Electronic Supplementary Material (ESI) for Dalton Transactions

Synthesis, Structure, Spectral and Electrochemical Properties of $B(OR)_2$-Smaragdyrin Complexes

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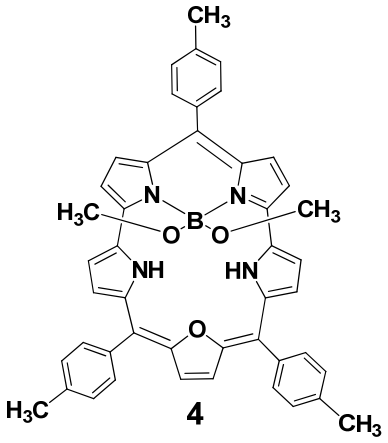

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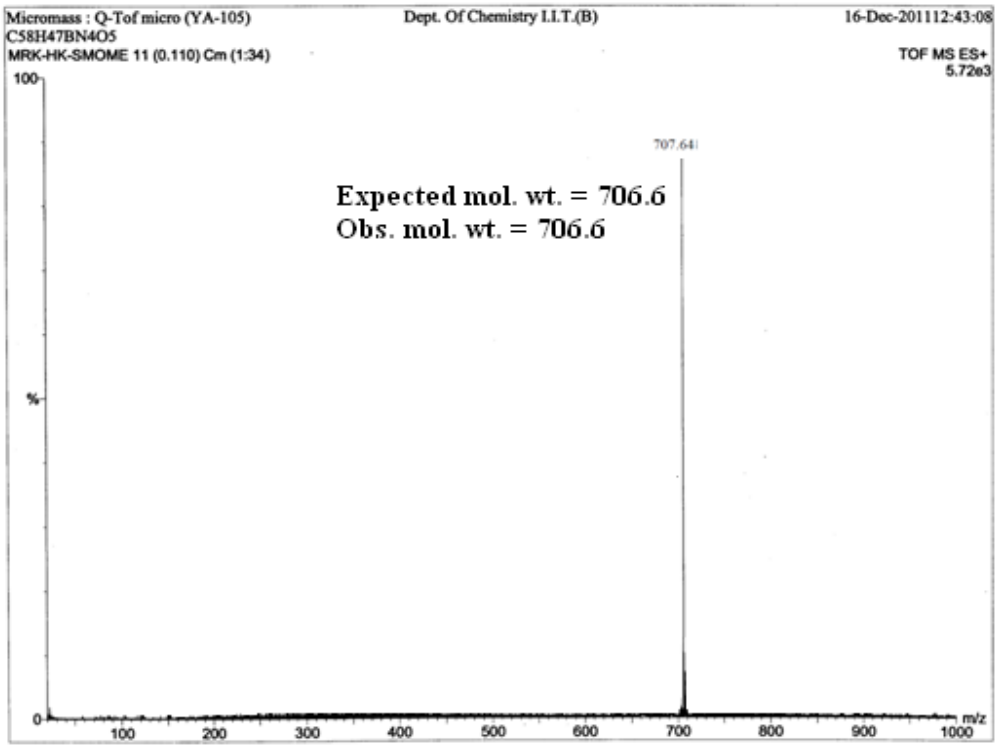
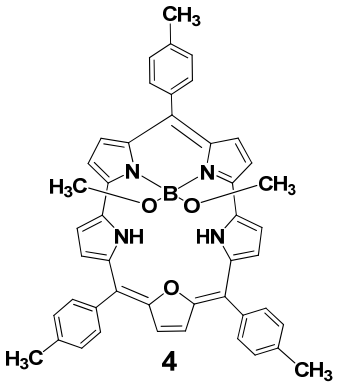


Figure S1. ES-MS spectrum of compound **4.**



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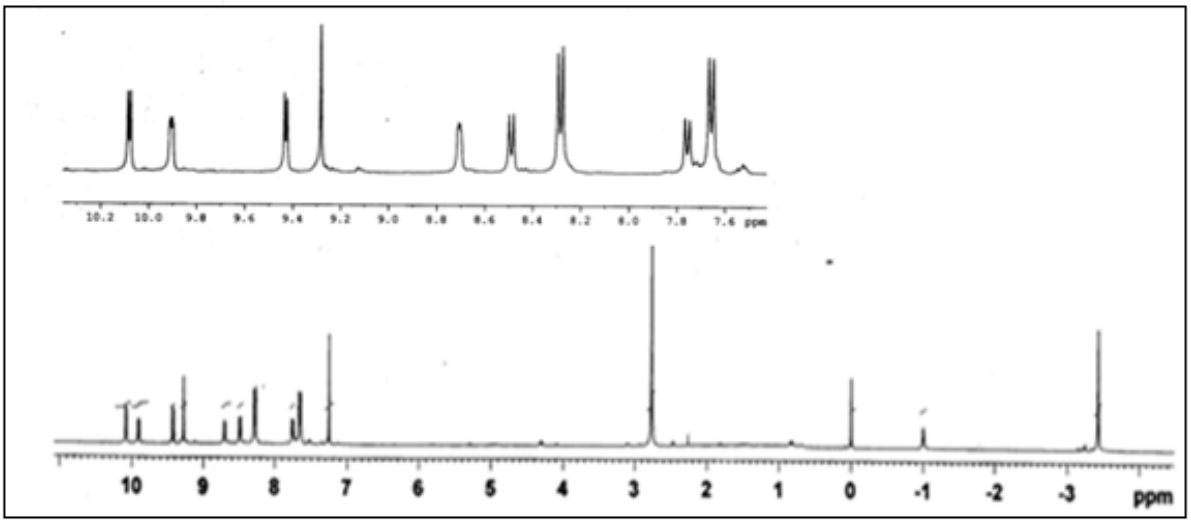


Figure S2. ^{1}H NMR spectrum of compound **4** recorded in $CDCl_3$**.**

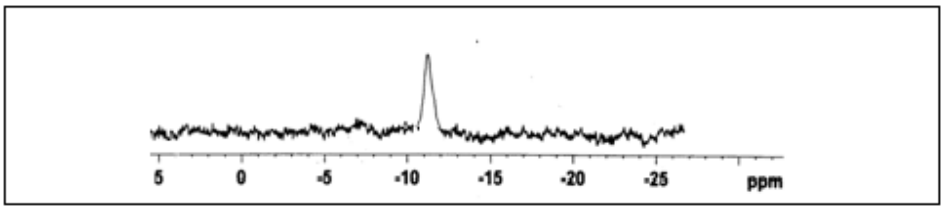


Figure S2. ^{11}B NMR spectrum of compound **4** recorded in $CDCl_3$**.**

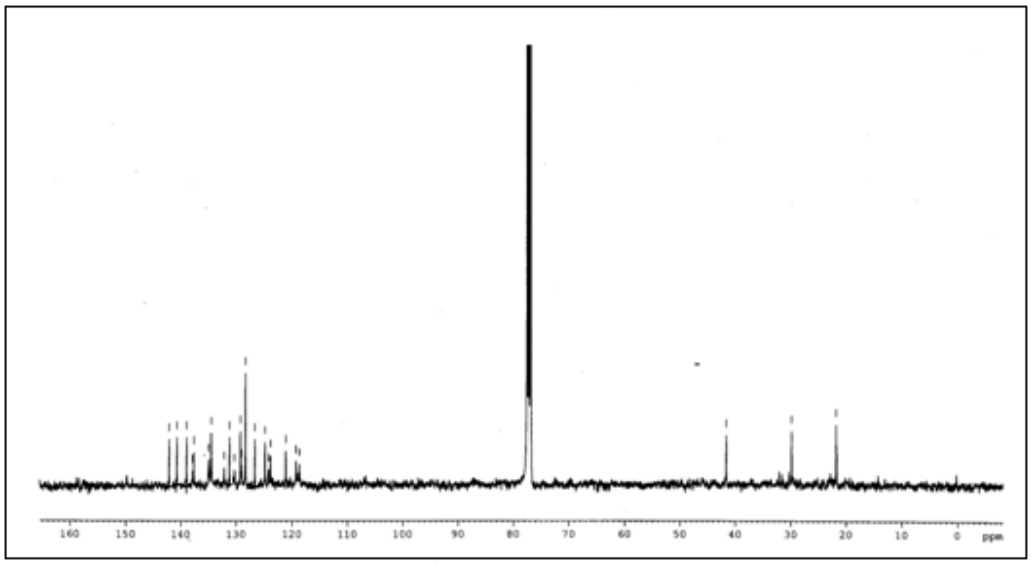
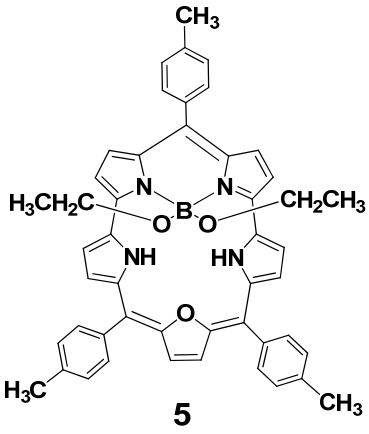


Figure S3. ^{13}C NMR spectrum of compound of **4** recorded in $CDCl_3$**.**



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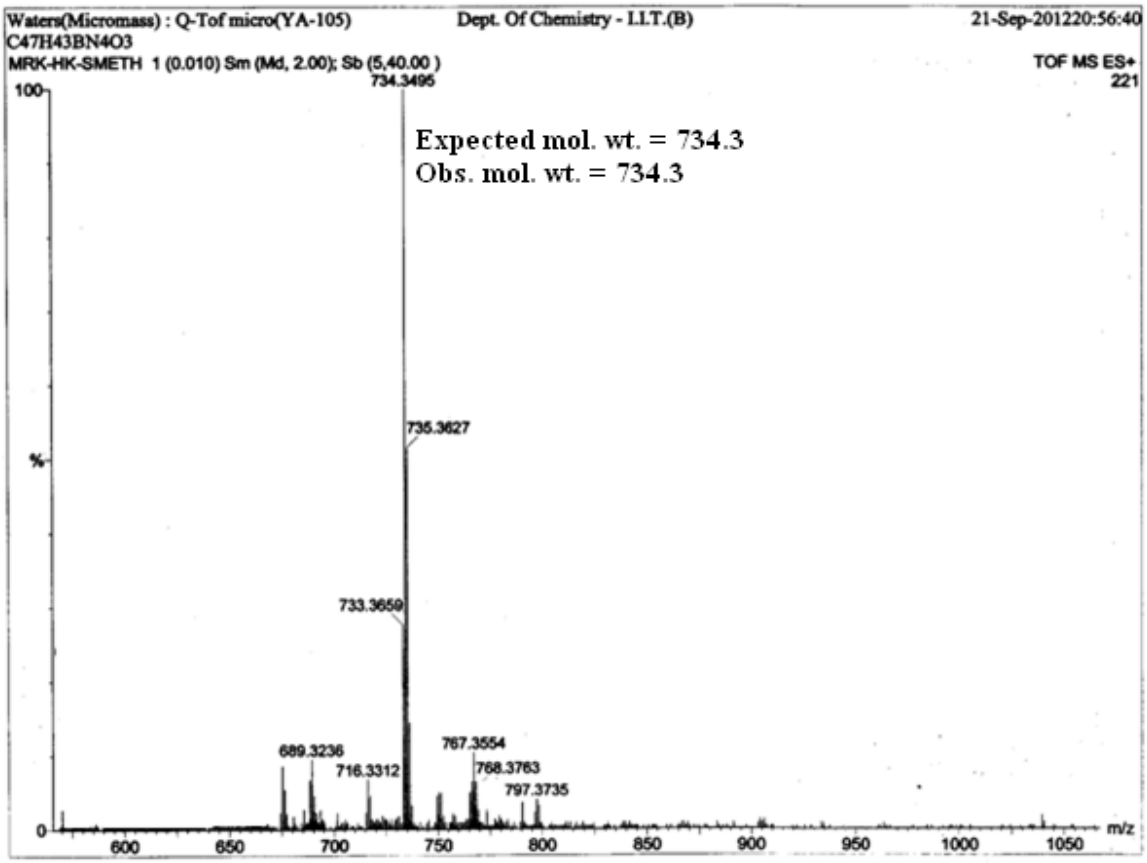
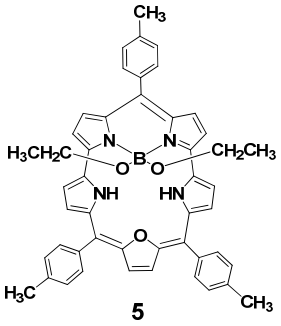


Figure S4. ES-MS spectrum of compound **5.**



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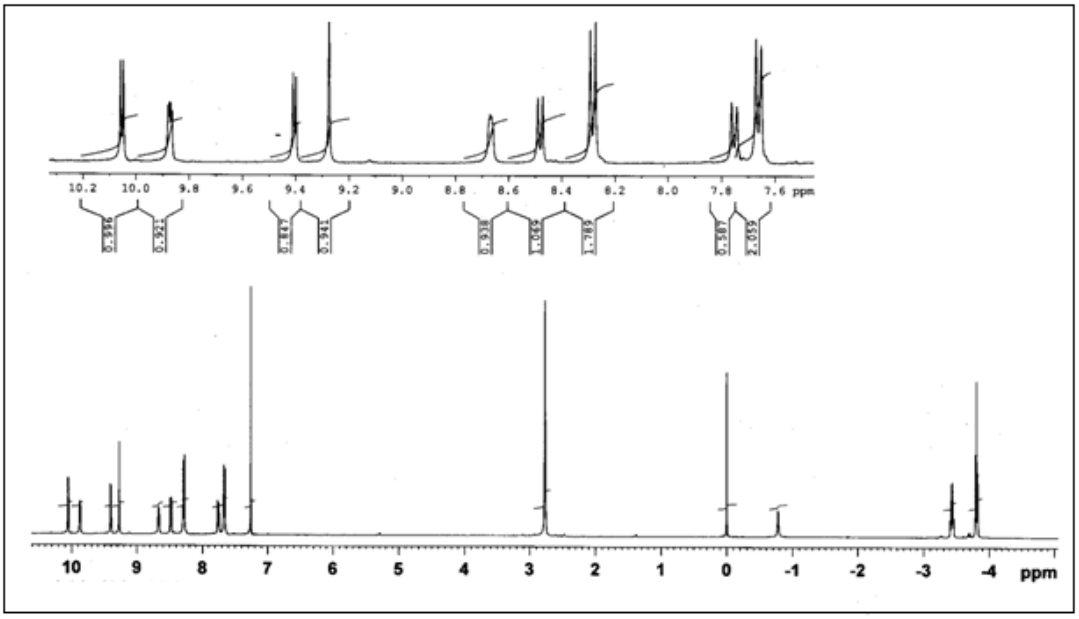


Figure S5. ^{1}H NMR spectrum of compound **5** recorded in $CDCl_3$**.**

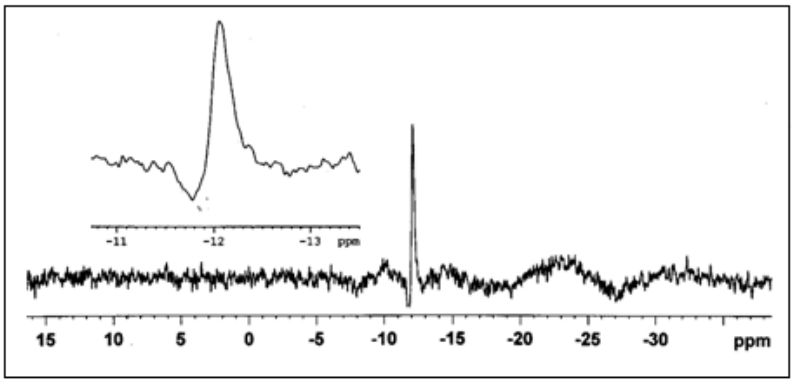


Figure S5. ^{11}B NMR spectrum of compound **5** recorded in $CDCl_3$**.**

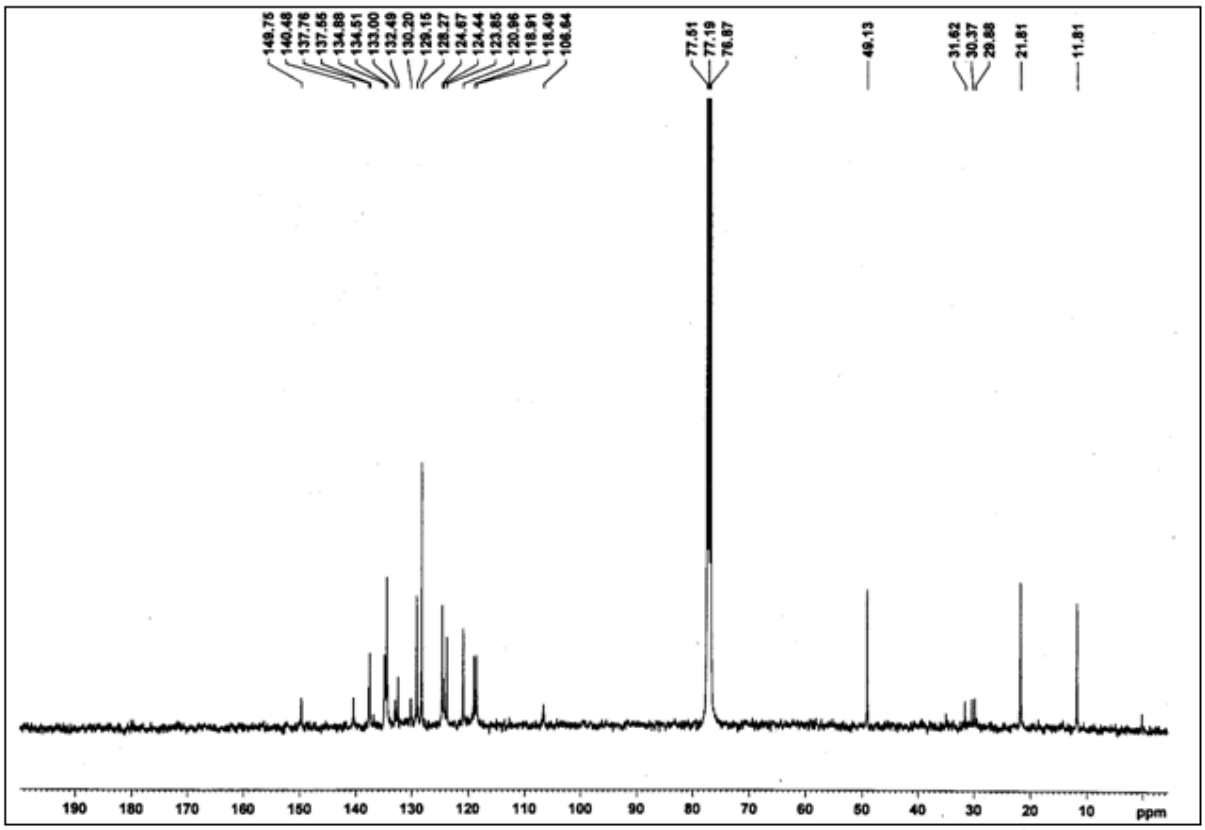
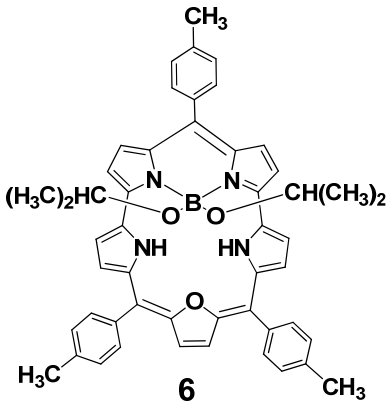


Figure S6. ^{13}C NMR spectrum of compound of **5** recorded in $CDCl_3$**.**



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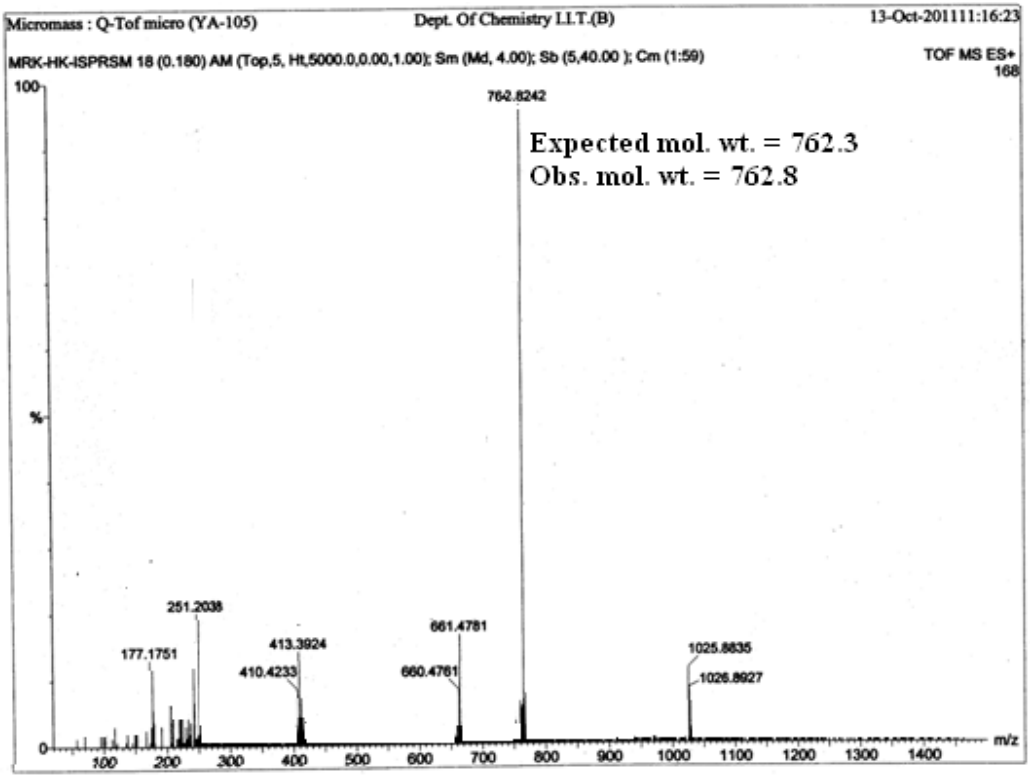
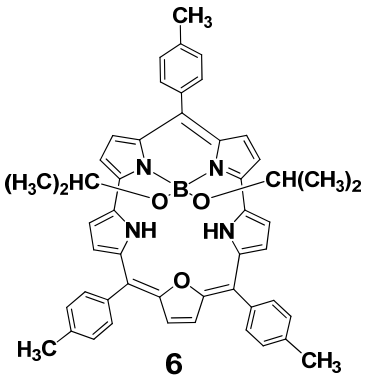


Figure S7. ES-MS spectrum of compound **6.**



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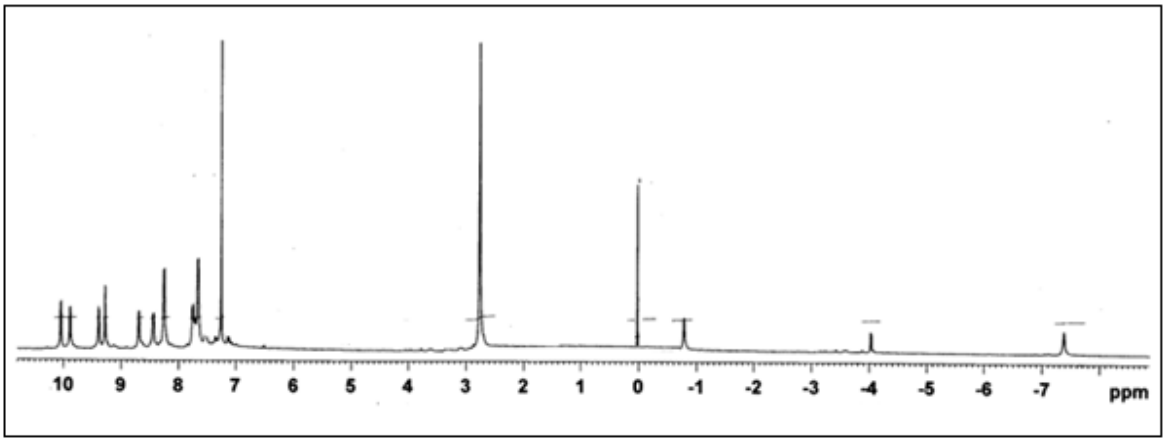


Figure S8. ^{1}H NMR spectrum of compound **6** recorded in $CDCl_3$**.**

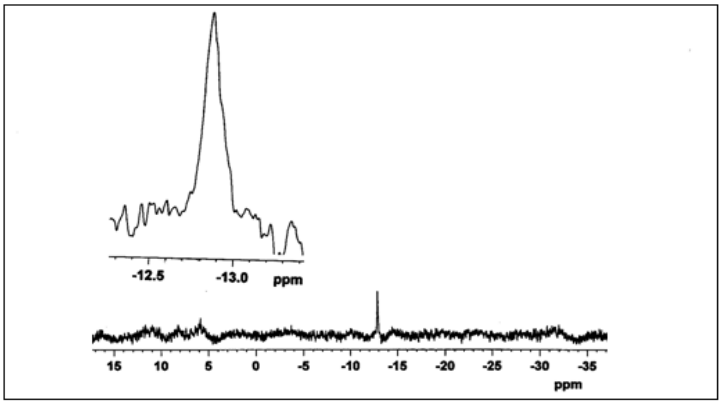


Figure S8. ^{11}B NMR spectrum of compound **6** recorded in $CDCl_3$**.**

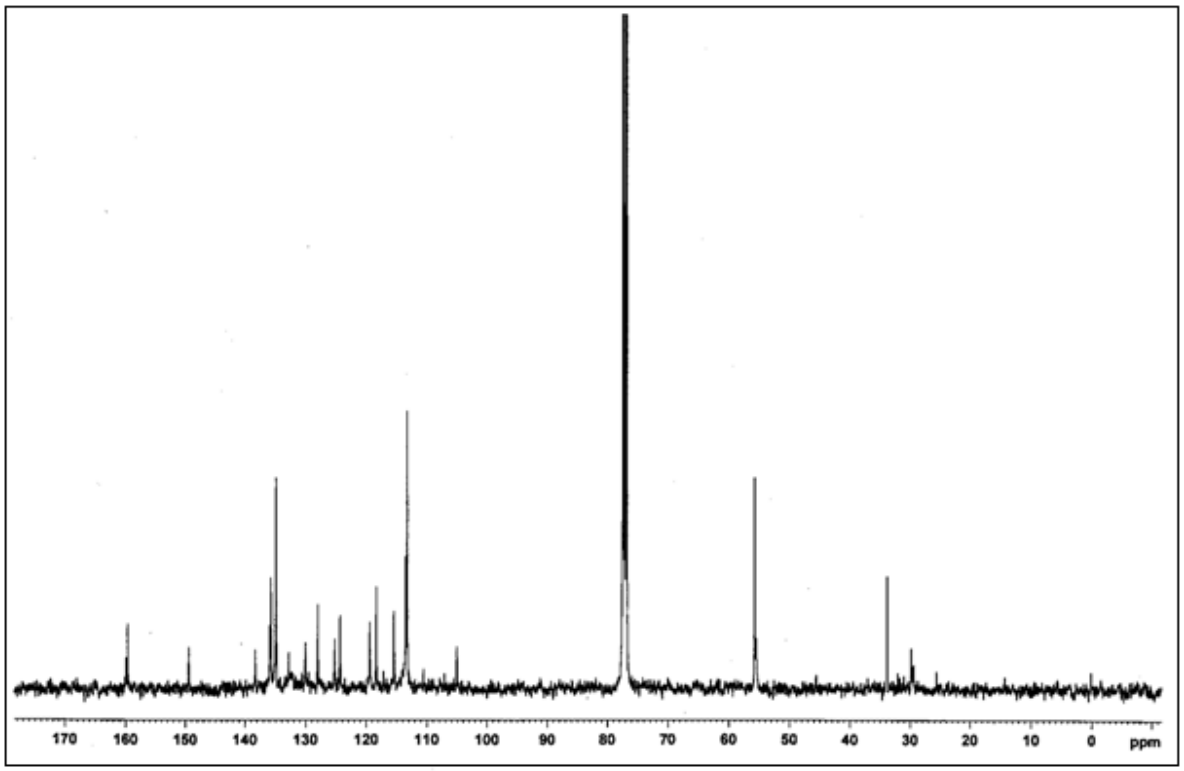
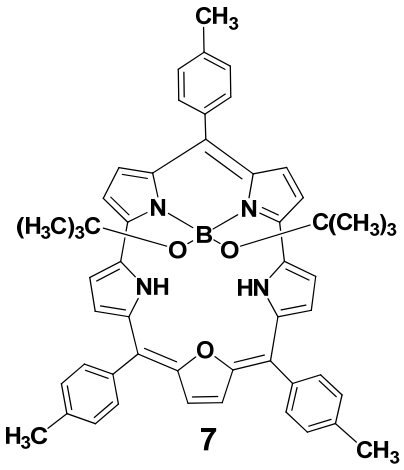


Figure S9. ^{13}C NMR spectrum of compound of **6** recorded in $CDCl_3$**.**



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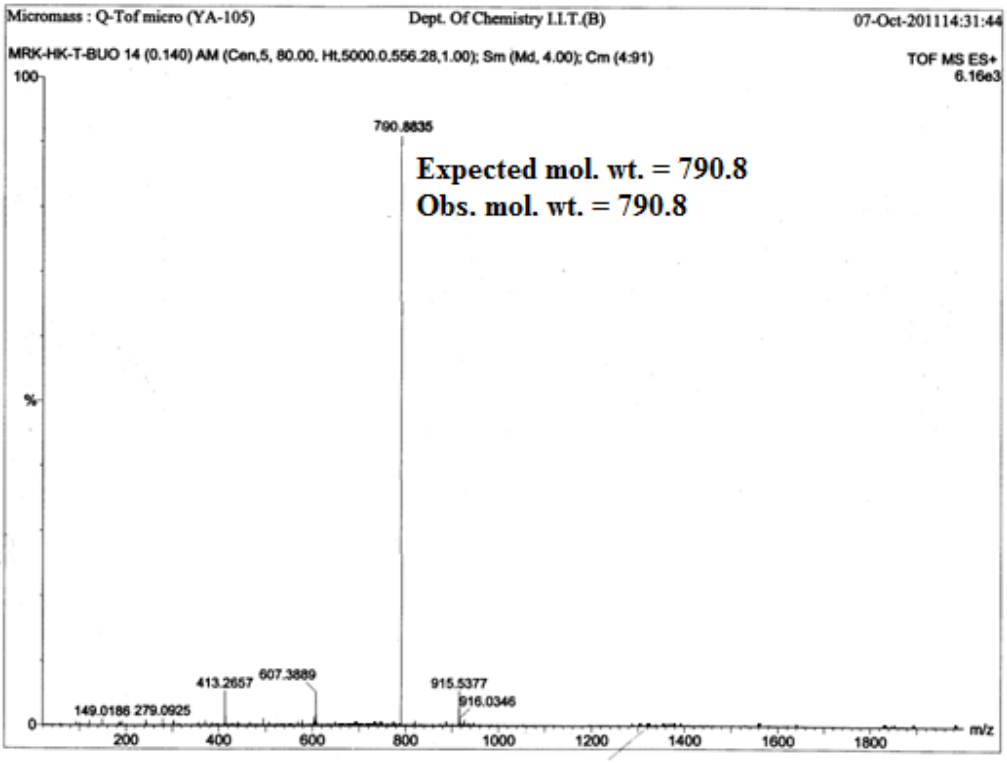
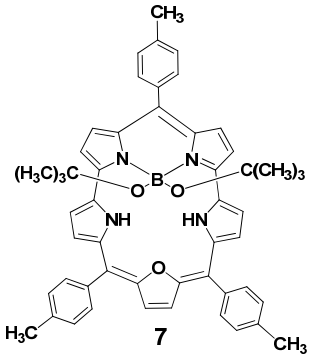


Figure S10. ES-MS spectrum of compound **7.**



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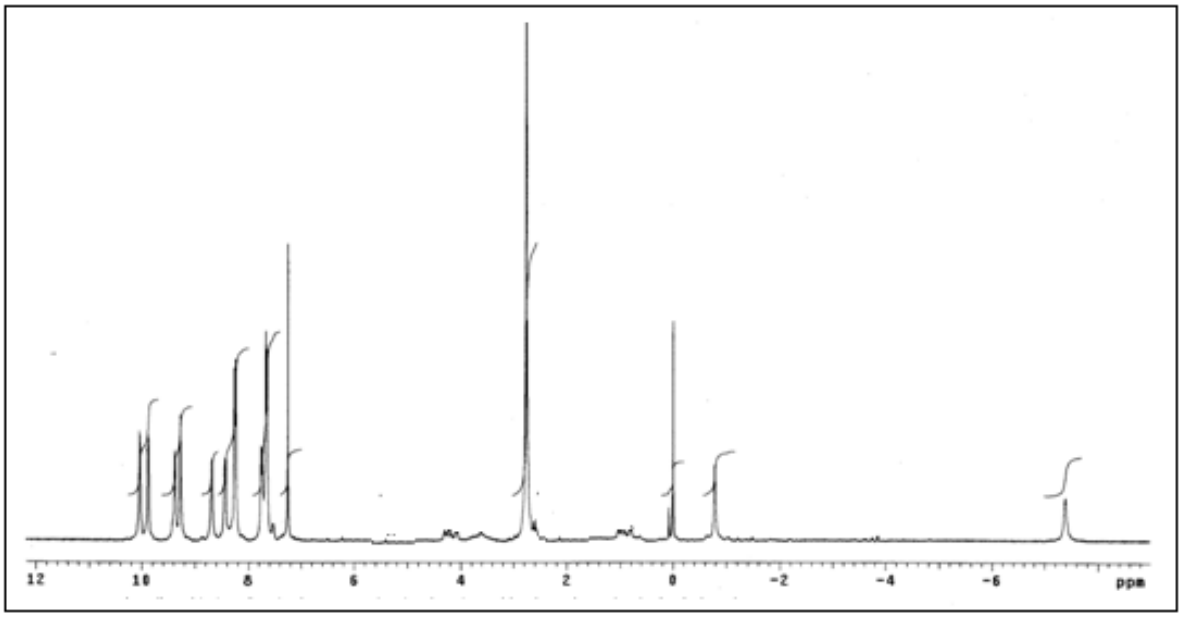


Figure S11. ^{1}H NMR spectrum of compound **7** recorded in $CDCl_3$**.**

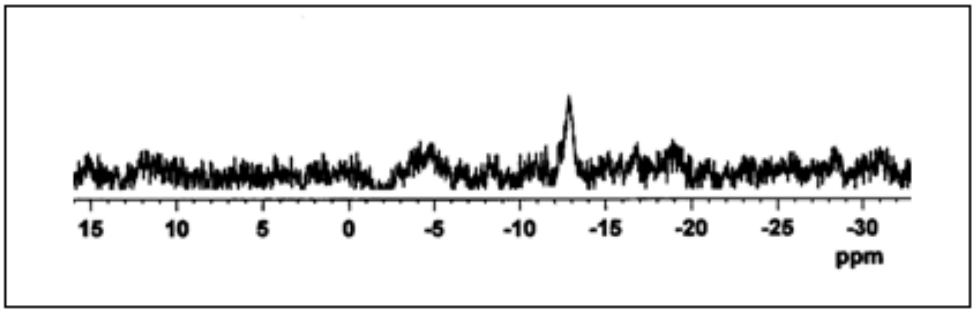


Figure S11. ^{11}B NMR spectrum of compound **7** recorded in $CDCl_3$**.**

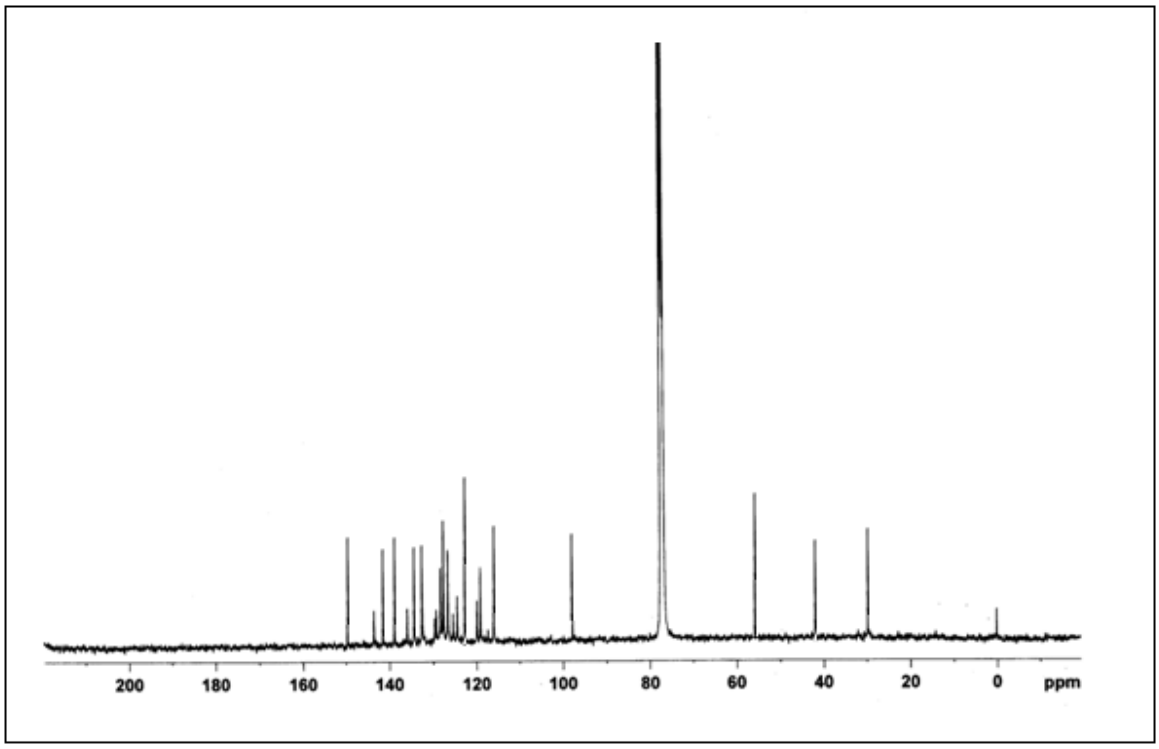
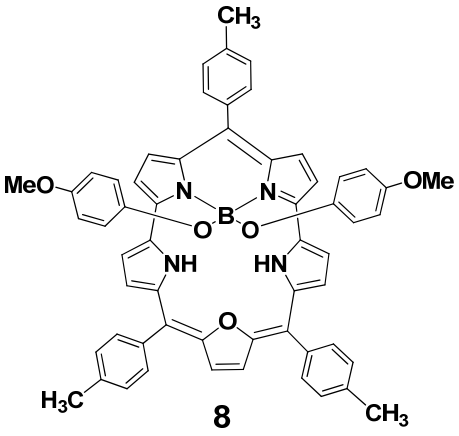


Figure S12. ^{13}C NMR spectrum of compound of **7** recorded in $CDCl_3$**.**



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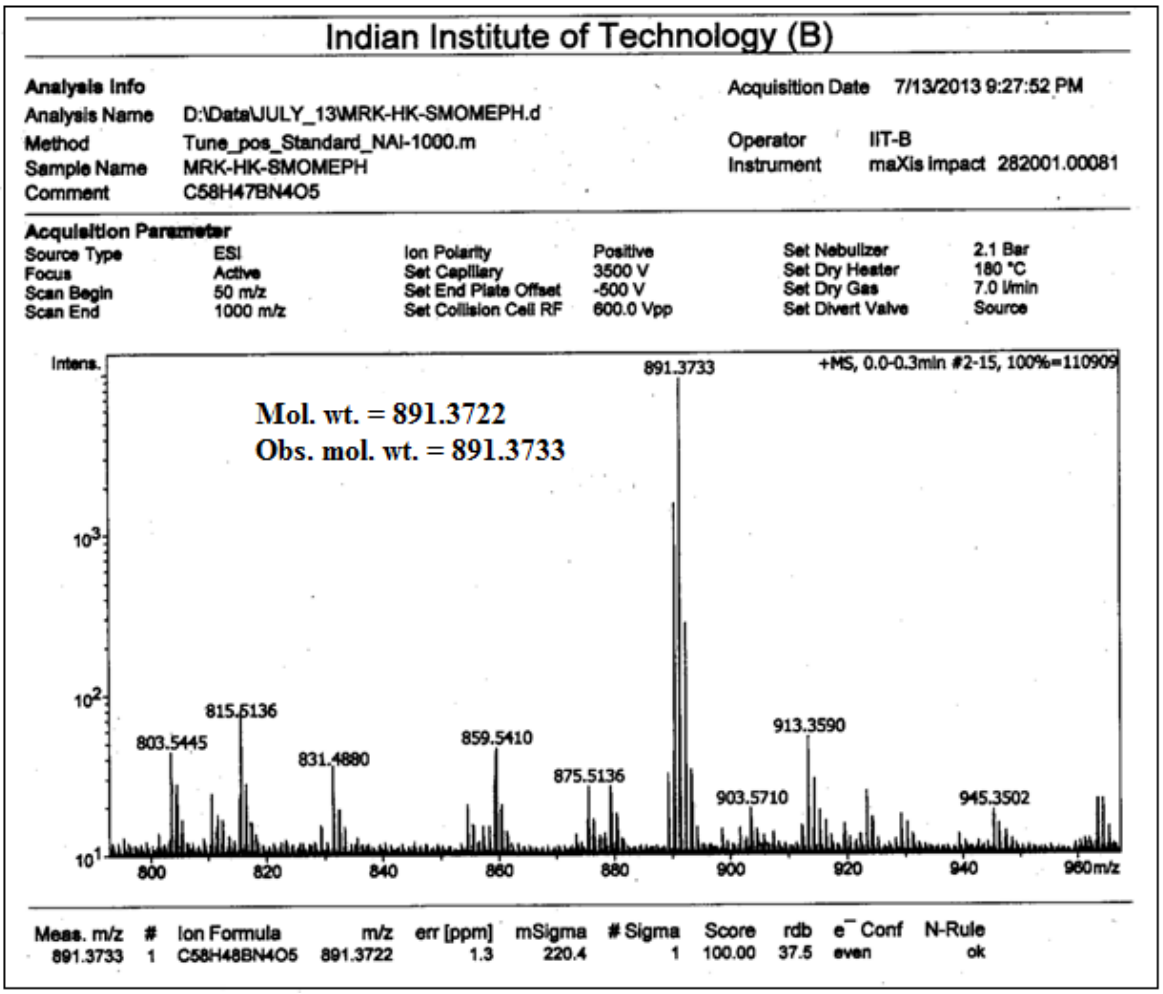
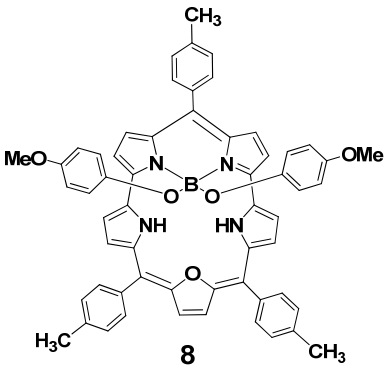


Figure S13. HR-MS spectrum of compound **8.**



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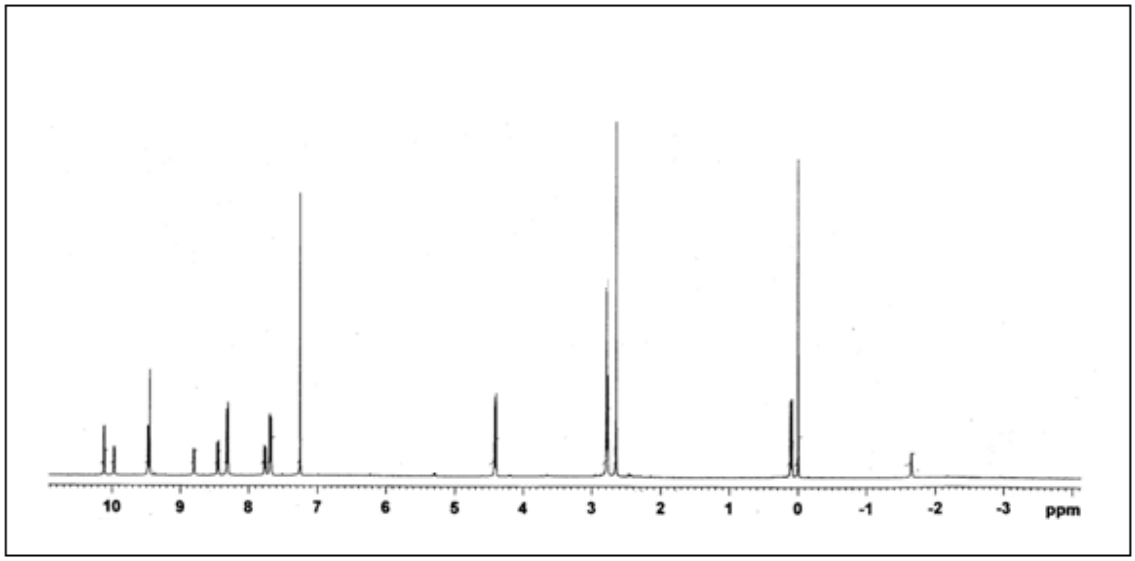


Figure S14. ^{1}H NMR spectrum of compound **8** recorded in $CDCl_3$**.**

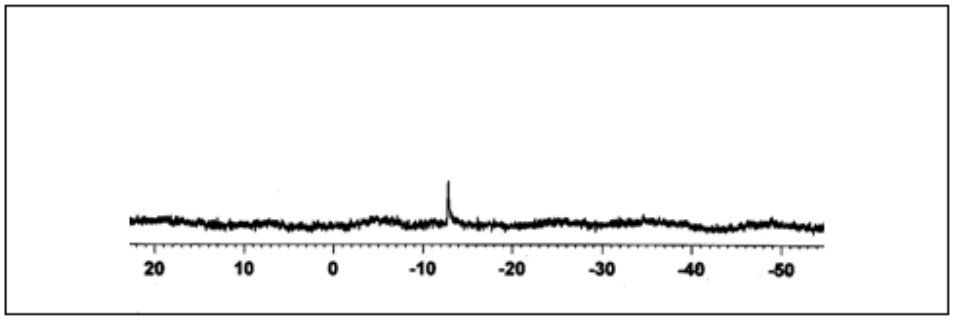


Figure S14. ^{11}B NMR spectrum of compound **8** recorded in $CDCl_3$**.**

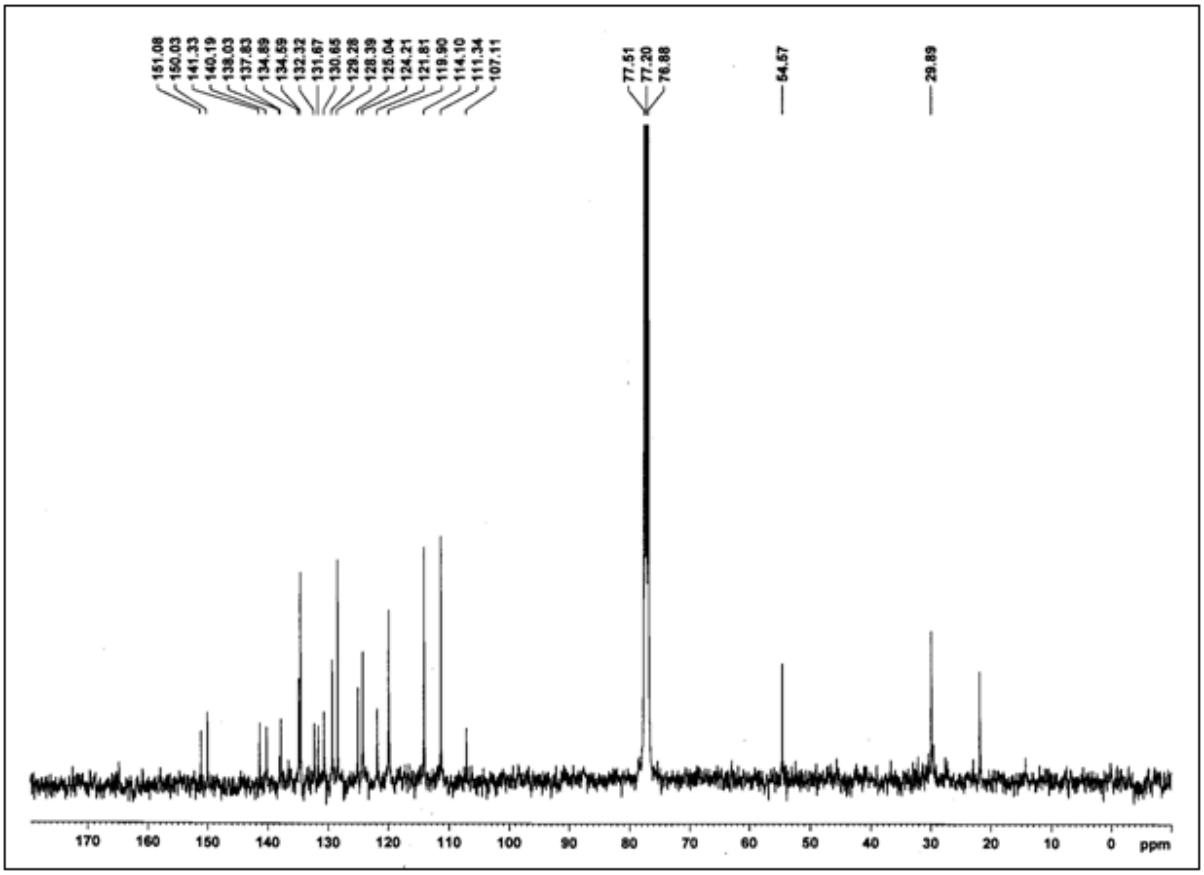
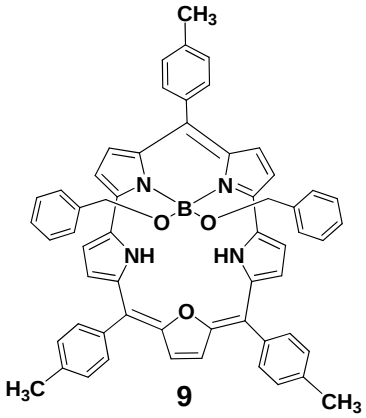


Figure S15. ^{13}C NMR spectrum of compound of **8** recorded in $CDCl_3$**.**



9

Mol. wt. = 858.3741

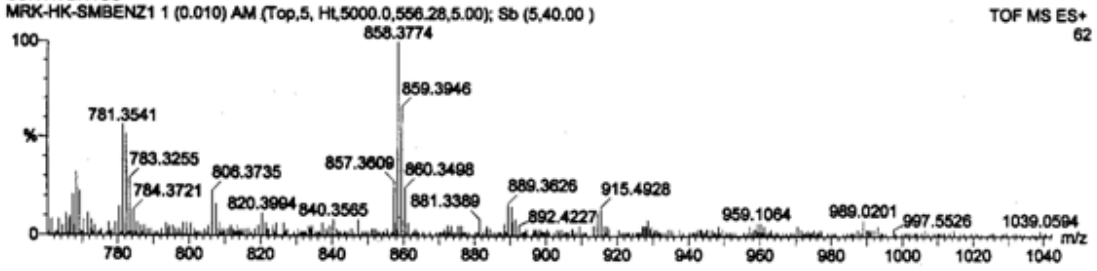
Obs. mol. wt. 858.3774

Elemental Composition Report

Single Mass Analysis (displaying only valid results)
Tolerance = 50.0 PPM / DBE: min = -1.5, max = 200.0
Isotope cluster parameters: Separation = 1.0 Abundance = 1.0%

Monoisotopic Mass, Odd and Even Electron Ions
10 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)

Waters(Micromass) : Q-Tof micro(YA-105) Dept. Of Chemistry - I.I.T.(B) 21-Sep-201219:38:46
C57H47BN4O3
MRK-HK-SMBENZ1 1 (0.010) AM (Top,5, Ht,5000.0,556.28,5.00); Sb (5,40.00) TOF MS ES+
62



Minimum:				-1.5		
Maximum:		200.0	50.0	200.0		
Mass	Calc. Mass	mDa	PPM	DBE	Score	Formula
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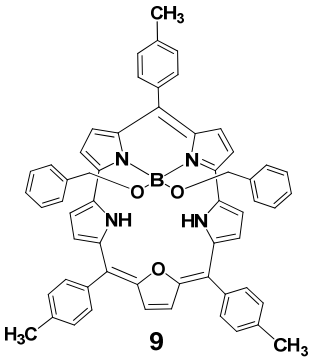
Figure S16. HR-MS spectrum of compound **9.**



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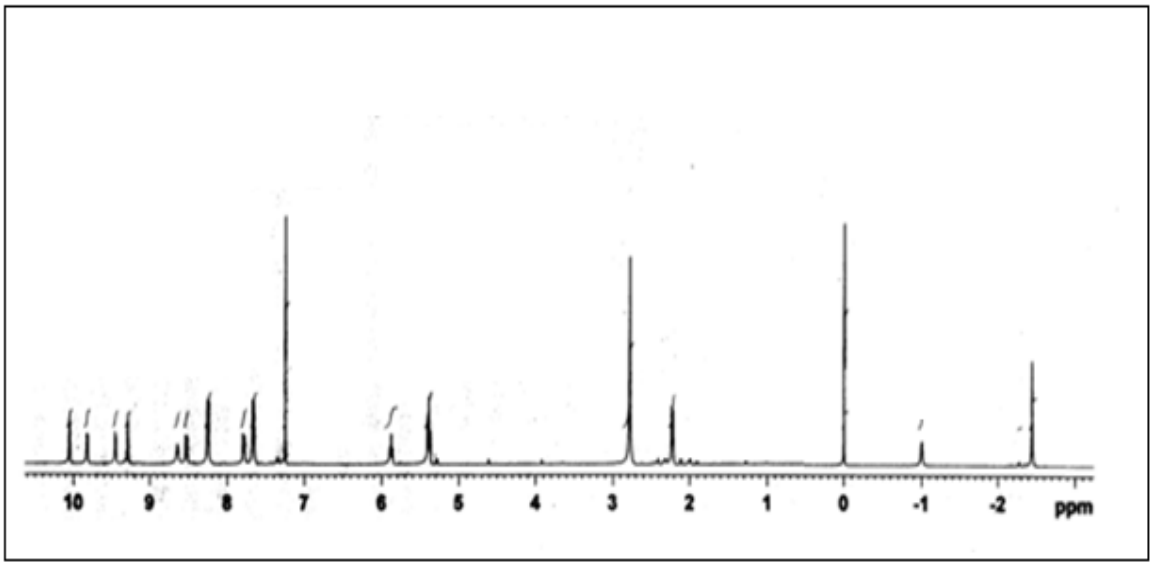


Figure S17. ^{1}H NMR spectrum of compound **9** recorded in $CDCl_3$**.**

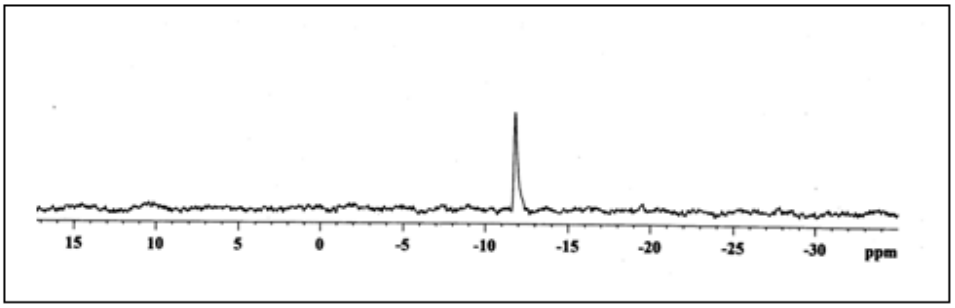


Figure S17. ^{11}B NMR spectrum of compound **9** recorded in $CDCl_3$**.**

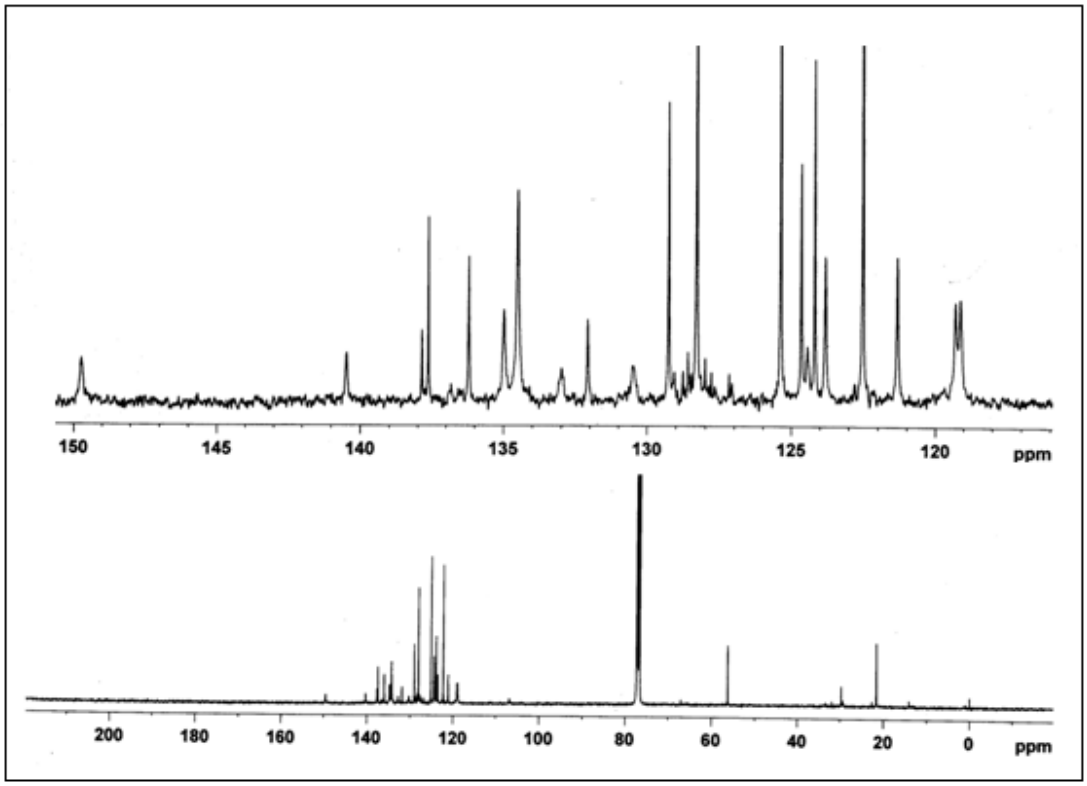
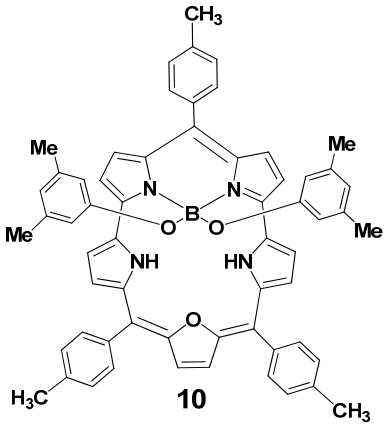


Figure S18. ^{13}C NMR spectrum of compound of **9** recorded in $CDCl_3$**.**



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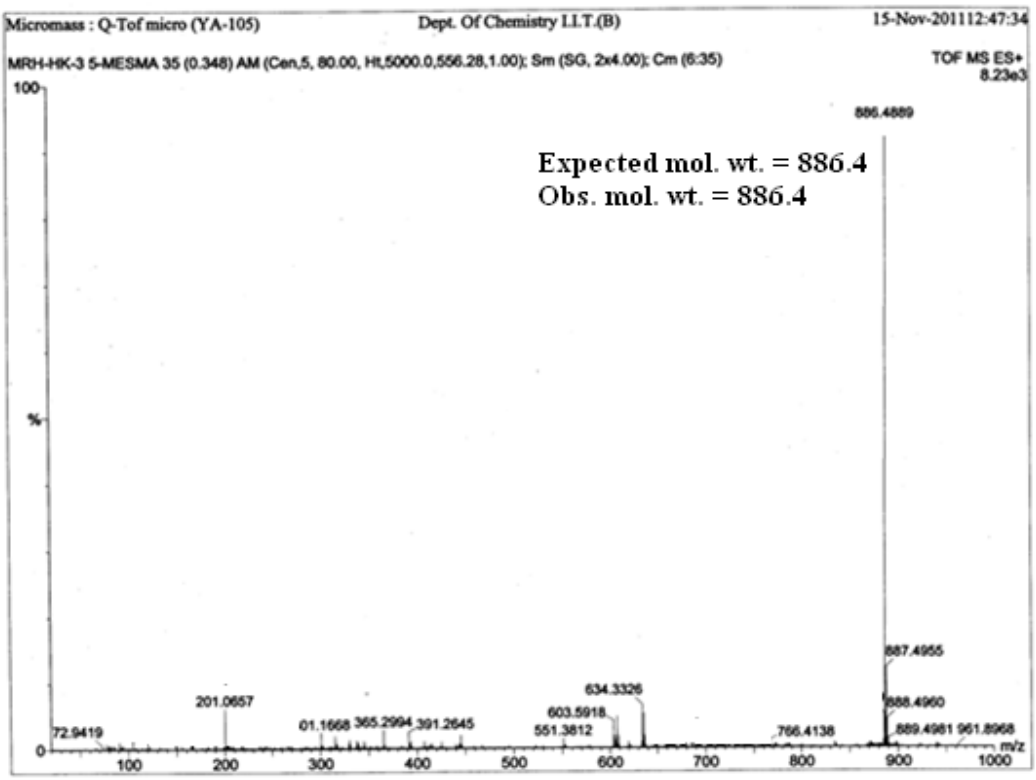
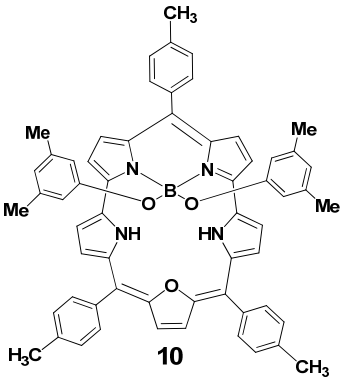


Figure S19. ES-MS spectrum of compound **10.**



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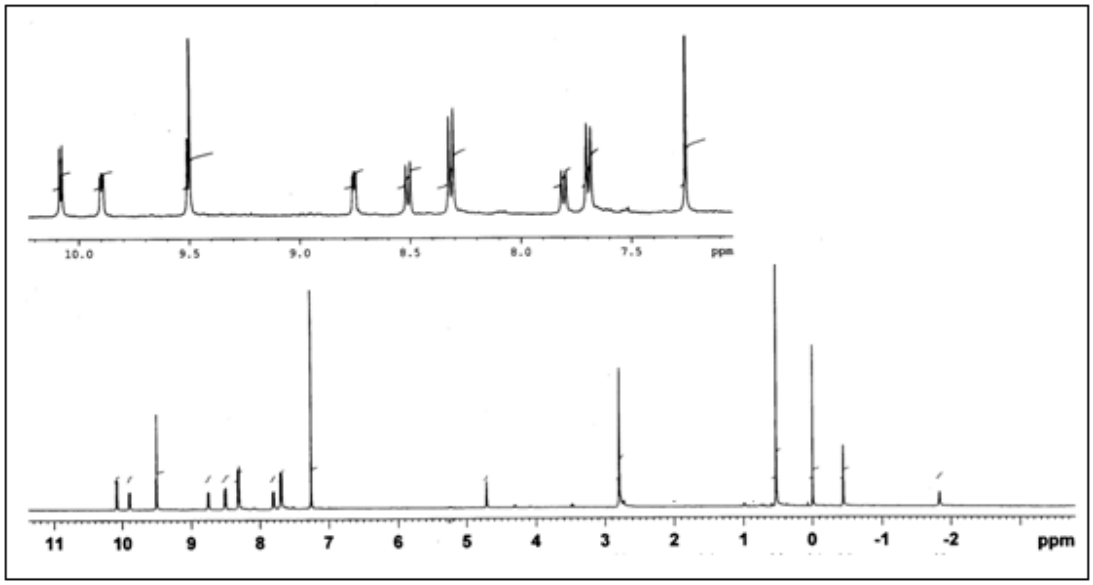


Figure S20. ^{1}H NMR spectrum of compound **10** recorded in $CDCl_3$**.**

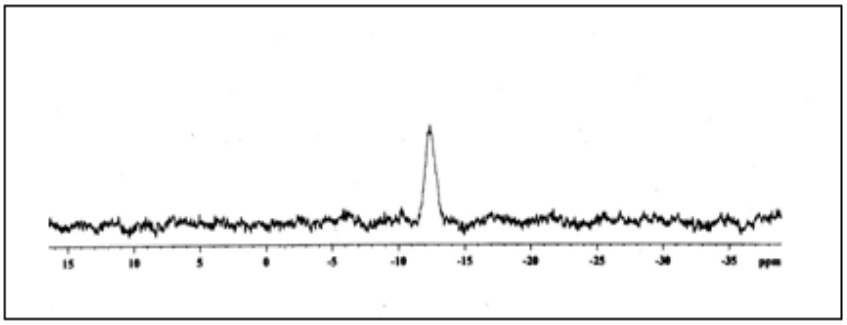


Figure S20. ^{11}B NMR spectrum of compound **10** recorded in $CDCl_3$**.**

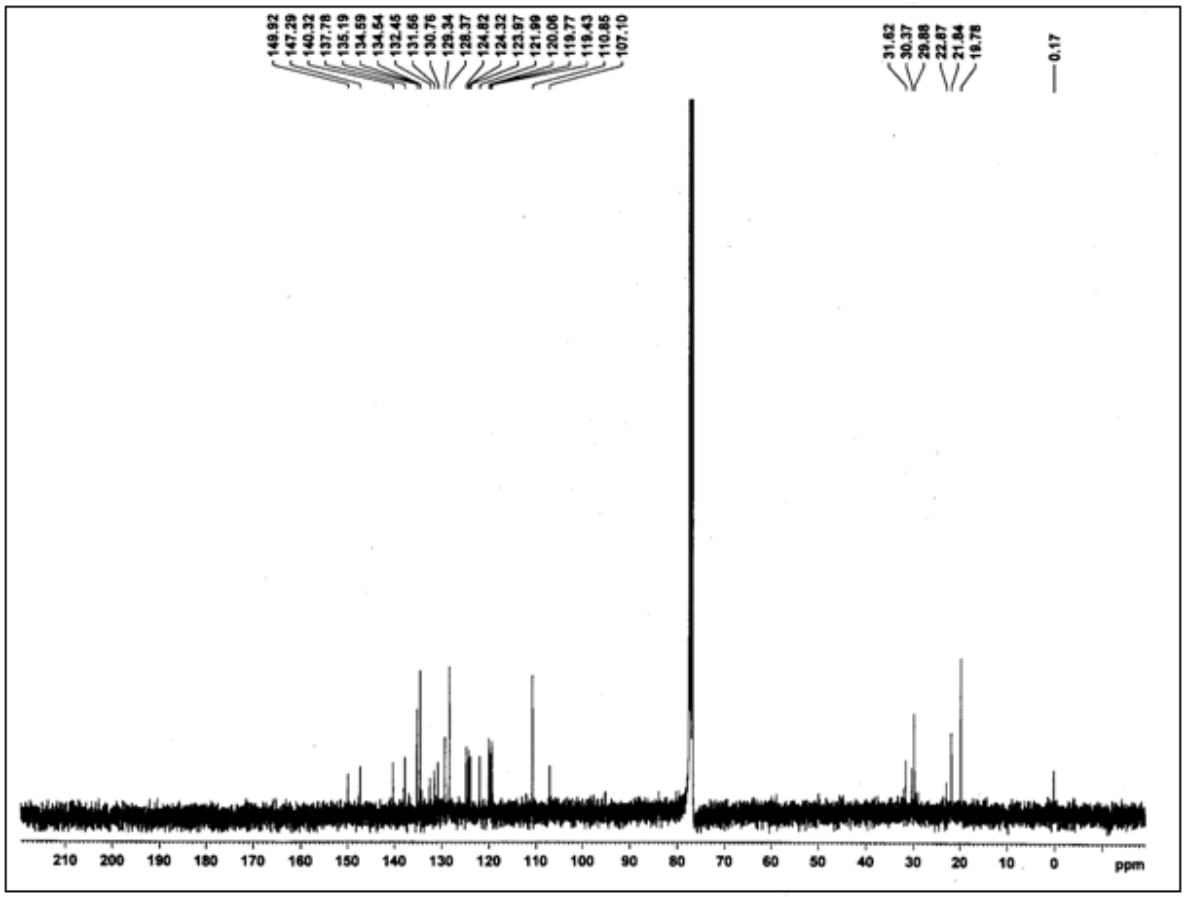
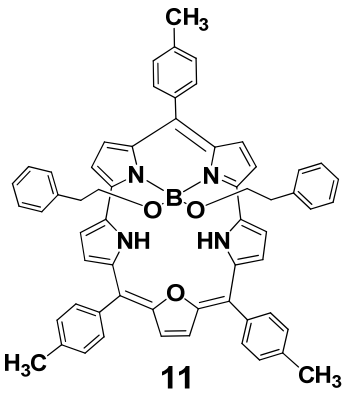


Figure S21. ^{13}C NMR spectrum of compound of **10** recorded in $CDCl_3$**.**



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Mol. wt. = 886.4054

Obs. mol. wt. = 886.4056

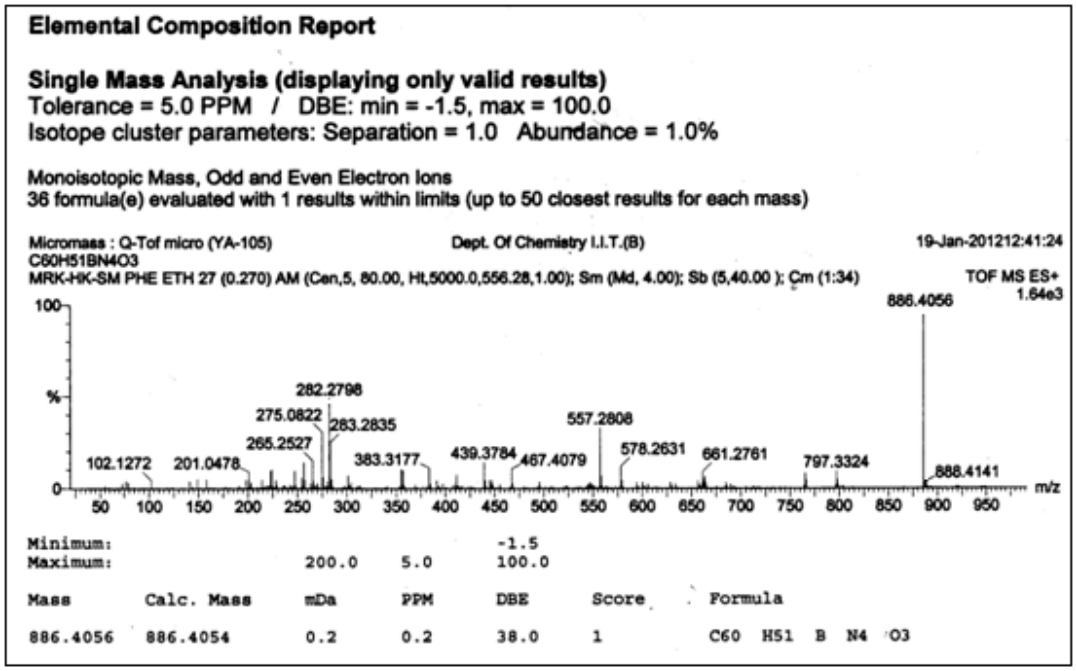
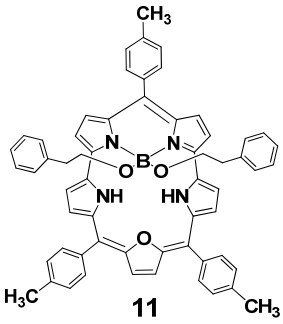


Figure S22. HR-MS spectrum of compound **11.**



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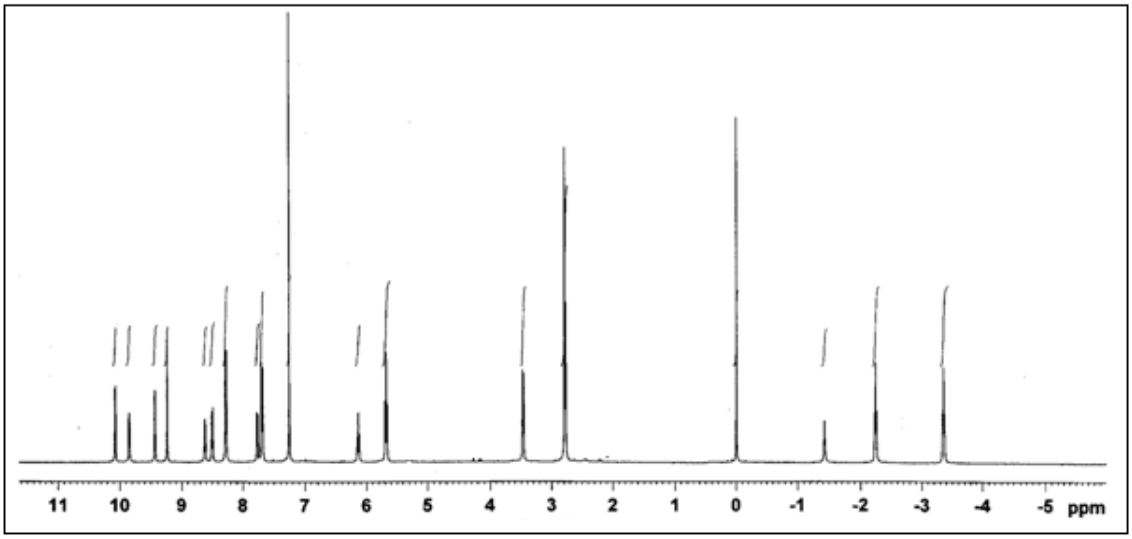


Figure S23. ^{1}H NMR spectrum of compound **11** recorded in $CDCl_3$**.**

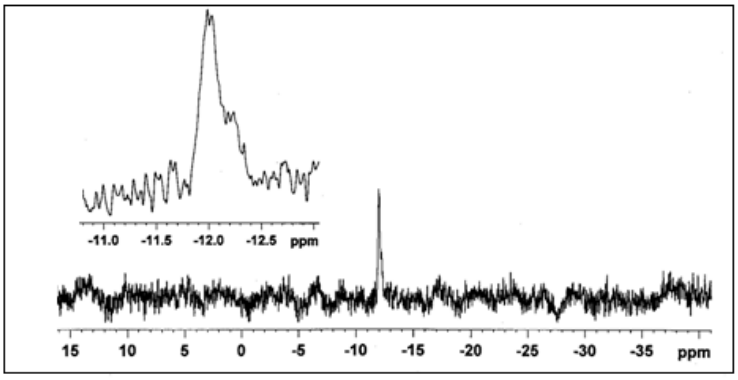


Figure S23. ^{11}B NMR spectrum of compound **11** recorded in $CDCl_3$**.**

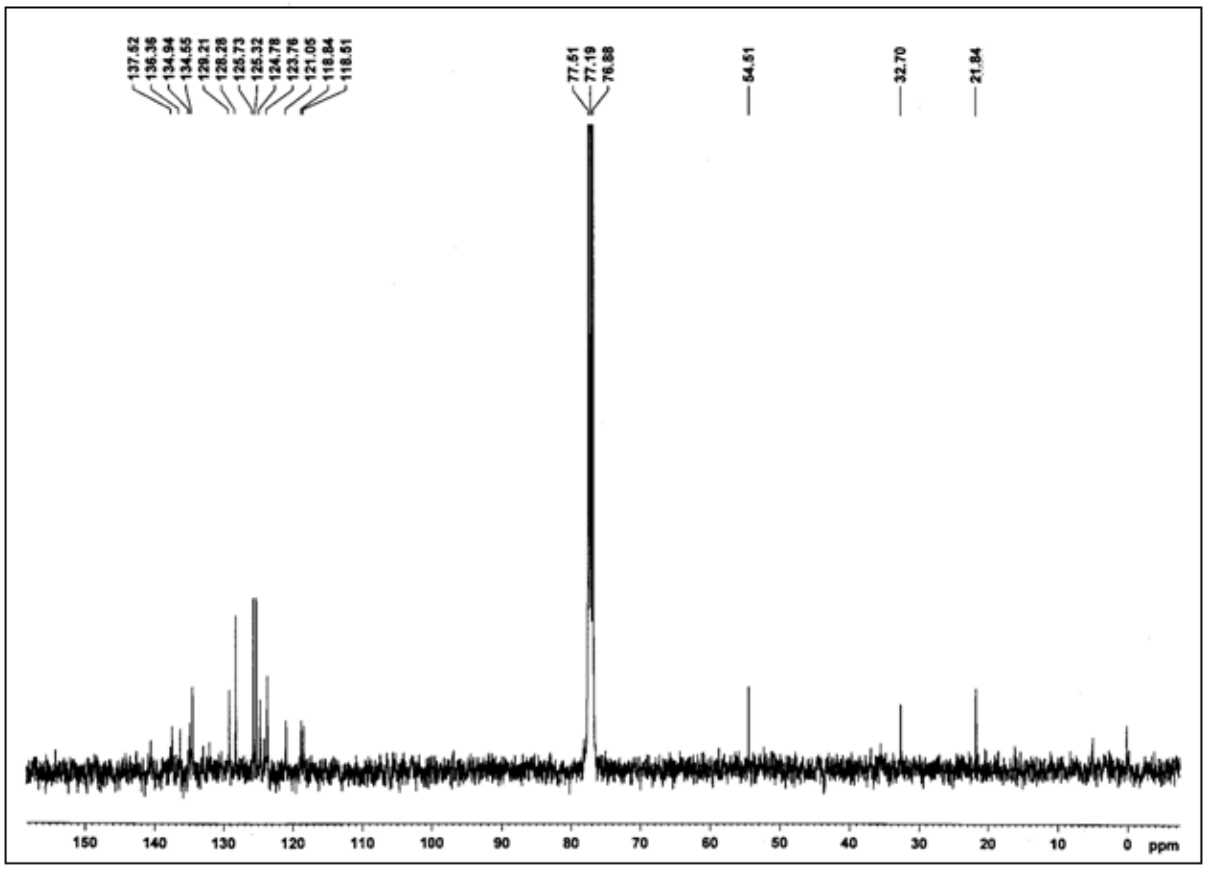
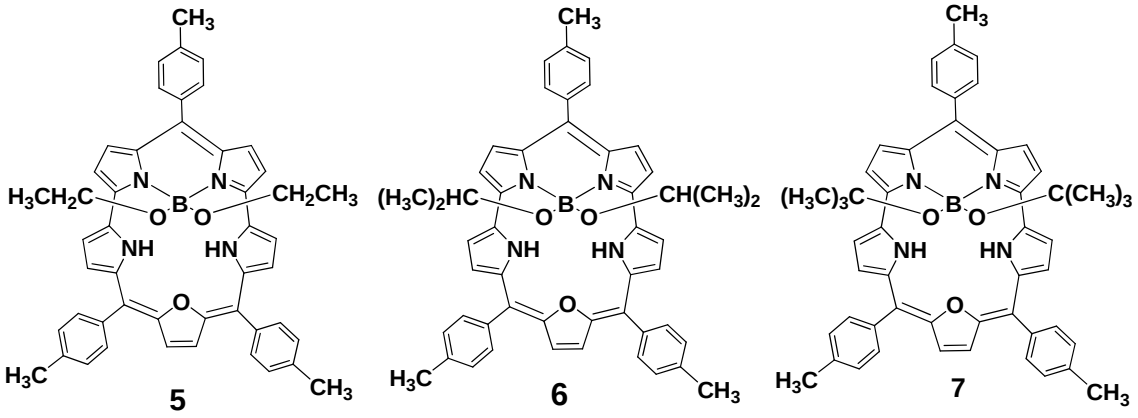


Figure S24. ^{13}C NMR spectrum of compound of **11** recorded in $CDCl_3$**.**



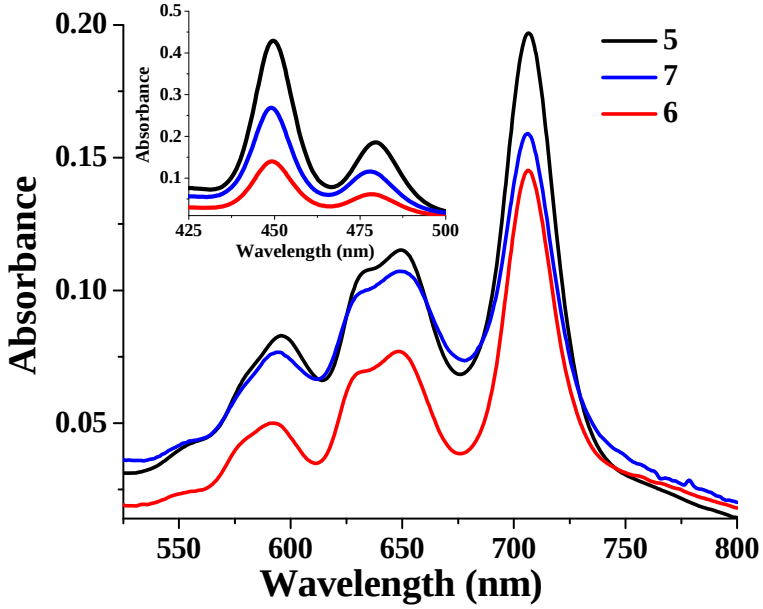


Figure S25. Q-bands absorption spectra of compounds of **5-7** recorded in $CHCl_3$. The inset shows the corresponding Soret bands. The concentrations were used 10^{-5} M and 10^{-6} M for Q and Soret bands respectively.

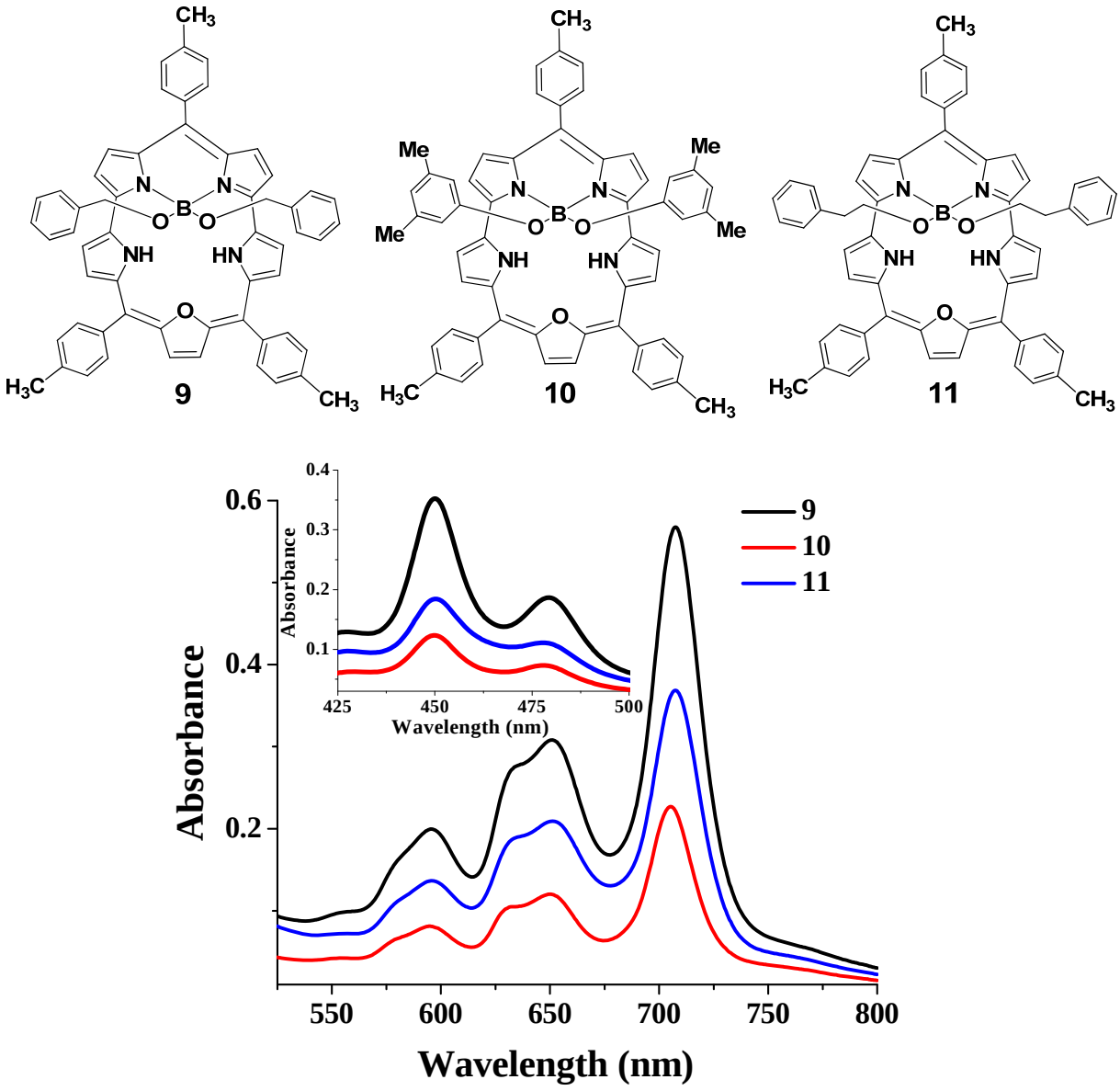


Figure S26. Q-bands absorption spectra of compounds of **9-11** recorded in $CHCl_3$. The inset shows the corresponding Soret bands. The concentrations were used 10^{-5} M and 10^{-6} M for Q and Soret bands respectively.

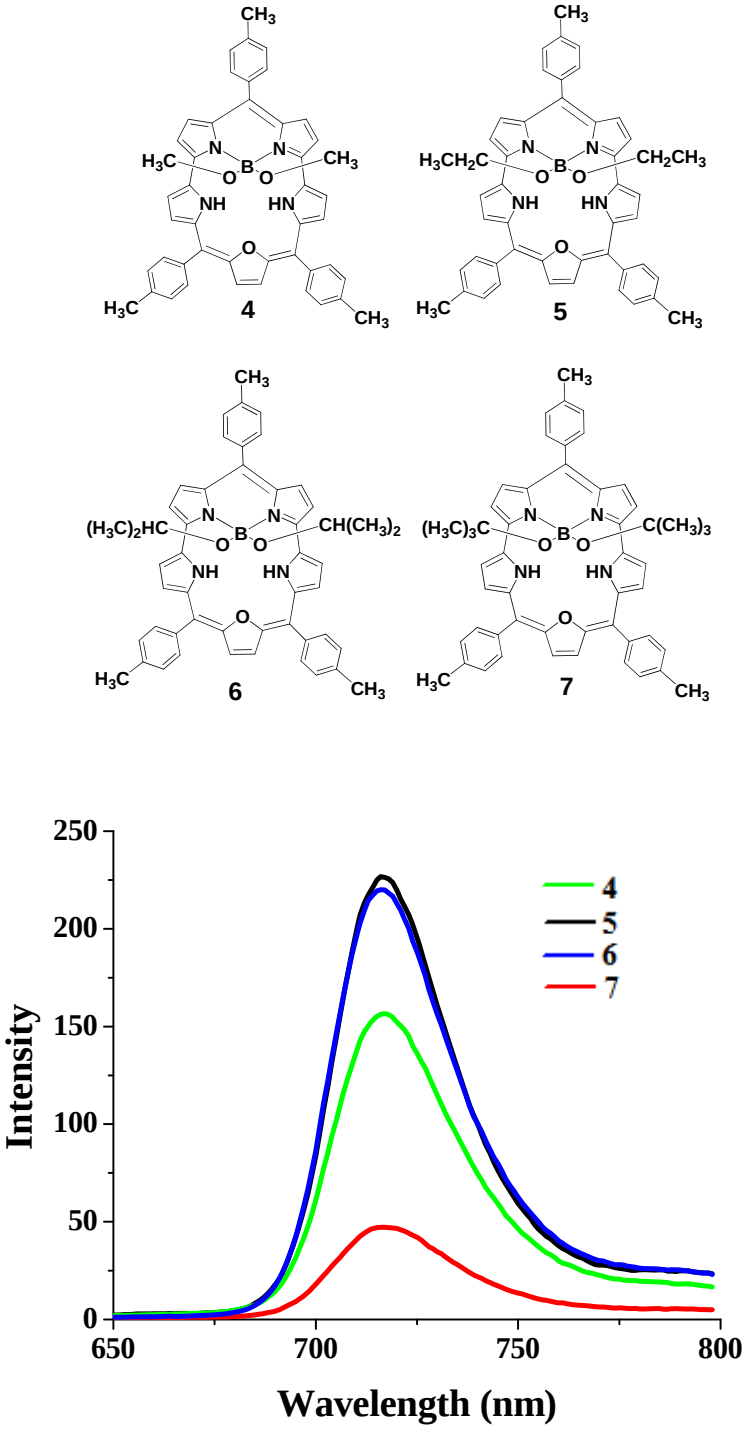
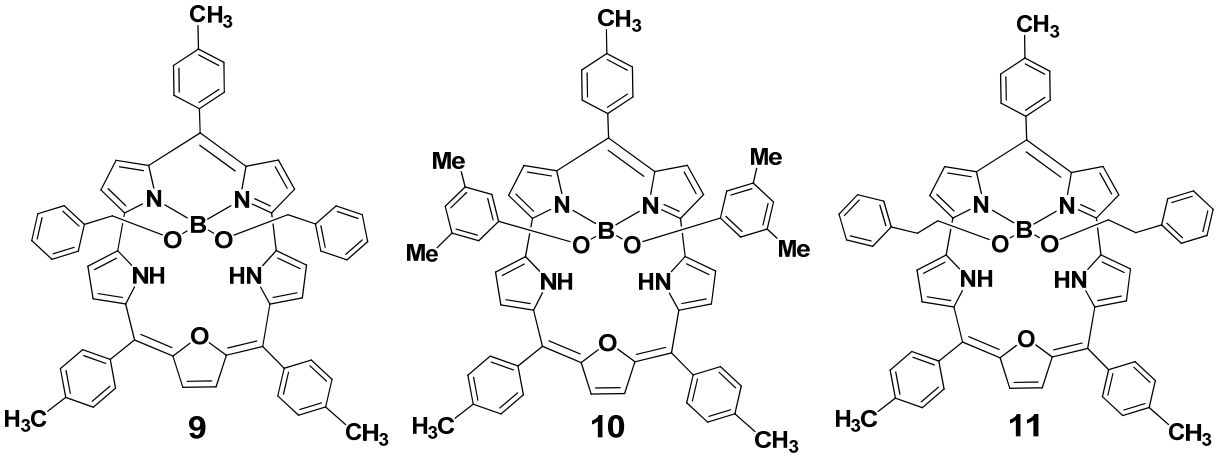


Figure S27. Emission spectra of compounds of **4-7** recorded in $CHCl_3$ by exciting at their corresponding absorption maxima.



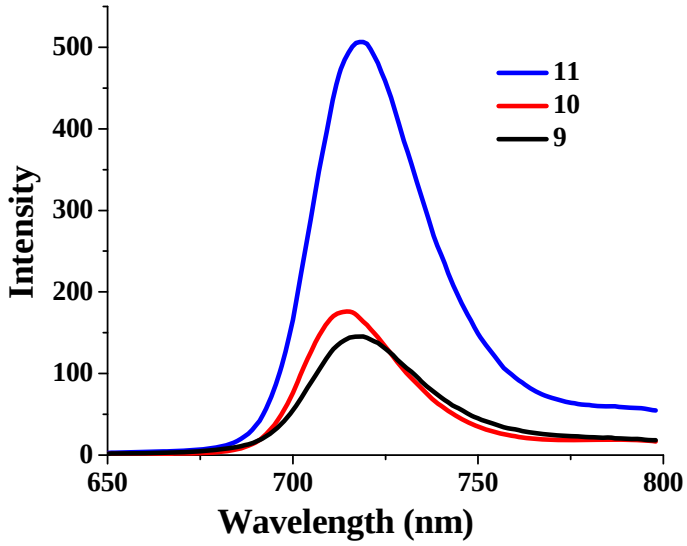
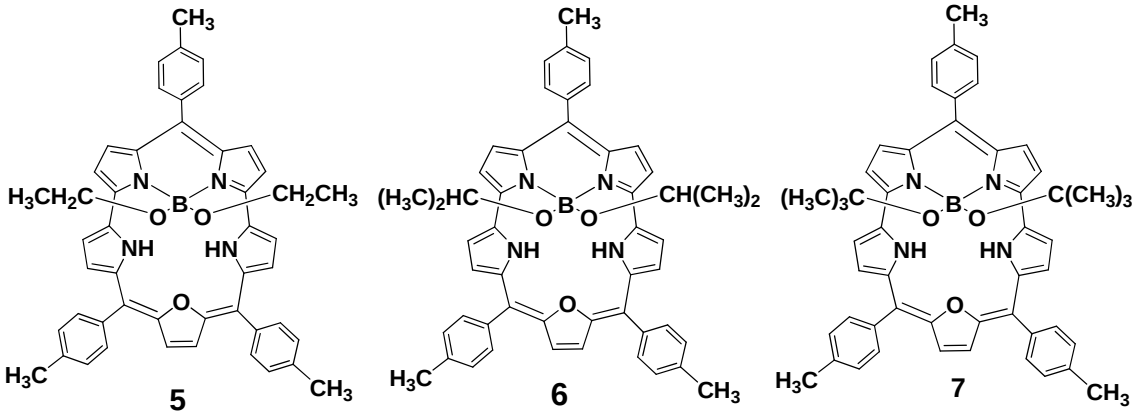


Figure S28. Emission spectra of compounds of **9-11** recorded in $CHCl_3$ by exciting at their corresponding absorption maxima.



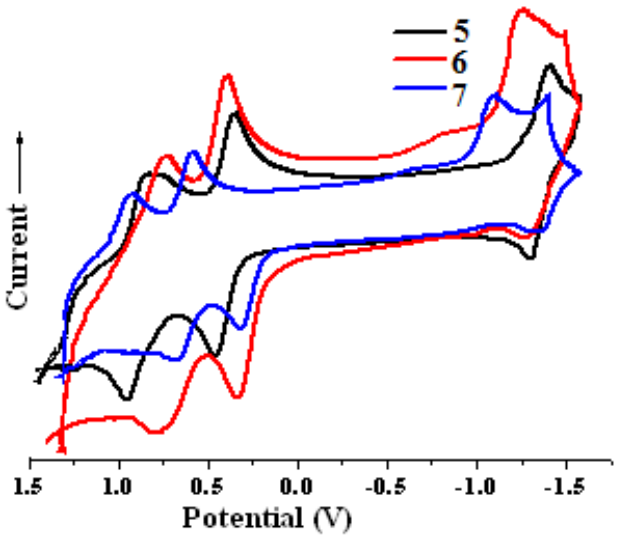
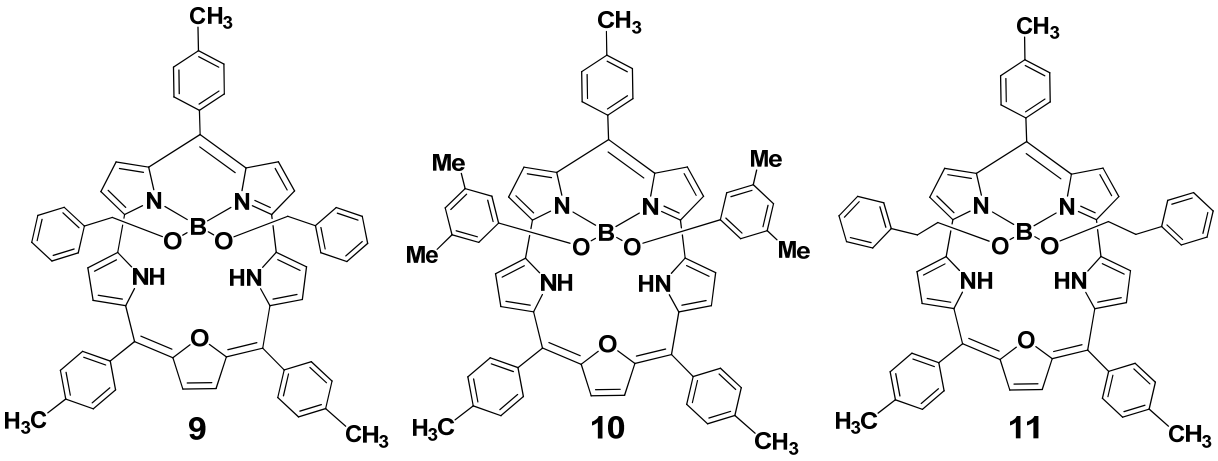


Figure S29. Cyclic voltammograms of compounds of **5-7** recorded in CH_2Cl_2 containing 0.1 M TBAP as supporting electrolyte using scan rate of 50 mV/sec.



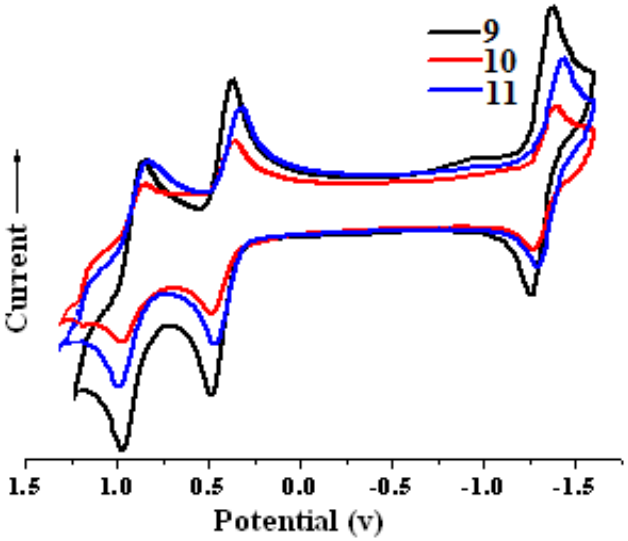


Figure S30. Cyclic voltammograms of compounds of **9-11** recorded in CH_2Cl_2 containing 0.1 M TBAP as supporting electrolyte using scan rate of 50 mV/sec.

Table S1: Crystallographic data for compound

Parameters	**Sm-3,5-MePh**
mol formula	C60 H51 B N4 O3
fw	886.86
cryst sym	Triclinic
Space group	P -1
a (Å)	11.795(2)
b (Å)	14.191(3)
c (Å)	15.317(4)
α (deg)	91.144(14)
β (deg)	107.536(13)
γ (deg)	90.403(11)
V (Å^3)	2444.1(9)
Z	2
μ (mm^{-1})	0.074
D_{calcd} (g cm^{-3})	1.205
F(000)	936
2θ range (deg)	1.81 - 25.12
Independent refections	8535 [R(int) = 0.1388]
R1, wR2 [$I > 2\sigma(I)$]	0.0865, 0.1620

R1, wR2 (all data)	0.2545, 0.2373
GOF	0.937
Largest diff. peak/hole, (e Å^{-3})	0.338, -0.384