Supplementary Material

A selective colorimetric and fluorescent chemosensor for Cu^{2+} in living cells

Meipan Yang, Wenfei Meng, Xiaojing Liu, Na Su, Jia Zhou, Bingqin Yang*

Key Laboratory of Synthetic and Natural Functional Molecule Chemistry, Ministry of Education, College of Chemistry and Materials Science, Northwest University, Xi'an 710069, PR China

* Corresponding author: Bingqin Yang
Tel.: +0086 29 88302217
Fax: +0086 29 88302617
E-mail: yangbq@nwu.edu.cn; ymp1111@163.com

Table of contents

Table S1 X-ray table of compound **MP**

Compound	**MP**
Formula	$C_{41}H_{40}N_6O_3$
Formula weight	664.79
Temperature (K)	296(2)
Wavelength (Å)	0.71073
Crystal system	Monoclinic
space group	P2(1)/c
Unit cell dimensions /(Å, °)	a = 12.160 (2) α= 90
	b =12.154(2) β= 96.593(4)
	c = 24.347(3) γ= 90
Volume ($Å^3$)	3574.5(10)
Z	4
Calculated density (Mg/m^3)	1.235
Absorption coefficient (mm^{-1})	0.080
F(000)	1408
Crystal size (mm^3)	0.31 x 0.26 x 0.14
Theta range for data collection (°)	1.88 - 25.10
Limiting indices	-14<=h<=14
	-11<=k<=14
	-23<=l<=29
Reflections collected / unique	16174 / 6369 [*R*(int) = 0.0437]
Completeness to θ = 25.10	99.9 %
Max. and min. transmission	0.9889 and 0.9759
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	6369 / 0 /456
Goodness-of-fit on F^2	1.052
Final R indices [I>2σ (I)]	R1 = 0.0699, wR2 = 0.1134
R indices (all data)	R1 = 0.1842, wR2 = 0.1488
Largest diff. peak and hole/(e. $Å^{-3}$)	0.327 and -0.192
CCDC	989882

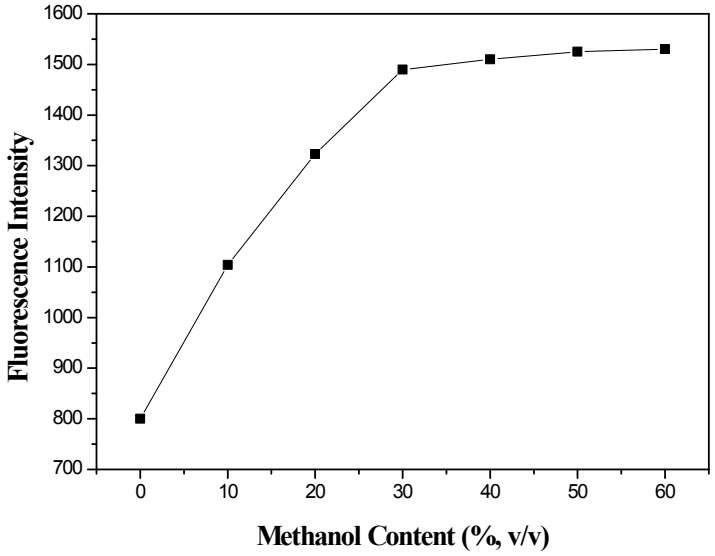

Fig. S1. Effect of the methanol content on the fluorescence intensity of **MP** (10 μM) with the presence of Cu^{2+} (10 μM) for 20 min, λ_{ex} = 535 nm.

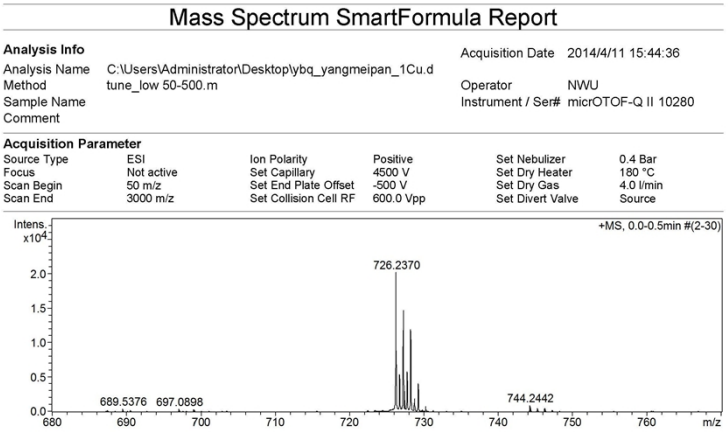

Fig. S2. Mass spectrum of **MP** in the presence of Cu^{2+}.

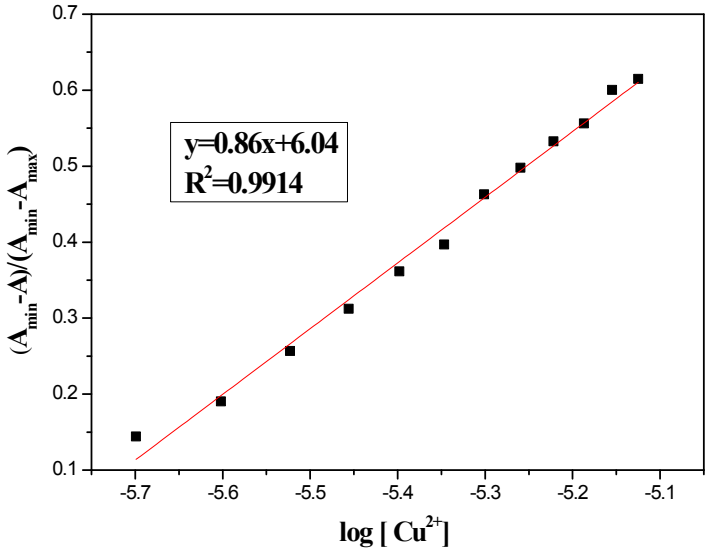

Fig. S3. The plot of absorption intensity at 552 nm of **MP** vs. Cu^{2+} concentrations.

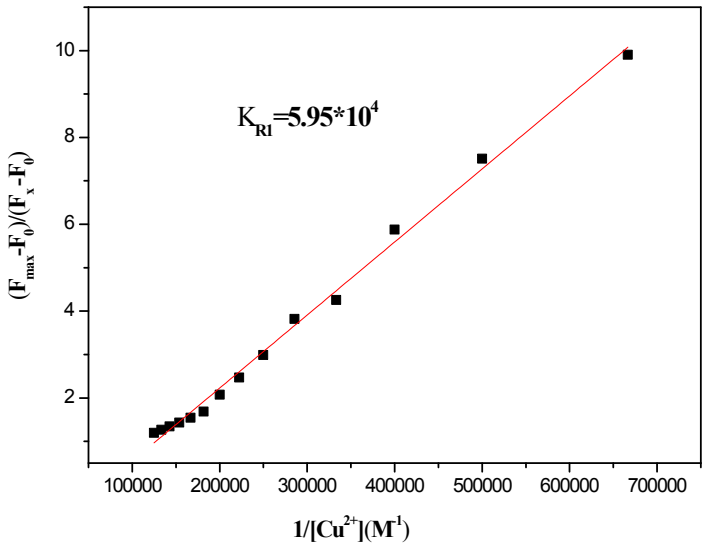

Fig. S4. Determination of binding constant of **MP** with Cu^{2+} using Benesi-Hildebrand equation

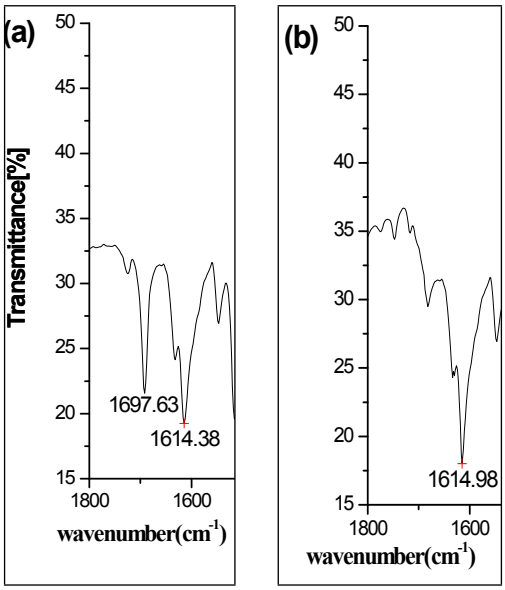

Fig. S5. IR spectra of **MP** (a), **MP** + Cu^{2+} (b).

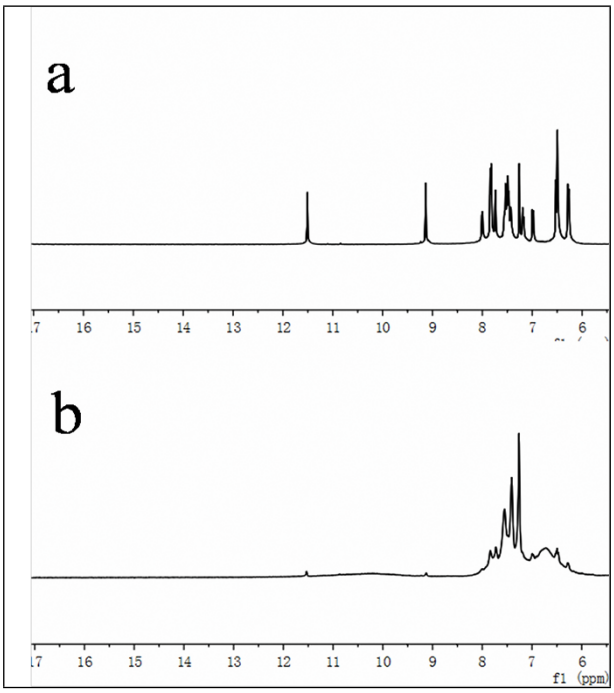

Fig. S6. ^{1}H NMR spectrum ($CDCl_3$) of **MP** before (a), after (b) addition of Cu^{2+}.

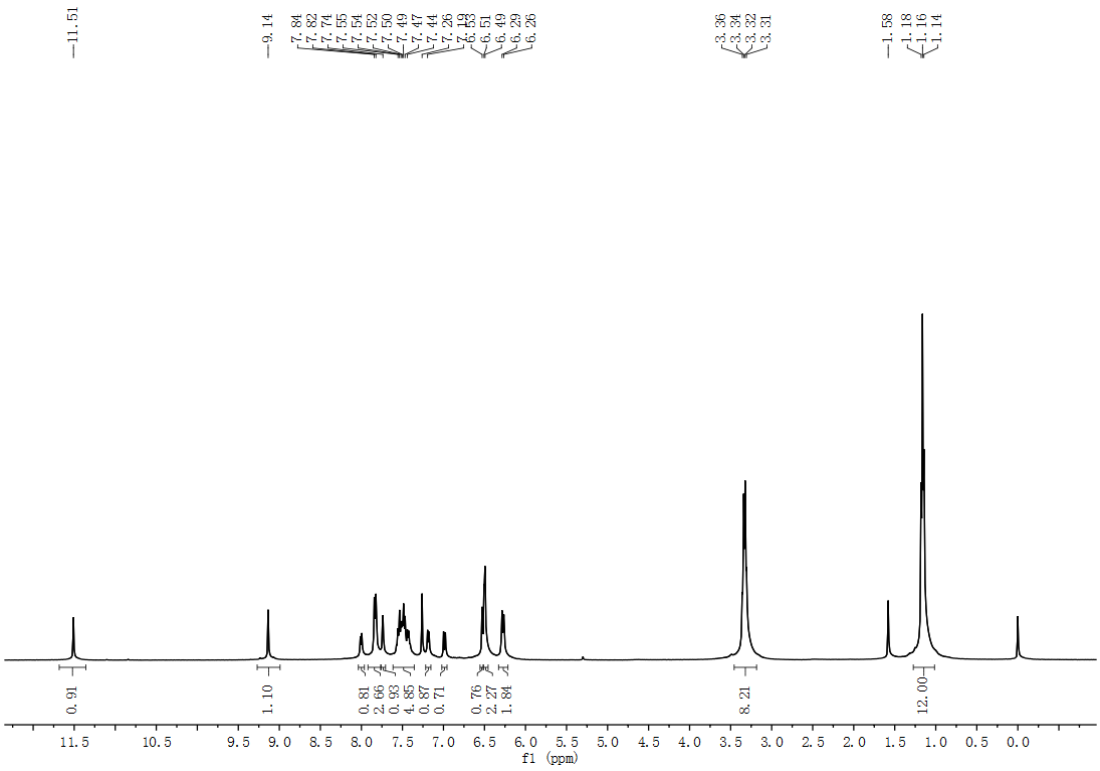

Fig. S7. ^{1}H NMR spectrum of **MP** in $CDCl_3$.

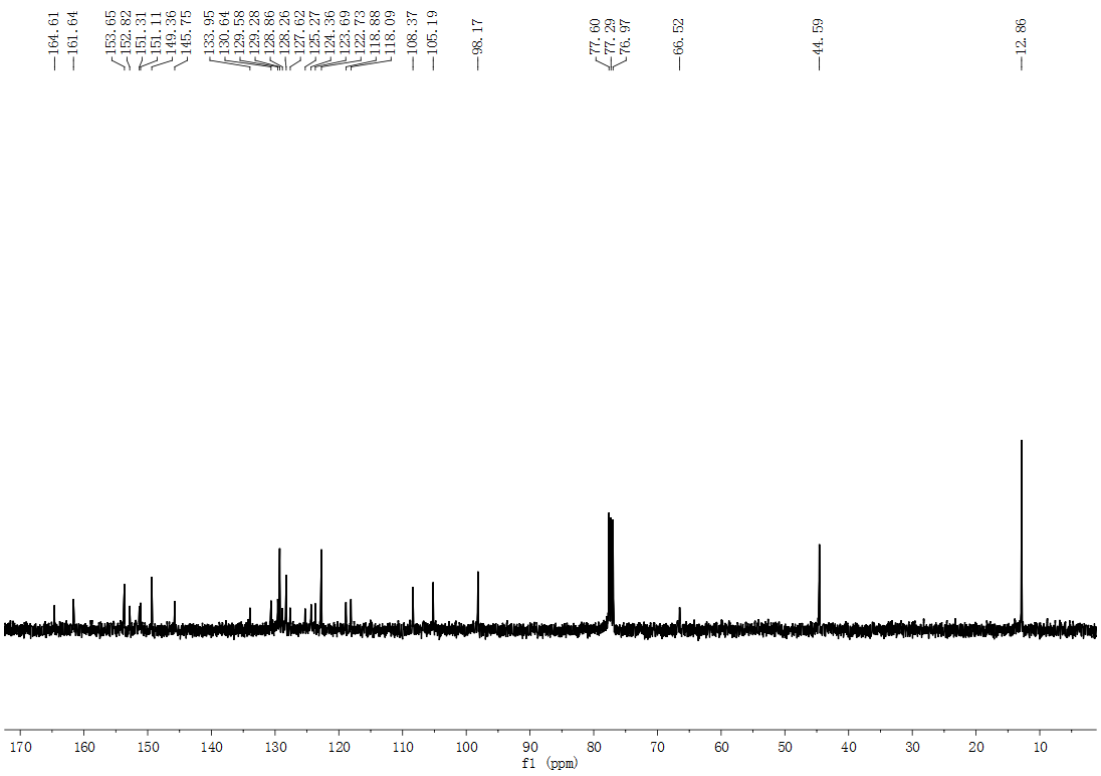

Fig. S8. ^{13}C NMR spectrum of **MP** in $CDCl_3$.

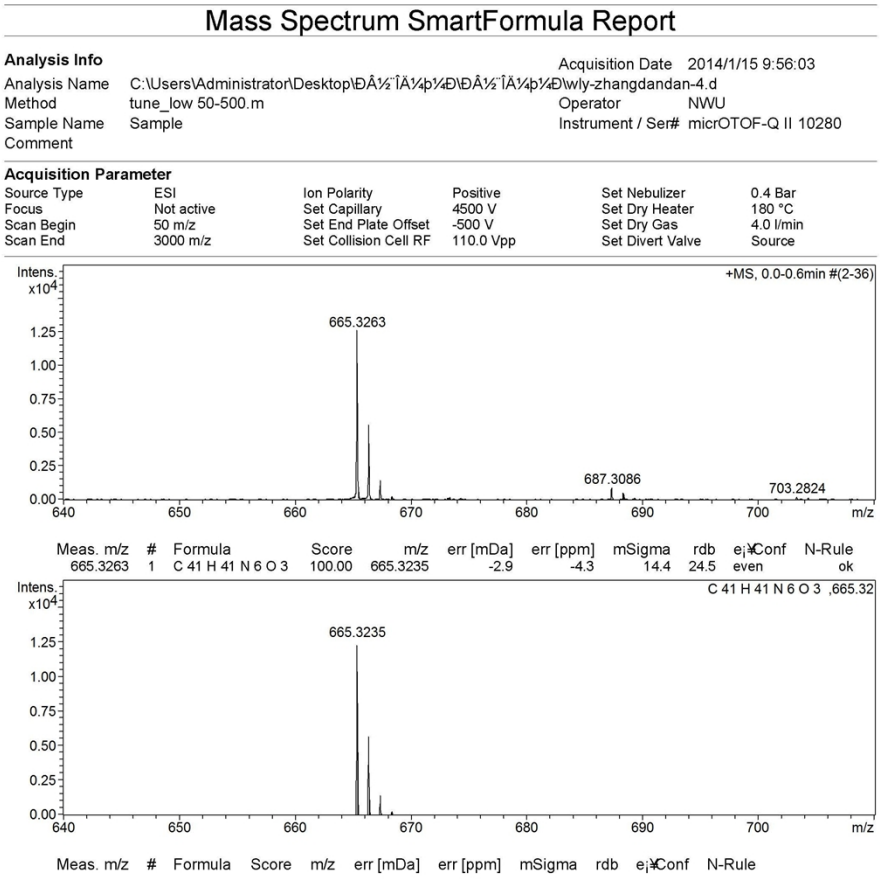

Fig. S9. Mass spectrum of **MP**.