3, 5-Diformyl-Borondipyrromethene for Selective Detection of Cyanide Anion

Sheri Madhu[a], Santanu Kumar Basu[b], Sameer Jadhav[b] and Mangalampalli Ravikanth[a*]

[a]Department of Chemistry, Indian Institute of Technology Bombay, Powai, Mumbai, 400 076, India. E-mail: ravikanth@chem.iitb.ac.in

[b]Department of Chemical Engineering, Indian Institute of Technology Bombay, Powai, Mumbai, 400 076, India.

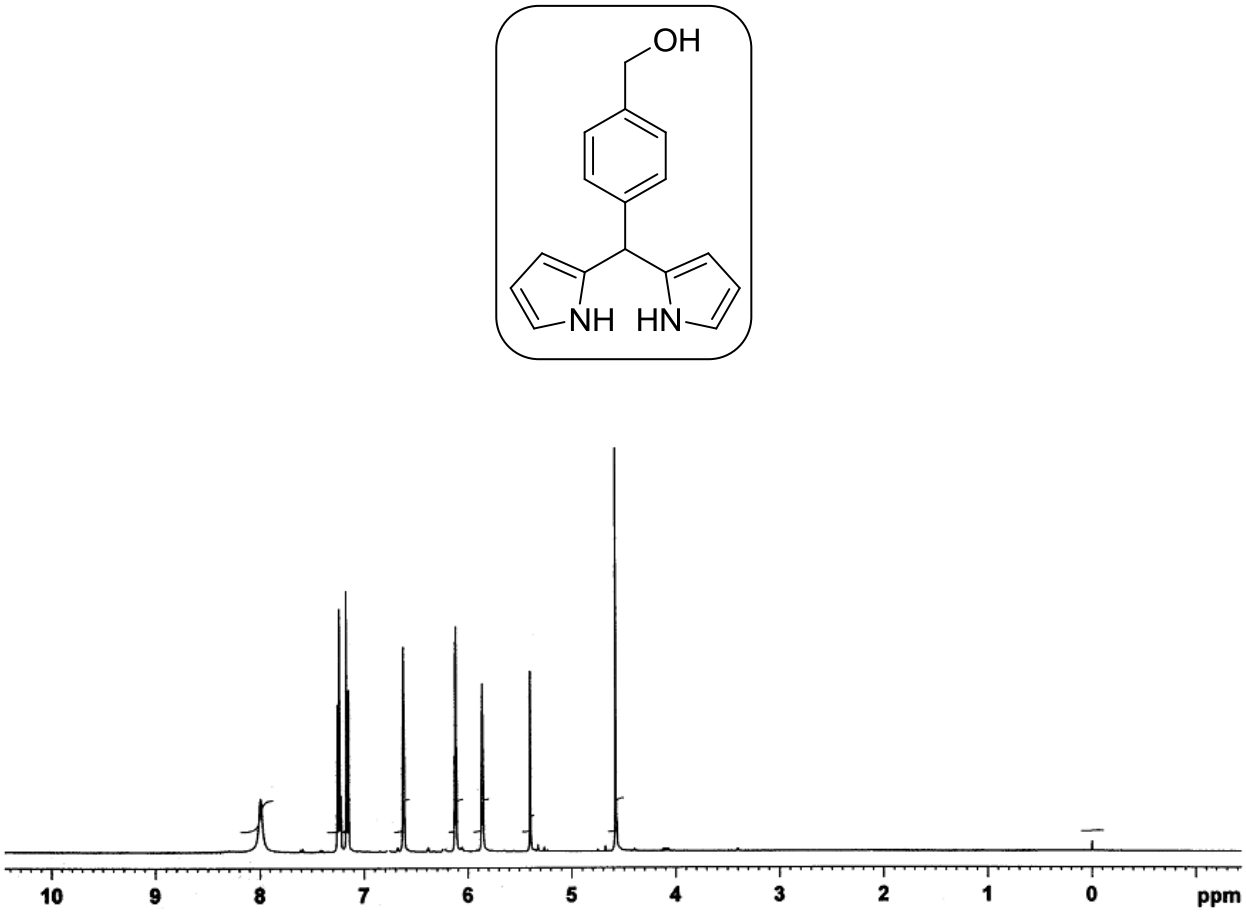


Figure S1: ^{1}H NMR spectrum of compound **4** recorded in $CDCl_3$

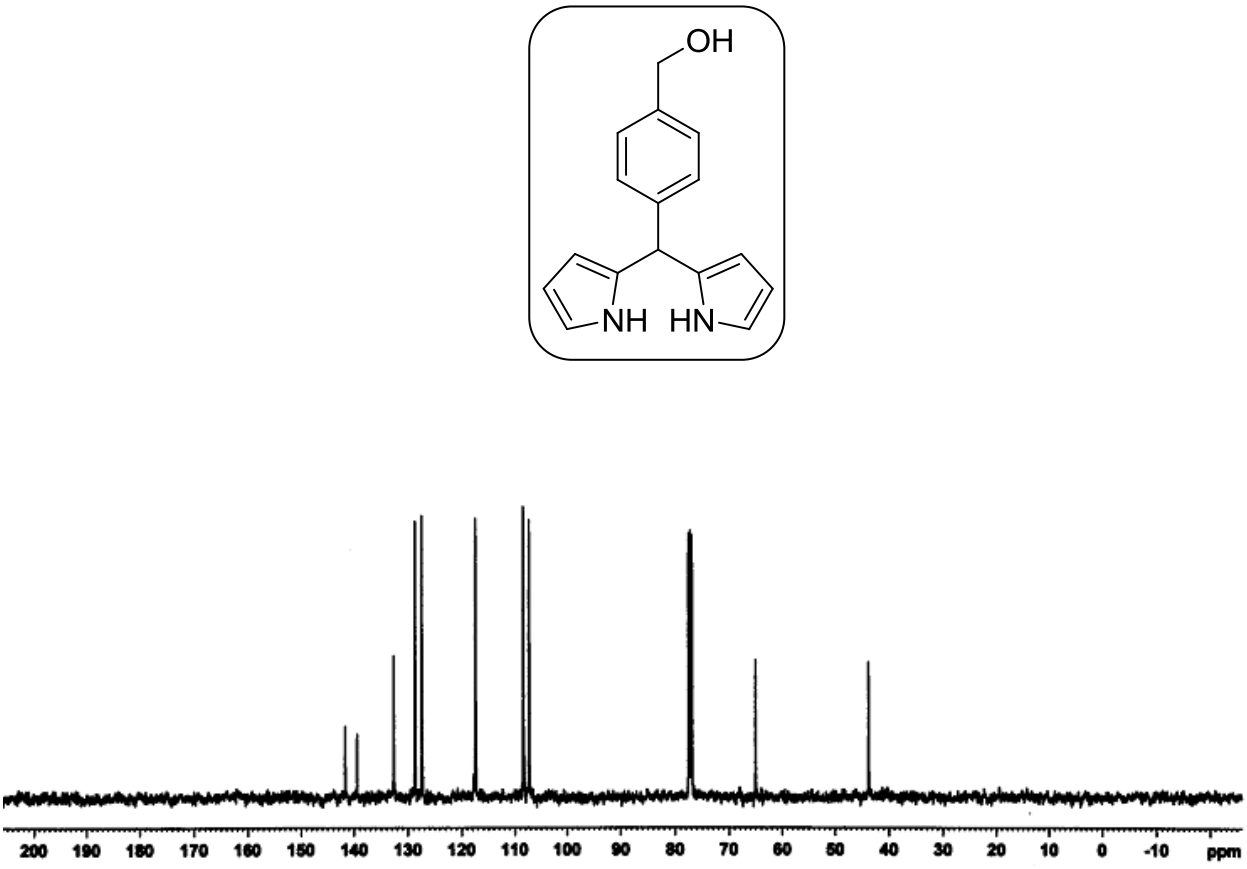
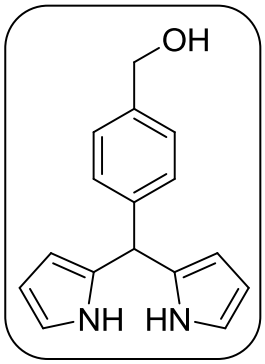


Figure S2: ^{13}C NMR spectrum of compound **4** recorded in $CDCl_3$

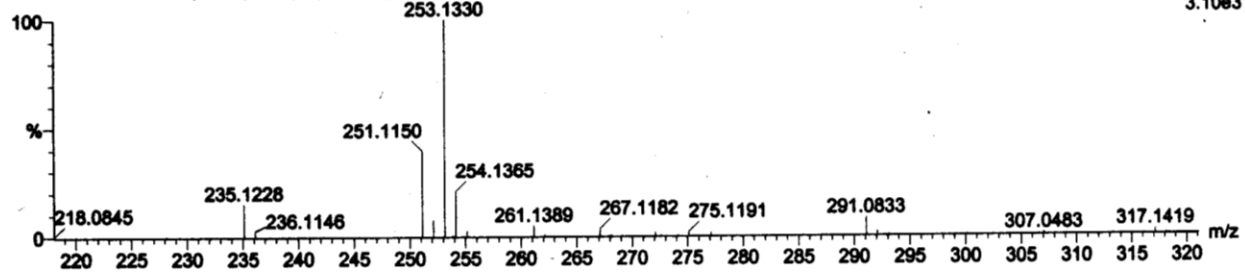


Elemental Composition Report **Page 1**

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
4 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) 11-Aug-201219:50:20
C16H16N2O
MRK-SM-OHDPM 28 (0.280) AM (Top,5, Ar,5000.0,556.28,1.00); Sm (Md, 4.00); Sb (5,40.00); Cm (26:51) TOF MS ES+
3.10e3



Minimum:				-1.5		
Maximum:		200.0	50.0	200.0		
Mass	Calc. Mass	mDa	PPM	DBE	Score	Formula
253.1330	253.1341	-1.1	-4.4	9.5	1	C16 H17 N2 O

Figure S3: HRMS spectrum of compound **4**

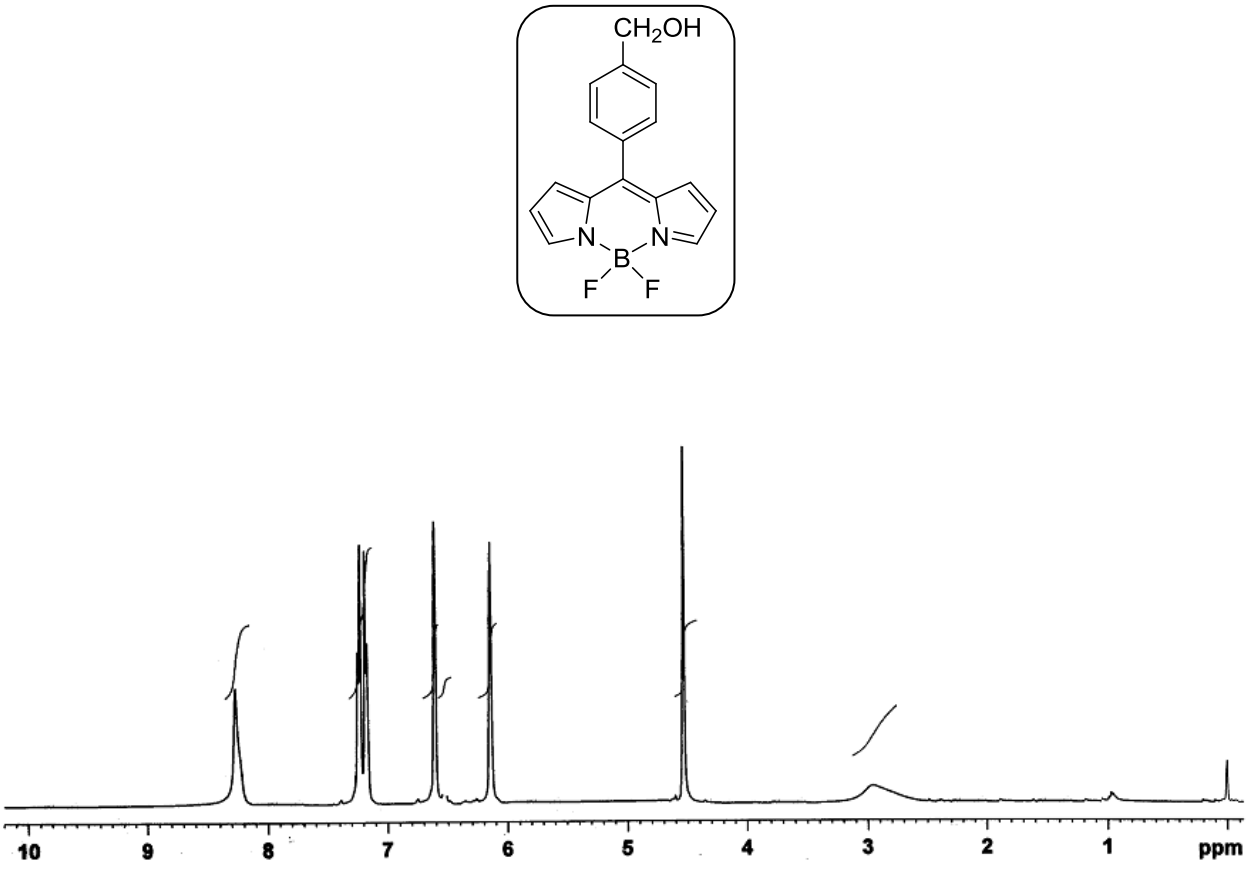


Figure S4: ^{1}H NMR spectrum of compound **5** recorded in $CDCl_3$

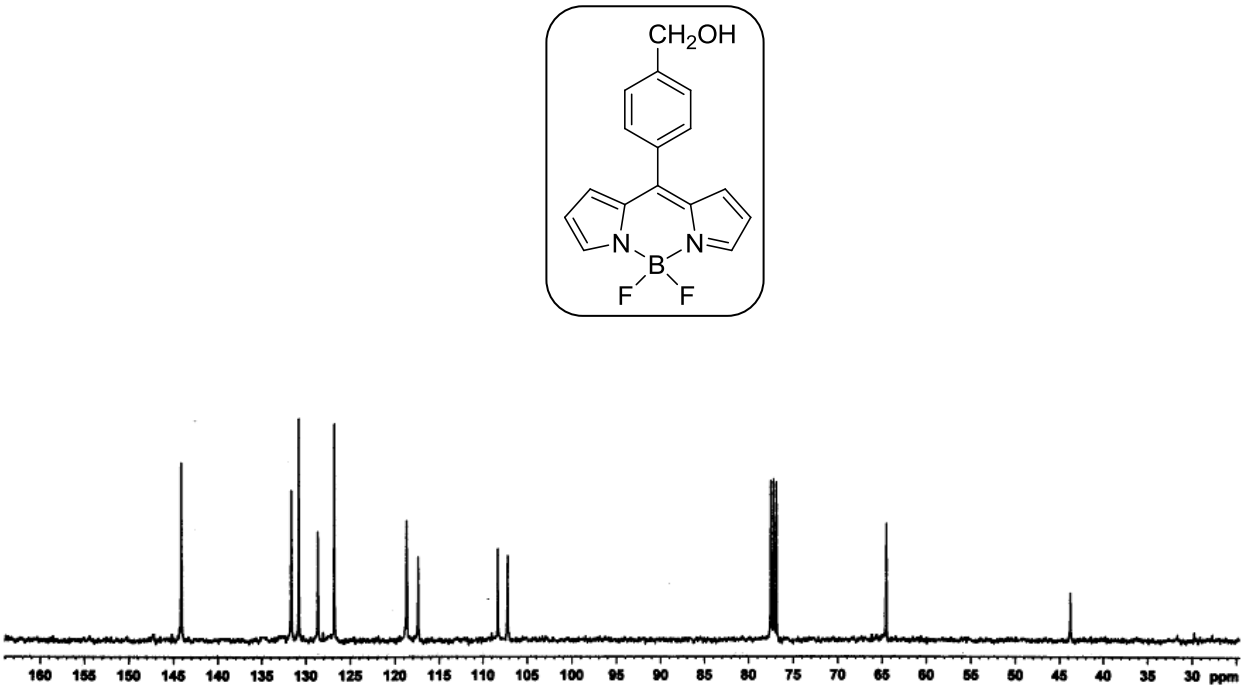


Figure S5: ^{13}C NMR spectrum of compound **5** recorded in $CDCl_3$

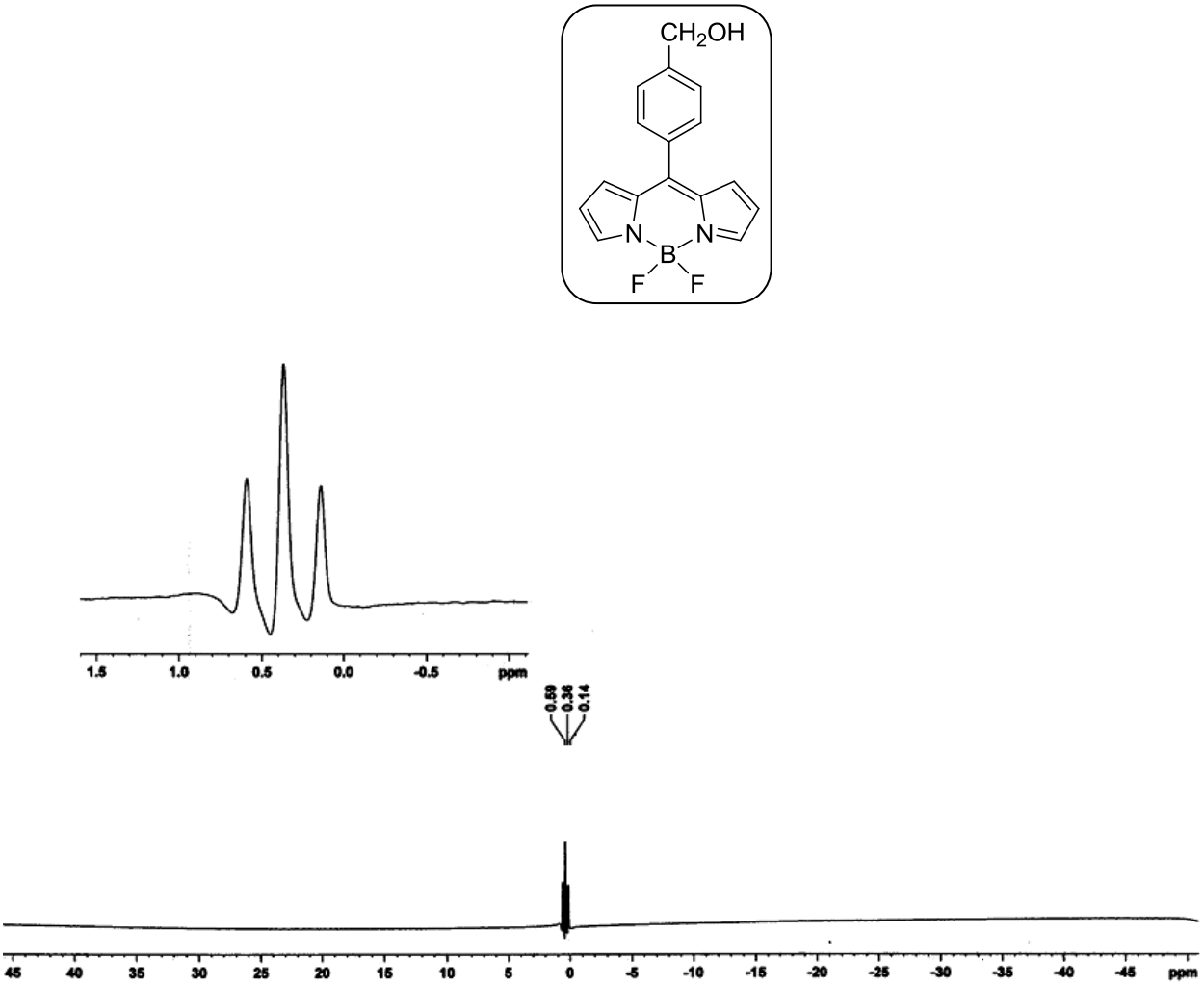


Figure S6: ^{11}B NMR spectrum of compound **5** recorded in $CDCl_3$**.** Inset shows the expansion

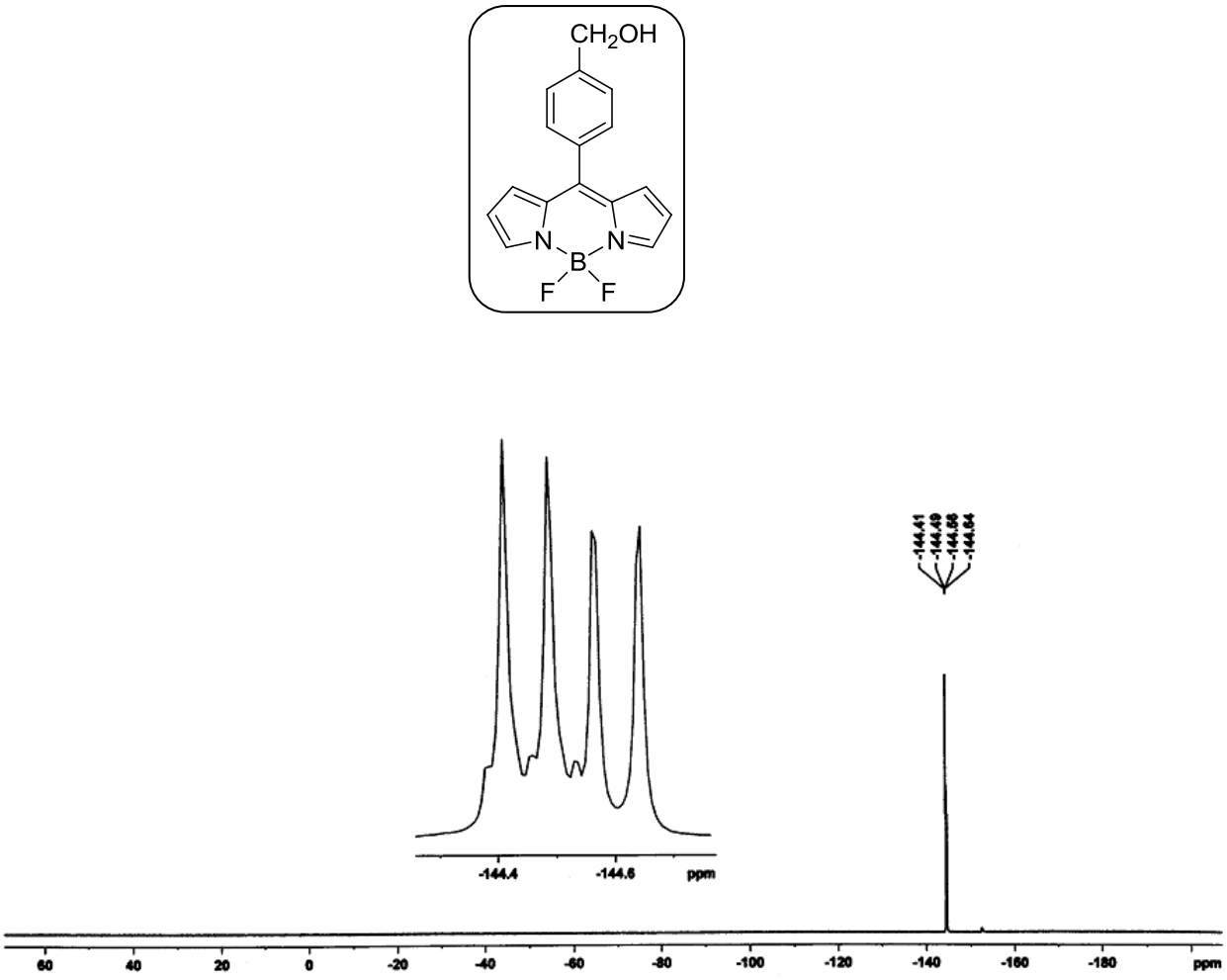
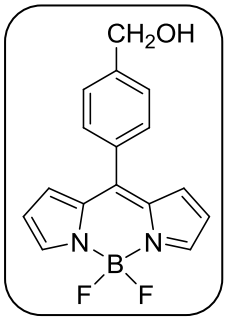


Figure S7: ^{19}F NMR spectrum of compound **5** recorded in $CDCl_3$**.** Inset shows the expansion

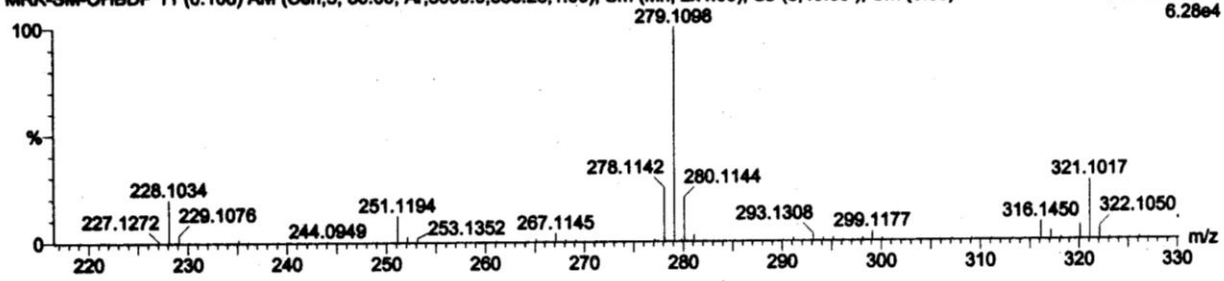


Elemental Composition Report Page 1

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
19 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) 11-Aug-201220:07:17
C16H13BF2N2O
MRK-SM-OHBDP 11 (0.108) AM (Cen,5, 80.00, Ar,5000.0,556.28,1.00); Sm (Mn, 2x4.00); Sb (5,40.00); Cm (6:33) TOF MS ES+
6.28e4



Minimum:				-1.5		
Maximum:		200.0	50.0	200.0		
Mass	Calc. Mass	mDa	PPM	DBE	Score	Formula
279.1098	279.1105	-0.7	-2.5	11.5	1	C16 H13 B N2 O F

Figure S8: HRMS spectrum of compound **5**

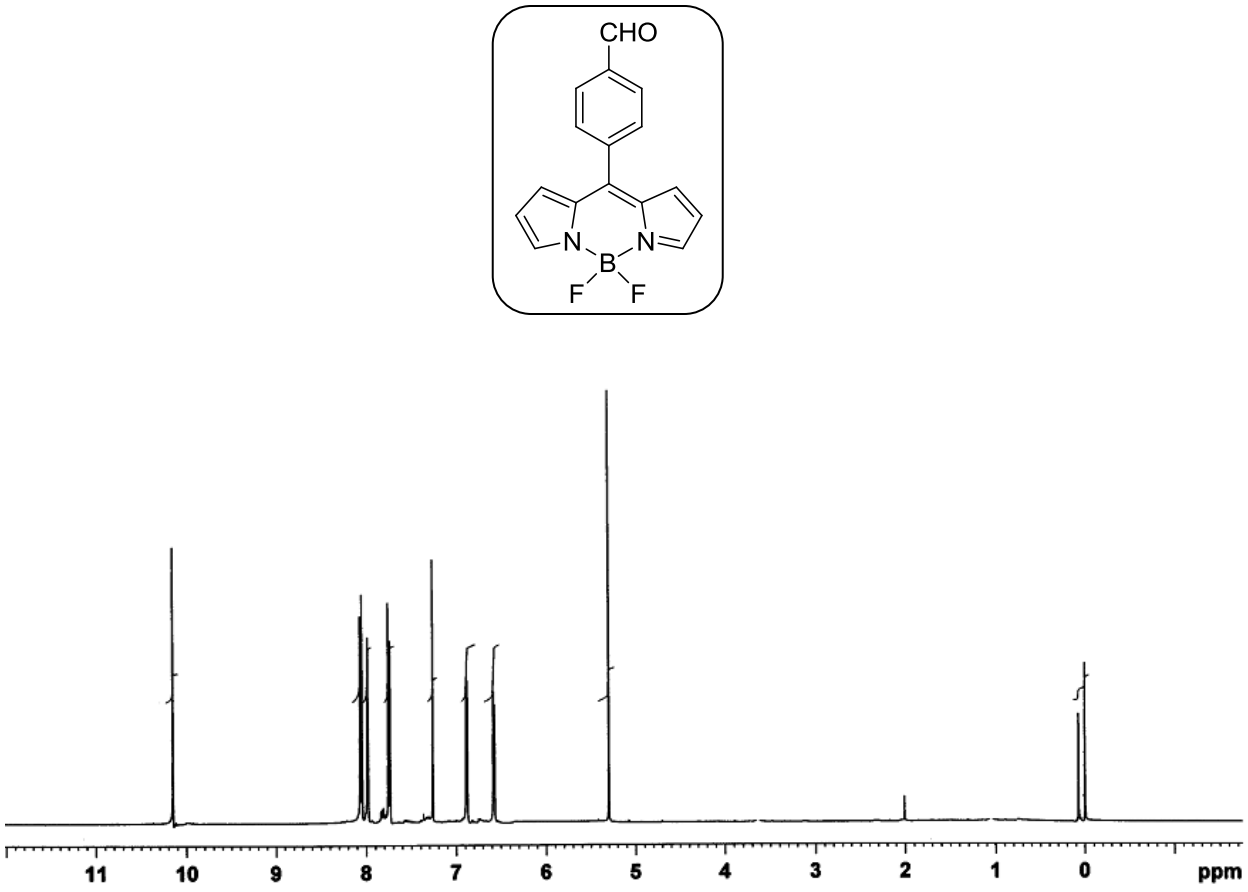


Figure S9: ^{1}H NMR spectrum of compound **3** recorded in $CDCl_3$

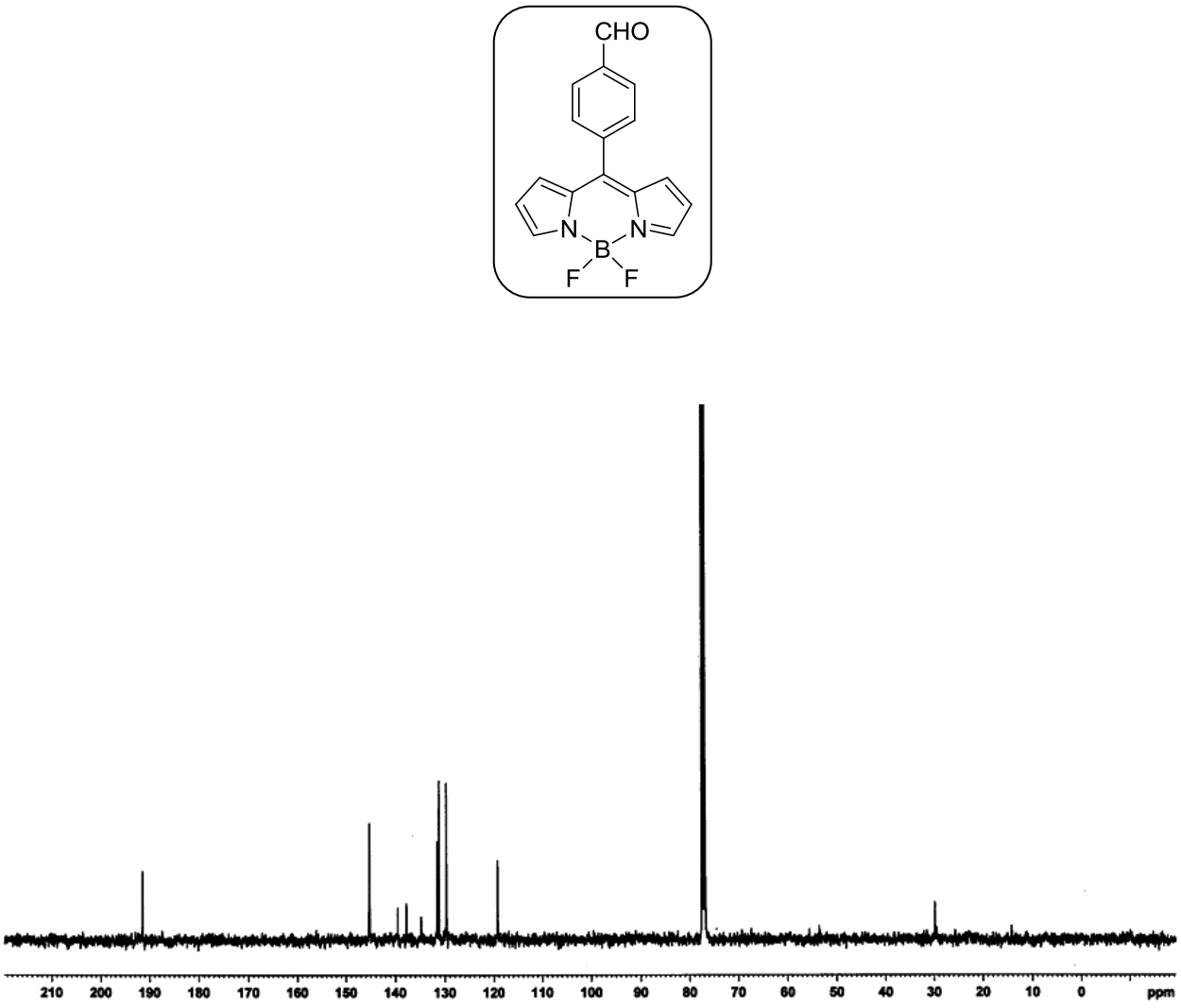


Figure S10: ^{13}C NMR spectrum of compound **3** recorded in $CDCl_3$

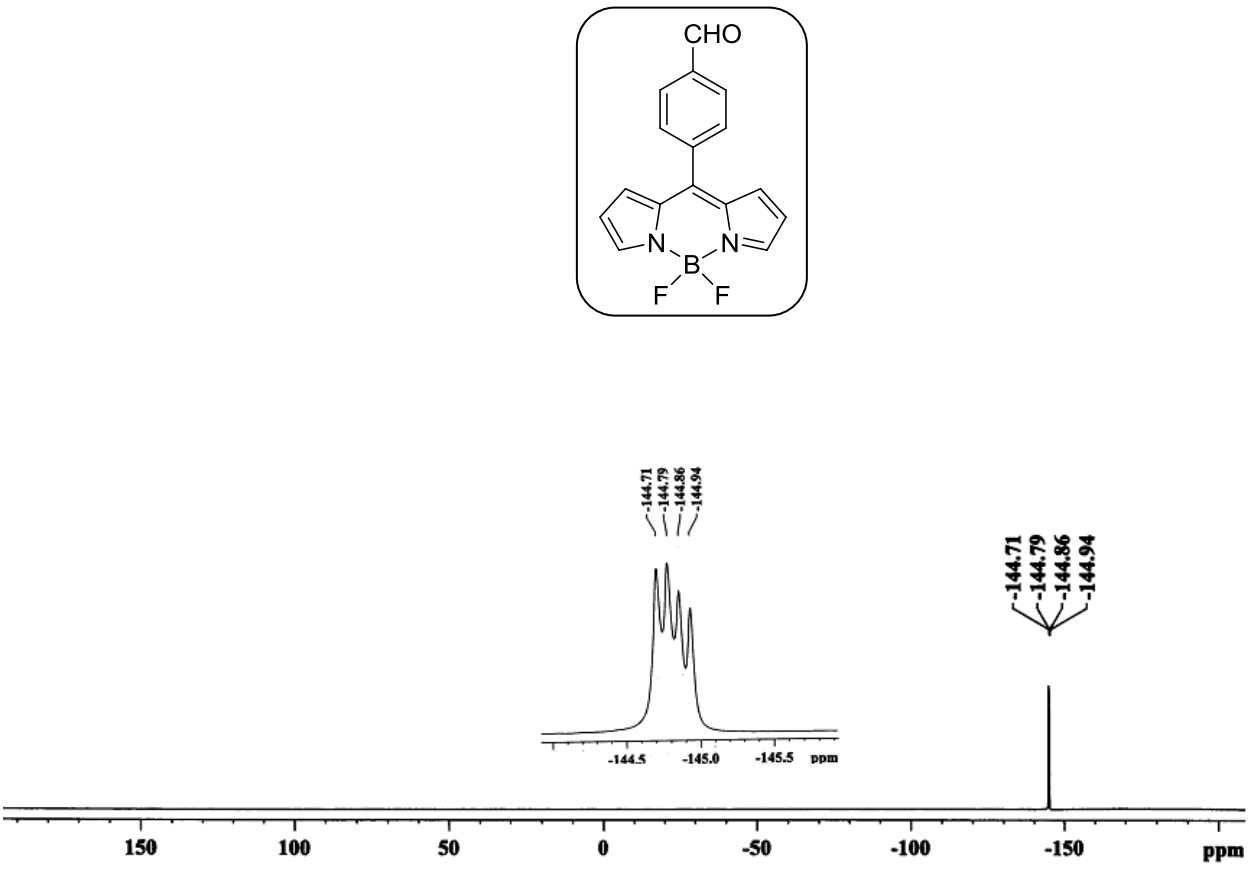


Figure S11: ^{19}F NMR spectrum of compound **3** recorded in $CDCl_3$. Inset shows the expansion

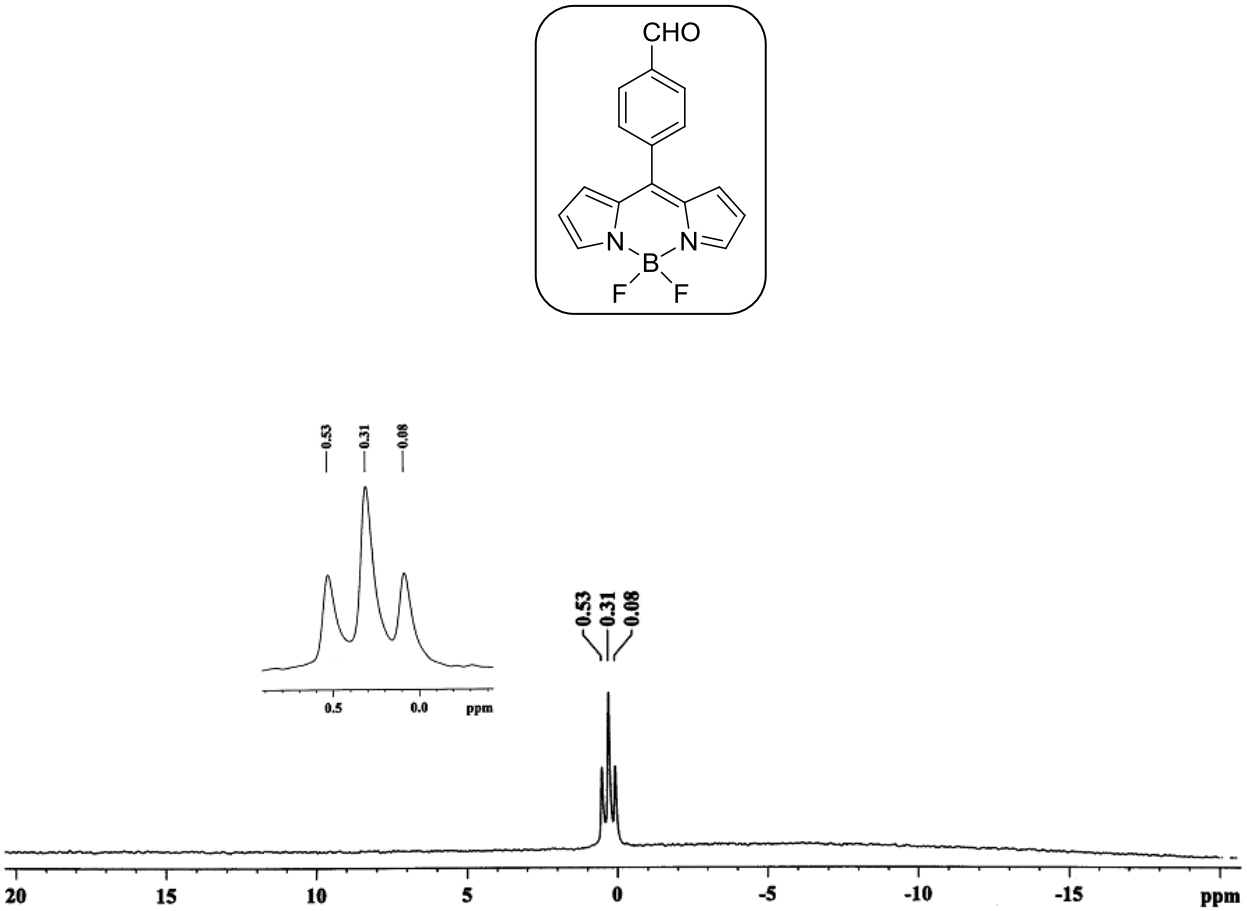
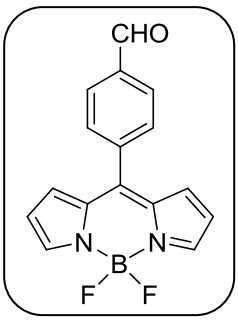


Figure S12: ^{11}B NMR spectrum of compound **3** recorded in $CDCl_3$. Inset shows the expansion

\

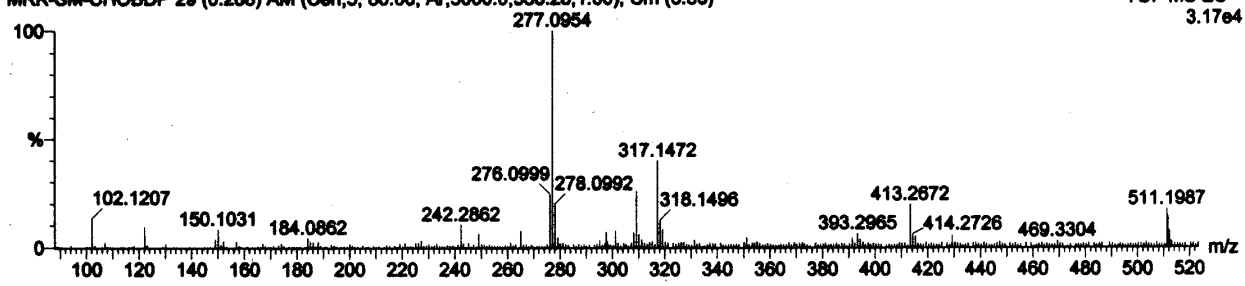


Elemental Composition Report **Page 1**

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
18 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) 11-Aug-201220:49:00
C16H11BF2N2O
MRK-SM-CHOBDP 29 (0.288) AM (Cen,5, 80.00, Ar,5000.0,556.28,1.00); Cm (6:36) TOF MS ES+
3.17e4



Minimum:				-1.5		
Maximum:		200.0	50.0	200.0		
Mass	Calc. Mass	mDa	PPM	DBE	Score	Formula
277.0954	277.0948	0.5	1.9	12.5	1	C16 H11 B N2 O F

Figure S13: HRMS spectrum of compound **3**

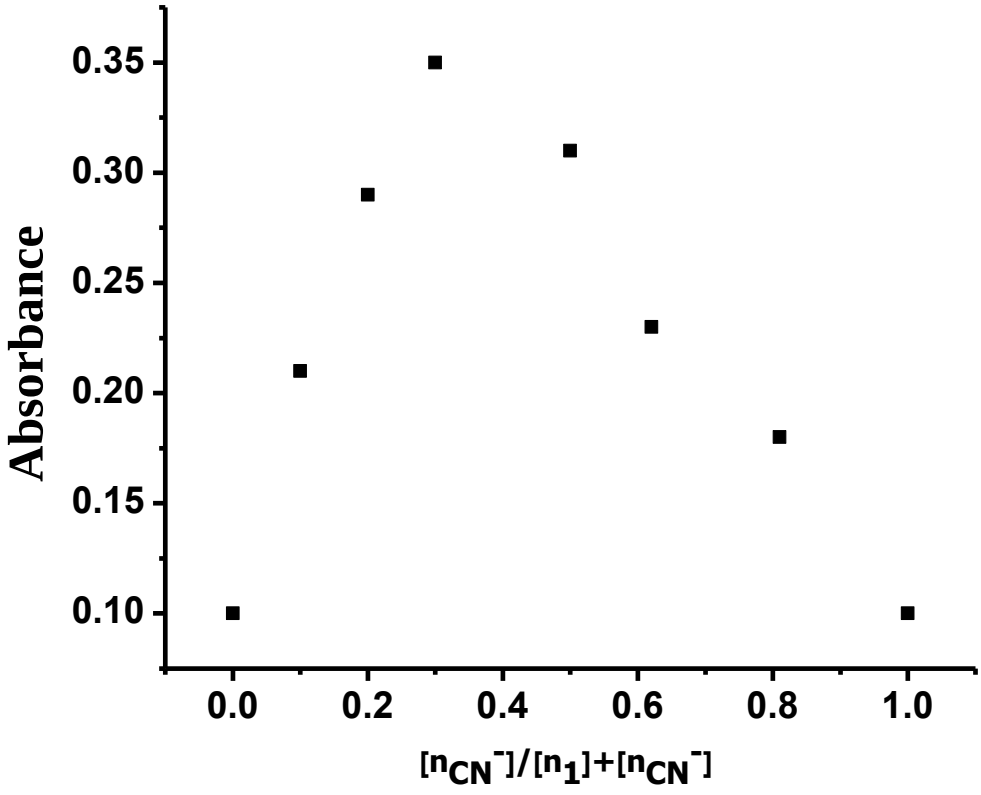


Figure S14: Job's plot for the **1** with CN^-. Where n_{CN}^-, n_1 are mole fractions of CN^- and **1** respectively which forms 1:2 complex.

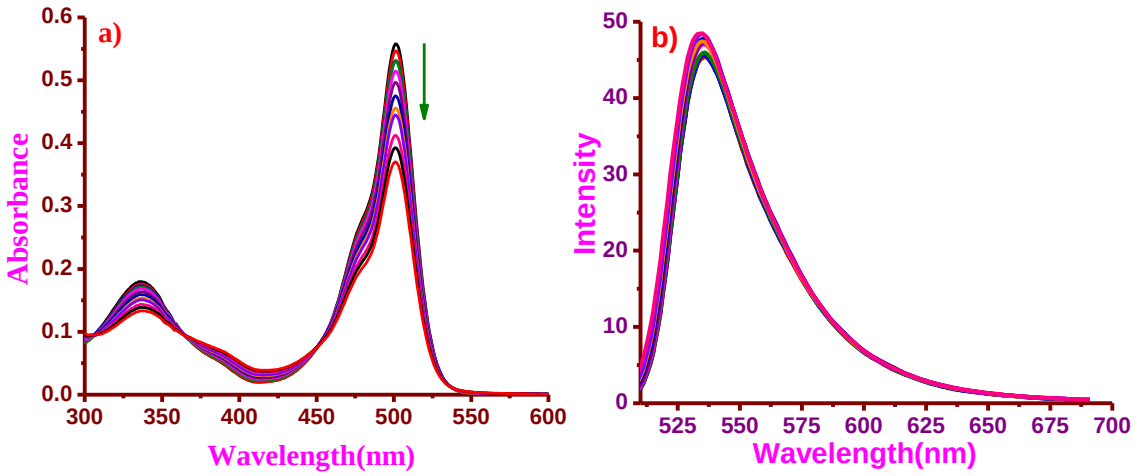


Figure S15: a) Absorption b) Emission spectra of compound **3** ($5x10^{-6}$ M) upon titration with different conc. of CN^- (TBACN) solution (0-50 equiv.) in CH_3CN.

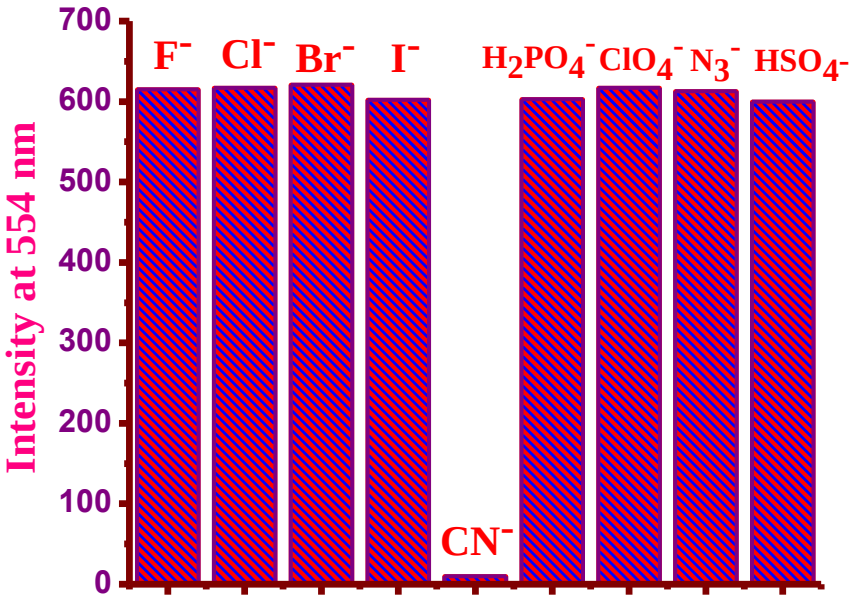


Figure S16: Histogram showing the changes in fluorescence intensity of compound **1** upon addition of various anions (excess of equivalents).

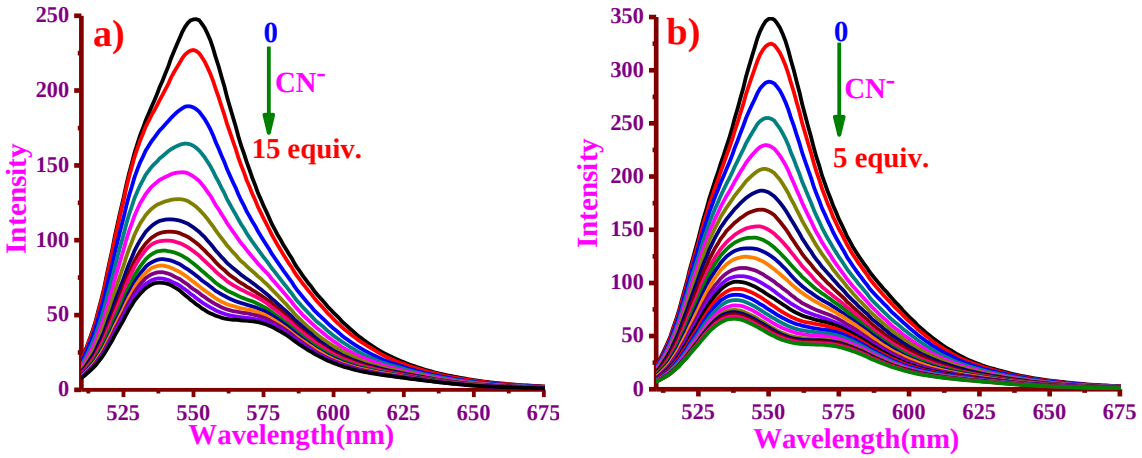


Figure S17: Emission spectra of compound **1** ($5x10^{-6}$ M), a) upon titration with different conc. of CN^- (TBACN) solution (0-15 equiv.) in ($CH_3CN:H_20$; 97:3 v/v), b) upon titration with different conc. of CN^- (TBACN) solution (0-5 equiv.) in ($CH_3CN:H_20$; 99:1 v/v).