

Supplementary Material

A novel ratiometric fluorescent sensor based on terpyridine derivatives for Zn²⁺ in aqueous solution

Qinghong Bai^A, Yangming Jiang^{B,C}, Enming Hu^{B,C}, Libin Lv^{A,}, Chenghui Wang^A and Xin Xiao^{A,*}*

^AKey Laboratory of Macrocyclic and Supramolecular Chemistry of Guizhou Province, Guiyang, 550025, PR China

^BState Key Laboratory of Functions and Applications of Medicinal Plants, Guizhou Medical University, Guiyang, 550014, PR China

^CNatural Products Research Center of Guizhou Province, Guiyang 550014, PR China

*Correspondence to: Email: llp6591@163.com, gyhxxiaoxin@163.com

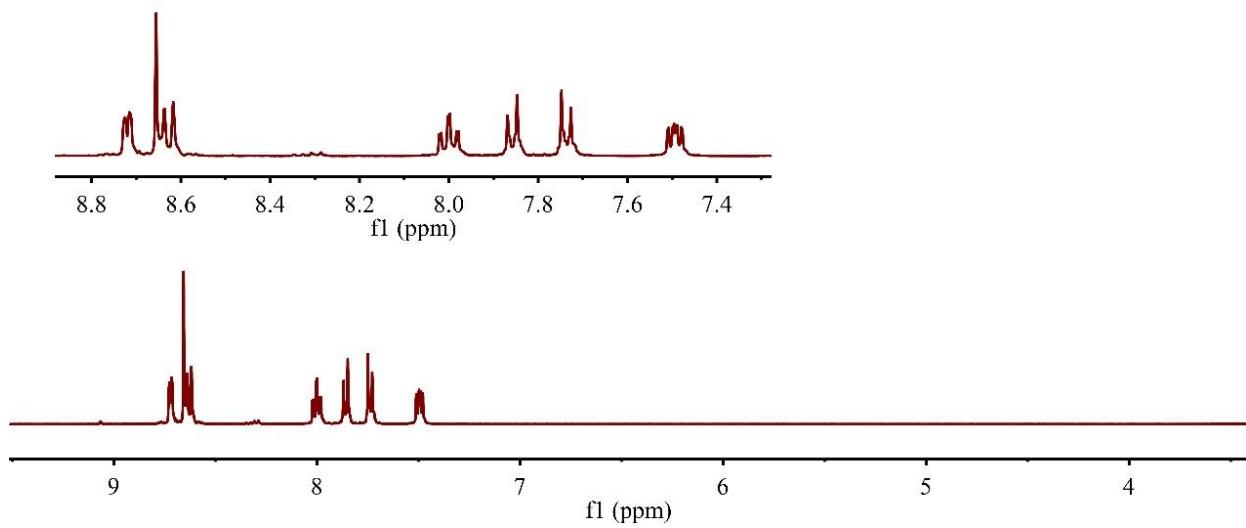


Fig. S1. ¹H NMR spectrum (400 MHz, DMSO-*d*₆) of **Compound G1**.

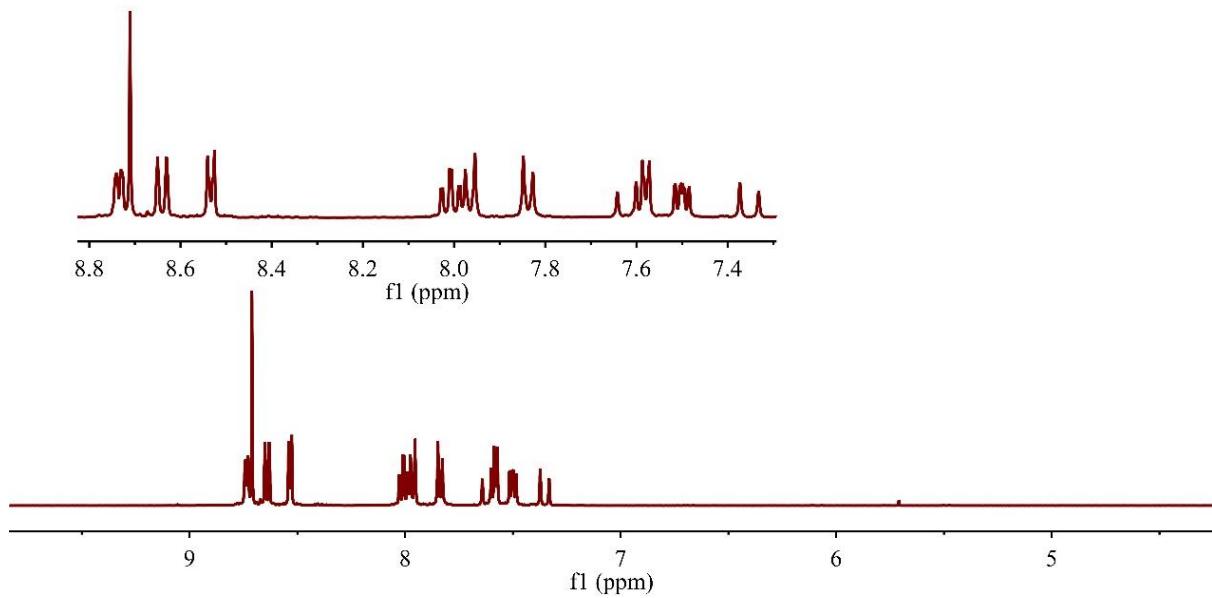


Fig. S2. ¹H NMR spectrum (400 MHz, DMSO-*d*₆) of **Compound G2**.

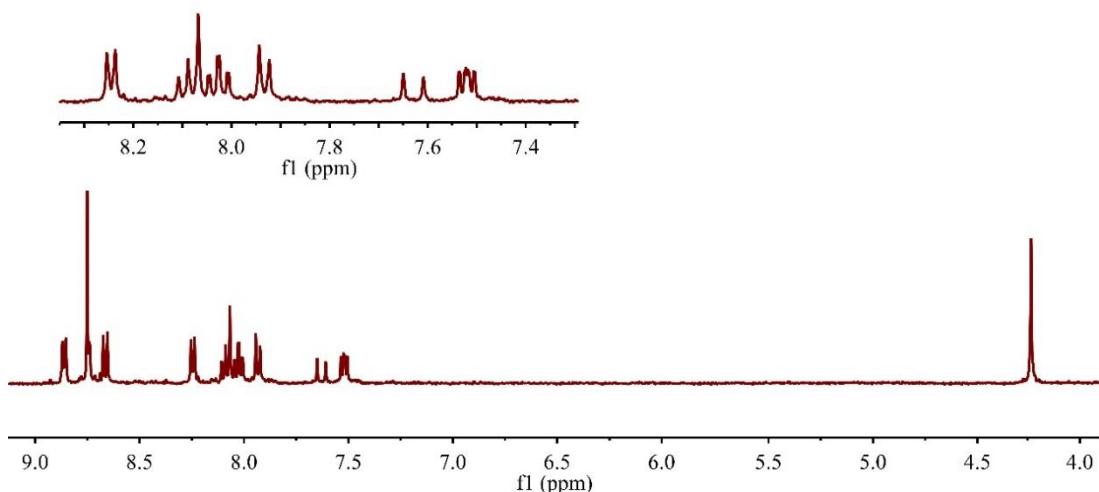


Fig. S3. ¹H NMR spectrum (400 MHz, DMSO-*d*₆) of **Compound G**.

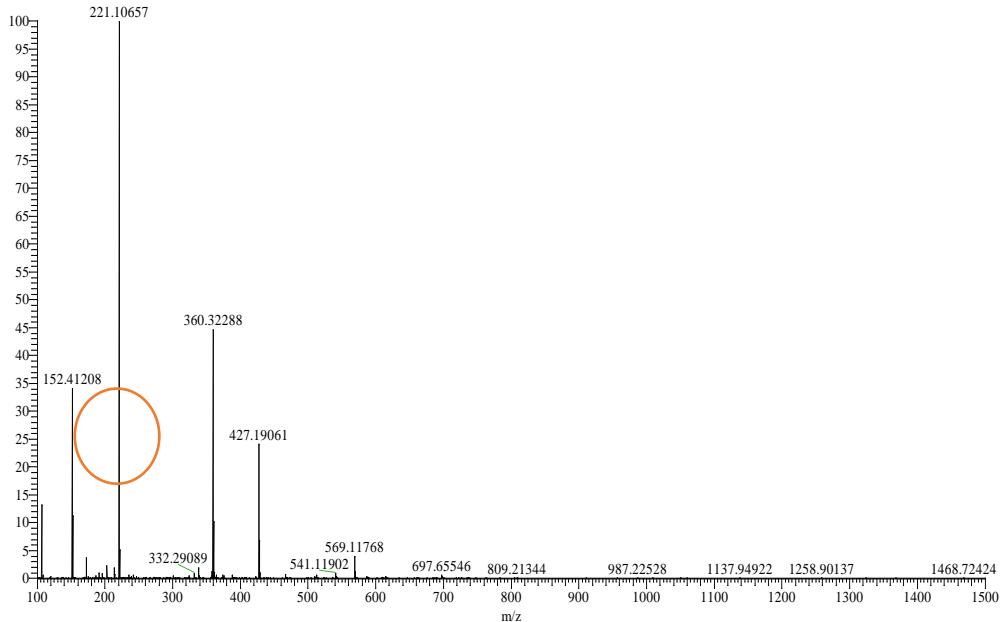


Fig. S4. Mass spectrum of **Compound G**.

The association constant of G with Zn²⁺

K_a is calculated by Kaleida Graph software. The custom formula is as follows:

$$0.5 * (m1 * ((1E-5) + M0 * (1E-5) + (1/m2)) - (((m1 * ((1E-5) + M0 * (1E-5) + (1/m2)))^2) - 4 * (m1^2) * (1E-5) * M0 * (1E-5)))^{(0.5)}; \text{ m1} = 1\text{e+7}; \text{ m2} = 2\text{e+5};$$

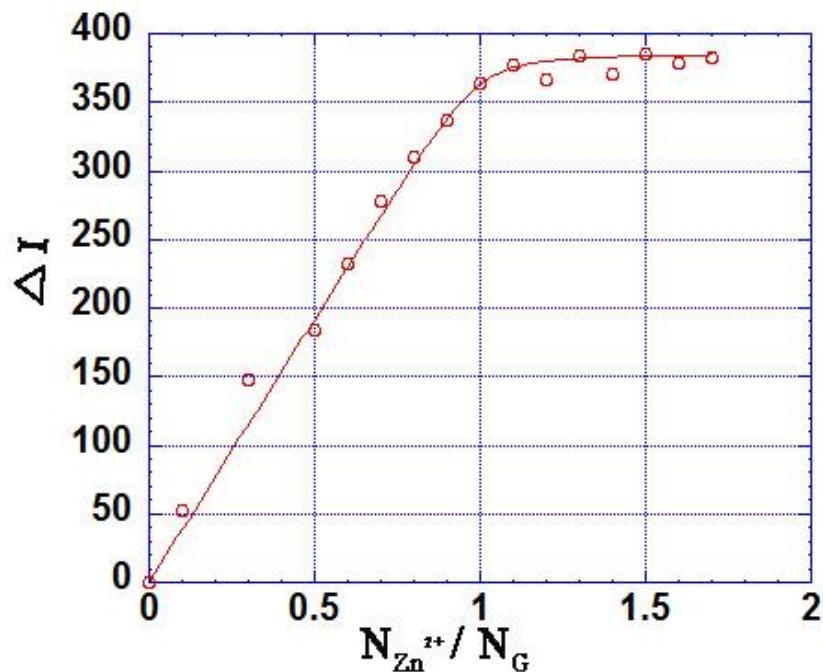


Fig. S5. The intensity changes of **G** upon addition of Zn²⁺ and the red solid line was obtained from the non-linear curve-fitting.

Table S1. The data from the Kaleida Graph.

$K_a(M^{-1})$	R^2
2.4627×10^5	0.993

Table S2. Standard deviation and detection limit calculation for Zn^{2+} .

Fluorescence Intensity	Standard deviation (σ)	Slope(K)	Detection limit ($(3\sigma/K)$)
165.211			
164.490			
165.487			
164.110			
163.890	2.15	$377.01 \times 10^5 M^{-1}$	$1.71 \times 10^{-7} M$
160.820			
163.006			
159.341			
162.466			
161.353			
159.895			

Table S3. Comparison of the solvents and detection limits (LOD) with recently reported fluorescent probes for Zn^{2+} .

Solvents	LOD (M)	References
C_2H_3N	4.82×10^{-7}	1
C_2H_5OH	2.5×10^{-5}	2
H_2O / THF (9:1, v/v)	3.7×10^{-7}	3
DMF / H_2O (2:3, v/v)	2.5×10^{-7}	4
H_2O	1.71×10^{-7}	This work

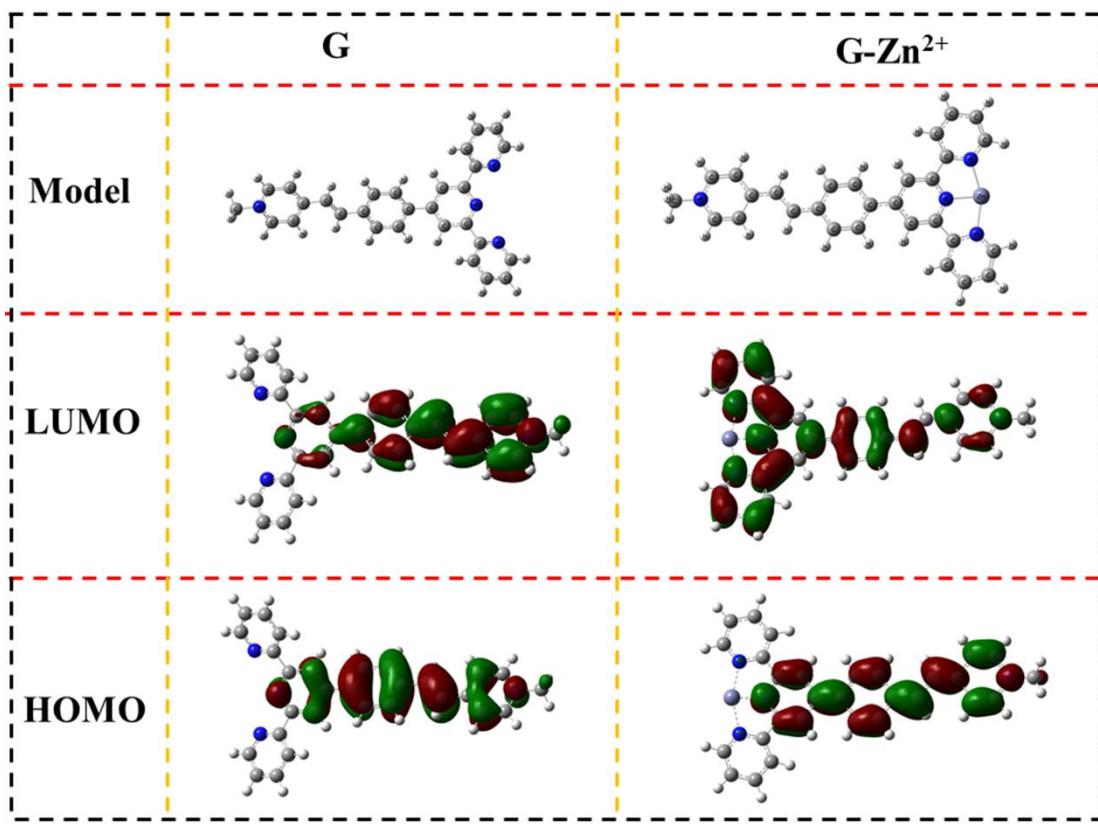


Fig. S6. HOMO and LUMO orbitals of probe G and G-Zn²⁺ complex.

Table S4 Excitation parameters of G and G-Zn²⁺

	D(A)	Sr	H(A)	t(A)	HDI	EDI
G	2.249	0.70027	3.716	-1.254	6.36	6.44
G-Zn ²⁺	3.566	0.73868	4.968	-1.04	5.45	5.13

References

1. Zhang X, Liu J, Wang J, Han L, Ma S, Zhao M, Xi G. Adenosine triphosphate (ATP) and zinc(II) ions responsive pyrene based turn-on fluorescent probe and its application in live cell imaging. *J Photochem Photobiol B* **2021**, 223, 112279.
2. Huo F, Wu Q, Kang J, Zhang Y, Yin C. A specific fluorescent probe for zinc ion based on thymolphthalein and it's application in living cells. *Sensors and Actuators B: Chemical* **2018**, 262, 263.
3. Li Y, Gu Z, He T, Yuan X, Zhang Y, Xu Z, Qiu H, Zhang Q, Yin S. Terpyridyl-based triphenylamine derivatives with aggregation-induced emission characteristics for selective detection of Zn²⁺, Cd²⁺ and CN⁻ ions and application in cell imaging. *Dyes and Pigments* **2020**, 173.
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