Supporting Information

A novel ferrocenyl−naphthalimide as a multichannel probe for the detection of Cu(II) and Hg(II) in aqueous media and living cells

Junyang Dong[a]， Jianfeng Hu[a],[b]， Huricha Baigude[a]，Hao Zhang[a],[b],[c]*

[a] School of Chemical & Chemical Engineering, Inner Mongolia University, Hohhot 010021, P. R. China.

[b] Inner Mongolia Key Laboratory of Fine Organic Synthesis, Hohhot 010021, P. R. China

[c] State Key Laboratory of Polymer Physics and Chemistry, Changchun Institute of Applied Chemistry, Chinese Academy of Sciences, Changchun 130022, P. R. China

*Corresponding Author, tel.: +86-471-4994406, fax: +86-471-4994406, e-mail: haozhang@imu.edu.cn; zh_hjf@hotmail.com

Table of Contents

Crystal data of 1

Crystal Structure Report for 1

Table 1. Sample and crystal data for 1.

Chemical formula	$C_{32}H_{33}FeN_3O_2S_2$	
Formula weight	609.57	
Temperature	296(2) K	
Wavelength	0.71073 Å	
Crystal system	monoclinic	
Space group	P 1 21/c 1	
Unit cell dimensions	a = 14.9241(19) Å	α = 90°
	b = 15.1194(19) Å	β = 110.093(2)°
	c = 13.5614(17) Å	γ = 90°
Volume	2873.8(6) $Å^3$	
Z	4	
Density (calculated)	1.409 g/cm^3	
Absorption coefficient	0.705 mm^{-1}	
F(000)	1272	

Table 2. Data collection and structure refinement for 1.

Theta range for data collection	1.45 to 28.30°
Index ranges	-19<=h<=10, -20<=k<=20, -17<=l<=18
Reflections collected	20377
Independent reflections	7094 [R(int) = 0.0348]

Coverage of independent reflections	99.6%	
Absorption correction	multi-scan	
Structure solution technique	direct methods	
Structure solution program	SHELXS-97 (Sheldrick, 2008)	
Refinement method	Full-matrix least-squares on F^2	
Refinement program	SHELXL-97 (Sheldrick, 2008)	
Function minimized	$\Sigma\ w(F_o^2 - F_c^2)^2$	
Data / restraints / parameters	7094 / 0 / 362	
Goodness-of-fit on F^2	1.027	
Final R indices	4545 data; $I>2\sigma(I)$	R1 = 0.0674, wR2 = 0.1622
	all data	R1 = 0.1145, wR2 = 0.1928
Weighting scheme	$w=1/[\sigma^2(F_o^2)+(0.0833P)^2+3.1808P]$ where $P=(F_o^2+2F_c^2)/3$	
Largest diff. peak and hole	1.001 and -0.523 eÅ^{-3}	
R.M.S. deviation from mean	0.069 eÅ^{-3}	

Table 3. Atomic coordinates and equivalent isotropic atomic displacement parameters (Å^2) for 1.

U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

x/a	y/b	z/c	U(eq)

	x/a	y/b	z/c	U(eq)
Fe1	0.39988(4)	0.33303(4)	0.90852(4)	0.04880(19)
S1	0.15066(7)	0.34705(8)	0.58838(7)	0.0595(3)
S2	0.97239(8)	0.31710(8)	0.63933(8)	0.0627(3)
O1	0.6770(2)	0.3212(2)	0.7500(2)	0.0762(9)
O2	0.8215(2)	0.5801(2)	0.7259(2)	0.0780(9)
N1	0.9776(2)	0.3688(3)	0.4560(3)	0.0655(10)
C18	0.7571(3)	0.3949(2)	0.9099(3)	0.0490(9)
N3	0.7543(3)	0.4475(2)	0.7388(3)	0.0620(9)
C1	0.4809(4)	0.3715(5)	0.0553(3)	0.0868(16)
C2	0.4817(4)	0.2808(4)	0.0486(3)	0.0862(17)
C3	0.3865(5)	0.2512(4)	0.0203(4)	0.0950(19)
C4	0.3281(4)	0.3263(4)	0.0115(4)	0.0786(15)
C5	0.3869(4)	0.3988(4)	0.0330(3)	0.0826(15)
C6	0.4501(4)	0.3955(4)	0.8058(3)	0.0783(15)
C7	0.4599(3)	0.3052(4)	0.7971(3)	0.0729(14)
C8	0.3698(3)	0.2667(3)	0.7693(3)	0.0600(11)
C9	0.3024(3)	0.3348(3)	0.7614(3)	0.0496(9)
C10	0.3522(3)	0.4153(3)	0.7834(3)	0.0666(12)
C11	0.1964(3)	0.3225(3)	0.7284(3)	0.0601(11)
C12	0.0249(3)	0.3449(2)	0.5547(3)	0.0488(9)
C13	0.0235(3)	0.4126(4)	0.3877(3)	0.0813(15)
C14	0.9773(3)	0.3911(4)	0.2804(3)	0.0710(13)
N2	0.8744(2)	0.4059(2)	0.2405(2)	0.0528(8)
C15	0.8306(3)	0.4039(3)	0.1309(3)	0.0490(9)
C16	0.8579(2)	0.4706(2)	0.0701(3)	0.0454(8)
C17	0.8205(2)	0.4641(2)	0.9589(3)	0.0443(8)

	x/a	y/b	z/c	U(eq)
C19	0.7269(3)	0.3380(3)	0.9706(3)	0.0580(10)
C20	0.7624(3)	0.3428(3)	0.0798(3)	0.0605(11)
C21	0.7252(3)	0.3837(3)	0.7956(3)	0.0573(10)
C22	0.8071(3)	0.5232(3)	0.7827(3)	0.0572(10)
C23	0.8451(3)	0.5290(2)	0.8978(3)	0.0485(8)
C24	0.9048(3)	0.5982(3)	0.9442(3)	0.0568(10)
C25	0.9400(3)	0.6053(3)	0.0534(3)	0.0597(10)
C26	0.9169(3)	0.5436(3)	0.1144(3)	0.0536(9)
C27	0.7291(4)	0.4357(4)	0.6228(3)	0.0754(13)
C28	0.6409(4)	0.4867(4)	0.5659(4)	0.0882(16)
C29	0.6238(5)	0.4898(4)	0.4469(4)	0.0987(18)
C30	0.5944(6)	0.4069(4)	0.3941(5)	0.107(2)
C31	0.8315(3)	0.3526(3)	0.3038(3)	0.0685(12)
C32	0.8727(3)	0.3776(4)	0.4156(3)	0.0775(15)

Table 4. Bond lengths (Å) for 1.

Fe1-C3	2.019(5)	Fe1-C5	2.025(5)
Fe1-C1	2.027(4)	Fe1-C6	2.028(5)
Fe1-C10	2.026(4)	Fe1-C9	2.026(3)
Fe1-C2	2.033(4)	Fe1-C4	2.033(5)
Fe1-C8	2.047(4)	Fe1-C7	2.048(4)
S1-C12	1.773(4)	S1-C11	1.822(4)
S2-C12	1.651(4)	O1-C21	1.220(5)
O2-C22	1.223(5)	N1-C12	1.330(4)
N1-C32	1.476(5)	N1-C13	1.484(5)
C18-C19	1.370(5)	C18-C17	1.415(5)
C18-C21	1.466(5)	N3-C21	1.393(5)

N3-C22	1.401(5)	N3-C27	1.498(5)
C1-C2	1.375(8)	C1-C5	1.393(7)
C1-H5	0.93	C2-C3	1.411(8)
C2-H4	0.93	C3-C4	1.411(8)
C3-H1	0.93	C4-C5	1.371(8)
C4-H2	0.93	C5-H3	0.93
C6-C7	1.383(7)	C6-C10	1.417(7)
C6-H31	0.93	C7-C8	1.394(6)
C7-H30	0.93	C8-C9	1.418(6)
C8-H6	0.93	C9-C10	1.404(6)
C9-C11	1.500(5)	C10-H7	0.93
C11-H28	0.97	C11-H29	0.97
C13-C14	1.417(6)	C13-H13A	0.97
C13-H13B	0.97	C14-N2	1.460(5)
C14-H14A	0.97	C14-H14B	0.97
N2-C15	1.404(4)	N2-C31	1.474(5)
C15-C20	1.373(5)	C15-C16	1.446(5)
C16-C26	1.412(5)	C16-C17	1.420(5)
C17-C23	1.411(5)	C19-C20	1.392(6)
C19-H8	0.93	C20-H9	0.93
C22-C23	1.468(5)	C23-C24	1.379(5)
C24-C25	1.395(6)	C24-H12	0.93
C25-C26	1.366(6)	C25-H10	0.93
C26-H11	0.93	C27-C28	1.493(7)
C27-H21	0.97	C27-H13	0.97
C28-C29	1.546(7)	C28-H14	0.97
C28-H15	0.97	C29-C30	1.436(8)

C29-H16	0.97	C29-H17	0.97
C30-H20	0.96	C30-H18	0.96
C30-H19	0.96	C31-C32	1.477(6)
C31-H31A	0.97	C31-H31B	0.97
C32-H32A	0.97	C32-H32B	0.97

Table 5. Bond angles (°) for 1.

C3-Fe1-C5	67.2(2)	C3-Fe1-C1	67.6(2)
C5-Fe1-C1	40.2(2)	C3-Fe1-C6	163.0(3)
C5-Fe1-C6	120.5(3)	C1-Fe1-C6	107.7(2)
C3-Fe1-C10	155.3(3)	C5-Fe1-C10	106.9(2)
C1-Fe1-C10	124.5(2)	C6-Fe1-C10	40.9(2)
C3-Fe1-C9	121.6(2)	C5-Fe1-C9	124.93(19)
C1-Fe1-C9	161.4(2)	C6-Fe1-C9	68.10(17)
C10-Fe1-C9	40.55(16)	C3-Fe1-C2	40.8(2)
C5-Fe1-C2	67.1(2)	C1-Fe1-C2	39.6(2)
C6-Fe1-C2	125.3(2)	C10-Fe1-C2	161.3(3)
C9-Fe1-C2	157.4(2)	C3-Fe1-C4	40.8(2)
C5-Fe1-C4	39.5(2)	C1-Fe1-C4	67.5(2)
C6-Fe1-C4	154.3(2)	C10-Fe1-C4	119.3(2)
C9-Fe1-C4	107.91(19)	C2-Fe1-C4	68.1(2)
C3-Fe1-C8	110.2(2)	C5-Fe1-C8	162.9(2)
C1-Fe1-C8	156.1(2)	C6-Fe1-C8	67.1(2)
C10-Fe1-C8	68.00(19)	C9-Fe1-C8	40.73(16)
C2-Fe1-C8	122.9(2)	C4-Fe1-C8	127.5(2)
C3-Fe1-C7	127.5(2)	C5-Fe1-C7	155.1(2)
C1-Fe1-C7	121.2(2)	C6-Fe1-C7	39.7(2)
C10-Fe1-C7	67.9(2)	C9-Fe1-C7	67.94(16)

C2-Fe1-C7	109.6(2)	C4-Fe1-C7	164.5(2)
C8-Fe1-C7	39.82(18)	C12-S1-C11	104.45(19)
C12-N1-C32	121.8(3)	C12-N1-C13	123.4(3)
C32-N1-C13	112.7(3)	C19-C18-C17	119.2(3)
C19-C18-C21	120.6(4)	C17-C18-C21	120.2(4)
C21-N3-C22	124.6(3)	C21-N3-C27	119.0(4)
C22-N3-C27	116.5(4)	C2-C1-C5	108.2(6)
C2-C1-Fe1	70.4(3)	C5-C1-Fe1	69.8(3)
C2-C1-H5	125.9	C5-C1-H5	125.9
Fe1-C1-H5	125.4	C1-C2-C3	107.7(5)
C1-C2-Fe1	70.0(3)	C3-C2-Fe1	69.1(3)
C1-C2-H4	126.2	C3-C2-H4	126.2
Fe1-C2-H4	126.3	C2-C3-C4	107.6(5)
C2-C3-Fe1	70.1(3)	C4-C3-Fe1	70.2(3)
C2-C3-H1	126.2	C4-C3-H1	126.2
Fe1-C3-H1	125.1	C5-C4-C3	107.1(5)
C5-C4-Fe1	69.9(3)	C3-C4-Fe1	69.1(3)
C5-C4-H2	126.5	C3-C4-H2	126.5
Fe1-C4-H2	126.1	C4-C5-C1	109.4(5)
C4-C5-Fe1	70.6(3)	C1-C5-Fe1	70.0(3)
C4-C5-H3	125.3	C1-C5-H3	125.3
Fe1-C5-H3	125.7	C7-C6-C10	108.8(4)
C7-C6-Fe1	70.9(3)	C10-C6-Fe1	69.4(3)
C7-C6-H31	125.6	C10-C6-H31	125.6
Fe1-C6-H31	125.6	C6-C7-C8	108.3(4)
C6-C7-Fe1	69.4(3)	C8-C7-Fe1	70.1(2)
C6-C7-H30	125.8	C8-C7-H30	125.8

Fe1-C7-H30	126.3	C7-C8-C9	108.1(4)
C7-C8-Fe1	70.1(2)	C9-C8-Fe1	68.8(2)
C7-C8-H6	125.9	C9-C8-H6	125.9
Fe1-C8-H6	126.6	C10-C9-C8	107.6(4)
C10-C9-C11	126.8(4)	C8-C9-C11	125.5(4)
C10-C9-Fe1	69.7(2)	C8-C9-Fe1	70.4(2)
C11-C9-Fe1	128.2(3)	C9-C10-C6	107.1(4)
C9-C10-Fe1	69.7(2)	C6-C10-Fe1	69.6(2)
C9-C10-H7	126.4	C6-C10-H7	126.4
Fe1-C10-H7	125.8	C9-C11-S1	105.4(3)
C9-C11-H28	110.7	S1-C11-H28	110.7
C9-C11-H29	110.7	S1-C11-H29	110.7
H28-C11-H29	108.8	N1-C12-S2	123.6(3)
N1-C12-S1	113.8(3)	S2-C12-S1	122.6(2)
C14-C13-N1	111.9(4)	C14-C13-H13A	109.2
N1-C13-H13A	109.2	C14-C13-H13B	109.2
N1-C13-H13B	109.2	H13A-C13-H13B	107.9
C13-C14-N2	115.1(4)	C13-C14-H14A	108.5
N2-C14-H14A	108.5	C13-C14-H14B	108.5
N2-C14-H14B	108.5	H14A-C14-H14B	107.5
C15-N2-C14	115.9(3)	C15-N2-C31	117.9(3)
C14-N2-C31	108.2(3)	C20-C15-N2	122.9(4)
C20-C15-C16	119.1(3)	N2-C15-C16	117.9(3)
C26-C16-C17	117.8(3)	C26-C16-C15	124.0(3)
C17-C16-C15	118.2(3)	C23-C17-C18	120.3(3)
C23-C17-C16	119.3(3)	C18-C17-C16	120.4(3)
C18-C19-C20	121.5(4)	C18-C19-H8	119.2

C20-C19-H8	119.2	C15-C20-C19	121.1(4)
C15-C20-H9	119.4	C19-C20-H9	119.4
O1-C21-N3	119.9(4)	O1-C21-C18	123.0(4)
N3-C21-C18	117.1(4)	O2-C22-N3	120.1(4)
O2-C22-C23	122.8(4)	N3-C22-C23	117.1(4)
C24-C23-C17	121.1(3)	C24-C23-C22	118.9(4)
C17-C23-C22	120.0(3)	C23-C24-C25	119.4(4)
C23-C24-H12	120.3	C25-C24-H12	120.3
C26-C25-C24	120.6(4)	C26-C25-H10	119.7
C24-C25-H10	119.7	C25-C26-C16	121.7(4)
C25-C26-H11	119.1	C16-C26-H11	119.1
N3-C27-C28	109.8(4)	N3-C27-H21	109.7
C28-C27-H21	109.7	N3-C27-H13	109.7
C28-C27-H13	109.7	H21-C27-H13	108.2
C27-C28-C29	110.7(5)	C27-C28-H14	109.5
C29-C28-H14	109.5	C27-C28-H15	109.5
C29-C28-H15	109.5	H14-C28-H15	108.1
C30-C29-C28	114.0(5)	C30-C29-H16	108.7
C28-C29-H16	108.7	C30-C29-H17	108.7
C28-C29-H17	108.7	H16-C29-H17	107.6
C29-C30-H20	109.5	C29-C30-H18	109.5
H20-C30-H18	109.5	C29-C30-H19	109.5
H20-C30-H19	109.5	H18-C30-H19	109.5
C32-C31-N2	110.4(4)	C32-C31-H31A	109.6
N2-C31-H31A	109.6	C32-C31-H31B	109.6
N2-C31-H31B	109.6	H31A-C31-H31B	108.1
C31-C32-N1	111.8(4)	C31-C32-H32A	109.3

N1-C32-H32A	109.3	C31-C32-H32B	109.3
N1-C32-H32B	109.3	H32A-C32-H32B	107.9

Table 6. Torsion angles (°) for 1.

C3-Fe1-C1-C2	38.2(4)	C5-Fe1-C1-C2	118.9(5)
C6-Fe1-C1-C2	-124.5(4)	C10-Fe1-C1-C2	-166.5(3)
C9-Fe1-C1-C2	161.7(6)	C4-Fe1-C1-C2	82.4(4)
C8-Fe1-C1-C2	-51.3(7)	C7-Fe1-C1-C2	-83.2(4)
C3-Fe1-C1-C5	-80.8(4)	C6-Fe1-C1-C5	116.6(4)
C10-Fe1-C1-C5	74.6(4)	C9-Fe1-C1-C5	42.8(9)
C2-Fe1-C1-C5	-118.9(5)	C4-Fe1-C1-C5	-36.5(4)
C8-Fe1-C1-C5	-170.2(5)	C7-Fe1-C1-C5	157.9(4)
C5-C1-C2-C3	0.8(5)	Fe1-C1-C2-C3	-59.0(3)
C5-C1-C2-Fe1	59.8(3)	C3-Fe1-C2-C1	-119.0(5)
C5-Fe1-C2-C1	-37.8(4)	C6-Fe1-C2-C1	74.2(4)
C10-Fe1-C2-C1	36.7(8)	C9-Fe1-C2-C1	-164.8(4)
C4-Fe1-C2-C1	-80.7(4)	C8-Fe1-C2-C1	157.9(3)
C7-Fe1-C2-C1	115.7(4)	C5-Fe1-C2-C3	81.2(4)
C1-Fe1-C2-C3	119.0(5)	C6-Fe1-C2-C3	-166.7(4)
C10-Fe1-C2-C3	155.8(6)	C9-Fe1-C2-C3	-45.8(6)
C4-Fe1-C2-C3	38.3(3)	C8-Fe1-C2-C3	-83.1(4)
C7-Fe1-C2-C3	-125.3(4)	C1-C2-C3-C4	-0.9(5)
Fe1-C2-C3-C4	-60.5(3)	C1-C2-C3-Fe1	59.6(3)
C5-Fe1-C3-C2	-80.8(4)	C1-Fe1-C3-C2	-37.1(3)
C6-Fe1-C3-C2	39.9(9)	C10-Fe1-C3-C2	-161.6(5)
C9-Fe1-C3-C2	161.1(3)	C4-Fe1-C3-C2	-118.1(5)
C8-Fe1-C3-C2	117.4(3)	C7-Fe1-C3-C2	75.9(4)
C5-Fe1-C3-C4	37.4(3)	C1-Fe1-C3-C4	81.1(3)

C6-Fe1-C3-C4	158.1(7)	C10-Fe1-C3-C4	-43.5(7)
C9-Fe1-C3-C4	-80.7(4)	C2-Fe1-C3-C4	118.1(5)
C8-Fe1-C3-C4	-124.5(3)	C7-Fe1-C3-C4	-165.9(3)
C2-C3-C4-C5	0.6(5)	Fe1-C3-C4-C5	-59.8(3)
C2-C3-C4-Fe1	60.5(3)	C3-Fe1-C4-C5	118.4(5)
C1-Fe1-C4-C5	37.1(3)	C6-Fe1-C4-C5	-47.1(6)
C10-Fe1-C4-C5	-80.9(3)	C9-Fe1-C4-C5	-123.6(3)
C2-Fe1-C4-C5	80.0(4)	C8-Fe1-C4-C5	-164.5(3)
C7-Fe1-C4-C5	164.5(6)	C5-Fe1-C4-C3	-118.4(5)
C1-Fe1-C4-C3	-81.2(4)	C6-Fe1-C4-C3	-165.4(4)
C10-Fe1-C4-C3	160.7(3)	C9-Fe1-C4-C3	118.0(3)
C2-Fe1-C4-C3	-38.4(3)	C8-Fe1-C4-C3	77.1(4)
C7-Fe1-C4-C3	46.2(8)	C3-C4-C5-C1	-0.1(5)
Fe1-C4-C5-C1	-59.4(3)	C3-C4-C5-Fe1	59.3(3)
C2-C1-C5-C4	-0.5(6)	Fe1-C1-C5-C4	59.8(3)
C2-C1-C5-Fe1	-60.2(3)	C3-Fe1-C5-C4	-38.5(3)
C1-Fe1-C5-C4	-120.3(5)	C6-Fe1-C5-C4	158.4(3)
C10-Fe1-C5-C4	115.9(3)	C9-Fe1-C5-C4	75.1(4)
C2-Fe1-C5-C4	-83.0(4)	C8-Fe1-C5-C4	46.1(9)
C7-Fe1-C5-C4	-170.3(4)	C3-Fe1-C5-C1	81.7(4)
C6-Fe1-C5-C1	-81.4(4)	C10-Fe1-C5-C1	-123.8(4)
C9-Fe1-C5-C1	-164.7(3)	C2-Fe1-C5-C1	37.3(4)
C4-Fe1-C5-C1	120.3(5)	C8-Fe1-C5-C1	166.4(6)
C7-Fe1-C5-C1	-50.0(7)	C3-Fe1-C6-C7	46.9(8)
C5-Fe1-C6-C7	159.9(3)	C1-Fe1-C6-C7	117.9(3)
C10-Fe1-C6-C7	-119.6(4)	C9-Fe1-C6-C7	-81.4(3)
C2-Fe1-C6-C7	77.8(4)	C4-Fe1-C6-C7	-167.3(4)

C8-Fe1-C6-C7	-37.2(3)	C3-Fe1-C6-C10	166.5(7)
C5-Fe1-C6-C10	-80.5(3)	C1-Fe1-C6-C10	-122.6(3)
C9-Fe1-C6-C10	38.1(3)	C2-Fe1-C6-C10	-162.6(3)
C4-Fe1-C6-C10	-47.8(6)	C8-Fe1-C6-C10	82.4(3)
C7-Fe1-C6-C10	119.6(4)	C10-C6-C7-C8	0.1(5)
Fe1-C6-C7-C8	59.5(3)	C10-C6-C7-Fe1	-59.4(3)
C3-Fe1-C7-C6	-164.4(3)	C5-Fe1-C7-C6	-44.6(6)
C1-Fe1-C7-C6	-80.0(4)	C10-Fe1-C7-C6	37.9(3)
C9-Fe1-C7-C6	81.8(3)	C2-Fe1-C7-C6	-122.2(3)
C4-Fe1-C7-C6	159.1(6)	C8-Fe1-C7-C6	119.6(4)
C3-Fe1-C7-C8	76.0(4)	C5-Fe1-C7-C8	-164.2(4)
C1-Fe1-C7-C8	160.4(3)	C6-Fe1-C7-C8	-119.6(4)
C10-Fe1-C7-C8	-81.6(3)	C9-Fe1-C7-C8	-37.7(3)
C2-Fe1-C7-C8	118.2(3)	C4-Fe1-C7-C8	39.6(8)
C6-C7-C8-C9	-0.5(5)	Fe1-C7-C8-C9	58.5(3)
C6-C7-C8-Fe1	-59.0(3)	C3-Fe1-C8-C7	-124.9(3)
C5-Fe1-C8-C7	157.1(7)	C1-Fe1-C8-C7	-44.9(7)
C6-Fe1-C8-C7	37.1(3)	C10-Fe1-C8-C7	81.5(3)
C9-Fe1-C8-C7	119.6(4)	C2-Fe1-C8-C7	-81.2(4)
C4-Fe1-C8-C7	-167.6(3)	C3-Fe1-C8-C9	115.4(3)
C5-Fe1-C8-C9	37.5(8)	C1-Fe1-C8-C9	-164.6(5)
C6-Fe1-C8-C9	-82.6(3)	C10-Fe1-C8-C9	-38.1(3)
C2-Fe1-C8-C9	159.1(3)	C4-Fe1-C8-C9	72.8(3)
C7-Fe1-C8-C9	-119.6(4)	C7-C8-C9-C10	0.7(4)
Fe1-C8-C9-C10	60.0(3)	C7-C8-C9-C11	177.1(3)
Fe1-C8-C9-C11	-123.6(4)	C7-C8-C9-Fe1	-59.3(3)
C3-Fe1-C9-C10	157.1(3)	C5-Fe1-C9-C10	74.3(4)

C1-Fe1-C9-C10	41.9(7)	C6-Fe1-C9-C10	-38.5(3)
C2-Fe1-C9-C10	-169.5(5)	C4-Fe1-C9-C10	114.5(3)
C8-Fe1-C9-C10	-118.3(4)	C7-Fe1-C9-C10	-81.4(3)
C3-Fe1-C9-C8	-84.6(3)	C5-Fe1-C9-C8	-167.4(3)
C1-Fe1-C9-C8	160.3(6)	C6-Fe1-C9-C8	79.8(3)
C10-Fe1-C9-C8	118.3(4)	C2-Fe1-C9-C8	-51.2(6)
C4-Fe1-C9-C8	-127.2(3)	C7-Fe1-C9-C8	36.9(3)
C3-Fe1-C9-C11	35.7(5)	C5-Fe1-C9-C11	-47.1(5)
C1-Fe1-C9-C11	-79.5(8)	C6-Fe1-C9-C11	-159.9(4)
C10-Fe1-C9-C11	-121.4(5)	C2-Fe1-C9-C11	69.1(7)
C4-Fe1-C9-C11	-6.9(4)	C8-Fe1-C9-C11	120.3(5)
C7-Fe1-C9-C11	157.2(4)	C8-C9-C10-C6	-0.6(4)
C11-C9-C10-C6	-176.9(4)	Fe1-C9-C10-C6	59.9(3)
C8-C9-C10-Fe1	-60.5(3)	C11-C9-C10-Fe1	123.2(4)
C7-C6-C10-C9	0.3(5)	Fe1-C6-C10-C9	-59.9(3)
C7-C6-C10-Fe1	60.3(3)	C3-Fe1-C10-C9	-52.4(6)
C5-Fe1-C10-C9	-124.4(3)	C1-Fe1-C10-C9	-165.0(3)
C6-Fe1-C10-C9	118.2(4)	C2-Fe1-C10-C9	167.5(6)
C4-Fe1-C10-C9	-83.4(3)	C8-Fe1-C10-C9	38.3(3)
C7-Fe1-C10-C9	81.4(3)	C3-Fe1-C10-C6	-170.6(5)
C5-Fe1-C10-C6	117.4(3)	C1-Fe1-C10-C6	76.8(4)
C9-Fe1-C10-C6	-118.2(4)	C2-Fe1-C10-C6	49.3(8)
C4-Fe1-C10-C6	158.4(3)	C8-Fe1-C10-C6	-79.9(3)
C7-Fe1-C10-C6	-36.8(3)	C10-C9-C11-S1	80.2(4)
C8-C9-C11-S1	-95.5(4)	Fe1-C9-C11-S1	172.3(2)
C12-S1-C11-C9	-173.3(3)	C32-N1-C12-S2	3.8(6)
C13-N1-C12-S2	165.8(4)	C32-N1-C12-S1	-175.3(4)

C13-N1-C12-S1	-13.3(6)	C11-S1-C12-N1	174.7(3)
C11-S1-C12-S2	-4.5(3)	C12-N1-C13-C14	149.6(5)
C32-N1-C13-C14	-47.0(6)	N1-C13-C14-N2	52.5(6)
C13-C14-N2-C15	166.5(4)	C13-C14-N2-C31	-58.4(6)
C14-N2-C15-C20	117.6(5)	C31-N2-C15-C20	-13.0(6)
C14-N2-C15-C16	-63.5(5)	C31-N2-C15-C16	165.9(4)
C20-C15-C16-C26	170.9(4)	N2-C15-C16-C26	-8.0(5)
C20-C15-C16-C17	-6.7(5)	N2-C15-C16-C17	174.3(3)
C19-C18-C17-C23	-173.5(4)	C21-C18-C17-C23	7.2(5)
C19-C18-C17-C16	4.7(5)	C21-C18-C17-C16	-174.5(3)
C26-C16-C17-C23	1.4(5)	C15-C16-C17-C23	179.2(3)
C26-C16-C17-C18	-176.8(3)	C15-C16-C17-C18	1.0(5)
C17-C18-C19-C20	-4.7(6)	C21-C18-C19-C20	174.5(4)
N2-C15-C20-C19	-174.1(4)	C16-C15-C20-C19	7.0(6)
C18-C19-C20-C15	-1.3(7)	C22-N3-C21-O1	177.8(4)
C27-N3-C21-O1	-2.7(6)	C22-N3-C21-C18	-3.5(6)
C27-N3-C21-C18	175.9(4)	C19-C18-C21-O1	-5.3(6)
C17-C18-C21-O1	173.9(4)	C19-C18-C21-N3	176.1(4)
C17-C18-C21-N3	-4.7(5)	C21-N3-C22-O2	-172.7(4)
C27-N3-C22-O2	7.8(6)	C21-N3-C22-C23	8.7(6)
C27-N3-C22-C23	-170.7(4)	C18-C17-C23-C24	178.3(3)
C16-C17-C23-C24	0.1(5)	C18-C17-C23-C22	-1.8(5)
C16-C17-C23-C22	179.9(3)	O2-C22-C23-C24	-4.5(6)
N3-C22-C23-C24	174.0(4)	O2-C22-C23-C17	175.6(4)
N3-C22-C23-C17	-5.8(5)	C17-C23-C24-C25	-1.3(6)
C22-C23-C24-C25	178.9(4)	C23-C24-C25-C26	1.0(6)
C24-C25-C26-C16	0.5(6)	C17-C16-C26-C25	-1.7(5)

C15-C16-C26-C25	-179.4(4)	C21-N3-C27-C28	96.4(5)
C22-N3-C27-C28	-84.1(5)	N3-C27-C28-C29	169.5(4)
C27-C28-C29-C30	71.3(7)	C15-N2-C31-C32	-167.3(4)
C14-N2-C31-C32	58.6(5)	N2-C31-C32-N1	-56.5(6)
C12-N1-C32-C31	-146.4(4)	C13-N1-C32-C31	49.8(6)

Table 7. Anisotropic atomic displacement parameters (Å^2) for 1.

The anisotropic atomic displacement factor exponent takes the form: $-2\pi^2[h^2 a^{*2} U_{11} + ... + 2 h k a^* b^* U_{12}]$

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Fe1	0.0451(3)	0.0616(4)	0.0323(3)	0.0029(2)	0.0038(2)	0.0076(2)
S1	0.0397(5)	0.0893(8)	0.0410(5)	0.0130(5)	0.0031(4)	0.0028(5)
S2	0.0520(6)	0.0819(8)	0.0512(5)	0.0172(5)	0.0136(4)	-0.0033(5)
O1	0.076(2)	0.075(2)	0.0632(18)	-0.0129(15)	0.0060(16)	-0.0192(17)
O2	0.077(2)	0.101(3)	0.0585(18)	0.0099(17)	0.0261(16)	-0.0190(18)
N1	0.0366(18)	0.104(3)	0.0483(18)	0.0236(18)	0.0051(14)	-0.0053(18)
C18	0.0369(19)	0.050(2)	0.052(2)	0.0017(16)	0.0050(15)	0.0038(16)
N3	0.061(2)	0.073(2)	0.0485(18)	-0.0024(16)	0.0141(16)	-0.0037(18)
C1	0.068(3)	0.133(5)	0.043(2)	-0.018(3)	-0.002(2)	0.009(3)
C2	0.089(4)	0.121(5)	0.040(2)	0.021(3)	0.012(2)	0.049(4)
C3	0.158(6)	0.083(4)	0.047(2)	0.015(2)	0.039(3)	-0.010(4)
C4	0.068(3)	0.119(5)	0.049(2)	0.009(3)	0.021(2)	0.010(3)
C5	0.085(4)	0.104(4)	0.053(3)	-0.018(3)	0.017(2)	0.022(3)
C6	0.063(3)	0.109(4)	0.053(2)	0.015(3)	0.008(2)	-0.021(3)
C7	0.049(3)	0.124(4)	0.041(2)	0.003(2)	0.0098(18)	0.017(3)
C8	0.061(3)	0.077(3)	0.0361(18)	-0.0051(18)	0.0089(17)	0.012(2)
C9	0.045(2)	0.066(2)	0.0316(16)	0.0057(15)	0.0046(14)	0.0047(18)
C10	0.066(3)	0.066(3)	0.053(2)	0.018(2)	0.001(2)	0.002(2)

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C11	0.045(2)	0.090(3)	0.0370(18)	0.0062(18)	0.0039(15)	0.003(2)
C12	0.044(2)	0.049(2)	0.0463(19)	0.0064(15)	0.0063(15)	-0.0016(16)
C13	0.047(3)	0.136(5)	0.055(2)	0.023(3)	0.0099(19)	-0.011(3)
C14	0.042(2)	0.116(4)	0.050(2)	0.012(2)	0.0090(17)	0.004(2)
N2	0.0375(17)	0.071(2)	0.0446(16)	0.0090(14)	0.0072(13)	0.0005(15)
C15	0.0366(19)	0.058(2)	0.0467(19)	0.0054(16)	0.0069(15)	0.0090(16)
C16	0.0357(19)	0.048(2)	0.0487(19)	0.0006(15)	0.0096(15)	0.0047(15)
C17	0.0333(18)	0.048(2)	0.0496(19)	0.0023(15)	0.0119(14)	0.0082(15)
C19	0.047(2)	0.056(2)	0.057(2)	0.0048(18)	-0.0006(17)	-0.0085(18)
C20	0.047(2)	0.064(3)	0.060(2)	0.0119(19)	0.0053(18)	-0.0047(19)
C21	0.043(2)	0.065(3)	0.055(2)	-0.0024(19)	0.0049(17)	0.0031(19)
C22	0.046(2)	0.074(3)	0.052(2)	0.001(2)	0.0167(17)	-0.0020(19)
C23	0.039(2)	0.053(2)	0.053(2)	-0.0012(16)	0.0149(16)	0.0035(16)
C24	0.057(3)	0.057(2)	0.060(2)	0.0003(18)	0.0257(19)	-0.0015(19)
C25	0.055(3)	0.055(2)	0.066(3)	-0.0092(19)	0.017(2)	-0.0096(19)
C26	0.050(2)	0.058(2)	0.050(2)	-0.0052(17)	0.0129(17)	0.0040(18)
C27	0.065(3)	0.095(4)	0.062(3)	-0.005(2)	0.018(2)	0.001(3)
C28	0.066(3)	0.121(5)	0.078(3)	0.013(3)	0.026(3)	0.009(3)
C29	0.100(4)	0.116(5)	0.070(3)	0.017(3)	0.017(3)	-0.007(4)
C30	0.153(6)	0.082(4)	0.094(4)	-0.006(3)	0.053(4)	-0.011(4)
C31	0.041(2)	0.100(3)	0.057(2)	0.022(2)	0.0071(18)	-0.007(2)
C32	0.040(2)	0.130(4)	0.056(2)	0.027(3)	0.0079(18)	-0.001(3)

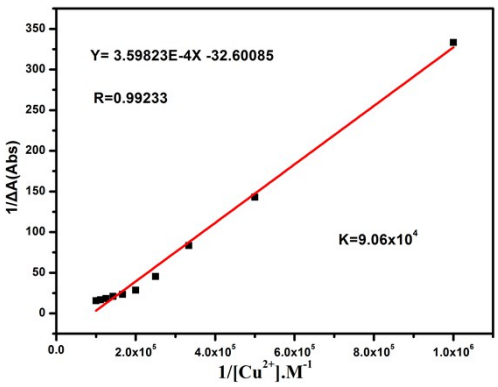
Table 8. Hydrogen atomic coordinates and isotropic atomic displacement parameters (Å^2) for 1.

	x/a	**y/b**	**z/c**	**U(eq)**

	x/a	y/b	z/c	U(eq)
H5	0.5340	0.4083	1.0718	0.104
H4	0.5353	0.2453	1.0607	0.103
H1	0.3659	0.1928	1.0093	0.114
H2	0.2622	0.3266	0.9944	0.094
H3	0.3671	0.4571	1.0327	0.099
H31	0.4995	0.4366	0.8234	0.094
H30	0.5170	0.2753	0.8080	0.088
H6	0.3562	0.2067	0.7579	0.072
H7	0.3260	0.4711	0.7833	0.08
H28	0.1693	0.3626	0.7665	0.072
H29	0.1810	0.2623	0.7414	0.072
H13A	0.0219	0.4762	0.3965	0.098
H13B	0.0898	0.3945	0.4091	0.098
H14A	-0.0106	0.3293	0.2703	0.085
H14B	0.0058	0.4259	0.2388	0.085
H8	-0.3184	0.2951	-0.0618	0.07
H9	-0.2605	0.3039	0.1187	0.073
H12	-0.0785	0.6398	-0.0969	0.068
H10	-0.0205	0.6524	0.0850	0.072
H11	-0.0592	0.5500	0.1870	0.064
H21	-0.2812	0.3734	-0.3949	0.09
H13	-0.2187	0.4562	-0.3985	0.09
H14	-0.3531	0.5465	-0.4065	0.106
H15	-0.4135	0.4592	-0.4226	0.106
H16	-0.4246	0.5339	-0.5854	0.118
H17	-0.3177	0.5086	-0.5631	0.118

	x/a	y/b	z/c	U(eq)
H20	-0.3555	0.3642	-0.5792	0.16
H18	-0.4191	0.4147	-0.6799	0.16
H19	-0.4619	0.3864	-0.5940	0.16
H31A	-0.2369	0.3620	0.2791	0.082
H31B	-0.1568	0.2904	0.2959	0.082
H32A	-0.1542	0.3402	0.4565	0.093
H32B	-0.1444	0.4384	0.4241	0.093

UV−Visible Absorption Spectra.



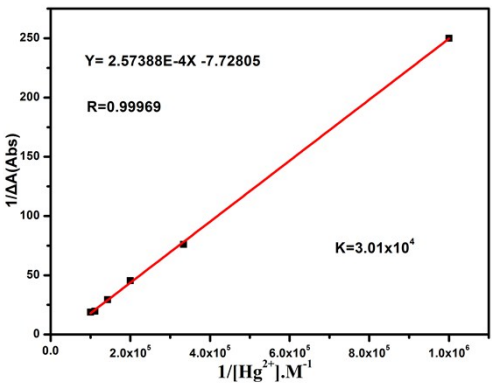


Figure S1. Benesi - Hildebrand plot obtained from the UV- vis absorption (absorption calculated from324 nm) for **1**-Cu^{2+} and (absorption calculated from 324 nm) **1**-Hg^{2+}.

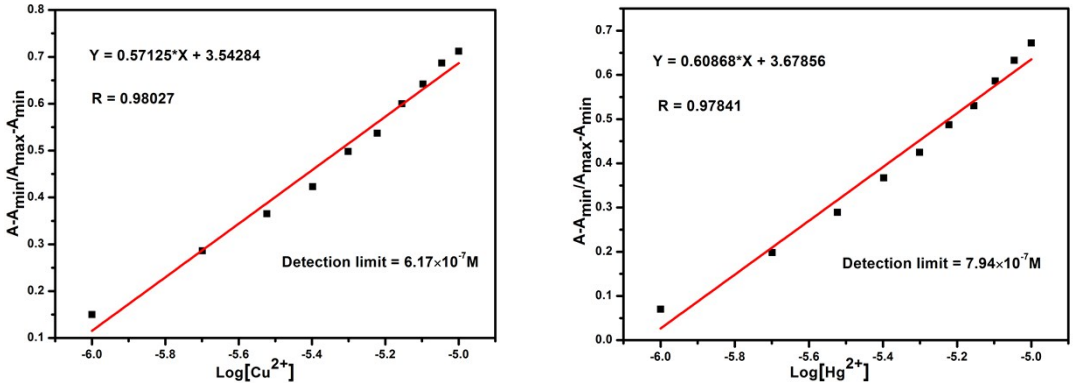
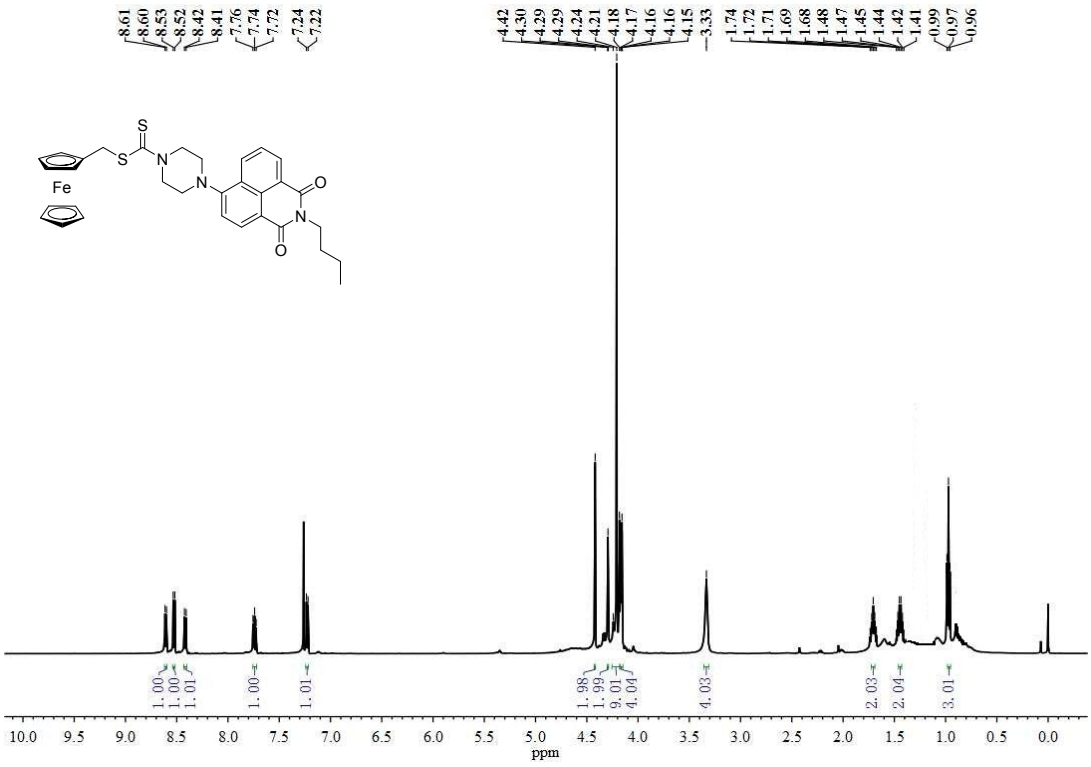
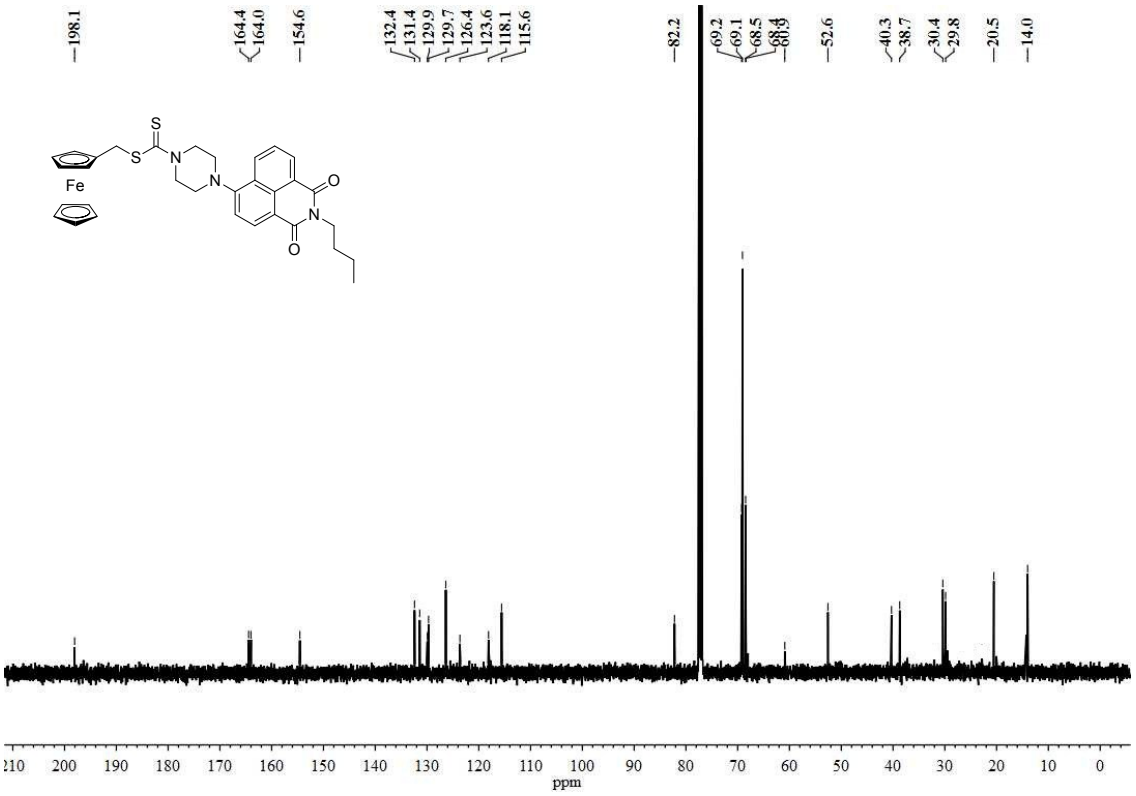


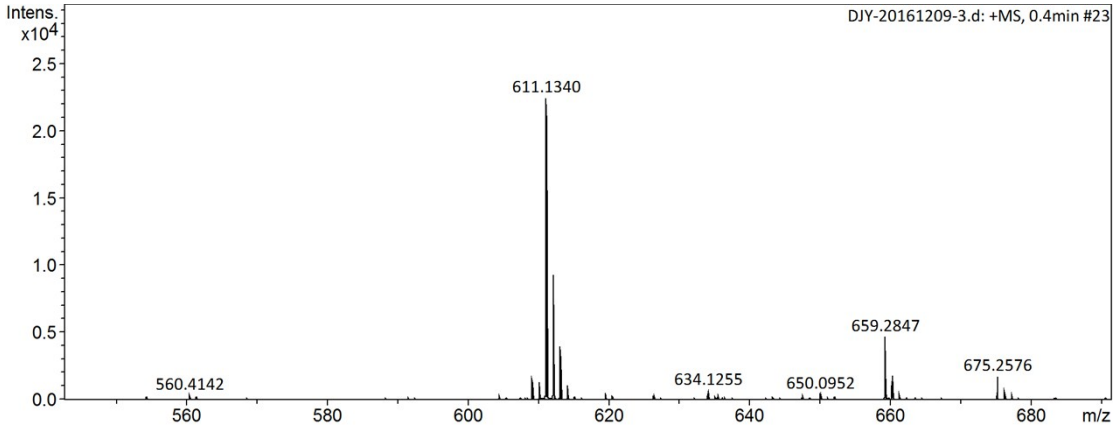
Figure S2. Benesi - Hildebrand plot obtained from the UV-vis absorption (absorption calculated from 324 nm) for **1**-Cu^{2+} and (absorption calculated from 324 nm) **1**-Hg^{2+}.

^{1}H NMR spectra and ^{13}C NMR spectra for 1.





HRMS (ESI-TOF) spectra for 1.



HRMS (ESI-TOF) spectra for 1-Cu^{2+}.

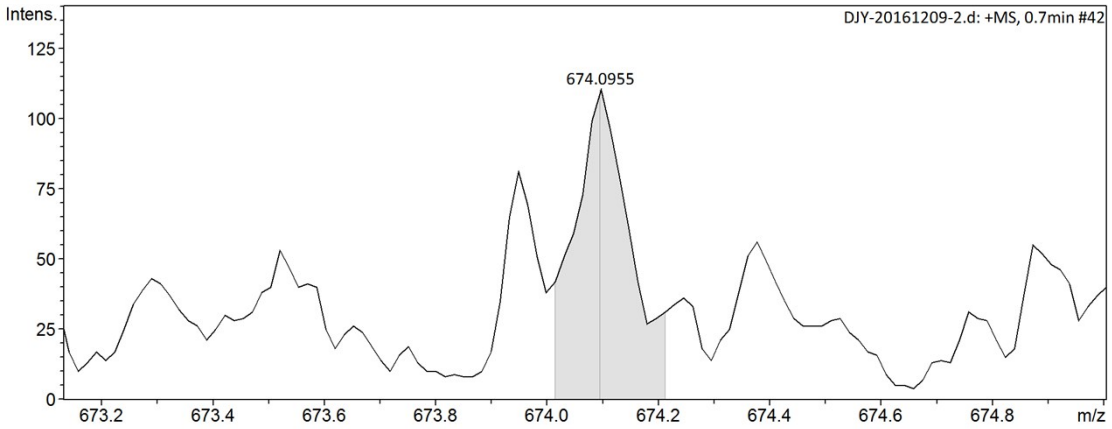


Figure S3. HRMS (ESI-TOF) spectra for 1-Cu^{2+}.

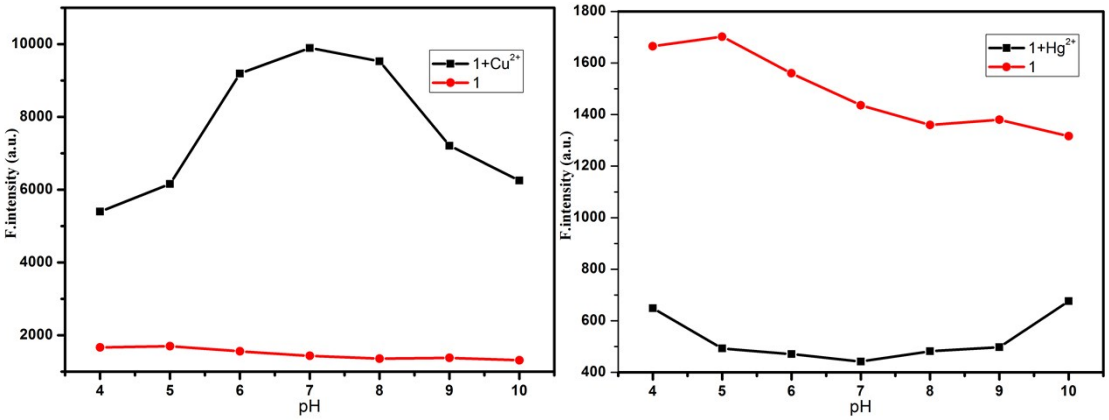


Figure S4. pH interference to the fluorescent detection for Cu^{2+} and Hg^{2+}.

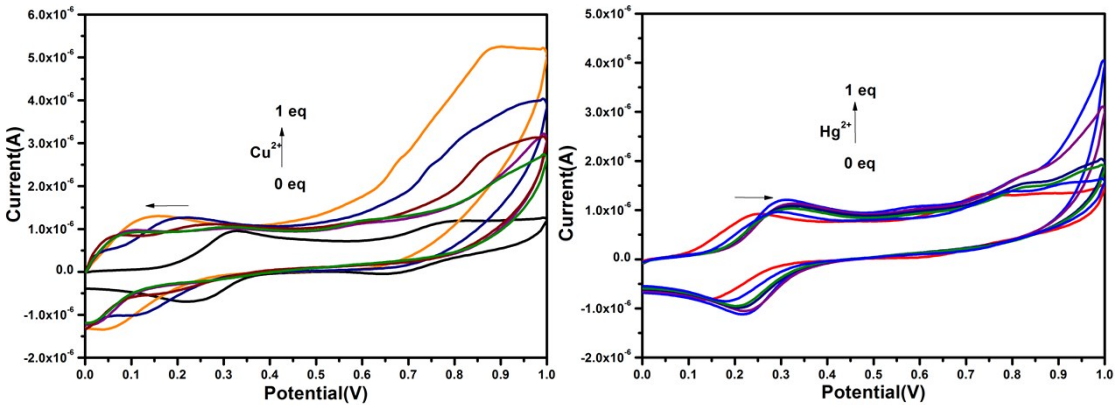


Figure S5. Cyclic Voltammetry of receptor **1** with $Cu(ClO_4)_2$ and $Hg(ClO_4)_2$ in CH_3CN/H_2O (7:3, v/v, 100 μM), containing 0.1 M [$(n\text{-}C_4H_9)_4NPF_6$] as supporting electrolyte and scanned at 0.1 V s^{-1}.

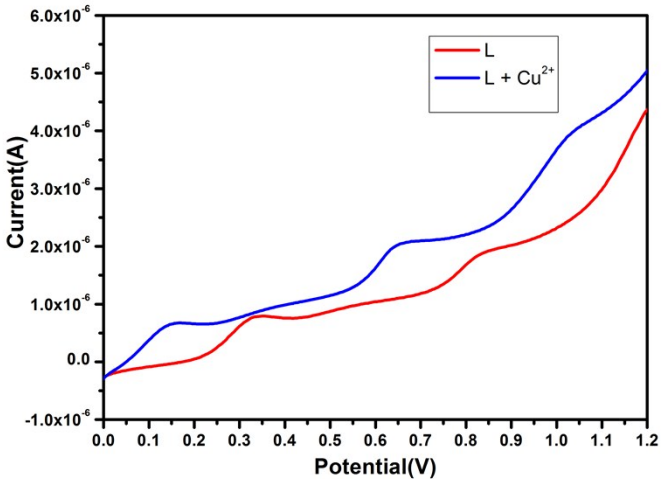


Figure S6. Linear Sweep Voltammetry of receptor **1** and receptor **1** with $Cu(ClO_4)_2$ in CH_3CN/H_2O (7:3, v/v, 100 μM), containing 0.1 M [$(n\text{-}C_4H_9)_4NPF_6$] as supporting electrolyte and scanned at 0.1 V s^{-1}.