

## **Supplementary Information**

# **Synthesis of an Unprecedented H-stitched Binuclear Crystal Structure Based on Selective Fluorescence Recognition of Zn<sup>2+</sup> in Newly Synthesized Schiff Base Ligand with DFT and Imaging Application in Living Cells**

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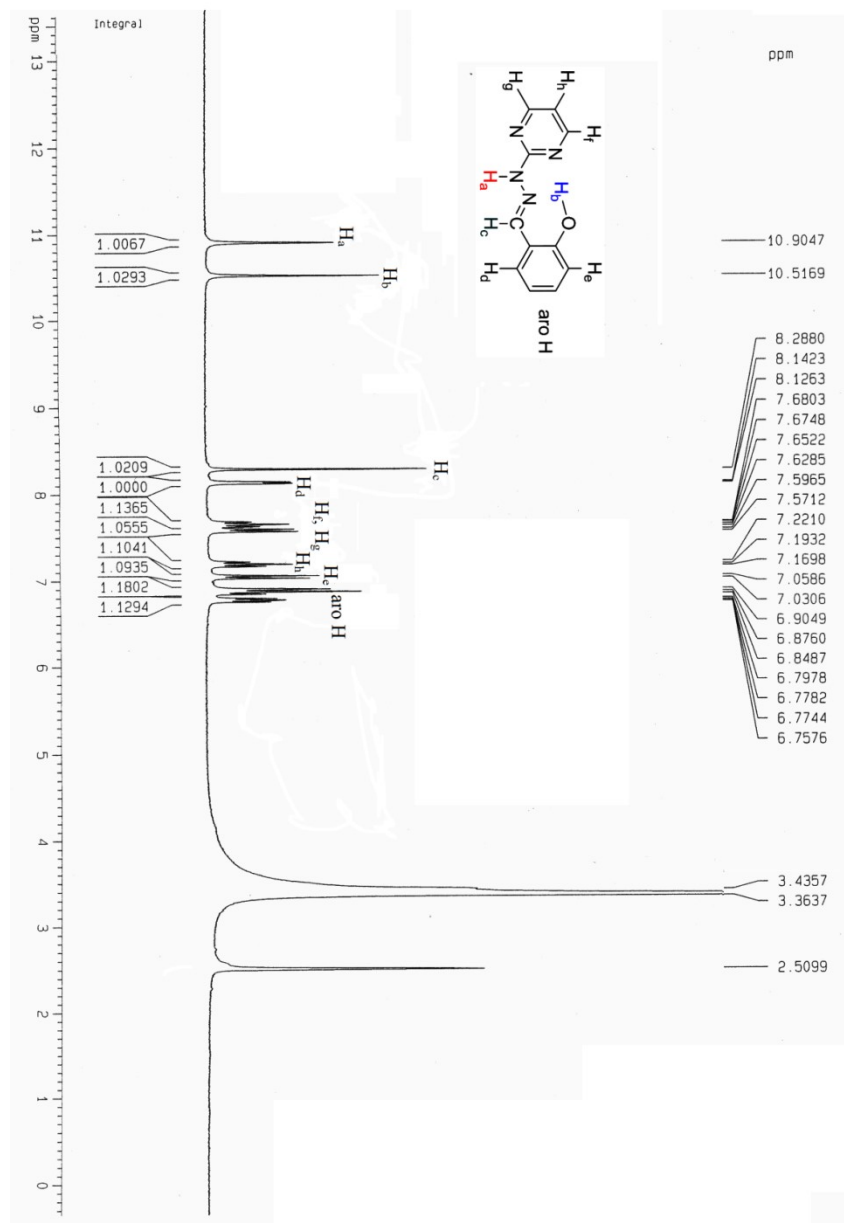
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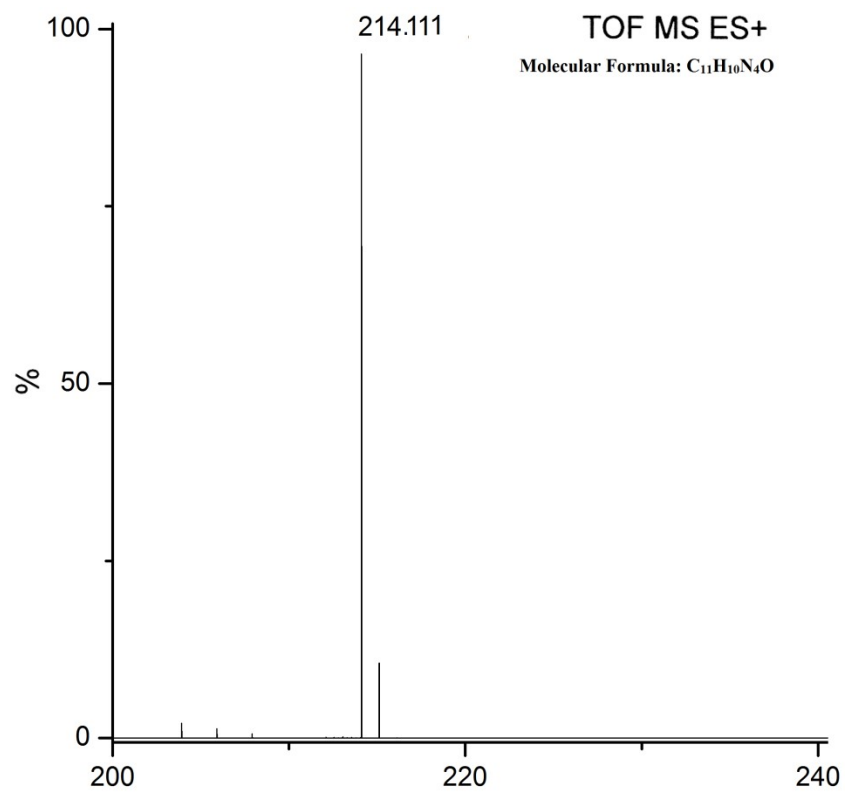
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1. <sup>1</sup>H NMR of ligand PHP (Figure S1),
2. HRMS of ligand PHP (Figure S2),
3. LOD Plot (Figure S3),
4. Selected bond distances from crystal structure (Table S1).
5. Mechanism of Complex formation (Scheme S1)



**Figure S1:** <sup>1</sup>H NMR of ligand PHP.



**Figure S2:** . HRMS of ligand PHP.

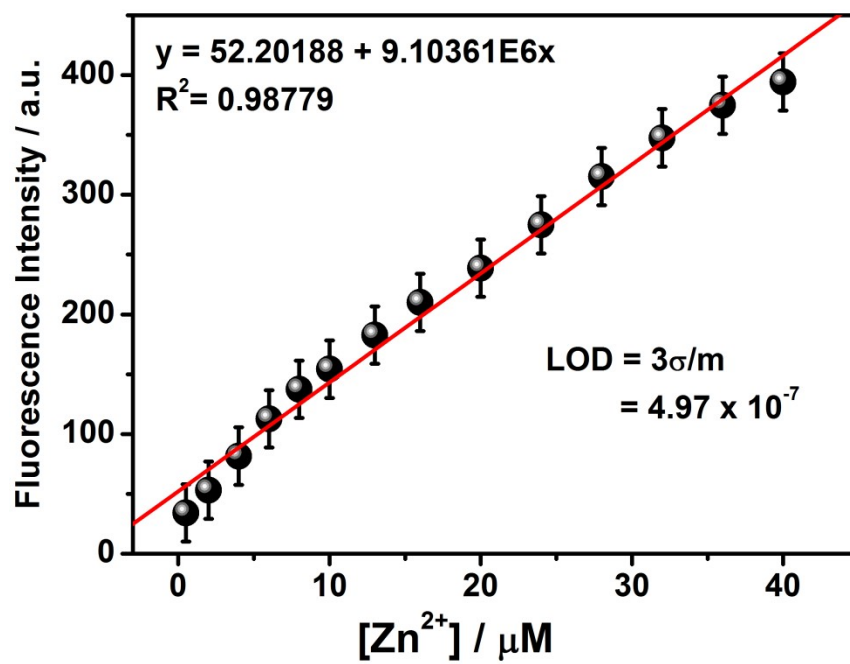


Figure S3: LOD plot for Zn<sup>2+</sup> sensing.

**Table S1.** Selected bond distance (Å) and angle (°) data for **1**

Selected Bonds	Value(Å)	Selected Angles	(°)
Zn01 -O3	2.155(2)	O3 -Zn01 -O4	85.31(9)
Zn01 -O4	2.059(2)	O3 -Zn01 -N9	81.19(10)
Zn01 -N9	2.149(3)	O3 -Zn01 -N13	107.35(10)
Zn01 -N11	2.142(3)	O4 -Zn01 -N9	98.25(10)
Zn01 -N13	2.138(3)	O4 -Zn01 -N11	97.01(10)
Zn01 -N15	2.126(3)	O4 -Zn01 -N13	84.00(10)
Zn02 -O1	2.162(2)	N9 -Zn01 -N11	76.31(11)
Zn02 -O2	2.060(2)	N9 -Zn01 -N13	171.36(10)
Zn02 -N1	2.117(3)	N11 -Zn01 -N13	95.16(11)
Zn02 -N4	2.136(3)	N13 -Zn01 -N15	75.91(10)
Zn02 -N5	2.127(3)	O1 -Zn02 -O2	83.93(9)
Zn02 -N7	2.133(3)	N4 -Zn02 -N7	99.64(11)
O4 -H202	1.34(5)	N5 -Zn02 -N7	76.13(11)
O1 -H202	1.16(5)	O1 -Zn02 -N1	81.82(10)
		N1 -Zn02 -N4	76.97(11)

**Scheme S1: Proposed Mechanism**

