Supporting Information for

Quinoline benzimidazole-conjugate for the highly selective detection of Zn(II) by dual colorimetric and fluorescent turn-on responses

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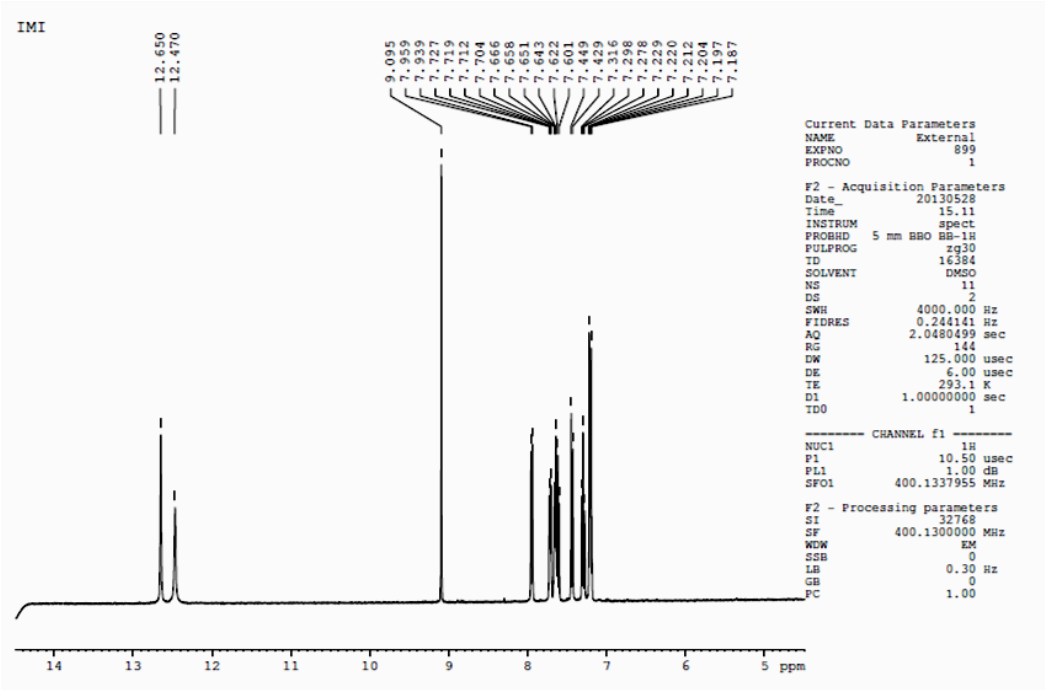


Fig. S1. ^{1}H-NMR Spectrum of **QBC**

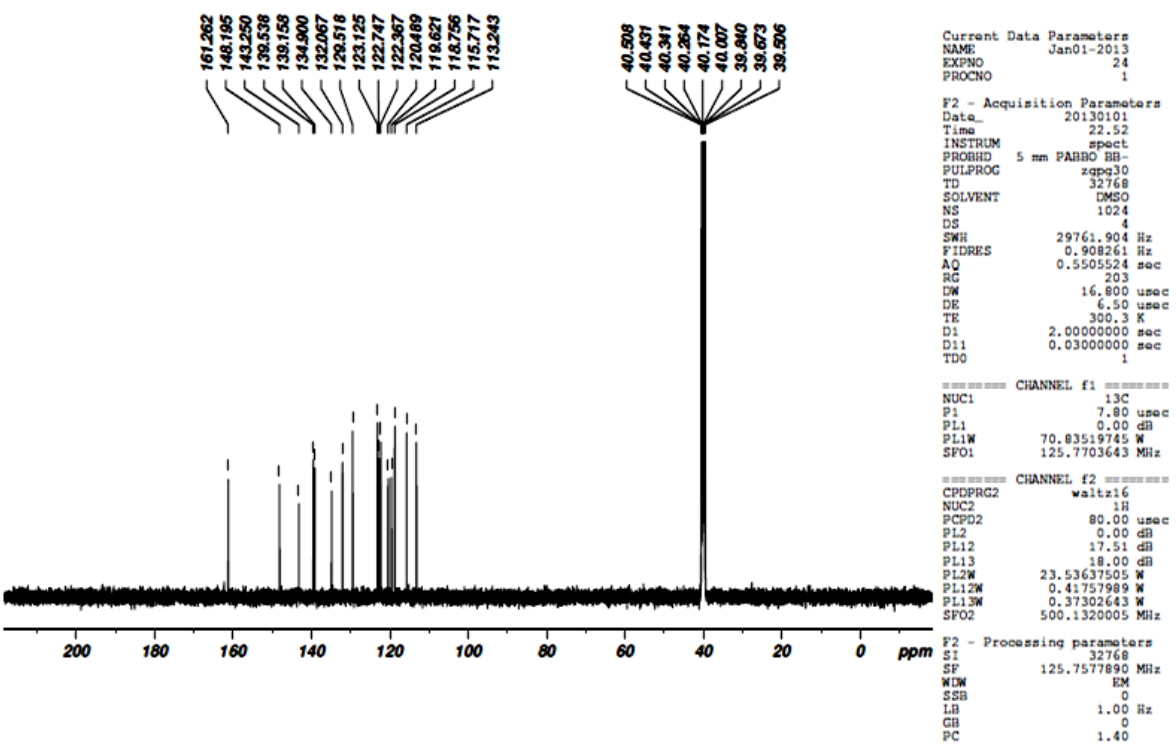


Fig. S2. ^{13}C-NMR Spectrum of **QBC**

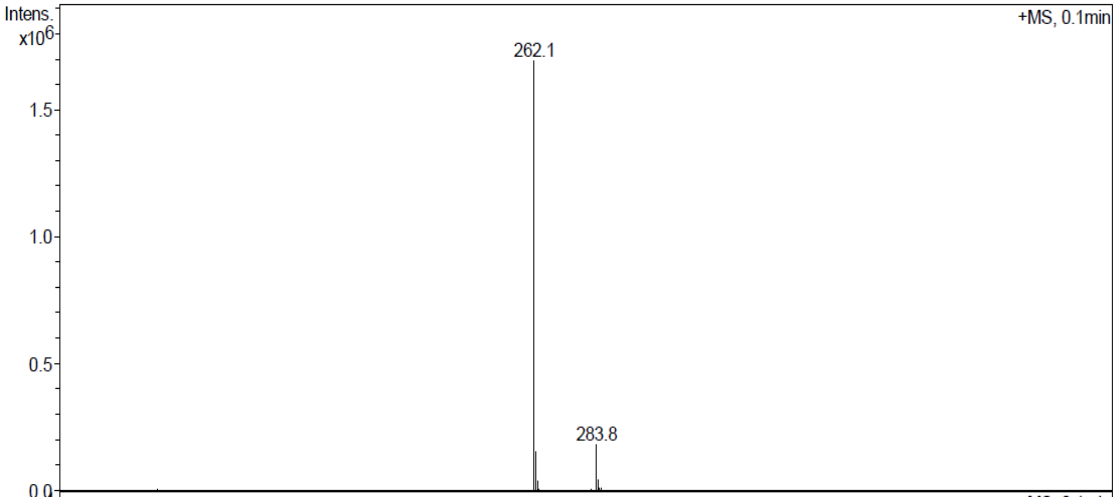


Fig. S3. LC- Mass spectrum of **QBC**

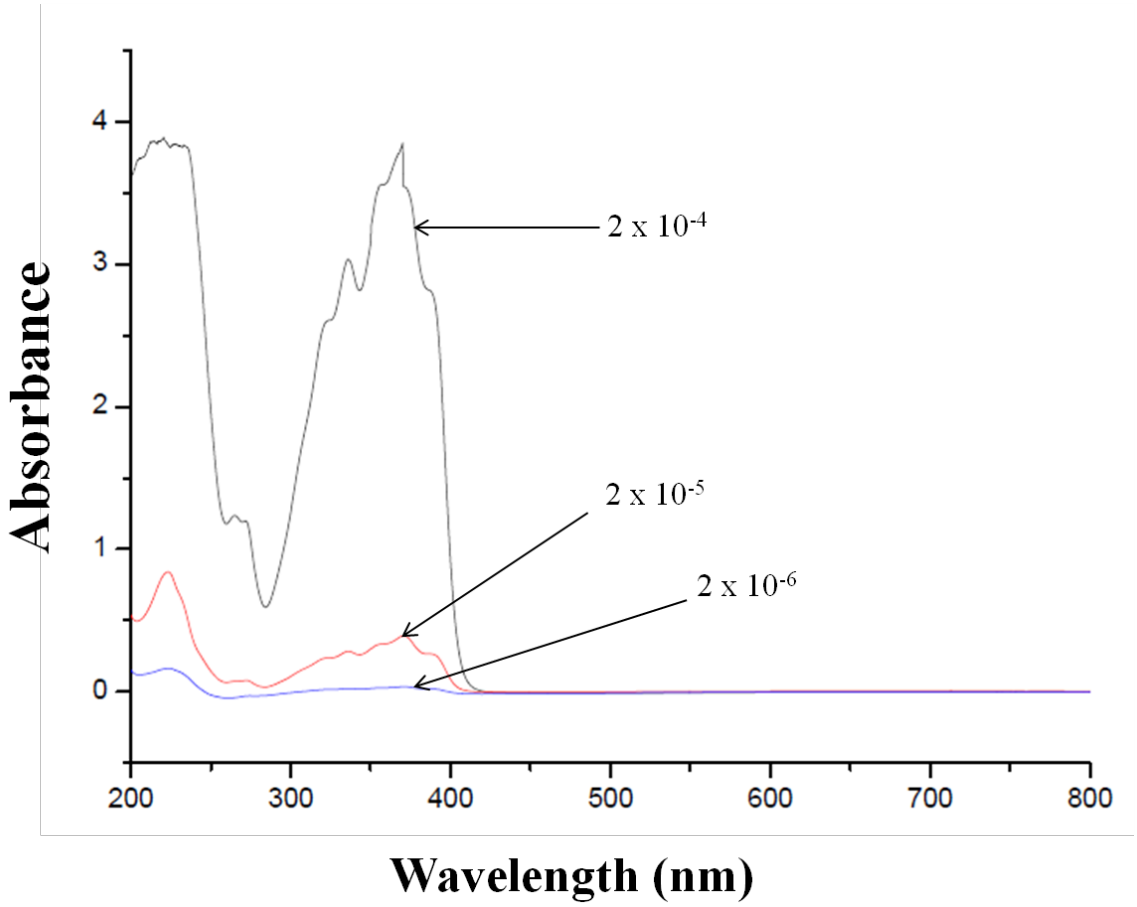


Fig. S4. Absorption spectrum of **QBC** in CH_3CN:H_2O (1:1 v/v) solution

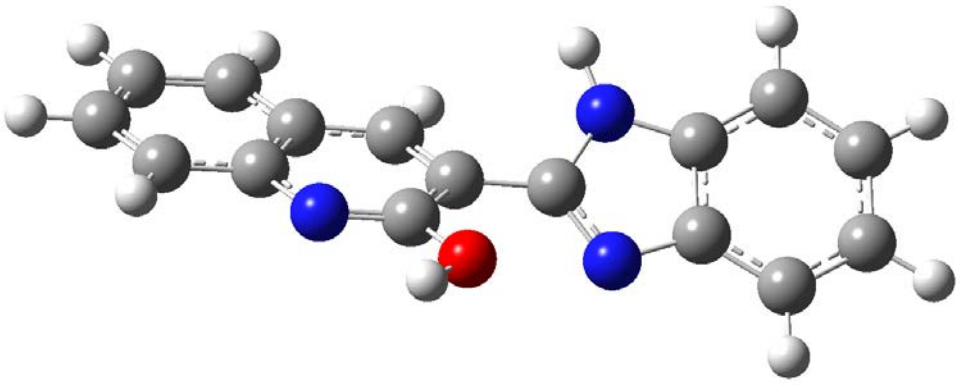


Fig. S5. Geometry of the **QBC** optimized using Gaussian 03 at B3LYP /6-31G level of theory

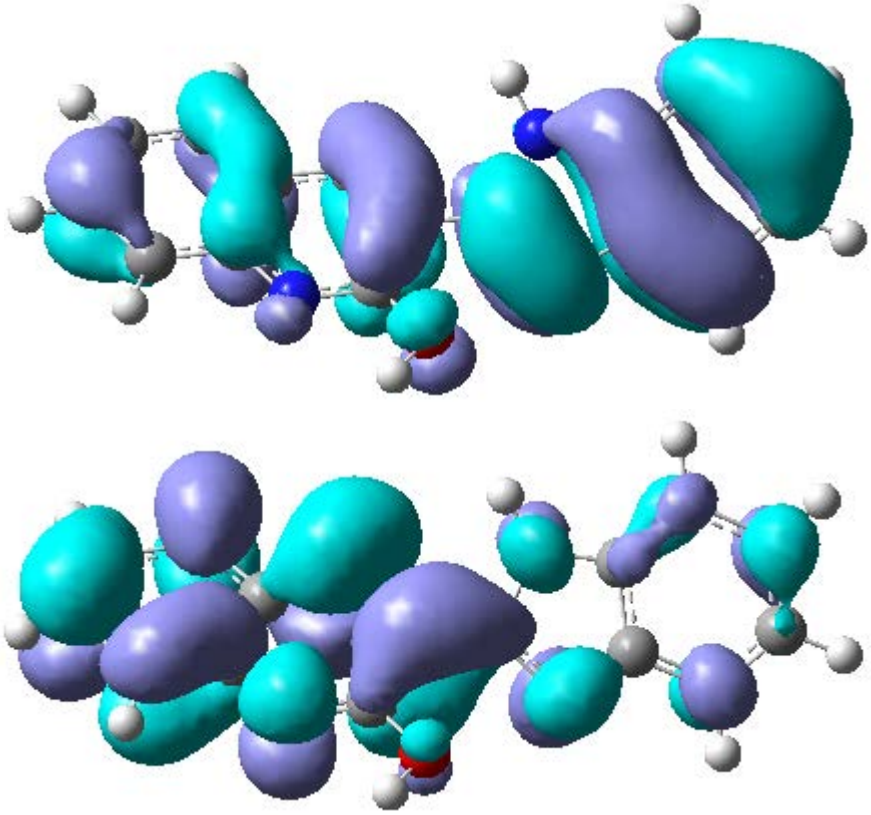


Fig. S6. Highest occupied molecular orbital (top) and Lowest Unoccupied Molecular Orbital (bottom) of **QBC** calculated using Gaussian 03 software at B3LYP /6-31G level of theory

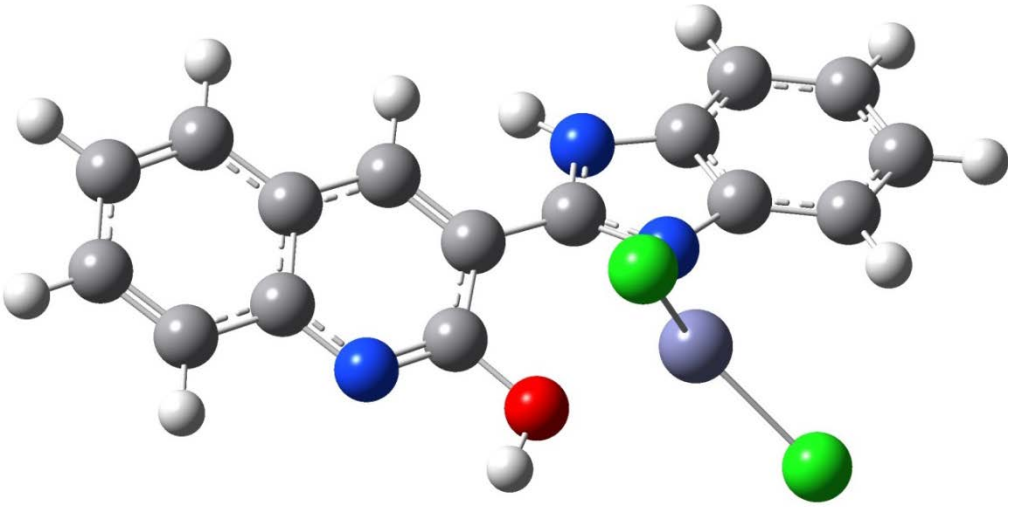


Fig. S7. Geometry of the **QBC**+Zn^{2+} optimized using Gaussian 03 at B3LYP /GenECP level of theory

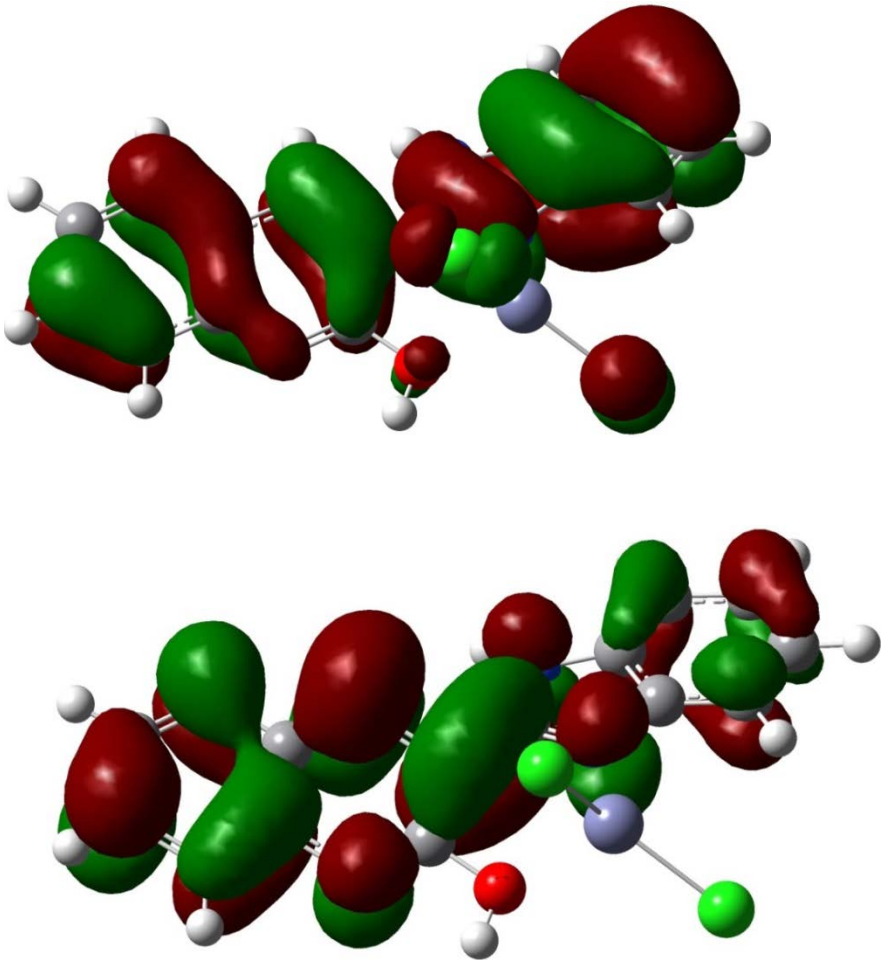


Fig. S8. Highest Occupied Molecular Orbital (top) Lowest Unoccupied Molecular Orbital (bottom) of **QBC**+Zn^{2+} calculated using Gaussian 03 at B3LYP /GenECP level of theory.

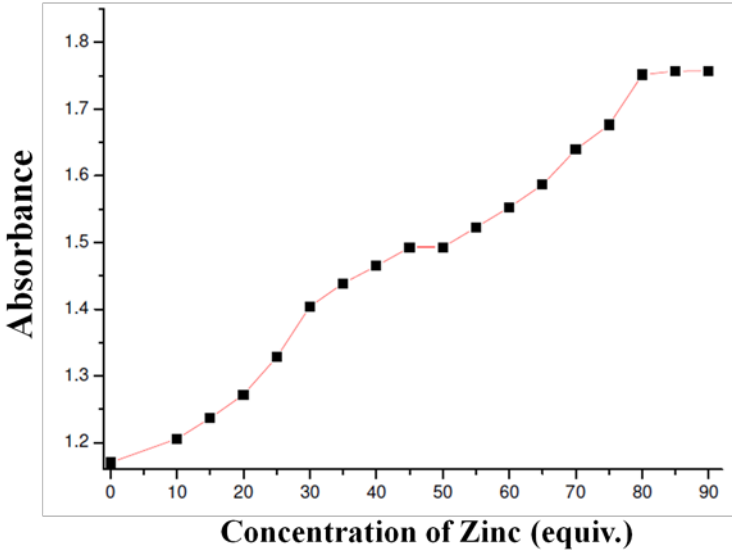


Fig. S9. Changes of absorption intensity of **QBC** (4 x 10^{-6} M) solution (CH_3CN-H_2O, 1:1 v/v, HEPES = 50 mM, pH=7.0) upon addition of different amount of Zn^{2+} (0-90 equiv.).

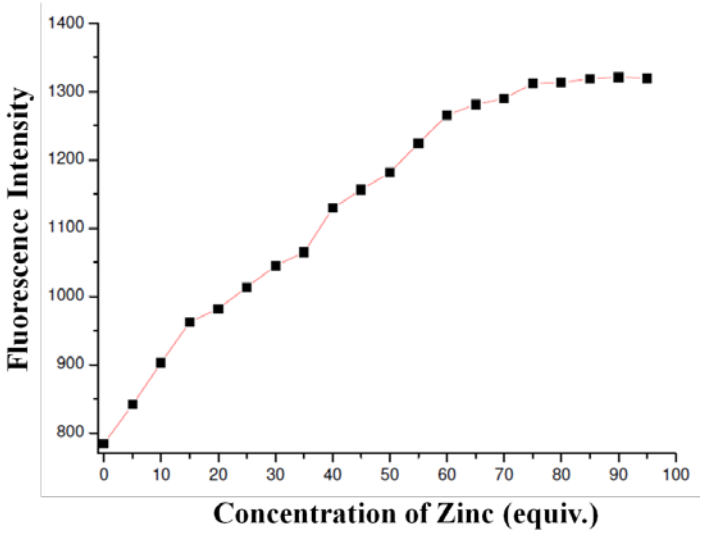


Fig. S10. Changes of fluorescence intensity of **QBC** (4 x 10^{-6} M) solution (CH_3CN-H_2O, 1:1 v/v, HEPES = 50 mM, pH=7.0) upon addition of different amount of Zn^{2+} (0-95 equiv. excited at 380 nm) emission = 425 nm.

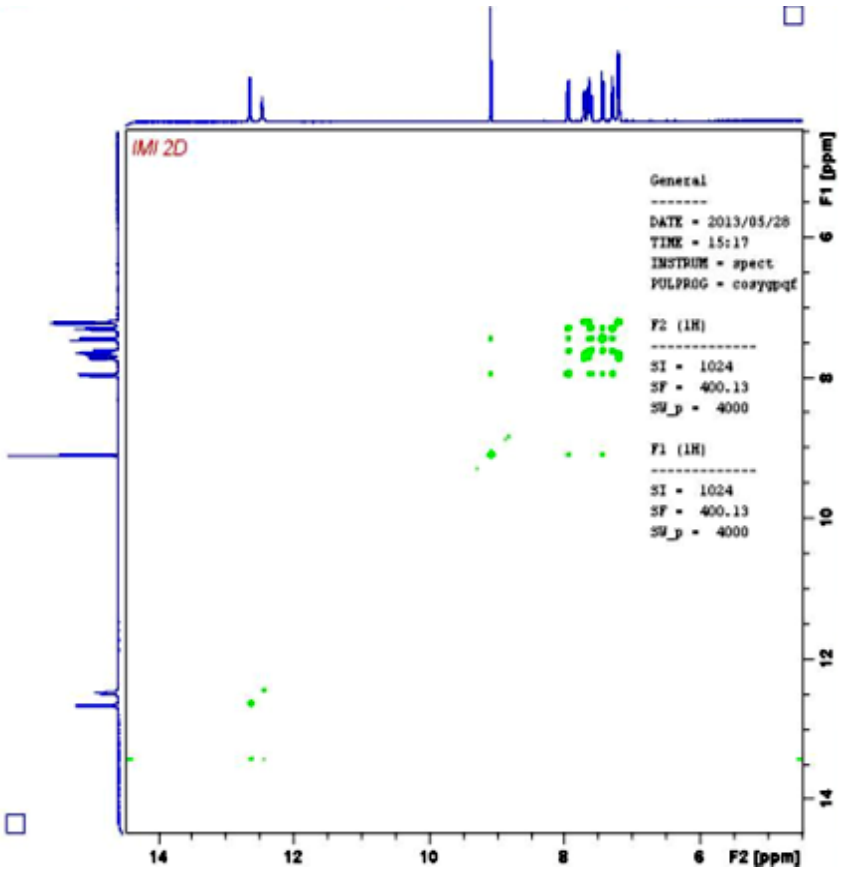


Fig. S11. 2D (^1H–^1H COSY) NMR Spectrum of **QBC**

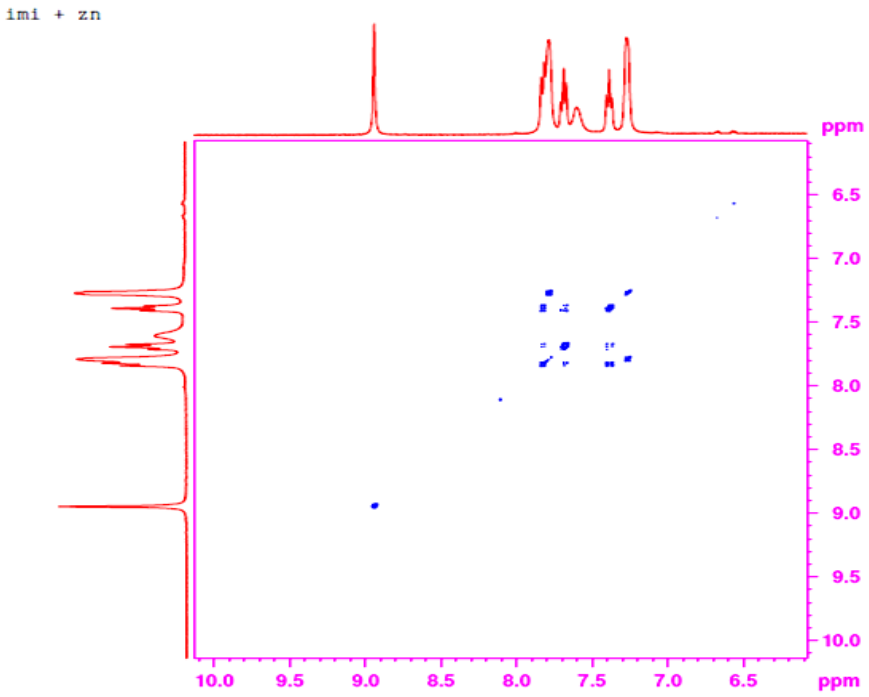


Fig. S12. 2D (^{1}H–^{1}H COSY) NMR Spectrum of **QBC**+Zn^{2+}

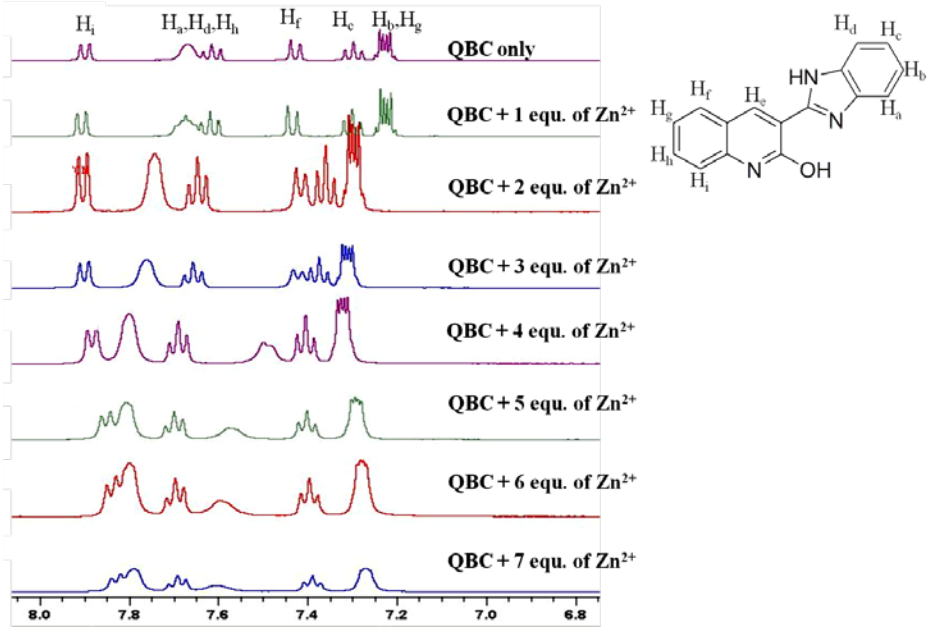


Fig. S13. Partial ^{1}H-NMR titration spectrum of **QBC** with different equ. of Zn^{2+}

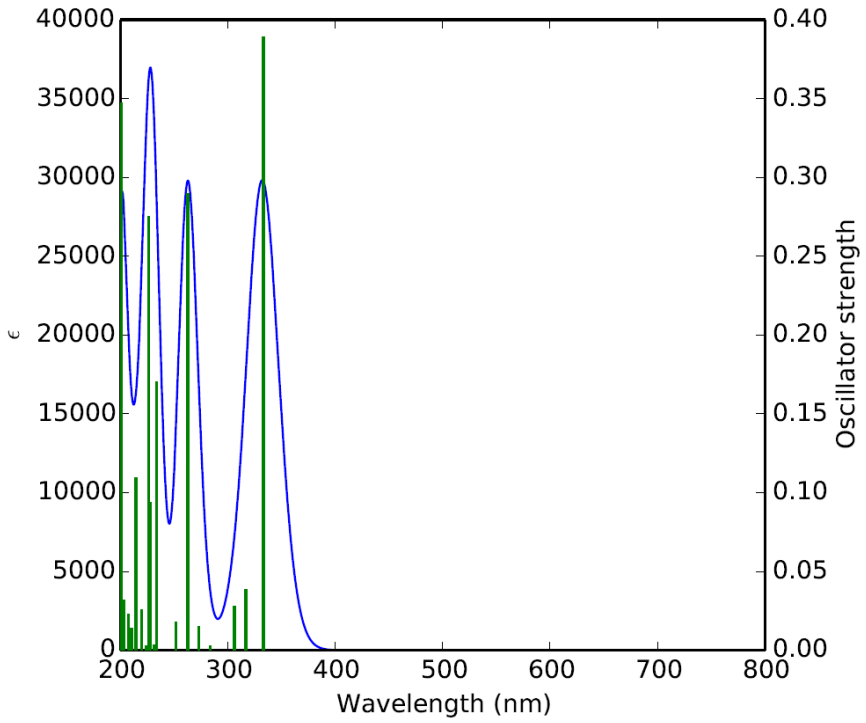


Fig. S14. TD spectra of **QBC** by Gaussian 03 at B3LYP /6-31G level of theory

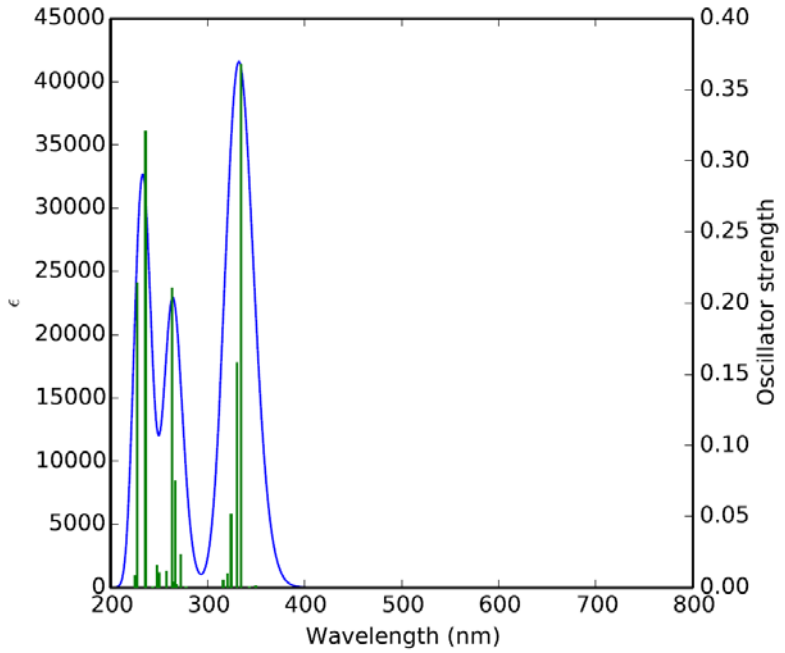
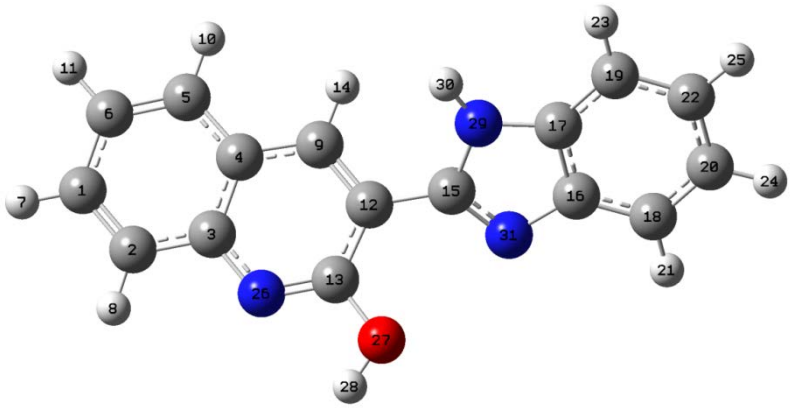


Fig. S15. TD spectra of **QBC**–Zn^{2+} by Gaussian 03 at B3LYP /6-31G level of theory



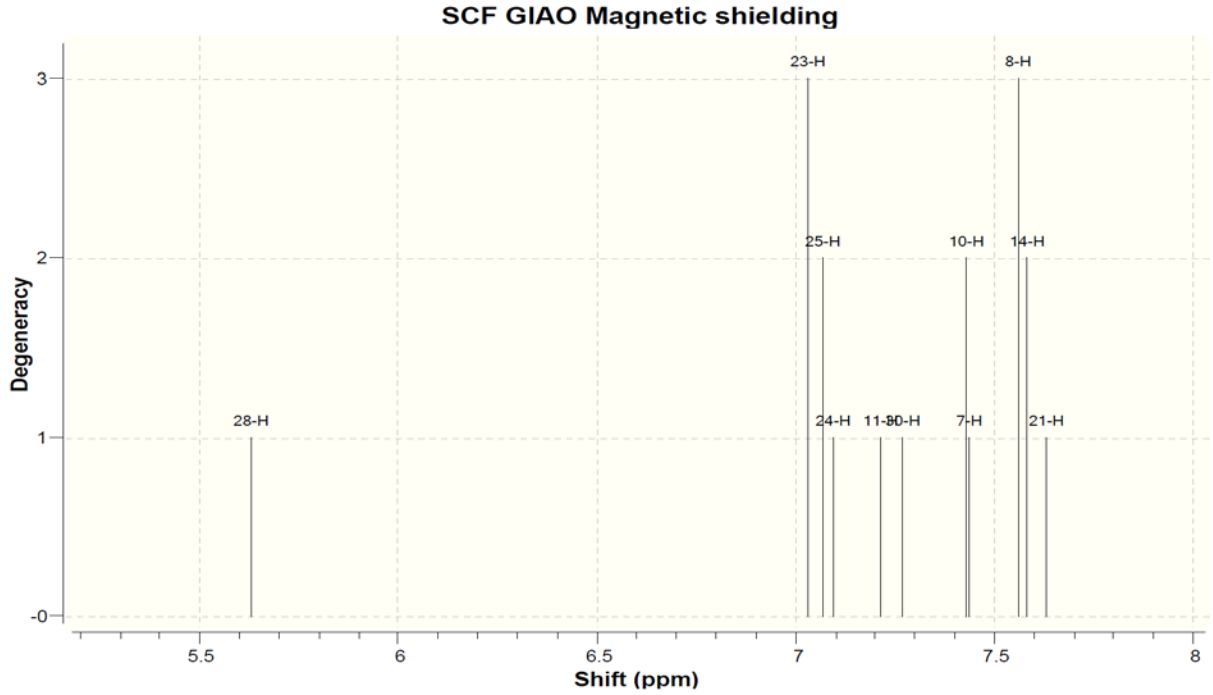


Fig. S16. ^{1}H NMR spectra of **QBC** by Gaussian 03 at SCF /6-31G level of theory.

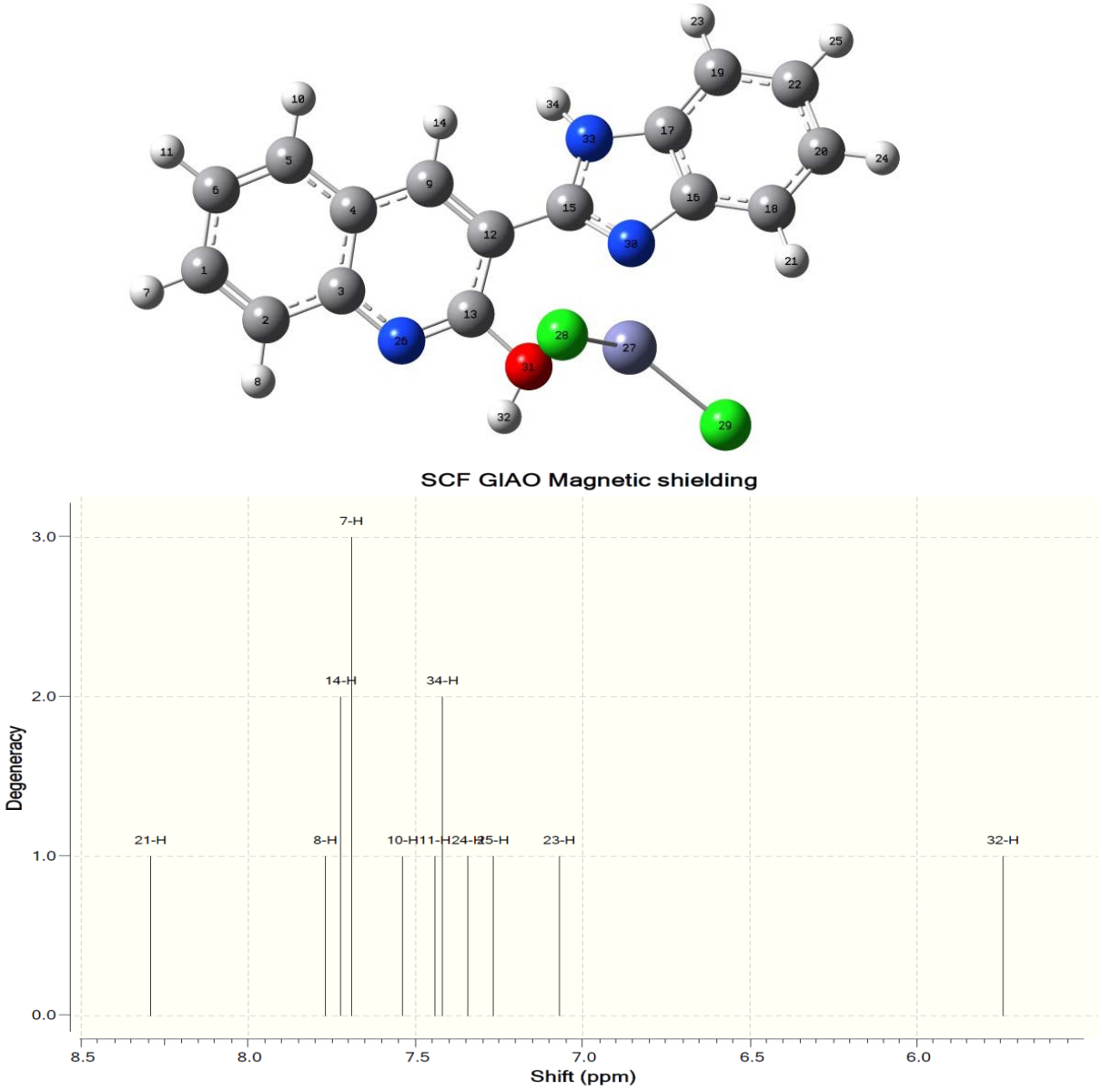


Fig. S17. ^{1}H NMR spectra of **QBC**+Zn^{2+} by Gaussian 03 at SCF /6-31G level of theory

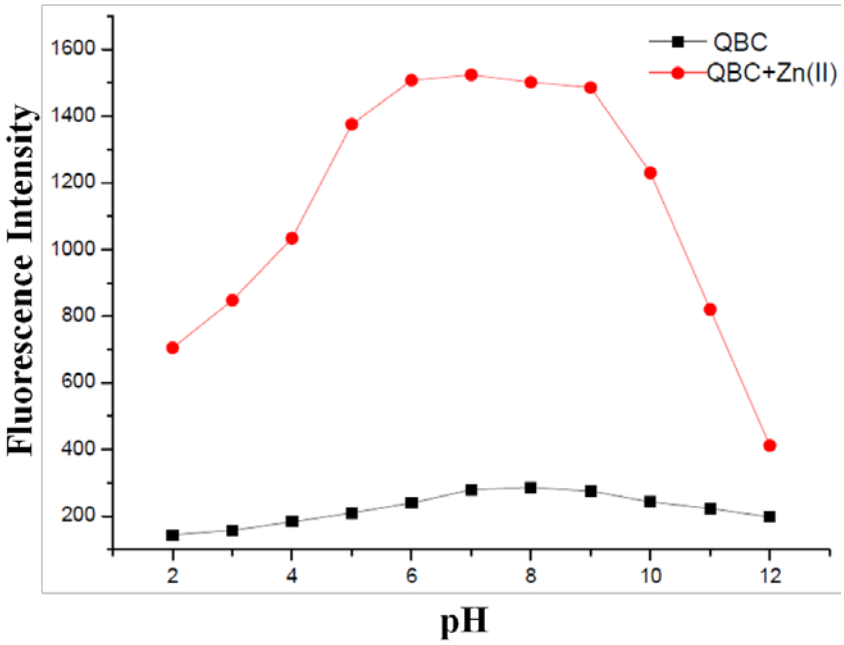


Fig. S18. The effect of pH **QBC** and **QBC** + Zn^{2+} in CH_3CN-H_2O (1;1 v/v) solutions at different pH values.

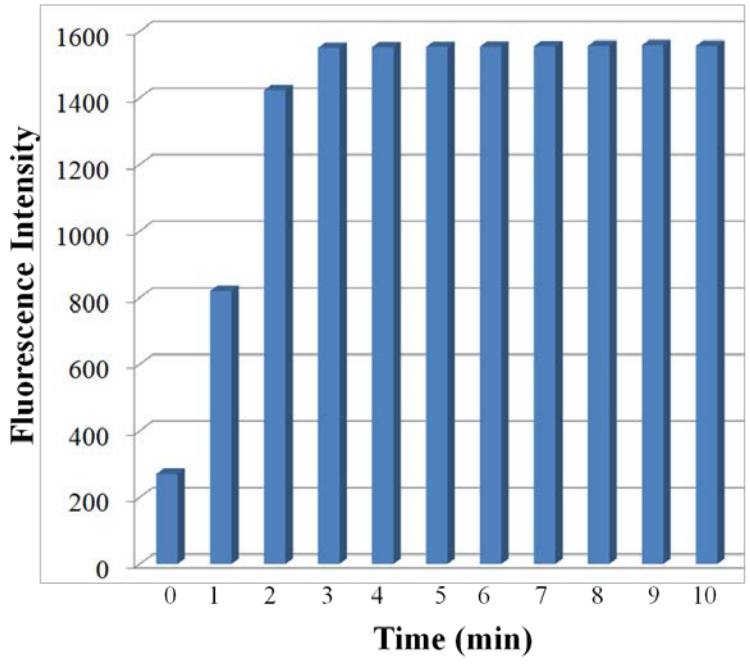


Fig. S19. The effective time response of **QBC** and **QBC** + Zn^{2+} in (CH_3CN-H_2O, 1;1 v/v, HEPES = 50 mM, pH=7.0)

Experimental Section

Materials and instruments

All solvents were purchased commercially with reagents grade quality. O-phenylenediamine was obtained from Merck and was used without further purification. 3-formyl-2-quinolone was prepared by literature procedure [29]. ^{1}H NMR and ^{13}C NMR spectra were recorded on a Brucker 400 MHz spectrometer, DMSO-d_6 solution with TMS as internal standard. LC-MS were determined on a LC-MSD-Trap-XCT Plus based on infusion methods. Absorption spectra were made on a Shimadzu UV-240 spectrophotometer. Fluorescence measurements were performed on a Jasco FP-8200 spectrofluorimeter equipped with quartz cuvettes of 1 cm path length. The excitation and emission slit widths were 5.0 nm. All absorption and emission spectra were recorded at 24 ±1 ^{0}C. Stock solutions for analysis were prepared (2 x 10^{-3}M for compound **QBC** (CH_3CN/H_2O, 1:1 (v/v), HEPES=50 mM, pH=7.0) immediately before the experiments. The solutions of metal ions were prepared from chloride and nitrate salts of Na^{+}, K^{+}, Mg^{2+}, Ca^{2+}, Zr^{2+}, Ba^{2+}, Cd^{2+}, Mn^{2+}, Co^{2+}, Ni^{2+}, Cu^{2+}, Cr^{3+}, Zn^{2+}, Pb^{2+}, Hg^{2+}, Al^{3+}, Fe^{3+}, Ce^{3+}, Fe^{2+} and Ag^{+}.

Absorption and fluorescence titration experiments

Stock solutions of Zn^{2+} ions (100 equiv.) and the receptor **QBC** (4 x 10^{-6} M) were prepared in CH_3CN-H_2O (1;1 v/v, HEPES=50 mM, pH=7.0) solutions and used for absorption and fluorescence titration experiments. The titration spectrum of **QBC** with Zn^{2+} (0–100 equiv.) was carried out in CH_3CN-H_2O solutions (1;1 v/v, HEPES=50 mM, pH=7.0) shown in Fig. 2 & 5. For the absorbance and fluorescence experiments 1 cm width and 4 cm height cuvette were used. The excitation was carried out at 380 nm for **QBC** with 5 nm emission slit widths in spectrofluorometer.