Electronic Supplementary Material (ESI) for RSC Advances.

Supporting Information

Boranil Dye Based "Turn-on" Fluorescent Probes for Detection of Hydrogen Peroxide and Their Cell Imaging Application

Jayabalan Shanmugapriya,[a‡] Kandasamy Rajaguru,[b‡] Gandhi Sivaraman,[c‡] Shanmugam Muthusubramanian,*[b] and Nattamai Bhuvanesh[d]

[a] *Department of Chemistry, Thiagarajar College of Engineering, Madurai – 625 01, India*

[b] *Department of Organic Chemistry, School of Chemistry, Madurai Kamaraj University, Madurai - 625 021, India*

[c] *Institute for Stem Cell Biology and Regenerative Medicine, National Centre for Biological Sciences, Bangalore – 560065, India*

[d] *X-ray Diffraction Laboratory, Department of Chemistry, Texas A & M University, College Station, Texas, 77842, USA*

[‡] *These authors have contributed equally*

e-mail: muthumanian2001@yahoo.com

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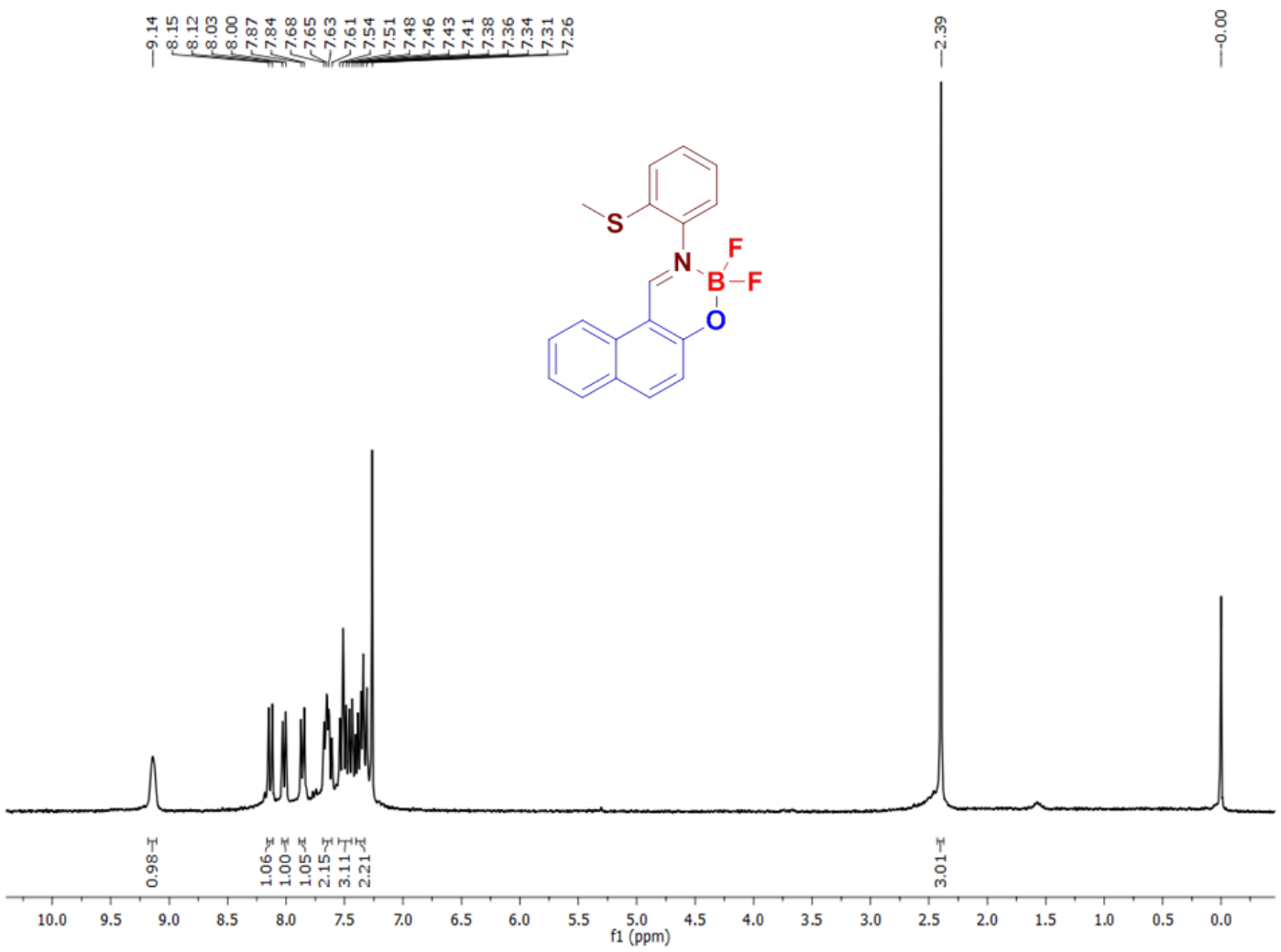


Figure S1. ^{1}H NMR spectrum of compound **SB-1**

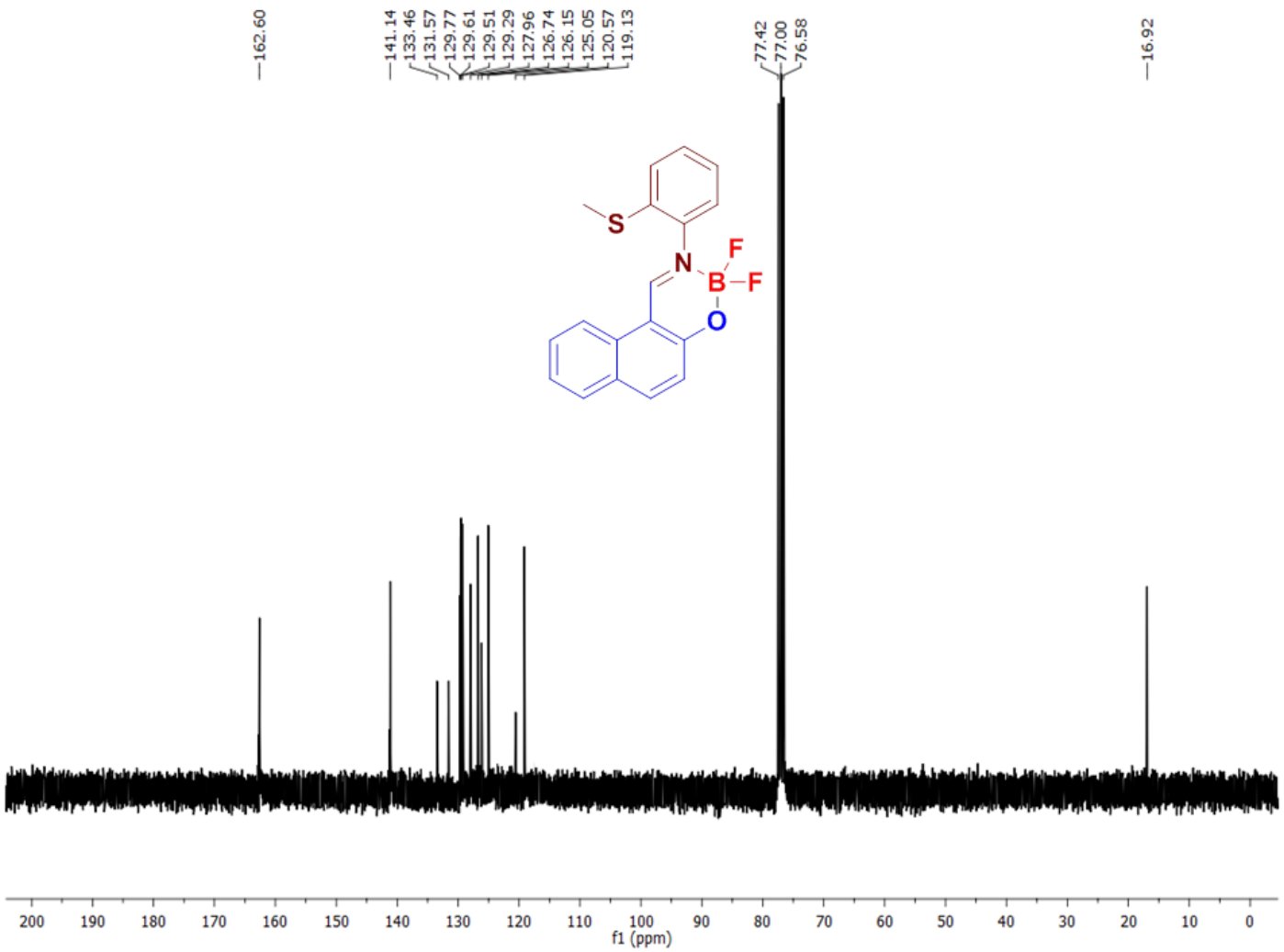


Figure S2. ^{13}C NMR spectrum of compound **SB-1**

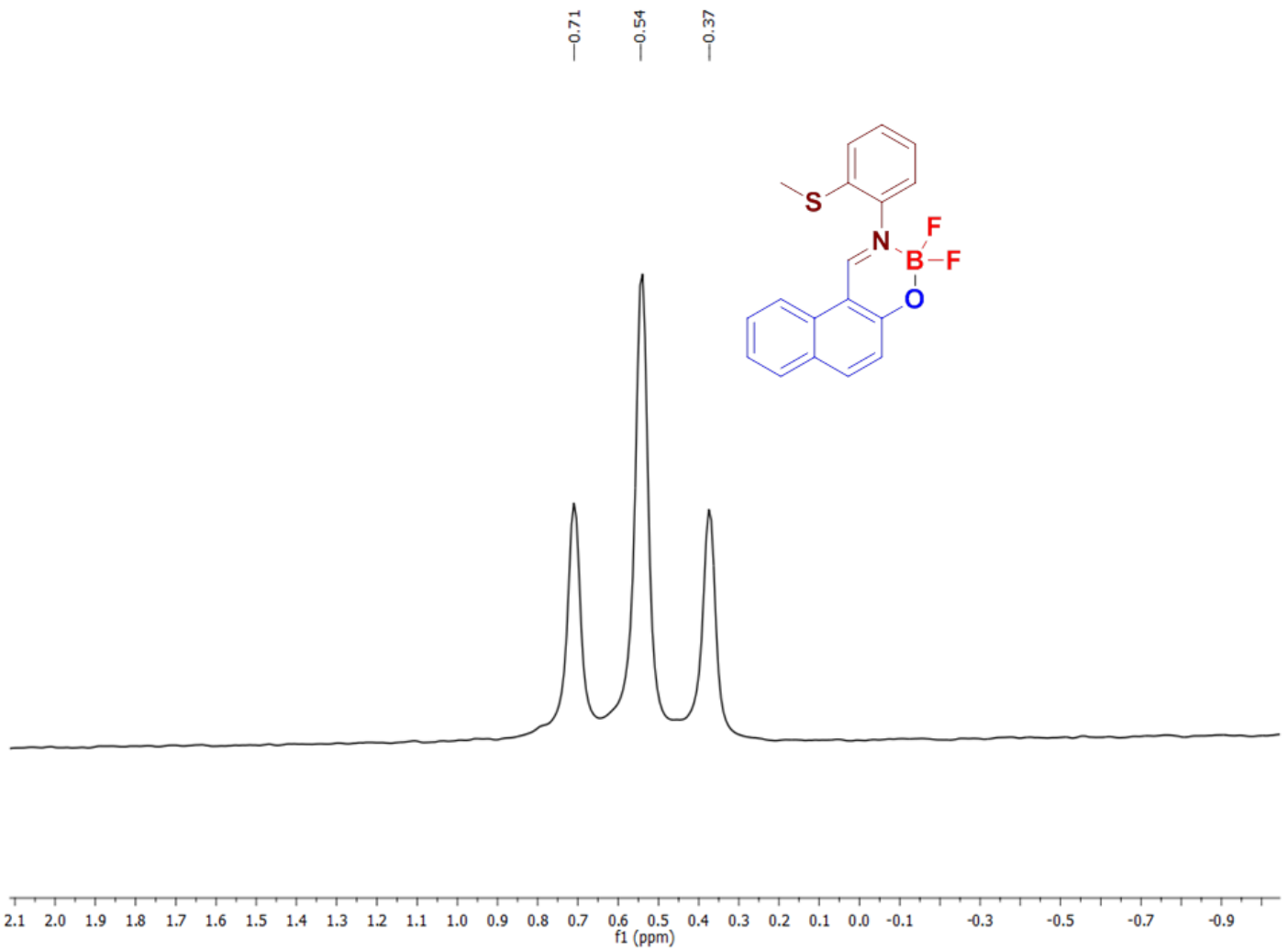


Figure S3. ^{11}B NMR spectrum of compound **SB-1**

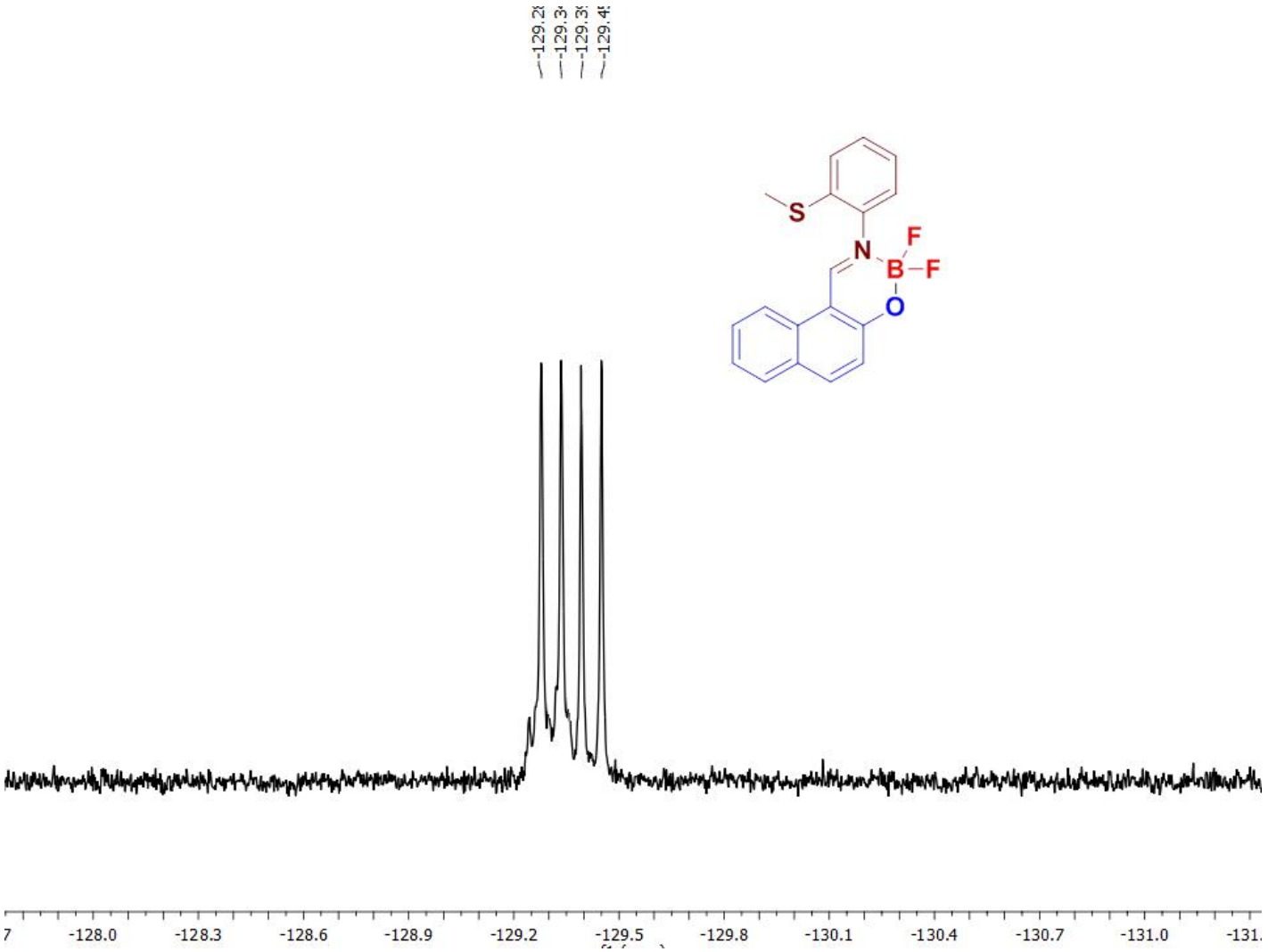


Figure S4. ^{19}F NMR spectrum of compound **SB-1**

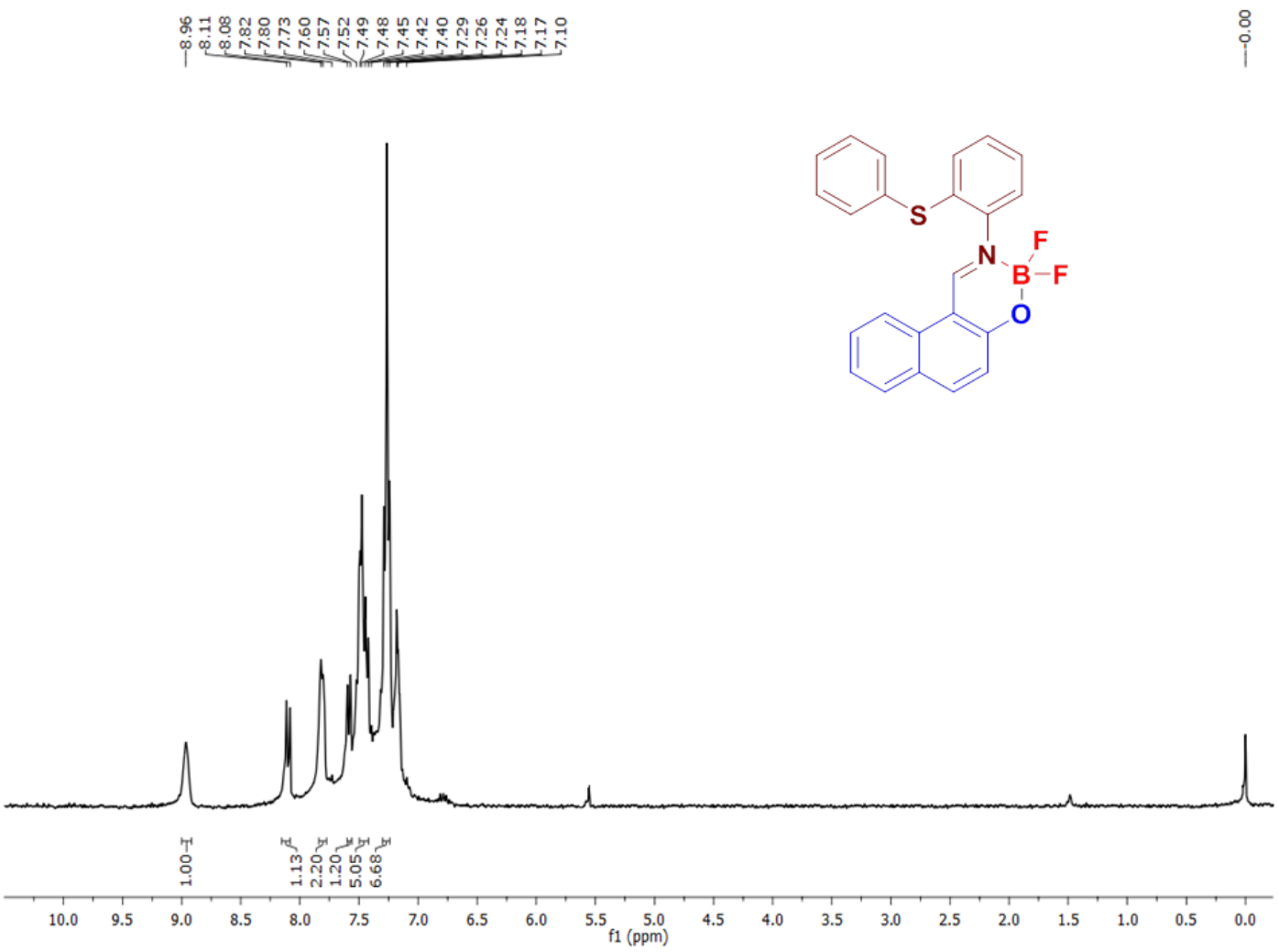


Figure S5. ^{1}H NMR spectrum of compound **SB-2**

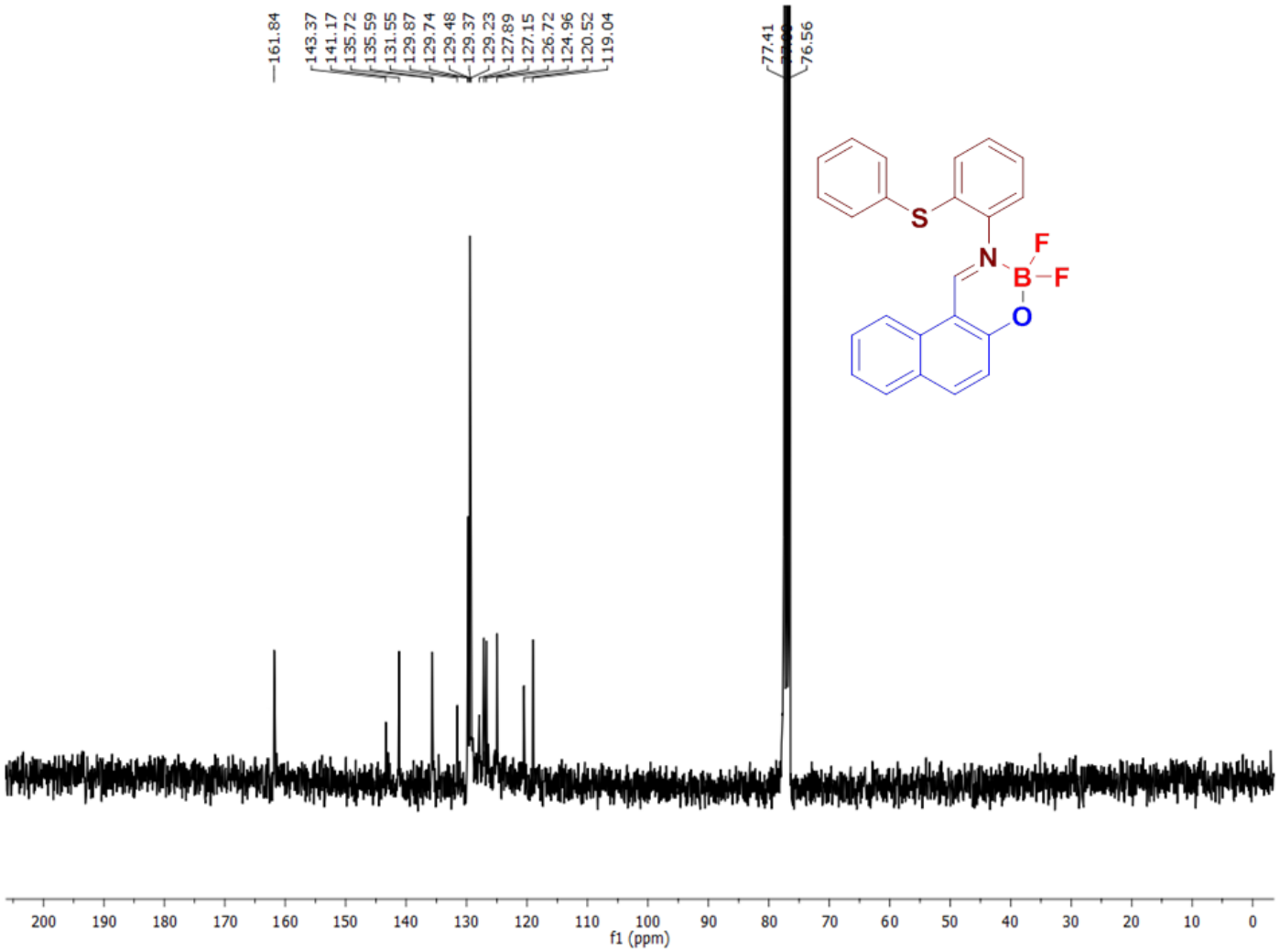


Figure S6. ^{13}C NMR spectrum of compound **SB-2**

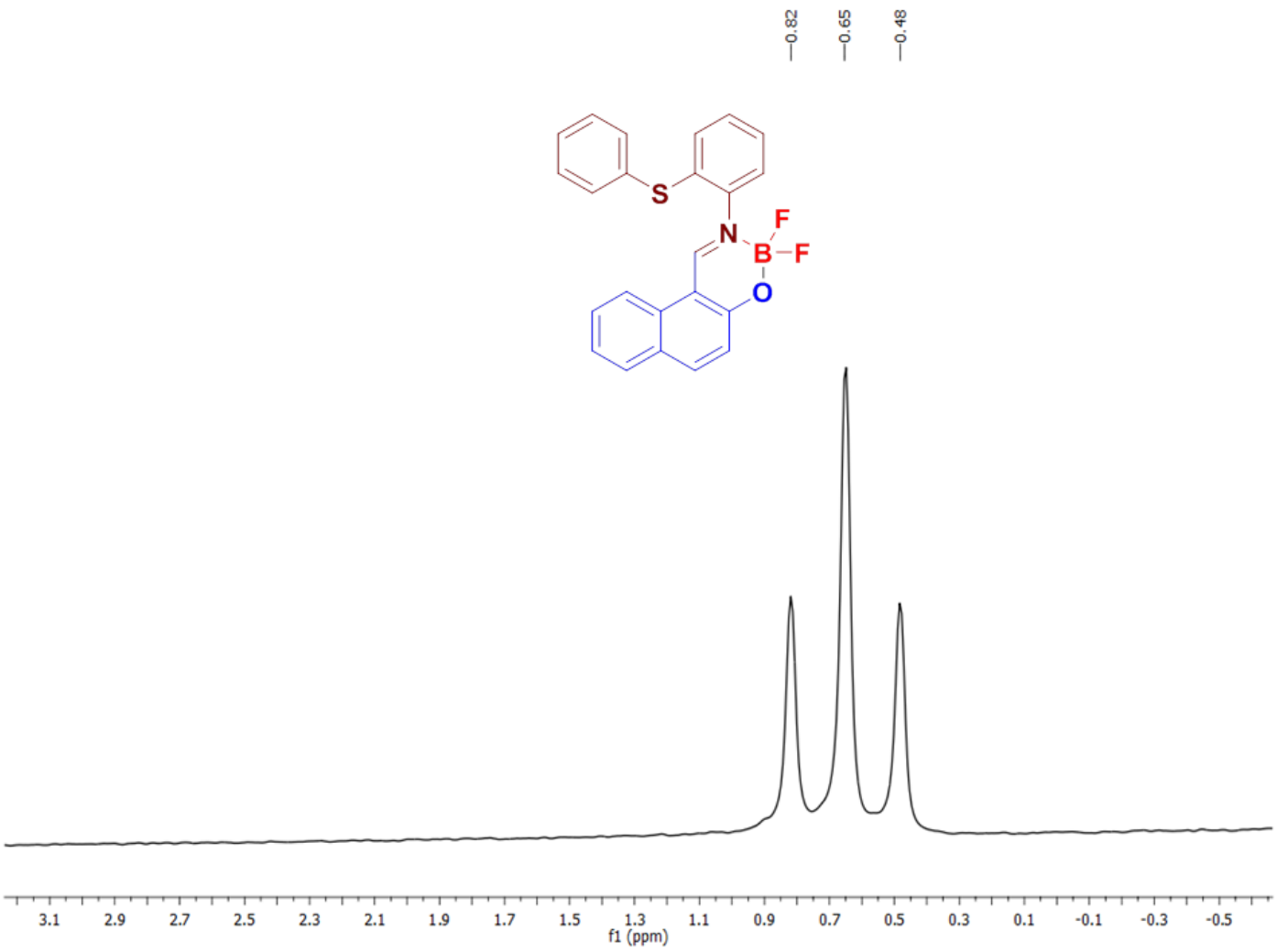


Figure S7. ^{11}B NMR spectrum of compound **SB-2**

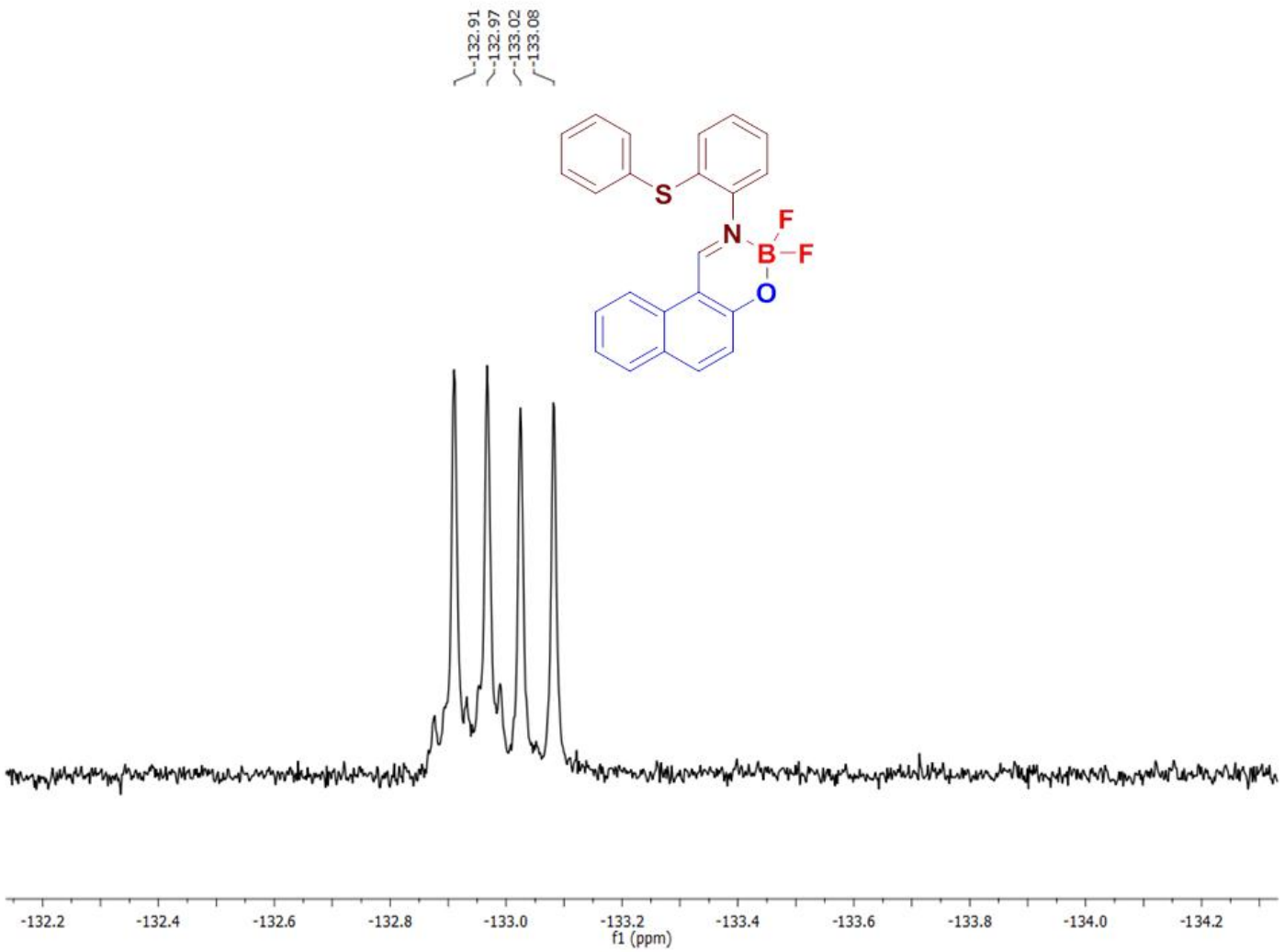


Figure S8. ^{19}F NMR spectrum of compound **SB-2**

Table S1. Selected Details about Data Collection and Crystal Refinement for boranil dyes SB-1 and SB-2

	SB-1	SB-2
CCDC number	1456040	1456041
Empirical formula	$C_{18}H_{14}BF_2NOS$	$C_{23}H_{16}BF_2NOS$
Formula weight	341.17	403.24
Temperature	110.15 K	110.15 K
Wavelength	0.71073 Å	0.71073 Å
Crystal system	Orthorhombic	Monoclinic
Space group	Pbca	P121/c1
Unit cell dimensions	a = 10.661(2) Å; α= 90°.	a = 15.06(2) Å; α= 90°.
	b = 11.234(2) Å; β= 90°.	b = 11.446(16) Å; β= 101.569(16)°.
	c = 25.712(5) Å; γ = 90°.	c = 10.980(16) Å; γ = 90°.
Volume	3079.5(11) $Å^3$	1855(5) $Å^3$
Z	8	4
Density (calculated)	1.472 Mg/m^3	1.444 Mg/m^3
Absorption coefficient	0.236 mm^{-1}	0.209 mm^{-1}
F(000)	1408	832
Crystal size	0.38 x 0.127 x 0.104 mm^3	0.522 x 0.148 x 0.074 mm^3

Theta range for data collection	2.482 to 24.998°.	2.252 to 27.550°.
Index ranges	-12<=h<=12, -13<=k<=13, -30<=l<=30	-19<=h<=19, -14<=k<=14, -14<=l<=14
Reflections collected	27275	21099
Independent reflections	2721 [R(int) = 0.0895]	4245 [R(int) = 0.0325]
Completeness to theta = 25.242°	97.8 %	99.9 %
Absorption correction	Semi-empirical from equivalents	Semi-empirical from equivalents
Max. and min. transmission	0.7456 and 0.6639	.7456 and 0.6822
Refinement method	Full-matrix least-squares on F^2	Full-matrix least-squares on F^2
Data / restraints / parameters	2721 / 0 / 218	4245 / 0 / 262
Goodness-of-fit on F^2	1.060	1.040
Final R indices [I>2sigma(I)]	R1 = 0.0458, wR2 = 0.0822	R1 = 0.0410, wR2 = 0.0910
R indices (all data)	R1 = 0.0675, wR2 = 0.0915	R1 = 0.0523, wR2 = 0.0972
Largest diff. peak and hole	0.277 and -0.304 e.Å^{-3}	0.351 and -0.317 e.Å^{-3}

Figure-S9: X-ray crystal structure of compound SB-1

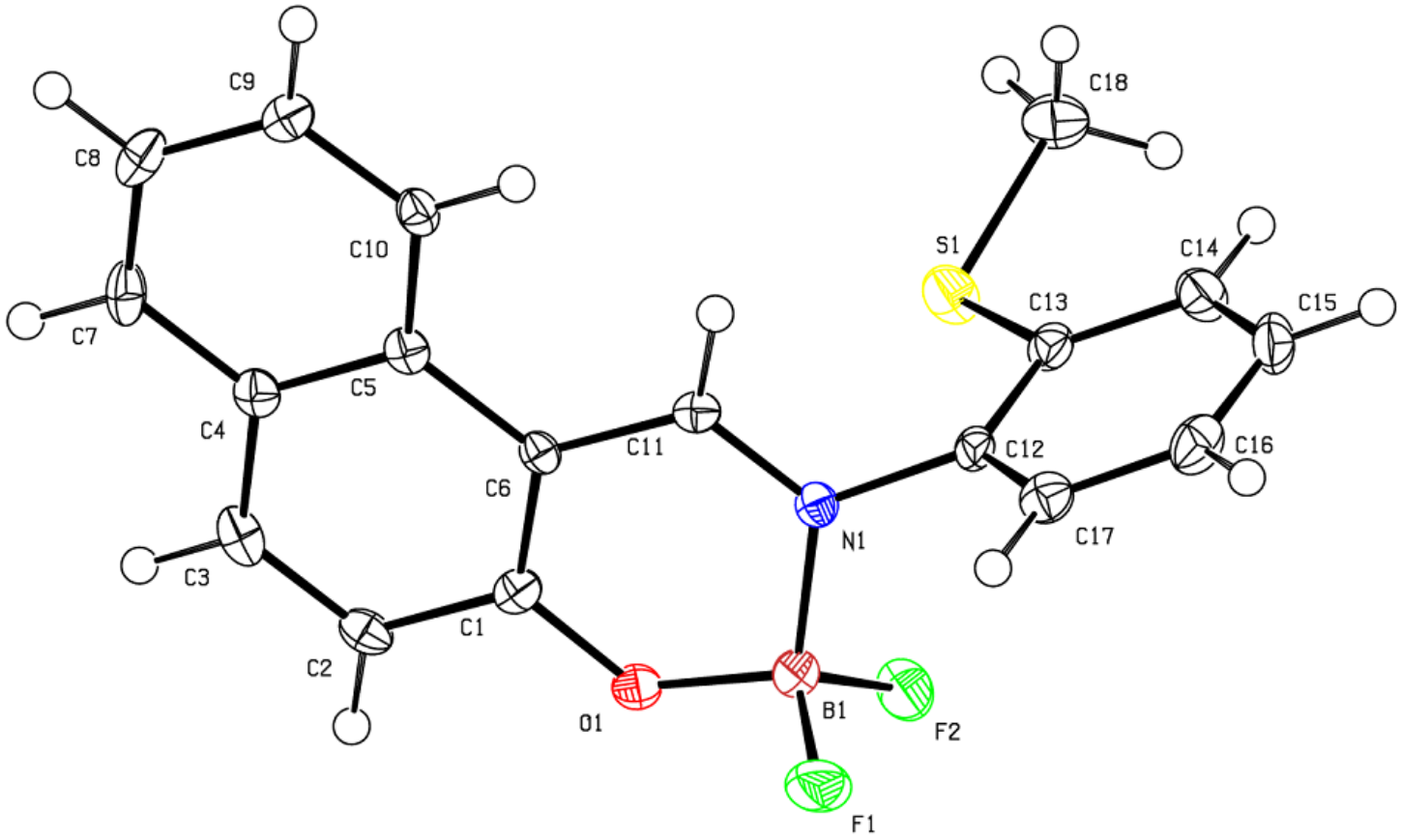


Figure-S10: X-ray crystal structure of compound SB-2

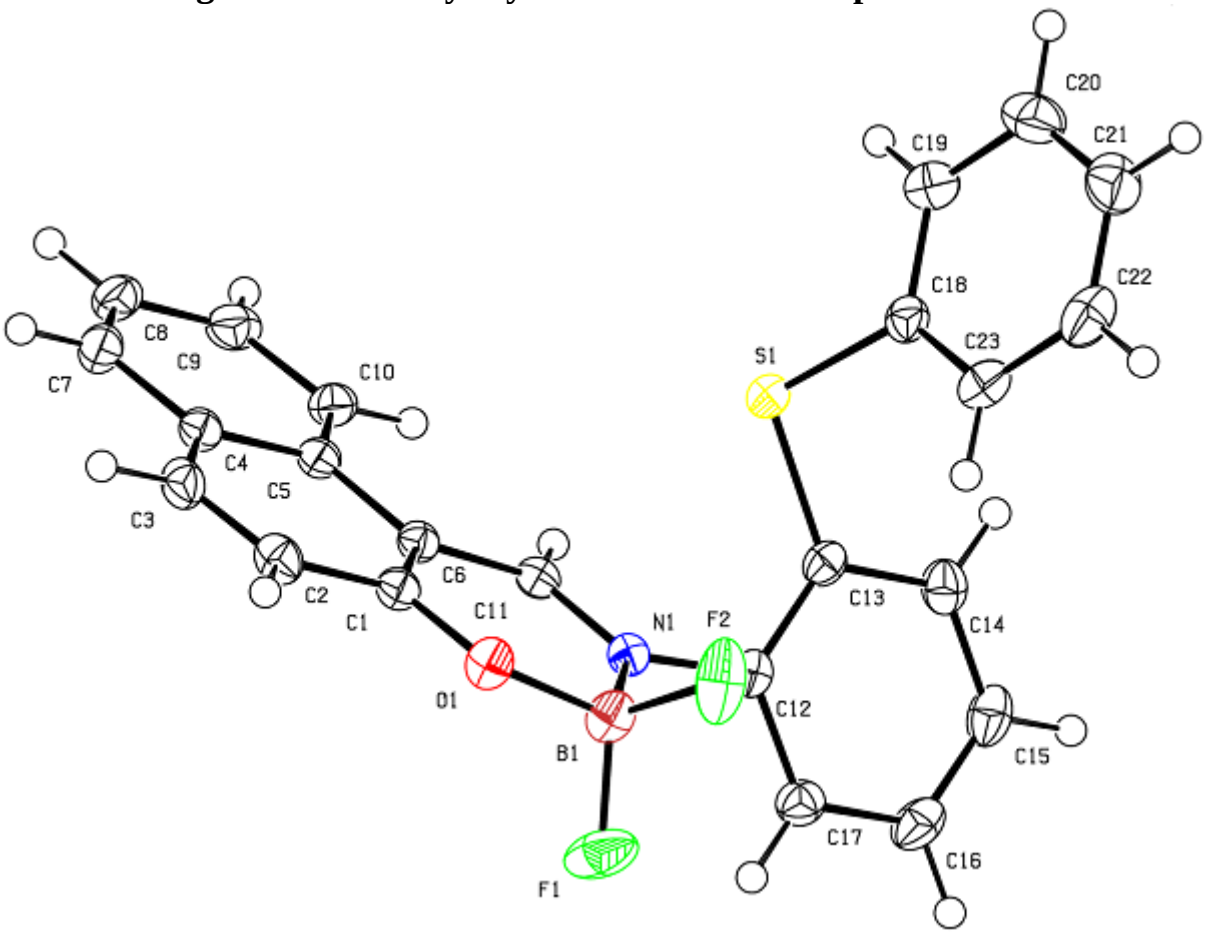


Figure S11.UV-Vis absorption spectra of **SB-1** (10 µM) in 100 mM Phosphate buffer (pH 7.54) in the presence of various RNS and ROS such as NO, H_2O_2, ClO^-, NO_3^-, NO_2^-, ROO^-, ONOO, O_2, t-BuOOH, ascorbic acid, GSH and HO^-(1mM) .

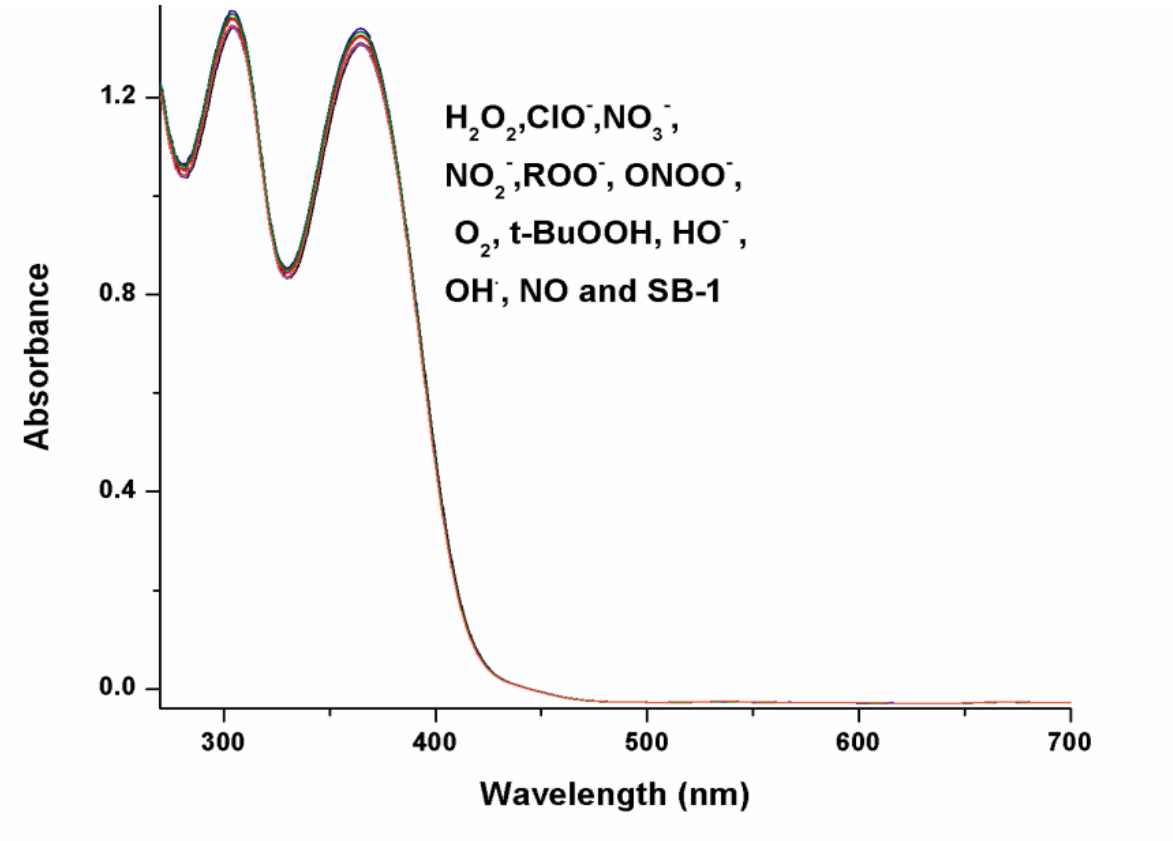


Figure S12. UV-Vis absorption spectra of **SB-2** (10 μM) in 100 mM phosphate buffer (pH 7.54) in the presence of various RNS and ROS such as NO, H_2O_2, ClO^-, NO_3^-, NO_2^-, ROO^-, ONOO, O_2, t-BuOOH, ascorbic acid, GSH and HO^- (1mM) .

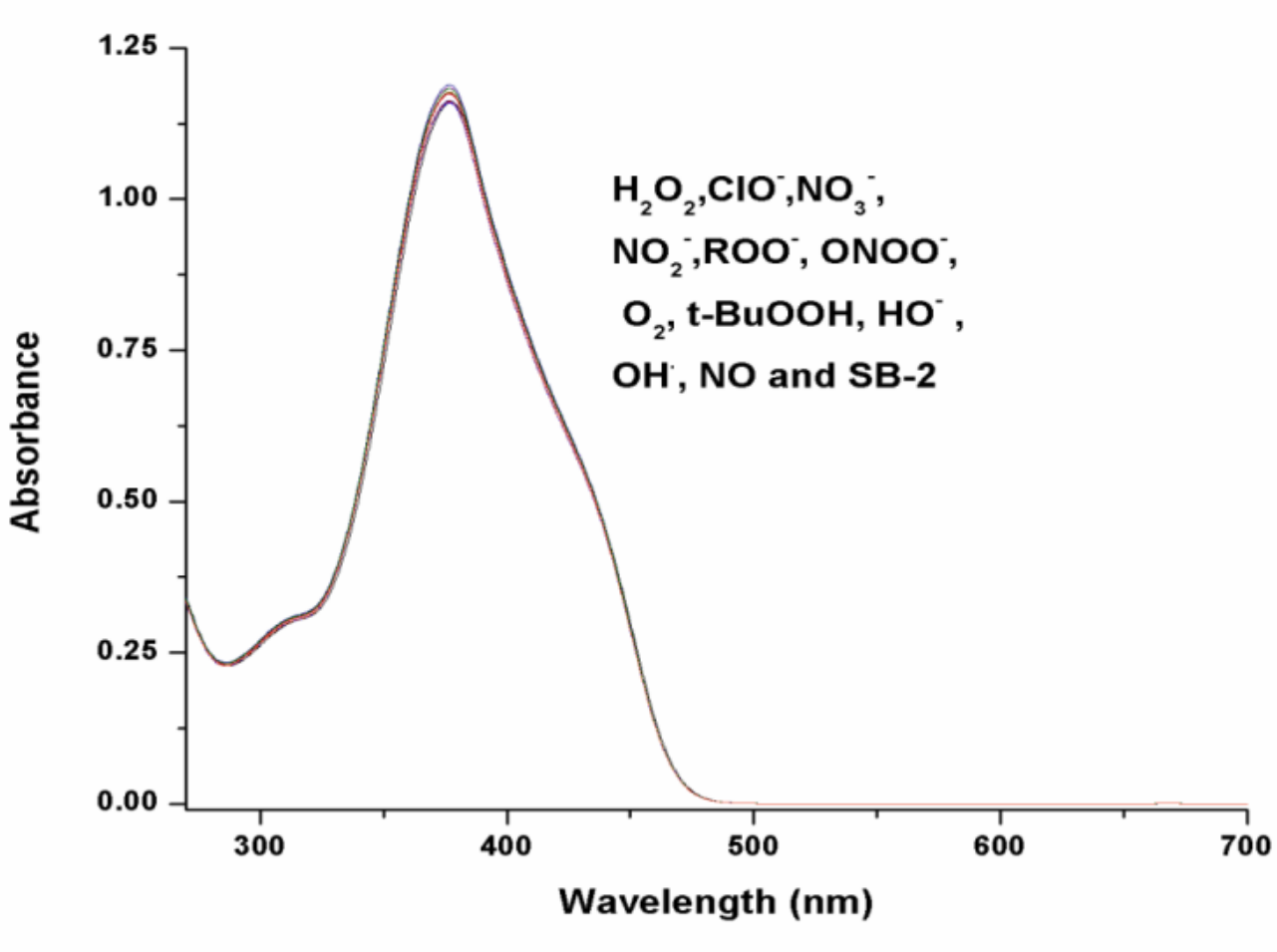


Figure S13. Time dependent fluorescence response of **SB-1** with H_2O_2.

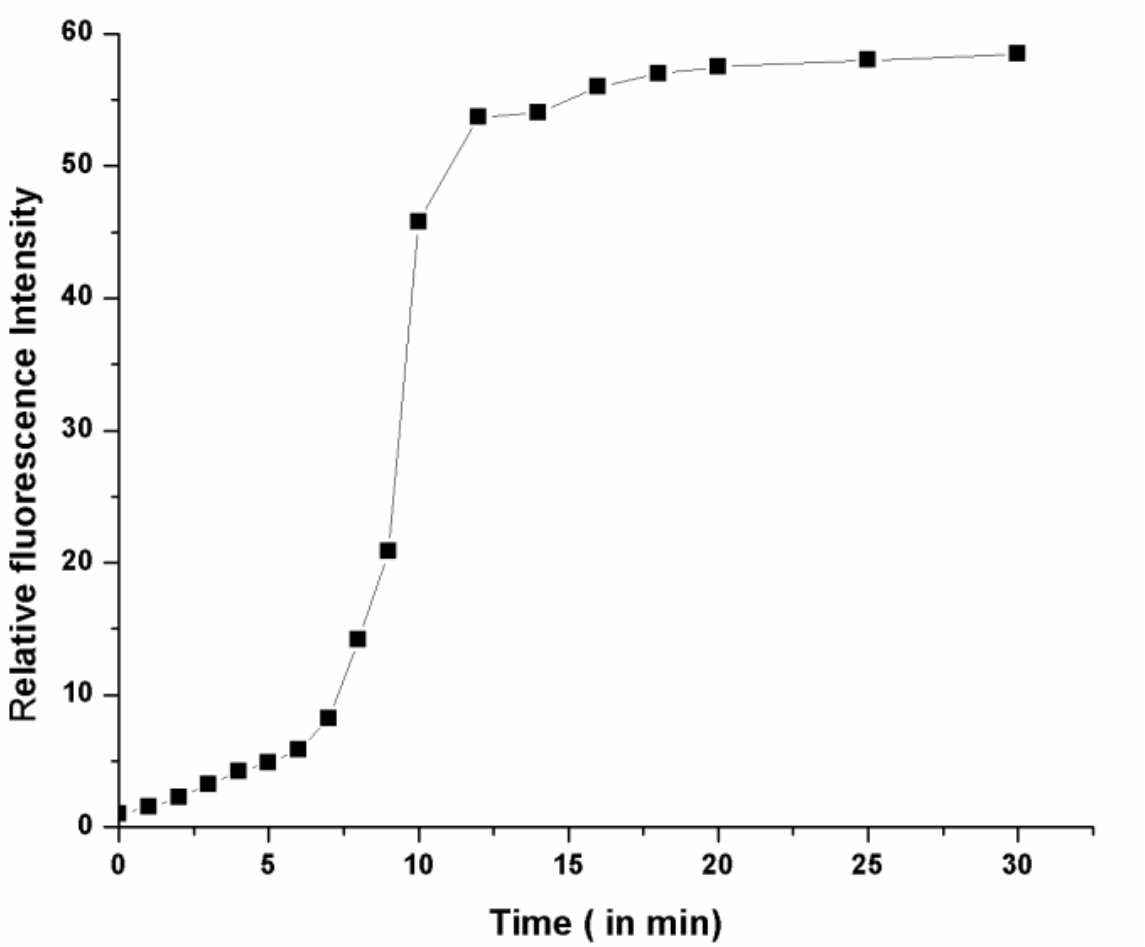


Figure S14. Time dependent fluorescence response of **SB-2** with H_2O_2.

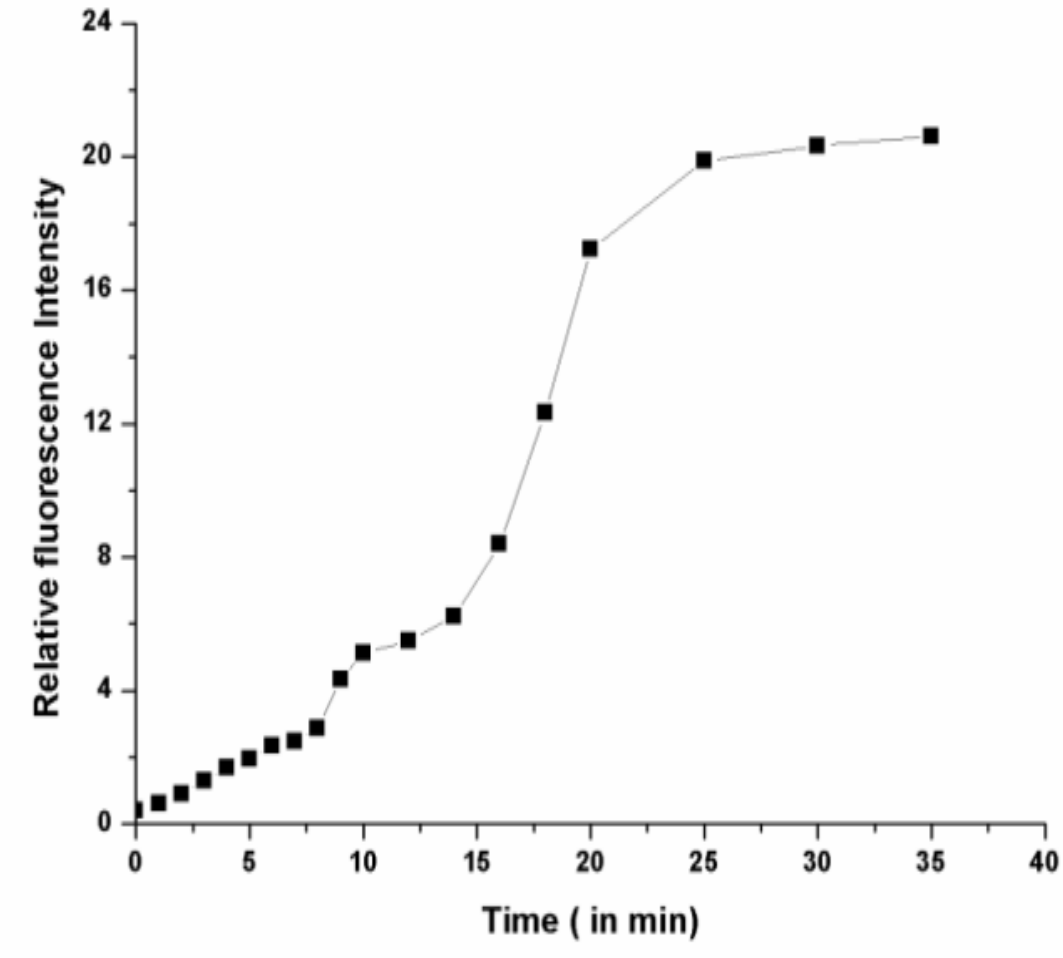


Figure S15. Linearity plot of change of fluorescence intensity at λ_{Emm} = 503 *vs* concentration of hydrogen peroxide added to the probe **SB-1**.

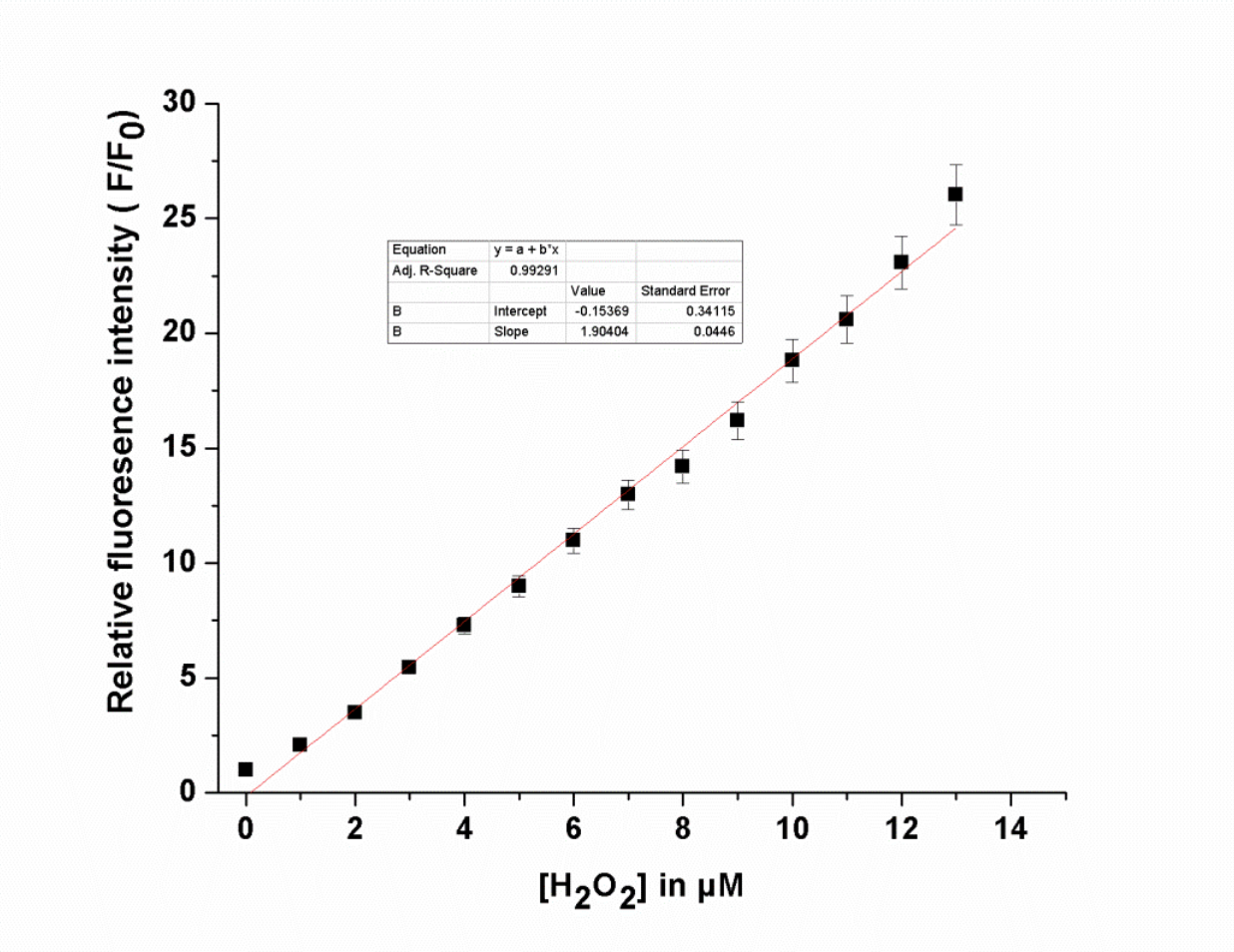


Figure S16. Linearity plot of change of fluorescence intensity at λ_{Emm} = 510 *vs* concentration of Hydrogen peroxide added to the probe **SB-2**.

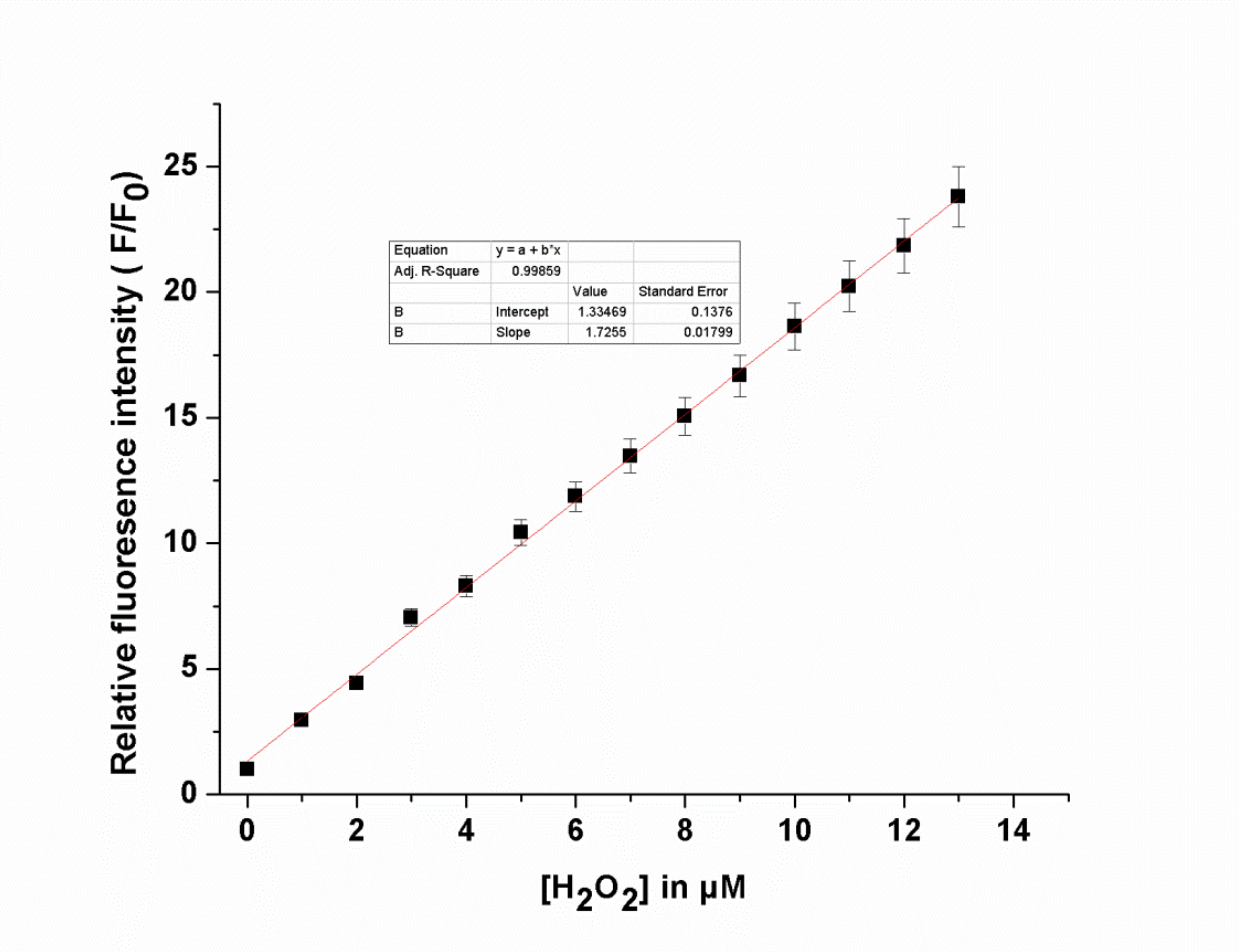


Figure S17. Effect of pH on the fluorescence of **SB-1** and SB-2

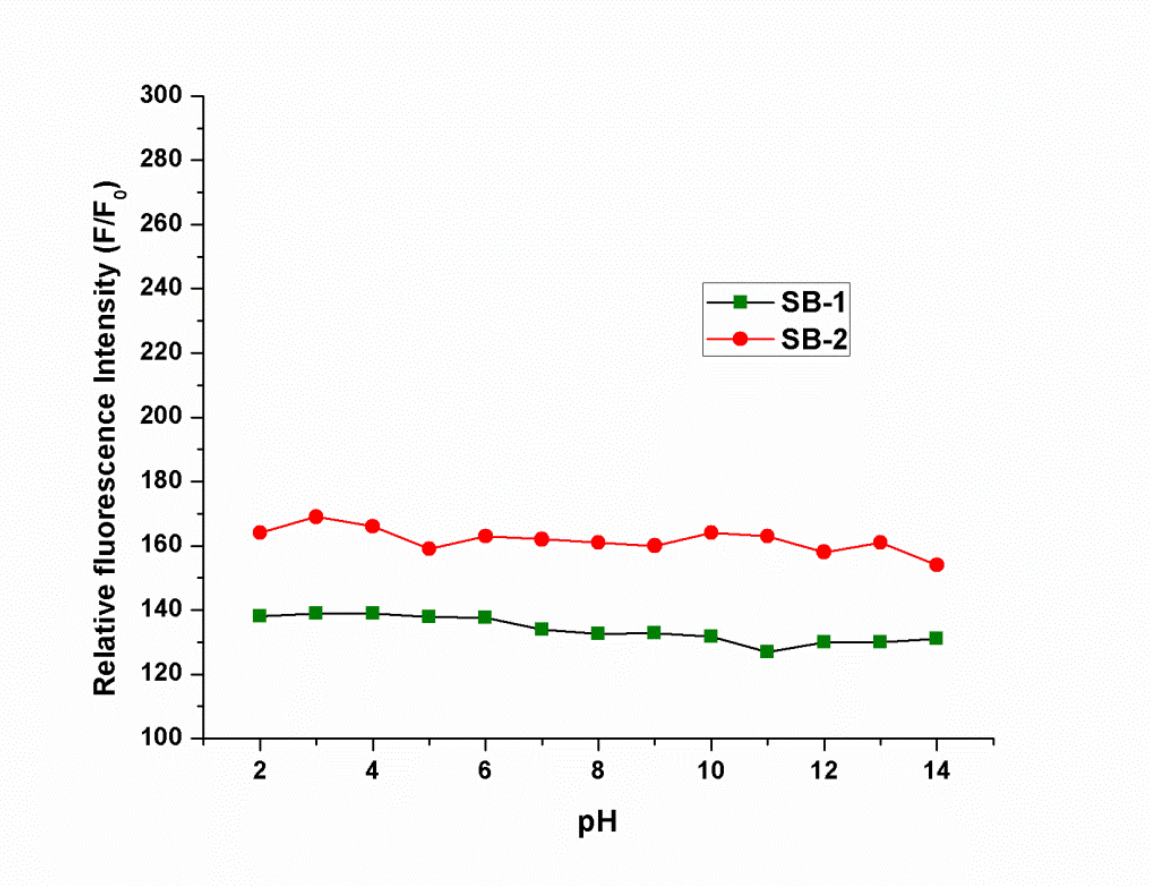


Figure S18. Cell viability assay- Plot of % of viable cells *vs* concentration of **SB-1** and **SB-2:**

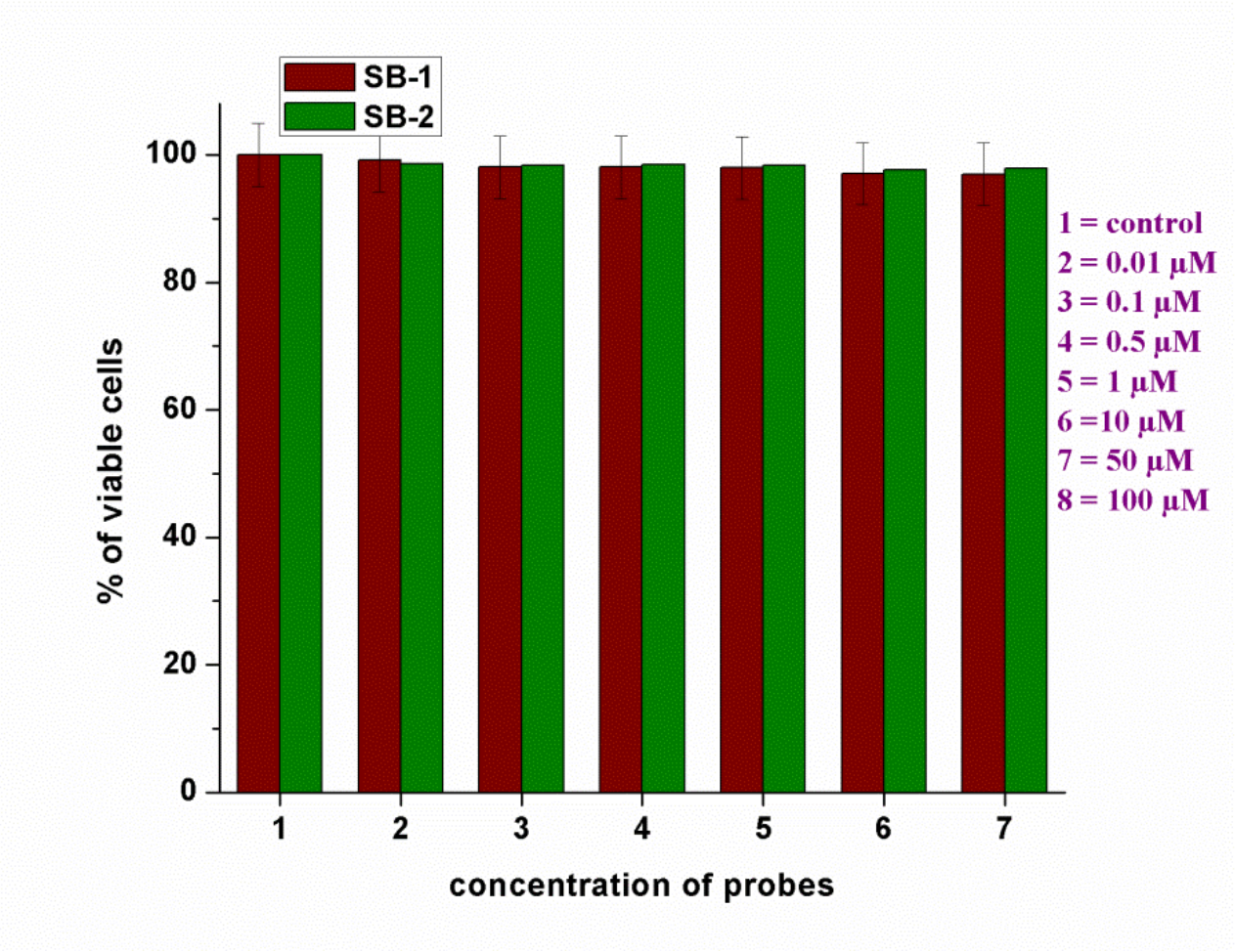
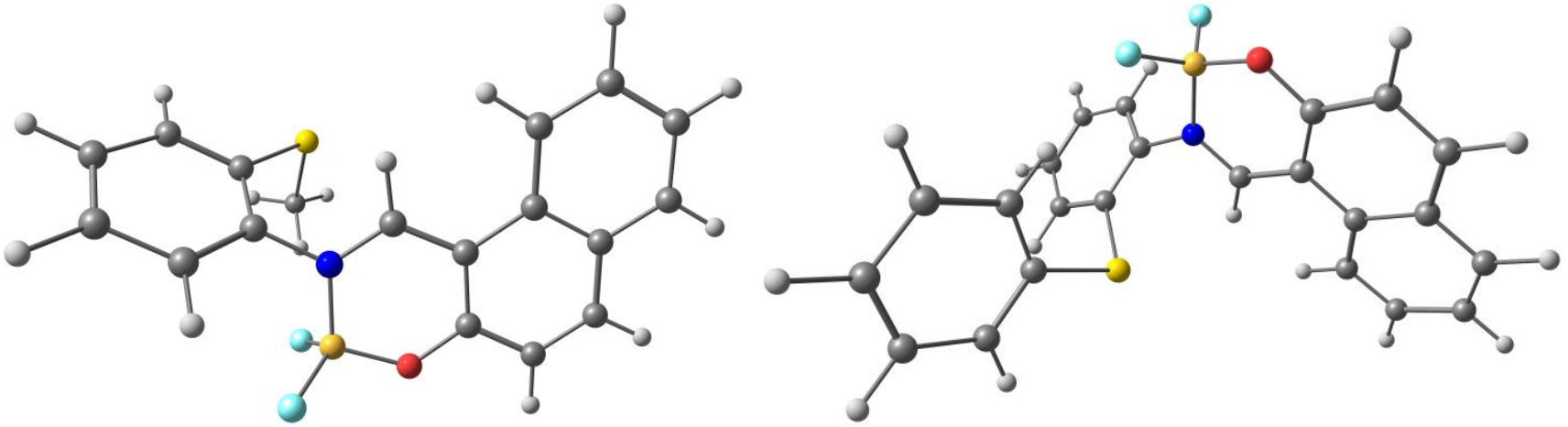
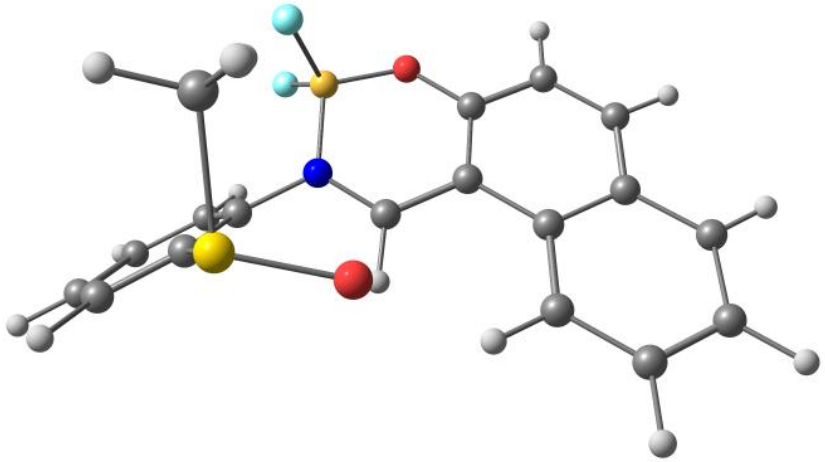


Figure S19. Optimized geometries of **SB-1** and **SB-2**

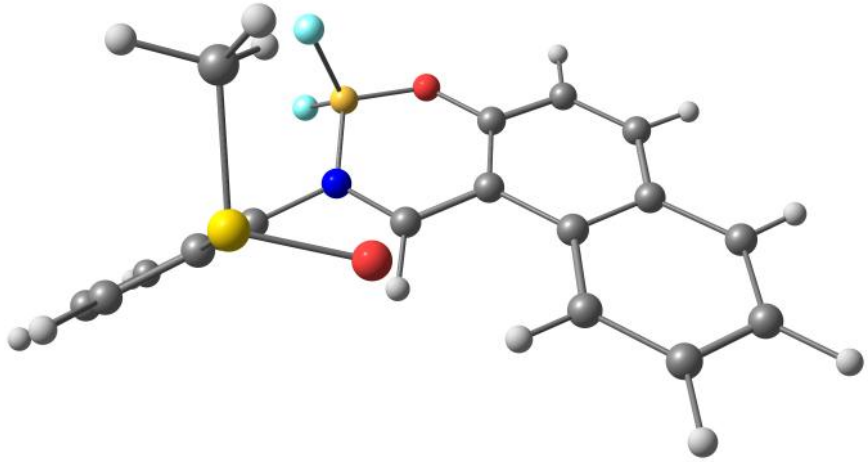


SB-1 **SB-2**

Figure S20. Optimized geometries of oxidized forms of **SB-1** and **SB-2**



Oxidized form of SB-1



Oxidized form of SB-2

Table S2: The comparison of the present H_2O_2 detection methods with the existing methods.

Boron based Probe	***Emission Maximum (λ in nm)***	***Turn on/off (fluorescence)***	***Detection limit***	***Ref***
Peroxy Lucifer	475	ON	Ratiometric	1
Cyaninefluorochrome	715	ON	1 μM	2
Mitochondria peroxy yellow 1	540	ON	NA	3
Ratio-Peroxyfluor-1	464	NA	Ratiometric	4
Prototype probe	440	NA	0.1 ~ 5 μM	5
MitoBoronic acid	NA	NA	1 μM	6
Tetraphenylethylene-Borolane (TPE-BO)	500	ON	0.52 μM	7
Naphthalimide fluorophore	528	ON	NA	8
Carbazole-Quinoline cationic based	527	ON	0.04 μM	9
meso-(4-pyridinyl)-substituted BODIPY	520	ON	0.1 - 40 μM	10
Boranil Dye **SB-1/SB-2**	503/510	ON	70.27 nM /31.27 nM	Present work

NA = Not available

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