

Supporting Information

Ratiometric detection of hypochlorite applying the restriction to 2-way-ESIPT : A Simple design for “naked-eye” tap water analysis

Shorter

Abhishek Manna and Shyamaprosad Goswami
Department of Chemistry, *Indian Institute of Engineering Science and Technology,*
Shibpur, West Bengal, India.

E-mail: spgoswamical@yahoo.com;

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1. Determination of fluorescence quantum yield:

Here, the quantum yield ϕ was measured by using the following equation,

$$\phi_x = \phi_s (F_x / F_s)(A_s / A_x)(n_x^2 / n_s^2)$$

Where,

X & S indicate the unknown and standard solution respectively, ϕ = quantum yield,

F = area under the emission curve, A = absorbance at the excitation wave length,

n = index of refraction of the solvent. Here ϕ measurements were performed using anthracene in ethanol as standard [$\phi = 0.27$] (error $\sim 10\%$).

The quantum yield of **BTHT** itself is 0.01 which changes into 0.65.

2. Calculation of detection limit:

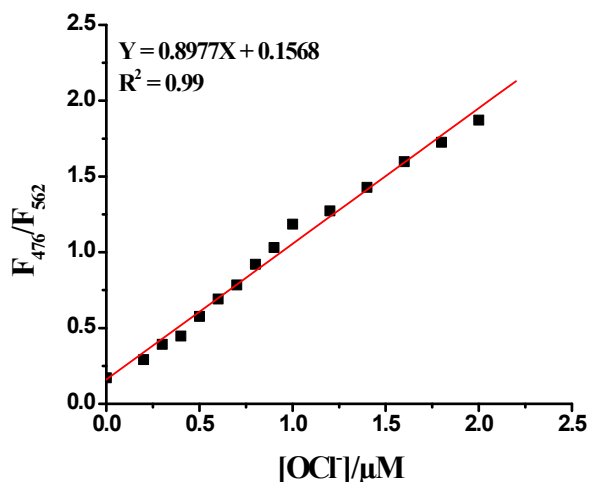


Fig. S1: Plot of intensity ratio (i.e. F_{476}/F_{562}) vs. $[OCl^-]$ in micromolar.

The detection limit DL of BTHT for OCl^- was determined from the following equation [S2]:

$DL = K * Sb1/S$. Where $K = 2$ or 3 (we take 2 in this case);

From the graph we get slope = 0.8977 , and $Sb1$ value is 0.066269 .

Thus using the formula we get the Detection Limit = 0.14μ M i.e. BTHT can detect OCl^- in this ppm level.

3. Fluorescence ratiometric responses of BTHT to OCl^- + metal ions anions and reactive species:

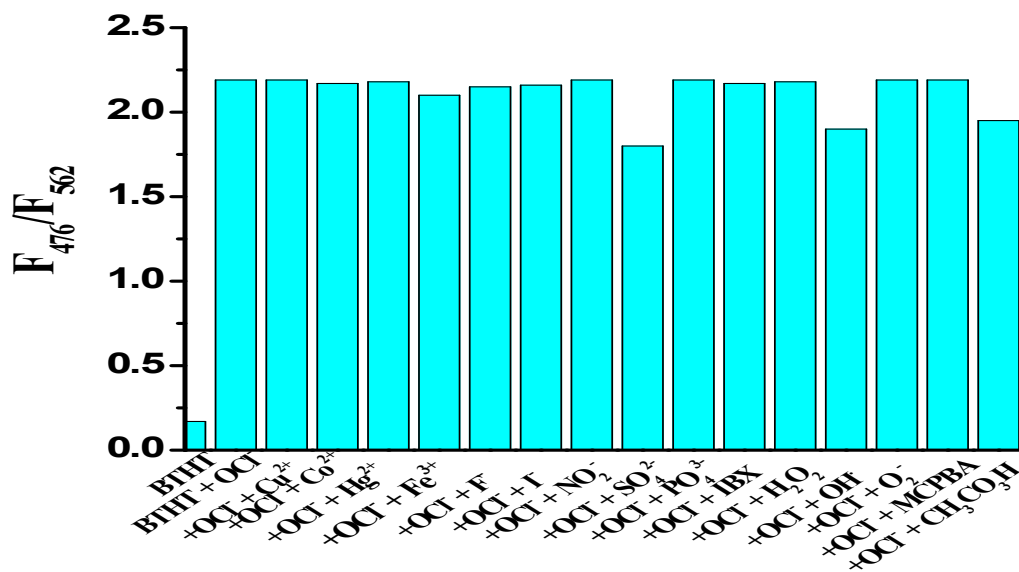
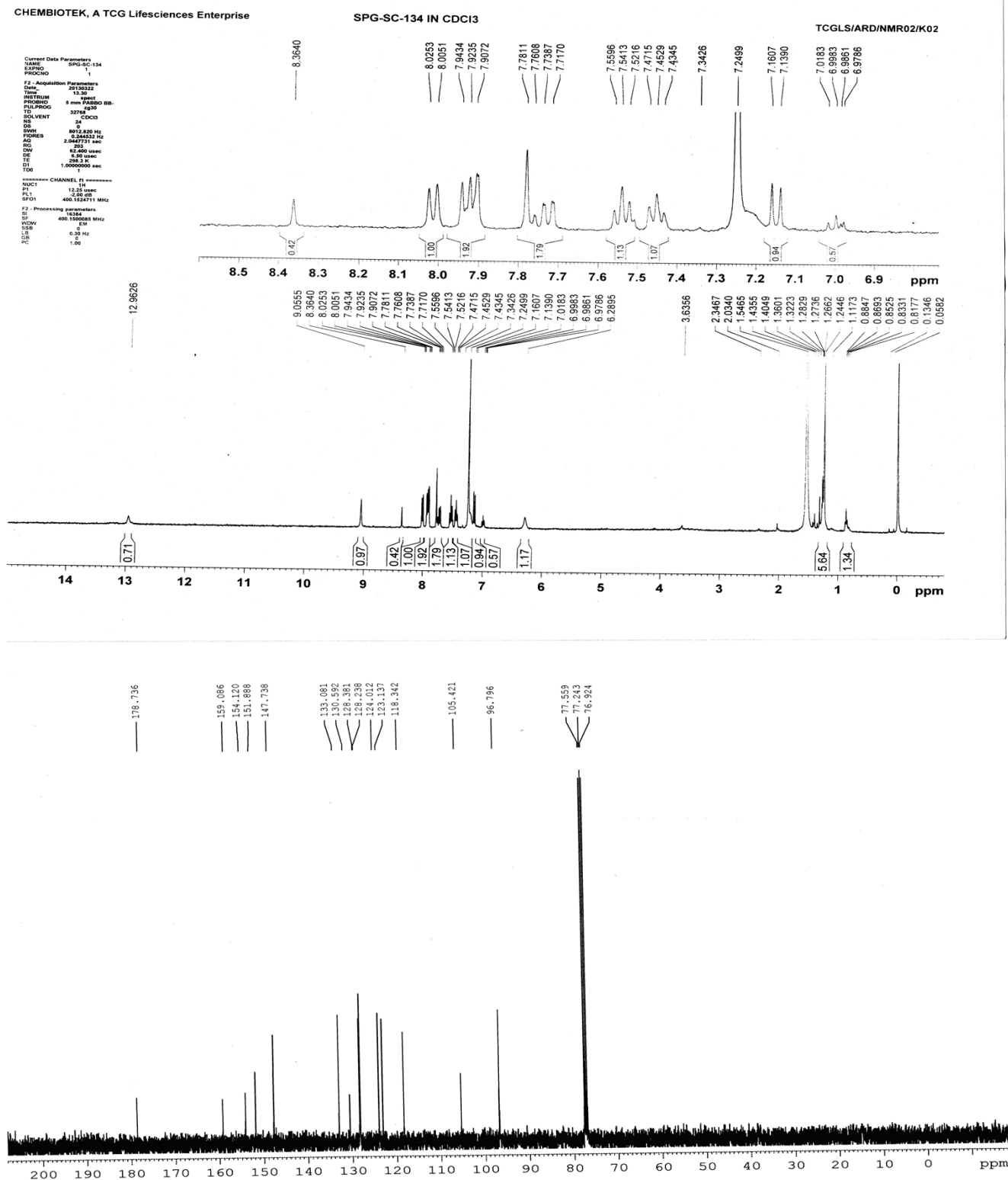


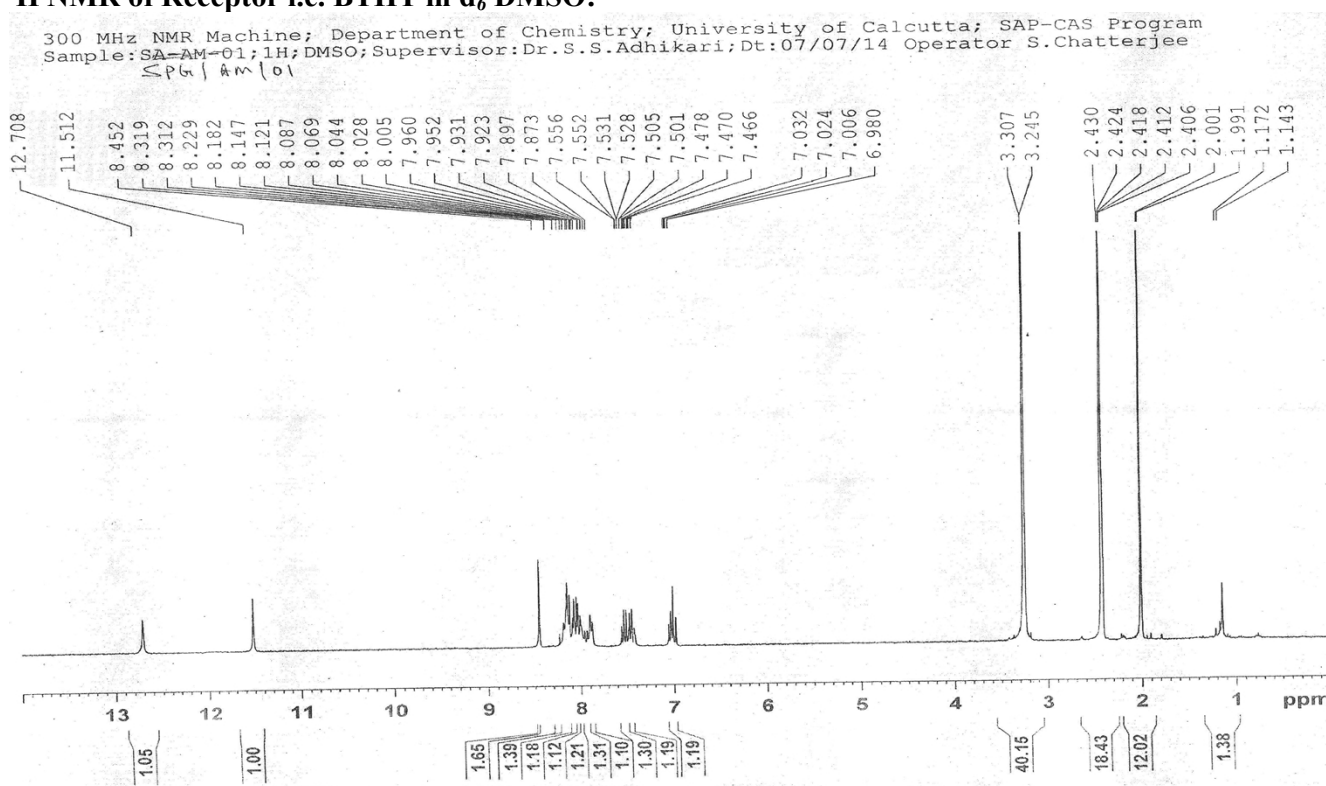
Fig S3: Fluorescence responses of BTHT ($c = 2.0 \times 10^{-5}$ M) to OCl^- (1 equiv) containing 10 equiv of various metal ions and anions ($\lambda_{\text{ex}} = 365$ nm).

4. ^1H NMR, ^{13}C NMR and ESI MS spectra of BTHT:

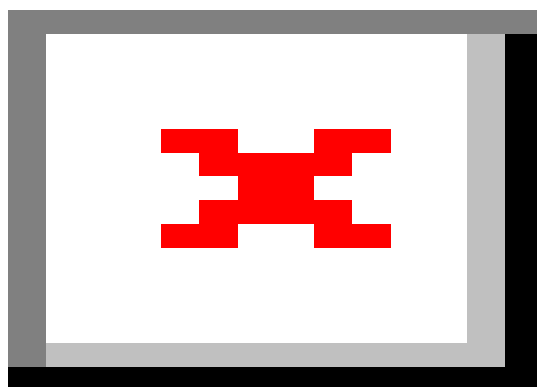
^1H NMR and ^{13}C NMR spectrum of Receptor i.e. BTHT in CDCl_3 :



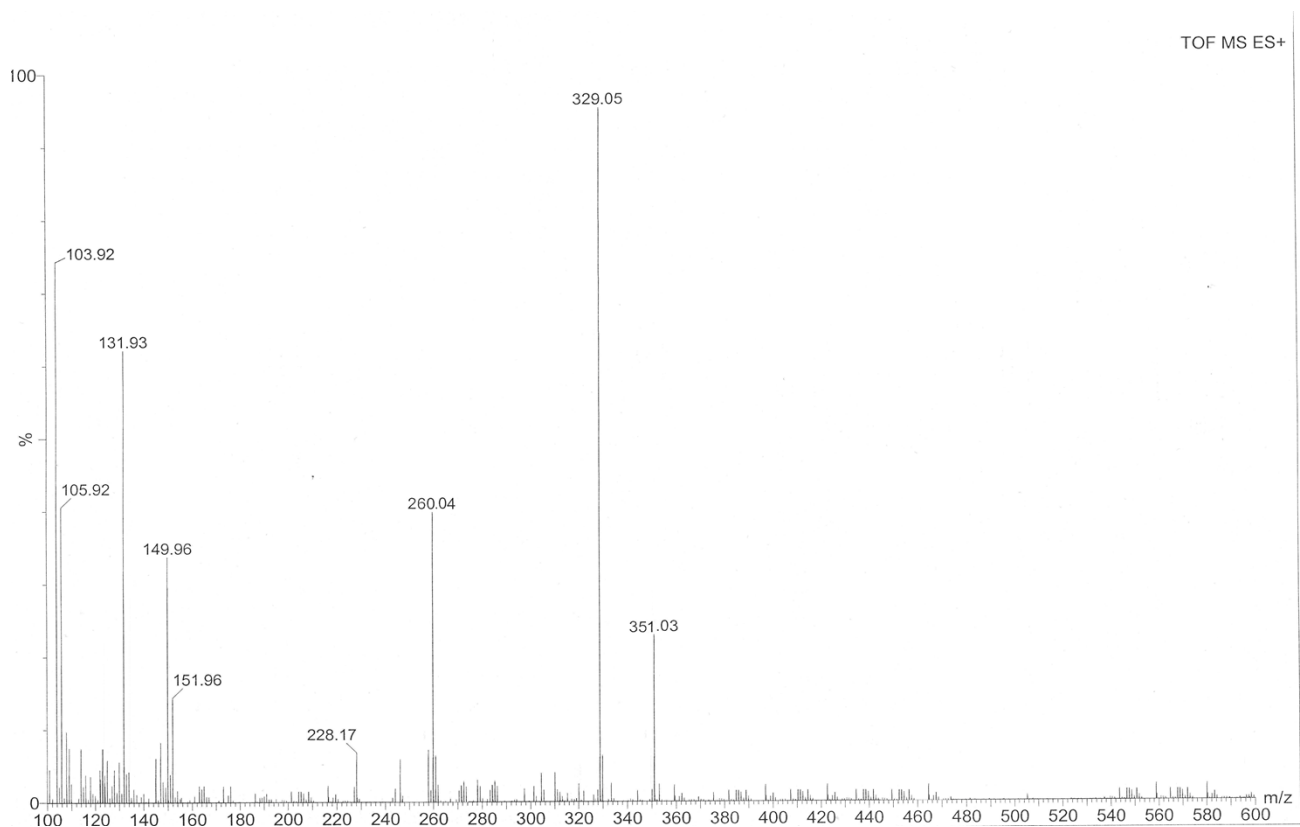
¹H NMR of Receptor i.e. BTHT in d₆ DMSO:



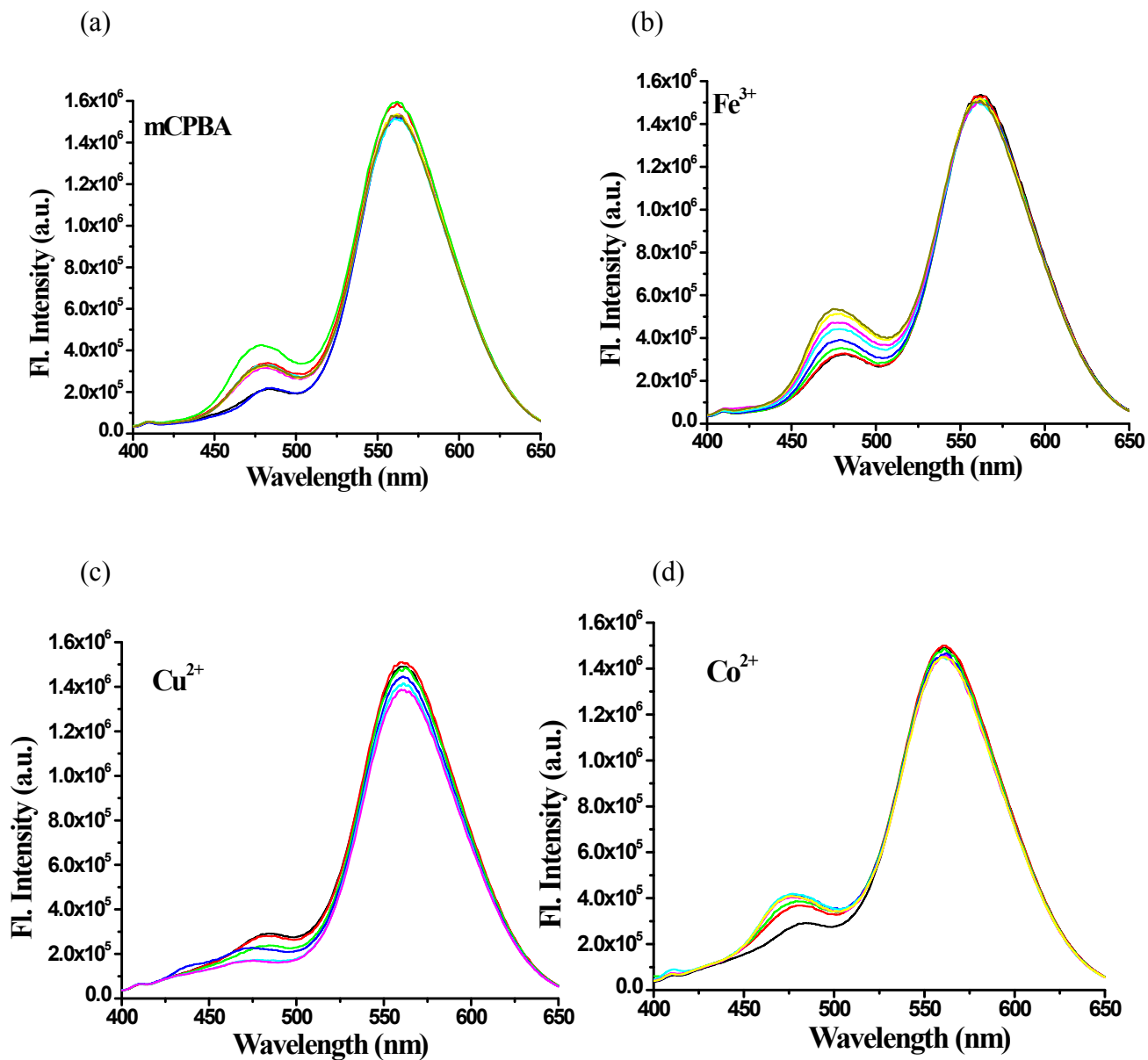
¹H NMR of BTHT + OCl⁻ in d₆ DMSO:

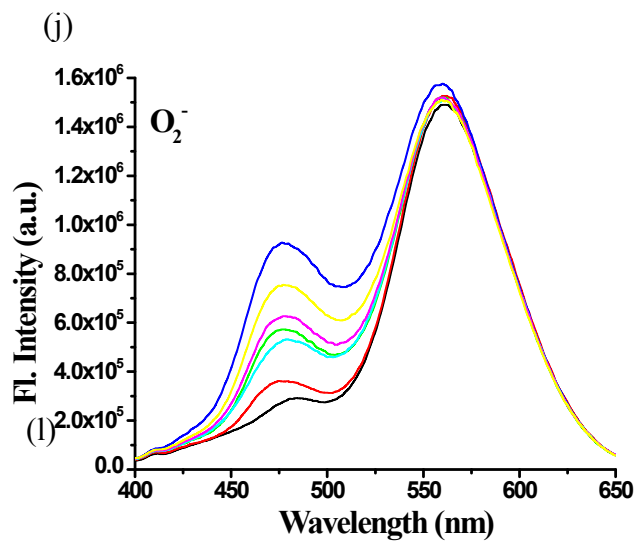
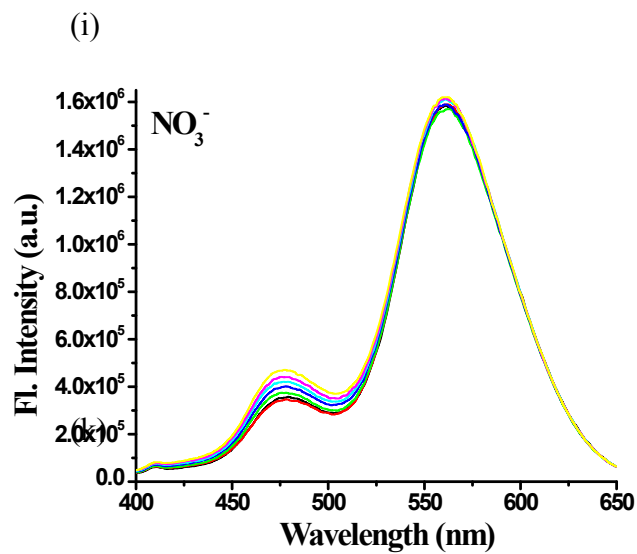
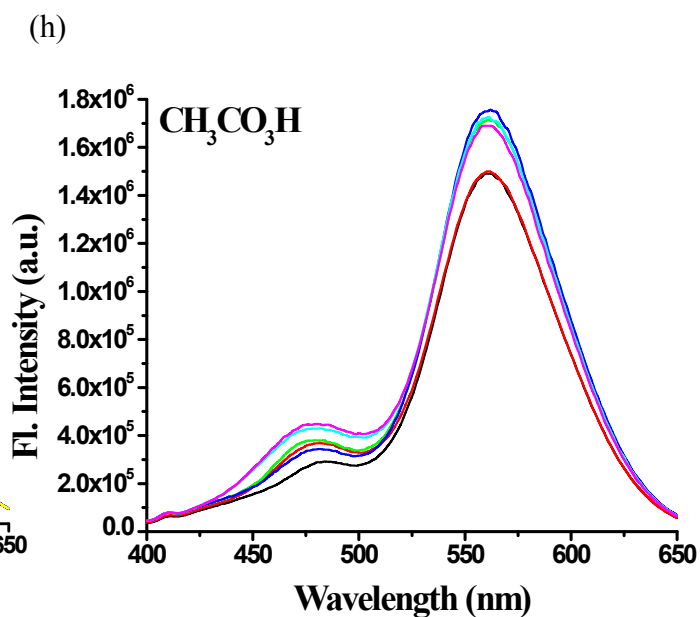
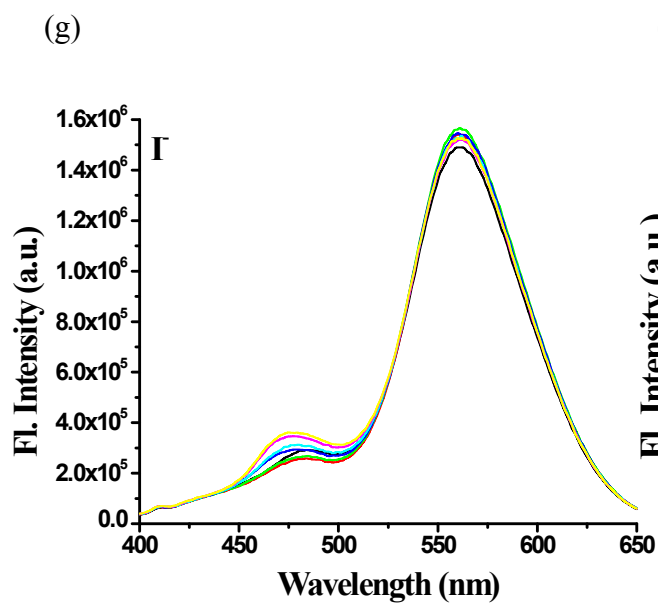
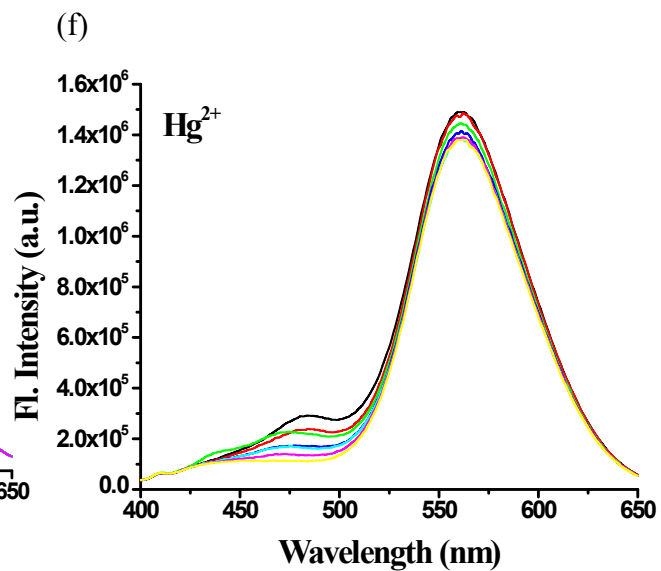
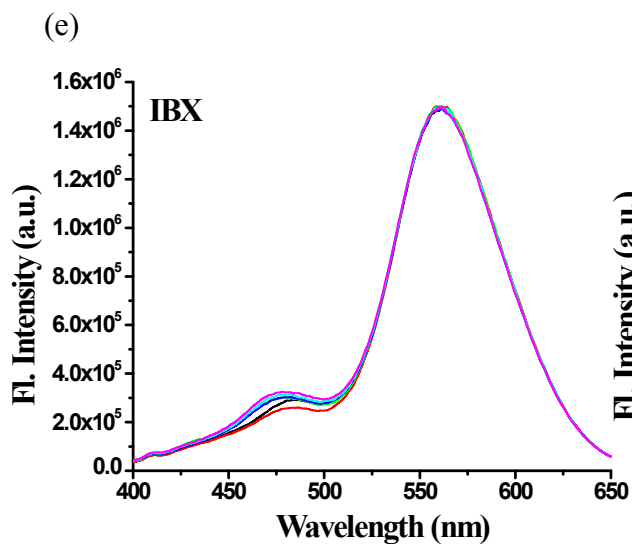


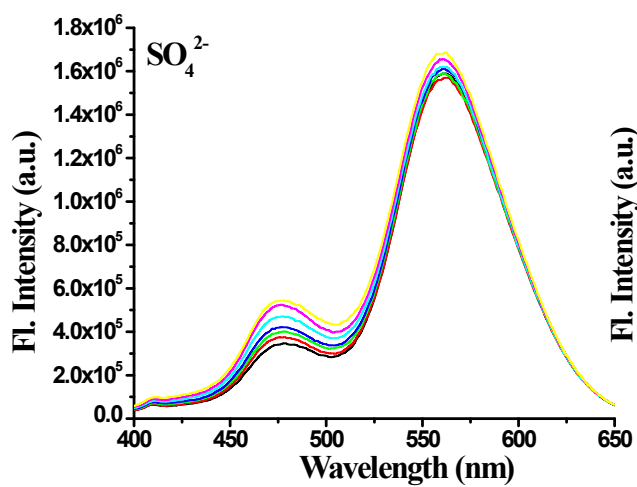
ESI-MS of Receptor i.e. BTHT:



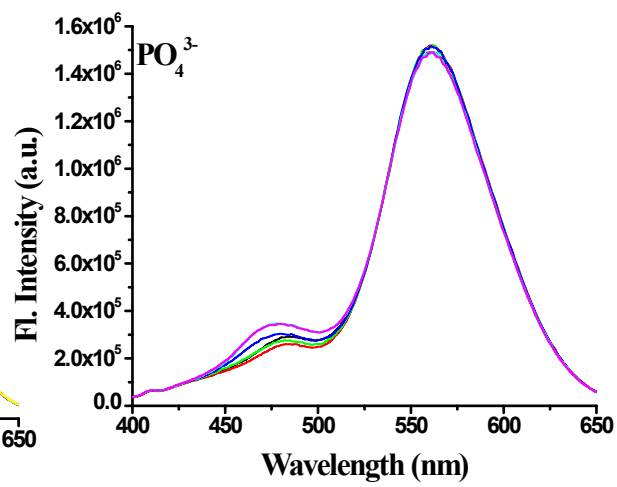
5. Fluorescence emission spectra of DPNO with different anions and oxidants as mCPBA, Fe^{3+} , Cu^{2+} , Co^{2+} , IBX, Hg^{2+} , I, CH_3COOOH , NO_3^- , Super oxide, SO_4^{2-} , PO_4^{3-} , H_2O_2 , Hydroxyl radical and F^- in $\text{CH}_3\text{CN} : \text{H}_2\text{O}$ (1:1, v/v) (The solutions of anions and oxidants were prepared from mCPBA, FeCl_3 , $\text{Cu}(\text{ClO})_2 \cdot 6\text{H}_2\text{O}$, $\text{Co}(\text{ClO})_2 \cdot 6\text{H}_2\text{O}$, IBX, HgCl_2 , KI, CH_3COOOH , NaNO_3 , K_2O , Na_2SO_4 , Na_3PO_4 , H_2O_2 , Femton's reagent and respectively in $\text{CH}_3\text{CN}-\text{H}_2\text{O}$).



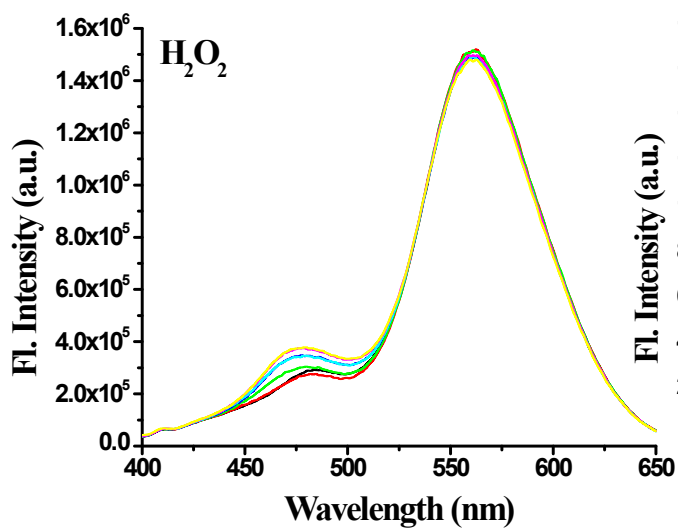




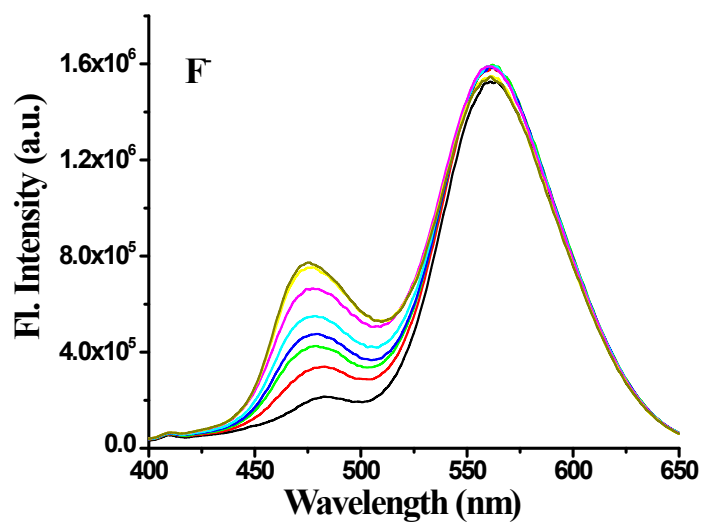
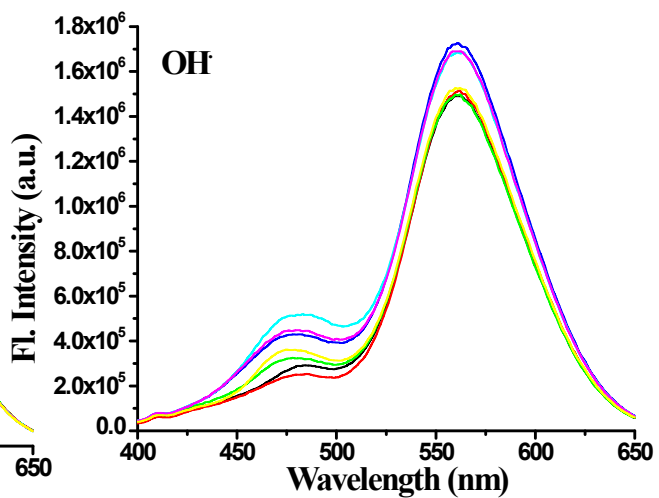
(m)



(n)



(o)



6. Fluorescence spectra of BTHT with different types of water samples:

Fluorescence emission spectra of BTHT ($c=2 \times 10^{-5}$ M) with different water samples (total volume 500 micro-litre for each) in $\text{CH}_3\text{CN} : \text{H}_2\text{O}$ (1:1, v/v).

