Electronic Supplementary Material (ESI) for RSC Advances.

Supporting information for

A highly efficient and selective coumarin based fluorescent probe for colorimetric detection of Fe^{3+} and fluorescence dual sensing of Zn^{2+} and Cu^{2+}

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Figure Captions:

Figure S1: Plot of log $((I-I_o) / (I_{max}-I))$ versus log $[M^{2+}]$ for titration of Zn^{2+} (a) and Cu^{2+} (b) with $\mathbf{H_{12}L}$ in CH_3OH/H_2O (40:60, v/v) solution indicating 1:1 complex formation.

Figure S2: Fluorescence emission spectra of $\mathbf{H_{12}L}$ in complexes with different substituents; **1**-ligand (free ion) and complexes (**2**-$Zn(SO_4)_2$, **3**-$Zn(NO_3)_2$, **4**-$Zn(CH_3COO)_2$, **5**-$ZnCl_2$ and **6**-$Zn(CO_3)$) in the solution phase at room temperature, respectively.

Figure S3: Fluorescence emission spectra of $\mathbf{H_{12}L}$ (1.5 x 10^{-4} M) in presence of Zn^{2+} ion (45μM) or EDTA (35μM) in CH_3OH/H_2O (40:60, v/v) solution at room temperature. Excitation was done at λ_{exc}= 370 nm.

Figure S4: Reversible changes in fluorescence intensity of $\mathbf{H_{12}L}$ at 484 nm after subsequent addition of Cu^{2+} and EDTA

Figure S5: ^1H NMR titration plot of $\mathbf{H_{12}L}$ **(1)** with Zn^{2+} (**2** = 0.25 eq., **3** = 0.50 eq. and **4** = 1.0 eq. of Zn^{2+}) ion in DMSO-d_6 solvent.

Figure S6: ^1H NMR titration plot of $\mathbf{H_{12}L}$ in different pH. Different pH values are: (**1**) 5.5, (**2**) 6.0, (**3**) 7.0, (**4**) 8.0, (**5**) 9.0, (**6**) 9.5 and (**7**) 10.0.

Figure S7: Fluorescence response of $\mathbf{H_{12}L}$ in presence of Cu^{2+} with different concentrations at different time. The concentrations of Cu^{2+} (μM) are: (i) 10.0, (ii) 20.0 and (iii) 35.0, respectively.

Figure S8: Truth table and the monomolecular circuit based on (a) Zn^{2+} and Cu^{2+} and (b) Zn^{2+} with EDTA and EDTA with Cu^{2+}.

Figure S9: DFT evaluated 3D isosurface HOMO and LUMO diagrams of $\mathbf{H_{12}L}$, $H_{12}L$-Zn^{2+} and $H_{12}L$-Cu^{2+} complexes, respectively.

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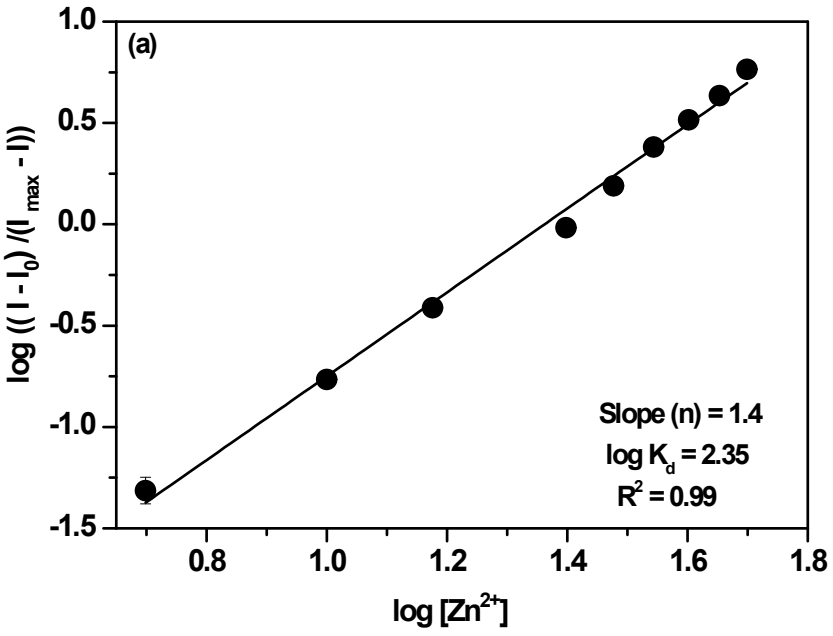

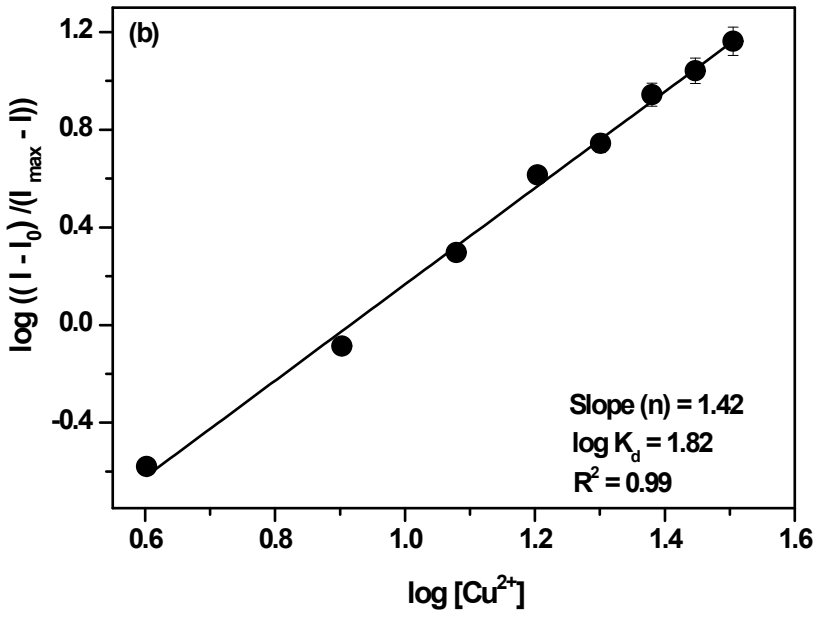

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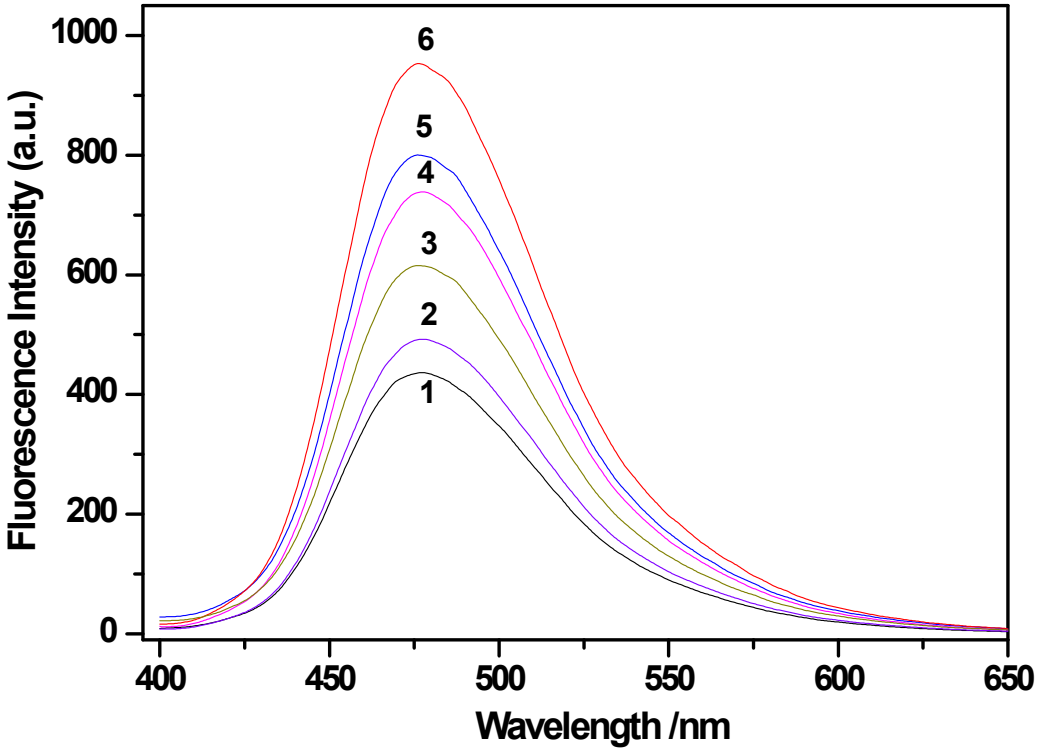

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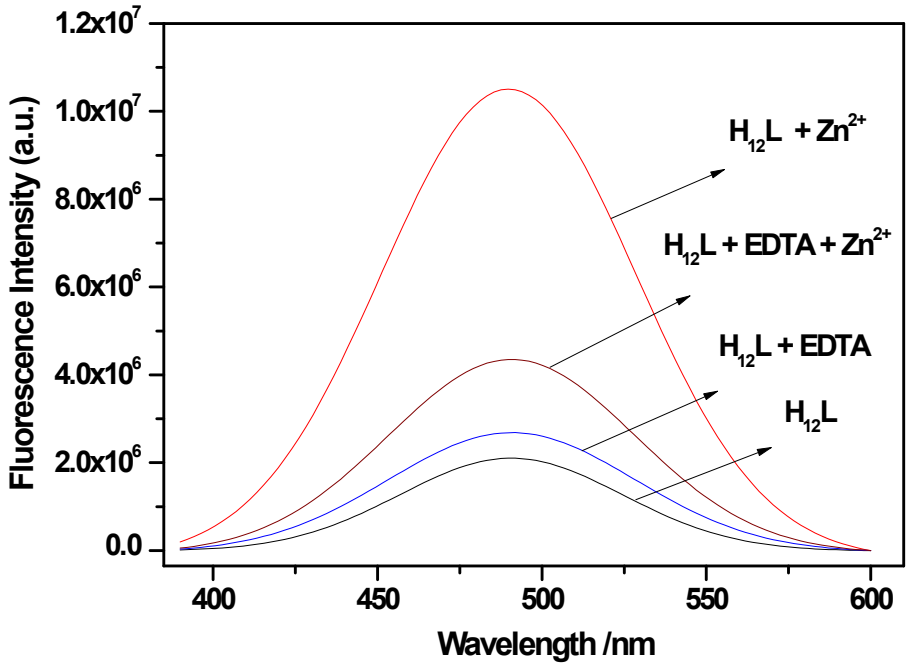

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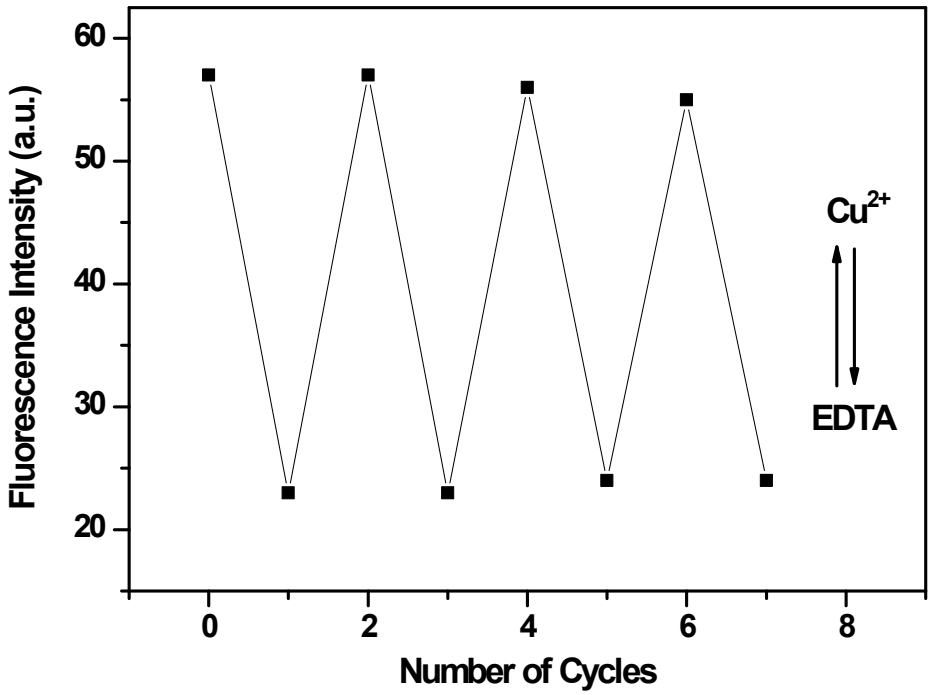

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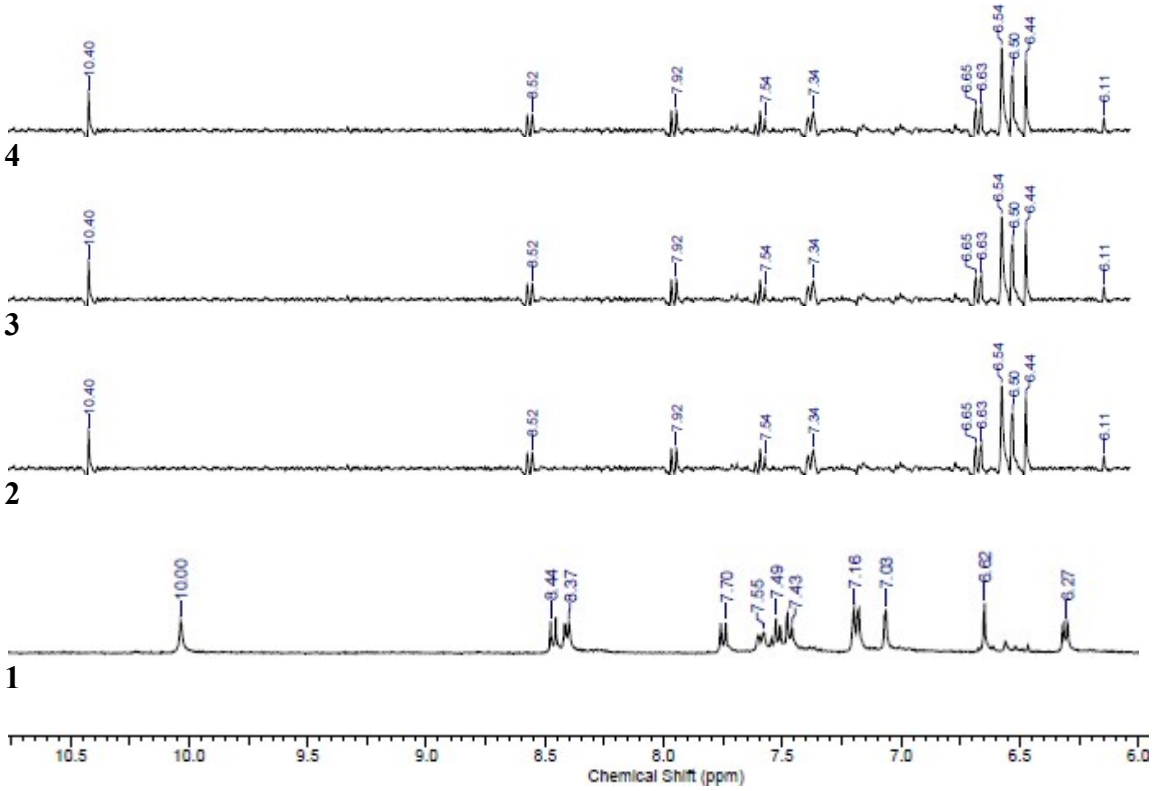

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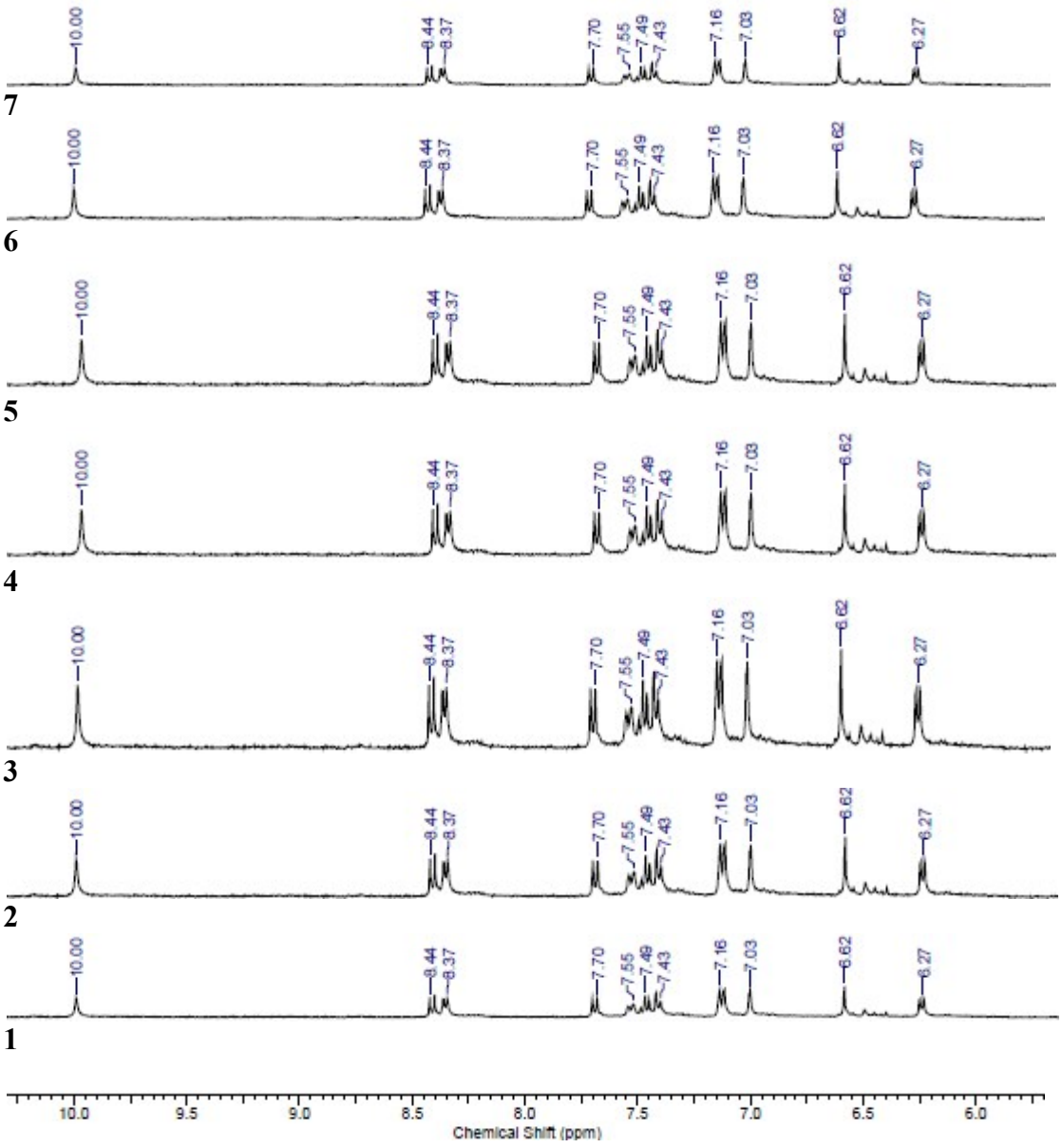

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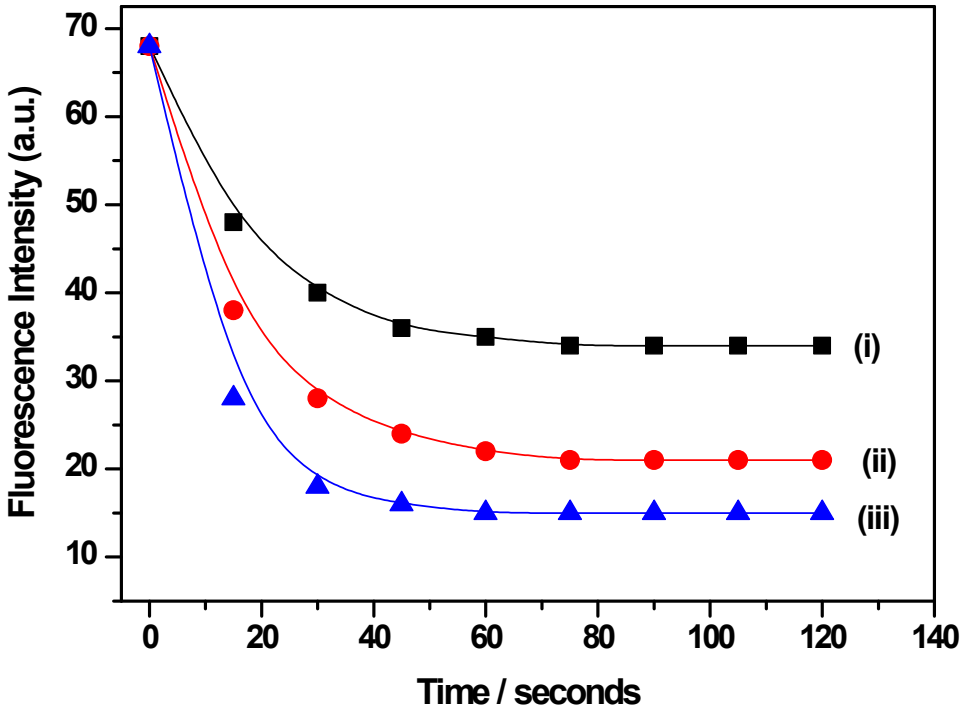
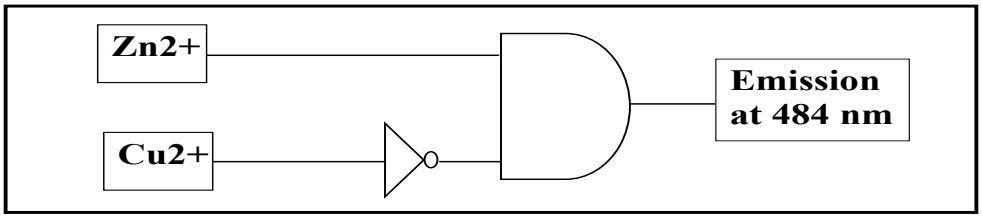


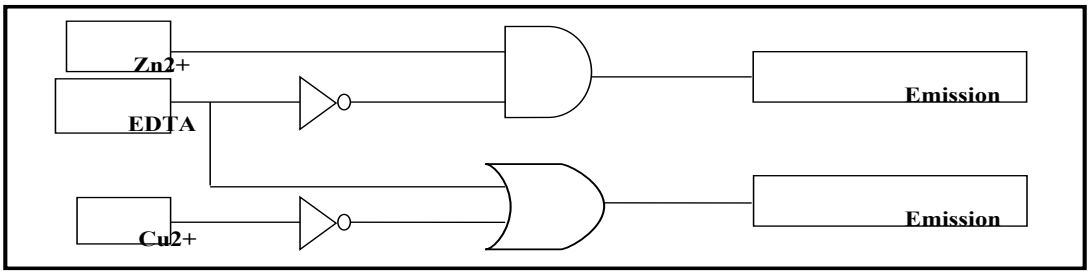
Figure S8: Truth table and the monomolecular circuit based on (a) Zn^{2+} and Cu^{2+} and (b) Zn^{2+} with EDTA and EDTA with Cu^{2+}.

INPUT		OUTPUT
IN1	**IN2**	**OUT**
Zn^{2+}	**Cu^{2+}**	**Emission at 484 nm**
0	0	0 (low)
0	1	0 (low)
1	0	1 (high)
1	1	0 (low)



(a) Zn^{2+} and Cu^{2+}

INPUT		OUTPUT
IN1	**IN2**	**OUT**
Zn^{2+}	**EDTA**	**Emission at 484 nm**
0	0	0 (low)
0	1	0 (low)
1	0	1 (high)
1	1	0 (low)
INPUT		**OUTPUT**
IN1	**IN2**	**OUT**
Cu^{2+}	**EDTA**	**Emission at 484 nm**
0	0	1 (high)
0	1	1 (high)
1	0	0 (low)
1	1	1 (high)



(b) Zn^{2+} with EDTA and EDTA with Cu^{2+}

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