Electronic Supplementary Material

for

A Fluorescent and Colorimetric Probe based on Naphthalene Diimide and High Sensitivity towards Copper Ions as Test Strips

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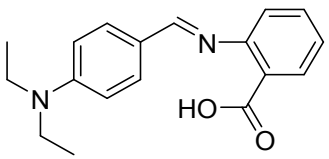
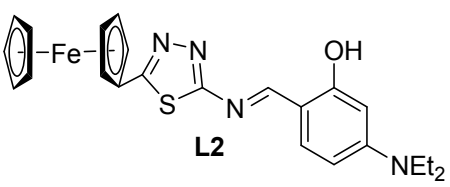
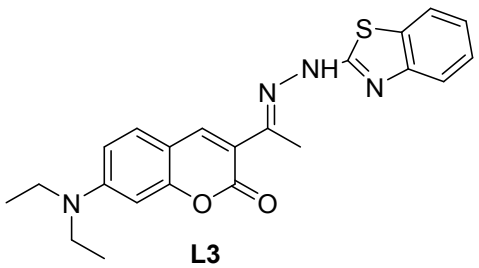
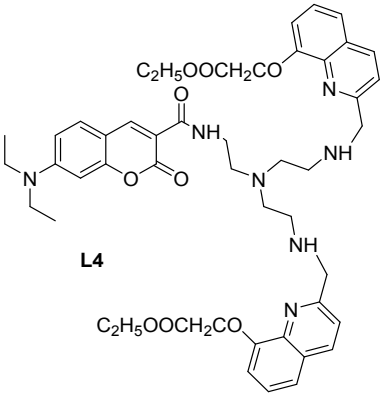
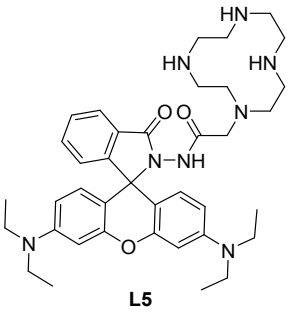
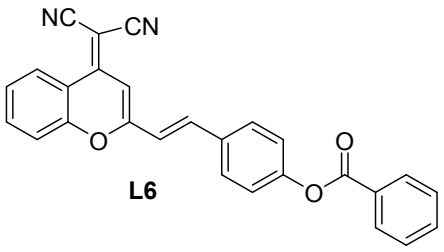
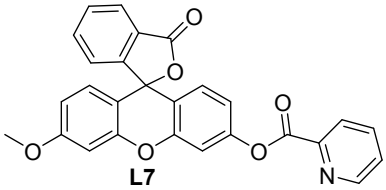
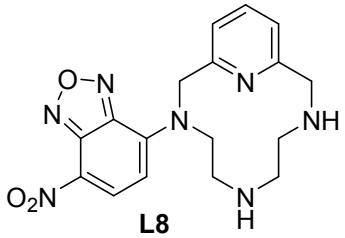
Table S1. Performance compared with available Cu^{2+}probes.

Ligand name	Fluorescence modes	Detection limit	Fluorophore	Issues
 **L1**	Quenching $\lambda_{ex}/\lambda_{em}$=341nm/393 nm	2.48 μM		Also complex with Fe^{2+}, Fe^{3+}
 **L2**	Enhancement $\lambda_{ex}/\lambda_{em}$=440 nm/510 nm	28 ppb	Salicylaldehyde derivative	Also complexes with Co^{2+}, Hg^{2+}

 **L3**	Enhancement $\lambda_{ex}/\lambda_{em}$=367 nm/457 nm	0.058 μM	Coumarin derivative	Also complexes with Hg^{2+} (response time= 1h)
 **L4**	Quenching $\lambda_{ex}/\lambda_{em}$=420 nm/468 nm	1.96 μM	Coumarin derivative	
 **L5**	Enhancement $\lambda_{ex}/\lambda_{em}$=552 nm/580 nm	126 ppb	Rhodamine derivative	Also complexes with Zn^{2+}
 **L6**	Enhancement λ_{em}=676 nm	0.023 μM	DCM derivative	Response time = 40 min
 **L7**	Enhancement $\lambda_{ex}/\lambda_{em}$=460 nm/514 nm	55 nM	Fluorescein derivative	Response time = 1 min
 **L8**	Quenching $\lambda_{ex}/\lambda_{em}$=470 nm/ 530 nm	0.84 μM		

Our Work	Quenching $\lambda_{ex}/\lambda_{em}$=602 nm/ 638 nm	0.97 μM	NDI derivative	Response time = 30 s

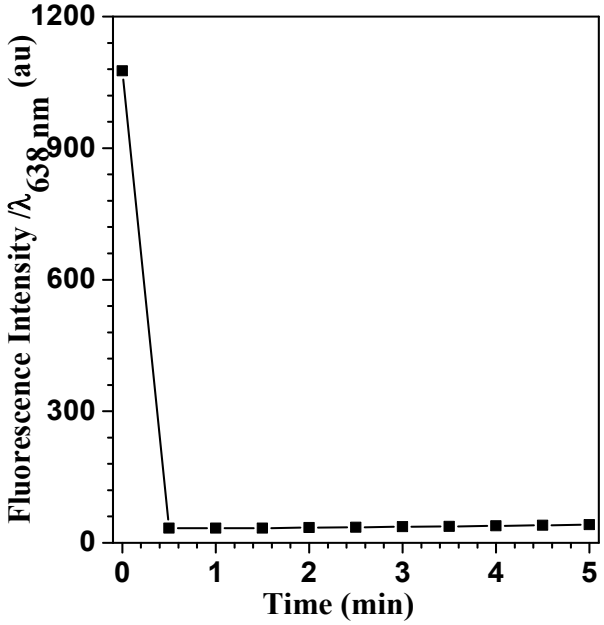


Fig.S1 Time-dependent quenching upon addition of a Cu ion source. The exicited wavelength was 605 nm.

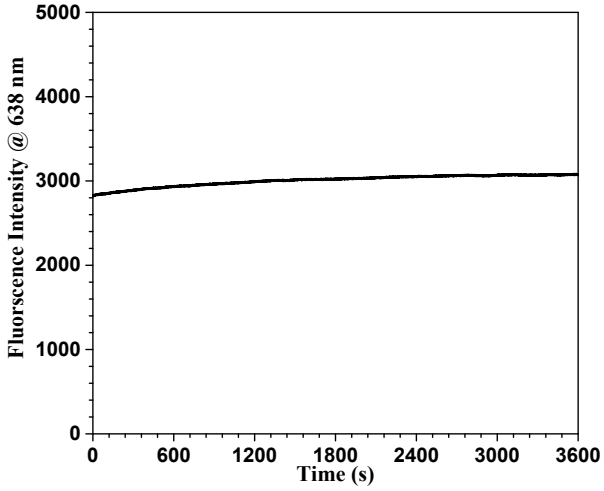


Fig. S2 The fluorescence intensity of NDI-Py in solution (concentration: 1×10^{-5} mol/L) with increasing scan (0–3600 s). Excitation wavelength: 605 nm.

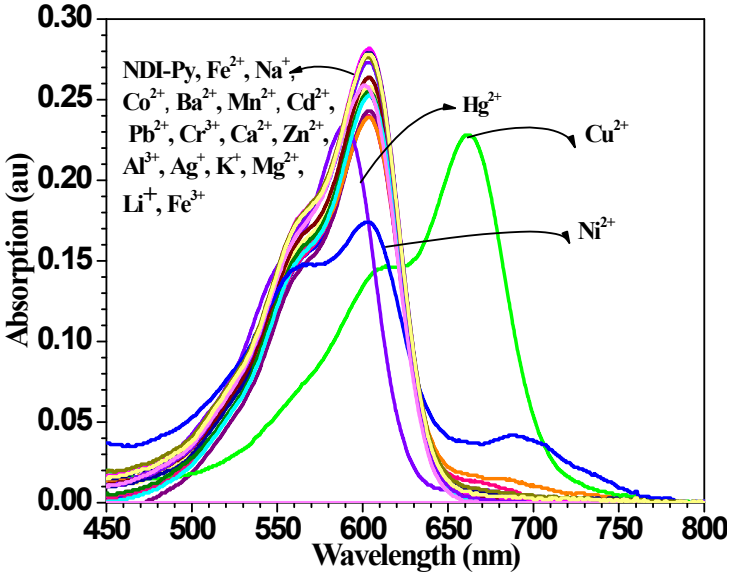


Fig. S3 The UV-visible spectra of **NDI-Py** in acetone (20 μM) towards 1.0 equiv. of various metal ions

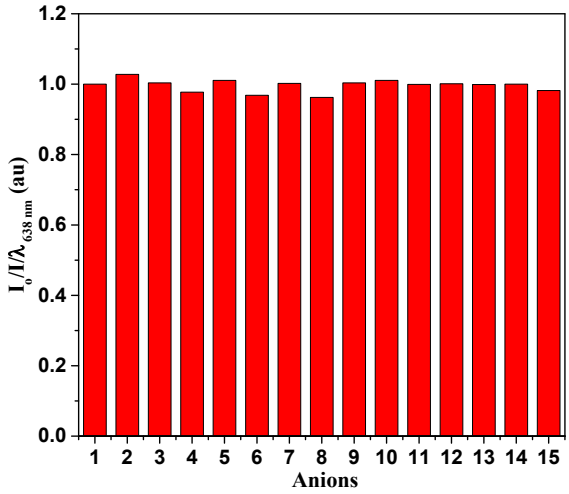


Fig. S4 The changes of fluorescence intensity of NDI-Py (10 μM in acetone) at 638 nm with 10 equiv of different anions. (1) Blank; (2) F^-; (3) Cl^-; (4) I^-; (5) Br^-; (6) ClO_3^-; (7) CO_3^{2-}; (8) HCO_3^-; (9) HSO_3^-; (10) $S_2O_3^{2-}$; (11) $S_2O_5^{2-}$; (12) SO_3^{2-}; (13) SO_4^{2-}; (14) NO_2^-; (15) NO_3^-.

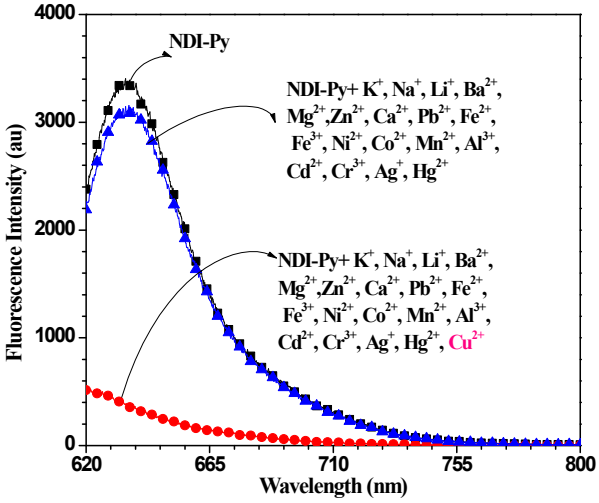


Fig. S5 Fluorescence spectra of **NDI-Py** (10 μM in acetone) with the addition of different metal ions (1 equiv.) at the same time.

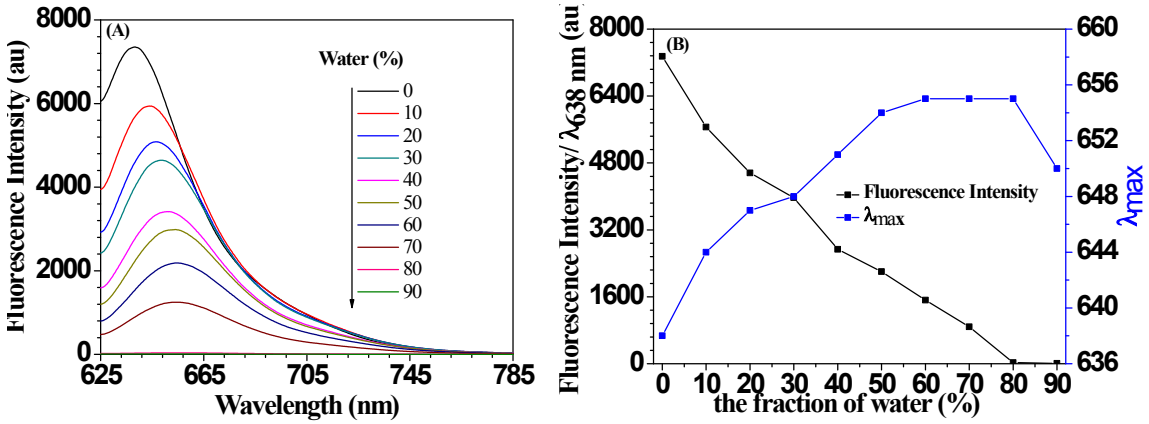


Fig. S6 (A) The changes of fluorescence intensity of **NDI-Py** in acetone with different HEPES buffer (10 μM, pH=7.0) contents; (B) Relationship between the HEPES buffer (10 μM, pH=7.0) contents and the corresponding fluorescence intensity and maximum emission wavelength of **NDI-Py** in acetone/HEPES mixed solvent

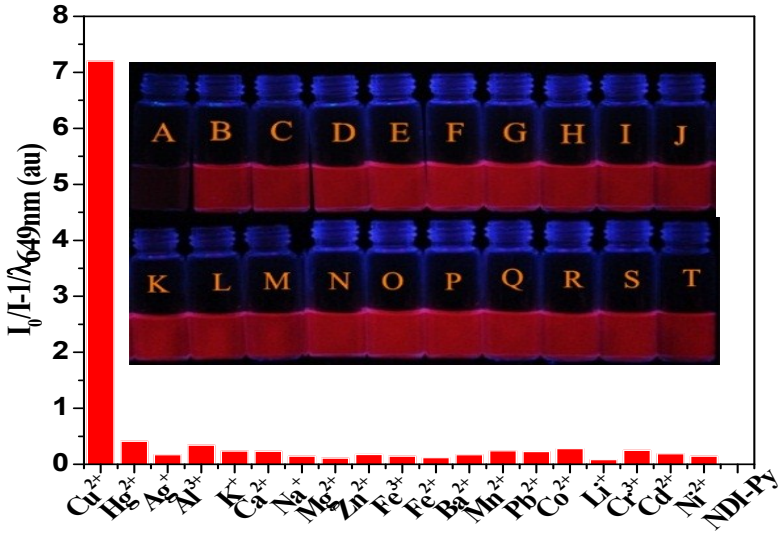


Fig. S7 Fluorescence spectra profiles of **NDI-Py** in acetone and HEPES solution (v/v: 7/3) (10 μM) towards 1.0 equiv of various metal ions. Inset: fluorescence photographs of compound **NDI-Py** with various metal ions : A) Cu^{2+}, B) Hg^{2+}, C) Ag^{+}, D) Al^{3+}, E) Na^{+}, F) K^{+}, G) Ca^{2+}, H) Mg^{2+}, I) Zn^{2+}, J) Fe^{3+}, K) Fe^{2+}, L) Ba^{2+}, M) Mn^{2+}, N) Pb^{2+}, O) Co^{2+}, P) Li^{+}, Q) Cr^{3+}, R) Cd^{2+}, S) Ni^{2+}, T) **NDI-Py**

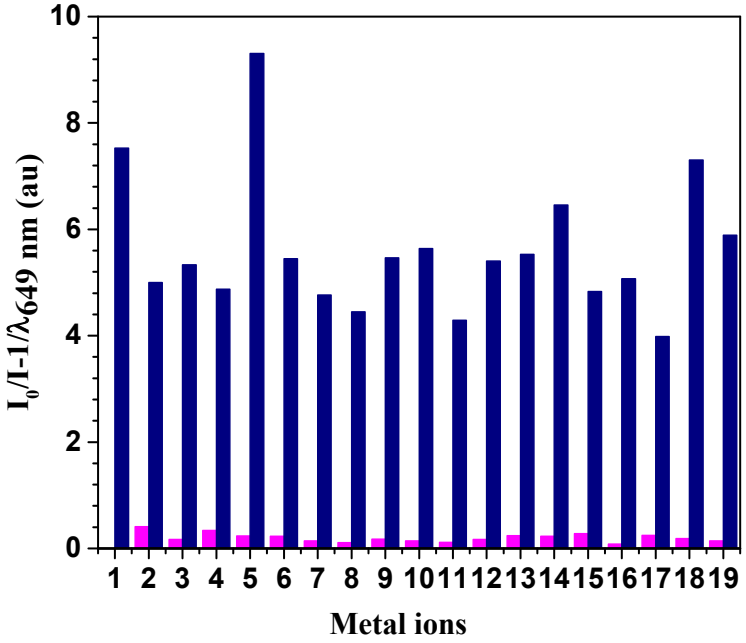


Fig. S8 Fluorescence spectra profiles of **NDI-Py** in acetone and HEPES solution (V/V: 7/3) (10 μM) towards 1 equiv. of copper ions in the presence of the same amount of

other metal ions. 1) **NDI-Py**, 2) Hg^{2+}, 3) Ag^{+}, 4) Al^{3+}, 5) Na^{+}, 6) K^{+}, 7) Ca^{2+}, 8) Mg^{2+}, 9) Zn^{2+},10) Fe^{3+},11) Fe^{2+}, 12) Ba^{2+}, 13) Mn^{2+}, 14) Pb^{2+}, 15) Co^{2+}, 16) Li^{+}, 17) Cr^{3+}, 18) Cd^{2+}, 19) Ni^{2+}. The magenta bars represent the relative fluorescence intensities of **NDI-Py** with various metal ions. The navy bars represent the relative fluorescence intensities of **NDI-Py** towards copper ions in the presence of other competing metal ions

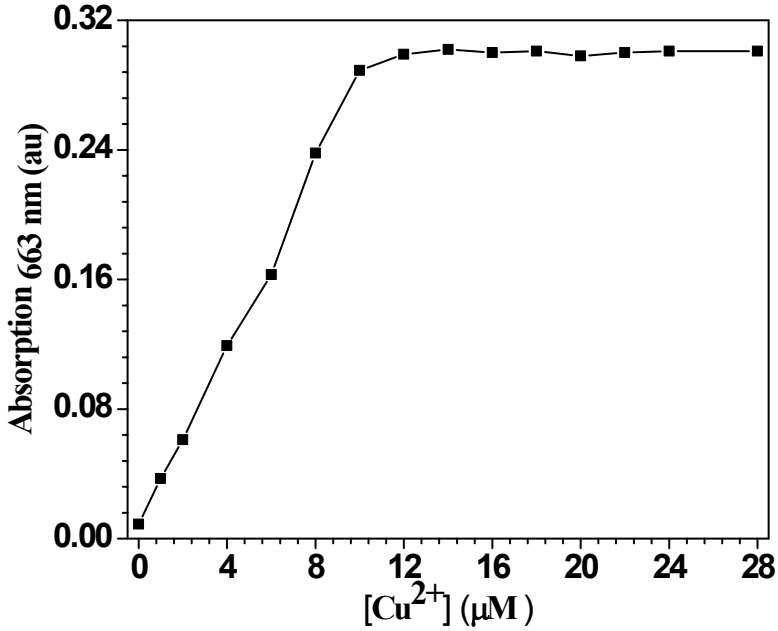


Fig. S9 The changes of absorption of **NDI-Py** at 663 nm in acetone (20 μM)

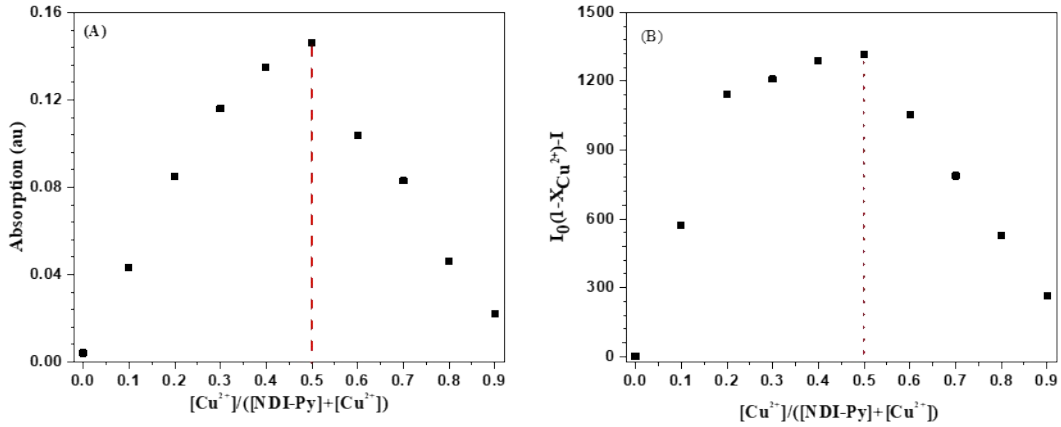


Fig. S10 (A) Job's plot of **NDI-Py** and copper ions ([**NDI-Py**] + [Cu^{2+}] = 40 μM) in acetone by UV-vis spectra, where the absorption at 663 nm was plotted against the mole fraction of [Cu^{2+}/[**NDI-Py**]+Cu^{2+}]. (B) Job's plot of **NDI-Py** and copper ions ([**NDI-Py**] + [Cu^{2+}] = 40 μM) in acetone by fluorescence spectra, where the fluorescence intensity at 638 nm was plotted against the mole fraction of [Cu^{2+}/[**NDI-Py**]+Cu^{2+}].

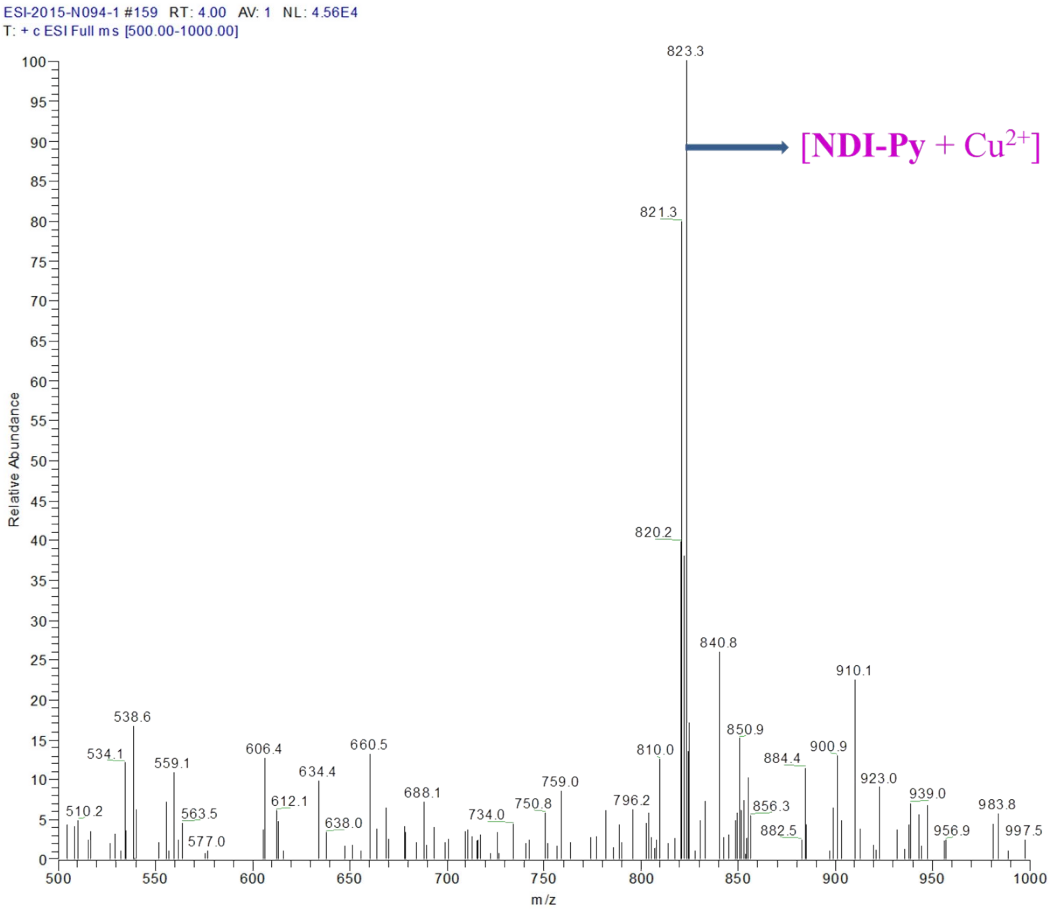


Fig. S11 ESI-MS spectrum of **NDI-Py** with copper ions.

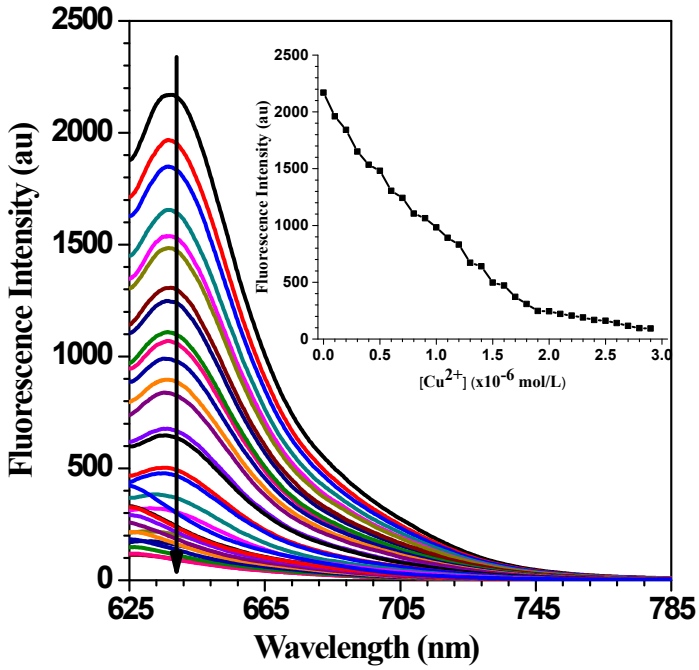


Fig. S12 Fluorescence titration curve of **NDI-Py** (2.0 μM) in acetone with different concentrations of copper ions

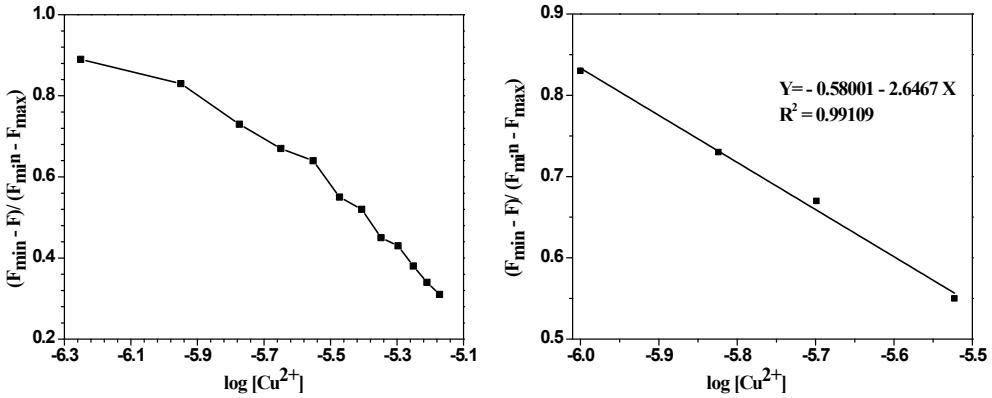


Fig. S13 The changes of fluorescence signal with different concentrations of copper ions

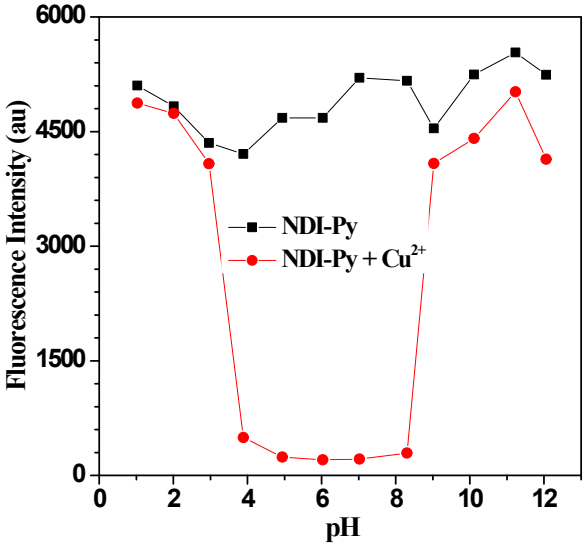


Fig. S14 The changes of fluorescence intensity of **NDI-Py** in the presence and absence of Cu^{2+} with variation of pH values.

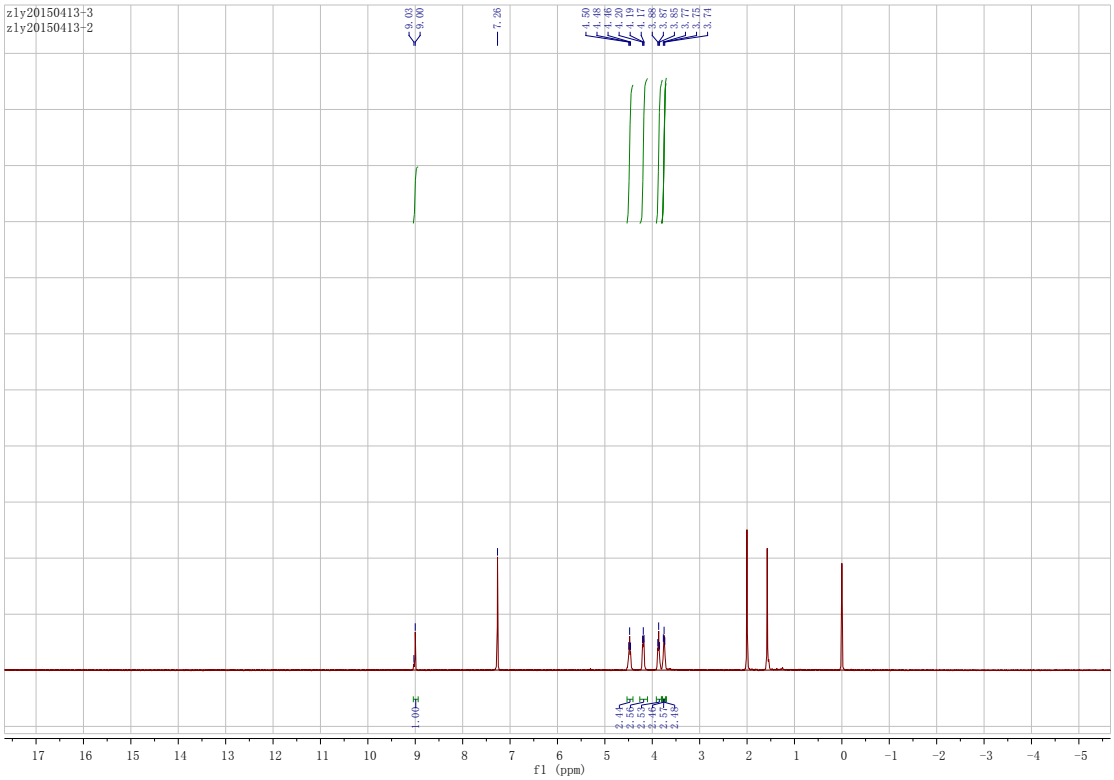


Fig. S15 The ^{1}H NMR spectrum of compound **2**

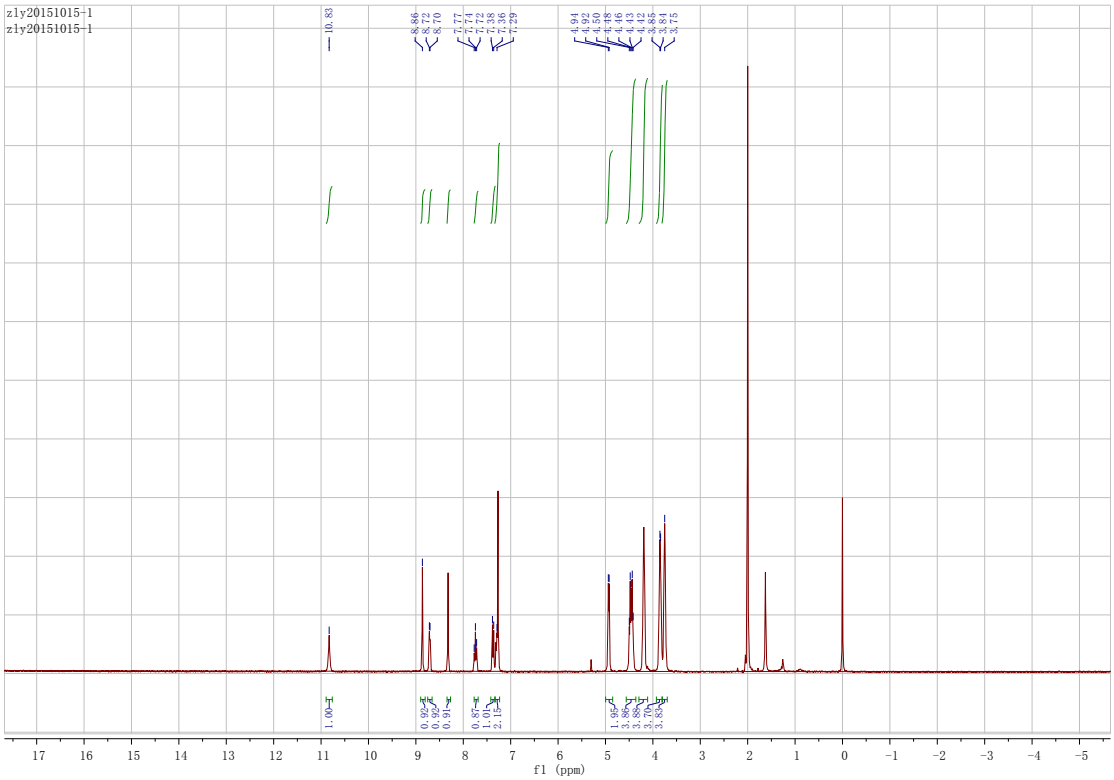


Fig.S16 The ^{1}H NMR spectrum of compound **3**

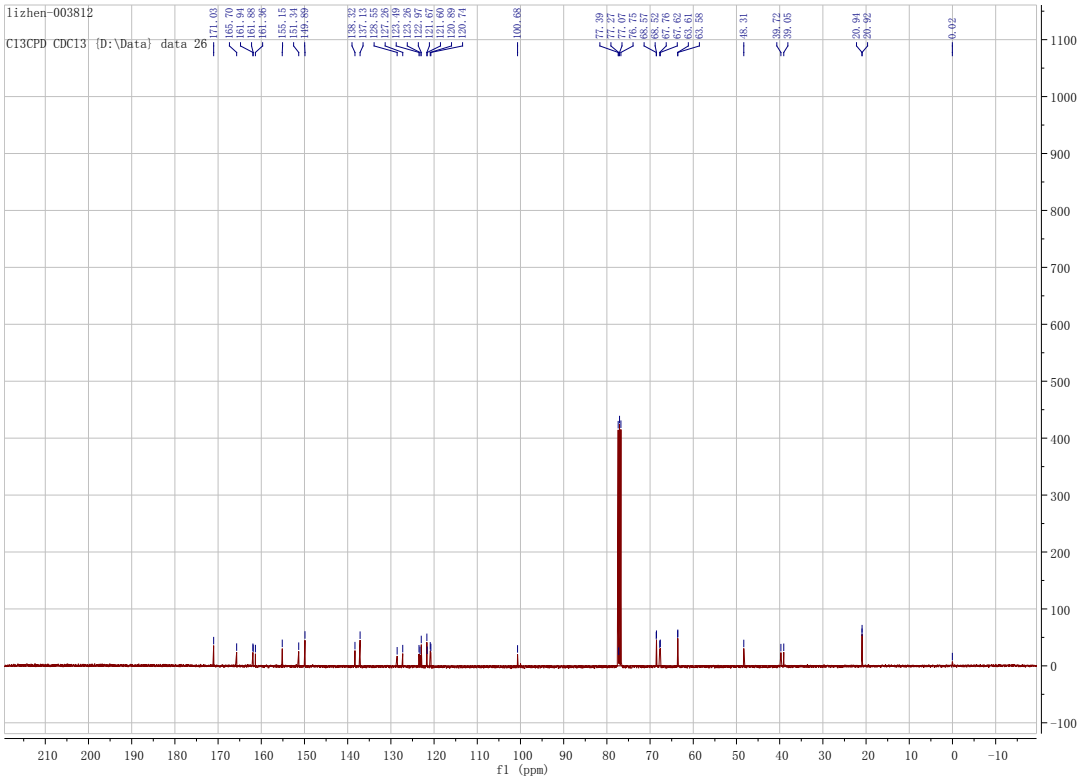


Fig.S17 The ^{13}C NMR spectrum of compound **3**.

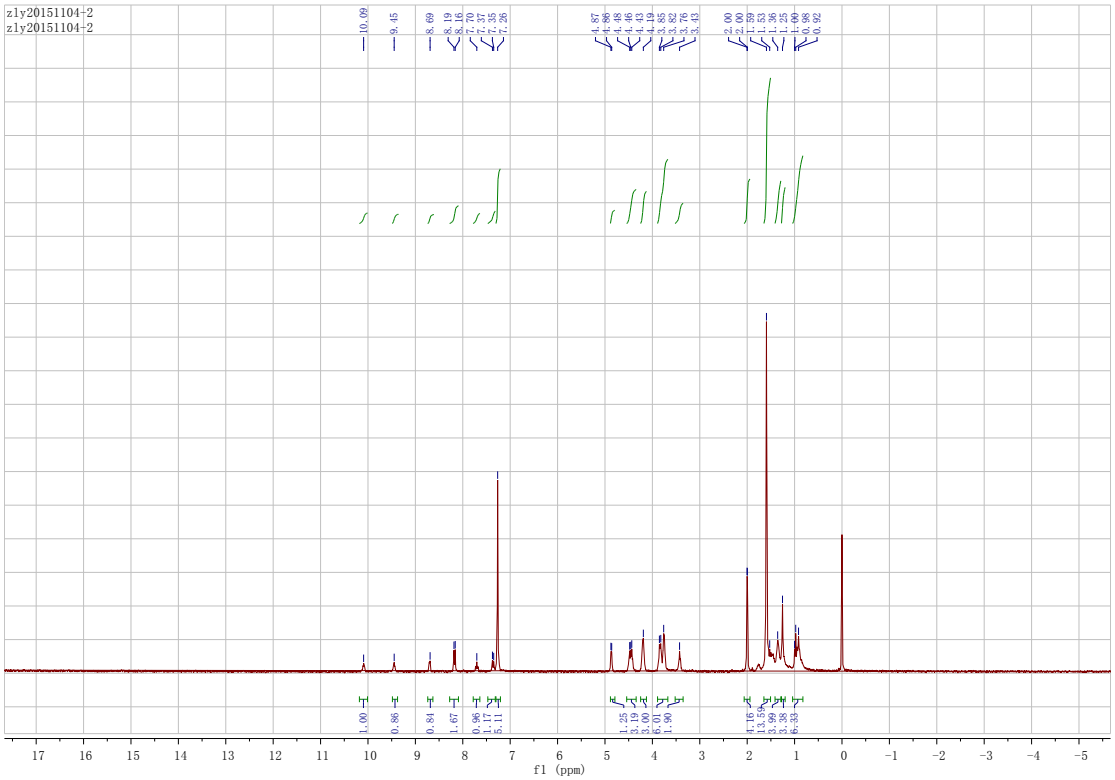


Fig. S18 The ^{1}H NMR spectrum of **NDI-Py**

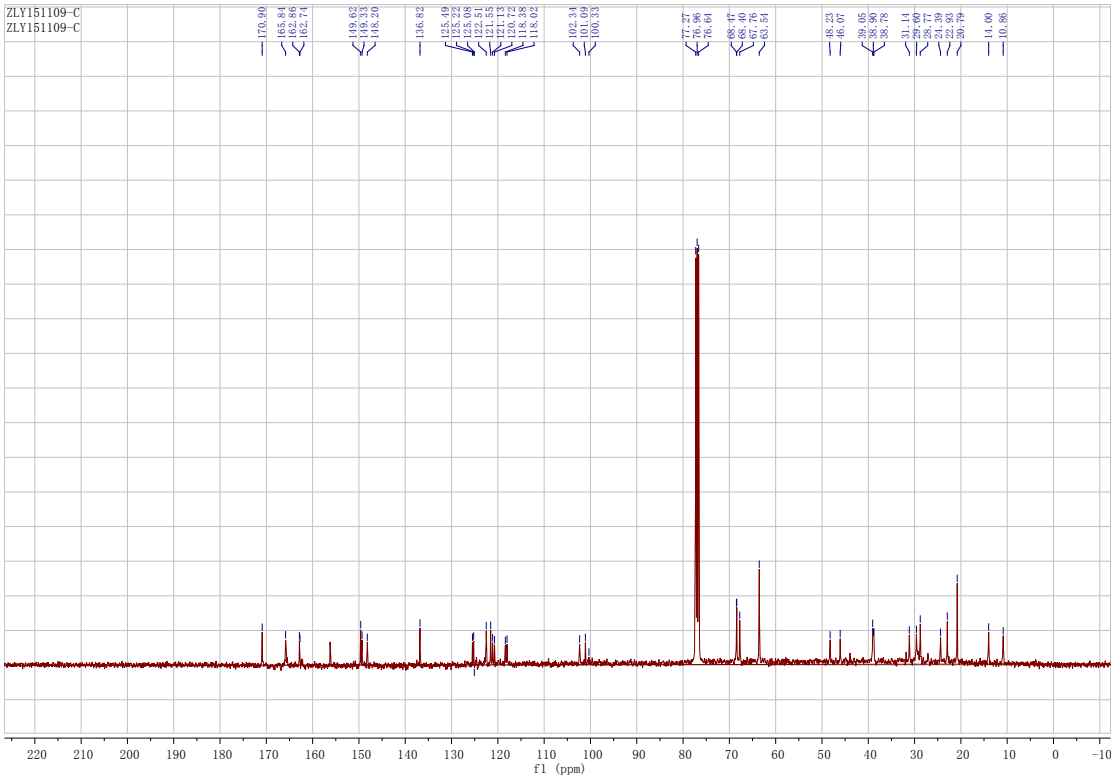


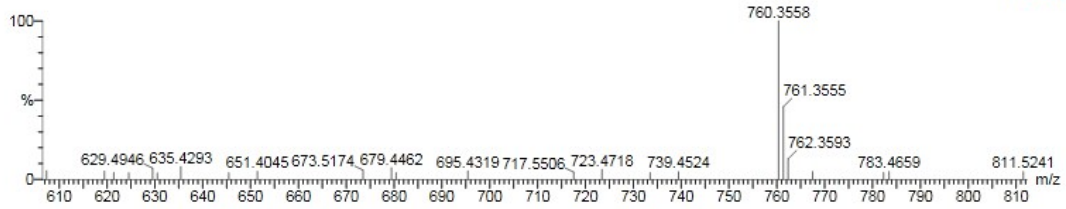
Fig. S19 The ^{13}C NMR spectrum of **NDI-Py**

Elemental Composition Report **Page 1**

Single Mass Analysis
Tolerance = 50.0 PPM / DBE: min = -1.5, max = 100.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
59 formula(e) evaluated with 4 results within limits (up to 1 closest results for each mass)
Elements Used:
C: 0-43 H: 0-54 N: 0-5 O: 0-10

WD ECUST institute of Fine Chem 08-Jan-2016 00:29:17
ZLY-1 89 (0.640) Cm (85:91) 1: TOF MS ES+ 1.10e+004



Minimum:				-1.5			
Maximum:		300.0	50.0	100.0			
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
760.3558	760.3558	0.0	0.0	18.5	12.1	0.0	C40 H50 N5 O10

Fig. 20 The HRMS spectrum of **NDI-Py**