ESI

9-*N*-alkylaminomethylanthracene probes for selective fluorescence sensing of pentafluorophenol

Anup Pandith, Ashwani Kumar and Hong-Seok Kim*

Department of Applied Chemistry, School of Applied Chemical Engineering, Kyungpook National University, Daegu 702-701, Republic of Korea

Corresponding author: Tel.:+82 53 9505588; fax: +82 53 9506594.

E-mail address: kimhs@knu.ac.kr

Contents:

Preparation of the buffer solution. The solid standard buffer was used without purification. Respective solid buffers dissolved in EtOH-H_2O mixture (9:1 v/v) and the exact pH value was obtained by adjusting the using solution of 0.001 M NaOH. All pH value was measured in digital pH meter instrument.

pH Dependent fluorescence studies: pH was maintained using the following solutions [all 0.01 M in EtOH-H_2O (9:1)] : trichloroacetate (pH 1); dichloroacetate (pH 2); chloroacetate (pH 3); acetate (pH 4 and 5); MES (pH 6); HEPES (pH 7 and 8); CHES (pH 9); CAPS (pH 10 and 11); TBAH (pH 12); NaOH (pH 13);

Abbreviations: Tetrabutylammoniumhydroxide (TBAH), 4-morpholineethanesulfonic acid sodium salt (MES), 4-(2-hydroxyethyl)piperazine-1-ethanesulfonicacid (HEPES), 2-(cyclohexylamino)ethanesulfonicacid (CHES), 3-cyclohexylamino-1-propanesulfonic acid (CAPS).

The fluorescence readings were obtained with maintaining constant pH using various standard buffer solutions*. Each fluorescence reading was taken and recorded after getting 3 concordant values.

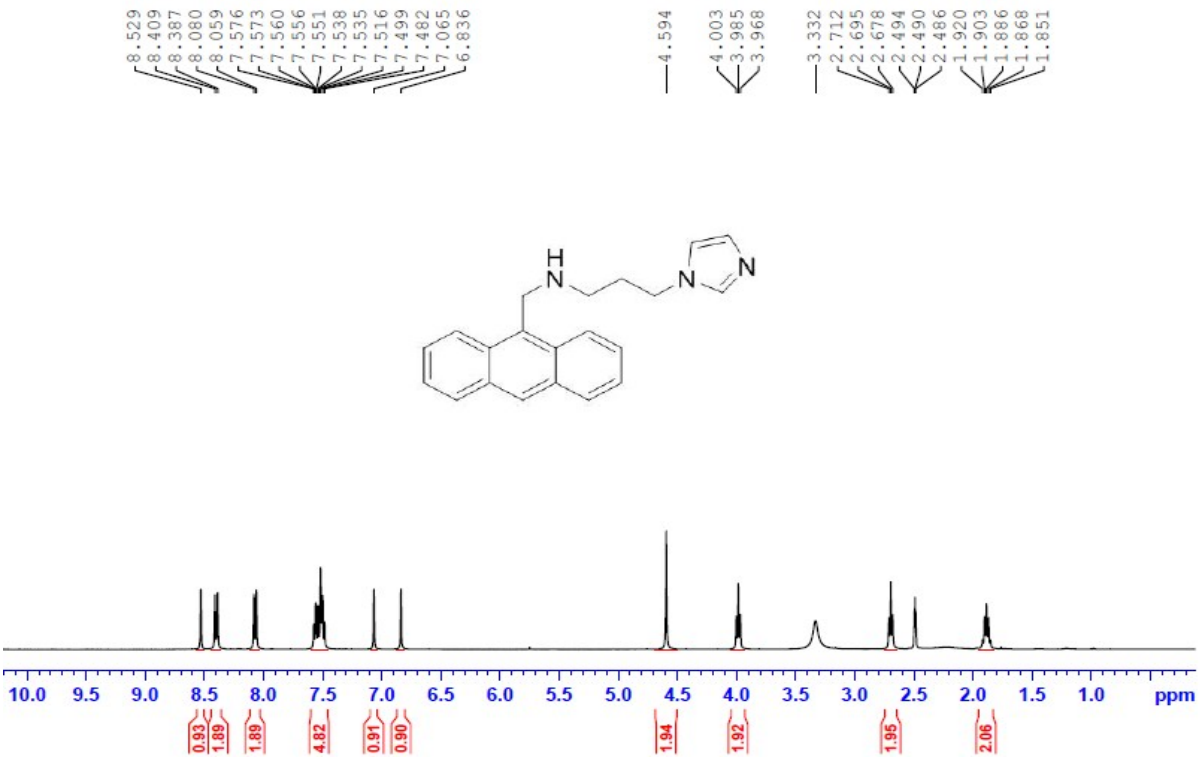


Fig. 1. ^{1}H NMR of probe **1**

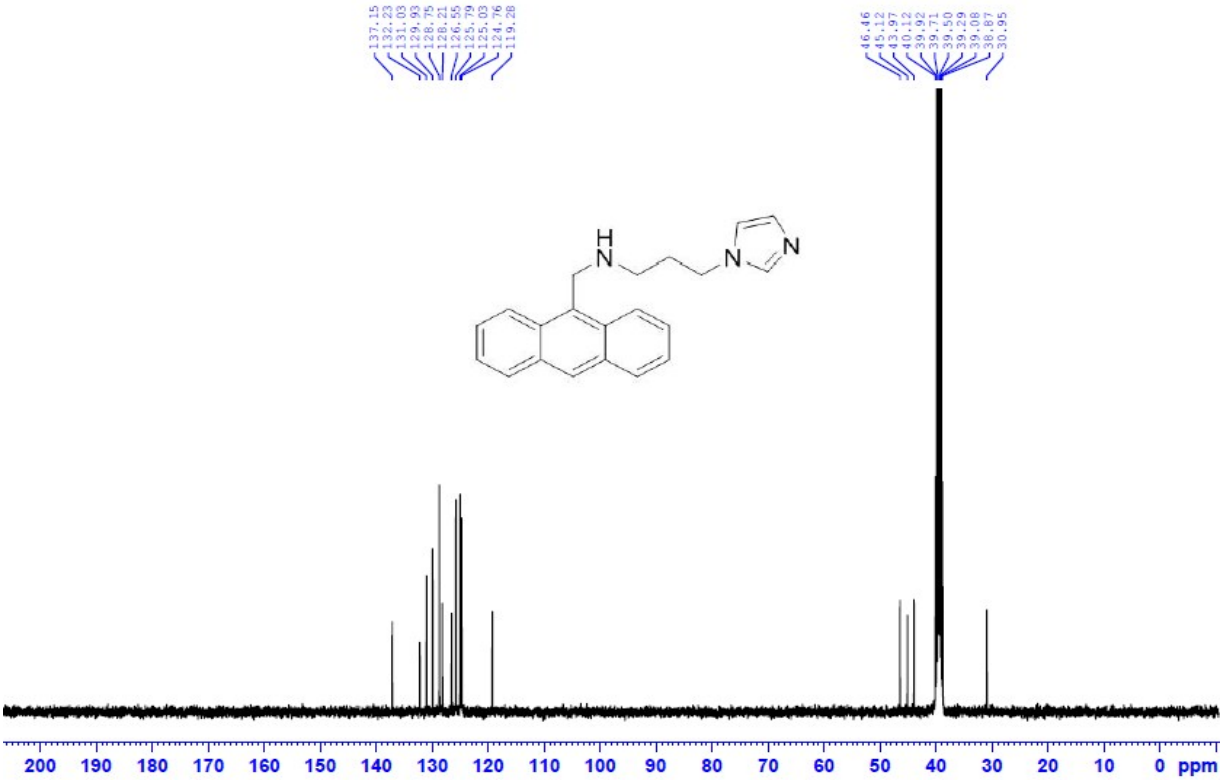


Fig. 2. ^{13}C NMR of probe **1**

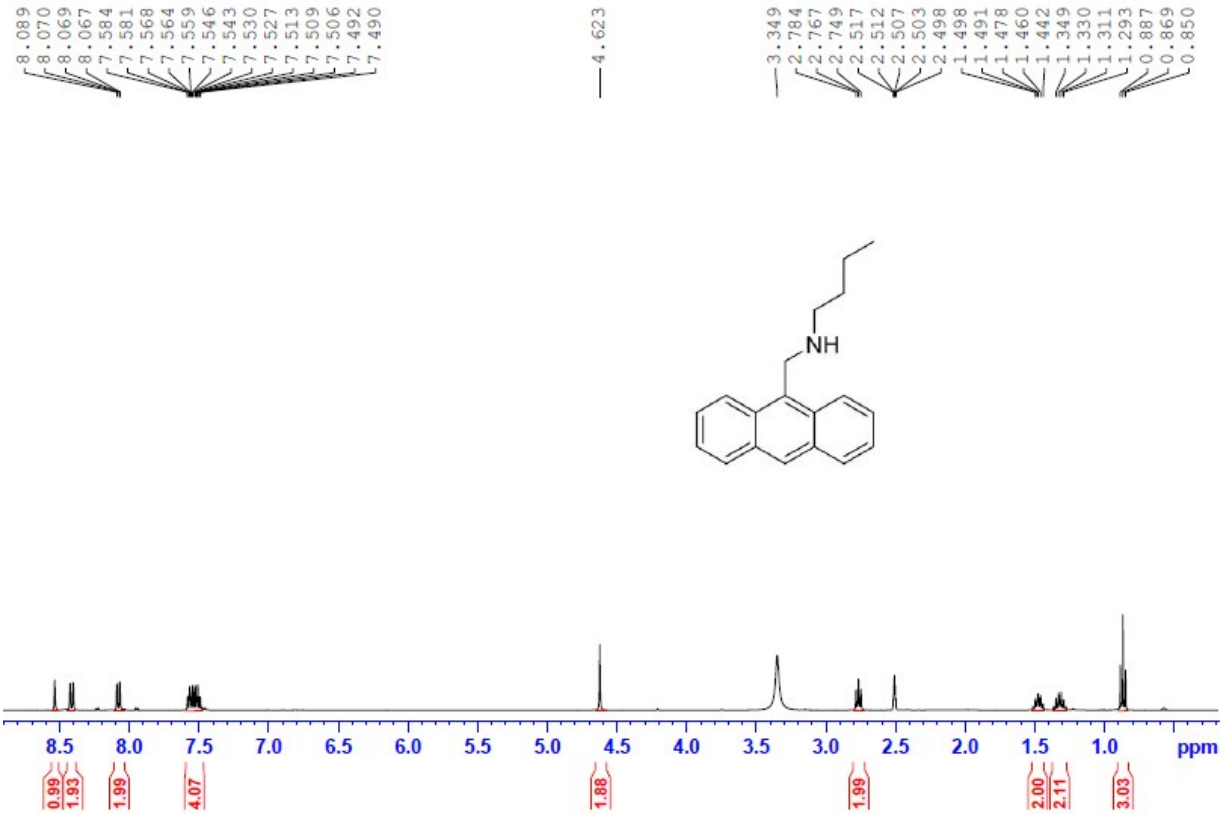


Fig. 3. ^{1}H NMR of probe **2**

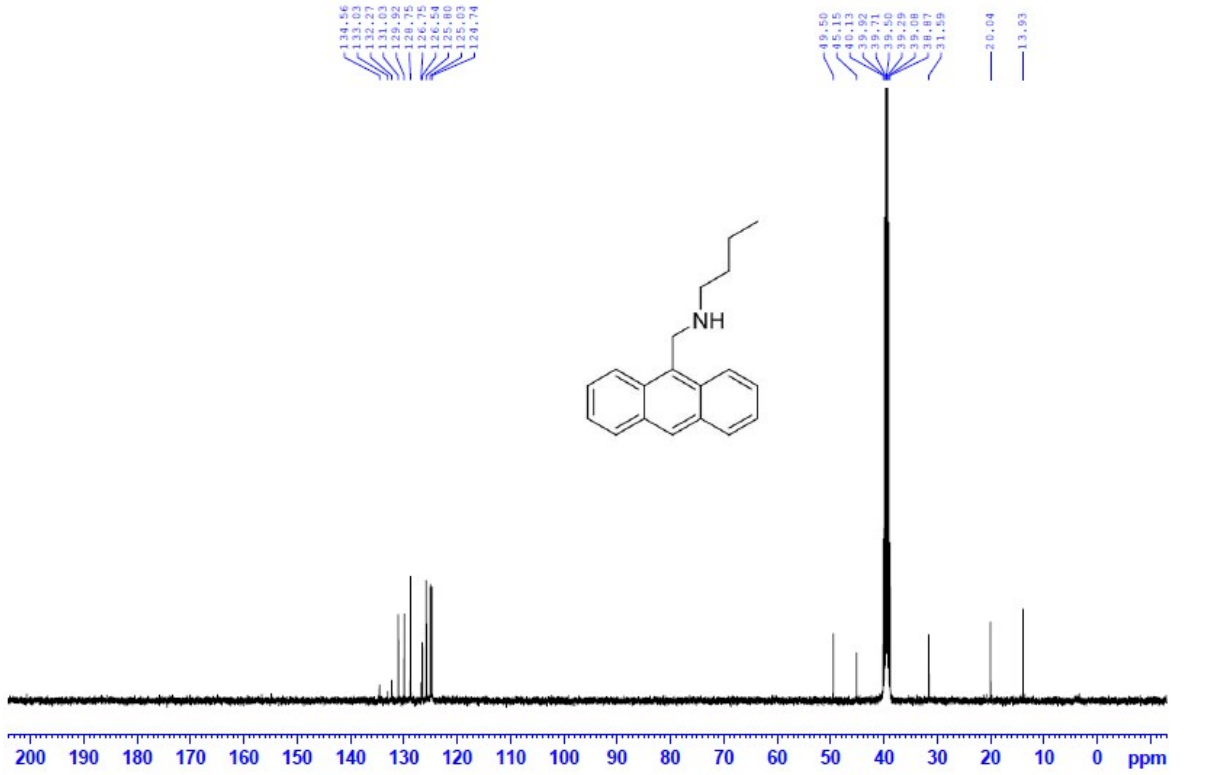


Fig. 4. ^{13}C NMR of probe **2**

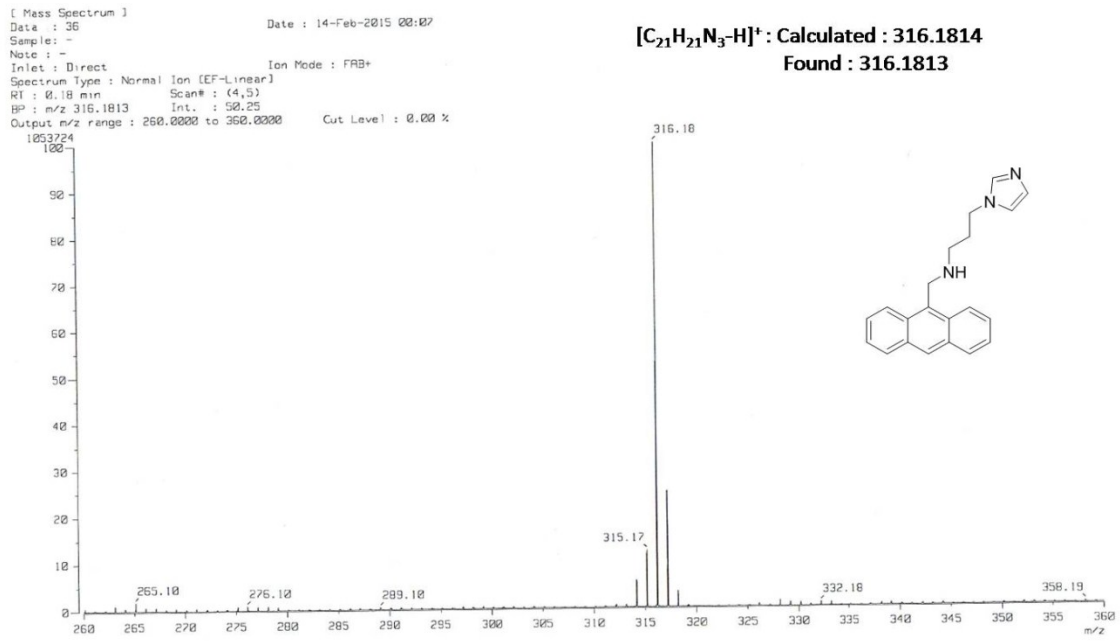


Fig. 5. HR-FAB mass of probe **1**

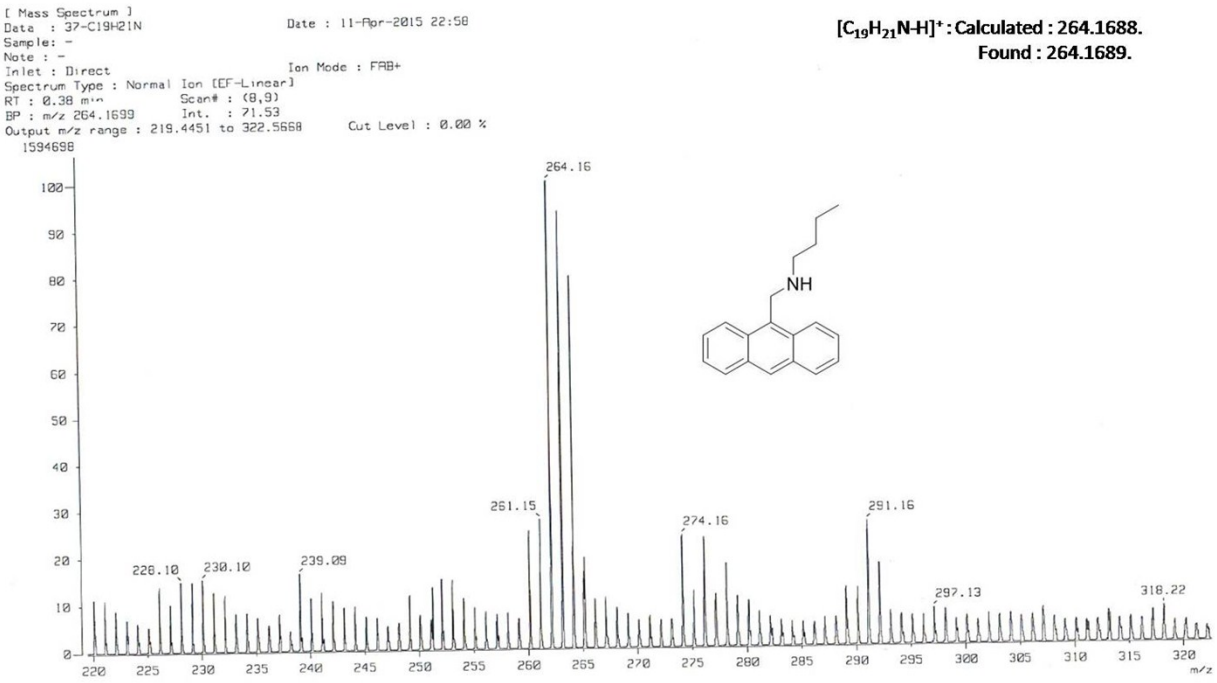


Fig. 6. HR-FAB mass of probe **2**

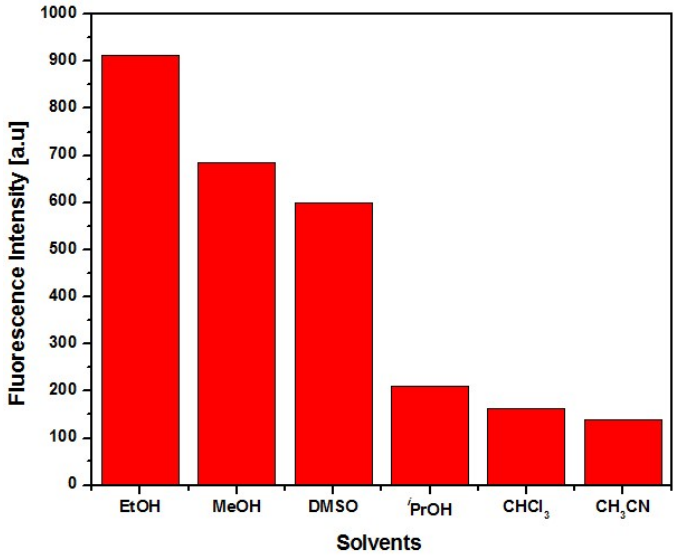


Fig. S1. Fluorescence enhancement of probe **1** (20 μM) with PFP (20 μM) in different solvent system: λ_{ex} = 365 nm, λ_{em} = 417 nm.

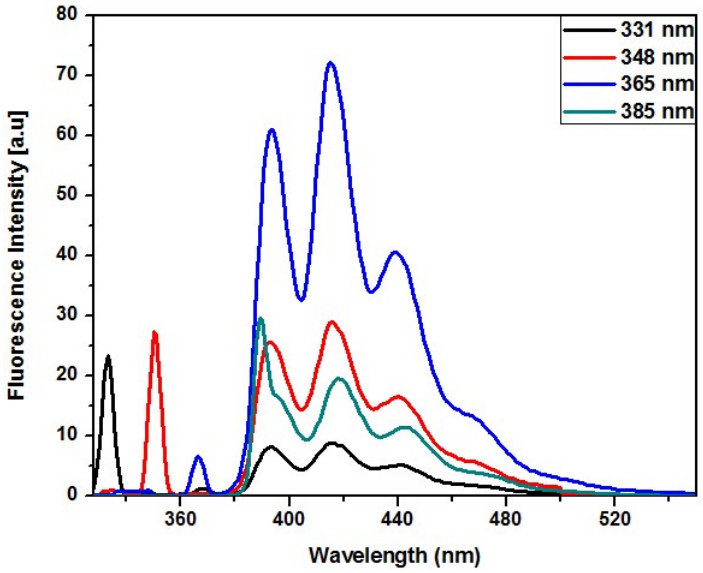


Fig. S2. Fluorescence emission behaviour of probe **1** (20 μM) at different excitation wavelength in EtOH.

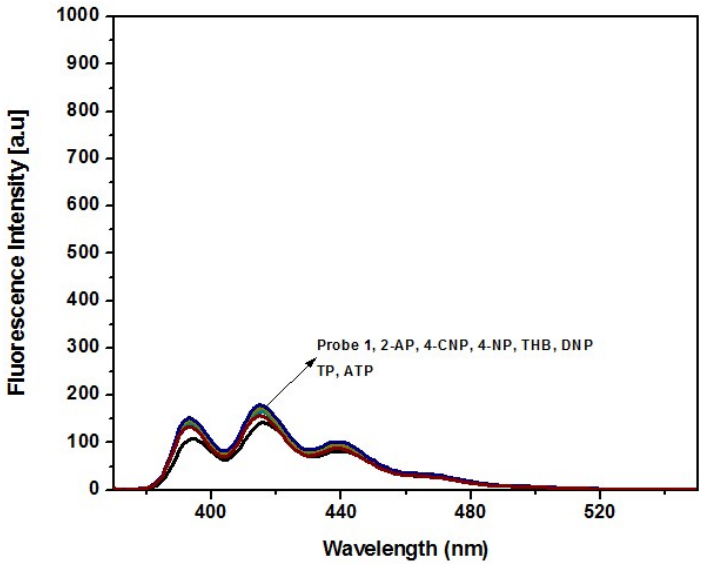


Fig. S3. Fluorescence studies of probe **1** (20 μM) with various miscellaneous phenol derivatives (200 μM) in EtOH: λ_{ex} = 365 nm.

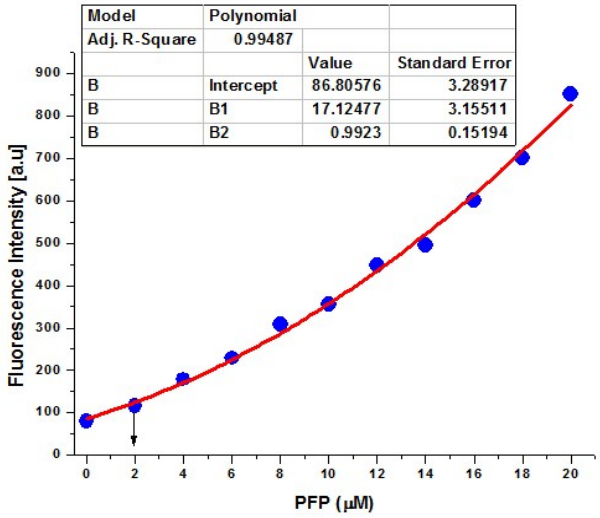


Fig. S4. Fluorescence enhancement response of probe **1** (20 μM) with various concentrations of PFP in EtOH at pH = 7.0 (HEPES): λ_{ex} = 365 nm and λ_{em} = 417 nm.

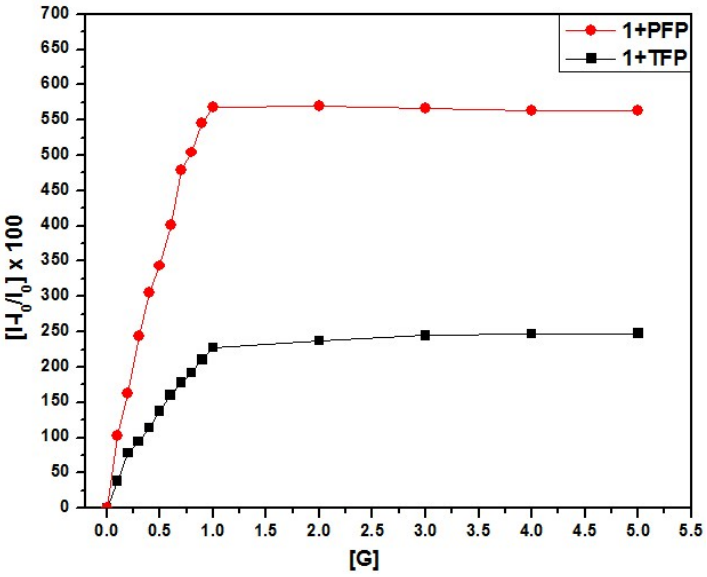


Fig. S5. Normalized fluorescence enhancement ratio $[I-I_0/I_0]$ x 100, vs [G]*, where I_0 represents the fluorescence emission of probe **1**, observed with 0.0 to 5.0 eq. of *PFP and *TFP at λ_{ex} = 365 nm, λ_{em} = 417 nm.

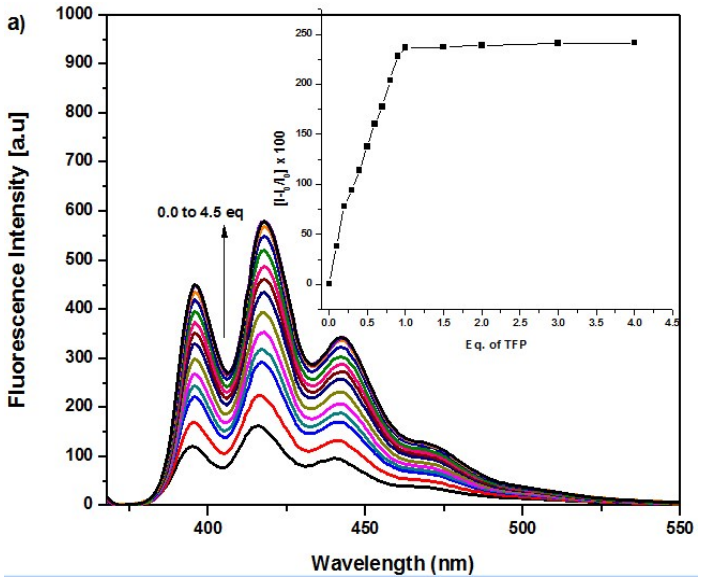


Fig. S6. a) Fluorescence titration studies of probe **1** (20 μM) with TFP (200 μM) at λ_{ex} = 365 nm in EtOH: Inset represents normalized fluorescence intensity vs eq. of TFP at λ_{em} = 417 nm.

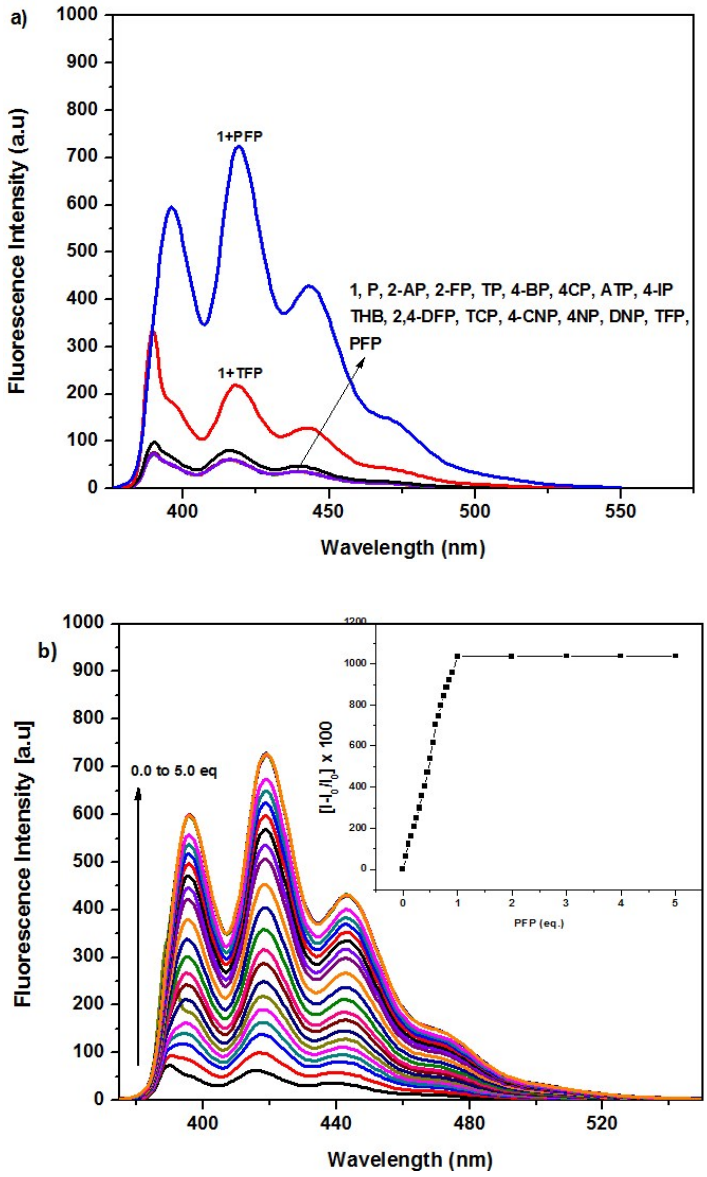


Fig. S7. a) Fluorescence spectra of probe **1** (20 μM) with various phenol derivatives (200 μM) at λ_{ex} = 385 nm in EtOH: b) Fluorescence titration spectra of probe **1** with PFP: Inset represents normalized fluorescence intensity *vs* equivalents of PFP at λ_{ex} = 385 nm and λ_{em} = 417 nm.

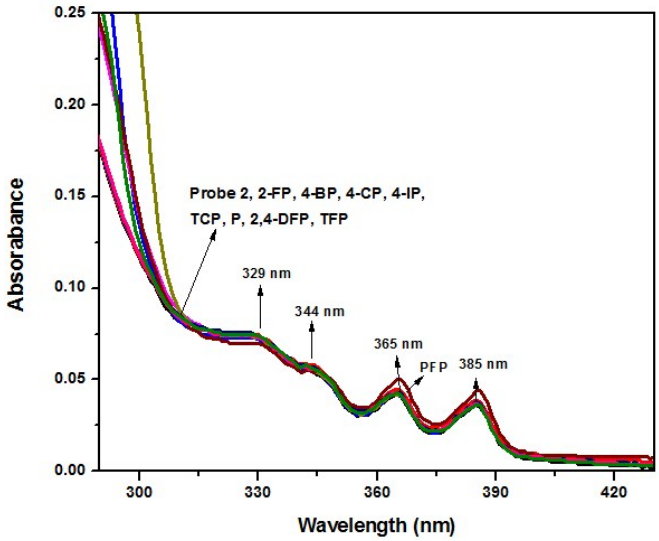


Fig. S8. a) UV-Visible spectra of probe **2** (20 μM) in EtOH with various halophenol derivatives (10 eq.)

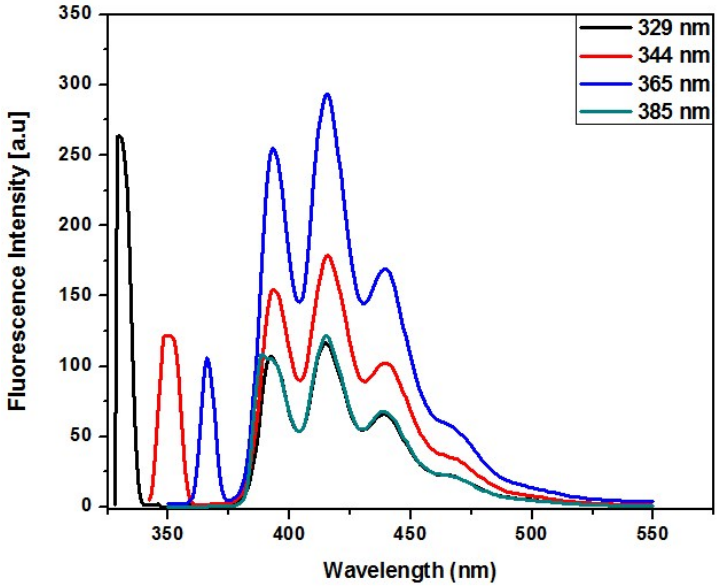


Fig. S9. Fluorescence emission behaviour of probe **2** (20 μM) at different excitation wavelength in EtOH.

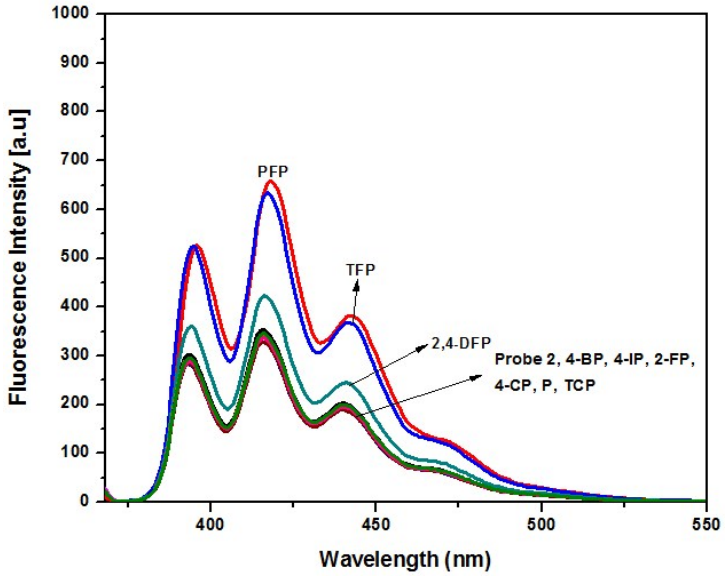
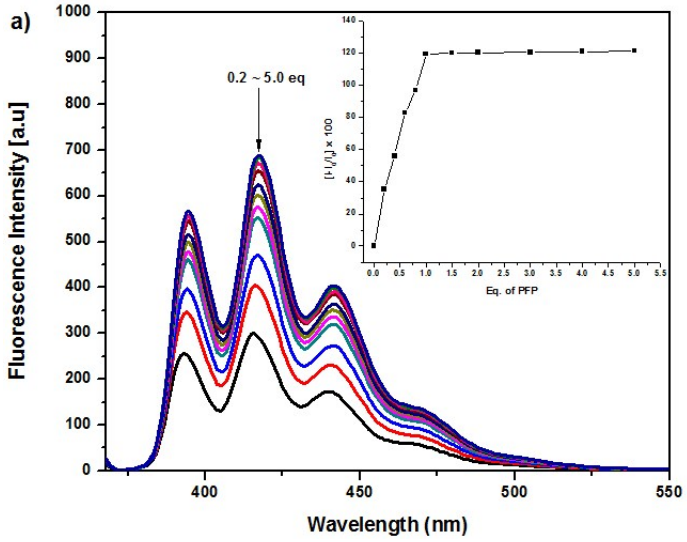


Fig. S10. Fluorescence spectra of probe **2** (20 μM) with halophenol derivatives (10 eq.): λ_{ex} = 365 nm in EtOH.



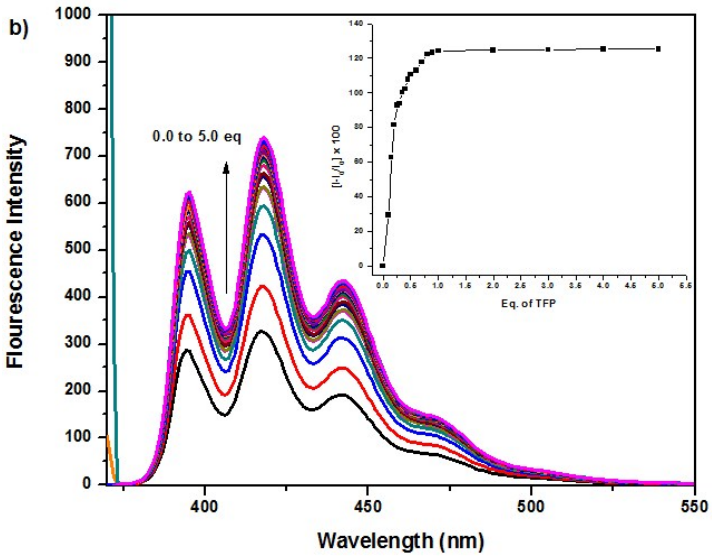


Fig. S11. a) Fluorescence titration studies of probe **2** (20 μM) with PFP (200 μM) at λ_{ex} = 365 nm in EtOH: Inset represents normalized fluorescence intensity of probe **2** *vs* equivalents of PFP at λ_{em} = 417 nm. b) Fluorescence titration studies of probe **2** (20 μM) with TFP (200 μM) at λ_{ex} = 365 nm in EtOH: Inset represent normalized fluorescence intensity of probe **2** *vs* equivalents of TFP at λ_{em} = 417 nm.

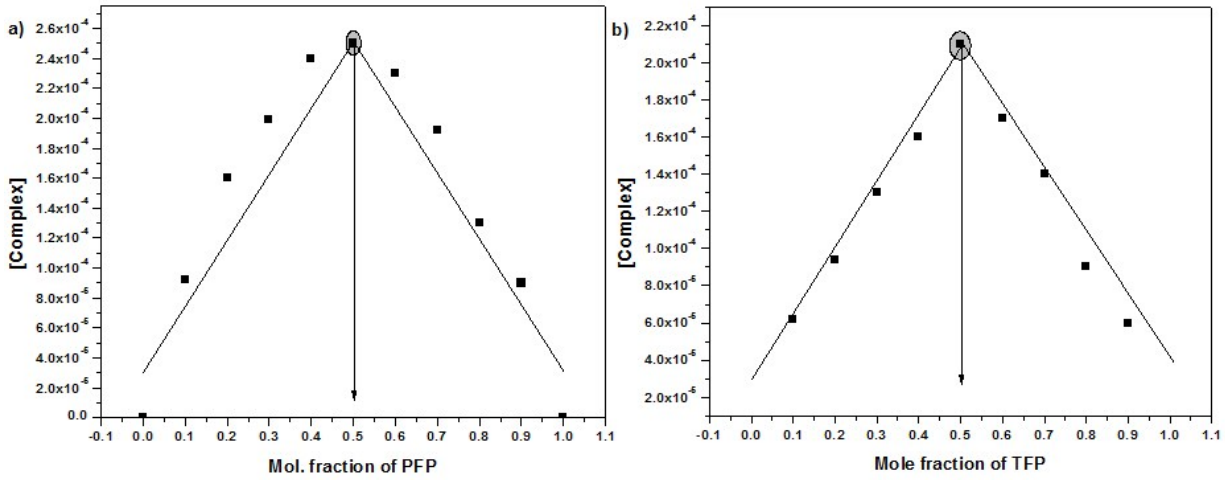


Fig. S12. Job's plot of probe **2** with a) PFP and b) TFP (20 μM) in EtOH: λ_{ex} = 365 nm, λ_{em} = 417 nm.

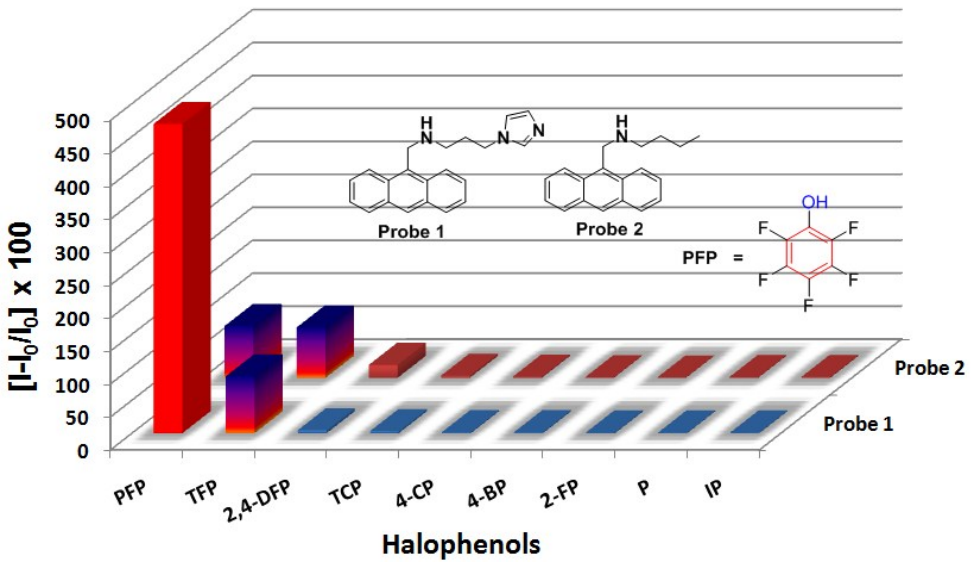


Fig. S13. Fluorescence enhancement ratio $[I-I_0/I_0]$ x 100 of probes **1** and **2** with a) PFP and b) TFP (20 μM) in EtOH: λ_{ex} = 365 nm, λ_{em} = 417 nm. I = Intensity of probe in presence of halophenols, I_0 = Intensity of probe in the absence of halophenol at 417 nm.

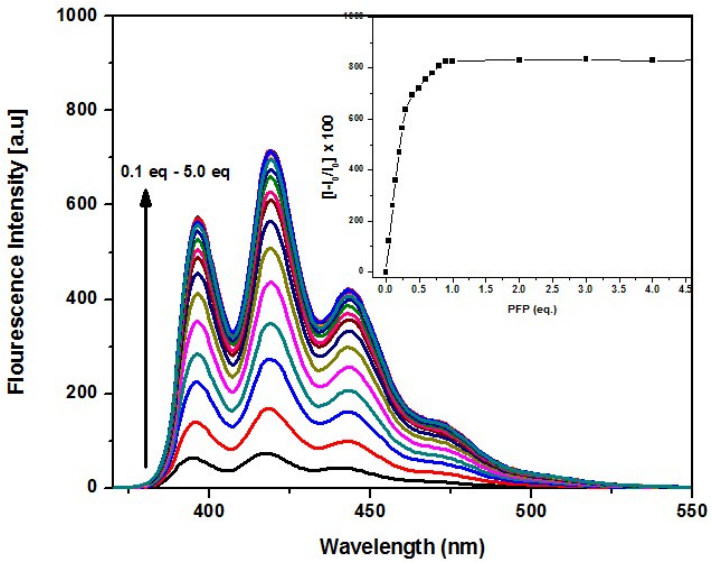


Fig. S14. Fluorescence titration spectra of probe **1** (20 μM) with PFP (200 μM) in DMSO: λ_{ex} = 365 nm: Inset represents normalised fluorescence intensity of probe **1** vs equivalents of PFP at λ_{em} = 417 nm.

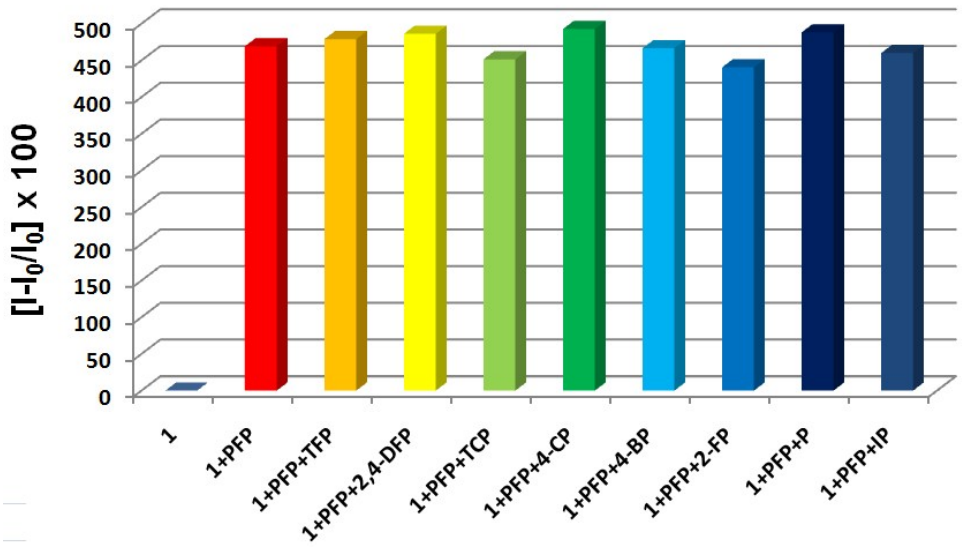


Fig. S15. Changes in relative fluorescence enhancement ratio $[I_0\text{-}I/I_0]$ x 100 of probe **1**•PFP complex in the presence of other halophenol derivatives: λ_{ex} = 365 nm, λ_{em} = 417 nm in EtOH.

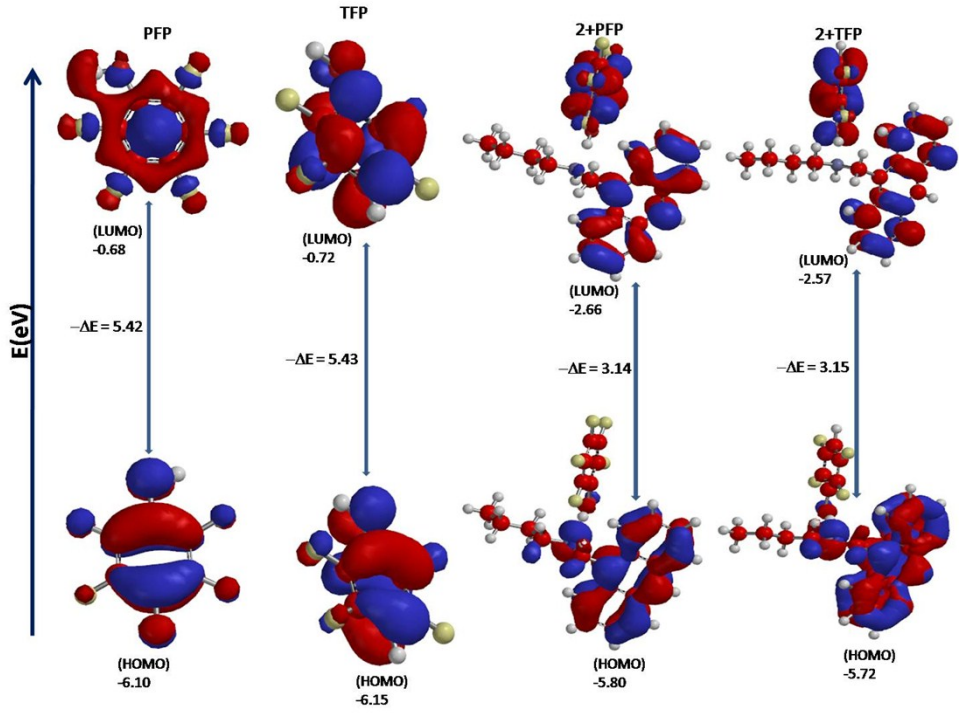


Fig. S16. HOMO and LUMO of PFP, TFP, probe **2**, **2**•PFP, and **2**•TFP calculated by the B3LYP/6-31G* method in EtOH medium.

Association constant calculations

The fluorescence titration data were programmed in *gnuplot ver. 4* software as mentioned below*.Thus obtained intensity was fitted automatically (reduced chisquare method) with least error bound.

***Equation 2.**

$$I = I_0 + I_\infty K_n [Guest]^n / 1 + K_n [Guest]^n$$

I = Intensity (calculated as a function of Y).
I_0 = Intensity at host only.
I_∞**=** Intensity at the saturation.
n value depending on the stoichiometric ratio's between host and guest ex: binding is 1:1 then n=1, 1:2 then n=2 and so on.