

## Electronic Supplementary Information

Qiang Guo<sup>a</sup>, Ru-Fen Zhang<sup>\*a</sup>, Xue-Wen Hua<sup>b</sup>, Qian-Li Li<sup>a</sup>, Xiu-Mei Du<sup>a</sup>, Jing Ru<sup>a</sup>, Chun-Lin Ma<sup>\*a</sup>

*a* Institution of Functional Organic Molecules and Materials, School of Chemistry and Chemical Engineering, Liaocheng University, Liaocheng, 252059, China.

*b* College of Agriculture, Liaocheng University, 252000, Liaocheng, Shandong, China

E-mail: macl856@163.com zhangrf856@163.com

## Table of contents

### 1. X-ray crystallography

**Table S1.** Selected bond lengths [Å] and angles [°] for complex 1

**Table S2.** Selected bond lengths [Å] and angles [°] for complex 2

**Table S3.** Selected bond lengths [Å] and angles [°] for complex 3

**Table S4.** Selected bond lengths [Å] and angles [°] for complex 4

**Table S5.** Comparison of Sn-O bond length of reported organotin(IV) complexes.

### 2. Percentage inhibition of complexes 2 and 4

**Figure S1.** Percentage inhibition of complex 2

**Figure S2.** Percentage inhibition of complex 4

### 3. <sup>1</sup>H NMR spectra of complexes 1-4

**Figure S3-S6.** <sup>1</sup>H NMR spectra data of complexes 1-4

**Figure S7-S8.** <sup>1</sup>H NMR spectra data of HL<sub>1</sub> and HL<sub>2</sub>

### 4. <sup>13</sup>C NMR spectra of complexes 2-4

**Figure S9-S11.** <sup>13</sup>C NMR spectra data of complexes 2-4

**Figure S12-S13.** <sup>13</sup>C NMR spectra data of HL<sub>1</sub> and HL<sub>2</sub>

### 5. <sup>119</sup>Sn NMR spectra

**Figure S14.** <sup>119</sup>Sn NMR spectra data of complexes 2

**Figure S15.** <sup>119</sup>Sn NMR spectra data of complexes 3

**Figure S16.** <sup>119</sup>Sn NMR spectra data of complexes 4

### 6. HSQC of complex 2-4 and ligands

**Figure S17.** HSQC spectrum for complex 2

**Figure S18.** HSQC spectrum for HL<sub>1</sub>

**Figure S19.** HSQC spectrum for complex 3

**Figure S20.** HSQC spectrum for complex 4

**Figure S21.** HSQC spectrum for HL<sub>2</sub>

### 7. ADPs of complexes 2-4

**Figure S22.** Molecular structure of complex 2 which the ellipsoids are represented at 30% probability

**Figure S23.** Molecular structure of complex 3 which the ellipsoids are represented at 30% probability

**Figure S24.** Molecular structure of complex 4 which the ellipsoids are represented at 30% probability

## 1. X-ray crystallography

**Table S1.** Bond lengths (Å) and Bond angles (°) of Complex 1.

Bond lengths (Å)			
Sn(1)-O(1)	2.335(5)	Sn(1)-C(4)	2.108(8)
Sn(1)-C(3)	2.099(8)	Sn(1)-O(7)	2.075(5)
Sn(1)-O(7A)	2.022(5)	Sn(2)-O(4)	2.209(5)
Sn(2)-O(3)	2.499(5)	Sn(2)-O(1)	2.421(5)
Sn(2)-O(6)	2.321(5)	Sn(2)-C(7)	2.105(8)
Sn(2)-C(6)	2.093(8)	Sn(2)-O(7A)	2.078(5)
O(7)-Sn(1A)	2.022(5)	O(7)-Sn(2A)	2.078(5)

Bond angles (°)			
O(1)-Sn(1)-Sn(1A)	107.96(12)	C(4)-Sn(1)-Sn(1A)	110.2(2)
C(4)-Sn(1)-O(1)	90.9(3)	C(3)-Sn(1)-Sn(1A)	110.4(2)
C(3)-Sn(1)-O(1)	91.6(3)	C(3)-Sn(1)-C(4)	136.3(3)
O(7)-Sn(1)-Sn(1A)	36.71(13)	O(7A)-Sn(1)-Sn(1A)	37.83(13)
O(7)-Sn(1)-O(1)	144.57(17)	O(7A)-Sn(1)-O(1)	70.19(18)
O(7)-Sn(1)-C(4)	99.6(3)	O(7A)-Sn(1)-C(4)	112.7(3)
O(7)-Sn(1)-C(3)	103.2(3)	O(7A)-Sn(1)-C(3)	109.2(3)
O(7A)-Sn(1)-O(7)	74.5(2)	O(4)-Sn(2)-O(3)	147.91(16)
O(4)-Sn(2)-O(1)	142.47(16)	O(4)-Sn(2)-O(6)	76.43(17)
O(1)-Sn(2)-O(3)	69.61(15)	O(6)-Sn(2)-O(3)	71.49(17)
O(6)-Sn(2)-O(1)	141.04(17)	C(7)-Sn(2)-O(4)	94.5(3)
C(7)-Sn(2)-O(3)	84.1(3)	C(7)-Sn(2)-O(1)	87.7(3)
C(7)-Sn(2)-O(6)	86.4(3)	C(6)-Sn(2)-O(4)	96.6(3)
C(6)-Sn(2)-O(3)	81.1(3)	C(6)-Sn(2)-O(1)	89.6(3)
C(6)-Sn(2)-O(6)	86.4(3)	C(6)-Sn(2)-C(7)	165.0(3)
O(7A)-Sn(2)-O(4)	74.94(18)	O(7A)-Sn(2)-O(3)	137.15(17)
O(7A)-Sn(2)-O(1)	67.57(17)	O(7A)-Sn(2)-O(6)	151.36(18)
O(7A)-Sn(2)-C(7)	95.4(3)	O(7A)-Sn(2)-C(6)	97.2(3)
Sn(1A)-O(7)-Sn(2A)	123.4(2)	Sn(1)-O(7)-Sn(2A)	130.9(2)

Symmetry code for complex 1: A: 1-x, 2-y, 1-z.

**Table S2.** Bond lengths (Å) and Bond angles (°) of Complex **2**.

Bond lengths (Å)			
Sn(1)-O(1)	2.094(3)	Sn(1)-O(3)	2.199(4)
Sn(1)-O(6)	2.176(4)	Sn(1)-O(4)	2.099(4)
Sn(1)-C(1)	2.146(7)	Sn(1)-C(7)	2.136(6)
Bond angles (°)			
C(7)-Sn(1)-O(6)	162.9(2)	C(7)-Sn(1)-O(3)	87.3(2)
C(7)-Sn(1)-C(1)	105.1(3)	O(1)-Sn(1)-O(4)	163.76(14)
O(6)-Sn(1)-O(3)	76.89(14)	O(1)-Sn(1)-C(7)	99.3(2)
O(1)-Sn(1)-O(6)	84.72(15)	O(1)-Sn(1)-O(3)	81.32(14)
O(1)-Sn(1)-C(1)	91.5(2)	O(4)-Sn(1)-C(7)	91.3(2)
O(4)-Sn(1)-O(3)	87.05(15)	C(1)-Sn(1)-O(3)	166.7(2)
O(4)-Sn(1)-O(6)	81.62(15)	O(6)-Sn(1)-O(3)	87.05(15)
O(4)-Sn(1)-C(1)	97.5(2)	C(1)-Sn(1)-O(6)	91.3(2)
C(8)-C(7)-Sn(1)	120.8(5)	C(12)-C(7)-Sn(1)	122.8(5)
C(30)-O(6)-Sn(1)	123.3(3)	C(13)-O(3)-Sn(1)	125.8(3)
C(44)-O(1)-Sn(1)	134.1(3)	C(28)-O(4)-Sn(1)	133.4(3)
C(6)-C(1)-Sn(1)	119.3(3)	C(2)-C(1)-Sn(1)	123.2(3)

**Table S3.** Bond lengths (Å) and Bond angles (°) of Complex **3**

Bond lengths (Å)			
Sn(3)-O(13)	2.024(9)	Sn(3)-O(14)	2.065(9)
Sn(3)-C(37)	2.069(19)	Sn(3)-C(38)	2.039(15)
Sn(2)-O(1)	2.353(11)	Sn(2)-O(3)	2.372(12)
Sn(2)-O(7)	2.339(12)	Sn(2)-O(9)	2.420(10)
Sn(2)-O(13)	2.055(8)	Sn(4)-O(14)	2.094(9)
Sn(2)-C(18)	2.071(17)	Sn(2)-C(19)	2.031(14)
Sn(4)-O(4)	2.375(11)	Sn(4)-O(6)	2.346(10)
Sn(4)-O(12)	2.338(12)	Sn(4)-O(10)	2.342(10)
Sn(4)-C(41)	2.011(16)	Sn(4)-C(42)	2.020(18)
Sn(1)-O(13)	2.064(9)	Sn(1)-O(14)	1.991(10)
Sn(1)-C(39)	2.045(17)	Sn(1)-C(40)	2.089(15)
Sn(3)-O(7)	2.575(9)	Sn(3)-O(10)	2.697(9)
Sn(1)-O(1)	2.733(10)	Sn(1)-O(4)	2.607(8)

Bond angles (°)			
O(13)-Sn(3)-O(14)	75.6(4)	O(13)-Sn(3)-C(37)	106.5(7)
O(13)-Sn(3)-C(38)	105.1(6)	O(14)-Sn(3)-C(37)	104.3(6)
C(38)-Sn(3)-O(14)	106.1(5)	C(38)-Sn(3)-C(37)	140.4(8)
O(1)-Sn(2)-O(3)	72.2(4)	O(1)-Sn(2)-O(9)	144.2(4)
O(3)-Sn(2)-O(9)	72.9(4)	O(7)-Sn(2)-O(1)	143.7(4)
O(7)-Sn(2)-O(3)	144.7(4)	O(7)-Sn(2)-O(9)	72.5(4)
O(13)-Sn(2)-O(1)	72.5(4)	O(13)-Sn(2)-O(3)	144.4(4)
O(13)-Sn(2)-O(7)	70.5(4)	O(13)-Sn(2)-O(9)	142.7(4)
O(13)-Sn(2)-C(18)	95.6(5)	C(18)-Sn(2)-O(1)	90.6(7)
C(18)-Sn(2)-O(3)	89.0(6)	C(18)-Sn(2)-O(7)	92.1(6)
C(18)-Sn(2)-O(9)	81.3(6)	C(19)-Sn(2)-O(1)	96.8(6)
C(19)-Sn(2)-O(3)	81.5(5)	C(19)-Sn(2)-O(7)	89.5(6)
C(19)-Sn(2)-O(9)	85.4(5)	C(19)-Sn(2)-O(13)	98.6(5)
C(19)-Sn(2)-C(18)	165.4(6)	O(14)-Sn(4)-O(4)	69.7(3)
O(14)-Sn(4)-O(6)	142.6(4)	O(14)-Sn(4)-O(12)	144.7(4)
O(14)-Sn(4)-O(10)	72.8(4)	O(6)-Sn(4)-O(4)	73.1(3)

O(12)-Sn(4)-O(4)	145.4(3)	O(12)-Sn(4)-O(6)	72.6(4)
O(12)-Sn(4)-O(10)	72.0(4)	O(10)-Sn(4)-O(4)	142.5(4)
O(10)-Sn(4)-O(6)	144.0(4)	C(41)-Sn(4)-O(14)	96.3(5)
C(41)-Sn(4)-O(4)	90.9(5)	C(41)-Sn(4)-O(6)	88.4(6)
C(41)-Sn(4)-O(12)	84.0(5)	C(41)-Sn(4)-O(10)	94.8(5)
C(41)-Sn(4)-C(42)	169.0(7)	C(41)-Sn(4)-O(14)	94.8(5)
C(41)-Sn(4)-O(4)	93.0(6)	C(41)-Sn(4)-O(6)	82.8(6)
C(41)-Sn(4)-O(12)	87.0(6)	C(41)-Sn(4)-O(10)	88.4(6)
O(13)-Sn(1)-C(40)	108.4(5)	O(14)-Sn(1)-O(13)	76.3(4)
O(14)-Sn(1)-C(39)	106.4(6)	O(14)-Sn(1)-C(40)	107.9(6)
C(39)-Sn(1)-O(13)	105.7(6)	C(39)-Sn(1)-C(40)	136.1(6)
C(80)-O(1)-Sn(2)	136.8(11)	C(13)-O(3)-Sn(2)	133.3(11)
C(81)-O(7)-Sn(2)	136.7(14)	C(29)-O(9)-Sn(2)	137.3(11)
Sn(3)-O(13)-Sn(2)	127.2(5)	Sn(3)-O(13)-Sn(1)	103.4(4)
Sn(2)-O(13)-Sn(1)	129.3(5)	Sn(3)-O(14)-Sn(4)	126.6(5)
Sn(1)-O(14)-Sn(3)	104.6(4)	Sn(1)-O(14)-Sn(4)	128.8(4)
C(43)-O(4)-Sn(4)	141.3(11)	C(45)-O(6)-Sn(4)	135.1(10)
C(62)-O(12)-Sn(4)	136.1(11)	C(61)-O(10)-Sn(4)	137.3(11)

**Table S4.** Bond lengths (Å) and Bond angles (°) of Complex 4.

Bond lengths (Å)			
Sn(1)-O(1)	2.082(15)	Sn(1)-O(3)	2.143(12)
Sn(1)-O(4)	2.120(2)	Sn(1)-O(6)	2.170(15)
Sn(1)-C(1)	2.140(2)	Sn(1)-C(7)	2.160(19)
Bond angles (°)			
O(1)-Sn(1)-O(3)	83.5(7)	O(1)-Sn(1)-O(4)	160.4(6)
O(1)-Sn(1)-O(6)	81.5(7)	O(1)-Sn(1)-C(1)	96.0(9)
O(1)-Sn(1)-C(7)	95.7(9)	O(3)-Sn(1)-O(6)	77.8(5)
O(3)-Sn(1)-C(1)	89.6(6)	O(3)-Sn(1)-C(7)	168.2(7)
O(4)-Sn(1)-O(3)	81.5(7)	O(4)-Sn(1)-O(6)	83.0(7)
O(4)-Sn(1)-C(1)	96.4(9)	O(4)-Sn(1)-C(7)	96.4(10)
C(1)-Sn(1)-O(6)	167.3(6)	C(1)-Sn(1)-C(7)	102.2(8)
C(7)-Sn(1)-O(6)	90.4(7)	C(80)-O(1)-Sn(1)	130.0(16)
C(13)-O(3)-Sn(1)	127.1(13)	C(31)-O(4)-Sn(1)	129.6(19)
C(33)-O(6)-Sn(1)	122.4(15)	C(2)-C(1)-Sn(1)	118.6(16)
C(6)-C(1)-Sn(1)	123.6(17)	C(8)-C(7)-Sn(1)	116.5(17)
C(12)-C(7)-Sn(1)	124(2)		

**Table S5.** Comparison of Sn-O bond length of reported organotin(IV) complexes.

Organotin complexes	Bond length of Sn-O	Ref
$[(\text{Me}_2\text{Sn})_2(\text{O}_2\text{CCH}_2\text{S})_2\text{C}_2\text{N}_2\text{S}(\text{I}_3\text{-O})]_n$	2.011-2.288 Å	41
$\{[\text{Me}_2\text{Sn}(\text{cycloCH}_2)_2\text{CHCOO}]_2\text{O}\}_2$	2.224-2.317 Å	42
$[(\text{CH}_3)_2\text{Sn}(\text{OOC}_6\text{H}_4\text{OH})_2]$	2.016-2.557 Å	48
$[(n\text{-C}_4\text{H}_9)_2\text{Sn}(\text{OOC}_6\text{H}_4\text{OH})_2]$	2.104-2.632 Å	
$\text{Bu}_2\text{Sn}[\text{HL}^2]_2(\text{L}=4\text{-}(2\text{-hydroxynaphthylazo)benzoic acid})$	2.060-2.647 Å	49
$[(\text{Me}_2\text{Sn})_4\text{O}_2(\text{C}_{16}\text{H}_{17}\text{FN}_3\text{O}_3)_4]$	2.075 -2.499Å	Complex 1
$[\text{Ph}_2\text{Sn}(\text{C}_{16}\text{H}_{17}\text{FN}_3\text{O}_3)_2]$	2.094-2.199 Å	Complex 2
$[(\text{Me}_2\text{Sn})_4\text{O}_2(\text{C}_{18}\text{H}_{19}\text{FN}_3\text{O}_4)_4]$	1.991-2.420 Å	Complex 3
$[\text{Ph}_2\text{Sn}(\text{C}_{18}\text{H}_{19}\text{FN}_3\text{O}_4)_2]$	2.082-2.170 Å	Complex 4

## 2. Percentage inhibition of complexes 2 and 4

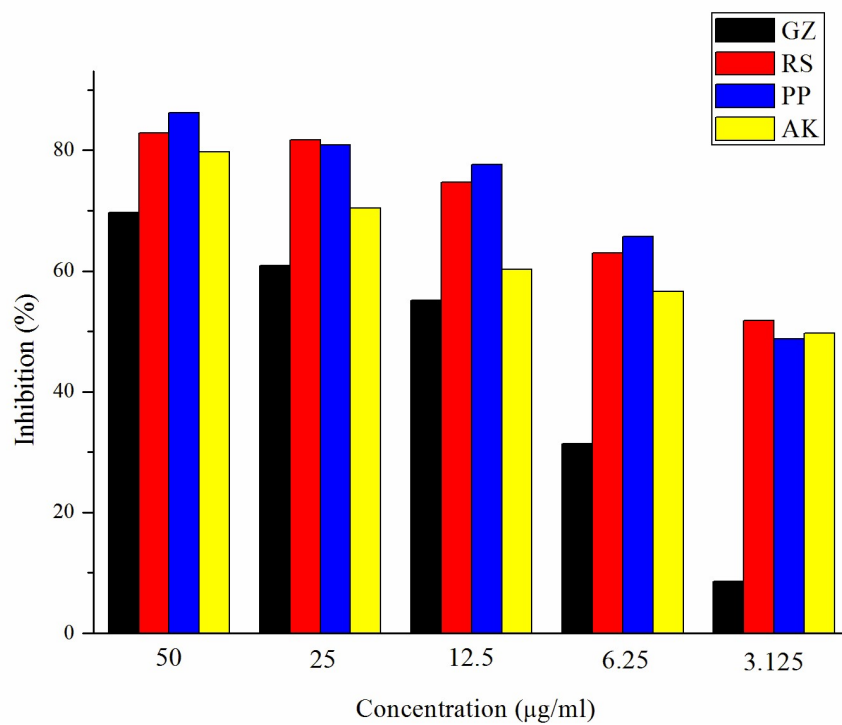


Figure S1. Percentage inhibition of complex 2

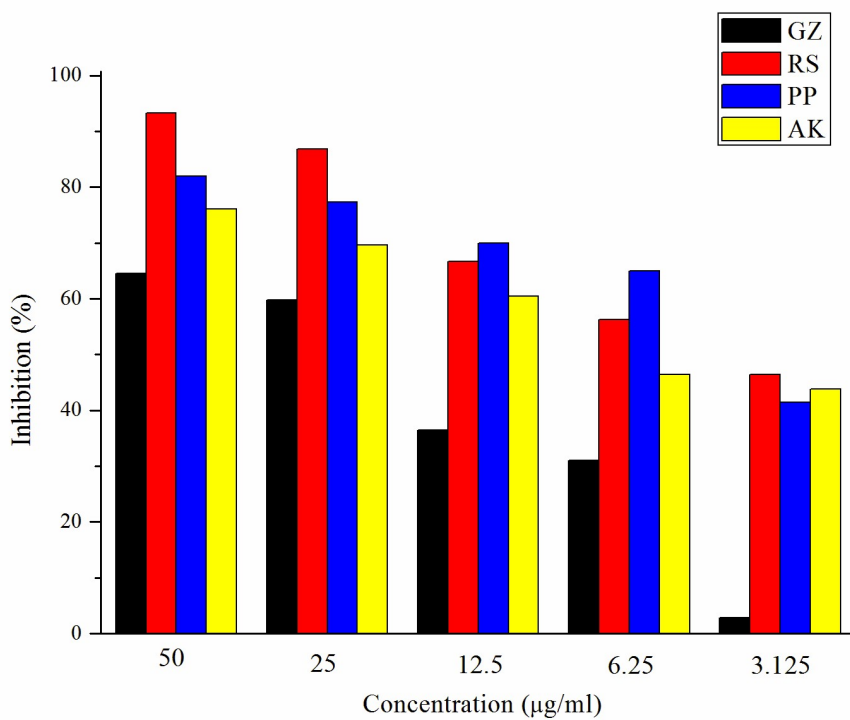


Figure S2. Percentage inhibition of complex 4

### 3. <sup>1</sup>H NMR spectra



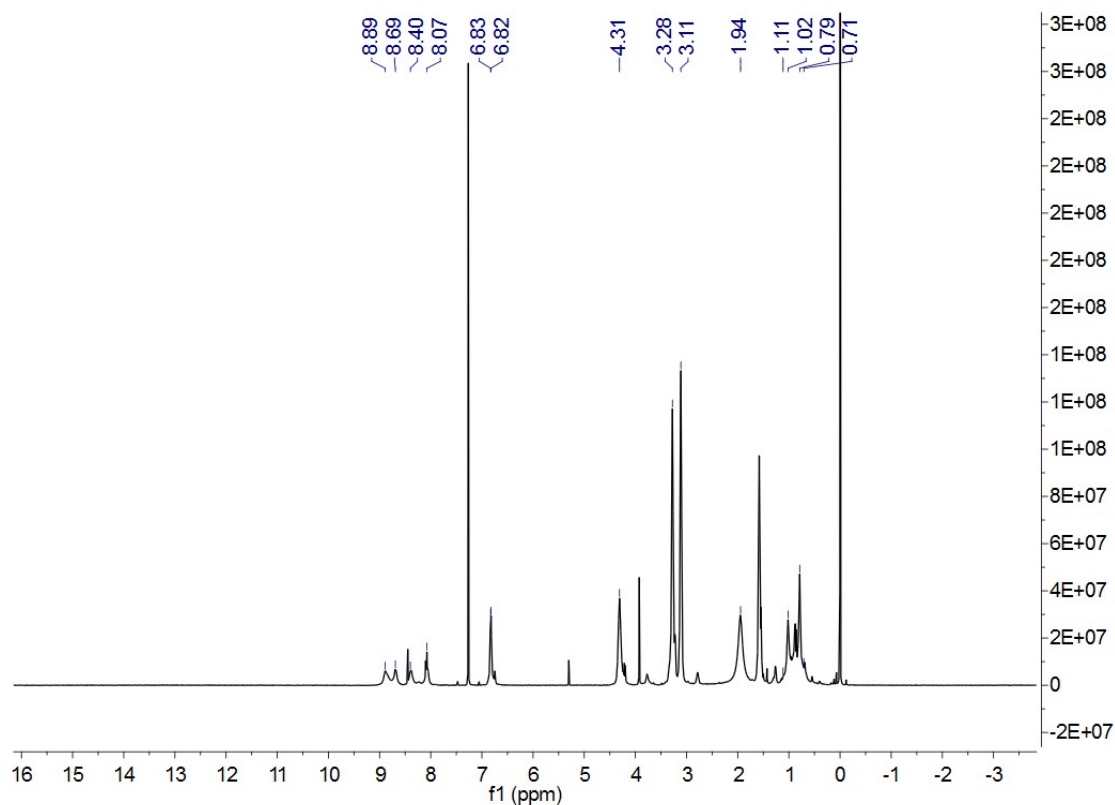


Figure S3.  $^1\text{H}$  NMR spectra( $\text{CDCl}_3$ , 500.00 MHz, ppm) data of complex 1

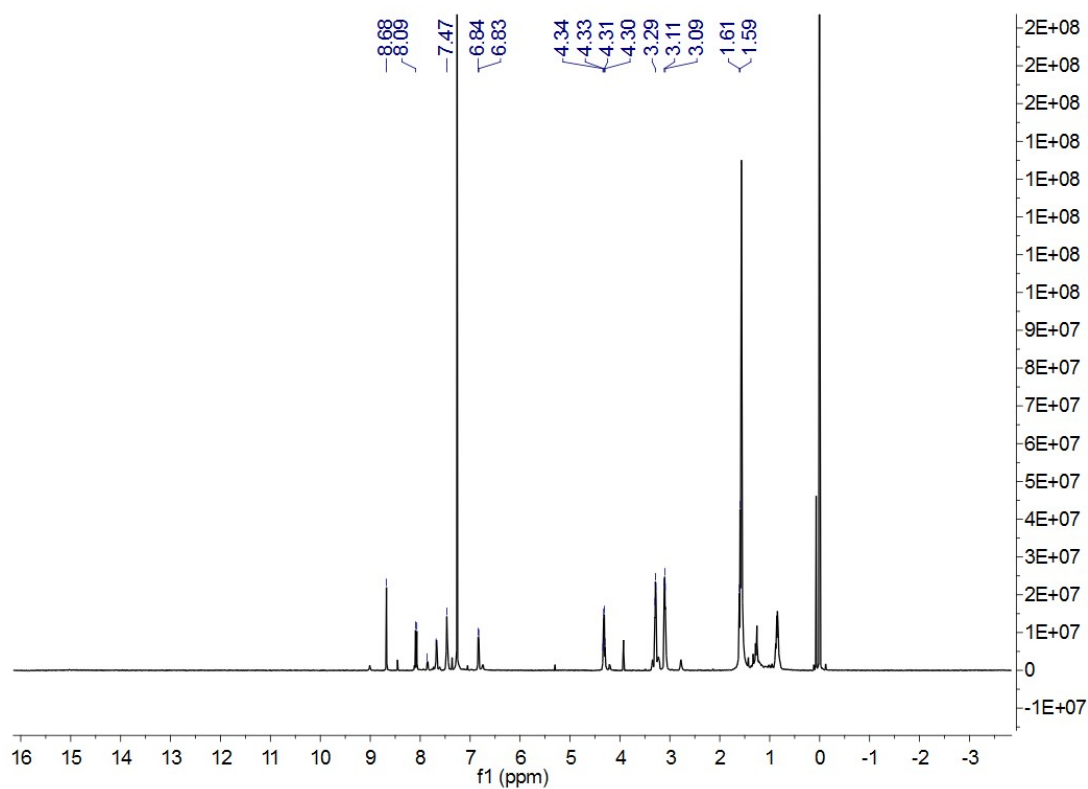


Figure S4.  $^1\text{H}$  NMR spectra( $\text{CDCl}_3$ , 500.00 MHz, ppm) data of complex 2

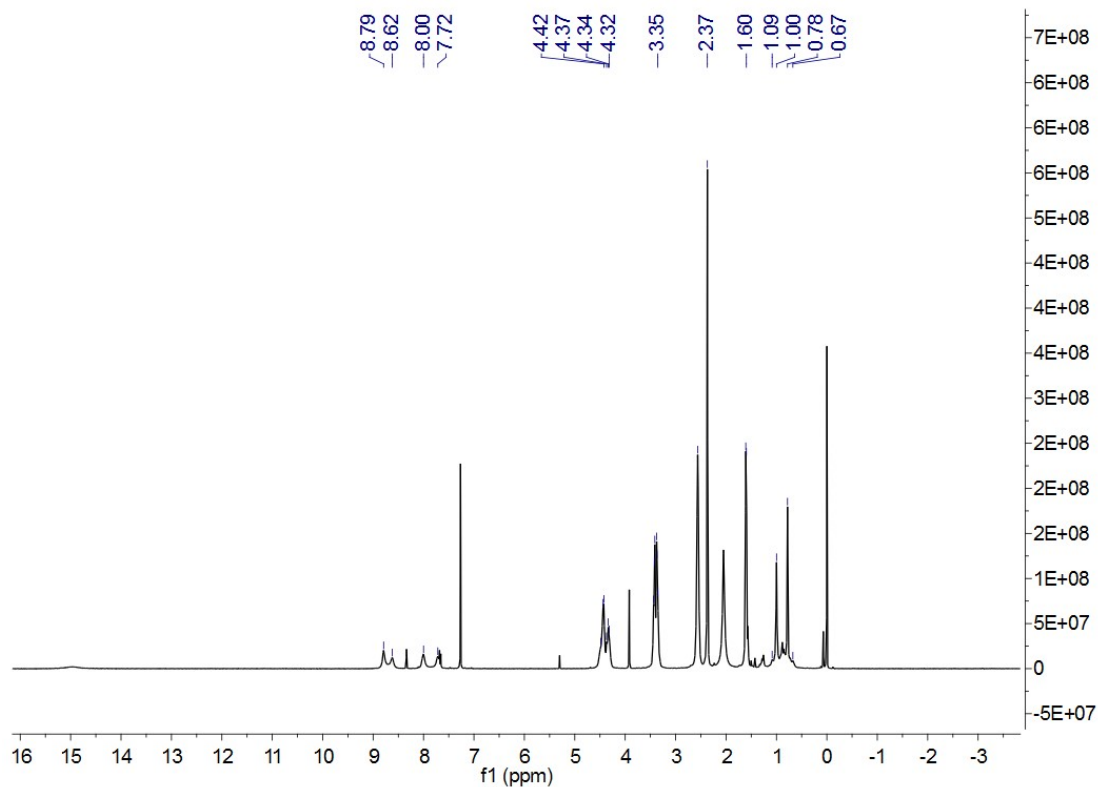


Figure S5.  $^1\text{H}$  NMR spectra( $\text{CDCl}_3$ , 500.00 MHz, ppm) data of complex 3

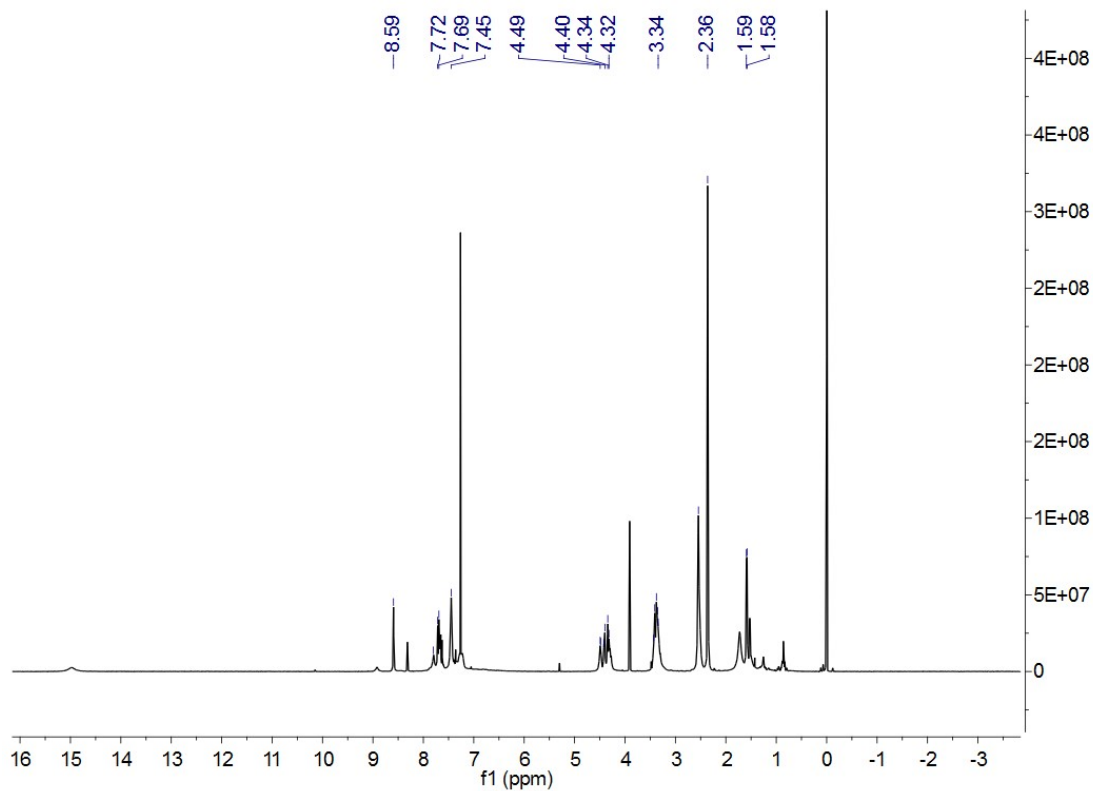


Figure S6.  $^1\text{H}$  NMR spectra( $\text{CDCl}_3$ , 500.00 MHz, ppm) data of complex 4

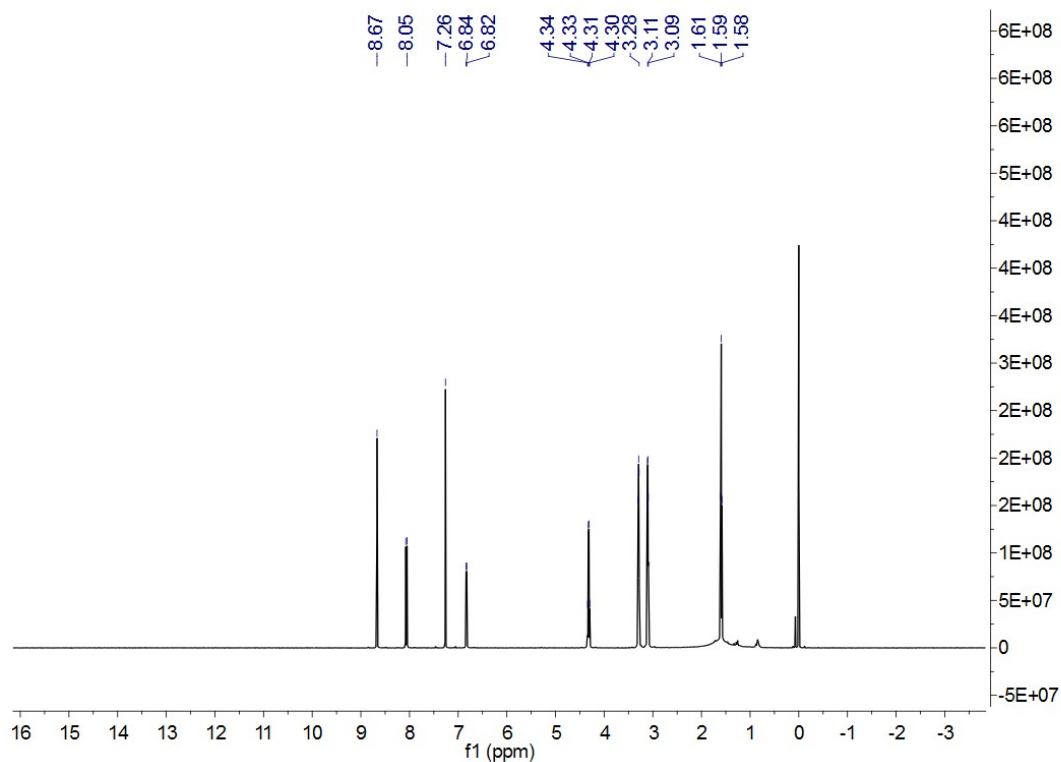


Figure S7. <sup>1</sup>H NMR spectra(CDCl<sub>3</sub>, 500.00 MHz, ppm) data of HL<sub>1</sub>

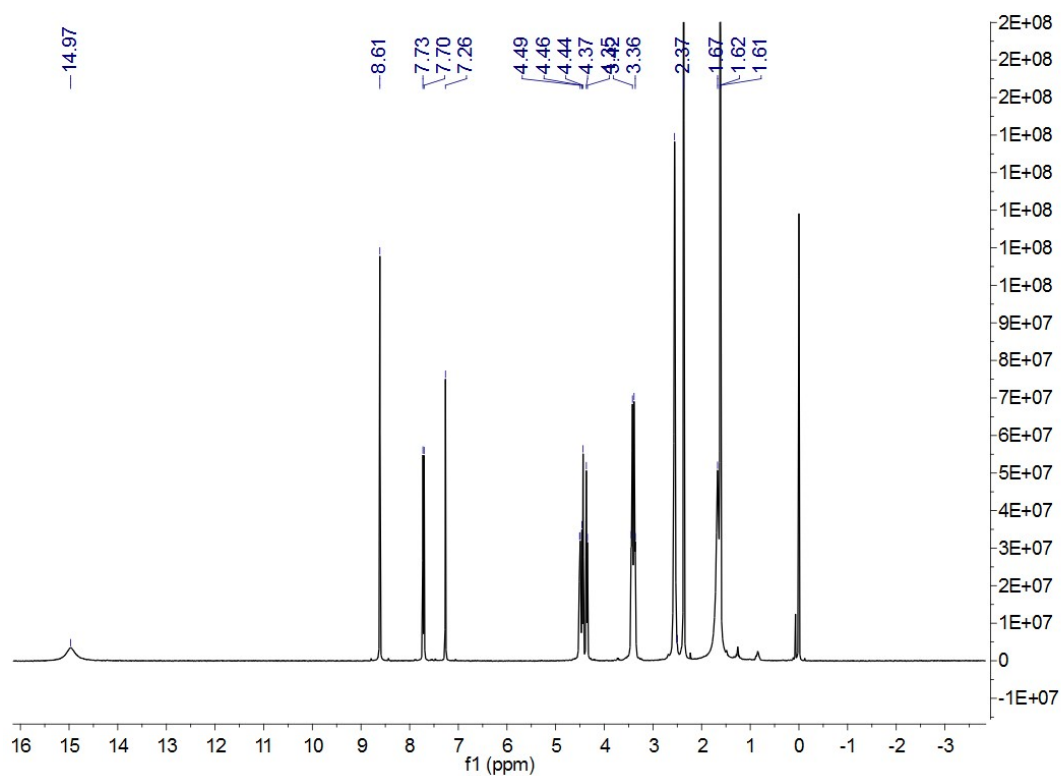


Figure S8. <sup>1</sup>H NMR spectra(CDCl<sub>3</sub>, 500.00 MHz, ppm) data of HL<sub>2</sub>

#### 4. $^{13}\text{C}$ NMR spectra

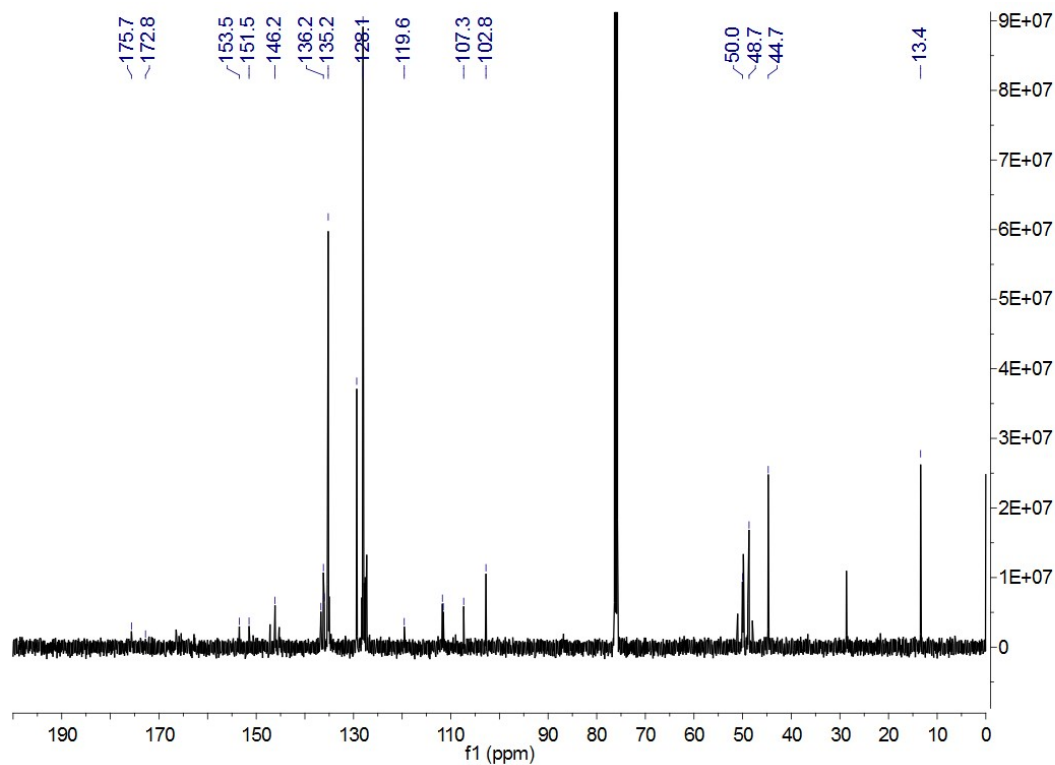


Figure S9.  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 125.7 MHz ppm) data of complex 2

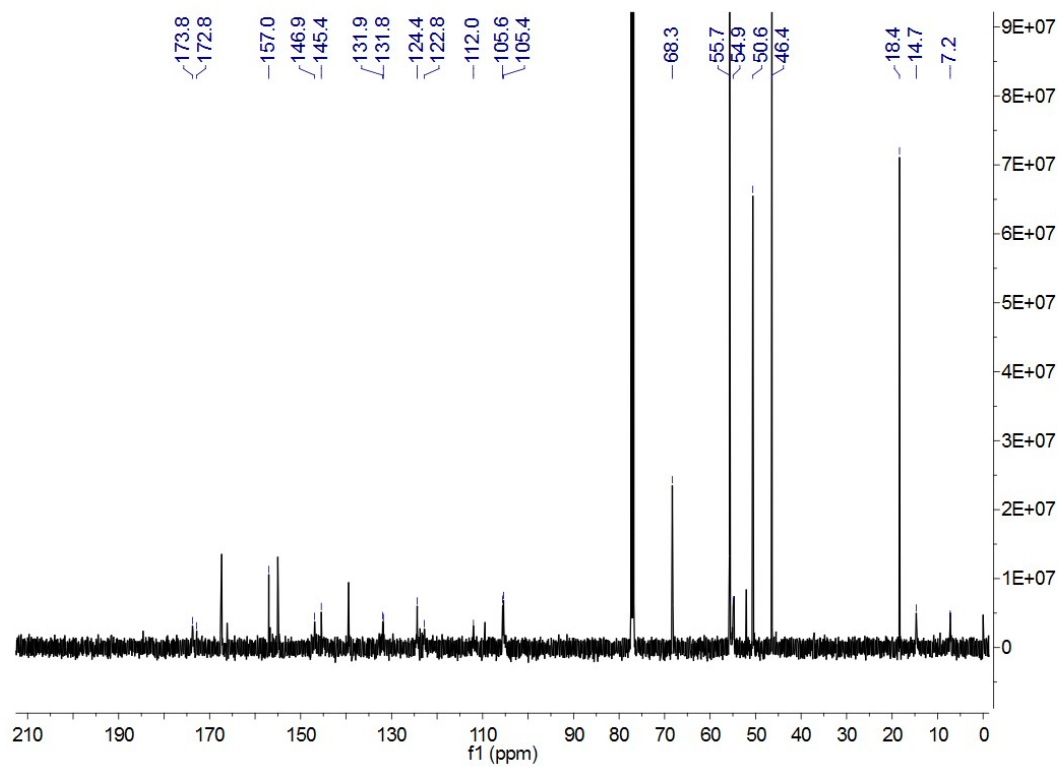


Figure S10.  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 125.7 MHz ppm) data of complex 3

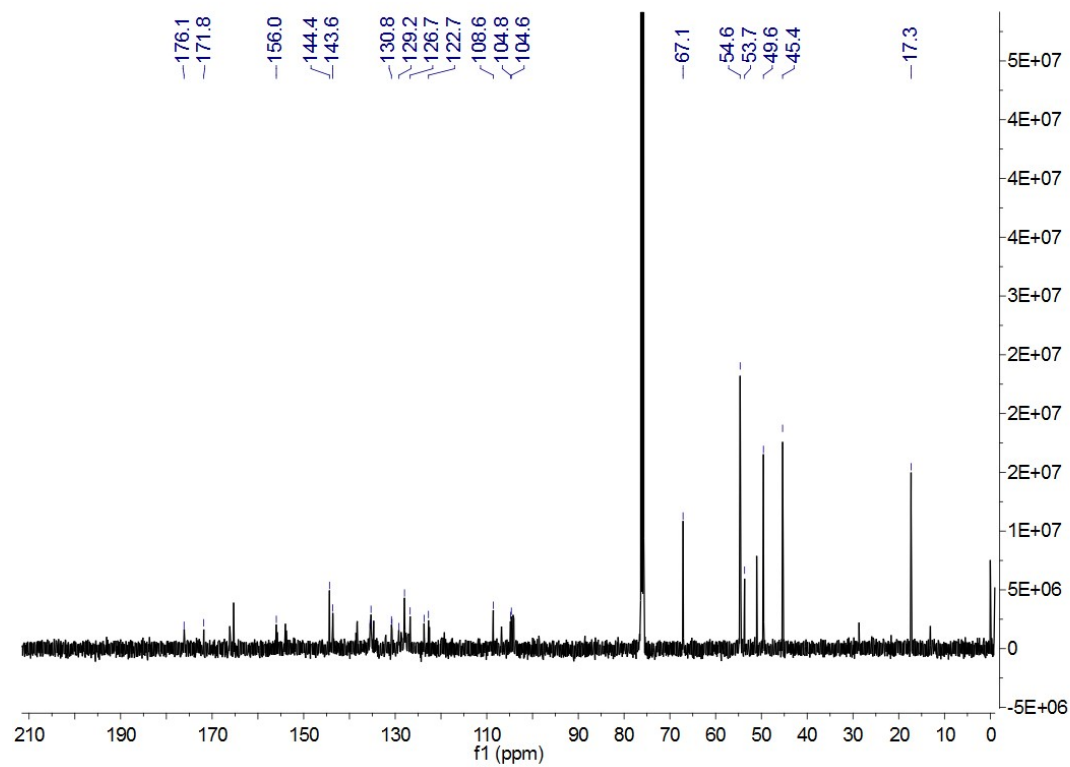


Figure S11.  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 125.7 MHz ppm) data of complex 4

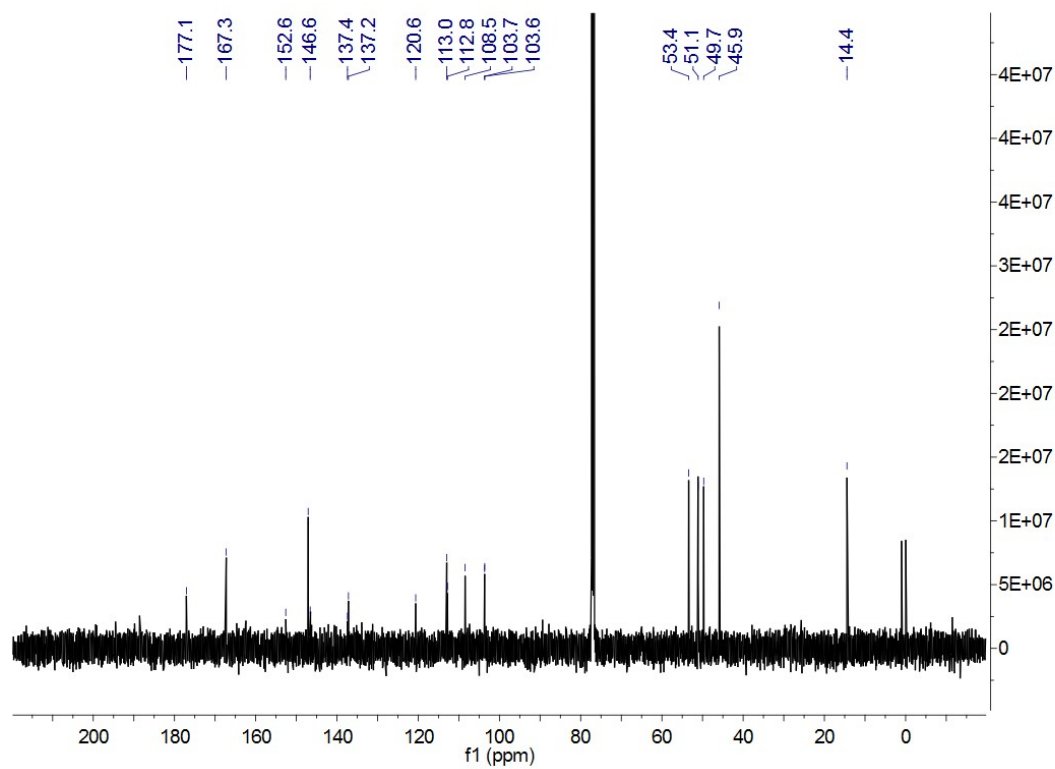


Figure S12.  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 125.7 MHz ppm) data of HL<sub>1</sub>

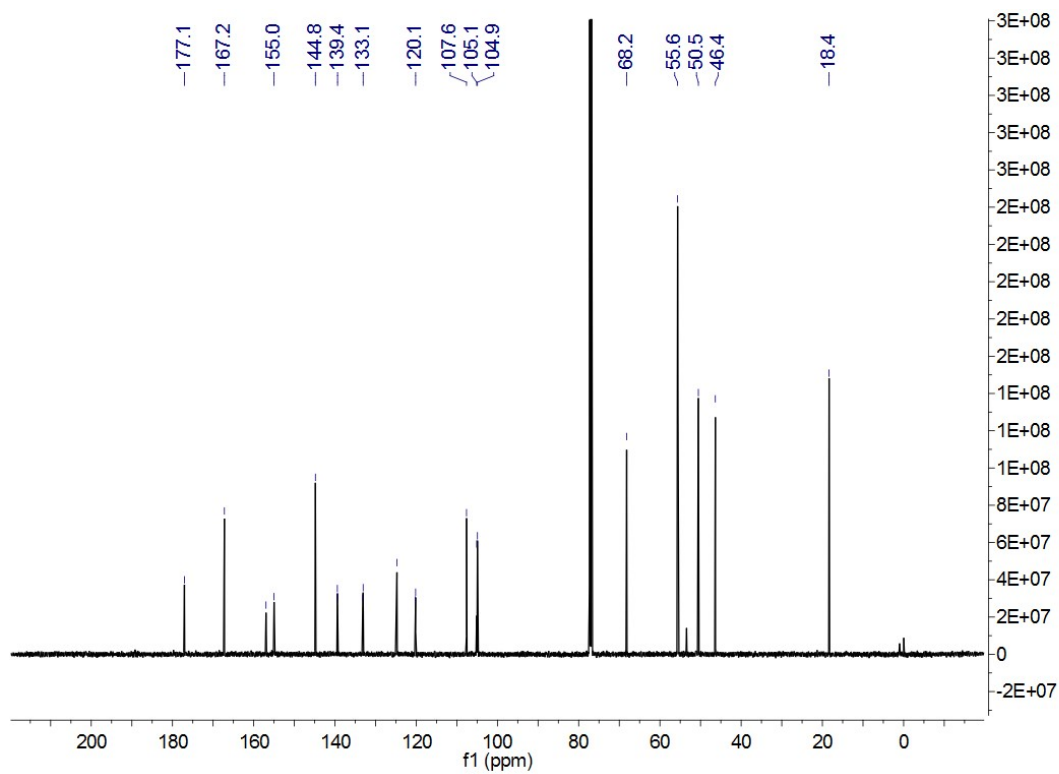


Figure S13.  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 125.7 MHz ppm) data of  $\text{HL}_2$

### 5. $^{119}\text{Sn}$ NMR spectra

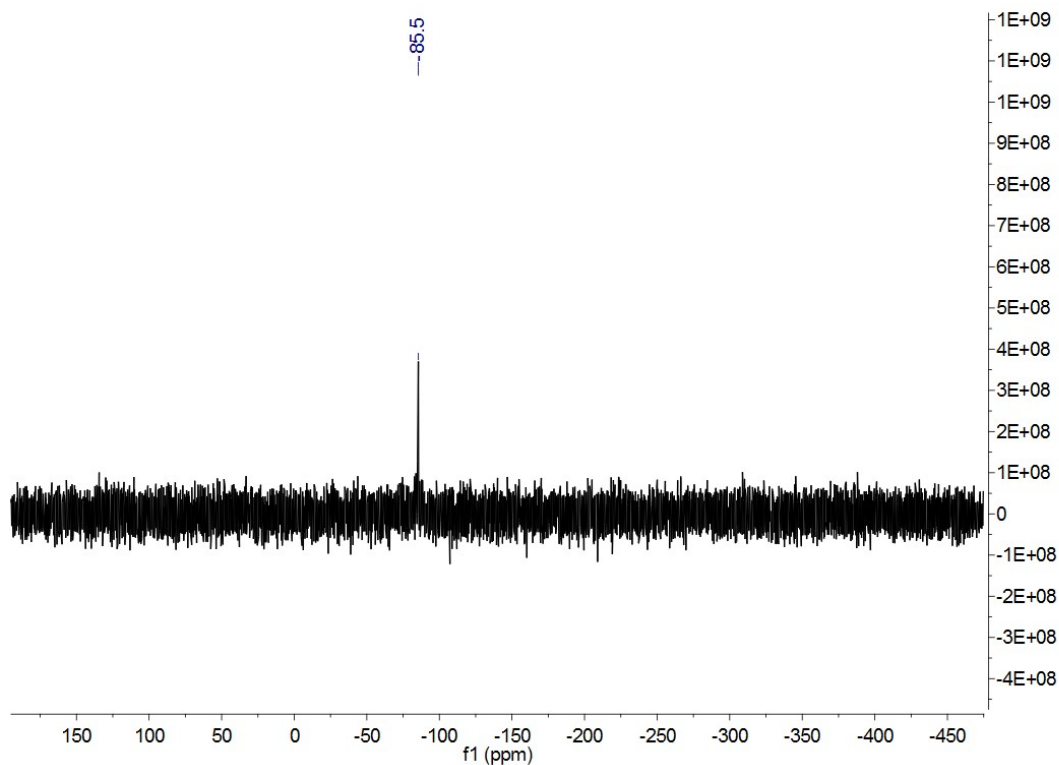
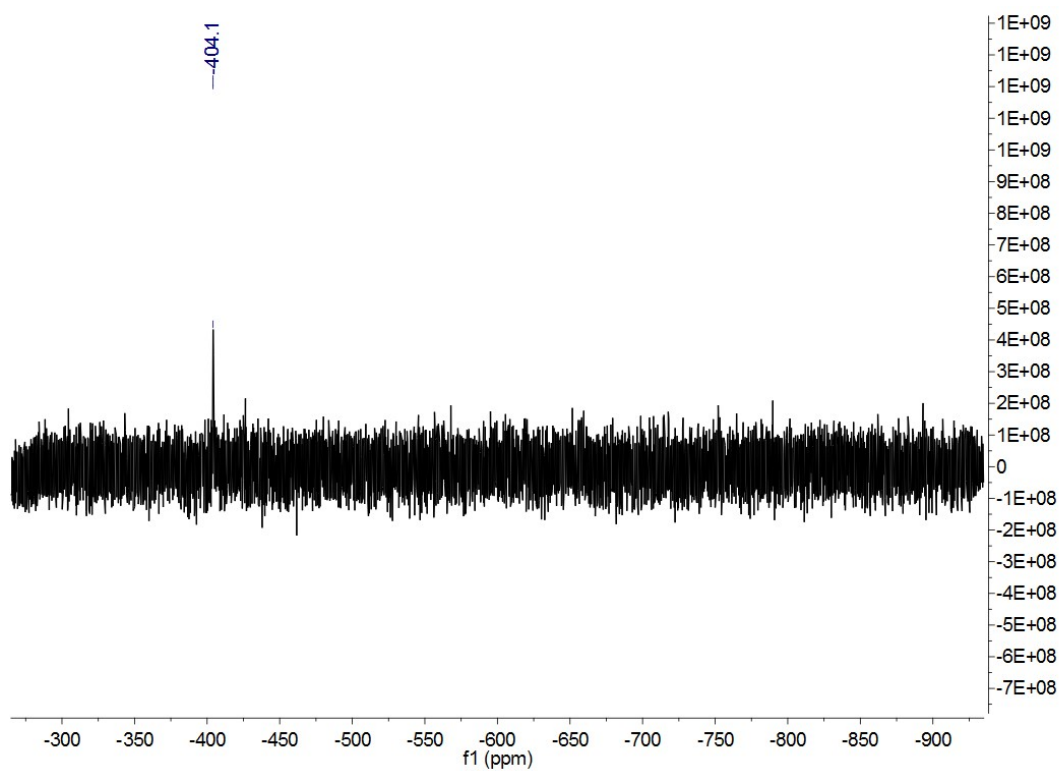
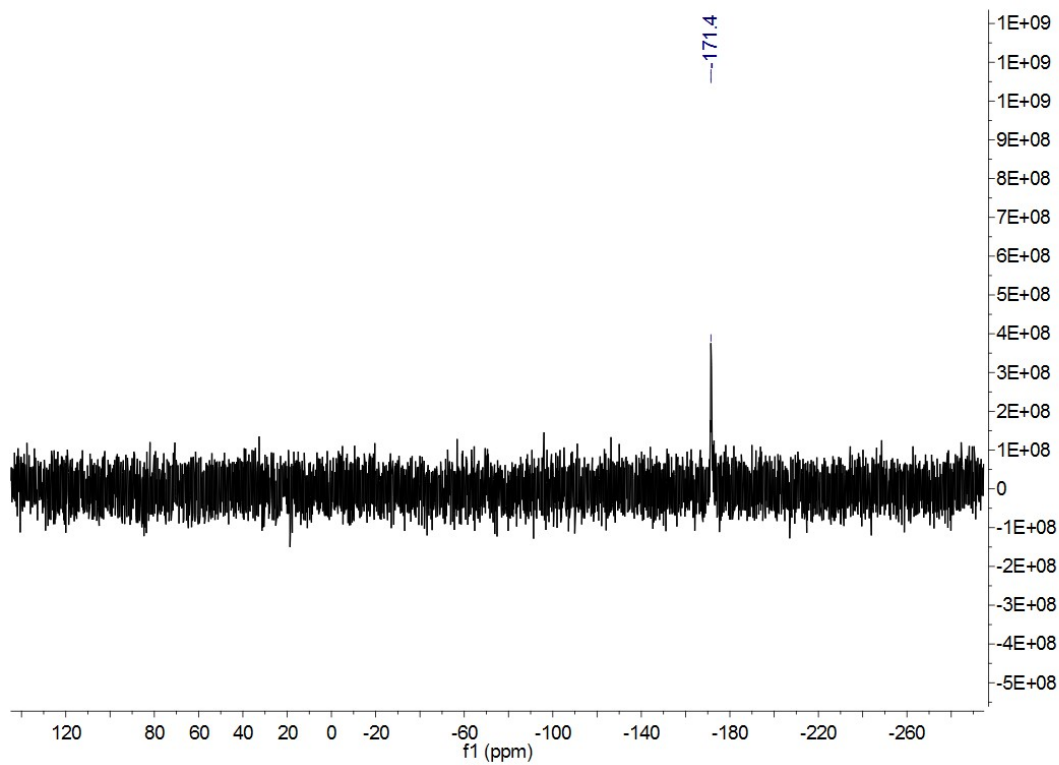
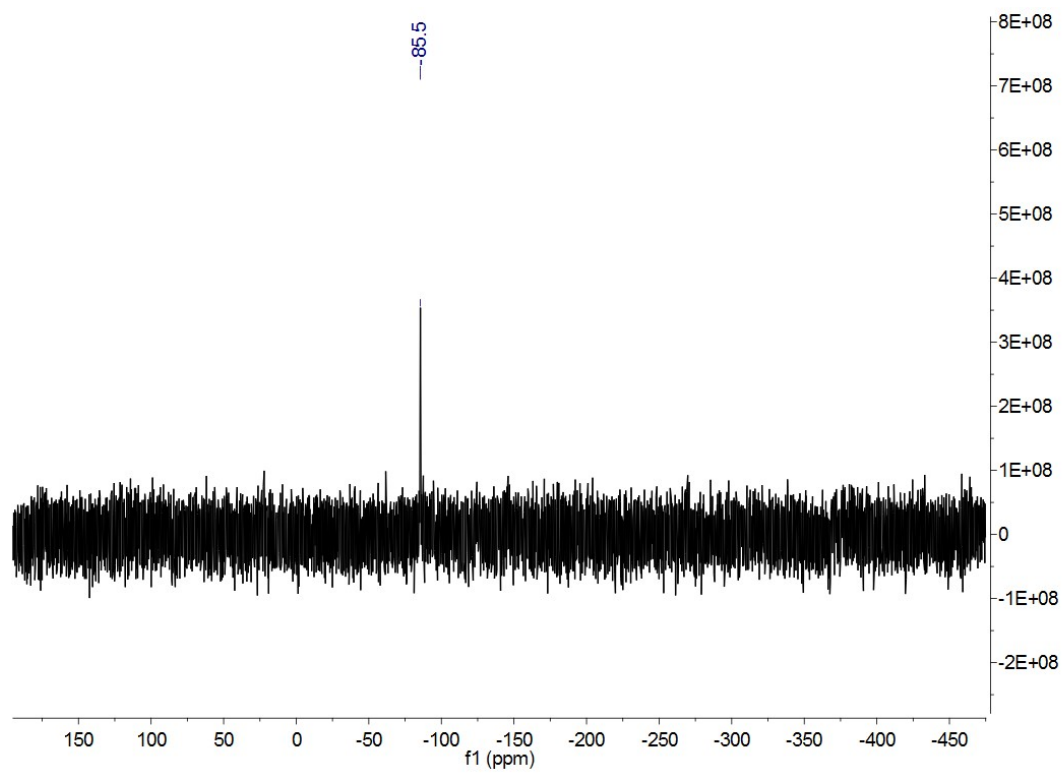


Figure S14.  $^{119}\text{Sn}$  NMR ( $\text{CH}_2\text{Cl}_2$ , 186.5 MHz ppm) spectra data of complex **2**



**Figure S15.**  $^{119}\text{Sn}$  NMR ( $\text{CH}_2\text{Cl}_2$ , 186.5 MHz ppm) spectra data of complexes **3**



**Figure S16.**  $^{119}\text{Sn}$  NMR ( $\text{CH}_2\text{Cl}_2$ , 186.5 MHz ppm) spectra data of complexes **4**



## 6. HSQC of HL<sub>1</sub> and complex 2

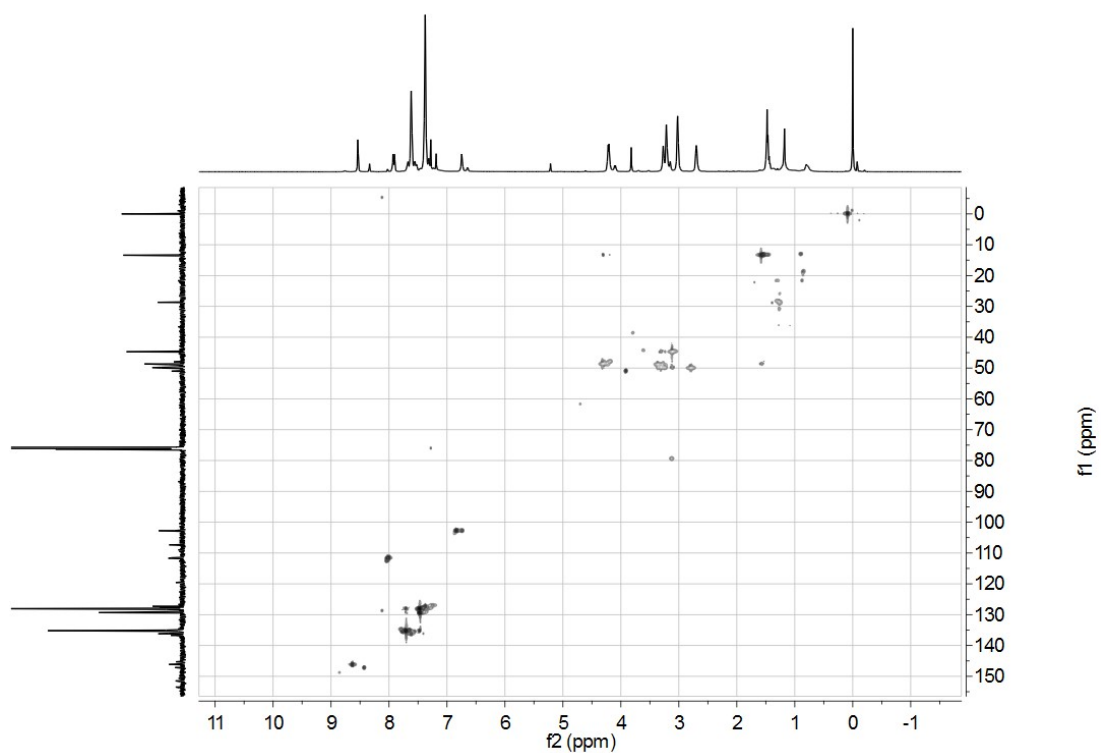


Figure S17. HSQC spectrum for complex 2

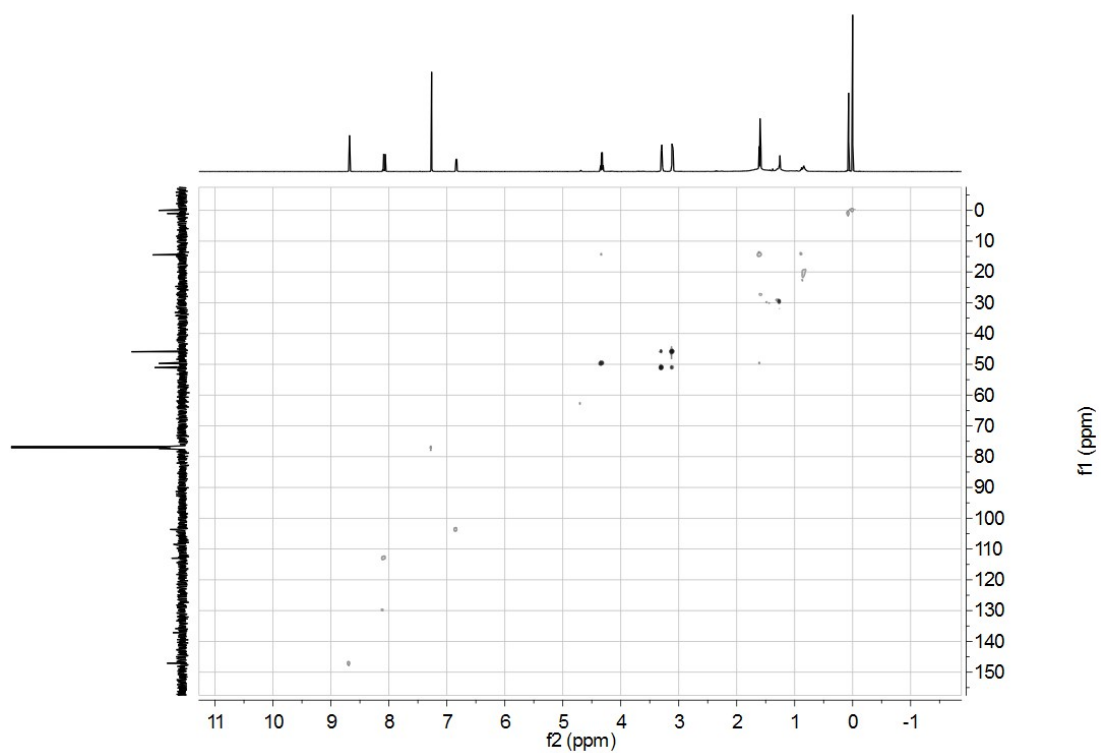
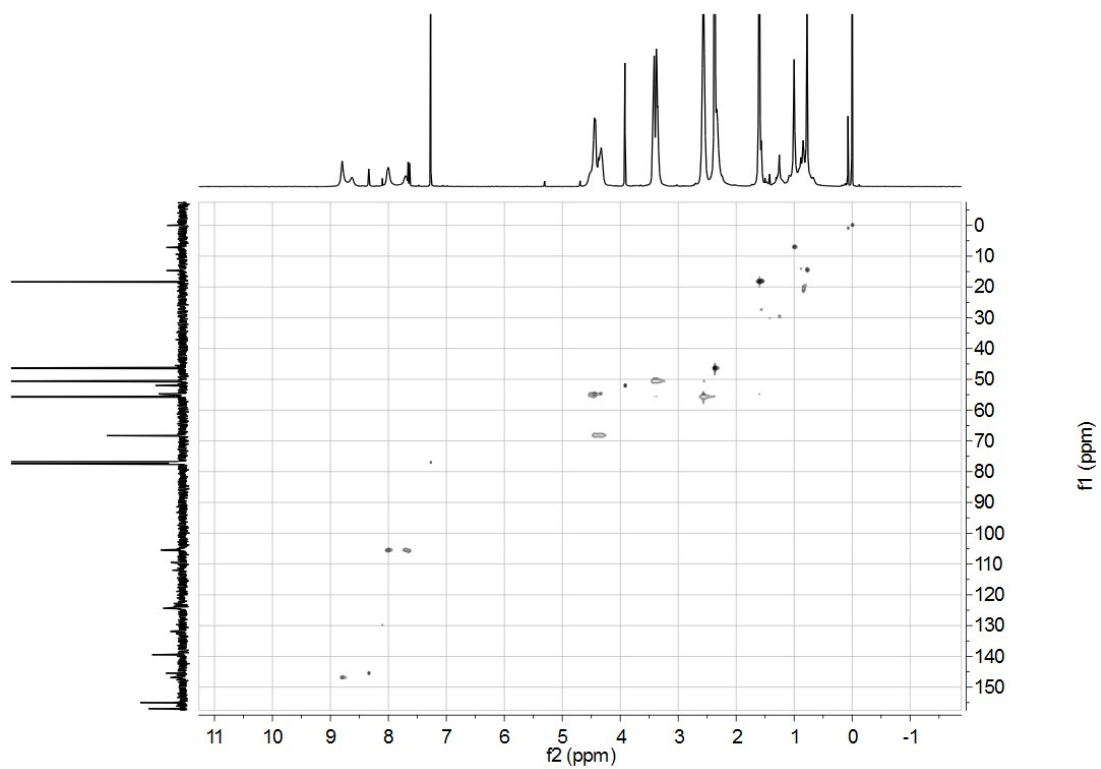
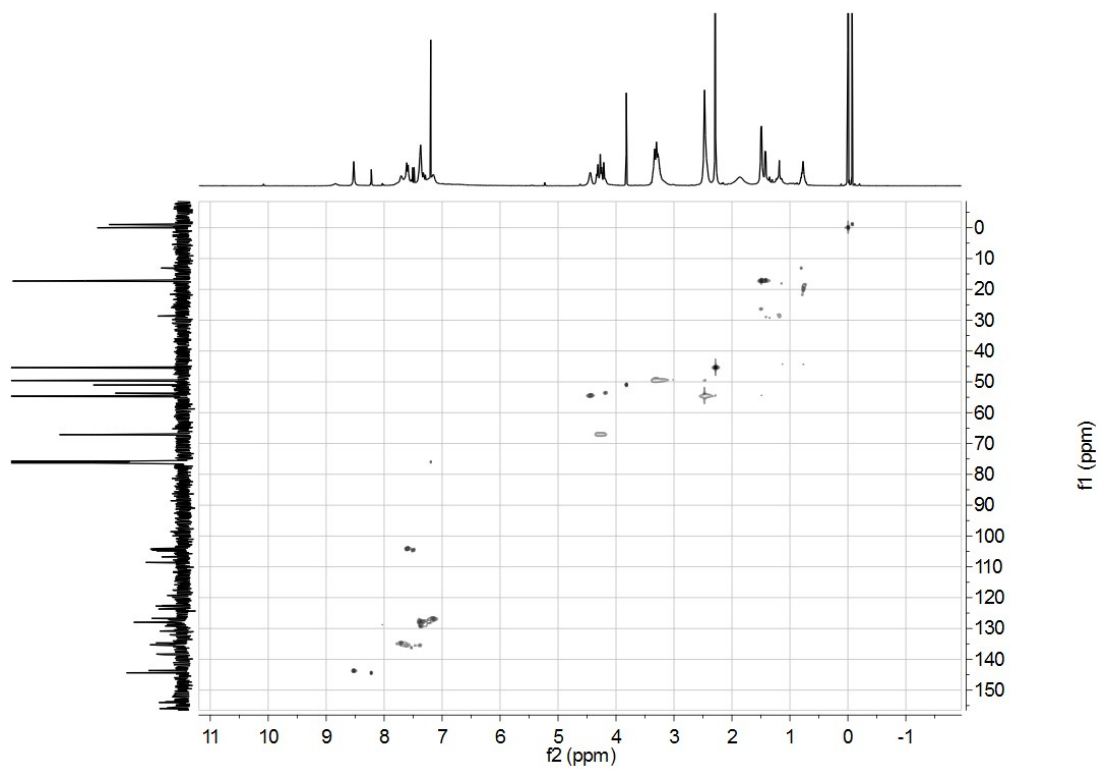


Figure S18. HSQC spectrum for HL<sub>1</sub>



**Figure S19.** HSQC spectrum for Complex 3



**Figure S20.** HSQC spectrum for Complex 4

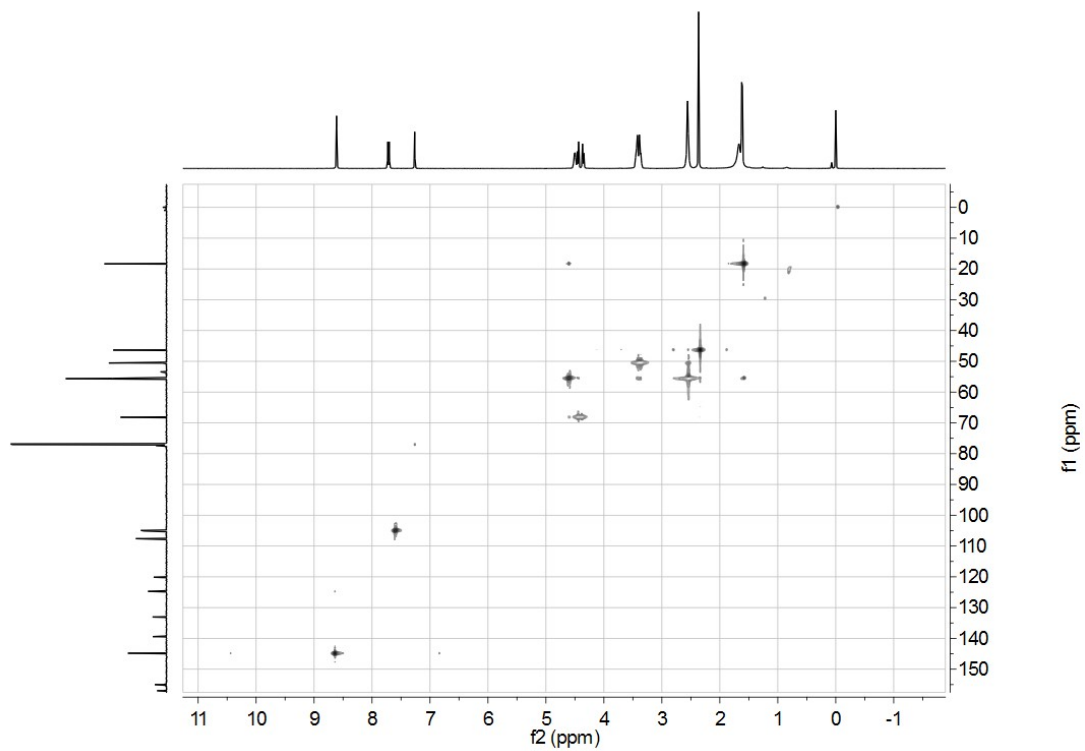


Figure S21. HSQC spectrum for HL<sub>2</sub>

### 7. ADPs of complexes 2-4

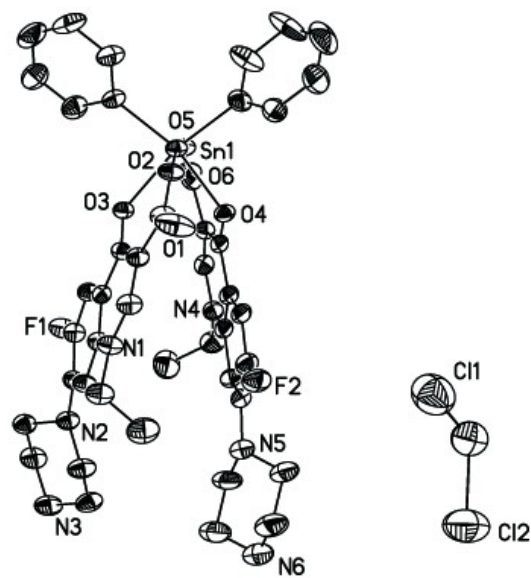
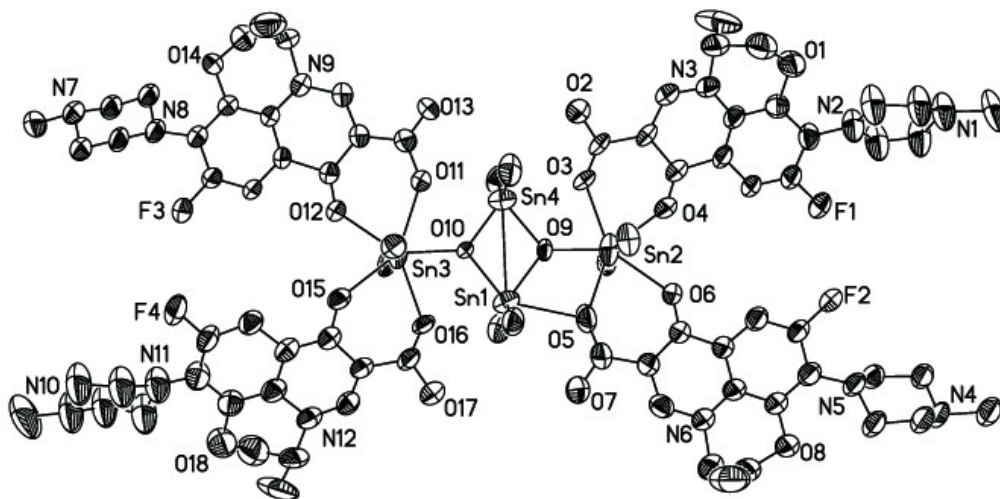
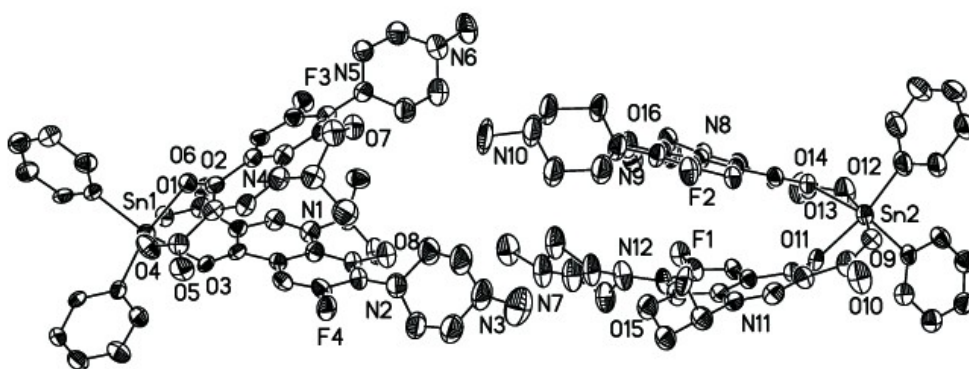


Figure S22. Molecular structure of complex 2 which the ellipsoids are represented at 30% probability



**Figure S23.** Molecular structure of complex **3** which the ellipsoids are represented at 30% probability



**Figure S24.** Molecular structure of complex **4** which the ellipsoids are represented at 30% probability