Supplementary Material

A selective colorimetric and fluorescent chemosensor for Cu²⁺ in

living cells

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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, °)	$a = 12.160 (2)$ $\alpha = 90$				
	$b = 12.154(2)$ $\beta = 96.593(4)$				
	$c = 24.347(3)$ $\gamma = 90$				
Volume (Å ³)	3574.5(10)				
Ζ	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<=1<=29				
Reflections collected / unique	16174 / 6369 [R(int) = 0.0437]				
Completeness to $\theta = 25.10$	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 $[I \ge 2\sigma(I)]$	R1 = 0.0699, wR2 = 0.1134				
R indices (all data)	R1 = 0.1842, wR2 = 0.1488				
Largest diff. peak and hole/(e. Å -	0.327 and -0.192				
3)					
CCDC	989882				

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Table S1 X-ray table of compound \boldsymbol{MP}



Fig. S1. Effect of the methanol content on the fluorescence intensity of MP (10 μ M) with the presence of Cu²⁺ (10 μ M) for 20 min, $\lambda_{ex} = 535$ nm.

Mass Spectrum SmartFormula Report									
Analysis Info					Acquisition Date 2014/4/11 15:44:36				
Analysis Name Method Sample Name Comment	C:\Users\AdministratonDesktop\ybq_yangmeipan_1Cu.d tune_low 50-500.m				Operator Instrument / Ser#	erator NWU trument / Ser# micrOTOF-Q II 10280			
Acquisition Par	rameter								
Source Type Focus Scan Begin Scan End	ESI Not act 50 m/z 3000 m	ive n/z	Ion Polarity Set Capillary Set End Plate Offset Set Collision Cell RF	Positive 4500 V -500 V 600.0 Vpp	Set Nebulizer Set Dry Heater Set Dry Gas Set Divert Valve		0.4 Bar 180 °C 4.0 l/min Source		
Intens. x10 ⁴							+MS, 0.0-0.5min	#(2-30)	
2.0				726.2370					
1.5				I.					
1.0									
0.5	689.5376 6	97.0898		ttill .	744.2442				
680	690	700	710 720) 730	740	750	760	m/z	

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. ¹H NMR spectrum (CDCl₃) of MP before (a), after (b) addition of Cu^{2+} .



Fig. S7. ¹H NMR spectrum of MP in CDCl_{3.}



Fig. S8. ¹³C NMR spectrum of MP in CDCl₃.



Fig. S9. Mass spectrum of MP.