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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

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**Preparation of the buffer solution.** The solid standard buffer was used without purification. Respective solid buffers dissolved in EtOH-\(\text{H}_2\text{O}\) 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-\(\text{H}_2\text{O}\) (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: $\lambda_{ex} = 365$ nm, $\lambda_{em} = 417$ 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: $\lambda_{ex} = 365$ nm.

<table>
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<th>Model</th>
<th>Polynomial</th>
<th>Adj. R-Square</th>
<th>$B$</th>
<th>$\text{Value}$</th>
<th>$\text{Standard Error}$</th>
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<td>B2</td>
<td>0.9323</td>
<td>0.15194</td>
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</tr>
</tbody>
</table>

Fig. S4. Fluorescence enhancement response of probe 1 (20 μM) with various concentrations of PFP in EtOH at pH = 7.0 (HEPES): $\lambda_{ex} = 365$ nm and $\lambda_{em} = 417$ nm.
Fig. S5. Normalized fluorescence enhancement ratio \([I-I_0/I_0] \times 100\), 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 \(\lambda_{ex} = 365\) nm, \(\lambda_{em} = 417\) nm.

Fig. S6. a) Fluorescence titration studies of probe 1 (20 \(\mu\)M) with TFP (200 \(\mu\)M) at \(\lambda_{ex} = 365\) nm in EtOH: Inset represents normalized fluorescence intensity vs eq. of TFP at \(\lambda_{em} = 417\) nm.
Fig. S7. a) Fluorescence spectra of probe 1 (20 μM) with various phenol derivatives (200 μM) at \( \lambda_{ex} = 385 \text{ nm} \) in EtOH: b) Fluorescence titration spectra of probe 1 with PFP: Inset represents normalized fluorescence intensity vs equivalents of PFP at \( \lambda_{ex} = 385 \text{ nm} \) and \( \lambda_{em} = 417 \text{ nm} \).
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.): $\lambda_{ex} = 365$ nm in EtOH.
**Fig. S11.** a) Fluorescence titration studies of probe 2 (20 μM) with PFP (200 μM) at $\lambda_{ex} = 365$ nm in EtOH: Inset represents normalized fluorescence intensity of probe 2 vs equivalents of PFP at $\lambda_{em} = 417$ nm. b) Fluorescence titration studies of probe 2 (20 μM) with TFP (200 μM) at $\lambda_{ex} = 365$ nm in EtOH: Inset represent normalized fluorescence intensity of probe 2 vs equivalents of TFP at $\lambda_{em} = 417$ nm.

**Fig. S12.** Job’s plot of probe 2 with a) PFP and b) TFP (20 μM) in EtOH: $\lambda_{ex} = 365$ nm, $\lambda_{em} = 417$ nm.
**Fig. S13.** Fluorescence enhancement ratio \([I-I_0/I_0] \times 100\) of probes 1 and 2 with a) PFP and b) TFP (20 μM) in EtOH: \(\lambda_{ex} = 365\) nm, \(\lambda_{em} = 417\) 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: \(\lambda_{ex} = 365\) nm: Inset represents normalised fluorescence intensity of probe 1 vs equivalents of PFP at \(\lambda_{em} = 417\) nm.
**Fig. S15.** Changes in relative fluorescence enhancement ratio \([I_0-I/I_0] \times 100\) of probe 1•PFP complex in the presence of other halophenol derivatives: \(\lambda_{ex} = 365\) nm, \(\lambda_{em} = 417\) 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.

\[ I = I_0 + I_\infty K_n [\text{Guest}]/[1 + K_n [\text{Guest}]] \]

\( I \) = Intensity (calculated as a function of \( Y \)).
\( I_0 \) = Intensity at host only.
\( I_\infty \) = 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.