

Supporting Information

Hypochlorite promoted inhibition of photo-induced electron transfer in phenothiazine-borondipyrromethene donor-acceptor dyad: A cost-effective and metal-free “turn-on” fluorescent chemosensor for hypochlorite

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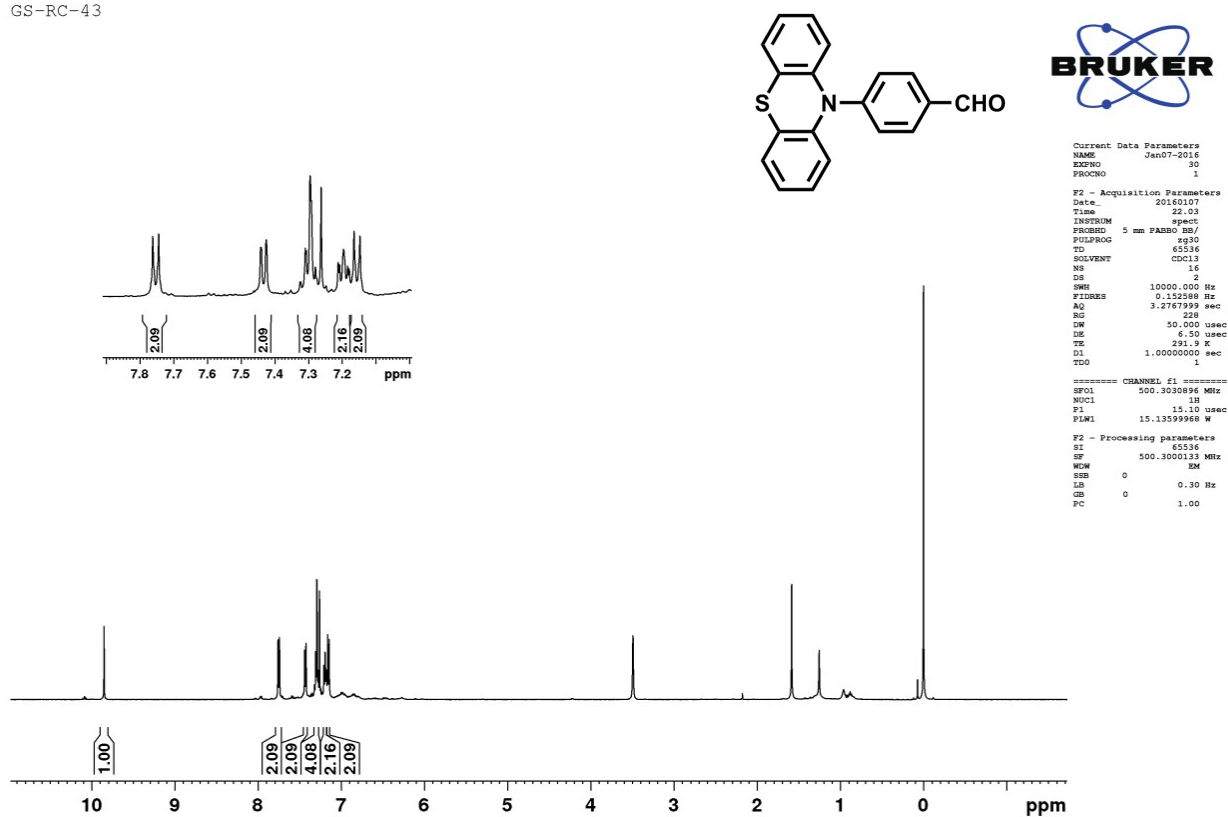
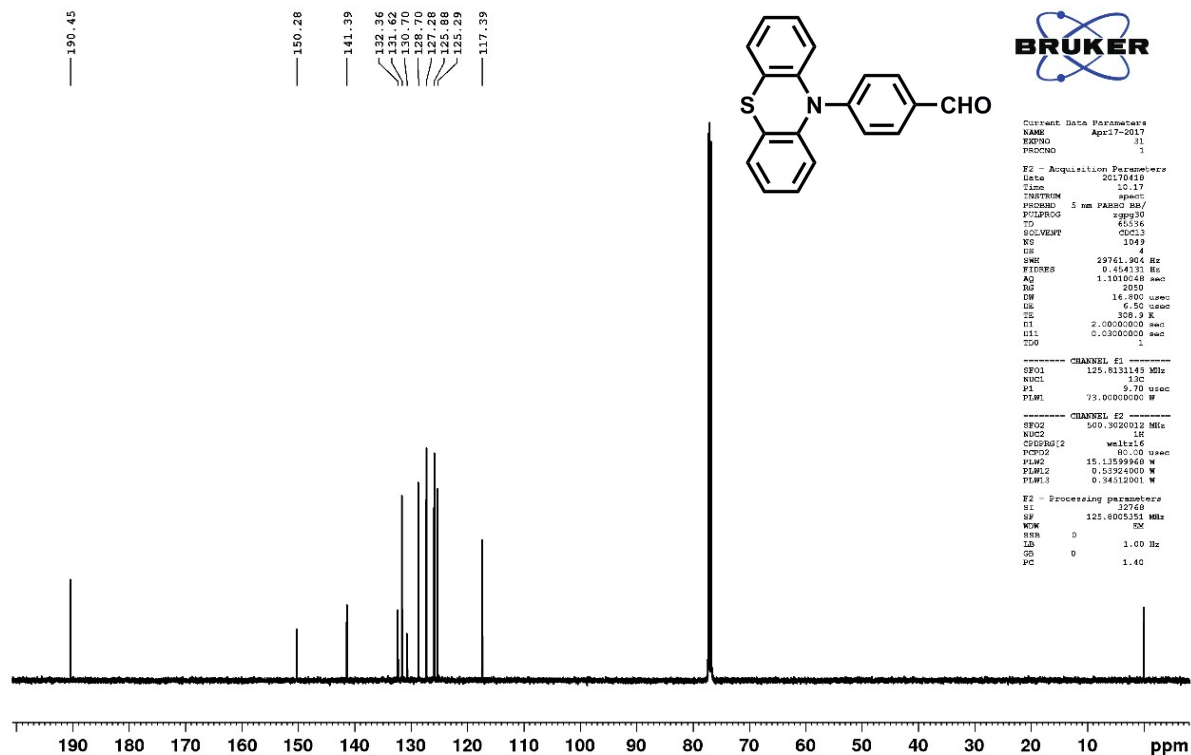
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Supporting Information

Table of Contents		Page No.
Fig. S1	^1H NMR spectrum of 10-(4-Formylphenyl)phenothiazine in CDCl_3 .	S3
Fig. S2	^{13}C NMR spectrum of 10-(4-Formylphenyl)phenothiazine in CDCl_3 .	S3
Fig. S3	^1H NMR spectrum of probe 1 in CDCl_3 .	S4
Fig. S4	^{13}C NMR spectrum of probe 1 in CDCl_3 .	S4
Fig. S5	ESI-MS spectrum of probe 1 in acetonitrile.	S5
Fig. S6	Absorbance changes in 1 (4.6×10^{-6} M) upon addition of increasing amounts of NaOCl in PBS buffer: ACN (9:1 v/v).	S5
Fig. S7	Solutions of probe 1 in PBS buffer with increasing amounts of NaOCl in presence of (a) visible light and (b) UV-light of $\lambda = 365$ nm.	S6
Fig. S8	Fluorescence changes in { 1 (2.3×10^{-6} M) + NaOCl (4.54×10^{-6} M)} w.r.t. time (in minutes) in PBS buffer: ACN (9:1 v/v).	S6
Fig. S9	Fluorescence changes of 1 (2.3×10^{-6} M) upon addition of increasing amounts of H_2O_2 in PBS buffer:ACN (9:1 v/v).	S7
Fig S10	Fluorescence changes in 1 (2.3×10^{-6} M) upon addition of increasing amounts of $\cdot\text{OH}$ in PBS buffer:ACN (9:1 v/v).	S7
Fig. S11	Fluorescence changes in 1 (2.3×10^{-6} M) upon addition of increasing amounts of $^1\text{O}_2$ in PBS buffer:ACN (9:1 v/v).	S8
Fig. S12	Fluorescence changes in 1 (2.3×10^{-6} M) upon addition of increasing amounts of O_2^- in PBS buffer:ACN (9:1 v/v).	S8
Fig. S13	Fluorescence changes in 1 (2.3×10^{-6} M) upon addition of increasing amounts of HCl in PBS buffer:ACN (9:1 v/v).	S9
Fig. S14	S \cdots N distance (brown), dihedral angle around S \cdots N axis (black), and natural bond orbital (NBO) charges (blue) of N, S, and O of (a) BODIPY, (b) phenyl phenothiazine and its oxidized products i.e., sulfoxide and sulfone, and (c) dyads 1 , 1+O , and 1+2O calculated using triple hybrid B3LYP method with 6-311+G* set.	S10
Fig. S15	Molecular Electron Potential maps (MEPs) and frontier orbitals of 1 , (1+O), and (1+2O) calculated using triple hybrid B3LYP method with 6-311 +G* set.	S11

Supporting Information

GS-RC-43

Fig. S1. ^1H NMR spectrum of 10-(4-Formylphenyl)phenothiazine in CDCl_3 .Fig. S2. ^{13}C NMR spectrum of 10-(4-Formylphenyl)phenothiazine in CDCl_3 .

Supporting Information

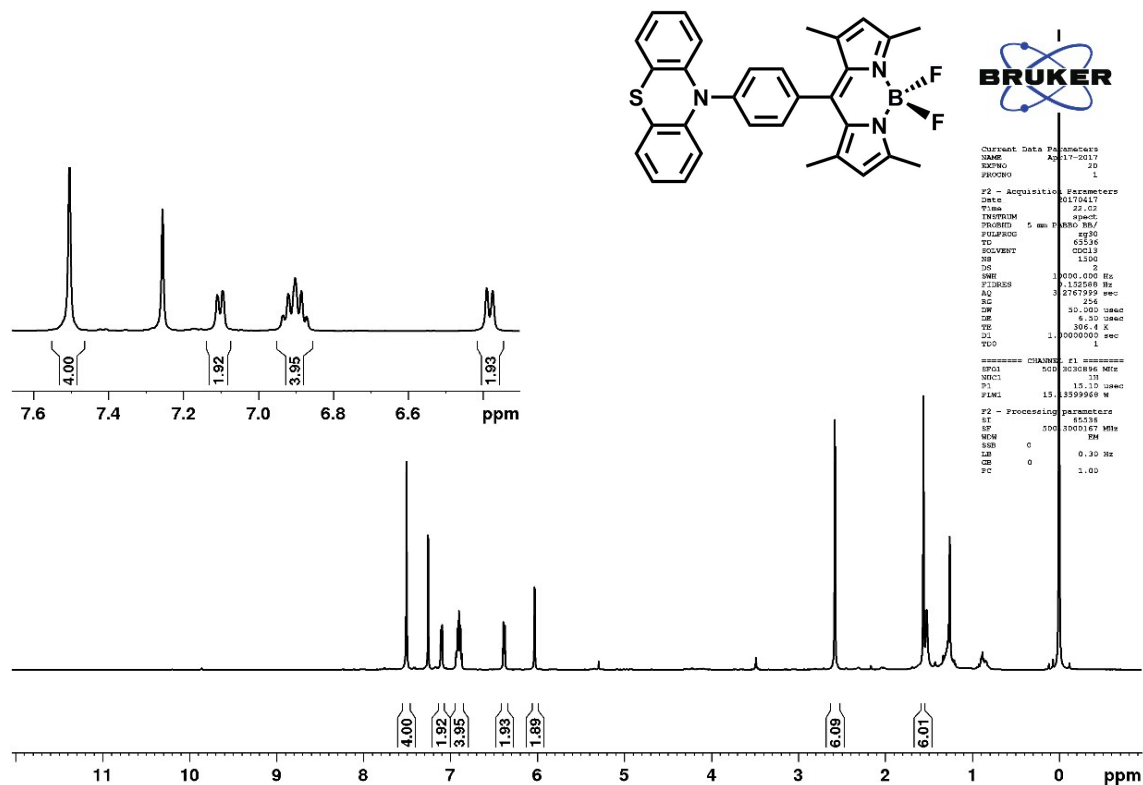


Fig. S3. ¹H NMR spectrum of probe 1 in CDCl₃.

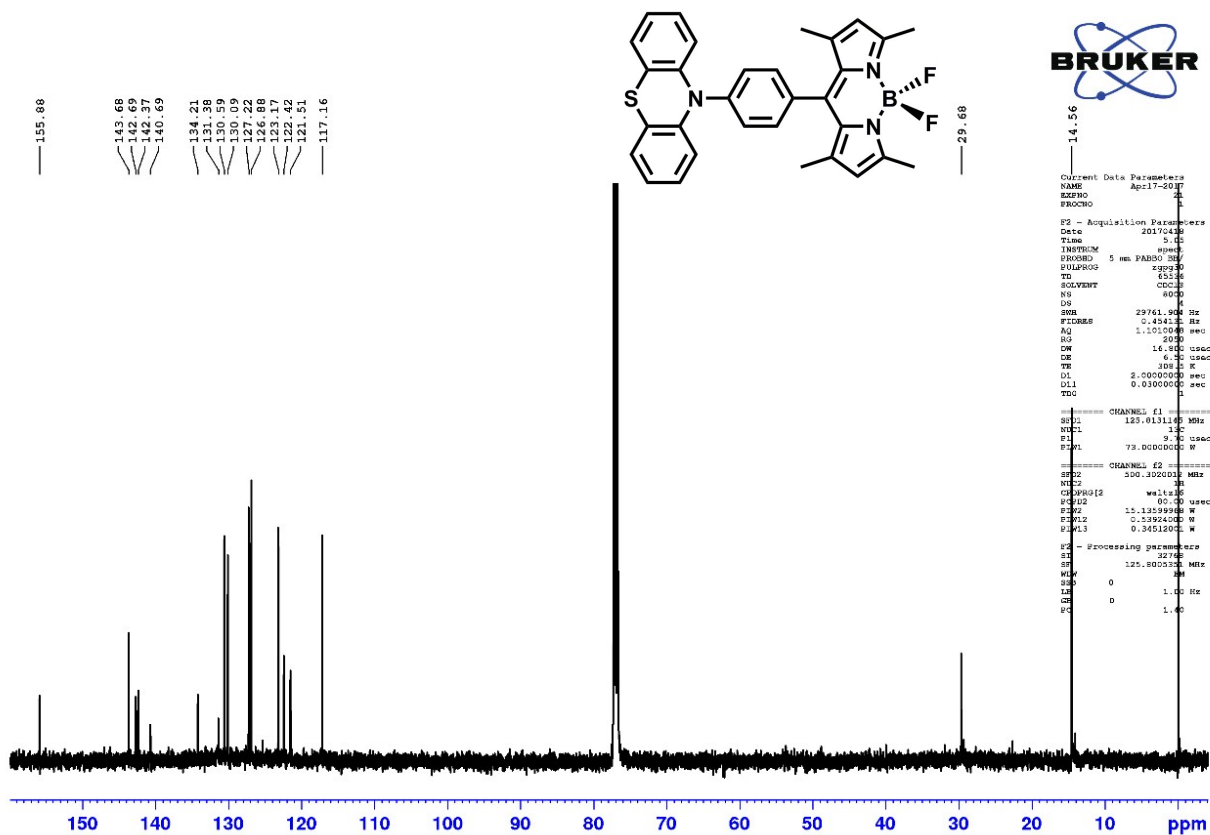


Fig. S4. ¹³C NMR spectrum of probe 1 in CDCl₃.

Supporting Information

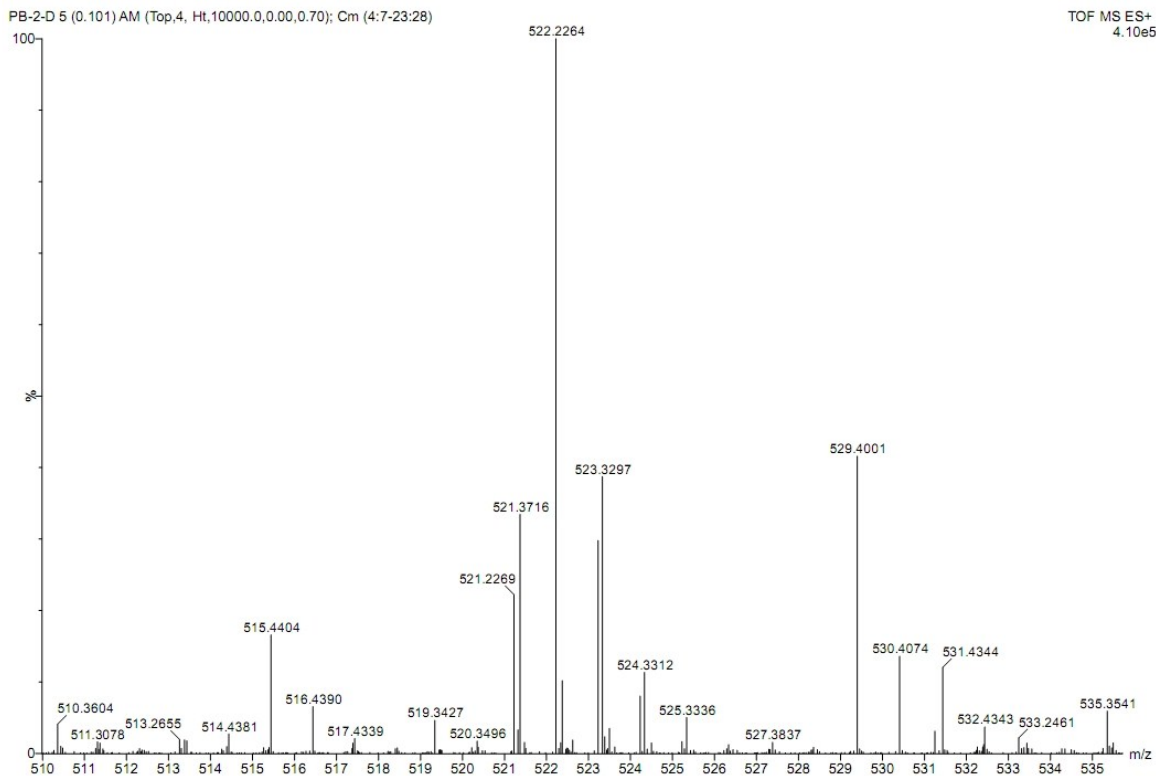


Fig. S5. ESI-MS spectrum of probe **1** in acetonitrile.

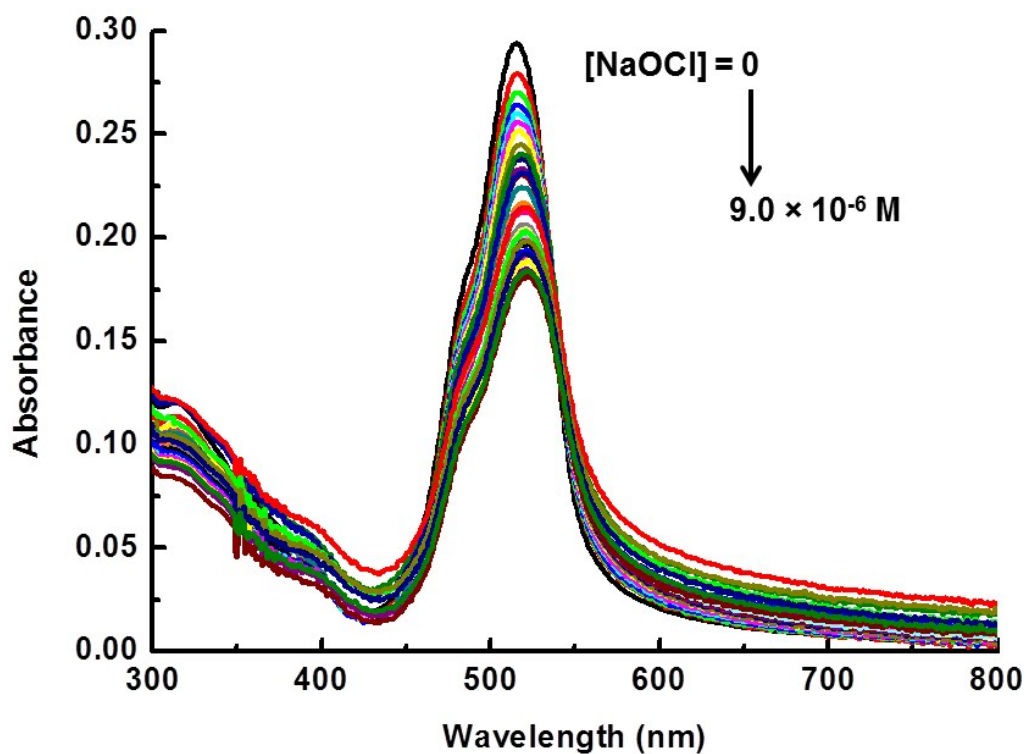


Fig. S6: Absorbance changes in **1** (4.6×10^{-6} M) upon addition of increasing amounts of NaOCl in PBS buffer: ACN (9:1 v/v).

Supporting Information

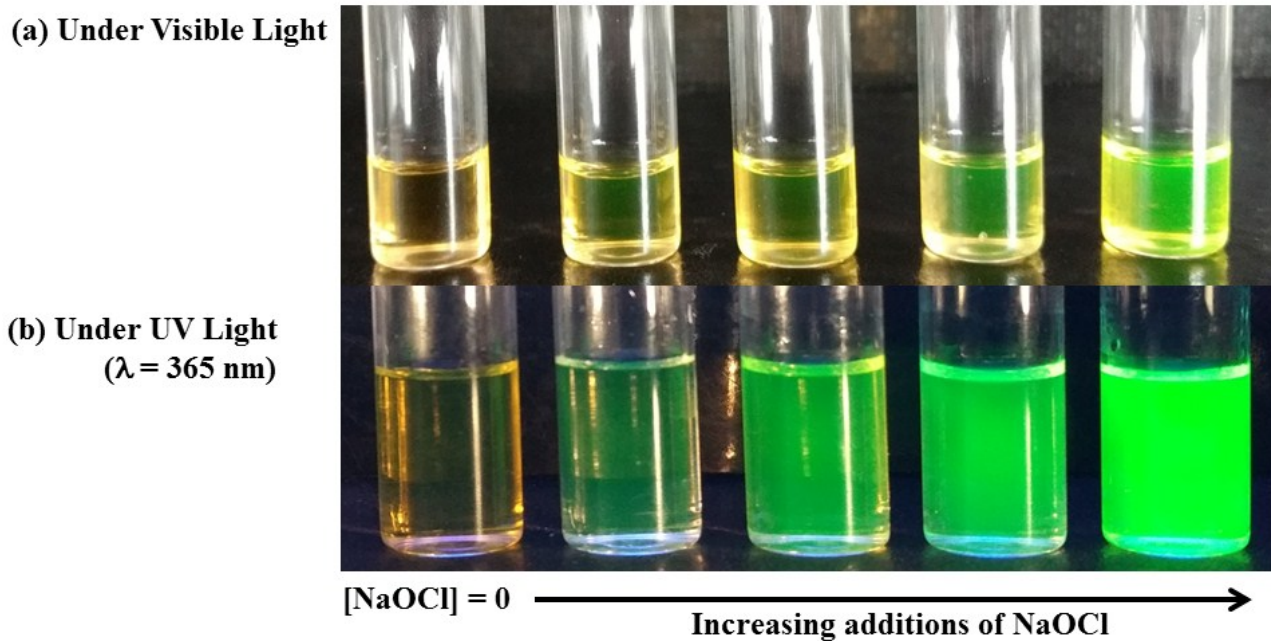


Fig. S7. Solutions of probe **1** in PBS buffer with increasing amounts of NaOCl in presence of (a) visible light and (b) UV-light of $\lambda = 365$ nm.

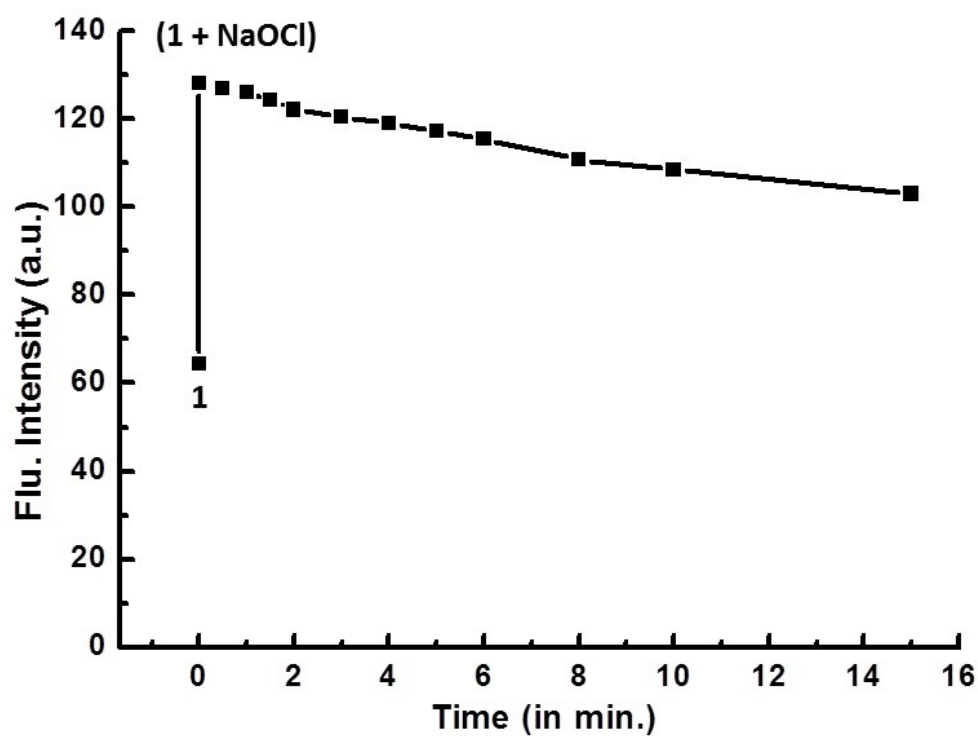


Fig. S8: Fluorescence changes in {**1** (2.3×10^{-6} M) + NaOCl (4.54×10^{-6} M)} w.r.t. time (in minutes) in PBS buffer:ACN (9:1 v/v).

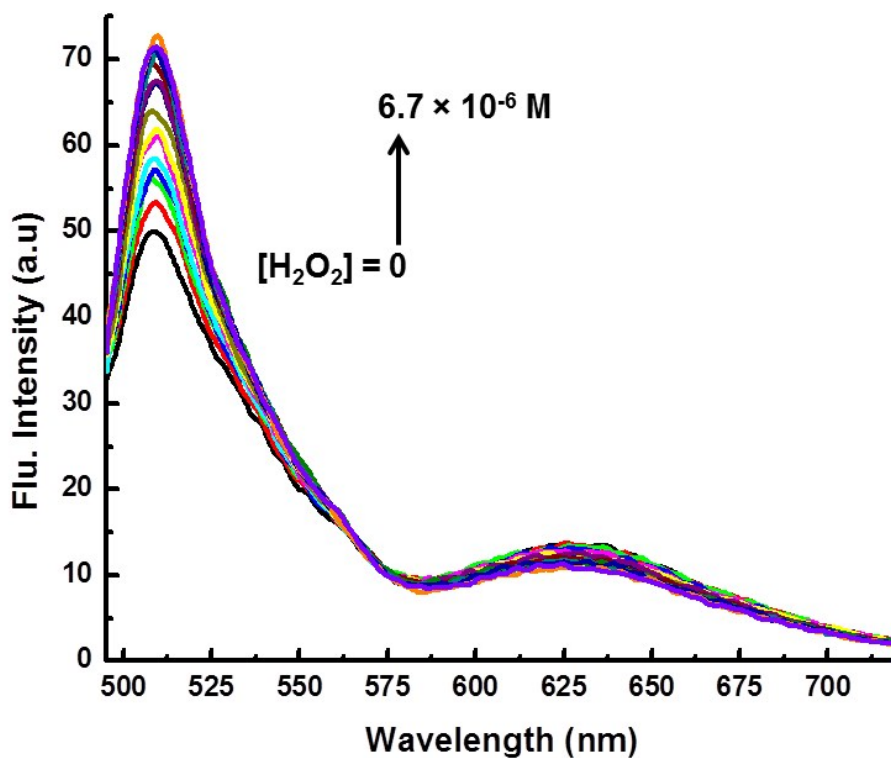
Supporting Information

Fig. S9: Fluorescence changes of **1** (2.3×10^{-6} M) upon addition of increasing amounts of H₂O₂ in PBS buffer:ACN (9:1 v/v).

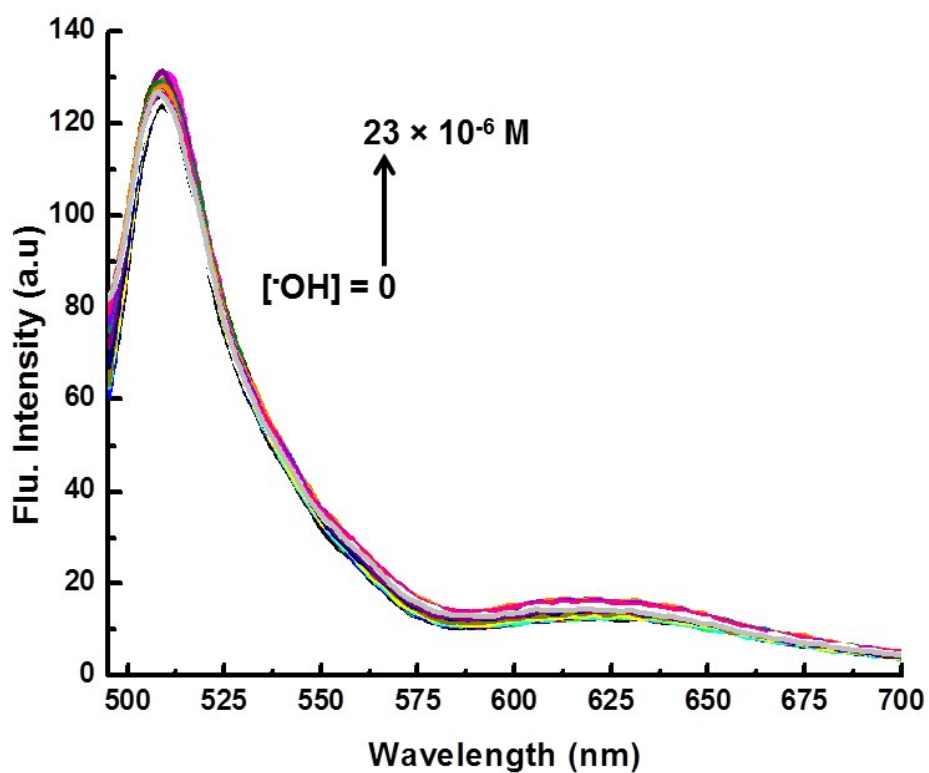


Fig. S10: Fluorescence changes in **1** (2.3×10^{-6} M) upon addition of increasing amounts of ·OH in PBS buffer:ACN (9:1 v/v).

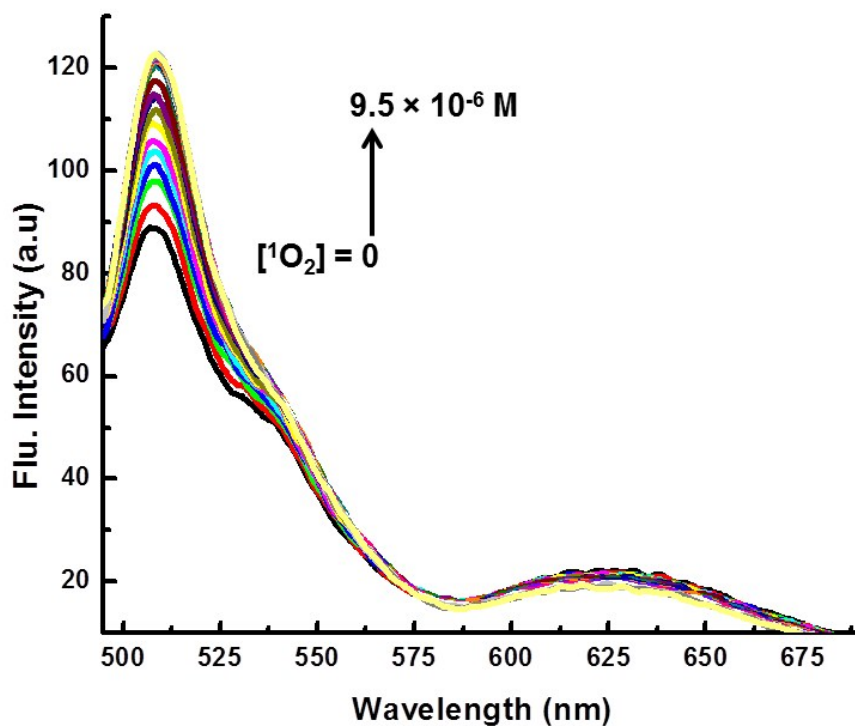
Supporting Information

Fig. S11: Fluorescence changes in **1** ($2.3 \times 10^{-6} \text{ M}$) upon addition of increasing amounts of $^1\text{O}_2$ in PBS buffer:ACN (9:1 v/v).

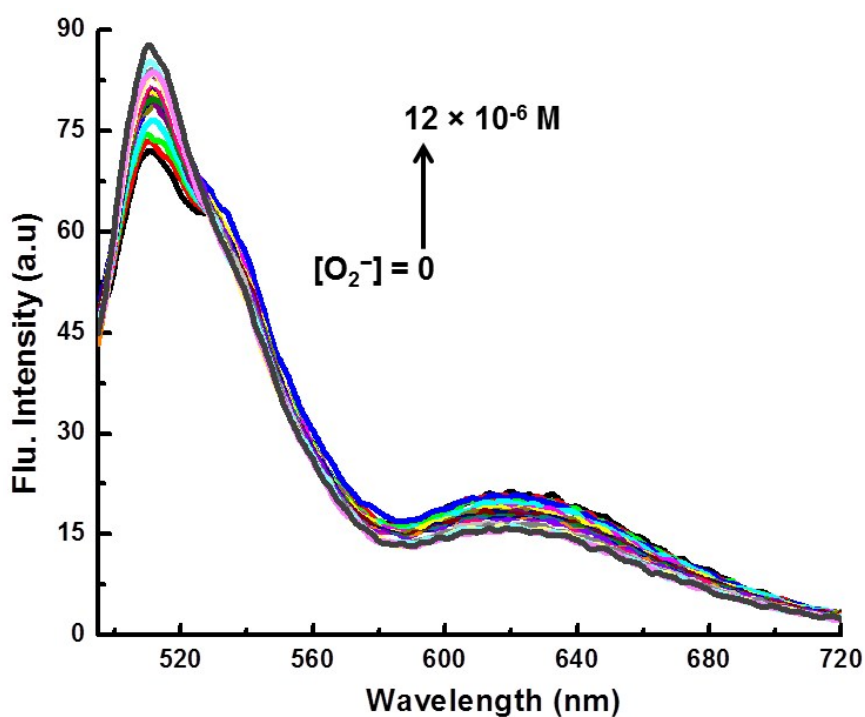


Fig. S12: Fluorescence changes in **1** ($2.3 \times 10^{-6} \text{ M}$) upon addition of increasing amounts of O_2^- in PBS buffer:ACN (9:1 v/v).

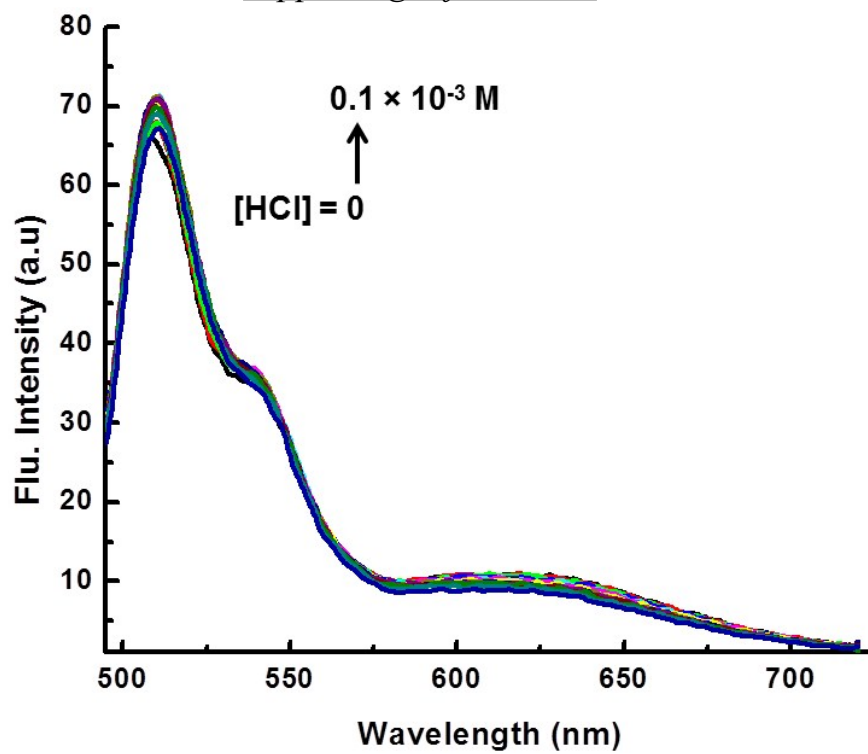
Supporting Information

Fig. S13: Fluorescence changes in **1** ($2.3 \times 10^{-6} M$) upon addition of increasing amounts of HCl in PBS buffer:ACN (9:1 v/v).

Supporting Information

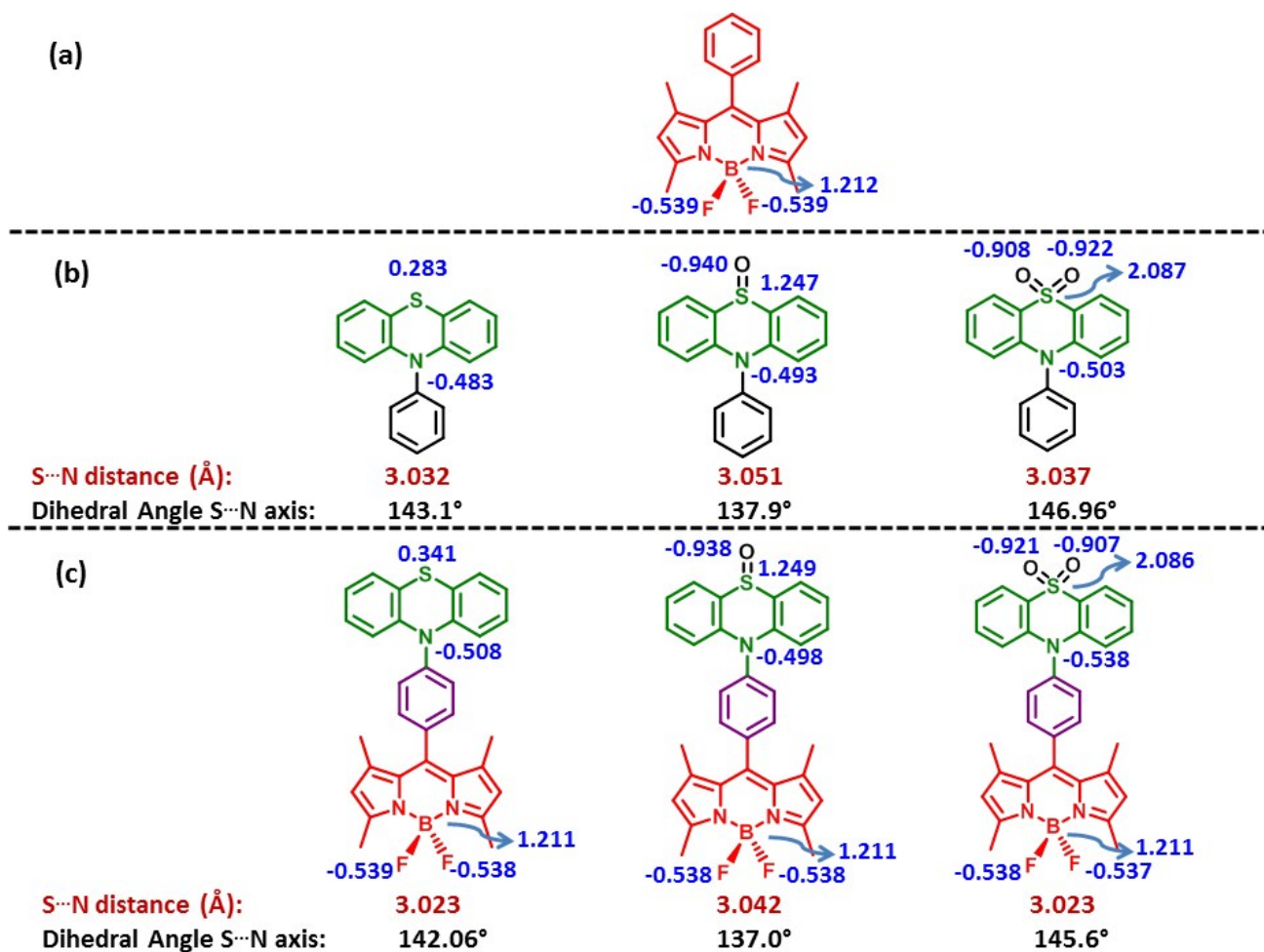


Fig. S14. S...N distance (**brown**), dihedral angle around S...N axis (**black**), and natural bond orbital (NBO) charges (**blue**) of N, S, and O of (a) BODIPY, (b) phenyl phenothiazine and its oxidized products i.e., sulfoxide and sulfone, and (c) dyads **1**, **1+O**, and **1+2O** calculated using triple hybrid B3LYP method with 6-311+G* set.

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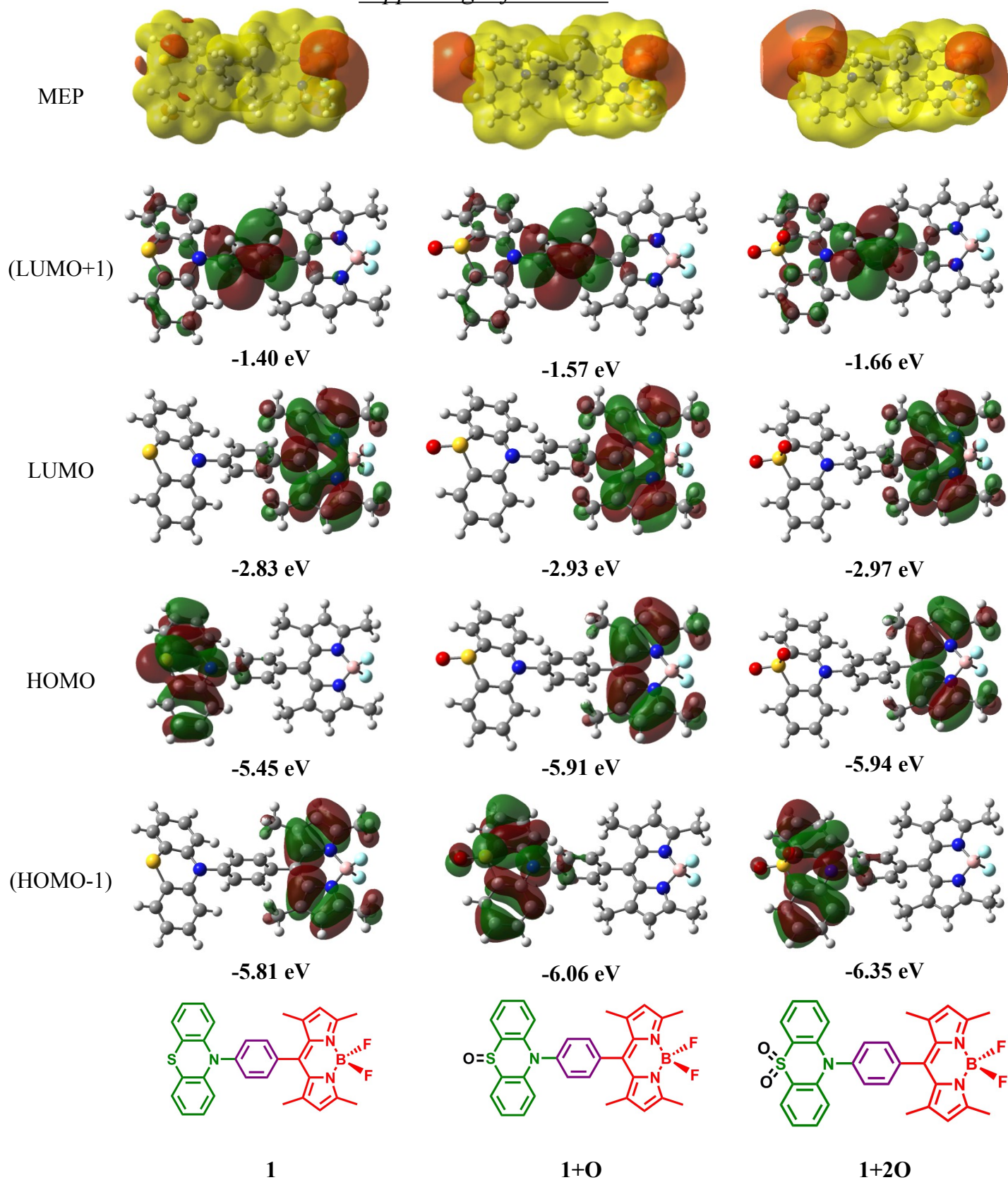


Fig. S15. Molecular Electrostatic Potential maps (MEPs) and frontier orbitals of **1**, (**1+O**), and (**1+2O**) calculated using triple hybrid B3LYP method with 6-311 +G* set.