

Thiophene-phenylquinazoline Probe for Selective Ratiometric Fluorescence and Visual Detection of Fe (III) and Turn-Off Fluorescence for I⁻ and its Applications

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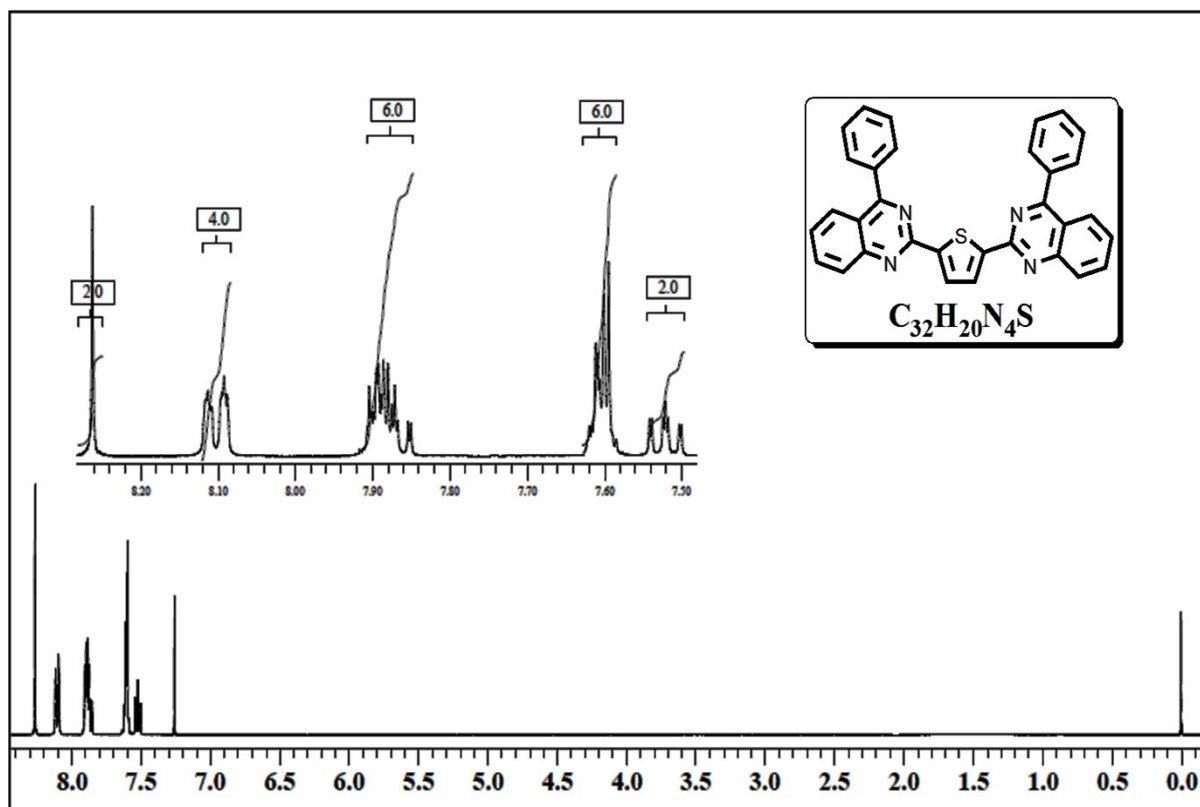


Fig. S1: ^1H NMR spectrum of BQT

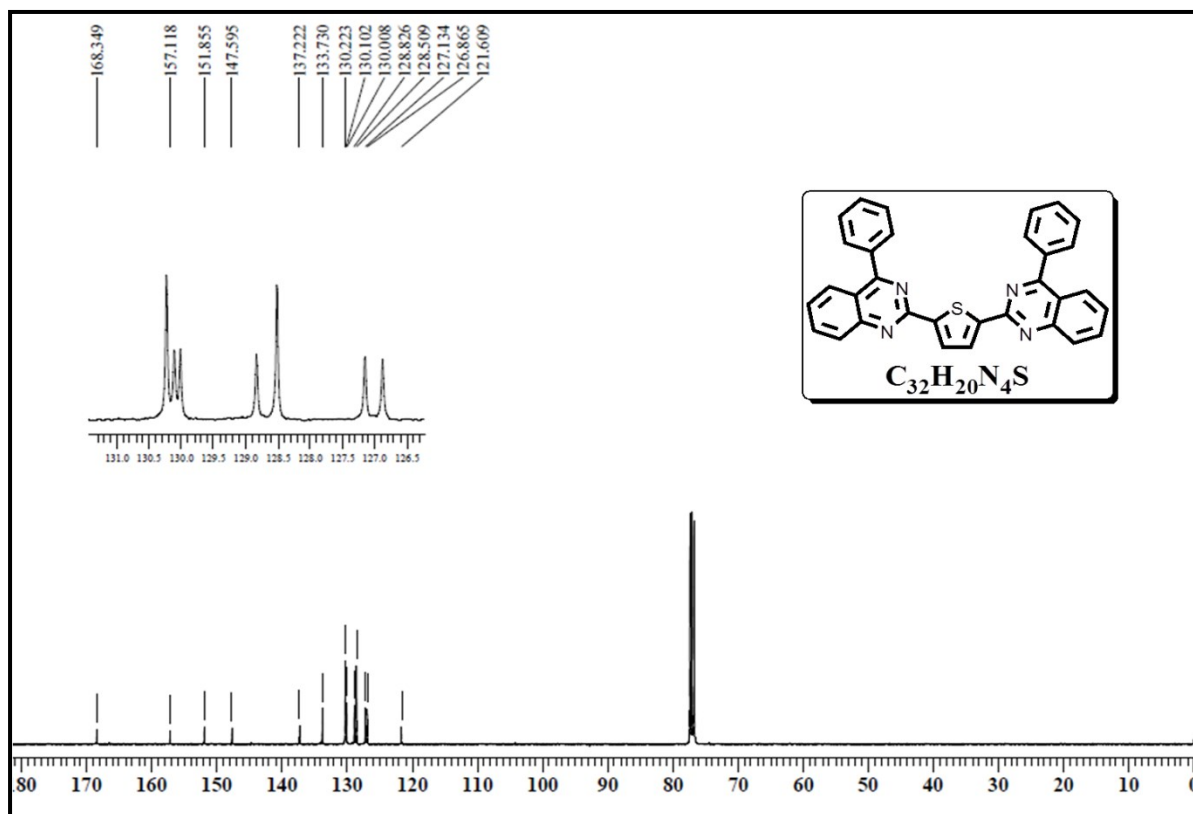


Fig. S2: ^{13}C NMR spectrum of BQT

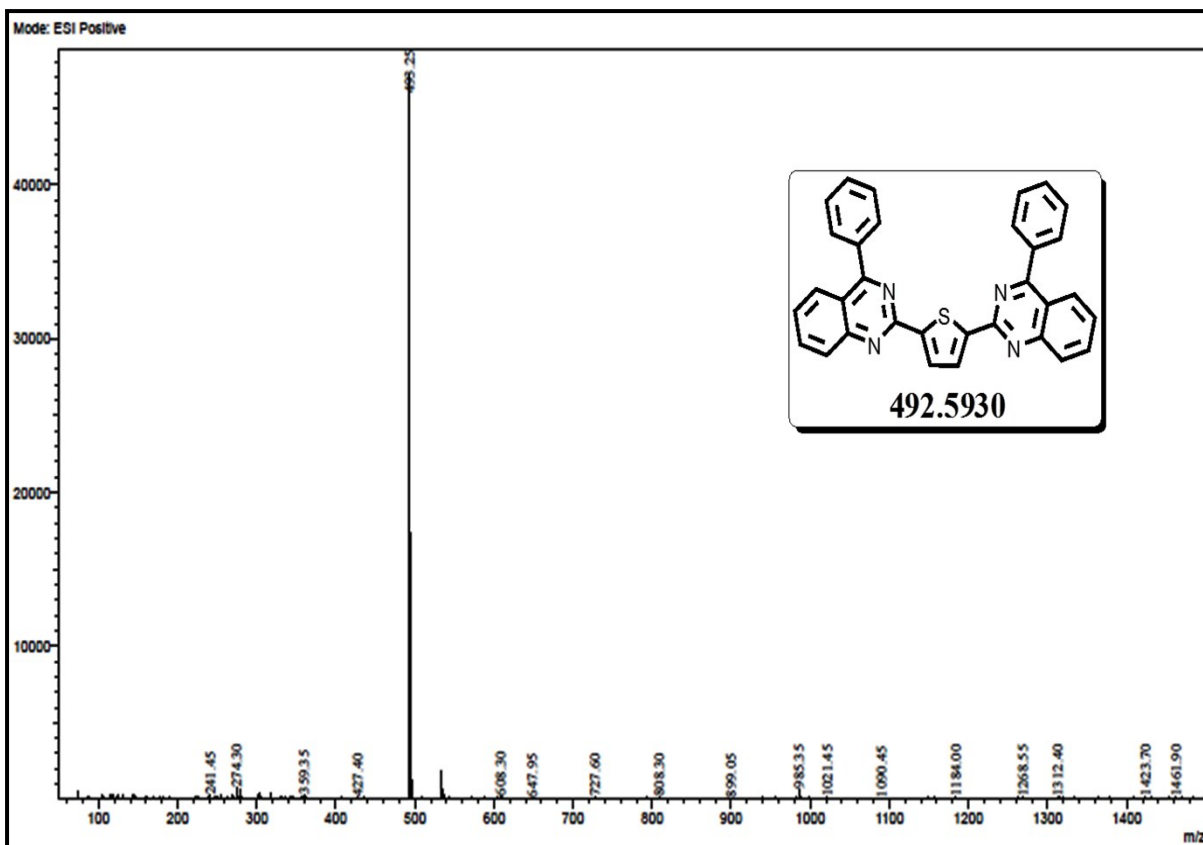


Fig. S3: ESI-Mass spectrum of BQT

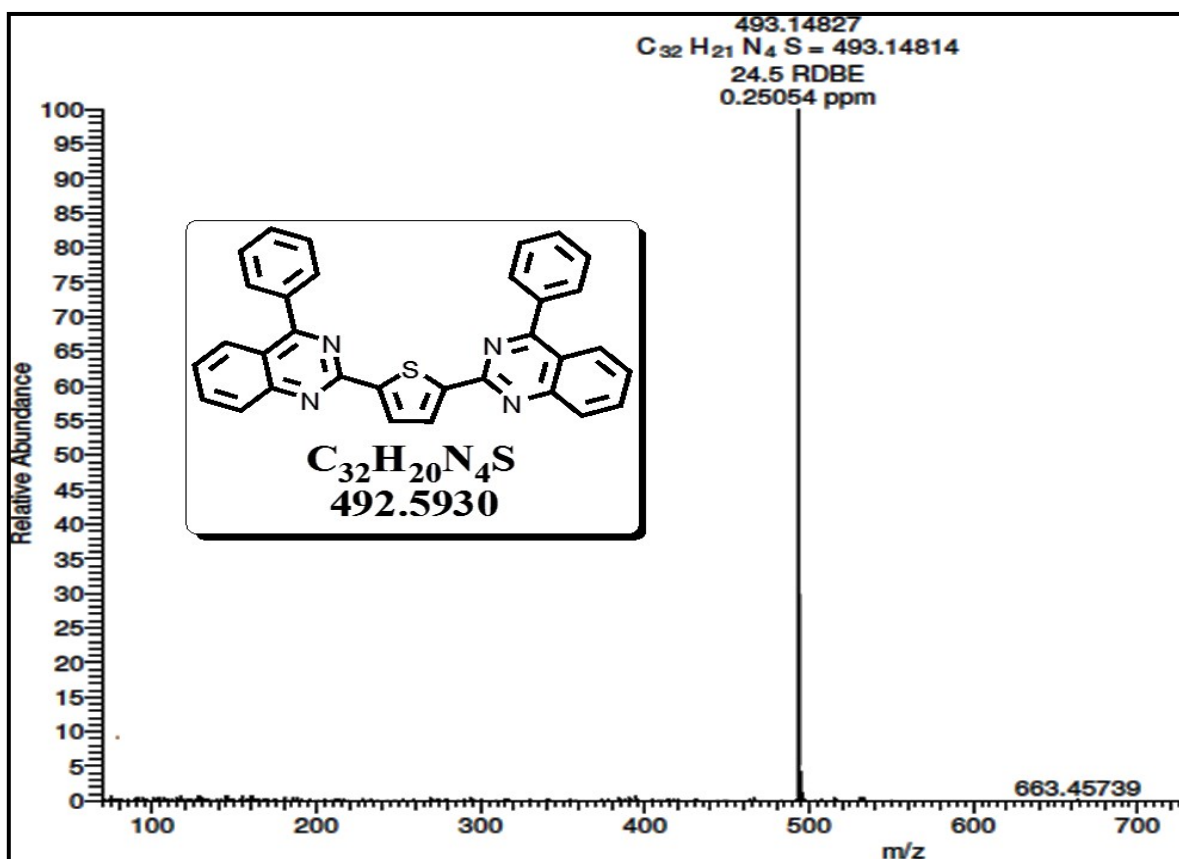


Fig. S4: ESI-HR Mass spectrum of BQT

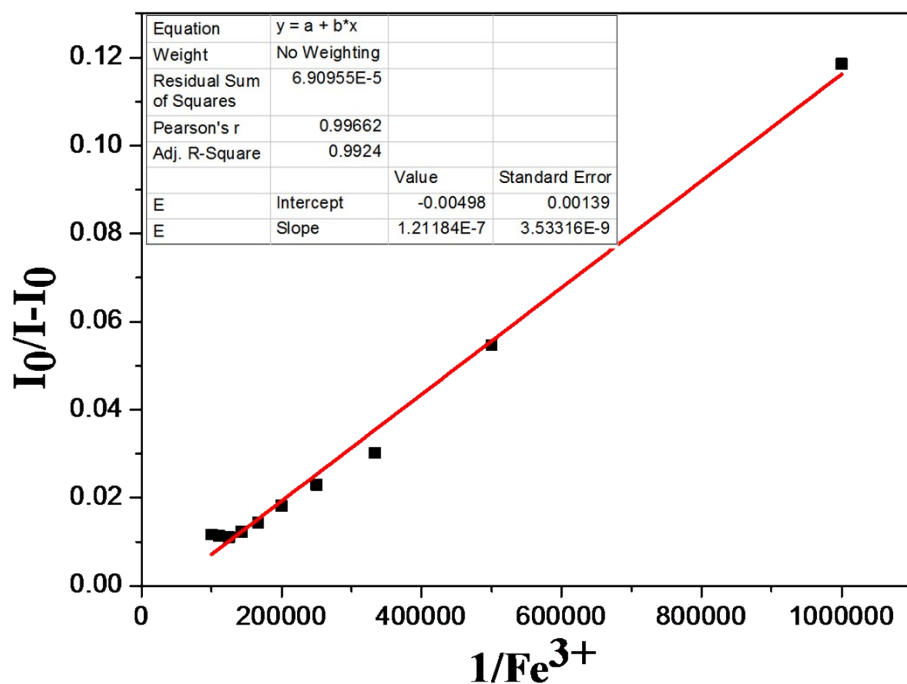
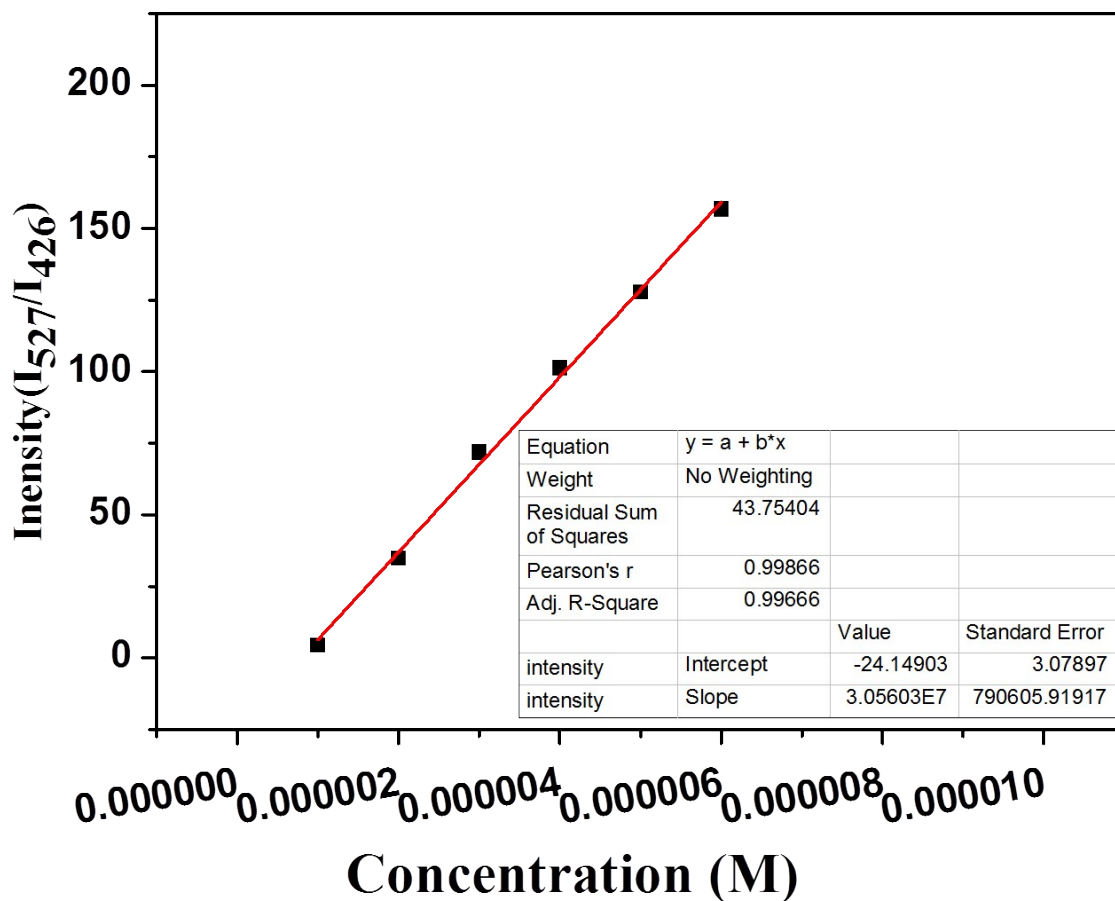
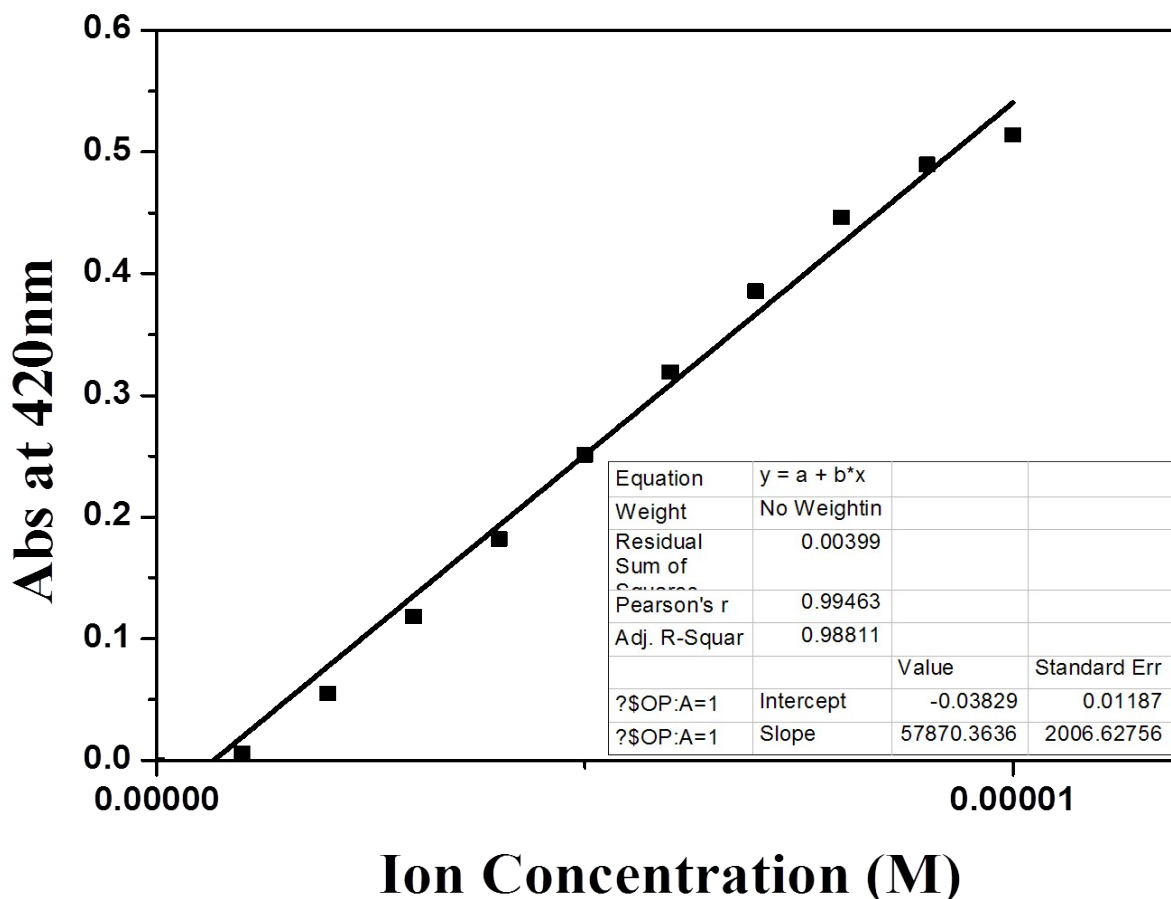


Fig. S5: Benesi–Hildebrand plots to determine binding constants for BQT-Fe³⁺
 Binding constant was calculated using the following equation
 Binding constant = Intercept/ Slope
 The calculated binding constant for BQT-Fe³⁺ is 4.1x 10⁻⁴ M⁻¹



LOD = $3\sigma/S$, where σ is the standard deviation and S is the slope of the linearity curve. σ is 0.21 and $S = 3.05603E7$. LOD is 2.0×10^{-8} M. LOQ = $3 \times \text{LOD} = 6.1 \times 10^{-8}$ M.

Fig. S6: Linearity curve from fluorescence titration for BQT-Fe³⁺ complex



LOD = $3\sigma/S$, where σ = standard deviation and S = slope of the linearity curve. S = 57870.3636 and σ is 0.00092. LOD of BQT for Fe = $1.6e-8$ M & LOQ of BQT for Fe = $4.8e-8$ M

Fig. S7: Linearity curve from UV-Vis titration for BQT-Fe³⁺ complex

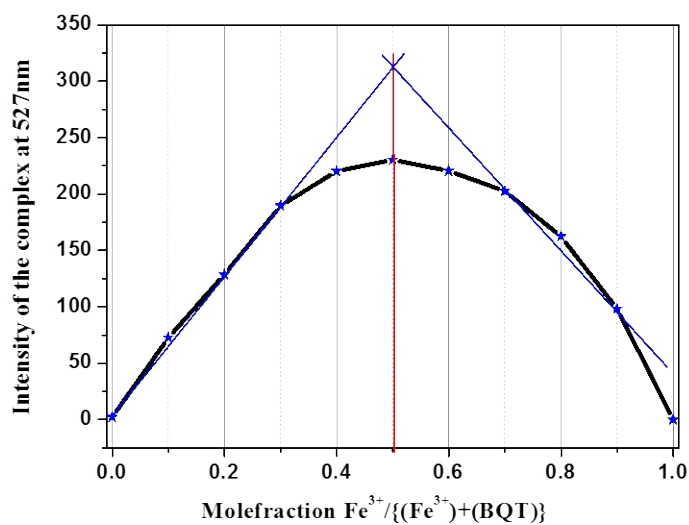


Fig. S8: Job's plot of BQT-Fe³⁺ complex

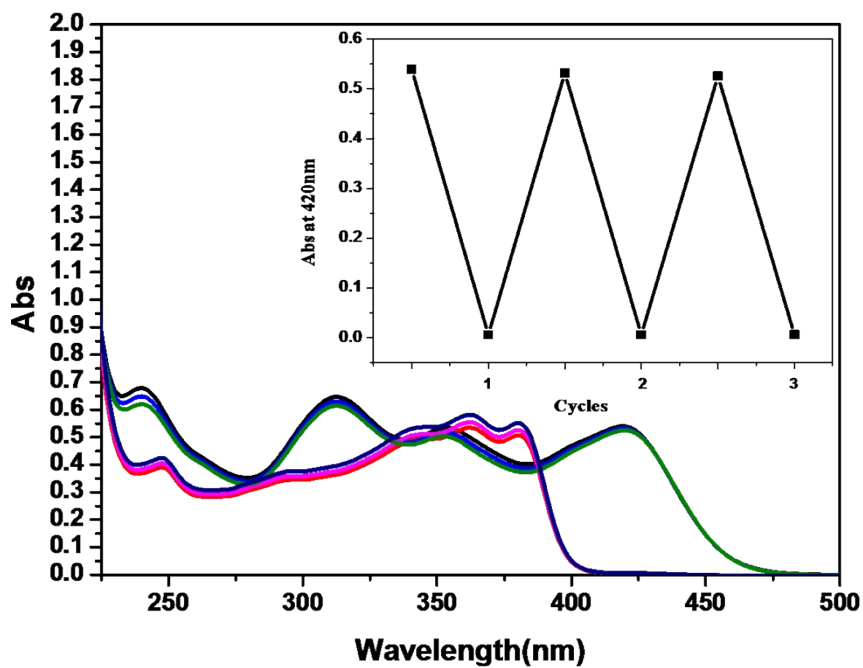


Fig. S9: Reversible cycles of absorption at 420 nm upon addition of Fe³⁺ and EDTA alternatively in CH₃CN solution of BQT.

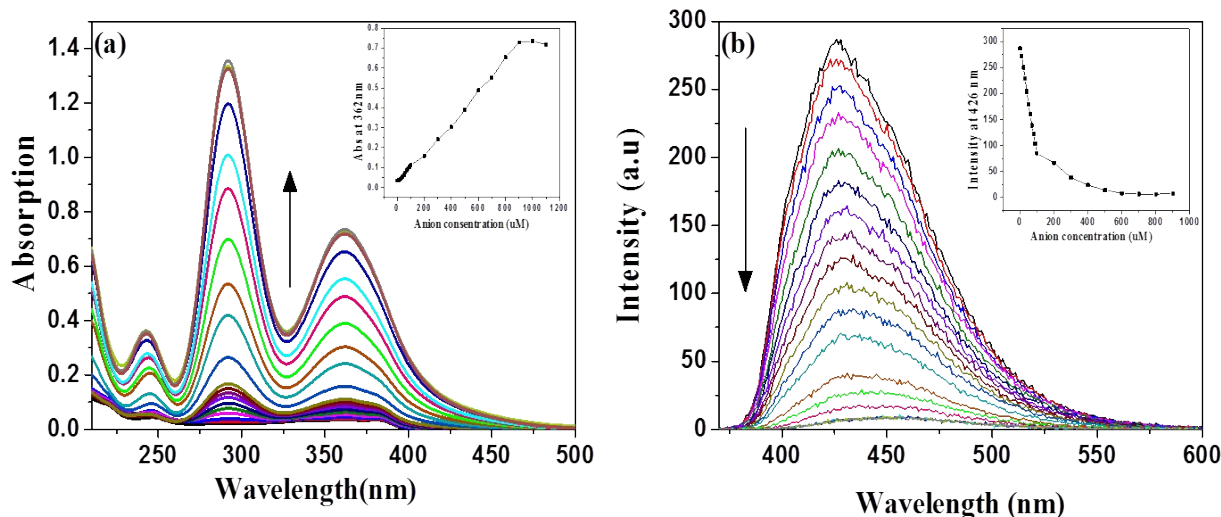


Fig. S10: The absorbance (a) spectra of I⁻ titration (0-1100μM) Insets: absorbance at 362 nm Vs concentration of I⁻ and fluorescence (b) spectra of I⁻ titration (0-900μM) Insets: intensity at 426 nm Vs concentration of I⁻ with the BQT (10 μM). Excitation wavelength is 362nm.

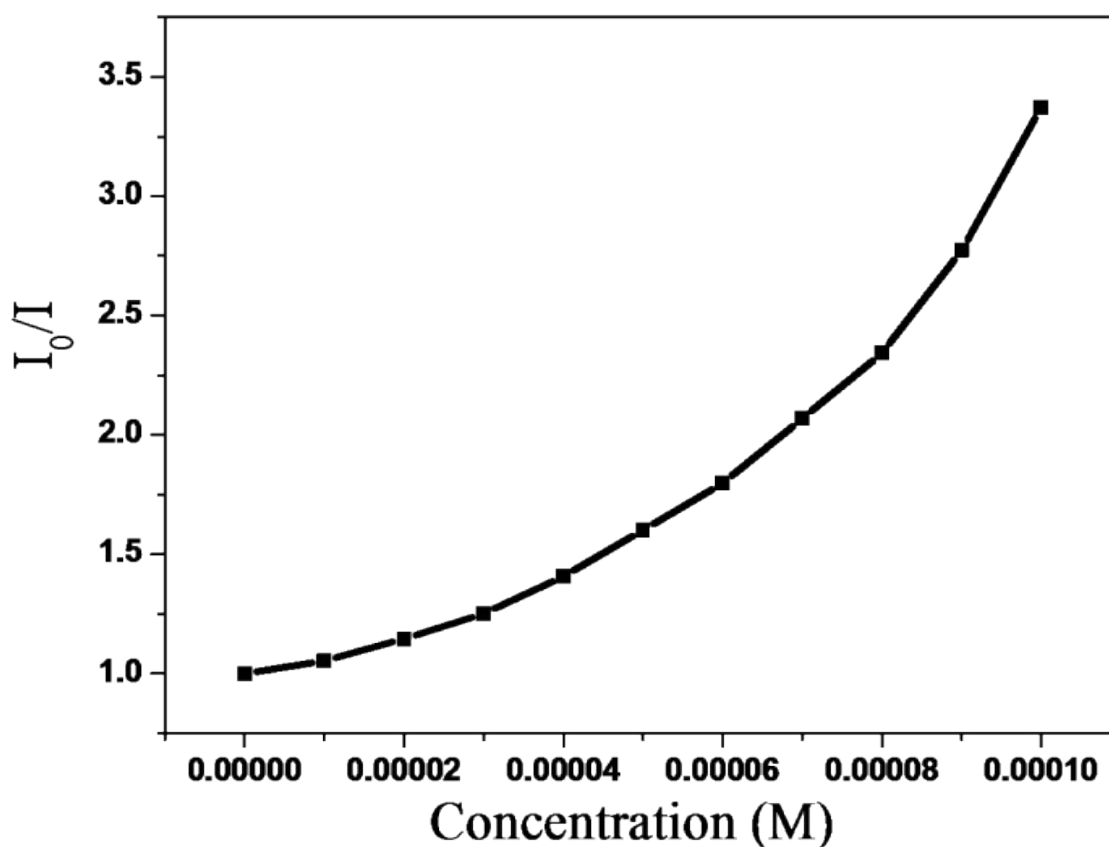


Fig.S11: Stern-Volmer plot for BQT quenching upon addition of iodide ion, here I₀ = BQT intensity without I⁻ ion and I = intensity with I⁻ ion.

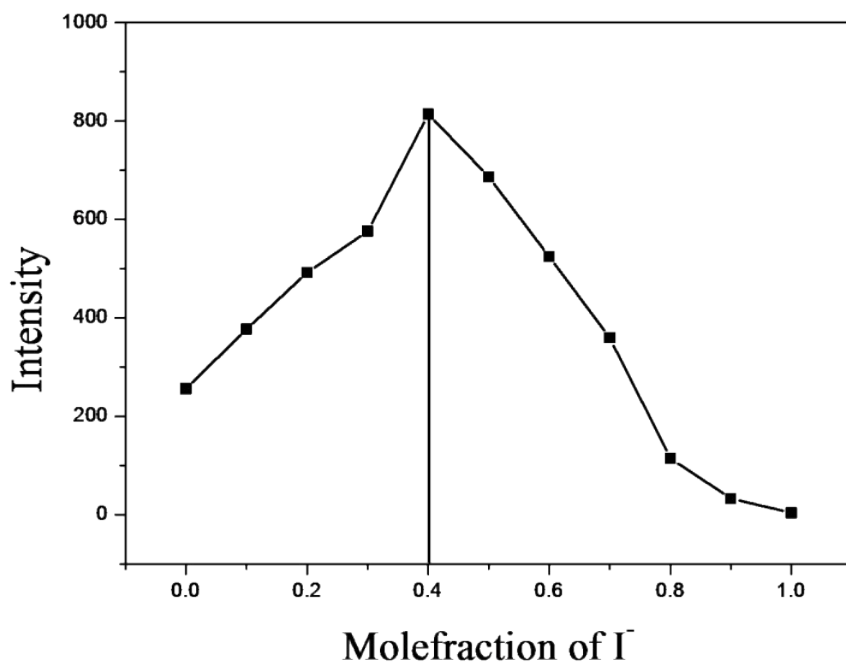
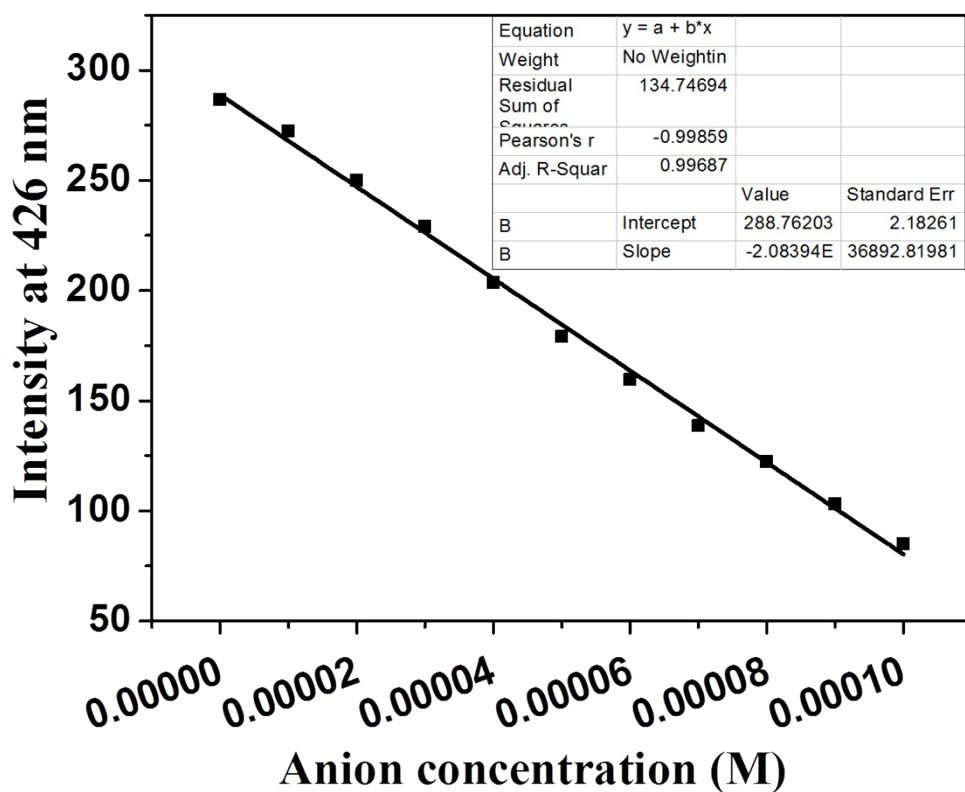


Fig.S12: Job's plot of BQT-I complex.



$LOD = 3\sigma/S$, where σ = standard deviation and S = slope of the linearity curve. σ is 0.12 and $S = 2083940$. LOD of BQT for $I^- = 1.7 \times 10^{-7}$ & LOQ of BQT for $I^- = 5.2 \times 10^{-7}$

Fig. S13: Linearity curve from fluorescence titration for BQT- I complex