Electronic Supplementary Material (ESI) for RSC Advances

Functionalized 3-Pyrrolyl Boron-Dipyrromethenes

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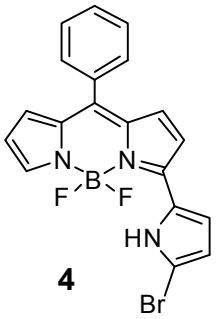
Mumbai 400 076, India. E-mail: ravikanth@chem.iitb.ac.in



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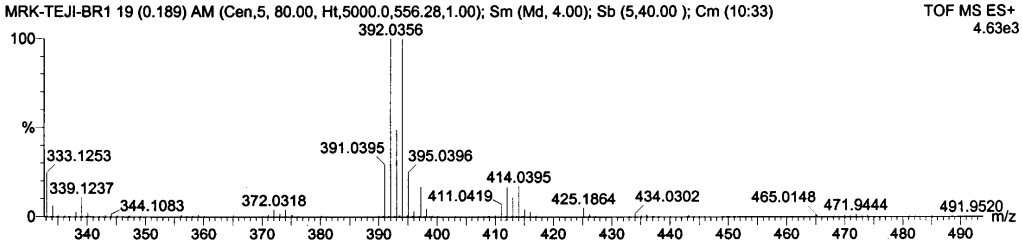
Elemental Composition Report **Page 1**

Single Mass Analysis (displaying only valid results)
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 100.0
Isotope cluster parameters: Separation = 1.0 Abundance = 1.0%

Monoisotopic Mass, Odd and Even Electron Ions
36 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

Micromass : Q-Tof micro (YA-105) Dept. Of Chemistry I.I.T.(B) 28-Nov-201112:47:24
C19H14BF2BrN3
MRK-TEJI-BR1 19 (0.189) AM (Cen,5, 80.00, Ht,5000.0,556.28,1.00); Sm (Md, 4.00); Sb (5,40.00); Cm (10:33) TOF MS ES+
4.63e3



Minimum:				-1.5		
Maximum:		200.0	5.0	100.0		
Mass	Calc. Mass	mDa	PPM	DBE	Score	Formula
392.0356	392.0370	-1.4	-3.7	14.5	1	C19 H13 B N3 F Br

Figure 1: HRMS mass spectrum of compound **4**

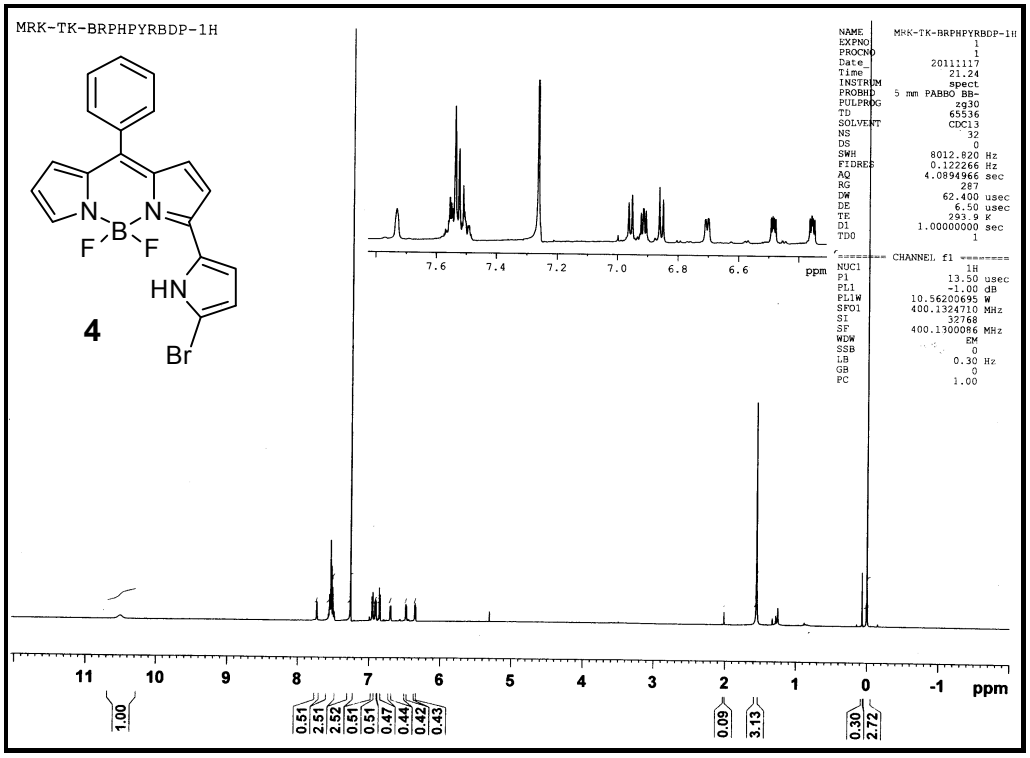


Figure 2: ^{1}H NMR spectrum of compound **4** recorded in $CDCl_3$

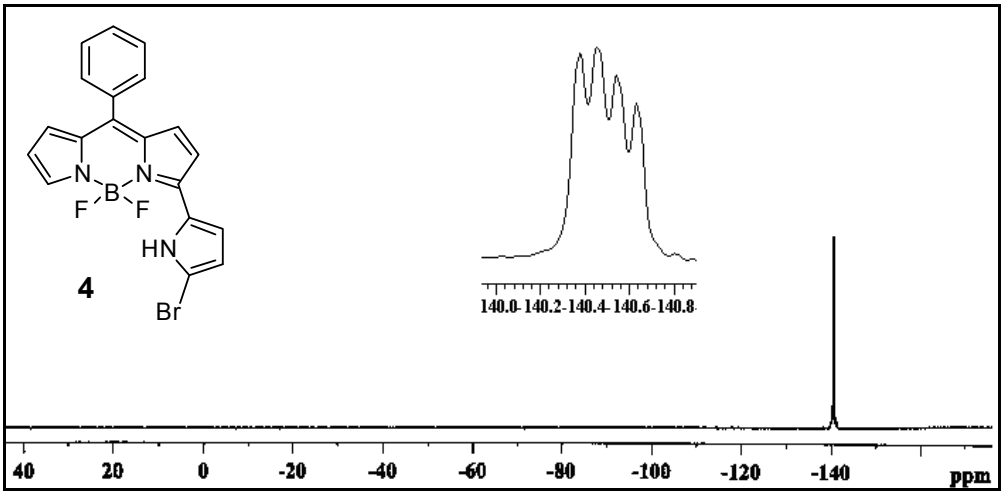


Figure 3: ^{19}F NMR spectrum of compound **4** recorded in $CDCl_3$

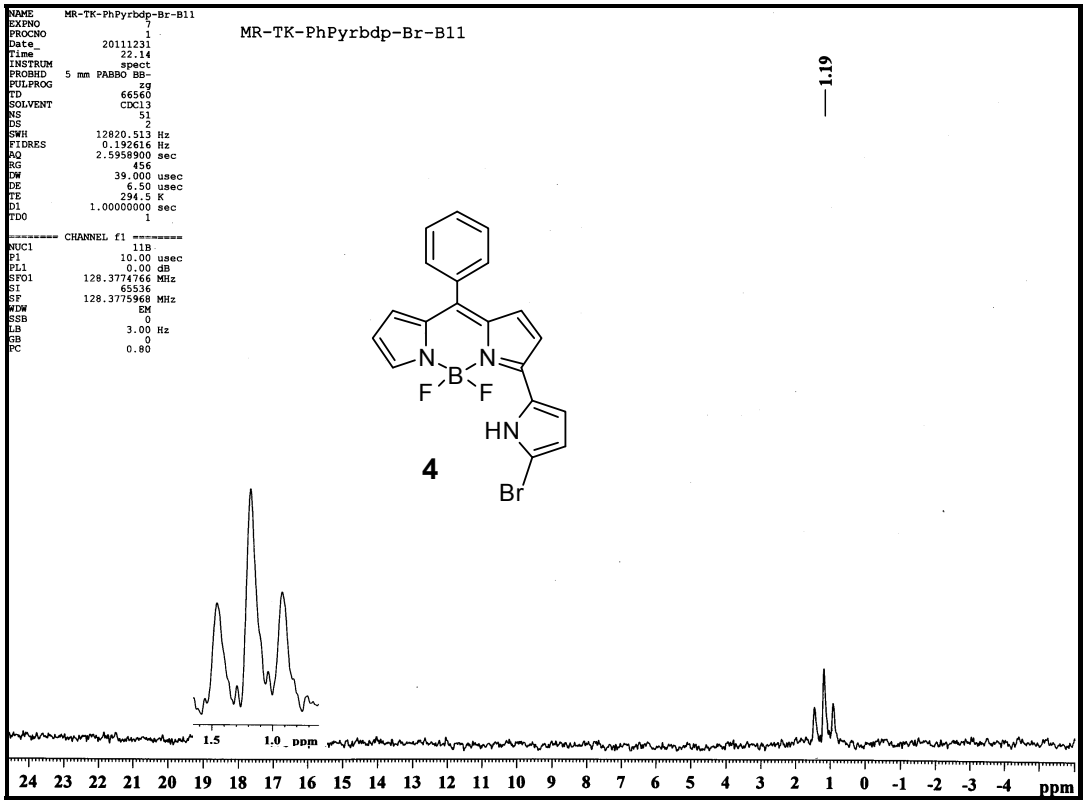


Figure 4: ^{11}B NMR spectrum of compound **4** recorded in $CDCl_3$

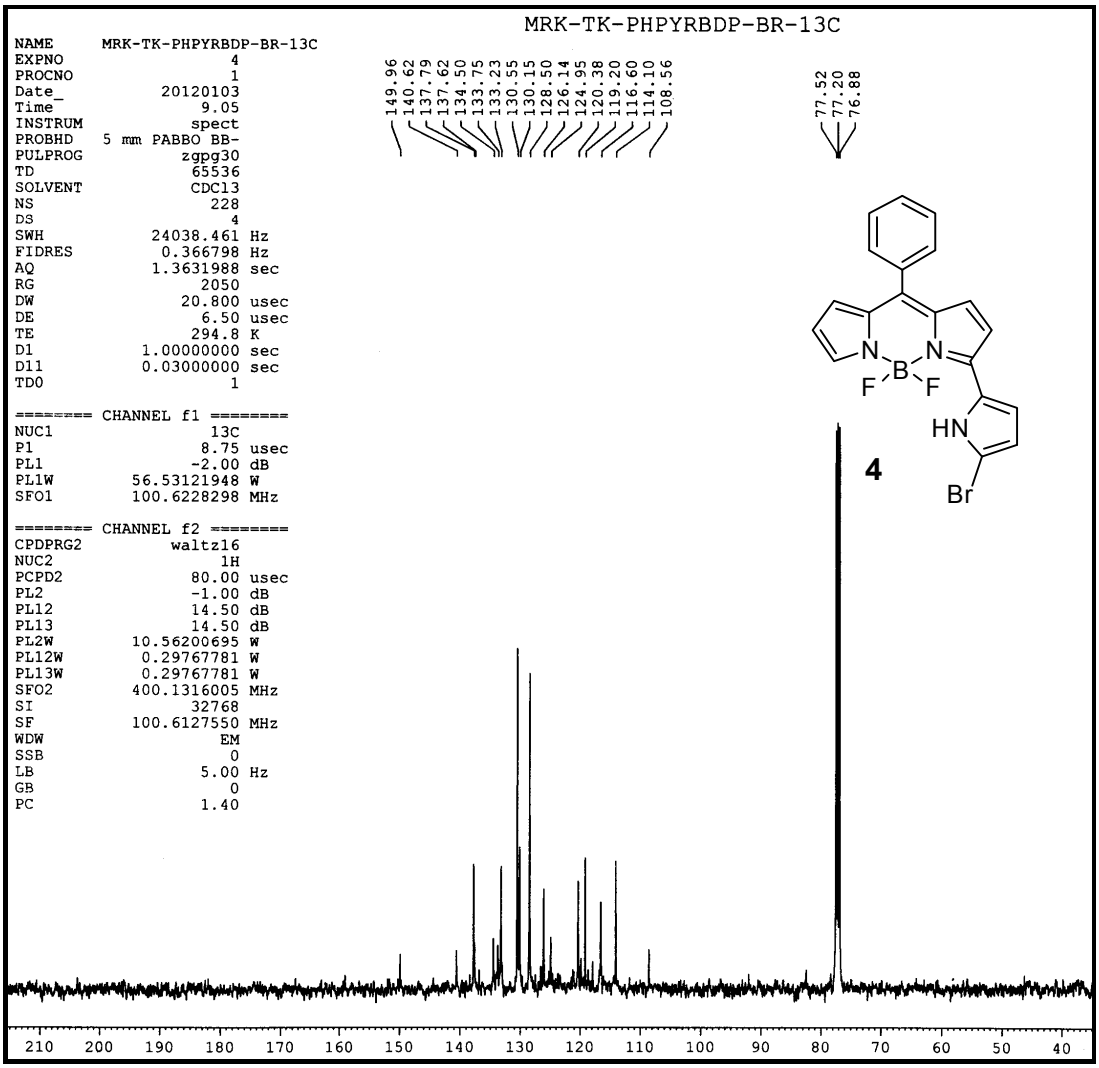
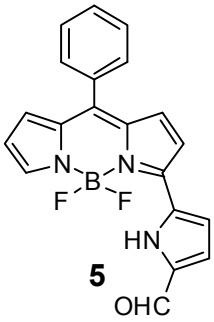


Figure 5: ^{13}C NMR spectrum of compound **4** recorded in $CDCl_3$ (δ in ppm)



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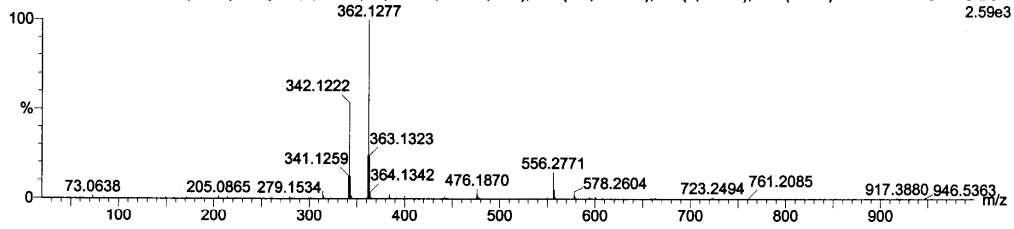
Elemental Composition Report Page:

Single Mass Analysis (displaying only valid results)
Tolerance = 4.0 PPM / DBE: min = -1.5, max = 100.0
Isotope cluster parameters: Separation = 1.0 Abundance = 1.0%

Monoisotopic Mass, Odd and Even Electron Ions
36 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

Micromass : Q-Tof micro (YA-105) Dept. Of Chemistry I.I.T.(B) 05-Dec-201114:04:55
C20H14BF2N3O
MRK-TK-PYBDP-CHO 35 (0.346) AM (Cen,5, 80.00, Ht,5000.0,556.28,1.00); Sm (SG, 2x9.00); Sb (5,40.00); Cm (10:40) TOF MS ES+
2.59e3



Minimum:				-1.5		
Maximum:		200.0	4.0	100.0		
Mass	Calc. Mass	mDa	PPM	DBE	Score	Formula
362.1277	362.1276	0.1	0.2	14.5	1	C20 H15 B N3 O F2

Figure 6: HRMS mass spectrum of compound **5**

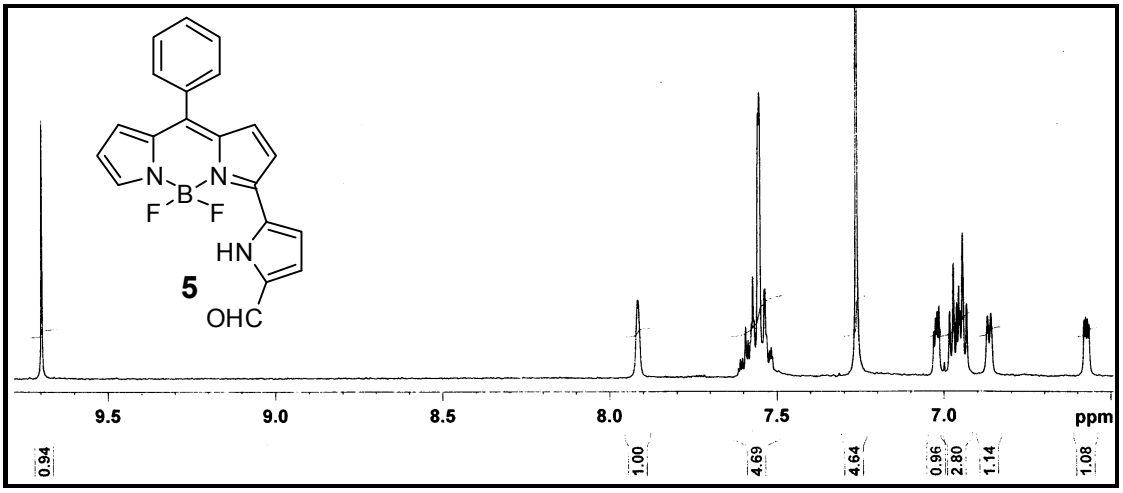


Figure 7: ^{1}H NMR spectrum of compound **5** in the selected region recorded in $CDCl_3$.

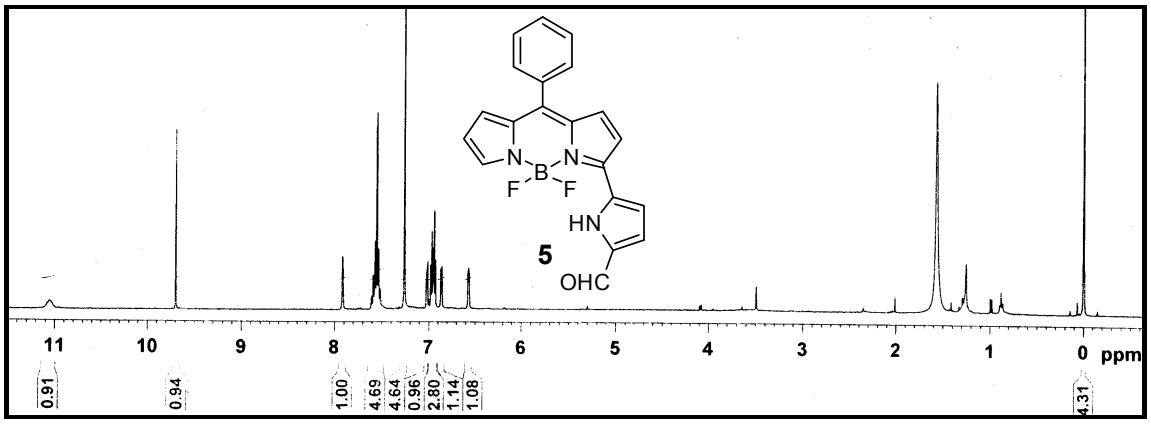


Figure 8: ^{1}H NMR spectrum of compound **5** recorded in $CDCl_3$.

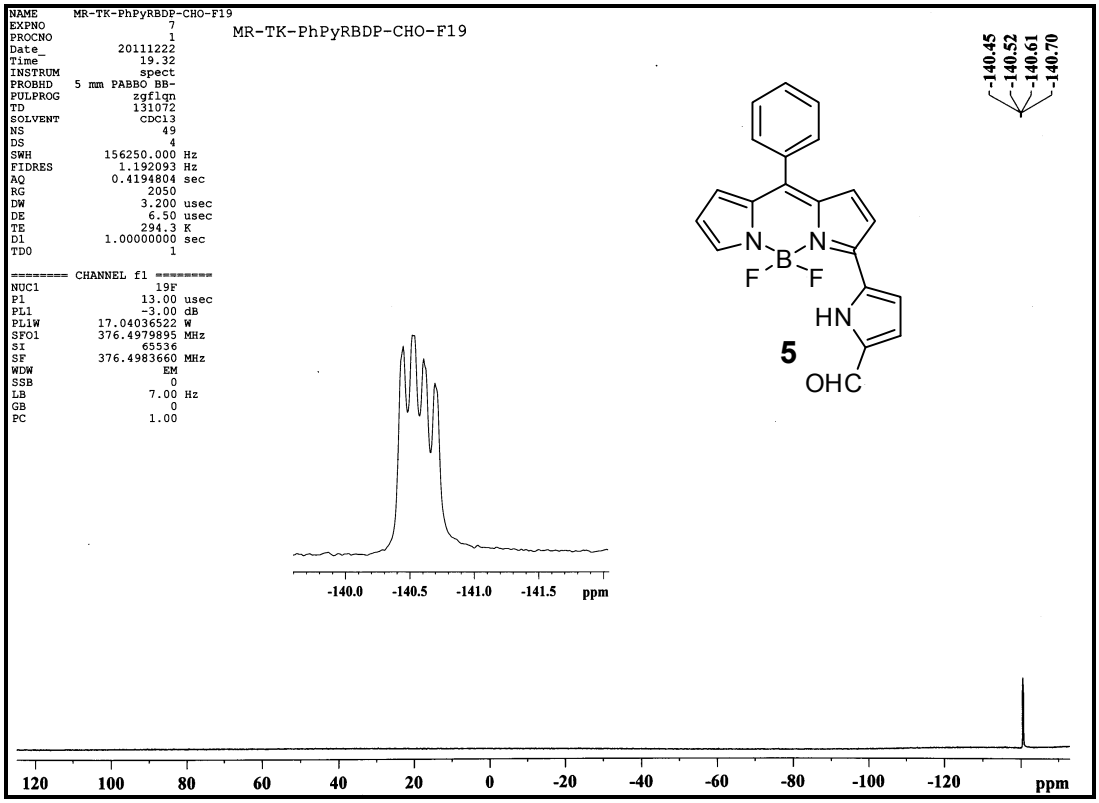


Figure 9: ^{19}F NMR spectrum of compound **5** recorded in $CDCl_3$

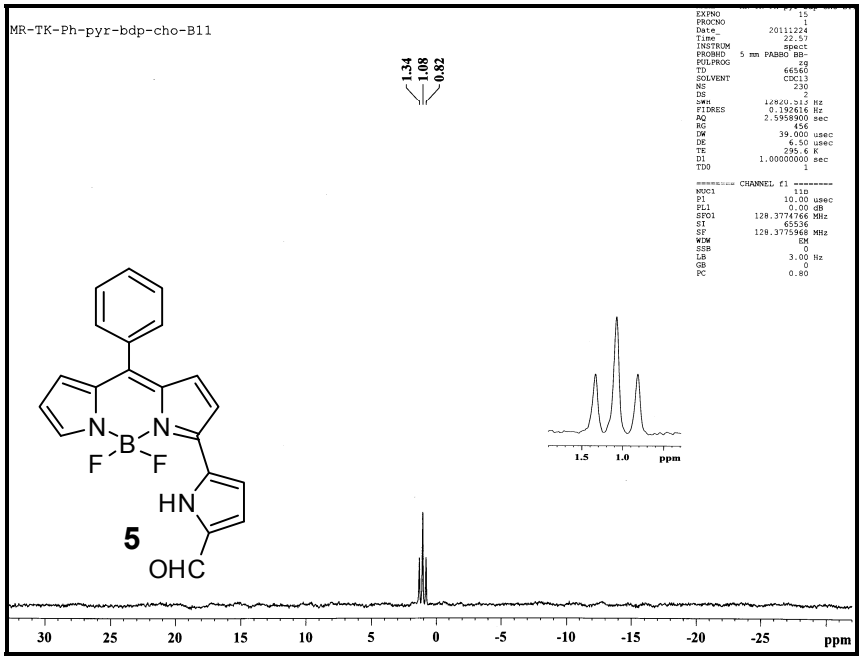


Figure 10: ^{11}B NMR spectrum of compound **5** recorded in $CDCl_3$

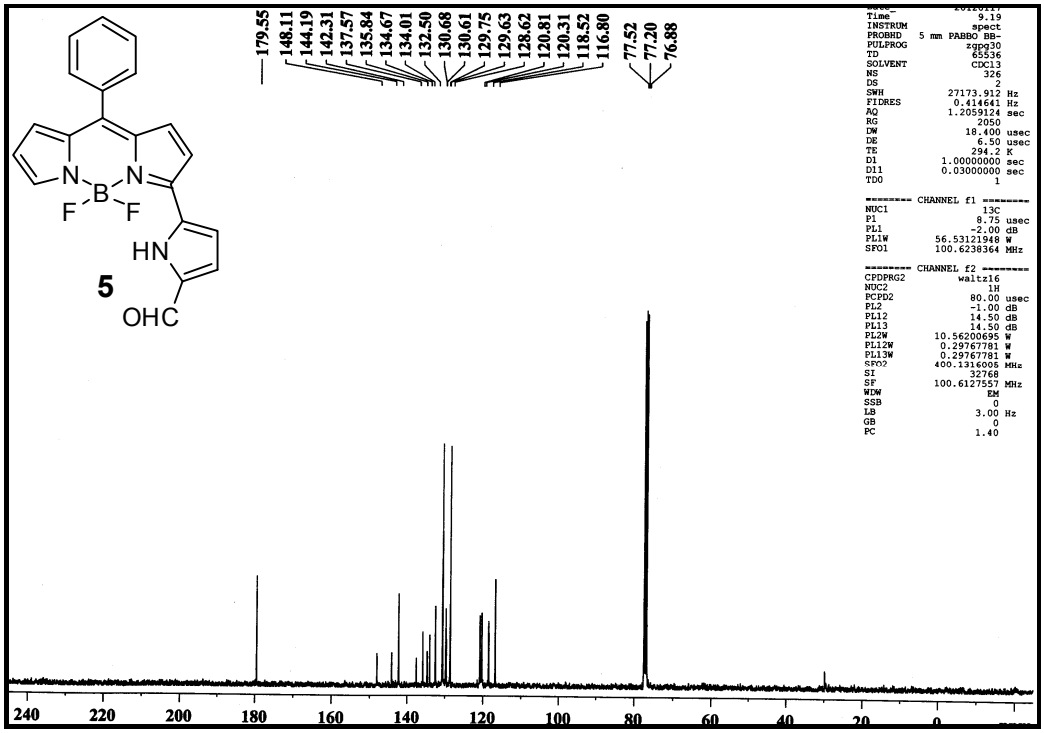
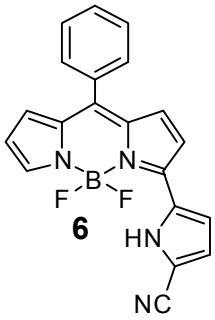


Figure 11: ^{13}C NMR spectrum of compound **5** recorded in $CDCl_3$ (δ□ in ppm)



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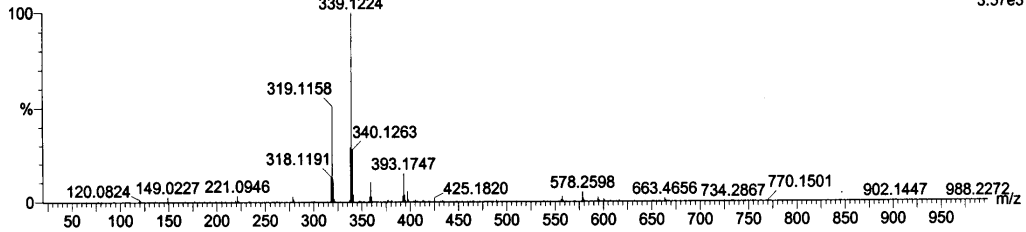
Elemental Composition Report **Page 1**

Single Mass Analysis (displaying only valid results)
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 100.0
Isotope cluster parameters: Separation = 1.0 Abundance = 1.0%

Monoisotopic Mass, Odd and Even Electron Ions
22 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

Micromass : Q-Tof micro (YA-105) Dept. Of Chemistry I.I.T.(B) 28-Nov-201114:00:14
C19H13BF2N4
MRK-TEJI-CN 2 (0.020) AM (Cen,5, 80.00, Ht,5000.0,556.28,1.00); Cm (1:8) TOF MS ES+
3.57e3



Minimum:				-1.5		
Maximum:		200.0	5.0	100.0		
Mass	Calc. Mass	mDa	PPM	DBE	Score	Formula
339.1224	339.1217	0.7	2.0	16.5	1	C20 H13 B N4 F

Figure 12: HRMS mass spectrum of compound **6**

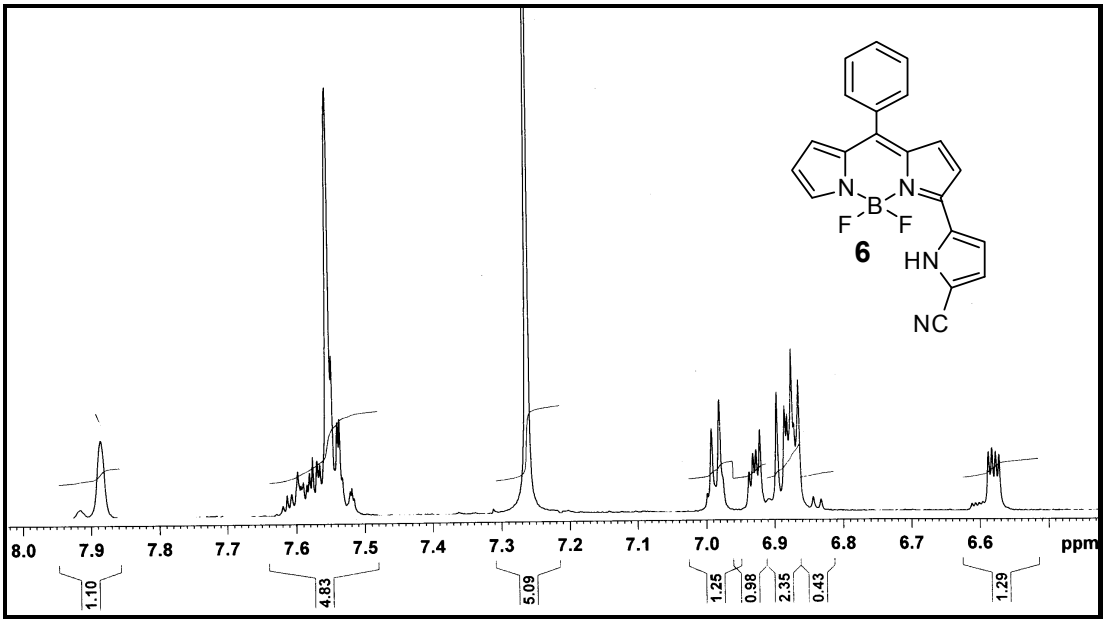


Figure 13: ^{1}H NMR spectrum of compound **6** in the selected region recorded in $CDCl_3$

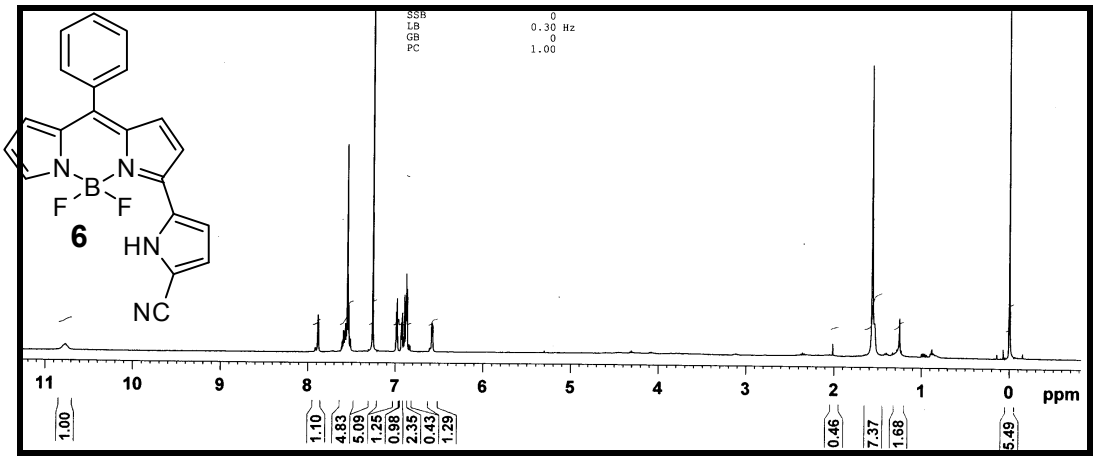


Figure 14: ^{1}H NMR spectrum of compound **6** recorded in $CDCl_3$

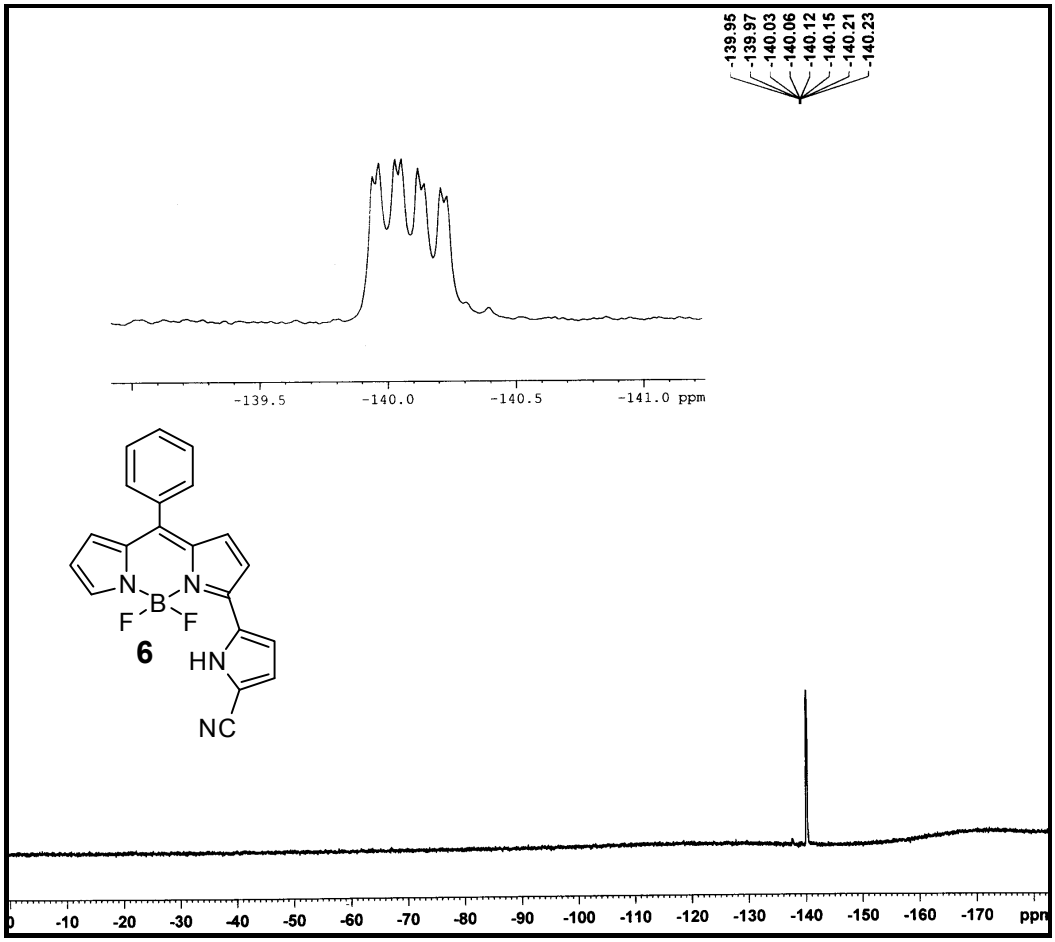


Figure 15: ^{19}F NMR spectrum of compound **6** recorded in $CDCl_3$

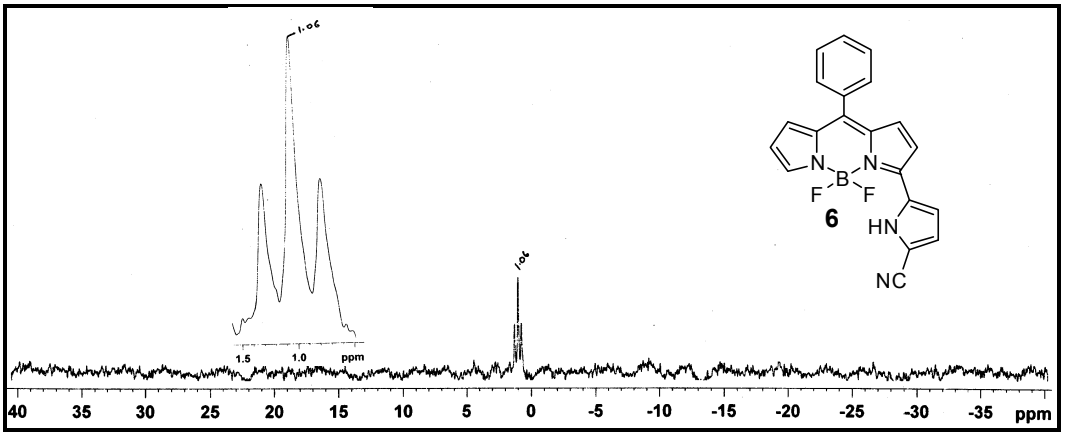


Figure 16: ^{11}B NMR spectrum of compound **6** recorded in $CDCl_3$

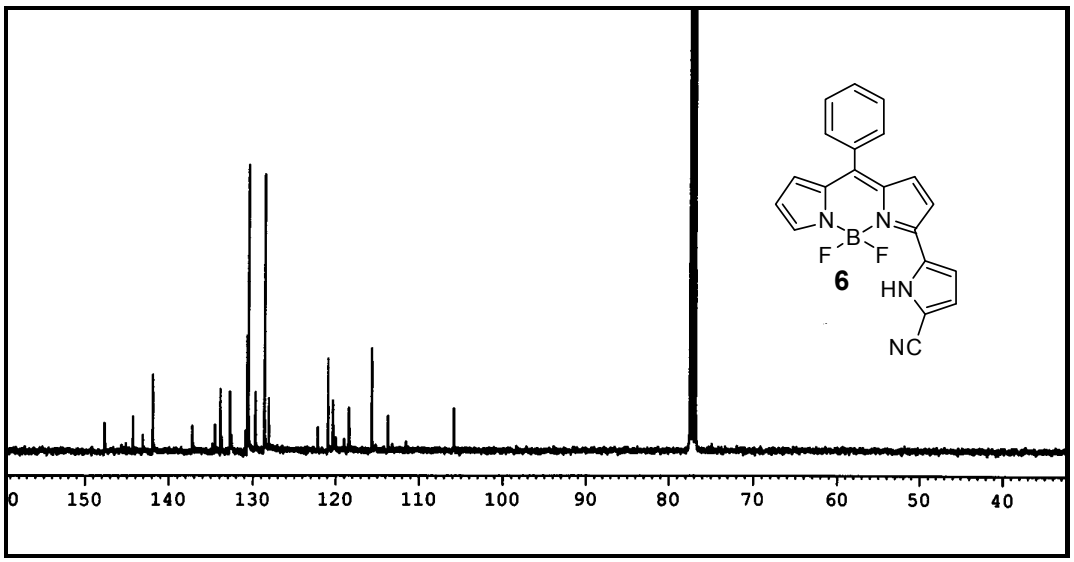
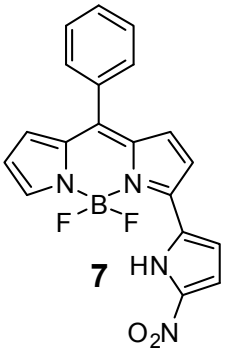


Figure 17: ^{13}C NMR spectrum of compound **6** recorded in $CDCl_3$



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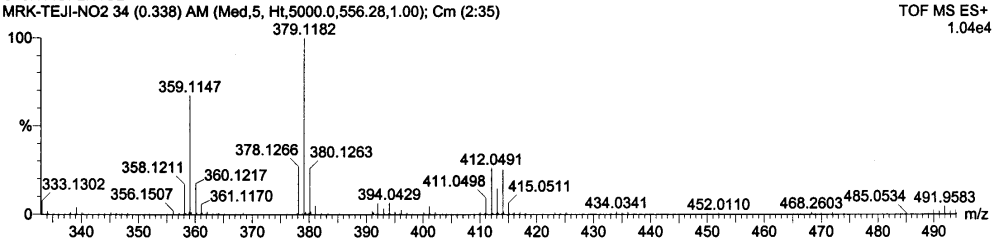
Elemental Composition Report **Page 1**

Single Mass Analysis (displaying only valid results)
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 100.0
Isotope cluster parameters: Separation = 1.0 Abundance = 1.0%

Monoisotopic Mass, Odd and Even Electron Ions
1783 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

Micromass : Q-Tof micro (YA-105) Dept. Of Chemistry I.I.T.(B) 28-Nov-201113:01:00
C19H14BF2N4O2
MRK-TEJI-NO2 34 (0.338) AM (Med,5, Ht,5000.0,556.28,1.00); Cm (2:35) TOF MS ES+
1.04e4



Minimum:				-1.5		
Maximum:		200.0	5.0	100.0		
Mass	Calc. Mass	mDa	PPM	DBE	Score	Formula
379.1182	379.1178	0.4	1.2	14.5	1	C19 H14 B N4 O2 F2

Figure 18: HRMS mass spectrum of compound **7**

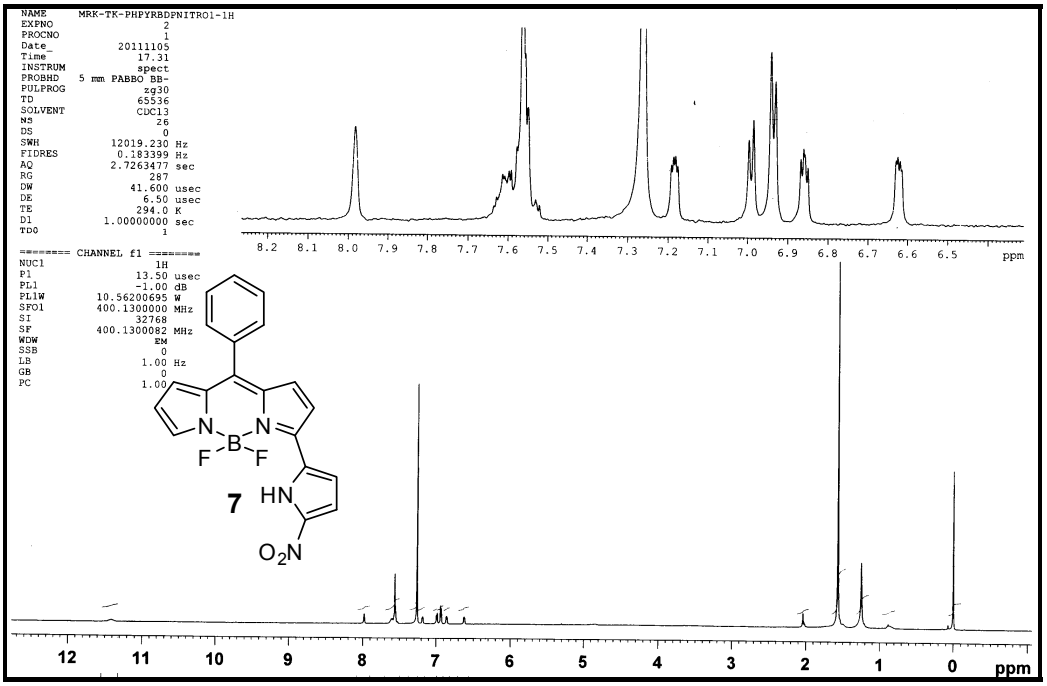


Figure 19: ^{1}H NMR spectrum of compound **7** recorded in $CDCl_3$. The inset shows ^{1}H NMR spectrum in selected region.

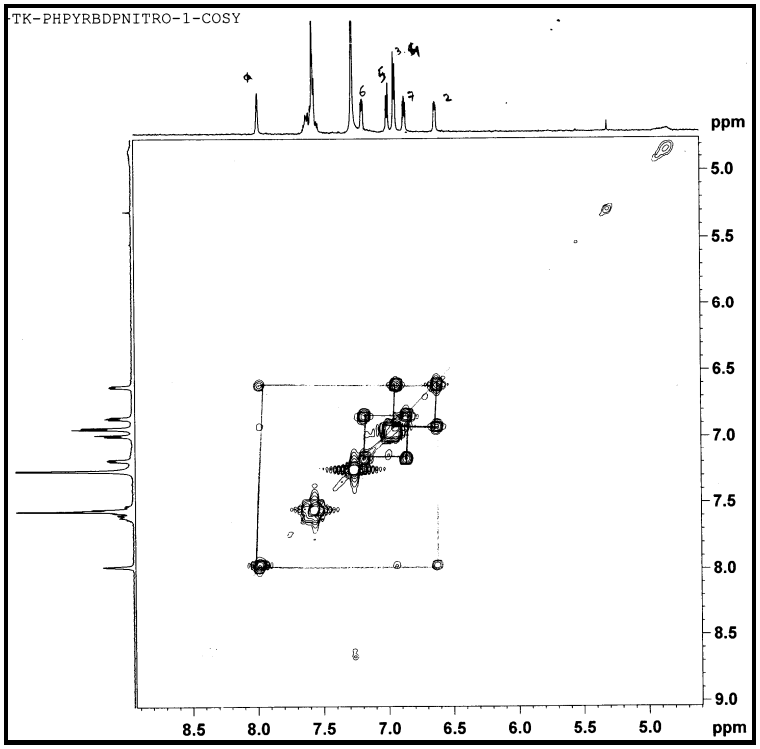


Figure 20: ^{1}H-^{1}H COSY NMR spectrum of compound **7** recorded in $CDCl_3$

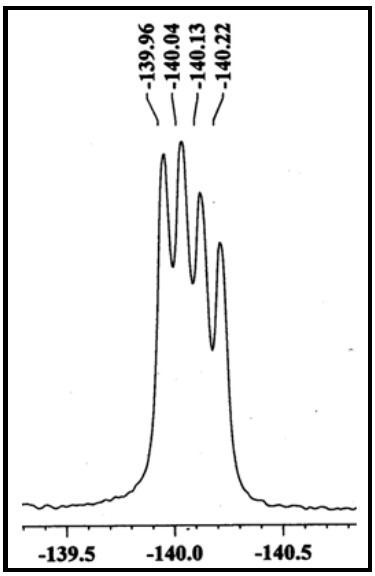


Figure 21: ^{19}F NMR spectrum of compound **7** recorded in $CDCl_3$ (δ □in ppm)

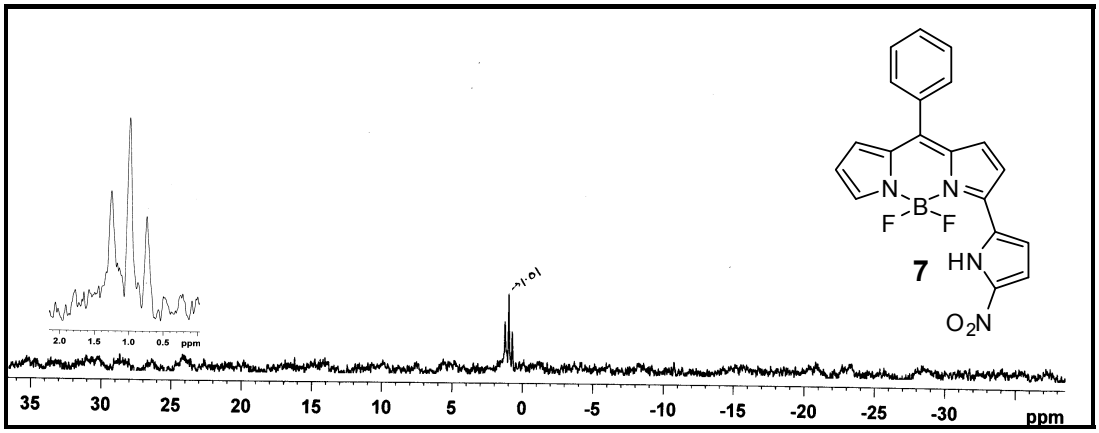


Figure 22: ^{11}B NMR spectrum of compound **7** recorded in $CDCl_3$

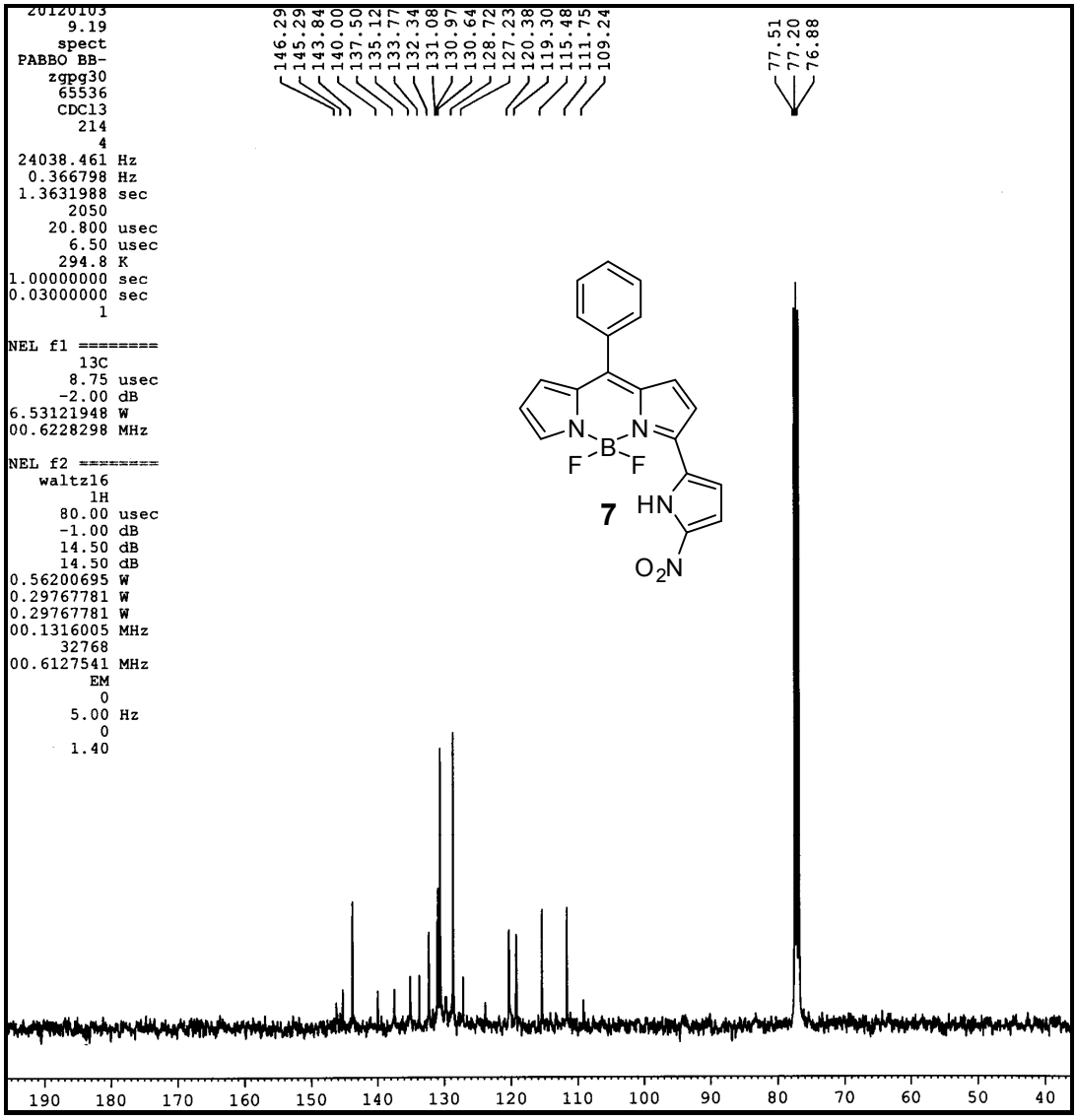
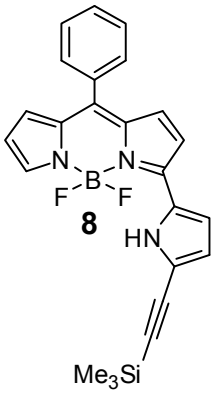


Figure 23: ^{13}C NMR spectrum of compound **7** recorded in $CDCl_3$ (δ in ppm)



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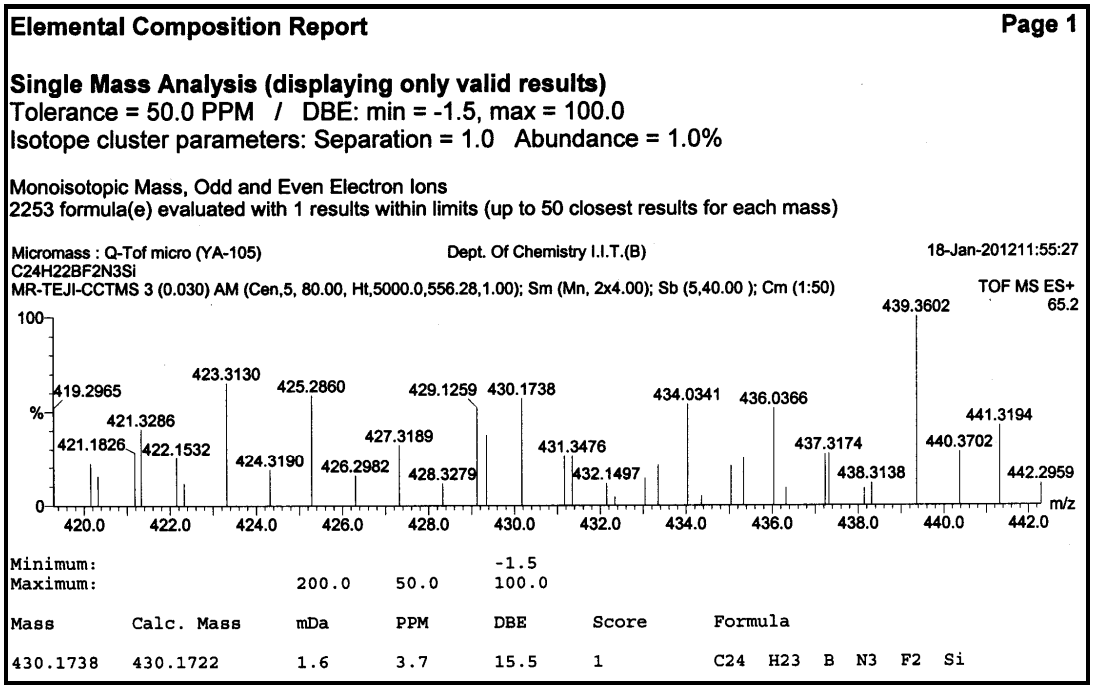

Elemental Composition Report **Page 1**

Single Mass Analysis (displaying only valid results)
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Isotope cluster parameters: Separation = 1.0 Abundance = 1.0%

Monoisotopic Mass, Odd and Even Electron Ions
2253 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

Micromass : Q-Tof micro (YA-105) Dept. Of Chemistry I.I.T.(B) 18-Jan-201211:55:27
C24H22BF2N3Si
MR-TEJI-CCTMS 3 (0.030) AM (Cen,5, 80.00, Ht,5000.0,556.28,1.00); Sm (Mn, 2x4.00); Sb (5,40.00); Cm (1:50) TOF MS ES+ 65.2

Minimum:				-1.5		
Maximum:		200.0	50.0	100.0		
Mass	Calc. Mass	mDa	PPM	DBE	Score	Formula
430.1738	430.1722	1.6	3.7	15.5	1	C24 H23 B N3 F2 Si

Figure 24: HRMS mass spectrum of compound **8**

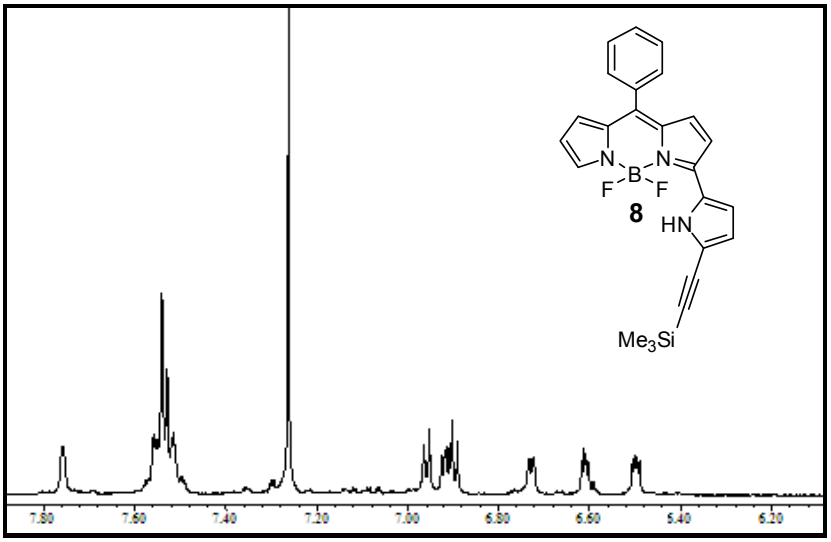


Figure 25: ^{1}H NMR spectrum of compound **8** in the selected region recorded in $CDCl_3$ (δ in ppm)

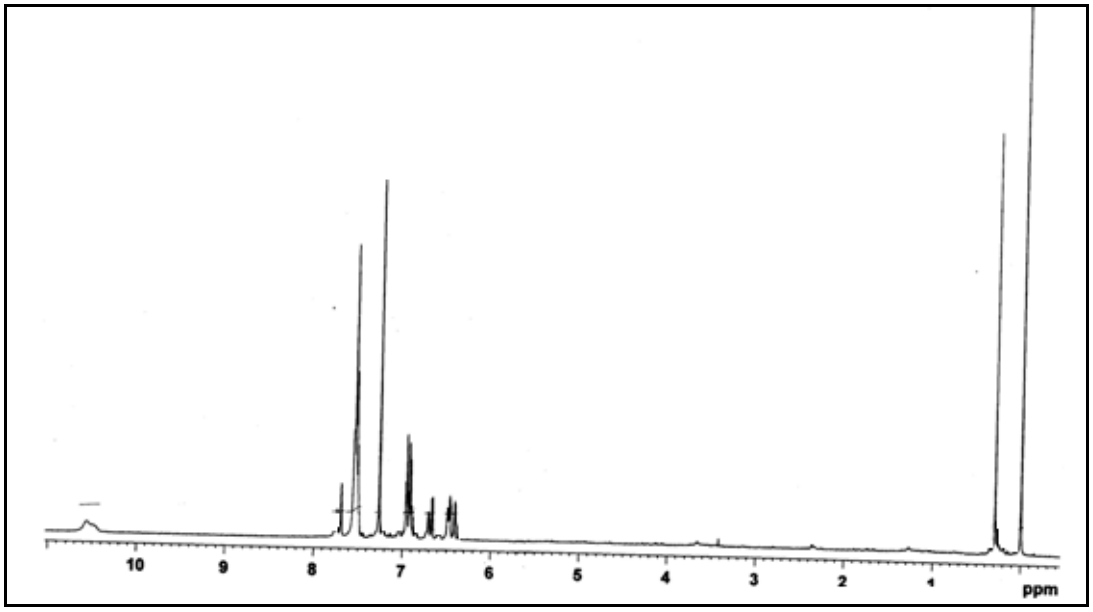


Figure 26: ^{1}H NMR spectrum of compound **8** recorded in $CDCl_3$

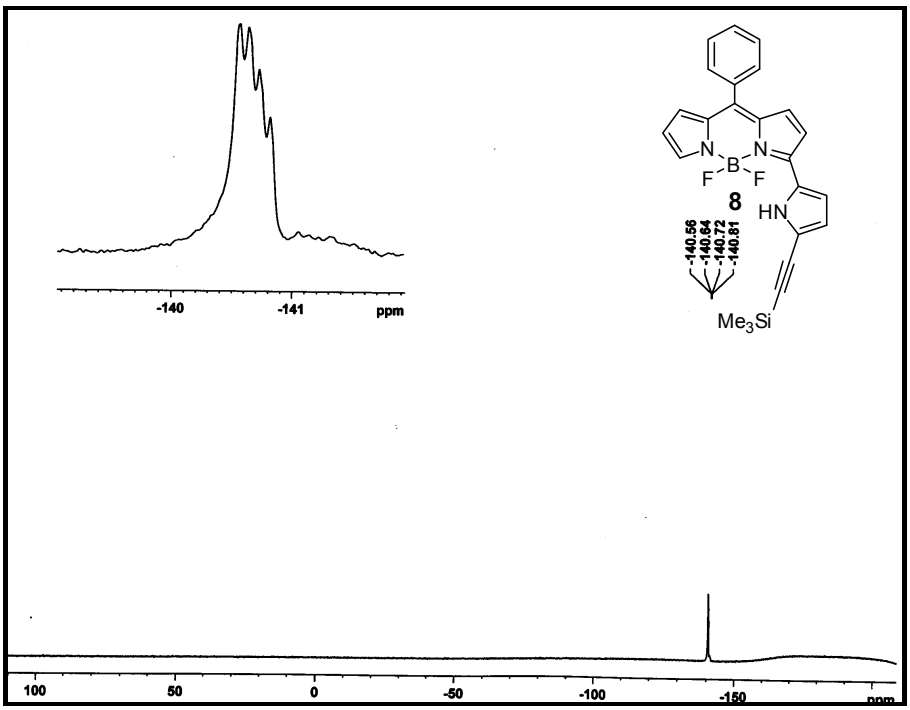


Figure 27: ^{19}F NMR spectrum of compound **8** recorded in $CDCl_3$ (δ□ in ppm)

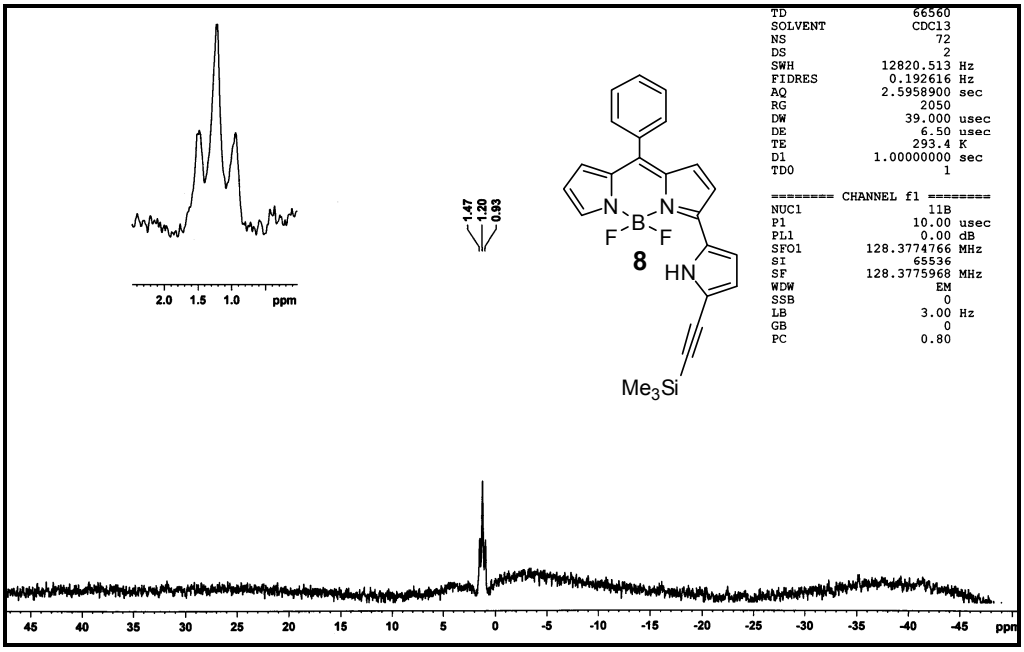


Figure 28: ^{11}B NMR spectrum of compound **8** recorded in $CDCl_3$

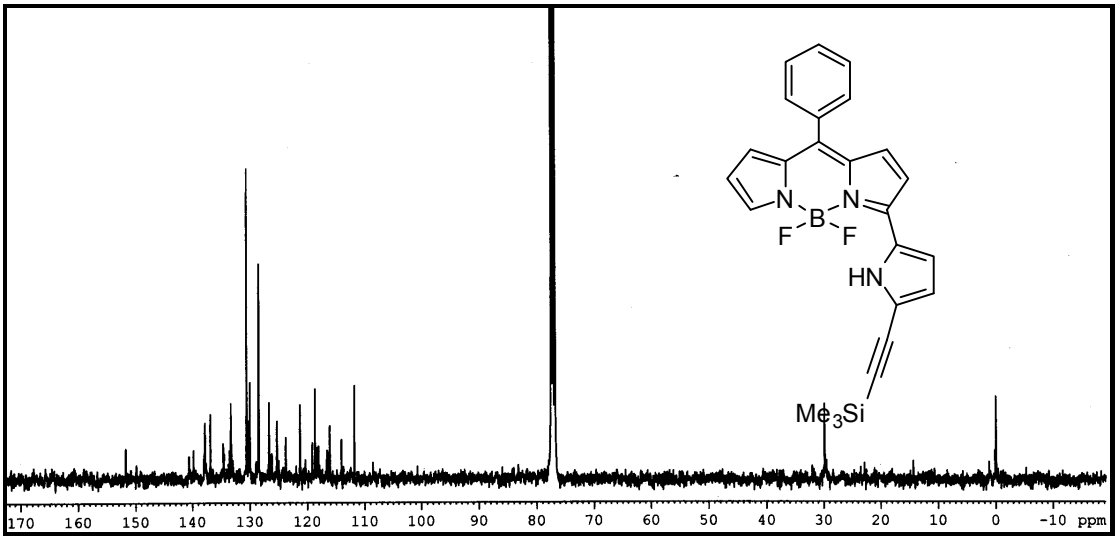
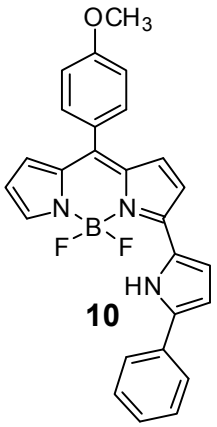


Figure 29: ^{13}C NMR spectrum of compound **8** recorded in $CDCl_3$



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Elemental Composition Report **Page 1**

Single Mass Analysis (displaying only valid results)
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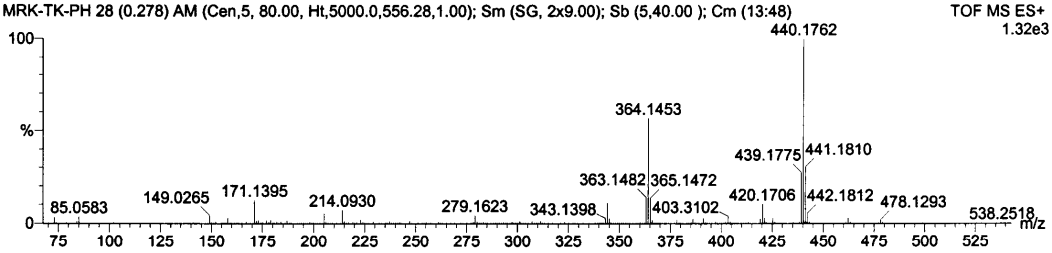
Isotope cluster parameters: Separation = 1.0 Abundance = 1.0%

Monoisotopic Mass, Odd and Even Electron Ions
32 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

Micromass : Q-Tof micro (YA-105) Dept. Of Chemistry I.I.T.(B) 05-Dec-201113:48:47
C26H20BF2N3O
MRK-TK-PH 28 (0.278) AM (Cen,5, 80.00, Ht,5000.0,556.28,1.00); Sm (SG, 2x9.00); Sb (5,40.00); Cm (13:48) TOF MS ES+
1.32e3



Minimum:				-1.5		
Maximum:		200.0	4.0	100.0		
Mass	Calc. Mass	mDa	PPM	DBE	Score	Formula
440.1762	440.1746	1.7	3.8	17.5	1	C26 H21 N3 O B F2

Figure 30: HRMS mass spectrum of compound **10**

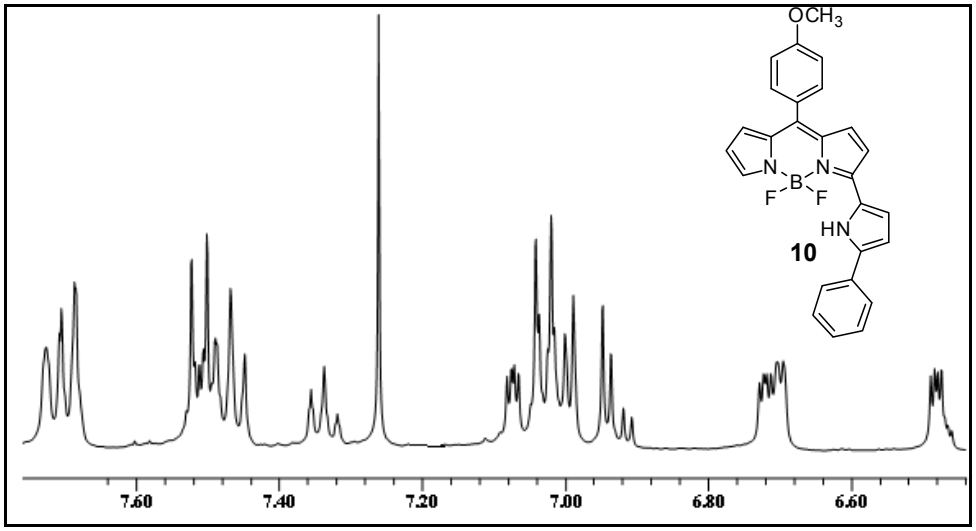


Figure 31: ^{1}H NMR spectrum of compound **10** in the selected region recorded in $CDCl_3$

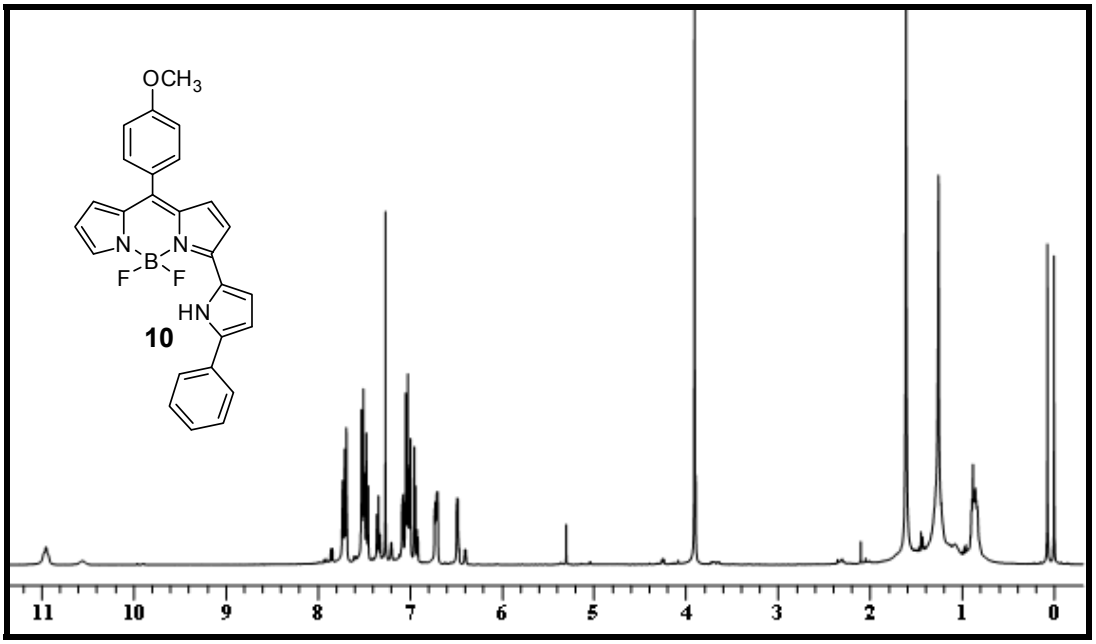


Figure 32: ^{1}H NMR spectrum of compound **10** recorded in $CDCl_3$

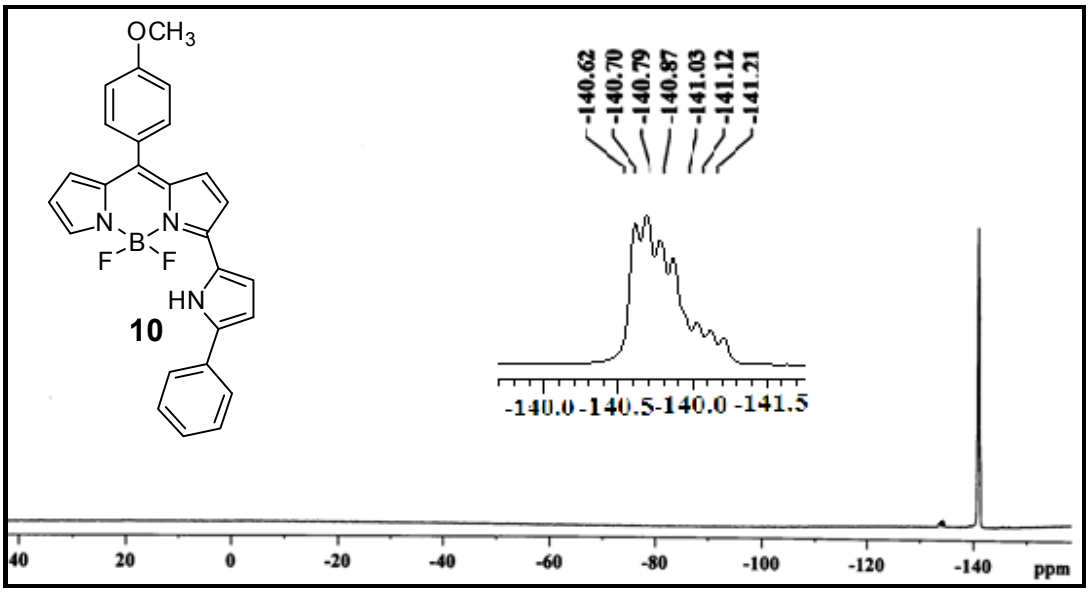


Figure 33: ^{19}F NMR spectrum of compound **10** recorded in $CDCl_3$

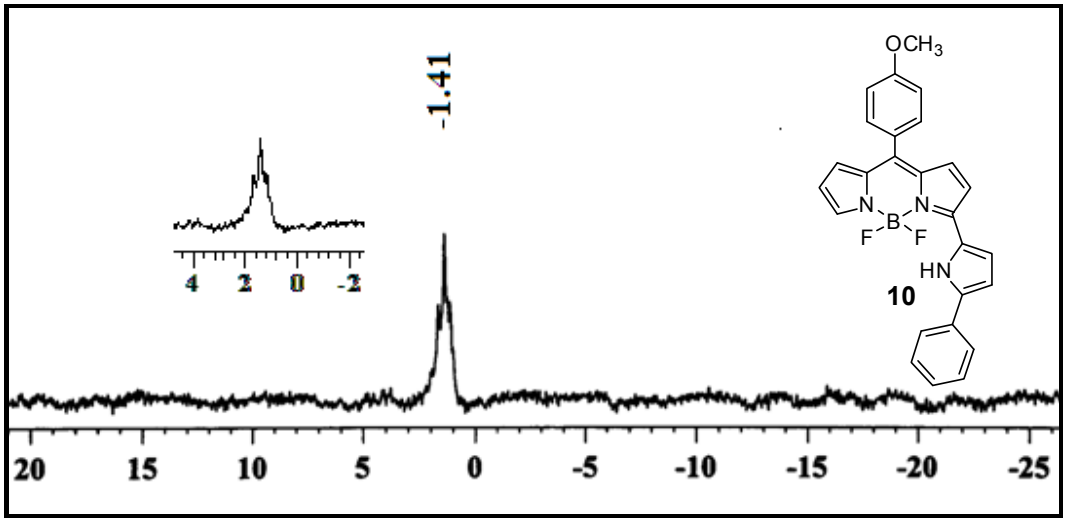


Figure 34: ^{11}B NMR spectrum of compound **10** recorded in $CDCl_3$ (δ in ppm)

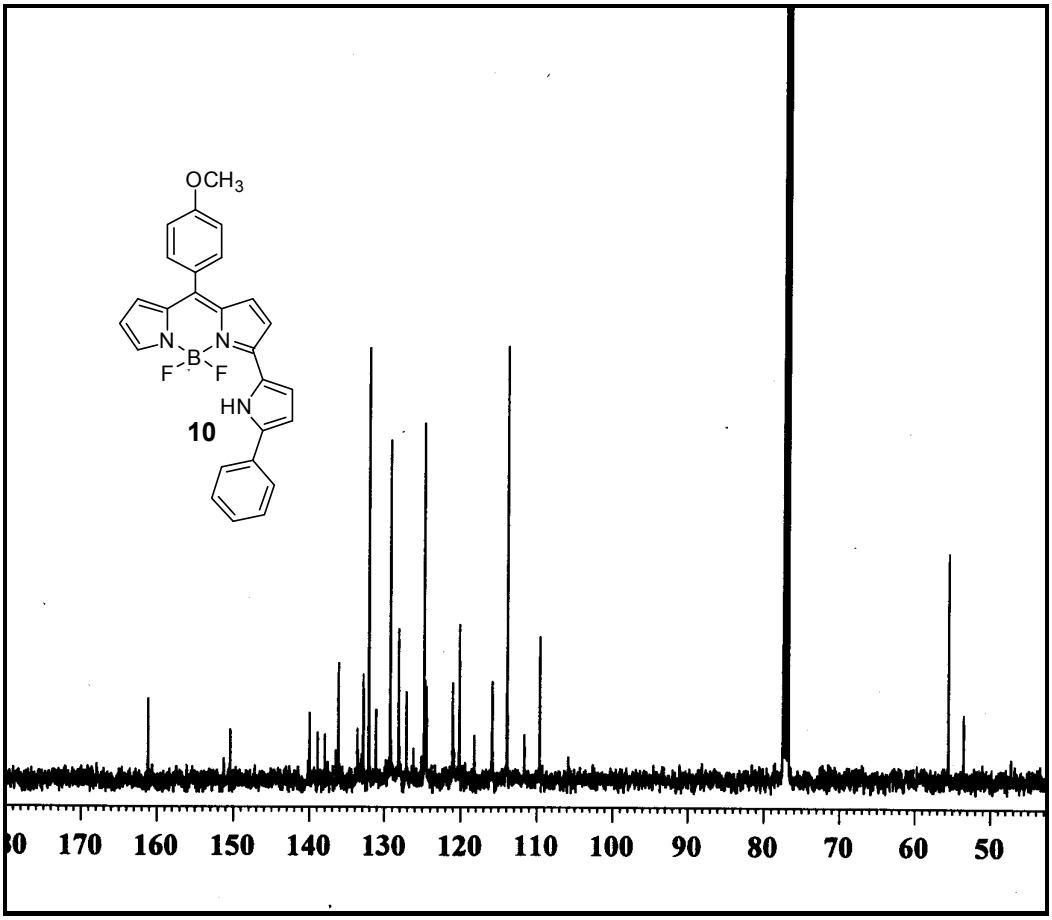
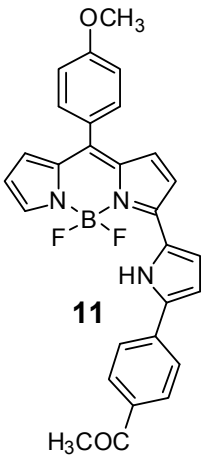


Figure 35: ^{13}C NMR spectrum of compound **10** recorded in $CDCl_3$ (δ in ppm)



11

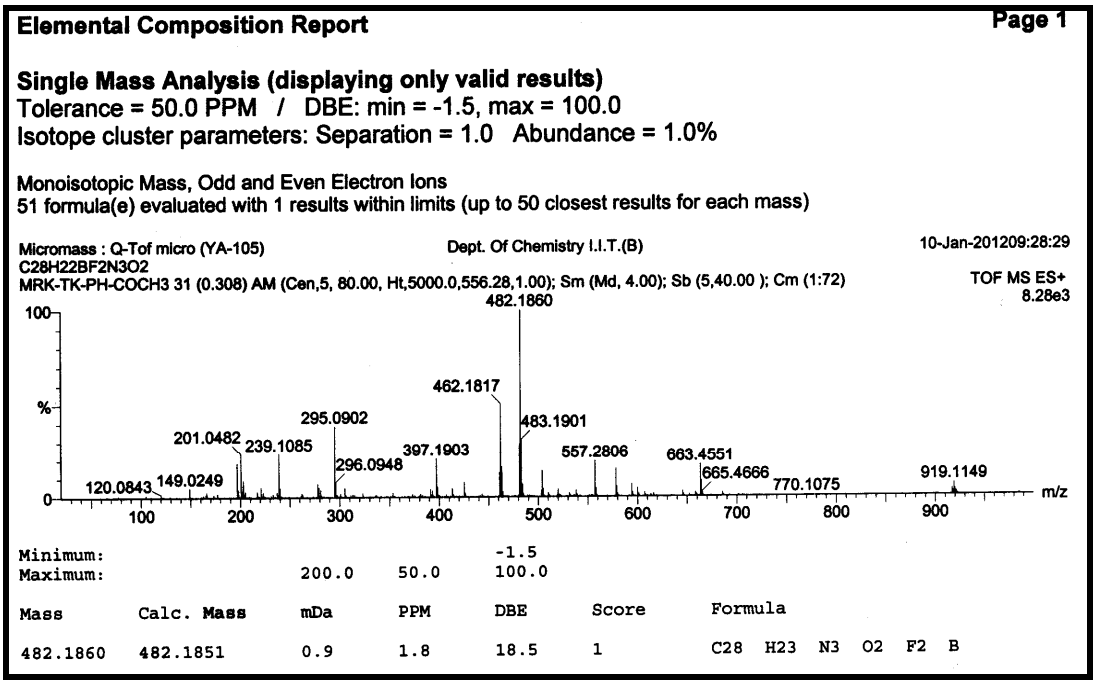


Figure 36: HRMS mass spectrum of compound **11**

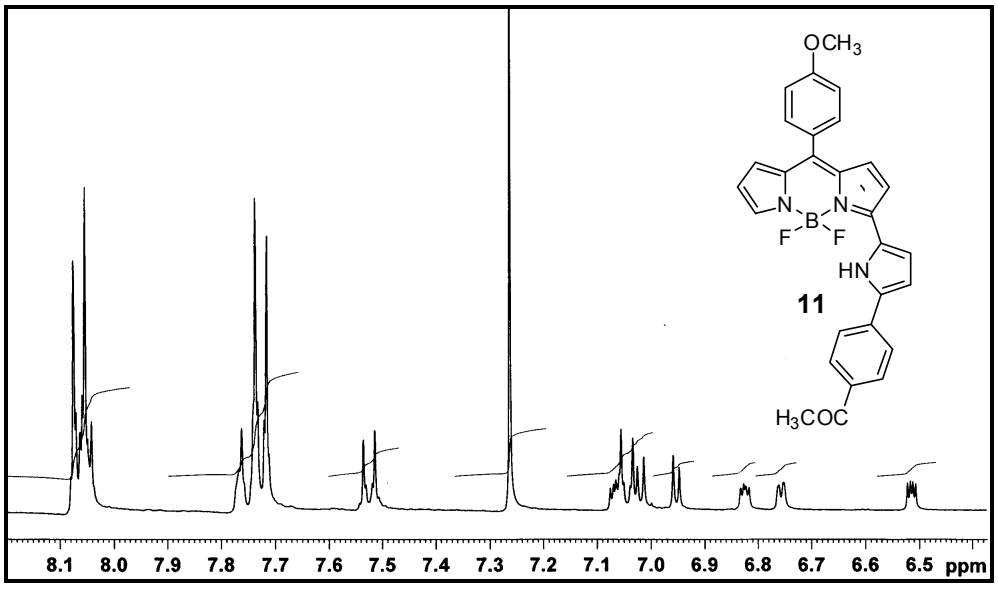


Figure 37: ^{1}H NMR spectrum of compound **11** in the selected region recorded in $CDCl_3$

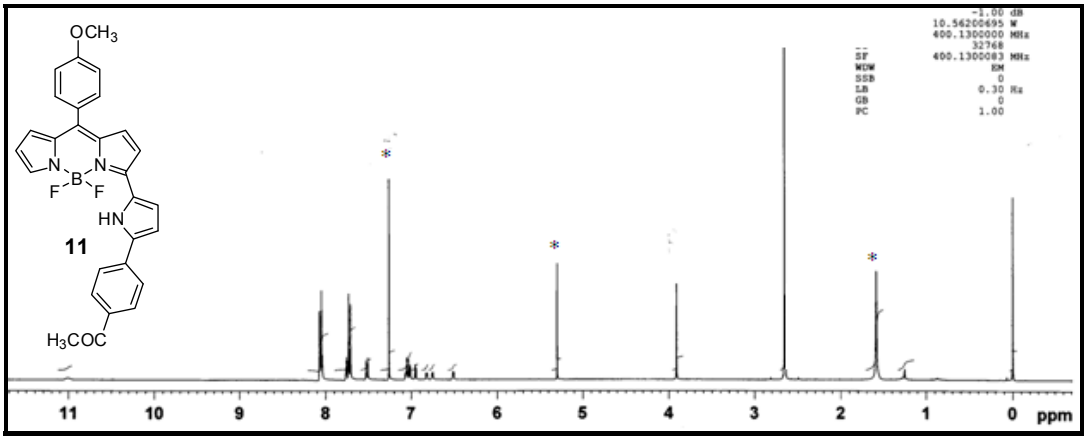


Figure 38: ^{1}H NMR spectrum of compound **11** recorded in $CDCl_3$

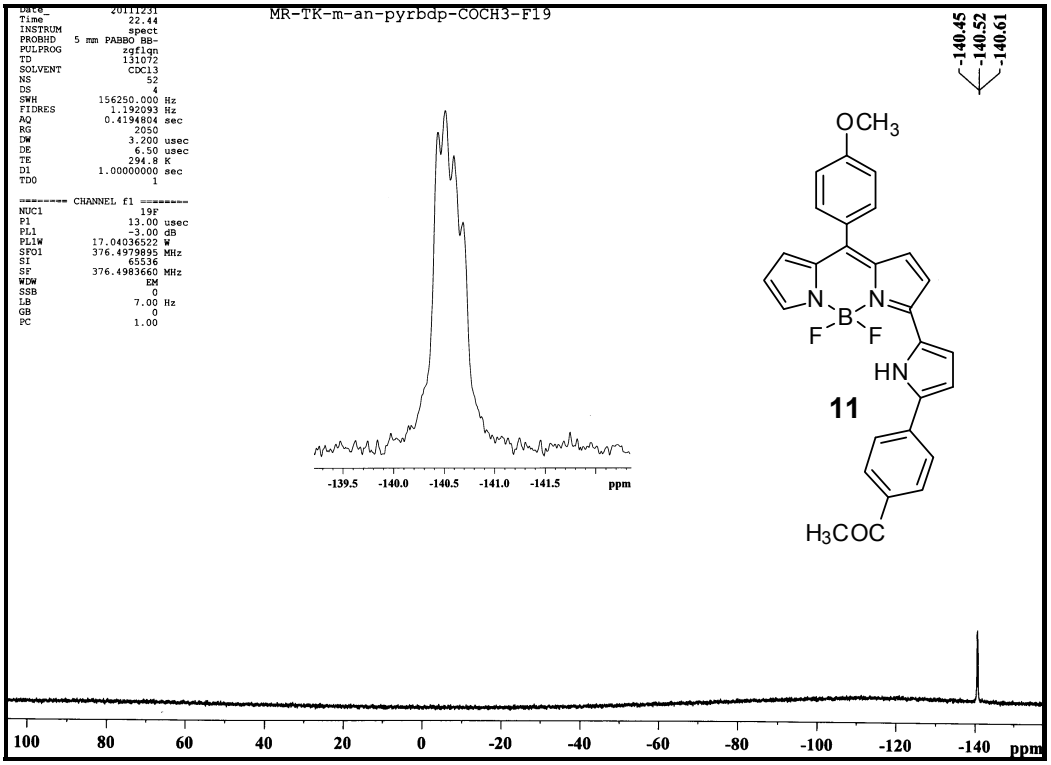


Figure 39: ^{19}F NMR spectrum of compound **11** recorded in $CDCl_3$

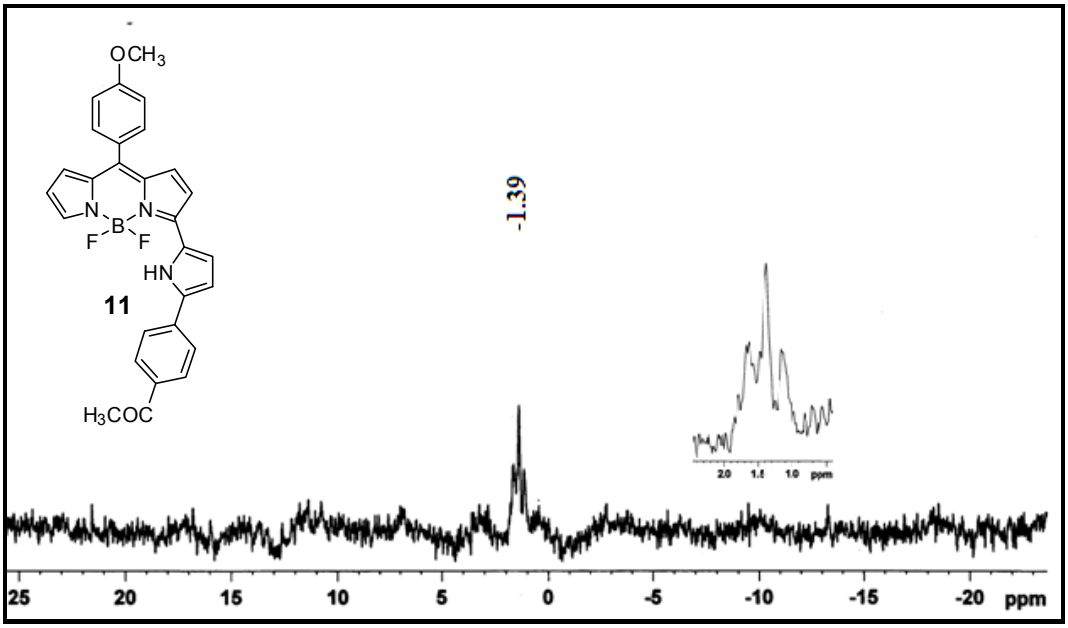


Figure 40: ^{11}B NMR spectrum of compound **11** recorded in $CDCl_3$

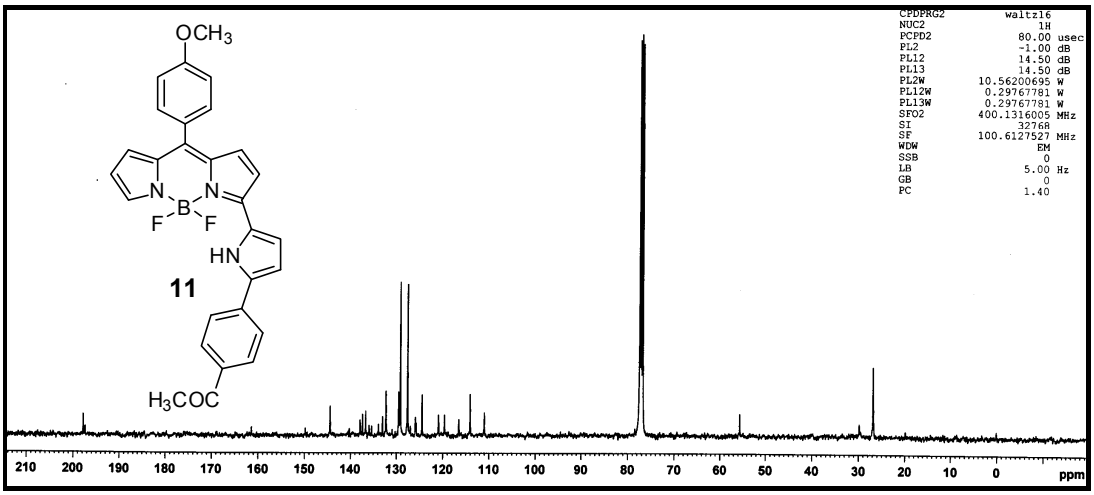
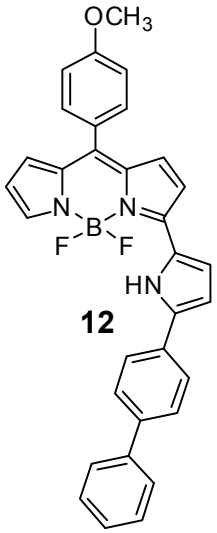


Figure 41: ^{13}C NMR spectrum of compound **11** recorded in $CDCl_3$



12

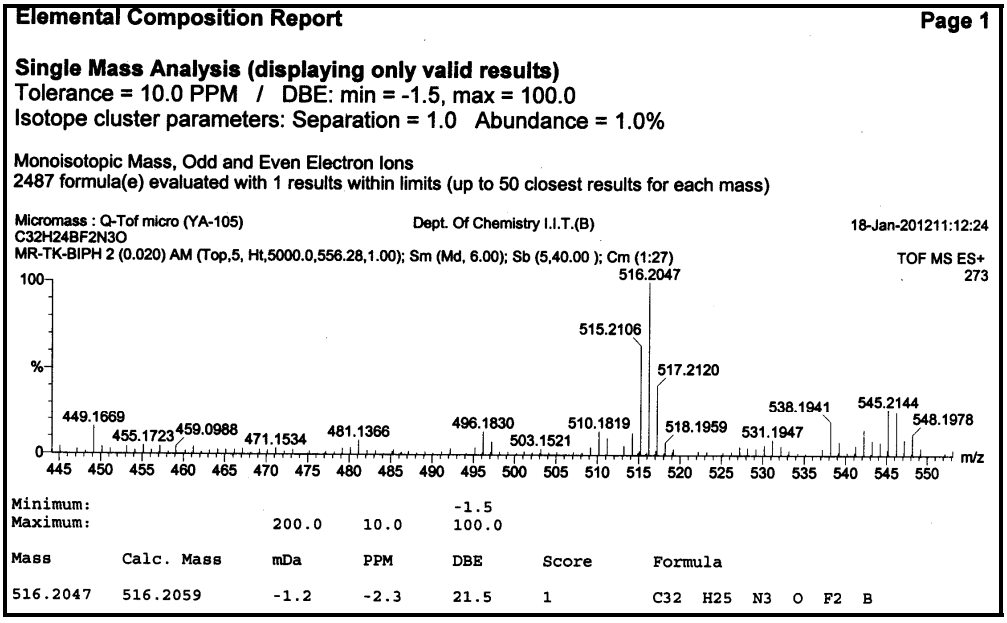


Figure 42: HRMS mass spectrum of compound **12**

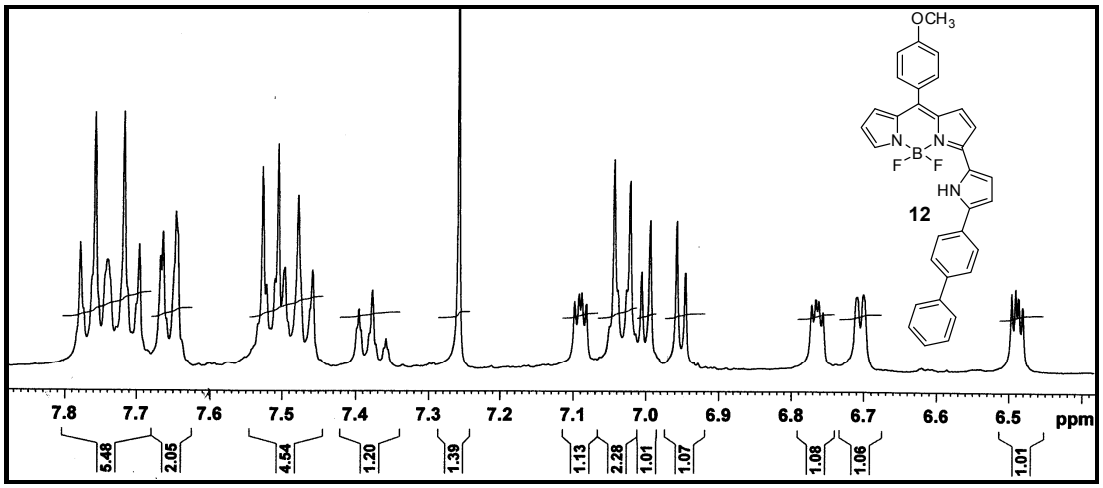


Figure 43: ^{1}H NMR spectrum of compound **12** in the selected region recorded in $CDCl_3$

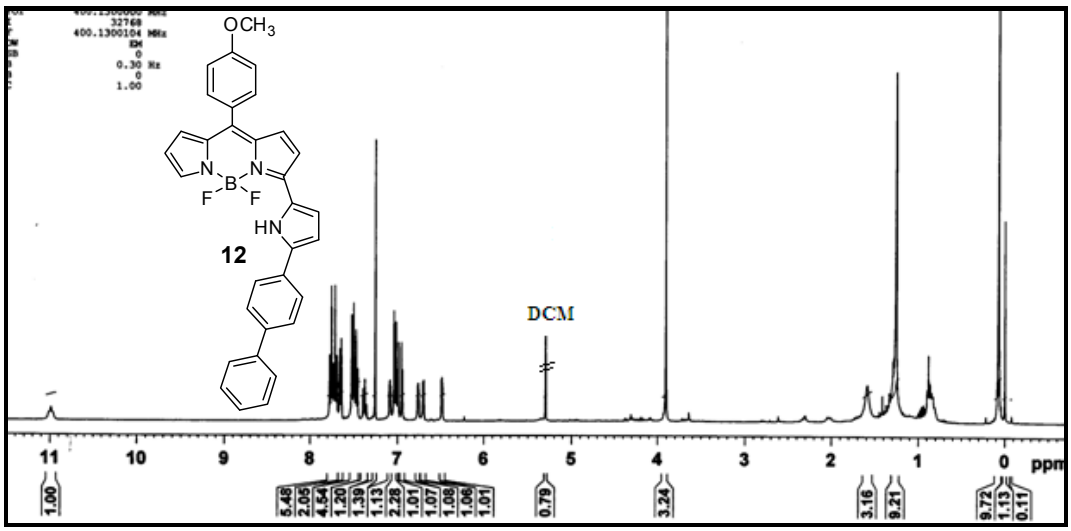


Figure 44: ^{1}H NMR spectrum of compound **12** recorded in $CDCl_3$

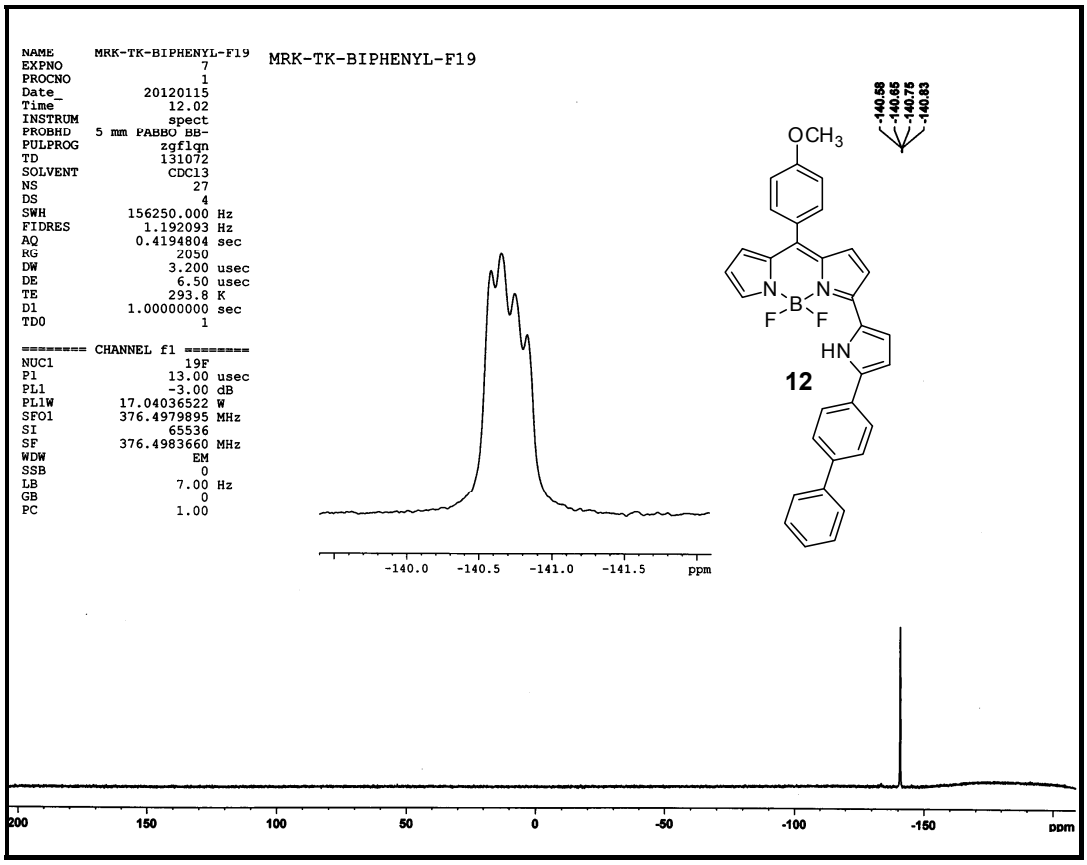


Figure 45: ^{19}F NMR spectrum of compound **12** recorded in $CDCl_3$

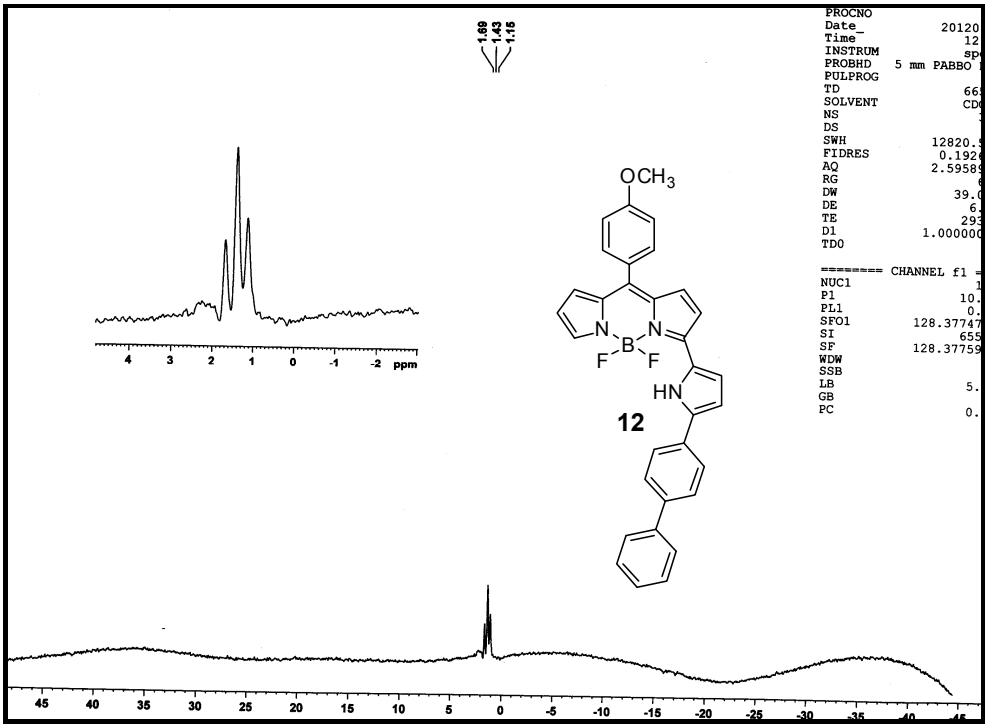


Figure 46: ^{11}B NMR spectrum of compound **12** recorded in $CDCl_3$

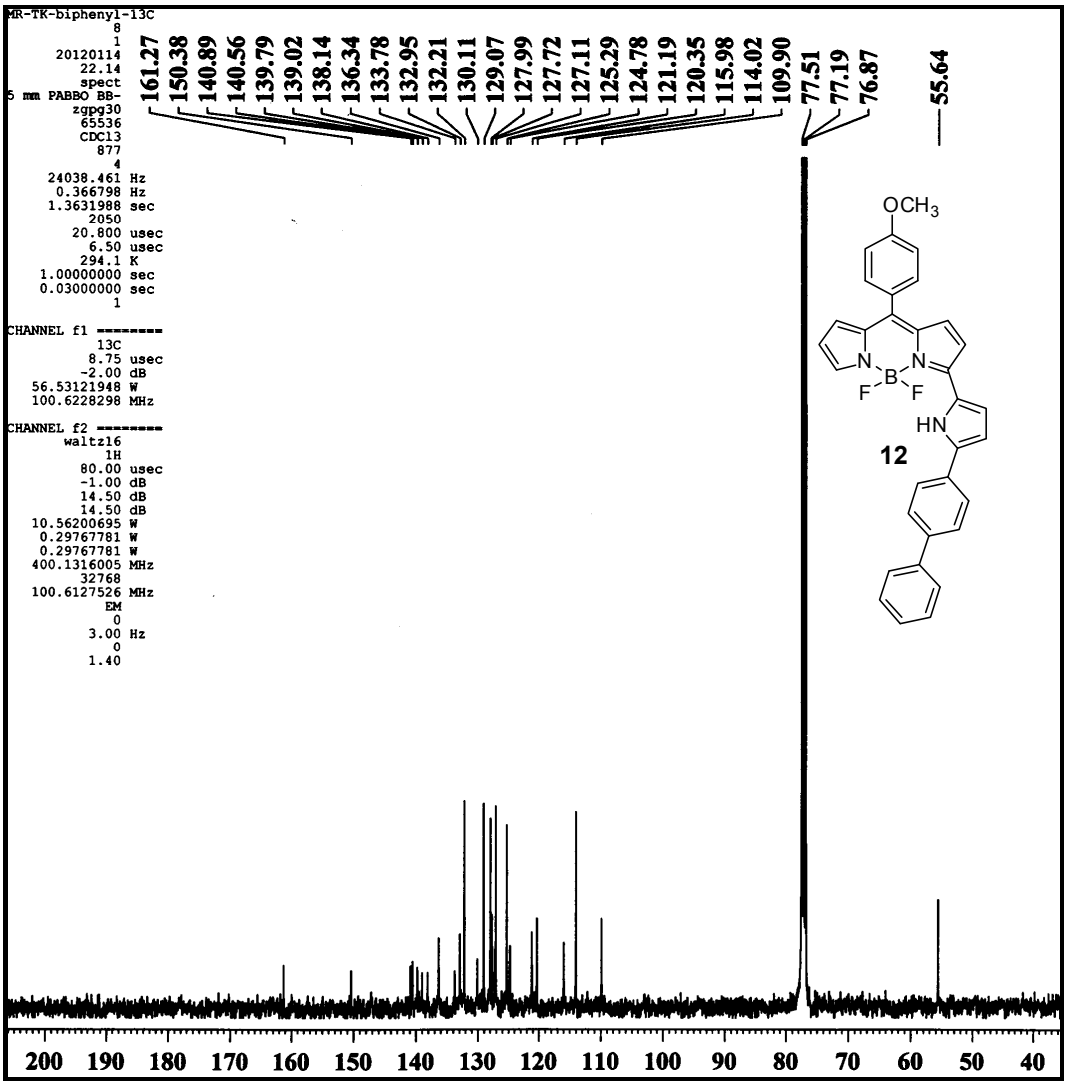
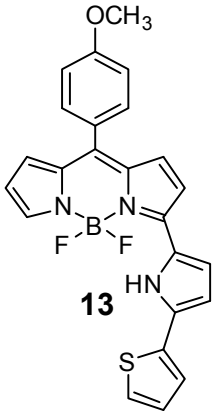


Figure 47: ^{13}C NMR spectrum of compound **12** recorded in $CDCl_3$ (δ in ppm)



13

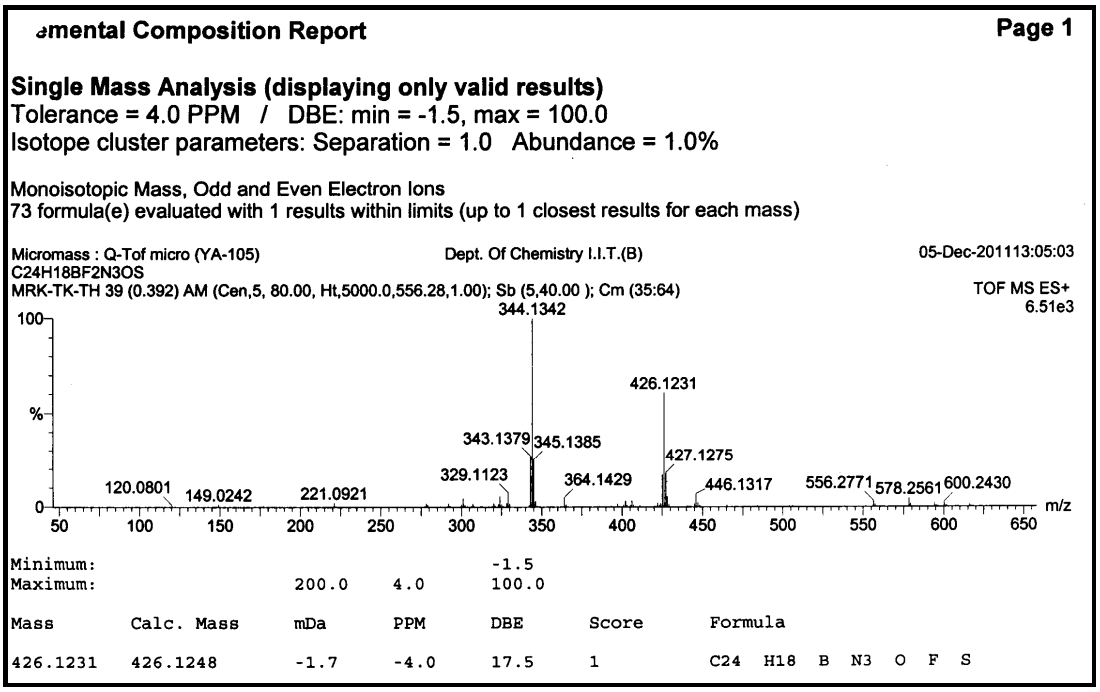


Figure 48: HRMS mass spectrum of compound **13**

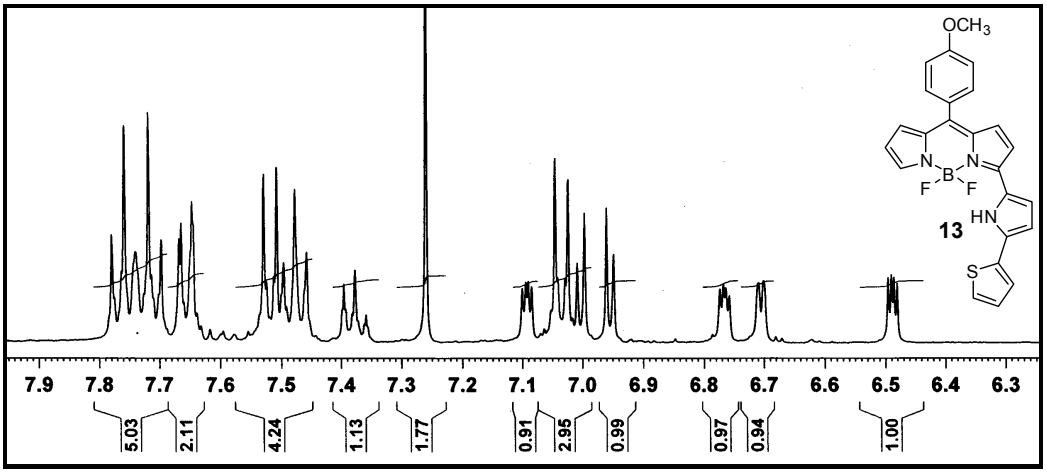


Figure 49: ^{1}H NMR spectrum of compound **13** in selected region recorded in $CDCl_3$

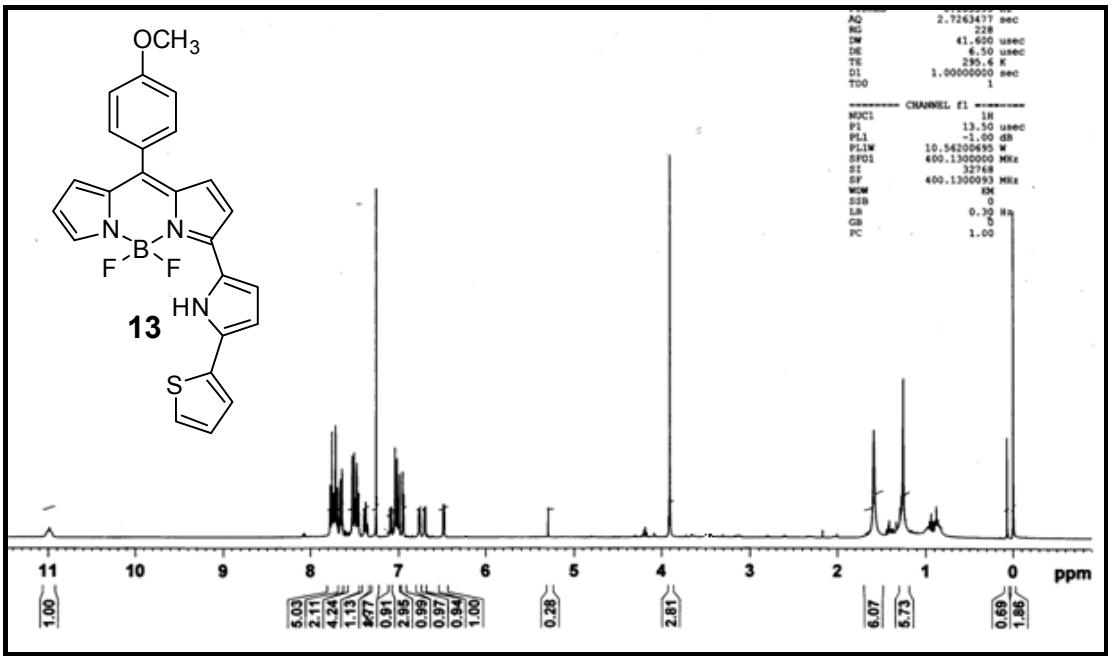


Figure 50: ^{1}H NMR spectrum of compound **13** recorded in $CDCl_3$

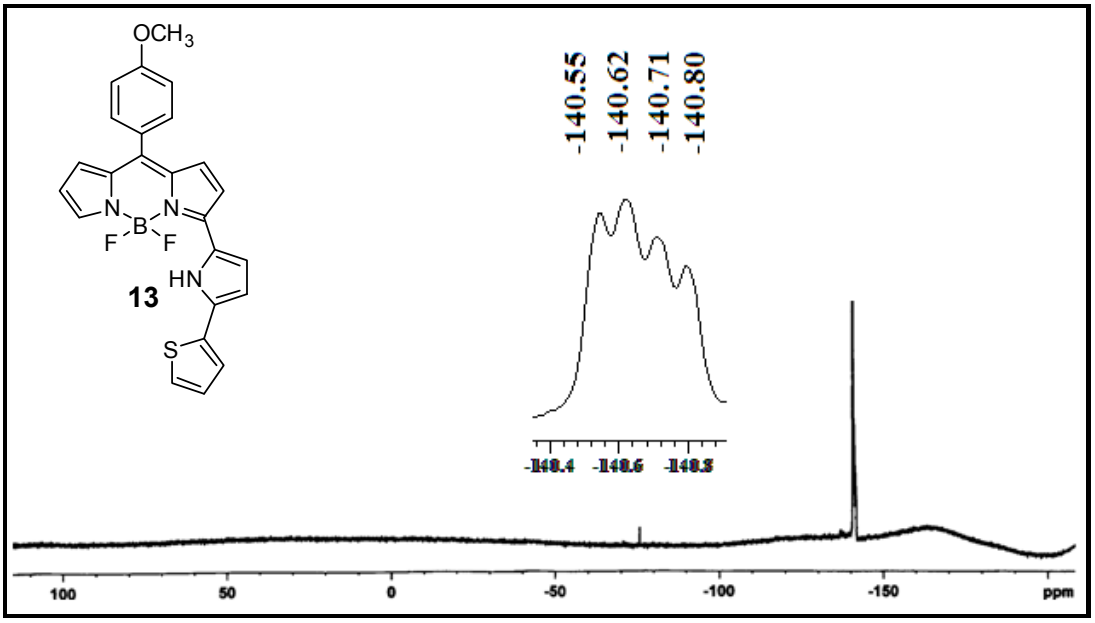


Figure 51: ^{19}F NMR spectrum of compound **13** recorded in $CDCl_3$

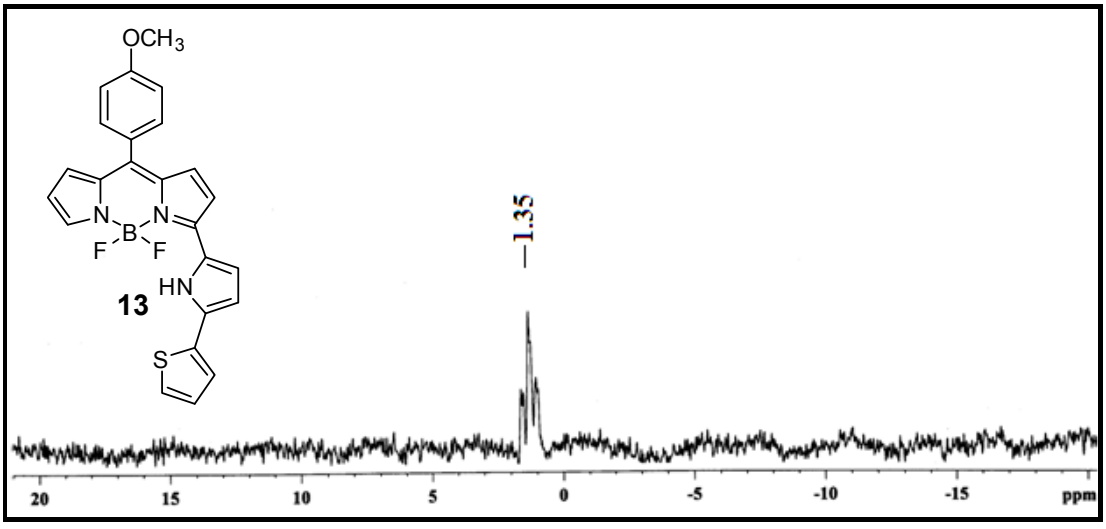


Figure 52: ^{11}B NMR spectrum of compound **13** recorded in $CDCl_3$

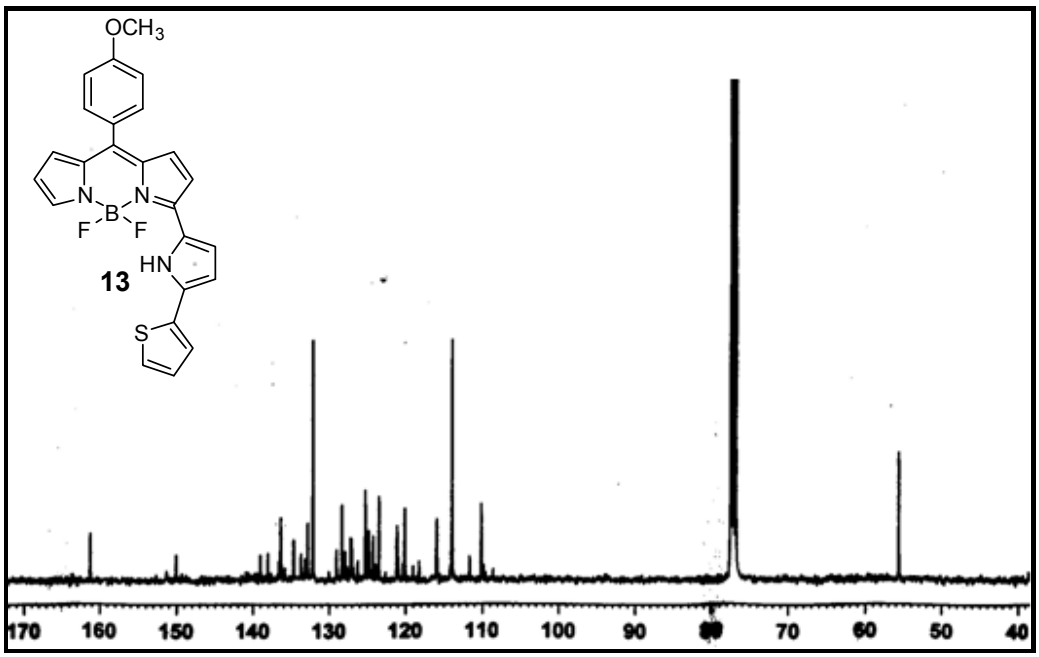
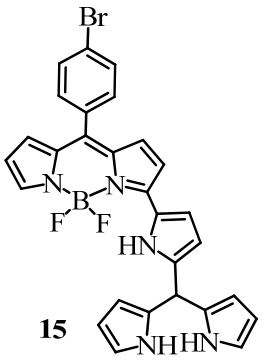


Figure 53: ^{13}C NMR spectrum of compound **13** recorded in $CDCl_3$



15

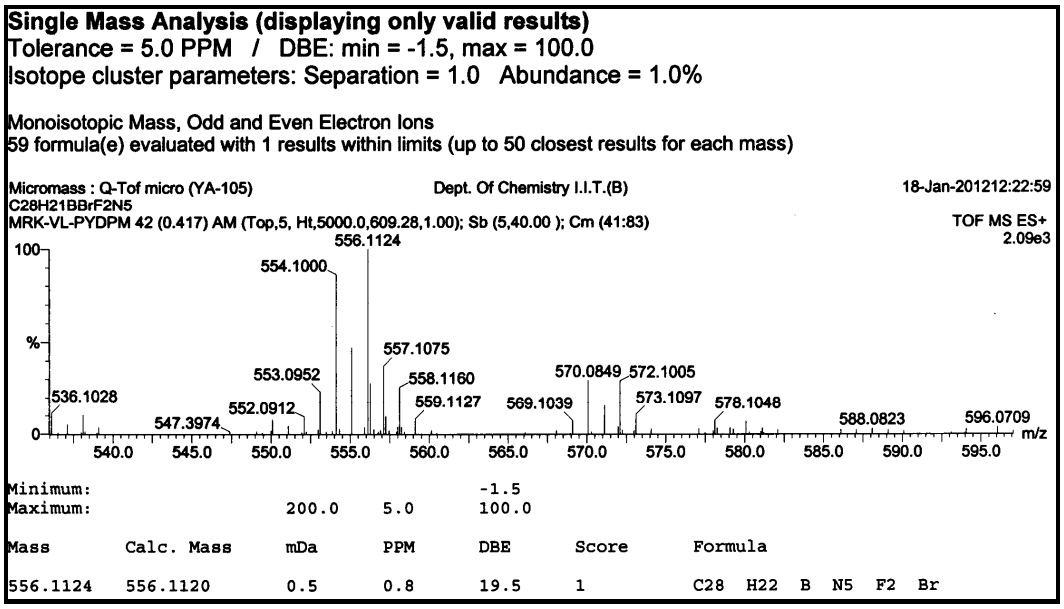


Figure 54: HRMS mass spectrum of compound **15**

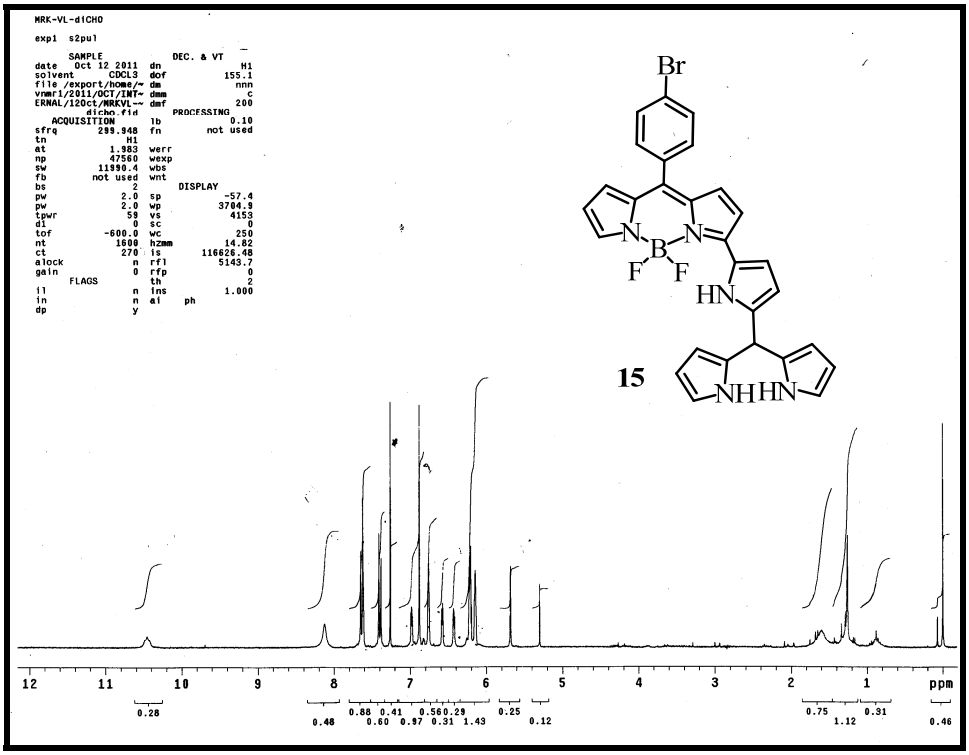


Figure 55 : ^{1}H NMR spectrum of compound **15** recorded in $CDCl_3$.

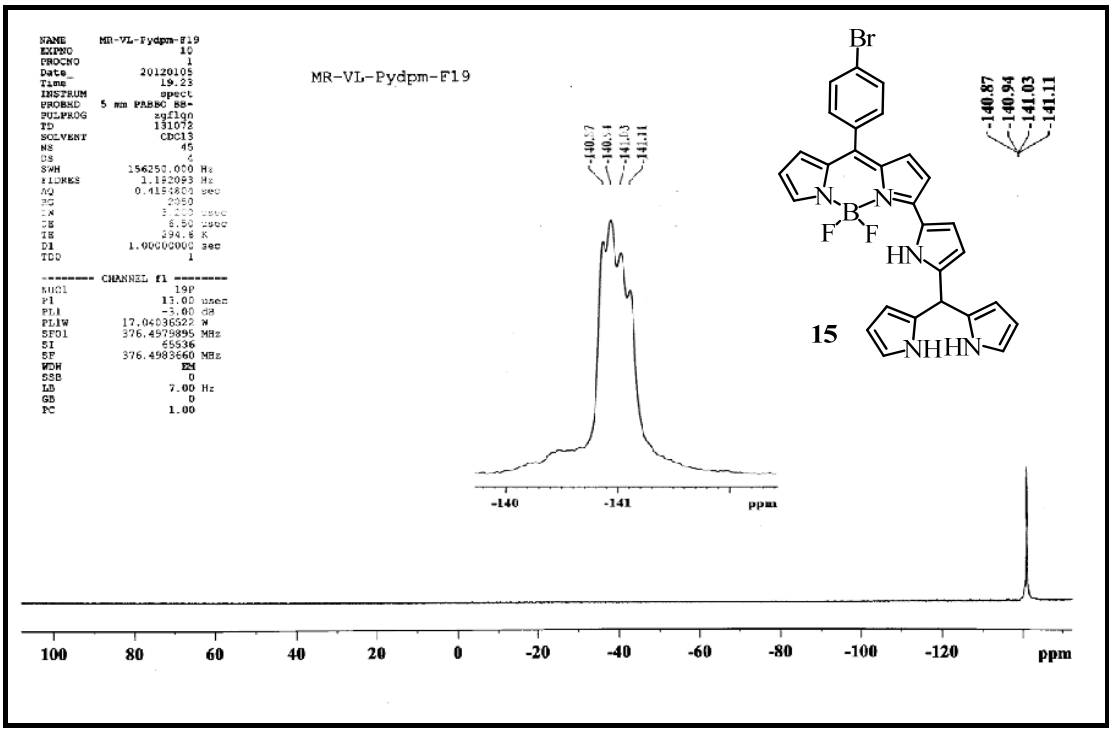


Figure 56 : ^{19}F NMR spectrum of compound **15** recorded in $CDCl_3$

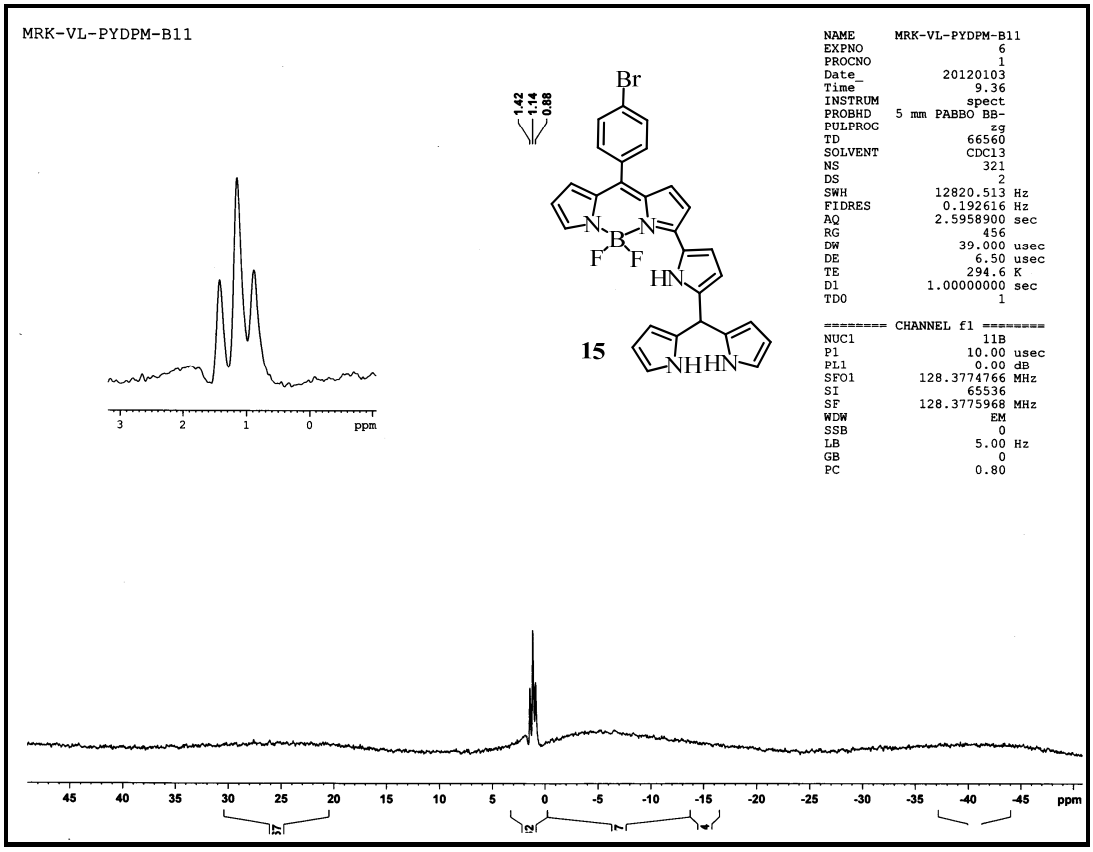


Figure 57 : ^{11}B NMR spectrum of compound **15** recorded in $CDCl_3$.

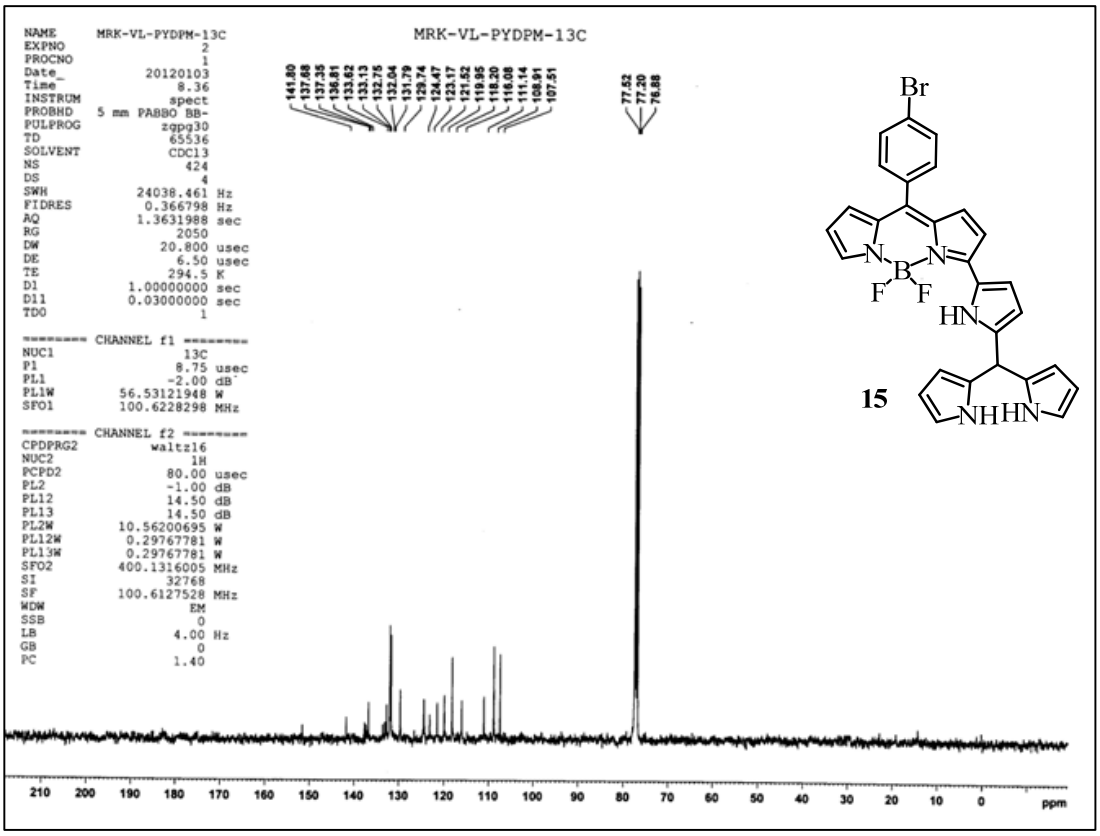
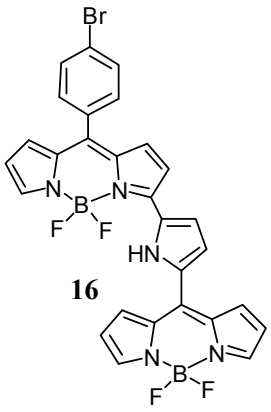


Figure 58 : ^{13}C NMR spectrum of compound **15** recorded in $CDCl_3$



16

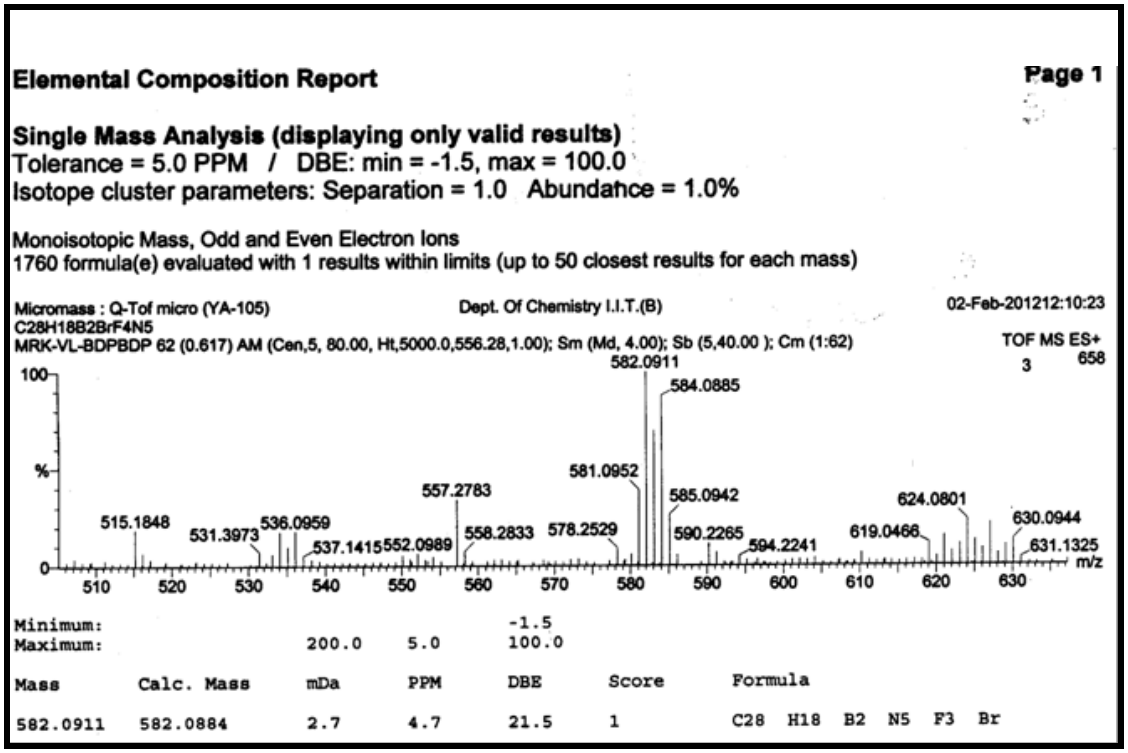


Figure 59 : HRMS spectrum of compound **16** recorded in $CDCl_3$

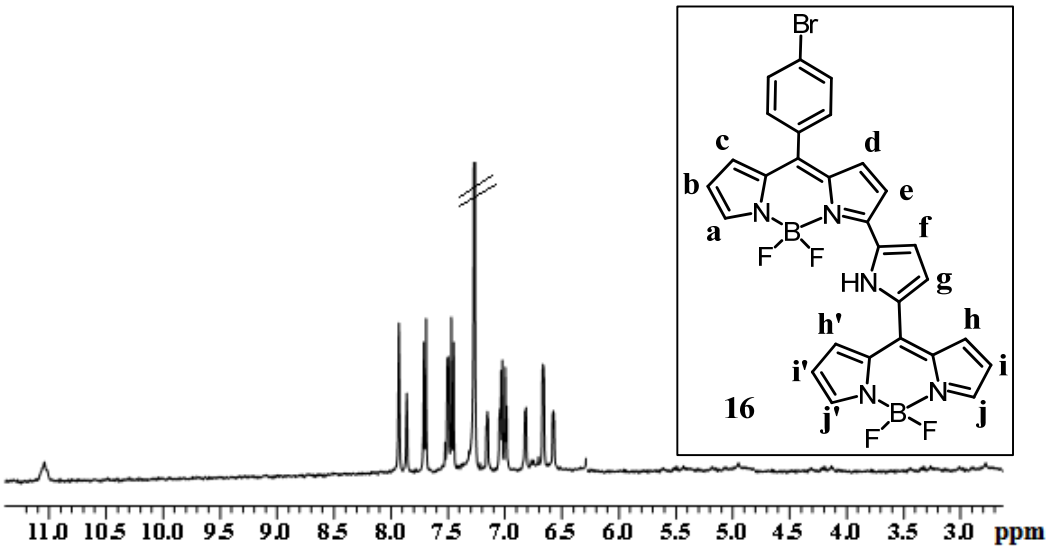


Figure 60 : ^{1}H NMR spectrum of compound **16** recorded in $CDCl_3$.

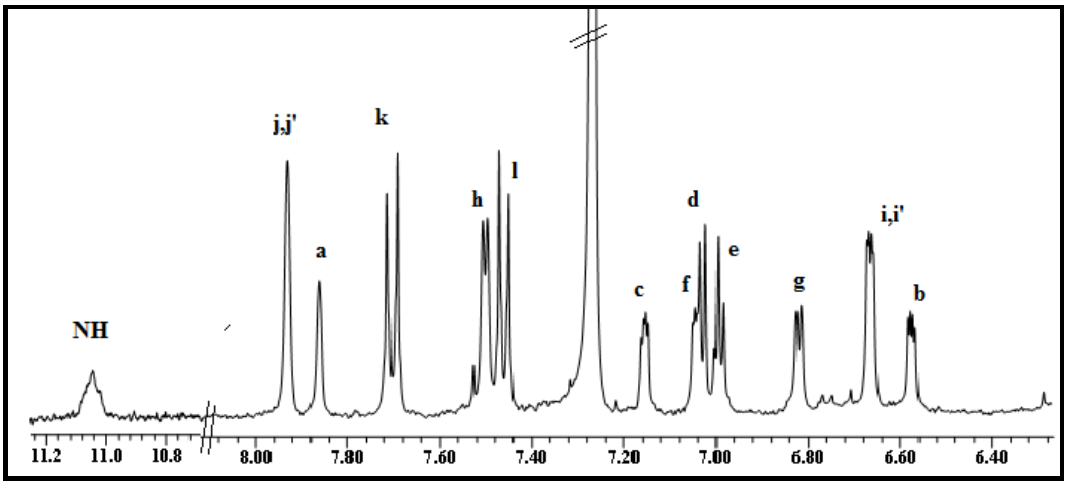


Figure 61 : ^{1}H NMR spectrum of compound **16** in selected region recorded in $CDCl_3$ (δ in ppm).

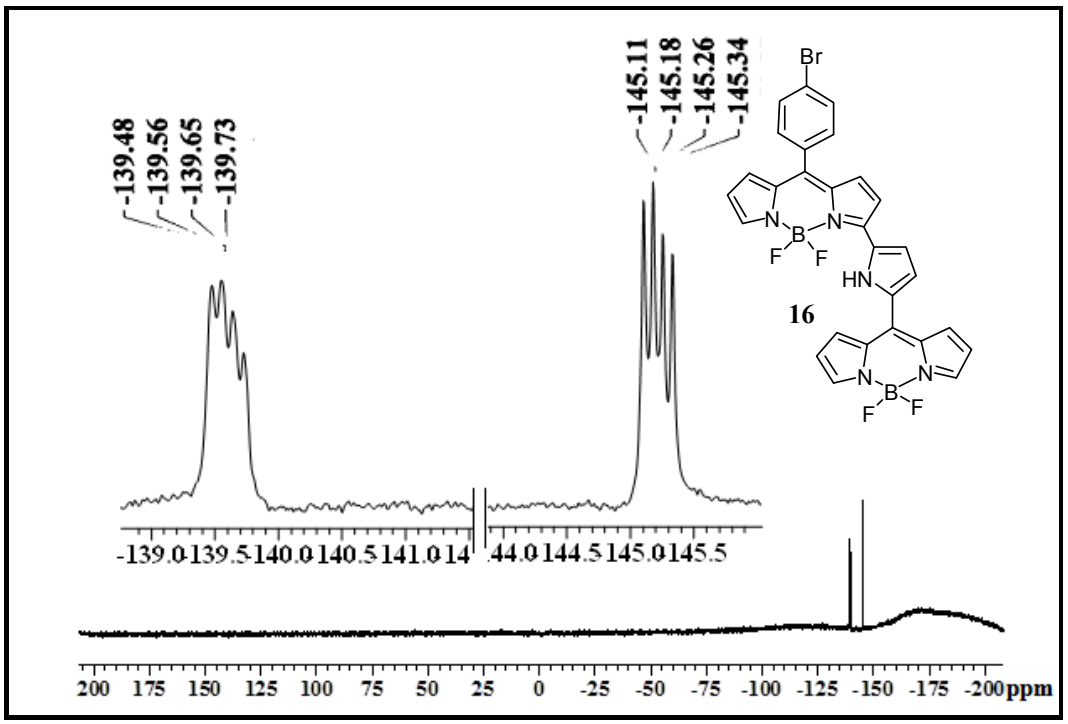


Figure 62: ^{19}F NMR spectrum of compound **16** recorded in $CDCl_3$.

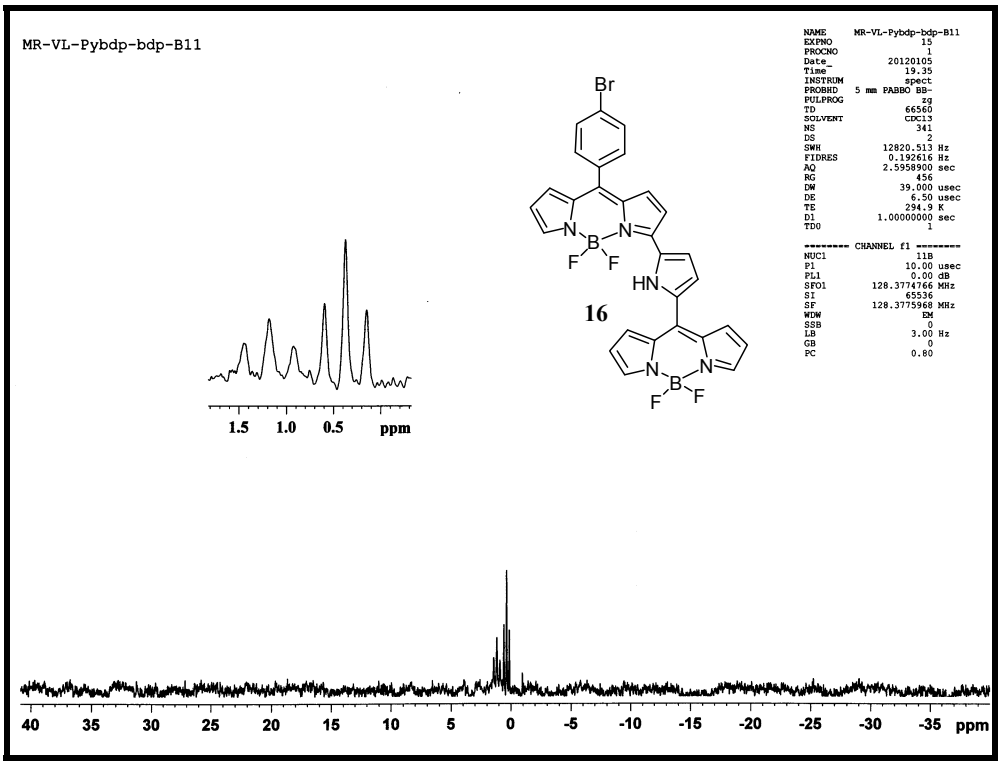


Figure 63: ^{11}B NMR spectrum of compound **16** recorded in $CDCl_3$.

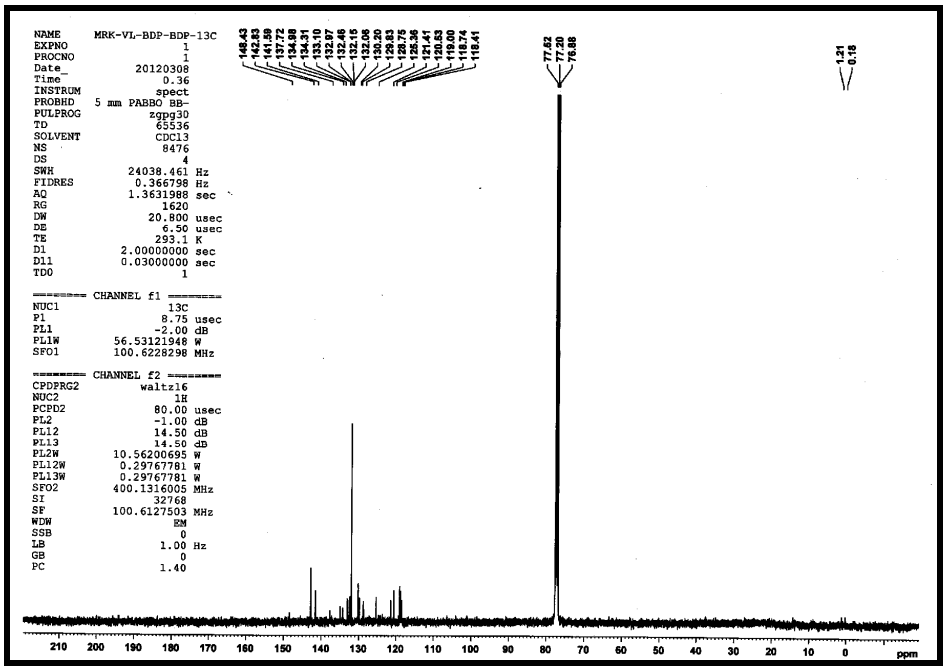


Figure 64 : ^{13}C NMR spectrum of compound **16** recorded in $CDCl_3$

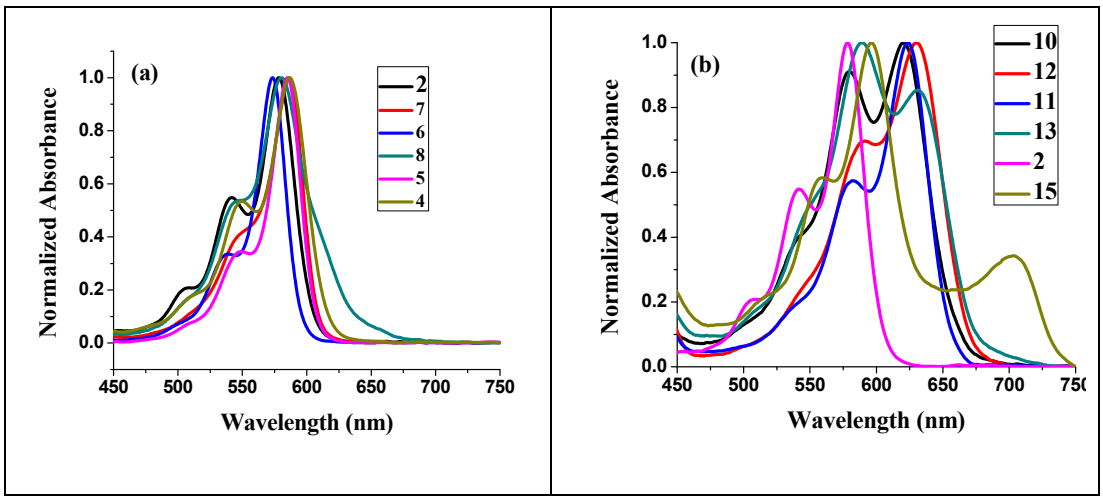


Figure 65: Comparison of normalized absorption spectra of (a) functionalized 3-pyrrolyl BODIPYs and (b) aryl substituted 3-pyrrolyl BODIPYs recorded in $CHCl_3$.

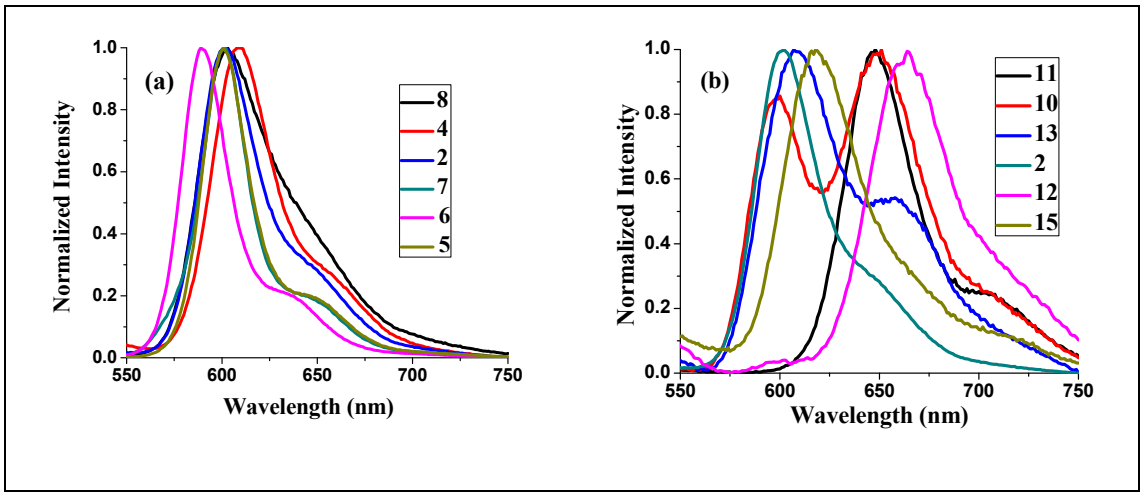


Figure 66: Comparison of normalized emission spectra of (a) functionalized 3-pyrrolyl BODIPYs and (b) aryl substituted 3-pyrrolyl BODIPYs recorded in $CHCl_3$ using λ_{exc} = 488 nm.

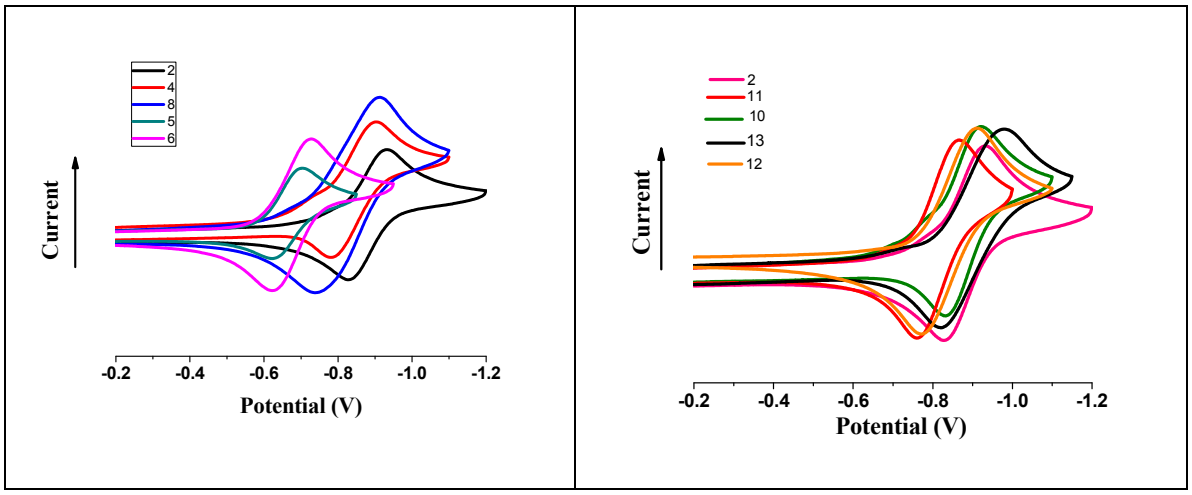


Figure 67: Comparison of the first reduction waves of cyclic voltammograms of compounds **2-13** at 50 mV s^{-1} scan rate recorded in CH_2Cl_2 containing 0.1 M Tetrabutylammonium perchlorate as supporting electrolyte.

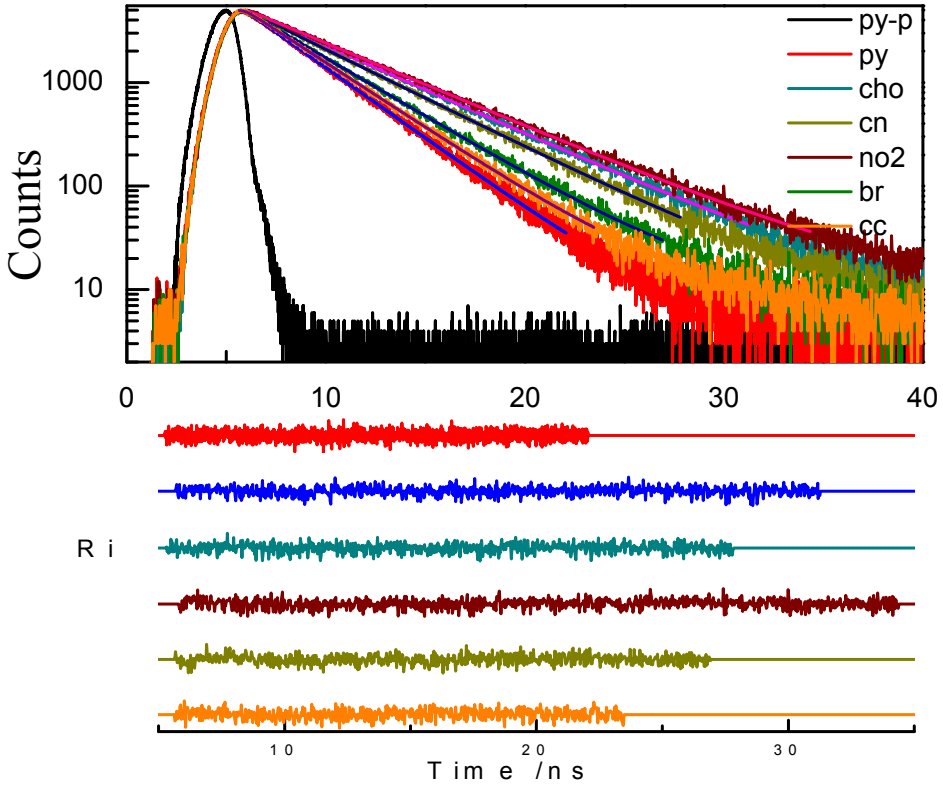


Figure 68: Fluorescence decay profile and weighted, residual, distribution fit of compounds **2** along with **4-8** in chloroform. The excitation wavelength used was 560 nm collected at corresponding wavelengths.

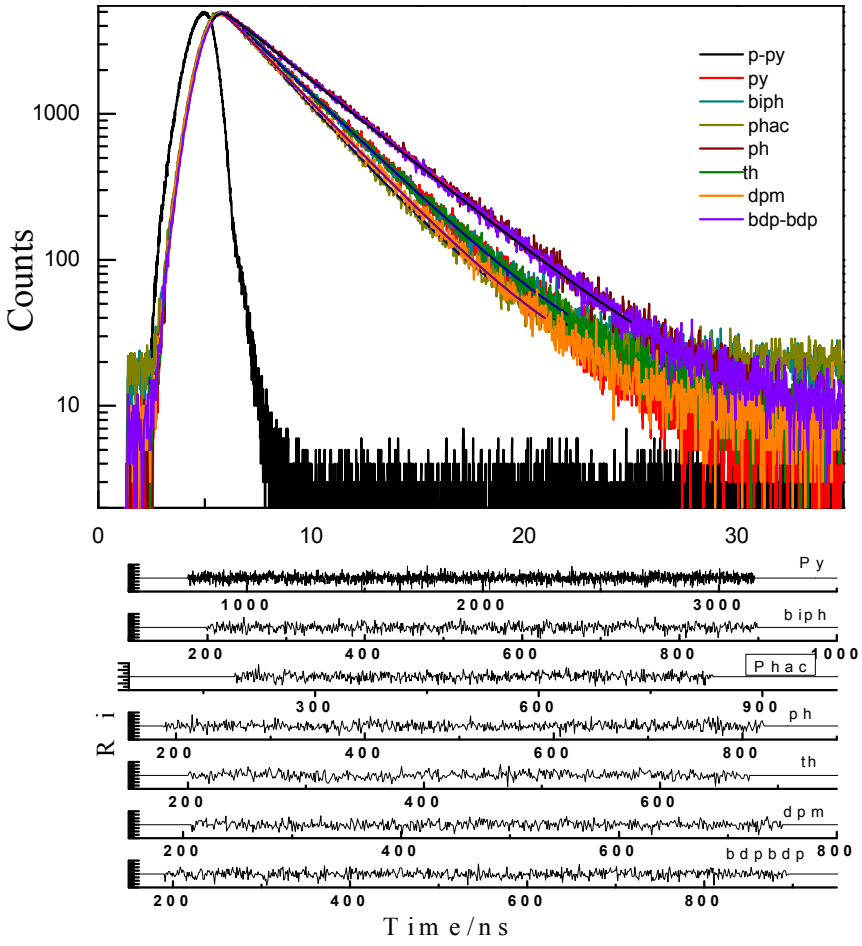


Figure 69: Fluorescence decay profile and weighted, residual, distribution fit of compounds **2** along with **10-16** in chloroform. The excitation wavelength used was 560 nm collected at corresponding wavelengths.