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ESI

A Pyrenesulfonyl imidazolium derivative as selective cyanide ion sensor in aqueous media

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Fig. SI 6: Fluorescence relative intensity bar diagram of probe **2** (1 μ M, PBS - EtOH (5:95), pH = 7.4) on addition of different anions viz. F⁻, Cl⁻, Br⁻, l⁻, NO₃⁻, ClO₄⁻, HSO₄⁻, H₂PO₄⁻, HP₂O₇³⁻, AcO⁻, CN⁻ -anions λ_{ex} = 336 nm, λ_{em} = 494 nm, slit width 3,3.

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Fig. SI 20: Fluorescence ratiometric response (I_{379}/I_{495}) of probe **2** (1 μ M, PBS - EtOH (5:95), pH = 7.4) with TBACN toward [CN⁻].



¹H NMR of probe $\mathbf{1}$ in DMSO-d₆



¹H NMR of probe **1** aliphatic reigion in DMSO-d₆







 ^{13}C NMR of probe $\boldsymbol{1}$ in DMSO-d_6



HRMS of probe 1



HRMS of probe 1



¹H NMR of probe **2** in DMSO-d₆



¹H NMR of probe **2** (aliphatic reigion) in DMSO-d₆





¹³C NMR of probe **2** in DMSO-d₆



HRMS of probe 2



Fig. SI 1: UV-vis study of probe **1** (10 μ M, PBS -EtOH (5:95), pH = 7.4) on addition of different anions viz. F⁻, Cl⁻, Br⁻, l⁻, NO₃⁻, ClO₄⁻, HSO₄⁻, H₂PO₄⁻, HP₂O₇³⁻, AcO⁻, CN⁻.



Fig. SI 2: UV-vis study of probe **2** (10 μ M, PBS -EtOH (5:95), pH = 7.4) on addition of different anions viz. F⁻, Cl⁻, Br⁻, l⁻, NO₃⁻, ClO₄⁻, HSO₄⁻, H₂PO₄⁻, HP₂O₇³⁻, AcO⁻, CN⁻.



Fig. SI 3: Fluorescence study of probe **1** (1 μ M, PBS -EtOH (5:95), pH = 7.4) on addition of different anions viz. F⁻, Cl⁻, Br⁻, l⁻, NO₃⁻, ClO₄⁻, HSO₄⁻, H₂PO₄⁻, HP₂O₇³⁻, AcO⁻, CN⁻ -anions λ_{ex} = 336 nm, slit width 3, 3.



Fig. SI 4: Fluorescence relative intensity bar diagram of probe **1** (1 μ M, PBS -EtOH (5:95), pH = 7.4) on addition of different anions viz. F⁻, Cl⁻, Br⁻, l⁻, NO₃⁻, ClO₄⁻, HSO₄⁻, H₂PO₄⁻, HP₂O₇³⁻, AcO⁻, CN⁻ -anions λ_{ex} = 336 nm, λ_{em} = 379 nm, slit width 3, 3.



Fig. SI 5: Fluorescence study of probe **2** (1 μ M, PBS -EtOH (5:95), pH = 7.4) on addition of different anions viz. F⁻, Cl⁻, Br⁻, l⁻, NO₃⁻, ClO₄⁻, HSO₄⁻, H2O₇⁻, HP₂O₇³⁻, AcO⁻, CN⁻ -anions λ_{ex} = 336 nm, slit width 3,3.



Fig. SI 6: Fluorescence relative intensity bar diagram of probe **2** (1 μ M, PBS -EtOH (5:95), pH = 7.4) on addition of different anions viz. F⁻, Cl⁻, Br⁻, l⁻, NO₃⁻, ClO₄⁻, HSO₄⁻, H₂PO₄⁻, HP₂O₇³⁻, AcO⁻, CN⁻ -anions λ_{ex} = 336 nm, λ_{em} = 494 nm, slit width 3,3.



Fig. SI 7: Fluorescence titration of probe **1** (1 μ M, PBS -EtOH (5:95), pH = 7.4) with CN⁻ ion, λ_{ex} = 336 nm, slit width 3, 3.



Fig. SI 8: The spectral fitting of the fluorescence titration data of probe **1** (1 μ M, PBS -EtOH (5:95), pH = 7.4) with CN⁻ ion, λ_{ex} = 336 nm, slit width 3, 3.



Fig. SI 9: Fluorescence titration of probe **2** (1 μ M, PBS -EtOH (5:95), pH = 7.4) with CN⁻ ion, λ_{ex} = 336 nm, slit width 3, 3.



Fig. SI 10: The spectral fitting of the fluorescence titration data of probe **2** (1 μ M, PBS -EtOH (5:95), pH = 7.4) with CN⁻ ion, λ_{ex} = 336 nm, λ_{em} = 495 nm, slit width 3, 3.



Fig. SI 11: (i) Partial ¹H NMR spectra of probe **2**; and (ii) upon addition of 1 eq. of TBACN; (iii) 2 eq. of TBACN; (iv) 3 eq. of TBACN; and (v) only TBACN in $D_2O-CD_3CD_2OD$ (1:6).



Fig. SI 12: (i) Partial ¹H NMR spectra of probe **2**; and (ii) upon addition of 1 eq. of TBACN; (iii) 2 eq. of TBACN; (iv) 3 eq. of TBACN; and (v) only TBACN in DMSO-d₆.



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Fig. SI 14: (i) Partial ¹H NMR spectra of probe **1**; and (ii) upon addition of 1 eq. of TBACN; (iii) 2 eq. of TBACN; and (iv) only TBACN in DMSO-d₆.



Fig. SI 15: (i) Partial ¹H NMR spectra of probe **1**; and (ii) upon addition of 1 eq. of TBACN; (iii) 2 eq. of TBACN; and (iv) only TBACN in DMSO-d₆.



Fig. SI 16: (i) Partial ¹H NMR spectra of probe **1**; and (ii) upon addition of 1 eq. of TBACN; (iii) 2 eq. of TBACN; and (iv) only TBACN in DMSO-d₆.



Fig. SI 17: "B3LYP/6-31G* calculated molecular orbitals of probe **1** and **1**•CN⁻ complex and their energy differences."



Fig. SI 18: "B3LYP/6-31G* calculated molecular orbitals of probe **2** and **2**•2(**CN**⁻) complex and their energy differences."



Fig. SI 19: Fluorescence ratiometric response (I_{495}/I_{379}) of probe **2** (1 μ M, PBS -EtOH (5:95), pH = 7.4) with TBACN toward [CN⁻].



Fig. SI 20: Fluorescence ratiometric response (I_{379}/I_{495}) of probe **2** (1 μ M, PBS -EtOH (5:95), pH = 7.4) with TBACN toward [CN⁻].