ESI

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

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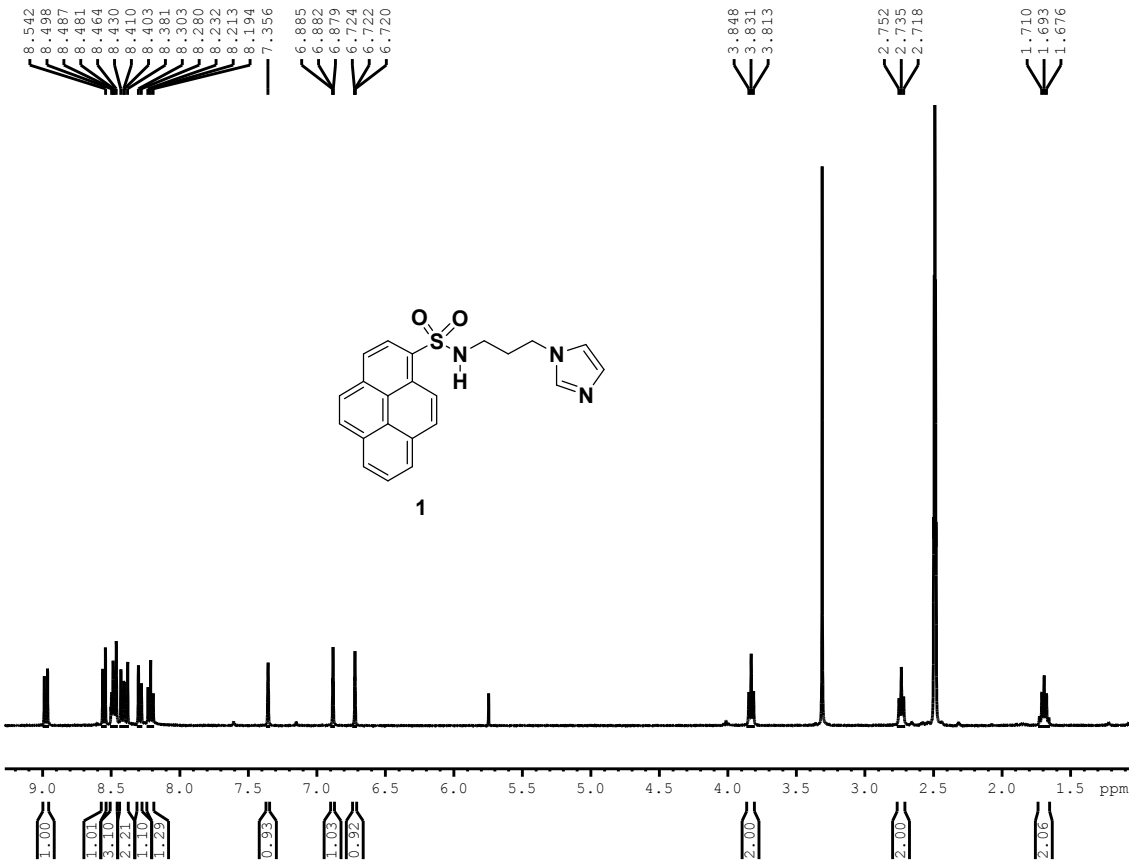
complex and their energy differences."



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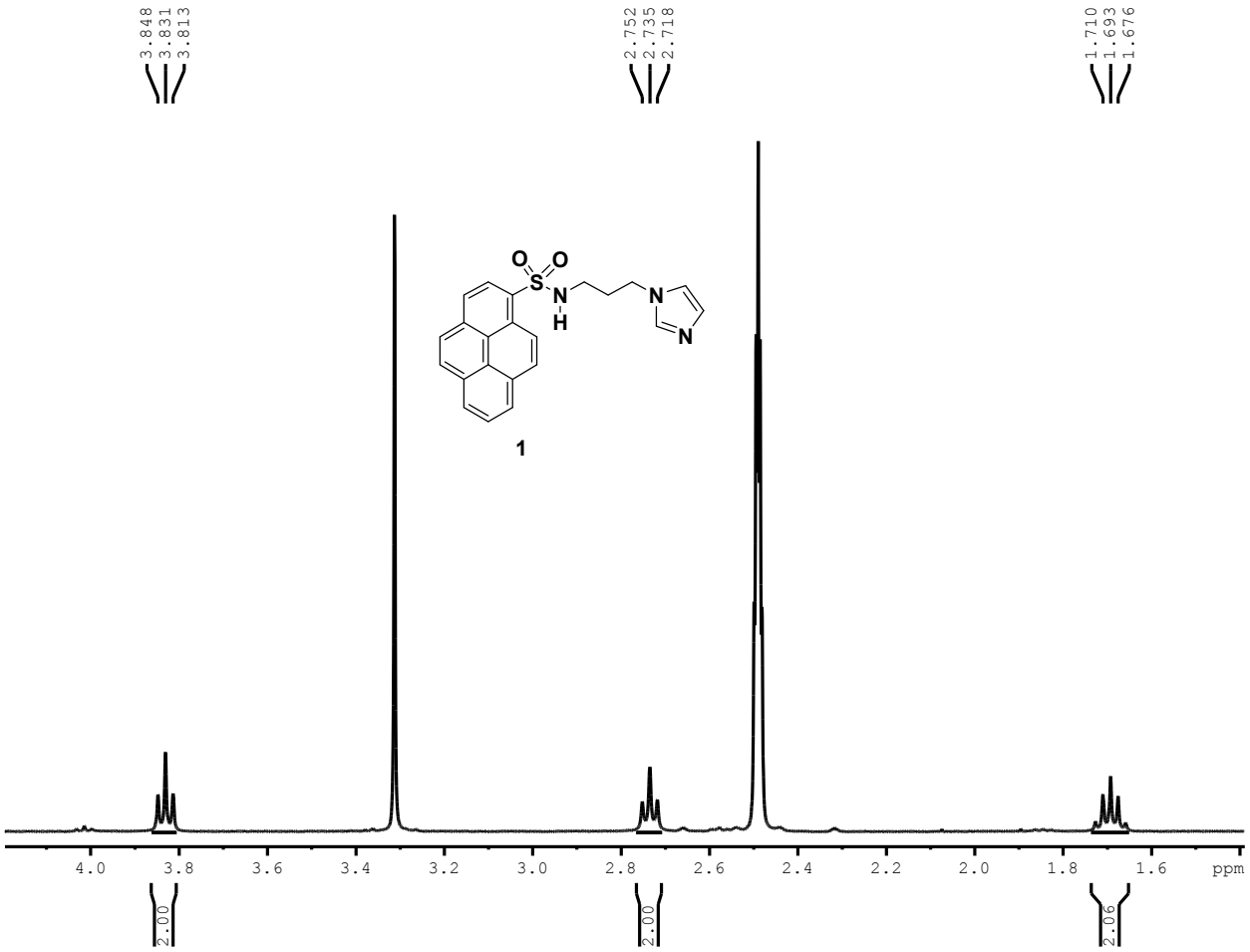

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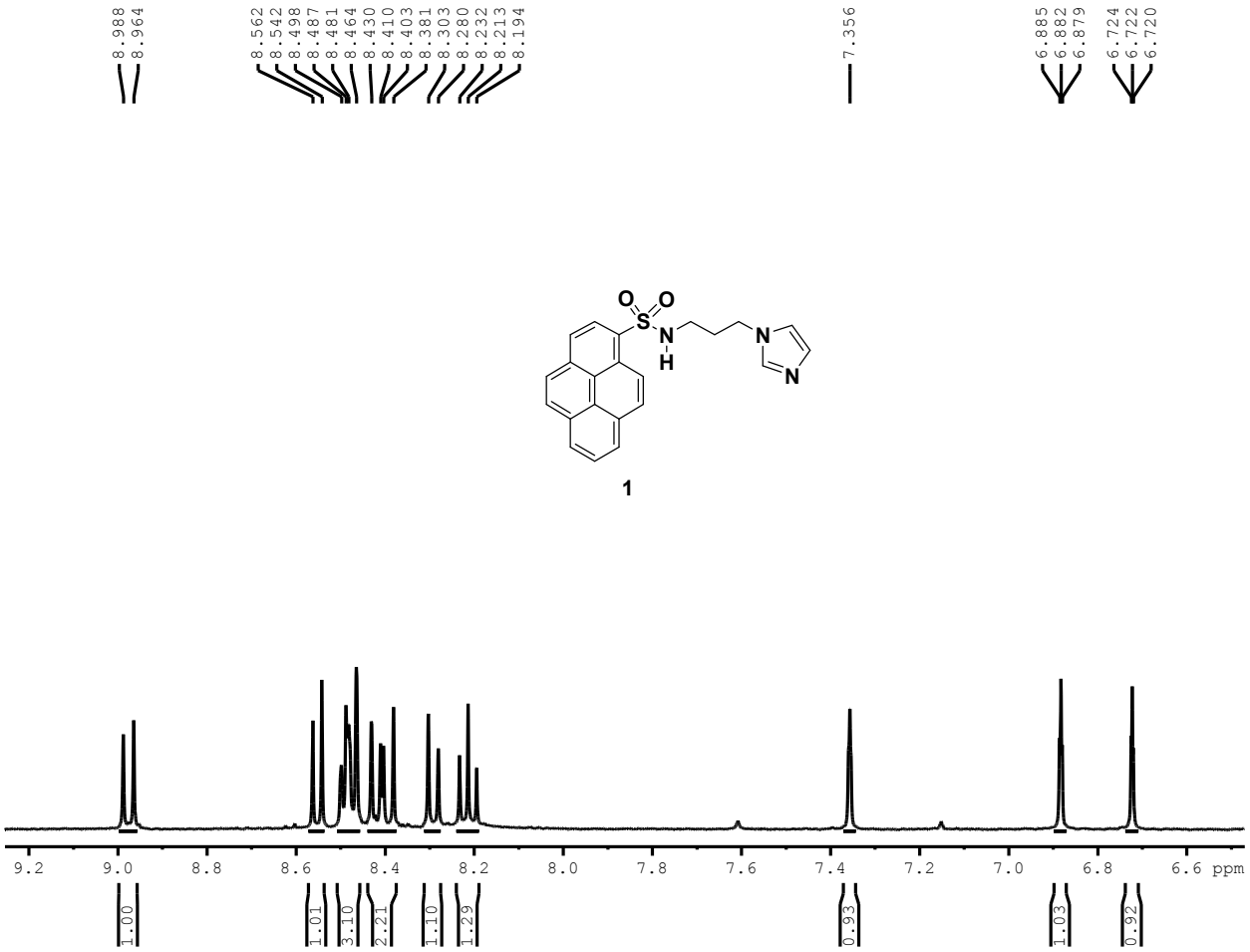

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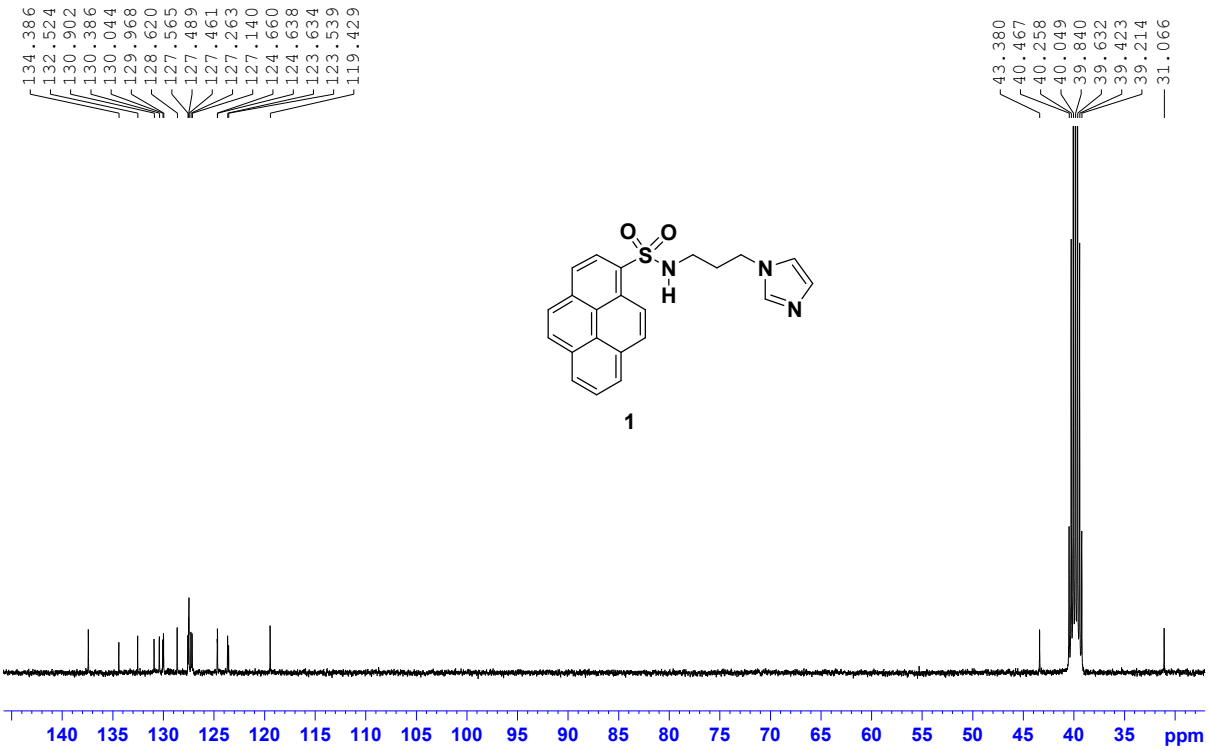

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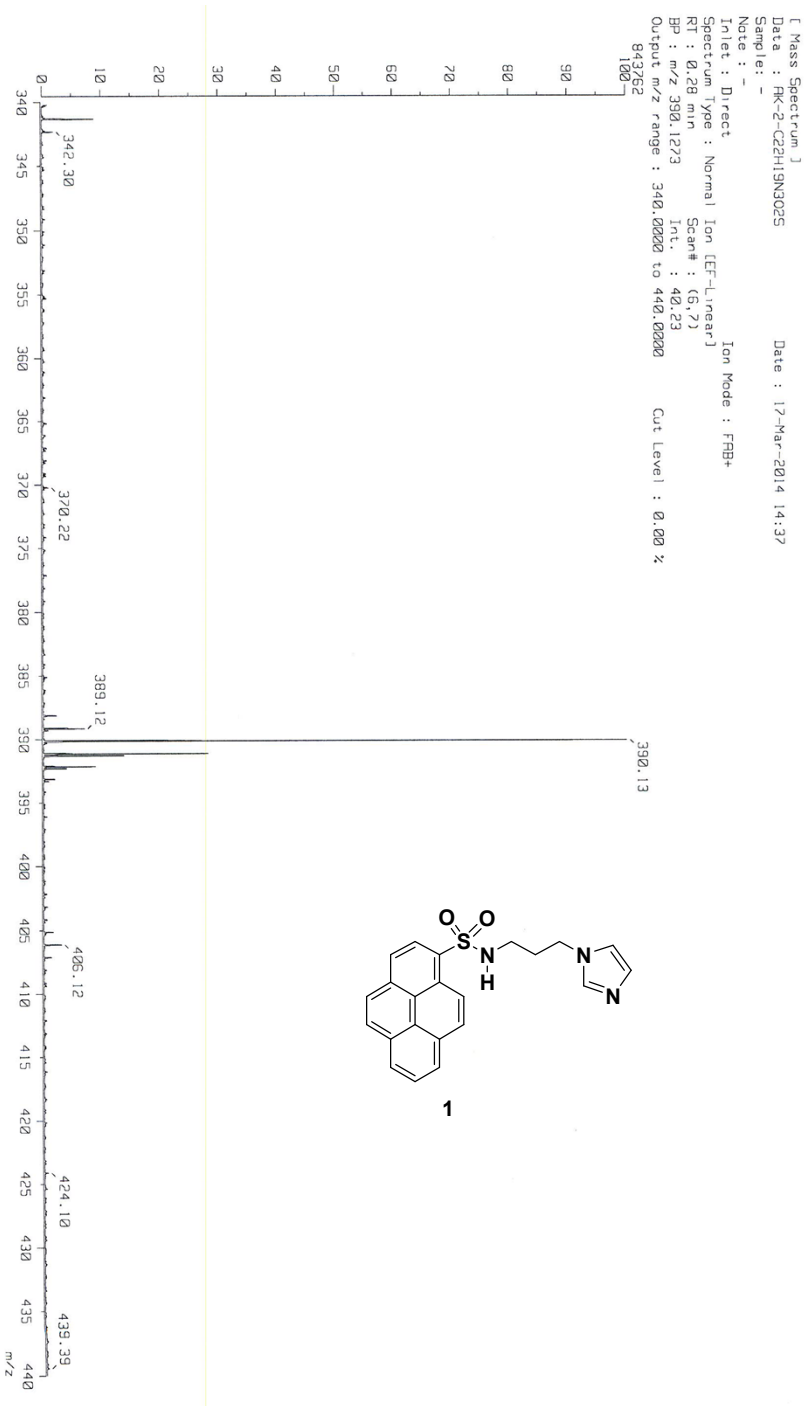

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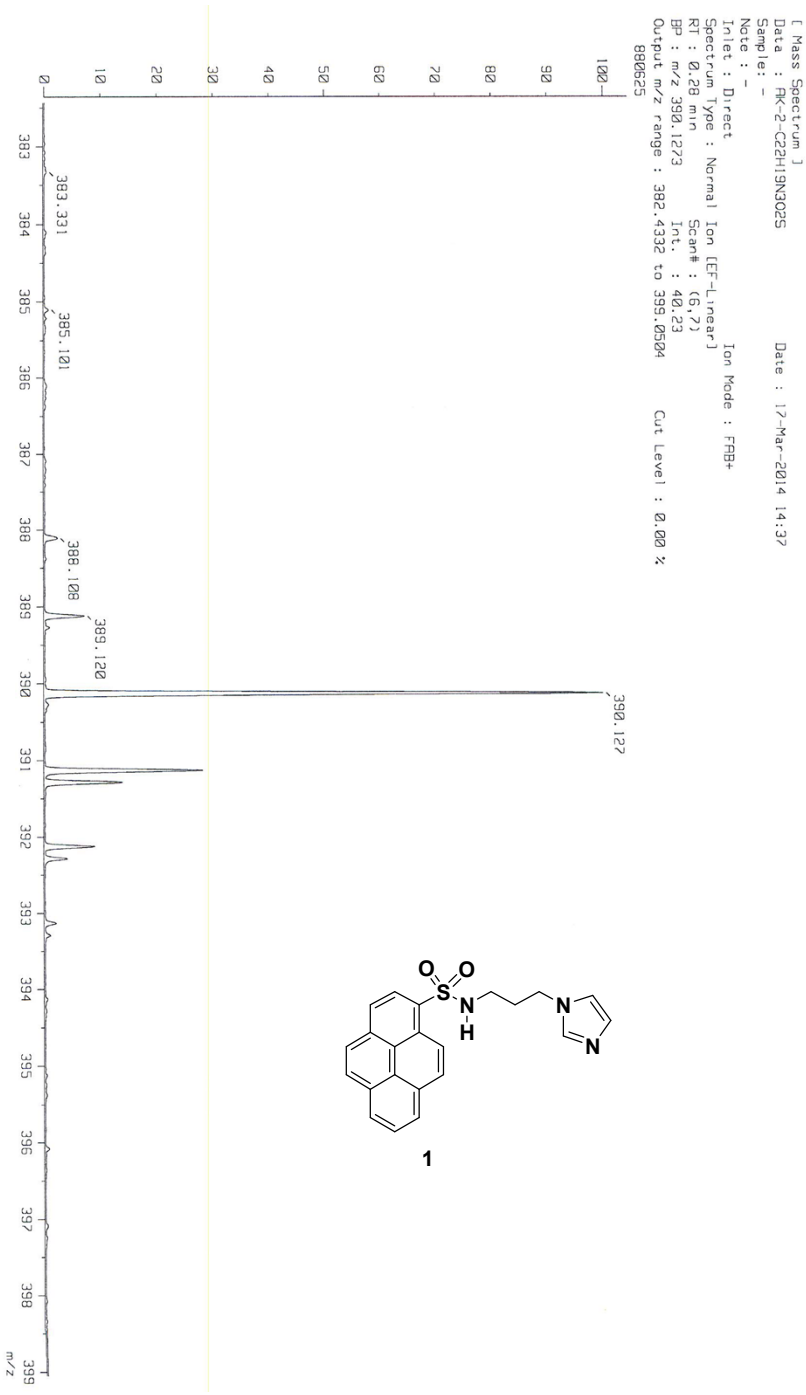

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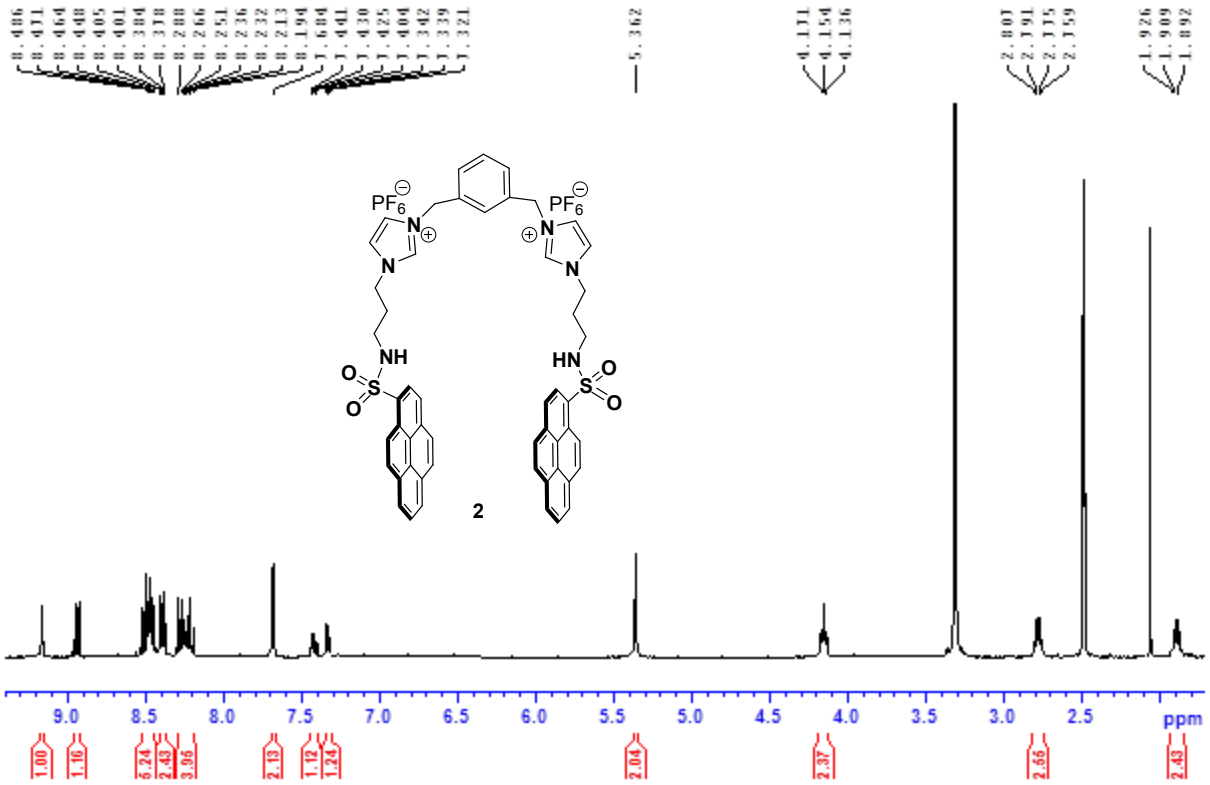

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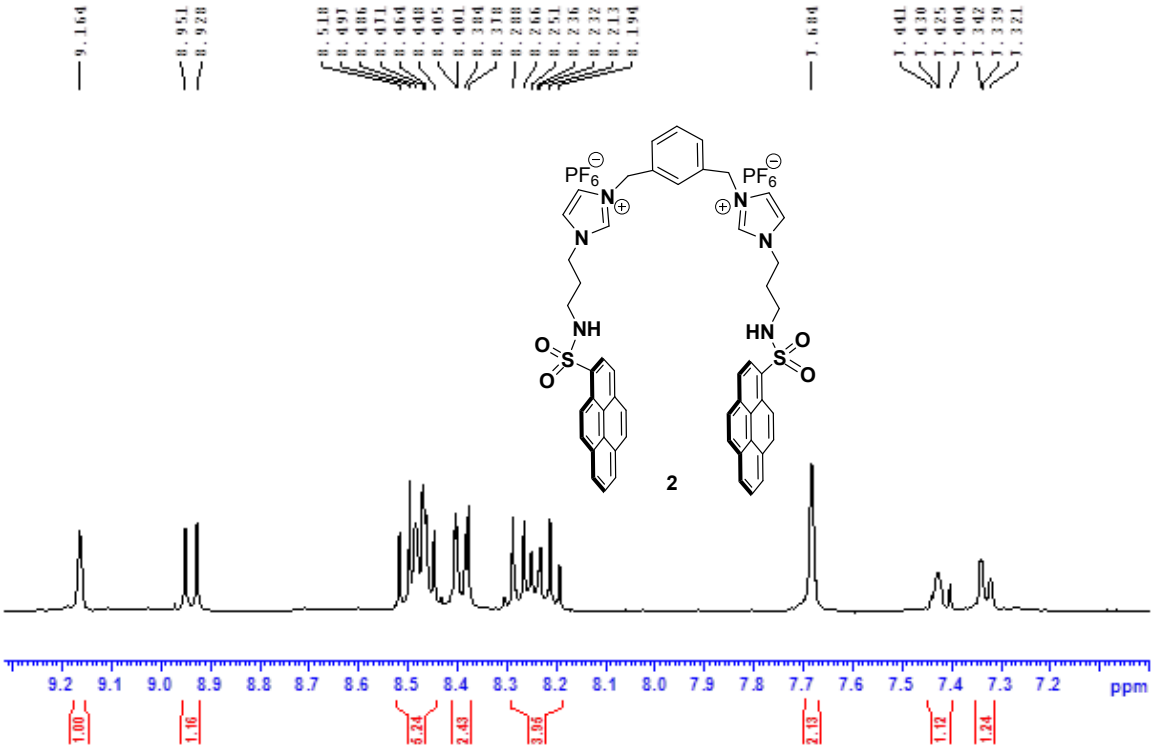
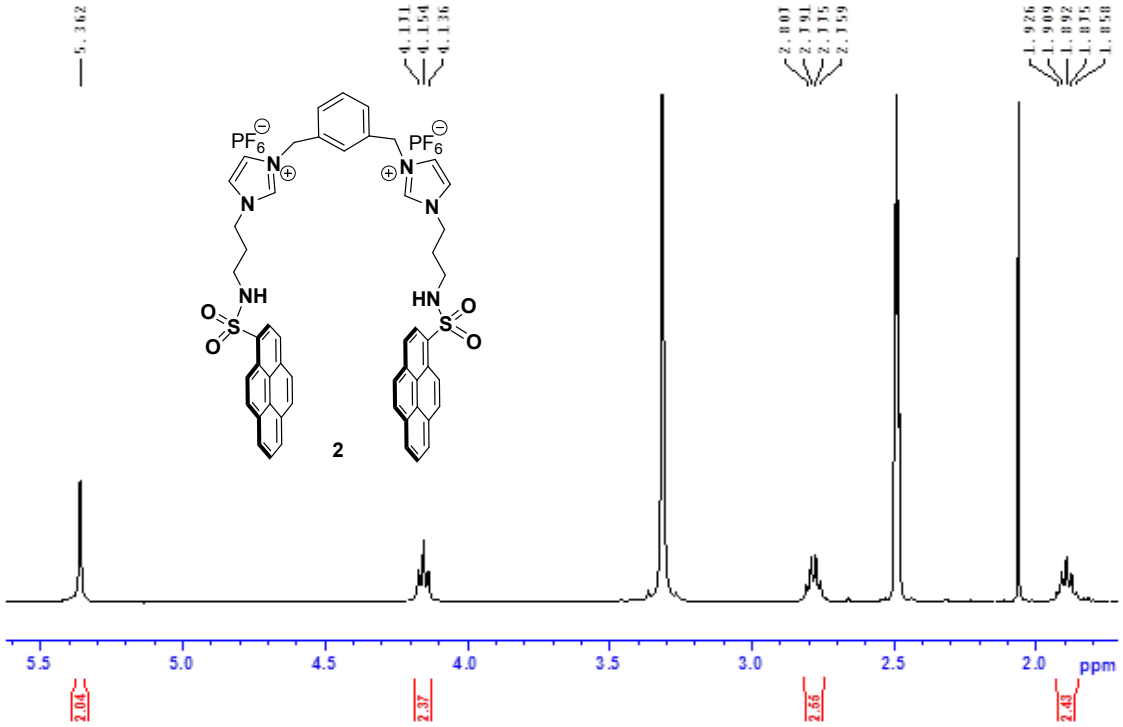


^{1}H NMR of probe **2** (aromatic reigion) in DMSO-d_6



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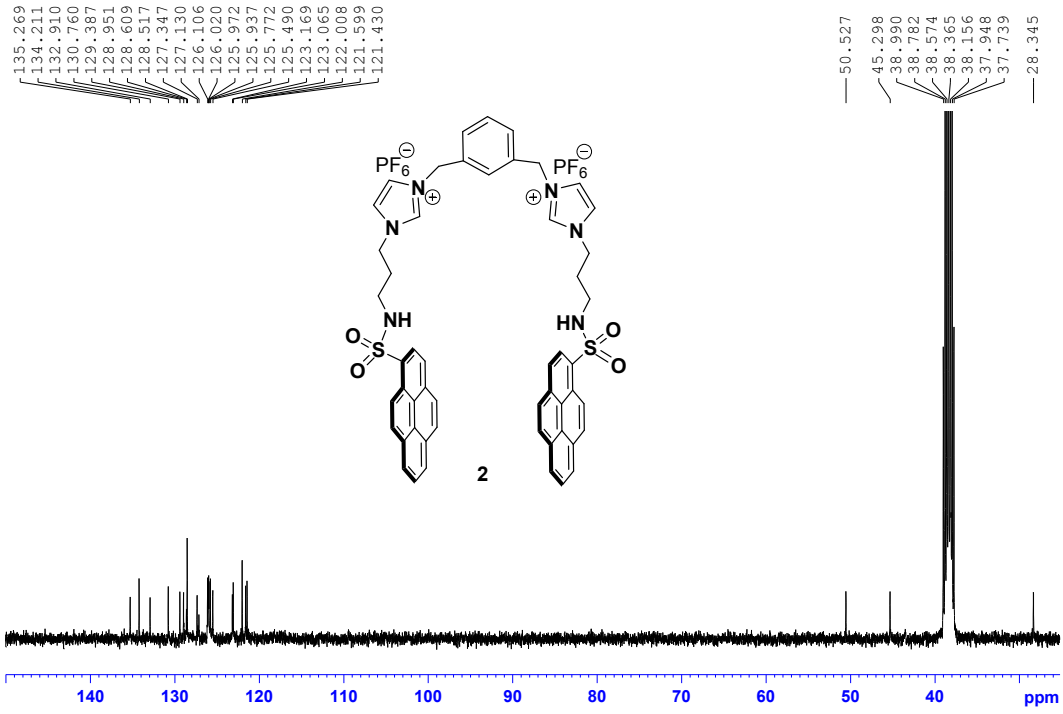

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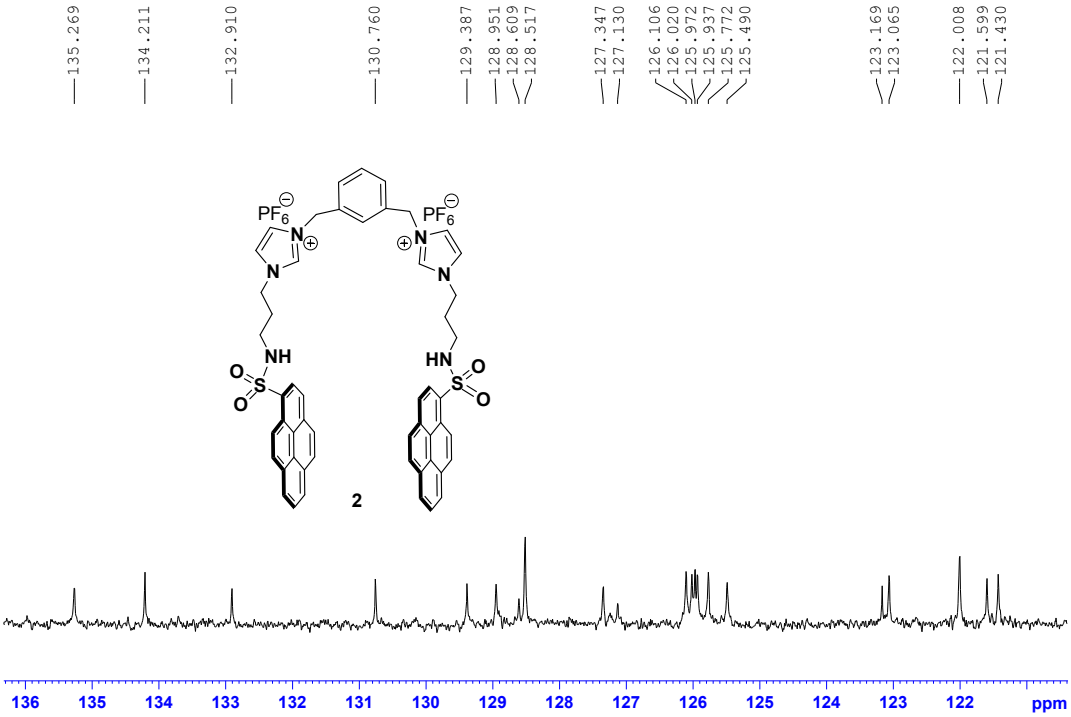

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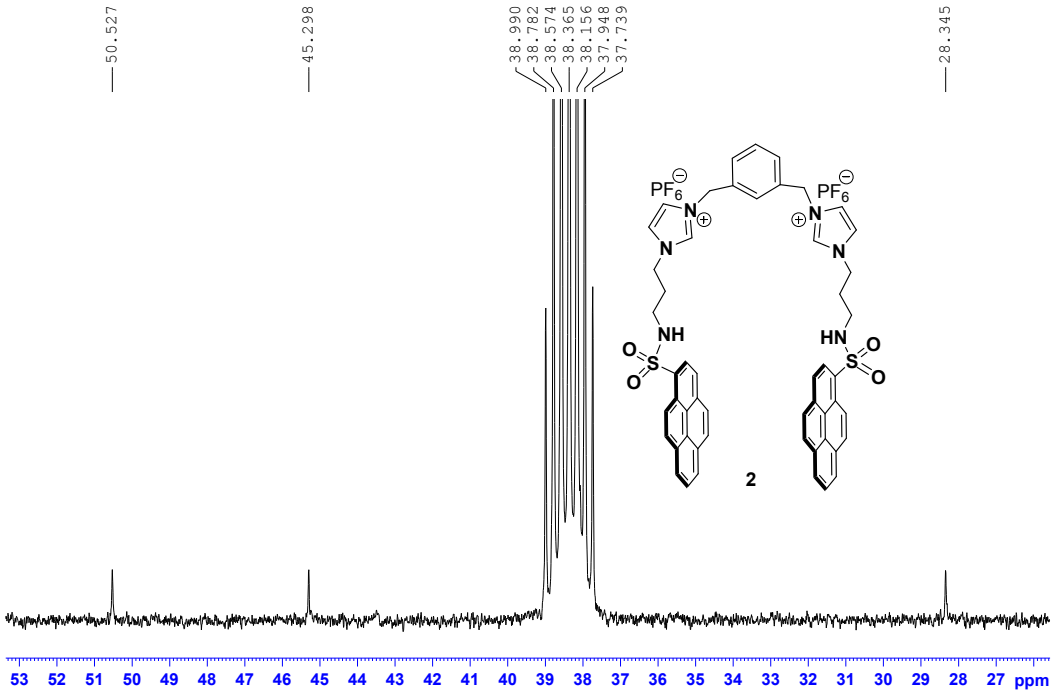

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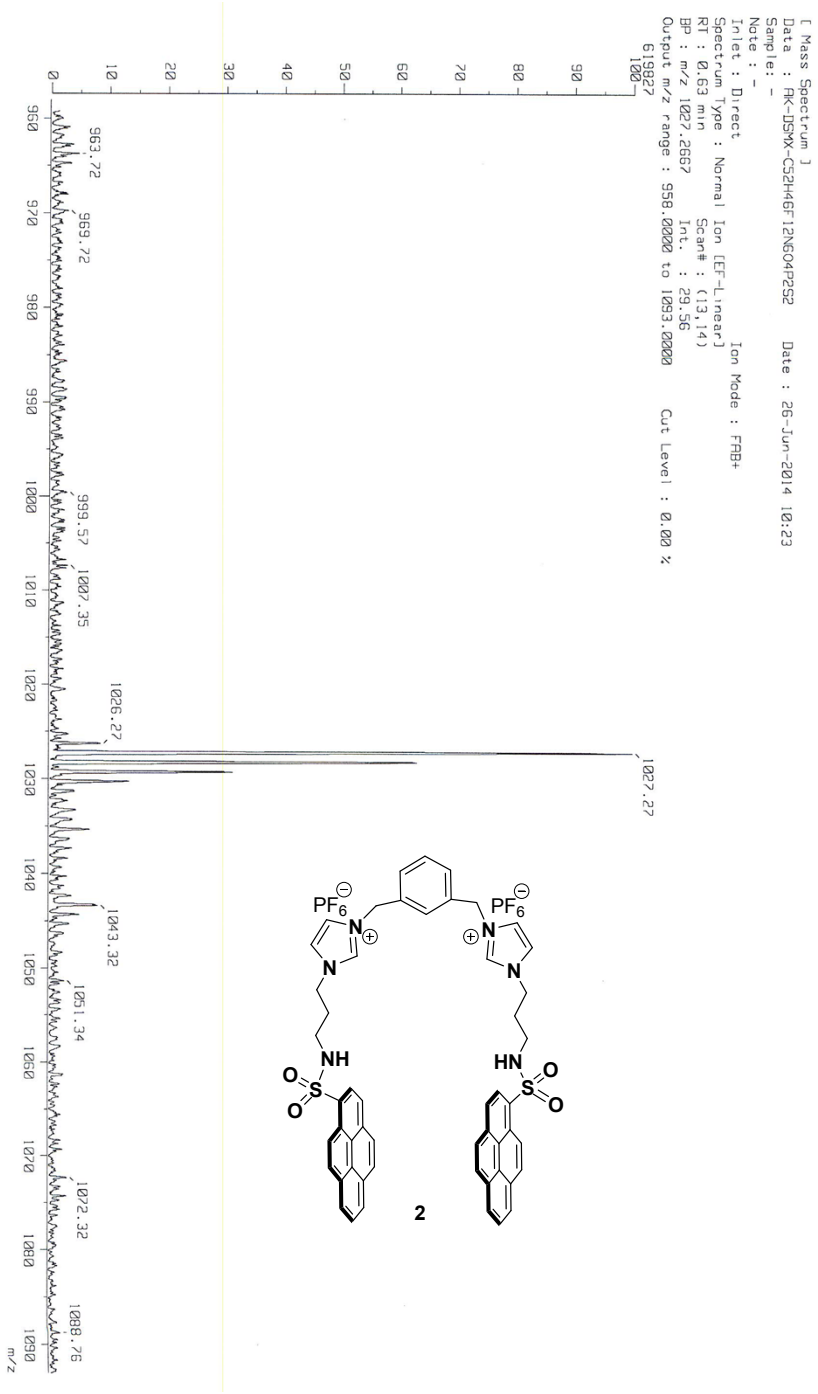

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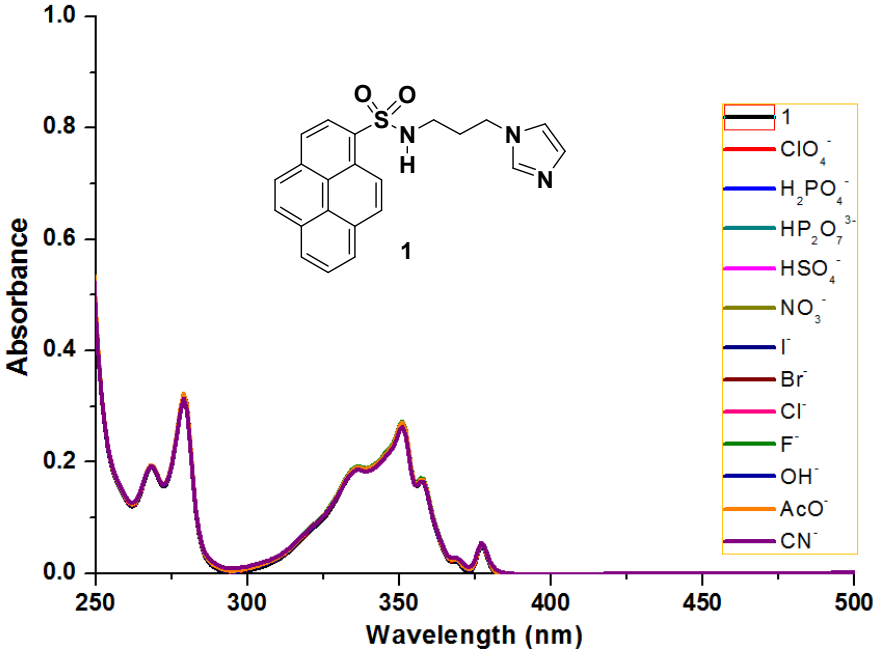


Fig. SI 1: UV-vis study of probe **1** (10 µM, PBS -EtOH (5:95), pH = 7.4) on addition of different anions viz. F^-, Cl^-, Br^-, I^-, NO_3^-, ClO_4^-, HSO_4^-, $H_2PO_4^-$, $HP_2O_7^{3-}$, AcO^-, CN^-.

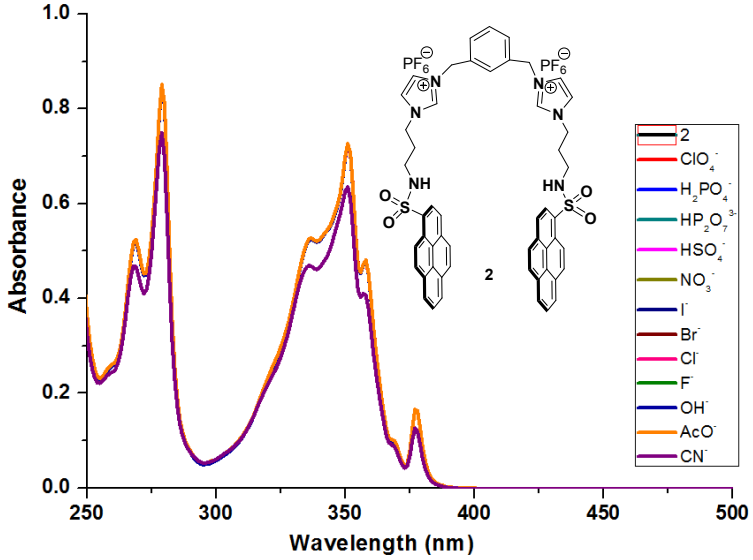


Fig. SI 2: UV-vis study of probe **2** (10 µM, PBS -EtOH (5:95), pH = 7.4) on addition of different anions viz. F^-, Cl^-, Br^-, I^-, NO_3^-, ClO_4^-, HSO_4^-, $H_2PO_4^-$, $HP_2O_7^{3-}$, AcO^-, CN^-.

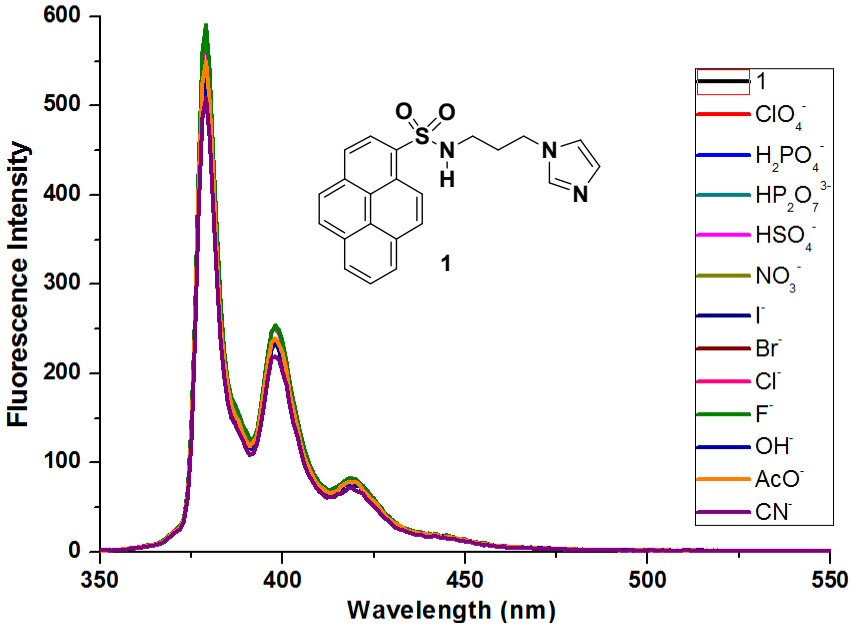


Fig. SI 3: Fluorescence study of probe **1** (1 µM, PBS -EtOH (5:95), pH = 7.4) on addition of different anions viz. F^-, Cl^-, Br^-, I^-, NO_3^-, ClO_4^-, HSO_4^-, $H_2PO_4^-$, $HP_2O_7^{3-}$, AcO^-, CN^- -anions λ_{ex} = 336 nm, slit width 3, 3.

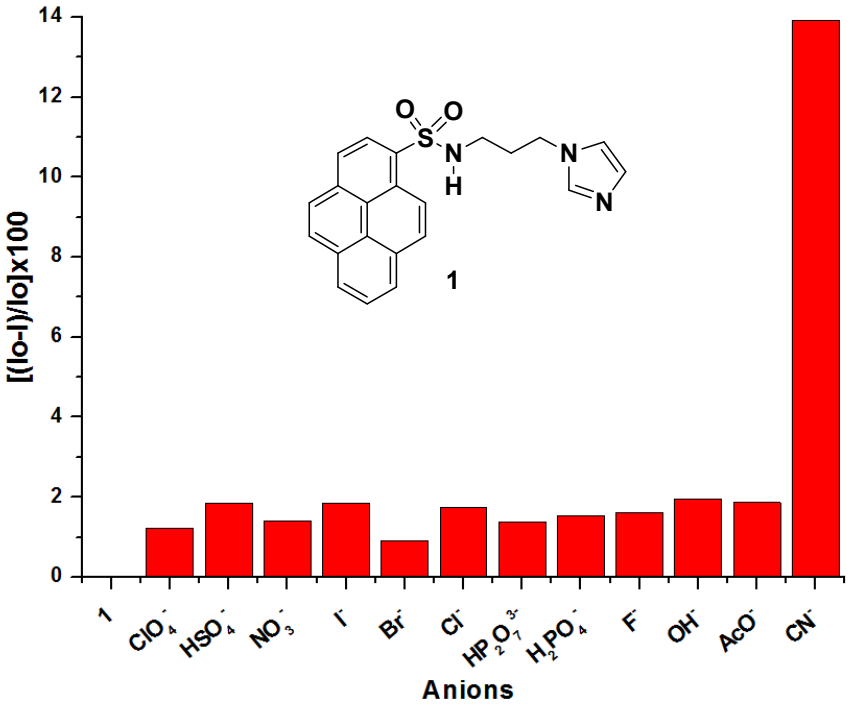


Fig. SI 4: Fluorescence relative intensity bar diagram of probe **1** (1 µM, PBS -EtOH (5:95), pH = 7.4) on addition of different anions viz. F^-, Cl^-, Br^-, I^-, NO_3^-, ClO_4^-, HSO_4^-, $H_2PO_4^-$, $HP_2O_7^{3-}$, AcO^-, CN^- -anions λ_{ex} = 336 nm, λ_{em} = 379 nm, slit width 3, 3.

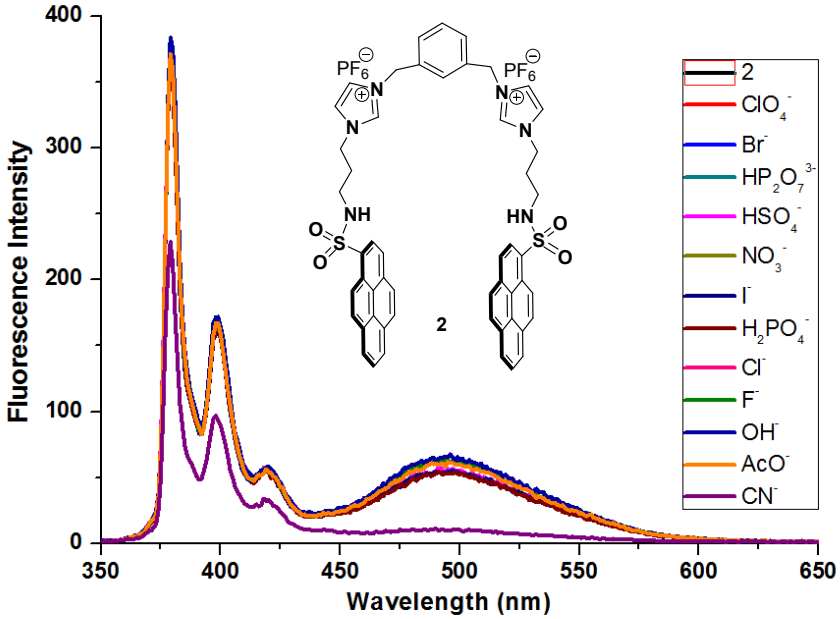


Fig. SI 5: Fluorescence study of probe **2** (1 µM, PBS -EtOH (5:95), pH = 7.4) on addition of different anions viz. F^-, Cl^-, Br^-, I^-, NO_3^-, ClO_4^-, HSO_4^-, $H_2PO_4^-$, $HP_2O_7^{3-}$, AcO^-, CN^- -anions λ_{ex} = 336 nm, slit width 3,3.

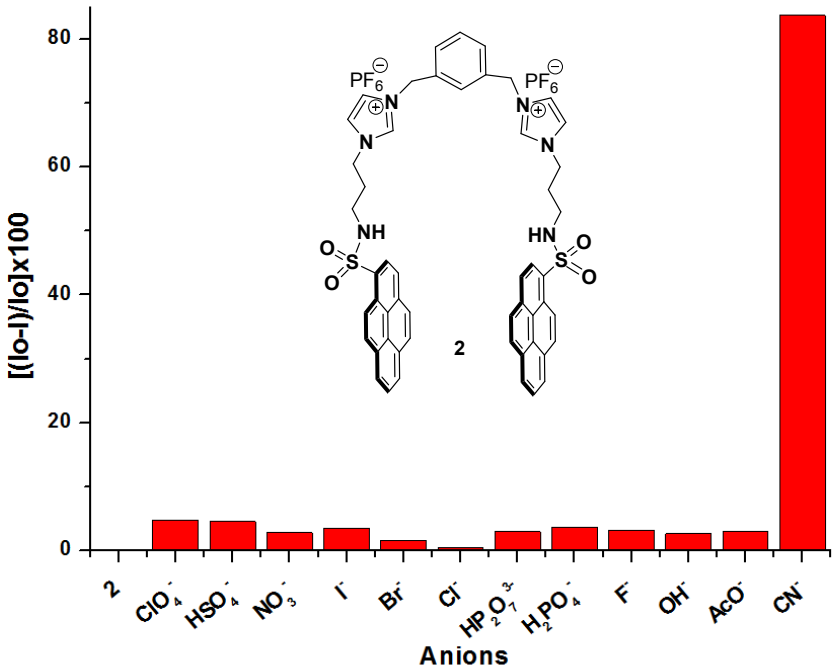


Fig. SI 6: Fluorescence relative intensity bar diagram of probe **2** (1 µM, PBS -EtOH (5:95), pH = 7.4) on addition of different anions viz. F^-, Cl^-, Br^-, I^-, NO_3^-, ClO_4^-, HSO_4^-, $H_2PO_4^-$, $HP_2O_7^{3-}$, AcO^-, CN^- -anions λ_{ex} = 336 nm, λ_{em} = 494 nm, slit width 3,3.

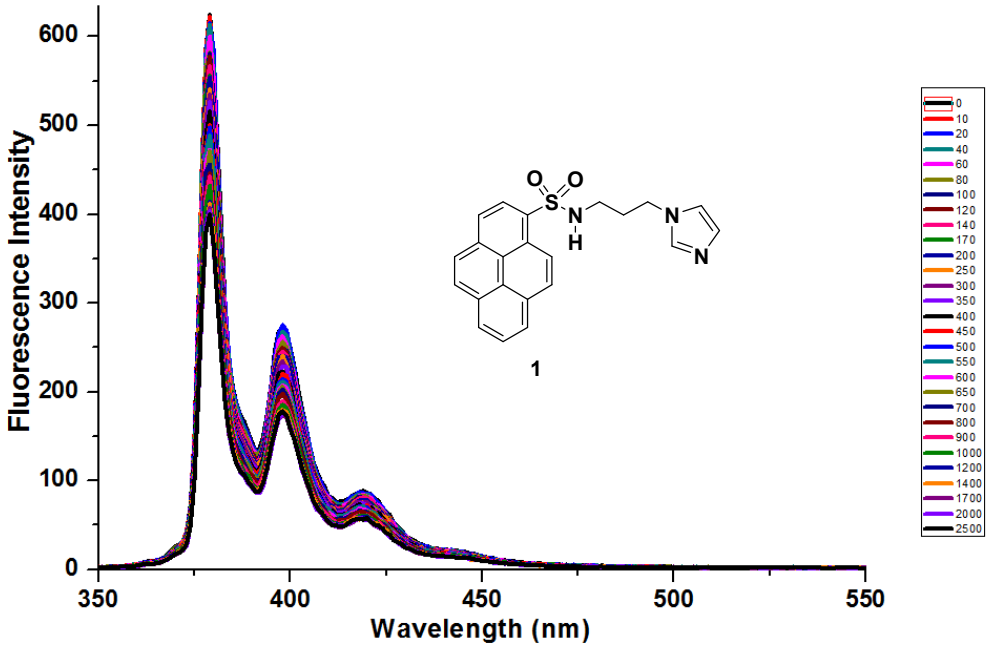


Fig. SI 7: Fluorescence titration of probe **1** (1 µM, PBS -EtOH (5:95), pH = 7.4) with CN^- ion, λ_{ex} = 336 nm, slit width 3, 3.

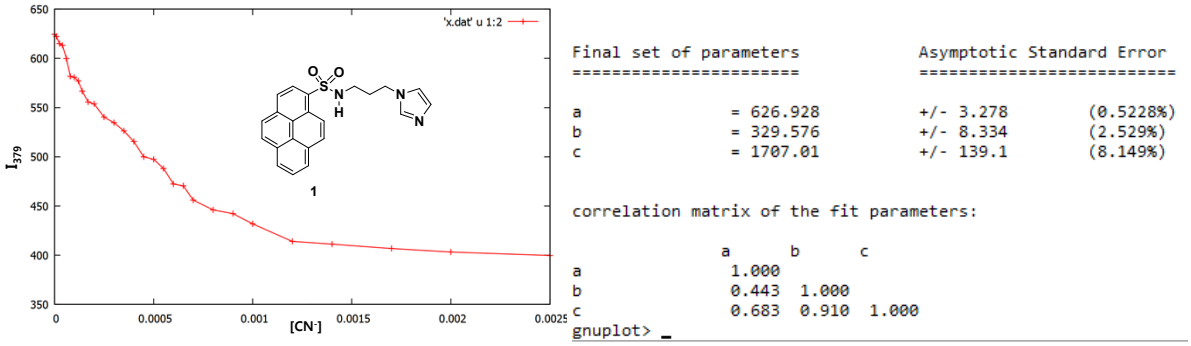


Fig. SI 8: The spectral fitting of the fluorescence titration data of probe **1** (1 µM, PBS -EtOH (5:95), pH = 7.4) with CN^- ion, λ_{ex} = 336 nm, slit width 3, 3.

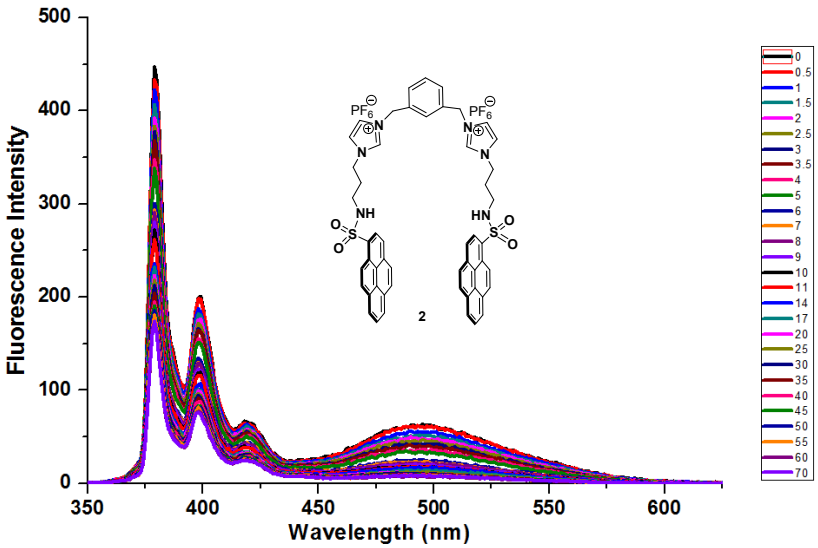
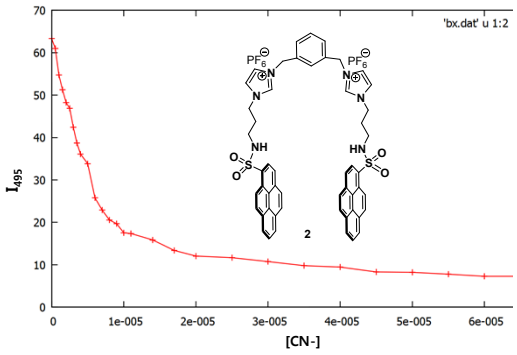


Fig. SI 9: Fluorescence titration of probe **2** (1 µM, PBS -EtOH (5:95), pH = 7.4) with CN^- ion, λ_{ex} = 336 nm, slit width 3, 3.

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Final set of parameters            Asymptotic Standard Error
=======================            ==========================

a               = 67.409           +/- 1.453        (2.156%)
b               = 53884.1          +/- 1.686e+004   (31.28%)
c               = 232550           +/- 1.398e+004   (6.011%)


correlation matrix of the fit parameters:

                a      b      c
a               1.000
b               0.199  1.000
c               0.803  0.367  1.000
gnuplot> _
```

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

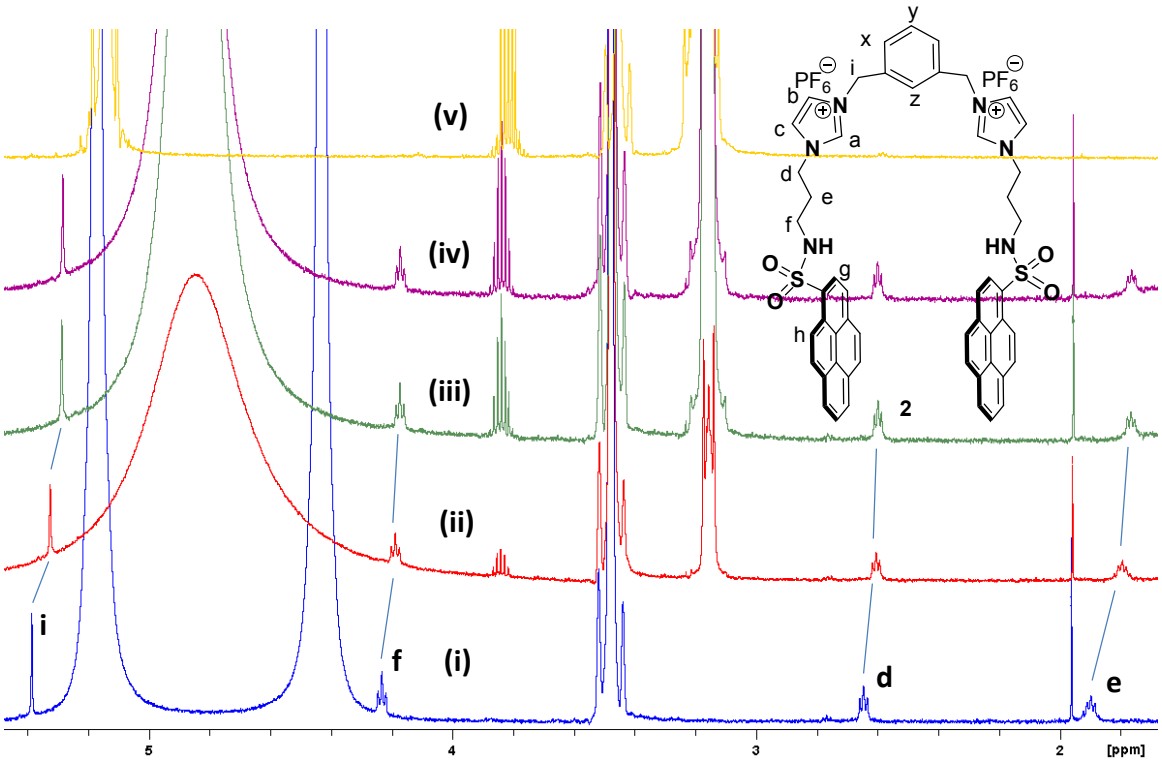

Fig. SI 11: (i) Partial ^{1}H NMR spectra of probe **2**; and (ii) upon addition of 1 eq. of TBACN; (iii) 2 eq. of TBACN; (iv) 3 eq. of TBACN; and (v) only TBACN in D_2O-CD_3CD_2OD (1:6).

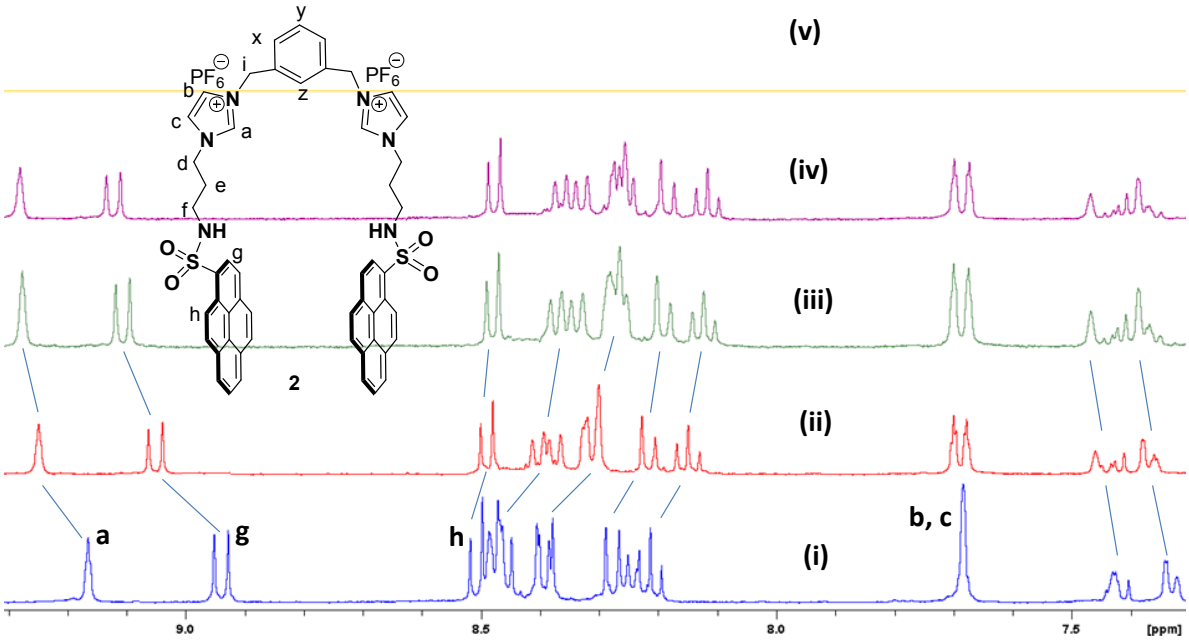

Fig. SI 12: (i) Partial ^{1}H NMR spectra of probe **2**; and (ii) upon addition of 1 eq. of TBACN; (iii) 2 eq. of TBACN; (iv) 3 eq. of TBACN; and (v) only TBACN in DMSO-d_6.

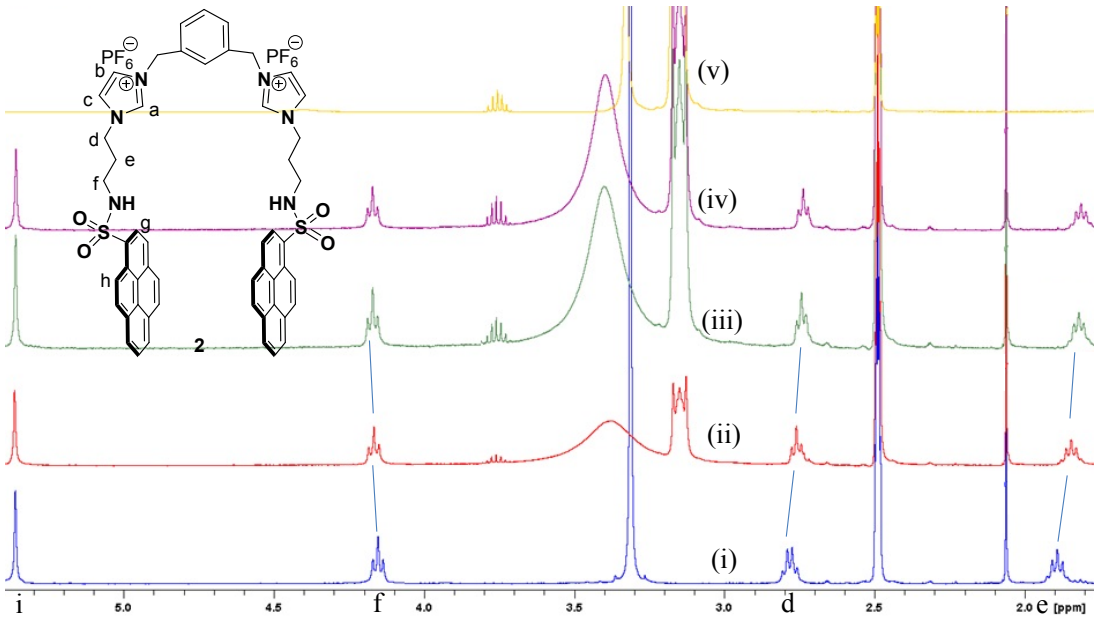

Fig. SI 13: (i) Partial ^{1}H NMR spectra of probe **2**; and (ii) upon addition of 1 eq. of TBACN; (iii) 2 eq. of TBACN; (iv) 3 eq. of TBACN; and (v) only TBACN in DMSO-d_6.

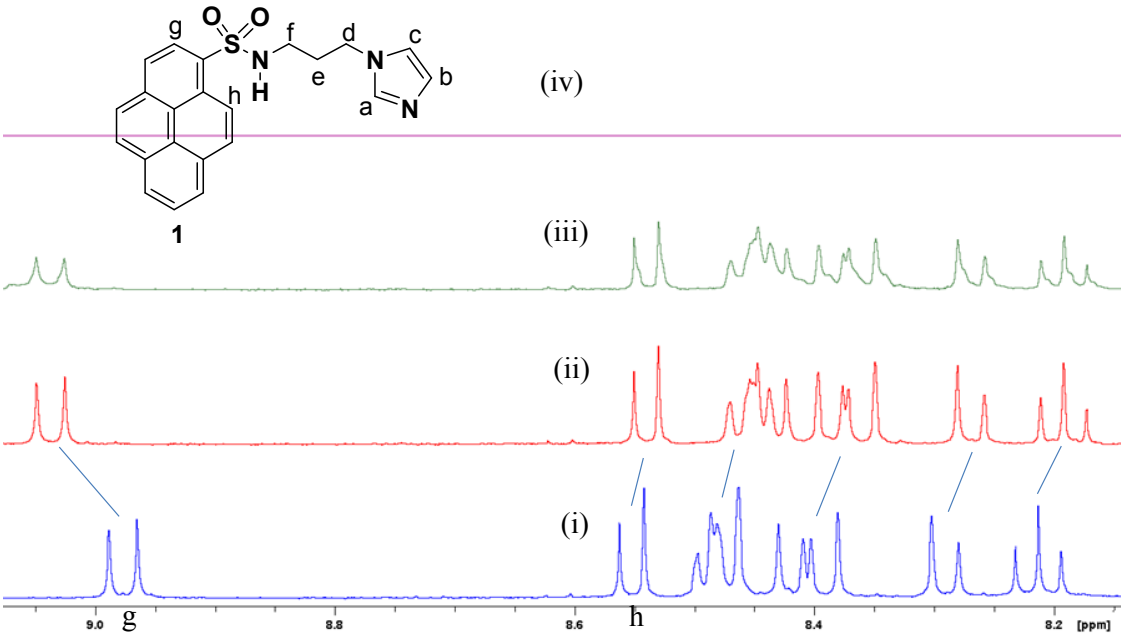

Fig. SI 14: (i) Partial ^{1}H NMR spectra of probe **1**; and (ii) upon addition of 1 eq. of TBACN; (iii) 2 eq. of TBACN; and (iv) only TBACN in DMSO-d_6.

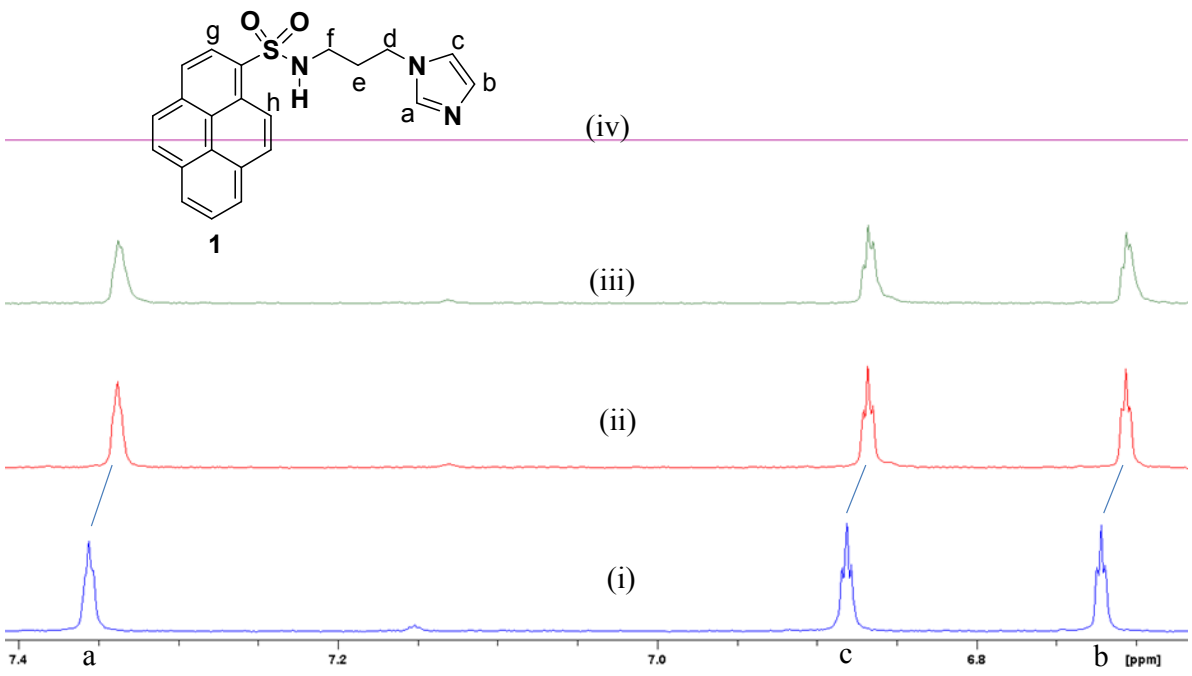

Fig. SI 15: (i) Partial ^{1}H NMR spectra of probe **1**; and (ii) upon addition of 1 eq. of TBACN; (iii) 2 eq. of TBACN; and (iv) only TBACN in DMSO-d_6.

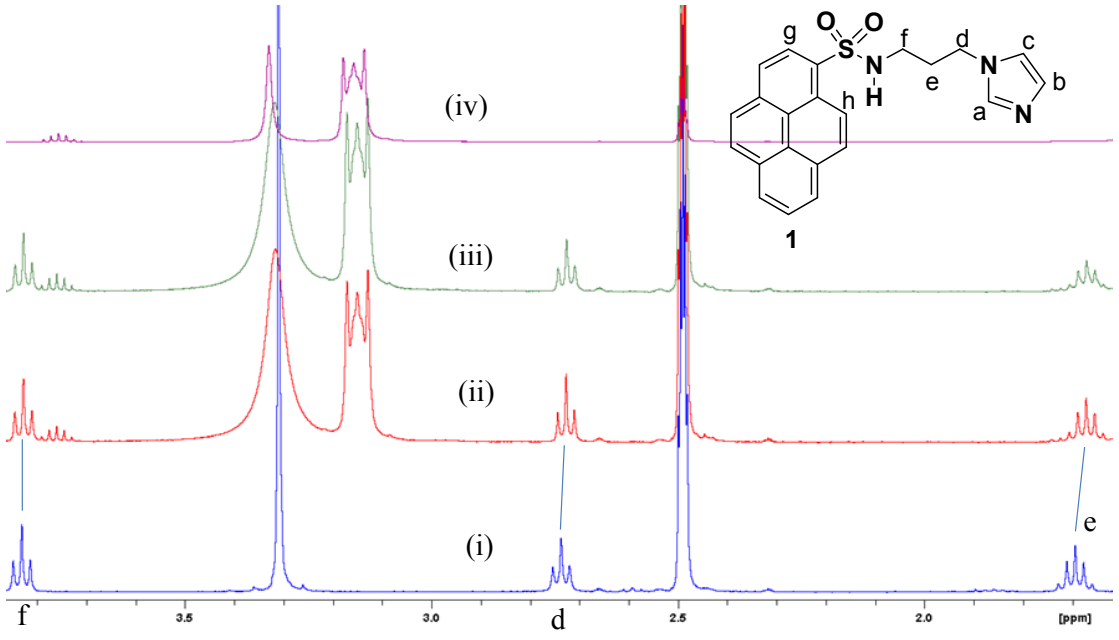

Fig. SI 16: (i) Partial ^{1}H NMR spectra of probe **1**; and (ii) upon addition of 1 eq. of TBACN; (iii) 2 eq. of TBACN; and (iv) only TBACN in DMSO-d_6.

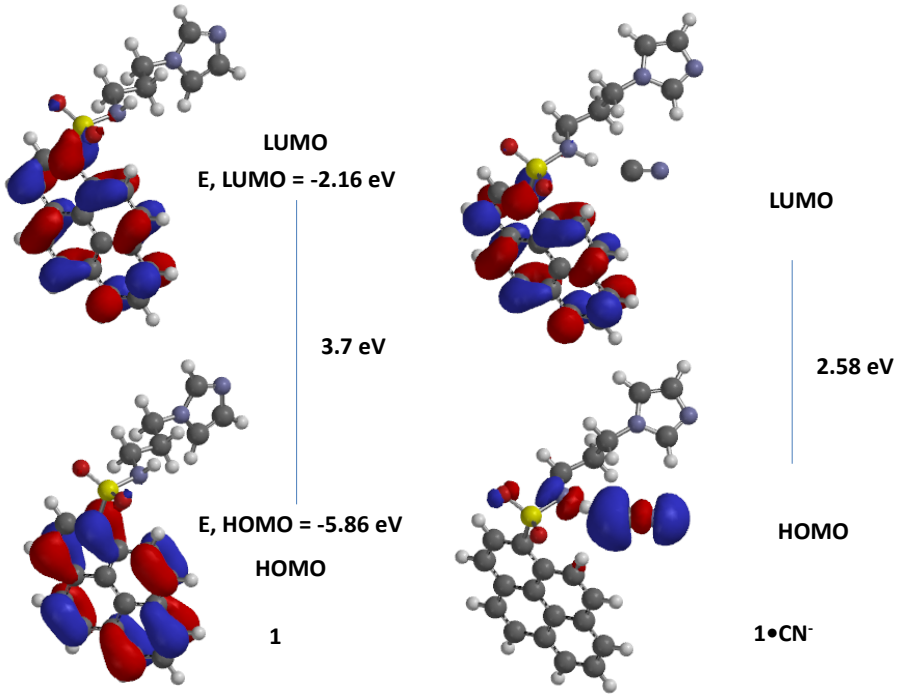

Fig. SI 17: "B3LYP/6-31G* calculated molecular orbitals of probe **1** and **1•CN**$^{-}$ complex and their energy differences."

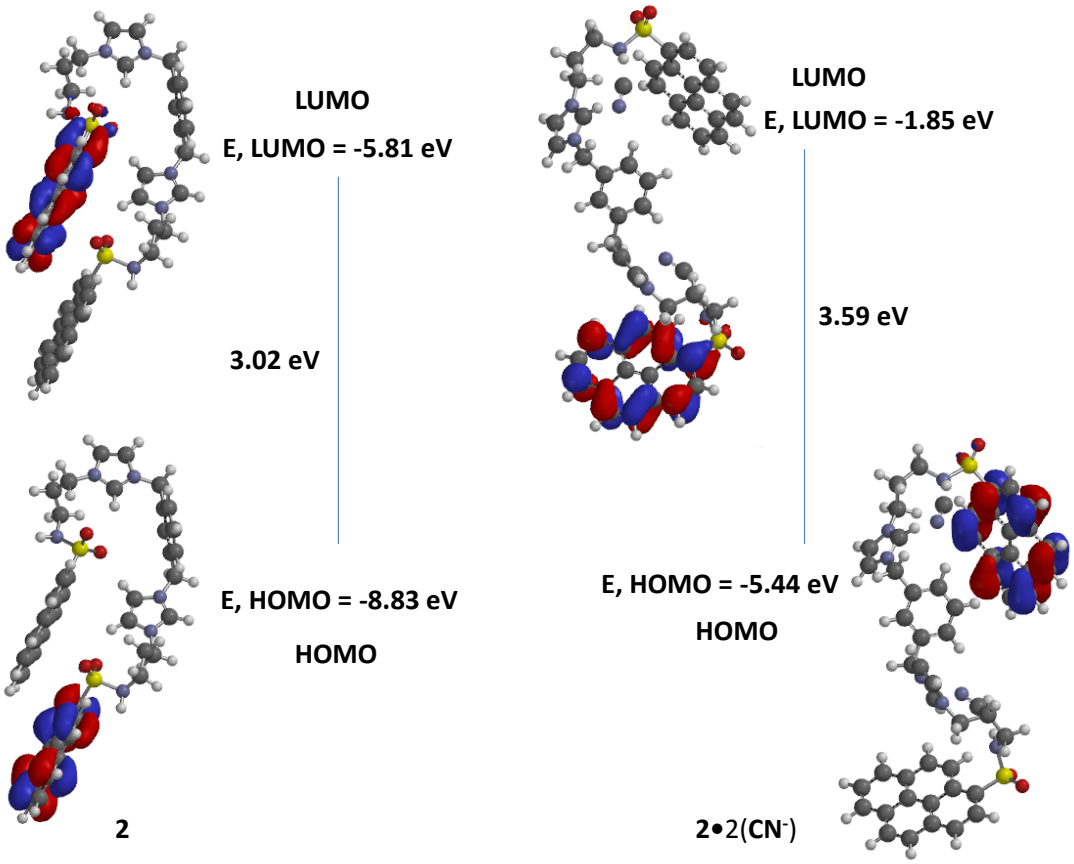

Fig. SI 18: "B3LYP/6-31G* calculated molecular orbitals of probe **2** and **2**•2(**CN**$^-$) complex and their energy differences."

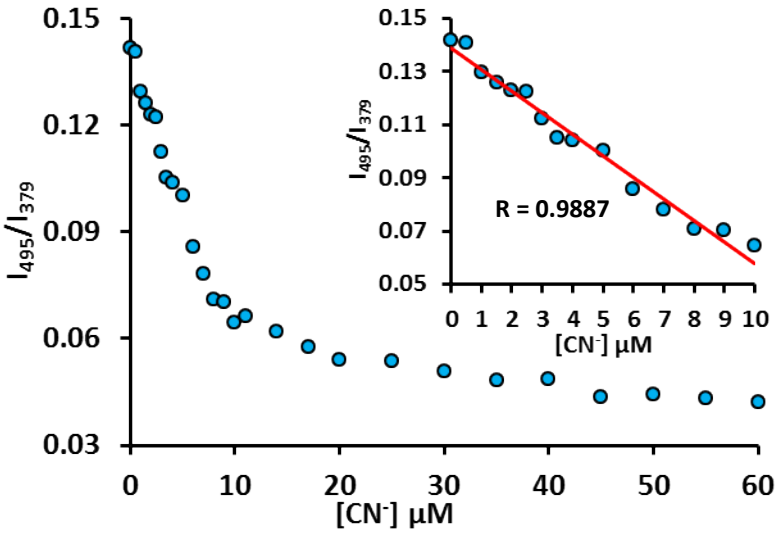

Fig. SI 19: Fluorescence ratiometric response (I_{495}/I_{379}) of probe **2** (1 µM, PBS -EtOH (5:95), pH = 7.4) with TBACN toward [CN^-].

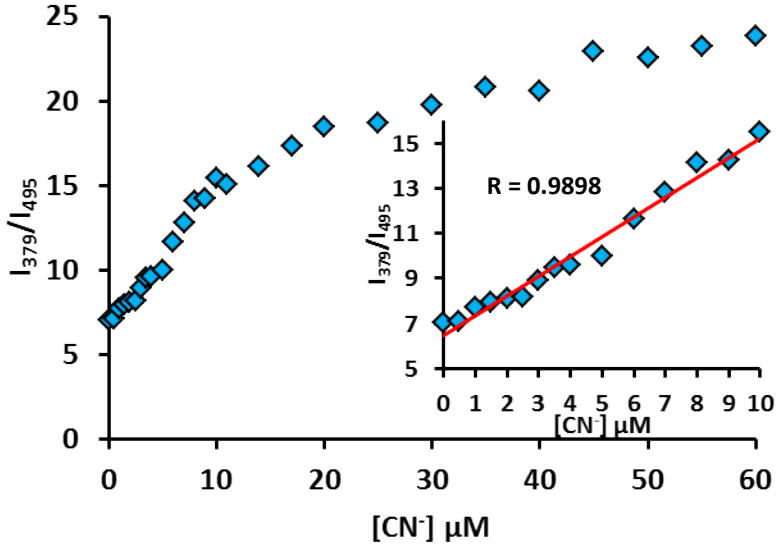

Fig. SI 20: Fluorescence ratiometric response (I_{379}/I_{495}) of probe **2** (1 µM, PBS -EtOH (5:95), pH = 7.4) with TBACN toward [CN^-].