Electronic Supplementary Material (ESI) for RSC Advances.

A quinoline based Schiff-base compound as *p*H sensor

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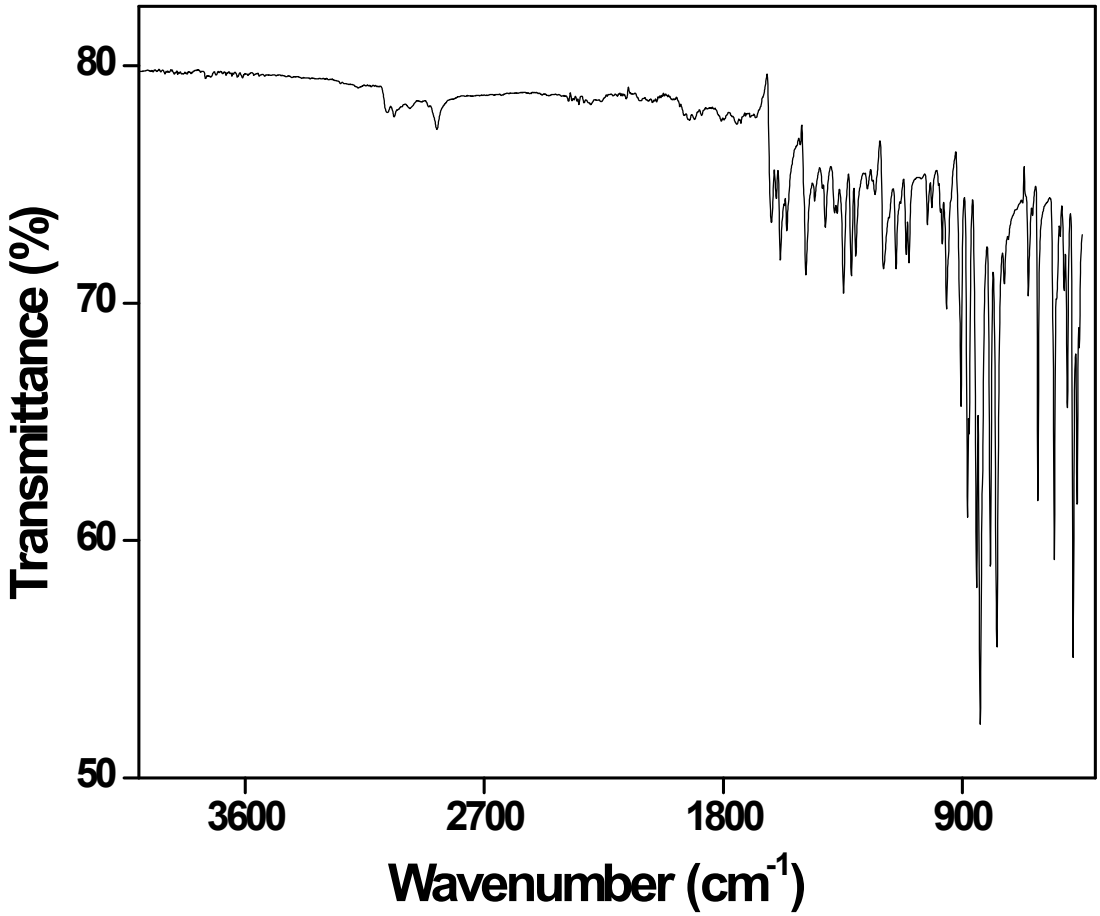

Fig. S1: FT-IR spectrum of **BQB**

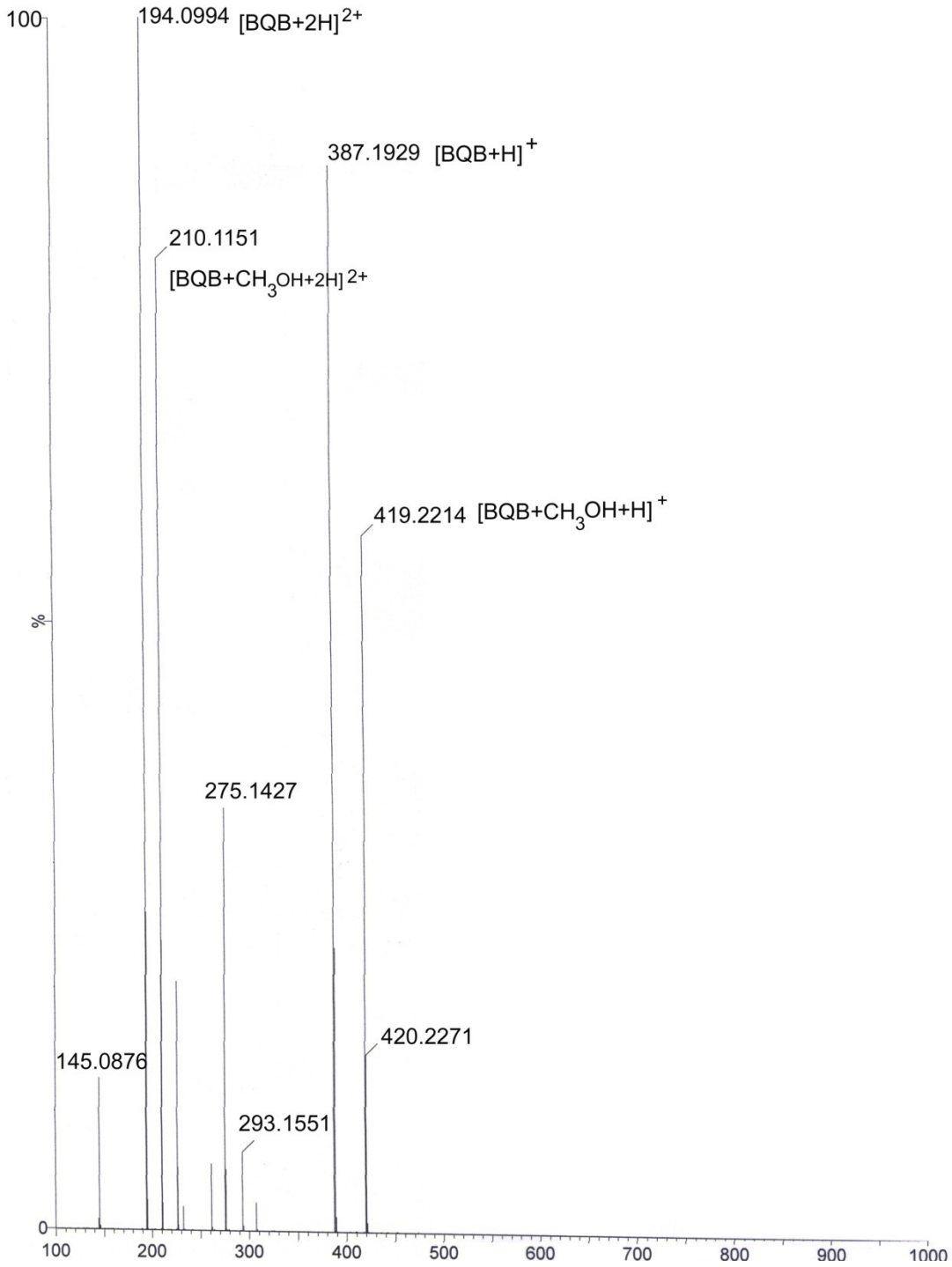

Fig. S2: ESI mass spectrum of **BQB** in methanol

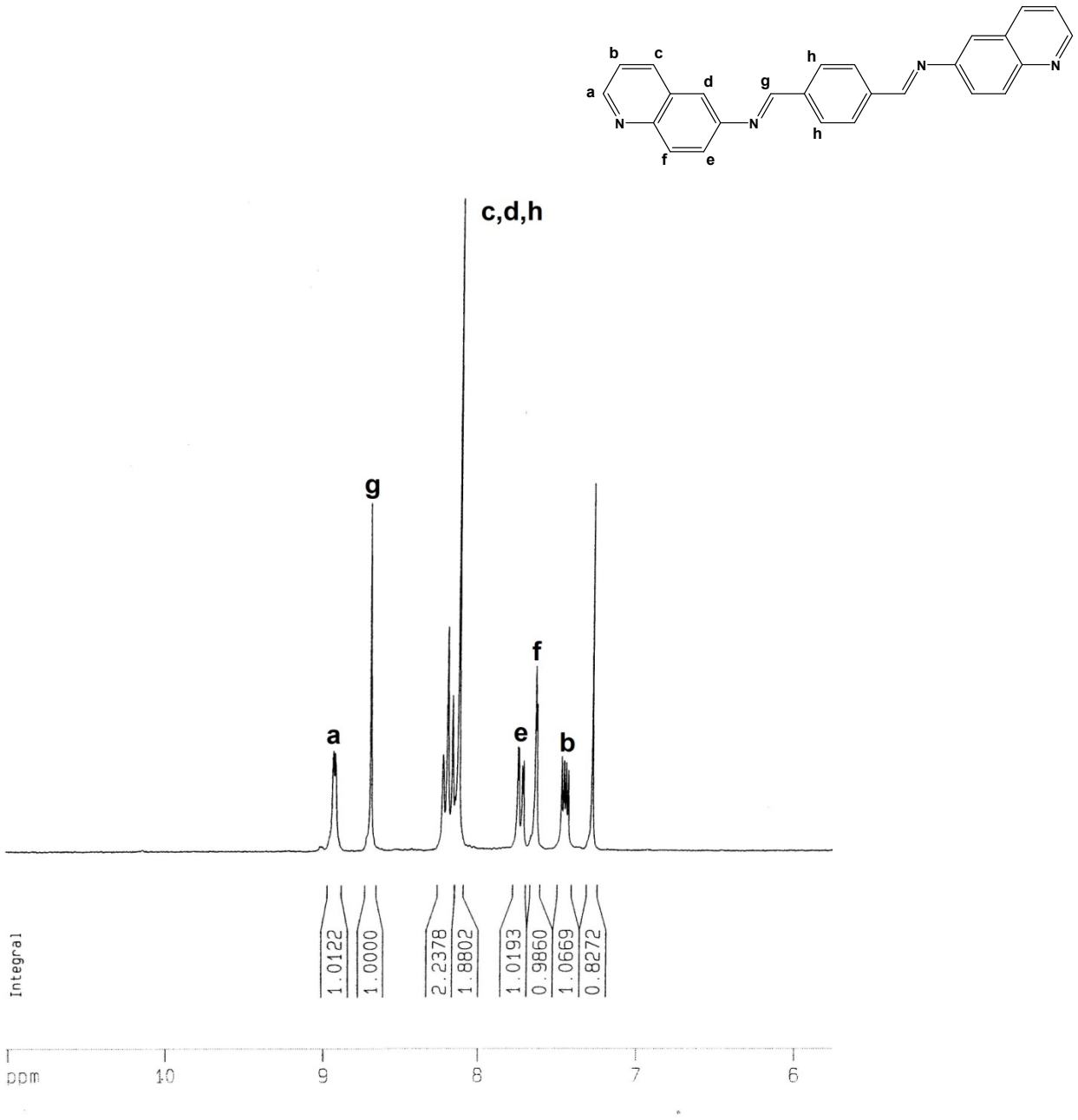

Fig. S3: ^{1}H NMR of **BQB** recorded in $CDCl_3$.

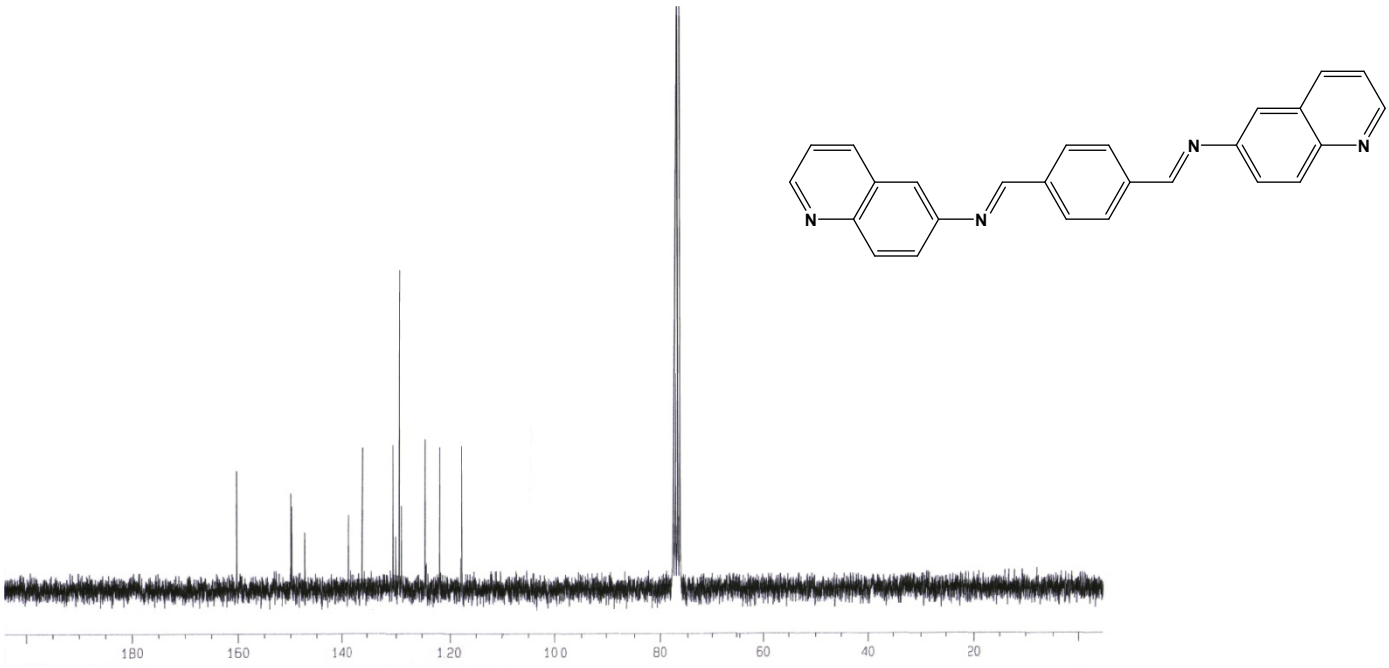

Fig. S4: ^{13}C NMR of **BQB** recorded in $CDCl_3$.

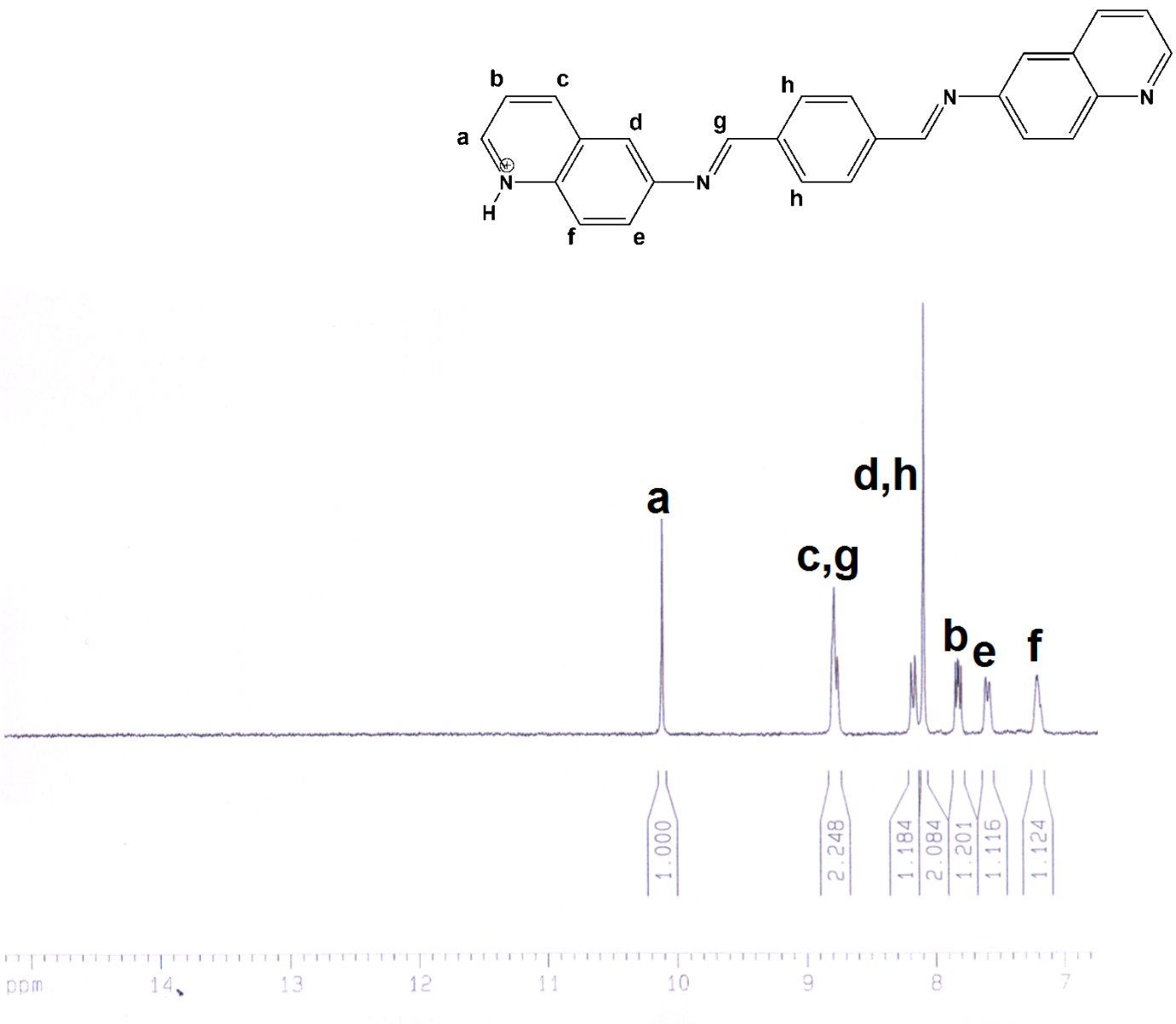

Fig. S5: ^{1}H NMR of **BQB** in the presence of H^{+} in DMSO-d_6.

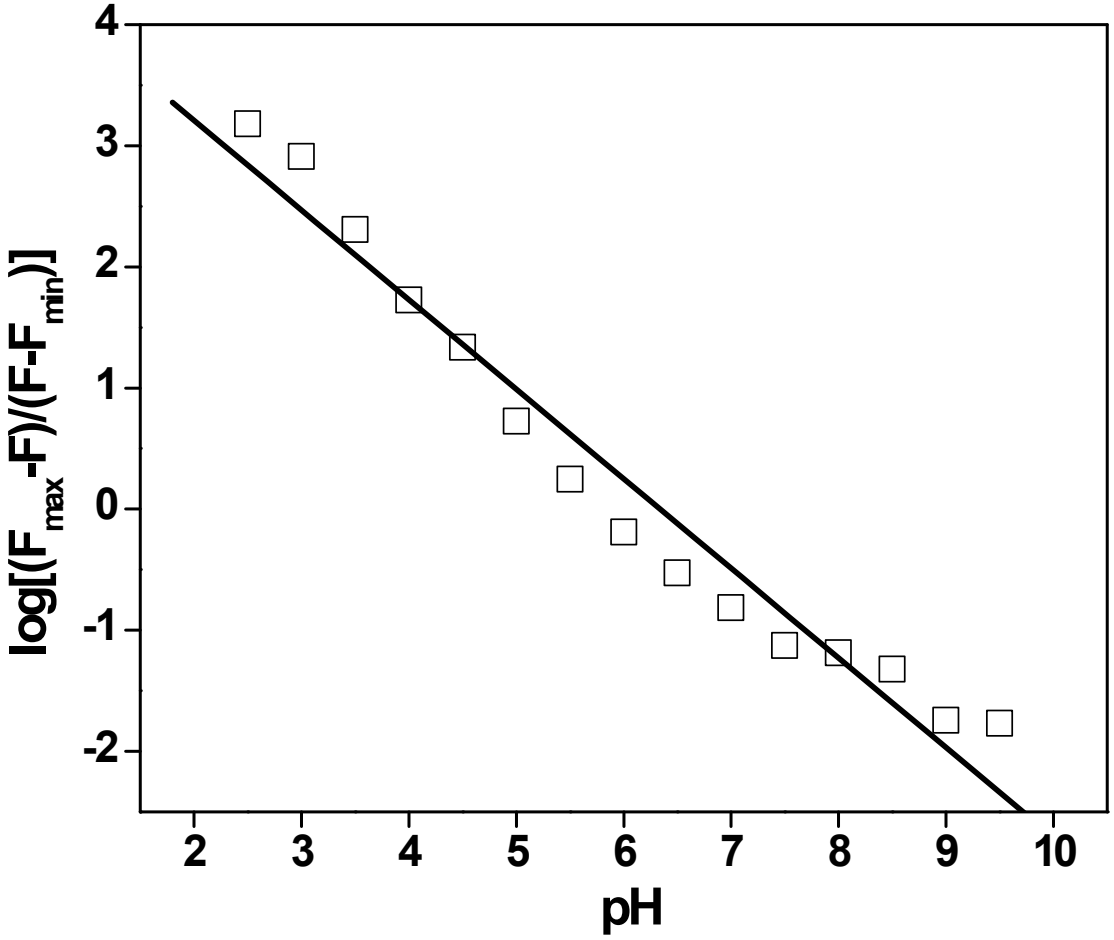

Fig. S6: Plot of $\log[(F_{max}-F)/(F-F_{min})]$ *vs* pH.

The pK_a of **BQB** has been measured using the Henderson–Hasselbach type mass action equation $\log\{(F_{max}–F)/(F–F_{min})\} = pH–pK_a$, where F_{max}, F_{min}, F represent the maximum, minimum and observed fluorescence intensity at a given pH value, respectively and it is found to be 6.3.

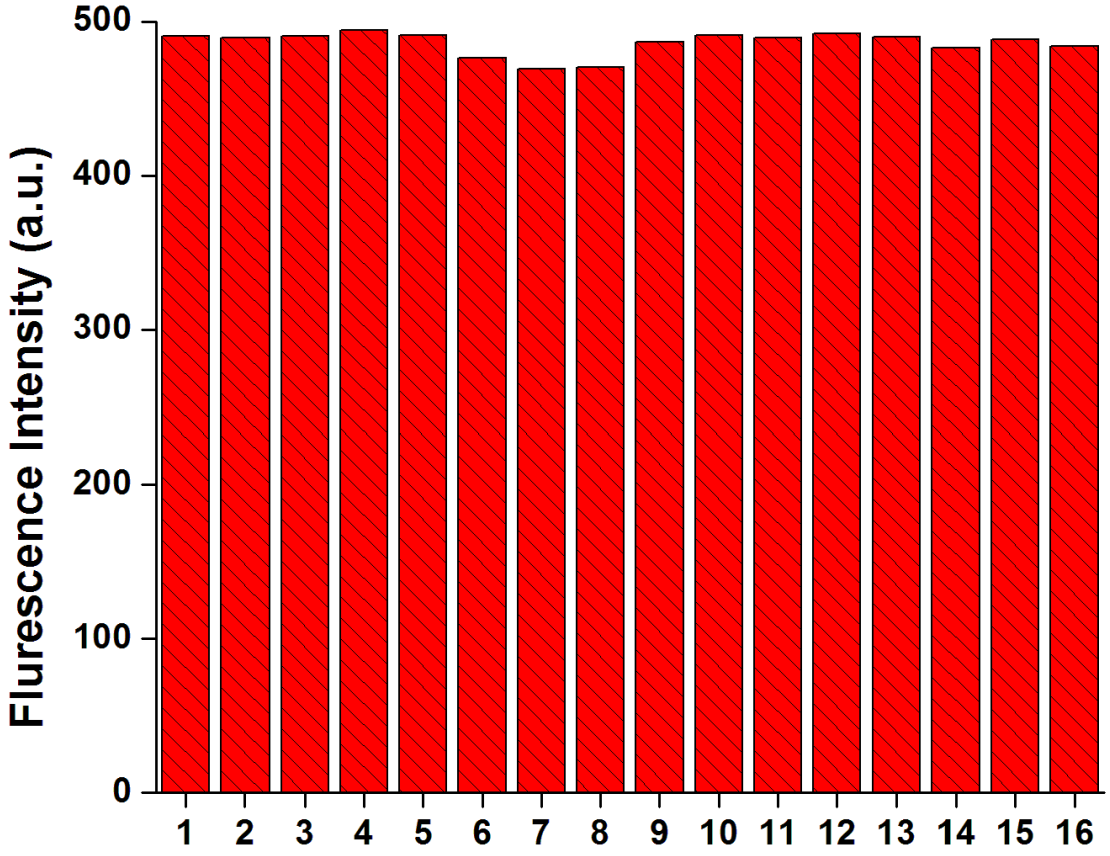

Fig. S7: Comparison of fluorescence response of **BQB** at pH 7.5 towards different ions at 25 ºC (λ_{ex}: 380 nm); 1, blank; 2, Na^{+}; 3, K^{+}; 4, Zn^{2+}; 5, Mg^{2+}; 6, Cu^{2+}; 7, Mn^{2+}; 8, Fe^{3+}; 9, Co^{2+}; 10, Ca^{2+}; 11, Ni^{2+}; 12, NO_3^{-}; 13, Cl^{-}; 14, SO_4^{2-}; 15, PO_4^{3-}; 16, BO_3^{3-}.

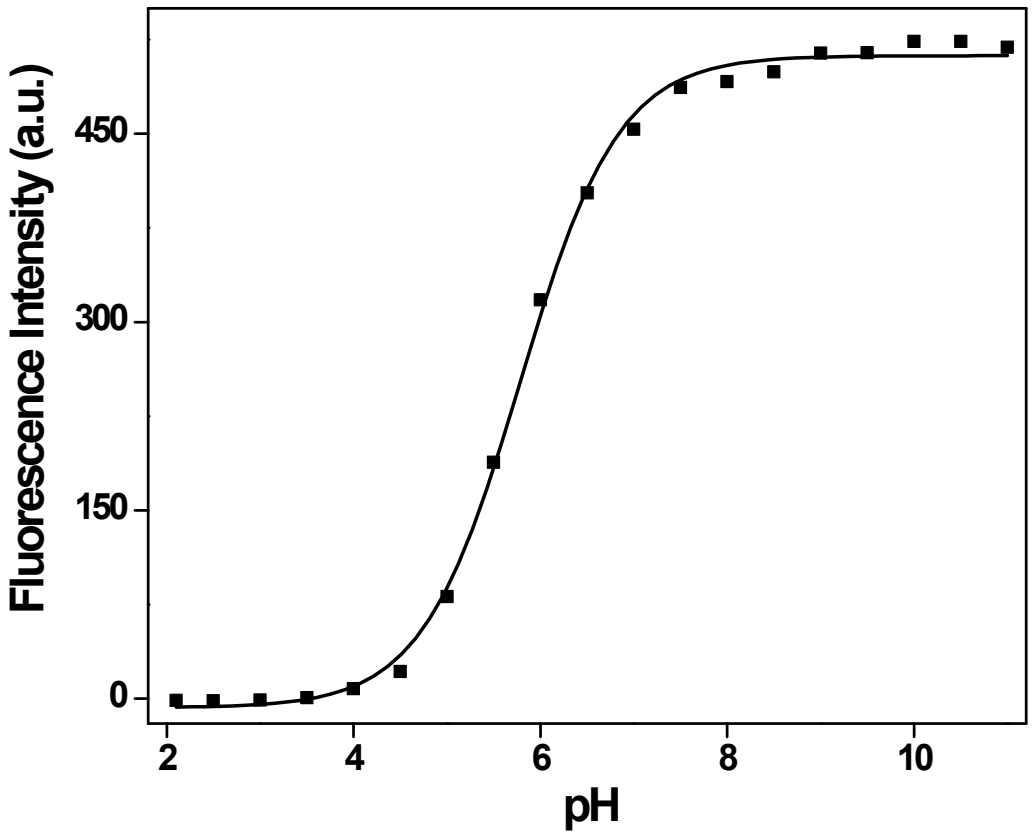

Fig. S8: Sigmoidal curve obtained by plotting Fluorescence Intensity of **BQB** against pH.

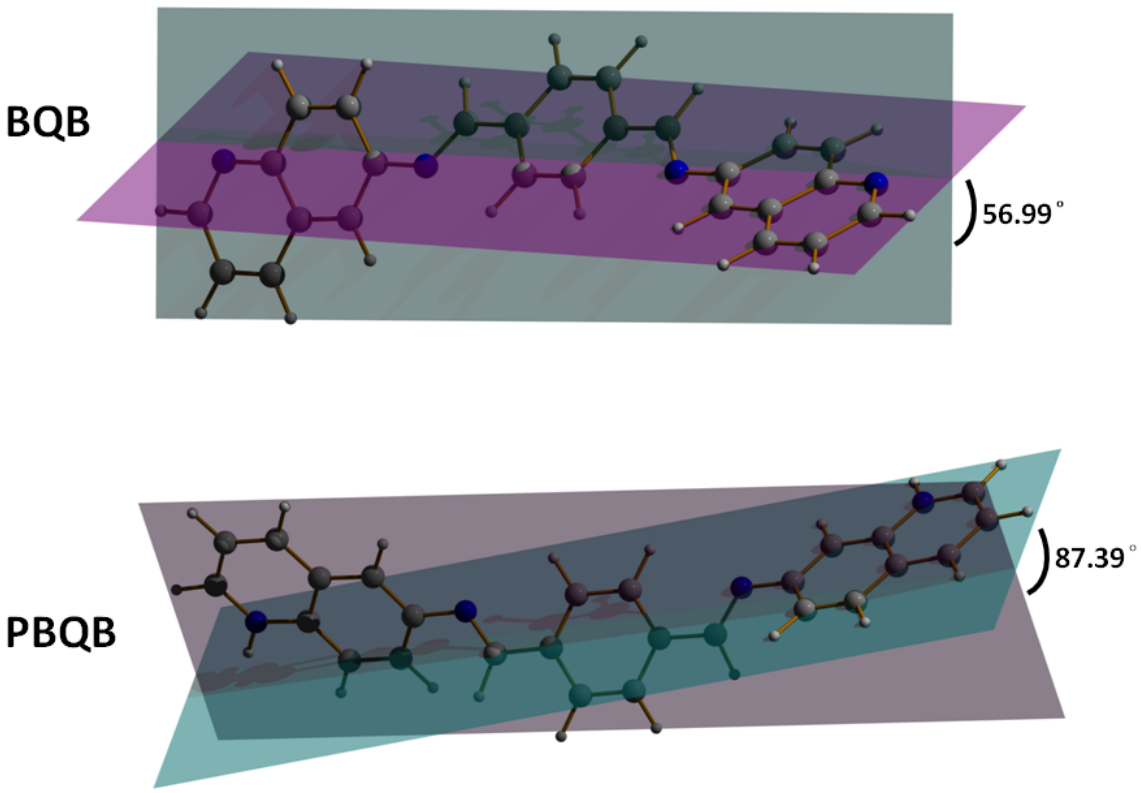

Fig. S9: Angle deviation between two optimized structures

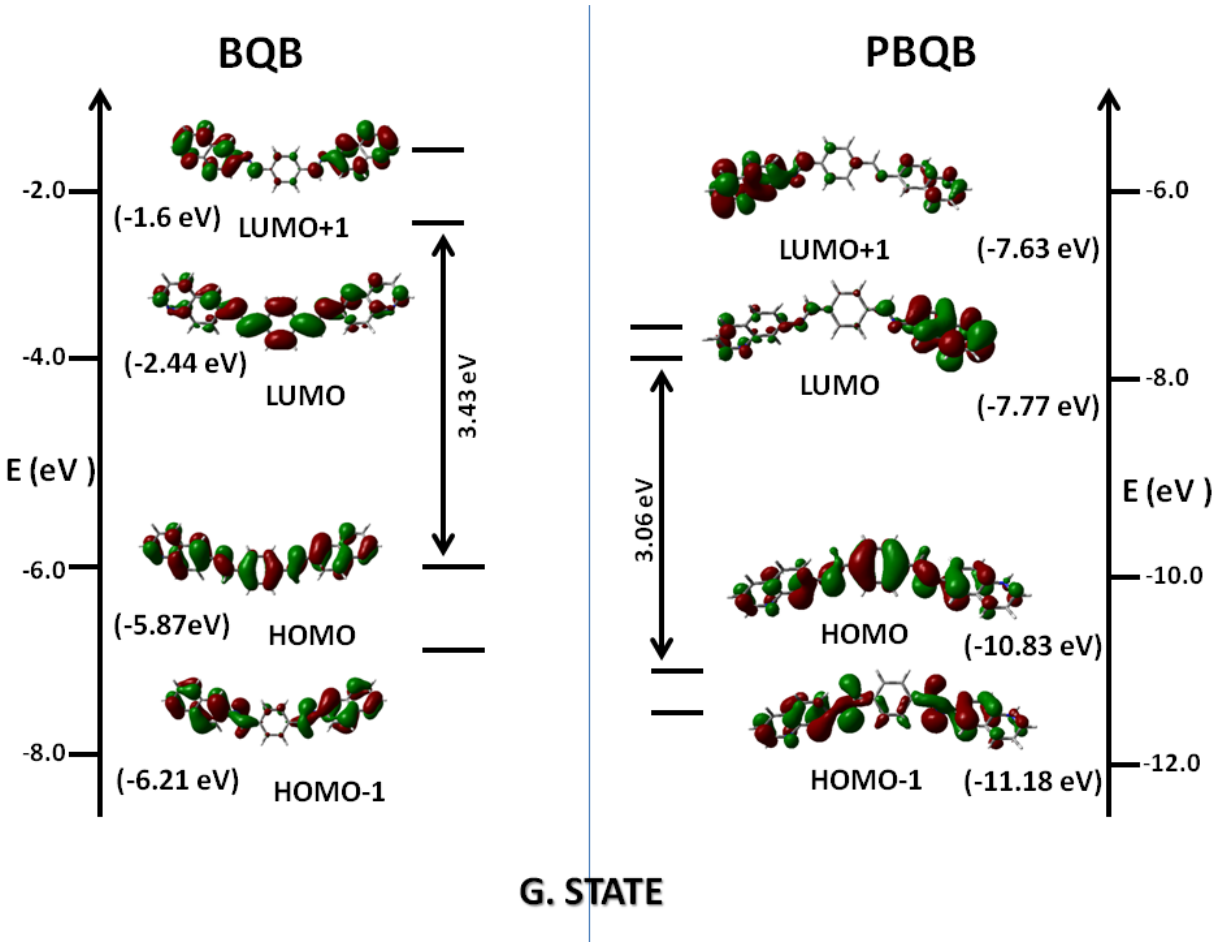

Fig. S10: Frontier MOs along with their HOMO LUMO energy gap of **BQB** and **PBQB**

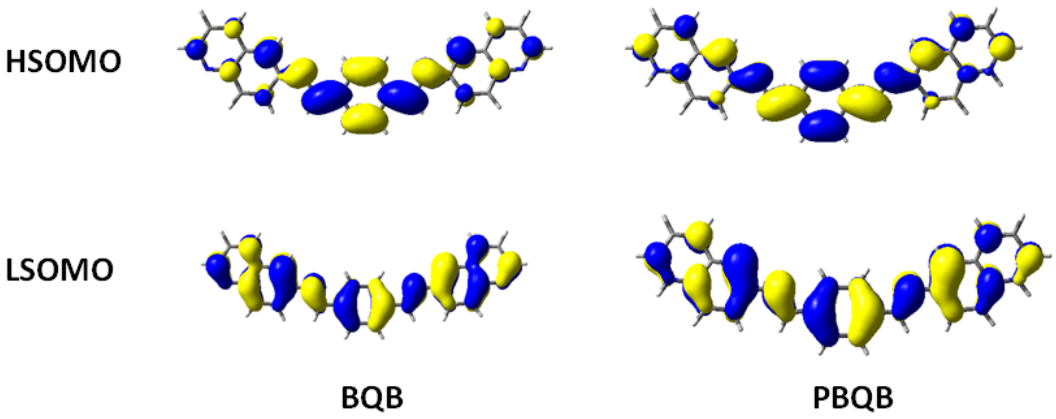

Fig. S11: Isodensity surface plots of the highest and lowest singly occupied molecular orbitals, HSOMO and LSOMO for the compounds BQB and PBQB at their T_1 state geometry

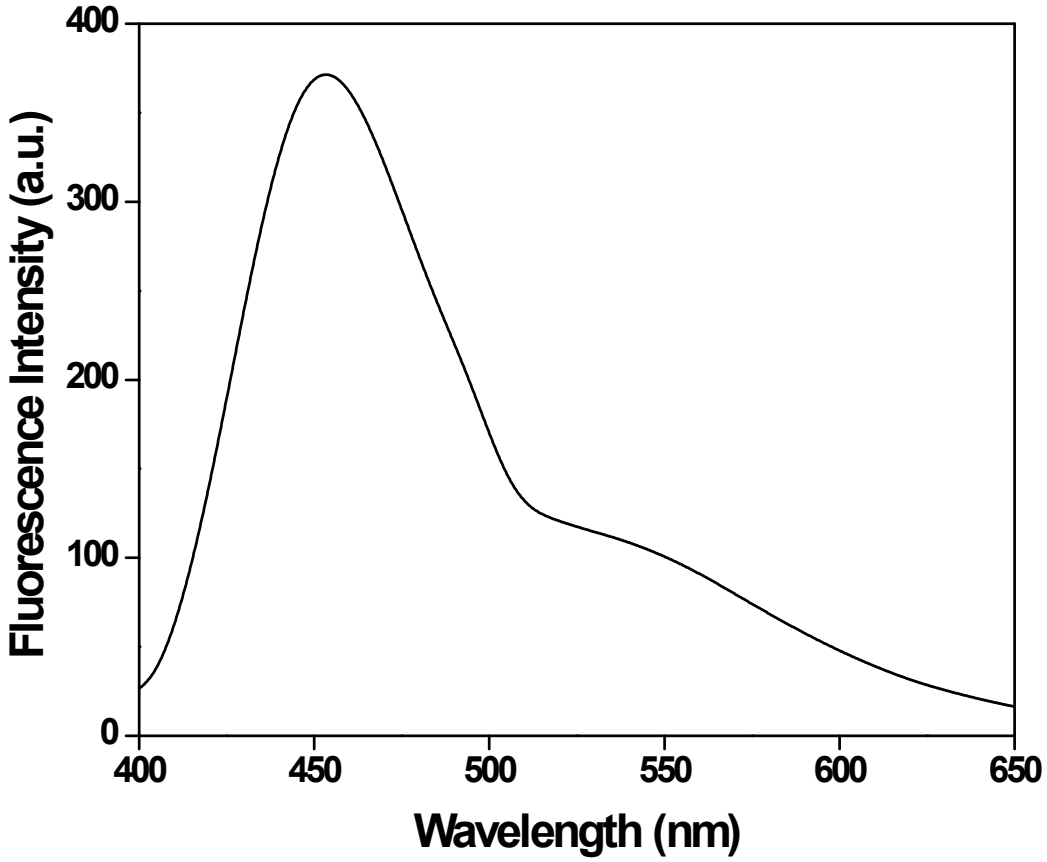

Fig. S12: Fluorescence spectrum of water of river Ganga in the presence of **BQB** (1×10^{-4} M) at room temperature (Excitation: 380 nm)

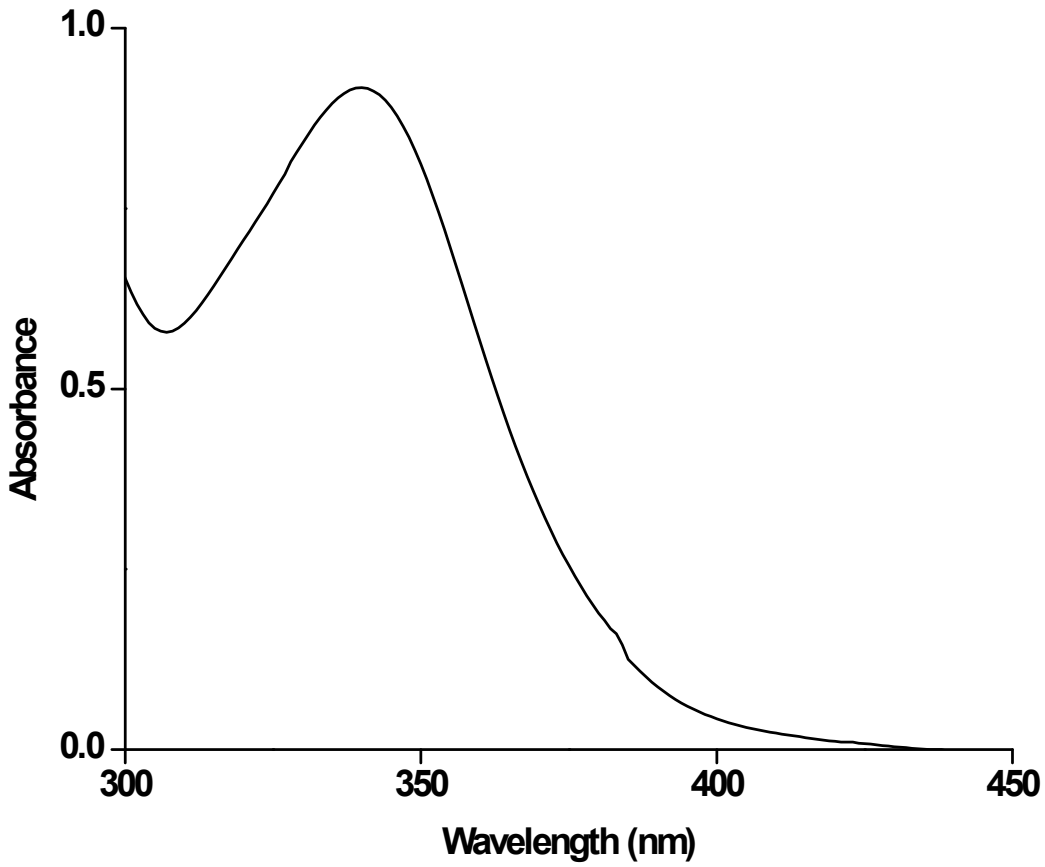

Fig. S13: Absorption spectrum of **BQB** (1×10^{-4} M) in water of river Ganga at room temperature

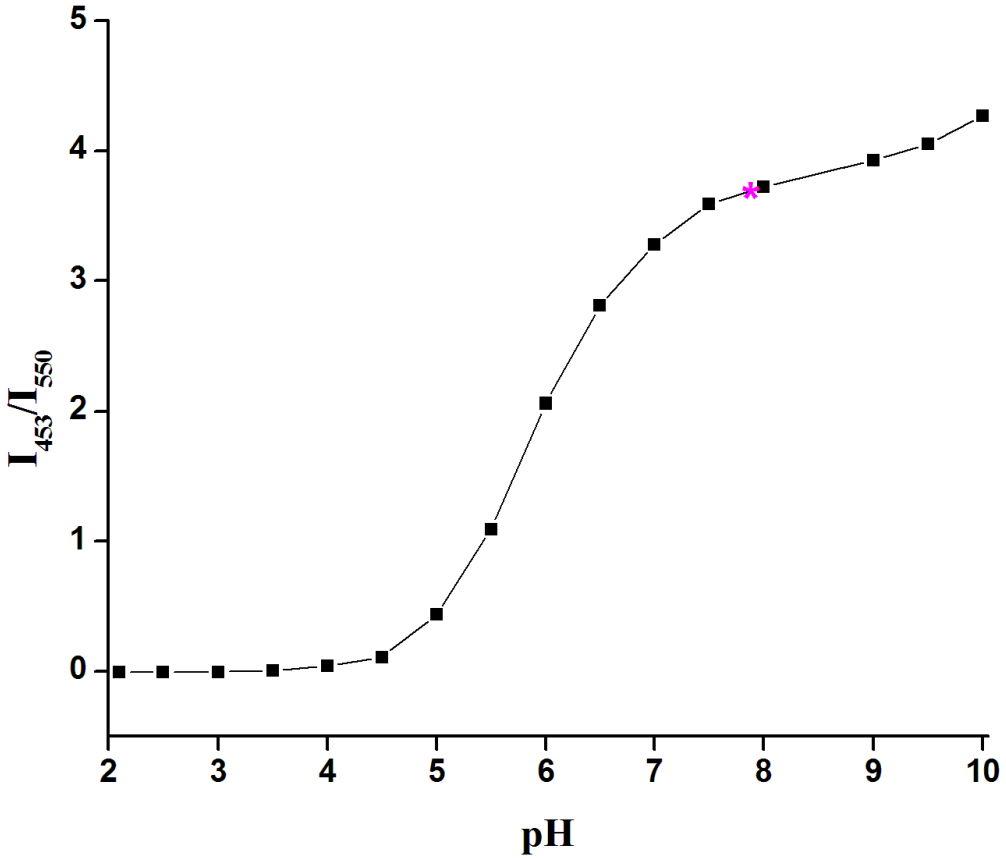

Fig. S14: Plot of ratio of fluorescence intensities of **BQB** in river water at 453 nm and 550 nm i.e. I_{435}/I_{550} *vs.* pH. I_{435}/I_{550} value of river water with **BQB** corresponds to pH 7.88