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Supporting Information

One-pot synthesis of ferrocenyl dithiocarbamates and its application for the detection of Cu²⁺

Junyang Dong^{a,b}, Jianfeng Hu^{a,c}, Hao Zhang^{a,c*}

^aSchool of Chemical & Chemical Engineering, Inner Mongolia University, Hohhot

010021, P. R. China.

^bState Key Laboratory of Solid Lubrication, Lanzhou Institute of Chemical Physics,

Chinese Academy of Sciences, Lanzhou 730000, P. R.China

^cInner Mongolia Key Laboratory of Fine Organic Synthesis, Hohhot 010021, P. R. China.

*Corresponding Author, tel: +86-471-4994406, fax: +86-471-4994406, e-mail: haozhang@imu.edu.cn; zh hjf@hotmail.com.

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1. General information.

All reagents were used as received from commercial sources, unless specified otherwise, or prepared as described in the references. N-tosylhydrazone and ammonium dithiocarbamate were prepared according to the literature method. Solvent dioxane was distilled over sodium. All Solvents were purified according to standard references procedures. For chromatography, 200-300 mesh silica gel (Qingdao, China) was employed. ¹H and ¹³C NMR spectra were recorded at 500 MHz and 125 MHz FT-NMR spectrometer. Chemical shifts are reported in ppm using tetramethylsilane as internal standard when CDCl₃ was used as solvent. The HRMS analysis was obtained on a QTOF mass spectrometer. Melting points were determined with melting points apparatus and are uncorrected. The data of **3a** and **3e** were collected on a Bruker APEX II CCD Mo-K α radiation ($\lambda = 0.71073$ Å) and measured at room temperature.

2.1H, 13C NMR spectra for all compounds



¹H NMR spectra and ¹³C NMR spectra for **3a**.



¹H NMR spectra and ¹³C NMR spectra for **3b**.



¹H NMR spectra and ¹³C NMR spectra for 3c.



 $^1\mathrm{H}$ NMR spectra and $^{13}\mathrm{C}$ NMR spectra for **3d**.



¹H NMR spectra and ¹³C NMR spectra for **3e**.



 $^1\mathrm{H}$ NMR spectra and $^{13}\mathrm{C}$ NMR spectra for **3f**.



 $^1\mathrm{H}$ NMR spectra and $^{13}\mathrm{C}$ NMR spectra for **3g**.



 $^1\mathrm{H}$ NMR spectra and $^{13}\mathrm{C}$ NMR spectra for **3h**.







 $^1\mathrm{H}$ NMR spectra and $^{13}\mathrm{C}$ NMR spectra for **3i**.





 $^1\mathrm{H}$ NMR spectra and $^{13}\mathrm{C}$ NMR spectra for **5a**.



 $^1\mathrm{H}$ NMR spectra and $^{13}\mathrm{C}$ NMR spectra for **5b**.



¹H NMR spectra and ¹³C NMR spectra for **5c**.

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140 130 120 110 100 90 80 70 60 50 40 30 20 10 0

200 190 180 170 160 150



 $^1\mathrm{H}$ NMR spectra and $^{13}\mathrm{C}$ NMR spectra for 5d.



¹H NMR spectra and ¹³C NMR spectra for **5e**.



Figure S1. Visual color changes of probe 3e upon addition of various metal ions (5 equiv) in CH₃CN/H₂O (7:3, v/v, 10 μ M).



Figure S2. Benesi - Hildebrand plot obtained from the UV- vis absorption (absorption calculated from 423 nm) **3e**-Cu²⁺.



Figure S3. Benesi - Hildebrand plot obtained from the UV- vis absorption (absorption calculated from 423 nm) **3e**-Cu²⁺.



Figure S4. The Job's plot of receptor 3e-Cu²⁺.