

Supporting Information:

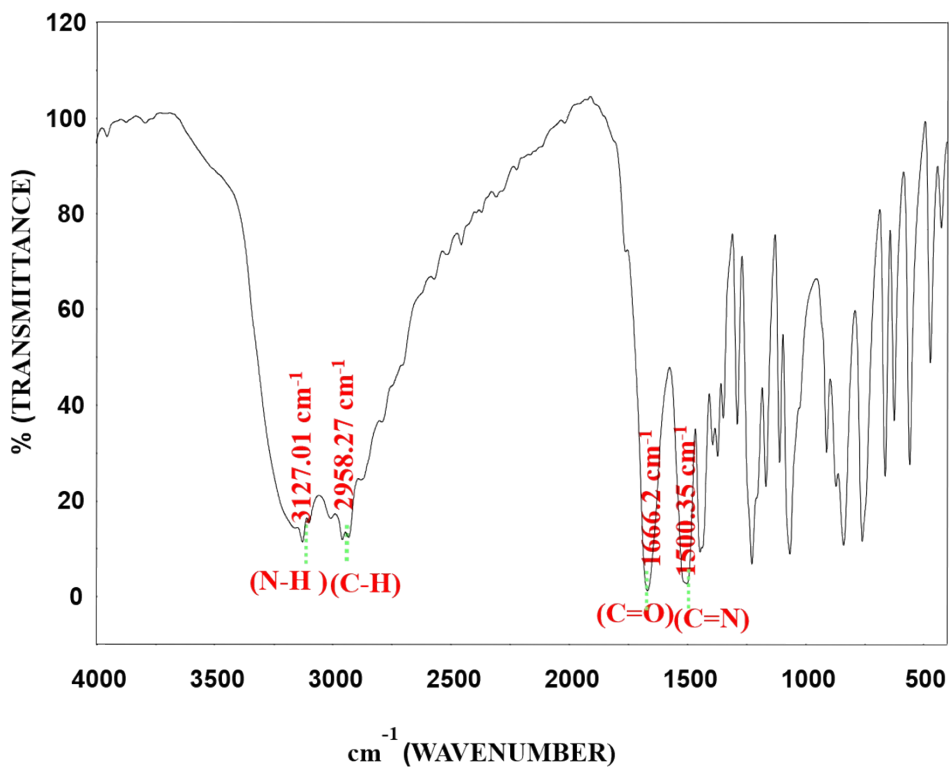


Fig.S1. FT-IR spectrum of OX(PID)₂

Santhosh-1

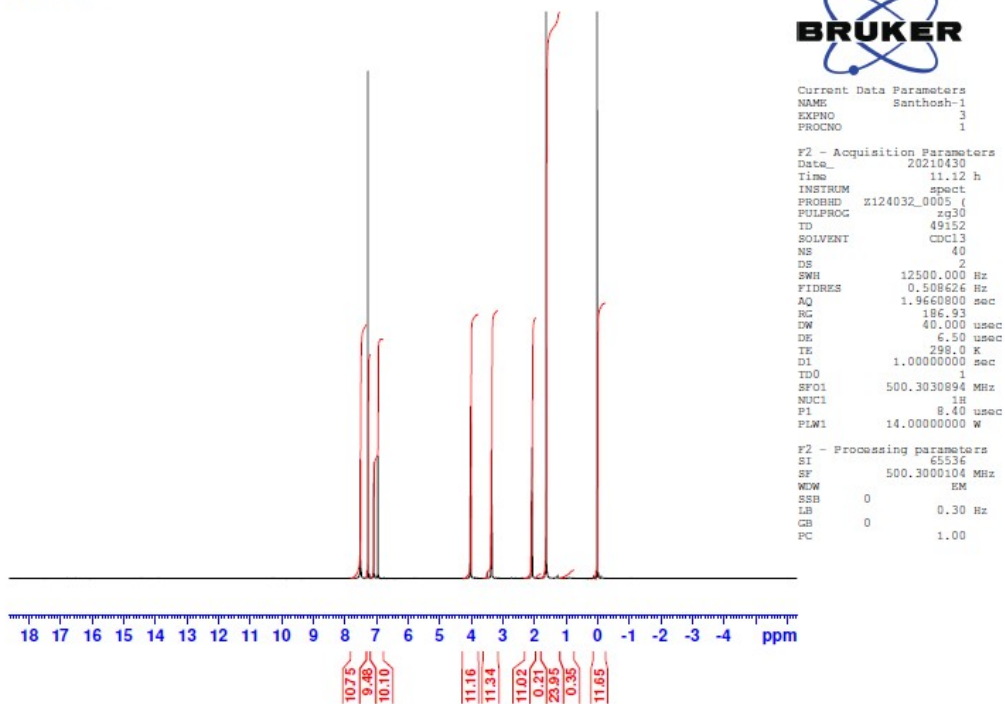
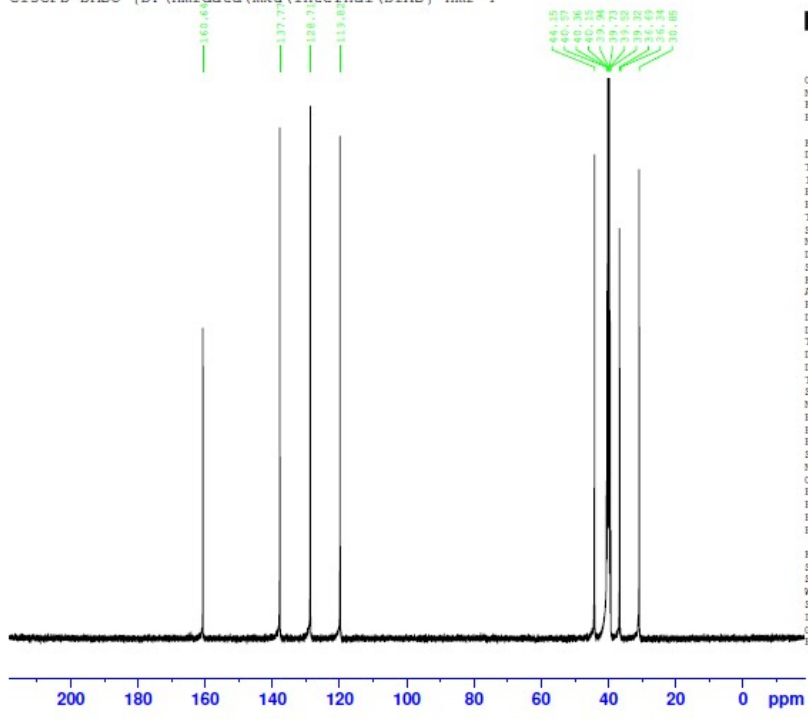


Fig.S2. ¹H NMR spectrum of OX(PID)₂

C13CPD DMSO {D:\nmrdata\mku\Internal\DrAS} nmr 4



Current Data Parameters
NAME 13C (X(PID)2
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20221114
Time 14.18 h
INSTRUM Avance NEO 400MHz
PROBHD z163739_0273 1
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 1024
DS 4
SWH 23809.523 Hz
FIDRES 0.726609 Hz
AQ 1.3762560 sec
RG 52.0123
DW 21.000 usec
DE 6.50 usec
TE 298.1 K
D1 2.0000000 sec
D11 0.0300000 sec
TD0 1
SFO1 100.6255806 MHz
NUC1 13C
P0 2.67 usec
P1 8.00 usec
PLW1 93.98000336 W
SFO2 400.3016012 MHz
NUC2 1H
CPDPRG2 waltz65
PCPD2 90.00 usec
PLW2 24.35899925 W
PLW12 0.19247000 W
PLW13 0.09681000 W

F2 - Processing parameters
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SF 100.62555151 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Fig.S3. ¹³C NMR spectrum of OX(PID)₂

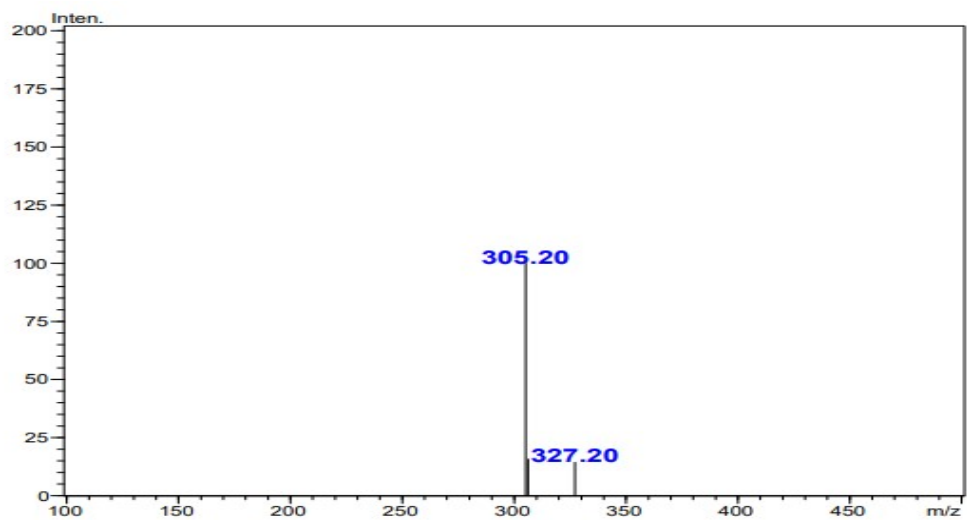


Fig.S4. ESI-Mass spectral data for OX(PID)₂

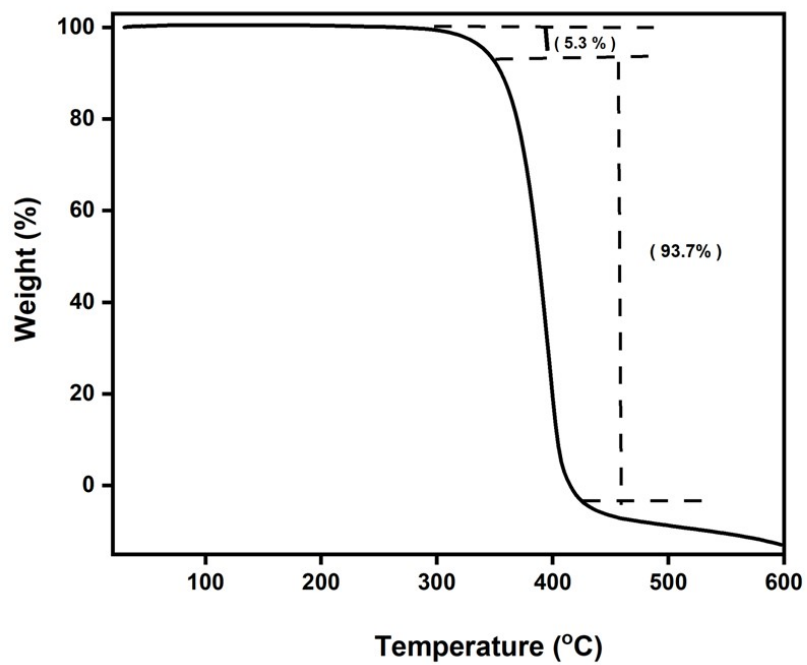


Fig.S5. TGA spectral data for OX(PID)₂

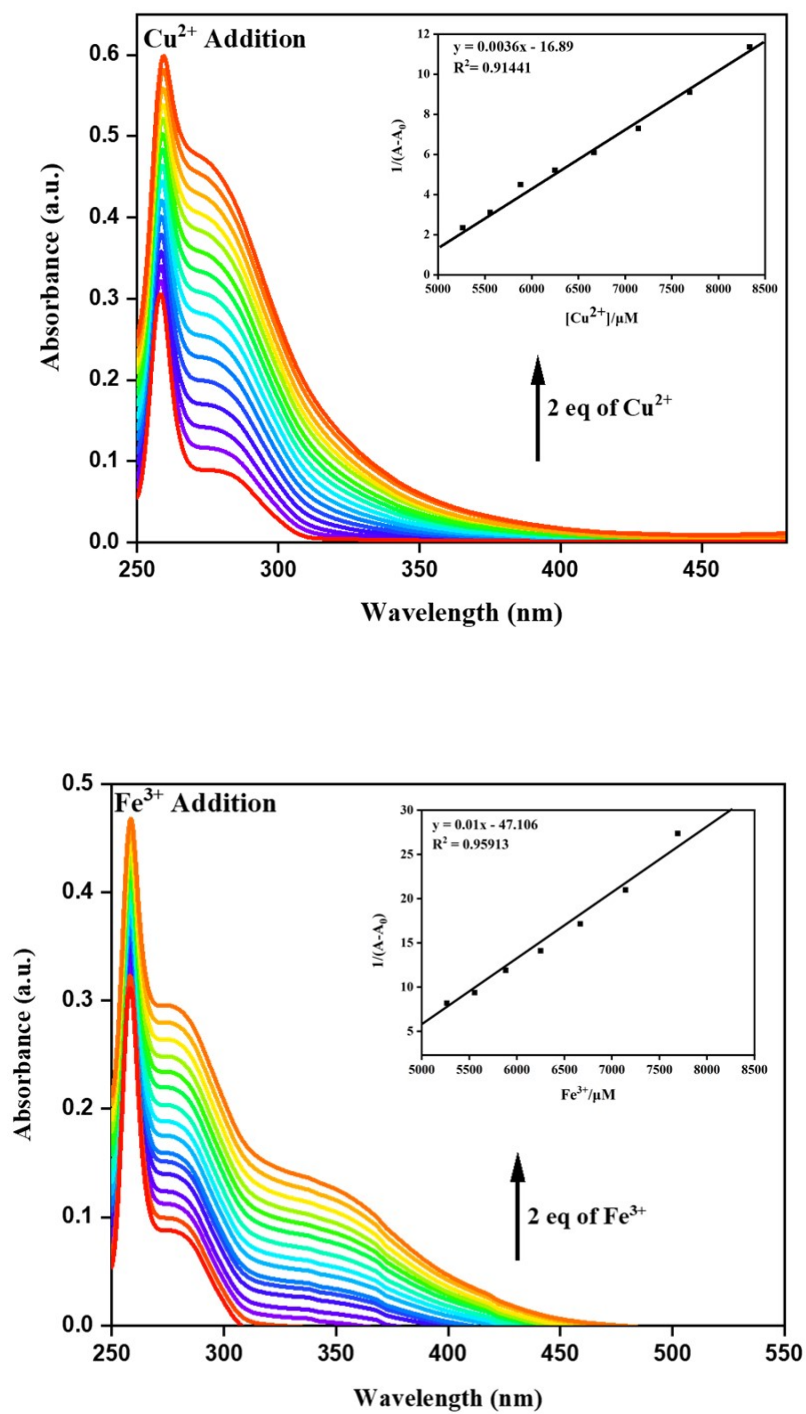


Fig. S6. UV-Vis absorption spectral changes of receptor OX(PID)₂ upon addition of various concentrations of (2 eq of Fe³⁺ and Cu²⁺) ions (2-20 μM).

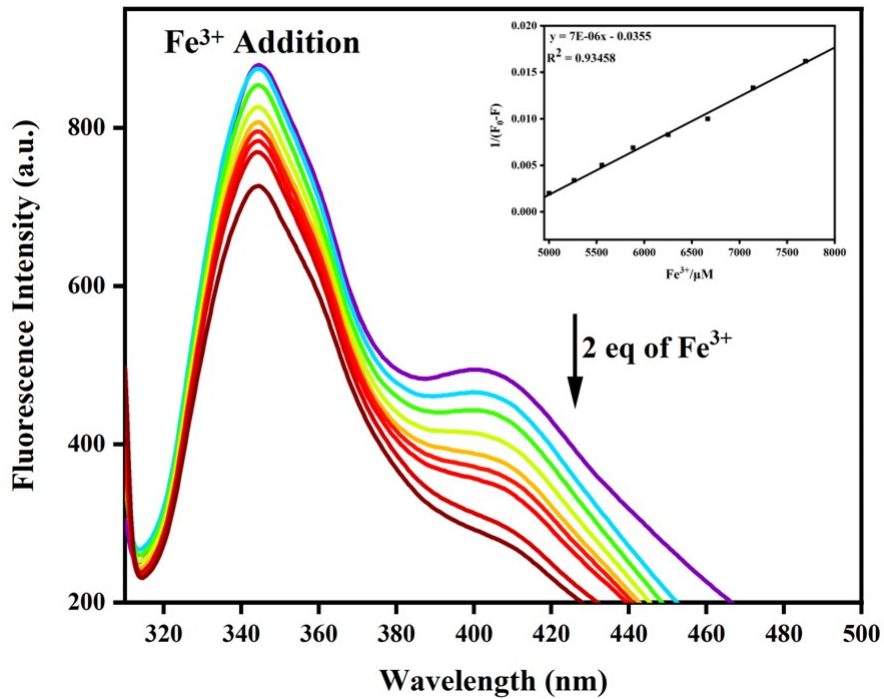
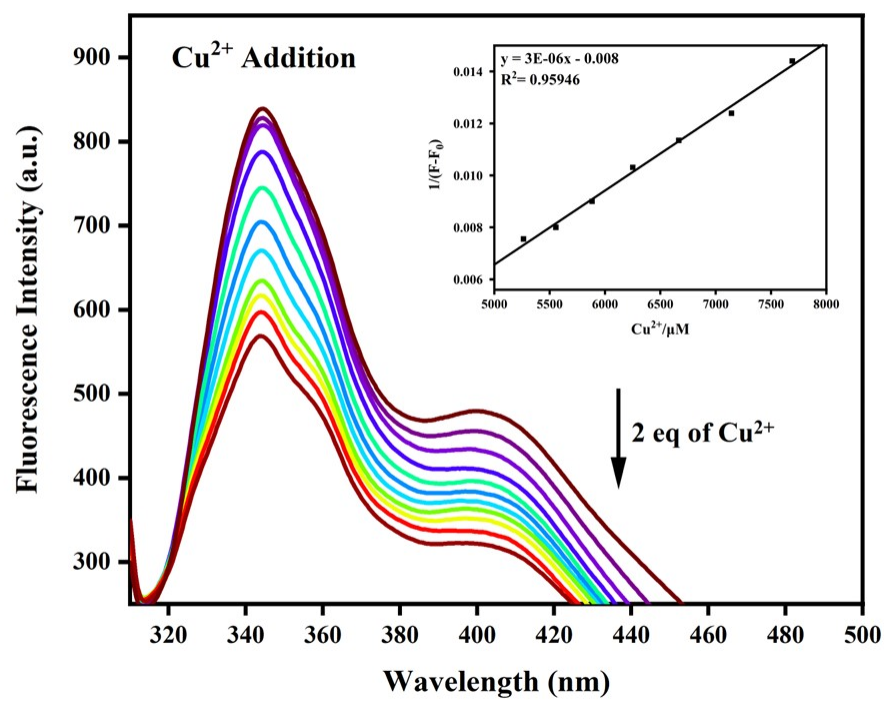


Fig.S7. Fluorescence emission spectra of receptor OX(PID)₂ with increasing concentration of Cu²⁺ and Fe³⁺ (2–20 μM) in DMSO.

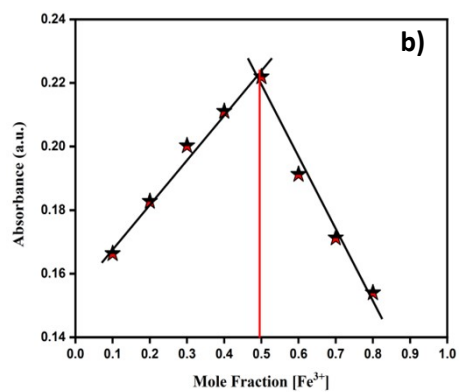
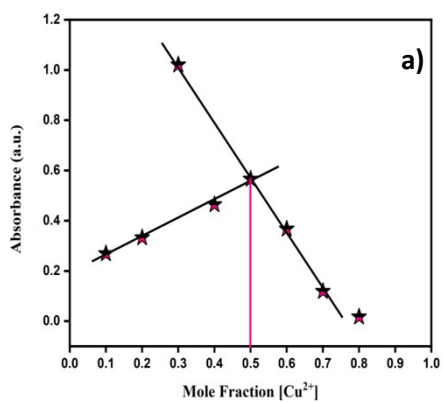


Fig.S8. (a) Job's plot analysis for OX(PID)₂ with Cu²⁺ **(b)** Job's plot analysis for OX(PID)₂ with Fe³⁺ ion

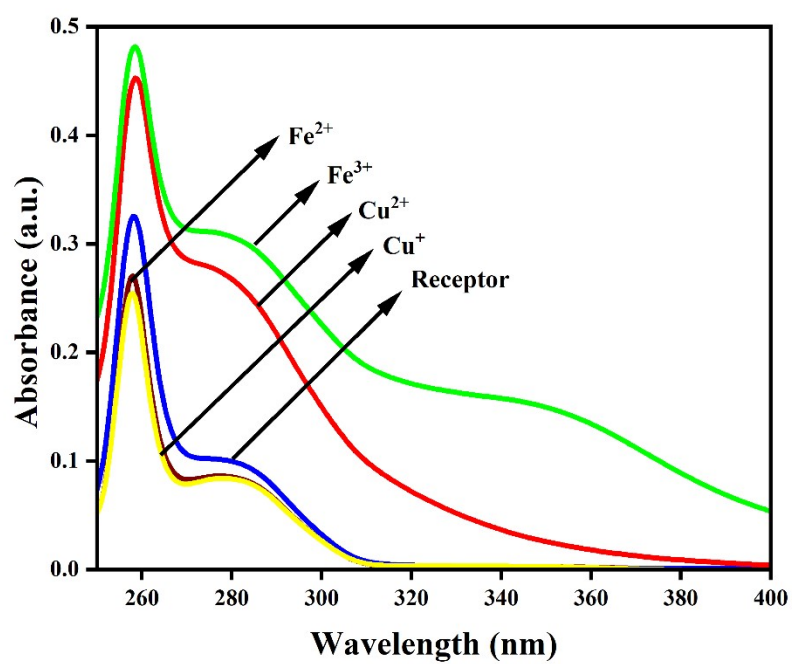
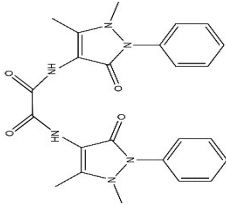
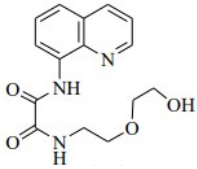
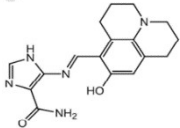
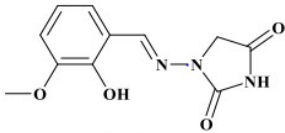
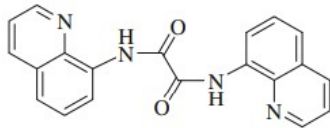
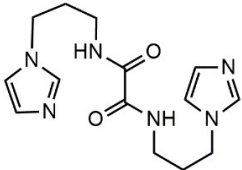


Fig. S9. UV-Vis absorption spectral changes of receptor OX(PID)₂ upon addition of 2 eq of Fe³⁺, Fe²⁺, and Cu⁺, Cu²⁺ ions (20 μM).

Table S1. Comparative binding constants and LODs of oxalamide-based compound

Oxalamide & Imidazole based receptors	Sensing analyte	Binding constant (M ⁻¹)	The detection limit (μM)	References
	Cu ²⁺	2.63 × 10 ³	0.42	31
	Zn ²⁺	2.5 × 10 ⁵	0.02	32
	Fe ²⁺	1.4 × 10 ⁴	0.32	33
	Fe ³⁺	2.8 × 10 ⁴	0.27	
	Cu ²⁺	3.3 × 10 ²	0.91	34
	Zn ²⁺	4.5 × 10 ³	11.9	
	Zn ²⁺	1.5 × 10 ⁴	2.4	35
	Cu ²⁺	2.58 × 10 ³	0.1	This work
	Fe ³⁺	7.15 × 10 ²	0.9	

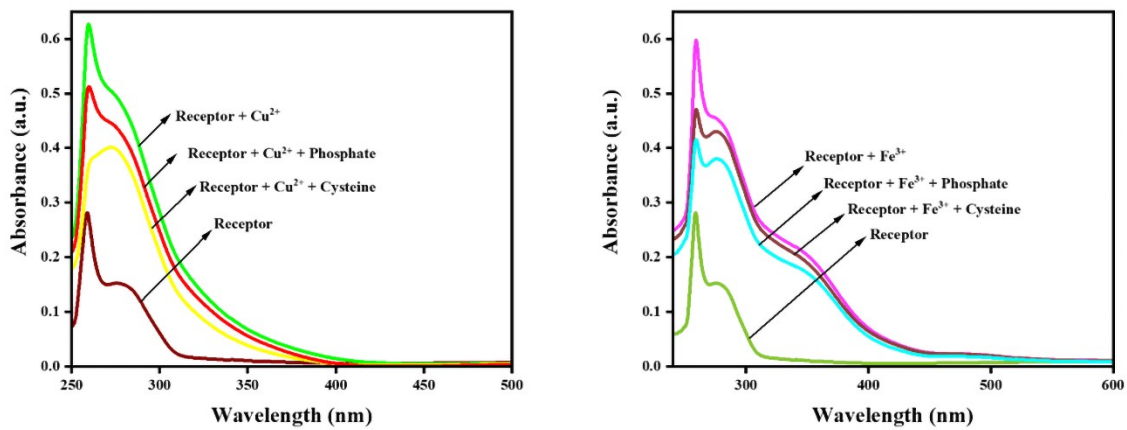


Fig. (S10, S11). Reversibility study for Receptor OX(PID)₂, Cu²⁺, and Fe³⁺ with Cysteine/Phosphate

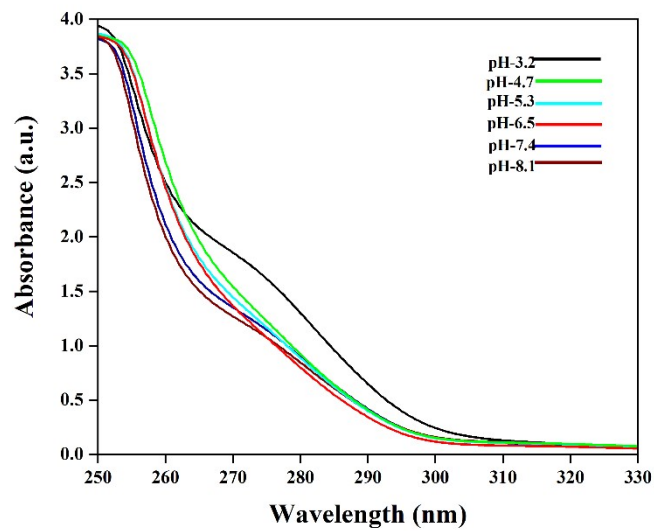


Fig.S12. Effects of pH on the absorbance spectral data of receptor OX(PID)₂ with different pH solutions.

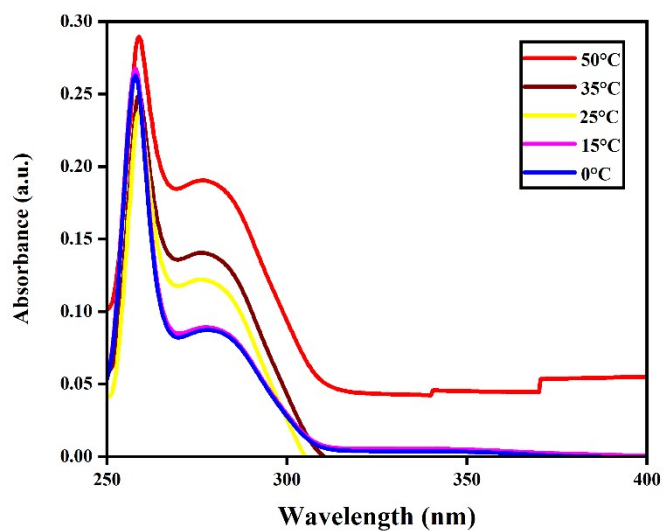


Fig.S13. Effects of temperature on the absorbance spectral data of receptor OX(PID)₂

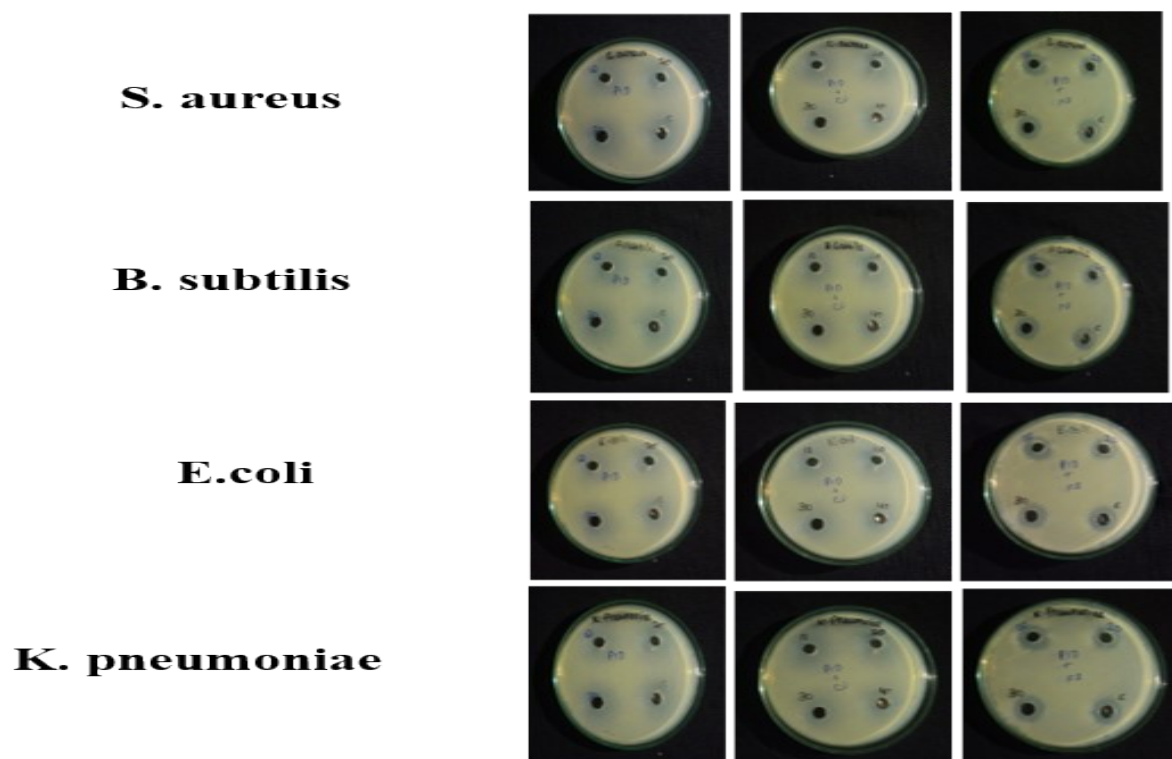


Fig. S14. Antibacterial activities of various concentrations of OX(PID)₂, OX(PID)₂ + Cu²⁺, and OX(PID)₂ + Fe³⁺ against *S. aureus*, *B. subtilis*, *E. coli*, and *K. pneumoniae*.

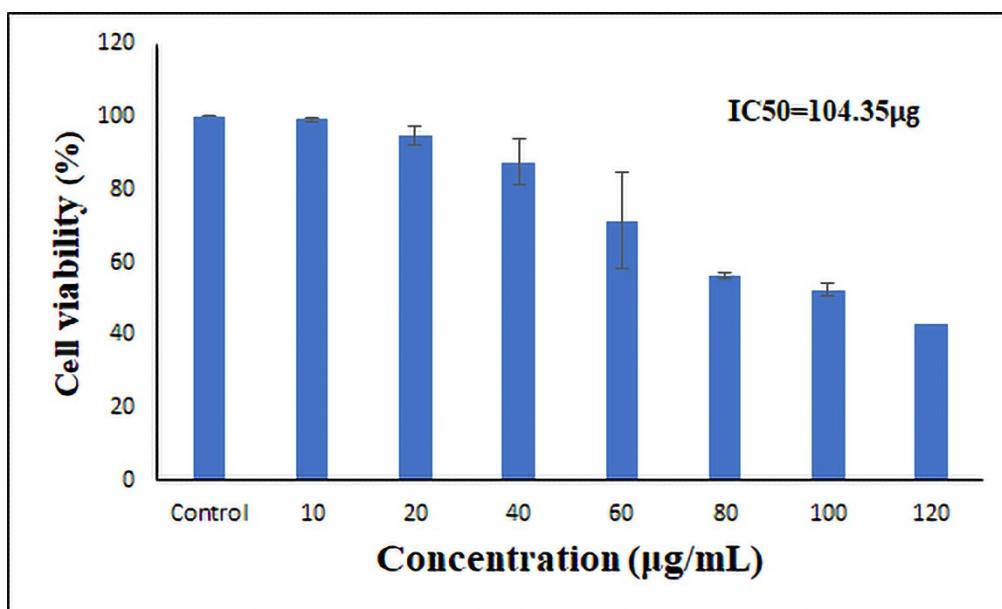


Fig. S15. Cytotoxicity MTT assay for Receptor OX(PID)₂ with MDA-MB-231 cells