Supporting Information

3,5-Bis(dithioacetal) *meso*-aryl BODIPYs: Selective Chemodosimeter for Hg(II) ion

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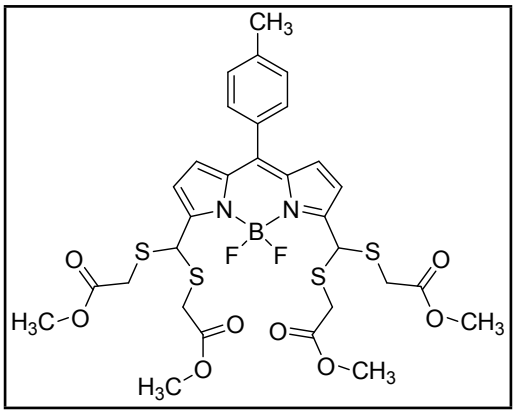


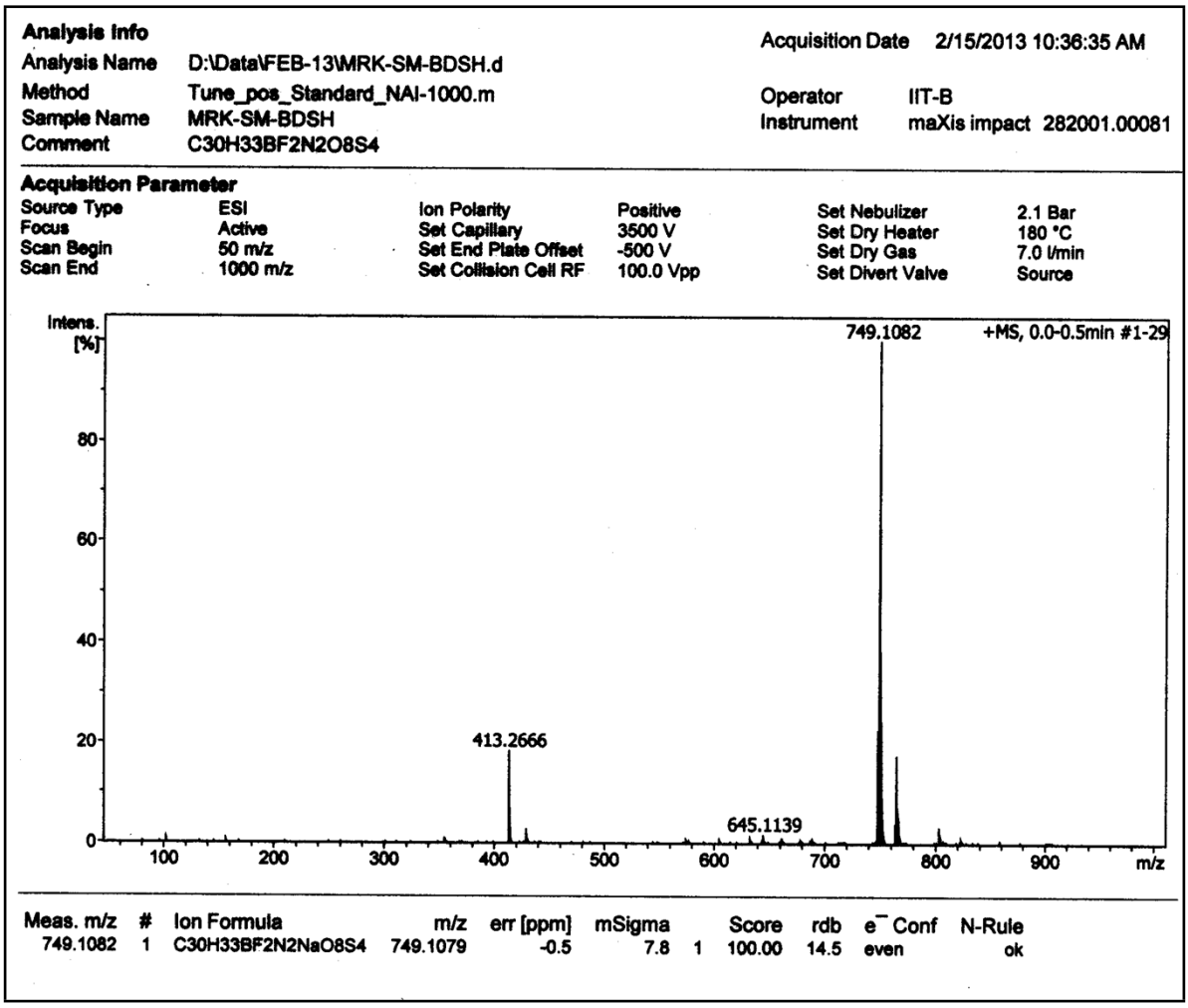
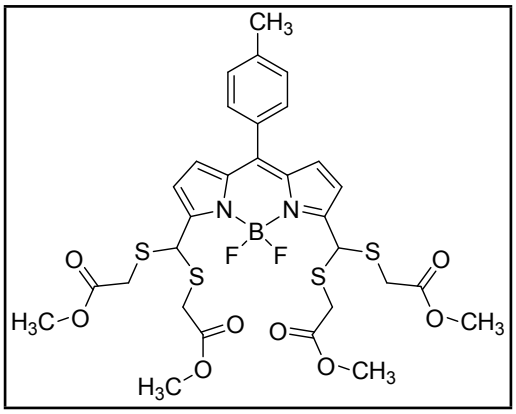


Figure S1: HR mass spectrum of BODIPY **1**



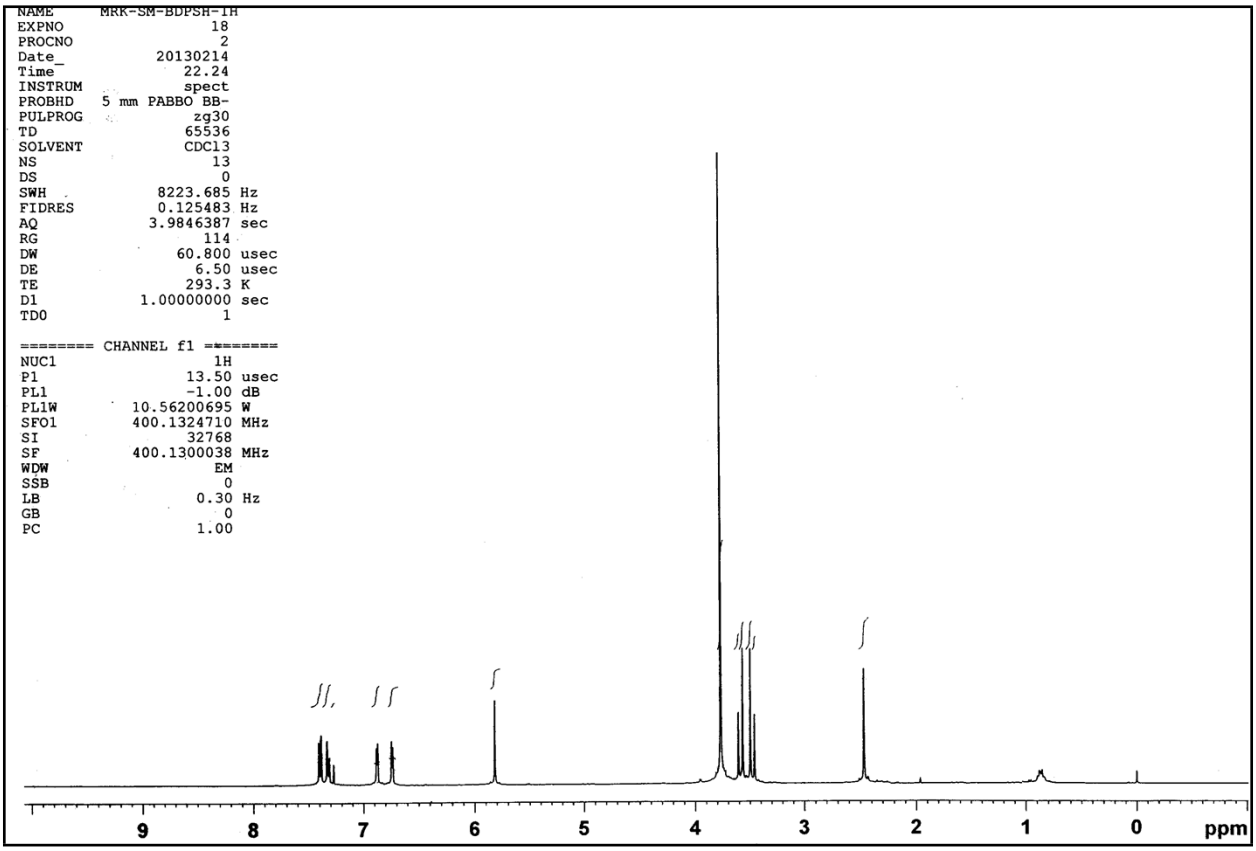
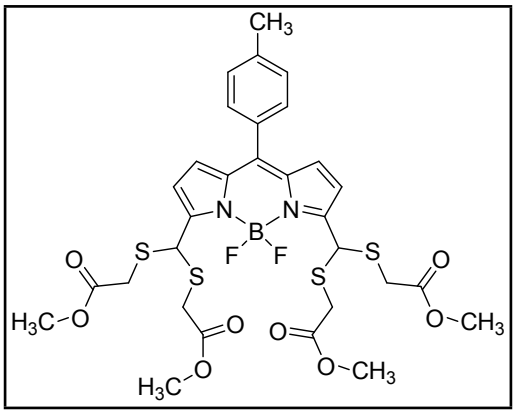


Figure S2: ^{1}H NMR spectrum of BODIPY **1** recorded in $CDCl_3$



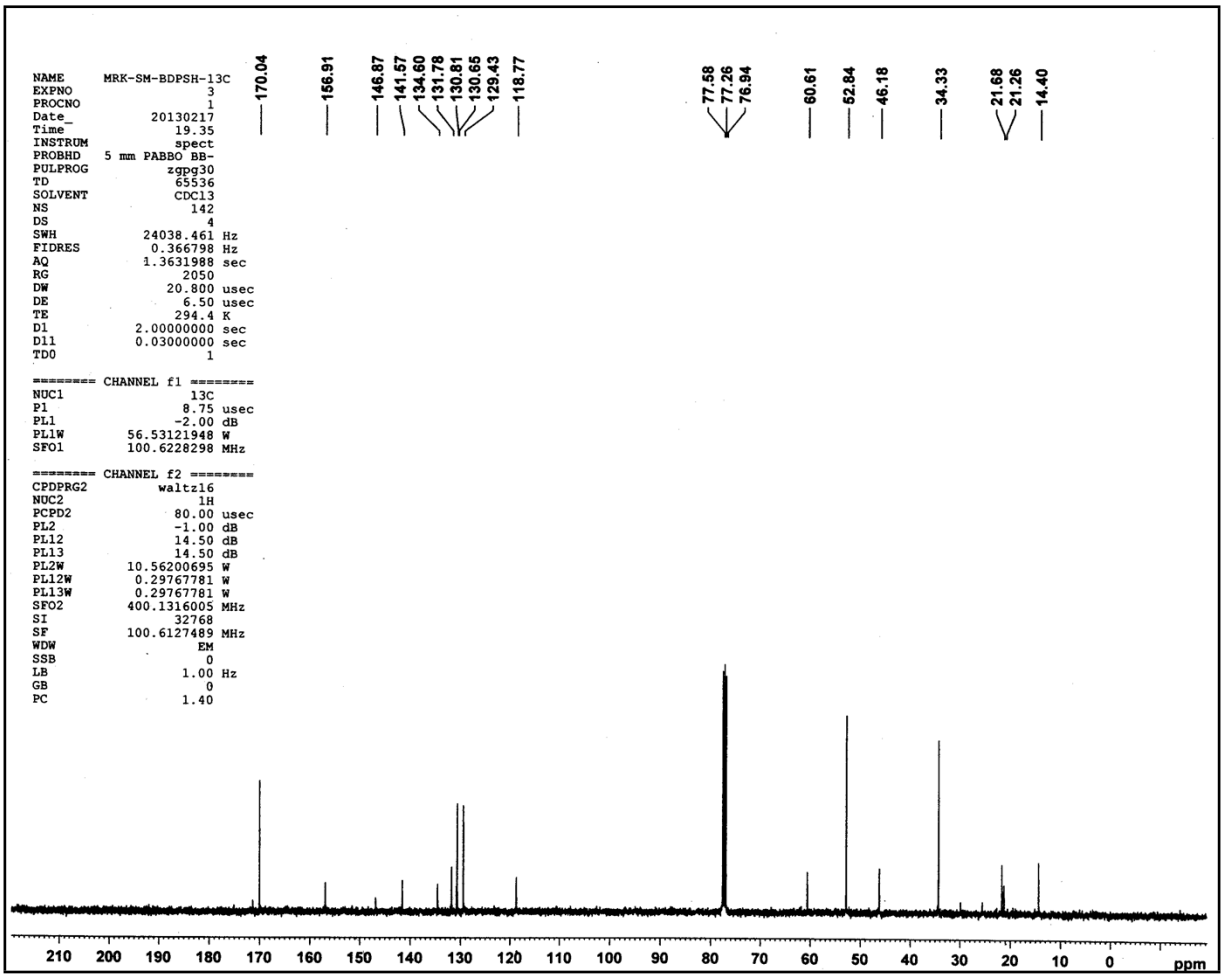
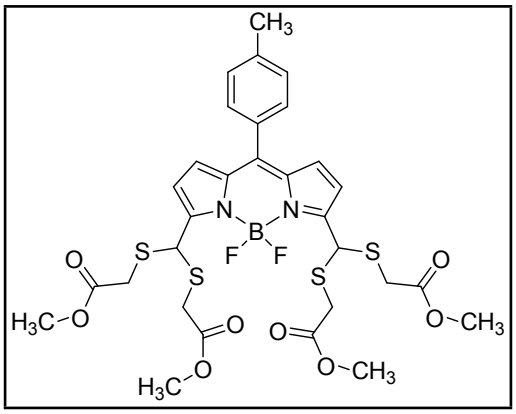


Figure S3: ^{13}C NMR spectrum of BODIPY **1** recorded in $CDCl_3$



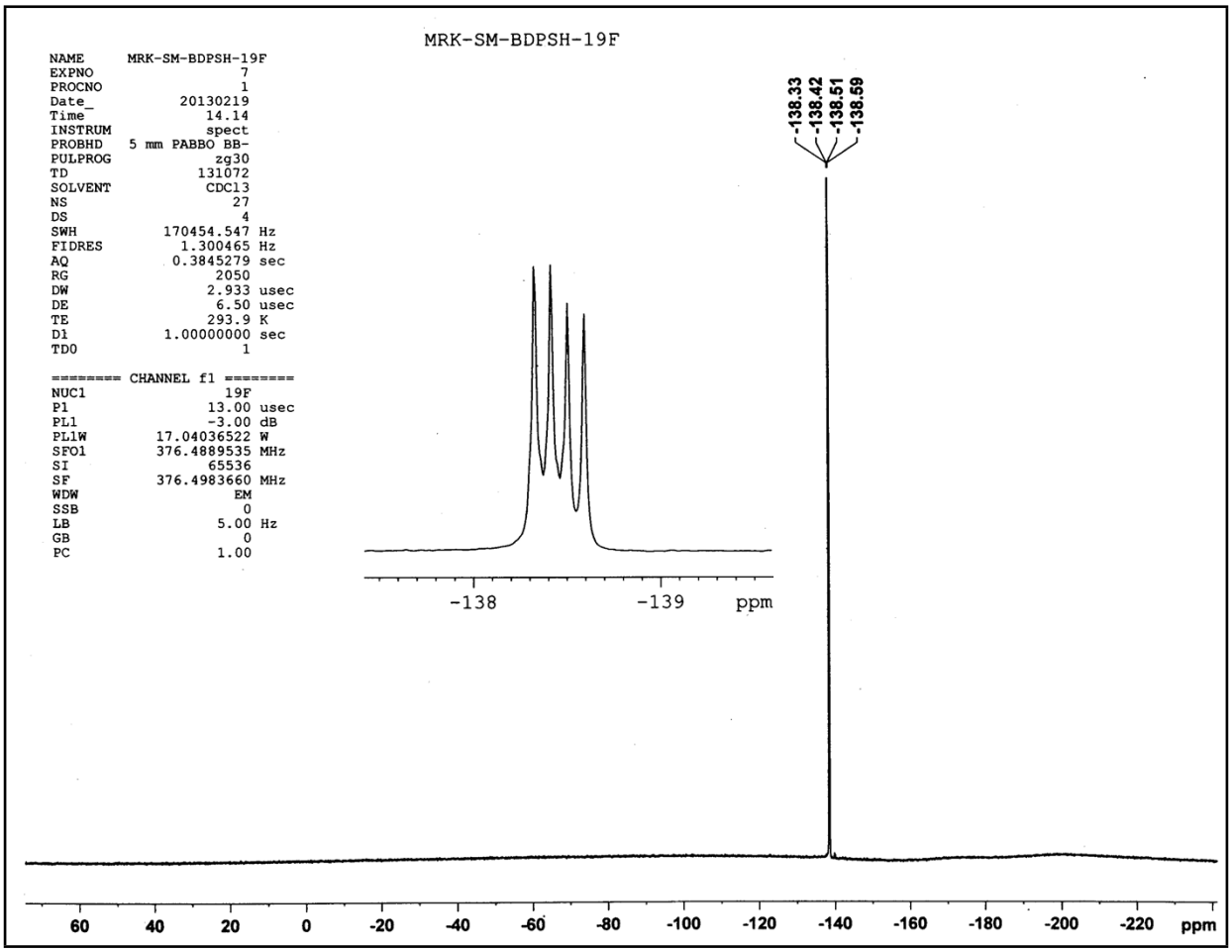
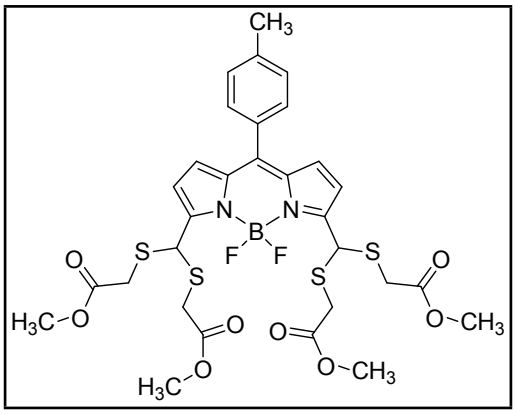


Figure S4: ^{19}F NMR spectrum of BODIPY **1** recorded in $CDCl_3$**.** Inset shows the expansion



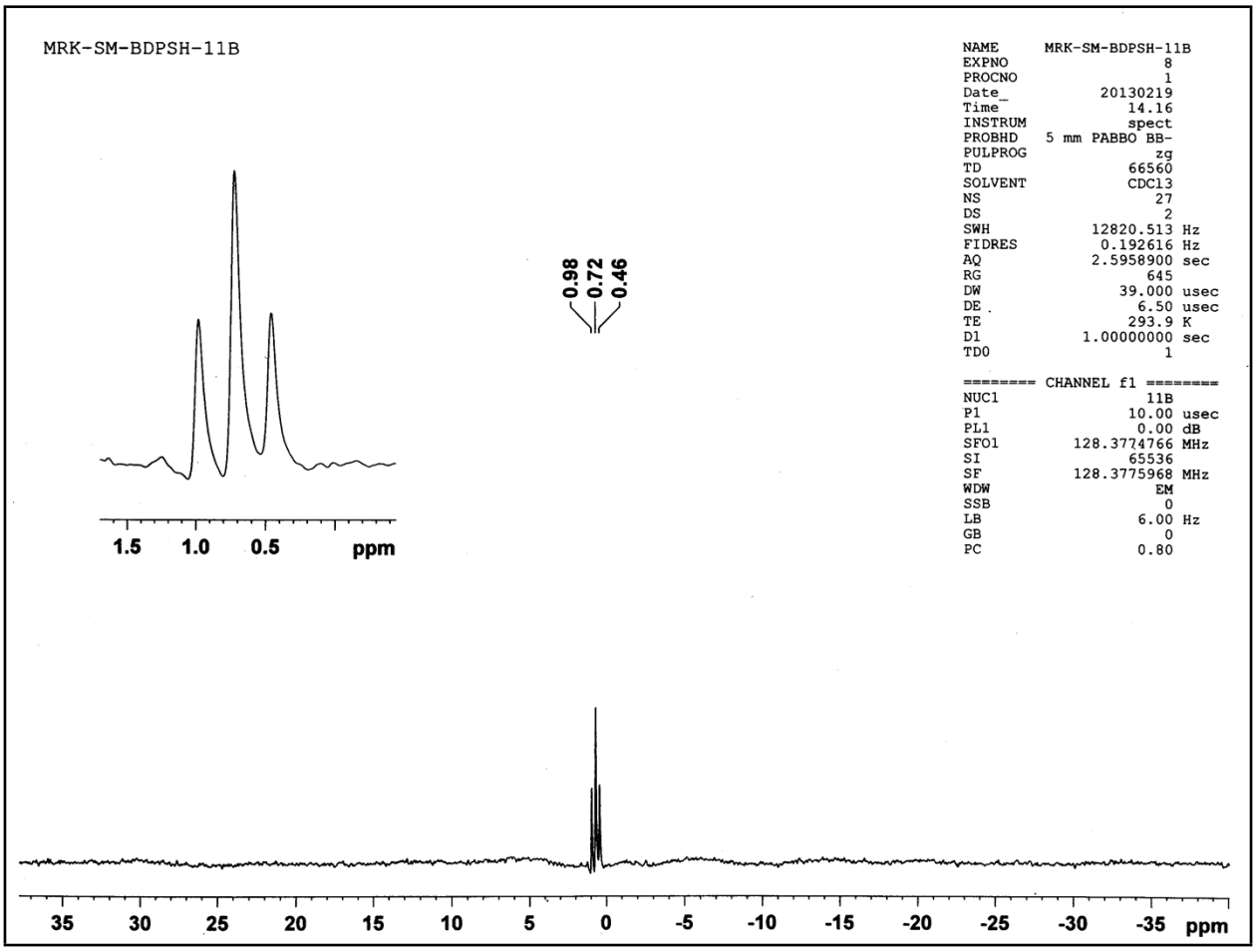
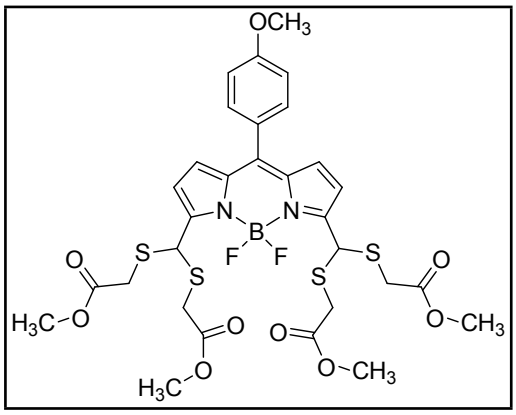


Figure S5: ^{11}B NMR spectrum of BODIPY **1** recorded in $CDCl_3$. Inset shows the expansion.

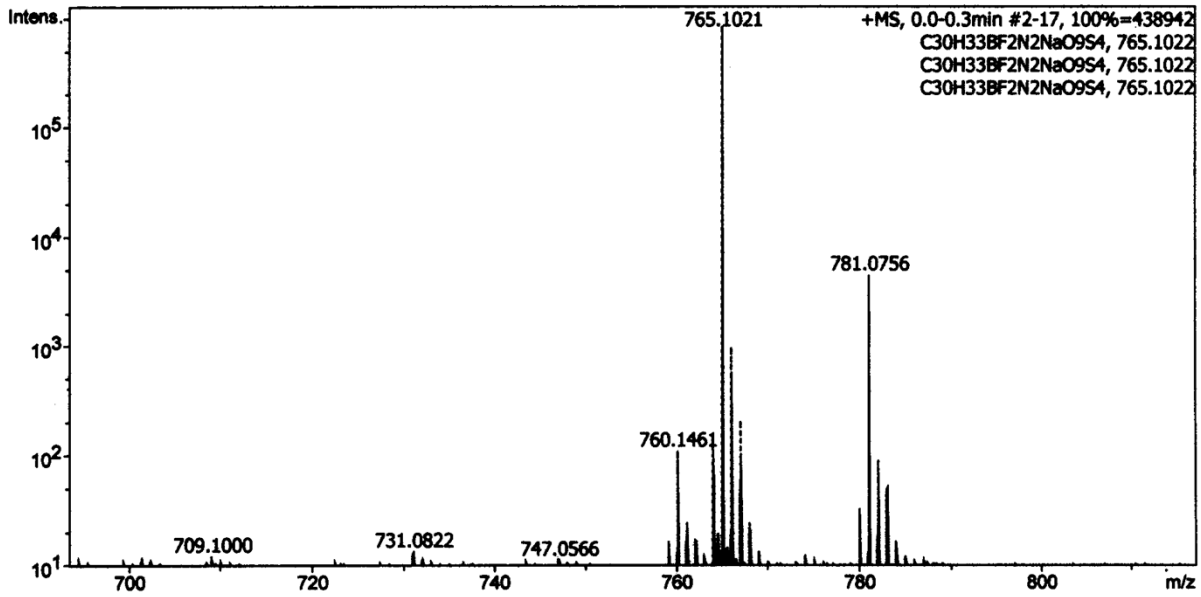


Analysis Info

Analysis Name	D:\Data\MAY-13\MR-SM-ABDPS.d	Acquisition Date	6/4/2013 2:42:34 PM
Method	Tune_pos_Standard_NAI-500.m	Operator	IIT-B
Sample Name	MR-SM-ABDPS	Instrument	maXis impact 282001.00081
Comment	C30H33BF2N2O9S4		

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	2.1 Bar
Focus	Active	Set Capillary	3200 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	7.0 l/min
Scan End	1000 m/z	Set Collision Cell RF	300.0 Vpp	Set Divert Valve	Source



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# Sigma	Score	rdb	e⁻ Conf	N-Rule
765.1021	1	C30H33BF2N2NaO9S4	765.1028	0.9	33.4	1	100.00	14.5	even	ok

Figure S6: HR mass spectrum of BODIPY **2**

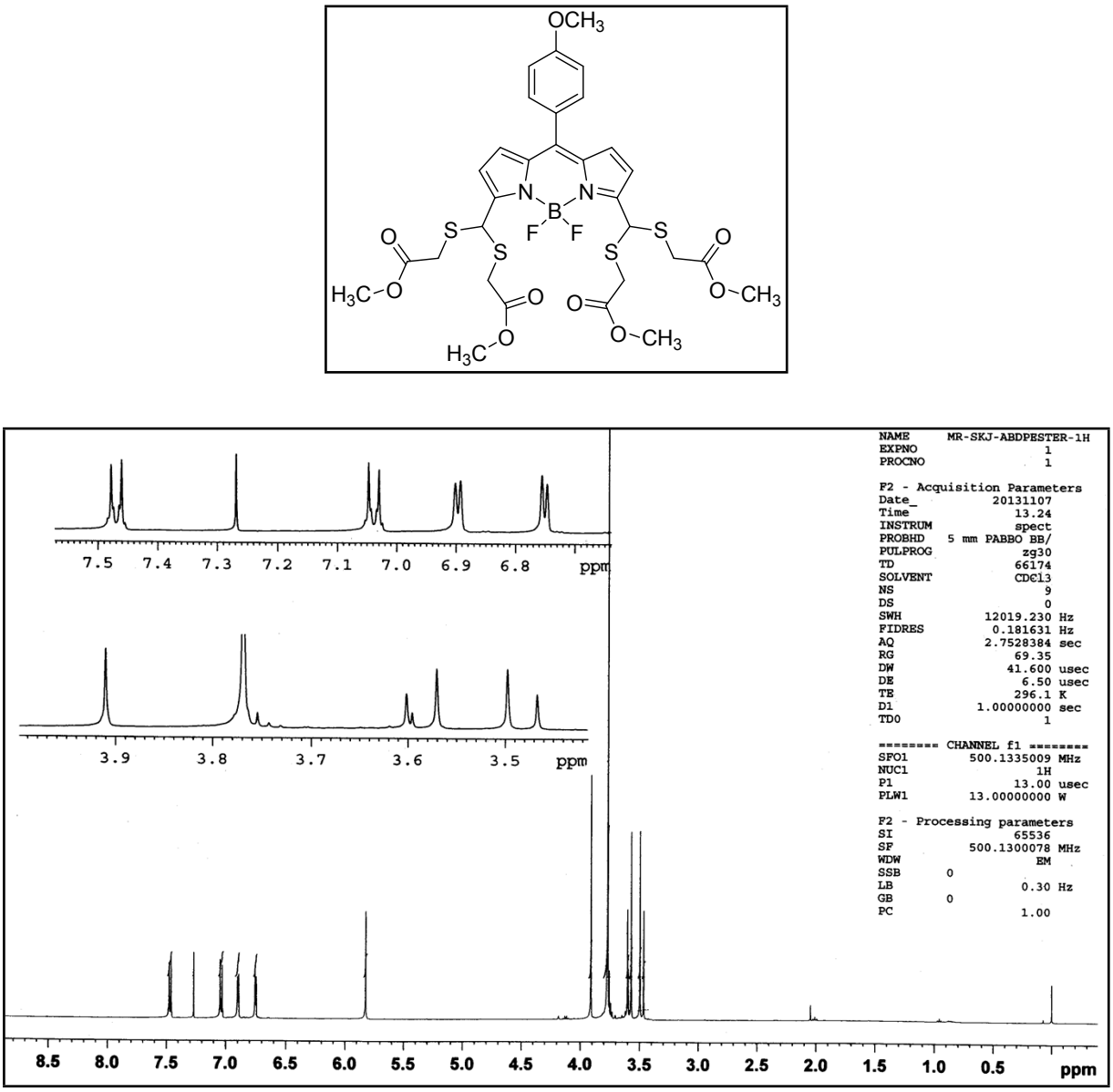
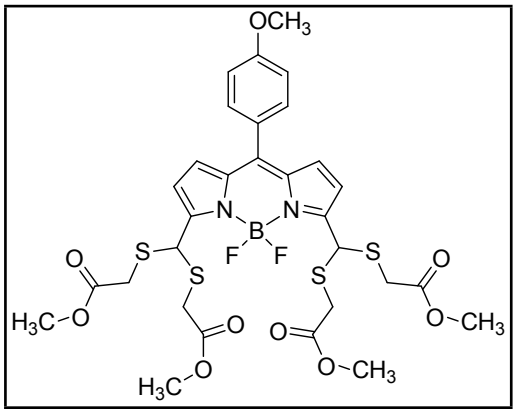


Figure S7: ^{1}H NMR spectrum of BODIPY **2** recorded in $CDCl_3$



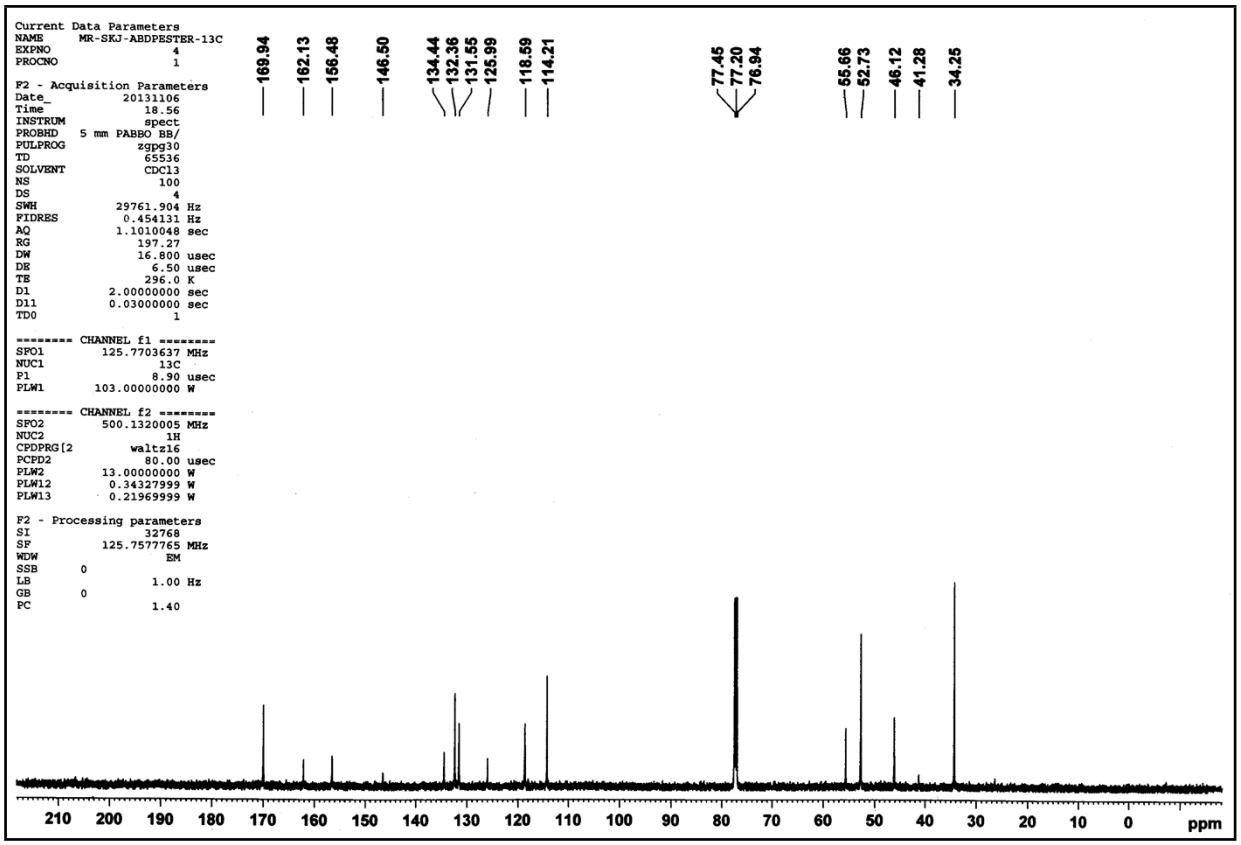
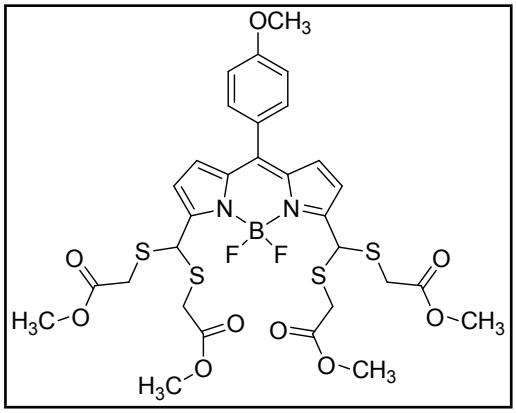


Figure S8: ^{13}C NMR spectrum of BODIPY **2** recorded in $CDCl_3$



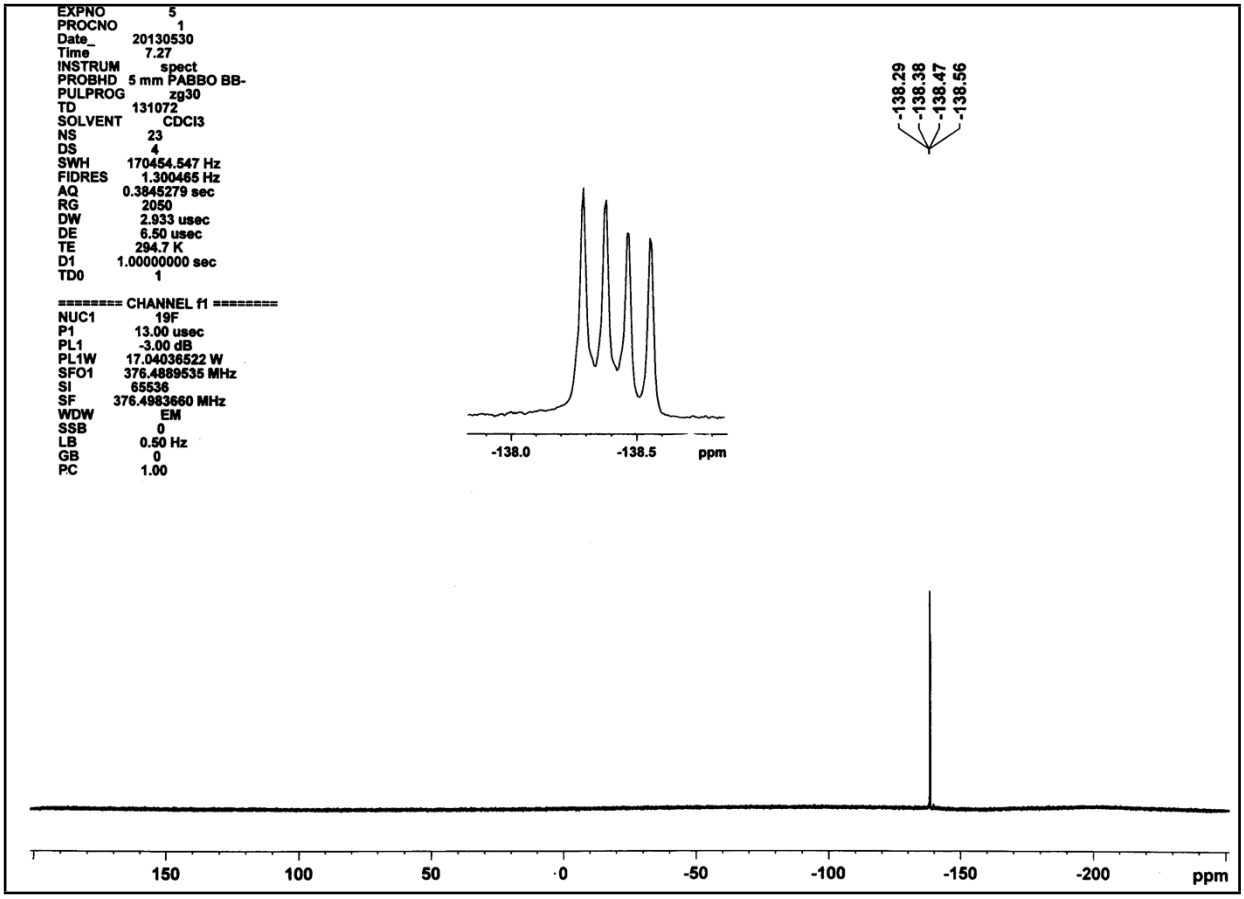
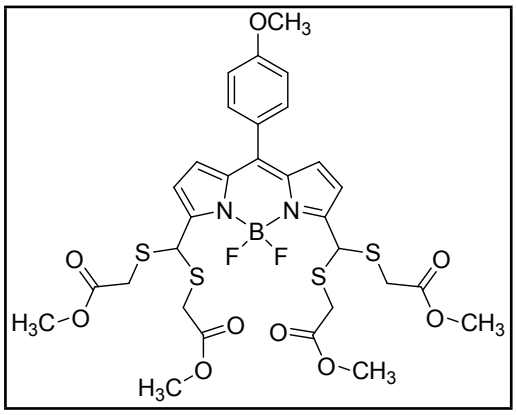


Figure S9: ^{19}F NMR spectrum of BODIPY **2** recorded in $CDCl_3$**.** Inset shows the expansion



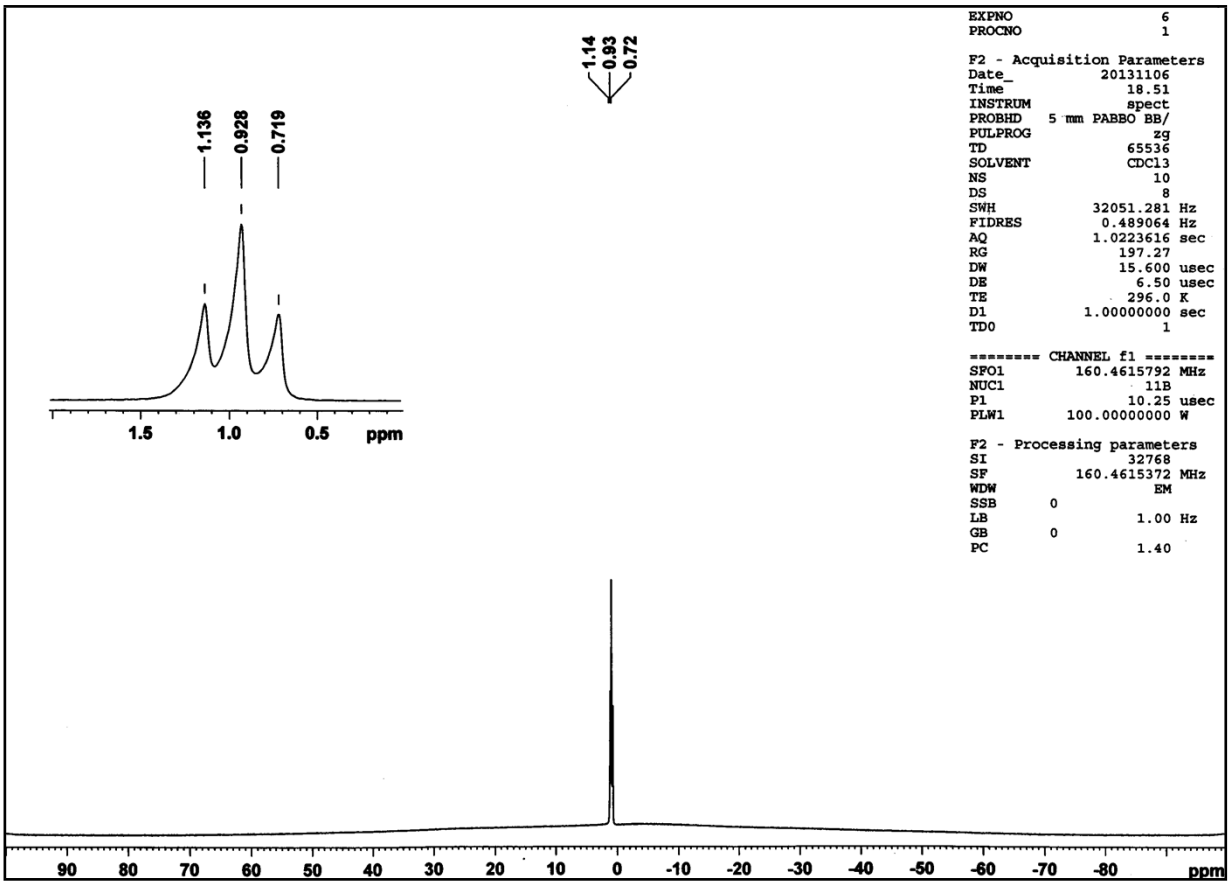


Figure S10: ^{11}B NMR spectrum of BODIPY **2** recorded in $CDCl_3$. Inset shows the expansion.

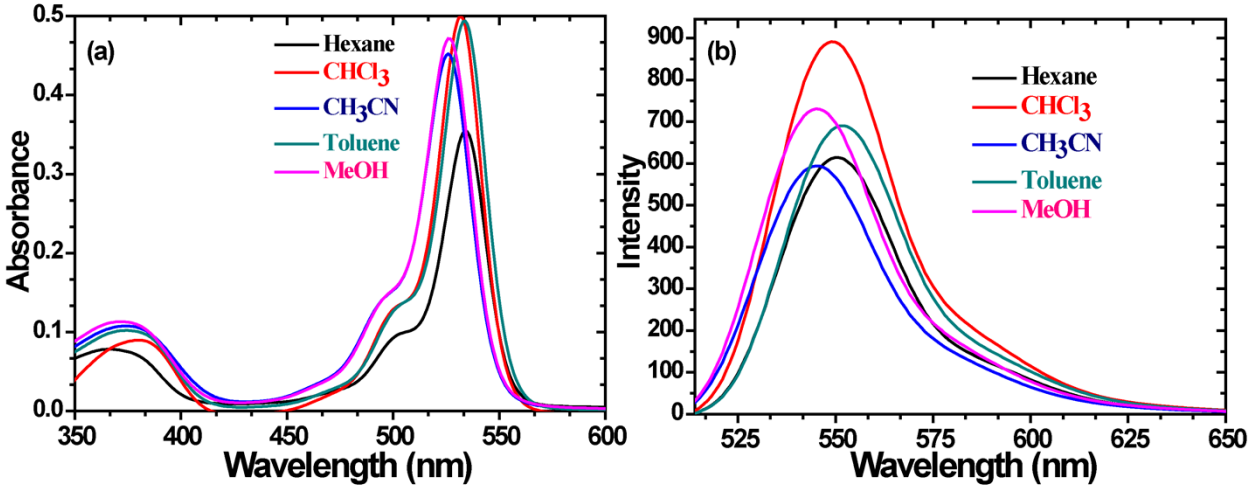


Figure S11: a) Absorption, b) emission spectra of BODIPY **1** (5 μM) recorded in different solvents. Excitation wavelength used was 488 nm.

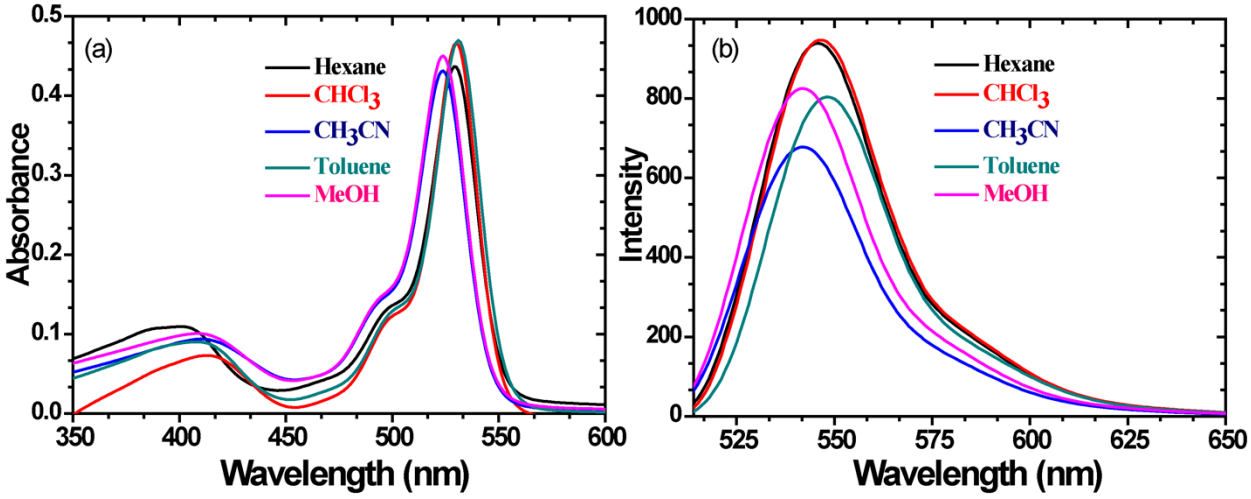


Figure S12: a) Absorption, b) emission spectra of BODIPY **2** (5 μM) recorded in different solvents. Excitation wavelength used was 488 nm.

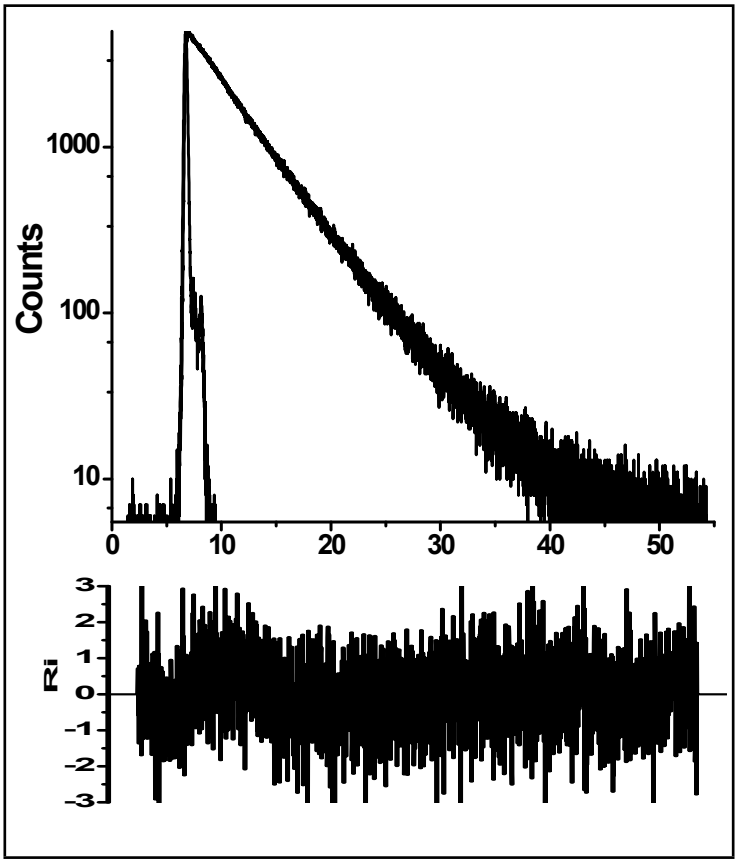


Figure S13: Fluorescence-decay profile and the corresponding weighted residual-distribution fit of the fluorescence decay of BODIPY **1** in $CHCl_3$. The excitation wavelength used was 440 nm and emission was detected at the emission-peak maxima (549 nm) of BODIPY **1**.

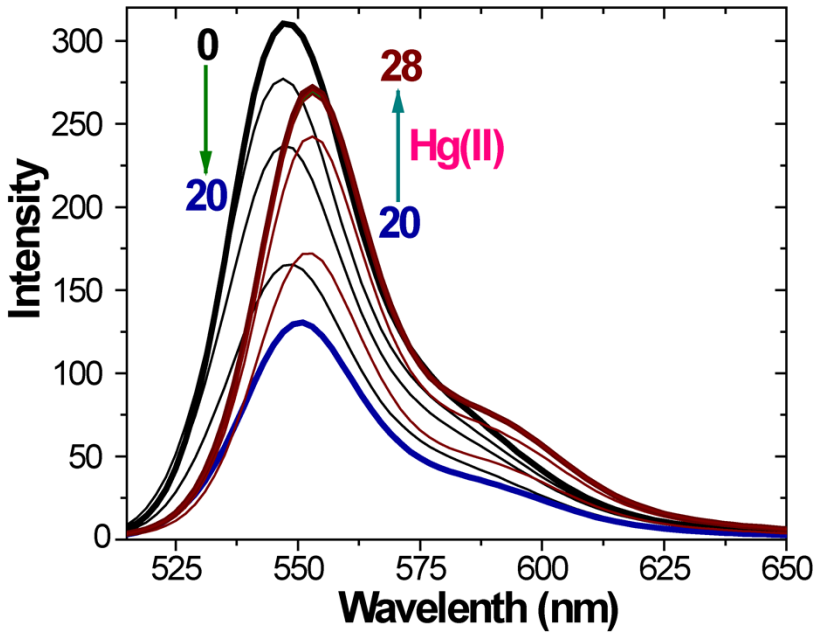


Figure S14: Emission spectral changes of BODIPY **1** (5 μM) upon addition of increasing equivalents of Hg^{2+} ions ($HgCl_2$) in CH_3CN/PBS (8:2; v/v, pH 7.4). The spectra were recorded after the addition of Hg^{2+} ion to BODIPY **1** for 10 min.

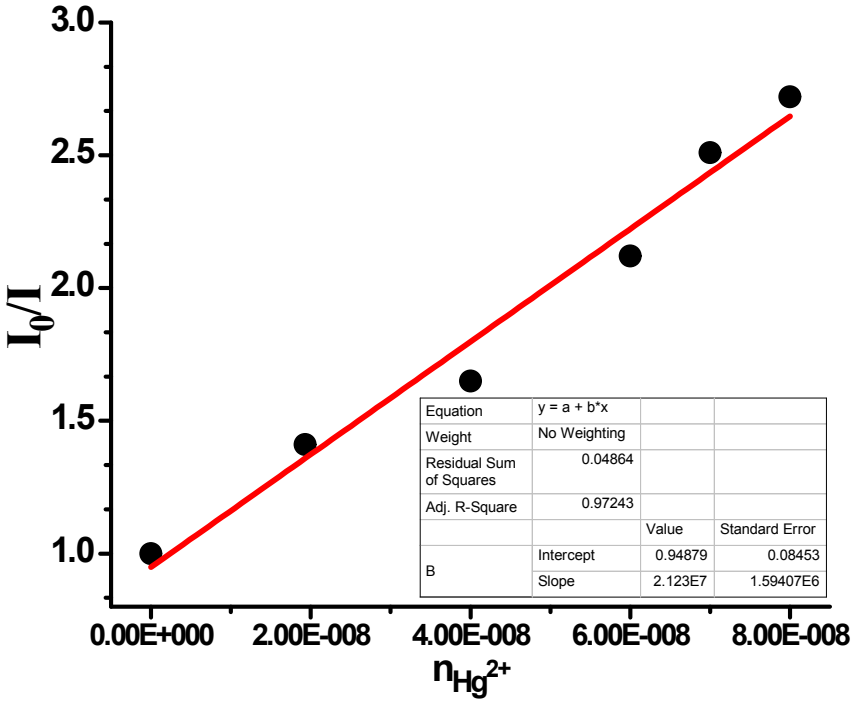


Figure S15: The linear dynamic fluorescence response for the titration of BODIPY **1** with F^- ion to determine the detection limit (LOD). The LOD was calculated using the formula 3σ/k, where σ = standard deviaition of blank (10 samples) and k = the slope of linear calibration curve.

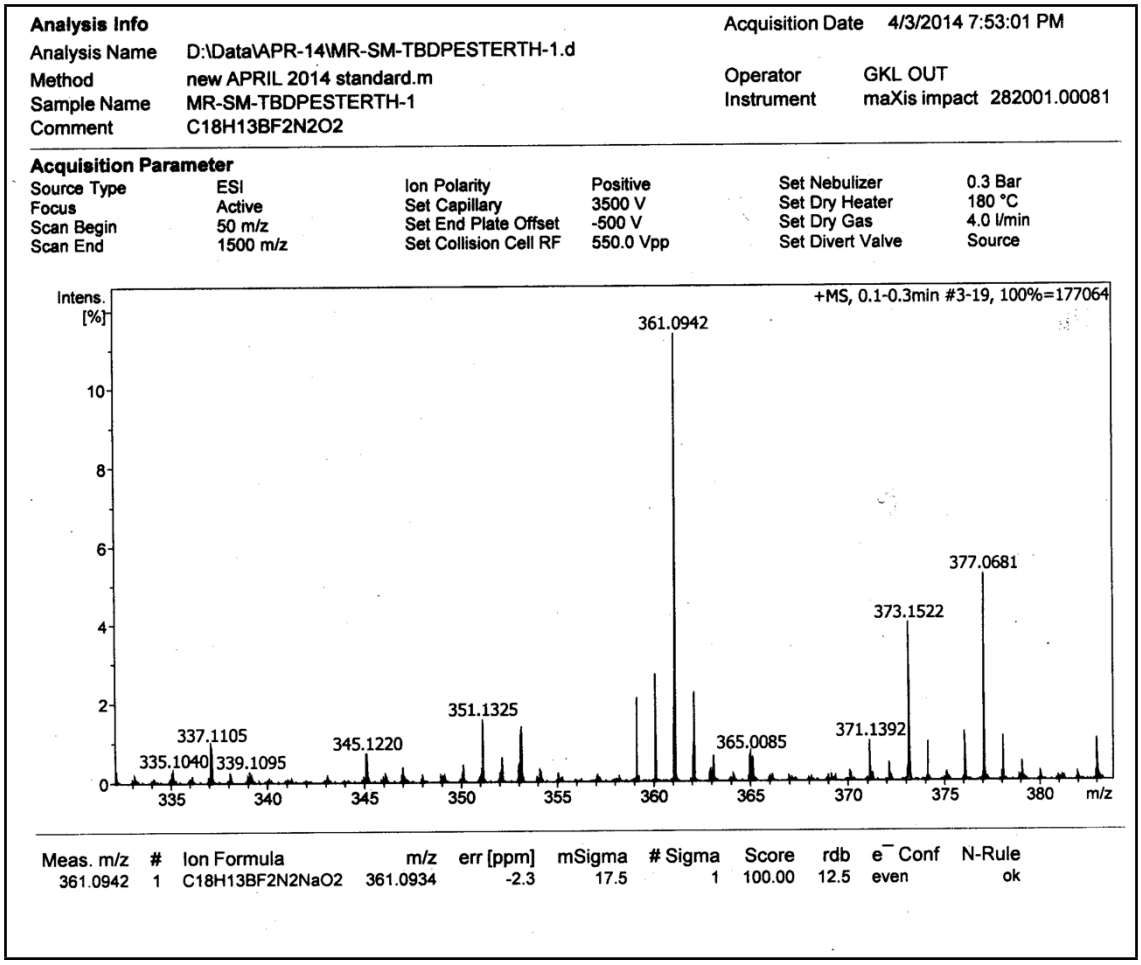


Figure S16: HR-MS spectrum showing the molecular ion peak for the formation of compound **3** during titration of BODIPY **1** with Hg(II) ion.