# *Meso*-Salicylaldehyde Substituted BODIPY as Chemodosimetric Sensor for Cyanide Anion

Avanish Dvivedi, Palanisamy Rajakannu 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

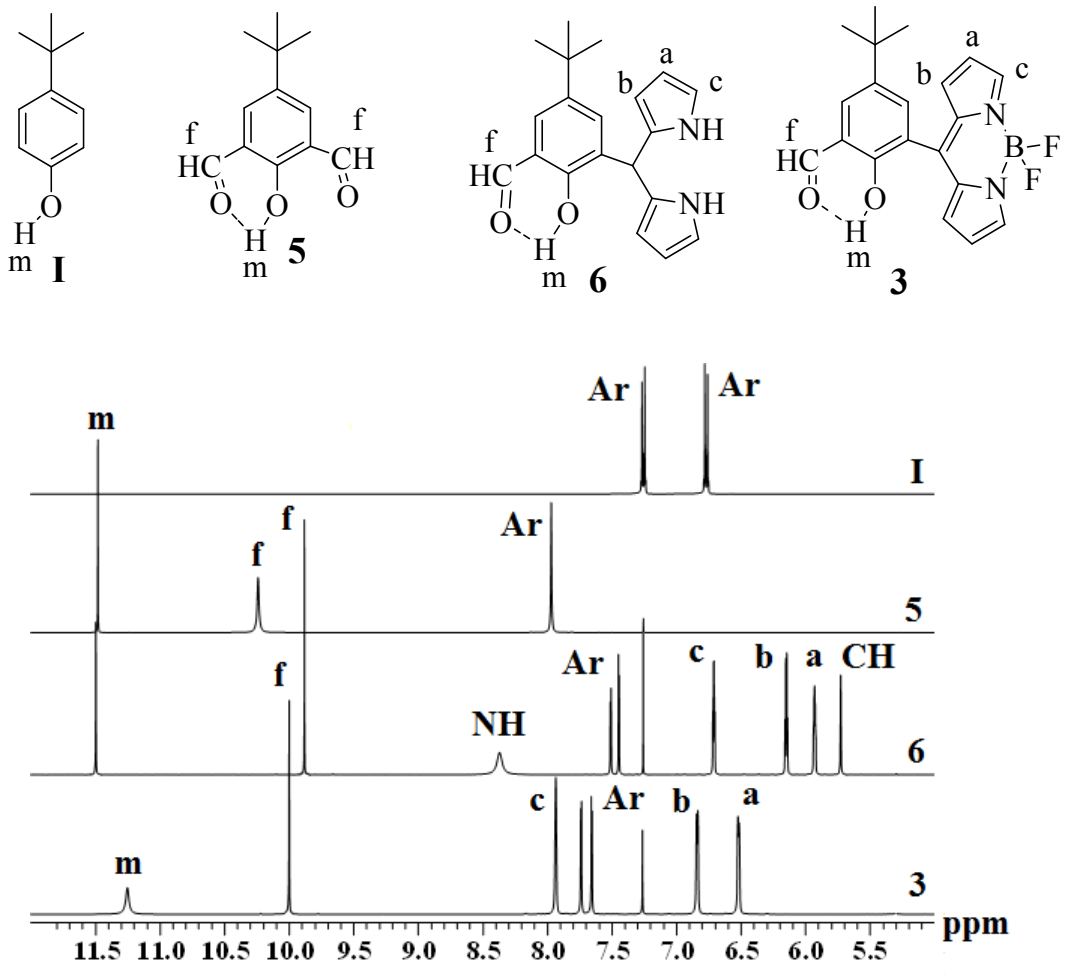



**Fig. S1** Comparison of $^{1}$H NMR spectra of **I, 5, 6** and compound **3**.

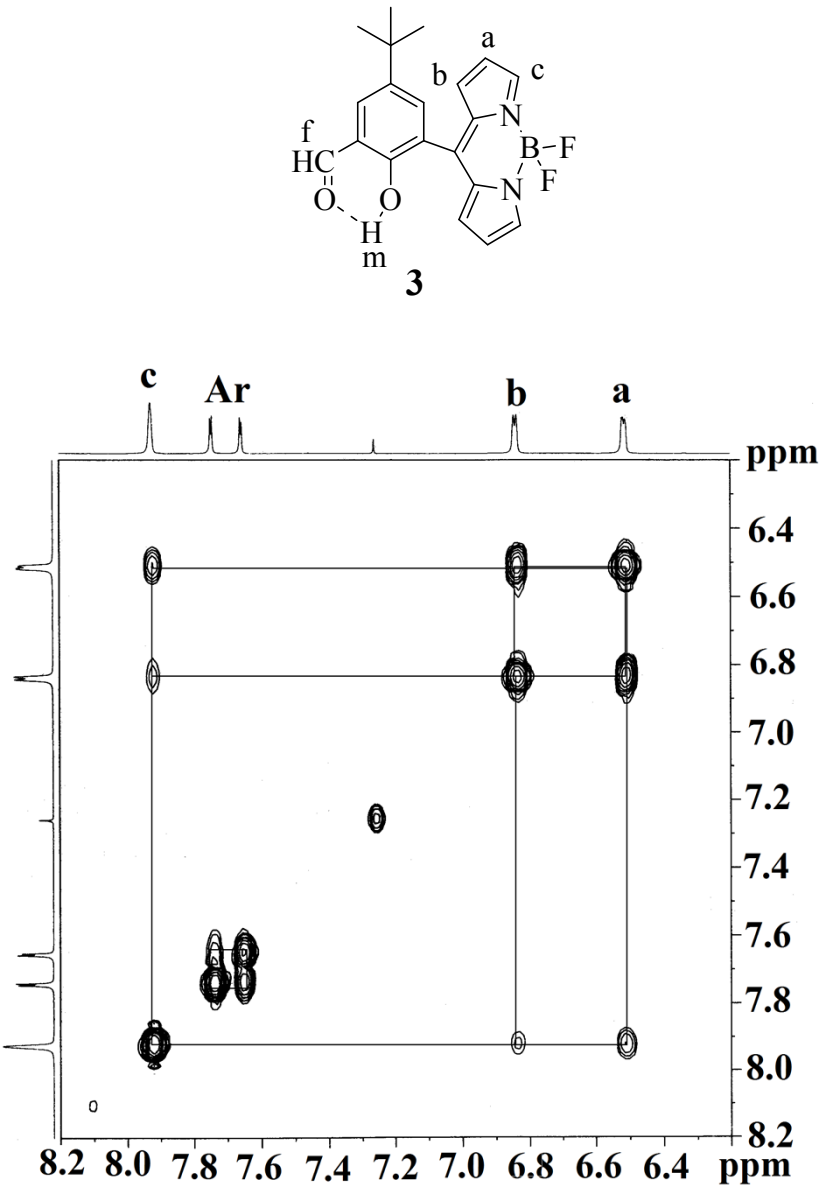
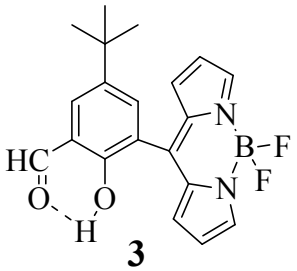



**Fig. S2** Sections of $^{1}$H-$^{1}$H COSY NMR spectra of BODIPY **3.**




**3**

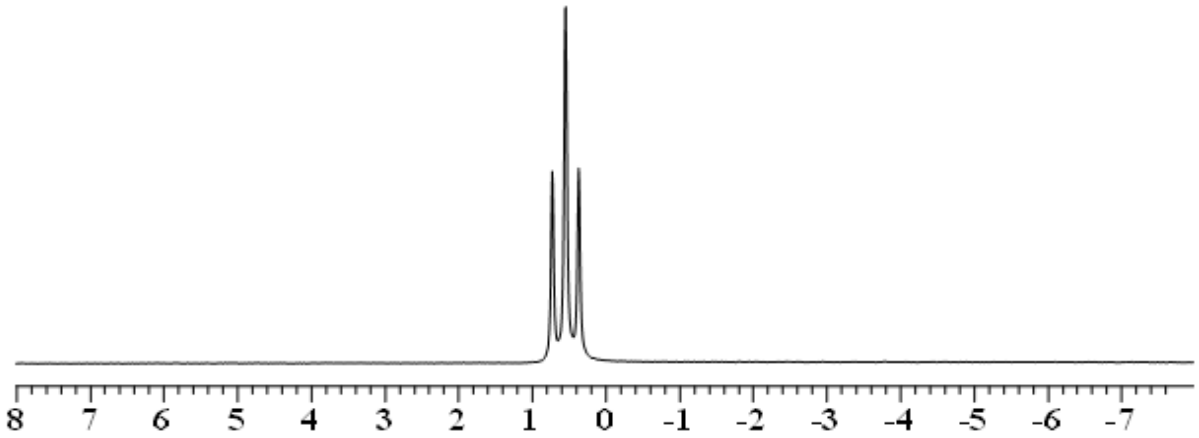



**Fig. S3** $^{11}$B NMR spectrum of BODIPY **3**.

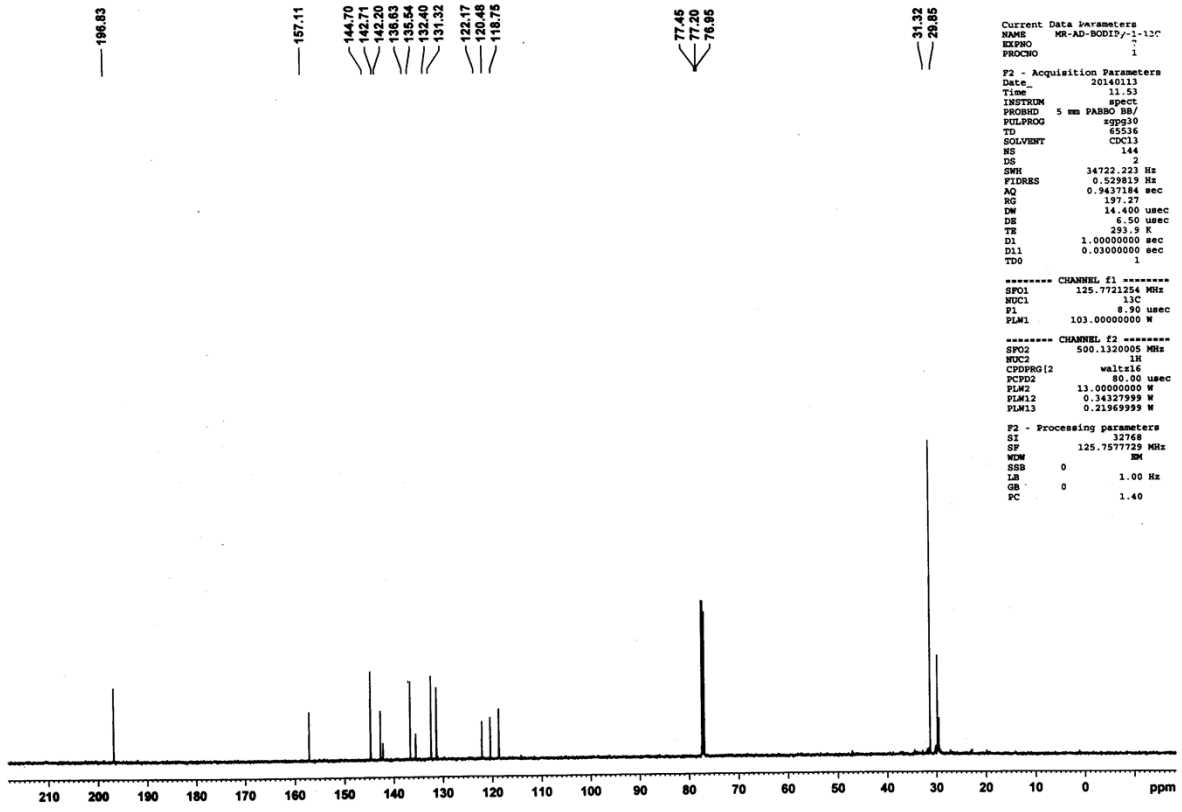



**Fig. S4** $^{13}$C NMR spectrum of BODIPY **3**.

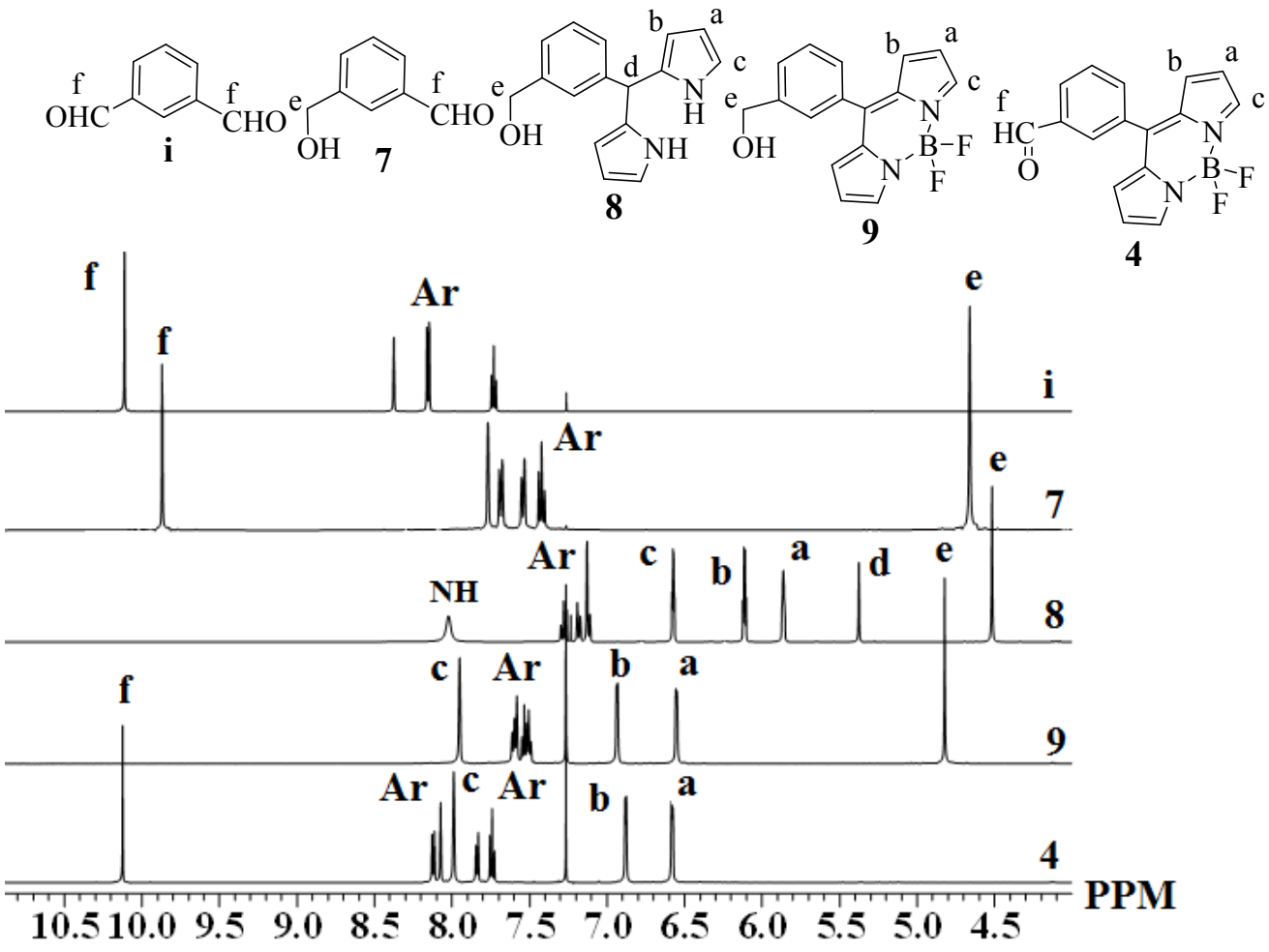



**Fig. S5** Comparison of $^{1}$H NMR spectra of **i, 7, 8, 9** and compound **4**.

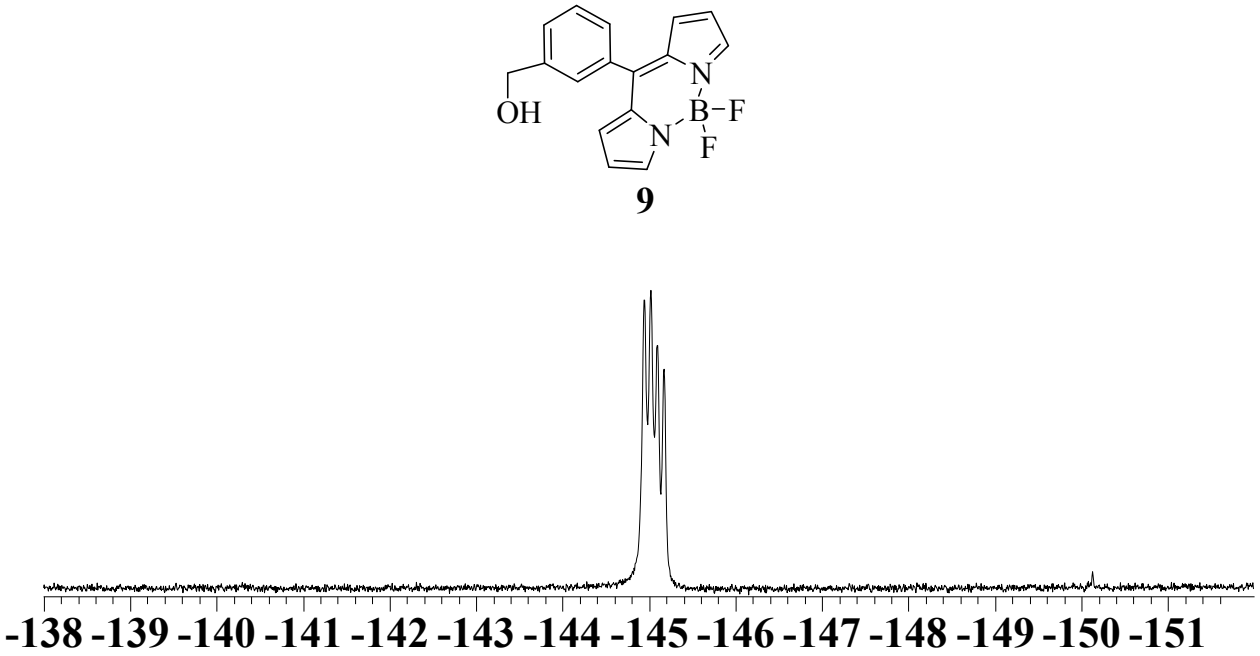
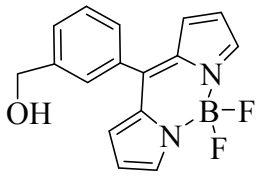



**Fig. S6** $^{11}$B NMR spectrum of BODIPY **9**.




**9**

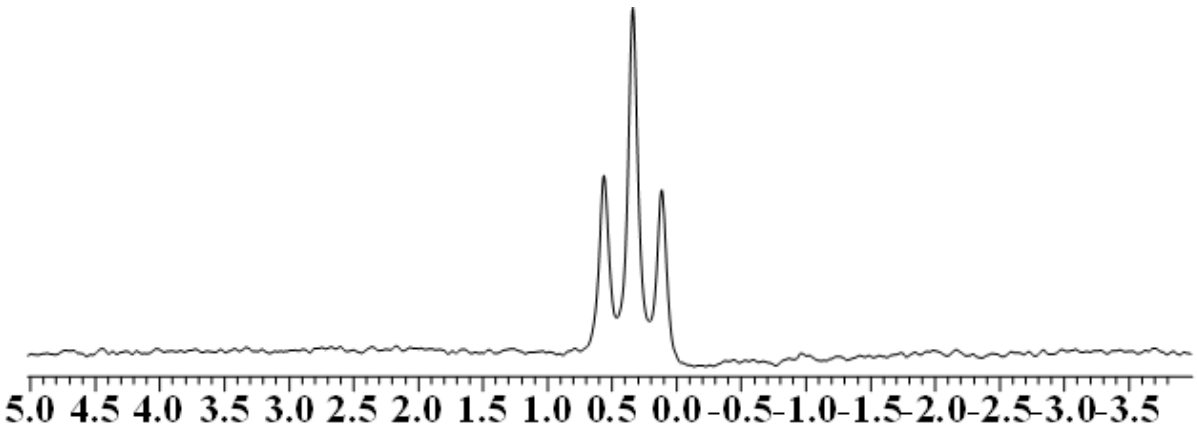



**Fig. S7** $^{19}$F NMR spectrum of BODIPY **9**.

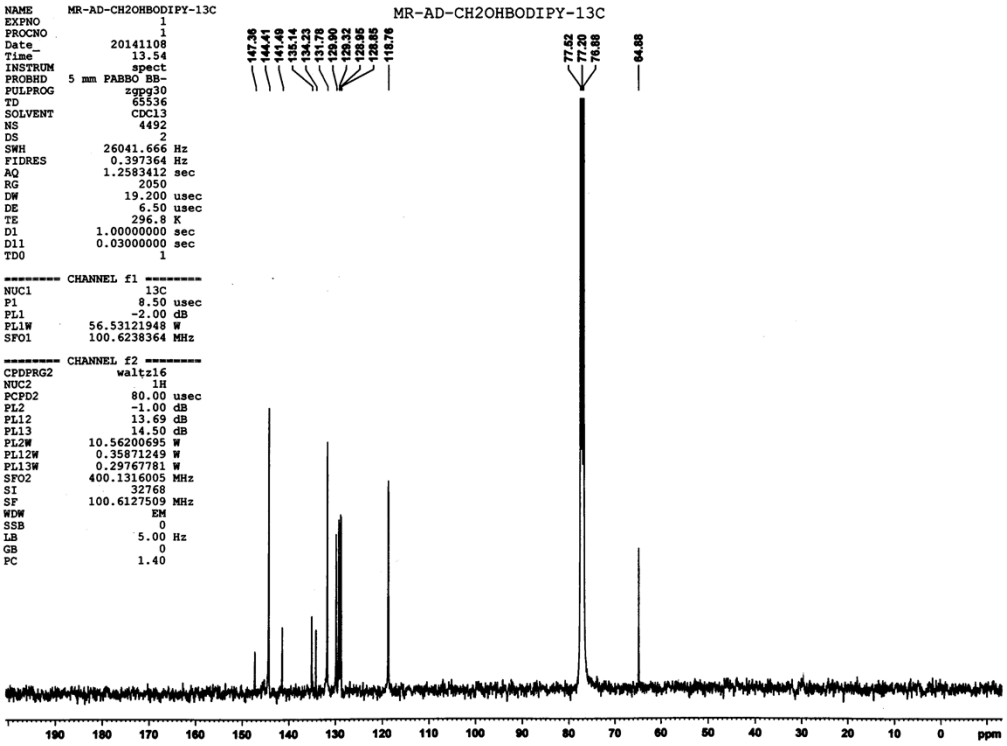
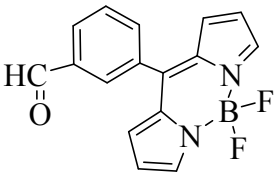



**Fig. S8** $^{13}$C NMR spectrum of BODIPY **9**.




**4**

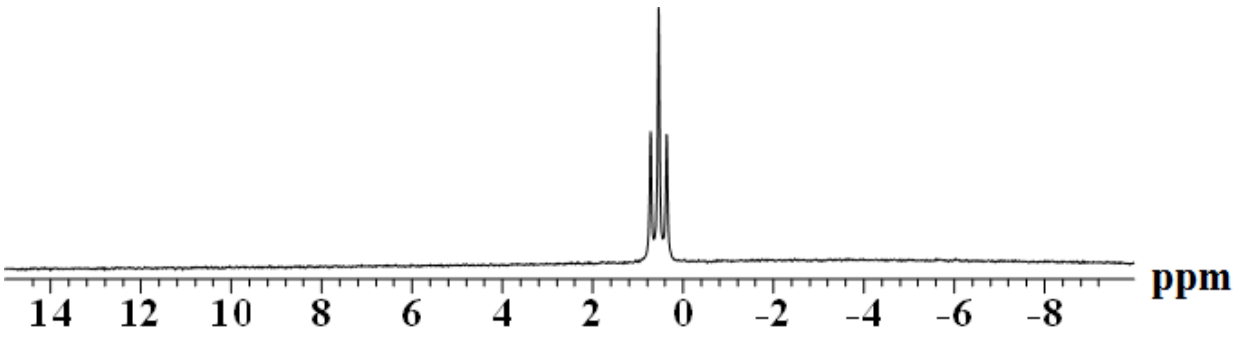



**Fig. S9** $^{11}$B NMR spectrum of BODIPY **4**.

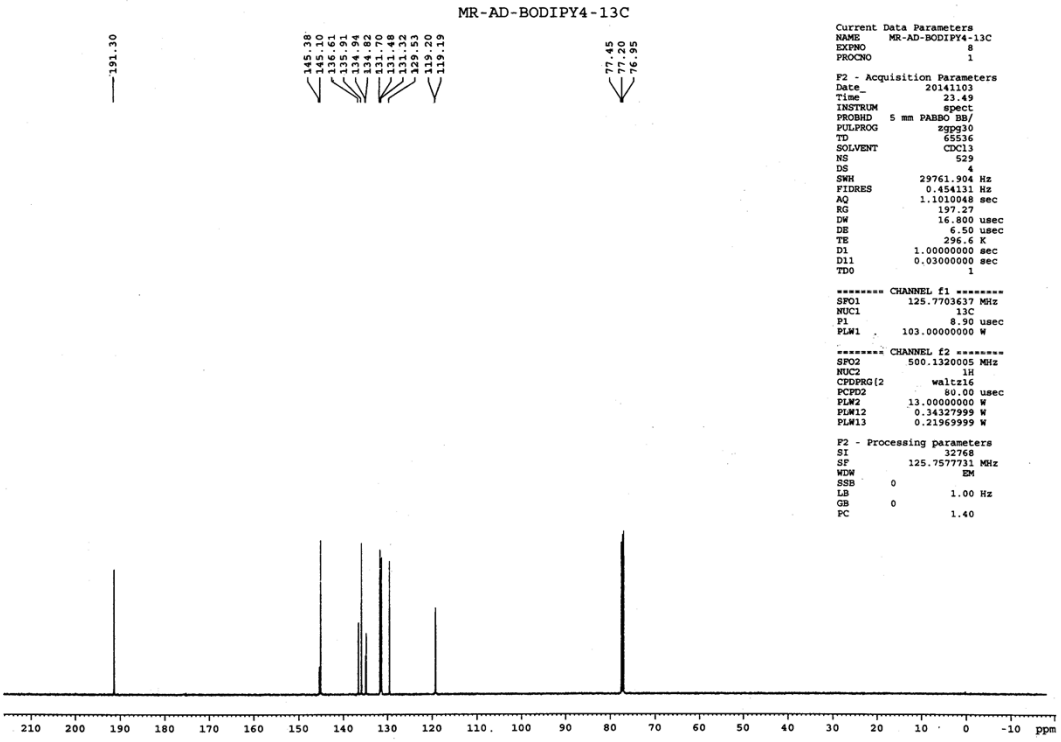
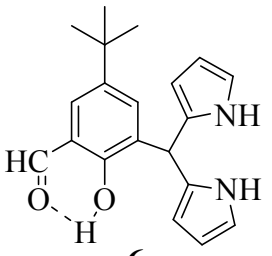



**Fig. S10** $^{13}$C NMR spectrum of BODIPY **4**.



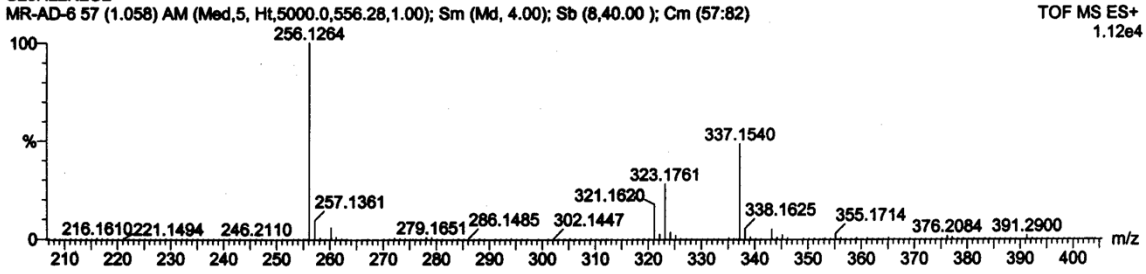

**6**

**Elemental Composition Report** **Page 1**

**Single Mass Analysis**
Tolerance = 10.0 PPM / DBE: min = -1.5, max = 50.0
Selected filters: None

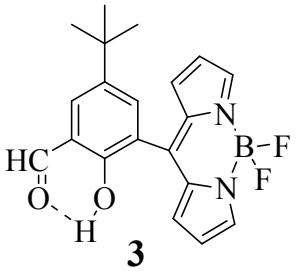
Monoisotopic Mass, Even Electron Ions
33 formula(e) evaluated with 1 results within limits (up to 6 closest results for each mass)
Elements Used:
C: 0-20 H: 0-23 N: 0-2 O: 0-2 S: 0-2

Q-Tof MICROMASS (YA-105) DEPARTMENT OF CHEMISTRY, I.I.T.(B) 07-Nov-201416:04:48
C20H22N2O2
MR-AD-6 57 (1.058) AM (Med,5, Ht,5000.0,556.28,1.00); Sm (Md, 4.00); Sb (8,40.00 ); Cm (57:82) TOF MS ES+
1.12e4




| | | | | | | |
|---|---|---|---|---|---|---|
| Minimum: | | | | -1.5 | | |
| Maximum: | | 5.0 | 10.0 | 50.0 | | |
| **Mass** | **Calc. Mass** | **mDa** | **PPM** | **DBE** | **i-FIT** | **Formula** |
| 323.1761 | 323.1760 | 0.1 | 0.3 | 10.5 | 143.9 | C20 H23 N2 O2 |

**Fig. S11** HR-MS of compound **6**.



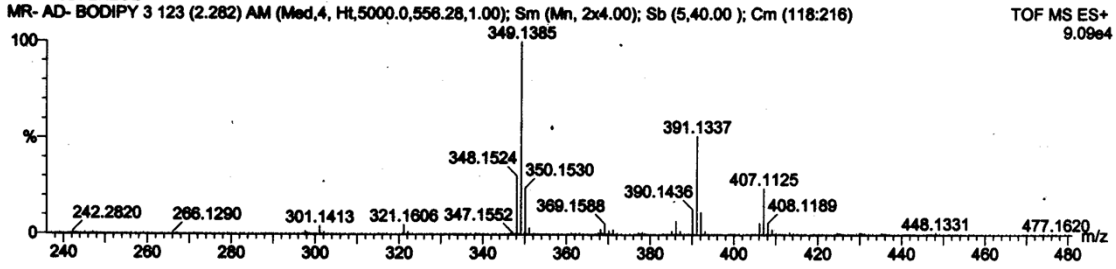
**3**

**Elemental Composition Report** **Page 1**

**Single Mass Analysis**
Tolerance = 10.0 PPM / DBE: min = -1.5, max = 50.0
Selected filters: None

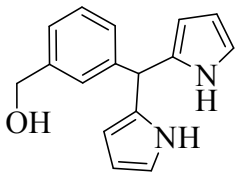
**Monoisotopic Mass, Even Electron Ions**
485 formula(e) evaluated with 1 results within limits (up to 6 closest results for each mass)
Elements Used:
C: 0-20 H: 0-19 B: 0-1 N: 0-2 O: 0-2 F: 0-2 K: 0-1 Cu: 0-1 Br: 0-1

Q-Tof MICROMASS (YA-105) DEPARTMENT OF CHEMISTRY, I.I.T.(B) 31-Oct-201416:35:10
C20H19BF2N2O2
MR- AD- BODIPY 3 123 (2.282) AM (Med,4, Ht,5000.0,556.28,1.00); Sm (Mn, 2x4.00); Sb (5,40.00 ); Cm (118:216) TOF MS ES+
9.09e4




| | | | | | | |
|---|---|---|---|---|---|---|
| Minimum: | | | | -1.5 | | |
| Maximum: | | 5.0 | 10.0 | 50.0 | | |
| Mass | Calc. Mass | mDa | PPM | DBE | i-FIT | Formula |
| 407.1125 | 407.1145 | -2.0 | -4.9 | 11.5 | 3.3 | C20 H19 B N2 O2 F2 K |

**Fig. S12** HR-MS of compound **3**.



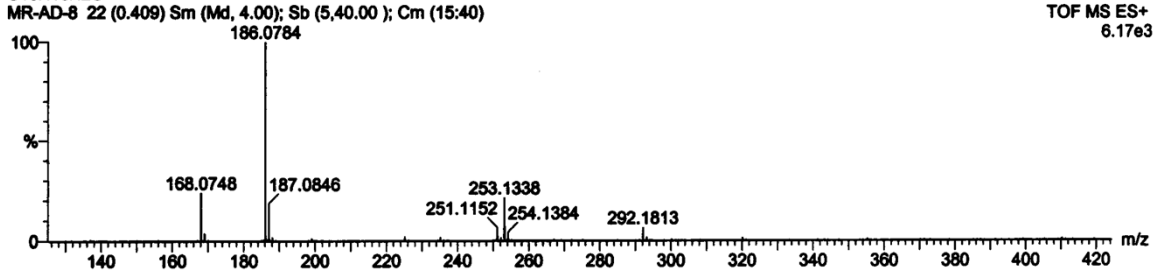

**8**

**Elemental Composition Report**

**Single Mass Analysis**
Tolerance = 10.0 PPM / DBE: min = -1.5, max = 50.0
Selected filters: None

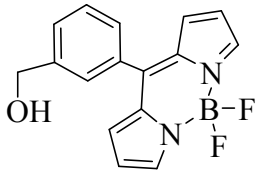
Monoisotopic Mass, Odd and Even Electron Ions
4 formula(e) evaluated with 1 results within limits (up to 6 closest results for each mass)
Elements Used:
C: 0-16 H: 0-17 N: 0-2 O: 0-1

Q-Tof MICROMASS (YA-105) DEPARTMENT OF CHEMISTRY, I.I.T.(B) 16-Dec-201412:28:39
C16H16N2O
MR-AD-8 22 (0.409) Sm (Md, 4.00); Sb (5,40.00 ); Cm (15:40) TOF MS ES+
6.17e3




| | | | | | |
|---|---|---|---|---|---|
| Minimum: | | | | -1.5 | |
| Maximum: | | 5.0 | 10.0 | 50.0 | |
| **Mass** | **Calc. Mass** | **mDa** | **PPM** | **DBE** | **Formula** |
| 253.1338 | 253.1341 | -0.3 | -1.2 | 9.5 | C16 H17 N2 O |

**Fig. S13** HR-MS of compound **8**.



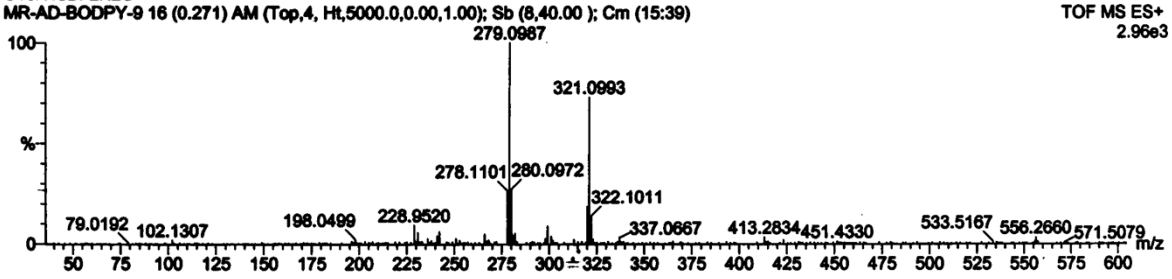

**9**

**Elemental Composition Report** **Page 1**

**Single Mass Analysis**
Tolerance = 10.0 PPM / DBE: min = -1.5, max = 50.0
Selected filters: None

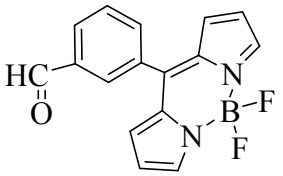
Monoisotopic Mass, Even Electron Ions
62 formula(e) evaluated with 1 results within limits (up to 6 closest results for each mass)
Elements Used:
C: 0-16 H: 0-13 B: 0-1 N: 0-2 O: 0-1 F: 0-2 Na: 0-1

Q-Tof MICROMASS (YA-105) DEPARTMENT OF CHEMISTRY, I.I.T.(B) 04-Nov-201412:05:07
C16H13BF2N2O
MR-AD-BODPY-9 16 (0.271) AM (Top,4, Ht,5000.0,0.00,1.00); Sb (8,40.00 ); Cm (15:39) TOF MS ES+
2.96e3




| | | | | | | |
|---|---|---|---|---|---|---|
| Minimum: | | | | -1.5 | | |
| Maximum: | | 5.0 | 10.0 | 50.0 | | |
| **Mass** | **Calc. Mass** | **mDa** | **PPM** | **DBE** | **i-FIT** | **Formula** |
| 321.0993 | 321.0987 | 0.6 | 1.9 | 10.5 | 5.5 | C16 H13 B N2 O F2 Na |

**Fig. S14** HR-MS of compound **9**.



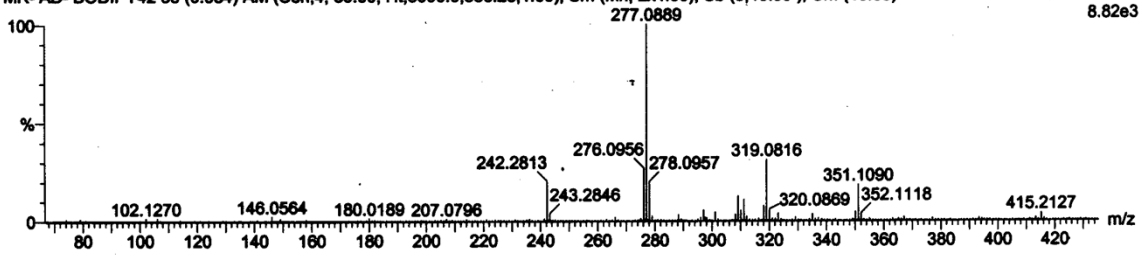
**4**

**Elemental Composition Report** **Page 1**

**Single Mass Analysis**
Tolerance = 100.0 PPM / DBE: min = -1.5, max = 50.0
Selected filters: None

Monoisotopic Mass, Odd and Even Electron Ions
61 formula(e) evaluated with 1 results within limits (up to 6 closest results for each mass)
Elements Used:
C: 0-16 H: 0-11 B: 0-1 N: 0-2 O: 0-1 F: 0-2 Na: 0-1

Q-Tof MICROMASS (YA-105) DEPARTMENT OF CHEMISTRY, I.I.T.(B) 31-Oct-201417:59:35
C16H11BF2N2O
MR- AD- BODIPY42 53 (0.984) AM (Cen,4, 80.00, Ht,5000.0,556.28,1.00); Sm (Mn, 2x4.00); Sb (5,40.00 ); Cm (46:65) TOF MS ES+
8.82e3




| | | | | | | |
|---|---|---|---|---|---|---|
| Minimum: | | | | -1.5 | | |
| Maximum: | | 5.0 | 100.0 | 50.0 | | |
| Mass | Calc. Mass | mDa | PPM | DBE | i-FIT | Formula |
| 319.0816+ | 319.0830 | -1.4 | -4.4 | 11.5 | 10.2 | C16 H11 B N2 O F2 Na |

**Fig. S15** HR-MS of compound **4**.

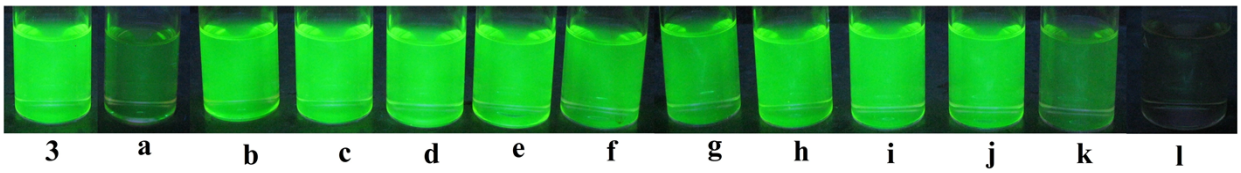



**Fig. 16** Fluorescence responses of chemodosimeter **3** ($1x10^{-5}$ M) in the presence of 10 eqv. of different anions and 4 eqv. of $CN^-$ ion under uv lamp in $CH_3CN$: (a) $F^-$, (b) $Cl^-$, (c) $Br^-$ (d) $I^-$, (e) $HSO_4^-$, (f)$ClO_4^-$, (g) $NO_3^-$, (h), $NO_2^-$, (i) $N_3^-$, (j) $CO_3^{--}$, (k) $H_2PO_4^-$, (l) $CN^-$

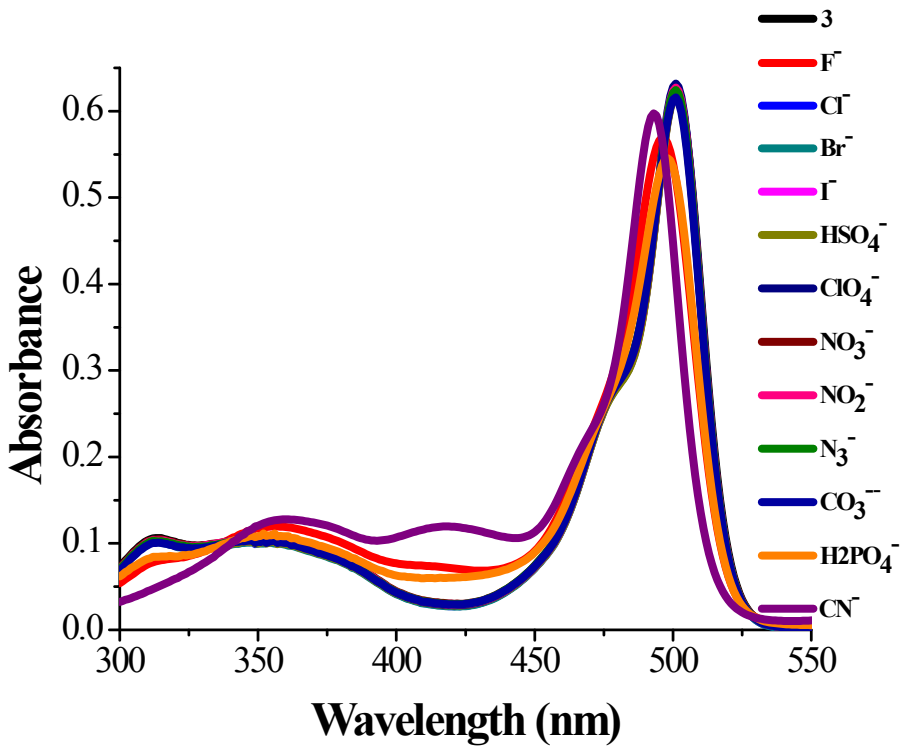



**Fig. S17** Absorption spectra of BODIPY **3** ($1x10^{-5}$ M) in presence of various anions (10 eqv.) and 4 eqv. of $CN^-$ ion in $CH_3CN$ solution.

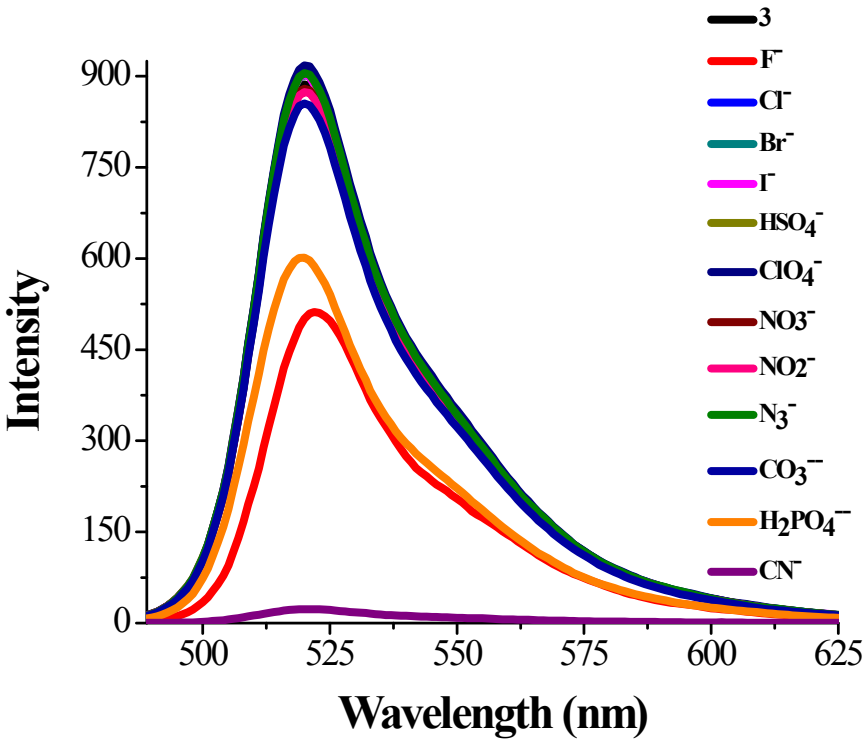



**Fig. S18** Fluorescence spectra of BODIPY **3** ($1x10^{-5}$ M) in presence of various anions (10 eqv.) and 4 eqv. of $CN^-$ ion in $CH_3CN$ solution.