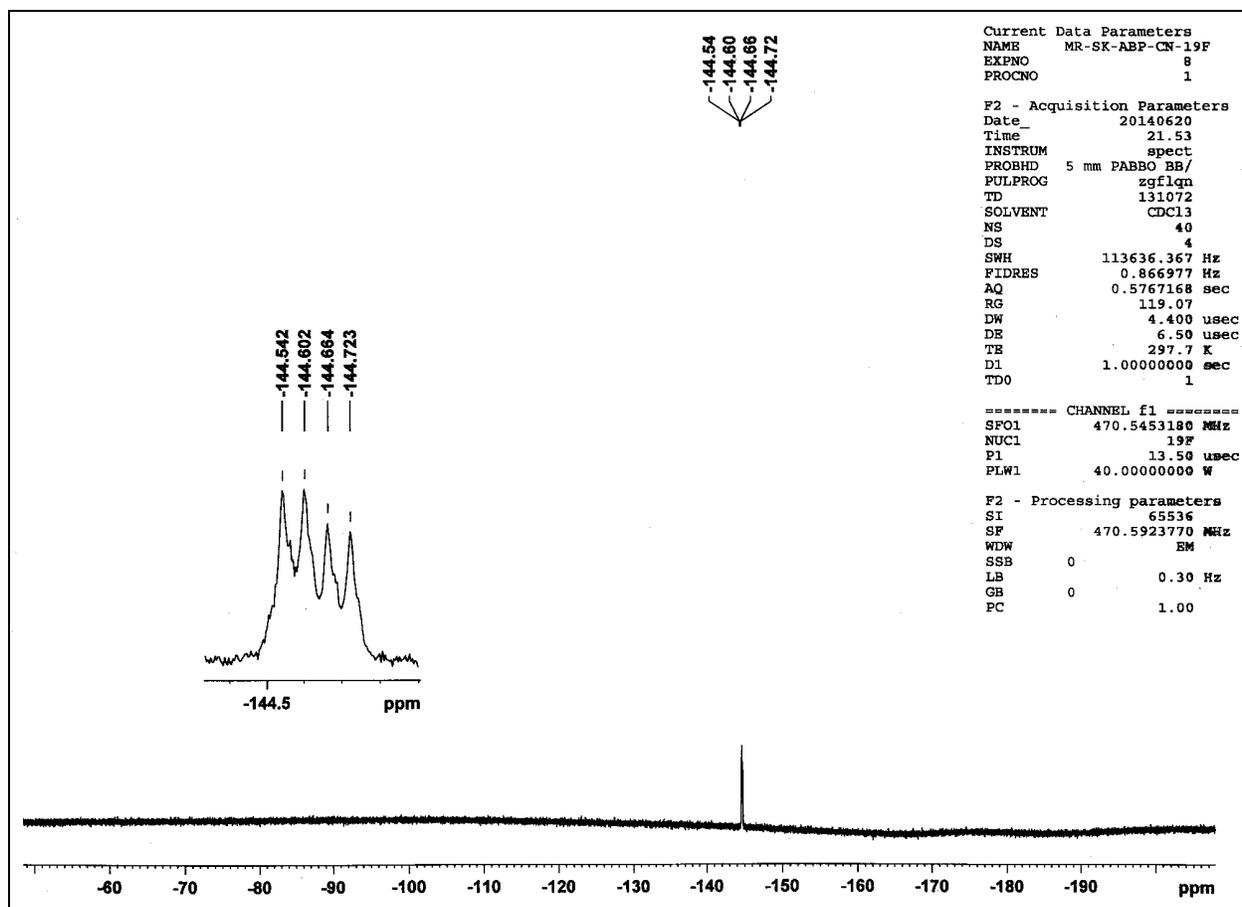
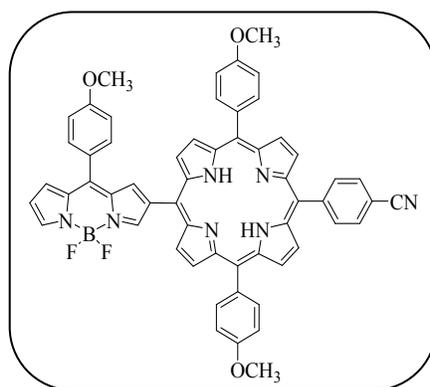


Figure S21: ^{19}F NMR spectrum of compound 4 recorded in CDCl_3 . Inset shows the expansion

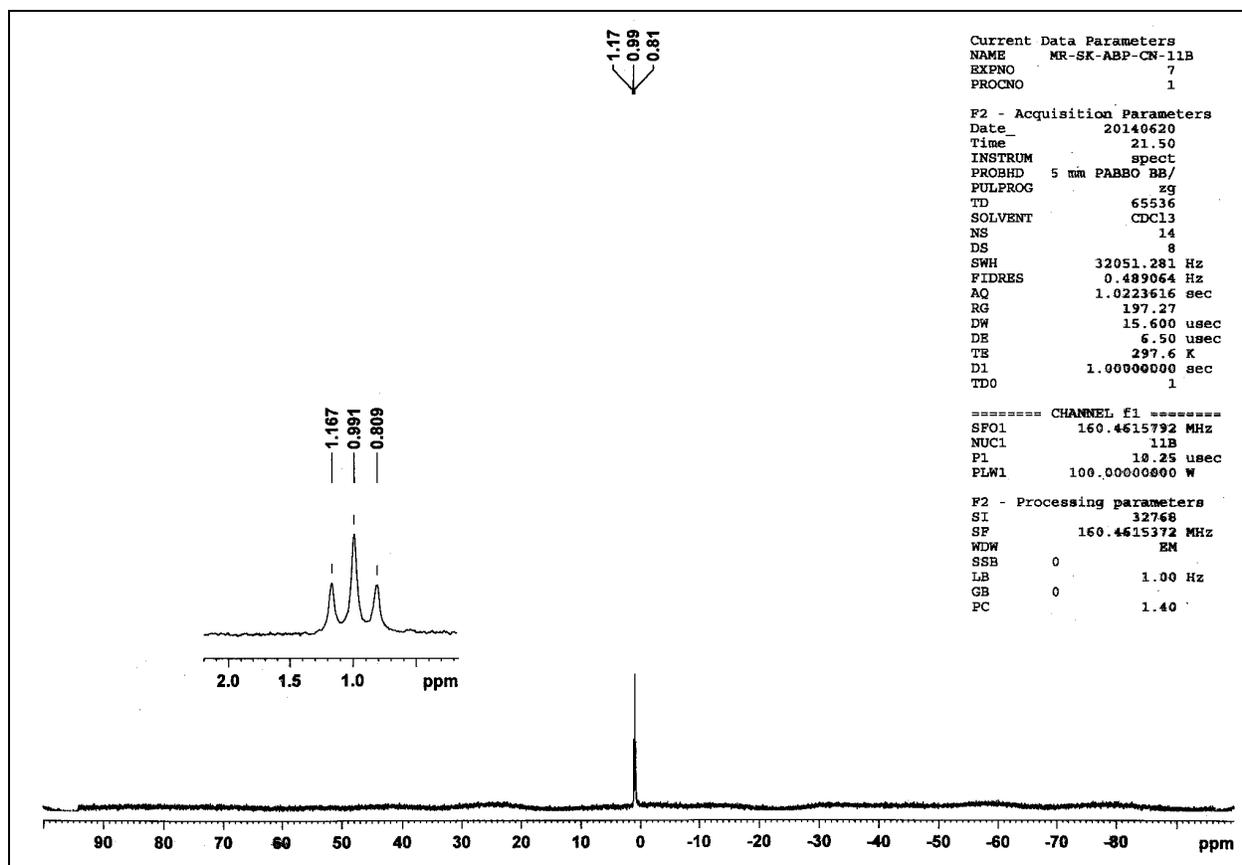
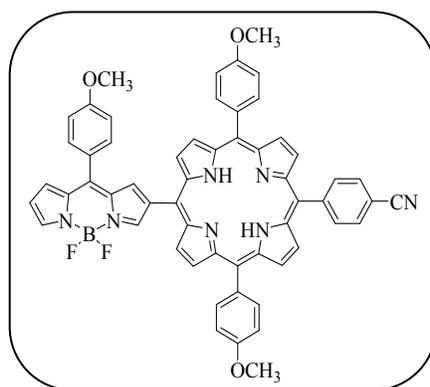


Figure S22: ^{11}B NMR spectrum of compound 4 recorded in CDCl_3 . Inset shows the expansion

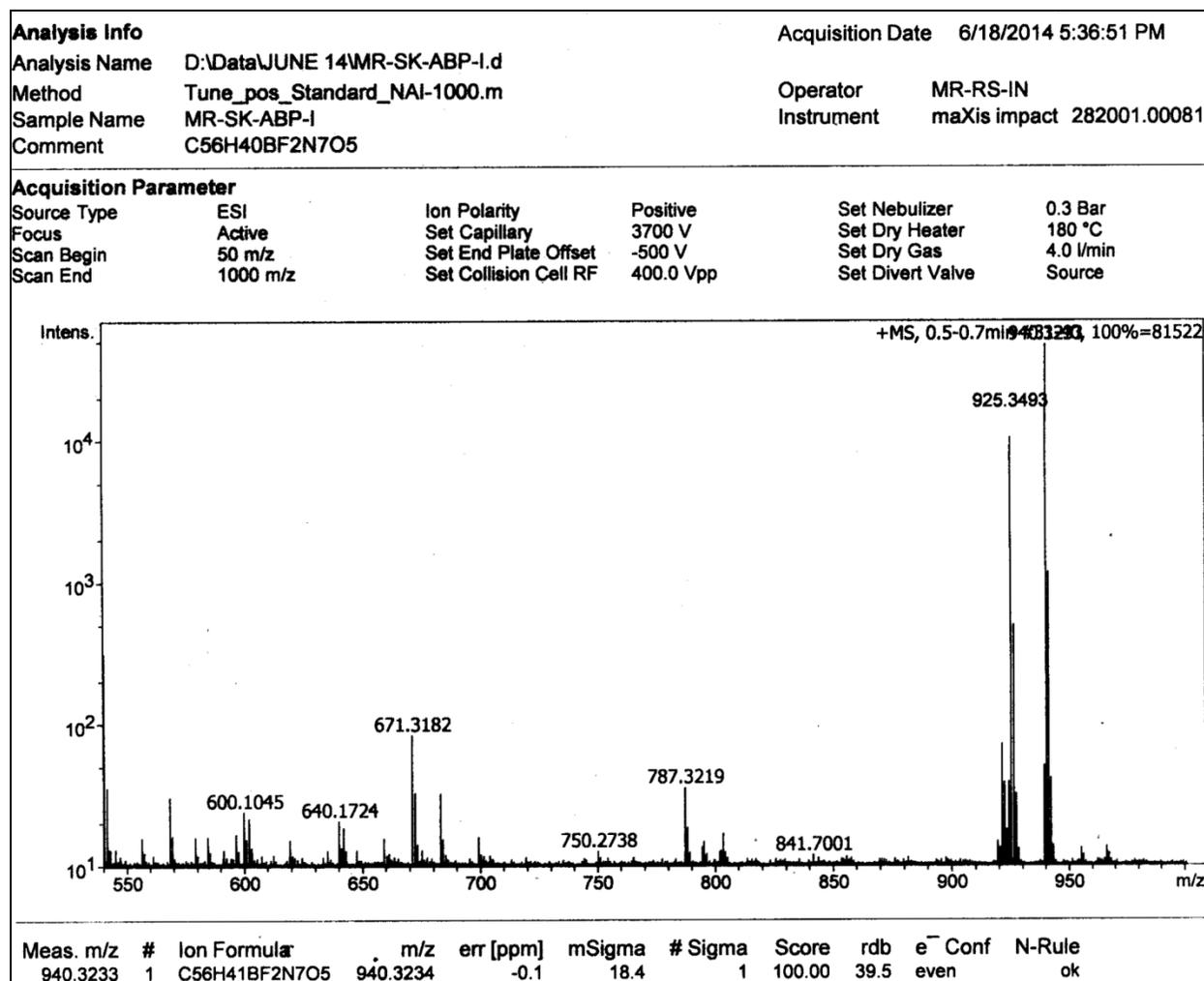
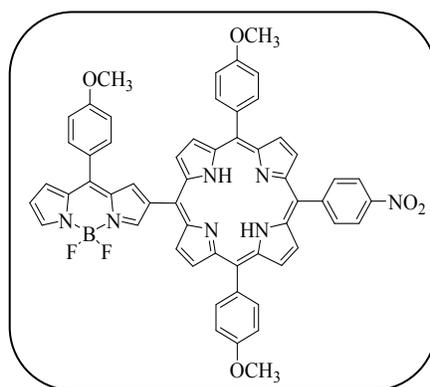


Figure S23: HR mass spectrum of compound 5

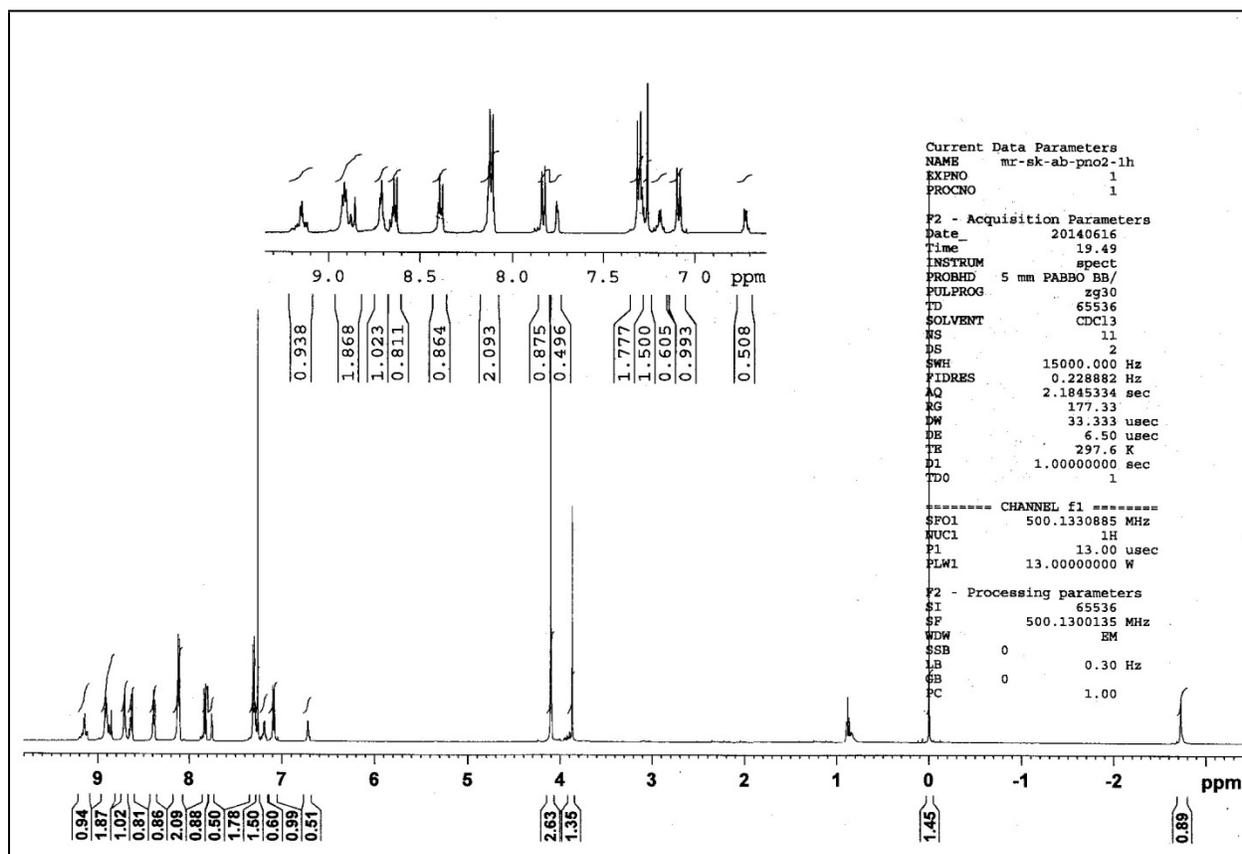
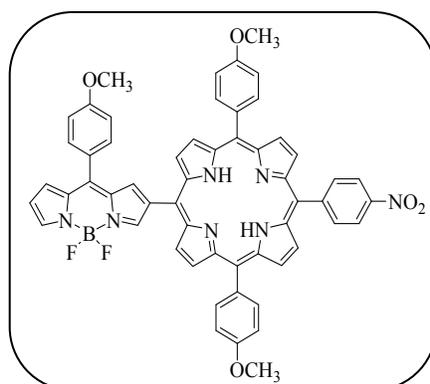


Figure S24: ^1H NMR spectrum of compound **5** recorded in CDCl_3

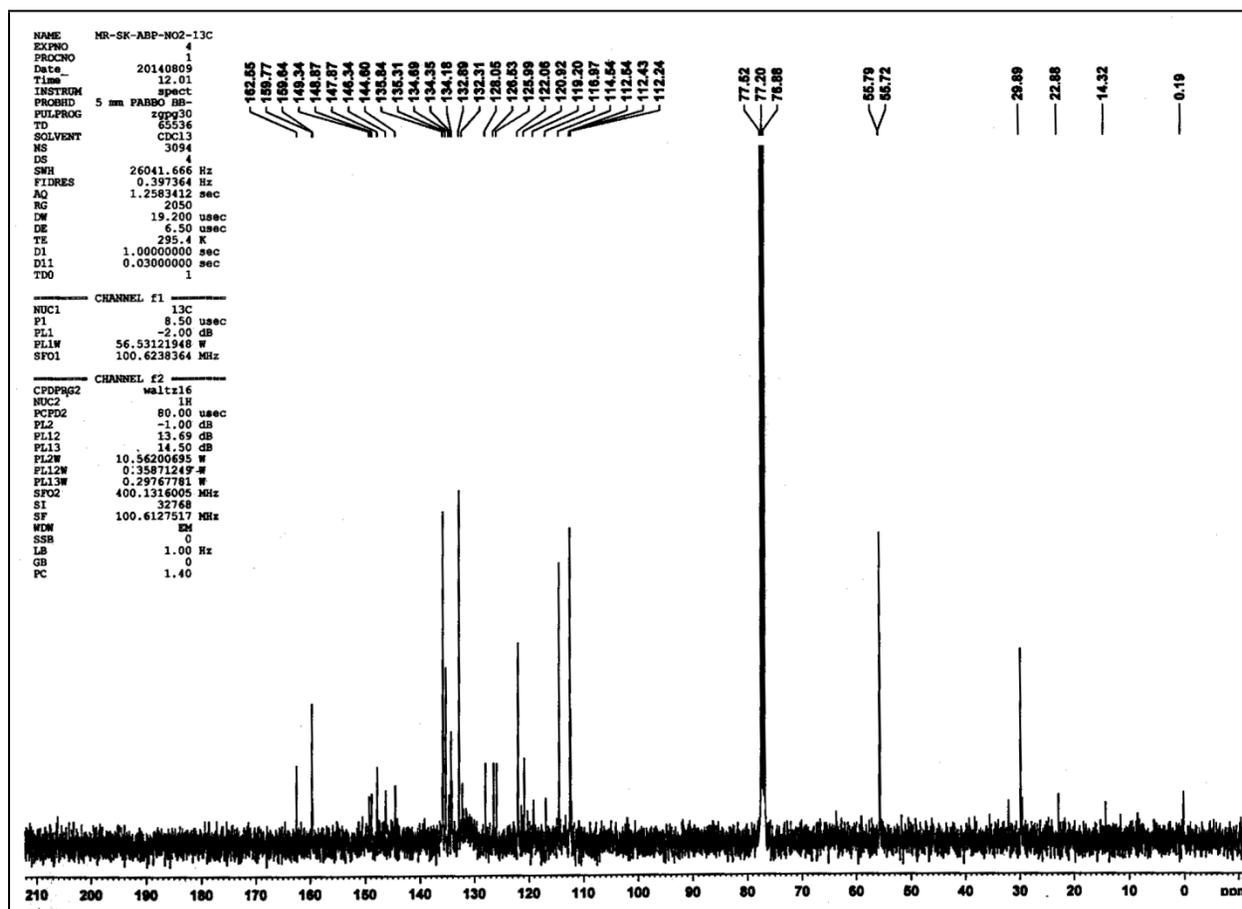
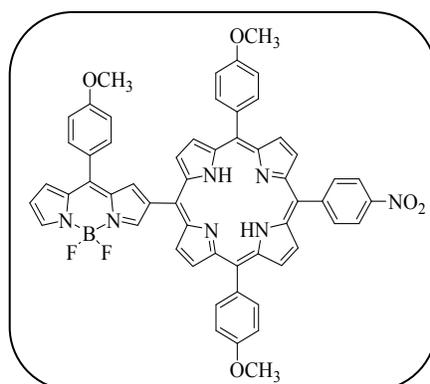


Figure S25: ^{13}C NMR spectrum of compound **5** recorded in CDCl_3

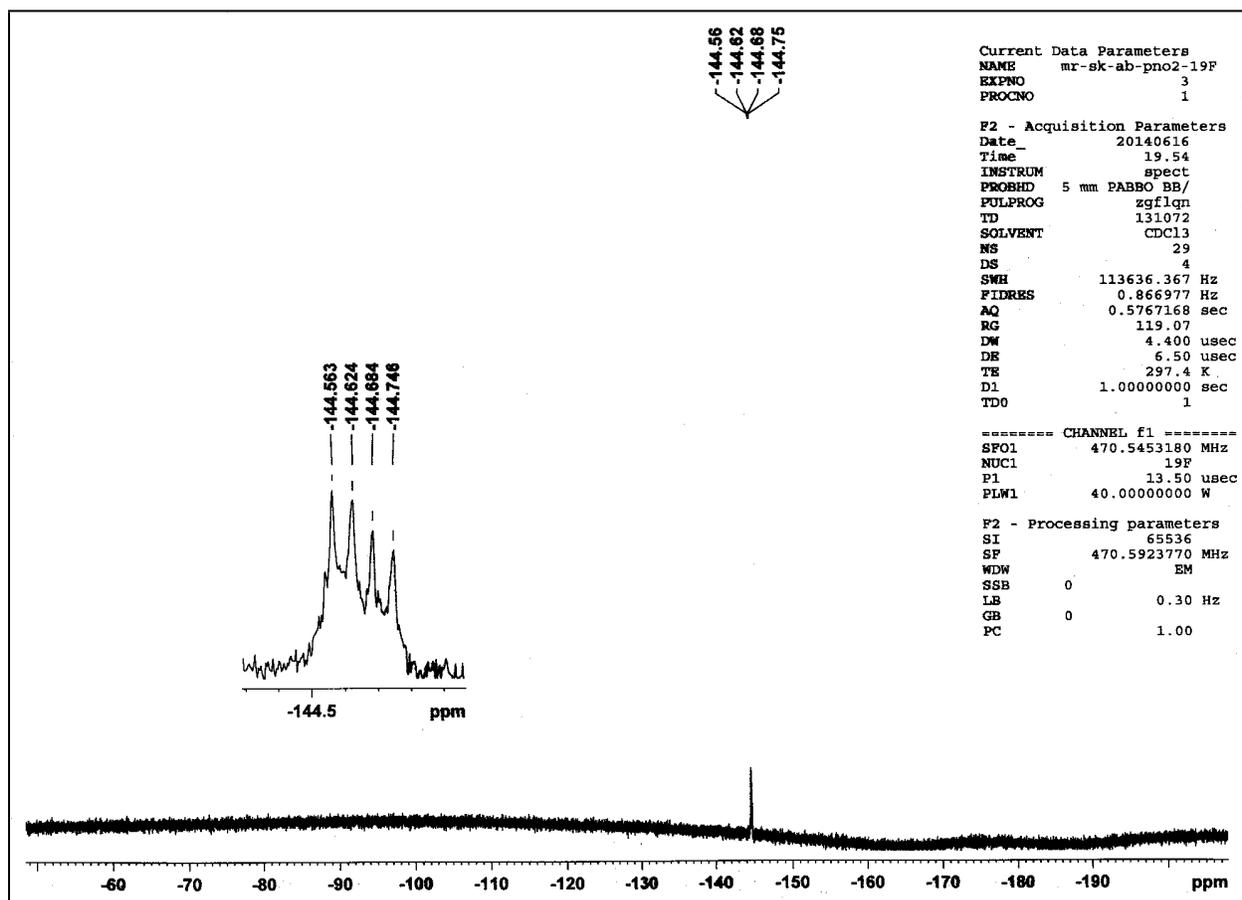
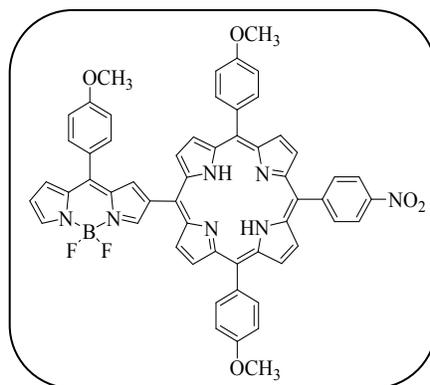


Figure S26: ^{19}F NMR spectrum of compound **5** recorded in CDCl_3 . Inset shows the expansion

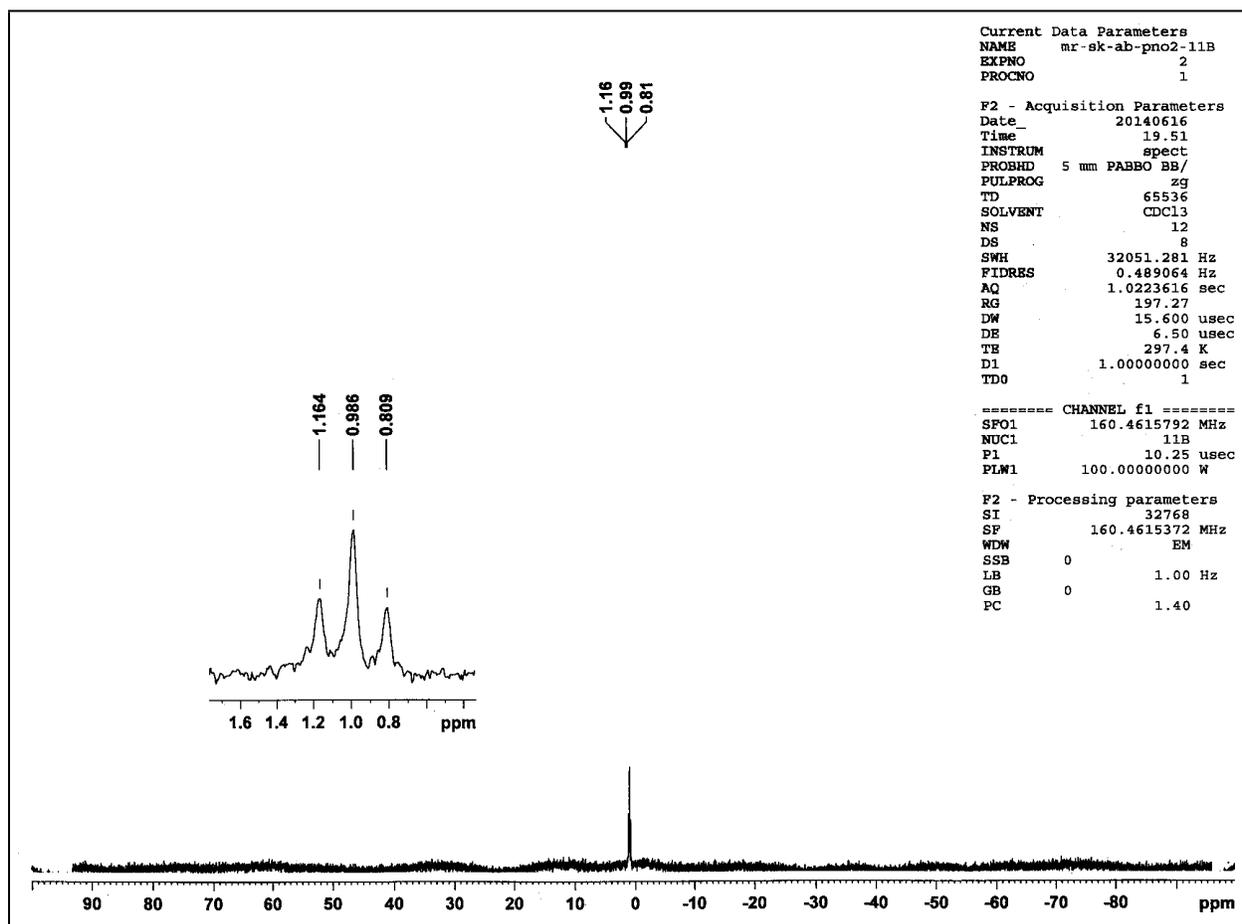
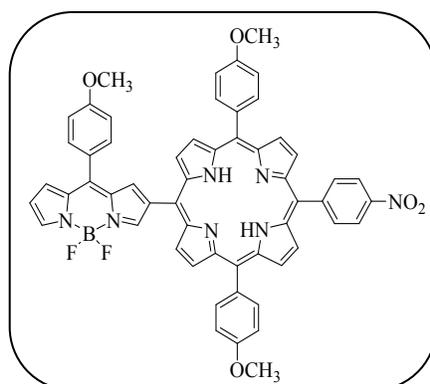


Figure S27: ^{11}B NMR spectrum of compound **5** recorded in CDCl_3 . Inset shows the expansion

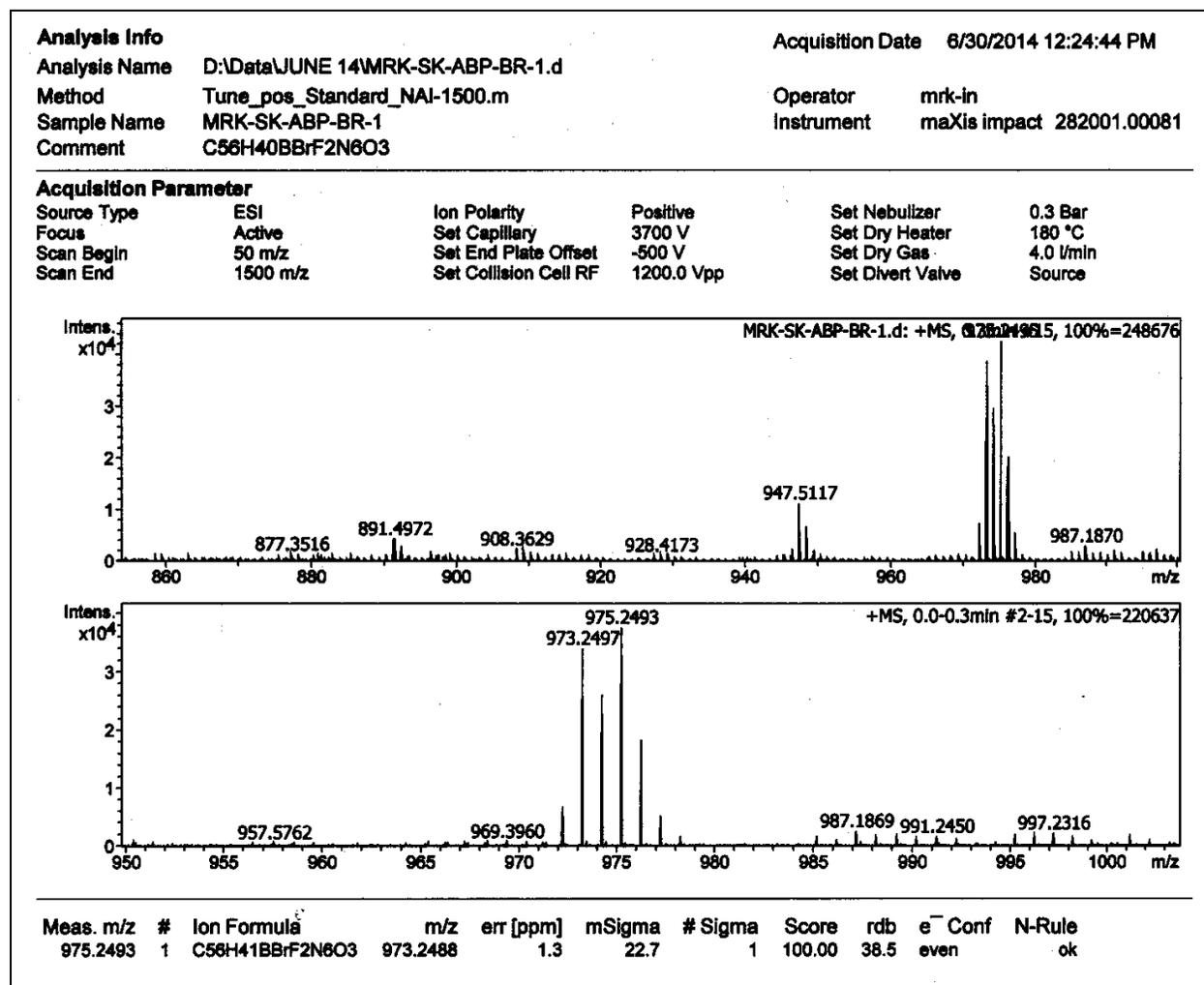
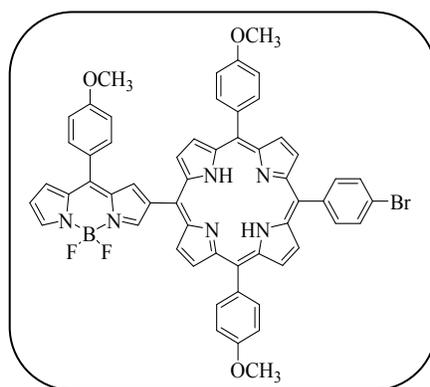


Figure S28: HR mass spectrum of compound 6

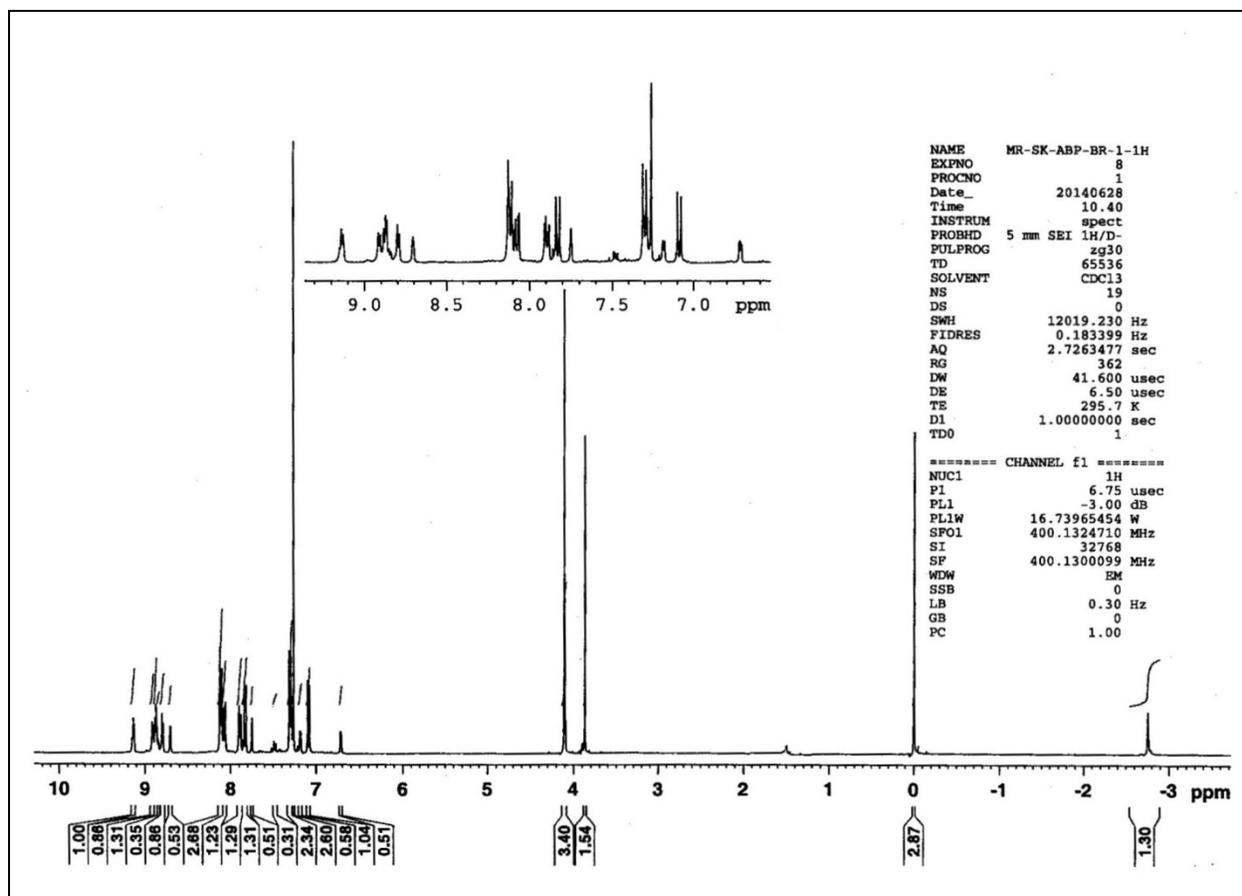
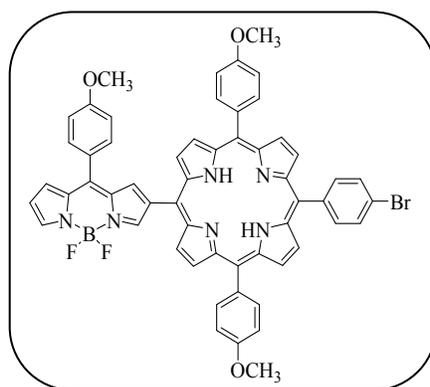


Figure S29: ^1H NMR spectrum of compound **6** recorded in CDCl_3

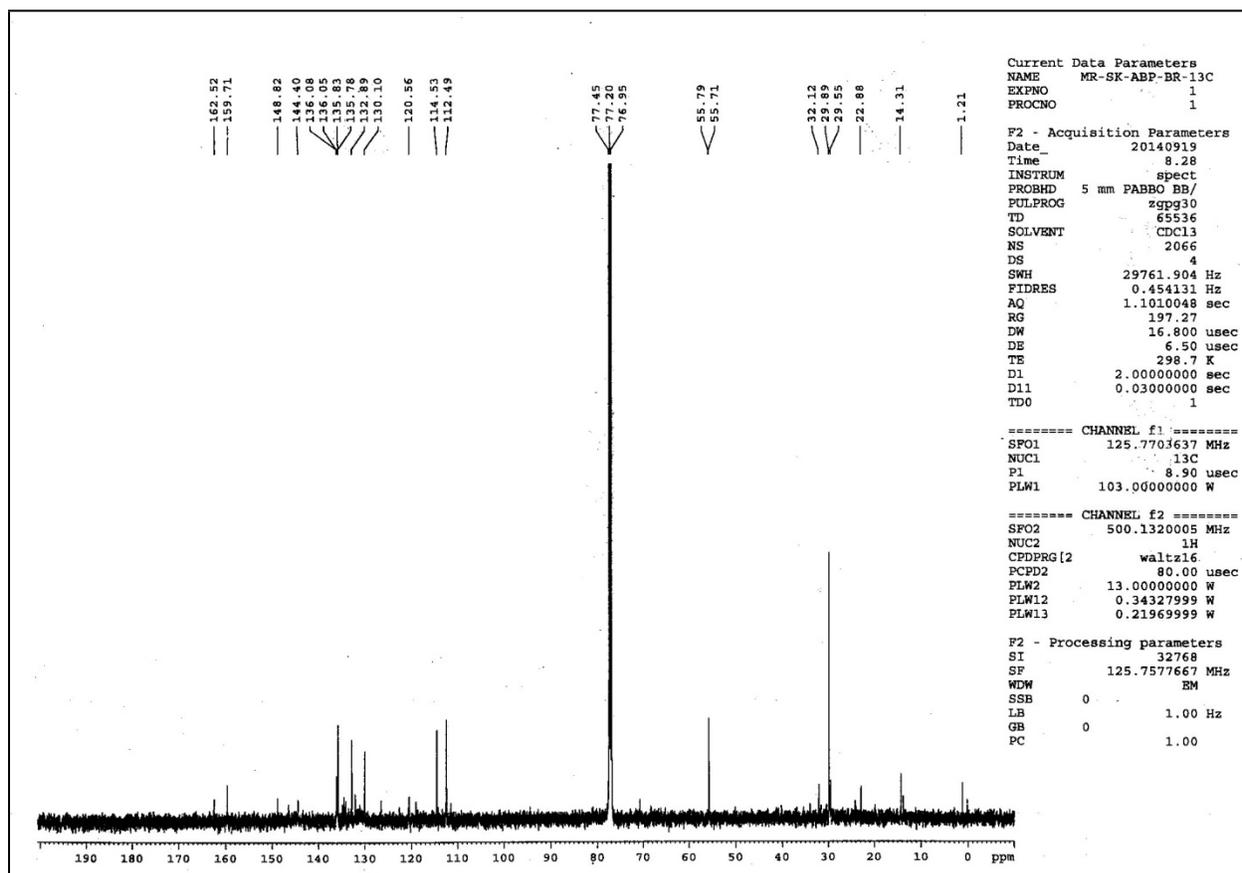
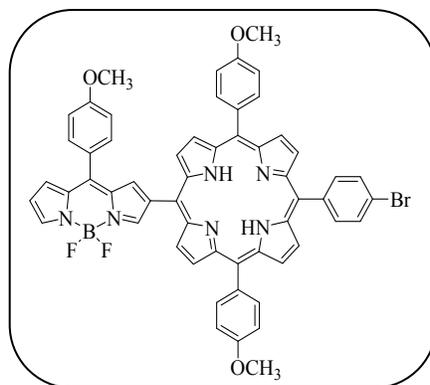


Figure S30: ^{13}C NMR spectrum of compound **6** recorded in CDCl_3

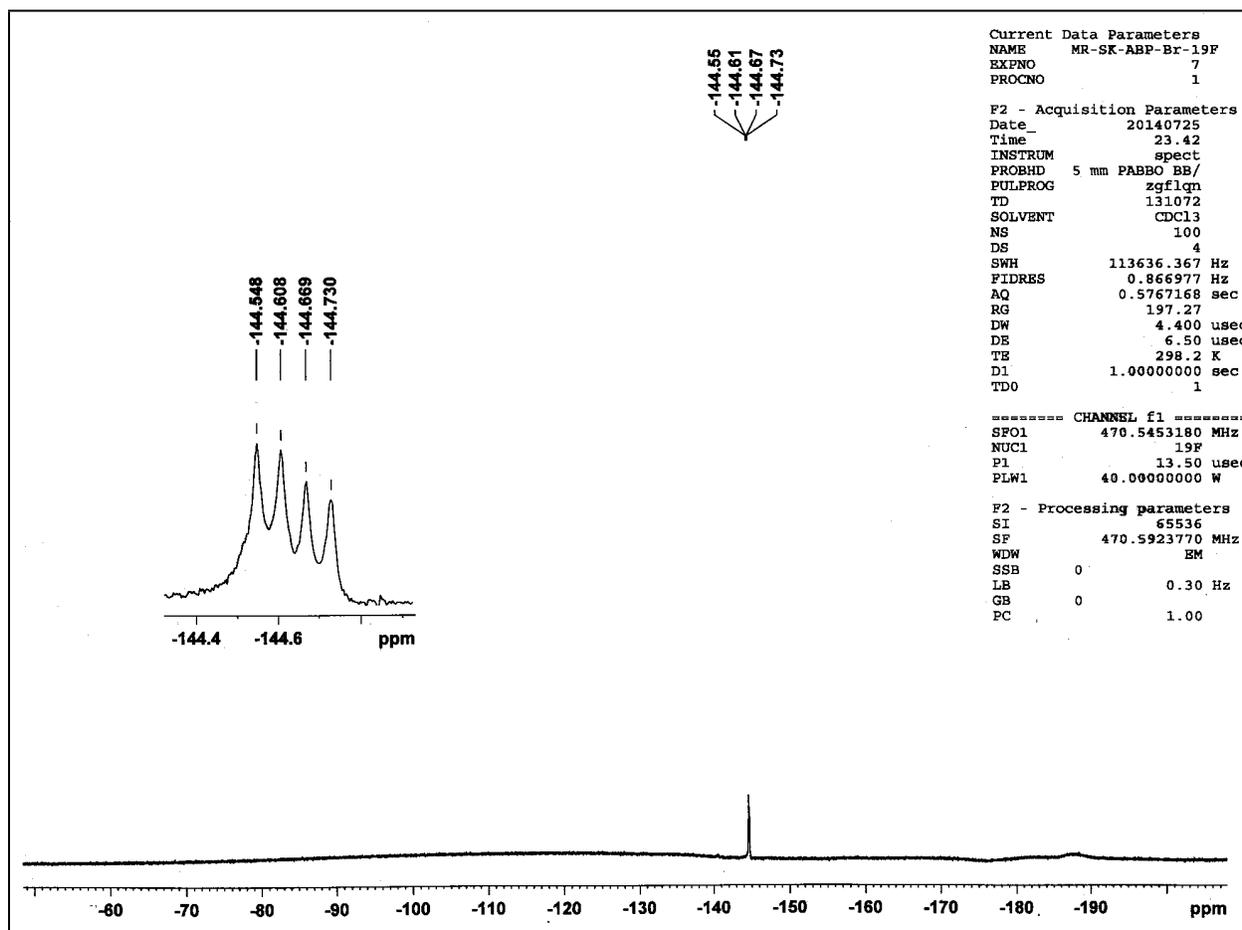
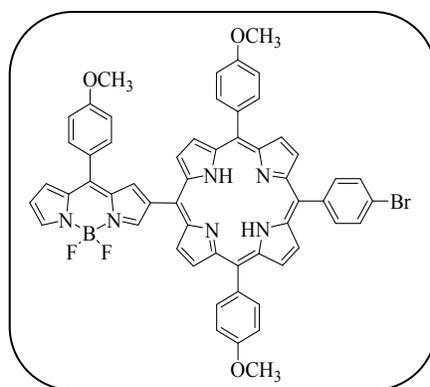


Figure S31: ^{19}F NMR spectrum of compound **6** recorded in CDCl_3 . Inset shows the expansion

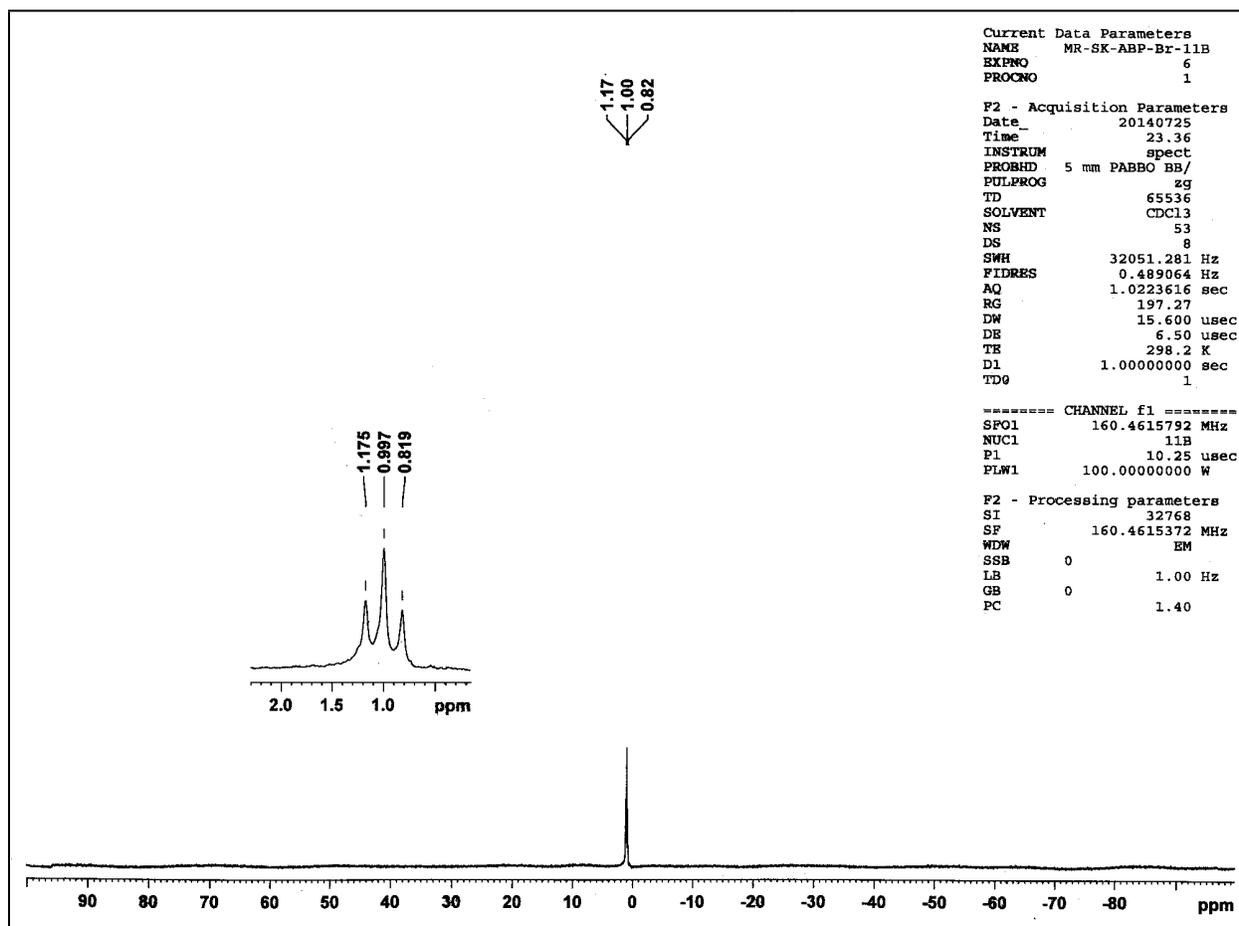
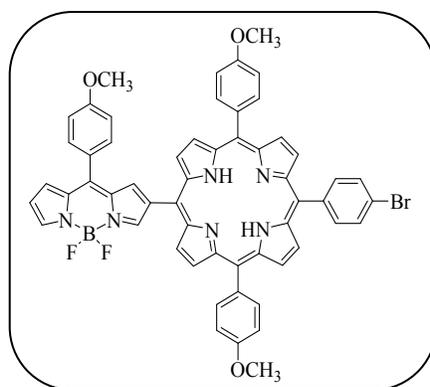


Figure S32: ^{11}B NMR spectrum of compound **6** recorded in CDCl_3 . Inset shows the expansion

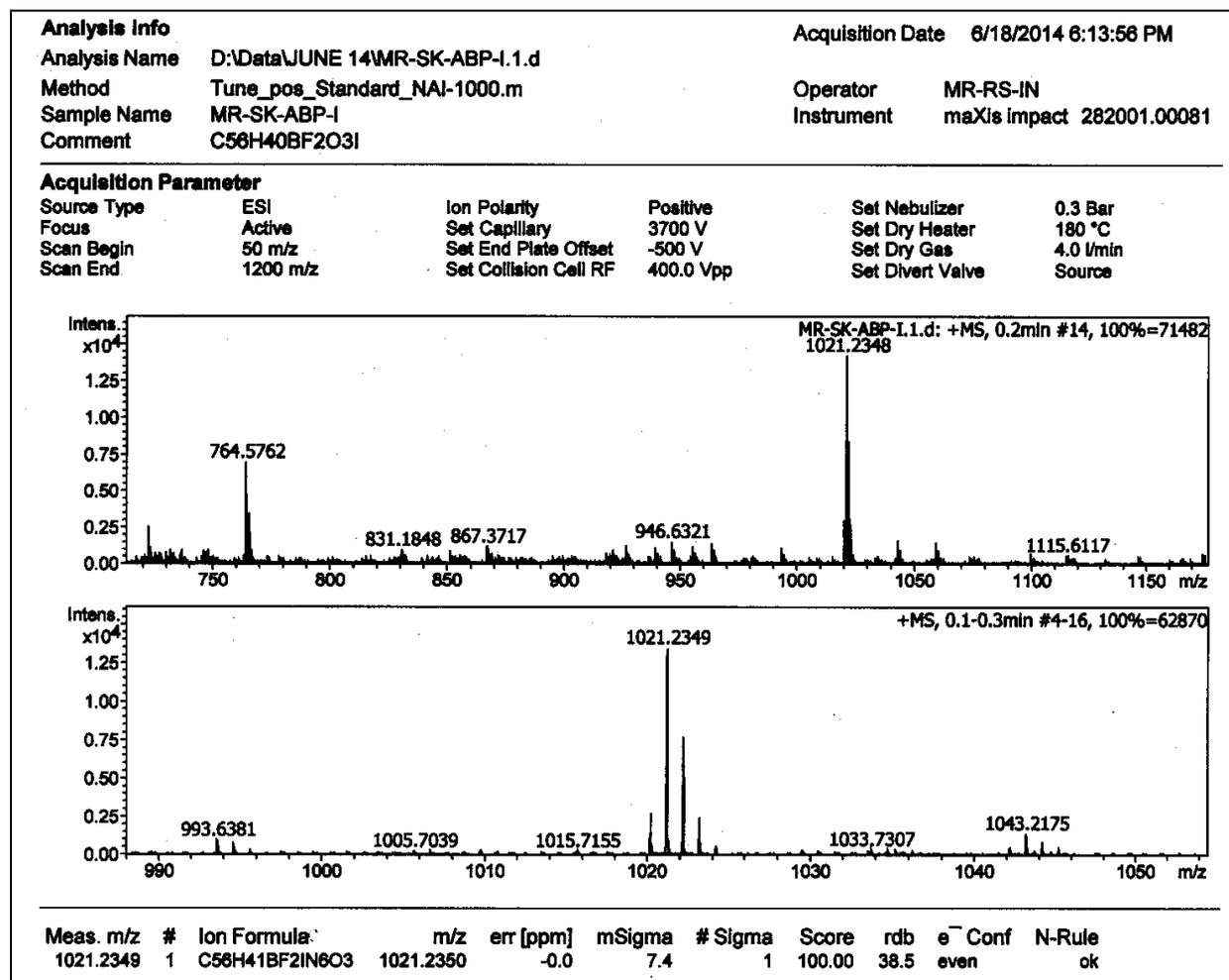
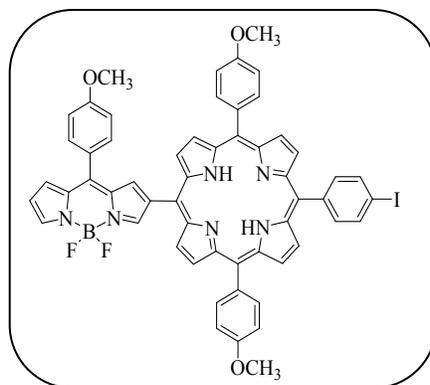


Figure S33: HR mass spectrum of compound 7

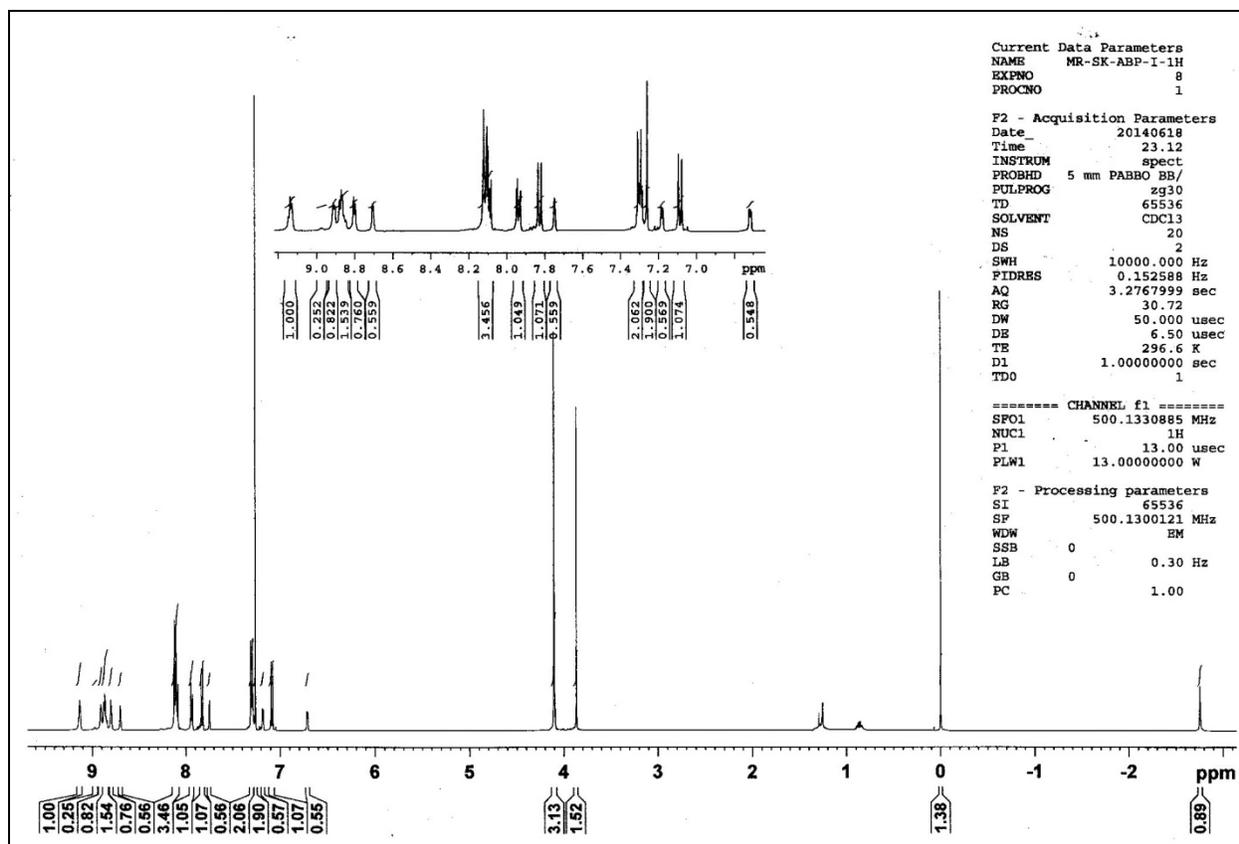
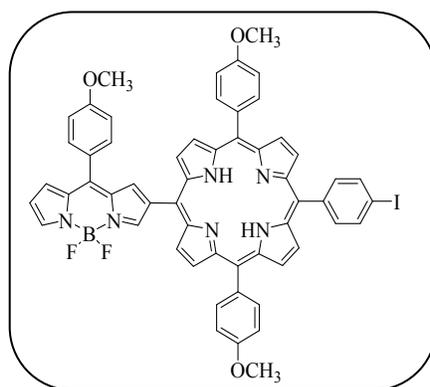


Figure S34: ^1H NMR spectrum of compound **7** recorded in CDCl_3

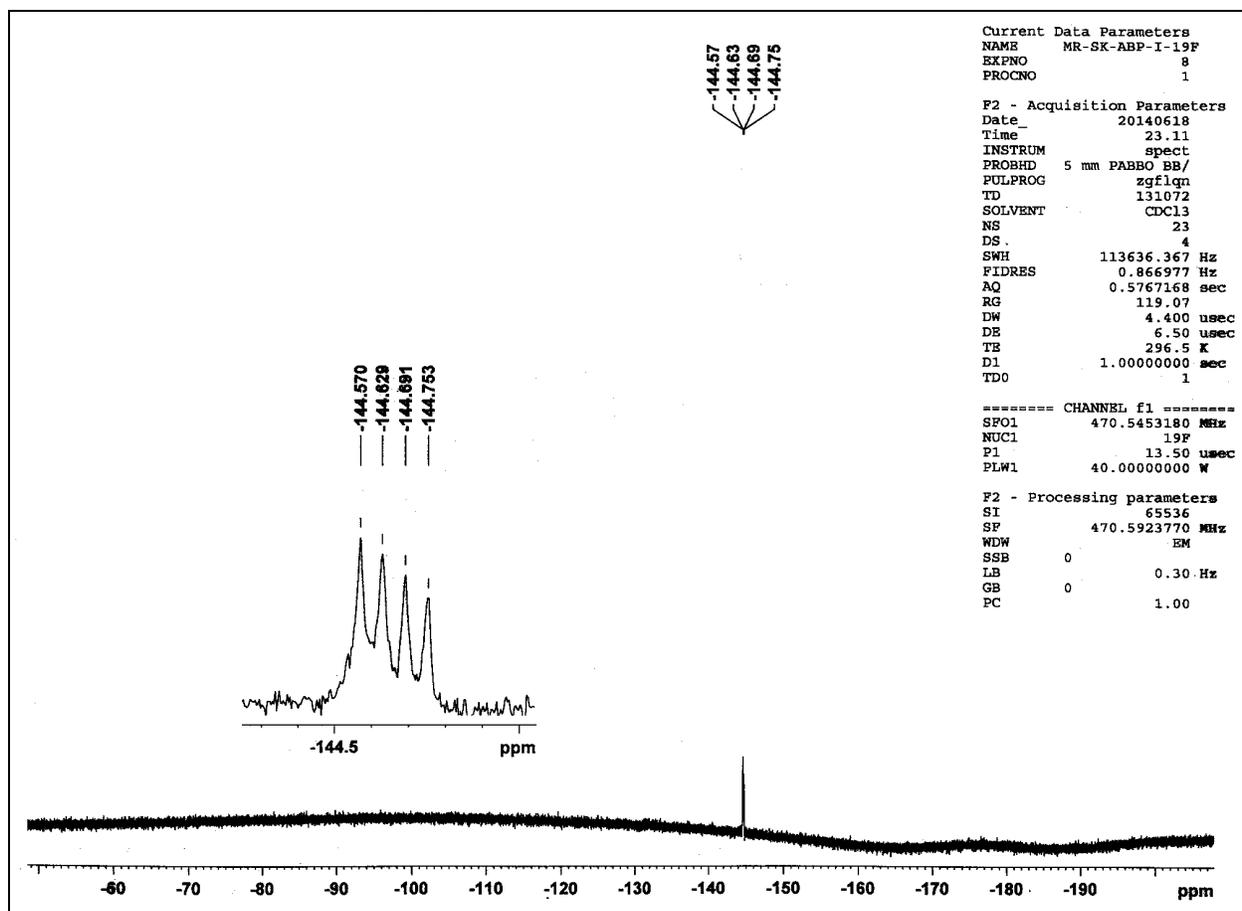
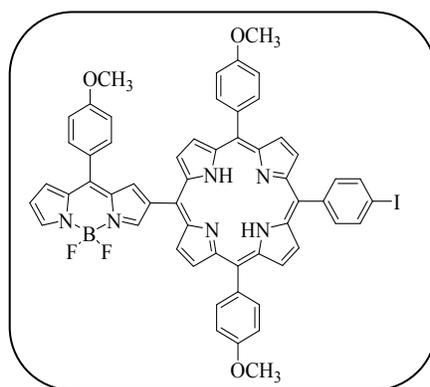


Figure S35: ^{19}F NMR spectrum of compound **7** recorded in CDCl_3 . Inset shows the expansion

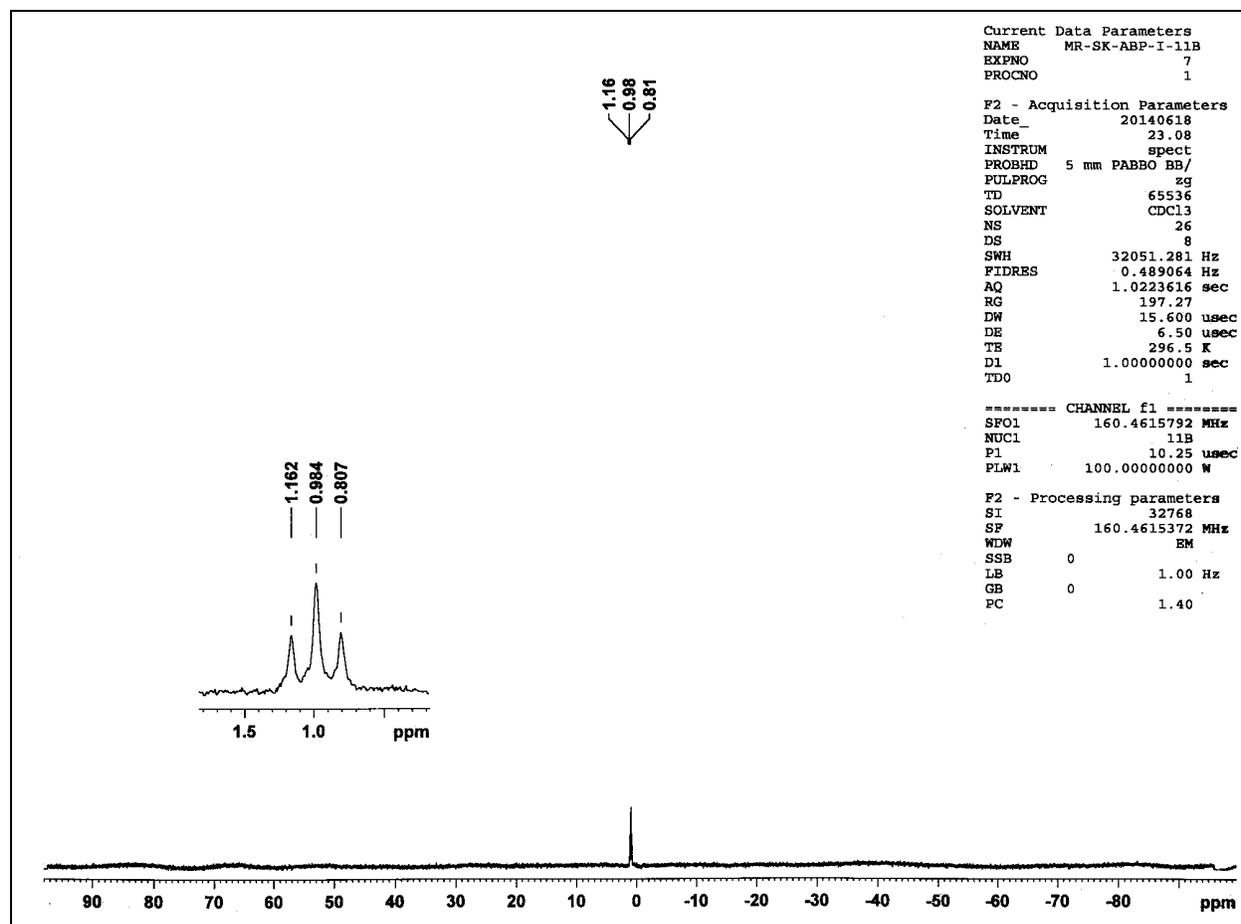
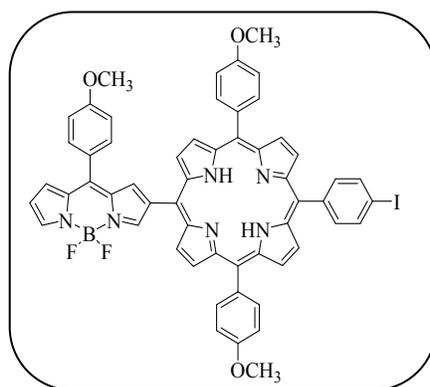
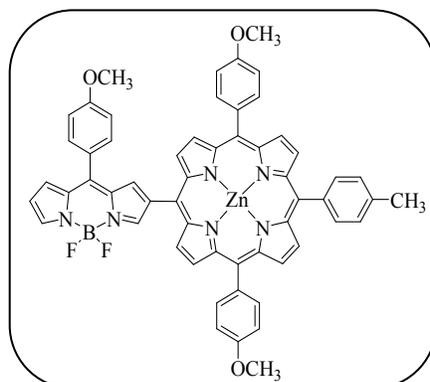


Figure S36: ^{11}B NMR spectrum of compound **7** recorded in CDCl_3 . Inset shows the expansion



Elemental Composition Report

Single Mass Analysis

Tolerance = 100.0 PPM / DBE: min = -1.5, max = 500.0

Selected filters: None

Monoisotopic Mass, Odd and Even Electron Ions

257 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

Elements Used:

C: 0-57 H: 0-42 B: 0-1 N: 0-6 O: 0-3 F: 0-2 64Zn: 0-1

Q-ToF MICROMASS (YA-105)

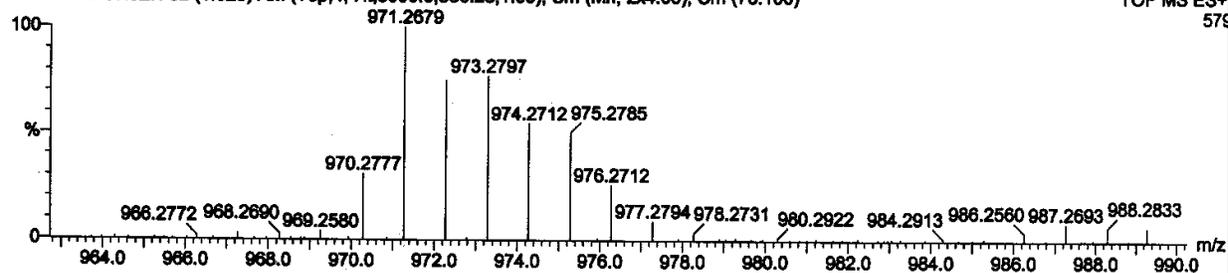
DEPARTMENT OF CHEMISTRY, I.I.T.(B)

18-Aug-2014 18:48:14

C57H41BF2N6O3Zn

MR-SK-PB-CH3ZN 82 (1.523) AM (Top,4, Ht,5000.0,556.28,1.00); Sm (Mn, 2x4.00); Cm (76:100)

TOF MS ES+
579



Minimum: -1.5
Maximum: 500.0 100.0 500.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
971.2679	971.2671	0.8	0.8	39.5	0.4	C57 H42 B N6 O3 F2 64Zn

Figure S37: HR mass spectrum of compound Zn1

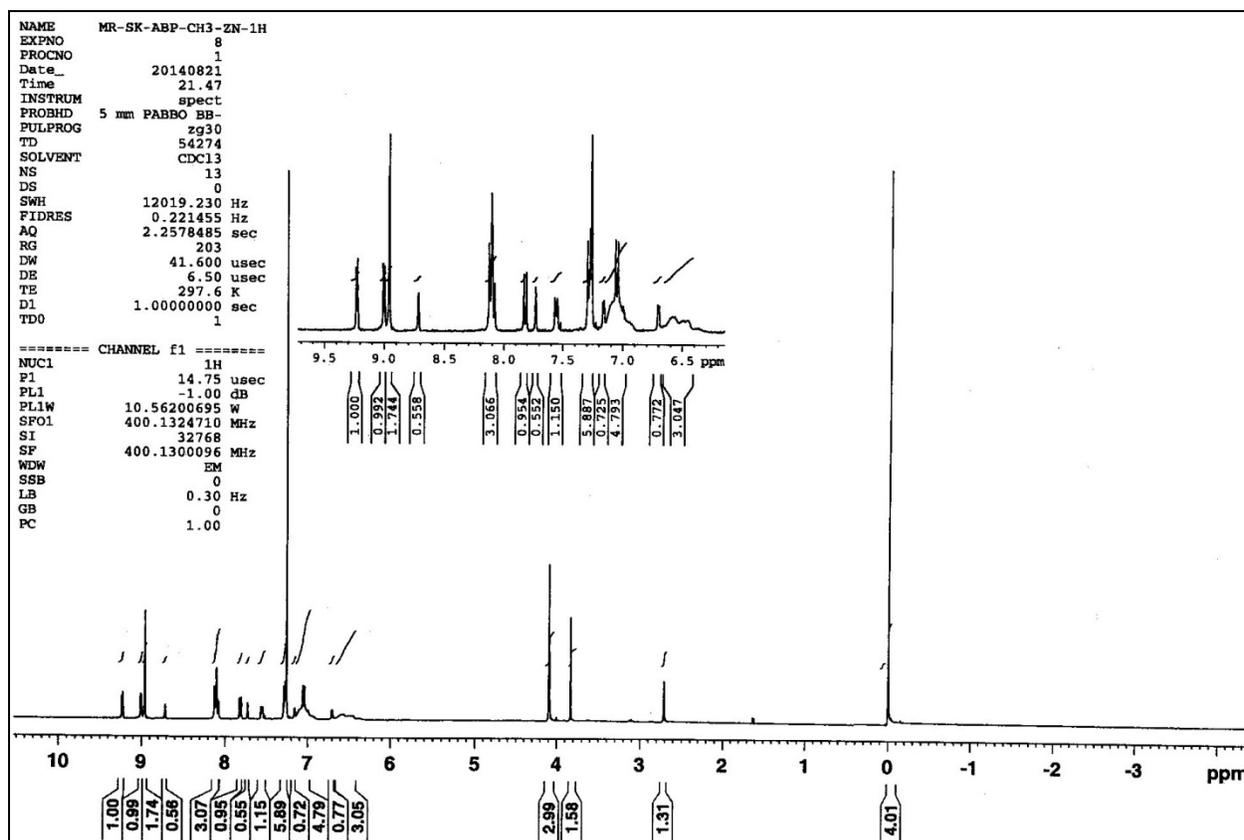
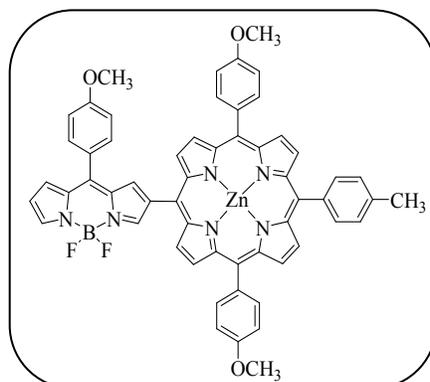


Figure S38: ^1H NMR spectrum of compound **Zn1** recorded in CDCl_3

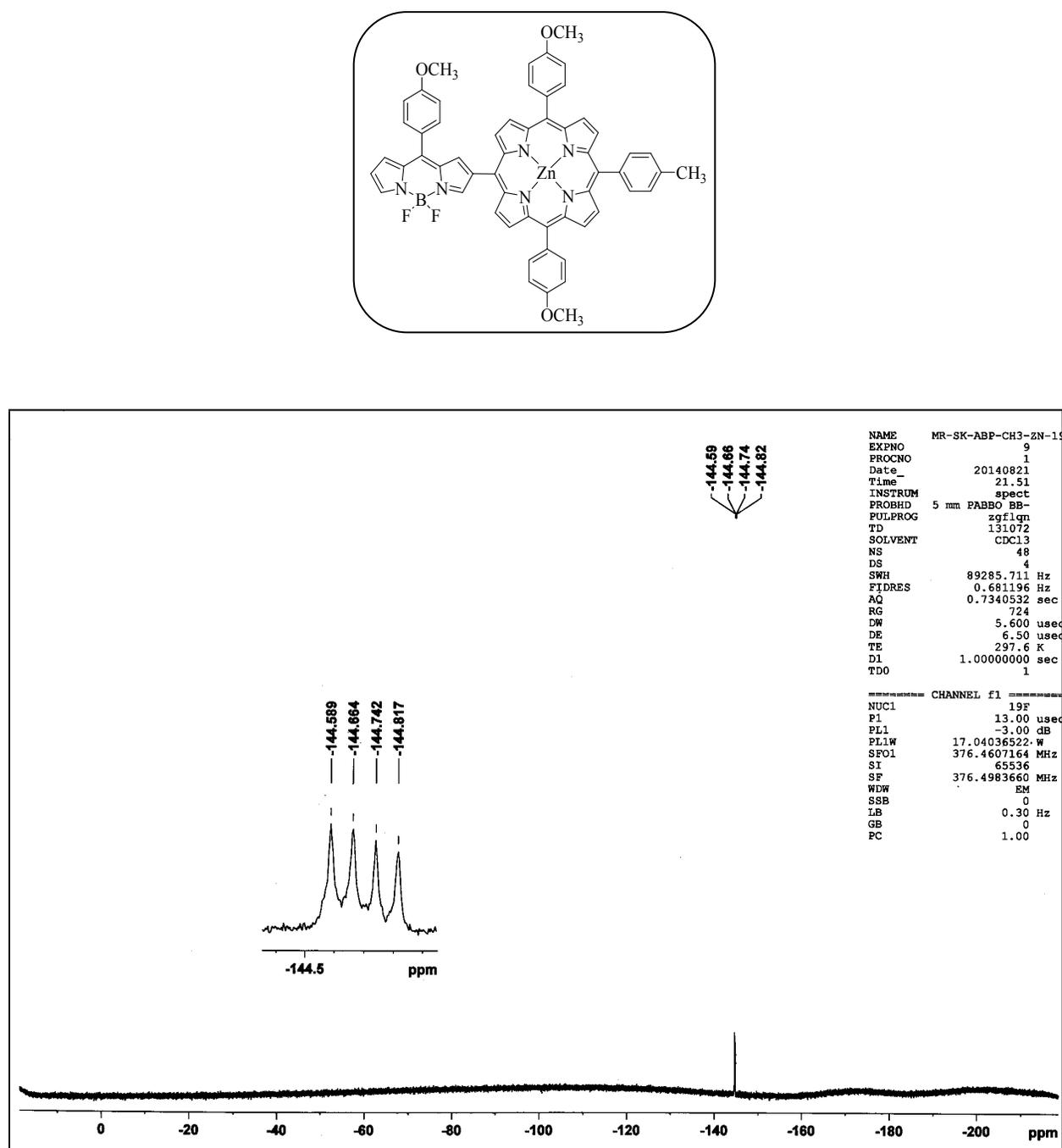


Figure S39: ^{19}F NMR spectrum of compound **Zn1** recorded in CDCl_3 . Inset shows the expansion

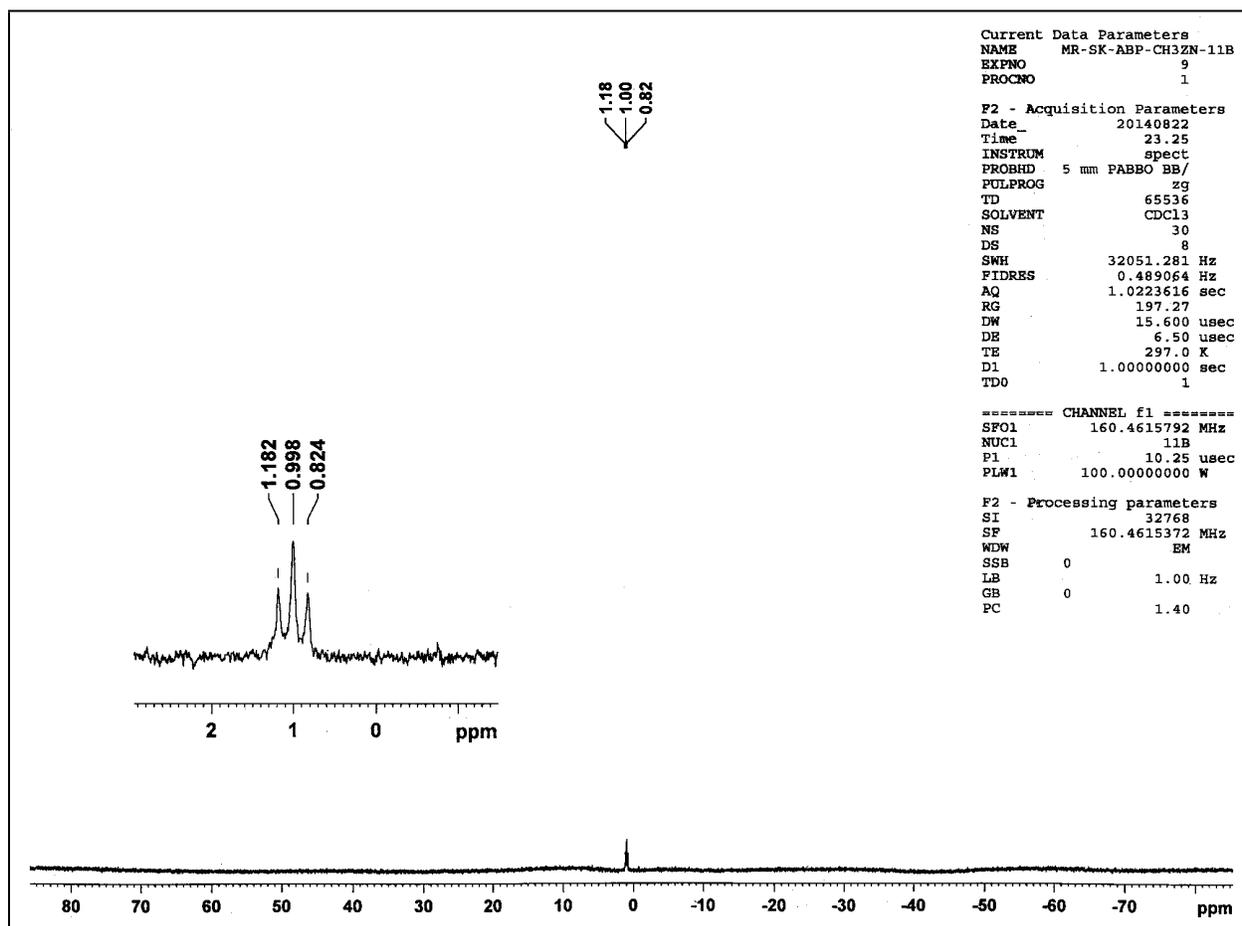
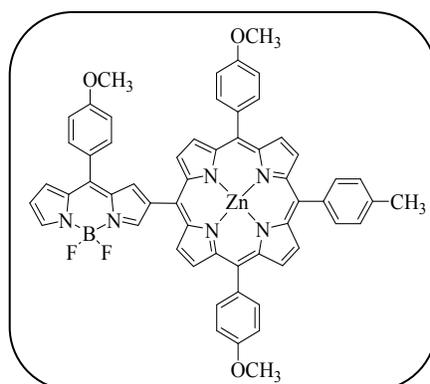


Figure S40: ^{11}B NMR spectrum of compound **Zn1** recorded in CDCl_3 . Inset shows the expansion

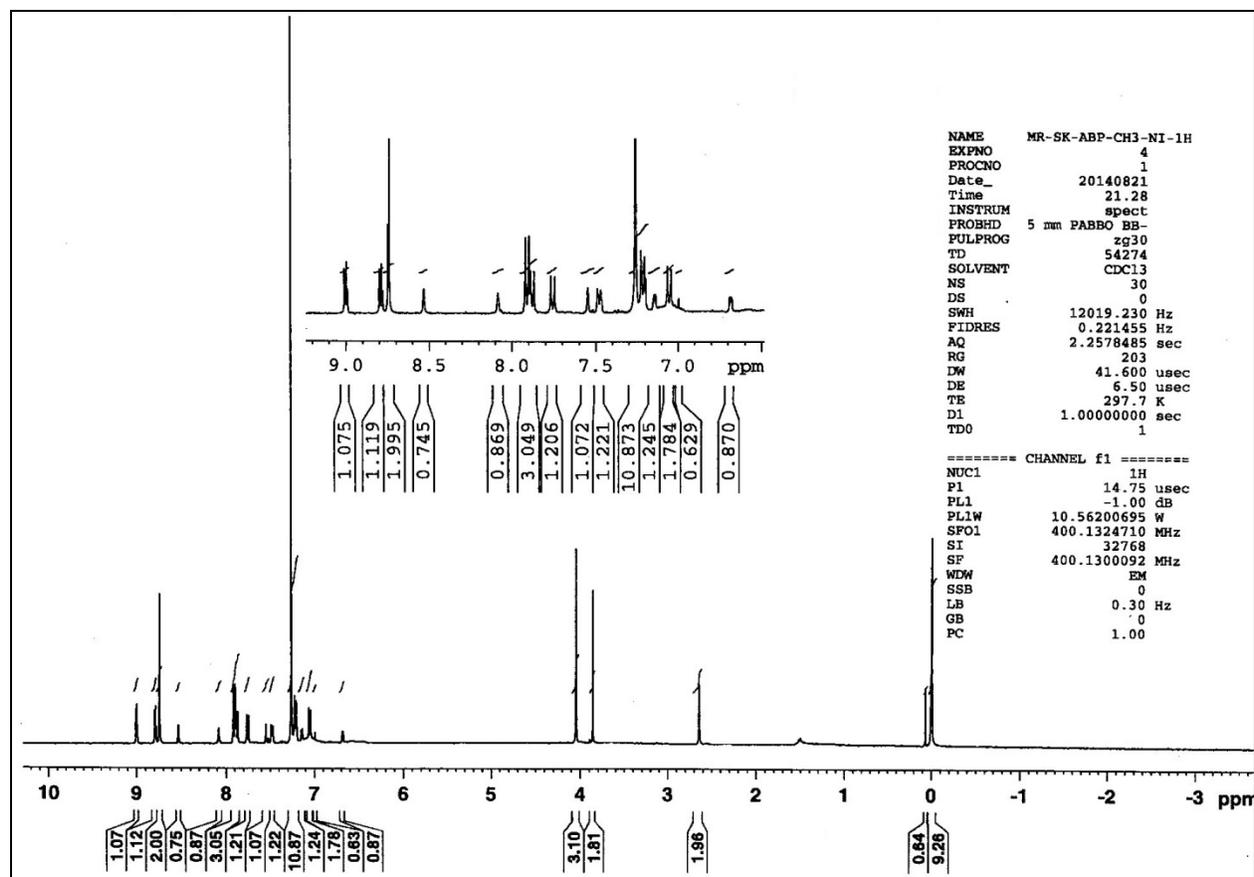
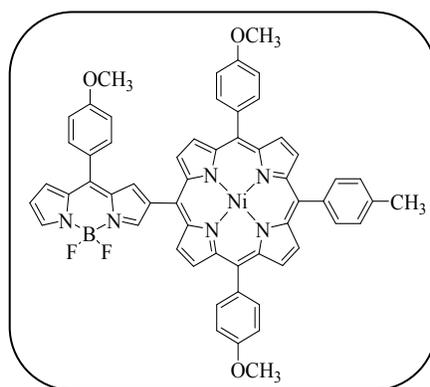


Figure S41: ^1H NMR spectrum of compound Ni1 recorded in CDCl_3

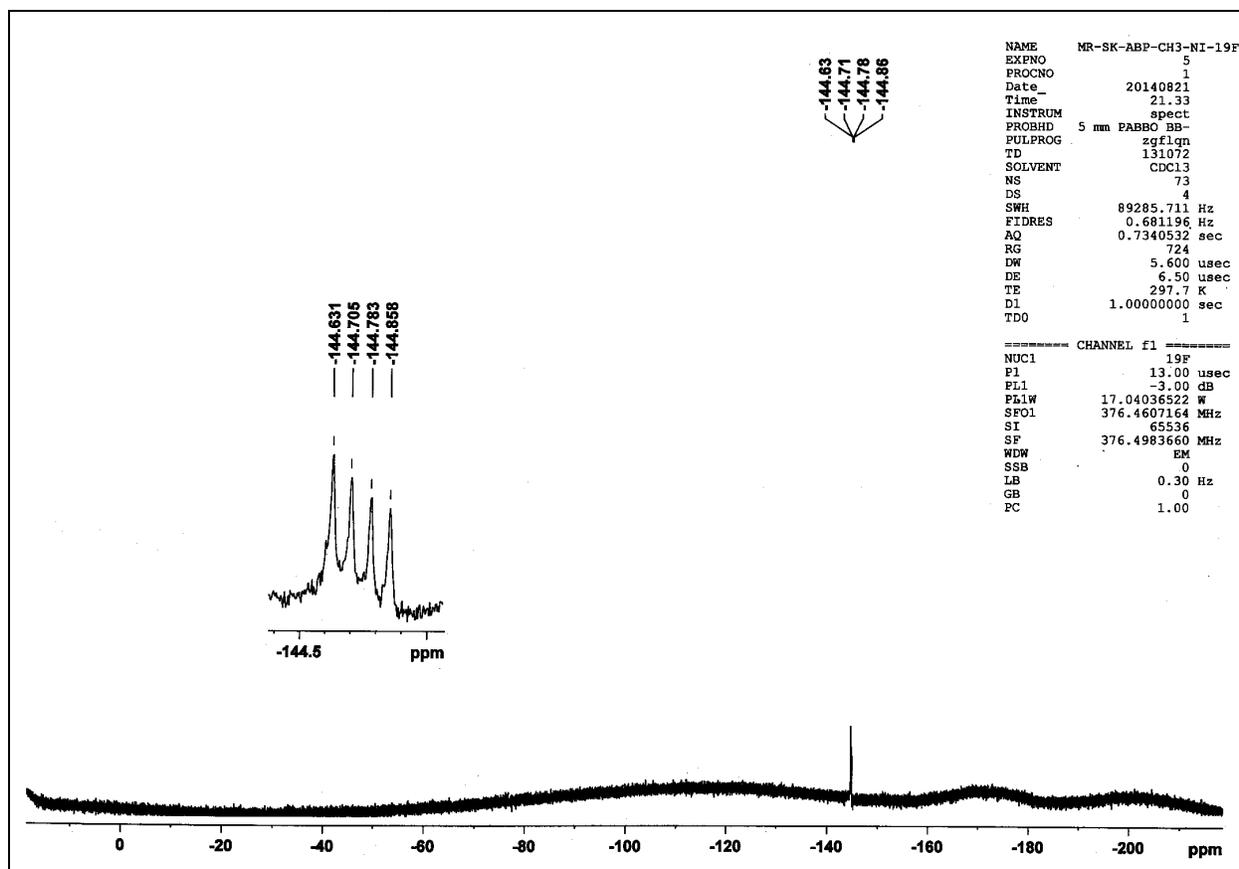
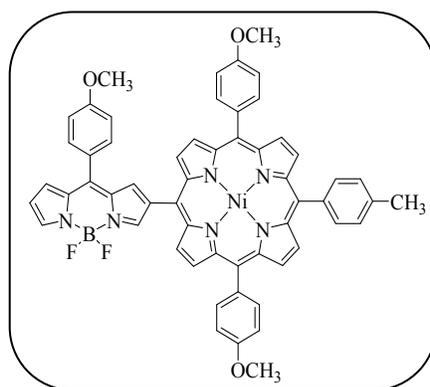


Figure S42: ¹⁹F NMR spectrum of compound NiI recorded in CDCl₃. Inset shows the expansion

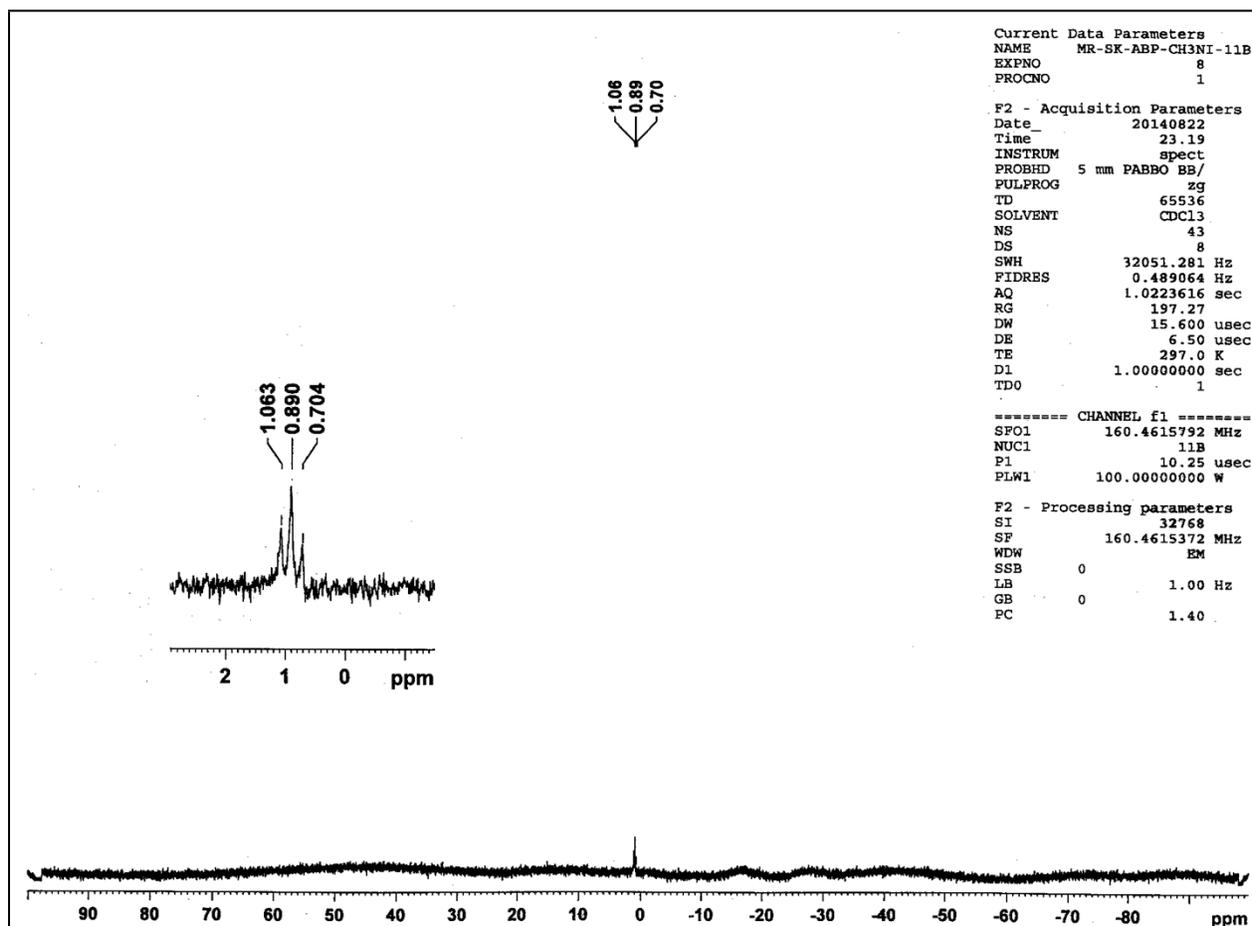
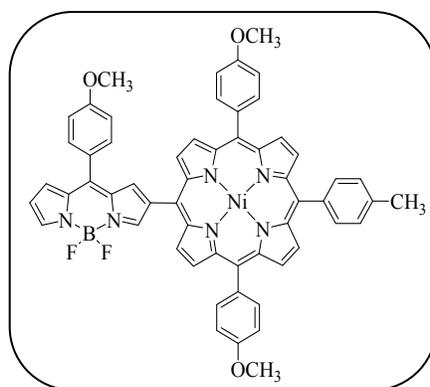


Figure S43: ^{11}B NMR spectrum of compound Ni1 recorded in CDCl_3 . Inset shows the expansion

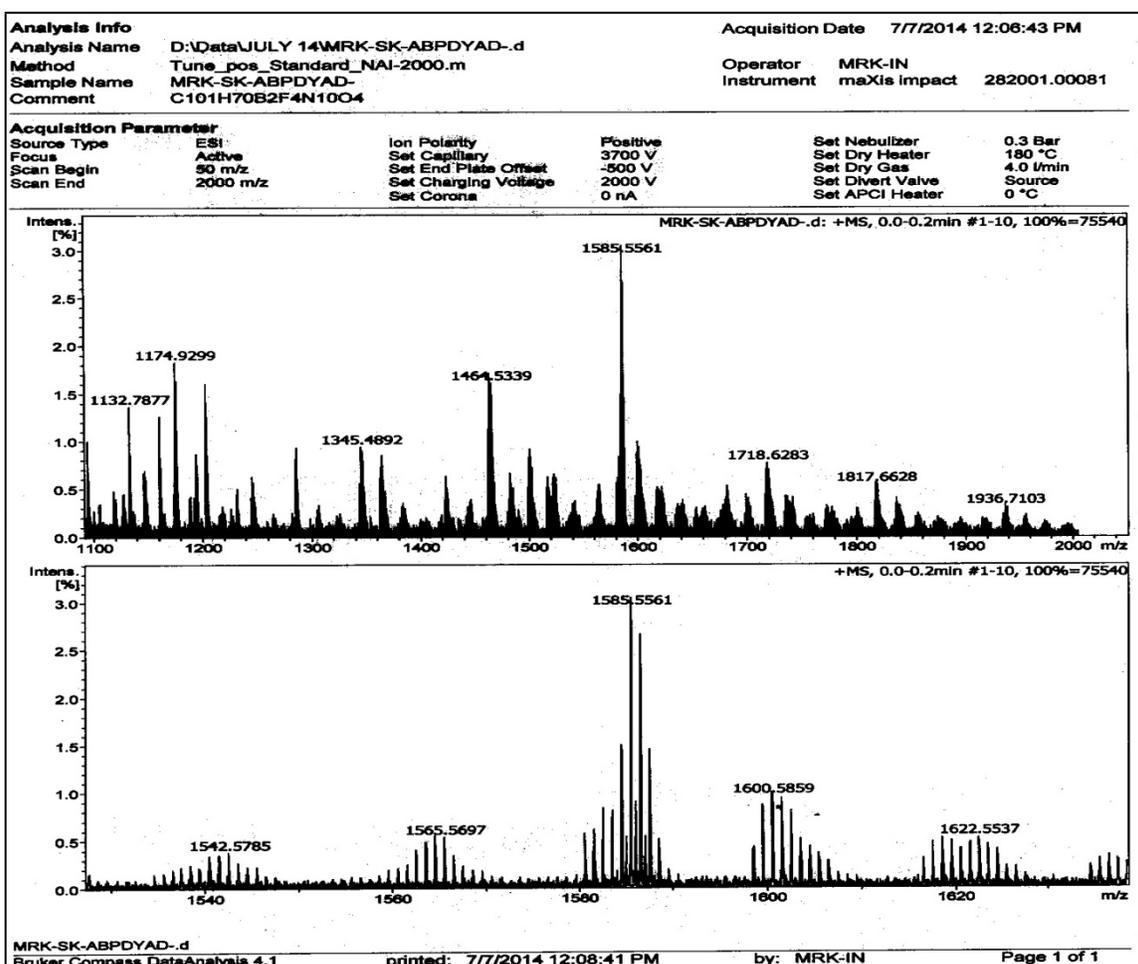
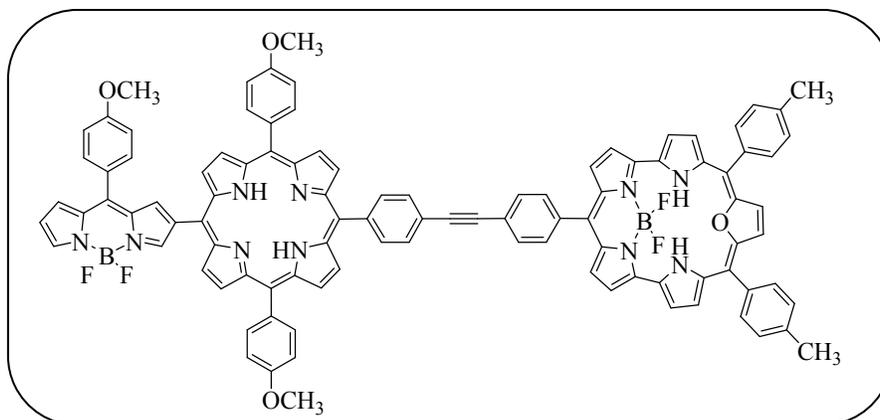


Figure S44: LR mass spectrum of compound 8

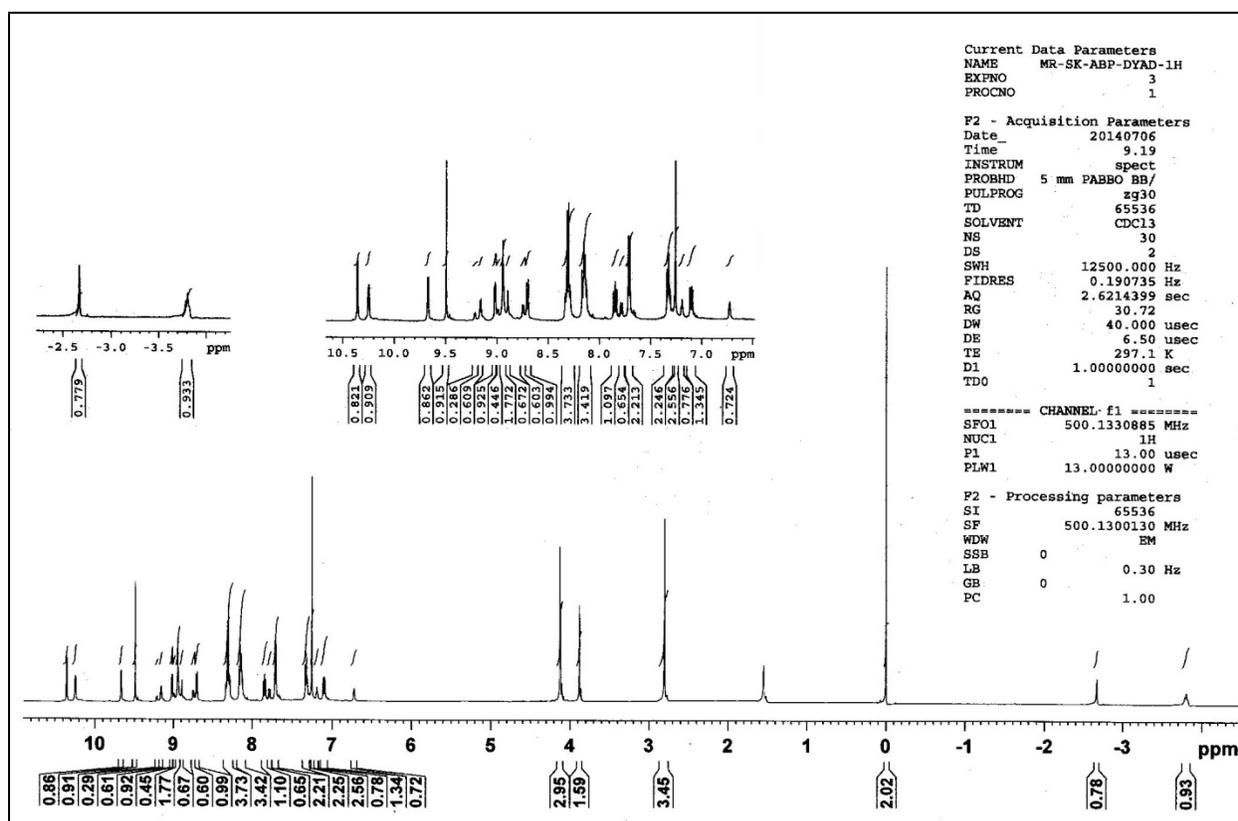
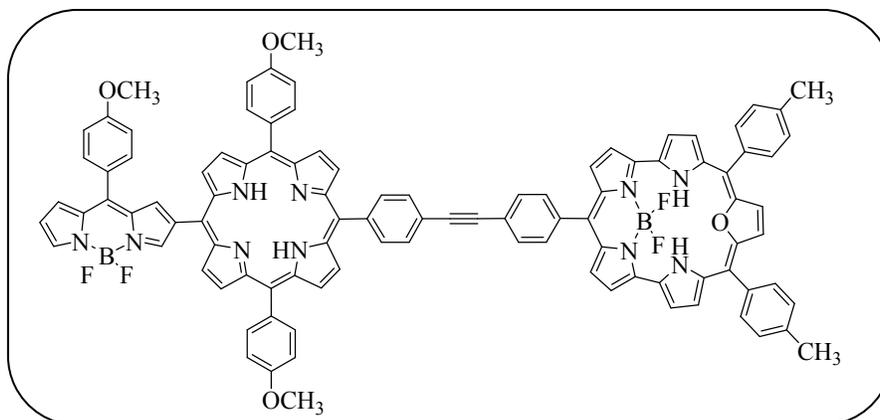


Figure S45: ^1H NMR spectrum of compound **1** recorded in CDCl_3

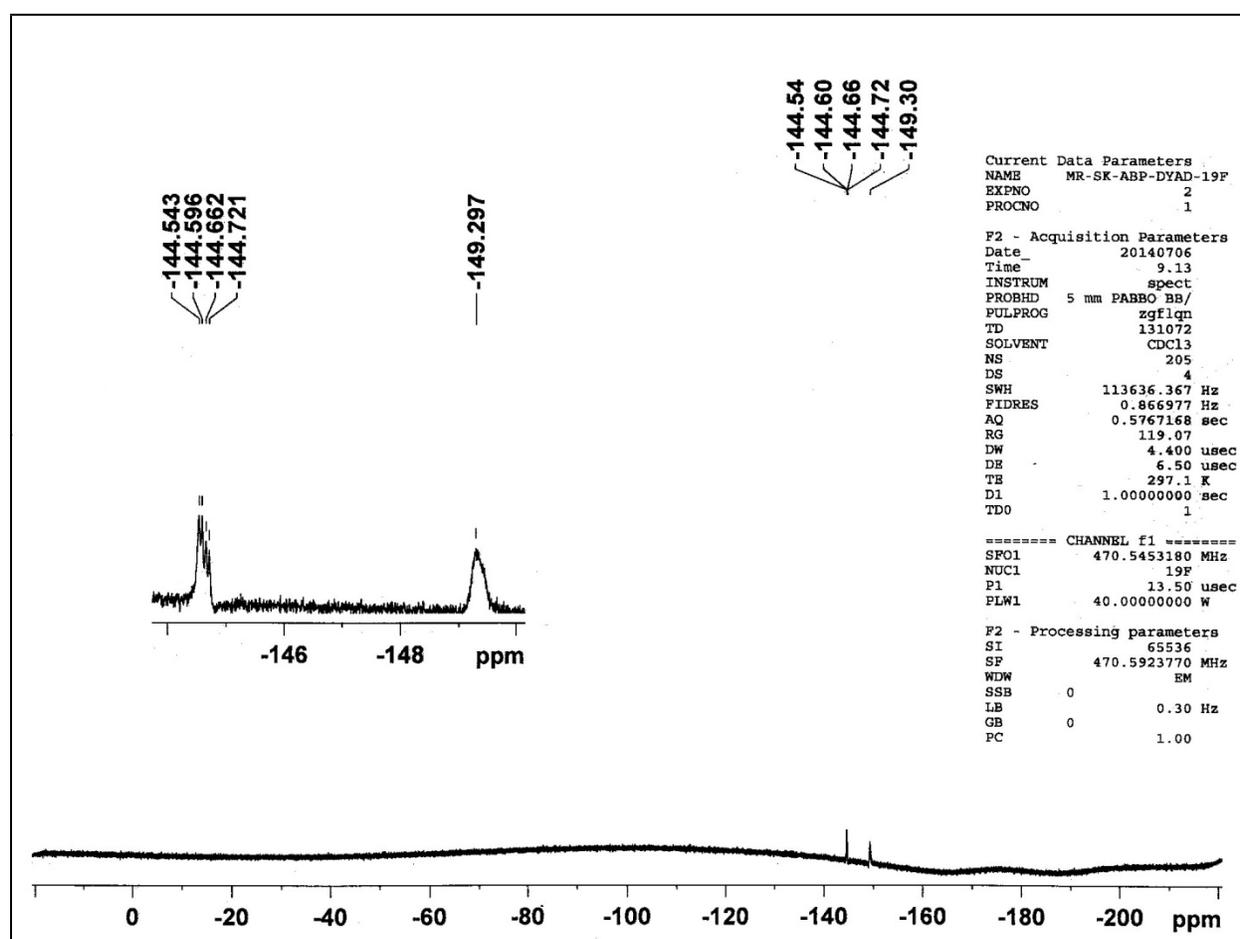
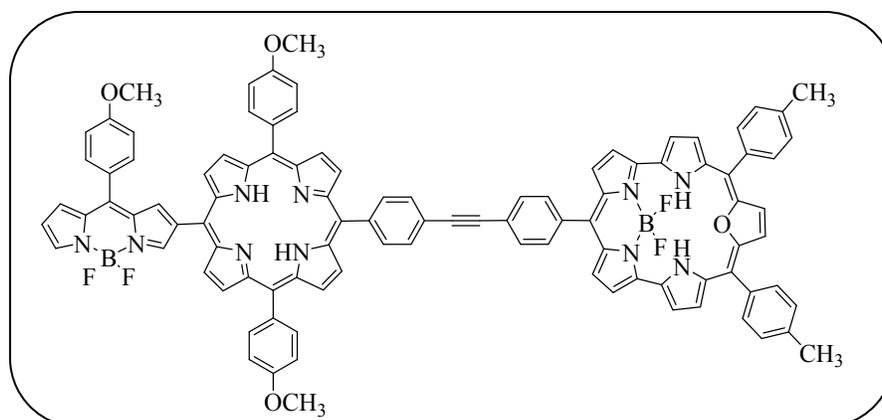


Figure S46: ^{19}F NMR spectrum of compound **8** recorded in CDCl_3 . Inset shows the expansion

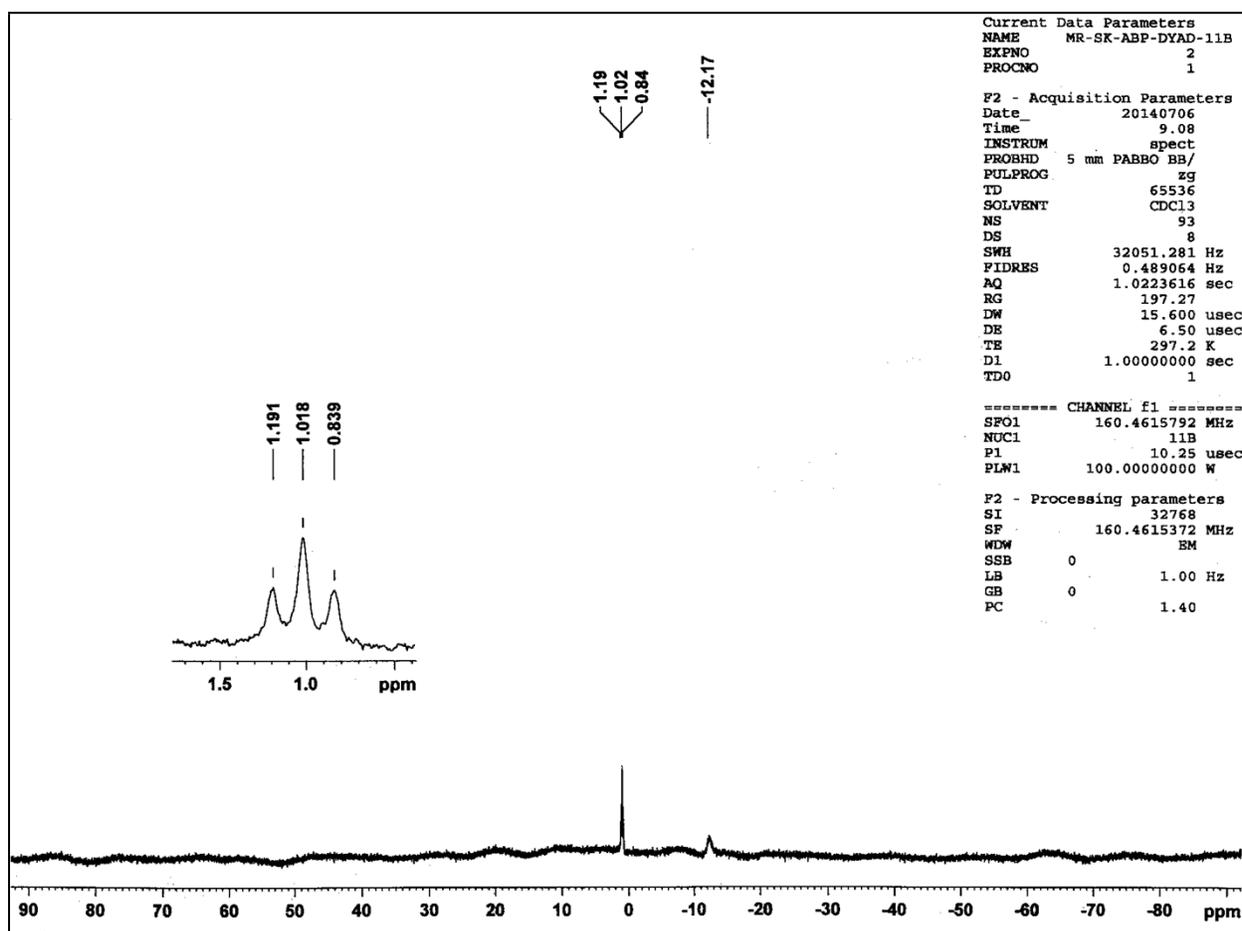
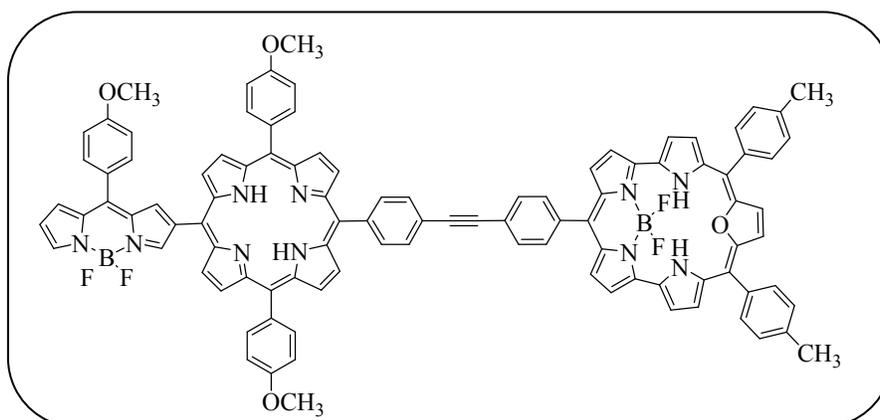


Figure S47: ^{11}B NMR spectrum of compound **8** recorded in CDCl_3 . Inset shows the expansion

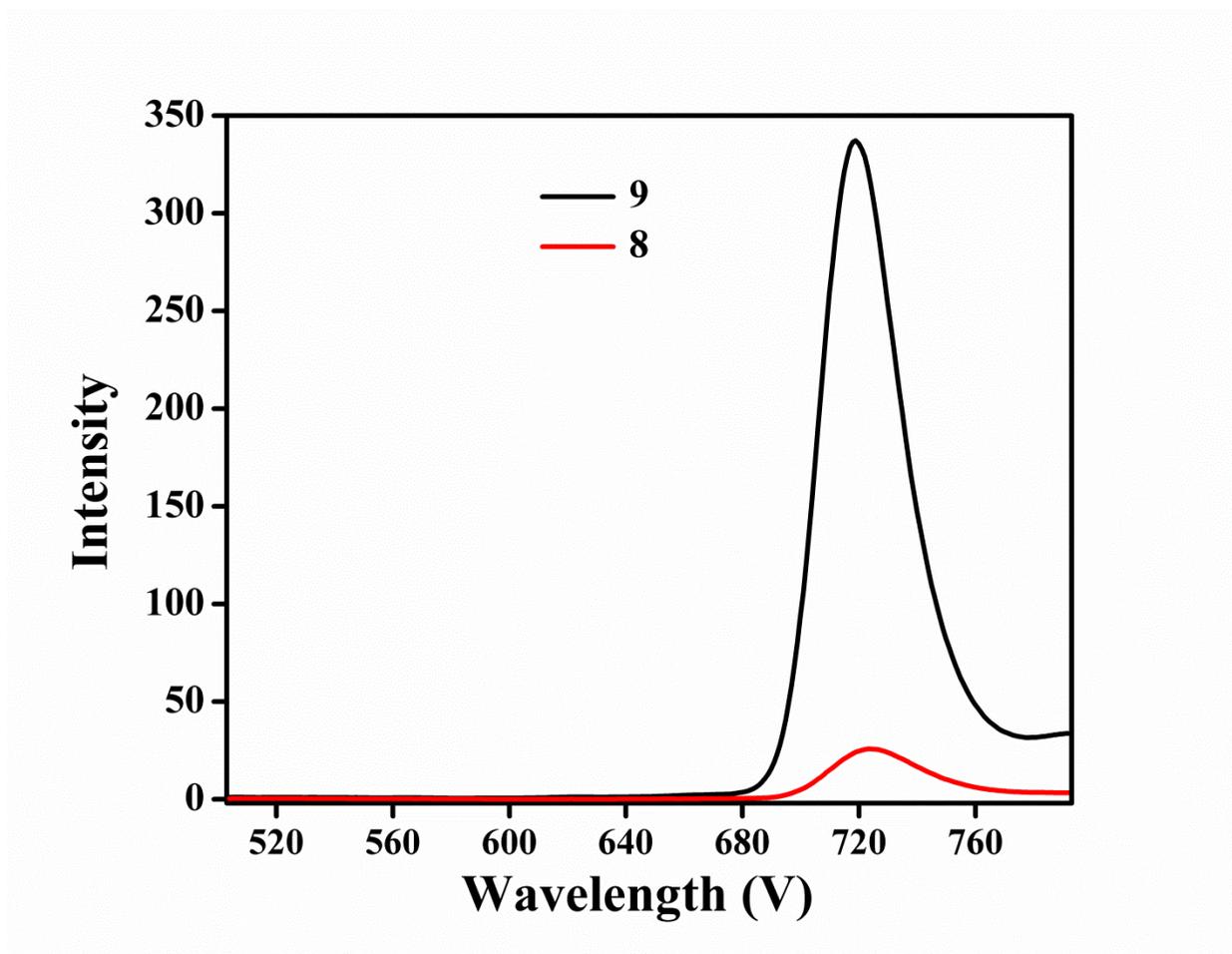


Figure S48: Comparison of Emission spectrum of compound **8** and compound **9** (5 μM) recorded in CHCl_3 solvents. Excitation wavelength used was 488 nm.