Electronic Supplementary Material (ESI) for New Journal of Chemistry.

Mono- and di-ferrocene conjugated 5-methyl benzimidazole based Multi-channel Receptor for Cation/Anion with their Antimicrobial and Anticancer studies

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Supporting information

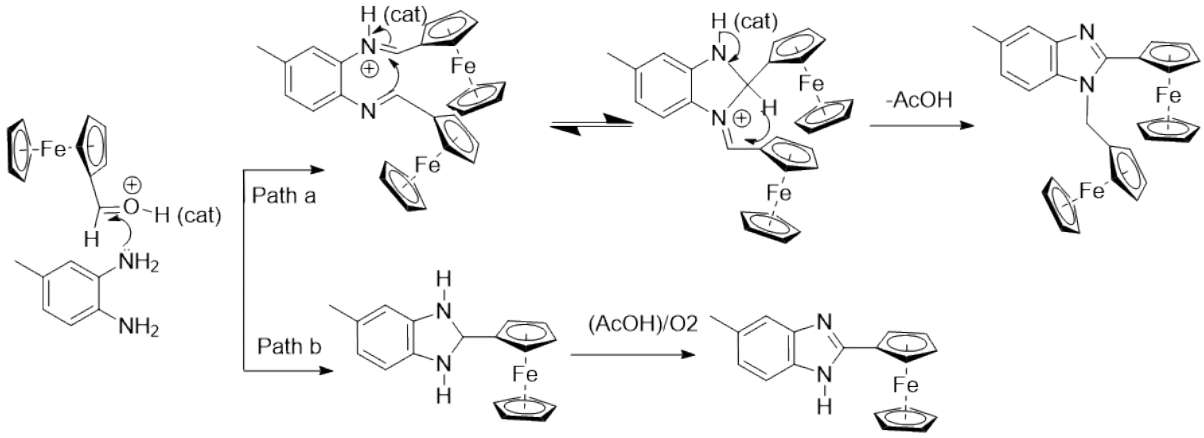

Fig. S1 A plausible mechanism for the synthetic route for the formation of receptors **1** and **2,** where nitrobenzene acts as the solvent and acetic acid (AcOH) the as catalyst.

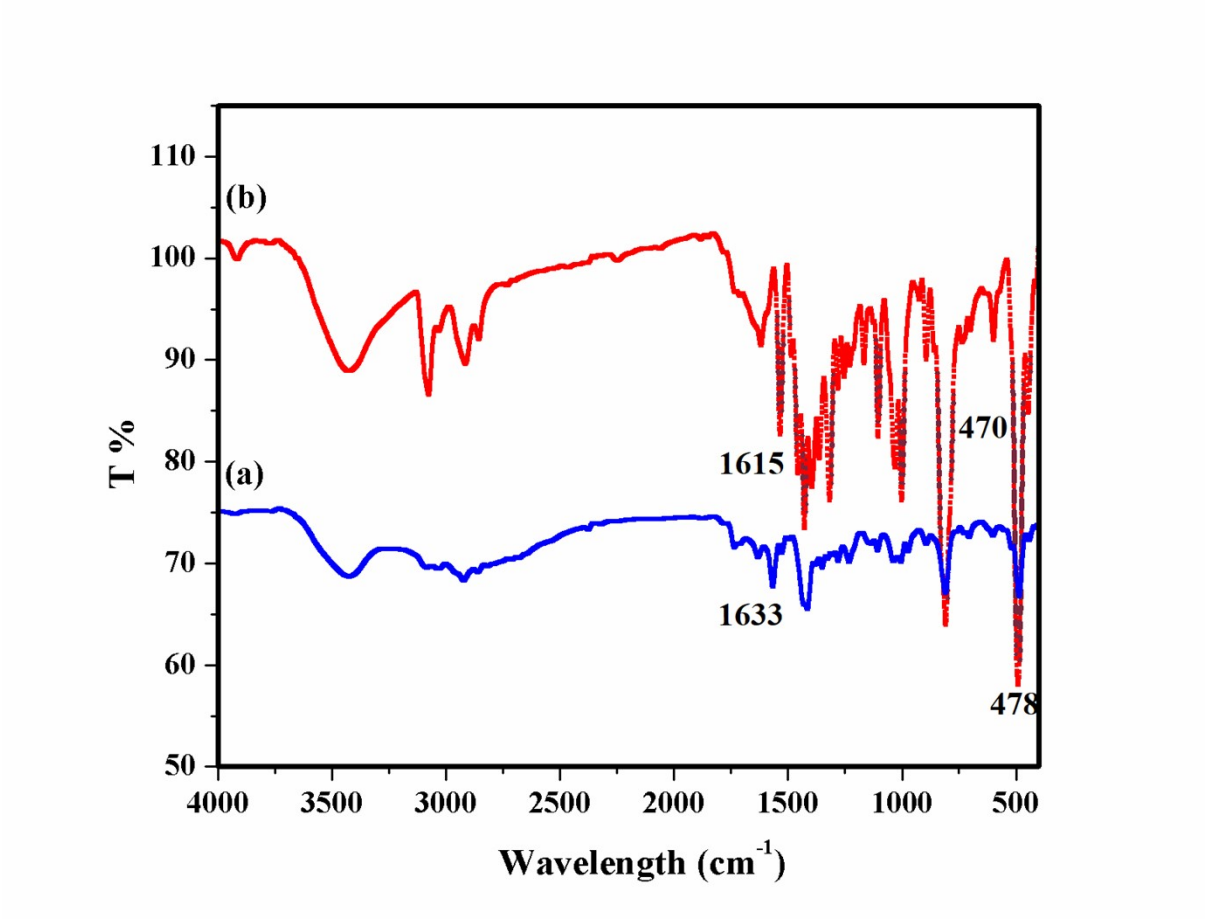

Fig. S2 FT-IR spectra he receptor **1 (a)** and receptor **2 (b)**

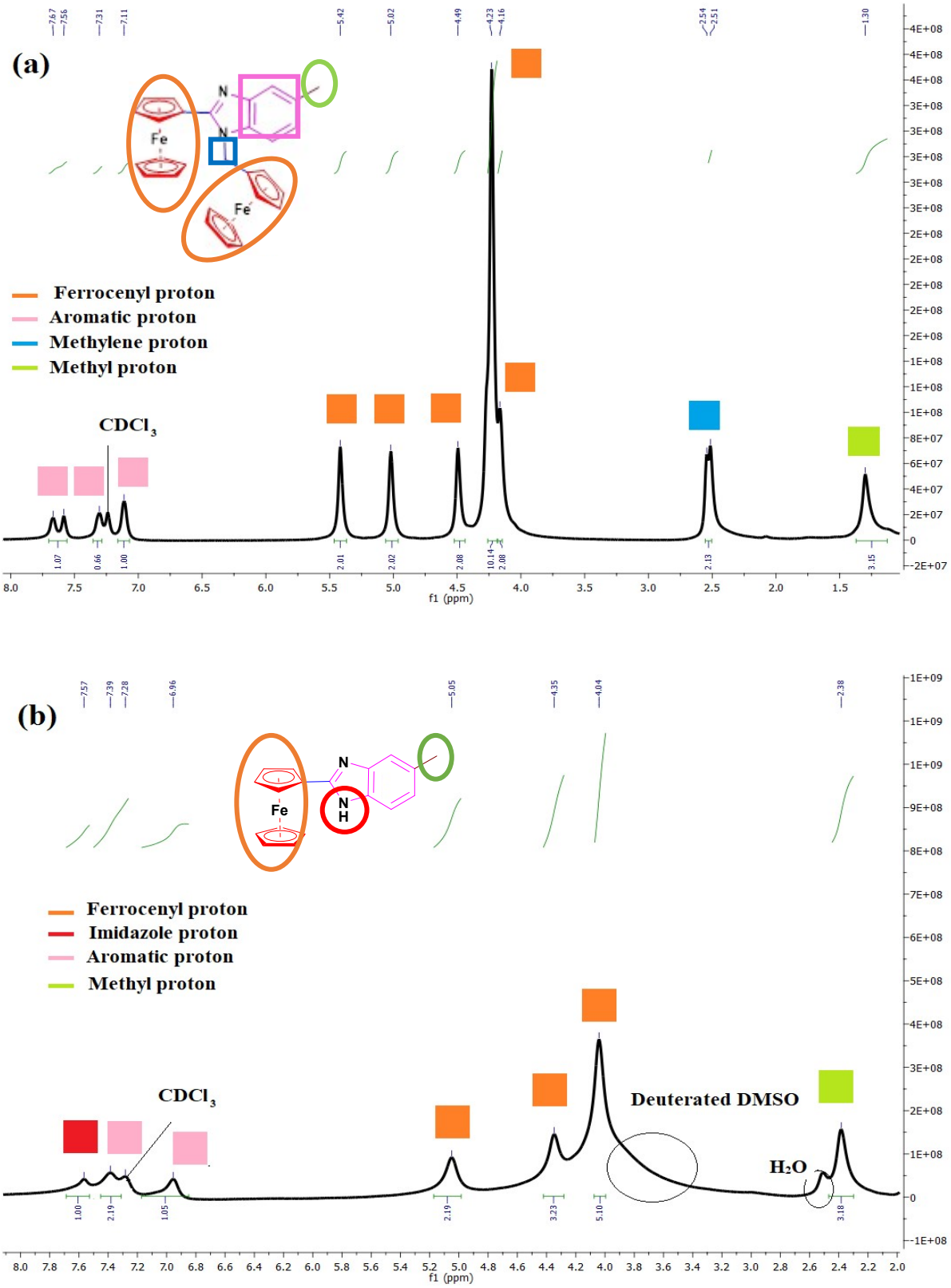

Fig. S3 ^{1}H NMR spectra for the **(a)** receptor **1** and **(b)** receptor **2**

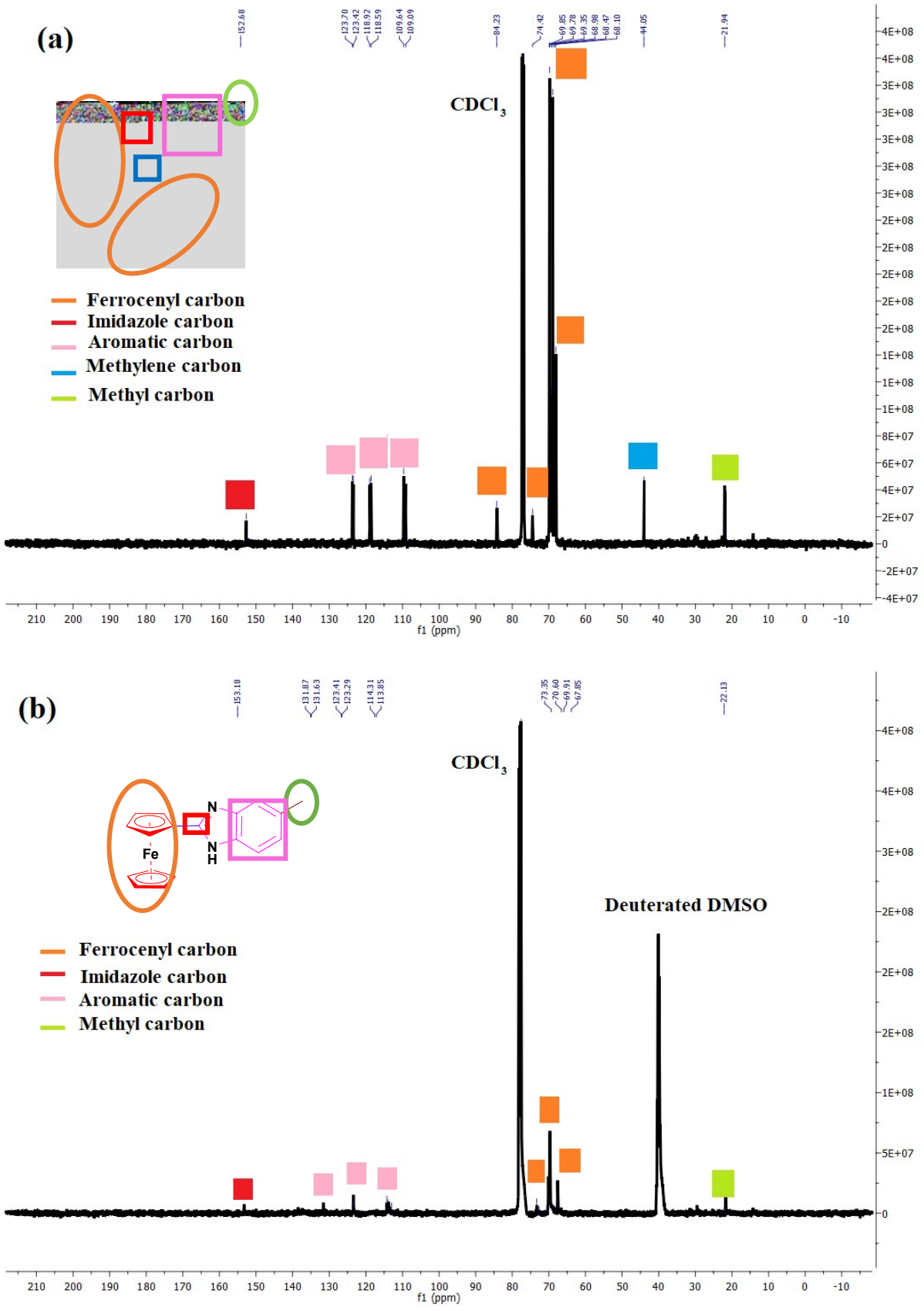

Fig. S4 ^{13}C NMR spectra **(a)** receptor and **(b)** receptor **2**

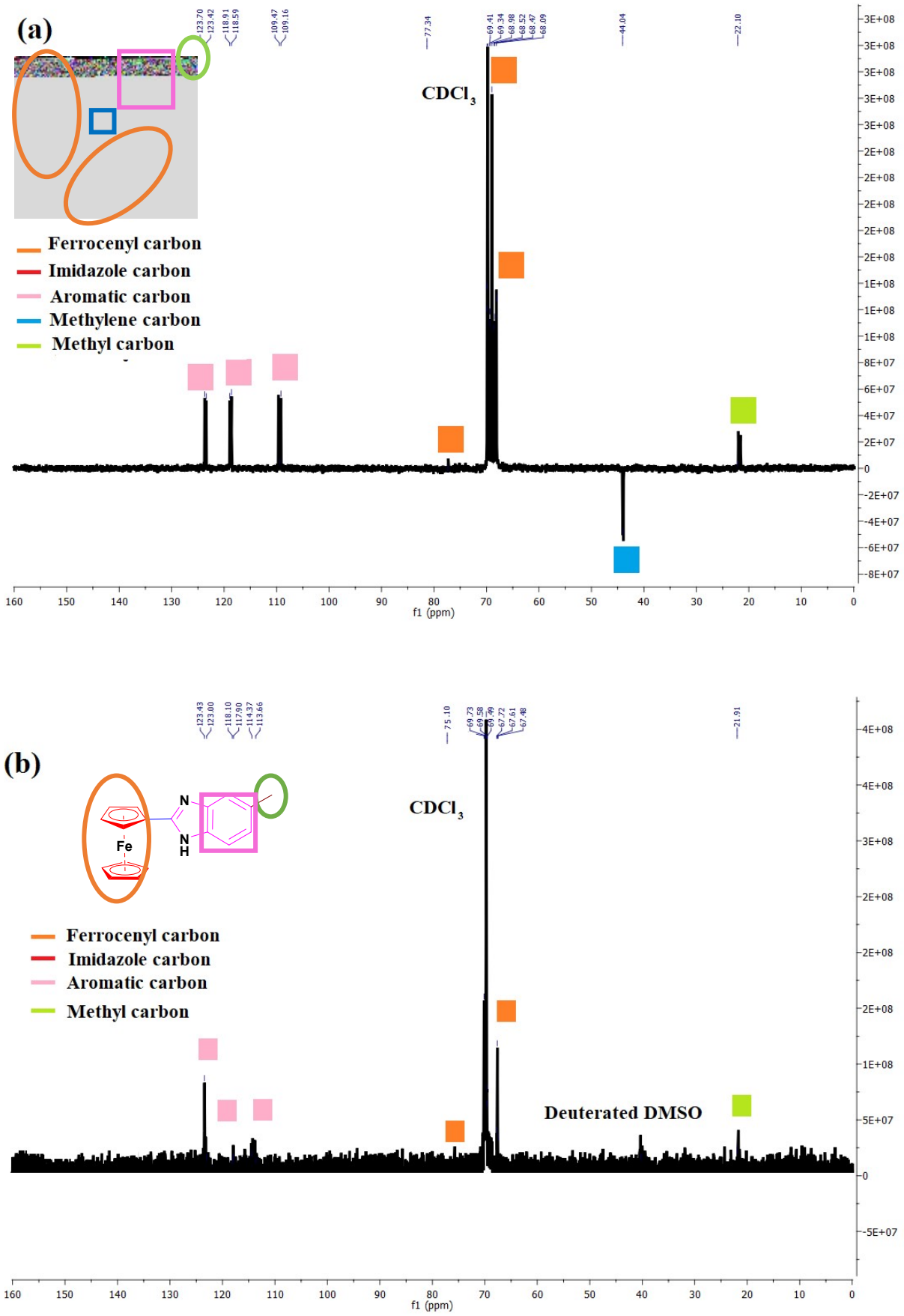

Fig. S5 DEPT 135 NMR spectra **(a)** receptor and **(b)** receptor **2**

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active	Set Capillary	4600 V	Set Dry Heater	180 °C
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Scan End	3000 m/z	Set Collision Cell RF	100.0 Vpp	Set Divert Valve	Waste

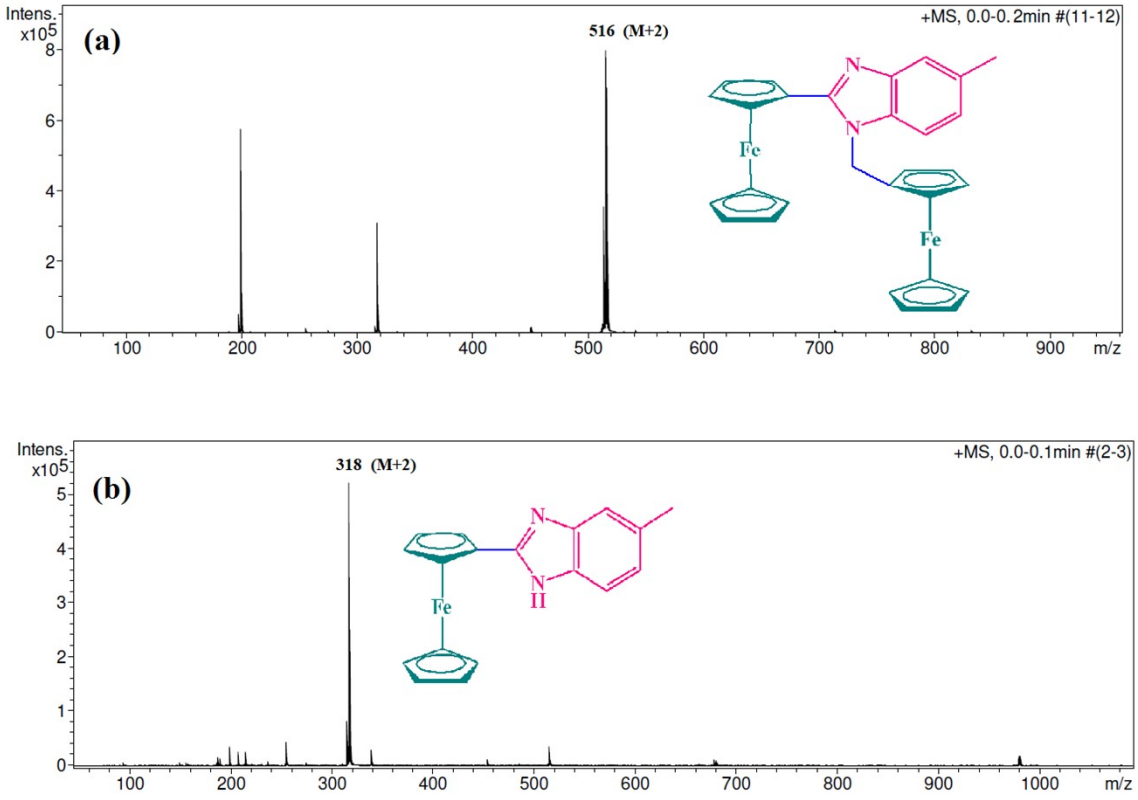


Fig. S6 ESI mass spectra for the receptor **1** (a) and receptor **2** (b)

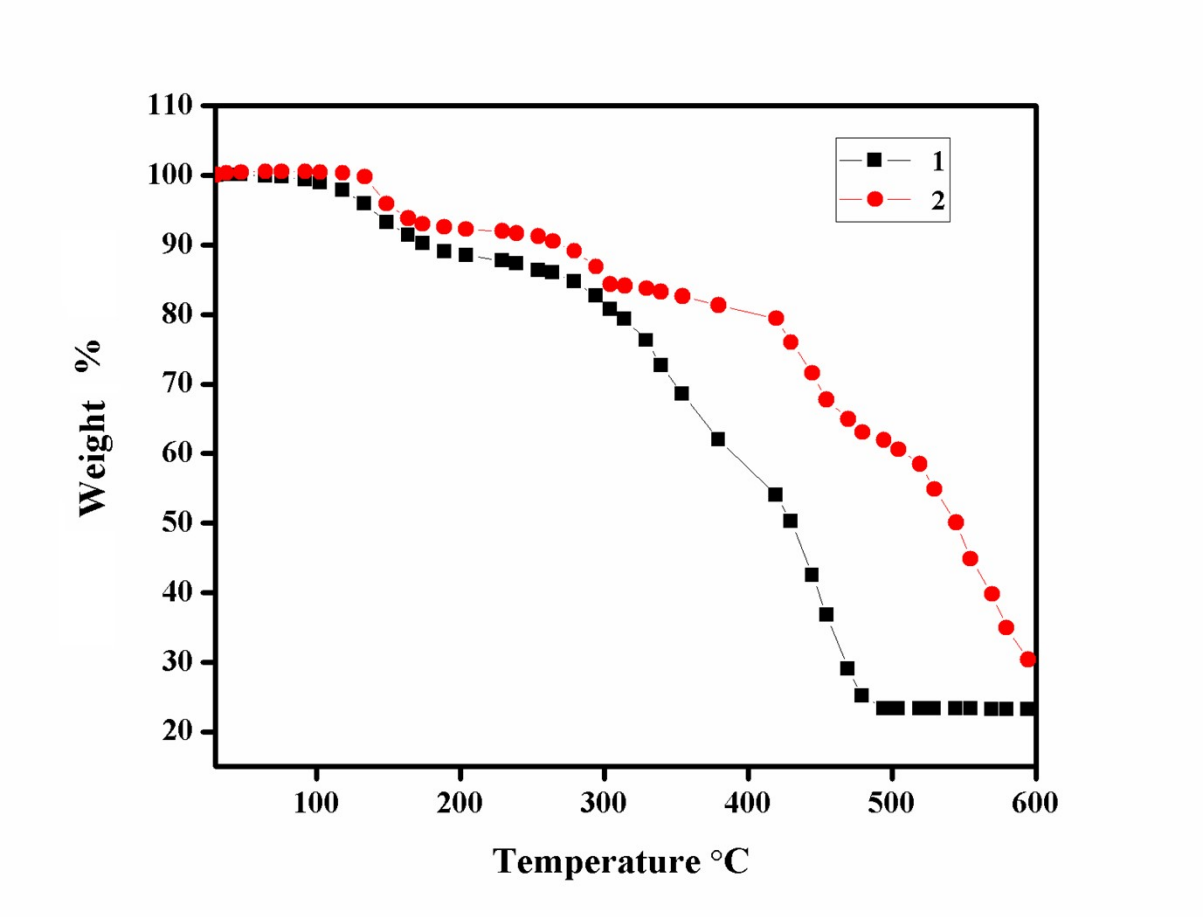
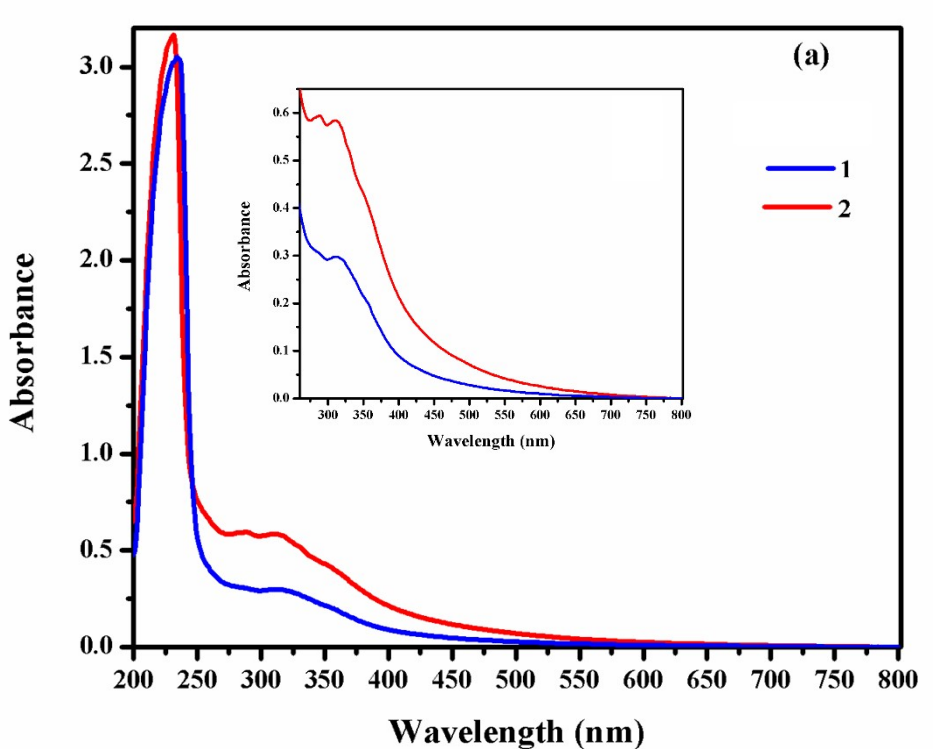


Fig. S7 Thermogram of receptors **1** (black) and **2**(red)



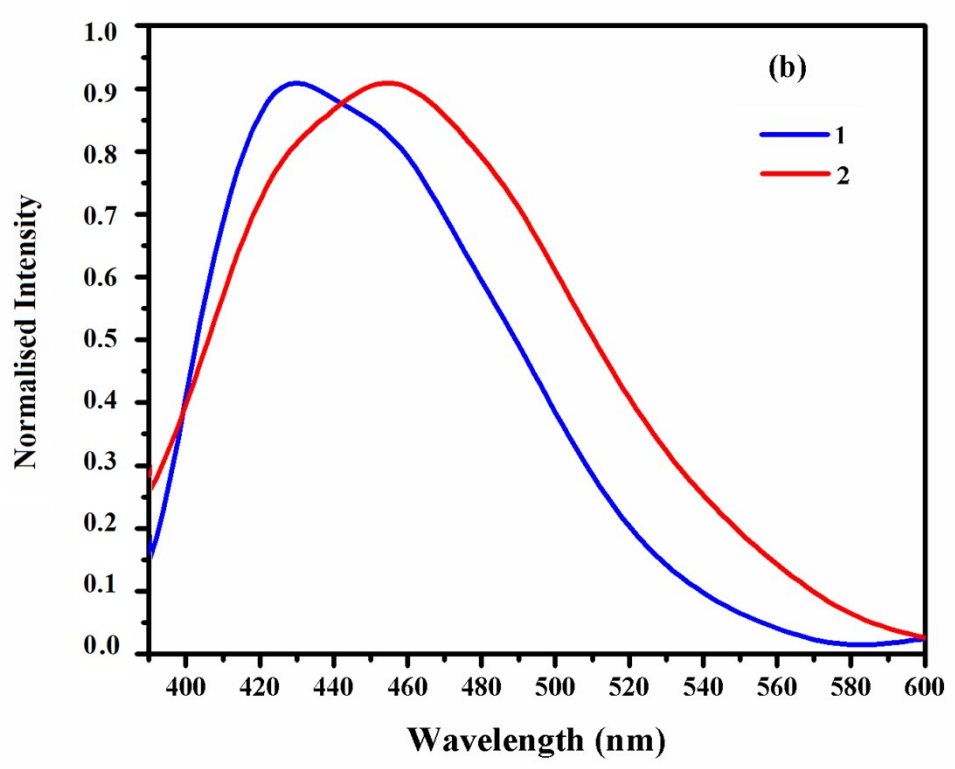


Fig. S8 (a) UV-visible spectroscopy (b) Fluorescence spectroscopy for receptor **1** and **2** (*c*= 10^{-5} M)

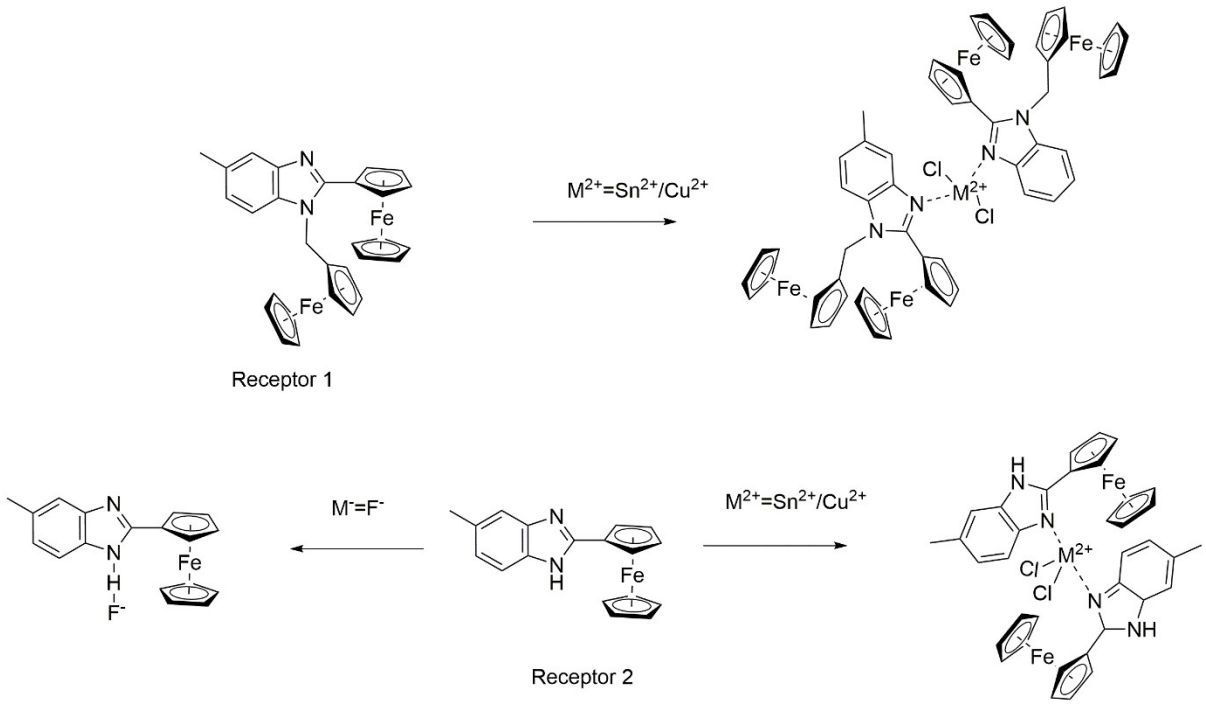


Fig. S9 Structural aspect for the formation of M^{2+} with receptors **1** M^{2+}/M^{-} with receptor **2**

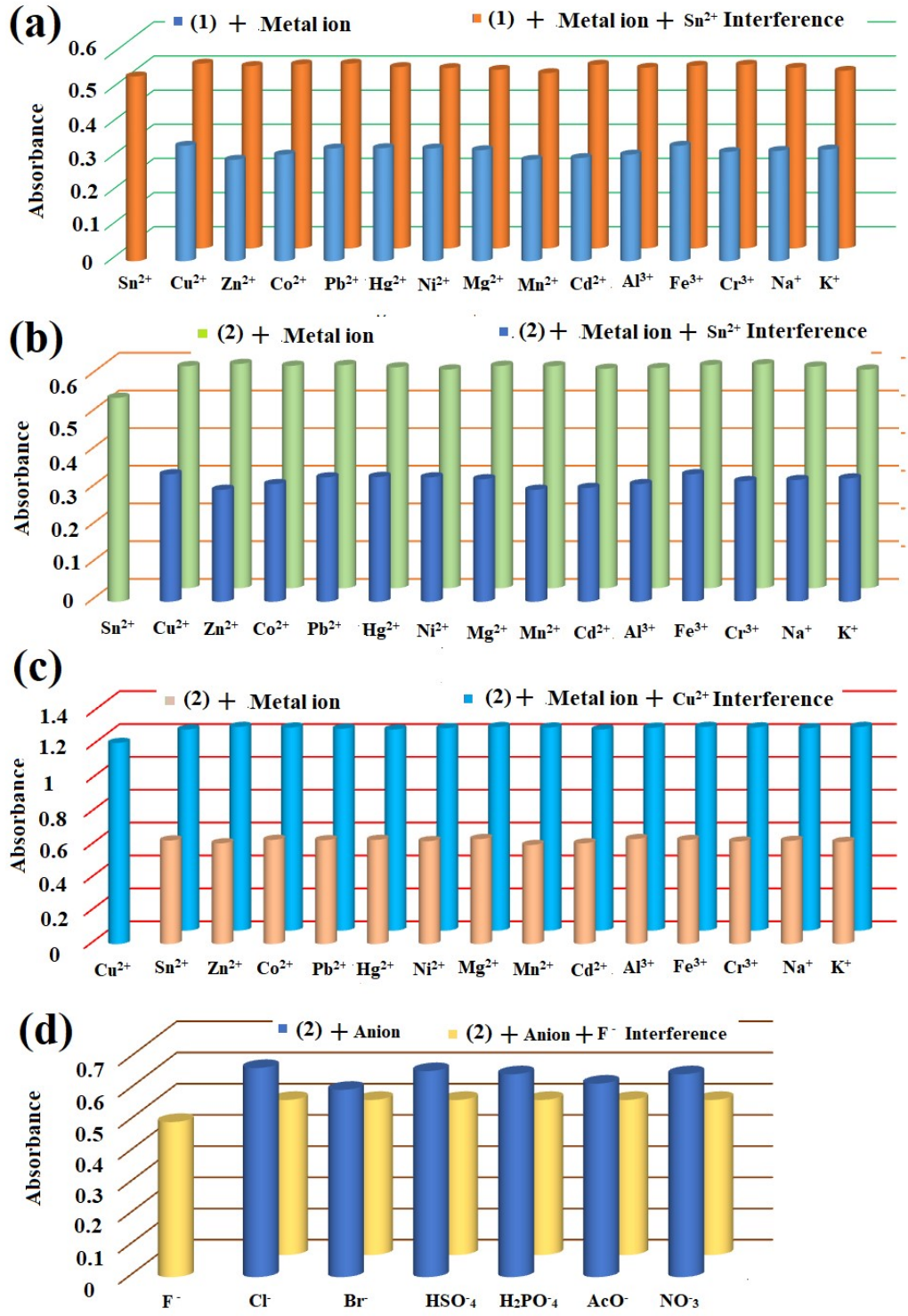


Fig. S10 (a) Interference studies **(a)** receptor **1** with Sn^{2+} at 358 nm **(b)** receptor **2** with Sn^{2+} at 356 nm**(c)** receptor **2** with Cu^{2+} at 310 nm **(d)** receptor **2** with F^- at 275 nm with various ions (c= 10^{-5} M)

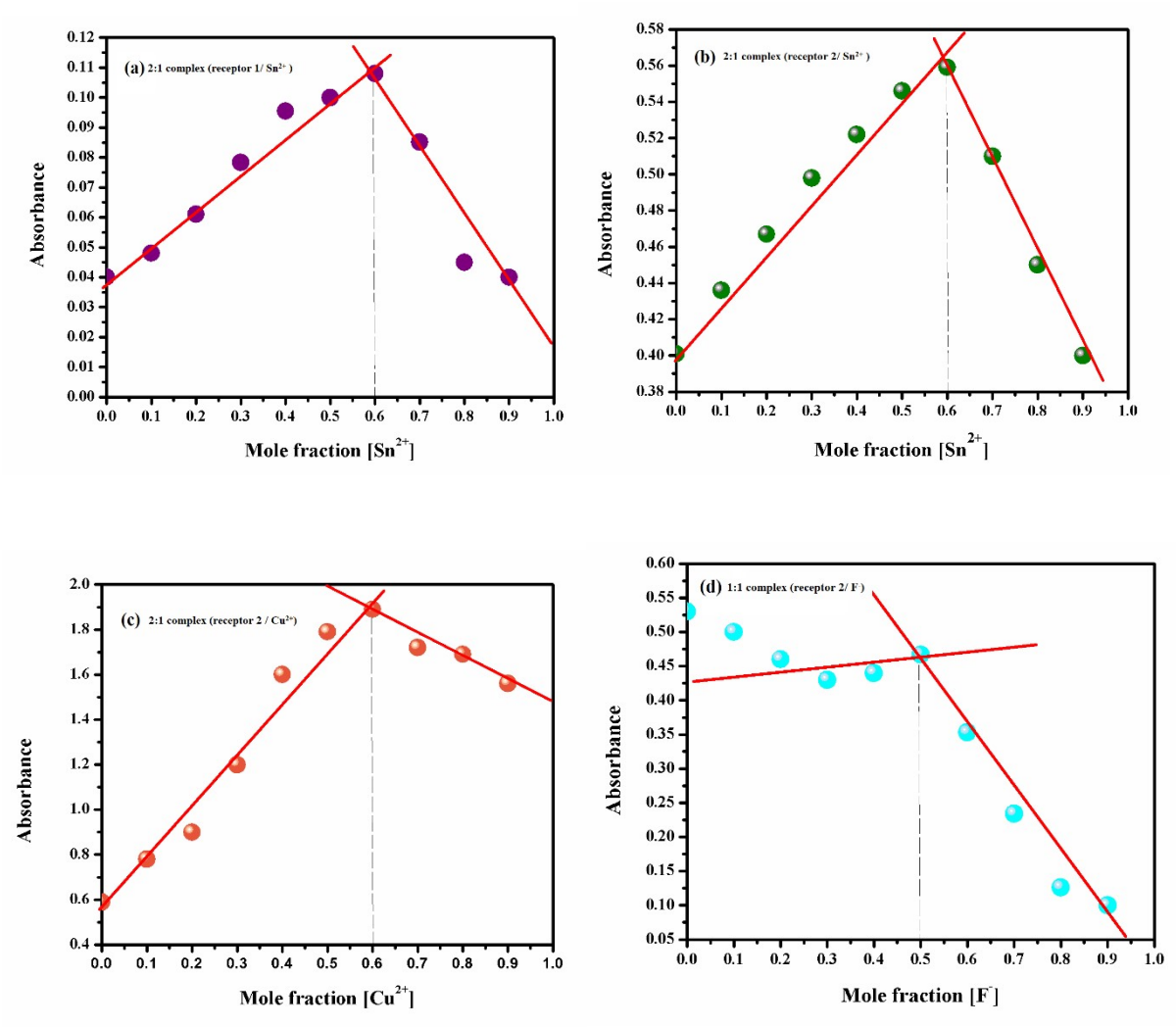
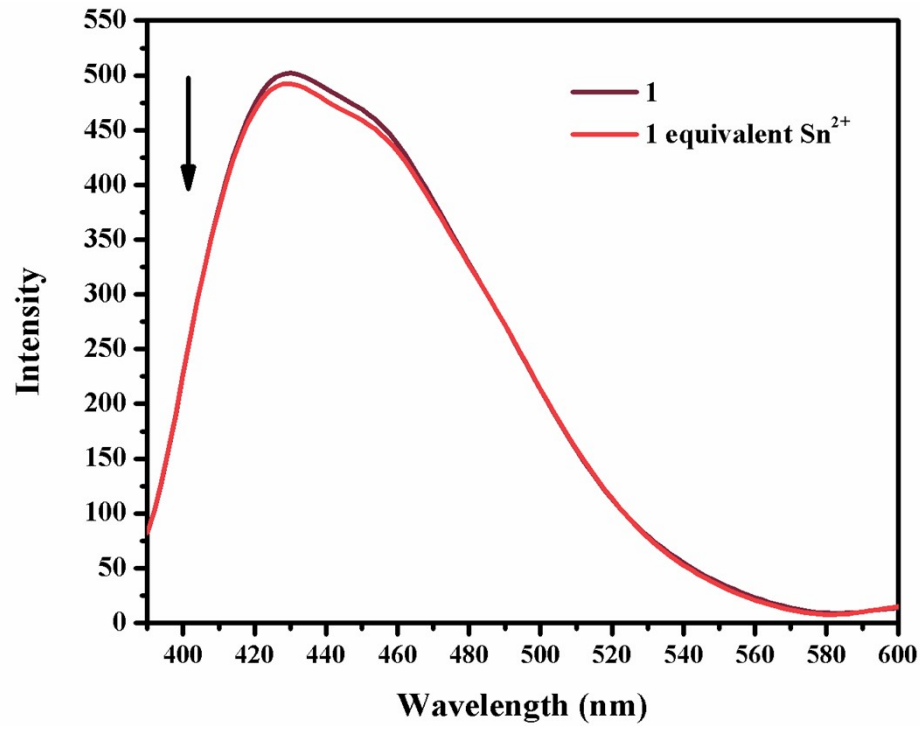


Fig. S11 Jobs plot for **(a)** receptor **1** with Sn^{2+} at 358 nm **(b)** receptor **2** with Sn^{2+} at 356 nm**(c)** receptor **2** with Cu^{2+} at 310 nm **(d)** receptor **2** with F^- at 275 nm



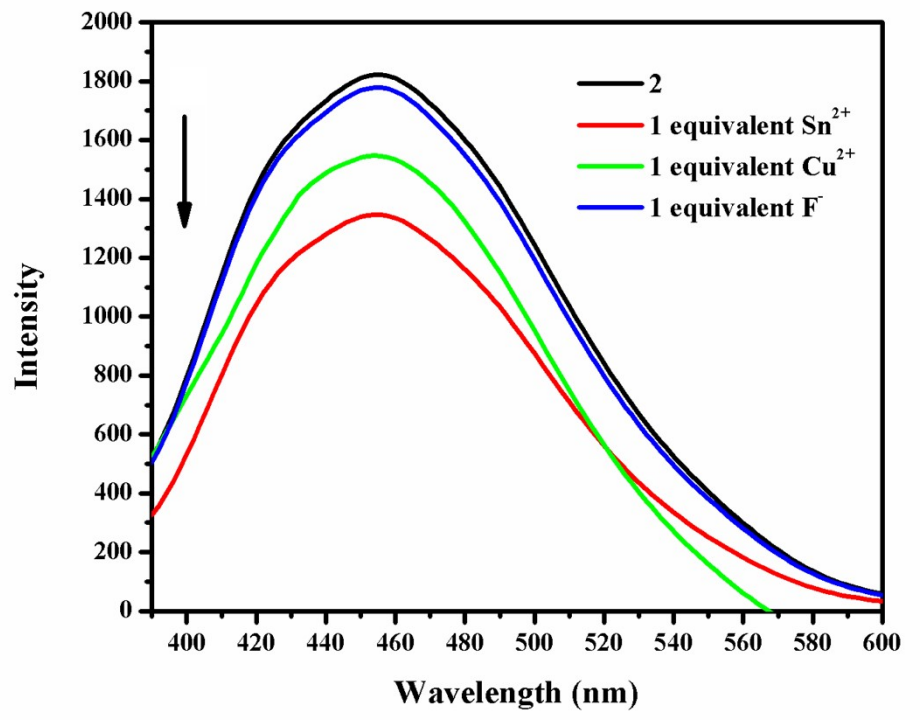


Fig. S12 Fluorescence spectroscopy for receptor **(1)** with 1 equivalent Sn^{2+} and receptor **(2)** with 1 equivalent Sn^{2+}, Cu^{2+} and F^- (c= 10^{-5} M).

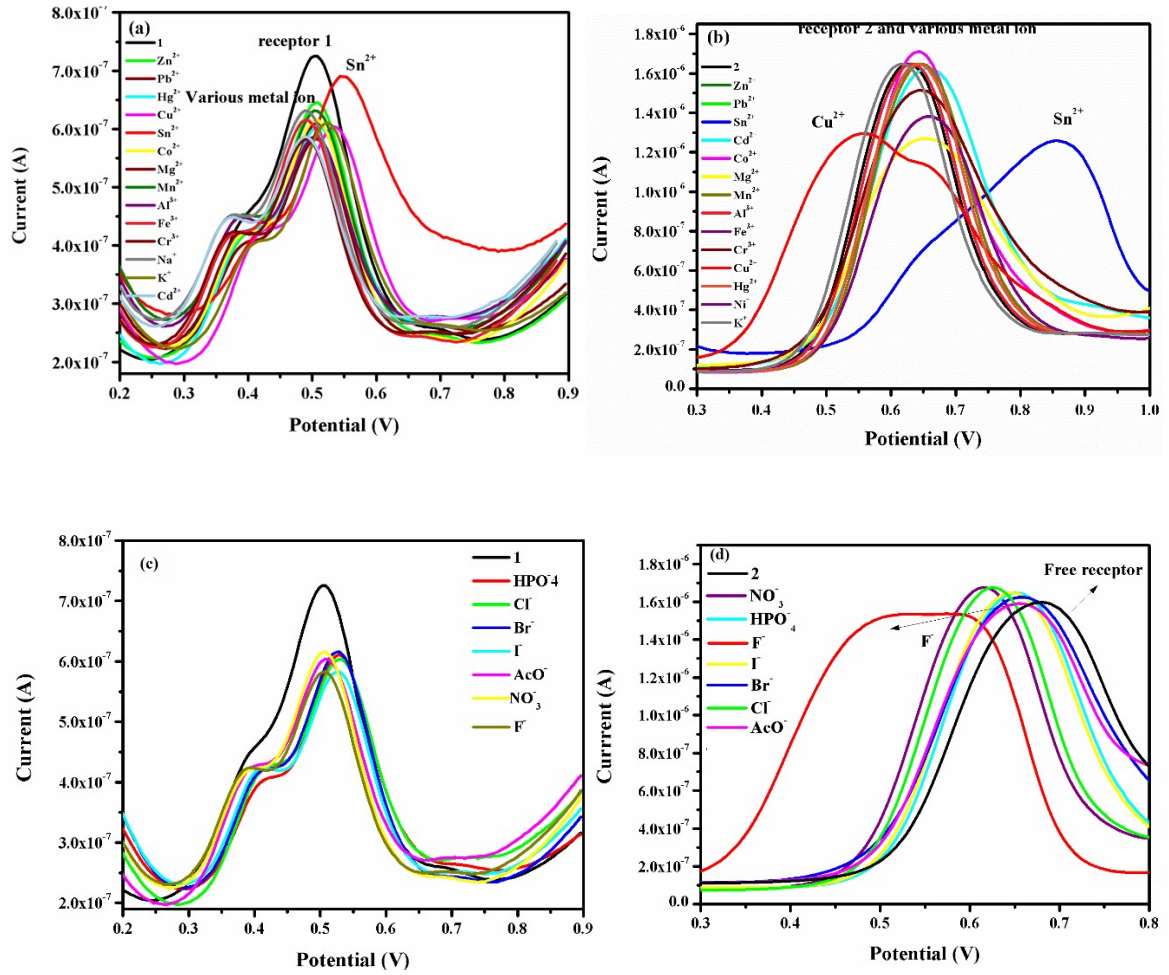


Fig. S13 Differential pulse voltammogram for **(a)** receptor **1** with various metal ion and **(b)** receptor **2** with various metal ion **(c)** receptor **1** with various anion and **(d)** receptor 2 with various anion (c = 1x10^{-3} M)

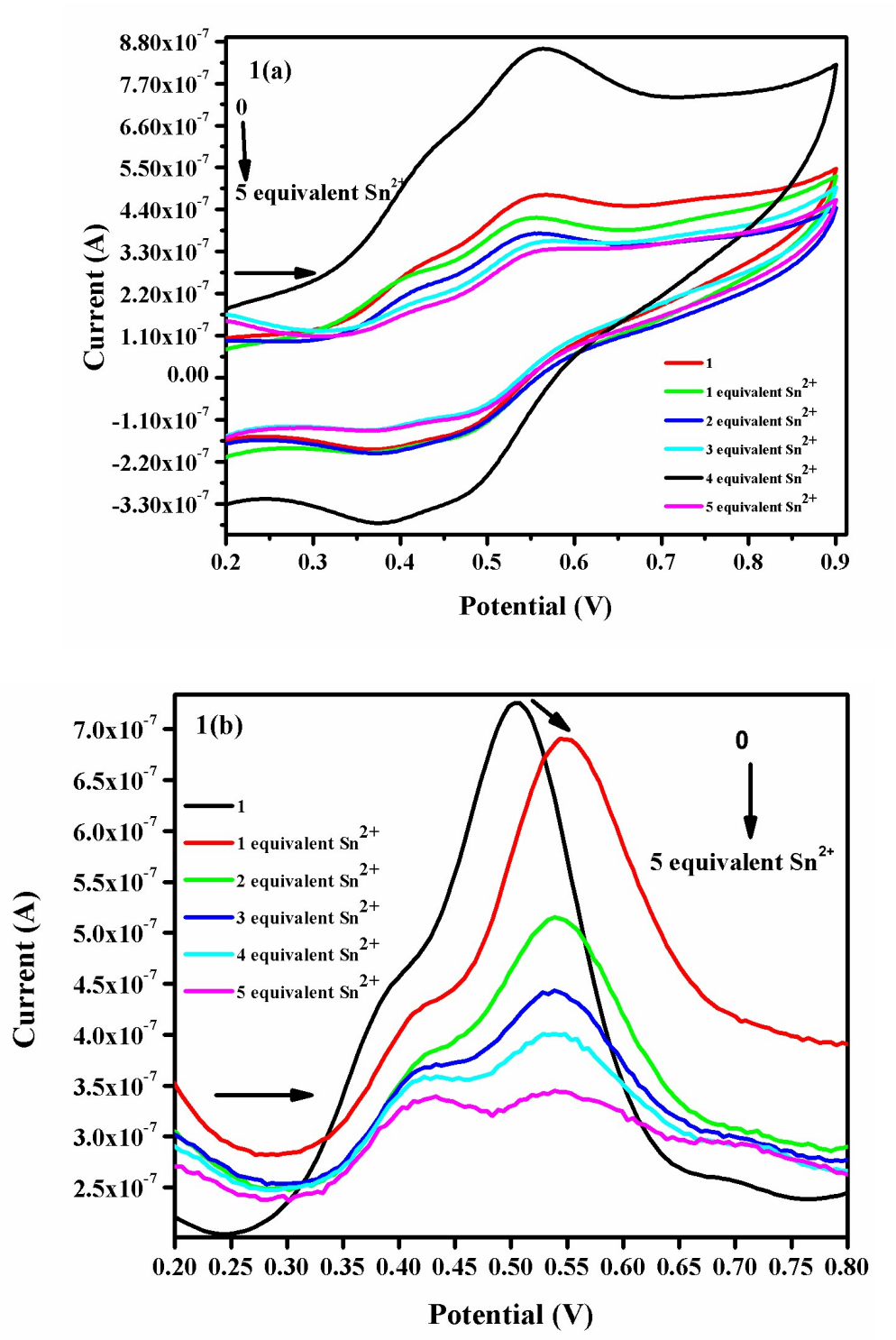


Fig. S14 (a) CV and **(b)** DPV of receptor **1** (black line) in CH_3CN (c = 1x10^{-3}M) using 0.1 M [(n-Bu)$_4$N] ClO_4 supporting electrolyte, by the sequential addition of 0 to 5.0 equivalent of Sn^{2+} ion.

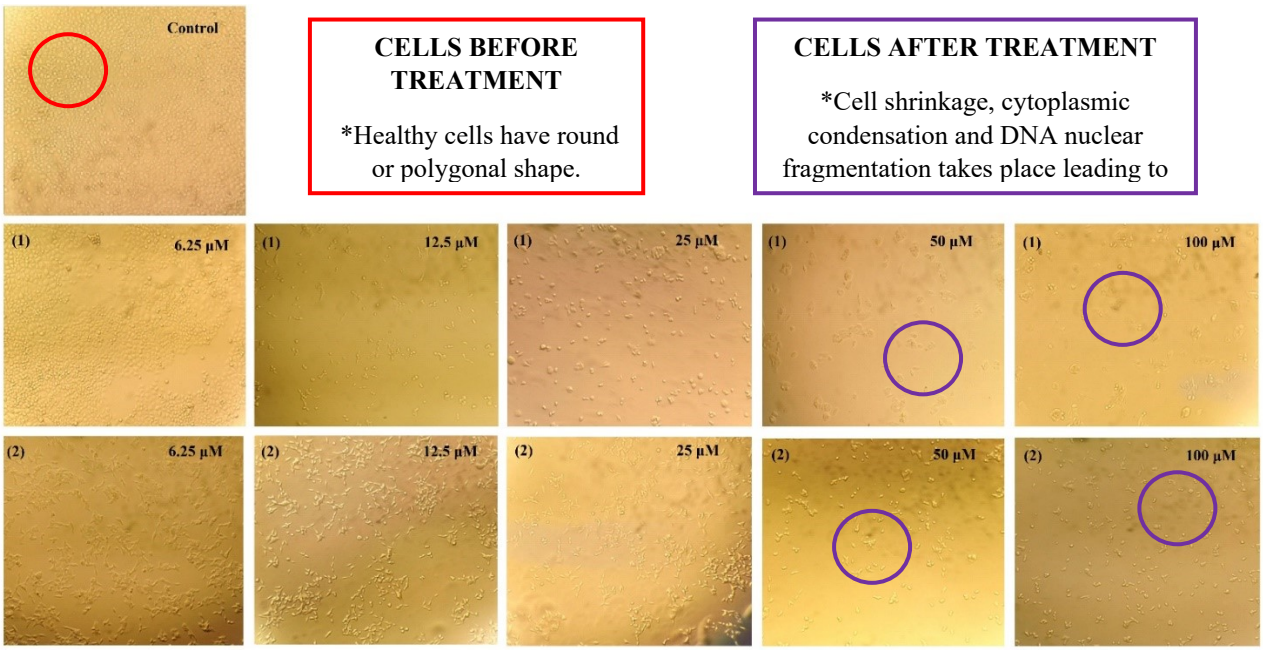


Fig. S15 *In vitro* cytotoxicity morphologies of HepG2 for receptor **(1)** and **(2)**

Table S1. Selected bond length and bond angle for receptor **1**

Bond length			Bond angle			
C1	C2	1.541	C3	C2	C7	121.34
C2	C3	1.368	C2	C3	C4	118.70
C3	C4	1.424	N2	C4	C5	111.49
C4	N2	1.376	N2	C4	C3	130.78
C5	N1	1.386	N1	C5	C4	104.49
C8	N2	1.323	C6	C5	C4	123.00
C8	N1	1.387	N2	C8	N1	112.74
C9	C10	1.435	N2	C8	C9	121.93
C9	Fe1	2.060	N1	C8	C9	125.27
C11	Fe1	2.024	C10	C9	C13	107.37
C11	C12	1.451	C10	C9	C8	122.45
C14	C18	1.397	C10	C9	Fe1	69.09
Fe1	C10	2.048	C8	C9	Fe1	131.16
Fe1	C17	2.061	C13	C9	Fe1	68.93
N1	C19	1.461	C11	C10	C9	108.31
C19	C20	1.510	C10	C11	Fe1	70.67
Fe2	C21	2.050	N1	C19	C20	110.81
C25	C26	1.390	C24	C20	C19	126.06
C29	C28	1.404	C24	C20	Fe2	69.06
Fe2	C28	2.011	C21	C20	C19	126.04

Table S2. Crystallographic data and structure refinement parameters of receptor **1**

Crystallographic data	**Receptor 1**
Formula	$C_{29}\ H_{26}\ Fe_2\ N_2$
Formula weight	514.22
T/K	304 K
Crystal system	Orthorhombic
Space group	P 2_1 2_1 2_1
Hall group	P 2ac, P 2ab
a/Å	9.6083(4)
b/Å	14.0301(6)
c/Å	17.6821(9)
α/°	90
β/°	90
γ/°	90
V	2383.64 (19)
Z/ Wavelength	4/0.71073
D_x [g cm^{-3}]	1.433
μ(Mo-Kα) mm^{-1}	1.237
F(000)	1064.0
Index ranges	-11 ≤ h ≤ 11, -16 ≤ k ≤ 16, -21≤ l ≤ 21
Reflections collected	4059
Unique reflections	299
GOF	1.013
θ (max)	25.027
Data completeness	1.61/0.91
R_1, wR_2 [$I > 2\sigma(I)$][a]	0.0591(2262)
R_1, wR_2 (all data)[b]	0.1204(4059)
$\Delta\rho_{min}$, $\Delta\rho_{max}$ (e $Å^{-3}$)	0.262, 1.000
CCDC No.	2124549

[a] $R = \sum||F_o| - |F_c||/\sum|F_o|$; $wR_2 = \{\sum[w(F_o^2 - F_c^2)^2]/\sum[w(F_o^2)^2]\}^{1/2}$. [b] $S = \{\sum[(F_o^2 - F_c^2)^2]/(n/p)\}^{1/2}$ where n is the number of reflections and p is the total number of parameters refined.

Table S3. Antimicrobial activity with zone of inhibition for the receptor **(1)** and **(2)**

Sample code	Sample name	Test Bacteria	Zone of Inhibition (mm)			
			10 µg/mL	20 µg/mL	30 µg/mL	Standard Drug
1a	1	*E. coli* ATCC-23848	0	19	30	31
1b	1	*S. aureus* ATCC-25923	0	20	31	32
1c	1	*C. albicans* ATCC-10231	0	0	32	29
2a	2	*E. coli* ATCC-23848	0	15	23	32
2b	2	*S. aureus* ATCC-25923	0	16	22	32
2c	2	*C. albicans* ATCC-10231	0	12	20	29

Standard drug: ampicillin, ciprofloxacin and fluconazole (30 µg/mL) for Gram-positive (1b, 2b), Gram-negative (1a, 2a) and fungi strains (1c, 2c) respectively