

Supporting Information

A γ -turn mimetic for selective sensing of Cu(II) and combinatorial multiple logic gate

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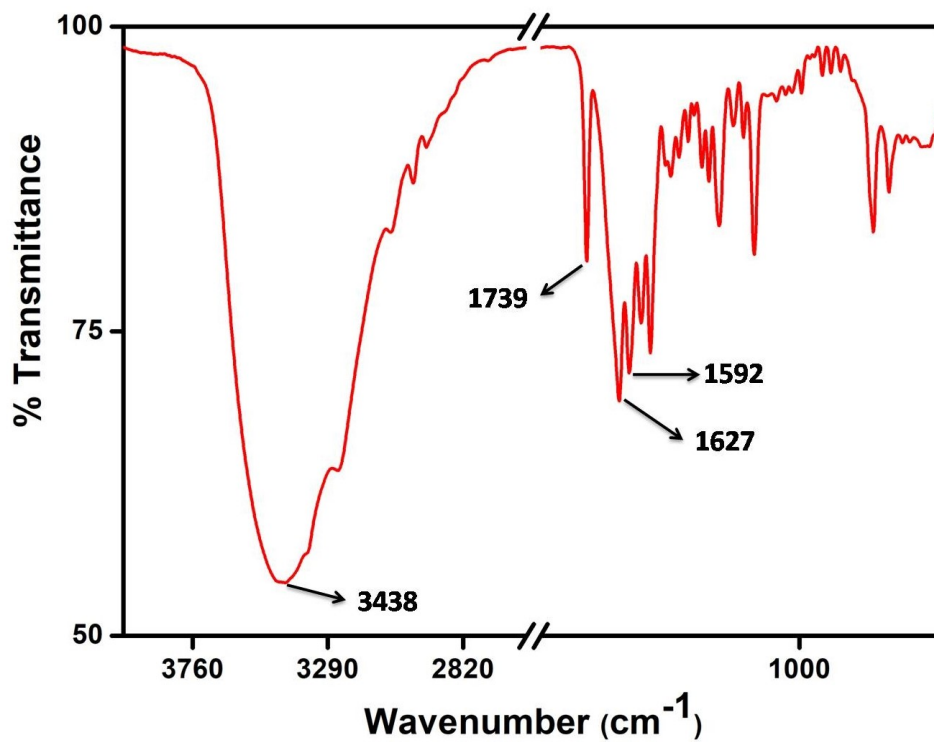


Figure S1: Solid- state FT-IR spectra of γ -turn mimetic **1**.

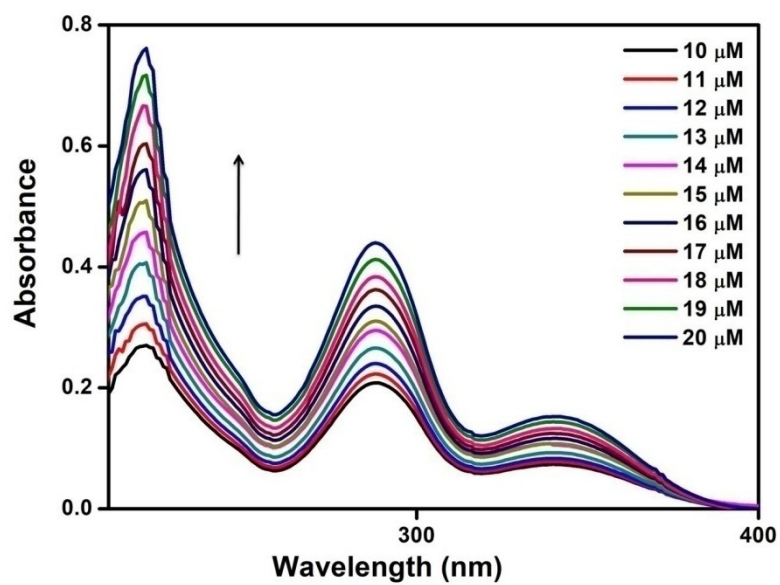


Figure S2: Concentration dependent UV-Vis spectra of γ -turn mimetic **1** in acetonitrile.

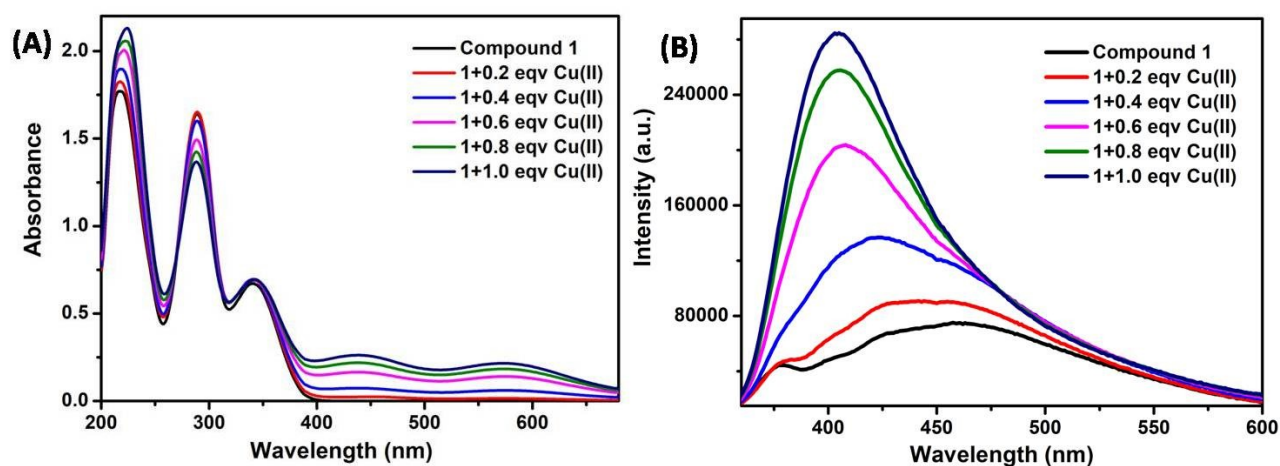


Figure S3: Change in (A) Absorption spectra and (B) Fluorescence spectra of γ -turn mimetic **1** ($c = 1.0 \times 10^{-4}$ M) upon addition of different concentration of Cu (II) salt in acetonitrile solution. (Excitation Wavelength = 340 nm)

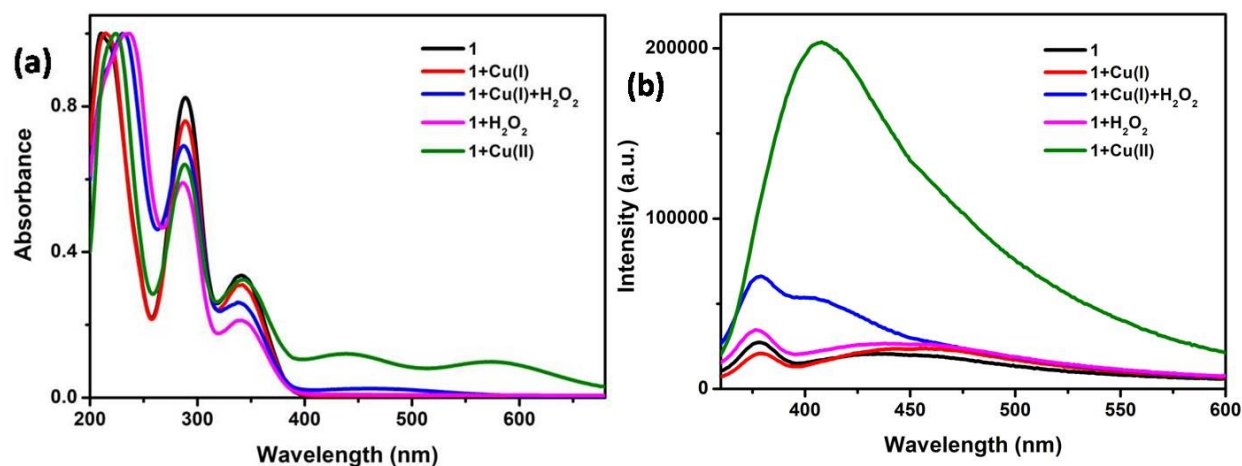


Figure S4: (a) Absorption and (b) Emission spectra of γ -turn mimetic **1** ($c = 1.0 \times 10^{-4}$ M) in the presence of Cu (II), Cu (I), H₂O₂ and a mixture of Cu (I) and H₂O₂ ($c = 1.0 \times 10^{-2}$ M) in acetonitrile solution. (Excitation Wavelength = 340 nm)

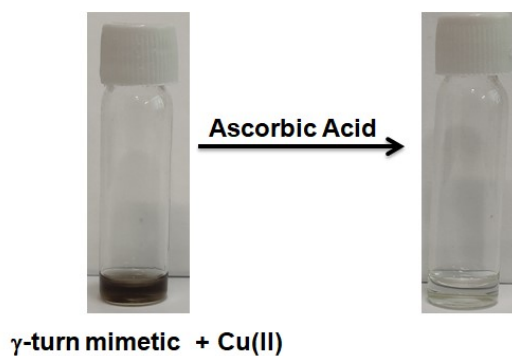


Figure S5: (a) Colour of γ -turn mimetic **1** ($c = 1.0 \times 10^{-4}$ M) in the presence of Cu (II) in acetonitrile solution and after addition of ascorbic acid ($c = 4.0 \times 10^{-4}$ M).

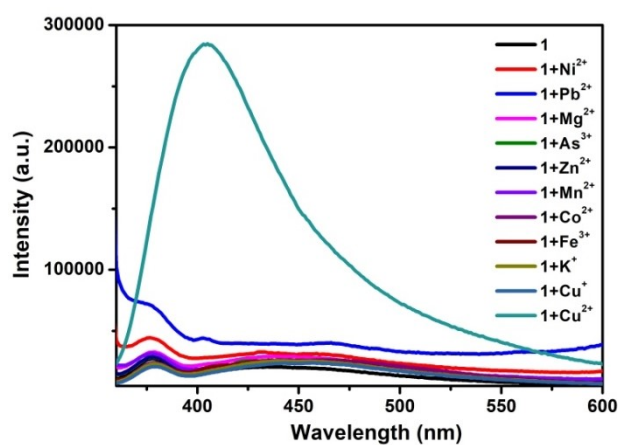
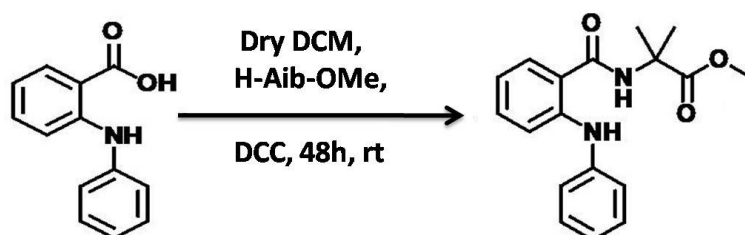


Figure S6: Emission spectra of γ -turn mimetic **1** ($c = 1.0 \times 10^{-4}$ M) in the presence of different metals in acetonitrile solution. (Excitation Wavelength = 340 nm)

Formula	C ₁₈ H ₂₀ N ₂ O ₃
Formula Weight	312.36
Crystal System	monoclinic
Space group	P2 ₁ /c
a, b, c [Angstrom]	16.8282(6), 10.4619(4), 9.5748(4)
alpha, beta, gamma [deg]	90, 100.788(4), 90
V [Ang**3]	1655.90(11)
Z	4
D(calc) [g/cm**3]	1.253
Mu(MoKa) [/mm]	0.086
F(000)	664
Crystal Size [mm]	0.01 x 0.02 x 0.03
Data Collection Temperature (K)	293
Radiation [Angstrom] MoKa	0.71073
Theta Min-Max [Deg]	2.3, 25.0
Dataset	20: 19 ; -12: 11 ; -11: 10
Tot., Uniq. Data, R(int)	8501, 2918, 0.048
Observed Data [I > 0.0 sigma(I)]	2455
Refinement Nref, Npar	2918, 211
R, wR2, S	0.0443, 0.1128, 1.10

Table S1: Crystal data and structure refinement of γ -turn mimetic **1**.

Synthesis of γ -turn mimetic **1:**



Scheme 1: The schematic representation for the synthesis of γ -turn mimetic **1**.

For concentration dependent absorption and emission spectroscopy study, 10^{-5} (M) γ -turn mimetic 1 solution was prepared in acetonitrile and then concentration increases gradually by addition of 10^{-3} (M) concentrated solution and every time the UV-Vis spectra was measured. For metal detection study, 10^{-4} (M) γ -turn mimetic 1 solution was prepared in acetonitrile and different metals have used in 1:1 equivalent and then the fluorescence and UV-Vis experiment were performed.

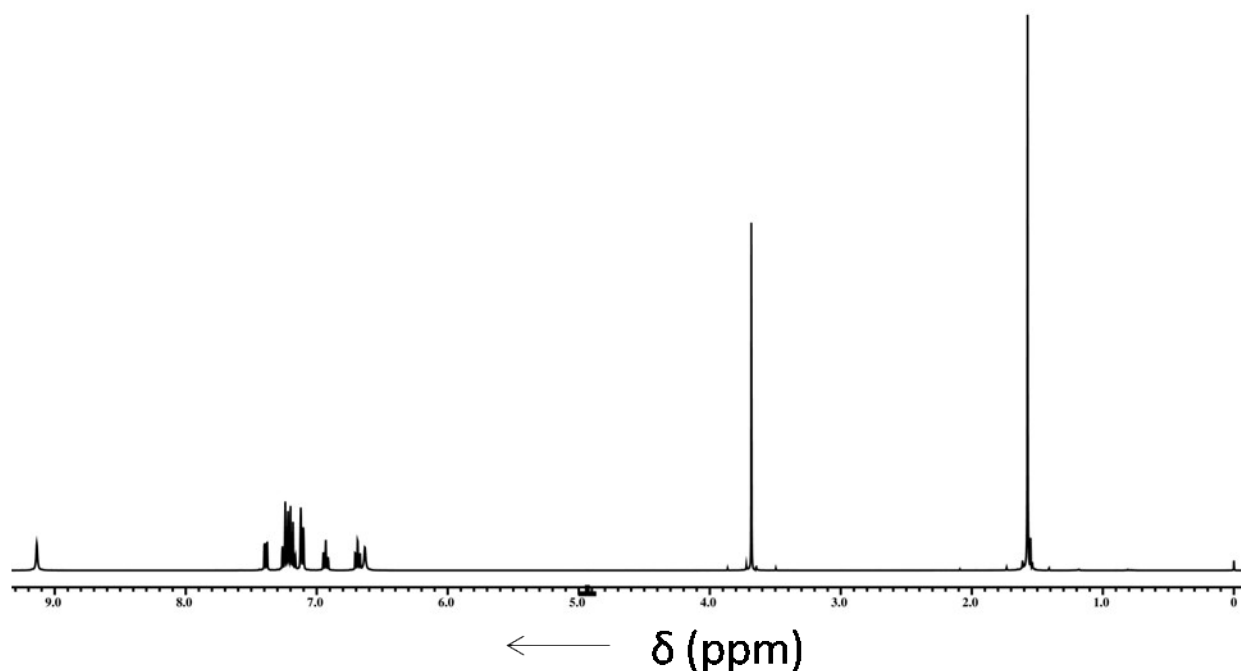


Figure S7: ^1H NMR spectra (400 MHz, CDCl_3 , δ ppm, 298K) of γ -turn mimetic 1.

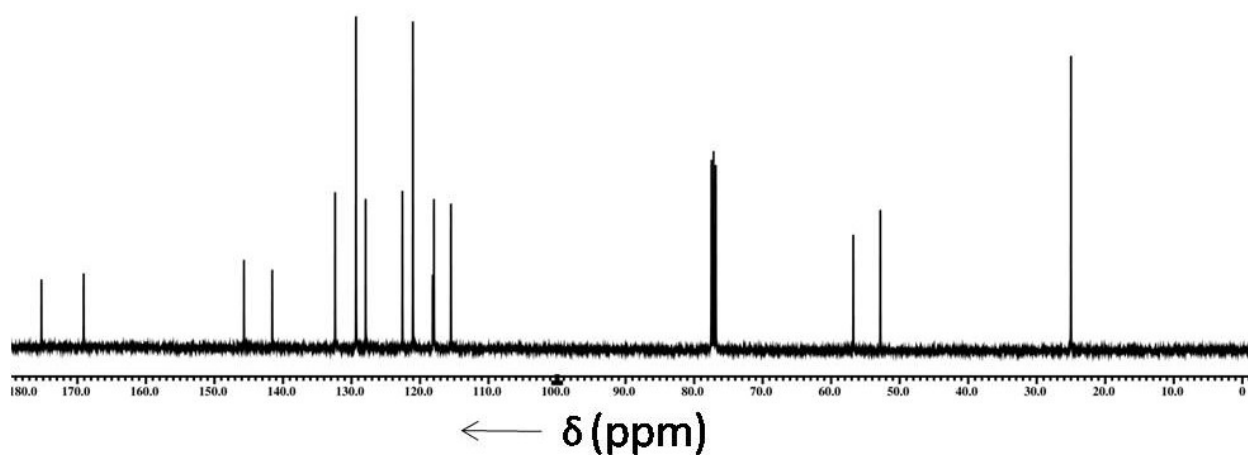


Figure S8: ^{13}C NMR spectra (100 MHz, CDCl_3 , δ ppm, 298K) of γ -turn mimetic 1.

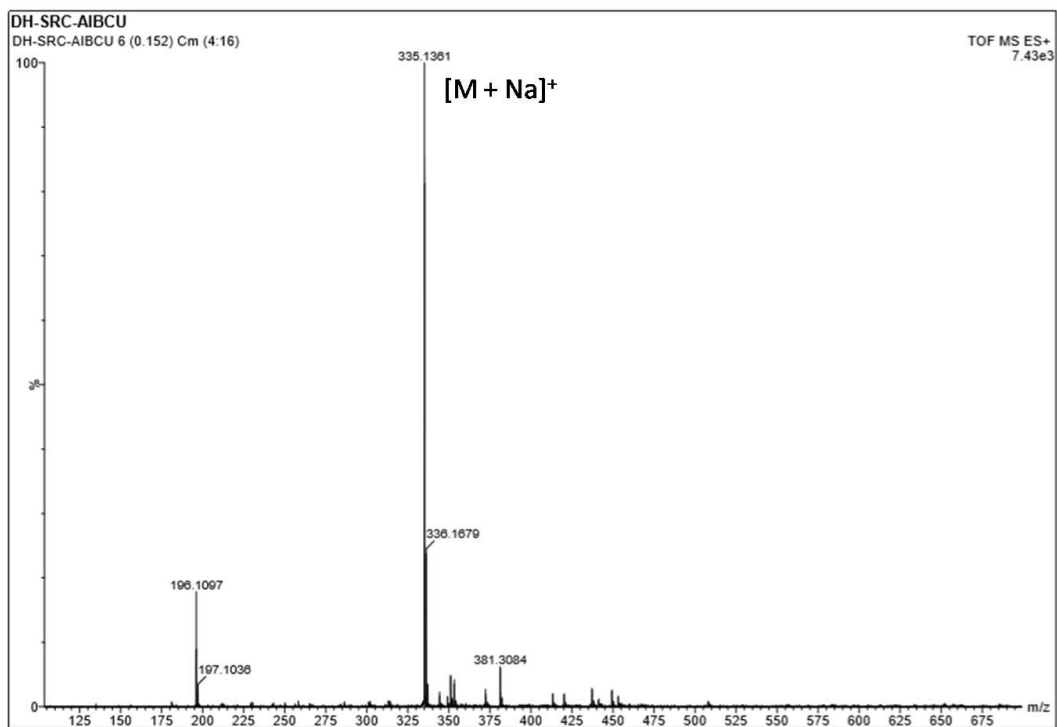


Figure S9: Mass spectra of γ -turn mimetic **1**.