

Supporting information

Highly selective colorimetric sensing of cyanide based on formation of dipyrromethane adducts

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Fig. S8. A plot of $(A - A_{\min}) / (A_{\max} - A_{\min})$ vs Log([CN⁻]), the calculated detection limit of sensor **3** is 7.1×10^{-6} M according to the literature method¹. A is the absorbance at 502 nm. The linear regression affords an R value of 0.994.

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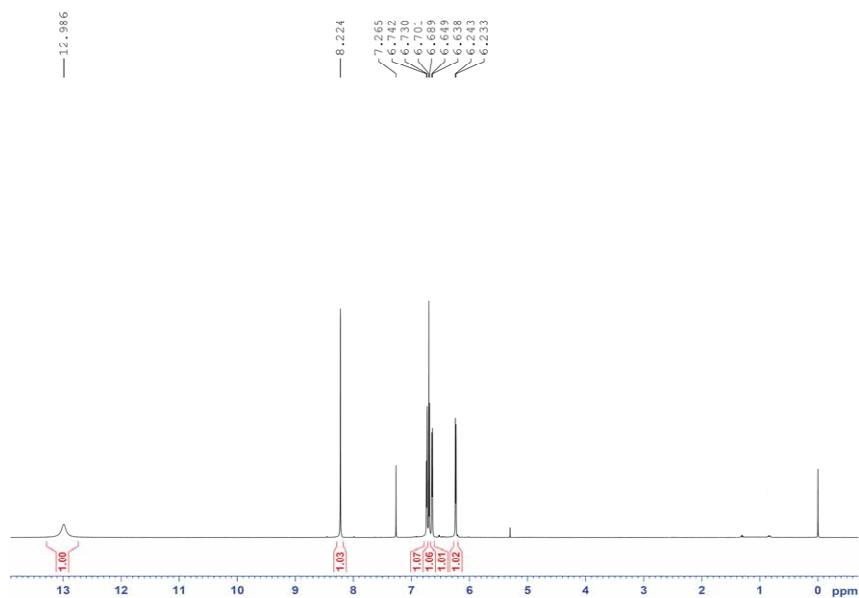


Fig. S1. The ^1H NMR spectrum of **1** in CDCl_3 .

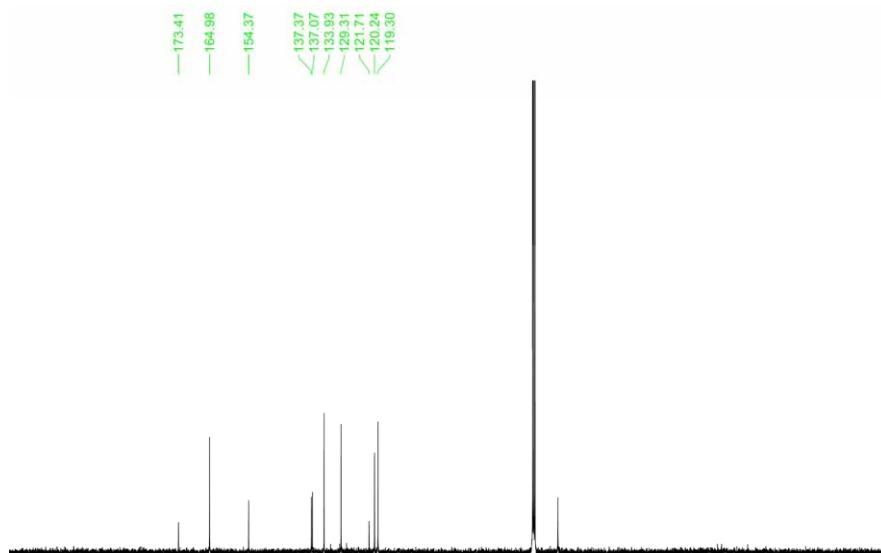


Fig. S2. The ^{13}C NMR spectrum of **1** in CDCl_3 .

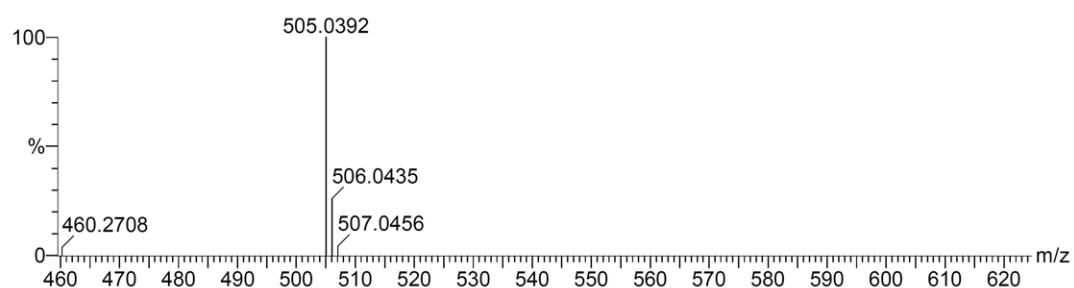


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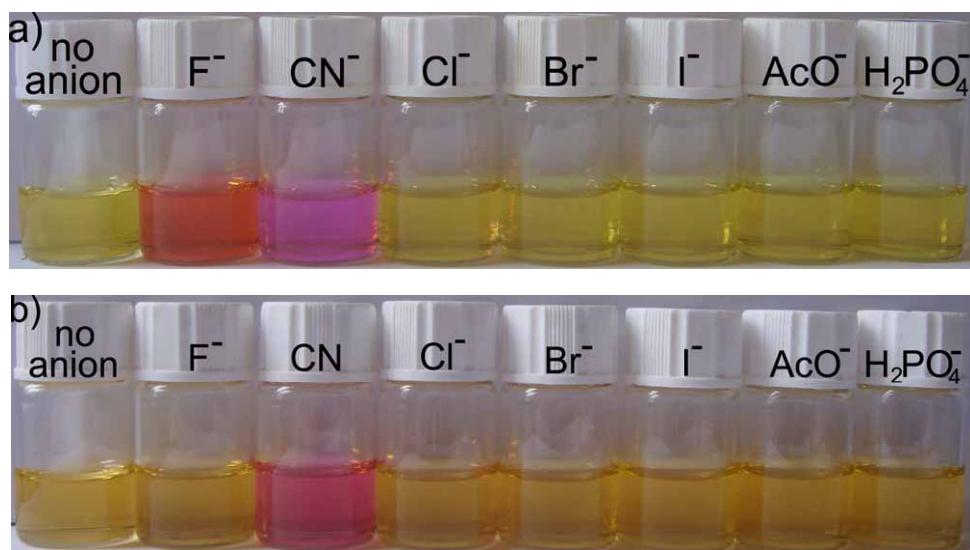


Fig. S4. A photograph showing the colour change of **2** (20 μM) upon addition of 800 μM of various anions: a) in CH_2Cl_2 ; b) in DMSO/ H_2O , 4/1, v/v.

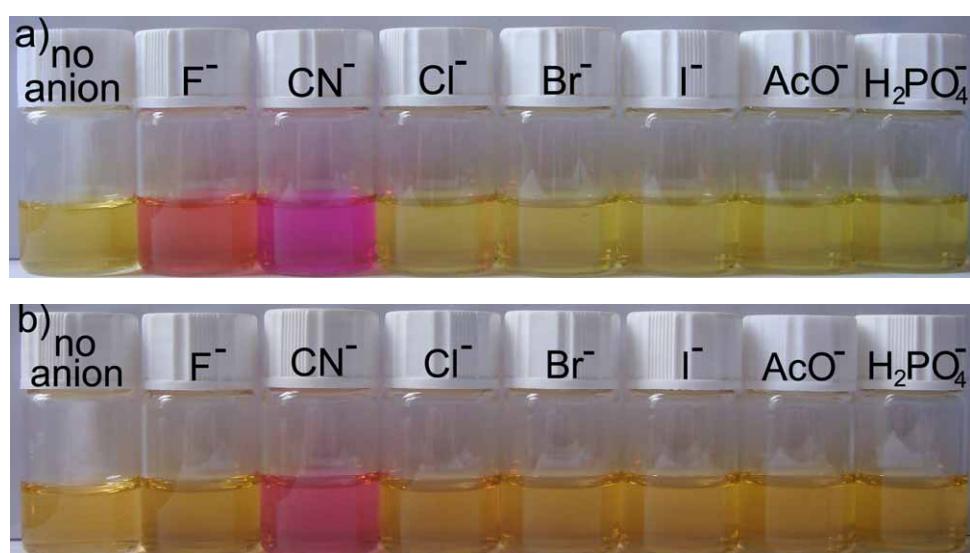


Fig. S5. A photograph showing the colour change of **3** (20 μM) upon addition of 800 μM of various anions: a) in CH_2Cl_2 ; b) in DMSO/ H_2O , 4/1, v/v.

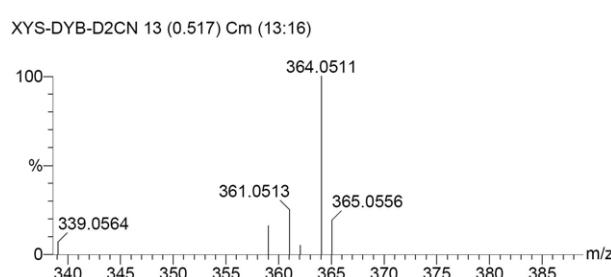


Fig. S6. HRMS of cyanide adduct of **3** in MeOH.

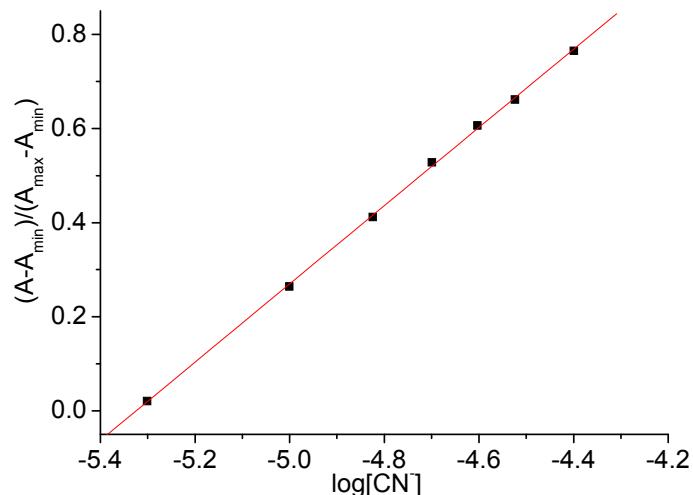


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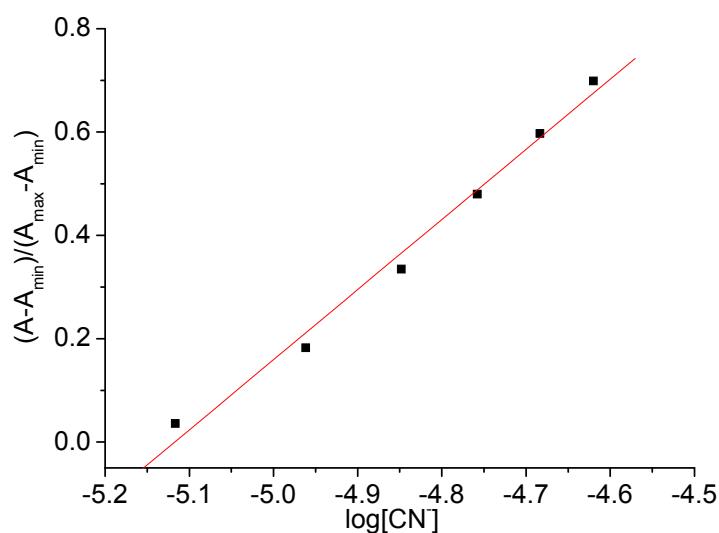


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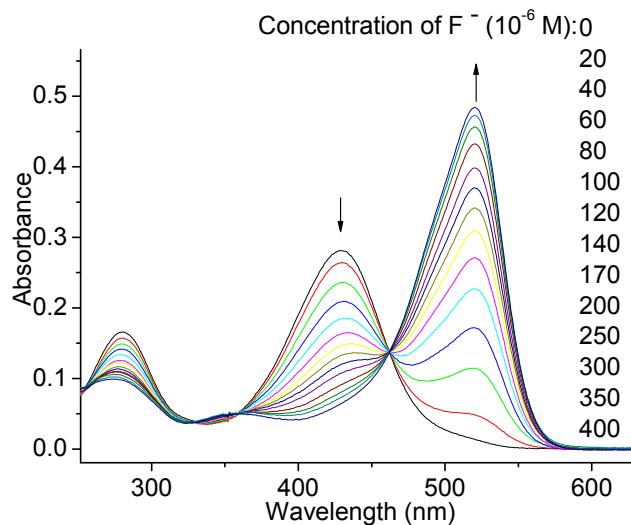


Fig. S9. UV-Vis spectral changes of **2** (10 μM) observed upon the addition of 0-400 μM F^- (TBA salt) in CH_2Cl_2 .

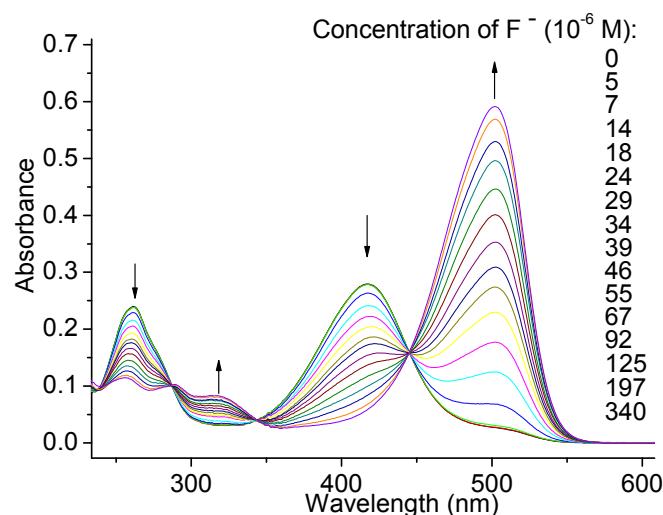


Fig. S10. UV-Vis spectral changes of **3** (12 μM) observed upon the addition of 0-340 μM F^- (TBA salt) in CH_2Cl_2 .

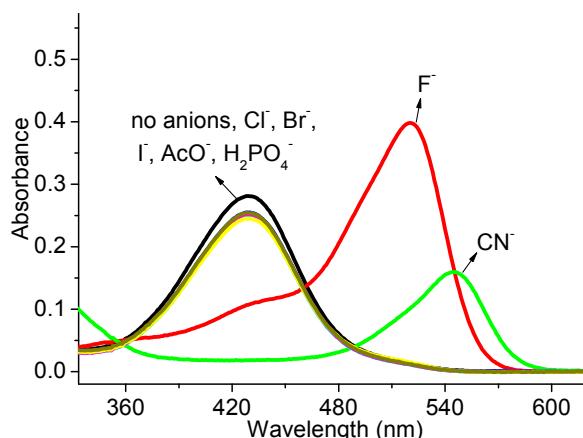


Fig. S11. UV-Vis spectral changes of **2** (10 μM) observed upon the addition of various anions (TBA salts, 38 μM for CN^- , 100 μM for F^- , 2000 μM for Cl^- , Br^- , I^- , AcO^- , H_2PO_4^-) in CH_2Cl_2 .

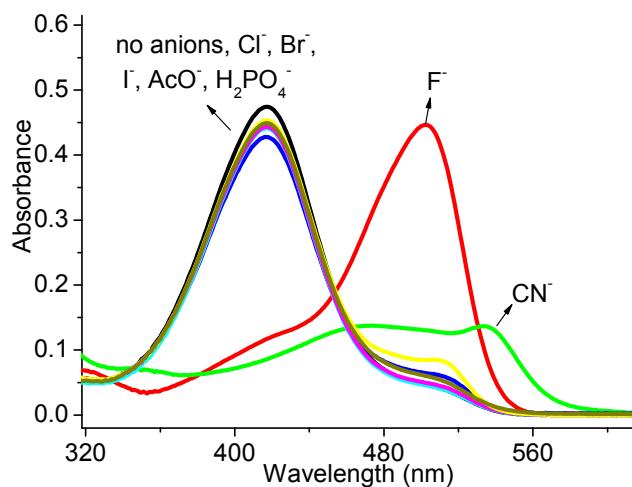


Fig. S12. UV-Vis spectral changes of **3** (12 μ M) observed upon the addition of various anions (TBA salts, 46 μ M for CN⁻, 120 μ M for F⁻, 2400 μ M for Cl⁻, Br⁻, I⁻, AcO⁻, H₂PO₄⁻) in CH₂Cl₂.

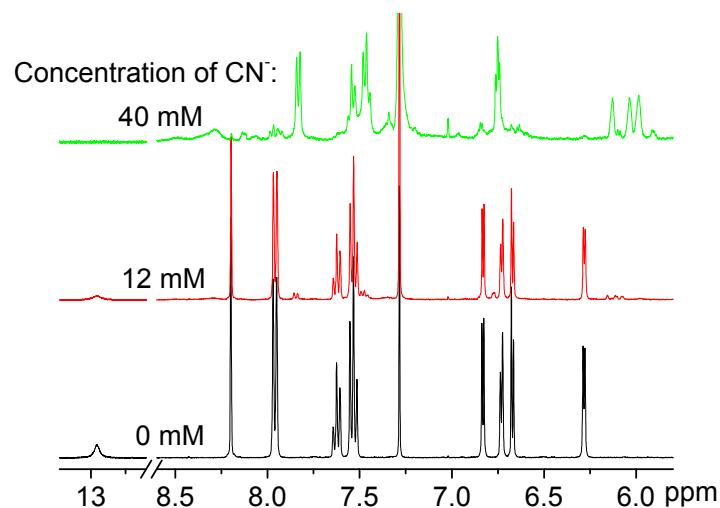


Fig. S13. Plots of ¹H NMR spectra of **2** (20 mM) on addition of CN⁻ in CDCl₃

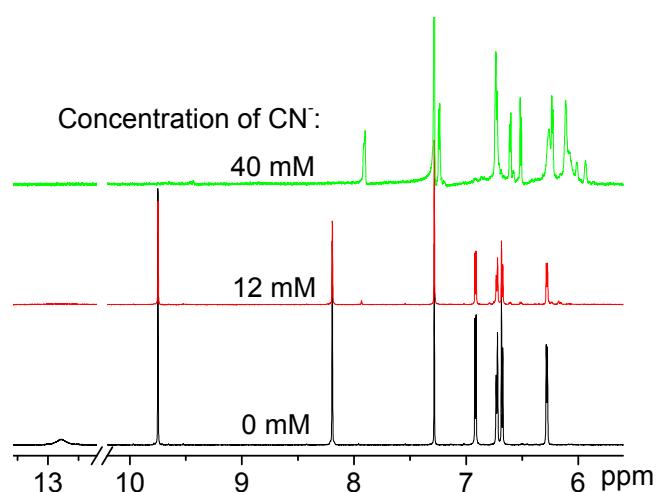


Fig. S14. Plots of ¹H NMR spectra of **3** (20 mM) on addition of CN⁻ in CDCl₃

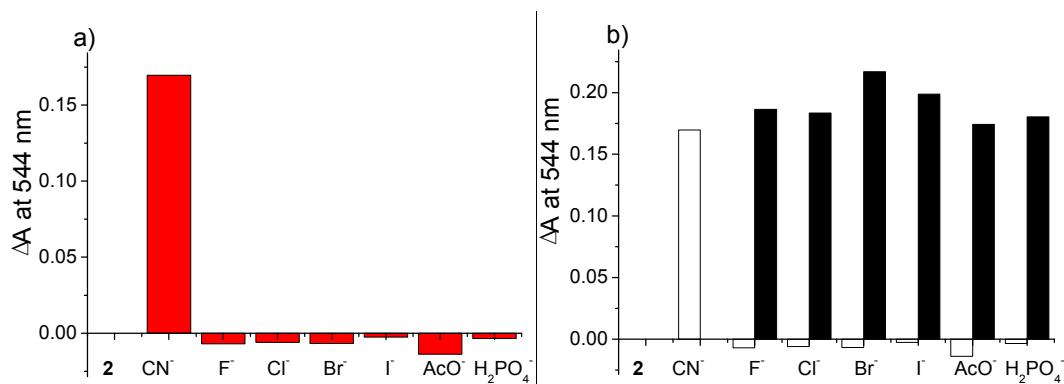


Fig. S15. Changes in the UV-Vis absorption spectrum of **2** (20 μ M) in the presence of the TBA salts of various anions (400 μ M for CN⁻, 4000 μ M for F⁻, Cl⁻, Br⁻, I⁻, AcO⁻, H₂PO₄⁻) in DMSO/H₂O, 4/1, v/v: (a) in the presence of various anions. (b) White bars represent the addition of various anions. Black bars represent the addition of 4000 μ M of indicated anions, followed by 400 μ M of CN⁻ anions.

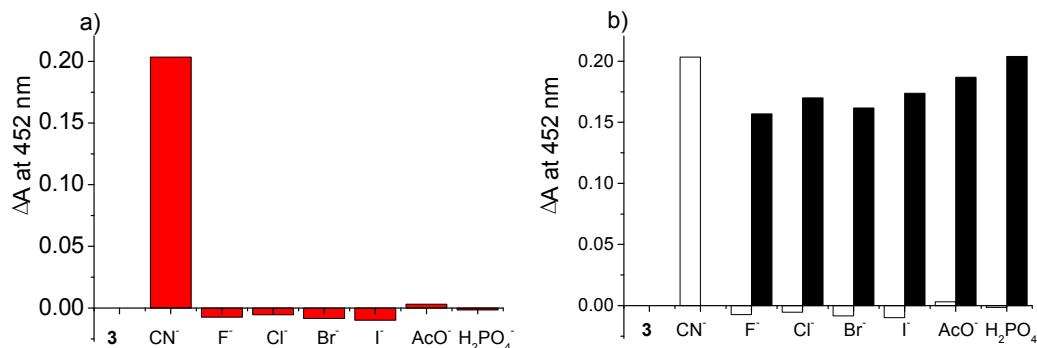


Fig. S16. Changes in the UV-Vis absorption spectrum of **3** (20 μ M) in the presence of the TBA salts of various anions (400 μ M for CN⁻, 4000 μ M for F⁻, Cl⁻, Br⁻, I⁻, AcO⁻, H₂PO₄⁻) in DMSO/H₂O, 4/1, v/v: (a) in the presence of various anions. (b) White bars represent the addition of various anions. Black bars represent the addition of 4000 μ M of indicated anions, followed by 400 μ M of CN⁻ anions.

References:

- [1] M. Shortreed, R. Kopelman, M. Kuhn and B. Hoyland, *Anal. Chem.*, 1996, **68**, 1414-1418.