

Supplementary Information

New Cu²⁺-specific “turn-on” fluorescent probe based on [5]helicene with very large Stokes shift and its potential in living cell

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Mass Spectrum List Report

Analysis Info

Analysis Name OSSUSK591108001.d
Method Tune_wide_POS_Tawatchai_05Feb2016.m
Sample Name M201NH
M201NH

Acquisition Date 11/8/2016 11:54:15 AM
Operator Administrator
Instrument micrOTOF 72

Acquisition Parameter

Source Type ESI
Scan Range n/a
Scan Begin 50 m/z
Scan End 3000 m/z

Ion Polarity Positive
Capillary Exit 150.0 V
Hexapole RF 400.0 V
Skimmer 1 70.0 V
Hexapole 1 25.0 V

Set Corrector Fill 50 V
Set Pulsar Pull 337 V
Set Pulsar Push 337 V
Set Reflector 1300 V
Set Flight Tube 9000 V
Set Detector TOF 2295 V

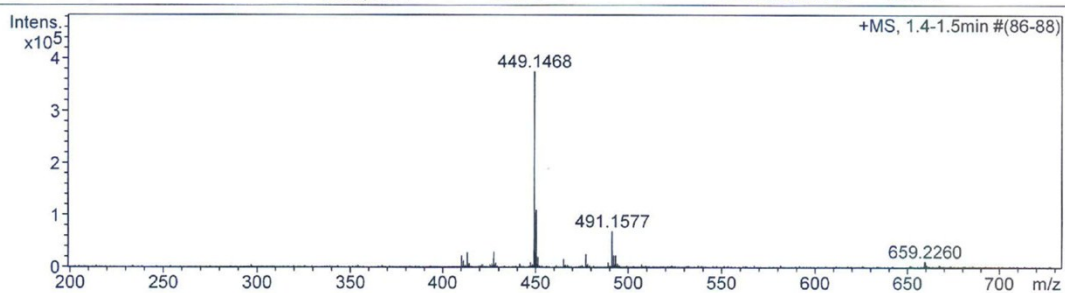


Fig. S1 HR-ESI MS of sensor 1: $C_{26}H_{22}N_2O_4Na^+$ calcd. 449.1472 ; m/z $[M+Na]^+$ found 449.1468.

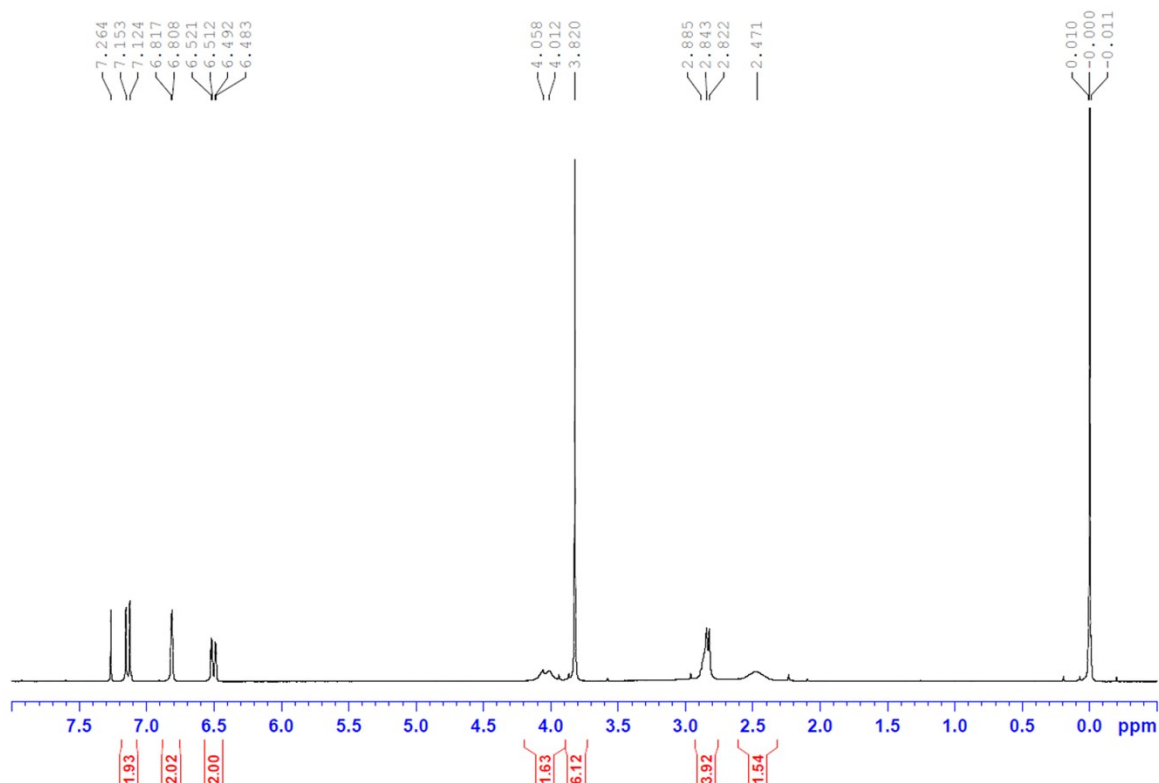


Fig. S2 ¹H-NMR spectrum of sensor 1 in CDCl₃.

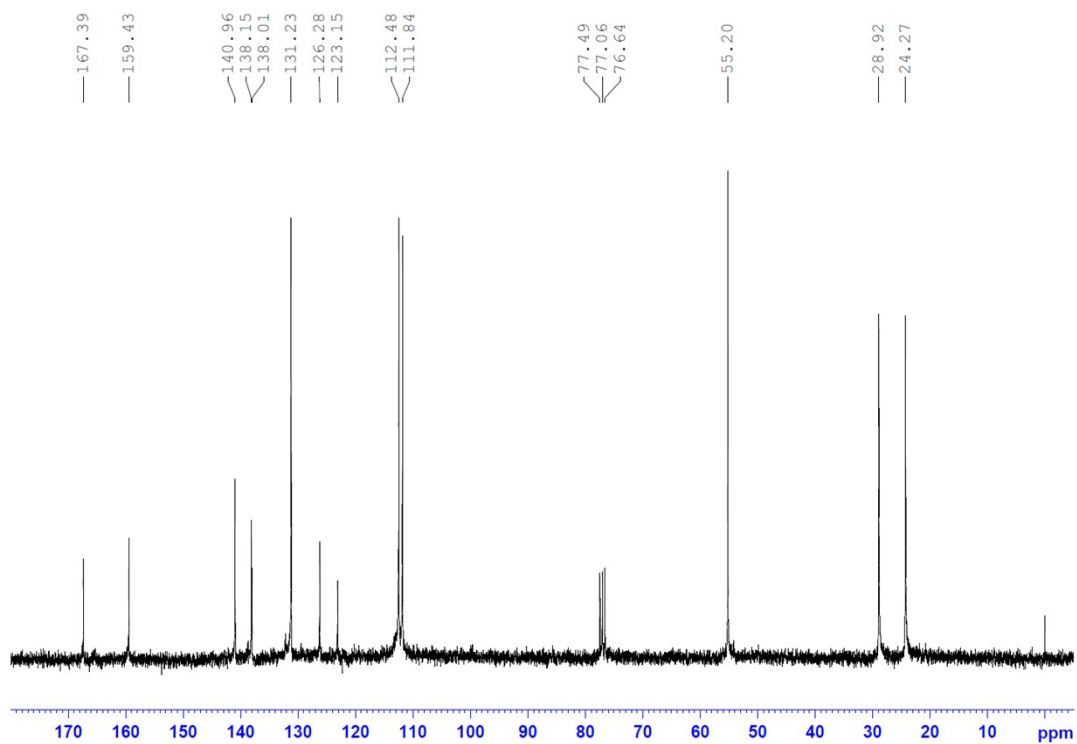


Fig. S3 ^{13}C -NMR spectrum of sensor **1** in CDCl_3 .

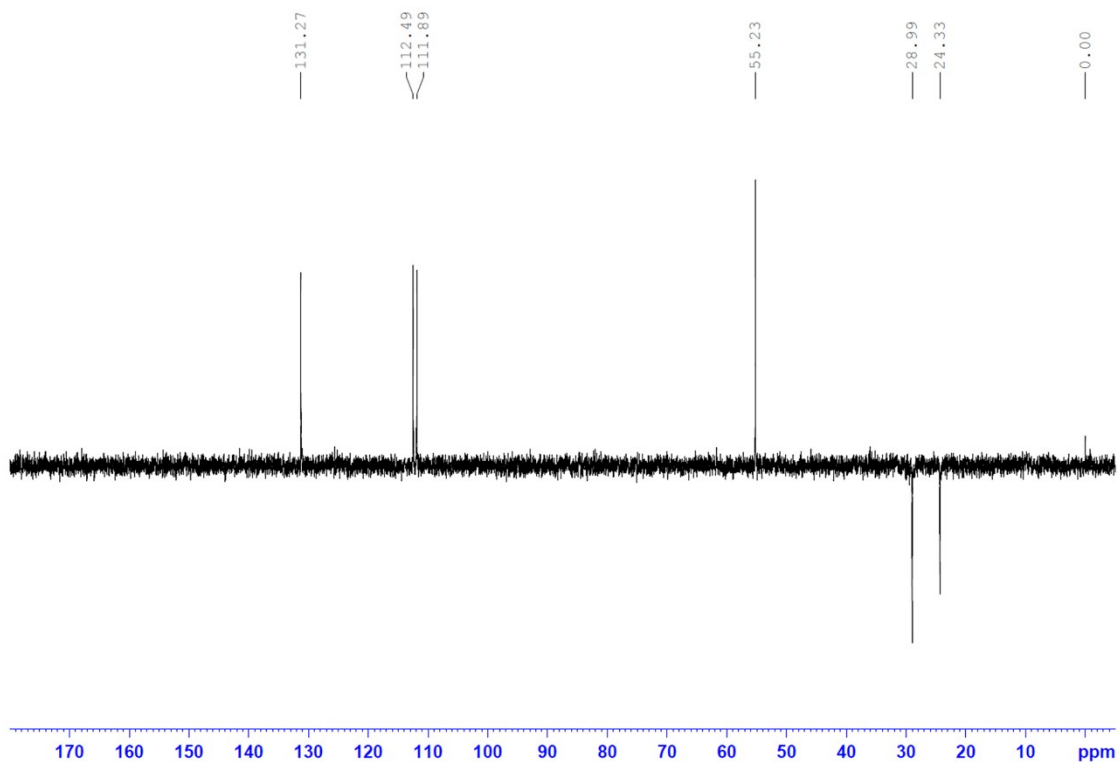


Fig. S4 DEPT-135 NMR spectrum of sensor **1** in CDCl_3 (75 MHz).

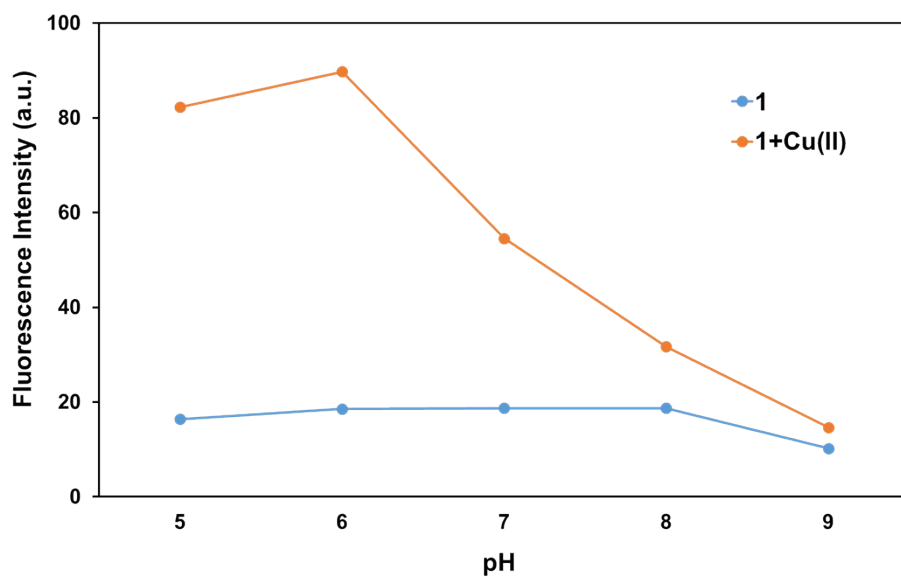


Fig. S5 Fluorescence emissions ($\lambda_{em}=556\text{ nm}$) of **1** ($2.40\ \mu\text{M}$) and the emissions after addition of Cu^{2+} ($66.7\ \mu\text{M}$) in HEPES buffer as function of pH ($\lambda_{ex}=373\text{ nm}$).

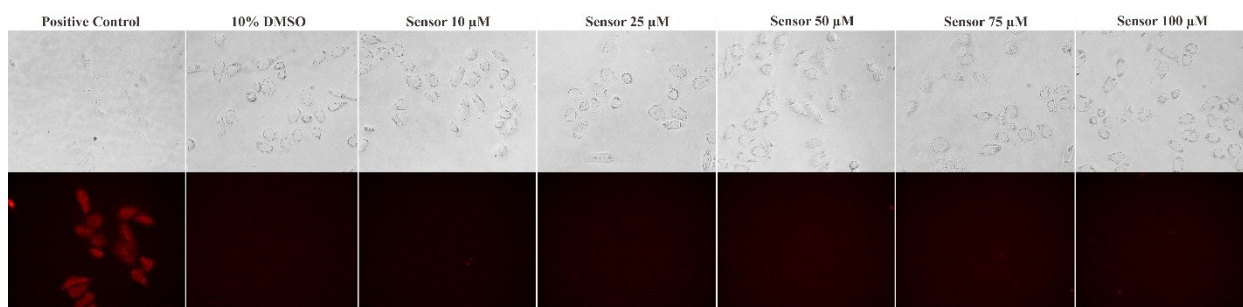


Fig. S6 Negative propidium iodide stain of HepG2 cells after sensor exposure showed that cells were viable with plasma membrane integrity. For positive control cells were treated with 10% TritonX-100. 10% DMSO the solvent of sensor was used as negative control.

Table S1. Crystallographic data for sensor 1

Bond precision:	C-C = 0.0020 Å	Wavelength=1.54178	
Cell:	a=21.755 (4) alpha=90	b=11.303 (2) beta=90	c=16.615 (3) gamma=90
Temperature:	273 K		
	Calculated	Reported	
Volume	4085.6 (13)	4085.8 (14)	
Space group	P b c n	P b c n	
Hall group	-P 2n 2ab	-P 2n 2ab	
Moiety formula	C26 H22 N2 O4	C26 H22 N2 O4	
Sum formula	C26 H22 N2 O4	C26 H22 N2 O4	
Mr	426.46	426.46	
Dx, g cm ⁻³	1.387	1.387	
Z	8	8	
Mu (mm ⁻¹)	0.766	0.766	
F000	1792.0	1792.0	
F000'	1797.56		
h,k,lmax	26,13,20	26,13,20	
Nref	4044	4010	
Tmin,Tmax	0.795,0.795	0.656,0.754	
Tmin'	0.795		
Correction method= # Reported T Limits: Tmin=0.656 Tmax=0.754			
AbsCorr = MULTI-SCAN			
Data completeness=	0.992	Theta(max)= 72.430	
R(reflections)=	0.0429(3276)	wR2(reflections)= 0.1221(4010)	
S =	1.036	Npar= 292	
