

Synthesis of Conjugated BODIPYs via the Wittig Reaction

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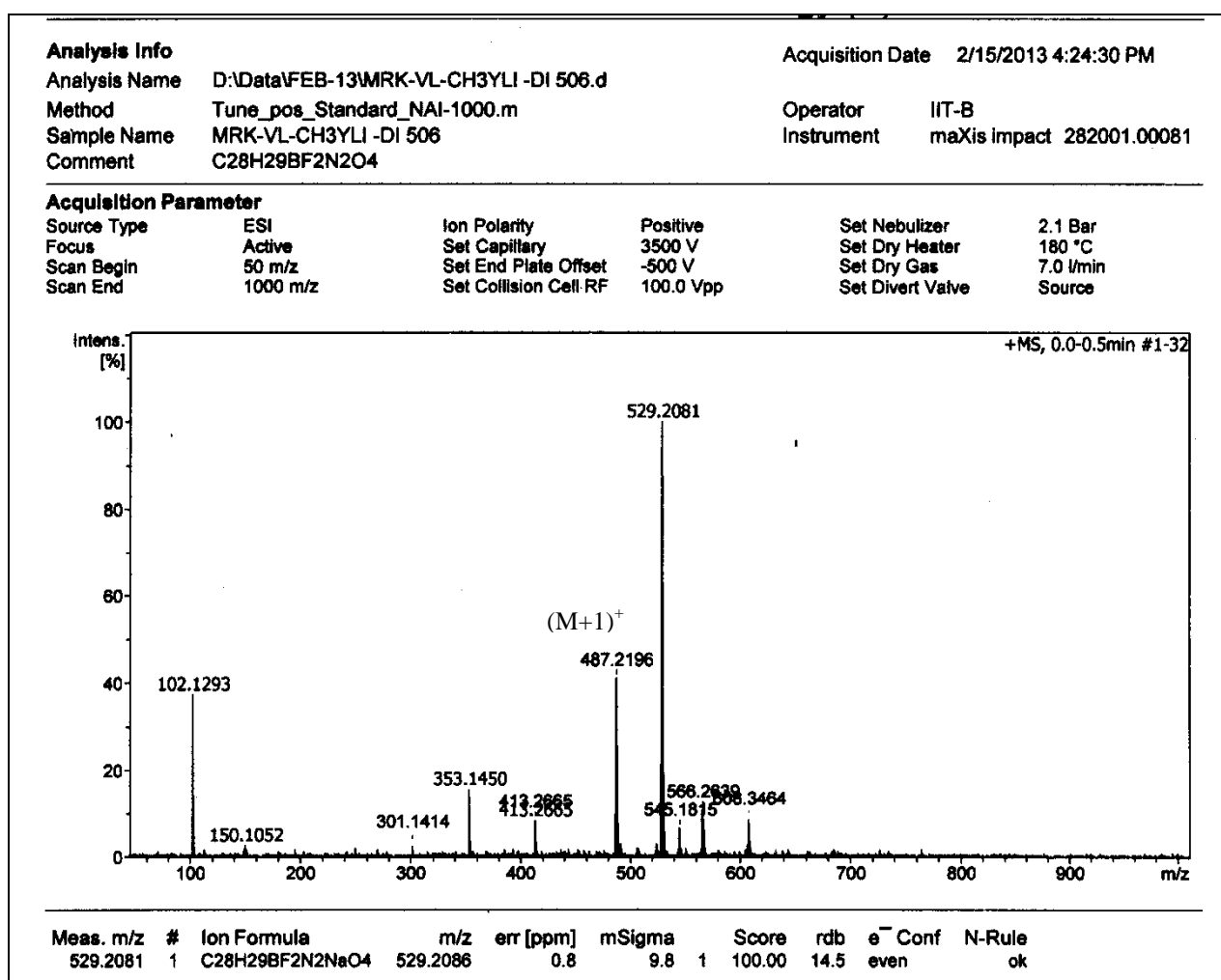
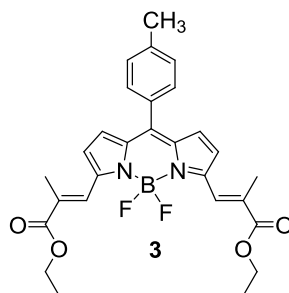


Figure 1: HRMS mass spectrum of compound 3

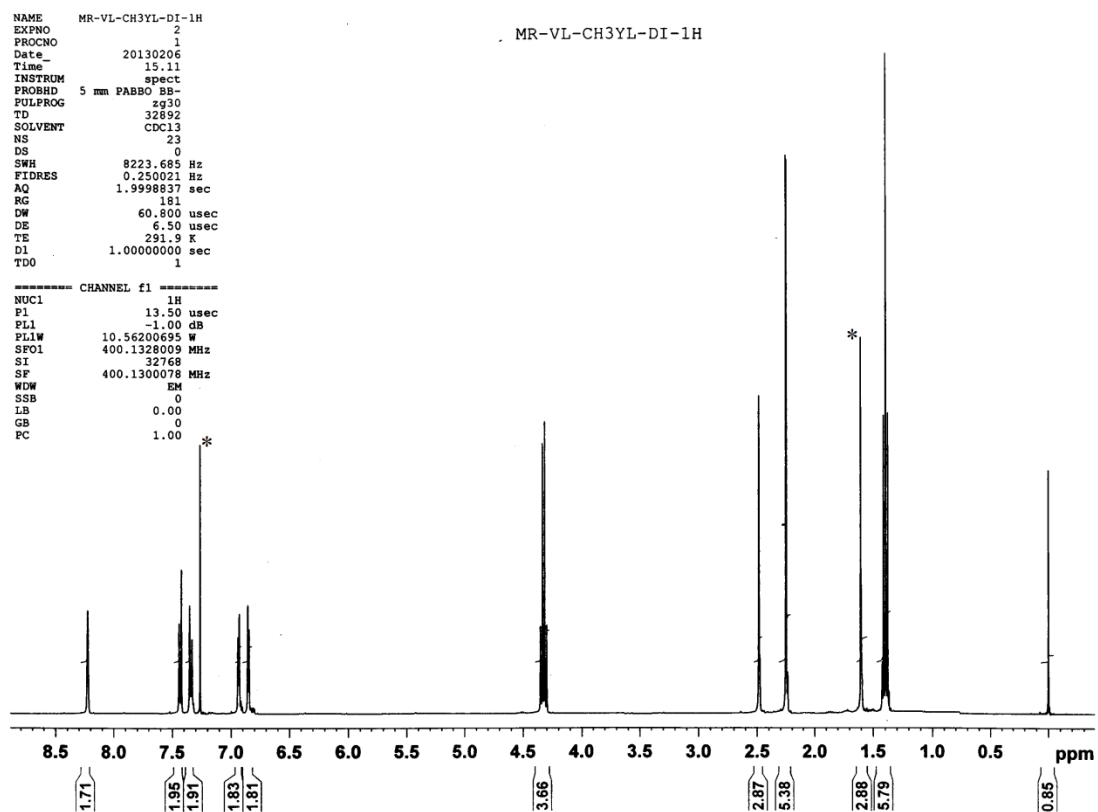


Figure 2: ^1H NMR spectrum of compound 3 in CDCl_3

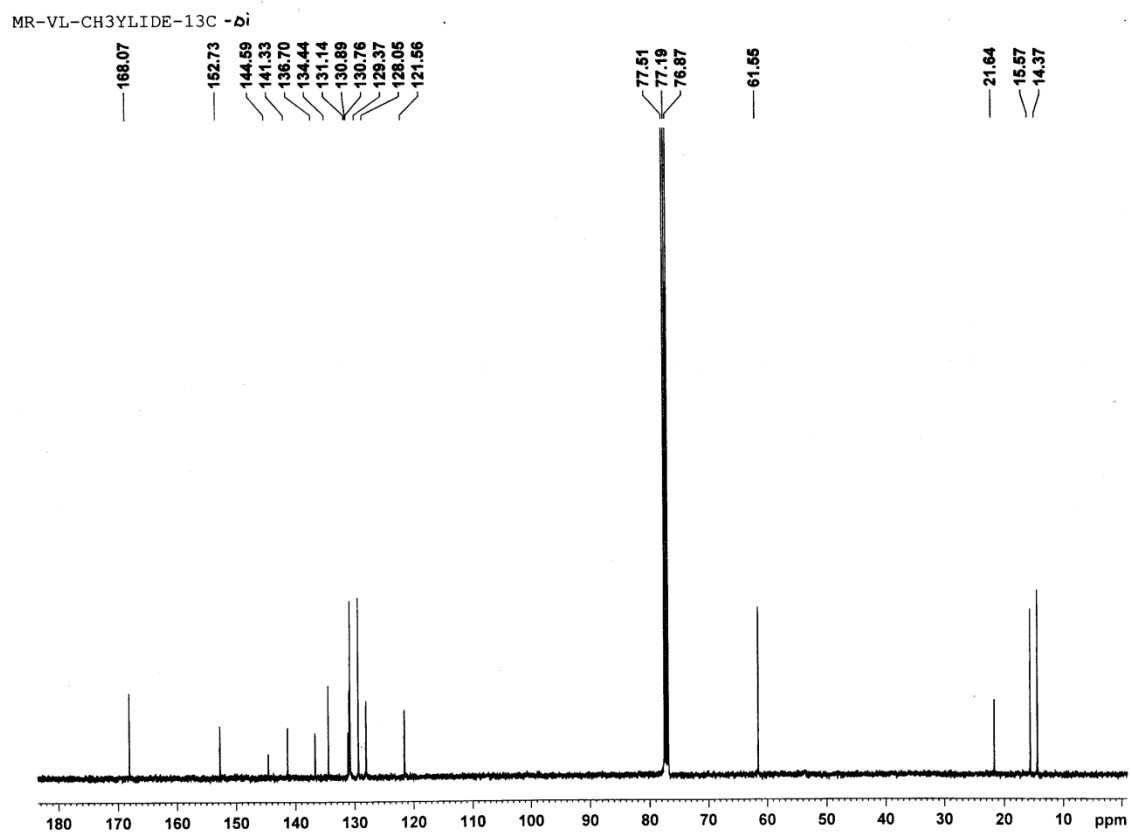


Figure 3: ^{13}C NMR spectrum of compound **3** in CDCl_3

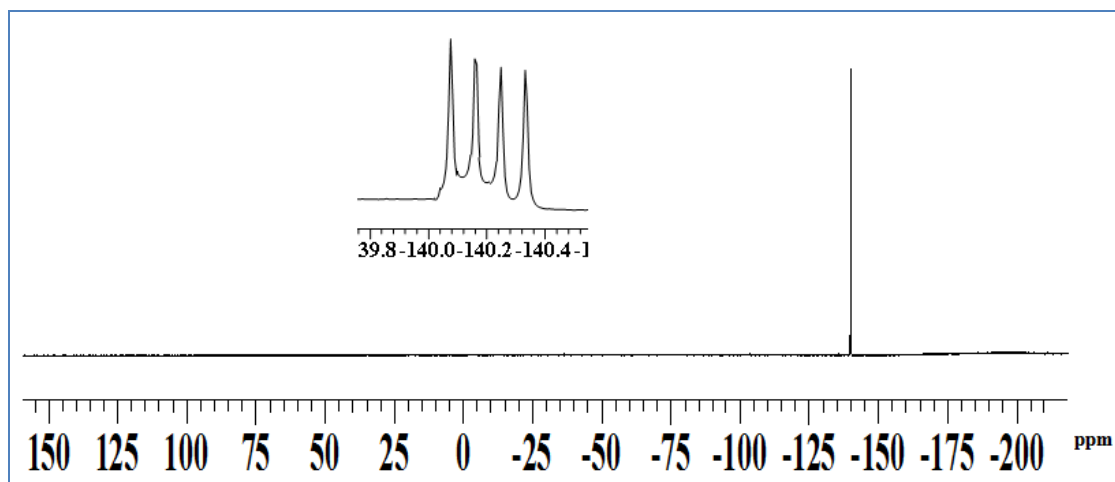


Figure 4: ^{19}F NMR spectrum of compound **3** in CDCl_3 . The inset shows the expansion

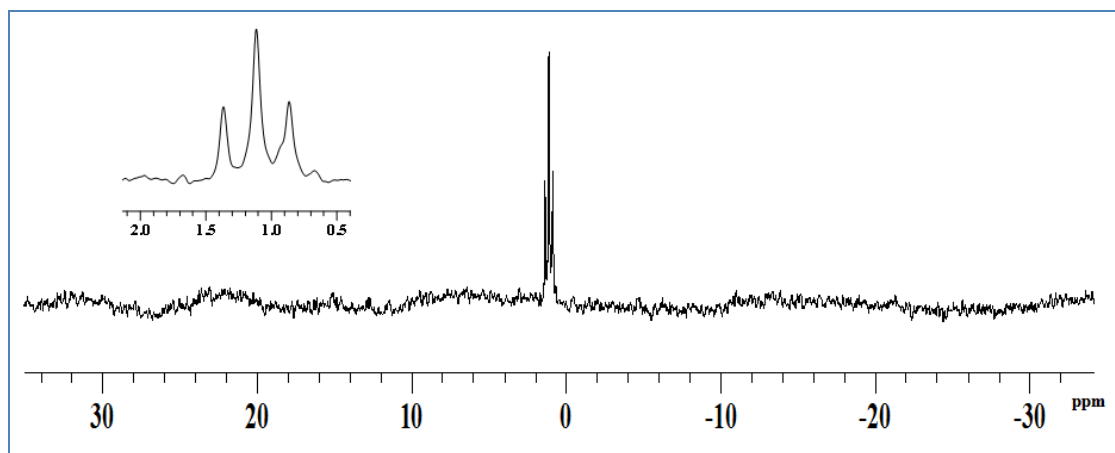


Figure 5: ^{11}B NMR spectrum of compound **3** in CDCl_3 . The inset shows the expansion

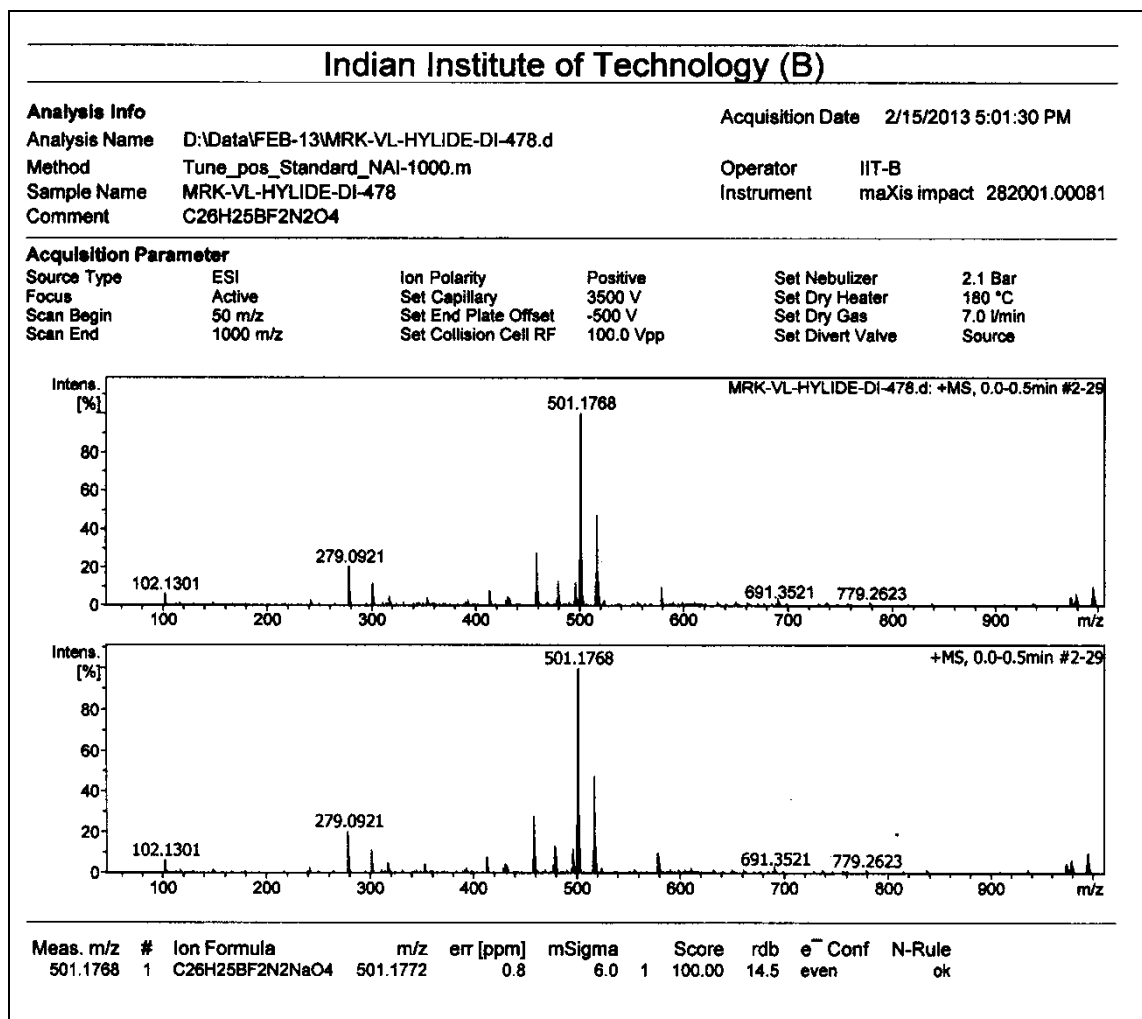
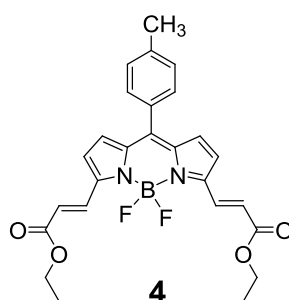


Figure 6: HRMS mass spectrum of compound 4

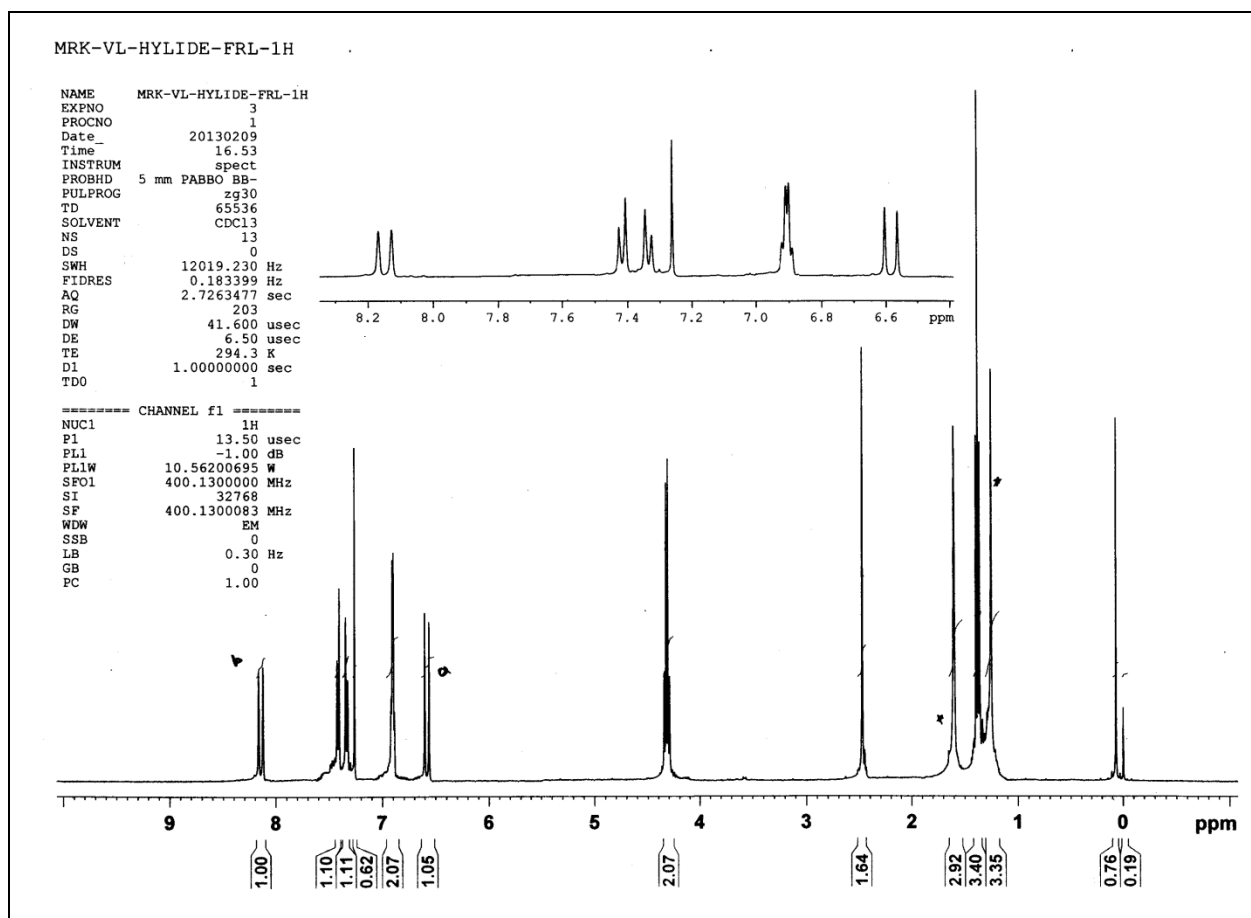


Figure 7: ^1H NMR spectrum of compound **4** in CDCl_3

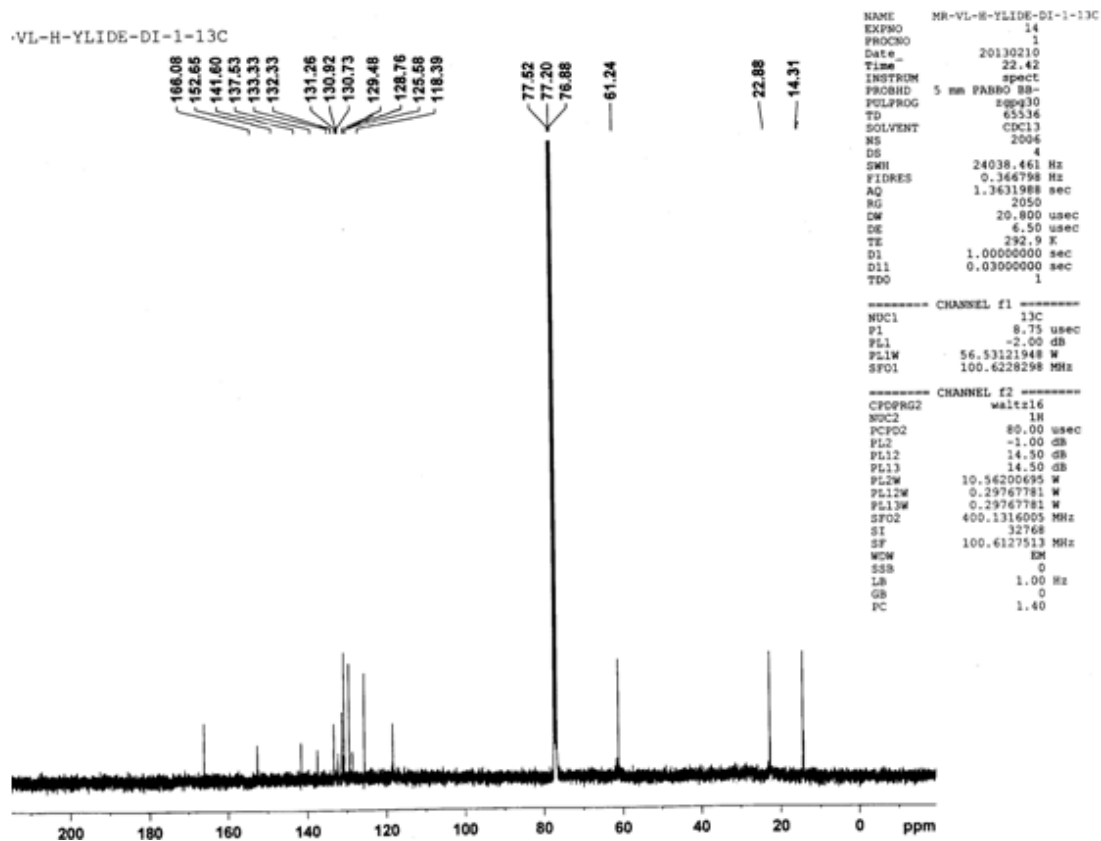


Figure 8: ^{13}C NMR spectrum of compound **4** in CDCl_3

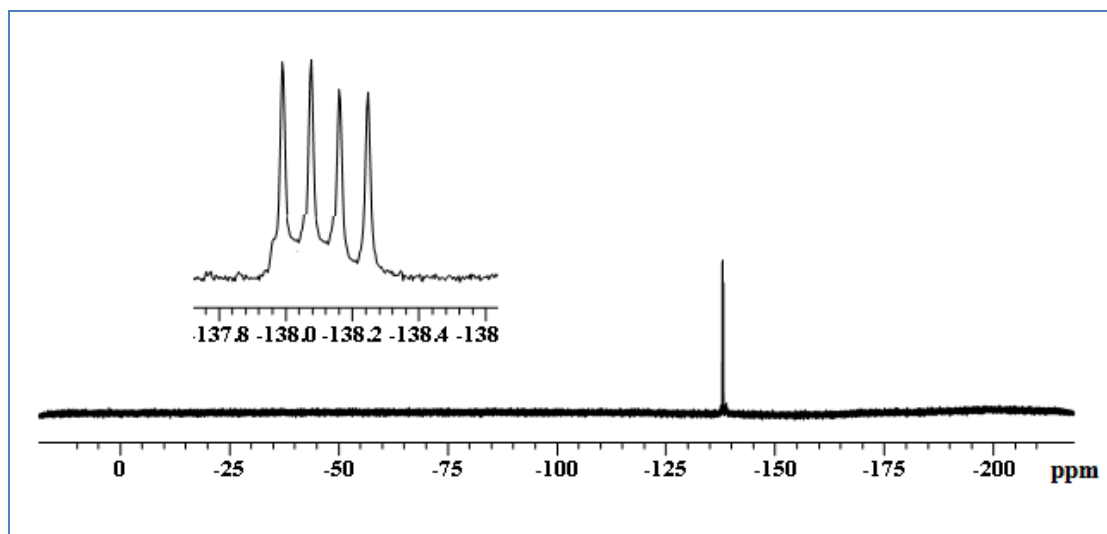


Figure 9: ^{19}F NMR spectrum of compound **4** in CDCl_3 . The inset shows the expansion

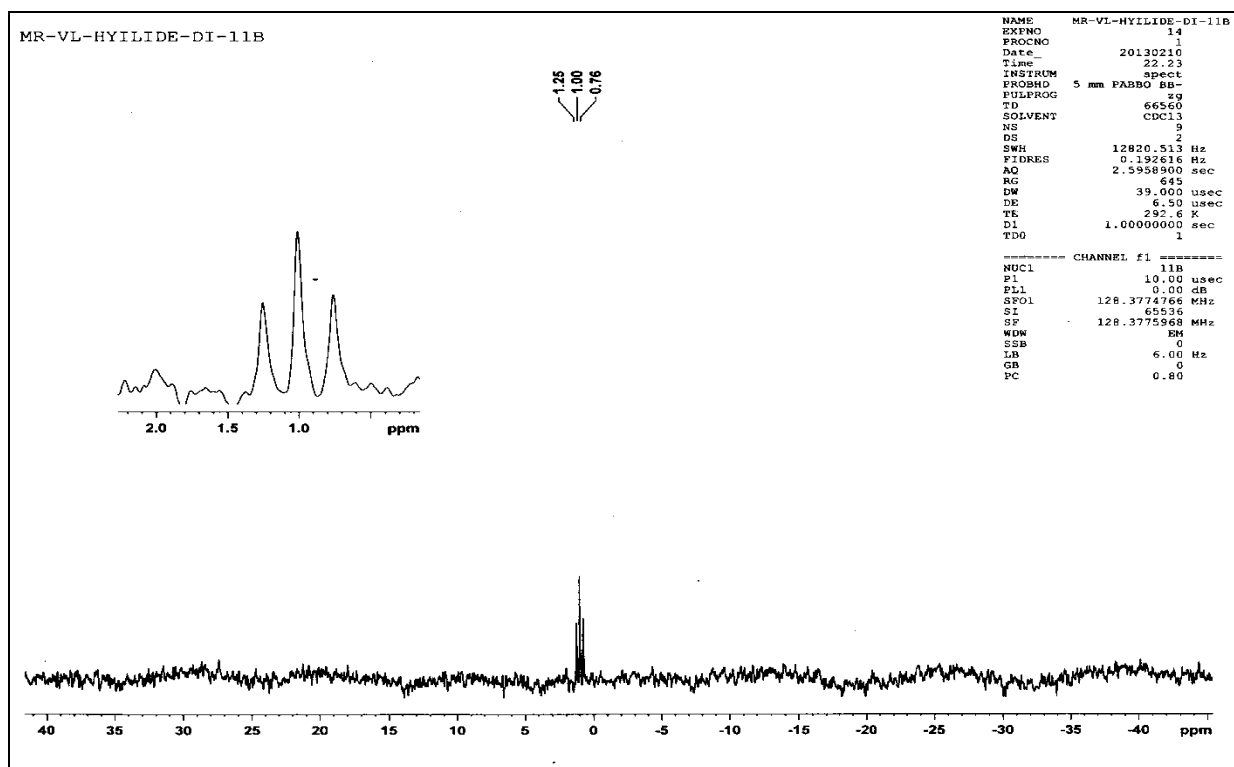


Figure 10: ^{11}B NMR spectrum of compound **4** in CDCl_3 . The inset shows the expansion

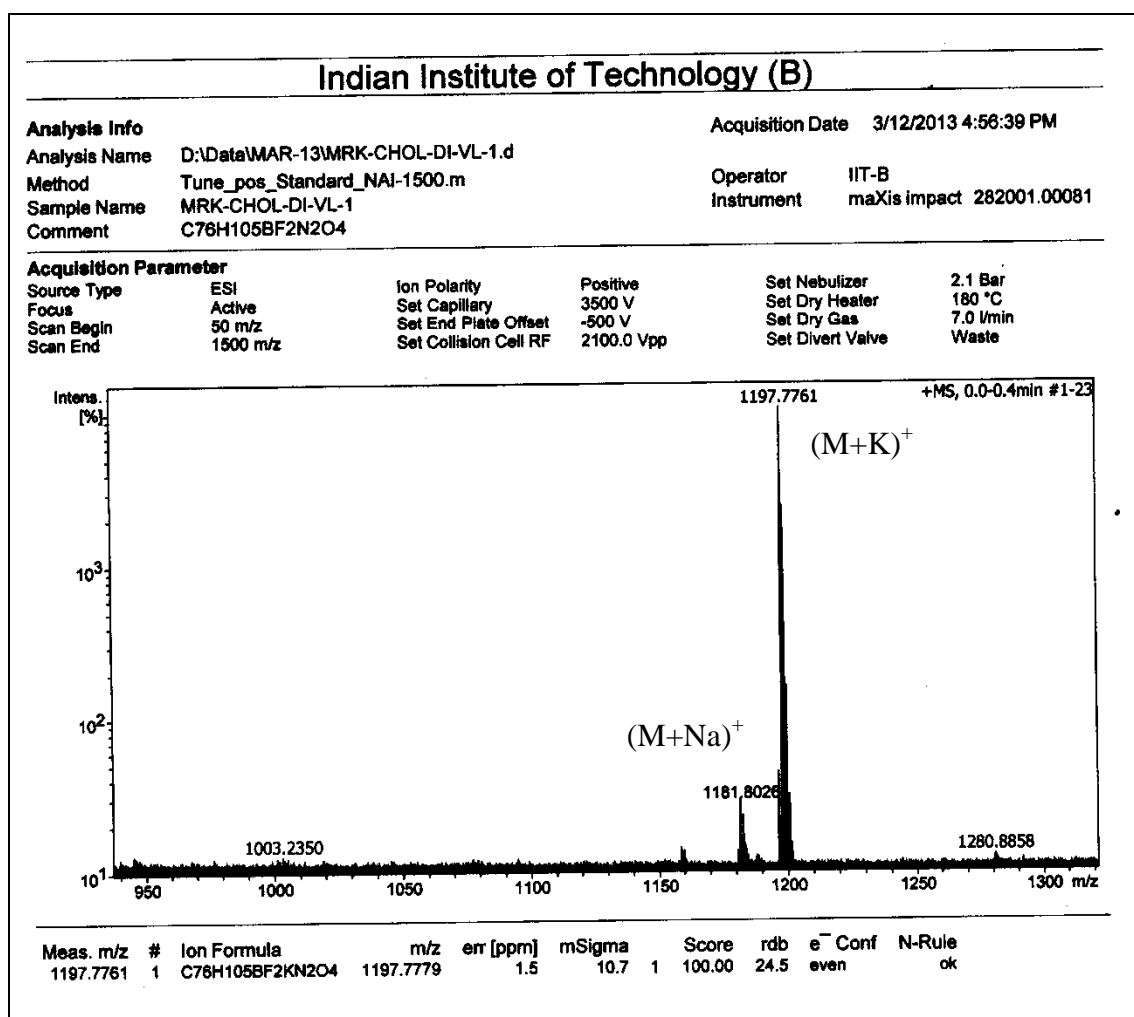
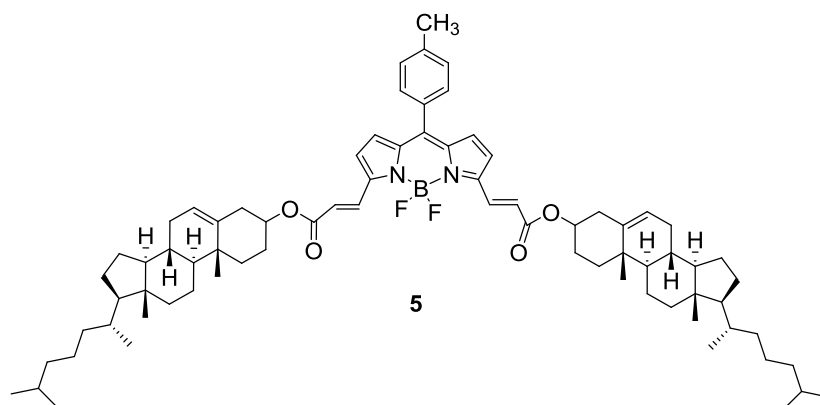


Figure 11: HRMS mass spectrum of compound 5 in CDCl₃.

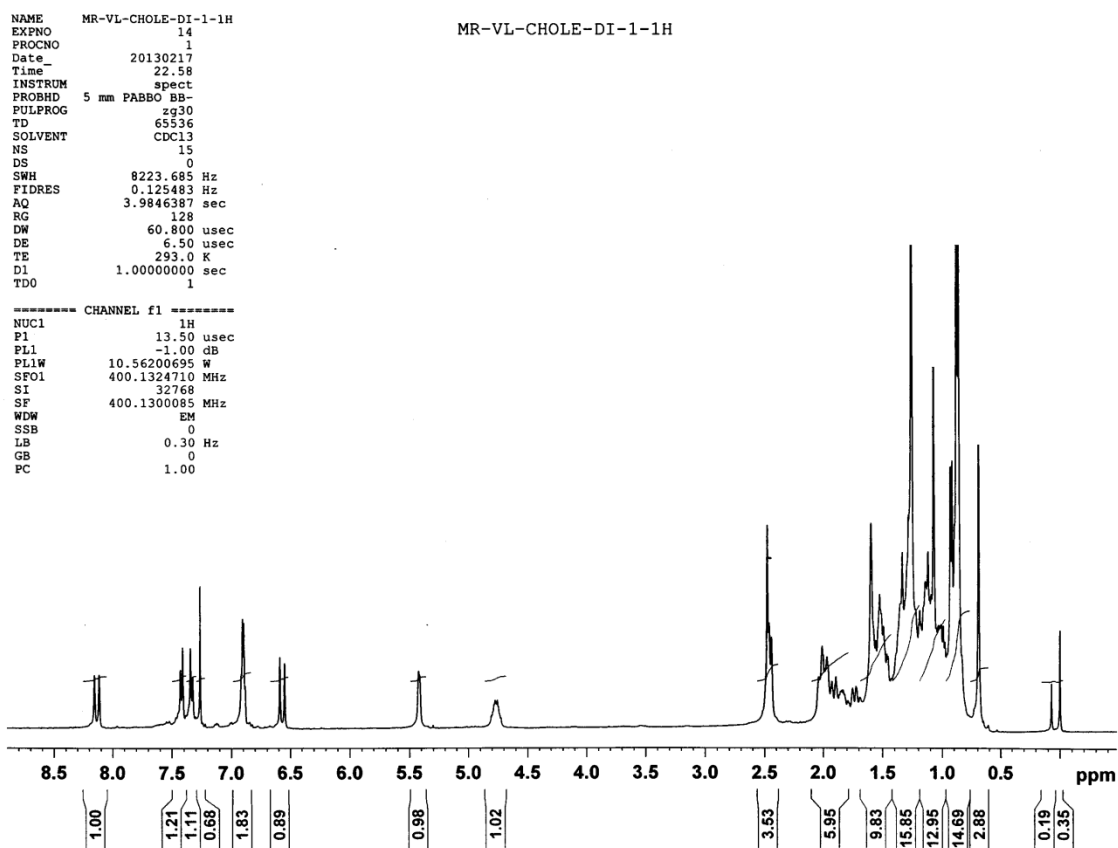


Figure 12: ^1H NMR spectrum of compound **5** in CDCl_3 .

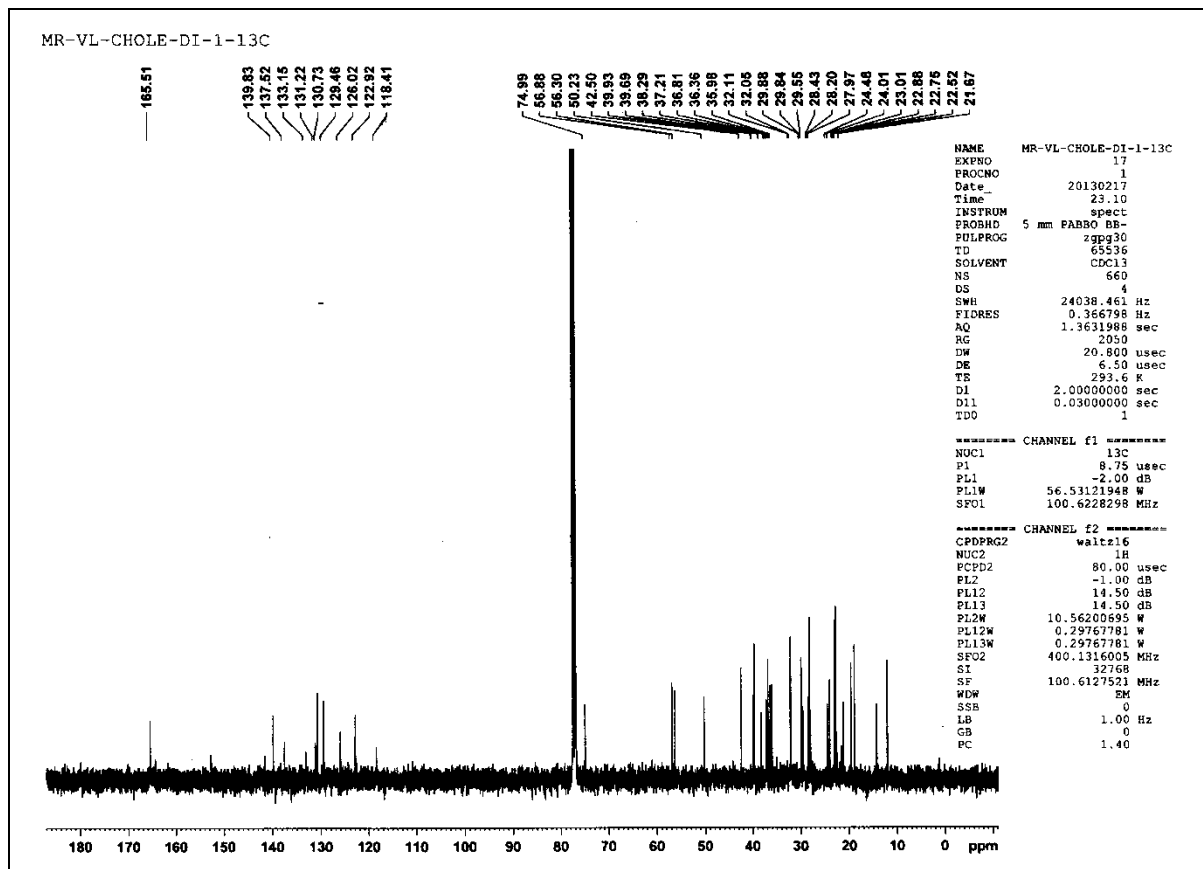


Figure 13: ^{13}C NMR spectrum of compound **5** in CDCl_3 .

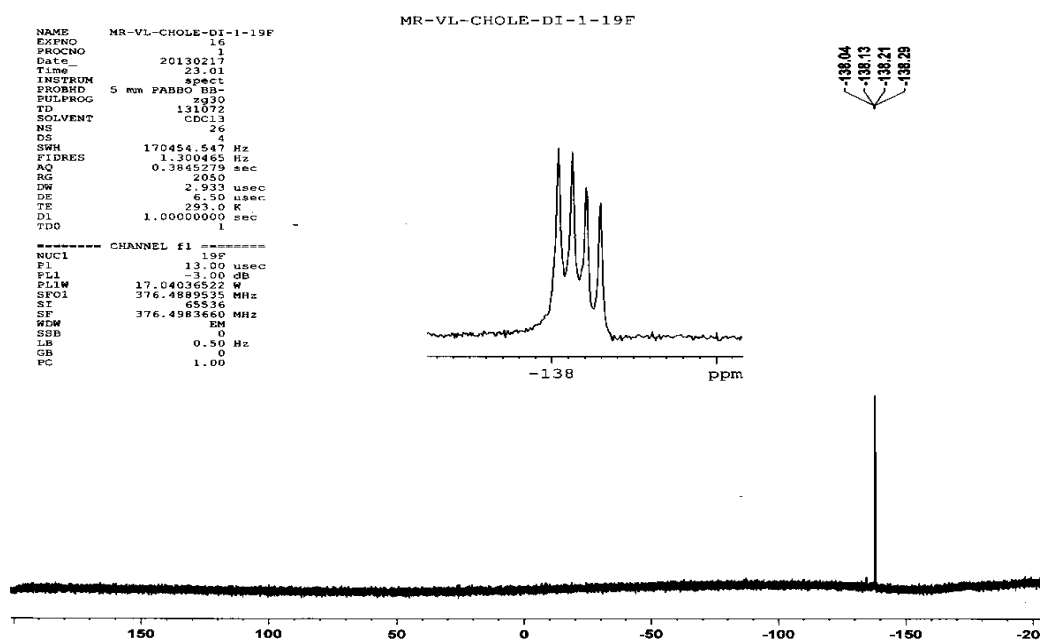


Figure 14: ^{19}F NMR spectrum of compound **5** in CDCl_3 . The inset shows the expansion

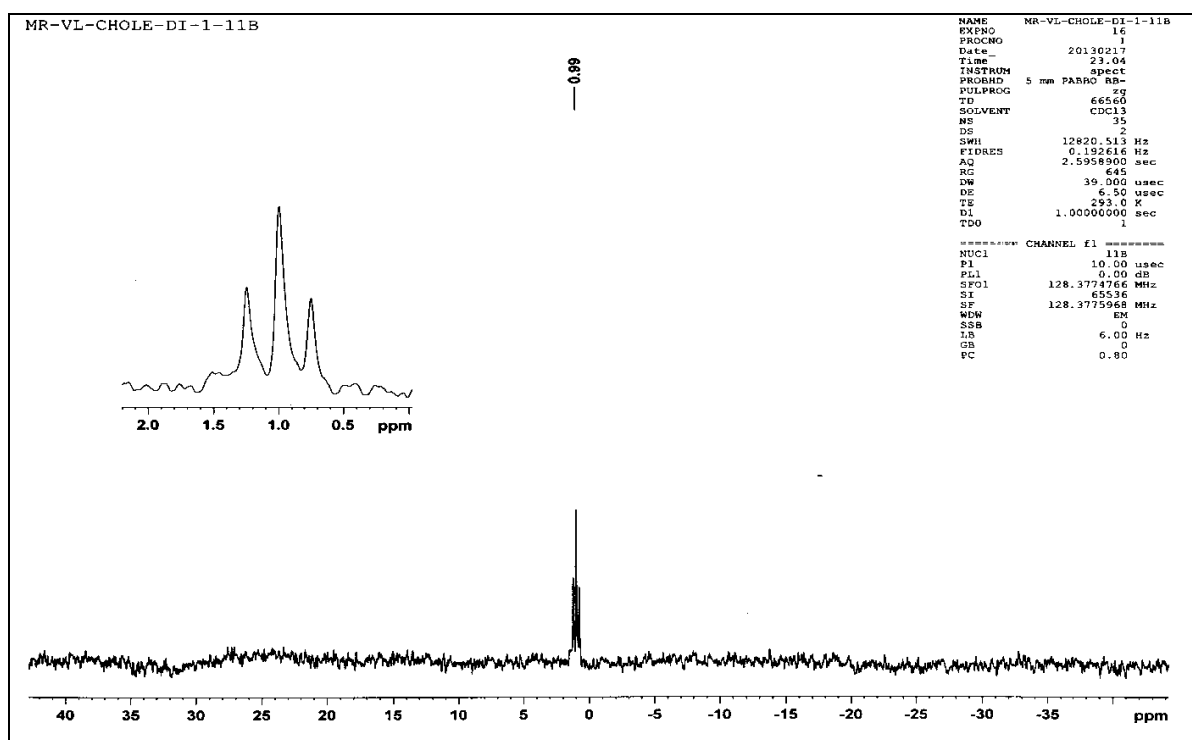


Figure 15: ^{11}B NMR spectrum of compound **5** in CDCl_3 . The inset shows the expansion

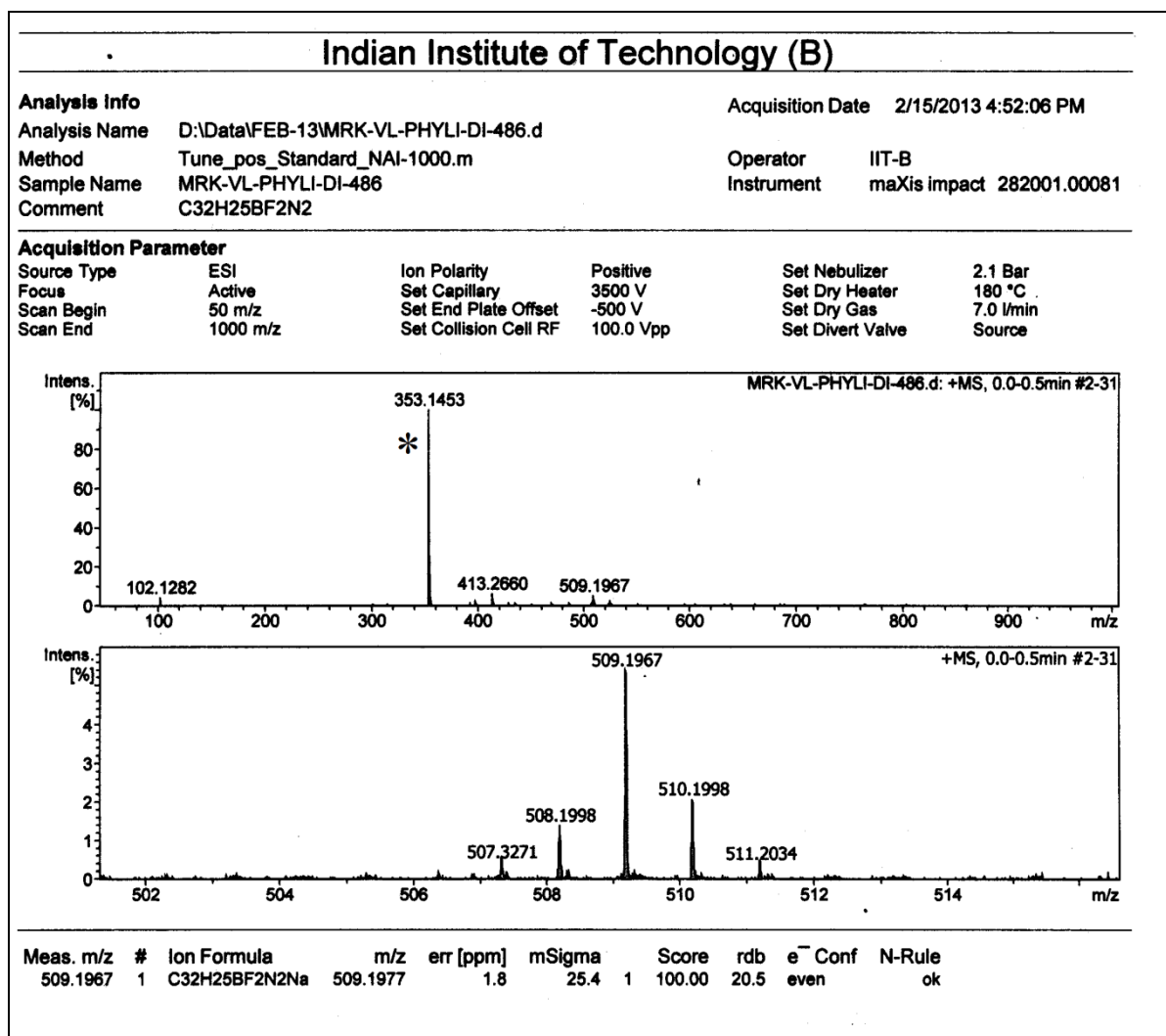
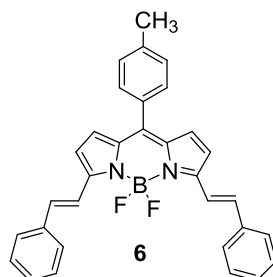


Figure 16: HRMS mass spectrum of compound 6

MRK-VL-DIPH-BDP-1H

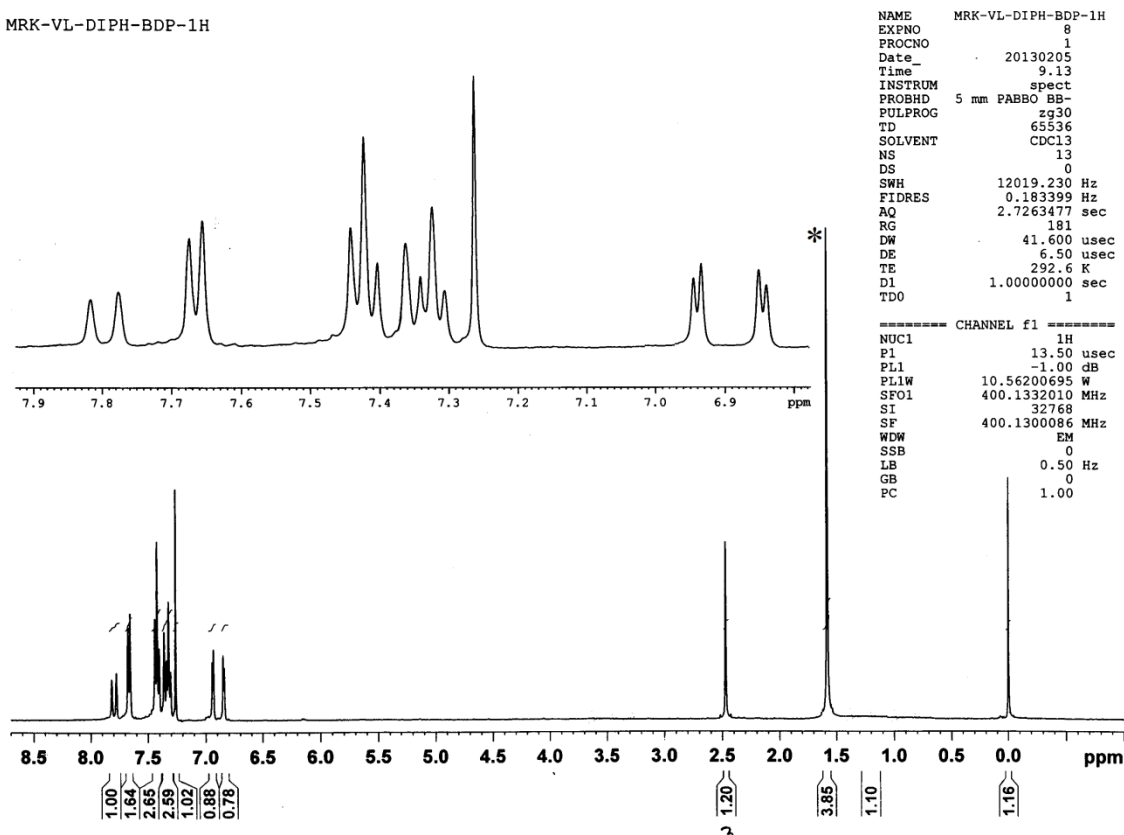


Figure 17: ^1H NMR spectrum of compound **6** in CDCl_3 .

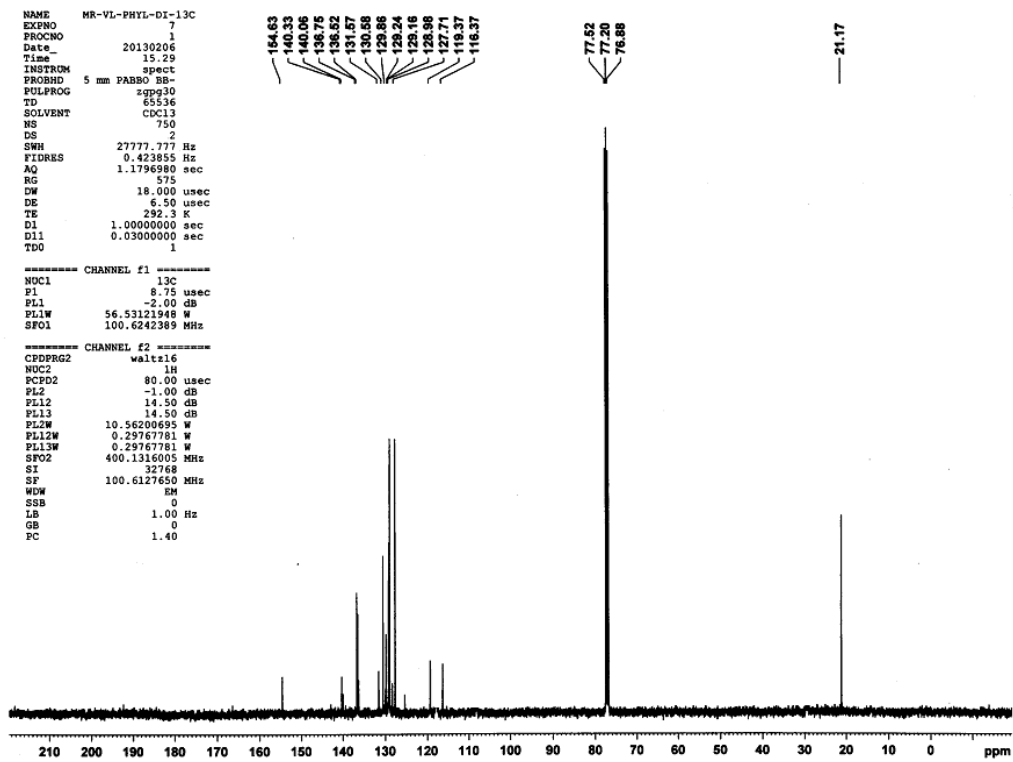


Figure 18: ^{13}C NMR spectrum of compound **6** recorded in CDCl_3 .

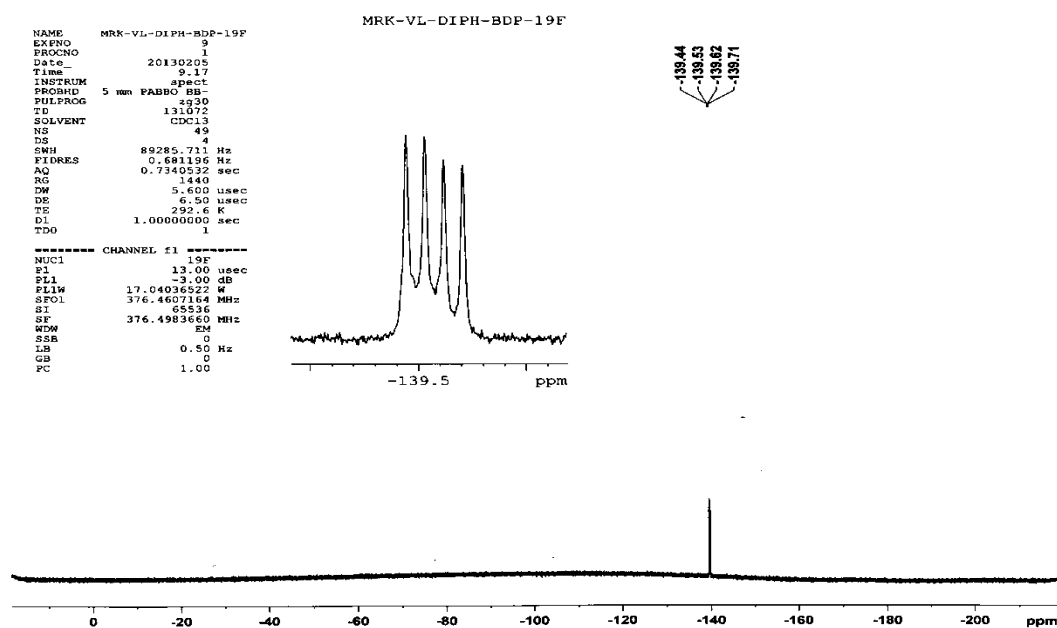


Figure 19: ^{19}F NMR spectrum of compound **6** in CDCl_3 . The inset shows the expansion

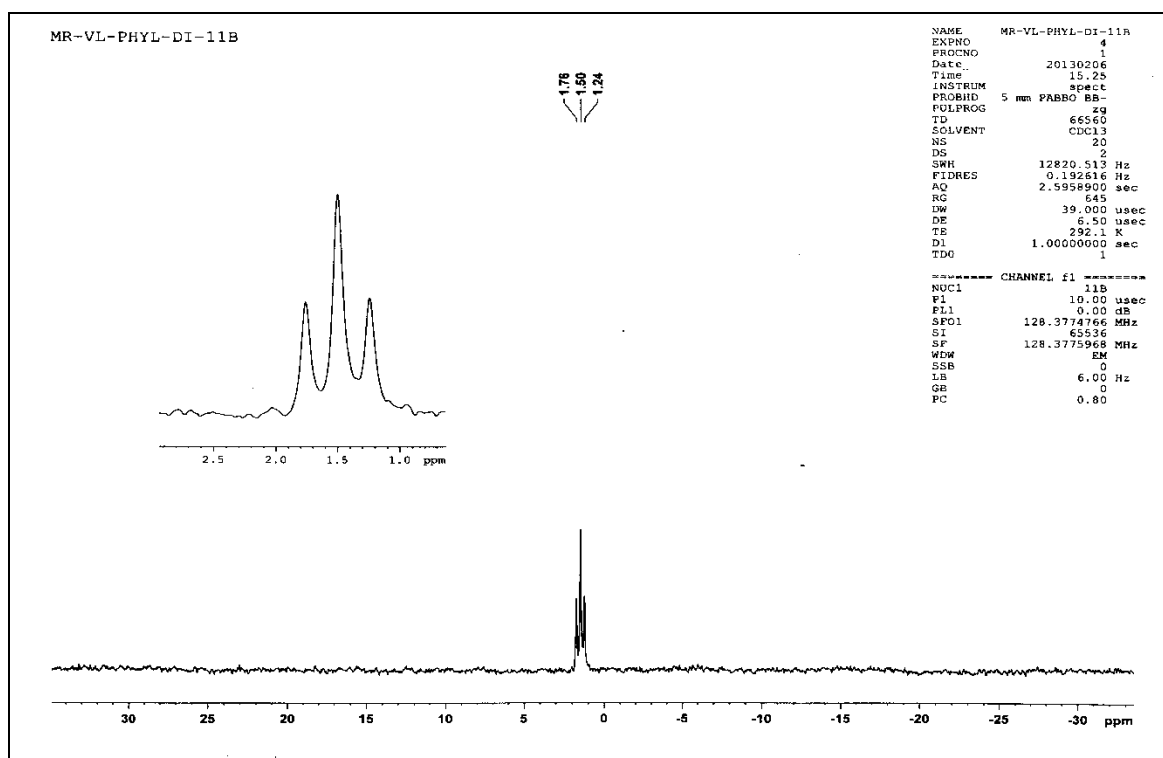


Figure 20: ^{11}B NMR spectrum of compound **6** in CDCl_3 . The inset shows the expansion

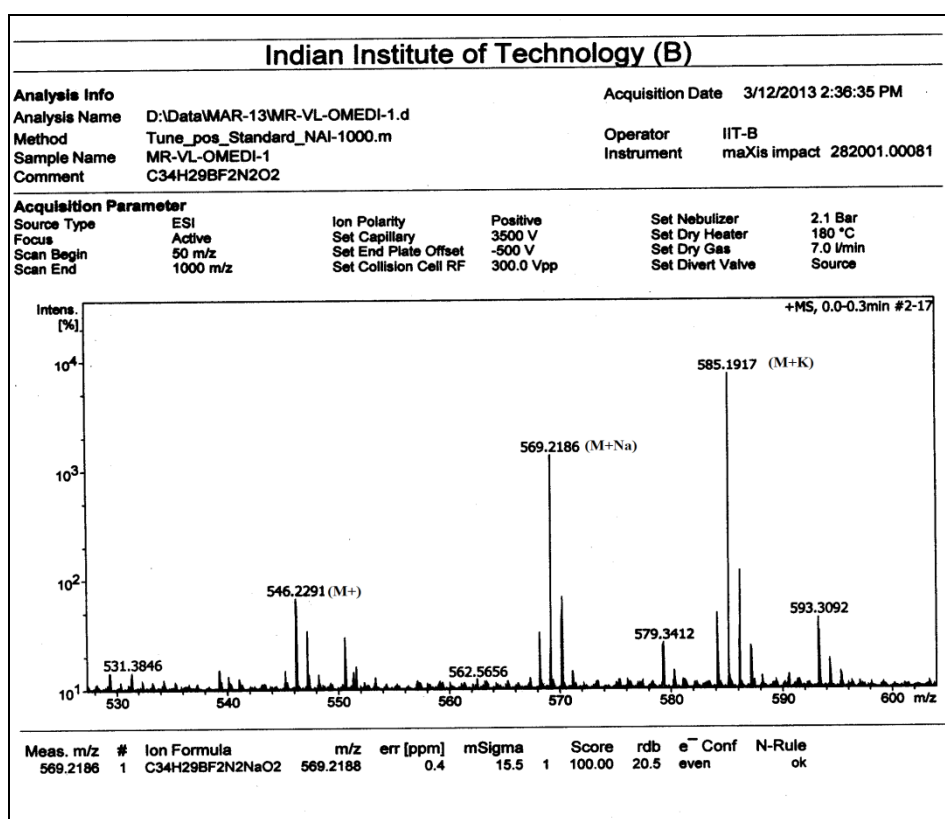
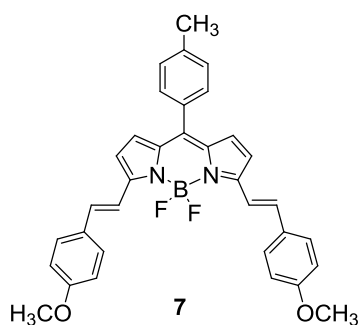


Figure 21: HRMS mass spectrum of compound 7

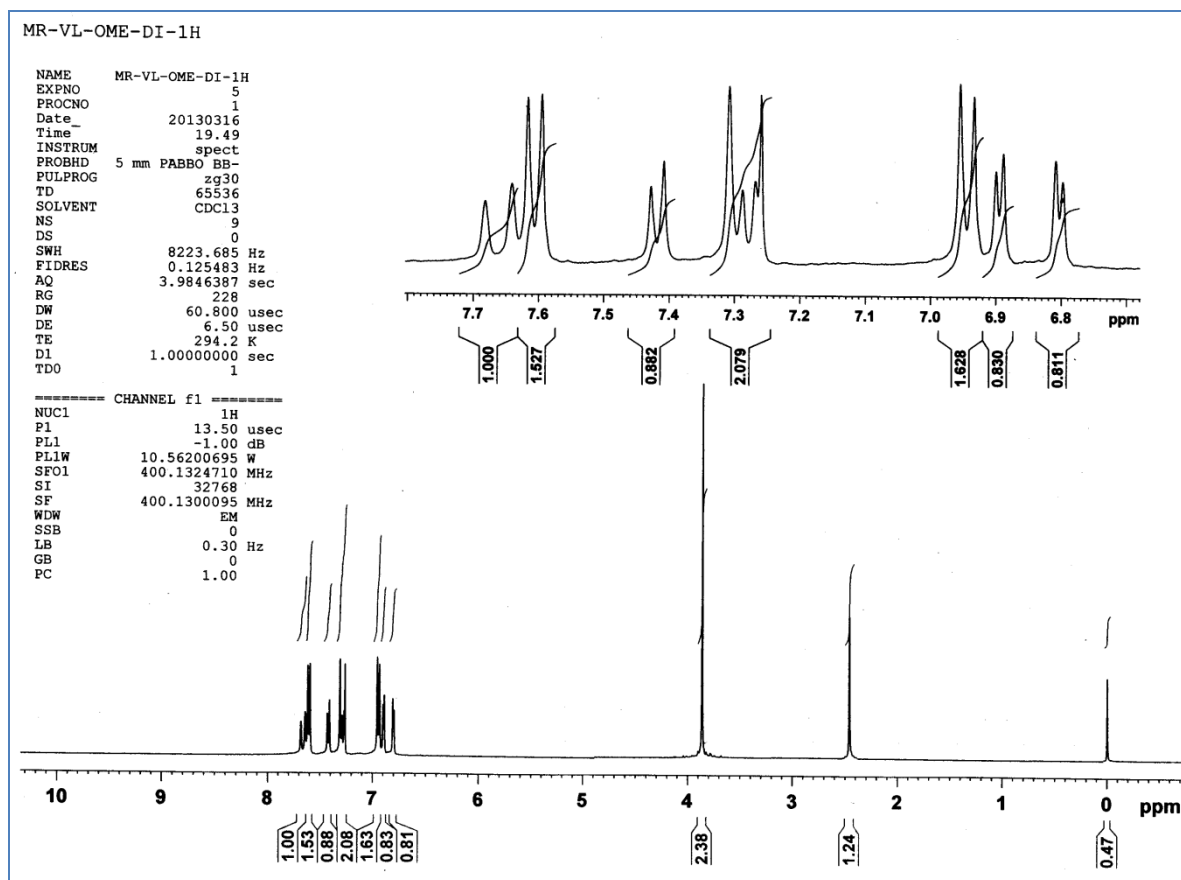


Figure 22: ^1H NMR spectrum of compound **7** in CDCl_3

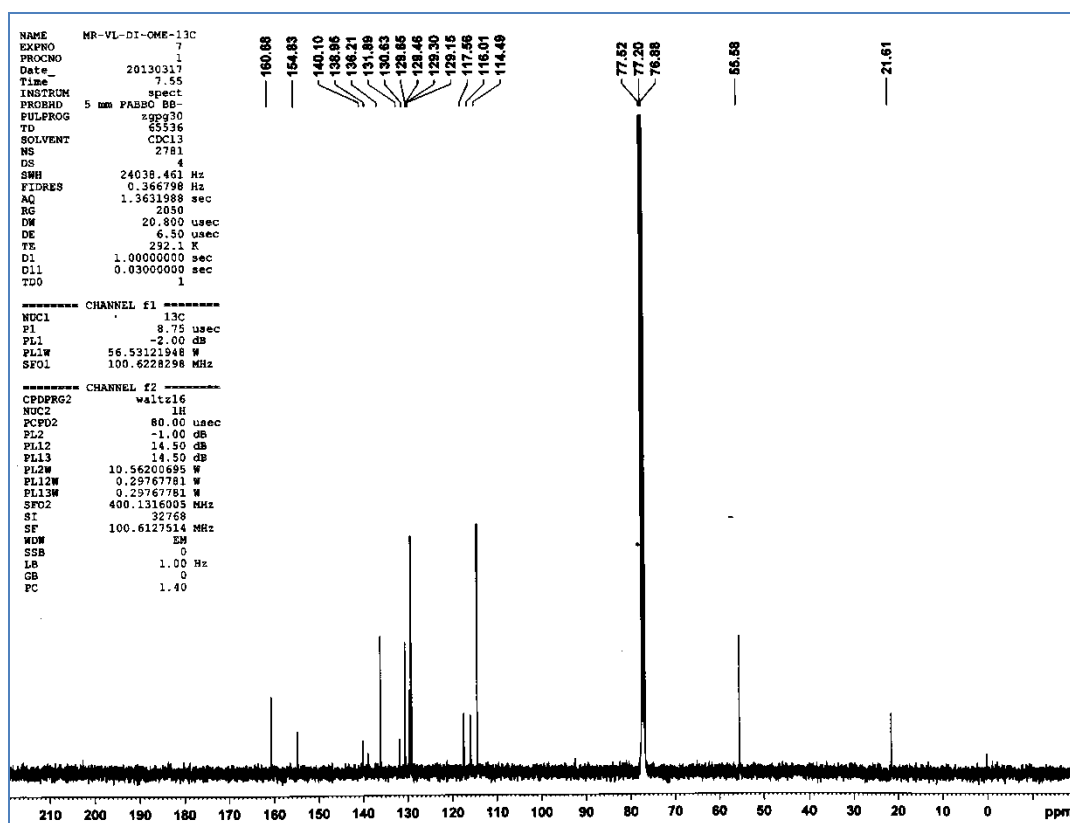


Figure 23: ^{13}C NMR spectrum of compound **7** in CDCl_3

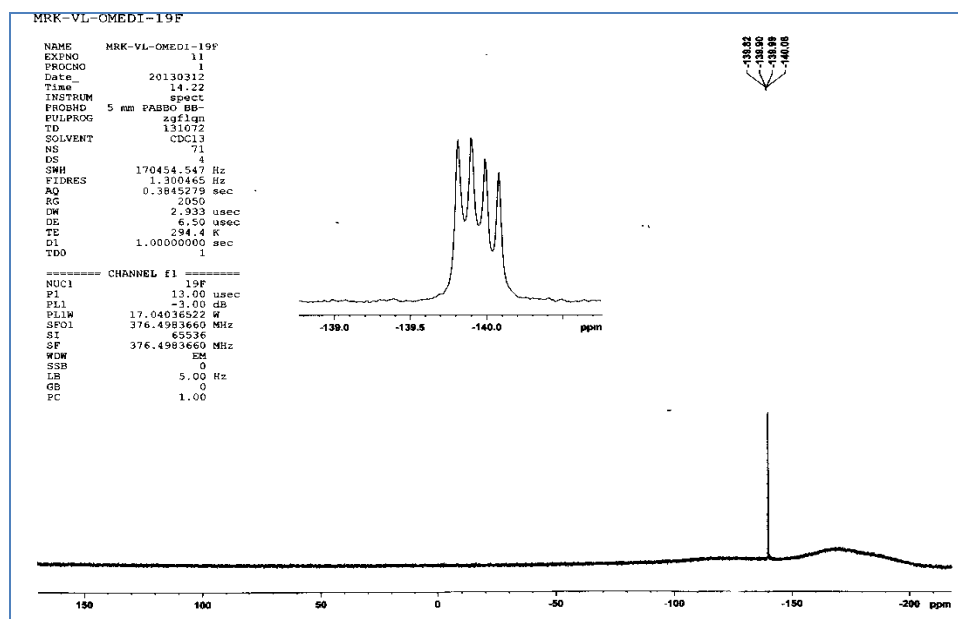


Figure 24: ^{19}F NMR spectrum of compound 7 in CDCl_3 . The inset shows the expansion

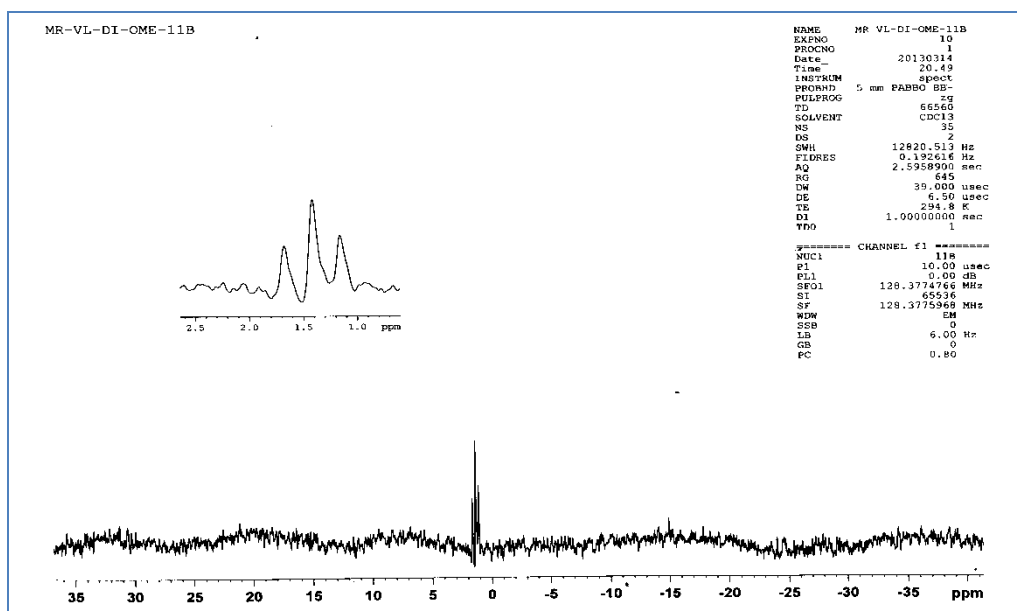


Figure 25: ^{11}B NMR spectrum of compound 7 in CDCl_3 . The inset shows the expansion

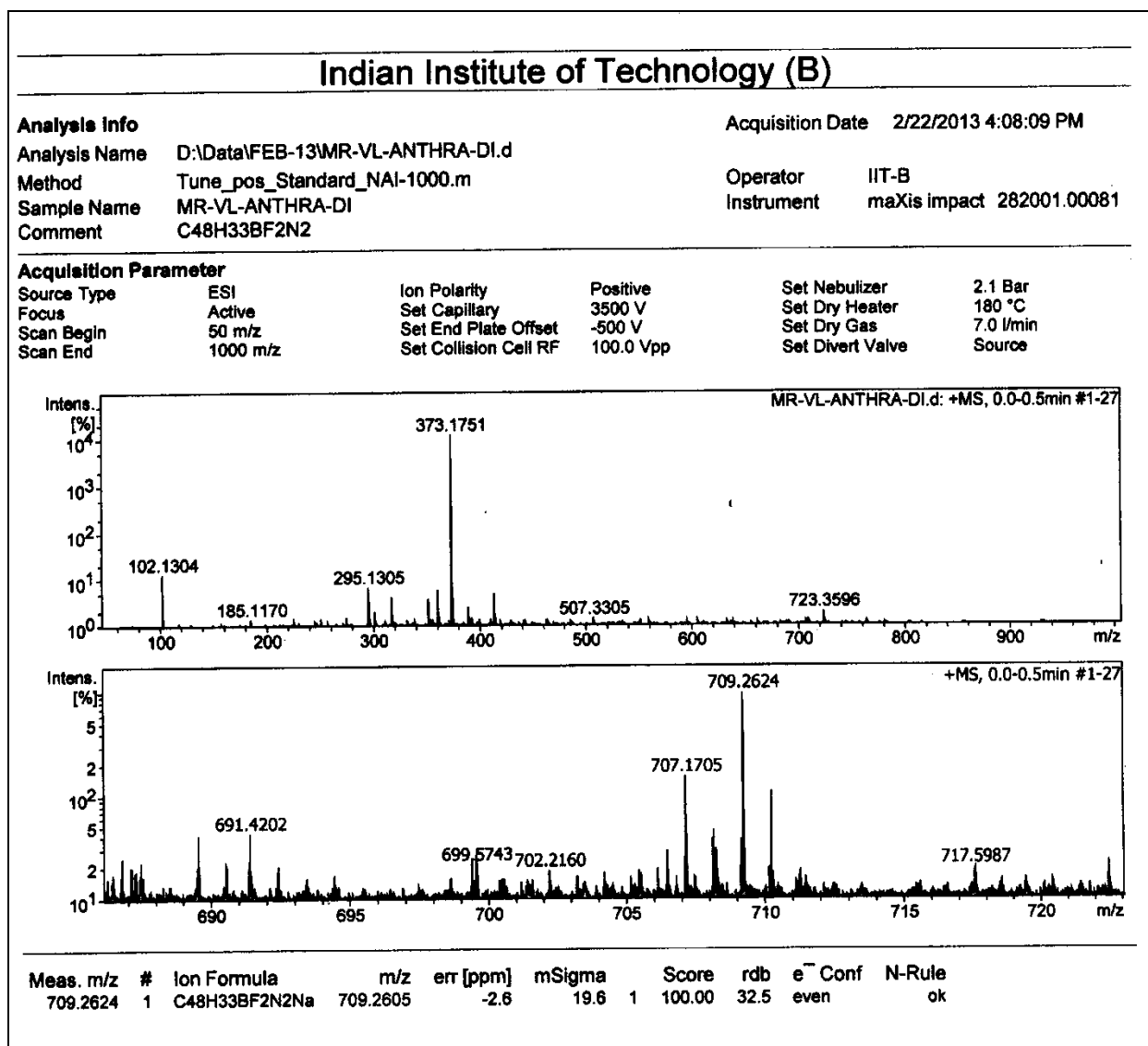
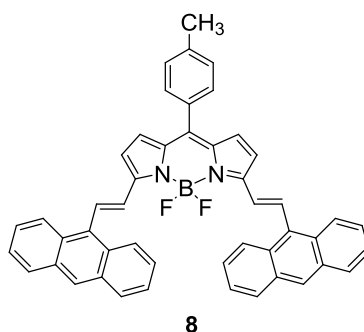


Figure 26: HRMS mass spectrum of compound 8 in CDCl₃

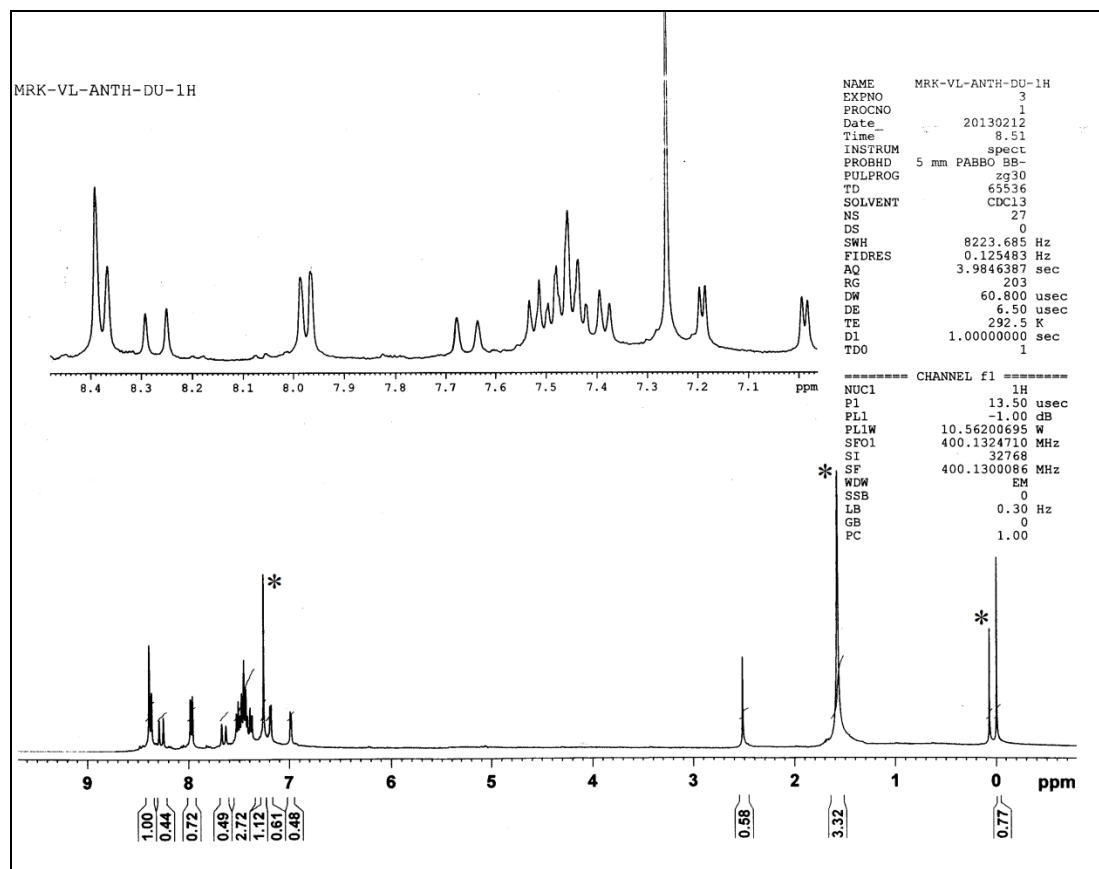


Figure 27: ^1H NMR spectrum of compound **8** in CDCl_3

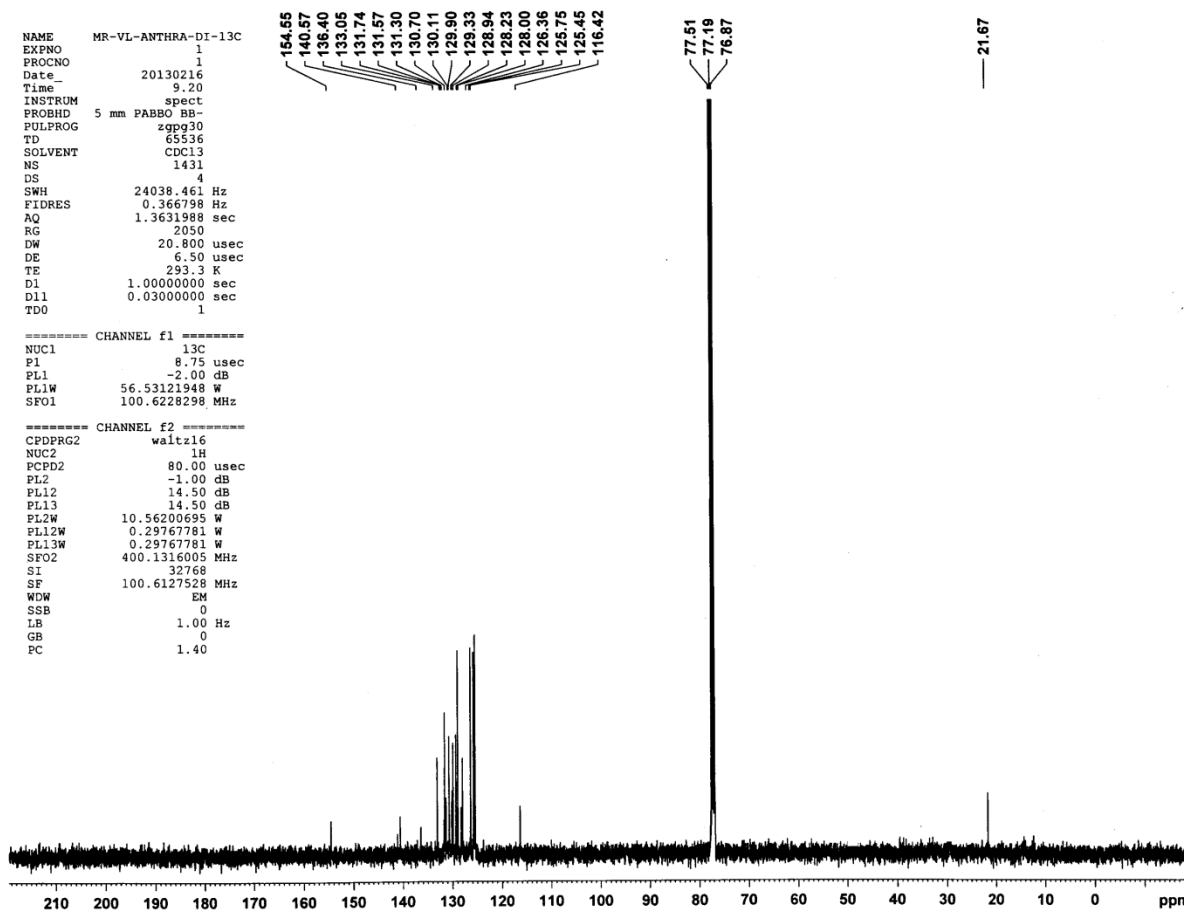
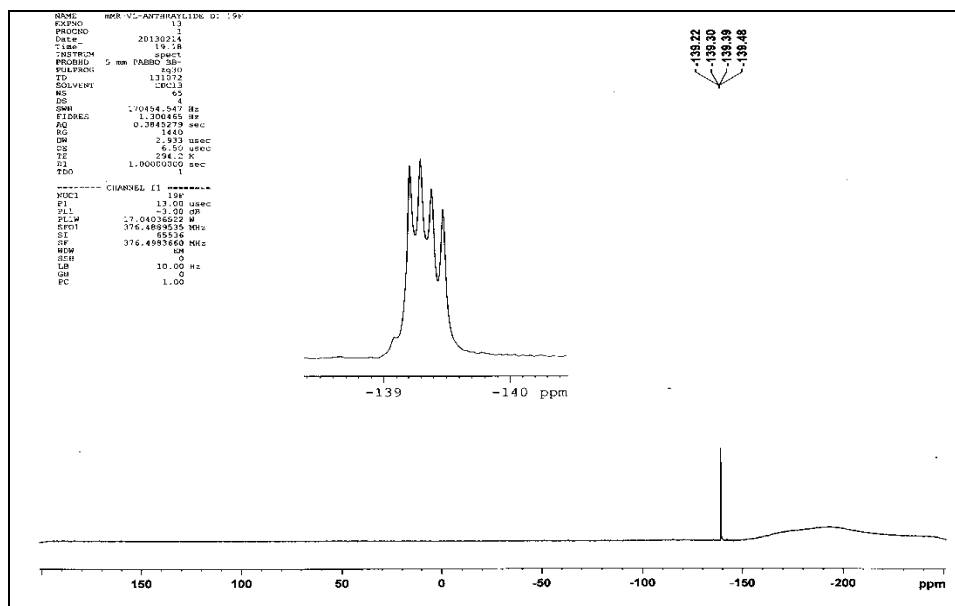


Figure 28: ^{13}C NMR spectrum of compound **8** in CDCl_3



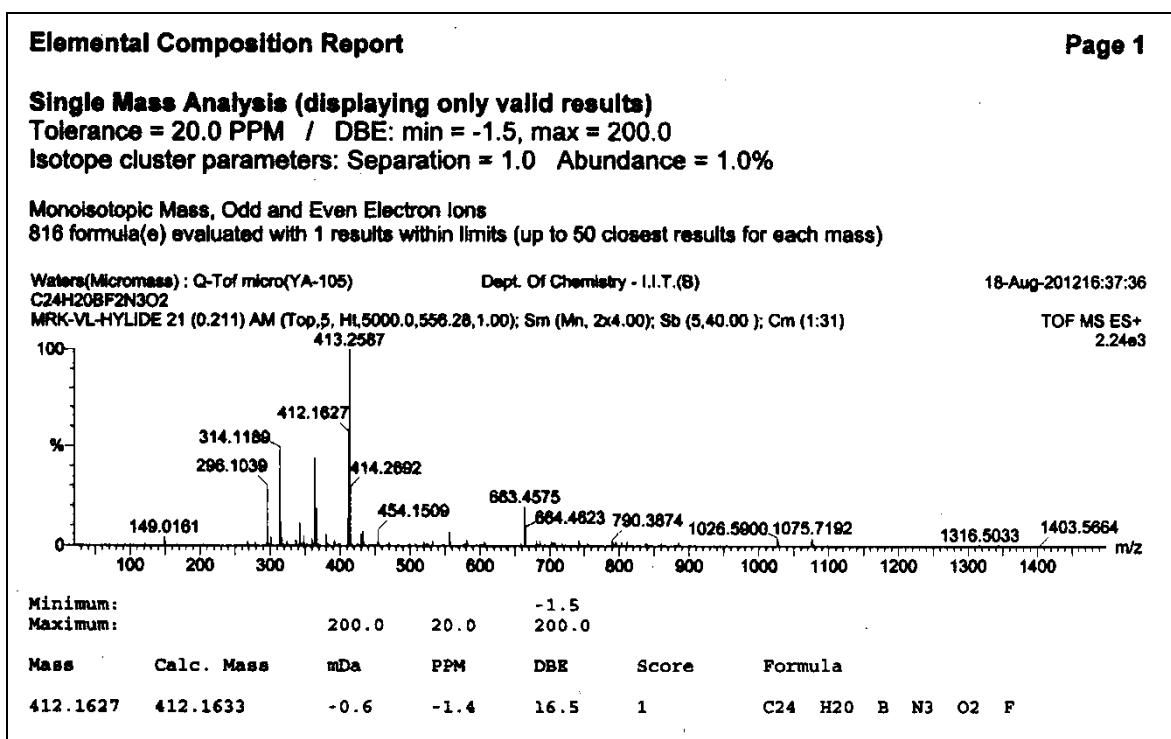
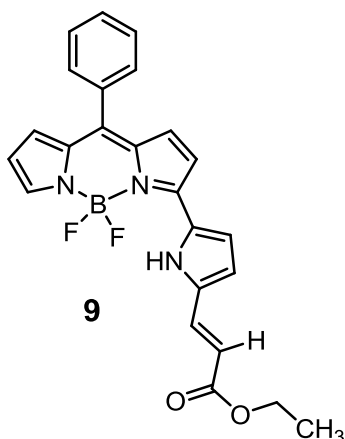


Figure 31: HRMS spectrum of compound 9

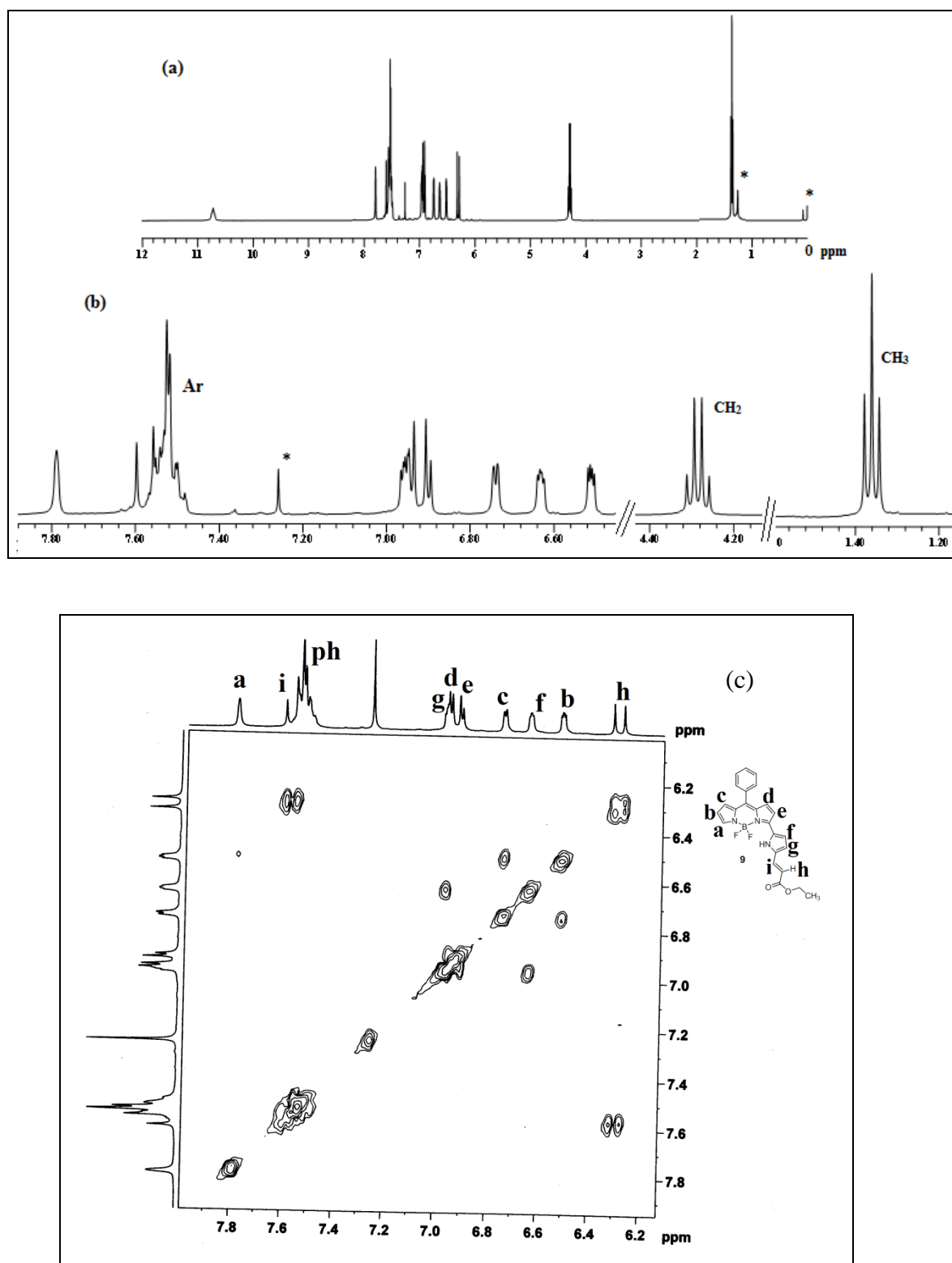


Figure 32: (a) ^1H NMR spectrum of compound **9** in CDCl_3 . (b) Expansion of the compound in the selected region. (c) ^1H - ^1H correlation spectrum of **9** in CDCl_3

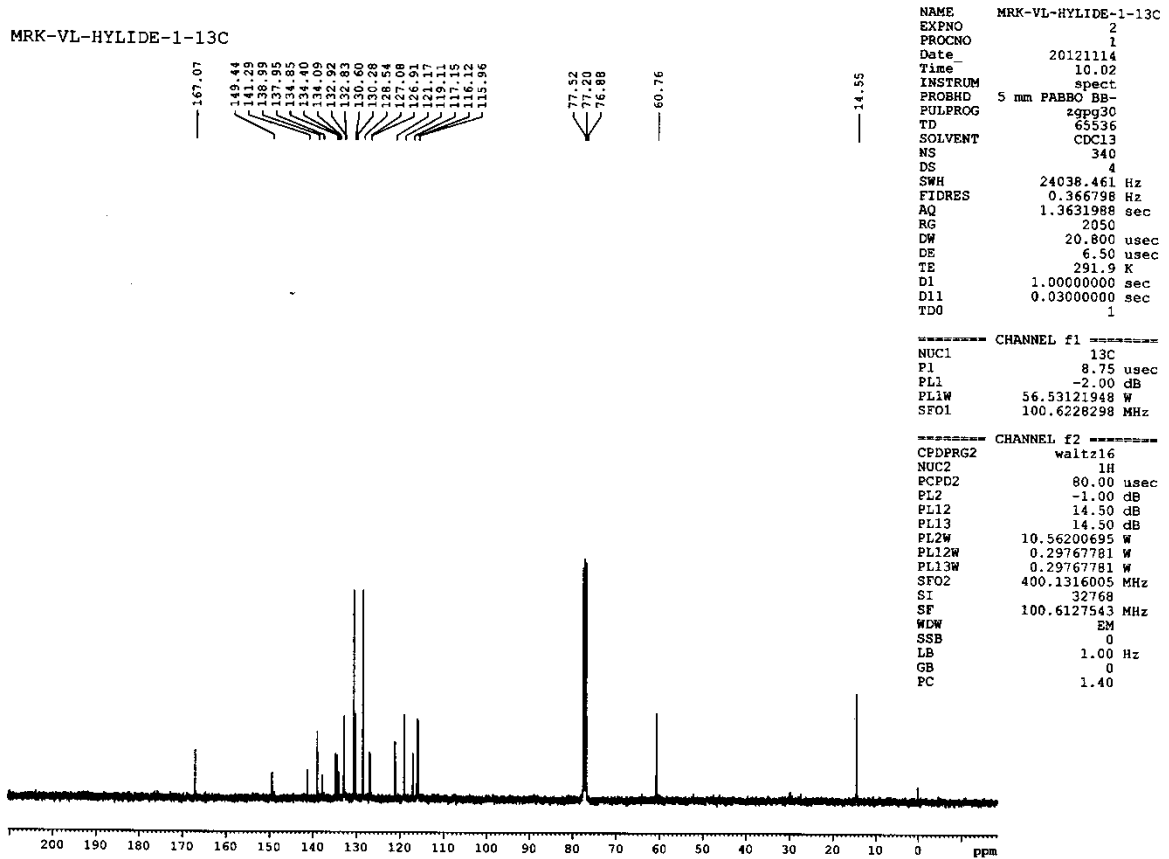


Figure 33: ^{13}C NMR spectrum of compound **9** in CDCl_3

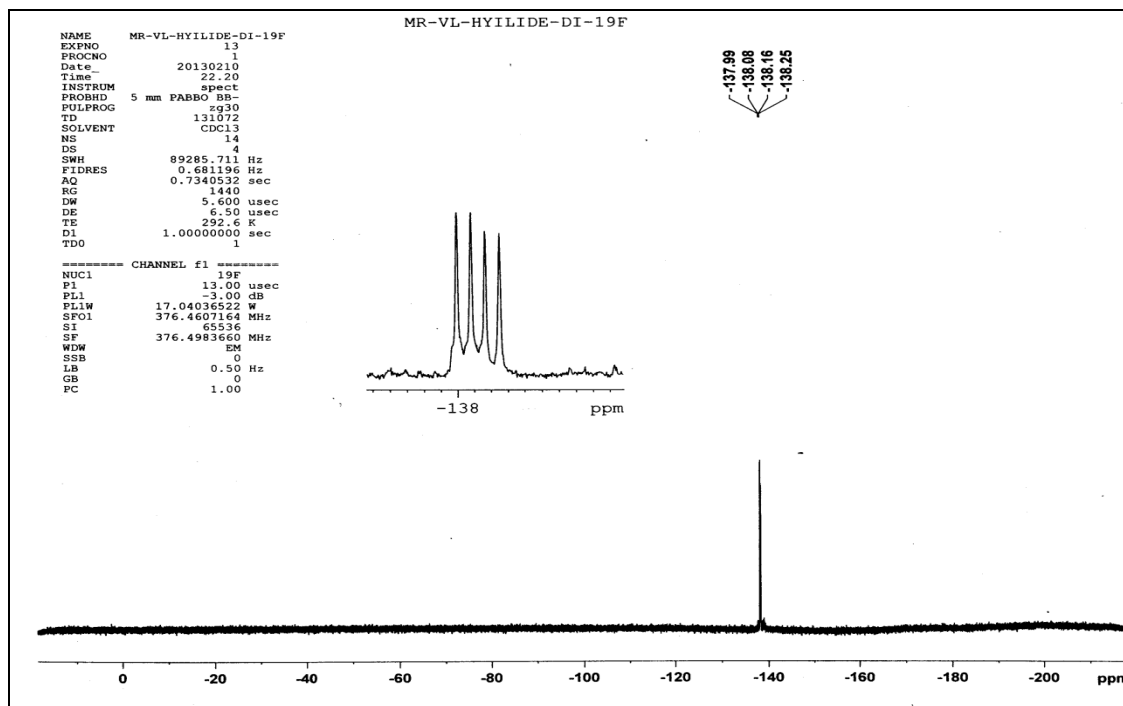


Figure 34: ^{19}F NMR spectrum of compound **9** in CDCl_3 . The inset shows the expansion

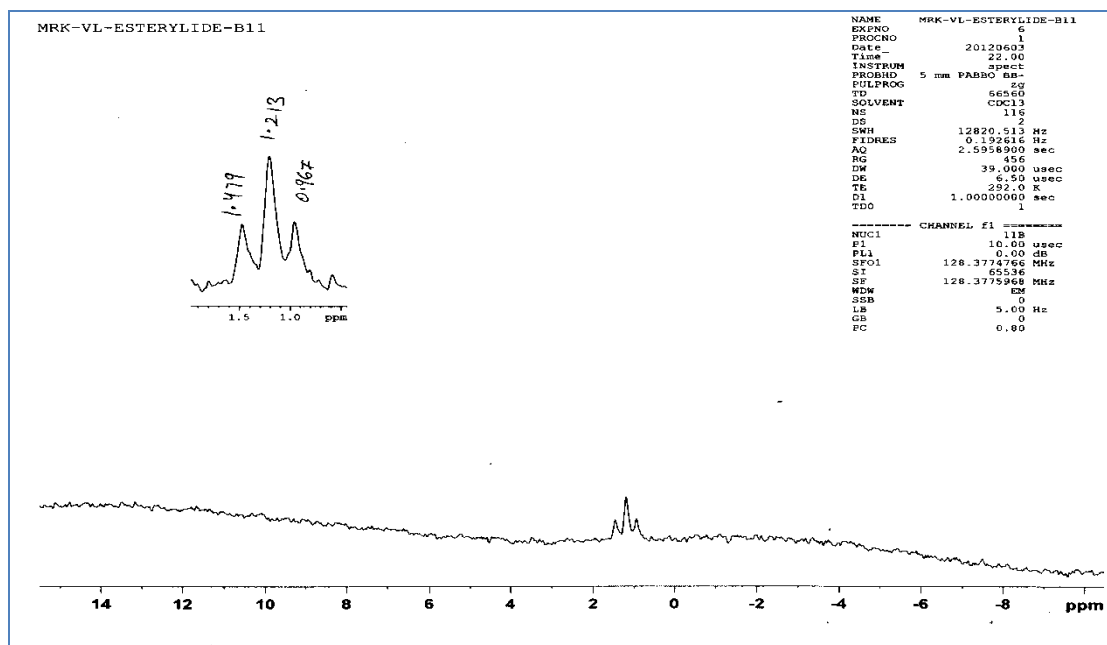
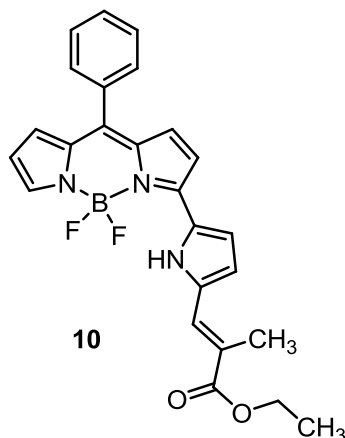


Figure 35: ^{11}B NMR spectrum of compound **9** in CDCl_3 . The inset shows the expansion



Elemental Composition Report

Page 1

Single Mass Analysis (displaying only valid results)

Tolerance = 20.0 PPM / DBE: min = -1.5, max = 200.0

Isotope cluster parameters: Separation = 1.0 Abundance = 1.0%

Monoisotopic Mass, Odd and Even Electron Ions

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

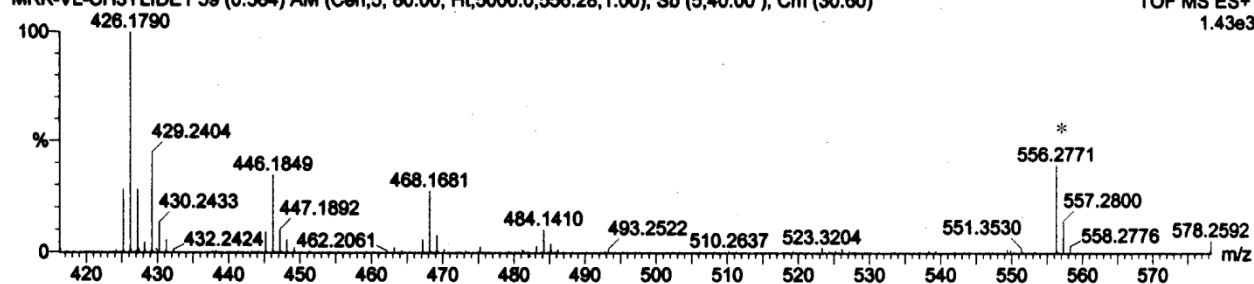
Waters(Micromass) : Q-ToF micro(YA-105)

Dept. Of Chemistry - I.I.T.(B)

18-Aug-201216:58:13

C₂₅H₂₂BF₂N₃O₂

MRK-VL-CH3YLIDE1 59 (0.584) AM (Cen,5, 80.00, Ht,5000.0,556.28,1.00); Sb (5,40.00); Cm (30:60)

TOF MS ES+
1.43e3

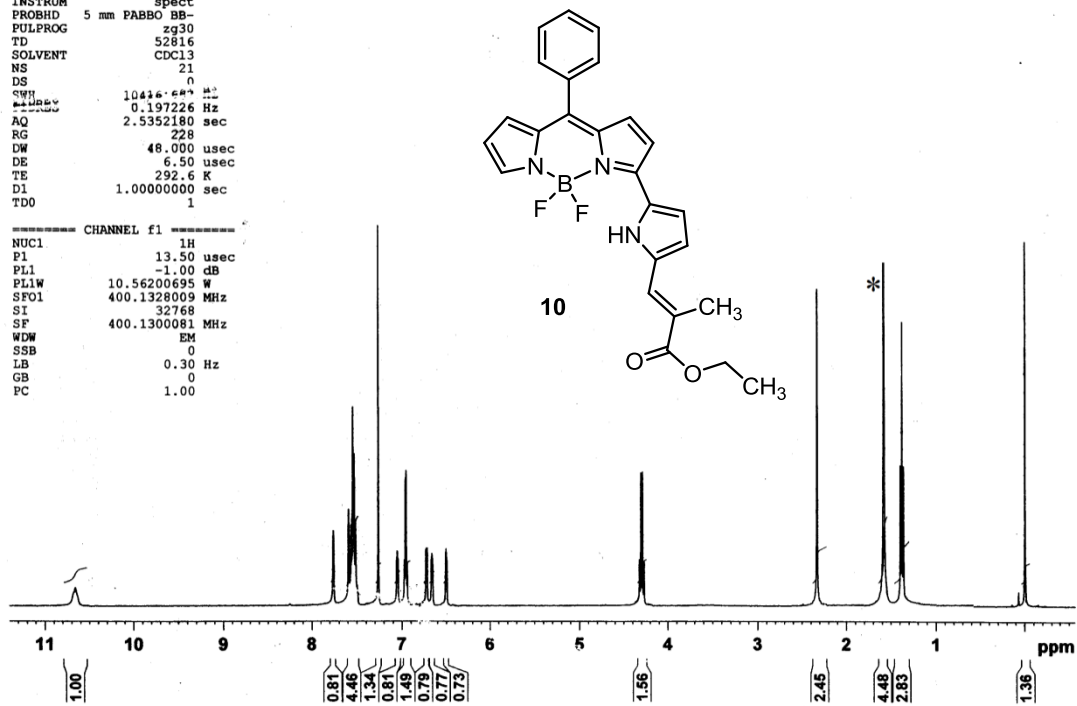
Minimum: -1.5
Maximum: 200.0 20.0 200.0

Mass	Calc. Mass	mDa	PPM	DBE	Score	Formula
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Figure 36: HRMS mass spectrum of compound 10

NAME MRK-VL-METHYLYLIDE-1H
 EXPNO 2
 PROCNO 2
 Date_ 20120701
 Time 18.30
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zg30
 TD 52816
 SOLVENT CDCl3
 NS 21
 DS 0
 SWH 10416.643 Hz
 FWHM 0.197226 Hz
 AQC 2.5352180 sec
 RG 228
 DW 48.000 usec
 DE 6.50 usec
 TE 292.6 K
 D1 1.00000000 sec
 TDO 1

MRK-VL-METHYLYLIDE-1H



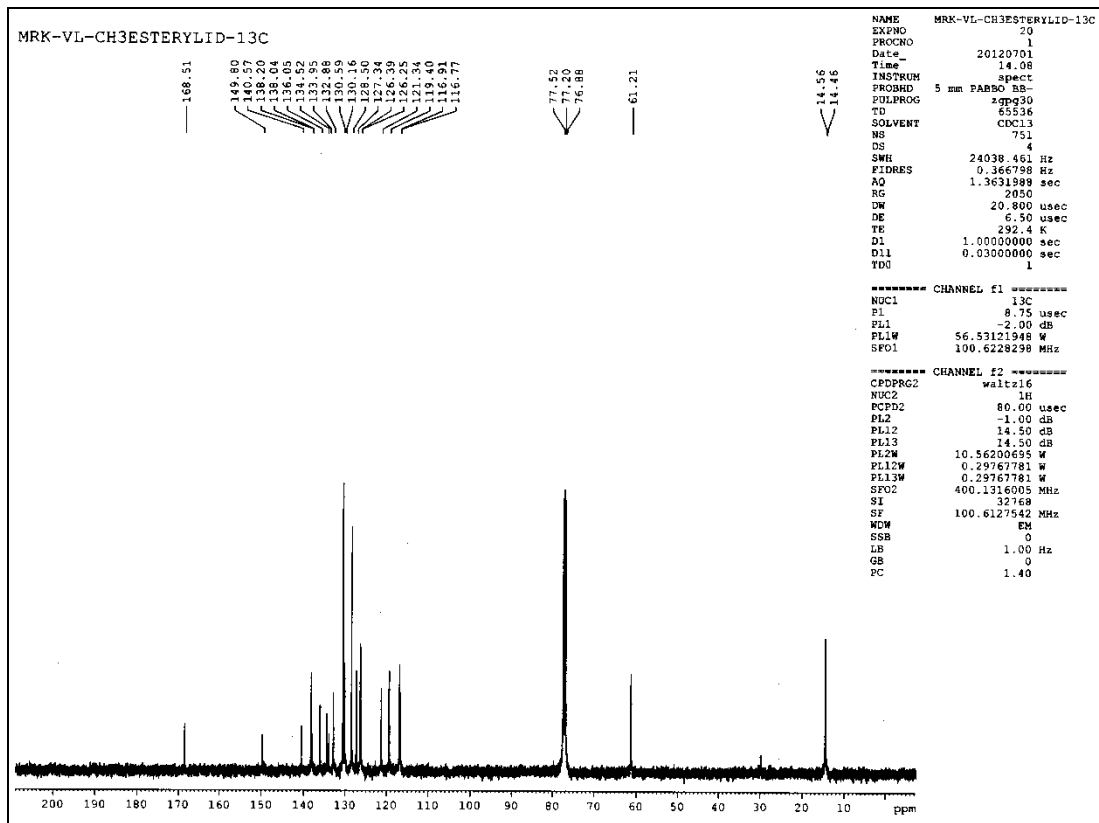


Figure 38: ^{13}C NMR spectrum of compound **10** in CDCl_3

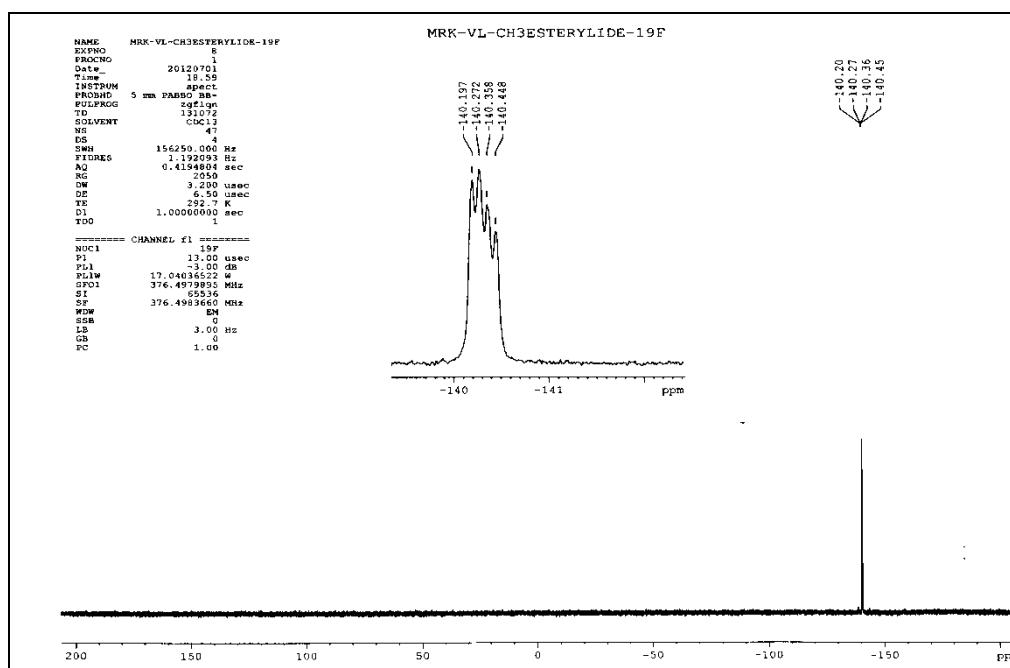


Figure 39: ^{19}F NMR spectrum of compound **10** in CDCl_3 . The inset shows the expansion

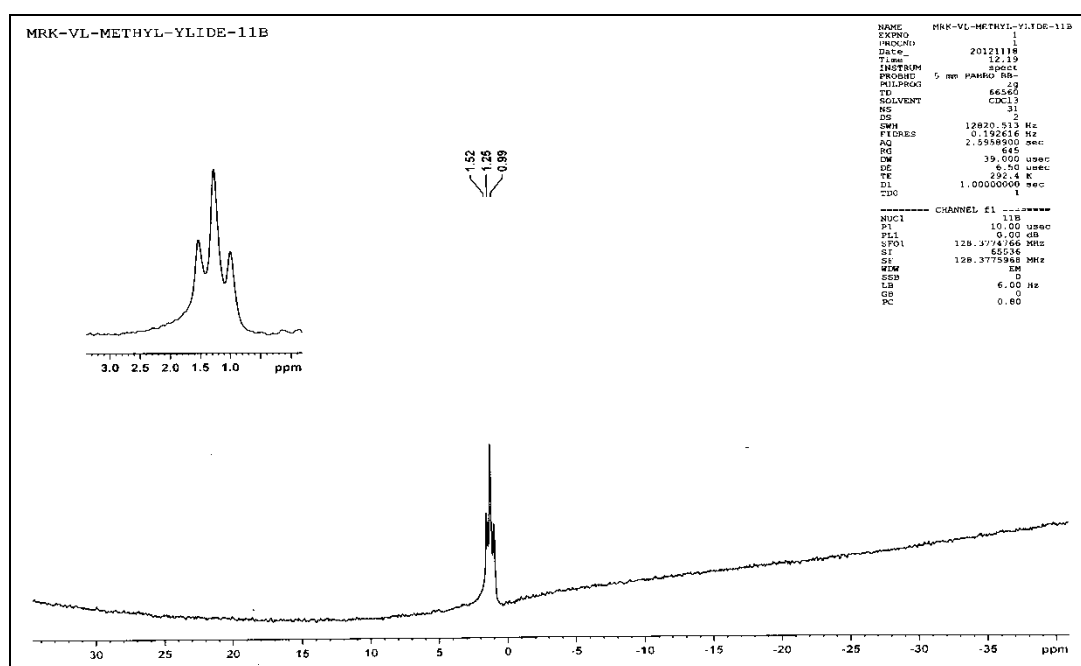


Figure 40: ^{11}B NMR spectrum of compound **10** in CDCl_3 . The inset shows the expansion

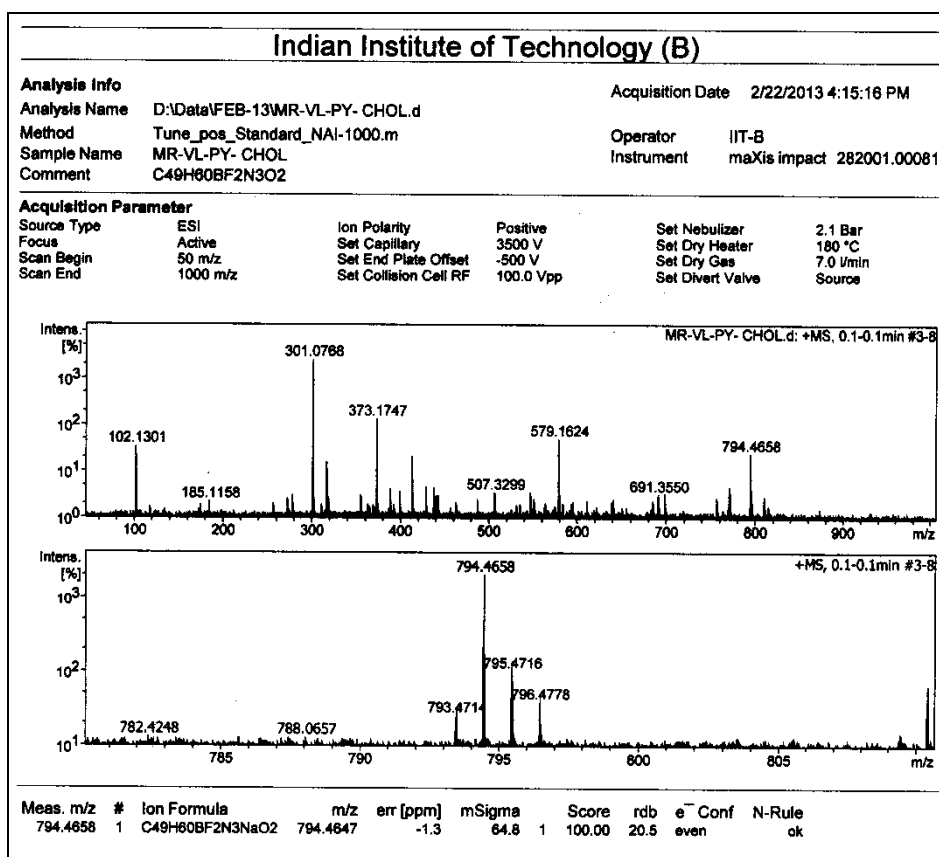
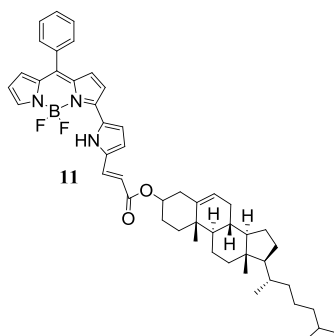


Figure 41: HRMS mass spectrum of compound 11

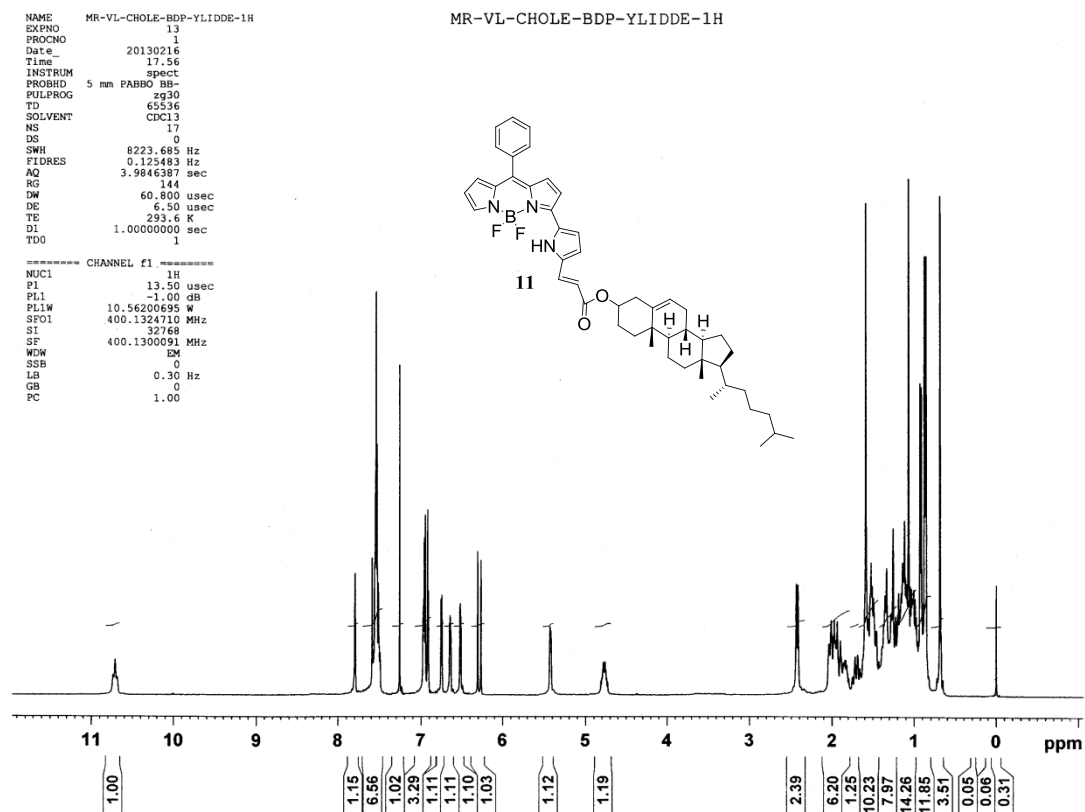


Figure 42: ^1H NMR spectrum of compound 11 in CDCl_3

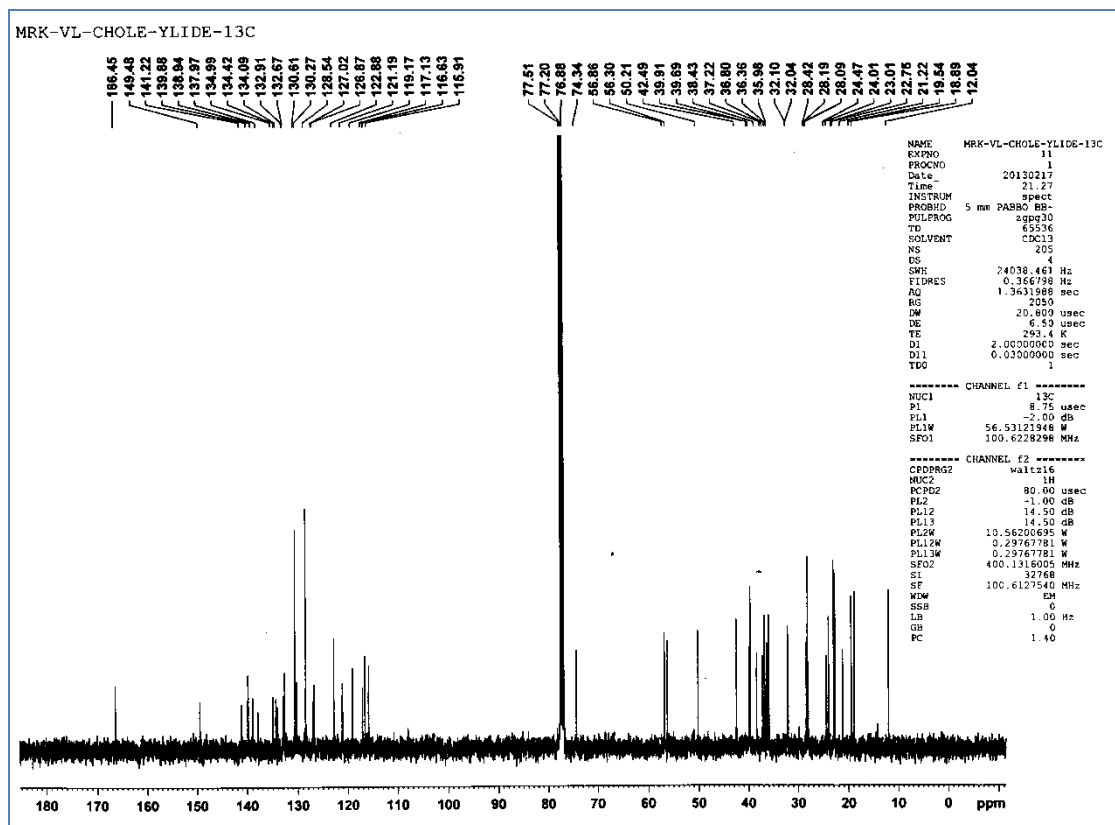


Figure 43: ^{13}C NMR spectrum of compound **11** in CDCl_3

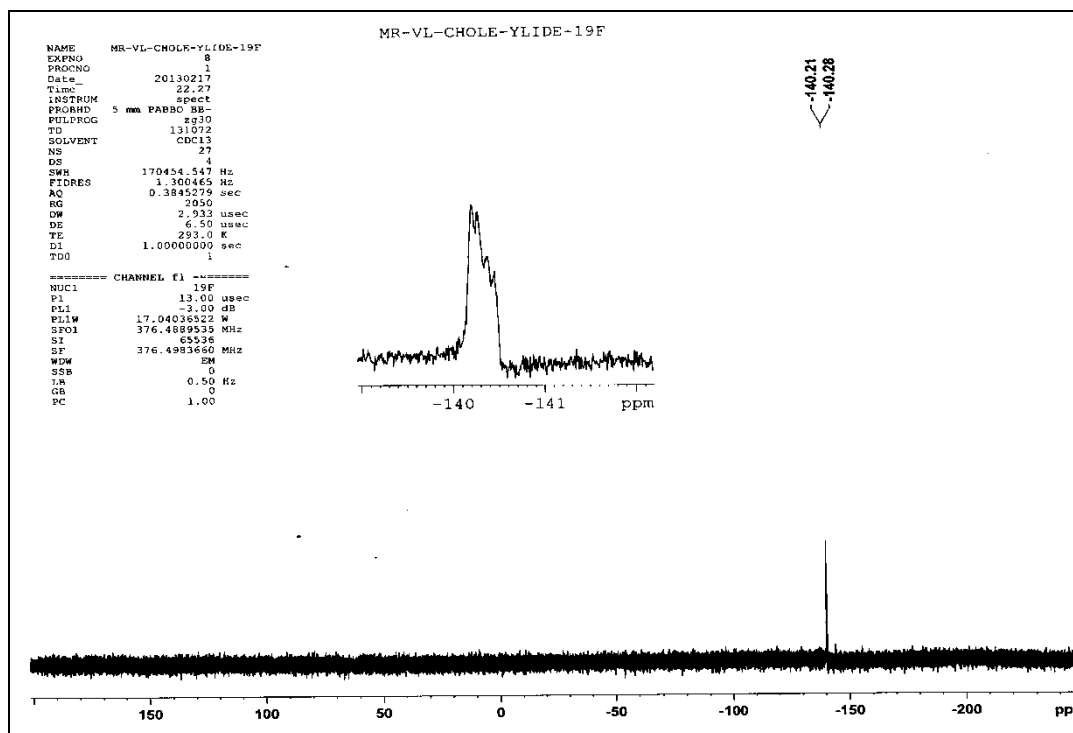


Figure 44: ^{19}F NMR spectrum of compound **11** in CDCl_3 . The inset shows the expansion

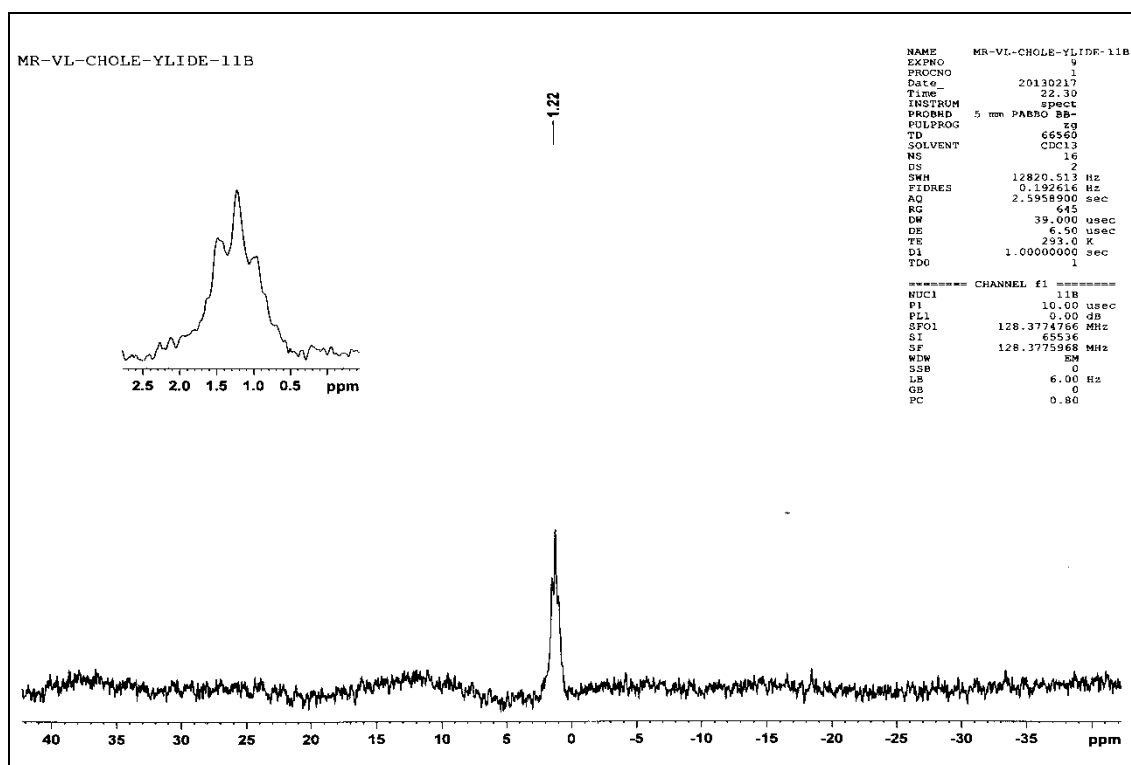


Figure 45: ^{11}B NMR spectrum of compound **11** in CDCl_3 . The inset shows the expansion

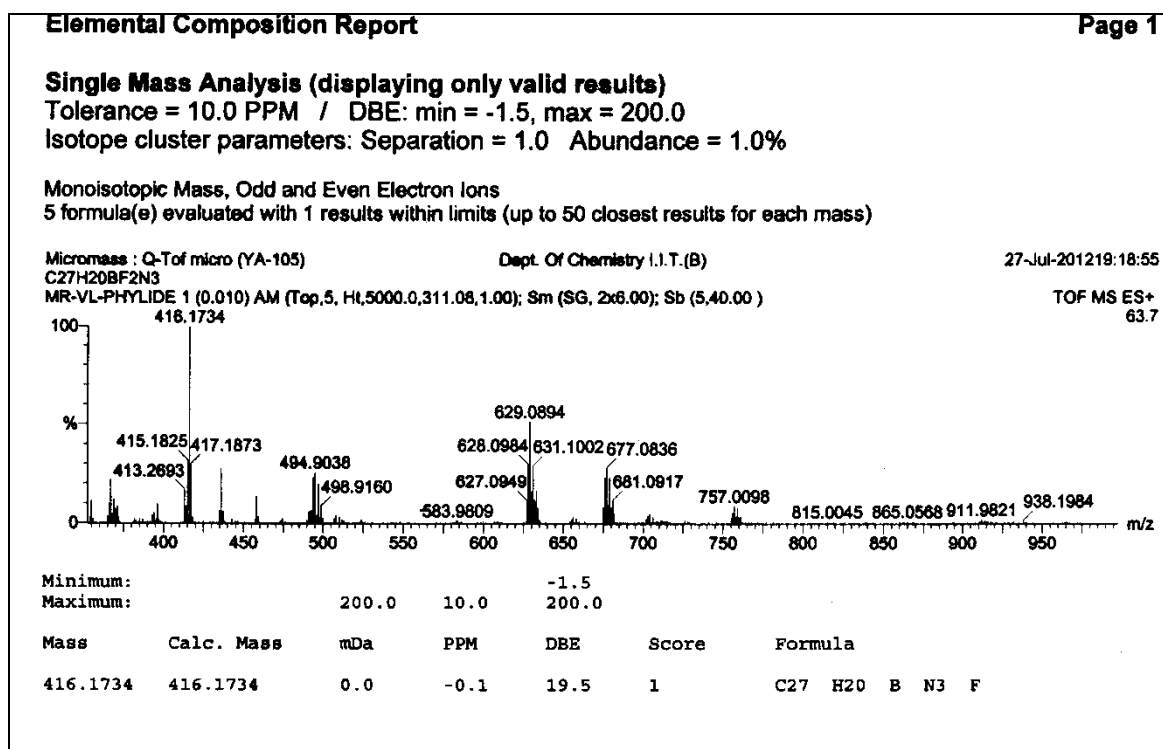
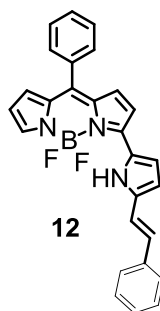


Figure 46: HRMS mass spectrum of compound 12

MR-VL-benzylilide-1H

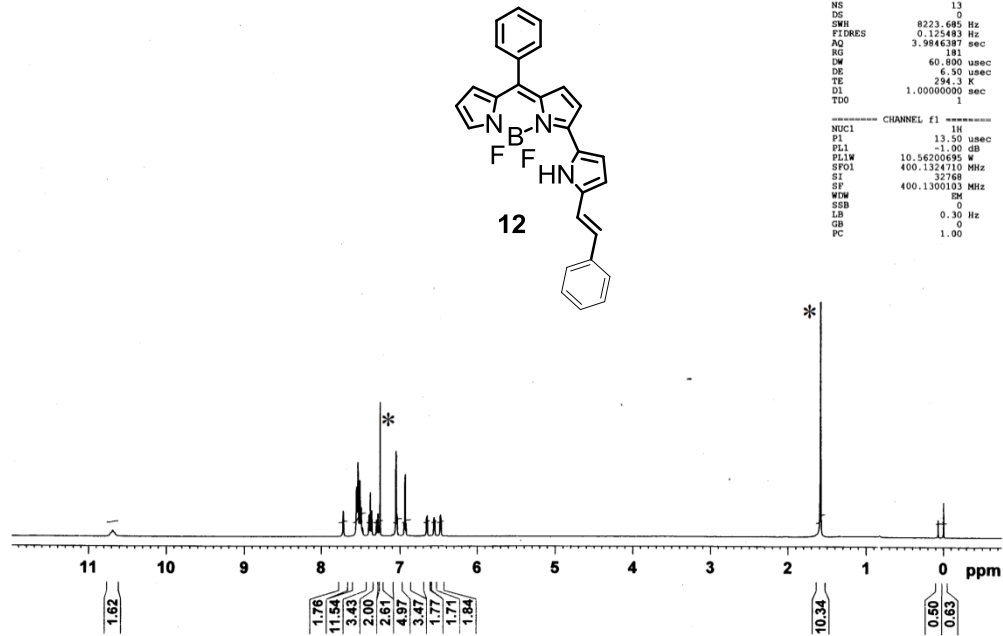


Figure 47: ^1H NMR spectrum of compound **12** in CDCl_3

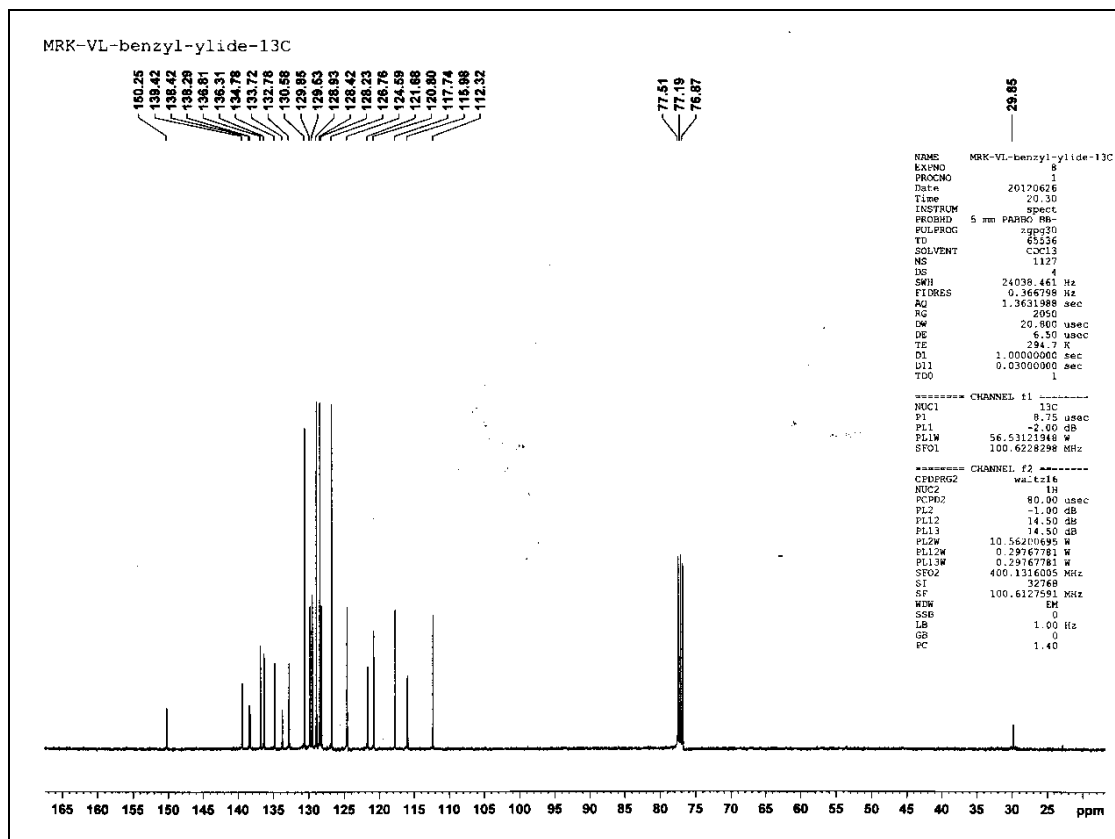


Figure 48: ^{13}C NMR spectrum of compound **12** in CDCl_3

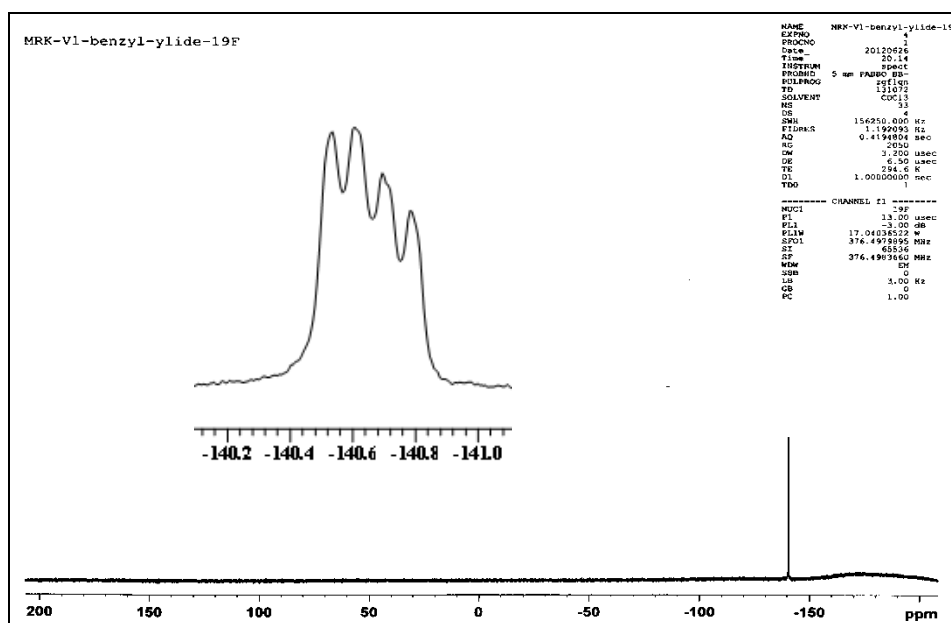


Figure 49: ^{19}F NMR spectrum of compound **12** in CDCl_3 . The inset shows the expansion

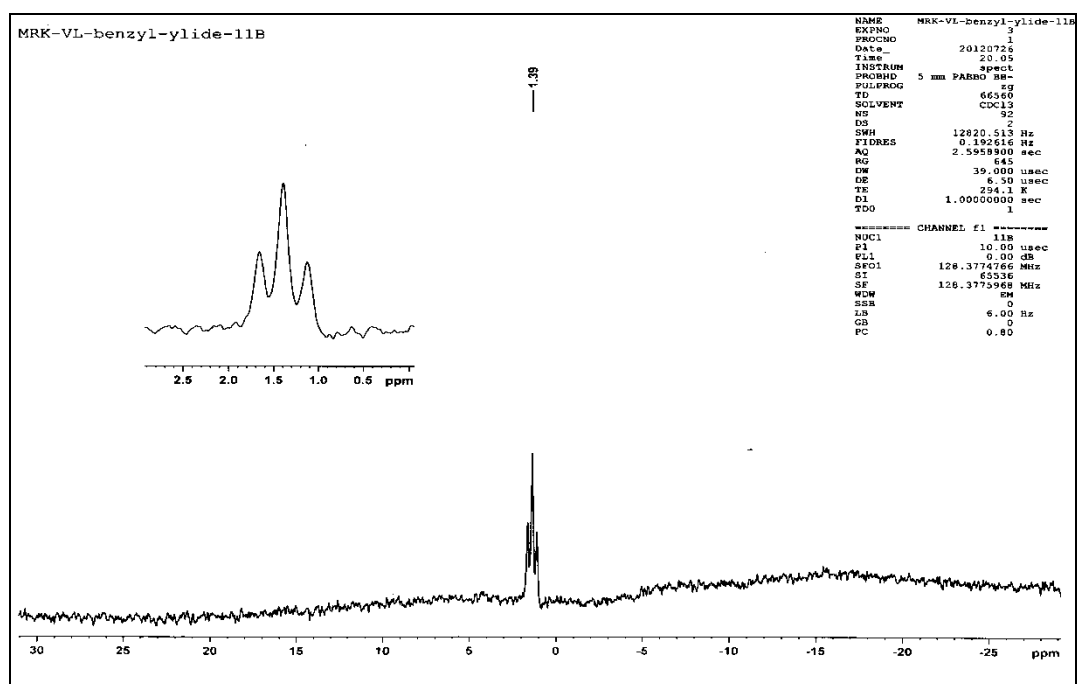


Figure 50: ^{11}B NMR spectrum of compound **12** in CDCl_3 . The inset shows the expansion

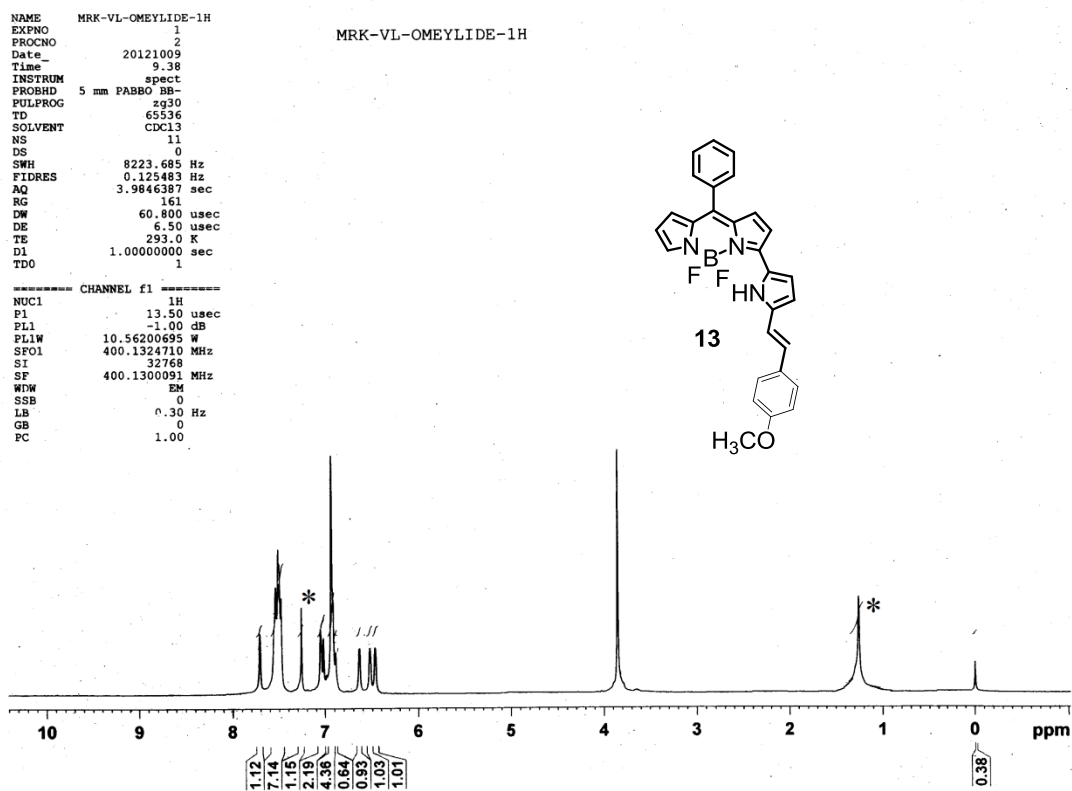


Figure 52: ¹H NMR spectrum of compound 13 in CDCl₃

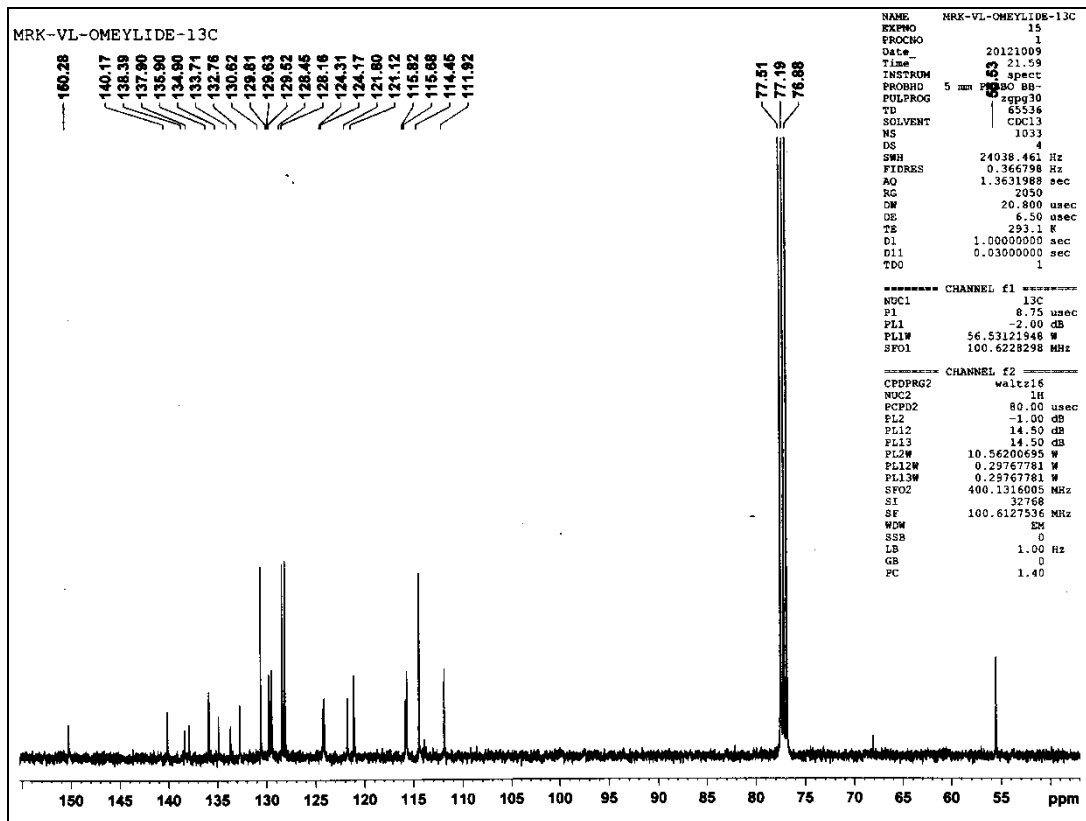


Figure 53: ^{13}C NMR spectrum of compound 13 in CDCl_3

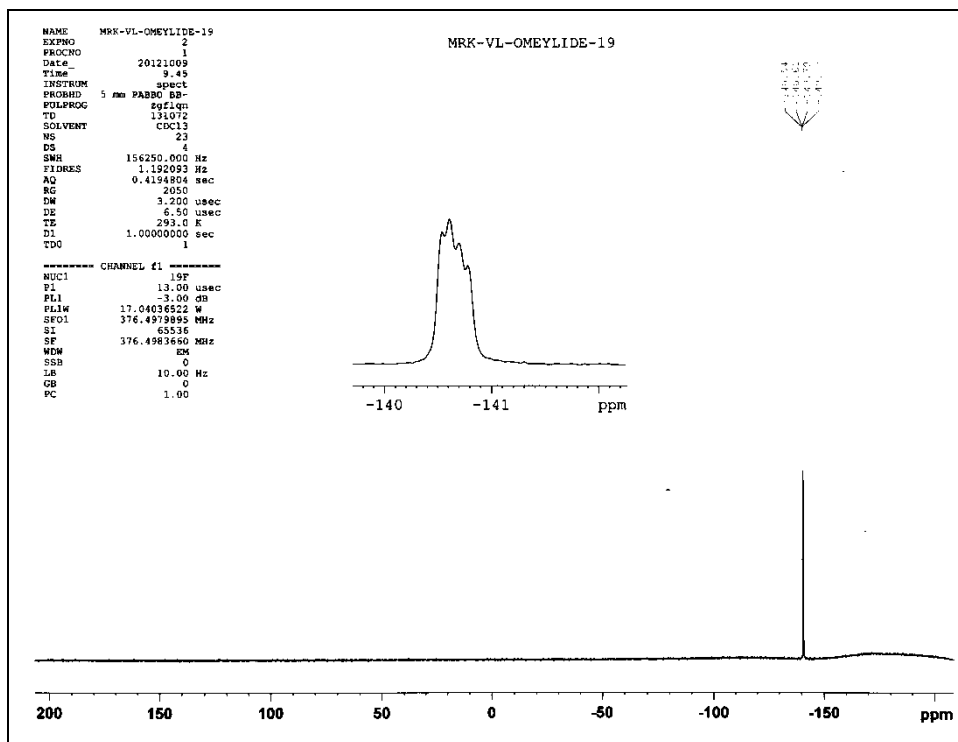


Figure 54: ^{19}F NMR spectrum of compound **13** in CDCl_3 . The inset shows the expansion

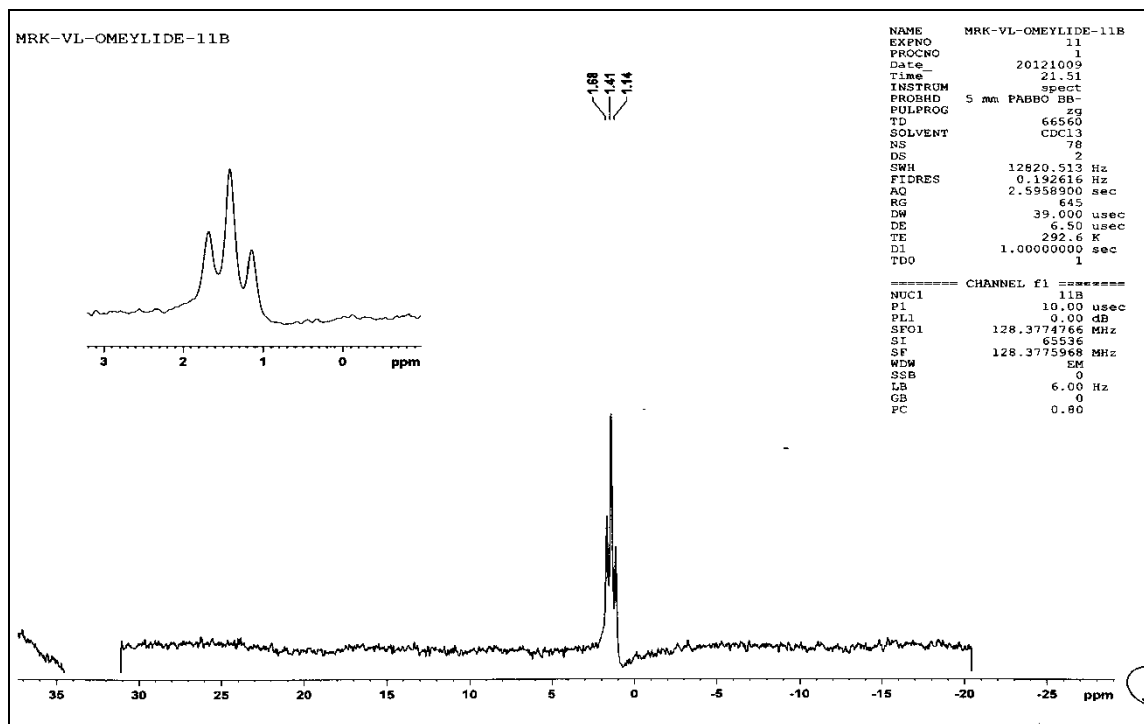


Figure 55: ^{11}B NMR spectrum of compound **13** in CDCl_3 . The inset shows the expansion

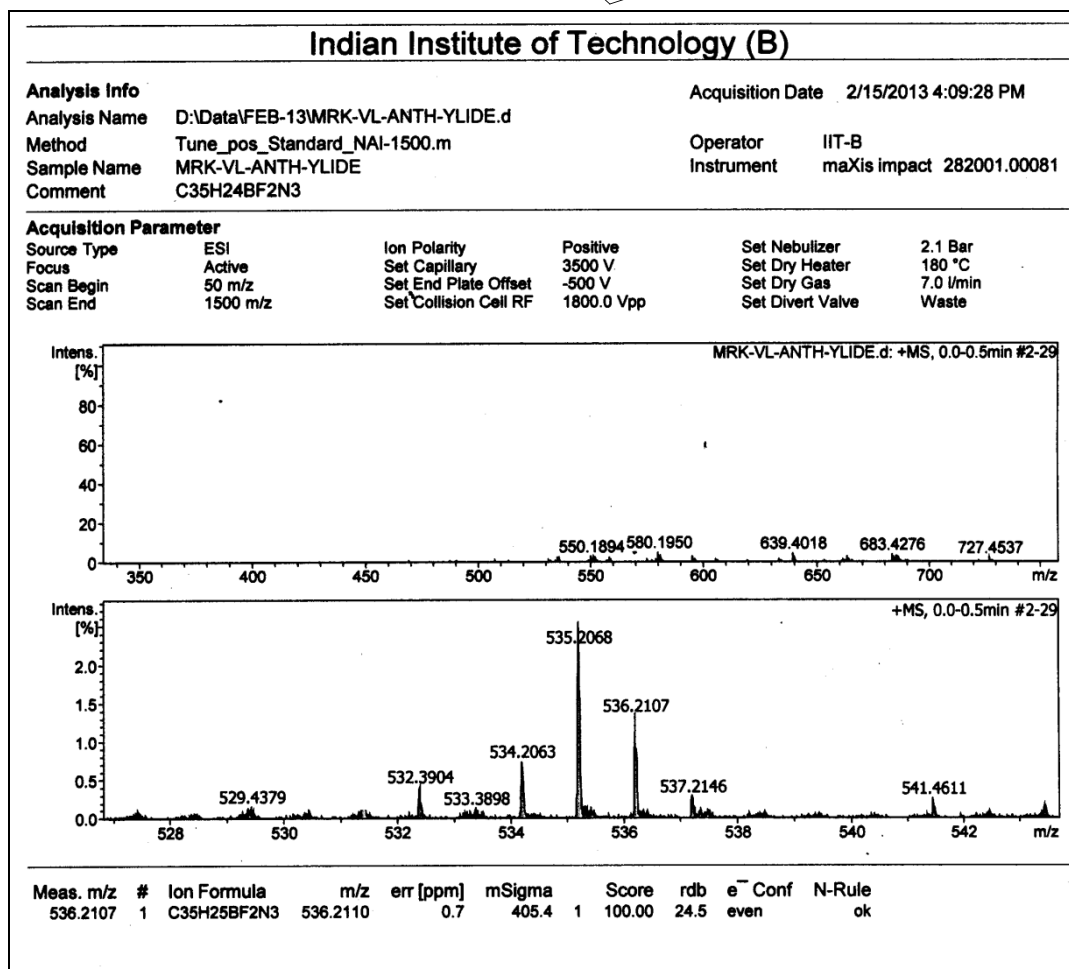
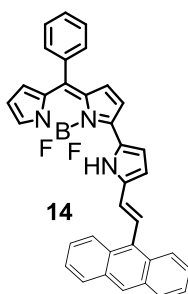


Figure 56: HRMS mass spectrum of compound **14**

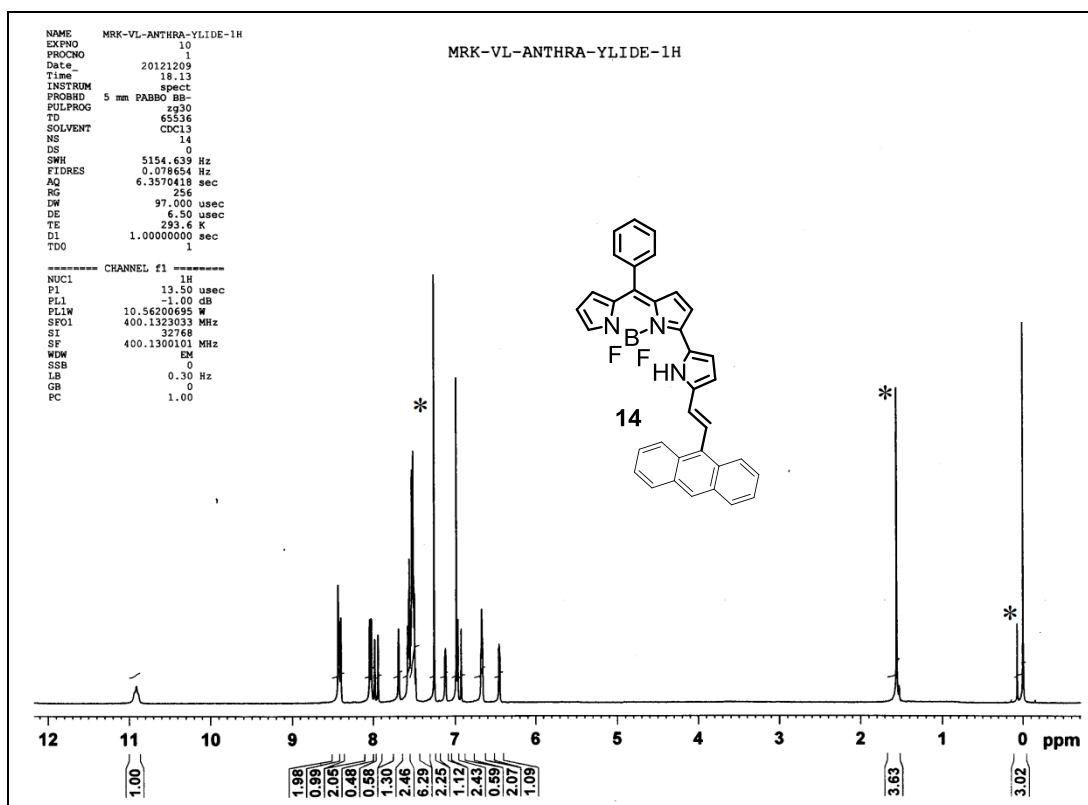


Figure 57: ^1H NMR spectrum of compound 14 in CDCl_3

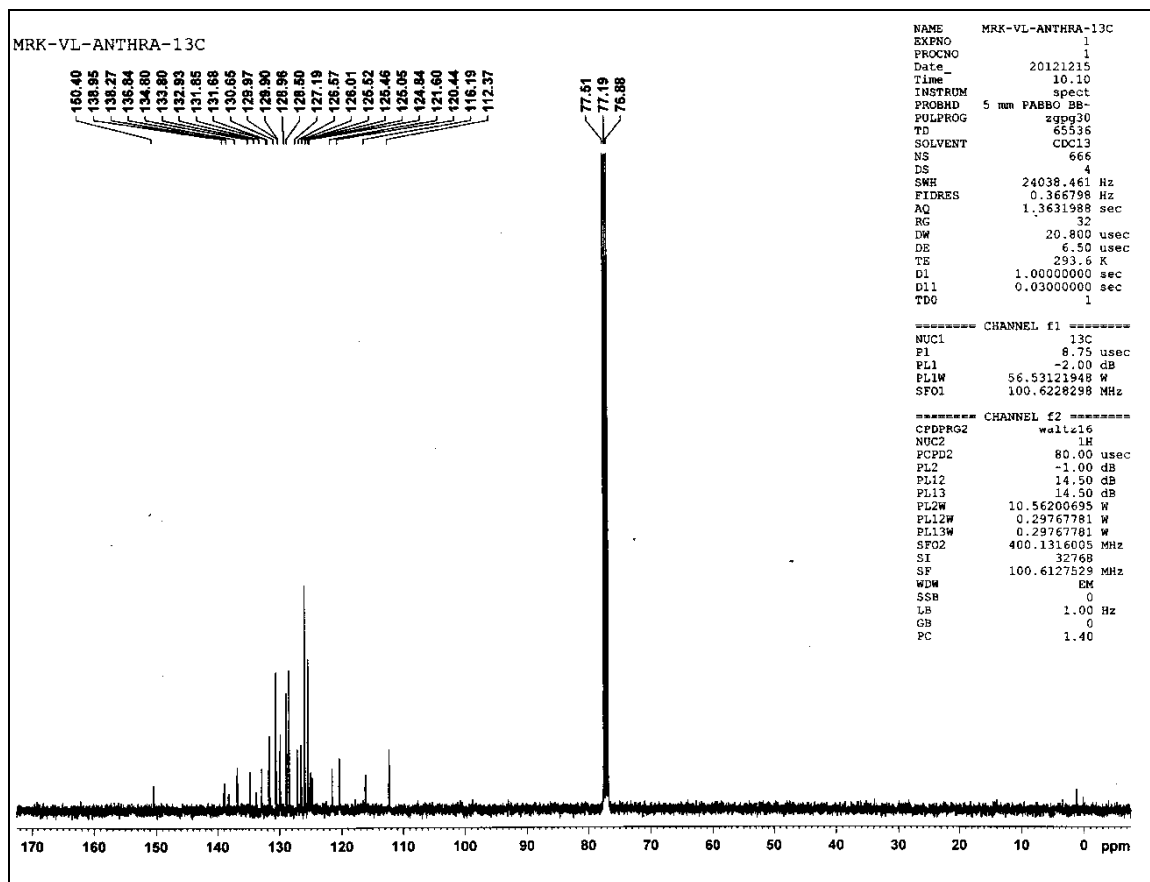


Figure 58: ^{13}C NMR spectrum of compound **14** in CDCl_3

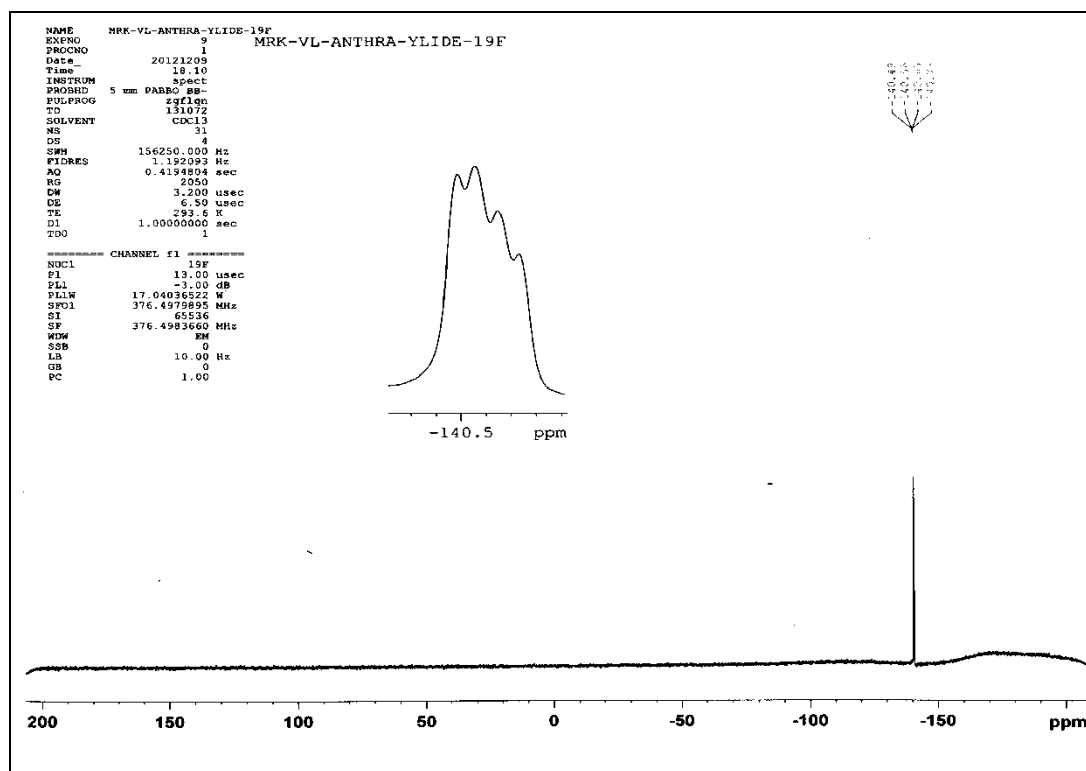


Figure 59: ^{19}F NMR spectrum of compound **14** in CDCl_3 . The inset shows the expansion

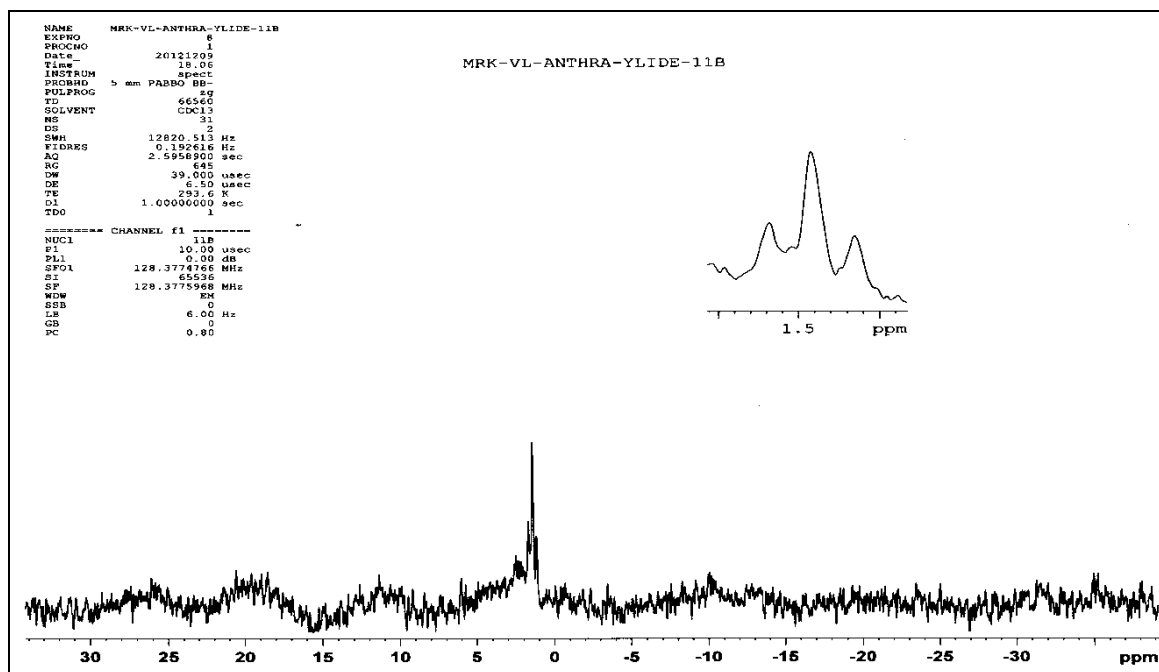


Figure 60: ^{11}B NMR spectrum of compound **14** in CDCl_3 . The inset shows the expansion

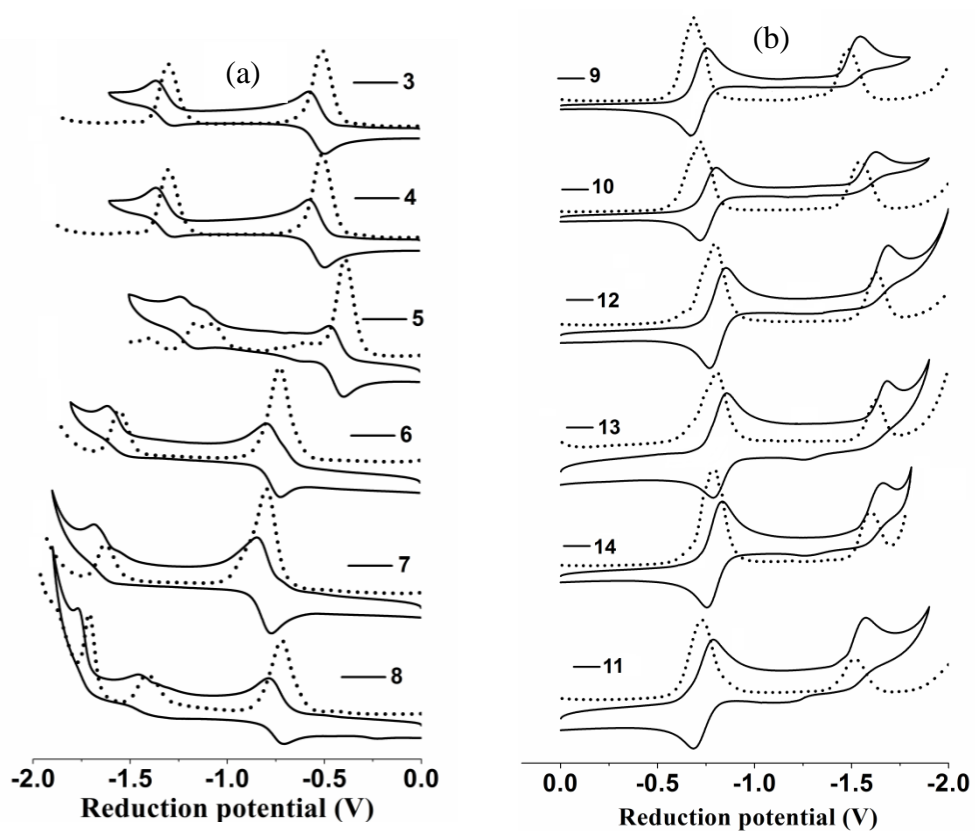


Figure 61: Comparison of reduction waves of compounds (a) **3-8** (b) **9-14** recorded in CH_2Cl_2 using TBAP as supporting electrolyte at 50 mV/sec scan rate.

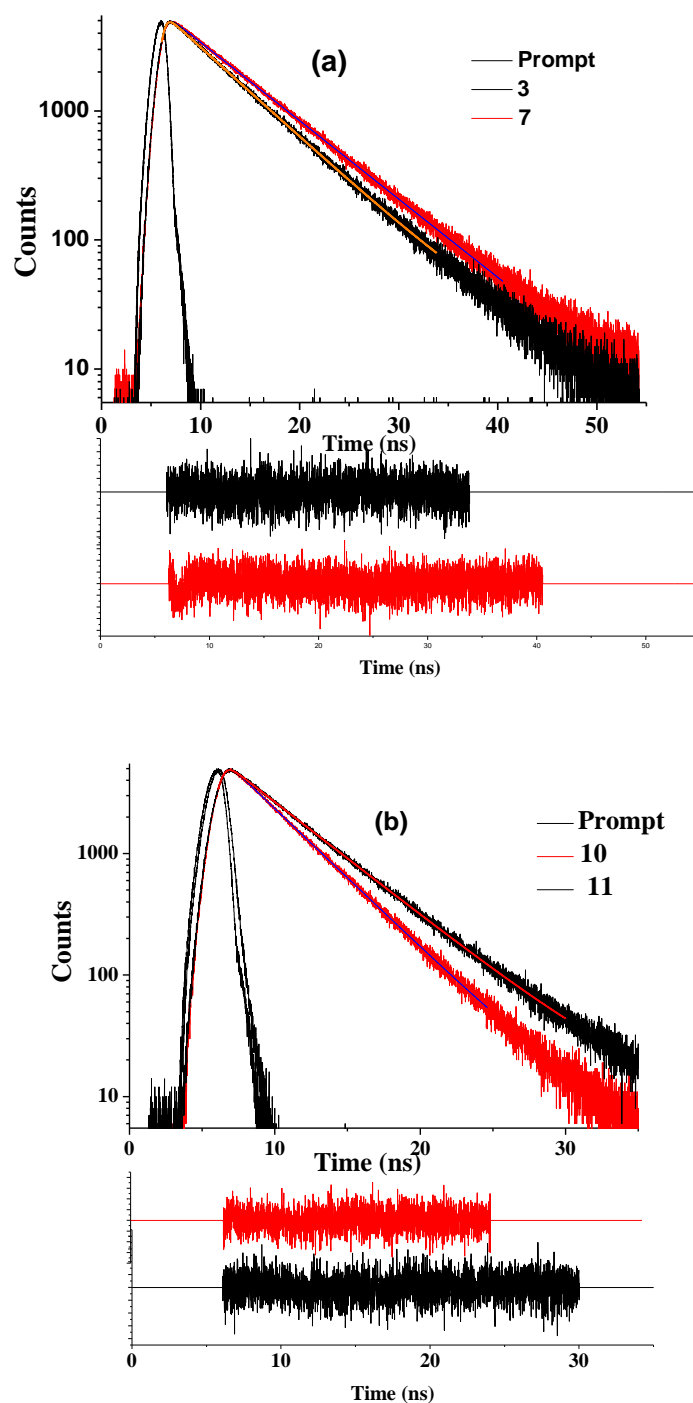


Figure 62: Fluorescence decay profile and weighted residual distribution fits of (a) compounds **3** and **8** (b) compounds **10** and **11** in chloroform. The excitation wavelength used was 560 nm and emission was detected at their corresponding wavelengths.