

Supporting information

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

Yubin Ding, Tong Li, Weihong Zhu,* and Yongshu Xie*

Key Laboratory for Advanced Materials and Institute of Fine Chemicals, East China University of Science and Technology, Shanghai, P. R. China.; E-mail: yshxie@ecust.edu.cn; Fax: (+86) 21-6425-2758. Tel: (+86) 21-6425-0772.

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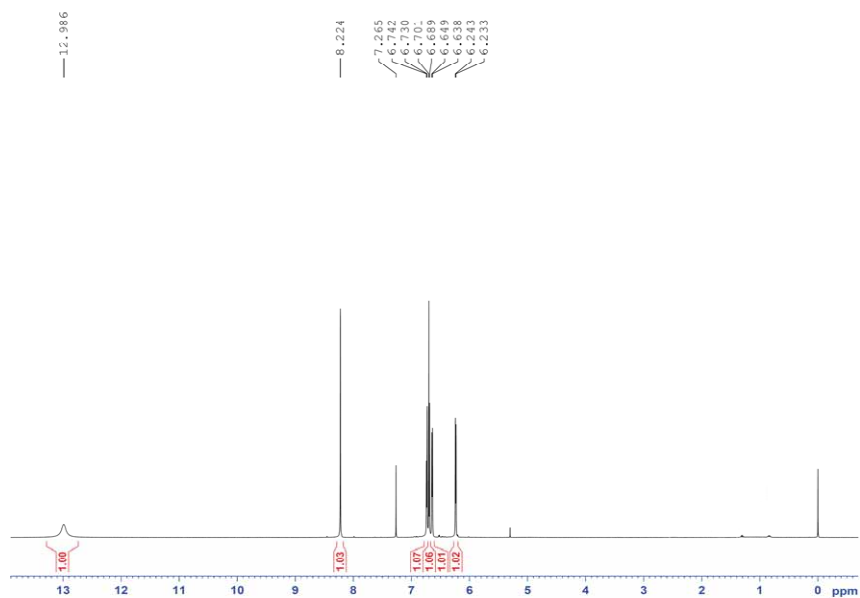


Fig. S1. The ^1H NMR spectrum of **1** in CDCl_3 .

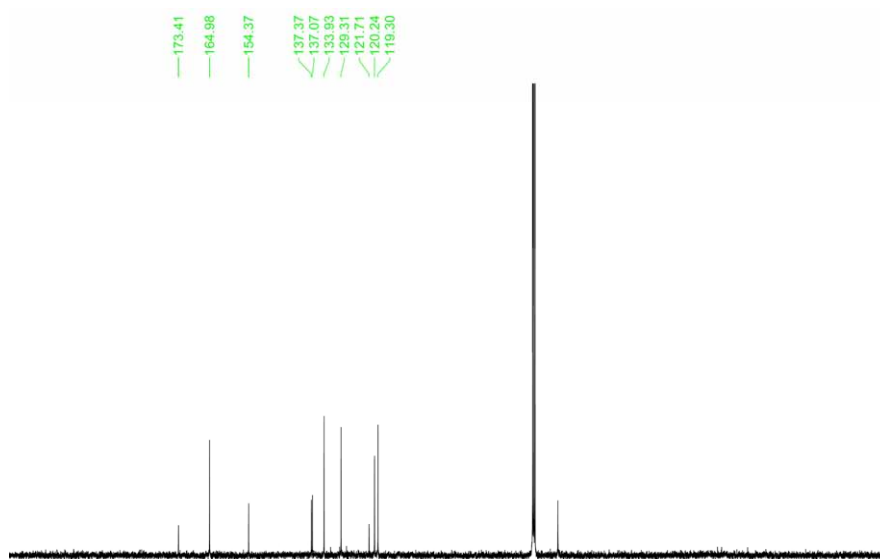


Fig. S2. The ^{13}C NMR spectrum of **1** in CDCl_3 .

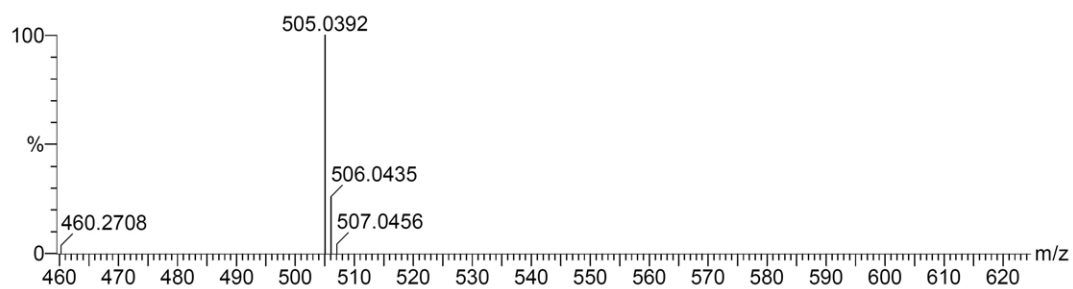


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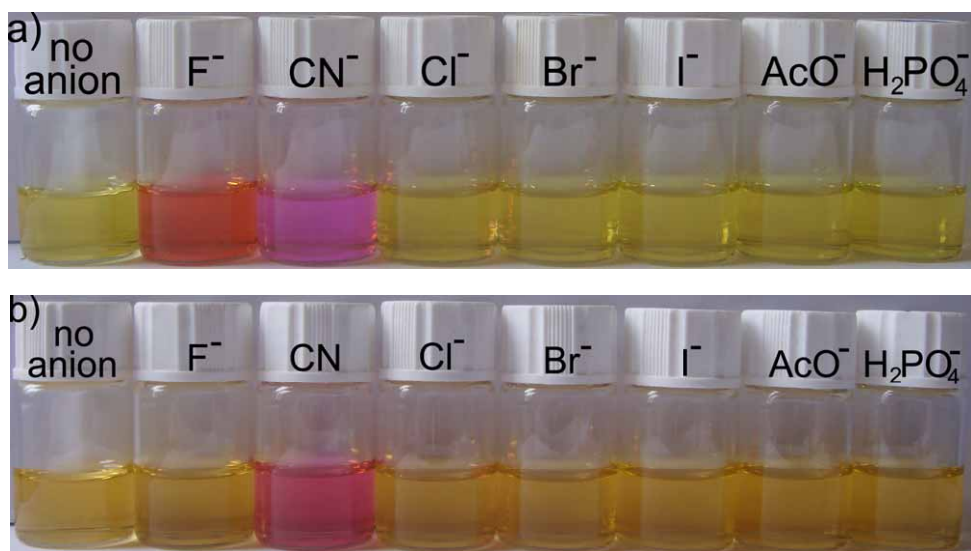


Fig. S4. A photograph showing the colour change of **2** (20 μM) upon addition of 800 μM of various anions: a) in CH₂Cl₂; b) in DMSO/H₂O, 4/1, v/v.

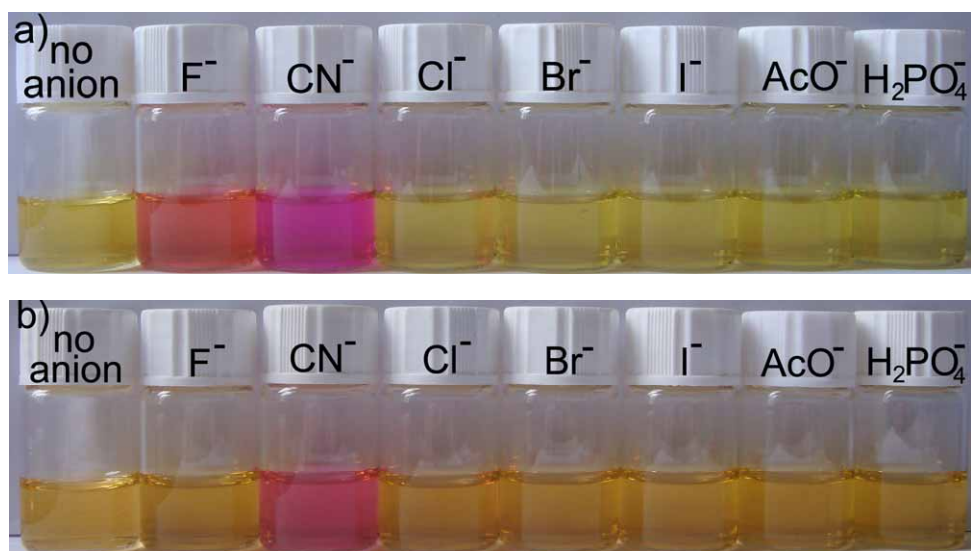


Fig. S5. A photograph showing the colour change of **3** (20 μM) upon addition of 800 μM of various anions: a) in CH₂Cl₂; b) in DMSO/H₂O, 4/1, v/v.

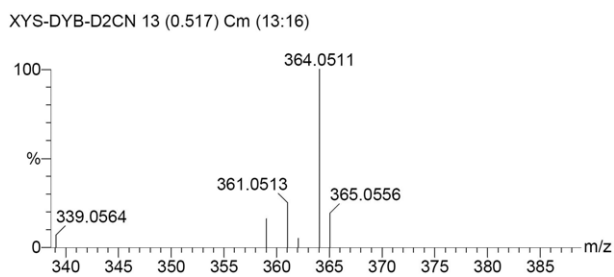


Fig. S6. HRMS of cyanide adduct of **3** in MeOH.

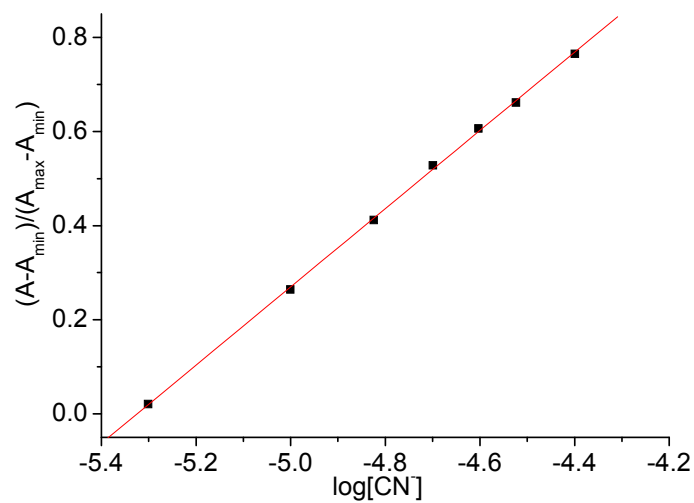


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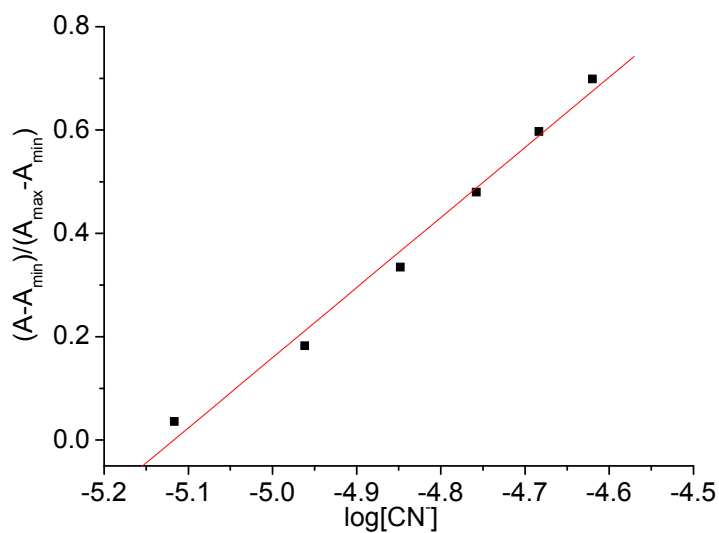


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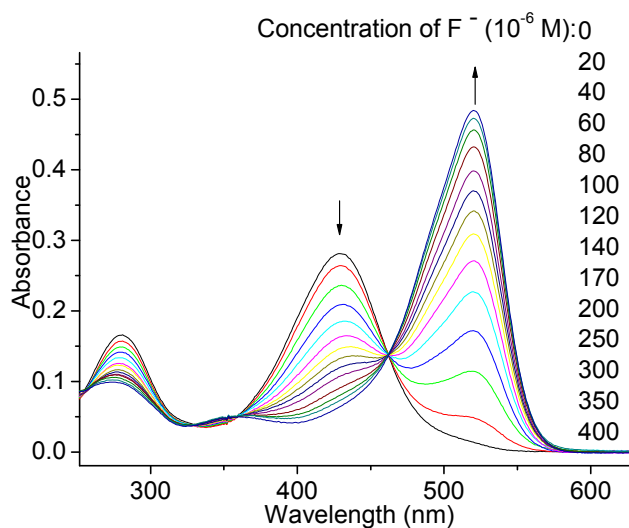


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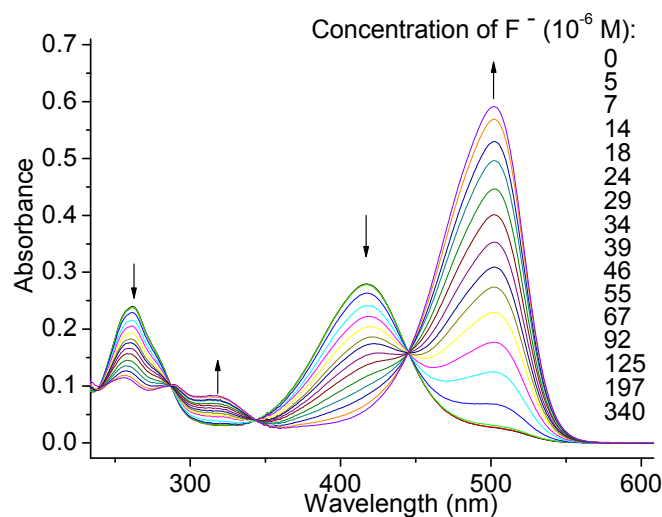


Fig. S10. UV-Vis spectral changes of **3** (12 μ M) observed upon the addition of 0-340 μ M F^- (TBA salt) in CH_2Cl_2 .

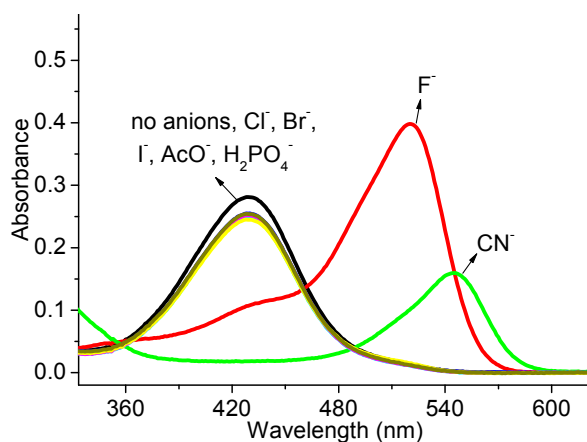


Fig. S11. UV-Vis spectral changes of **2** (10 μ M) observed upon the addition of various anions (TBA salts, 38 μ M for CN^- , 100 μ M for F^- , 2000 μ M for Cl^- , Br^- , I^- , AcO^- , $H_2PO_4^-$) in CH_2Cl_2 .

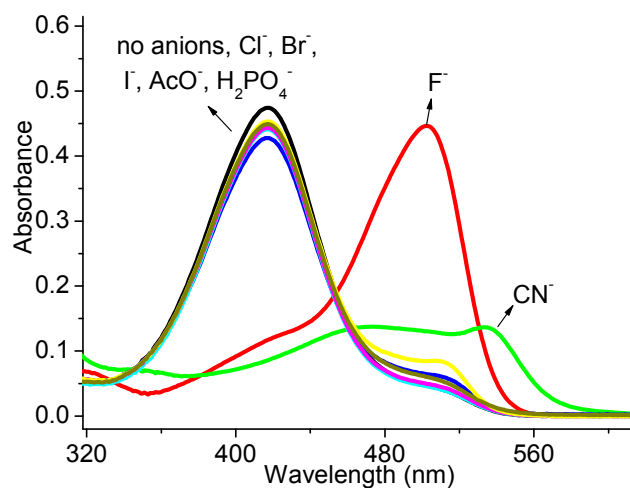


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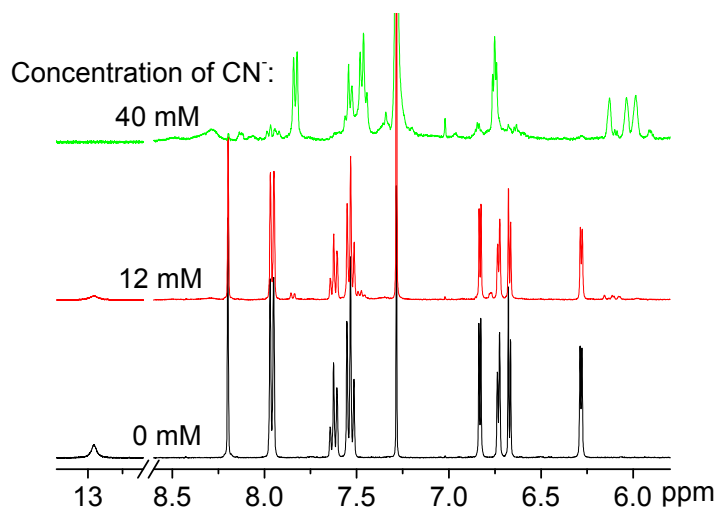


Fig. S13. Plots of ¹H NMR spectra of **2** (20 mM) on addition of CN⁻ in CDCl₃

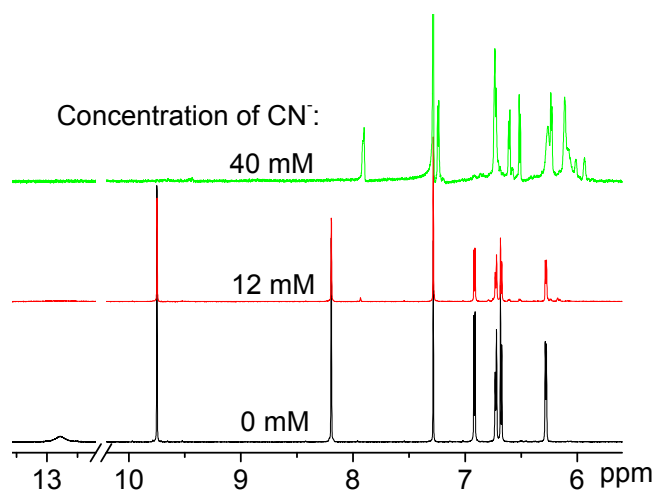


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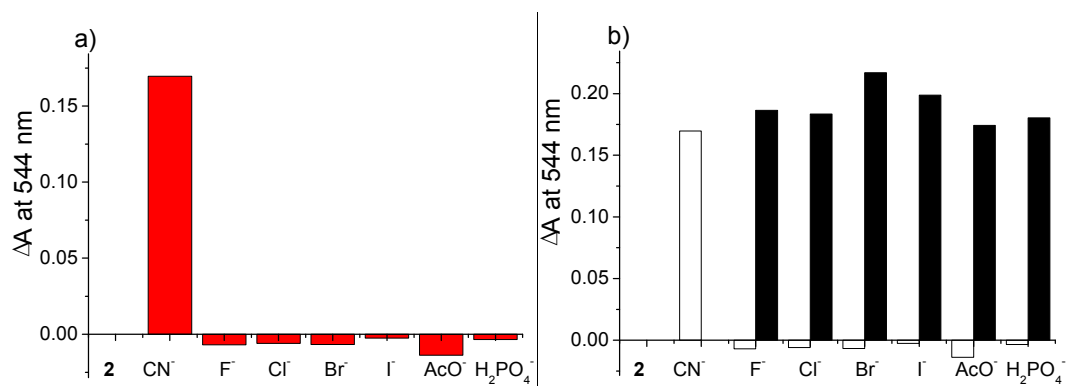


Fig. S15. Changes in the UV-Vis absorption spectrum of **2** (20 μM) in the presence of the TBA salts of various anions (400 μM for CN^- , 4000 μM for F^- , Cl^- , Br^- , I^- , AcO^- , H_2PO_4^-) in DMSO/ H_2O , 4/1, v/v: (a) in the presence of various anions. (b) White bars represent the addition of various anions. Black bars represent the addition of 4000 μM of indicated anions, followed by 400 μM of CN^- anions.

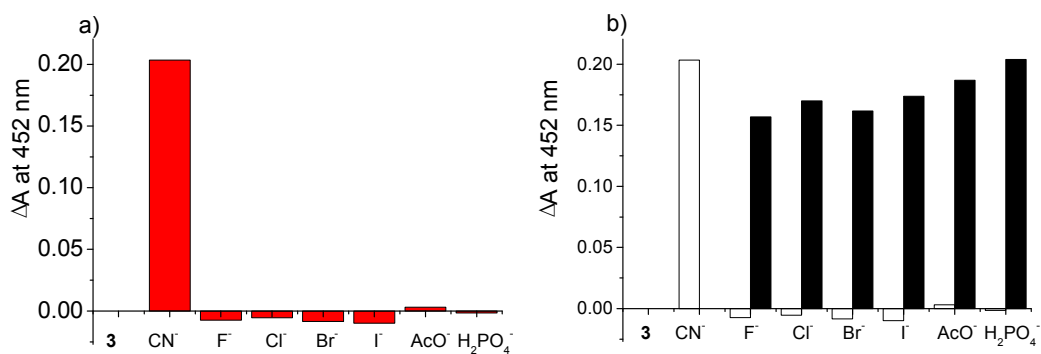


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References:

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