Boron-Dipyrromethene Based Multi Anionic Sensor and a Specific Cationic Sensor for Fe^{3+}

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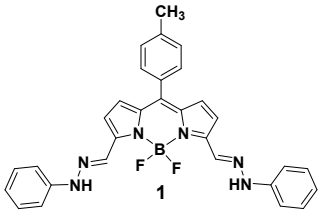
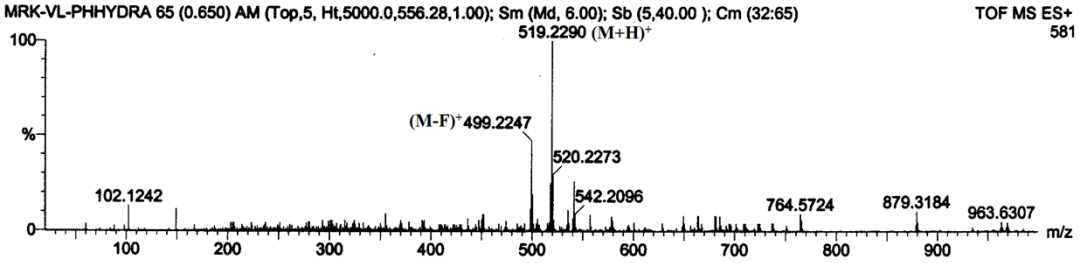


Elemental Composition Report **Page 1**

Single Mass Analysis (displaying only valid results)
Tolerance = 50.0 PPM / DBE: min = -1.5, max = 100.0
Isotope cluster parameters: Separation = 1.0 Abundance = 1.0%

Monoisotopic Mass, Odd and Even Electron Ions
28 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) 10-Apr-201212:59:45
C30H25BF2N6
MRK-VL-PHHYDRA 65 (0.650) AM (Top,5, Ht,5000.0,556.28,1.00); Sm (Md, 6.00); Sb (5,40.00); Cm (32:65) TOF MS ES+
581



Minimum:				-1.5		
Maximum:		200.0	50.0	100.0		
Mass	Calc. Mass	mDa	PPM	DBE	Score	Formula
519.2290	519.2280	1.0	1.9	20.5	1	C30 H26 B N6 F2

Figure S1: The HRMS of compound **1.**

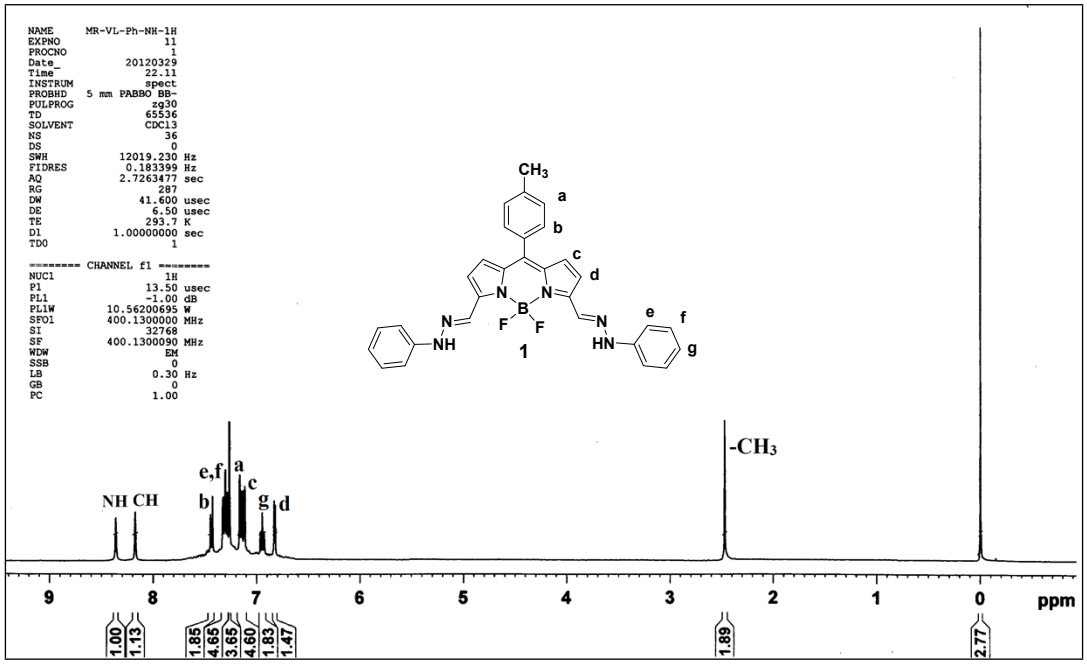


Figure S2: The ^{1}H-NMR spectrum of compound **1** recorded in $CDCl_3$

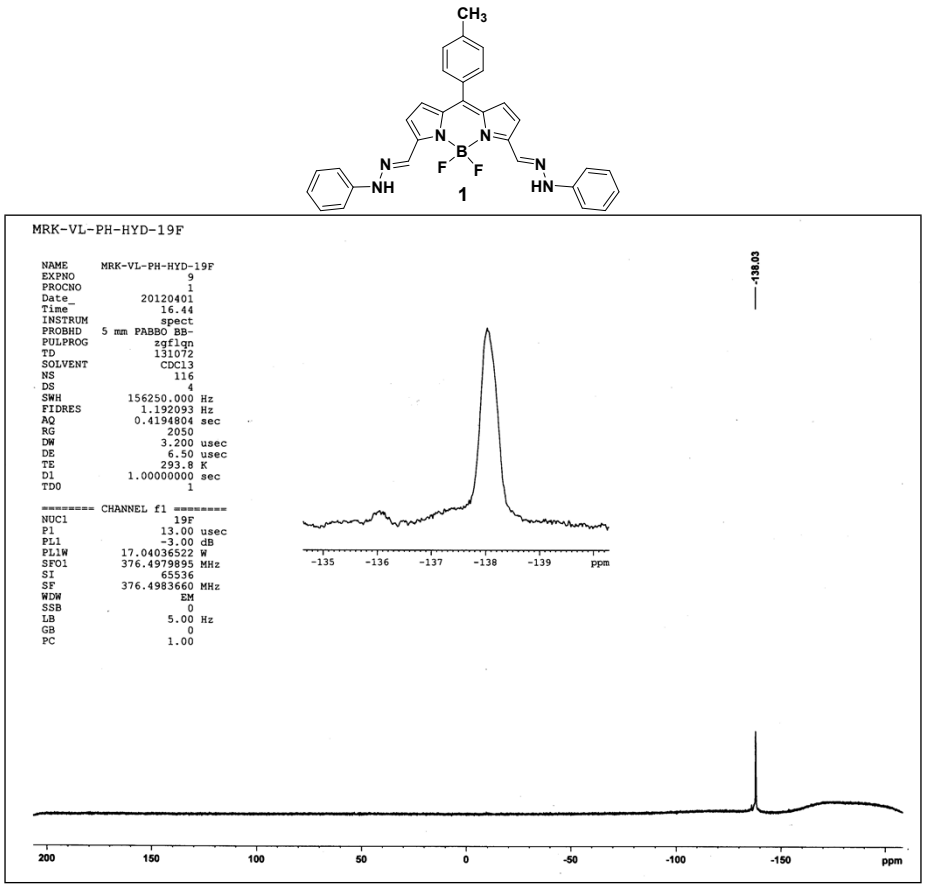


Figure S3: ^{19}F NMR spectrum of compound **1** in $CDCl_3$. The inset shows the expansion

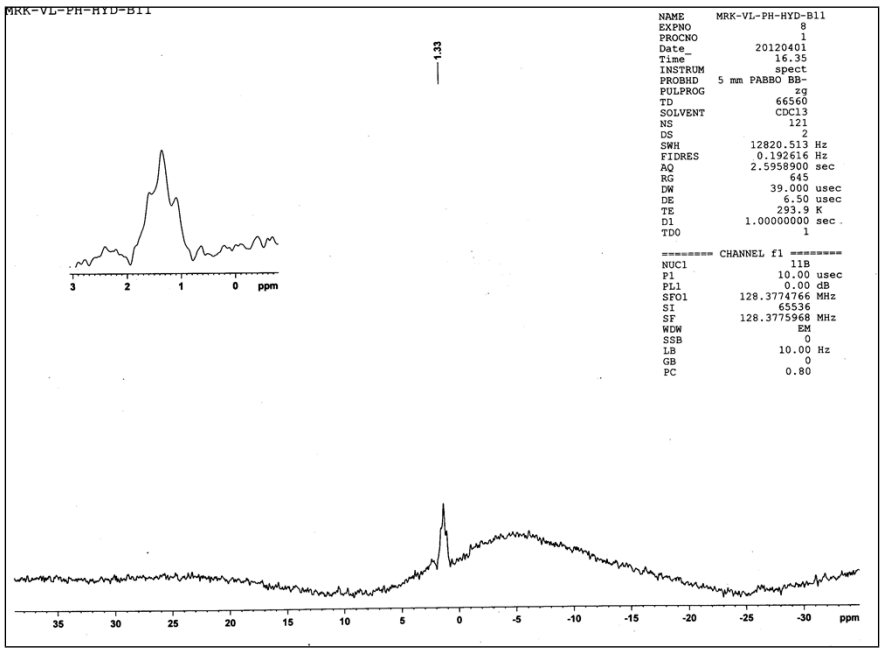
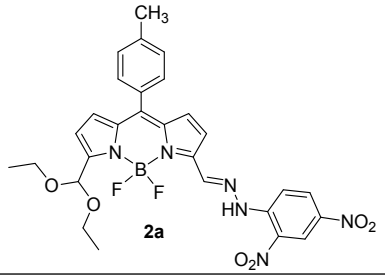


Figure S4: ^{11}B NMR spectrum of compound **1** in $CDCl_3$. The inset shows the expansion.

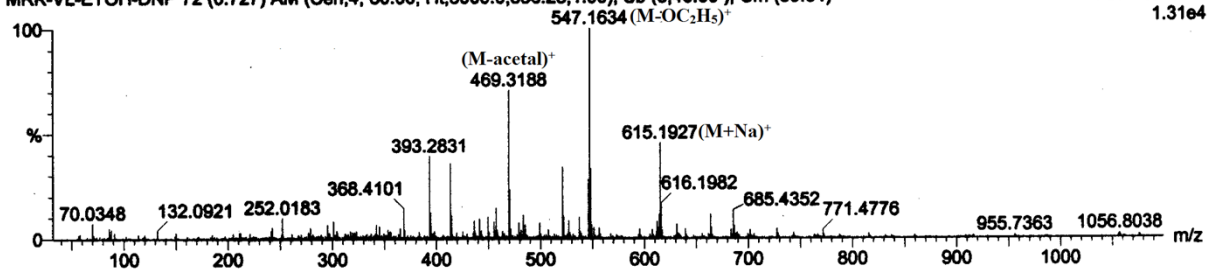


Elemental Composition Report **Page 1**

Single Mass Analysis (displaying only valid results)
Tolerance = 10.0 PPM / DBE: min = -1.5, max = 200.0
Isotope cluster parameters: Separation = 1.0 Abundance = 1.0%

Monoisotopic Mass, Odd and Even Electron Ions
12022 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) 06-Nov-201215:13:23
C28H27BF2N6O6
MRK-VL-ETOH-DNP 72 (0.727) AM (Cen,4, 80.00, Ht,5000.0,556.28,1.00); Sb (5,40.00); Cm (39:84) TOF MS ES+
1.31e4



Minimum:				-1.5		
Maximum:		50.0	10.0	200.0		
Mass	Calc. Mass	mDa	PPM	DBE	Score	Formula
615.1927	615.1951	-2.3	-3.8	17.5	1	C28 H27 B N6 O6 F2 Na

Figure S5: The HRMS mass spectrum of compound **2a.**

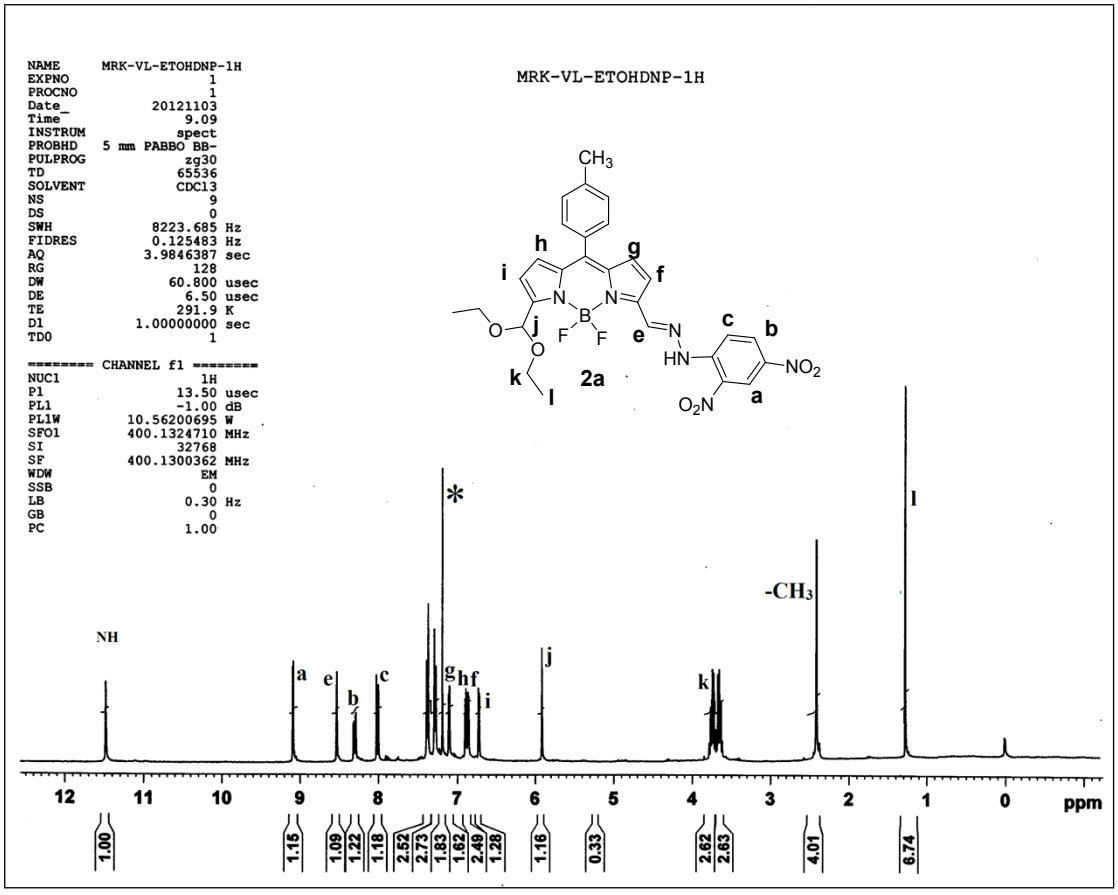


Figure S6: The ^{1}H-NMR spectrum of compound **2a** recorded in $CDCl_3$.

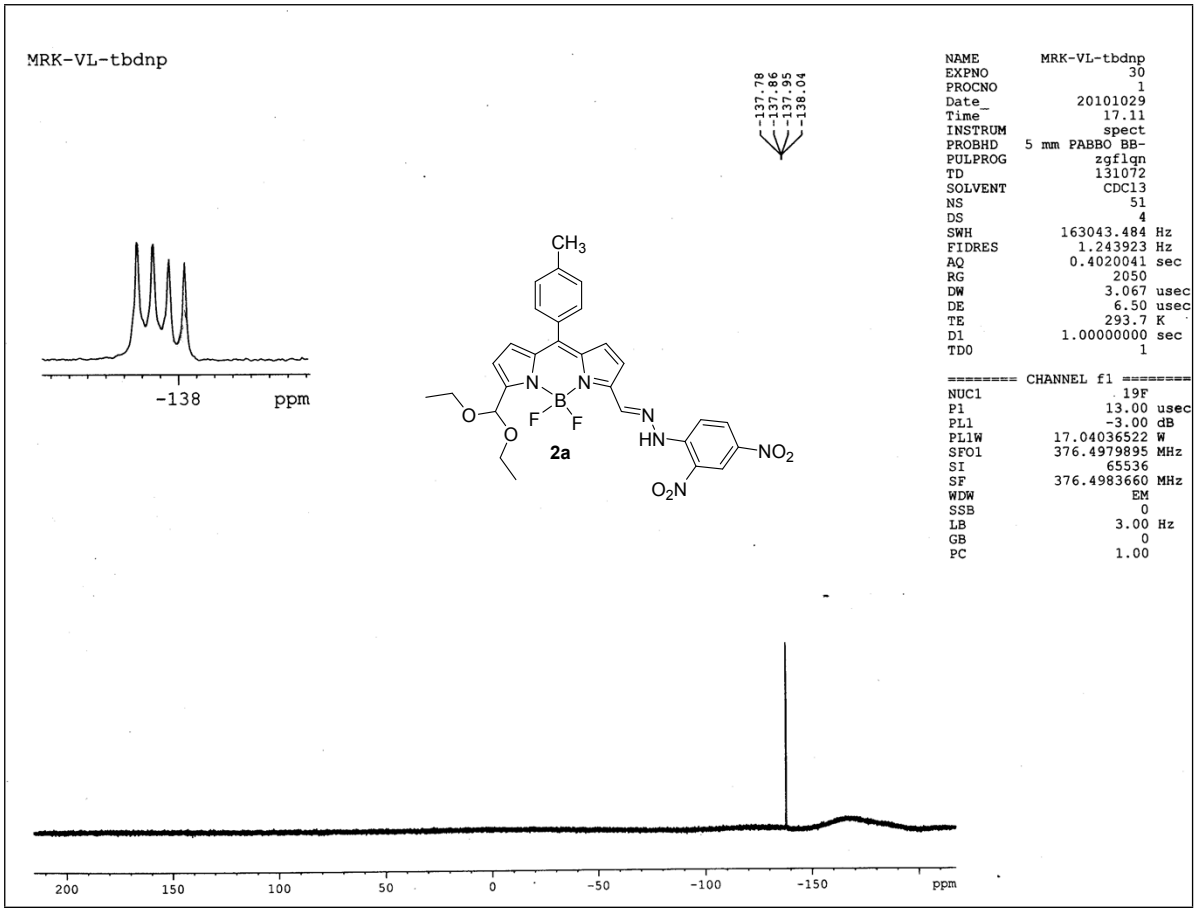
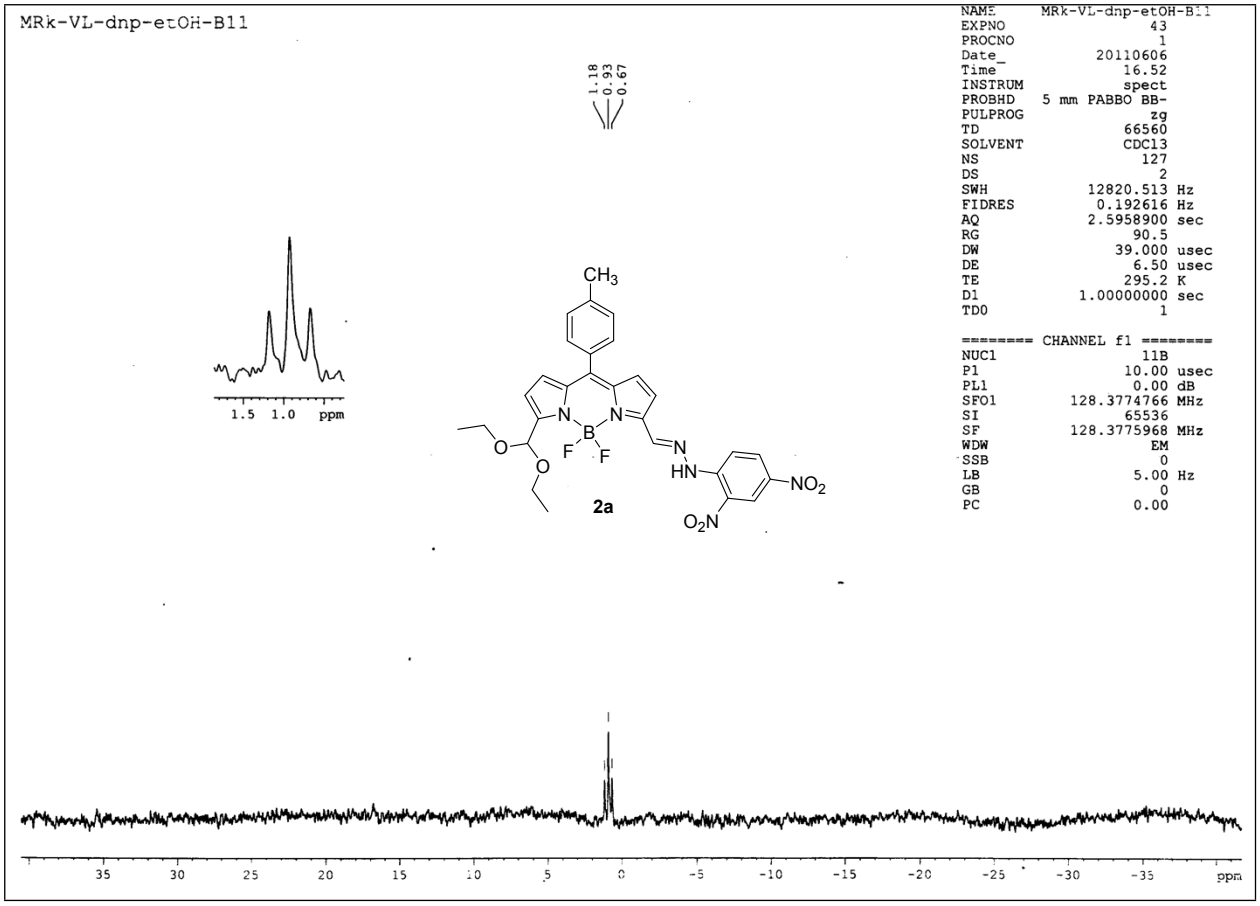
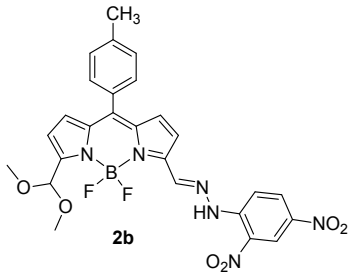


Figure S7: ^{19}F NMR spectrum of compound **2a** in $CDCl_3$. The inset shows the expansion



NAME	MRk-VL-dnp-etOH-B11
EXPNO	43
PROCNO	1
Date_	20110606
Time	16.52
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zg
TD	66560
SOLVENT	CDCl3
NS	127
DS	2
SWH	12820.513 Hz
FIDRES	0.192616 Hz
AQ	2.5958900 sec
RG	90.5
DW	39.000 usec
DE	6.50 usec
TE	295.2 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	11B
P1	10.00 usec
PL1	0.00 dB
SFO1	128.3774766 MHz
SI	65536
SF	128.3775968 MHz
WDW	EM
SSB	0
LB	5.00 Hz
GB	0
PC	0.00

Figure S8: ^{11}B NMR spectrum of compound **2a** in $CDCl_3$. The inset shows the expansion



2b

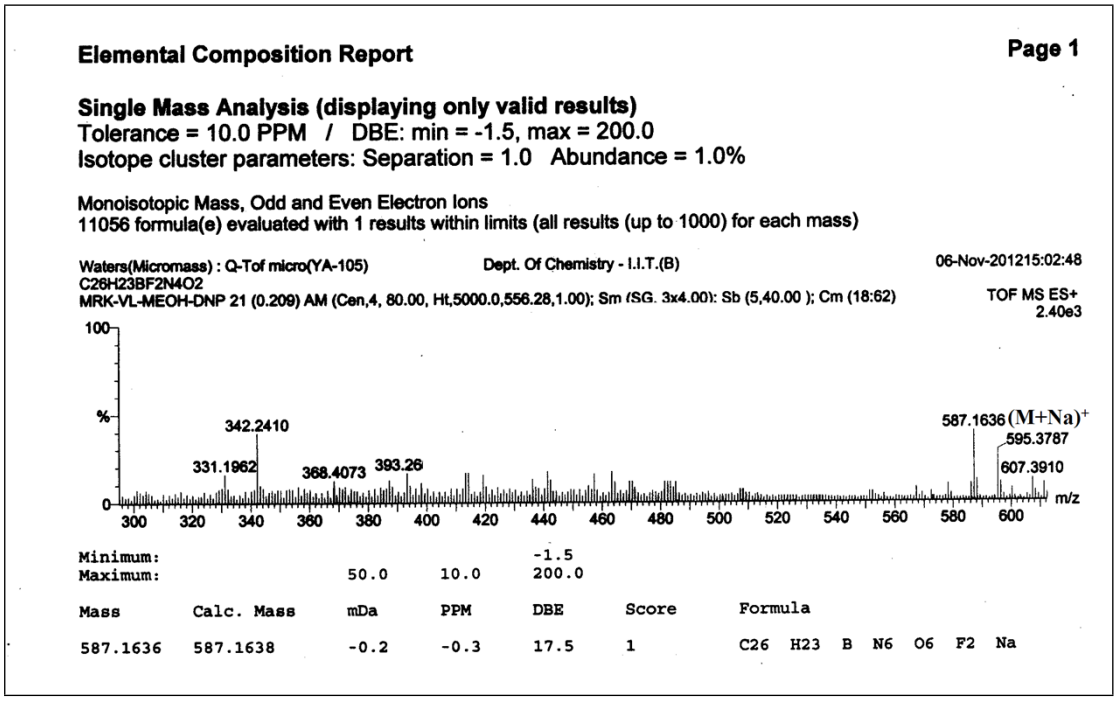


Figure S9: The HR-MS of compound **2b**

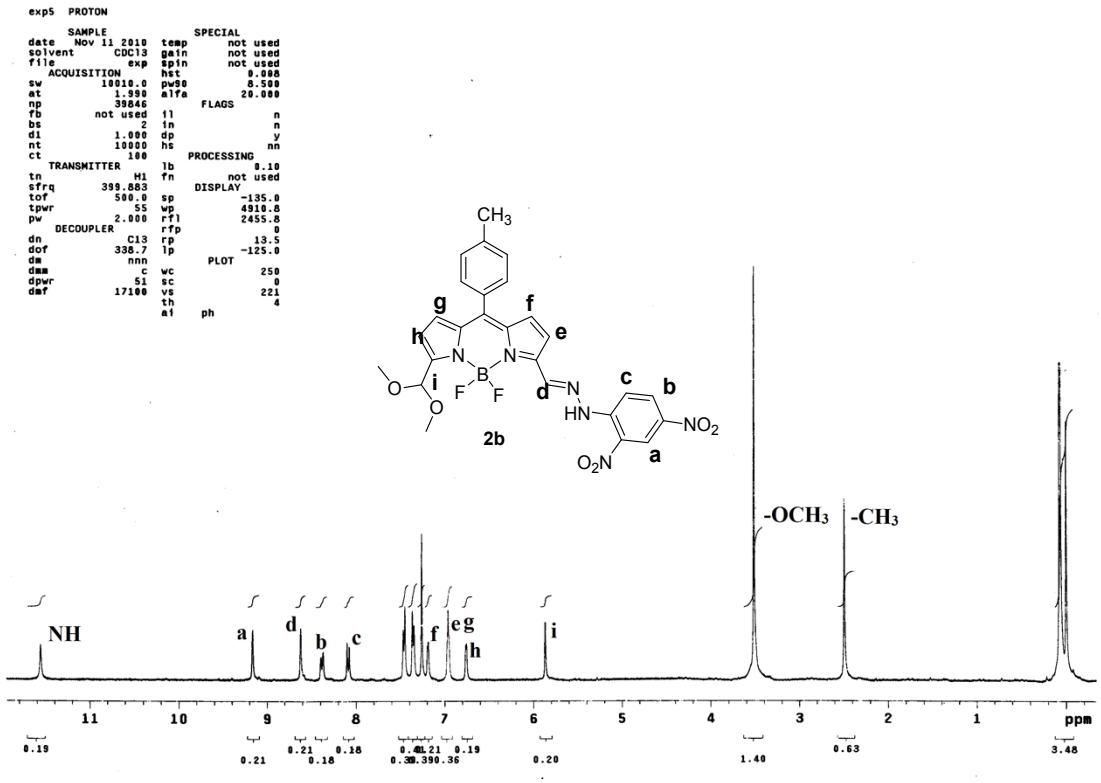


Figure S9: The ^{1}H NMR spectrum of compound **2b** recorded in $CDCl_3$.

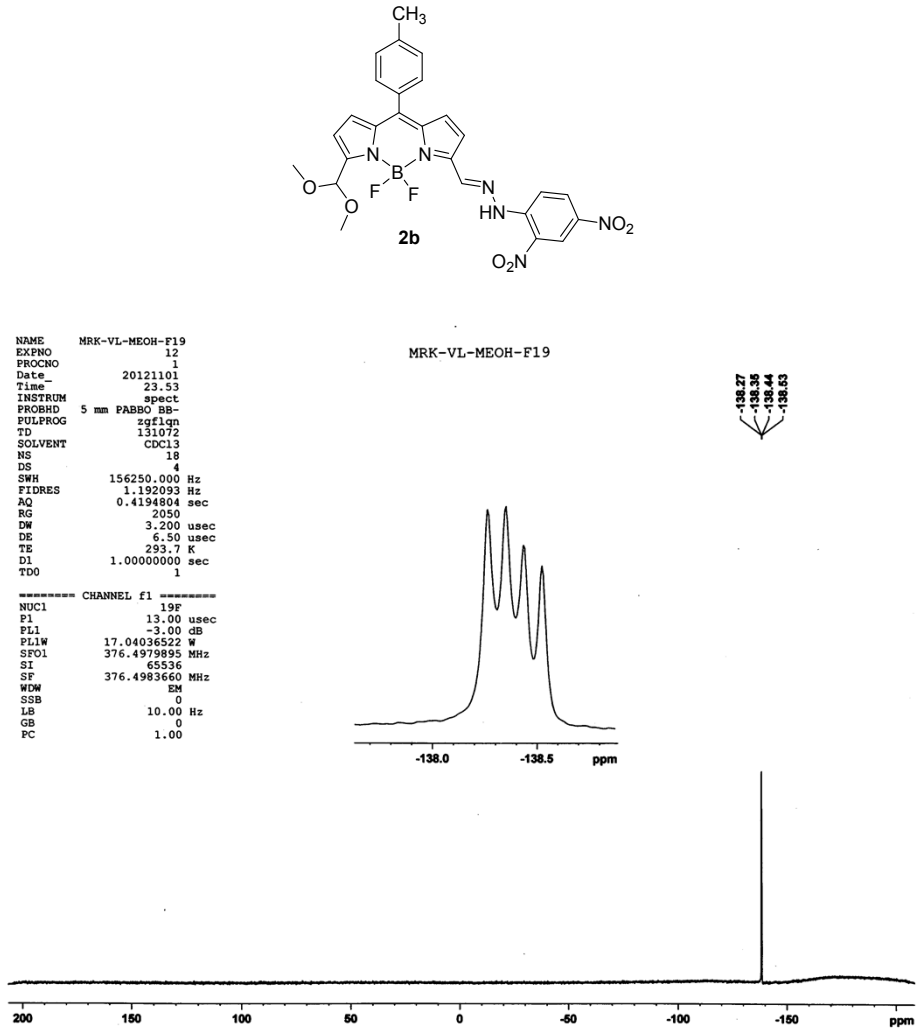


Figure S10: ^{19}F NMR spectrum of compound **2b** in $CDCl_3$. The inset shows the expansion

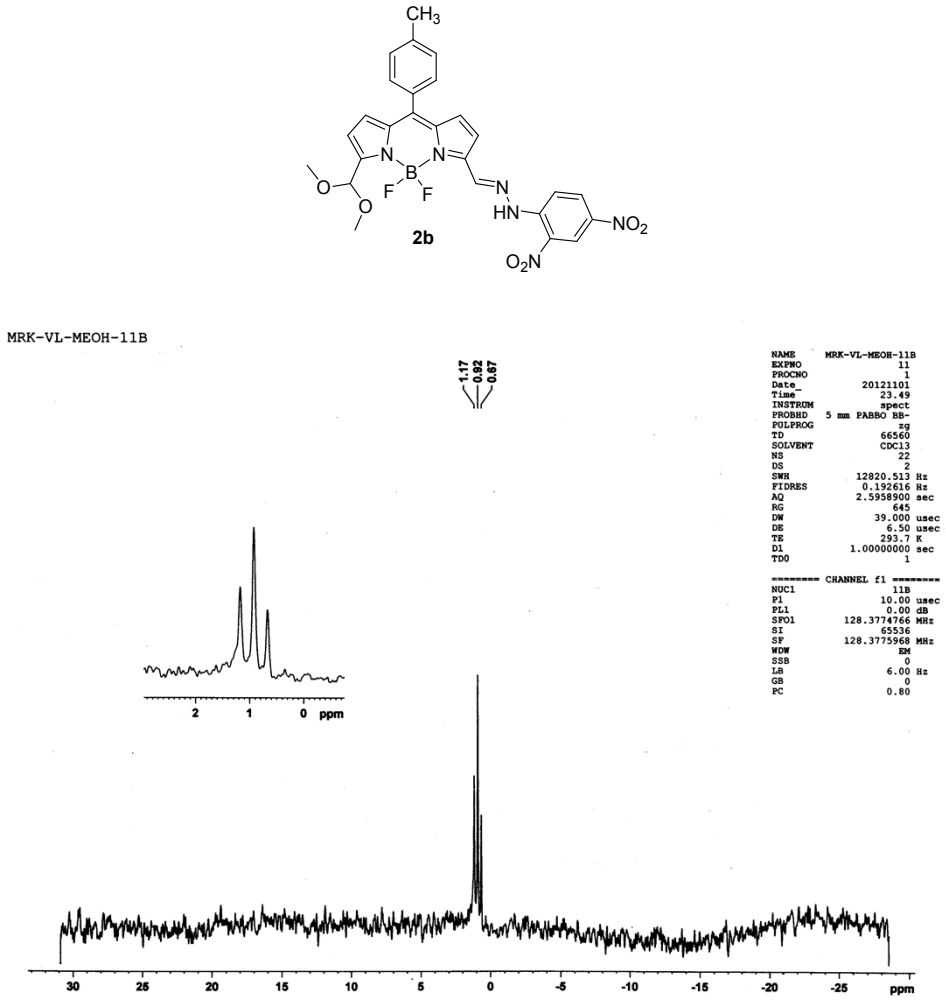


Figure S11: ^{11}B NMR spectrum of compound **2b** in $CDCl_3$. The inset shows the expansion

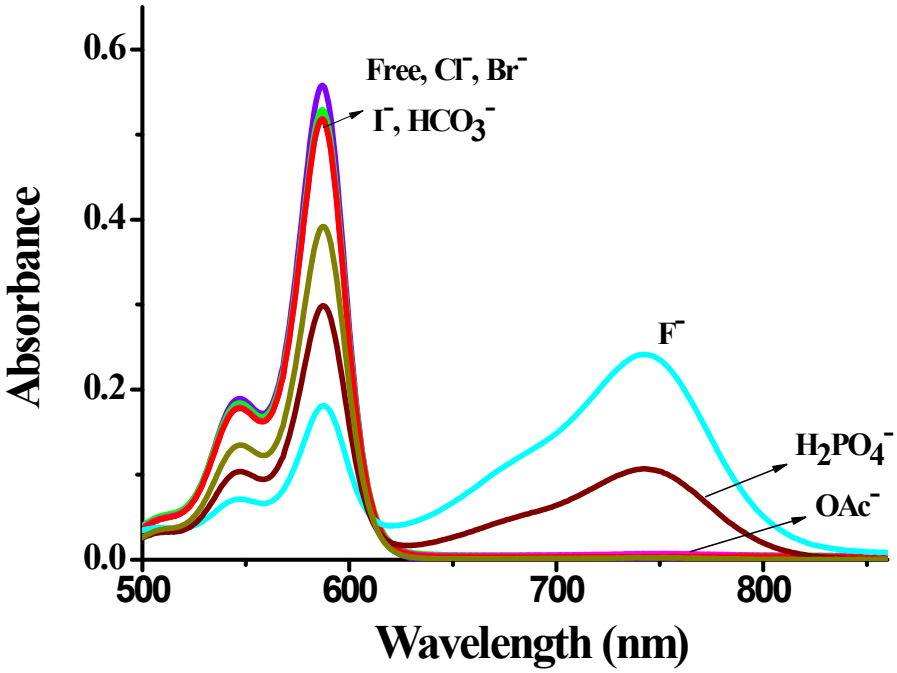


Figure S13: Absorption spectra of compound **2a** (5 x 10^{-6} M) in the presence of various anions (50 equivalents) in 9:1 ratio of CH_3CN:H_2O.

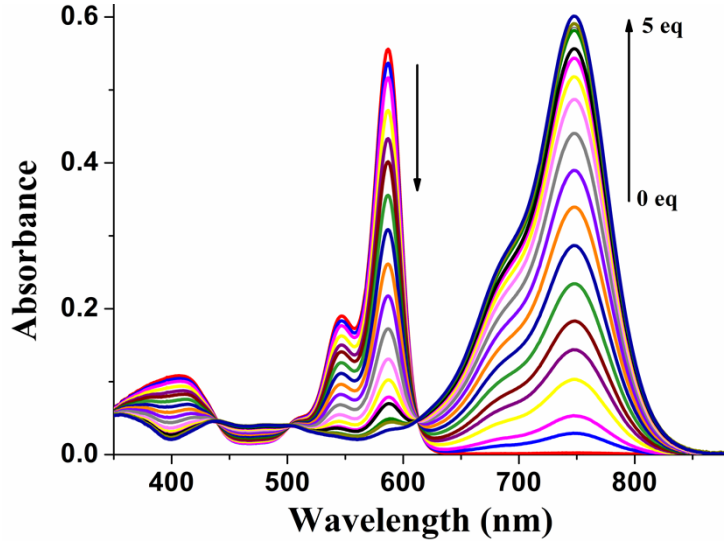


Figure S14: Absorption spectra of compound **2a** (5 x 10^{-6} M), with different conc. of CH_3COO^- solution (0–5 equivalents) in CH_3CN.

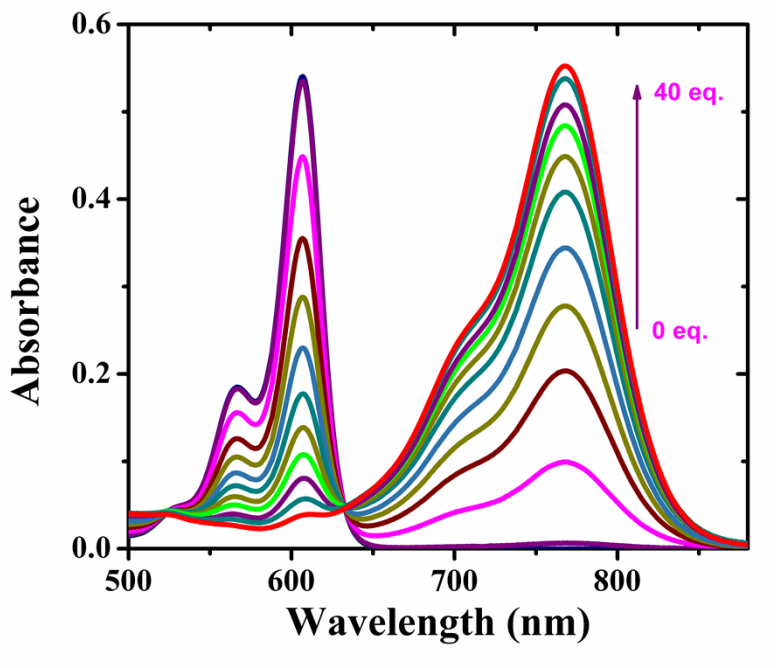
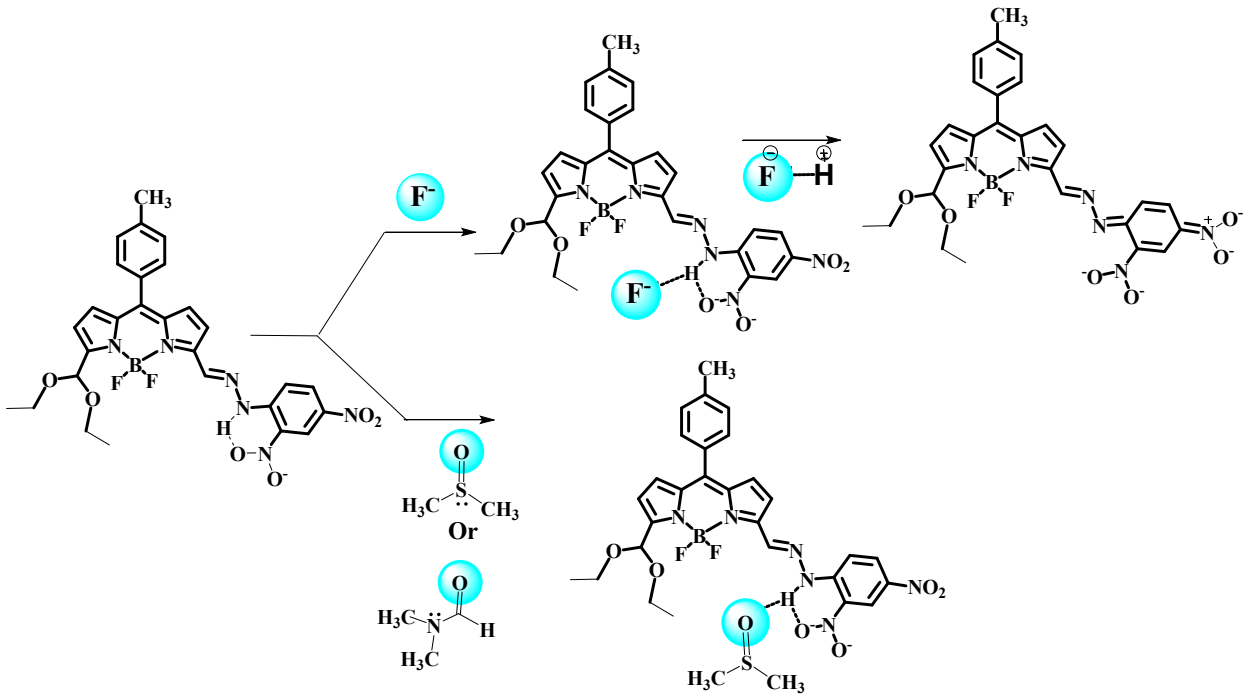
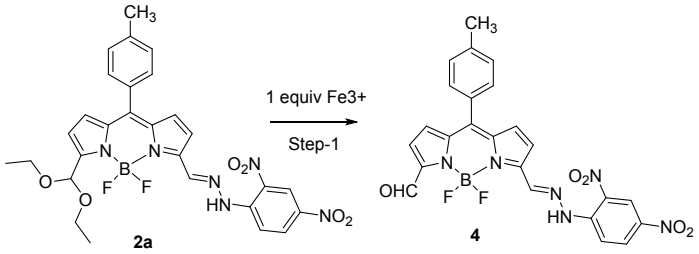


Figure S15: Absorption spectra of compound **2a** (5 x 10^{-6} M), with different conc. of $H_2PO_4^-$ solution (0–40 equivalents) in CH_3CN.



Scheme S1: Intermolecular hydrogen bonding interactions of compound **2a** with anion and solvents.



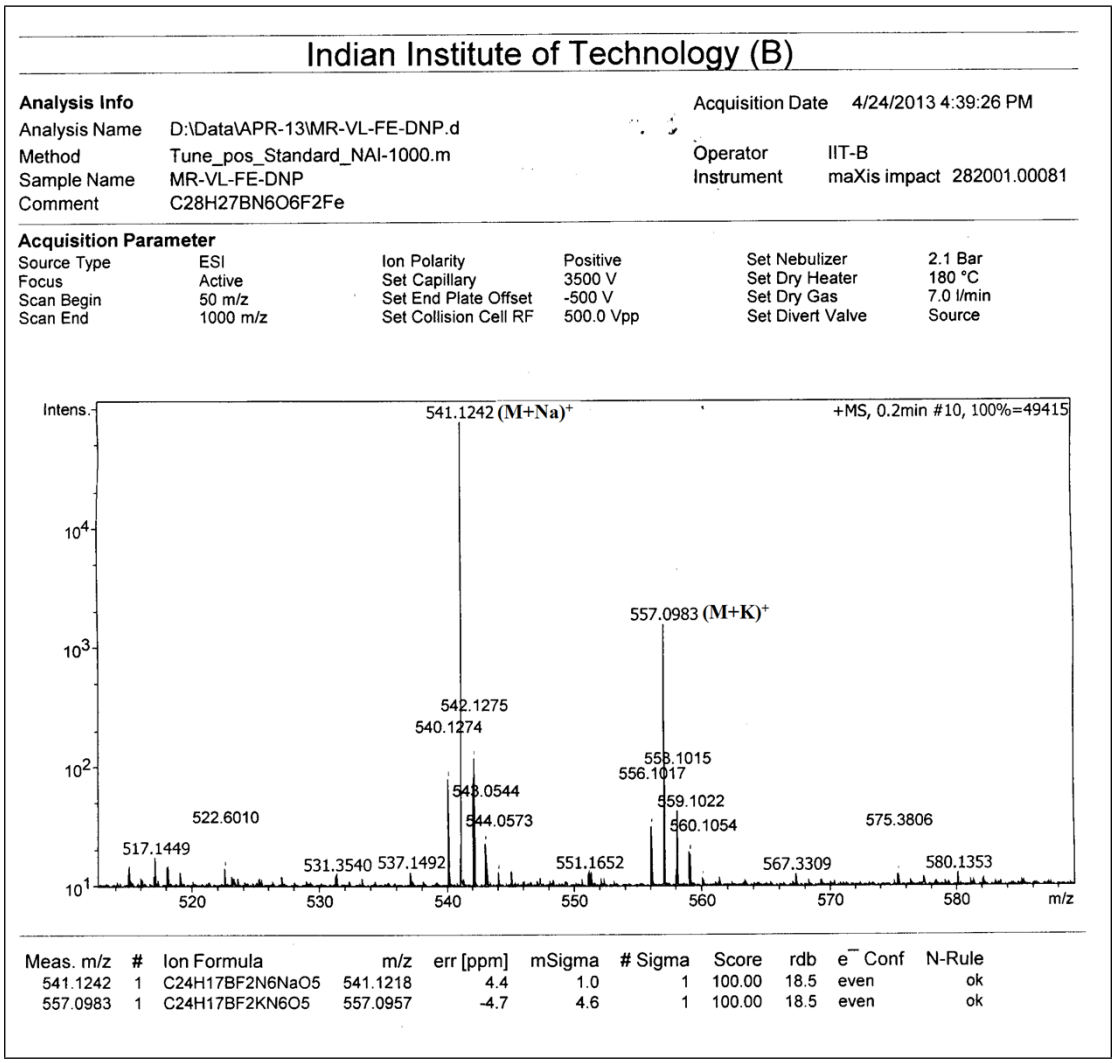
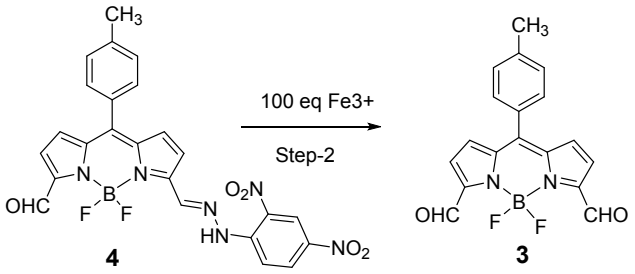


Figure S16: The HRMS of compound **4** generated by addition of 1 equivalent of Fe^{3+} to compound **2a**.



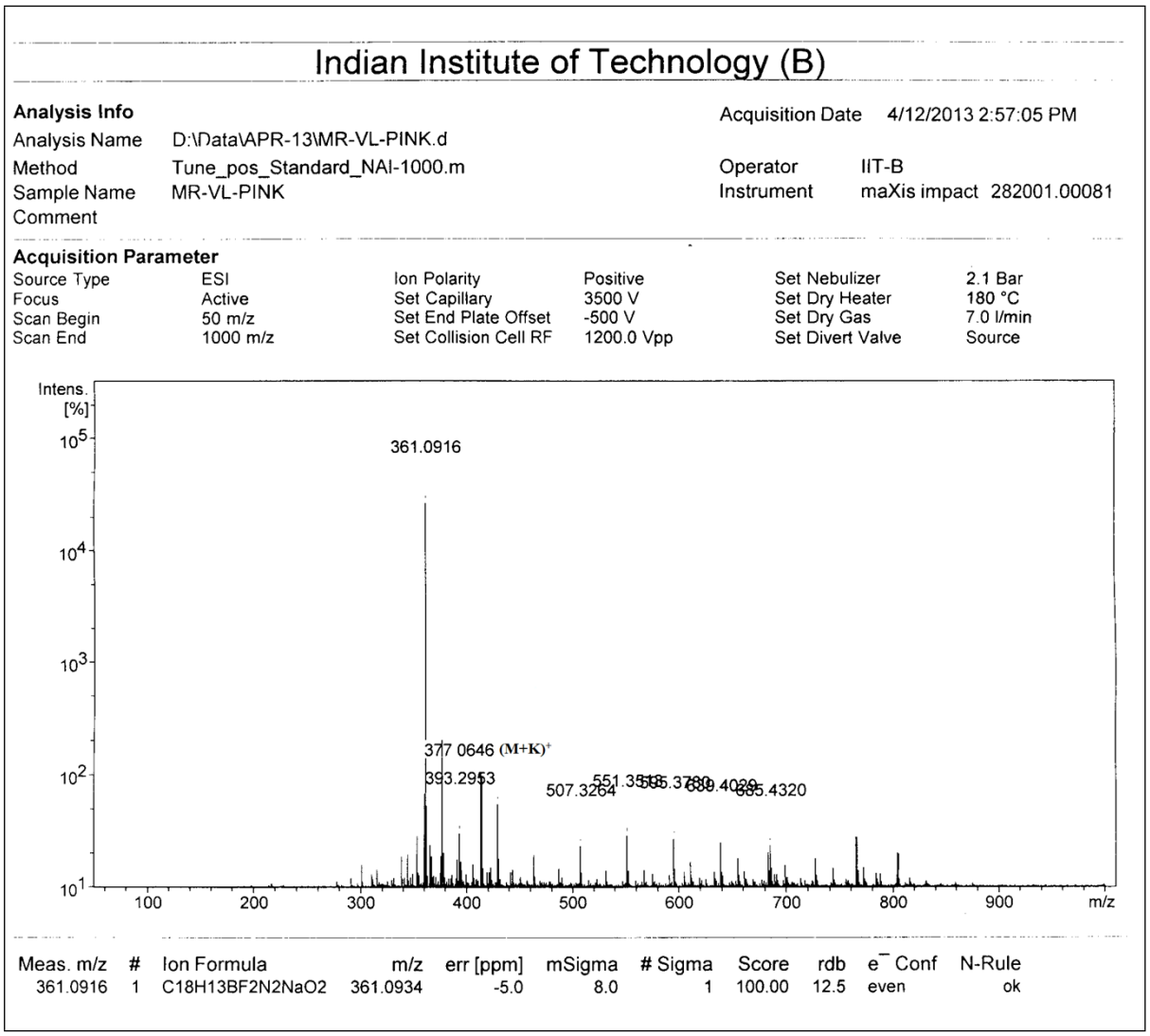


Figure S17: The HRMS of compound **3** generated by the addition of 100 equivalents of Fe^{3+}.

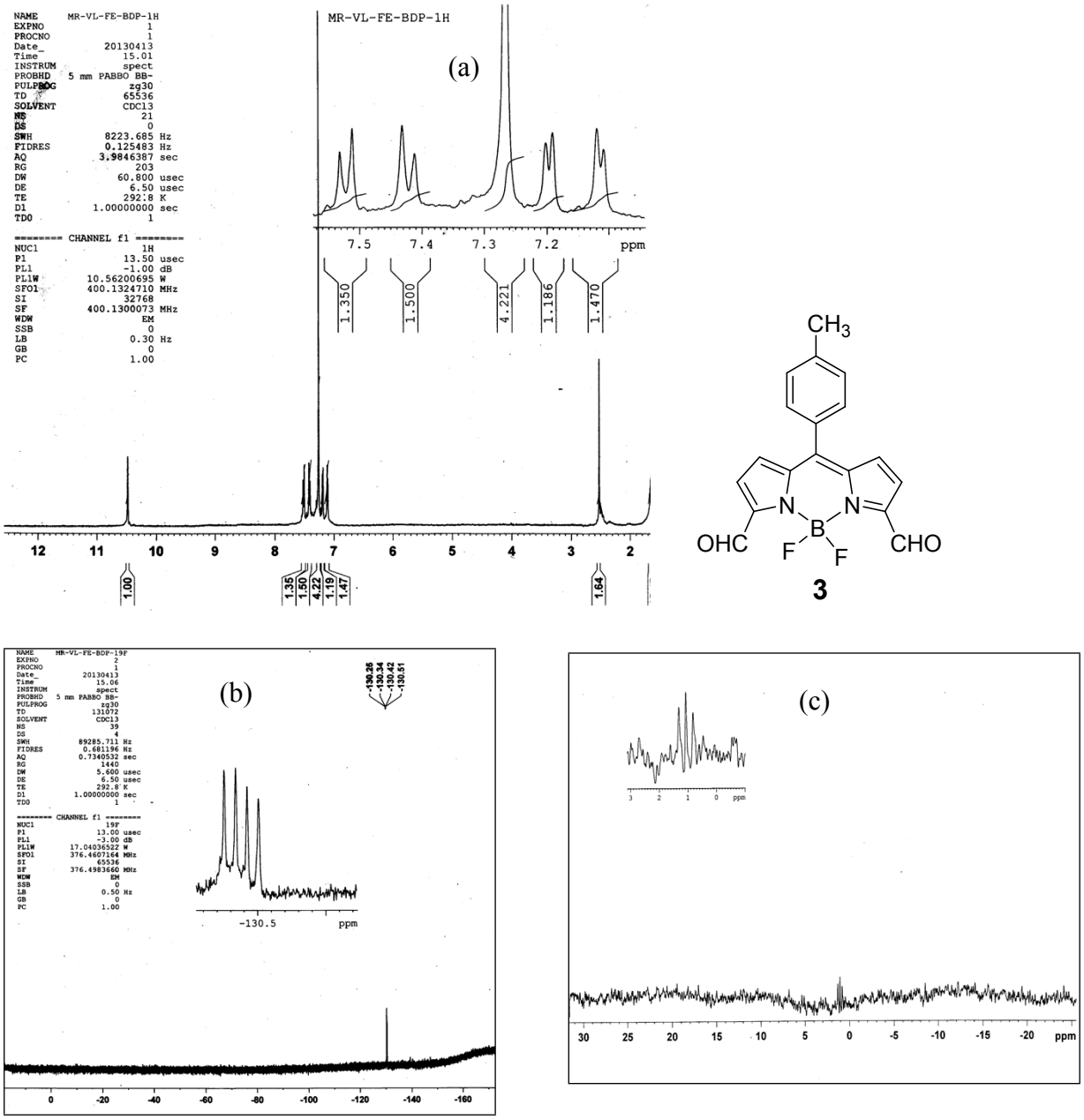


Figure S18: (a) ^{1}H NMR spectrum, (b) ^{19}F NMR and (c) ^{11}B NMR spectrum of compound **3** generated by addition of 100 equivalents of Fe^{3+} to compound **2a**.

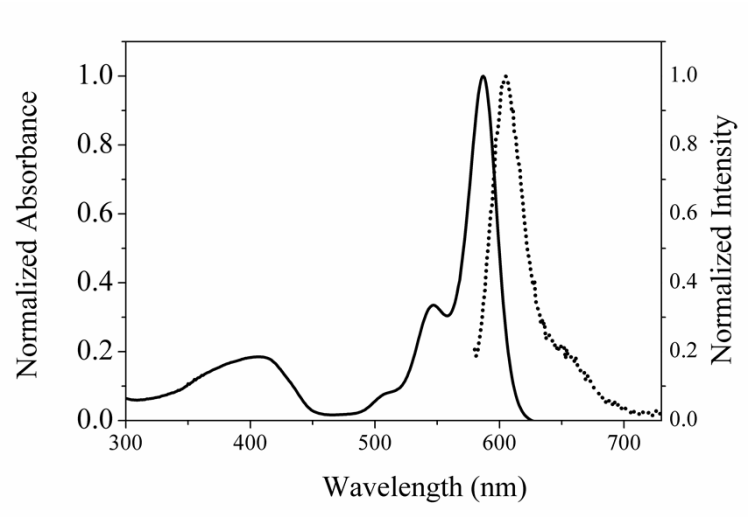


Figure S19: The overlay of normalized absorption (solid line) and emission spectra (dotted line) of compound **2a** in CH_3CN.

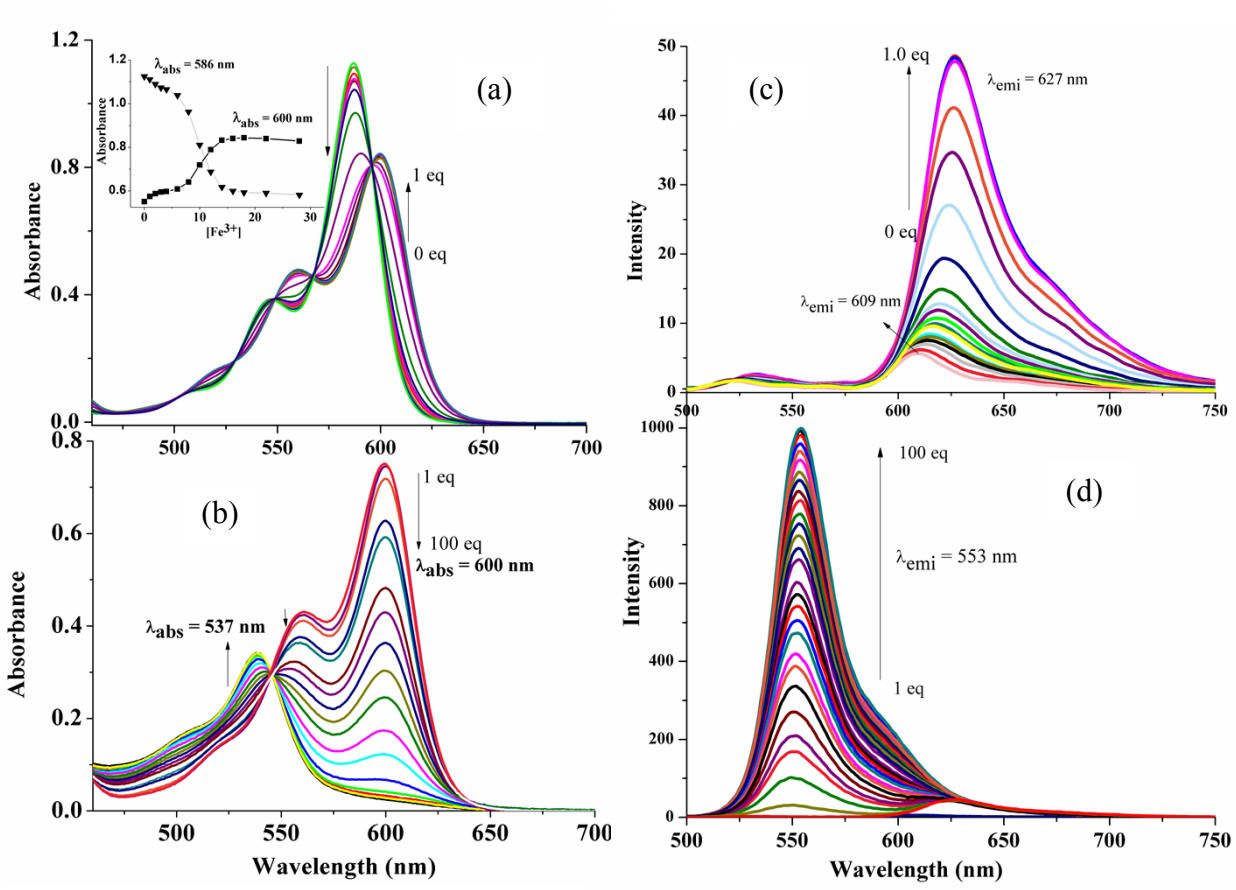


Figure S20: (a) Absorption spectrum of compound **2a** in the presence of Fe^{3+}: (a) 0 to 1 equivalent The inset shows the plot of I/I_{max} vs. $[Fe^{3+}]$; (b) 1 to 100 equivalents. Emission spectra of compound **1** (10^{-5} M) in the presence of Fe^{3+} excited at 488 nm: (c) 0 to 1 equivalent (d) 1 to 100 equivalents in CH_3CN.

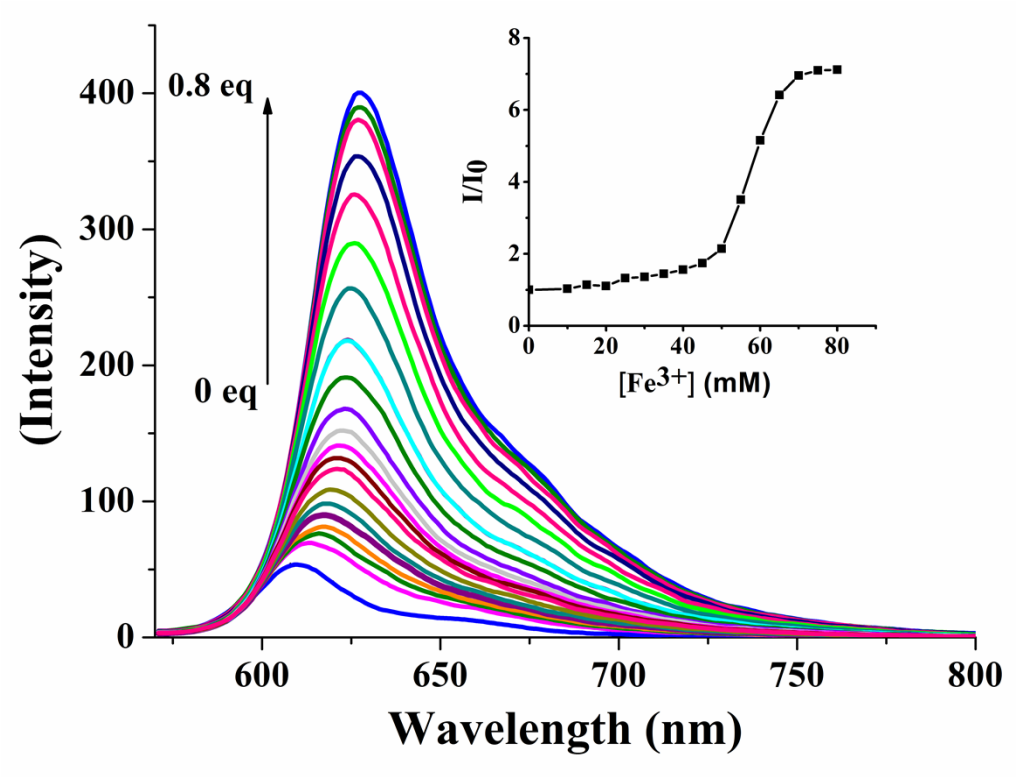


Figure S21: Emission spectra (λ_{ex} = 560 nm) of compound **2a** (10^{-5} M) upon titration with 0-1 equiv. of Fe^{3+} solution in CH_3CN. The inset shows the plot of I/I_{max} vs. $[Fe^{3+}]$

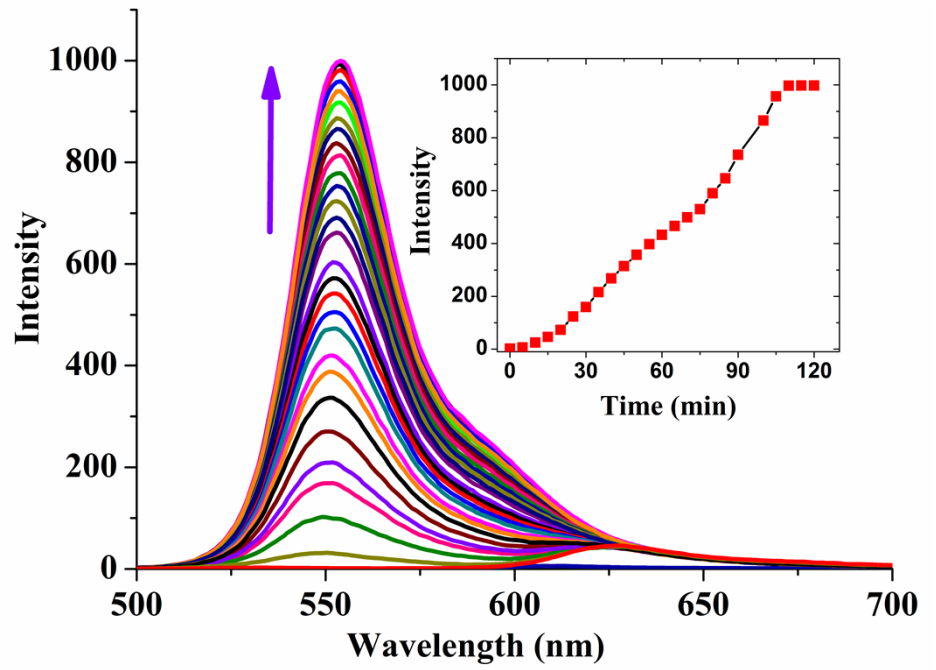


Figure S22: Emission spectral changes of BODIPY **2a** (10 μM) upon titration with 45 equivalents of Fe^{3+} (λ_{ex} = 488 nm) in CH_3CN. (Inset: Plot between the time and fluorescence intensity with 45 equivalents of Fe^{3+}). Each spectrum was recorded after 1 min from addition of Fe^{3+}.

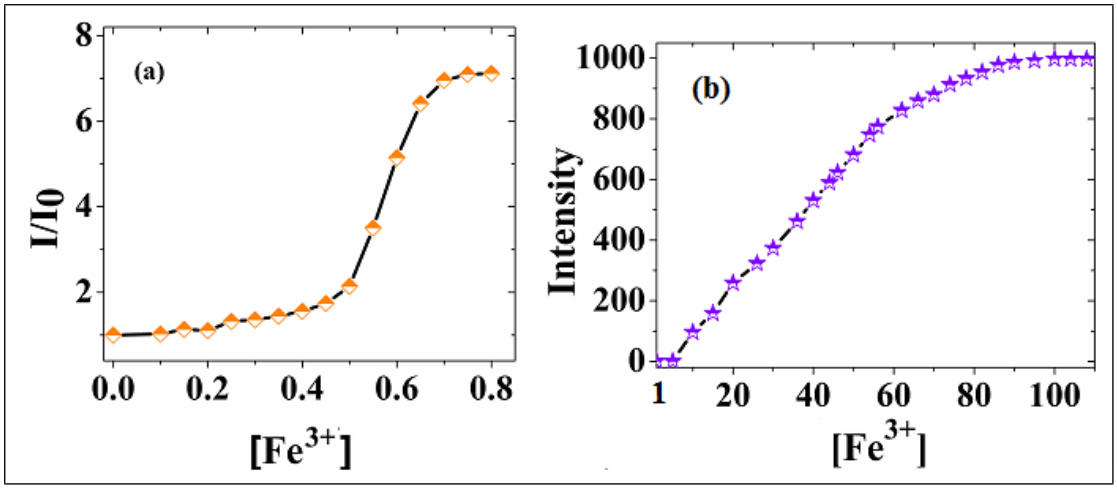


Figure S23: Relative emission changes of compound **2a** (10^{-5} M) in the presence of Fe^{3+} excited at 488 nm: (c) 0 to 1 equivalent (d) 1 to 100 equivalents in CH_3CN.

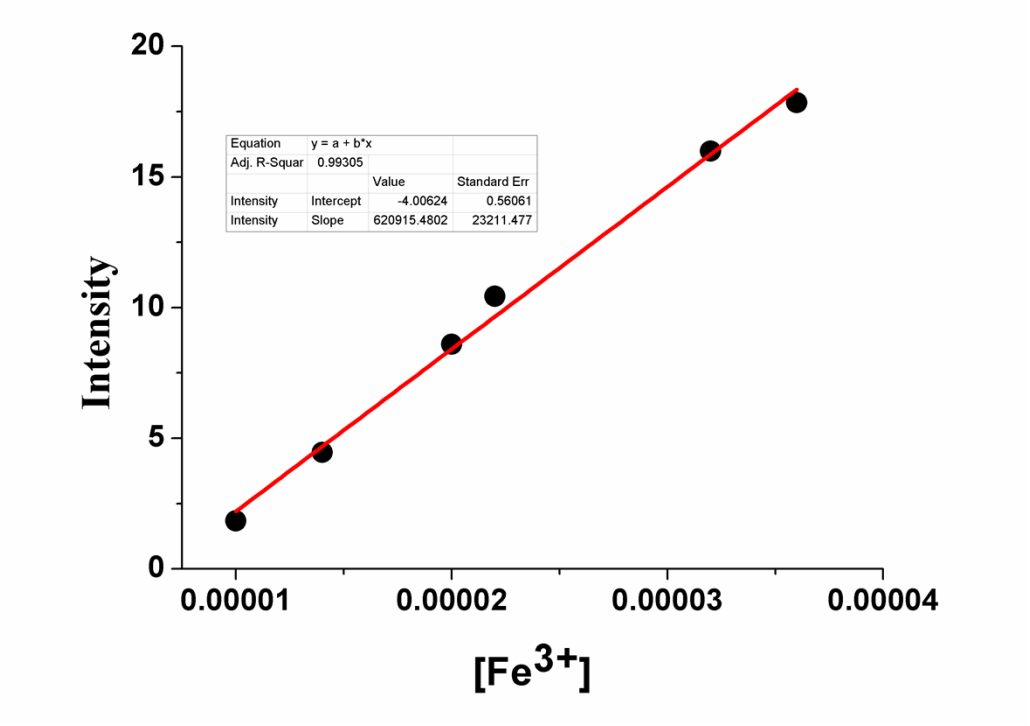


Figure S24: The linear dynamic fluorescence response for the titration of BODIPY **2a** with Fe^{3+} ion to determine the limit of detection (LOD). The LOD was calculated using the formula 3σ/k, where σ = standard deviation for 10 blank samples and k = slope of the linear calibration curve.

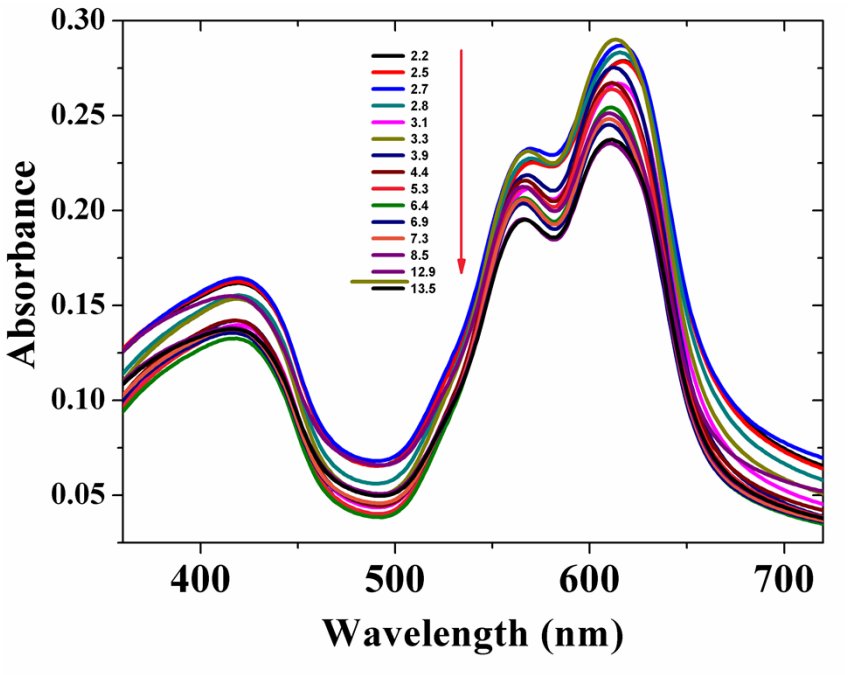


Figure S25: Absorption spectra of compound **2a** (10 μM) in an aqueous acetate buffer solution (0.1 M) as a function of the pH.

Table S1: Crystal data for compound **2a**

Parameters	**2a**
Mol. formula	$C_{28}H_{26}BF_2N_6O_8$
For. weight	623.36
Temp, K	150(2) K
cryst sym	Monoclinic,
space group	*C 2/c*
λ, Å	0.71073
a, Å	9.6447(9)
b, Å	23.900(3)
c, Å	27.692(3)
α, °	90.00
β, °	91.735(8)
γ, °	90.00
volume, Å^3	6380.3(12)
Z	8
μ (mm^{-1})	0.103
D_{calcd} (Mg m^{-3})	1.298
F(000)	444
θ range (deg)	3.32 to 25.00
e data / unique	18398 / 5627
R_{int}	=0.0983
Data / restraints / parameters	5627 / 0 / 409
GOF on F^2	0.742
R1, wR2 [$I > 2\sigma(I)$]	0.0636, 0.1574
R1, wR2 (all data)	0.2179, 0.1861
Largest diff. peak/hole, (e Å^{-3})	0.305 and -0.196