Supporting Information

Cd(II)-Terpyridine-based complex as a ratiometric fluorescent probe for pyrophosphate detection in solution and as an imaging agent in living cells

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Figure S1. Fluorescence spectra of **L1** (10 μM) in CH_3CN in the presence of various metal ions (50 μM): (1) Ni^{+}; (2) Mn^{2+}; (3) Cu^{2+}; (4) Fe^{3+}; (5) Co^{2+}; (6) Ag^{+}; (7) Ca^{2+}; (8) Na^{+}; (9) K^{+}; (10) Li^{+}; (11) Zn^{2+}; (12) Cd^{2+}; (13) $Al3^{+}$; (14) Host.

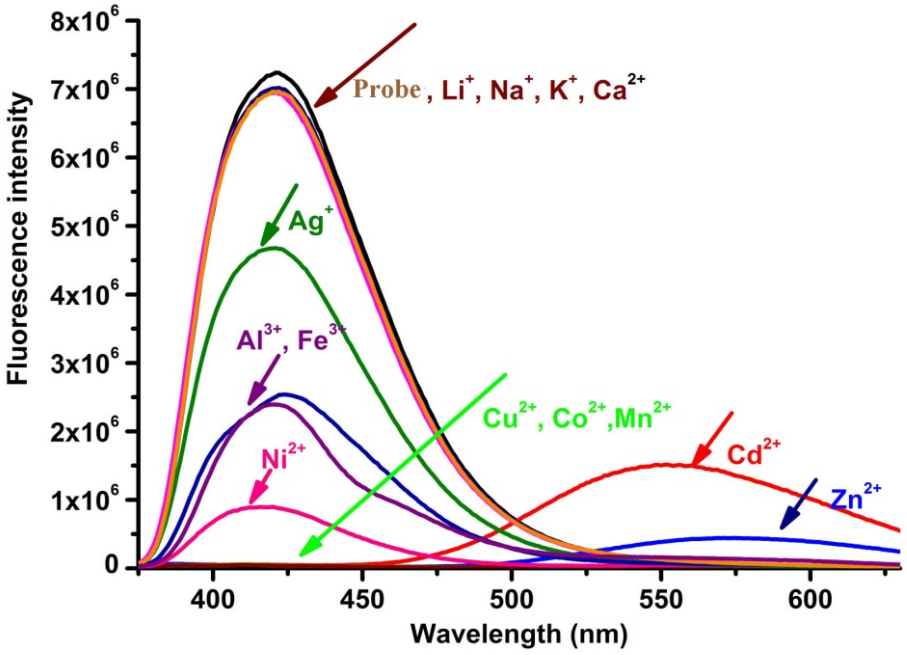
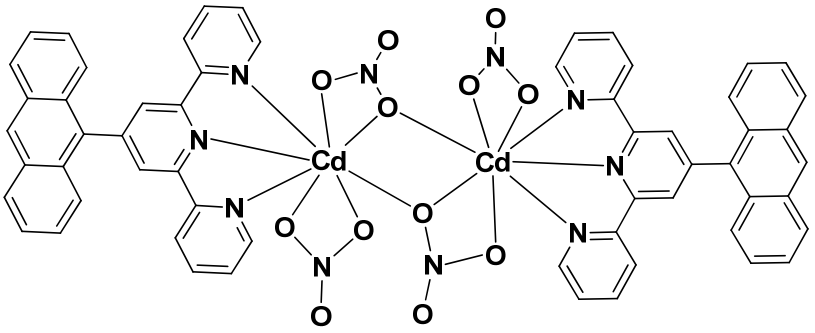


Figure S2. Structure of **L1-Cd(II) complex** and Mass spectrometry (HRMS) of **L1-Cd(II)** complex



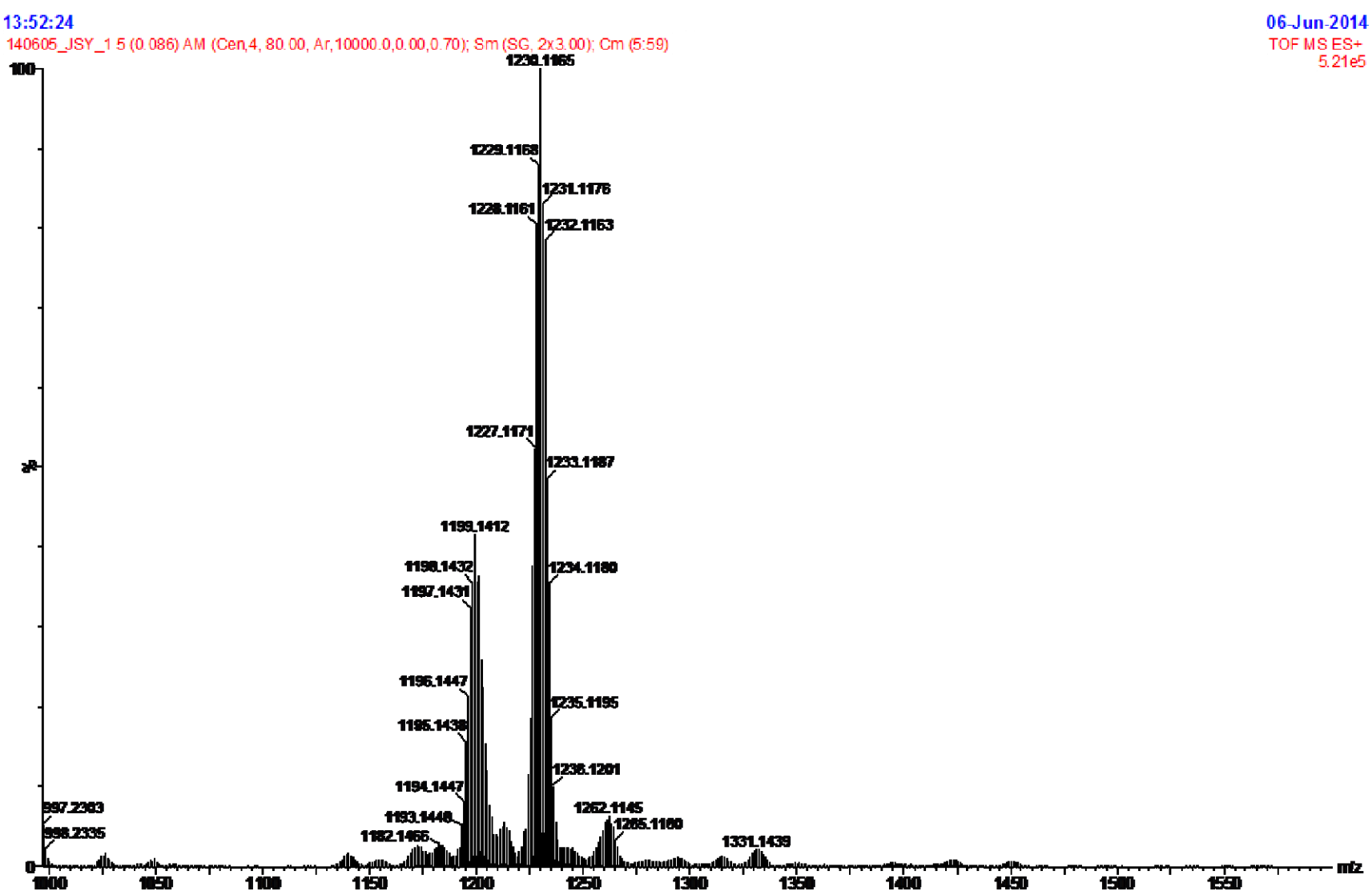

13:52:24
06-Jun-2014
140605_JSY_1 5 (0.086) AM (Cen,4, 80.00, Ar,10000.0,0.00,0.70); Sm (SG, 2x3.00); Cm (5:59)
TOF MS ES+
5.21e5
100
%
0
1238.1165
1229.1168
1231.1176
1228.1161
1232.1163
1227.1171
1233.1187
1199.1412
1198.1432
1234.1189
1197.1431
1196.1447
1235.1195
1195.1438
1236.1201
1194.1447
997.2363
1193.1448
1262.1145
998.2335
1265.1160
1192.1466
1331.1439
m/z
1000
1050
1100
1150
1200
1250
1300
1350
1400
1450
1500
1550

Figure S3. Absorption spectra of L1(10 μM) titration of Cd^{2+}

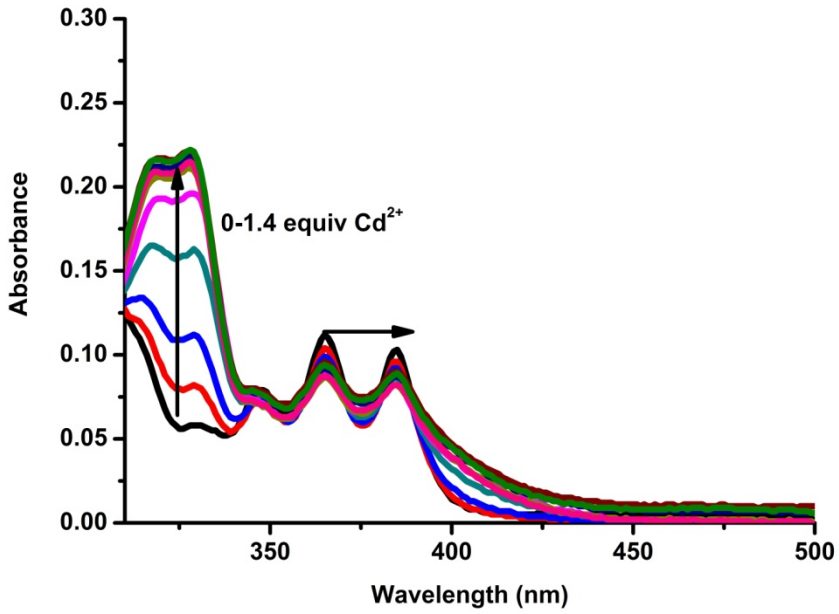


Figure S4. The determination **L1-Cd(II)** complex of the detection limit (LOD) for PPi

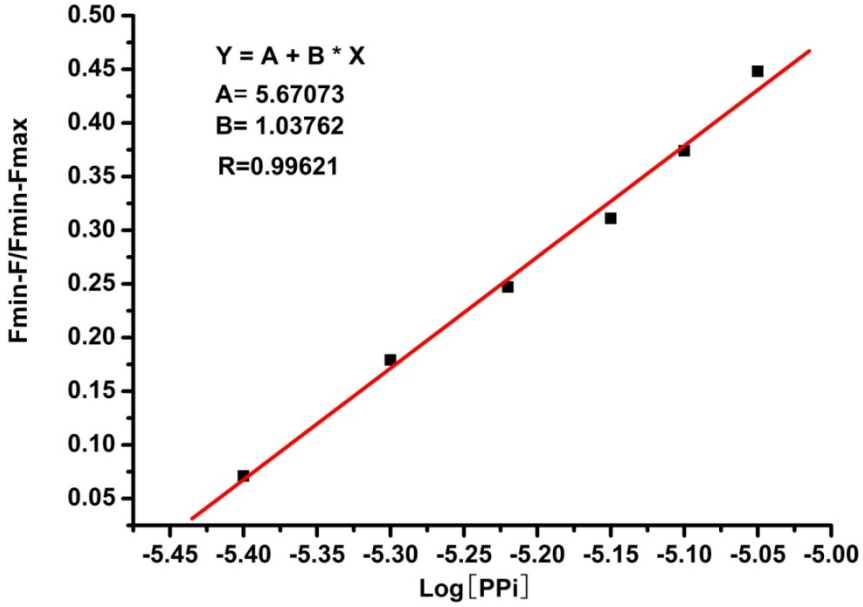


Figure S5. Mass spectral analysis for **L1-Cd(II)** interaction with PPi

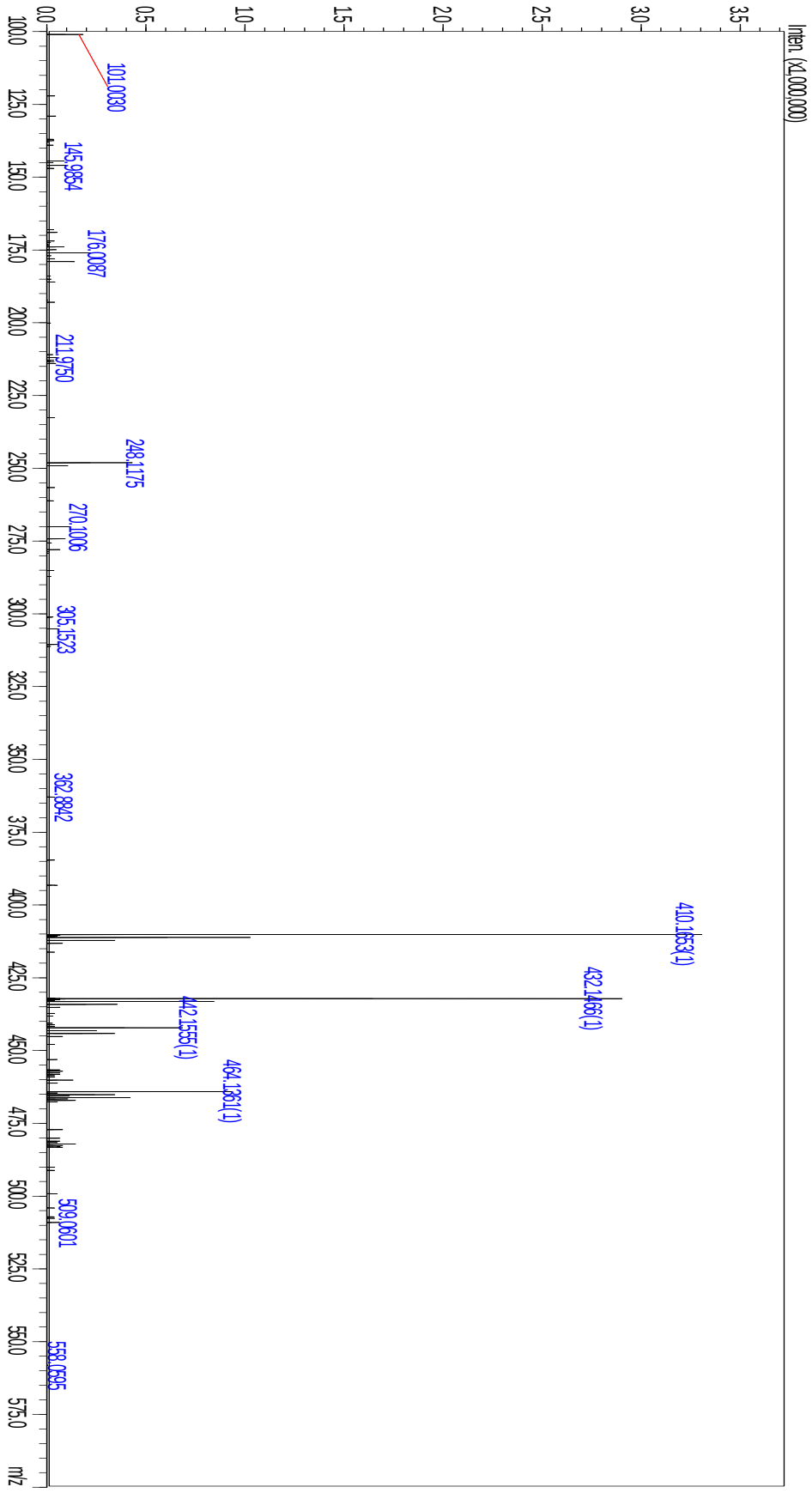


Figure S6. Absorption spectra of **L1** (10 μM), **L1-Cd(II)** complex(10 μM), and **L1-Cd(II)** complex (10 μM) with PPi (10 μM)

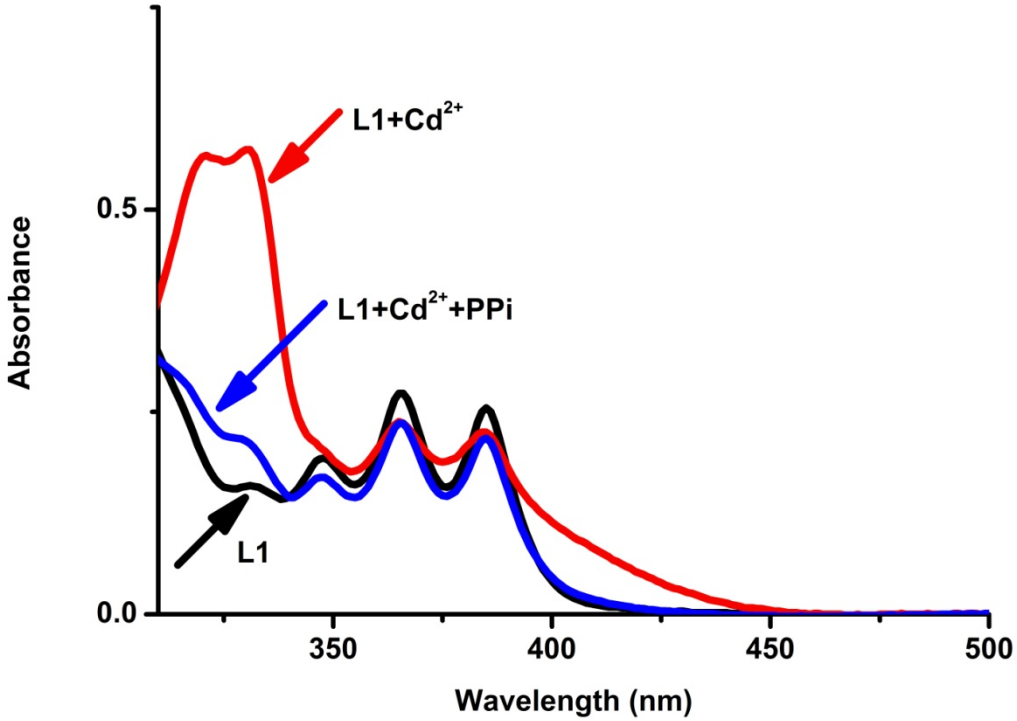


Figure S7. ^{1}H NMR spectra of **L1**

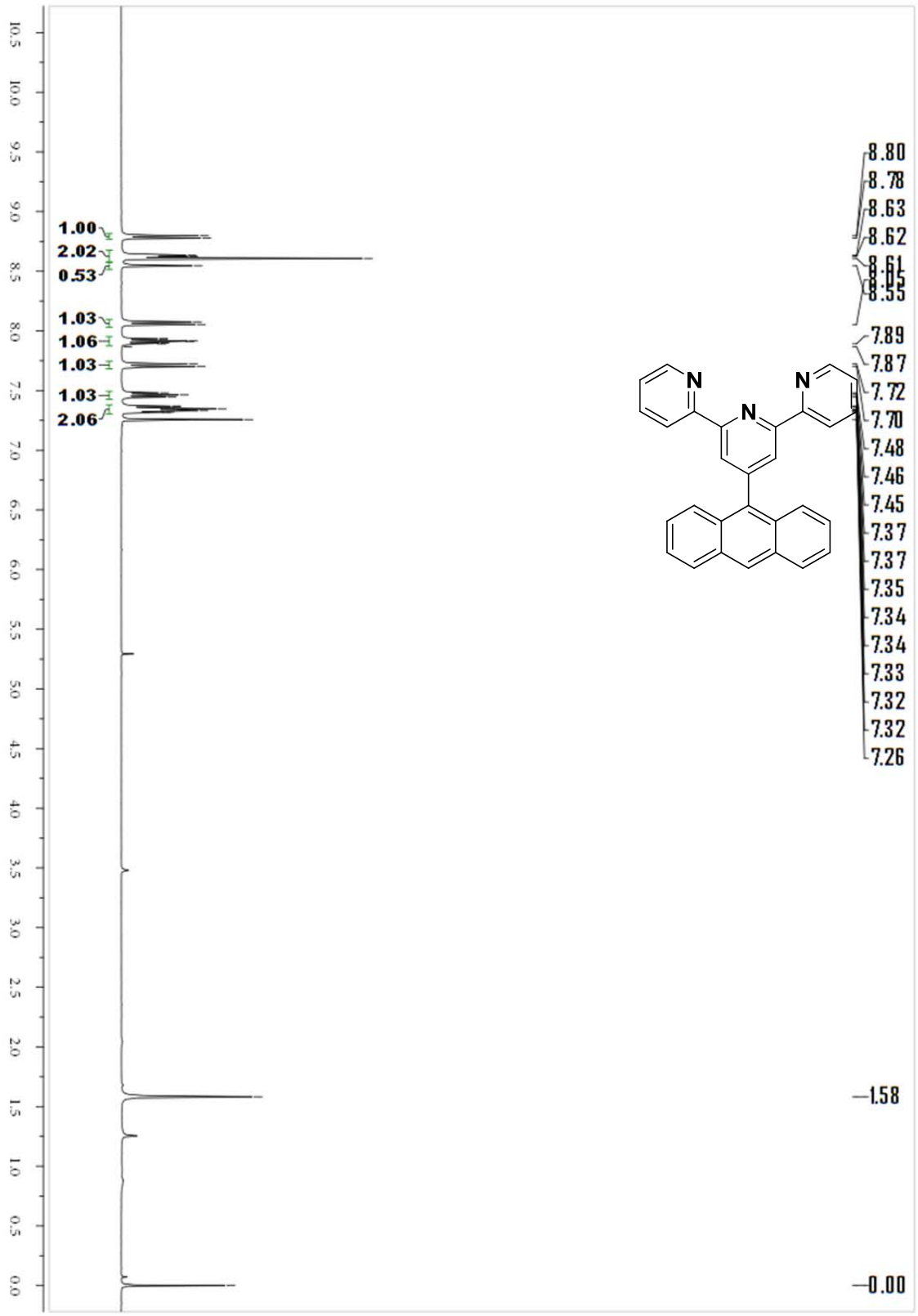


Figure S8. ^{13}C NMR spectra of **L1**

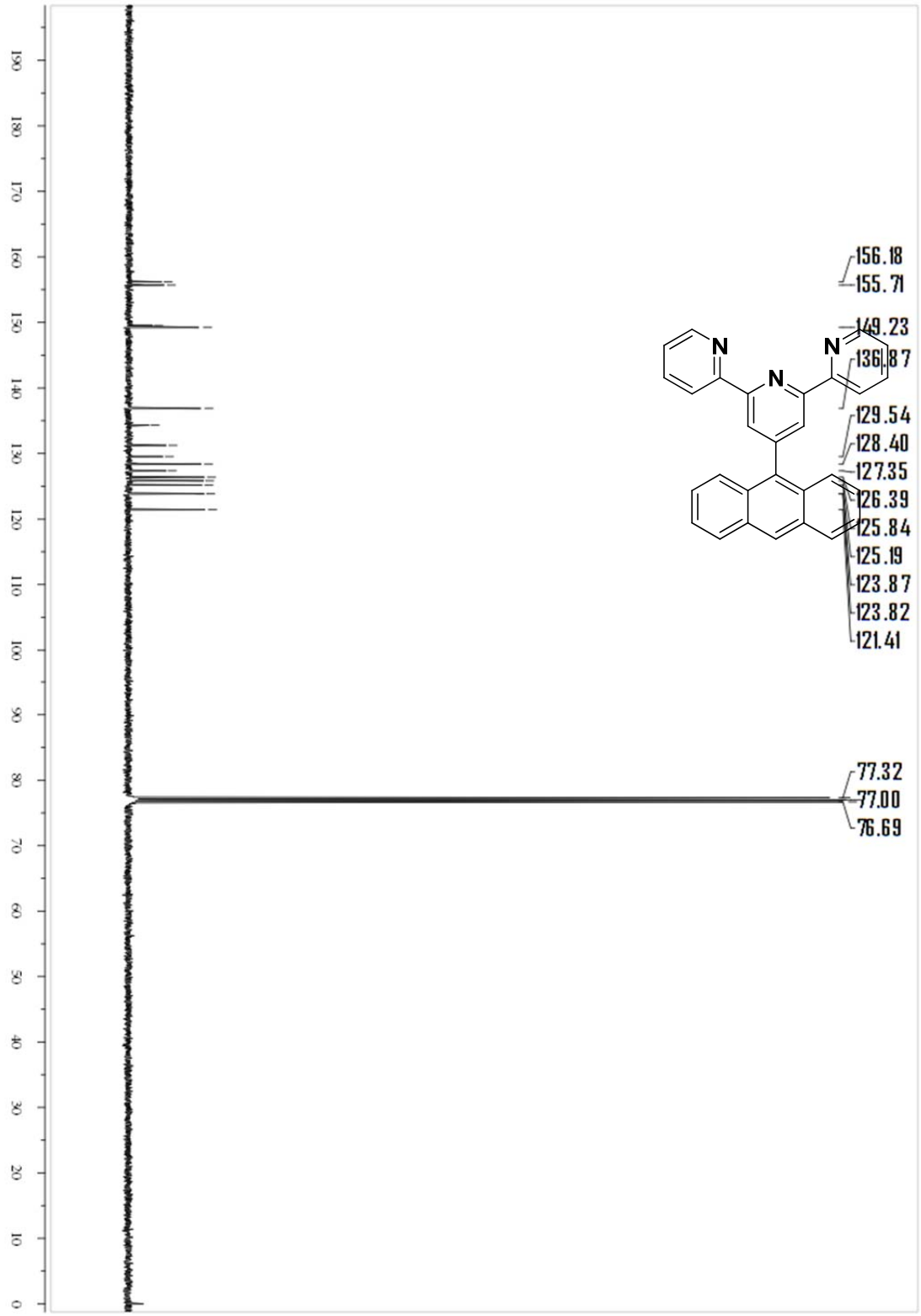


Figure S9. Mass spectrometry (HRMS) of **L1**

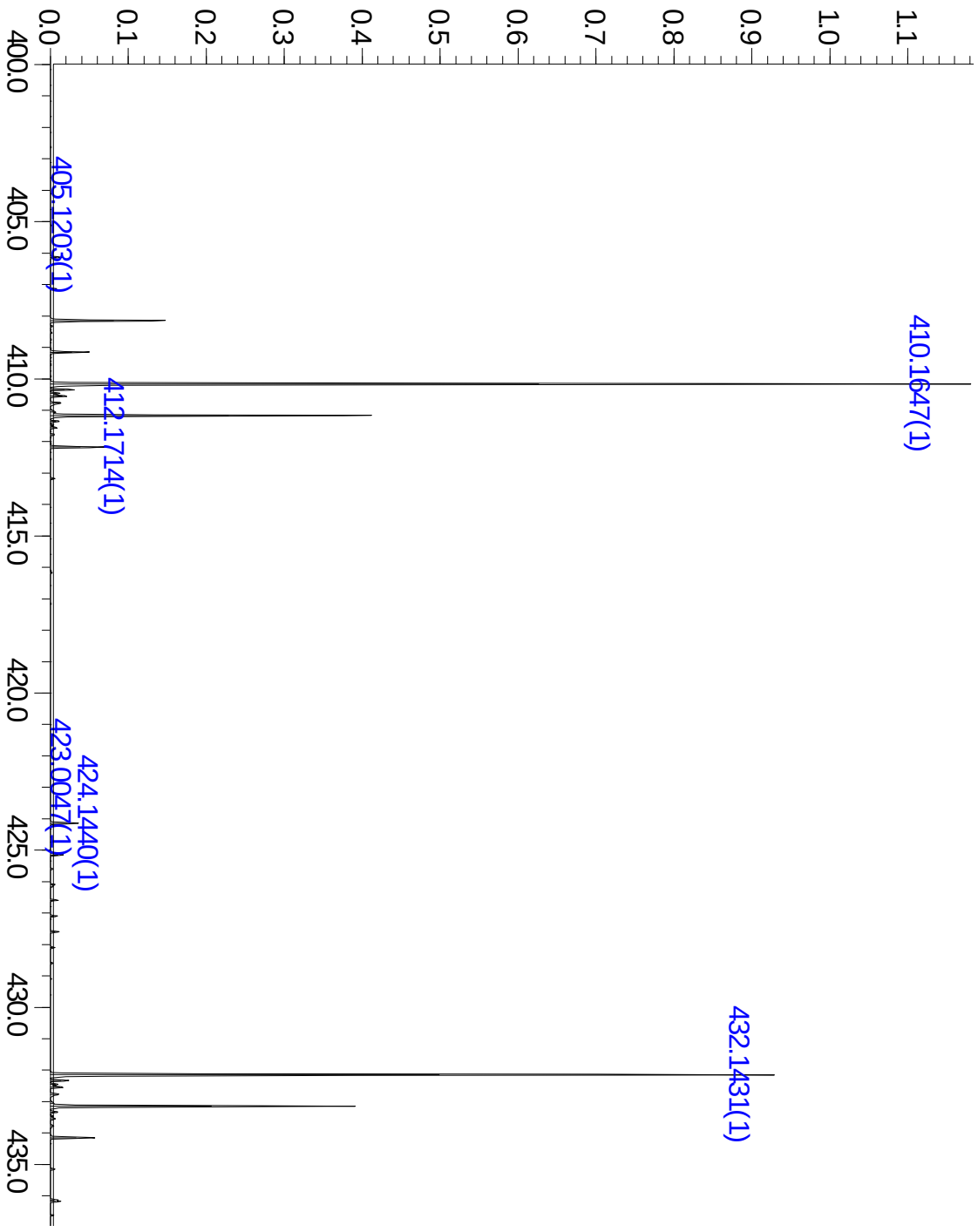


Figure S10. ^{1}H NMR spectra of **L1-Cd(II)** complex

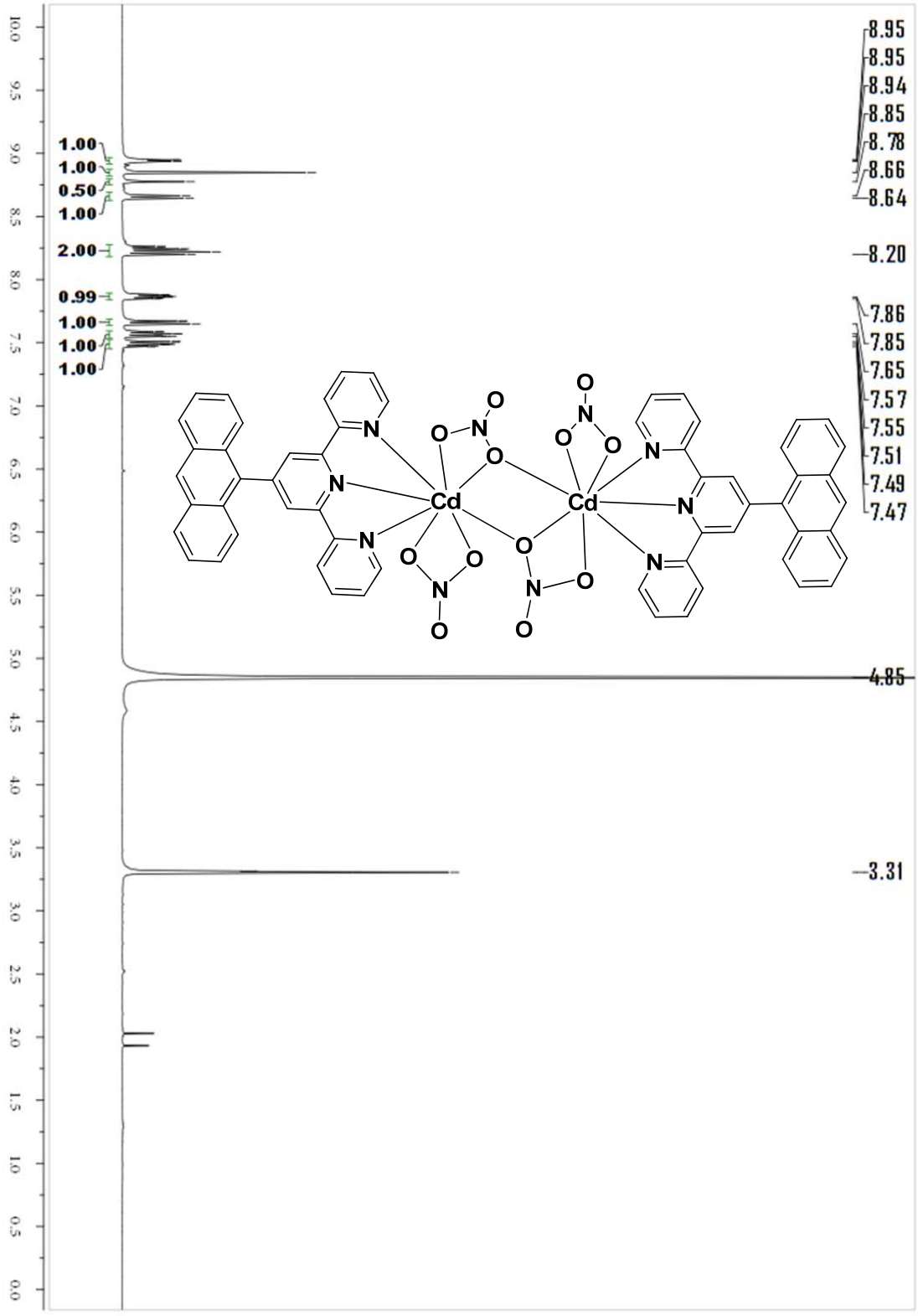


Figure S11. ^{13}C NMR spectra of **L1-Cd(II)** complex

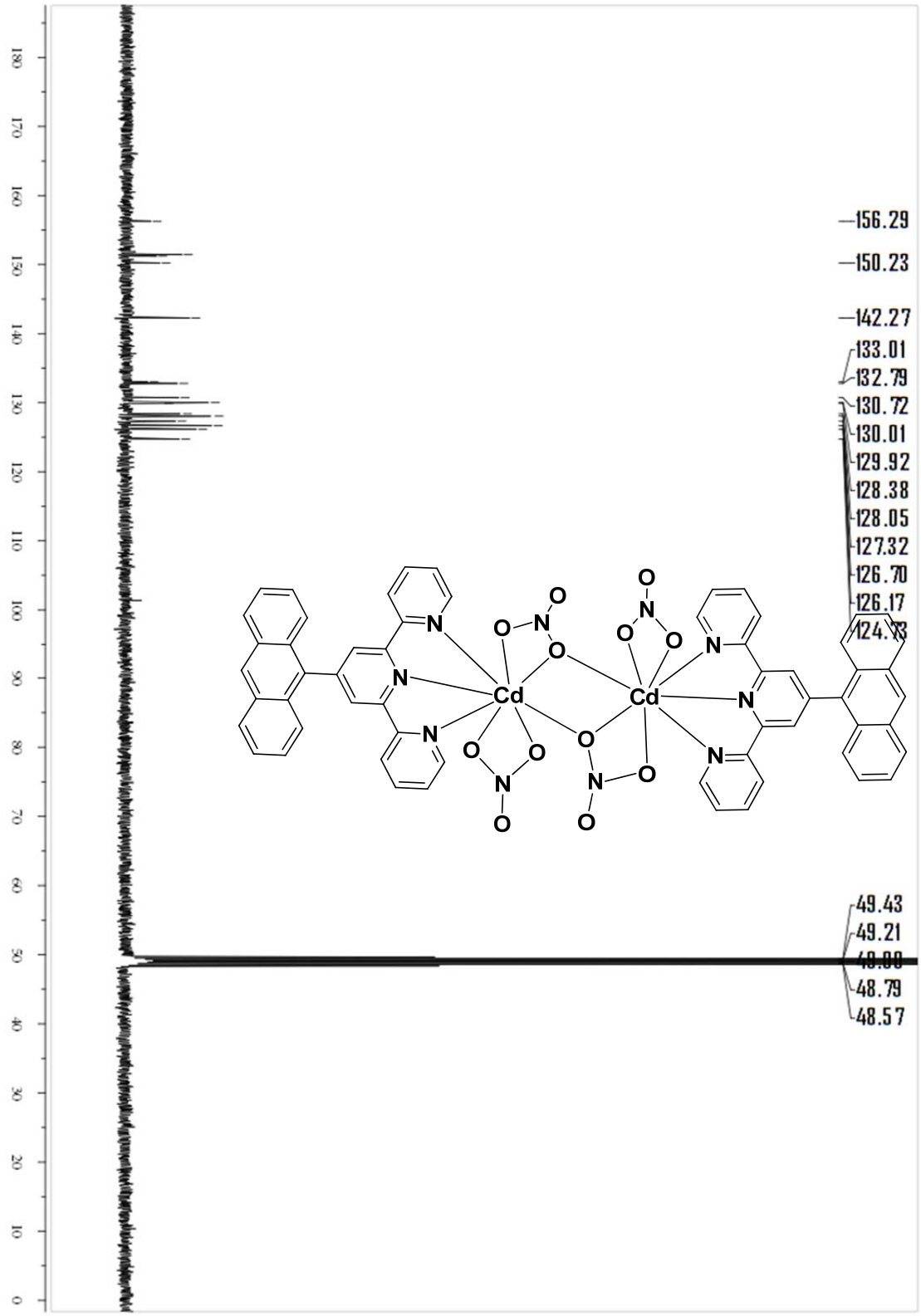


Figure S12. XRD structure of **L1-Cd(II)** complex, details of band angles, bond lengths

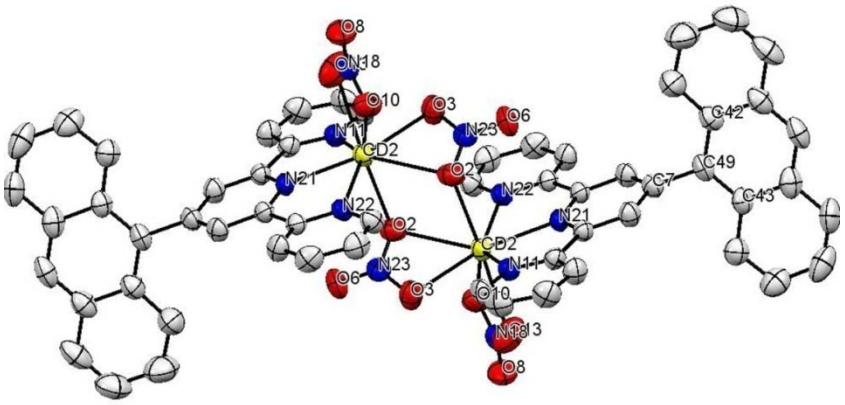


Table S1. Bond Lengths for L1-Cd(II) complex.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
Cd2	$O2^1$	2.544(4)	C44	C9	1.391(9)
Cd2	O2	2.591(3)	C44	C25	1.363(7)
Cd2	$O3^1$	2.352(3)	C46	C43	1.422(7)
Cd2	O10	2.462(4)	C46	C47	1.402(8)
Cd2	O13	2.504(4)	N11	C6	1.331(6)
Cd2	N21	2.311(3)	N11	C29	1.335(6)
Cd2	N22	2.359(3)	C43	C25	1.419(7)
Cd2	N11	2.363(3)	C47	C12	1.370(8)
O2	$Cd2^1$	2.544(4)	C48	C33	1.365(9)
O2	N23	1.256(5)	C1	C6	1.505(6)
O3	$Cd2^1$	2.352(3)	C1	C20	1.367(6)
O3	N23	1.274(5)	C4	C18	1.373(7)
O6	N23	1.214(5)	C6	C13	1.391(6)
O8	N18	1.210(5)	C7	C16	1.378(6)
O10	N18	1.246(5)	C7	C20	1.399(6)
O13	N18	1.242(6)	C12	C22	1.426(8)
N21	C1	1.339(5)	C13	C40	1.377(6)
N21	C38	1.335(5)	C16	C38	1.377(6)
N22	C4	1.348(6)	C18	C24	1.360(7)
N22	C35	1.331(5)	C22	C41	1.339(9)
C45	C46	1.418(8)	C24	C32	1.369(7)
C45	C9	1.352(9)	C27	C29	1.378(7)
C49	C42	1.404(7)	C27	C40	1.354(7)
C49	C43	1.410(6)	C32	C35	1.385(6)
C49	C7	1.499(6)	C33	C41	1.409(10)
C42	C48	1.426(7)	C35	C38	1.505(6)

C42	C12	1.438(7)	

Table S2. Bond Angles for L1-Cd(II) complex.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
O2[1]	Cd2	O2	69.48(13)	C48	C42	C12	117.4(5)
O3[1]	Cd2	O2	92.88(12)	C25	C44	C9	120.5(6)
O3[1]	Cd2	O2[1]	51.92(11)	C45	C46	C43	118.7(5)
O3[1]	Cd2	O10	81.05(13)	C47	C46	C45	121.6(5)
O3[1]	Cd2	O13	77.49(15)	C47	C46	C43	119.7(5)
O3[1]	Cd2	N22	134.02(12)	C6	N11	Cd2	117.4(3)
O3[1]	Cd2	N11	86.94(12)	C6	N11	C29	118.4(4)
O10	Cd2	O2	149.37(12)	C29	N11	Cd2	124.3(3)
O10	Cd2	O2[1]	83.58(11)	C49	C43	C46	118.7(4)
O10	Cd2	O13	50.23(12)	C49	C43	C25	123.2(4)
O13	Cd2	O2	157.21(13)	C25	C43	C46	118.1(4)
O13	Cd2	O2[1]	117.02(13)	C12	C47	C46	121.9(5)
N21	Cd2	O2[1]	147.04(11)	O8	N18	O10	121.0(4)
N21	Cd2	O2	87.24(11)	O8	N18	O13	123.0(5)
N21	Cd2	O3[1]	156.53(12)	O13	N18	O10	115.9(4)
N21	Cd2	O10	110.02(12)	C33	C48	C42	120.6(6)
N21	Cd2	O13	93.56(14)	N21	C1	C6	115.4(3)
N21	Cd2	N22	69.45(11)	N21	C1	C20	121.3(4)
N21	Cd2	N11	70.05(11)	C20	C1	C6	123.2(4)
N22	Cd2	O2[1]	86.00(11)	N22	C4	C18	122.8(5)
N22	Cd2	O2	87.48(11)	N11	C6	C1	117.0(4)
N22	Cd2	O10	76.04(12)	N11	C6	C13	121.1(4)
N22	Cd2	O13	114.14(13)	C13	C6	C1	121.9(4)
N22	Cd2	N11	137.65(12)	C16	C7	C49	121.6(4)
N11	Cd2	O2	78.73(11)	C16	C7	C20	117.9(4)
N11	Cd2	O2[1]	124.39(11)	C20	C7	C49	120.5(4)
N11	Cd2	O10	130.34(12)	C45	C9	C44	120.5(5)
N11	Cd2	O13	80.15(12)	C47	C12	C42	119.4(5)
Cd2[1]	O2	Cd2	110.52(13)	C47	C12	C22	121.7(5)
N23	O2	Cd2[1]	91.3(3)	C22	C12	C42	118.9(5)
N23	O2	Cd2	112.6(2)	C40	C13	C6	119.5(4)
N23	O3	Cd2[1]	100.0(3)	C38	C16	C7	119.7(4)
N18	O10	Cd2	97.9(3)	C24	C18	C4	119.0(4)
O2	N23	O3	116.4(4)	C1	C20	C7	119.6(4)
O6	N23	O2	123.3(4)	C41	C22	C12	121.9(6)
O6	N23	O3	120.3(4)	C18	C24	C32	119.1(4)
N18	O13	Cd2	96.0(3)	C44	C25	C43	121.0(5)
C1	N21	Cd2	119.8(3)	C40	C27	C29	118.3(4)
C38	N21	Cd2	120.3(3)	N11	C29	C27	123.4(5)

C38	N21	C1	119.9(3)	C24	C32	C35	119.3(5)
C4	N22	Cd2	123.6(3)	C48	C33	C41	121.6(6)
C35	N22	Cd2	117.8(3)	N22	C35	C32	122.1(4)
C35	N22	C4	117.6(4)	N22	C35	C38	116.0(3)
C9	C45	C46	121.1(5)	C32	C35	C38	121.8(4)
C42	C49	C43	121.1(4)	N21	C38	C16	121.4(4)
C42	C49	C7	119.4(4)	N21	C38	C35	115.1(3)
C43	C49	C7	119.5(4)	C16	C38	C35	123.4(4)
C49	C42	C48	123.4(5)	C27	C40	C13	119.3(4)
C49	C42	C12	119.1(4)	C22	C41	C33	119.6(6)