Electronic Supplementary Material (ESI) for RSC Advances.

Supporting Information

for

Development and cell imaging applications of a novel fluorescent probe for Cu^{2+}

Yuehua Yuan, Maozhong Tian,* Junling Wang, Hai Xie, Jun Qin, Feng Feng*

College of Chemistry and Environmental Engineering, Shanxi Datong University, Datong 037009, P. R. China

Contents:

1. Interfere of anions

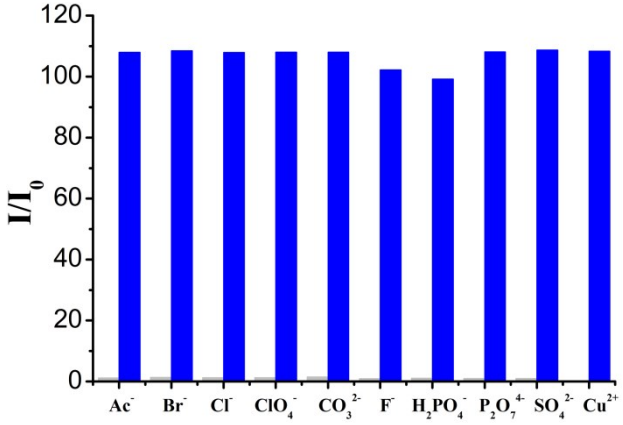

Fig. S1. Histogram showing selectivity of **1** (10 μM) for Cu^{2+} in HEPES buffer (50 mM, containing 0.1M KNO_3, pH=7.4) solution. The light gray bars represent the I/I_0 value in the presence of various anions (10 equivalents). The blue bars indicate the change in the emission intensity upon subsequent addition of Cu^{2+} (5 equivalents) to the solution containing **1** and the anions of interest. For all measurements, λ_{ex}=350 nm; T =298 K. The signal intensity at λ=488 nm (=I) was normalized with that of the sensor-only sample (=I_0). Excitation and emission slit widths were 3 and 6 nm, respectively.

2. Competitive experiments of Cu^{2+}

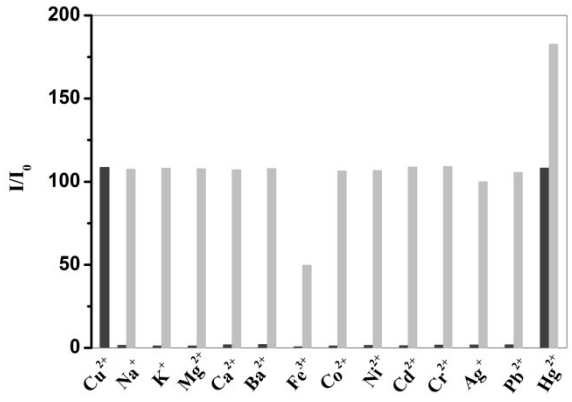

Fig. S2 Normalized fluorescence responses of **1** (10 μM) to various metal ions in HEPES buffer (50 mM, containing 0.1M KNO_3, pH=7.4) solution. The dark bars represent the I/I_0 value in the presence of various metal ions. The light gray bars indicate the change in the emission intensity

upon subsequent addition of Cu^{2+} (5 equivalents) to the solution containing **1** (10 μM) and the metal ions of interest (5 equivalents). For all measurements, λ_{ex}=350 nm; T =298 K. The signal intensity at λ=488 nm (=I) is normalized with that of the sensor-only sample (=I_0). Excitation and emission slit widths were 3 and 6 nm, respectively.

3. UV–vis spectral reponses of 1

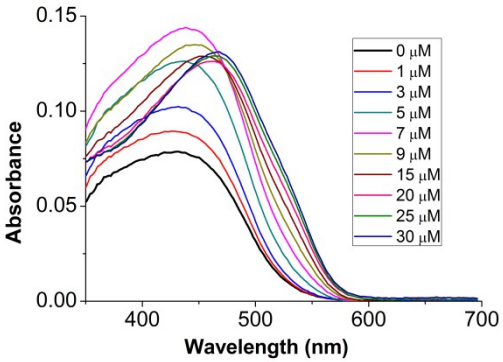

Fig. S3 Cu^{2+} (0-30 μM) induced variations in the absorption spectra of **1** (10 μM) in HEPES solution (50 mM, pH = 7.4)

4. MALDI-TOF mass spectrum of 1+Cu^{2+} (BDAT)

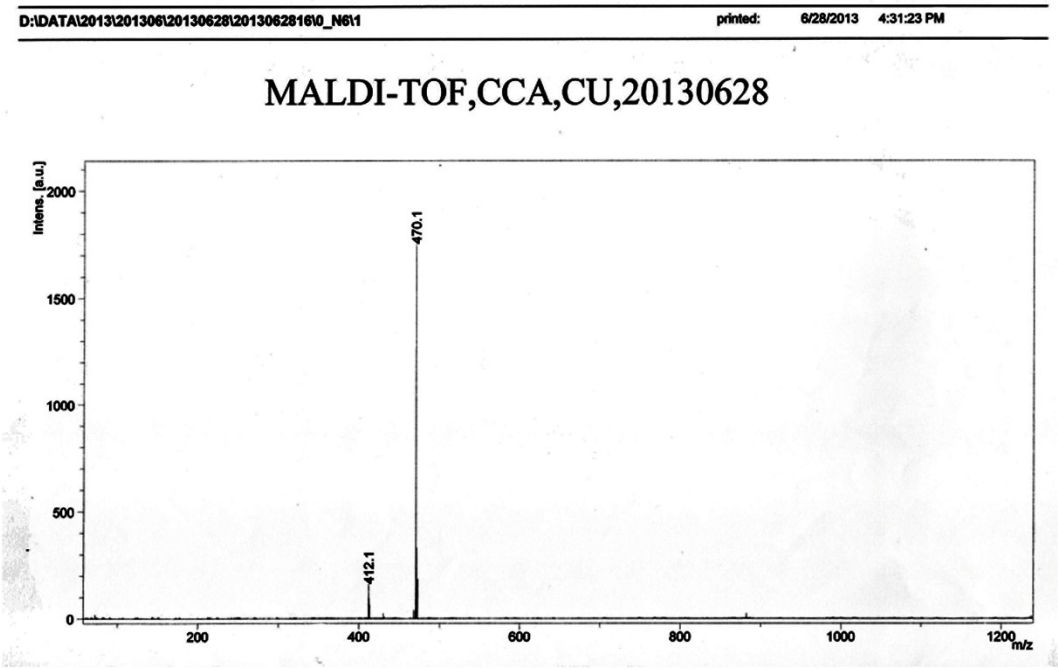

Fig. S4. MALDI-TOF mass spectrum of **1**+Cu^{2+} (**BDAT**)

5. Infrared spectra of 1 and 1+Cu^{2+}

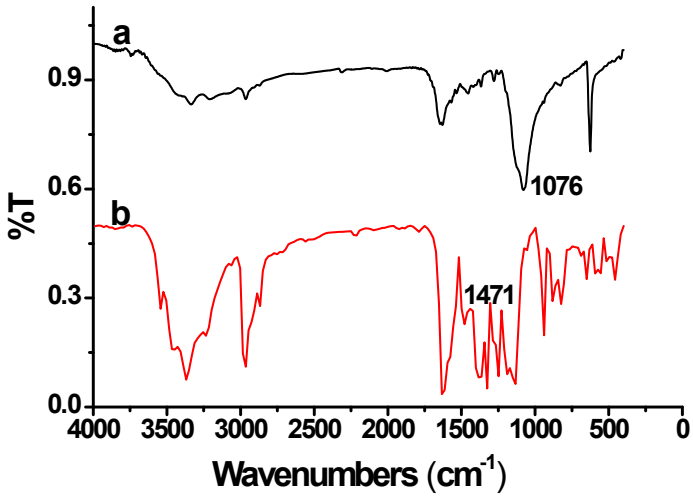

Fig. S5. IR spectra of **1** and **1+Cu^{2+}** (a: **1+Cu^{2+}**; b: probe **1**)

6. pH titration of free probe 1 and 1+Cu^{2+}

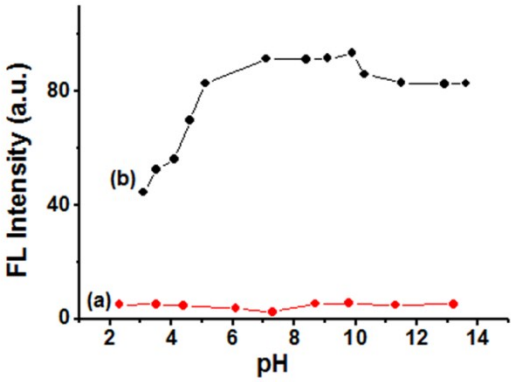

Fig. S6. Fluorescence intensity (488 nm) of free **1** (10 μM) (a) and after addition of 50 μM of Cu^{2+} (b) in 50 mM of HEPES buffer solution (pH = 7.4) as a function of different pH values. Excitation at 350 nm.

7. Crystal structure determination of 1.

Red crystals of **1** were grown upon EtOAc/Hexane mixture solution at 25 °C. The data collection of **1** was performed on a CrysAlisPro diffractometer using mirror monochromated Cu-K_α radiation (λ = 1.5418 Å). Intensities were measured by ω-scans and corrected for background, polarization and Lorentz effects. A semi-empirical absorption correction was applied for the

data sets. The structure was solved by direct methods and refined anisotropically by the least-squares procedure implemented in the SHELX program system [1]. Crystallographic data for the structure reported in this paper have been deposited with the Cambridge Crystallographic Data Centre as supplementary publication CCDC NO. 961622, Copies of the data can be obtained free of charge via www.ccdc.cam.ac.uk/conts/retrieving.html (or from the Cambridge Crystallographic Data centre, 12 Union Road, Cambridge CN21EZ, U; fax. (+44) 1223-33603 3; e-mail: deposit@ccdc.cam.ac.uk).

Table S1. Selected Crystallographic and Data Collection Parameters for probe **1**

empirical formula	$C_{26}H_{32}N_4O_2$
formula weight	432.56
crystal system	triclinic
space group	$P\bar{1}$
a (Å)	11.7693(5)
b (Å)	19.6839(10)
c (Å)	22.7064(7)
α (deg)	112.090(4)
β (deg)	90.068(3)
γ (deg)	99.006(4)
volume (Å^3)	4803.7(3)
Z	8
density (calcd) (g · cm^{-3})	1.196
absorption coeff (mm^{-1})	0.609
F(000)	1856
crystal color and shape	Red and needle
θ range for data collection	3.80°–63.69°
reflections collected	23886
independent reflections	23886
observed reflections [$I > 2\sigma(I)$]	15961
data/restraints/parameters	23886/0/1190
goodness-of-fit on F^2	1.086
final R indices [$I > 2\sigma(I)$]	$R_1 = 0.0749$, w$R_2 = 0.2076$
R indices (all data)	$R_1 = 0.1106$, w$R_2 = 0.2388$
Largest diff. peak and hole (e · Å^{-3})	0.530 and -0.489

8. The characterization data of probe 1

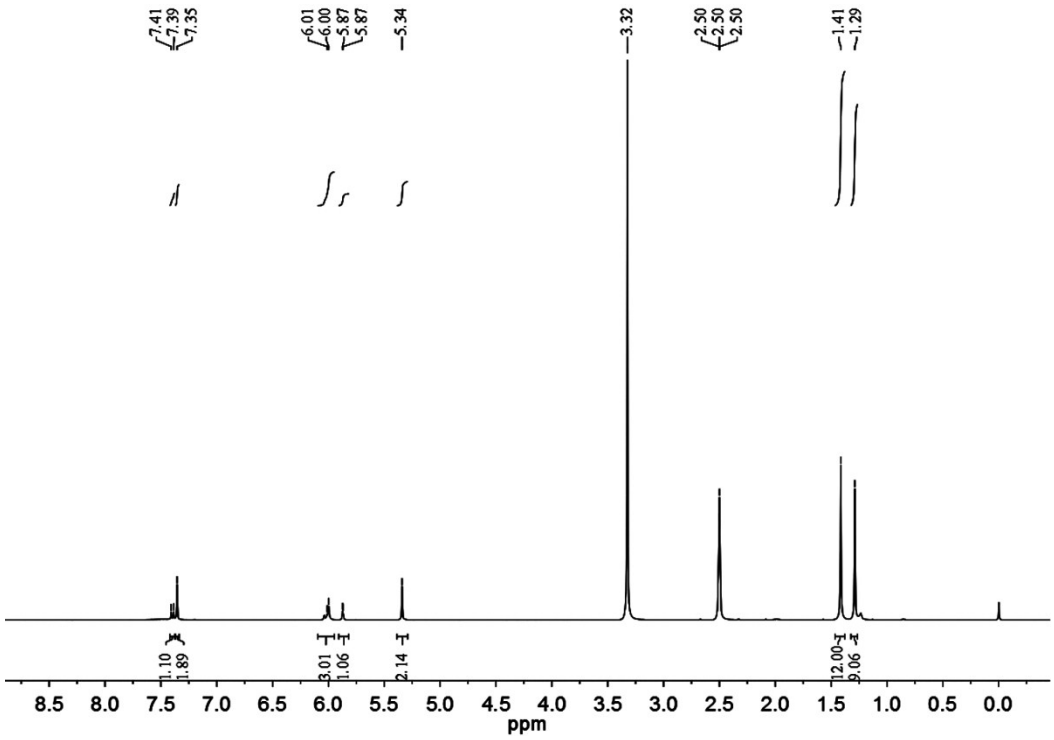

Fig. S7.[1]H NMR spectra of **1** in DMSO-d_6

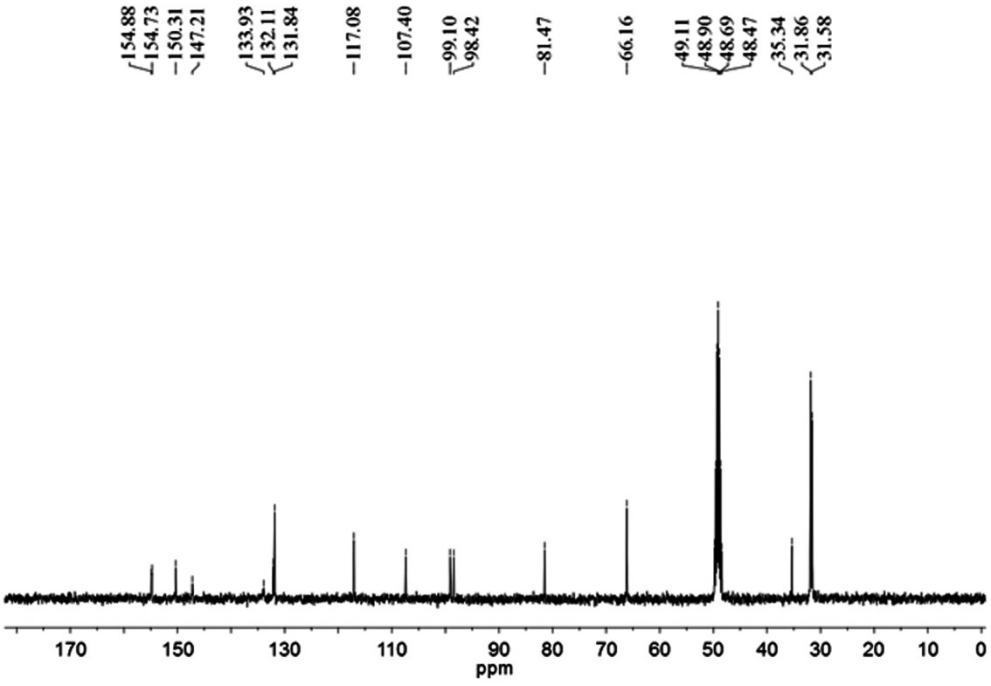

Fig. S8. **[13]C** NMR spectra of **1** in DMSO-d_6

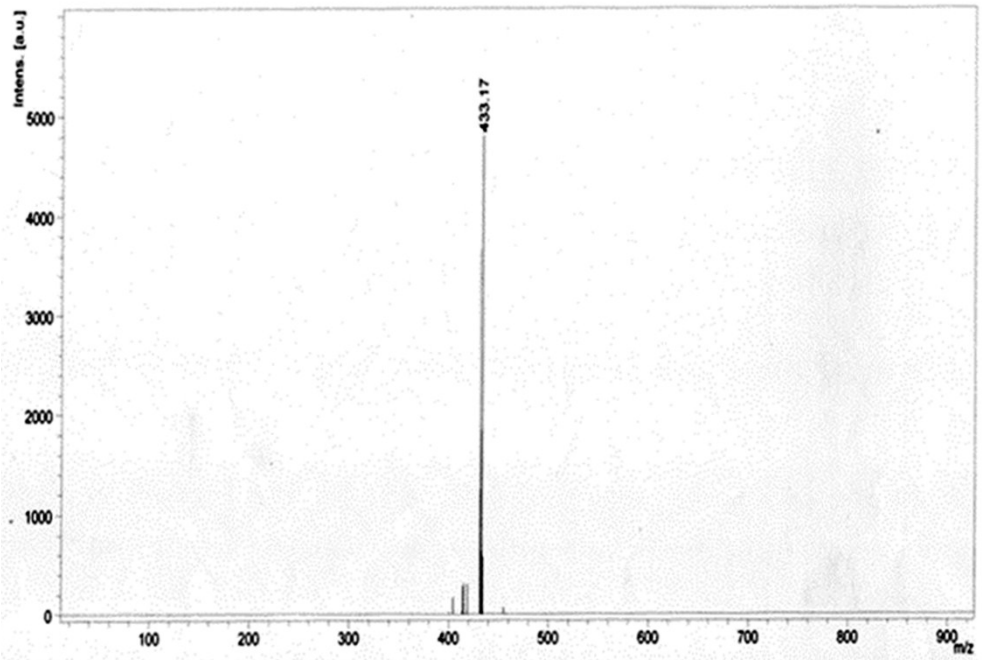

Fig. S9. MALDI-TOF mass spectrum of probe **1.**

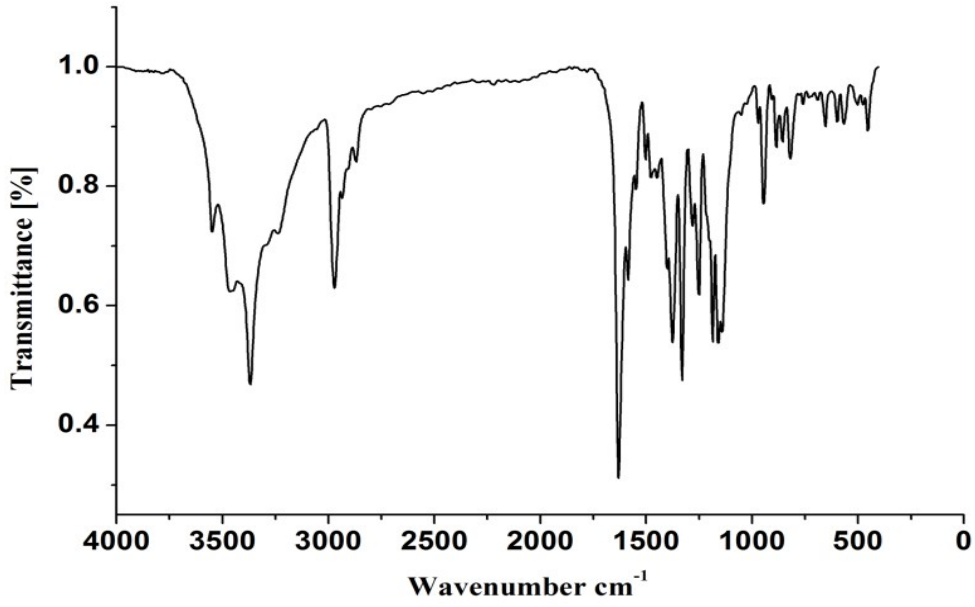

Fig. S10. IR spectrum of probe **1.**

9. References

[1] G. M. Sheldrick, SHELXS97 and SHELXL97, University of Gottingen, Germany, 1997.