

## Electronic Supplementary Information (ESI)

### A highly selective coumarin-based chemosensor for dual sensing of Cu<sup>2+</sup> and Zn<sup>2+</sup> ions with logic gate integration and live cell imaging

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## Methods and measurements

### Limit of detection (LOD)

The limit of detection for **CIH** was determined using fluorescence titration data and the IUPAC definition based on a plot of emission intensity vs. increasing  $Zn^{2+}/Cu^{2+}$  concentration. We repeated our observations eight times, measuring the emission intensity of **CIH** without  $Zn^{2+}/Cu^{2+}$  at every repetition and calculated the standard deviation of blank data. Fluorescence intensity data at 509 nm against  $Zn^{2+}/Cu^{2+}$  concentration were plotted to determine the slope. The detection limit is established using the following equation:<sup>1</sup>

$$\text{Limit of detection (LOD)} = \frac{3SD}{\text{Slope}(m)}$$

Where, the variables  $m$ , stands for the slope of intensity vs. sample concentration, and  $SD$ , stands for the standard deviation of blank readings.

### Binding constant ( $K_a$ )

Using the Job's plot, the binding ratio of **CIH** to metal ions was calculated. The Benesi-Hildebrand equation was used to determine the binding constants ( $K_a$ ) of **CIH** for  $Zn^{2+}$  and  $Cu^{2+}$ .<sup>2</sup>

$$\frac{I_o}{I - I_o} = \frac{a}{b - a} \left( \frac{1}{K_a [\text{Metal}]} + 1 \right)$$

Where,  $I$  and  $I_0$  represent the intensity of **CIH** fluorescence at 509 nm in the presence and absence of  $Zn^{2+}/Cu^{2+}$ , respectively;  $a$  and  $b$  are constants; and  $[\text{Metal}]$  represents the concentration of  $Zn^{2+}/Cu^{2+}$ .

### Fluorescence quantum yield measurements

The following equation was used to calculate quantum yield:<sup>3</sup>

$$Q = Q_r \left( \frac{I}{I_r} \right) \left( \frac{OD}{OD_r} \right) \left( \frac{n^2}{n_r^2} \right)$$

Where  $Q$  is the fluorescence quantum yield,  $I$  is the integrated fluorescence intensity,  $n$  is the refractive index of liquid, and  $OD$  is the optical density (absorption). The subscript  $r$  is used to represent the known quantum yield of reference quinine sulfate, which is 0.54 in 0.1 M  $H_2SO_4$ .

### Fluorescence decay measurements

To explore sensing properties, time-resolved fluorescence spectra were taken. The following equation has been used to calculate dynamic parameters:

$$y = A_1 * \exp\left(-\frac{x}{\tau_1}\right) + A_2 * \exp\left(-\frac{x}{\tau_2}\right) + y_0$$

The following equation was used for calculating the weighted mean lifetime:

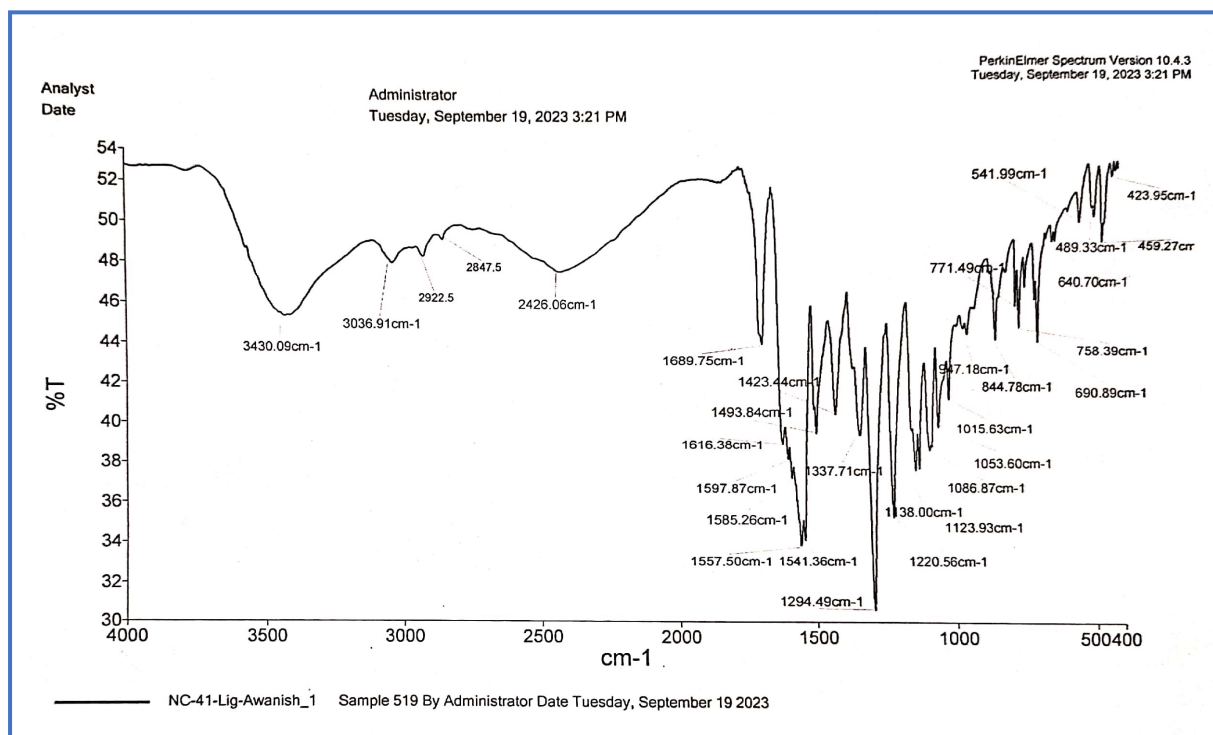
$$\langle \tau \rangle = (A_1\tau_1 + A_2\tau_2)/(A_1 + A_2)$$

Where,  $\tau_1/\tau_2$  and  $A_1/A_2$  are lifetimes ( $\tau$ ) and the fractions or amplitudes (A), respectively.

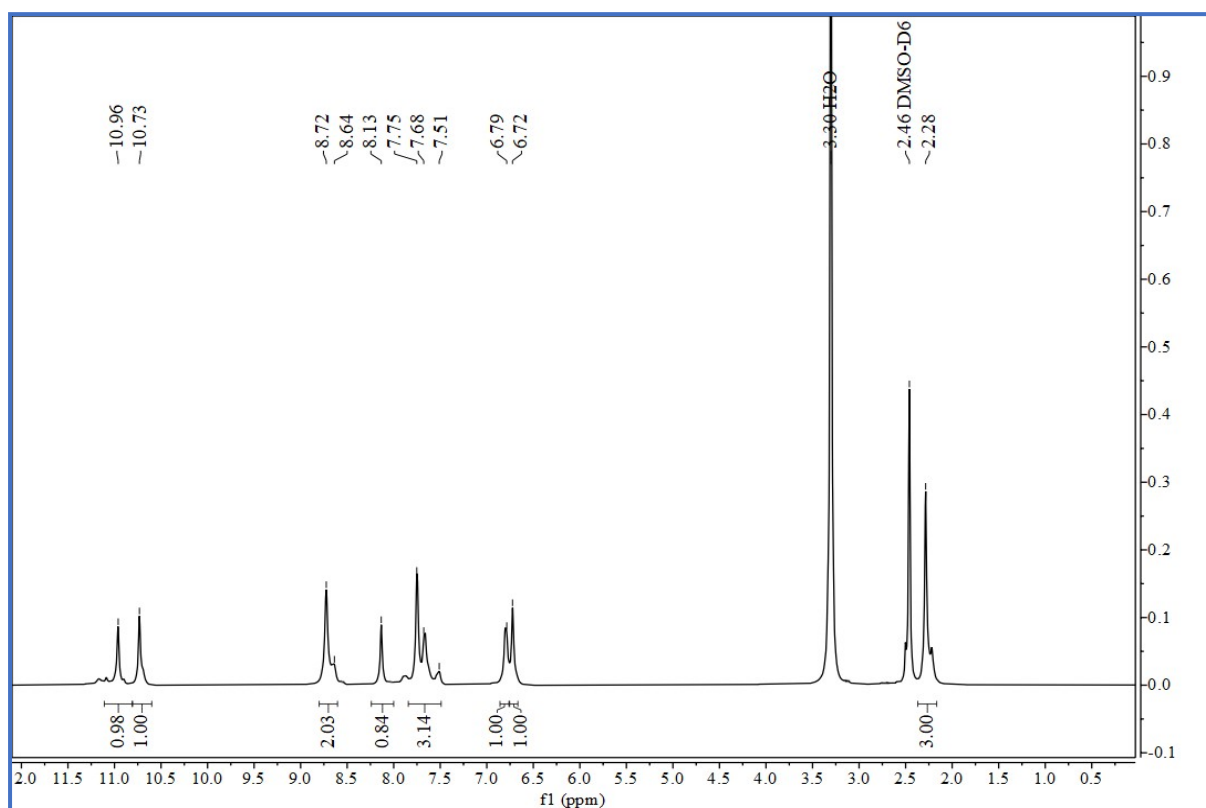
The following equations are used to compute the radiative rate constant ( $K_r$ ) and non-radiative rate constant ( $K_{nr}$ ):<sup>4</sup>

$$\langle \tau \rangle^{-1} = (K_r + K_{nr})$$

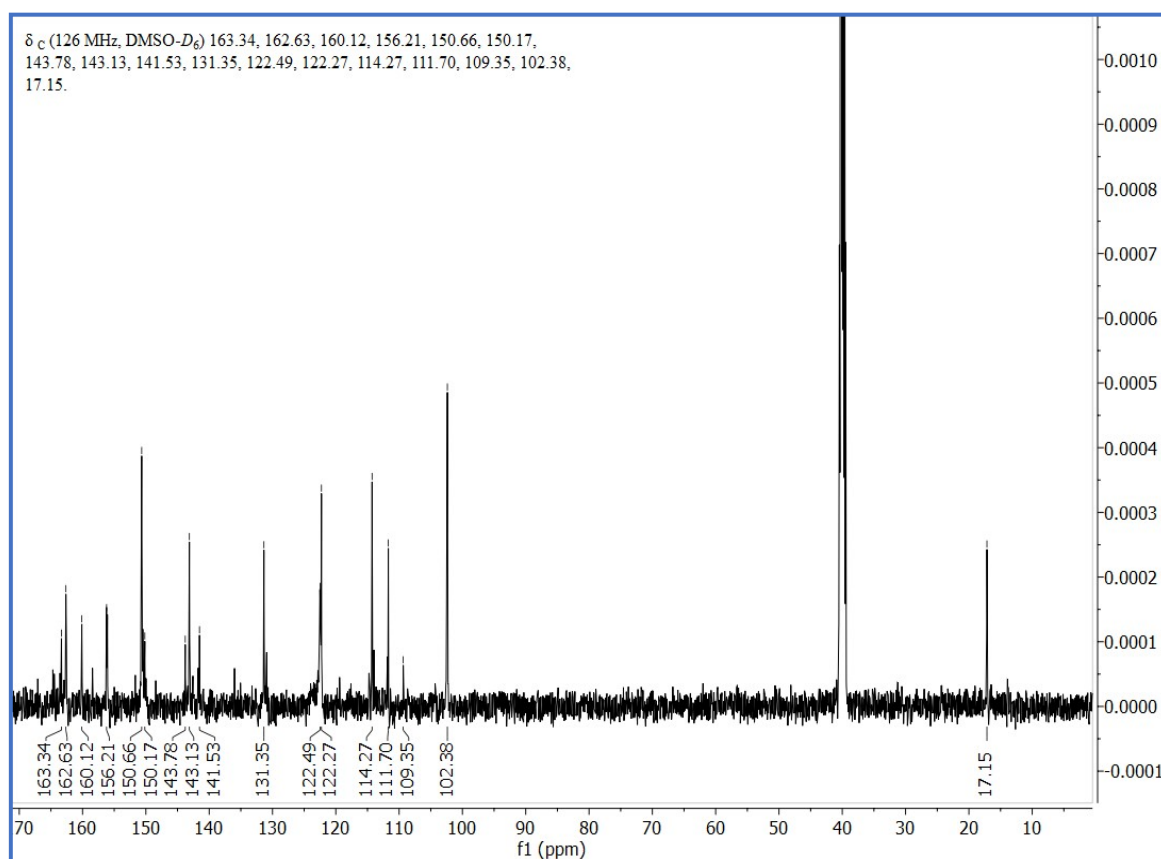
$$K_r = \frac{\Phi}{\langle \tau \rangle}$$



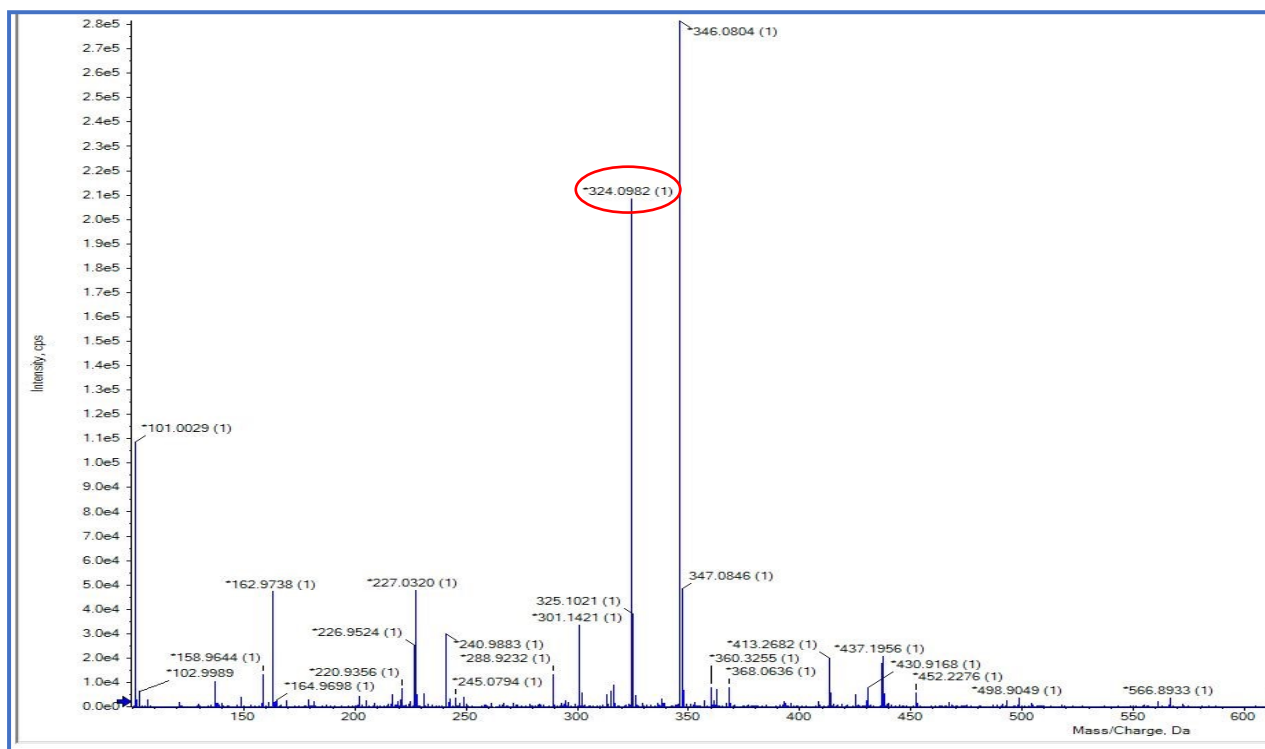
**Fig. S1** IR spectrum of CIH.



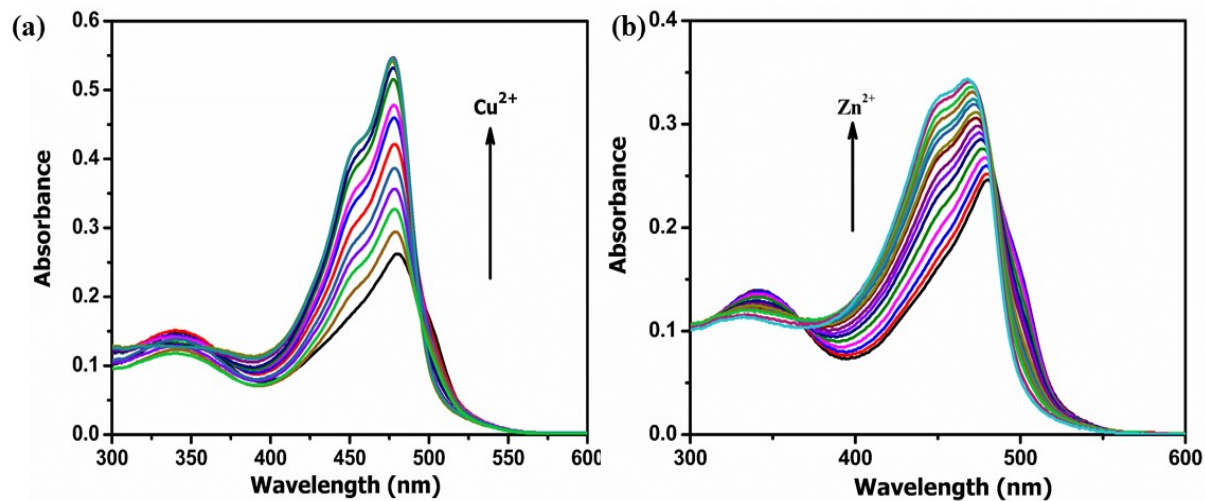
**Fig. S2** <sup>1</sup>H NMR spectrum of CIH



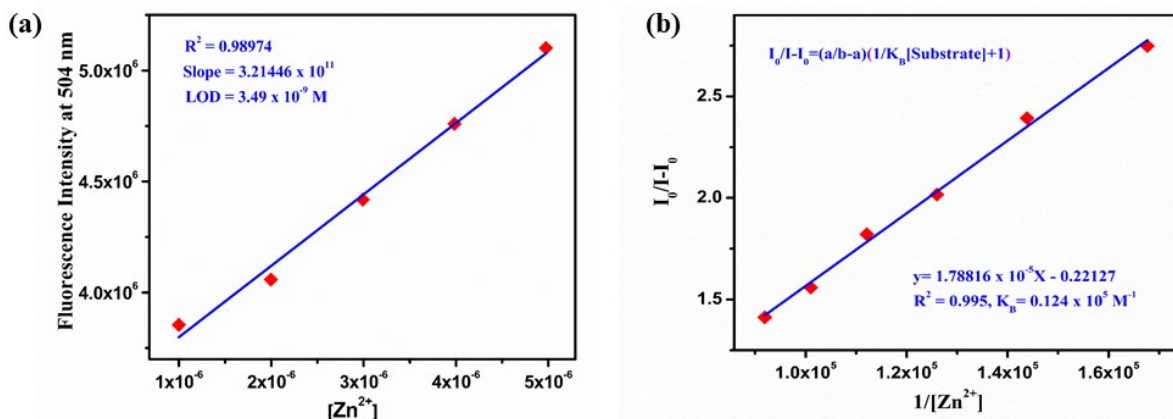
**Fig. S3**  $^{13}\text{C}$  NMR spectrum of CIH



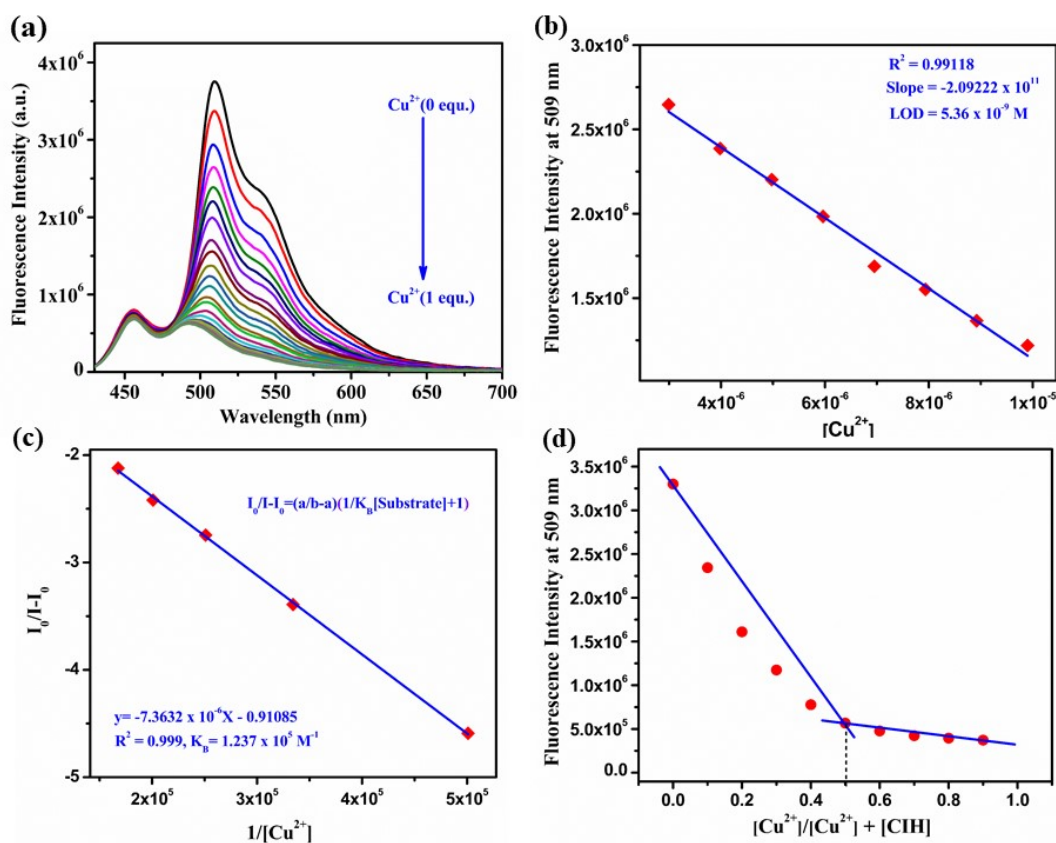
**Fig. S4** Mass spectrum of CIH



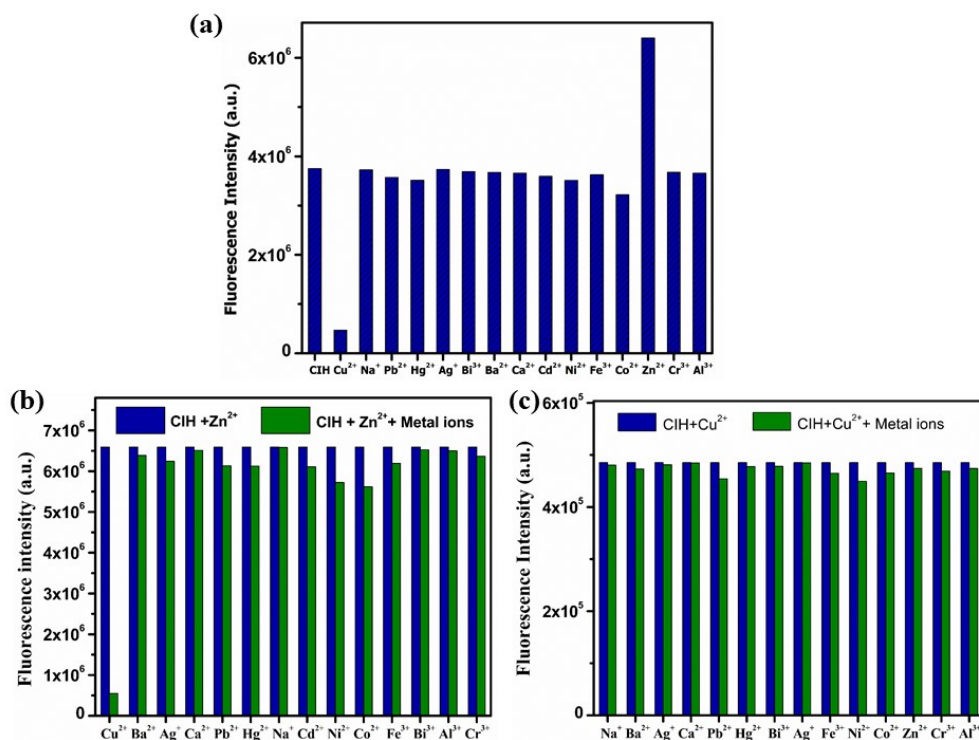
**Fig. S5** UV-Vis titration spectra of CIH (20  $\mu\text{M}$ ) in DMF:H<sub>2</sub>O (7:3, v/v, pH 7.4) HEPES buffer solution (a) in the presence of increasing concentration of  $\text{Cu}^{2+}$  (0-1equiv.); (b) in the presence of increasing concentration of  $\text{Zn}^{2+}$  (0-1equiv.).



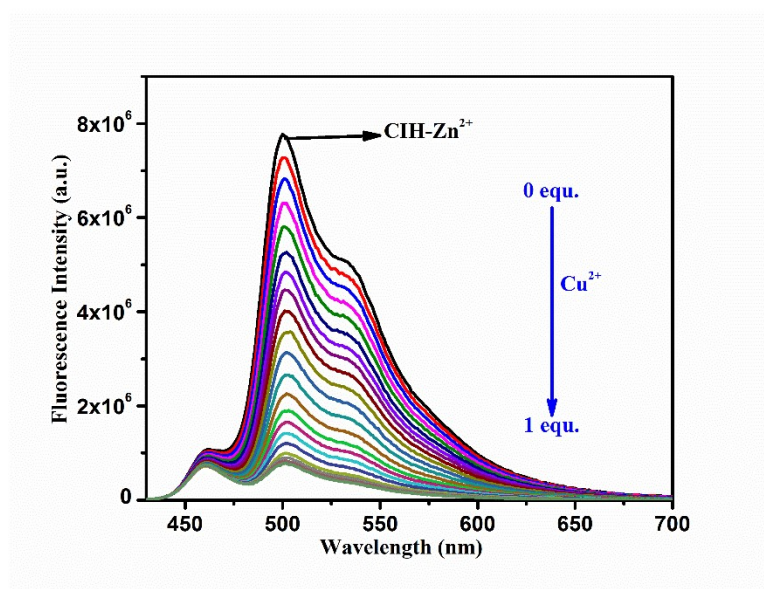
**Fig. S6** (a) Limit of detection (LOD) plot, the change in fluorescence intensity at 504 nm of **CIH** (20  $\mu$ M) as a function of  $Zn^{2+}$  ions concentration (b) Benesi-Hildebrand plot of **CIH** for determination of binding constant with  $Zn^{2+}$ .



**Fig. S7** (a) Fluorescence titration spectra of **CIH** (20  $\mu$ M,  $\lambda_{ex} = 420$  nm) in DMF:H<sub>2</sub>O (7:3, v/v, pH 7.4) HEPES buffer solution in the presence of  $Cu^{2+}$  (0- 1 equiv.) (b) Limit of detection (LOD) plot, the change in fluorescence intensity at 509 nm of **CIH** (20  $\mu$ M) as a function of  $Cu^{2+}$  ion concentration (c) Benesi-Hildebrand plot of **CIH** for evaluation of binding constant with  $Cu^{2+}$  and (d) Job's plot for determination of binding stoichiometry for **CIH**- $Cu^{2+}$ .

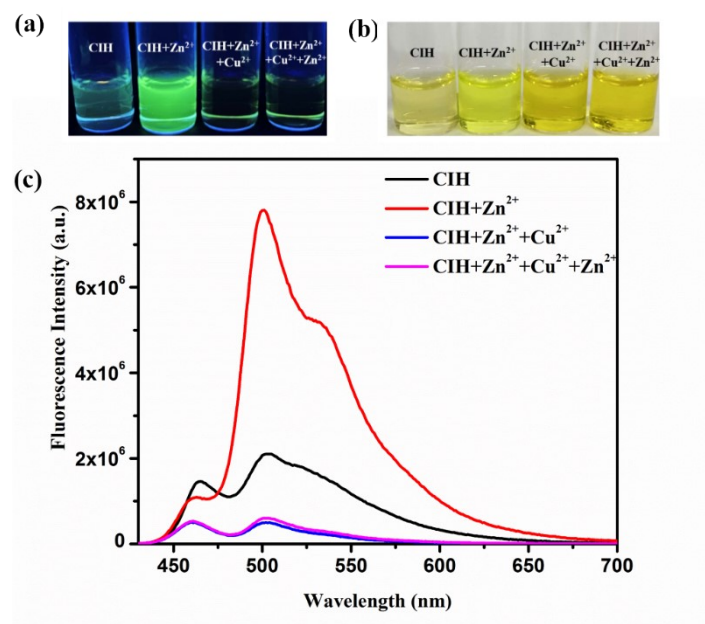


**Fig. S8** Fluorescence intensity measurement of **CIH** (20  $\mu\text{M}$ ) **(a)** after addition of various metal ions (20  $\mu\text{M}$ ) in DMF:H<sub>2</sub>O (7:3, v/v, pH 7.4) HEPES buffer solution **(b)** in the presence of  $\text{Cu}^{2+}$  + other metal ions (20  $\mu\text{M}$ ) in DMF:H<sub>2</sub>O (7:3, v/v, pH 7.4) HEPES buffer solution **(c)** in the presence of  $\text{Zn}^{2+}$  + other metal ions (20  $\mu\text{M}$ ) in DMF:H<sub>2</sub>O (7:3, v/v, pH 7.4) HEPES buffer solution. ( $\lambda_{\text{ex}} = 420 \text{ nm}$ ).

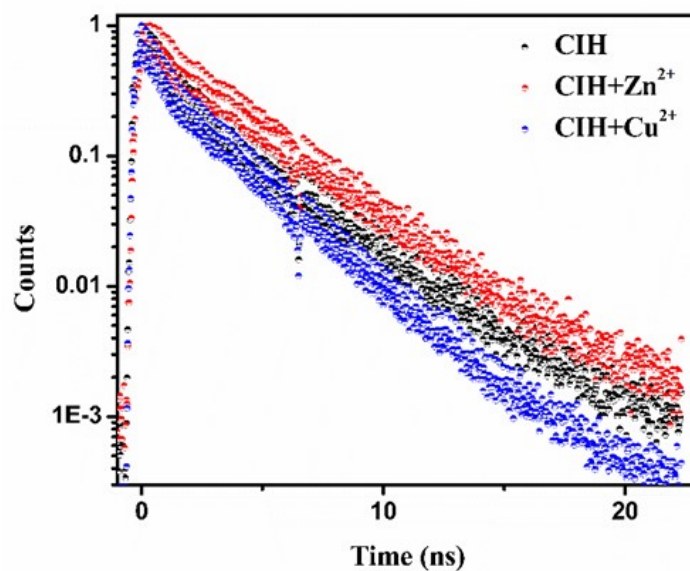


**Fig. S9** Fluorescence titration spectra of **CIH-Zn<sup>2+</sup>** (20  $\mu\text{M}$ ) with  $\text{Cu}^{2+}$  (0-1equiv.) in DMF:H<sub>2</sub>O (7:3, v/v, pH 7.4) HEPES buffer solution.

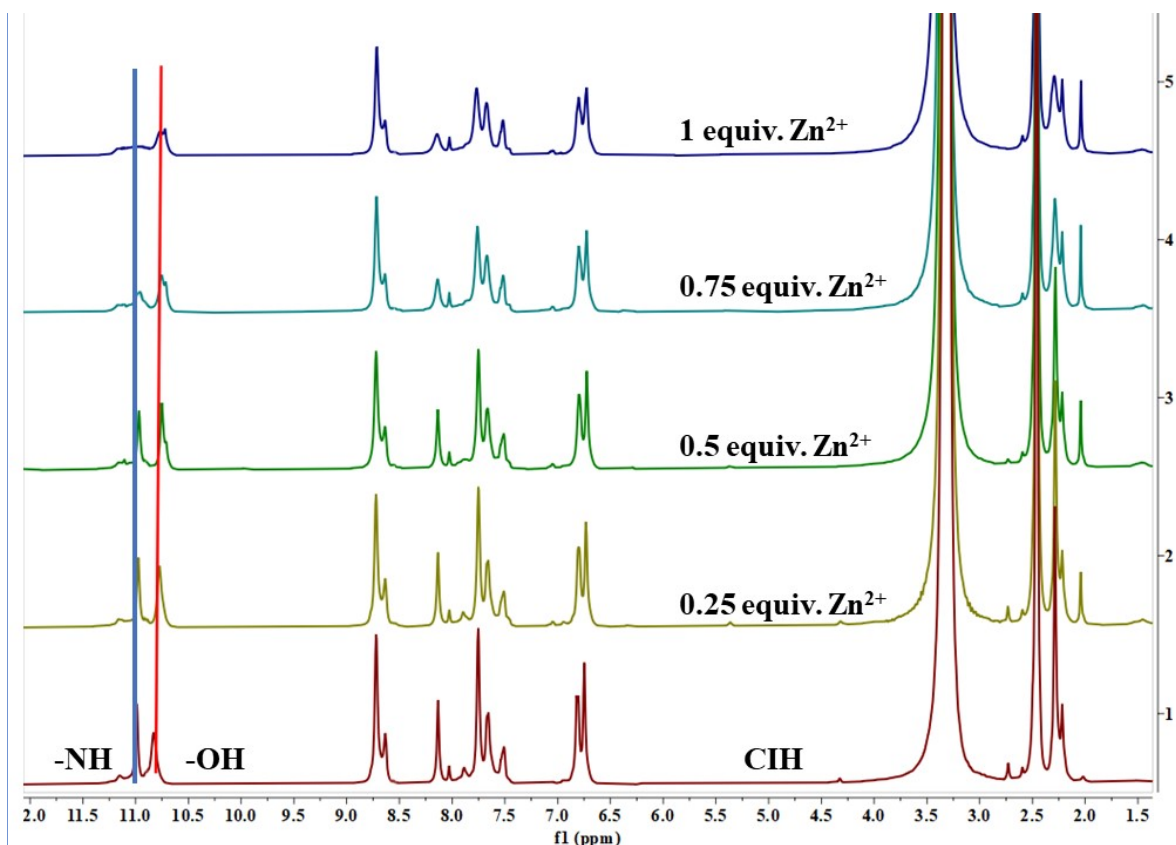




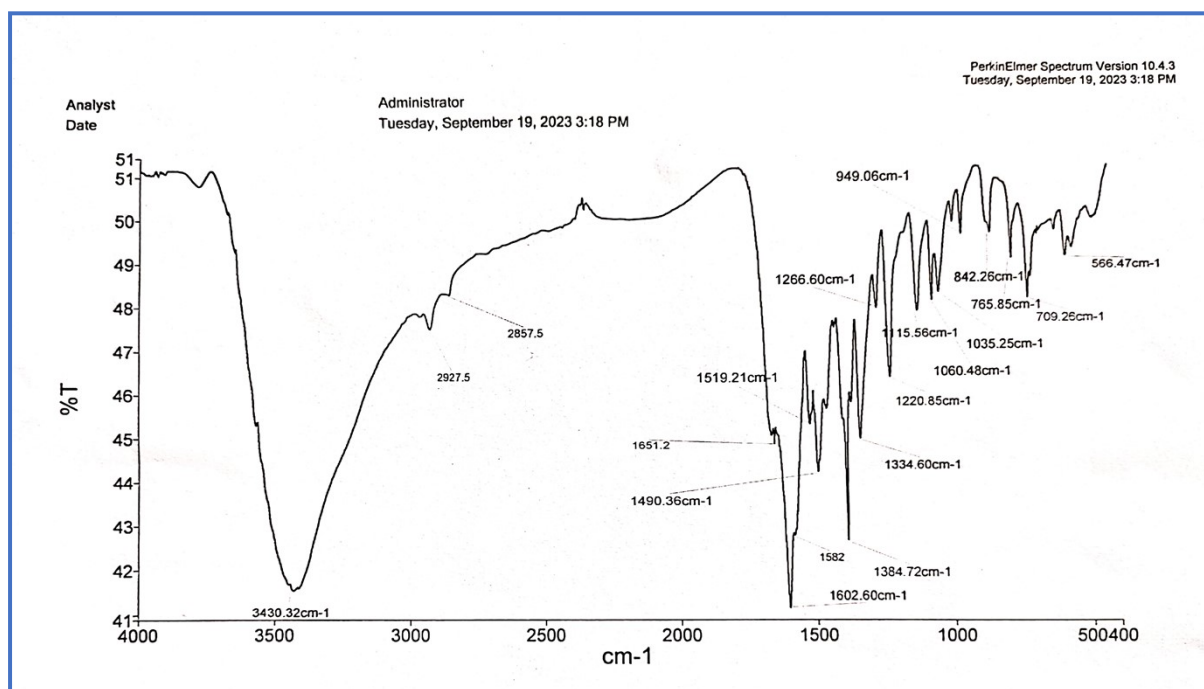
**Fig. S10** Images of **CIH**, **CIH-Zn<sup>2+</sup>**, **CIH-Zn<sup>2+</sup>-Cu<sup>2+</sup>** and **CIH-Zn<sup>2+</sup>-Cu<sup>2+</sup>-Zn<sup>2+</sup>** in DMF:H<sub>2</sub>O (7:3, v/v, pH 7.4) HEPES buffer solution under (a) UV- illumination and (b) Visible light. (c) Fluorescence spectra of **CIH** upon subsequent addition of Zn<sup>2+</sup> and Cu<sup>2+</sup>.



**Fig. S11** Time-resolved fluorescence decay profile of **CIH** in presence and absence of Zn<sup>2+</sup>/Cu<sup>2+</sup>, respectively in DMF:H<sub>2</sub>O (7:3, v/v, pH 7.4) HEPES buffer solution.



**Fig. S12**  $^1\text{H}$  NMR titration of CIH after addition of  $\text{Zn}^{2+}$  (0-1 equiv.) in  $\text{DMSO-d}_6$ .



**Fig. S13** IR spectrum of CIH- $\text{Zn}^{2+}$  complex.

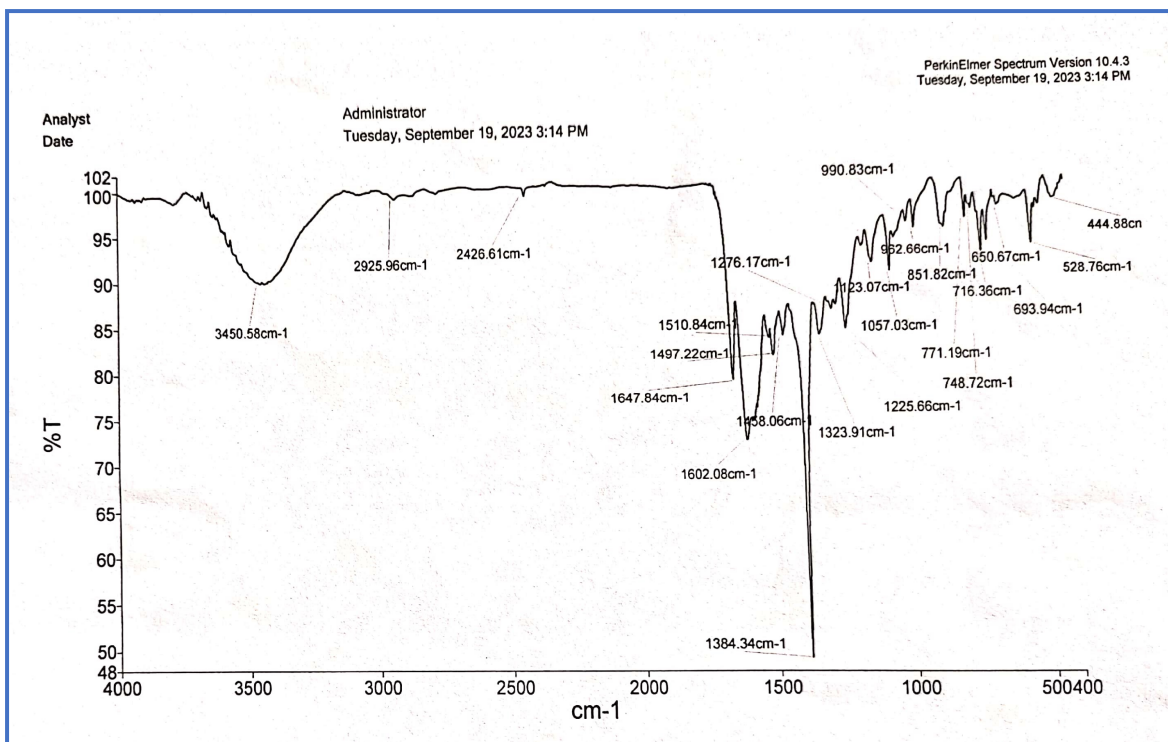


Fig. S14 IR spectrum of CIH-Cu<sup>2+</sup> complex.

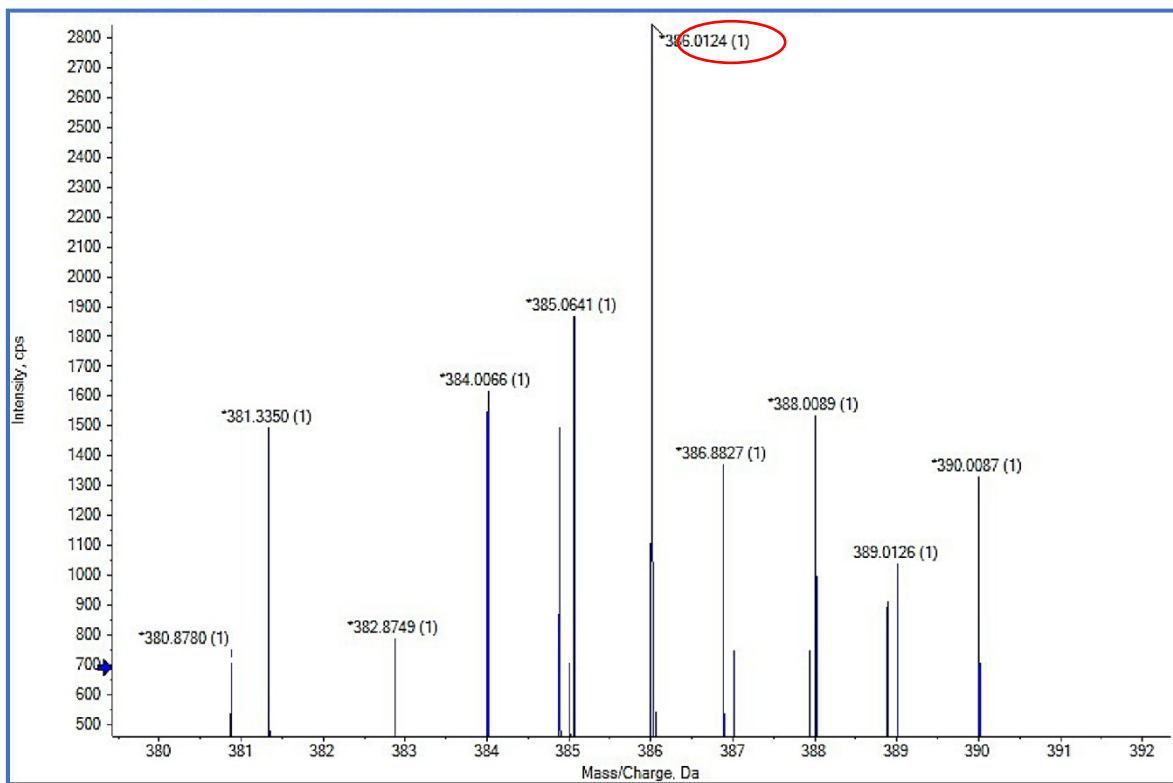
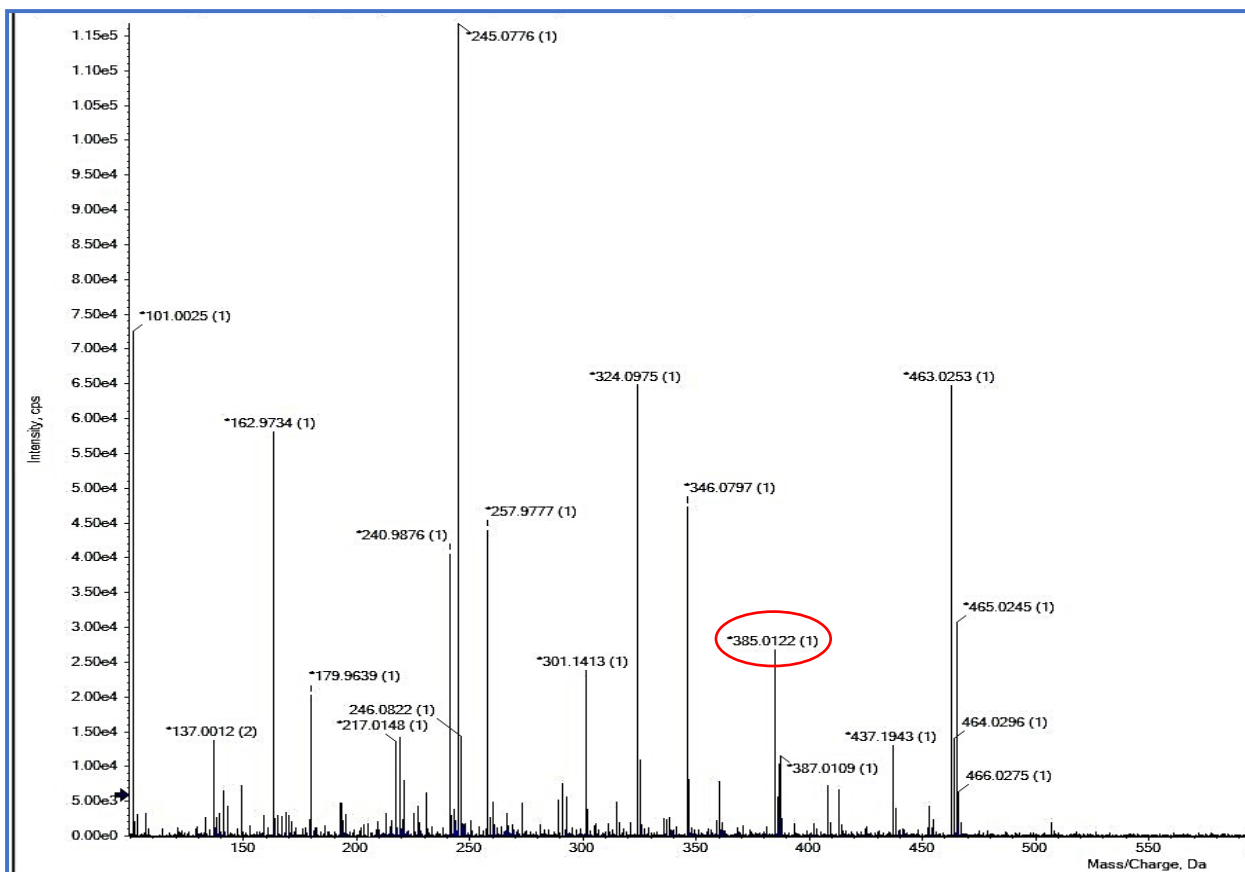
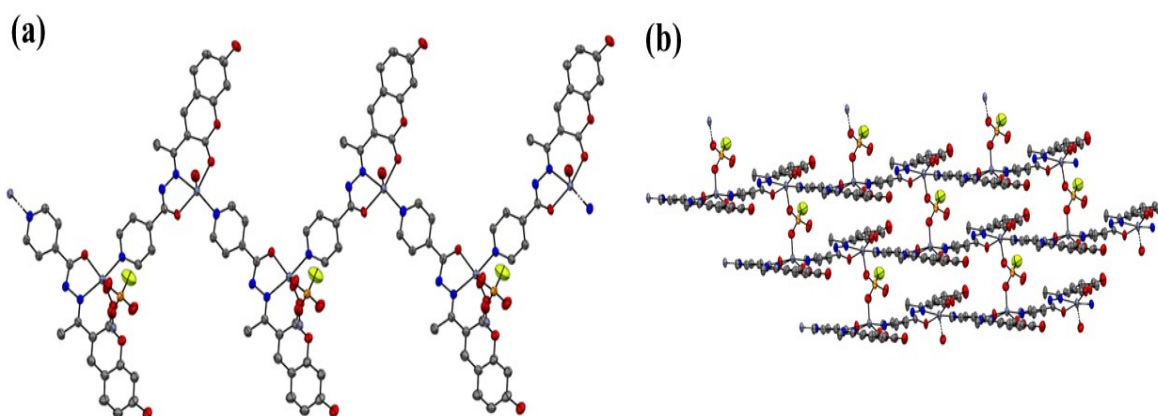


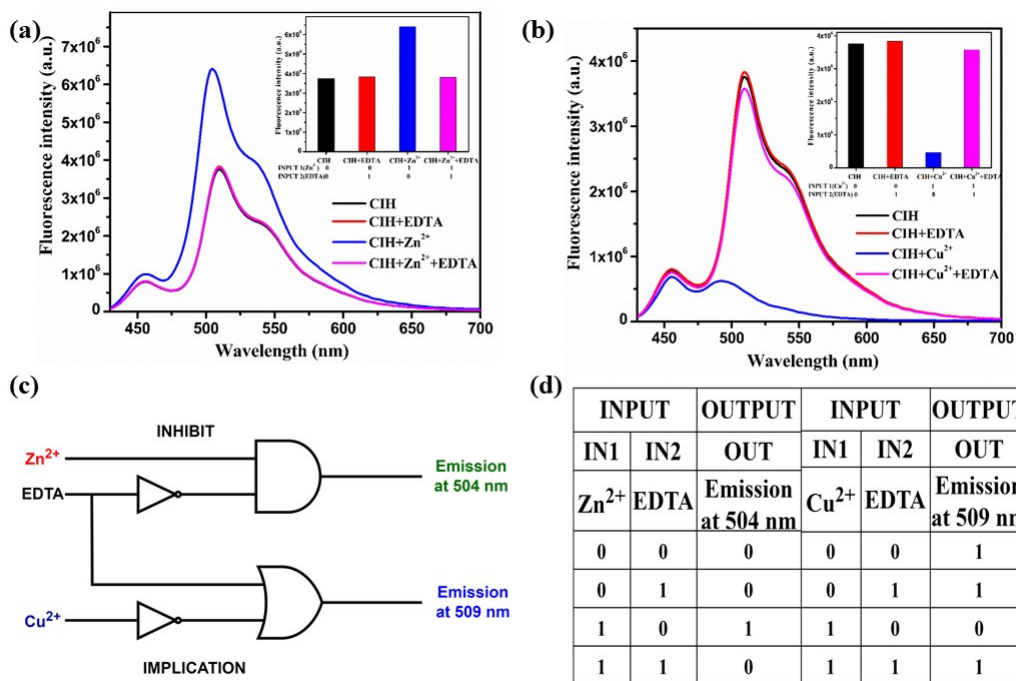
Fig. S15 Mass spectrum of CIH-Zn<sup>2+</sup>



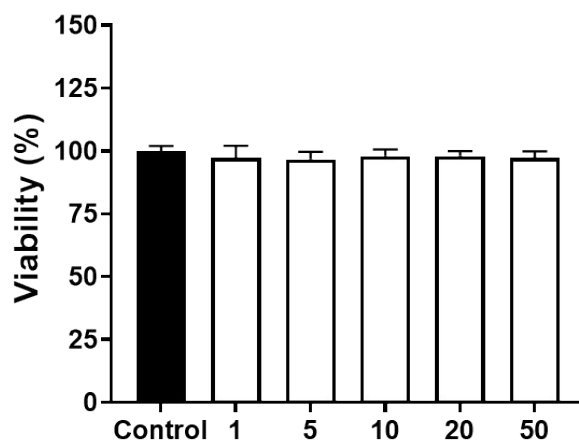
**Fig. S16** Mass spectrum of CIH-Cu<sup>2+</sup>



**Fig. S17** (a) A one-dimensional supramolecular structure of CIH-Zn<sup>2+</sup> complex in a coordination polymer framework (b) three-dimensional structure of CIH-Zn<sup>2+</sup> complex.



**Fig. S18** (a) Changes in emission intensity of CIH ( $\lambda_{ex} = 420$  nm) in the presence and absence of Zn<sup>2+</sup> and EDTA. Inset: Diagram depicting the emission output at 504 nm. (b) Changes in the emission intensity of CIH ( $\lambda_{ex} = 420$  nm) in the presence and absence of Cu<sup>2+</sup> and EDTA. Inset: Diagram depicting the emission output at 509 nm. (c) Schematic illustration of INHIBIT and the IMPLICATION logic gate. (d) truth table.



**Fig. S19** MTT assay plot showing treatment of SiHa cells with various concentration of CIH (1, 5, 10, 20 and 50  $\mu$ M) for 4 h.

**Table S1** Quantum yields and fluorescence decay parameters of **CIH** before and after treatment with  $Zn^{2+}/Cu^{2+}$  in DMF:H<sub>2</sub>O (7:3, v/v, pH 7.4) HEPES buffer solution.

Sample	A	$\tau$ (ns)	$\langle \tau \rangle$ (ns)	$\Phi$	Kr(s)	Knr(s)
<b>CIH</b>	0.521 (A1)	1.075( $\tau$ 1)	2.055	$10.41 \times 10^{-3}$	$5.07 \times 10^6$	$4.81 \times 10^8$
	0.348 (A2)	3.526 ( $\tau$ 2)				
<b>CIH-Zn<sup>2+</sup></b>	0.146 (A1)	0.99395( $\tau$ 1)	2.966	$24.72 \times 10^{-3}$	$8.33 \times 10^6$	$3.29 \times 10^8$
	0.637 (A2)	3.41947( $\tau$ 2)				
<b>CIH-Cu<sup>2+</sup></b>	0.482 (A1)	0.691 ( $\tau$ 1)	1.658	$2.70 \times 10^{-3}$	$1.63 \times 10^6$	$6.01 \times 10^8$
	0.403 (A2)	2.815 ( $\tau$ 2)				

**Table S2**  
Important crystallographic data of **CIH-Zn<sup>2+</sup>** complex

CCDC No.	<u>2305336</u>
Empirical formula	C <sub>34</sub> H <sub>24</sub> FN <sub>6</sub> O <sub>11</sub> PZn <sub>2</sub>
Formula weight	873.30
Temperature (K)	293
Crystal system	triclinic
Space group	P-1
a (Å)	11.6235(3)
b (Å)	12.0608(5)
c (Å)	16.9201(7)
$\alpha$ (°)	77.785(4)
$\beta$ (°)	87.986(3)
$\gamma$ (°)	77.824(3)
Volume (Å <sup>3</sup> )	2266.04(15)
Z	2
Density (g/cm <sup>3</sup> )	1.280
$\mu$ (mm <sup>-1</sup> )	2.155

F(000)	884.0
Crystal size (mm <sup>3</sup> )	0.025 × 0.02 × 0.01
Radiation	Cu Kα (λ = 1.54184)
2Θ range for data collection (°)	5.344 to 144.238
Reflections collected	29742
Independent reflections	8843 [R <sub>int</sub> = 0.0494, R <sub>sigma</sub> = 0.0489]
Data/restraints/parameters	8843/0/502
Goodness-of-fit on F <sup>2</sup>	1.054
Final R indexes [I ≥ 2σ (I)]	R <sub>1</sub> = 0.0665, wR <sub>2</sub> = 0.1947
Final R indexes [all data]	R <sub>1</sub> = 0.0821, wR <sub>2</sub> = 0.2047

$${}^a R_1 = \frac{\sum ||F_o| - |F_c||}{\sum |F_o|}$$

$${}^b R_2 = \left[ \frac{\sum w(|F^2_o| - |F^2_c|)^2}{\sum w|F^2_o|} \right]^{1/2}$$

**Table S3** List of bond lengths for **CIH-Zn<sup>2+</sup>**

Atom	Atom	Length/Å	Atom	Atom	Length/Å
Zn1	O4	1.989(3)	O8	C32	1.323(6)
Zn1	O3	2.055(3)	C13	C12	1.493(6)
Zn1	N4	2.053(4)	C13	C14	1.395(6)
Zn1	O9	1.965(4)	C13	C15	1.386(7)
Zn1	N1	2.092(4)	C26	C27	1.454(6)
Zn2	O6	2.144(3)	C26	C28	1.373(6)
Zn2	O5	2.068(3)	C26	C24	1.454(6)
Zn2	O10 <sup>1</sup>	2.075(4)	C23	C22	1.501(6)
Zn2	N3 <sup>2</sup>	2.071(4)	C28	C29	1.413(7)
Zn2	N6	2.088(4)	C24	C25	1.507(6)
P1	O10	1.450(4)	C17	C15	1.387(6)
P1	O9	1.448(4)	C22	C21	1.391(6)
P1	O11	1.454(4)	C22	C20	1.394(7)
P1	F1	1.473(5)	C29	C34	1.385(7)
O7	C27	1.355(5)	C29	C30	1.408(7)
O7	C34	1.377(6)	C34	C33	1.389(7)
O6	C27	1.235(5)	C5	C3	1.379(7)

Atom	Atom	Length/Å	Atom	Atom	Length/Å
O5	C23	1.265(5)	C5	C6	1.386(7)
O2	C5	1.379(6)	C21	C19	1.383(6)
O2	C9	1.357(6)	C8	C10	1.486(7)
O4	C12	1.274(5)	C8	C9	1.449(7)
O3	C9	1.216(6)	C8	C7	1.363(7)
N5	N6	1.391(5)	C10	C11	1.499(7)
N5	C23	1.306(6)	C14	C16	1.380(7)
O1	C1	1.343(6)	C1	C3	1.385(7)
N3	C17	1.327(6)	C1	C2	1.405(8)
N3	C16	1.349(6)	C30	C31	1.354(7)
N6	C24	1.299(6)	C7	C6	1.415(7)
N2	N1	1.395(5)	C31	C32	1.394(8)
N2	C12	1.312(6)	C6	C4	1.405(7)
N4	C19	1.333(6)	C20	C18	1.352(7)
N4	C18	1.349(6)	C32	C33	1.410(7)
N1	C10	1.301(6)	C2	C4	1.359(8)

**Table S4** List of bond angles for **CIH-Zn<sup>2+</sup>**

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
O4	Zn1	O3	148.18(17)	C28	C26	C24	119.8(4)
O4	Zn1	N4	96.27(15)	O5	C23	N5	128.0(4)
O4	Zn1	N1	78.41(14)	O5	C23	C22	117.7(4)
O3	Zn1	N1	83.86(15)	N5	C23	C22	114.3(4)
N4	Zn1	O3	90.24(15)	O7	C27	C26	119.1(4)
N4	Zn1	N1	157.78(18)	O6	C27	O7	113.3(4)
O9	Zn1	O4	99.50(17)	O6	C27	C26	127.6(4)
O9	Zn1	O3	109.76(18)	C26	C28	C29	123.9(4)
O9	Zn1	N4	101.15(19)	N6	C24	C26	120.3(4)
O9	Zn1	N1	101.01(19)	N6	C24	C25	121.9(4)
O5	Zn2	O6	161.42(12)	C26	C24	C25	117.9(4)
O5	Zn2	O10 <sup>1</sup>	94.16(16)	N3	C17	C15	122.2(4)
O5	Zn2	N3 <sup>2</sup>	95.87(14)	C21	C22	C23	120.9(4)
O5	Zn2	N6	77.52(13)	C21	C22	C20	117.6(4)



Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
O10 <sup>1</sup>	Zn2	O6	91.56(15)	C20	C22	C23	121.5(4)
O10 <sup>1</sup>	Zn2	N6	98.27(15)	C34	C29	C28	116.9(4)
N3 <sup>2</sup>	Zn2	O6	101.45(14)	C34	C29	C30	118.1(4)
N3 <sup>2</sup>	Zn2	O10 <sup>1</sup>	93.24(17)	C30	C29	C28	124.8(4)
N3 <sup>2</sup>	Zn2	N6	167.08(16)	O7	C34	C29	120.7(4)
N6	Zn2	O6	84.17(13)	O7	C34	C33	117.1(4)
O10	P1	O11	112.1(2)	C29	C34	C33	122.2(5)
O10	P1	F1	109.4(3)	O2	C5	C3	116.9(5)
O9	P1	O10	107.5(3)	O2	C5	C6	119.0(4)
O9	P1	O11	110.0(3)	C3	C5	C6	124.1(5)
O9	P1	F1	107.9(3)	C19	C21	C22	119.2(4)
O11	P1	F1	109.9(3)	C9	C8	C10	121.3(4)
C27	O7	C34	122.7(4)	C7	C8	C10	121.1(5)
C27	O6	Zn2	124.5(3)	C7	C8	C9	117.7(5)
C23	O5	Zn2	109.1(3)	N1	C10	C8	119.7(4)
C9	O2	C5	123.4(4)	N1	C10	C11	122.3(4)
C12	O4	Zn1	111.0(3)	C8	C10	C11	117.9(4)
C9	O3	Zn1	126.8(3)	O2	C9	C8	118.7(4)
P1	O10	Zn2 <sup>3</sup>	143.0(3)	O3	C9	O2	112.4(4)
C23	N5	N6	111.0(4)	O3	C9	C8	128.9(5)
C17	N3	Zn2 <sup>4</sup>	121.9(3)	C16	C14	C13	119.8(4)
C17	N3	C16	118.8(4)	N3	C16	C14	122.0(4)
C16	N3	Zn2 <sup>4</sup>	119.3(3)	O1	C1	C3	116.9(5)
N5	N6	Zn2	112.0(3)	O1	C1	C2	122.4(5)
C24	N6	Zn2	132.6(3)	C3	C1	C2	120.7(5)
C24	N6	N5	115.4(4)	C13	C15	C17	120.0(4)
C12	N2	N1	109.7(4)	C31	C30	C29	121.0(5)
C19	N4	Zn1	118.2(3)	N4	C19	C21	122.3(4)
C19	N4	C18	118.2(4)	C8	C7	C6	122.5(5)
C18	N4	Zn1	122.6(3)	C30	C31	C32	120.7(5)
P1	O9	Zn1	140.6(3)	C5	C3	C1	117.3(5)
N2	N1	Zn1	111.6(3)	C5	C6	C7	118.7(5)
C10	N1	Zn1	130.1(3)	C5	C6	C4	116.5(5)

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
C10	N1	N2	116.7(4)	C4	C6	C7	124.8(5)
C14	C13	C12	123.1(4)	C18	C20	C22	119.8(5)
C15	C13	C12	119.6(4)	O8	C32	C31	120.8(5)
C15	C13	C14	117.3(4)	O8	C32	C33	119.2(5)
O4	C12	N2	127.7(4)	C31	C32	C33	120.0(5)
O4	C12	C13	116.4(4)	C34	C33	C32	118.0(5)
N2	C12	C13	115.9(4)	C4	C2	C1	119.8(5)
C27	C26	C24	123.4(4)	N4	C18	C20	122.8(5)
C28	C26	C27	116.7(4)	C2	C4	C6	121.6(6)

**Table S5** Comparison of CIH with the previously reported sensors.

S. No.	Working media	Analyte	Detection limit (M)	Applications	Reversibility	Ref.
1	CH <sub>3</sub> OH: H <sub>2</sub> O (9:1, pH 7.4)	Zn <sup>2+</sup> , Cu <sup>2+</sup>	Zn <sup>2+</sup> : $3.21 \times 10^{-8}$ Cu <sup>2+</sup> : $2.13 \times 10^{-8}$	Logic gates, live cell imaging	Yes	5
2	CH <sub>3</sub> CN	Zn <sup>2+</sup> , Cu <sup>2+</sup>	Zn <sup>2+</sup> : $2.41 \times 10^{-6}$ Cu <sup>2+</sup> : $4.23 \times 10^{-6}$	Logic gates	Yes	6
3	THF:H <sub>2</sub> O (5:95)	Zn <sup>2+</sup> , Cu <sup>2+</sup>	Zn <sup>2+</sup> : $1.8 \times 10^{-6}$ Cu <sup>2+</sup> : $2.3 \times 10^{-7}$	live cell imaging	No	7
4	DMSO:water (1:1)	Zn <sup>2+</sup> , Cu <sup>2+</sup>	Zn <sup>2+</sup> : $3.5 \times 10^{-8}$ Cu <sup>2+</sup> : $1.46 \times 10^{-6}$	Logic gates, live cell imaging	Yes	8
5	DMSO/H <sub>2</sub> O (4:1, v/v)	Zn <sup>2+</sup> , Cu <sup>2+</sup>	Zn <sup>2+</sup> : $6.8 \times 10^{-8}$ Cu <sup>2+</sup> : $2.3 \times 10^{-8}$	Logic gates	No	9
6	HEPES Buffer	Zn <sup>2+</sup> , Cu <sup>2+</sup>	Zn <sup>2+</sup> : $2.29 \times 10^{-9}$ Cu <sup>2+</sup> : $3.67 \times 10^{-9}$	Logic gates, live cell imaging	Yes	10
7	HEPES Buffer	Zn <sup>2+</sup> , Cu <sup>2+</sup>	Zn <sup>2+</sup> : $13.2 \times 10^{-9}$ Cu <sup>2+</sup> : $4.1 \times 10^{-9}$	Logic gates, live cell imaging	No	11
8	EtOH: H <sub>2</sub> O (1:99)	Zn <sup>2+</sup> , Cu <sup>2+</sup>	Zn <sup>2+</sup> : $72 \times 10^{-9}$ Cu <sup>2+</sup> : $141 \times 10^{-9}$	Logic gates, live cell imaging	Yes	12
9	DMF:H <sub>2</sub> O (7:3, pH 7.4) HEPES	Zn <sup>2+</sup> , Cu <sup>2+</sup>	Zn <sup>2+</sup> : $3.49 \times 10^{-9}$ Cu <sup>2+</sup> : $5.36 \times 10^{-9}$	Logic gates, live cell imaging, mitotracking	Yes	This Work

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