

Supporting Information

A Highly Selective Turn-On Fluorescent Probe for the Detection of Zinc

Ling-Yi Shen ^{1,2,†}, Xiao-Li Chen ^{2,†}, Xian-Jiong Yang ^{1,2,*}, Hong Xu ², Ya-Li Huang ², Xing Zhang ², Carl Redshaw ³ and Qi-Long Zhang ^{1,2,*}

¹ School of Public Health, the key Laboratory of Environmental Pollution Monitoring and Disease Control, Ministry of Education, Guizhou Medical University, Guiyang 550014, China; shenly@stumail.nwu.edu.cn

² School of Basic Medical Science, Guizhou Medical University, Guiyang 550004, China; C13885297112@163.com (X.C.); xuhong@gmc.edu.cn (H.X.); ylh6401@gmc.edu.cn (Y.-L.H.); zhangxing11207115@126.com (X.Z.)

³ Department of Chemistry, University of Hull, Cottingham Road, Hull, Yorkshire HU6 7RX, UK; c.redshaw@hull.ac.uk

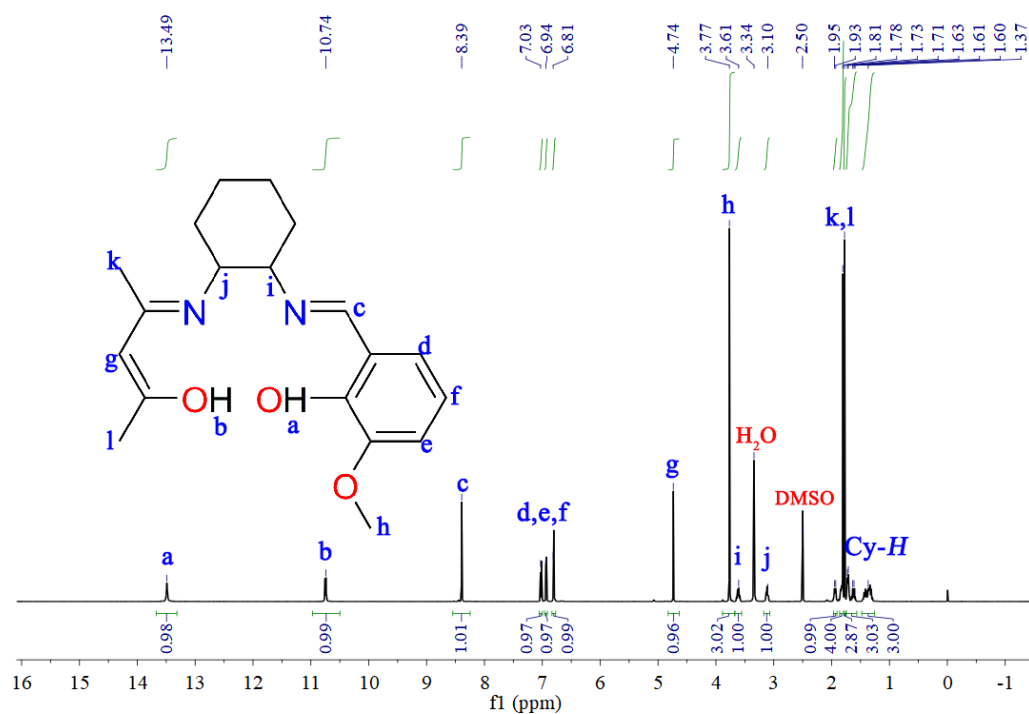
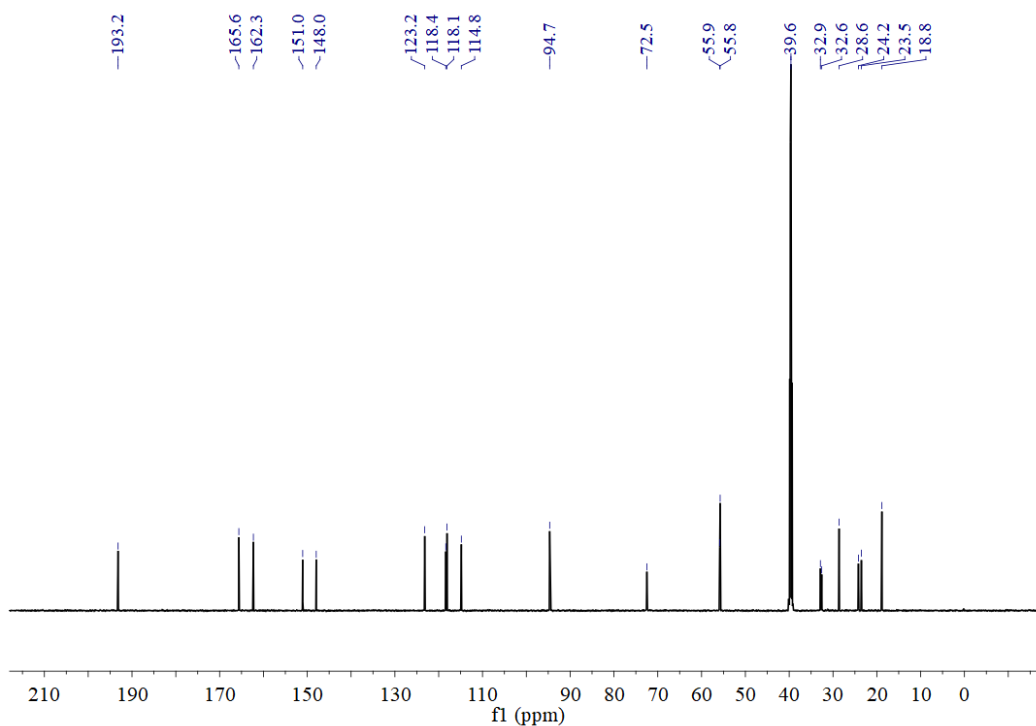
* Correspondence: yangxianjiong@gmc.edu.cn (X.-J.Y.); sciqzhang@gmc.edu.cn (Q.-L.Z.); Fax: +86-0851-88174017 (Q.-L.Z.)

† These authors contributed equally to this work.

Contents:

¹ H-NMR spectrum of probe L	S1
¹³ C-NMR spectrum of probe L	S2
HR ESI-MS spectrum of probe L	S3
Absorbance of L as a function of [Zn ²⁺]/[L].	S4
Job's plot of probe L with Zn ²⁺ .	S5
¹ H-NMR spectra of probe L with 0–1 equiv. of ZnCl ₂	S6
Crystallographic data and refinement details.	Table S1
Selected bond lengths and bond angles for complex L, Cu-complex and Cu-Zn complex	Table S2

NMR spectrum

Figure S1. ^1H -NMR spectrum of probe L (600 MHz, $\text{DMSO}-d_6$, 298 K).Figure S2. ^{13}C -NMR spectrum of probe L in (150.9 MHz, $\text{DMSO}-d_6$, 298 K).

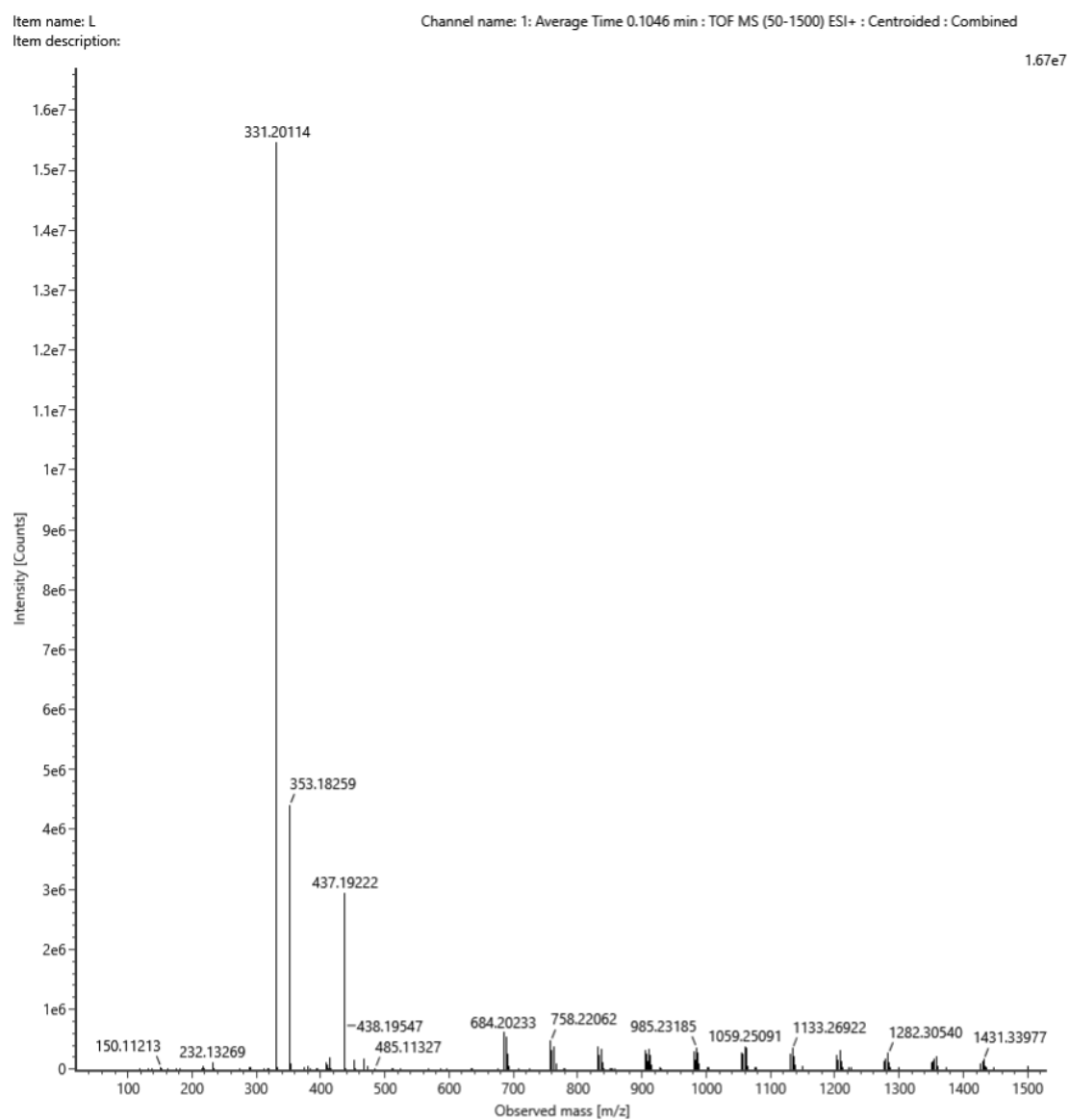


Figure S3. HR ESI-MS spectrum of probe **L**. The m/z peaks at 331.2011 and 353.1826 correspond to $[M + H]^+$ and $[M + Na]^+$.

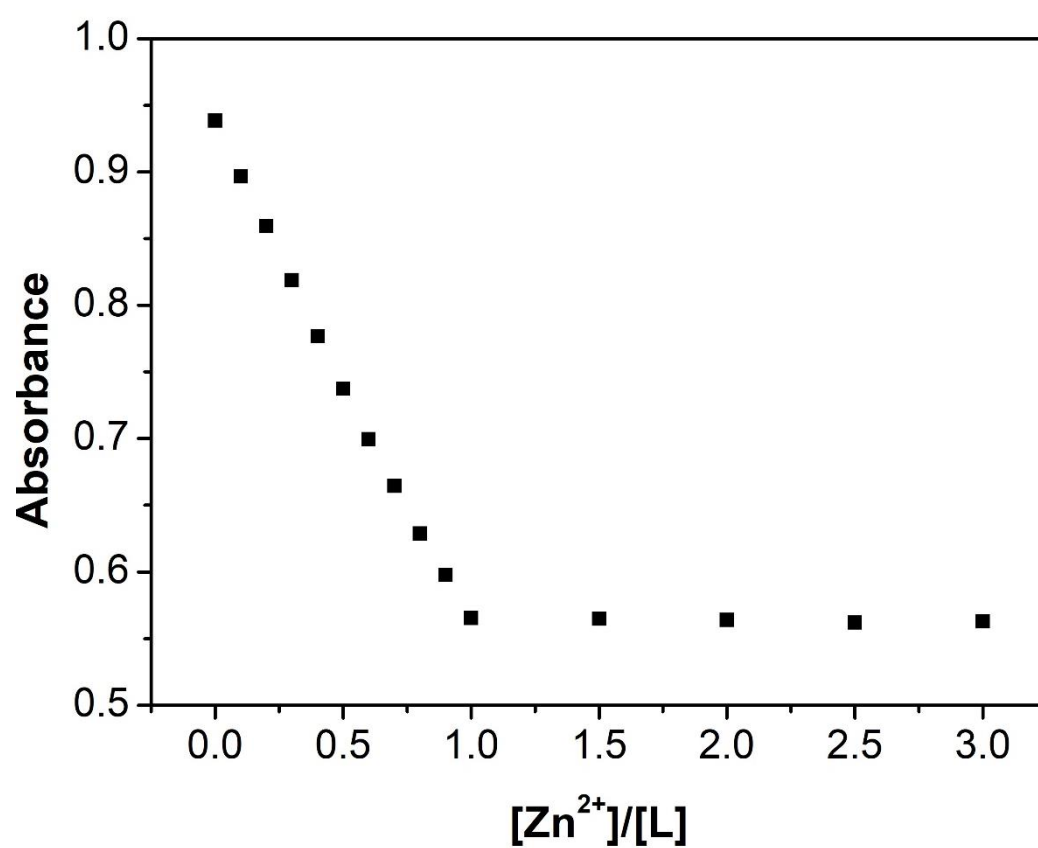


Figure S4. Absorbance of L at 312 nm as a function of $[Zn^{2+}]/[L]$.

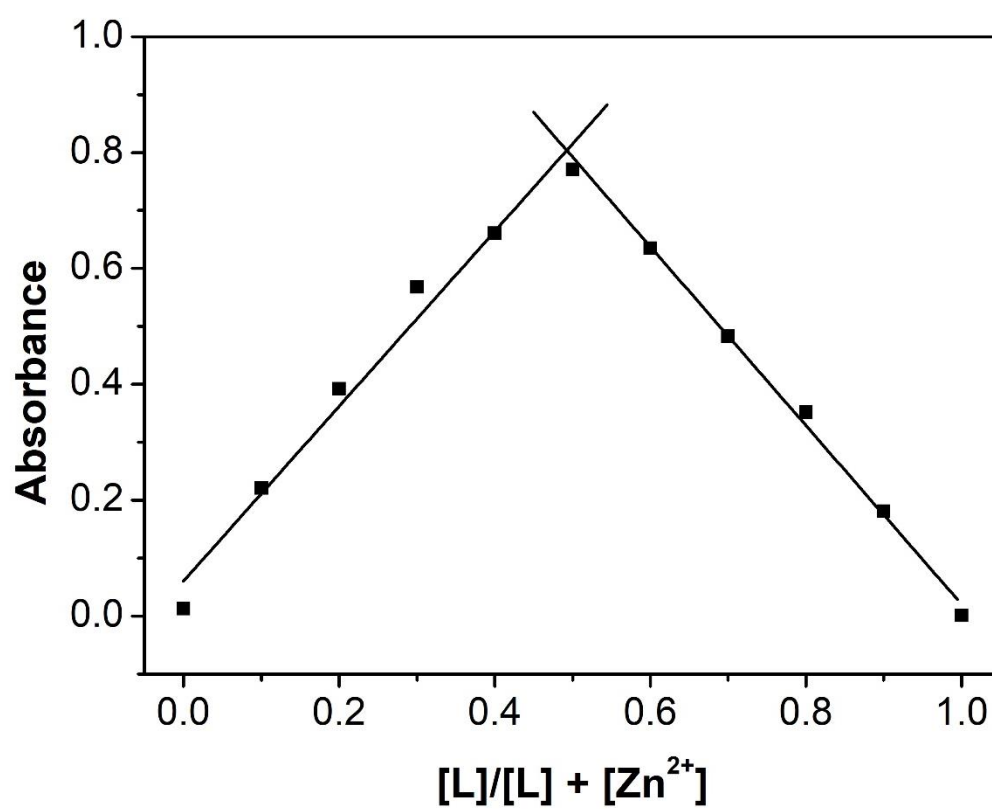


Figure S5. Job's plot of probe L with Zn^{2+} .

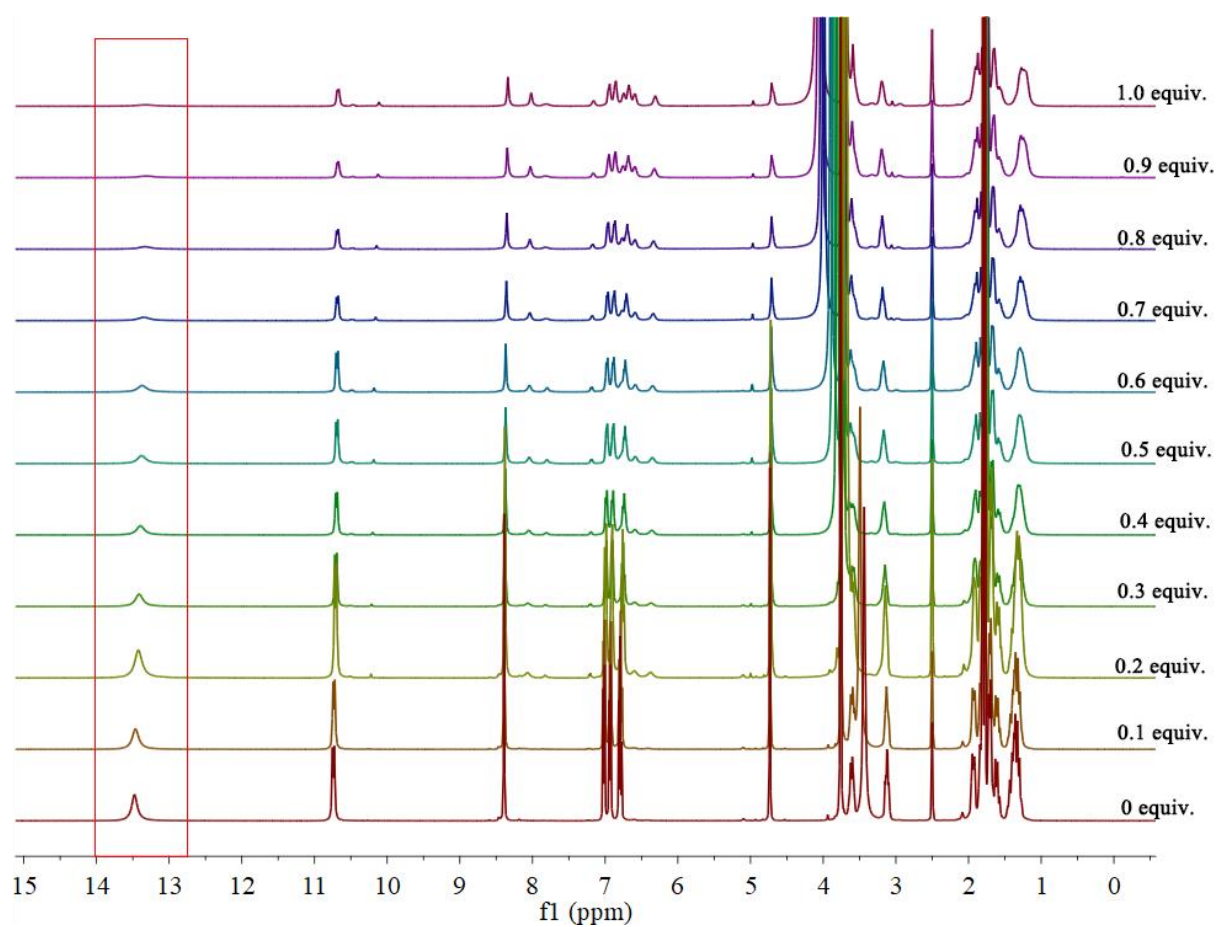


Figure S6. ¹H-NMR spectra of probe L with 0–1 equiv. of ZnCl₂ in DMSO-*d*₆.

X-ray crystallography Analysis

Table S1. Crystallographic data and refinement details for L, Cu-complex and Cu-Zn complex.

Complex	L	Cu-complex	Cu-Zn complex
CCDC Number	2067620	2067621	2067622
Formula	C ₁₉ H ₂₇ N ₂ O _{3.50}	C ₁₉ H ₂₄ CuN ₃ O ₃	C ₃₈ H ₅₀ Cl ₄ Cu ₂ N ₄ O ₆ Zn ₂
Formula weight	339.42	405.95	1058.44
Crystal system,	Tetragonal	Orthorhombic	Monoclinic
space group	<i>P</i> 4 ₂ 2 ₁ 2	<i>P</i> 2 ₁ 2 ₁ 2 ₁	<i>P</i> 2 ₁
<i>a</i> /Å	17.989(2)	7.6261(8)	9.9812(11)
<i>b</i> /Å	17.989(2)	12.8842(15)	19.966(2)
<i>c</i> /Å	12.862(2)	19.144(2)	11.0609(12)
α /deg	90	90	90
β /deg	90	90	105.840(4)
γ /deg	90	90	90
<i>V</i> /Å ³	4162.2(11)	1881.1(4)	2120.6(4)
<i>Z</i>	8	4	2
<i>D</i> _{calcd} /g cm ^{−3}	1.083	1.433	1.658
<i>F</i> (000)	1464	848	1080
μ /mm ^{−1}	0.075	1.184	2.408
θ range	2.264–24.992	2.875–28.348	1.914–24.996
<i>R</i> _{int}	0.1916	0.0351	0.1772
Final <i>R</i> ₁ , <i>wR</i> ₂ values (<i>I</i> > 2 σ (<i>I</i>))	0.1018, 0.2793	0.0382, 0.0668	0.0718, 0.1716
<i>R</i> ₁ , <i>wR</i> ₂ (all data)	0.2233, 0.3231	0.0657, 0.0761	0.0830, 0.1799
GOF (<i>F</i> ²)	1.024	1.029	0.999

Table S2. Selected bond lengths(nm) and bond angles (°) for complex L, Cu-complex and Cu-Zn complex.

L					
C1–N1	1.489(10)	C6–N2	1.466(11)	C15–C16	1.348(15)
N1–C17	1.319(10)	N2–C7	1.310(12)	C15–C16	1.348(15)
C15–O1	1.293(14)				
C1–N1–C17	127.0(7)	C6–N2–C7	120.2(8)	N1–C17–C16	121.5(9)
N2–C7–C8	121.9(10)				
Cu-complex					
C1–N1	1.480(5)	C6–N2	1.460(5)	C15–C16	1.352(6)
N1–C17	1.309(5)	N2–C7	1.290(5)	N1–Cu1	1.959(3)
N2–Cu1	1.916(3)	O1–Cu1	1.913(3)	O2–Cu1	1.909(3)
C15–O1	1.292(5)				
C1–N1–C17	123.2(3)	C6–N2–C7	123.4(3)	N1–Cu1–O1	95.25(13)
C1–N1–Cu1	112.6(2)	C6–N2–Cu1	110.1(2)	N1–Cu1–N2	85.22(13)
N2–Cu1–O2	92.44(12)	O1–Cu1–O2	87.78(11)		
Cu-Zn complex					
C1–N1	1.472(11)	C6–N2	1.479(10)	C15–C16	1.372(15)
N1–C17	1.297(12)	N2–C7	1.258(10)	N1–Cu1	1.946(7)
N2–Cu1	1.923(7)	C15–O1	1.267(11)	O1–Cu1	1.917(6)
O2–Cu1	1.934(6)	O1–Zn1	2.146(6)	O2–Zn1	2.002(6)
O3–Zn1	2.441(7)	Cl1–Zn1	2.223(3)	Cl2–Zn1	2.219(3)
Cu1.....Zn1	3.1062(13)				

N1–Cu1–O1	97.4(3)	N2–Cu2–O2	93.4(3)	N1–Cu1–N2	87.2(3)
O1–Cu1–O2	81.5(2)	O1–Zn–O2	74.5(2)	Cl1–Zn–Cl2	116.96(11)
