

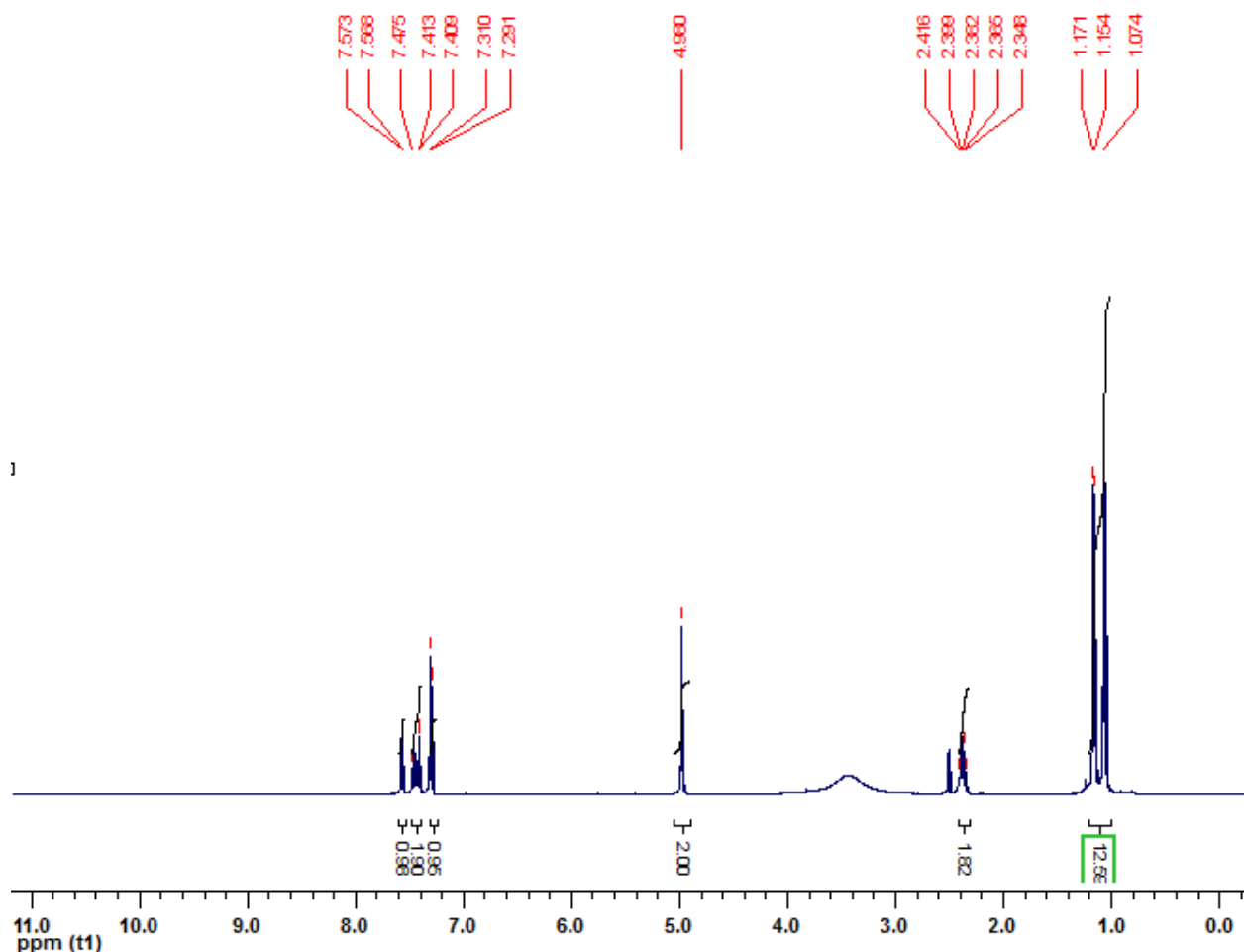
## Supporting Information-I

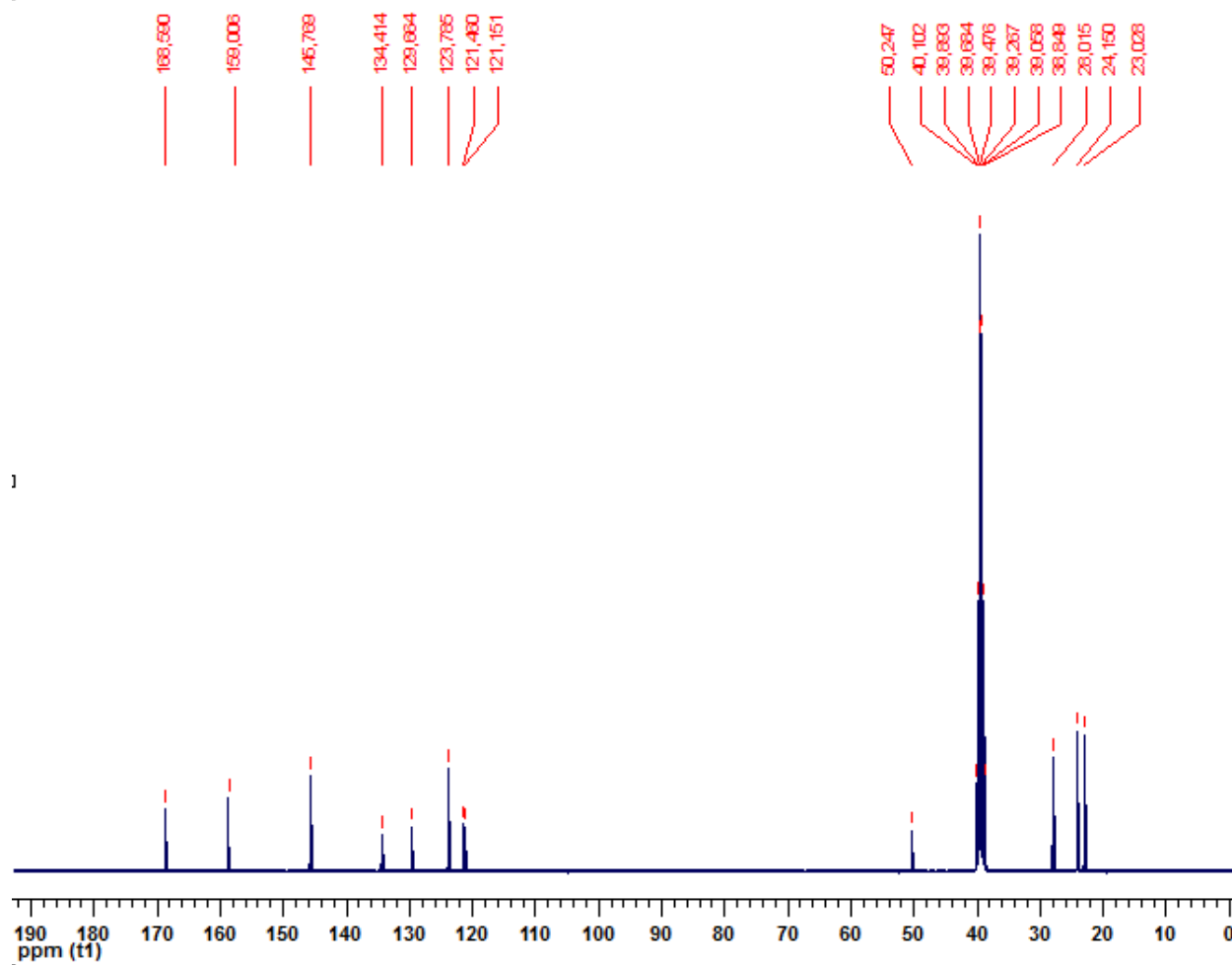
### Facile Access to Zinc and Cadmium Selones: Highly Active Catalysts for Barbier Reactions in Aqueous Media

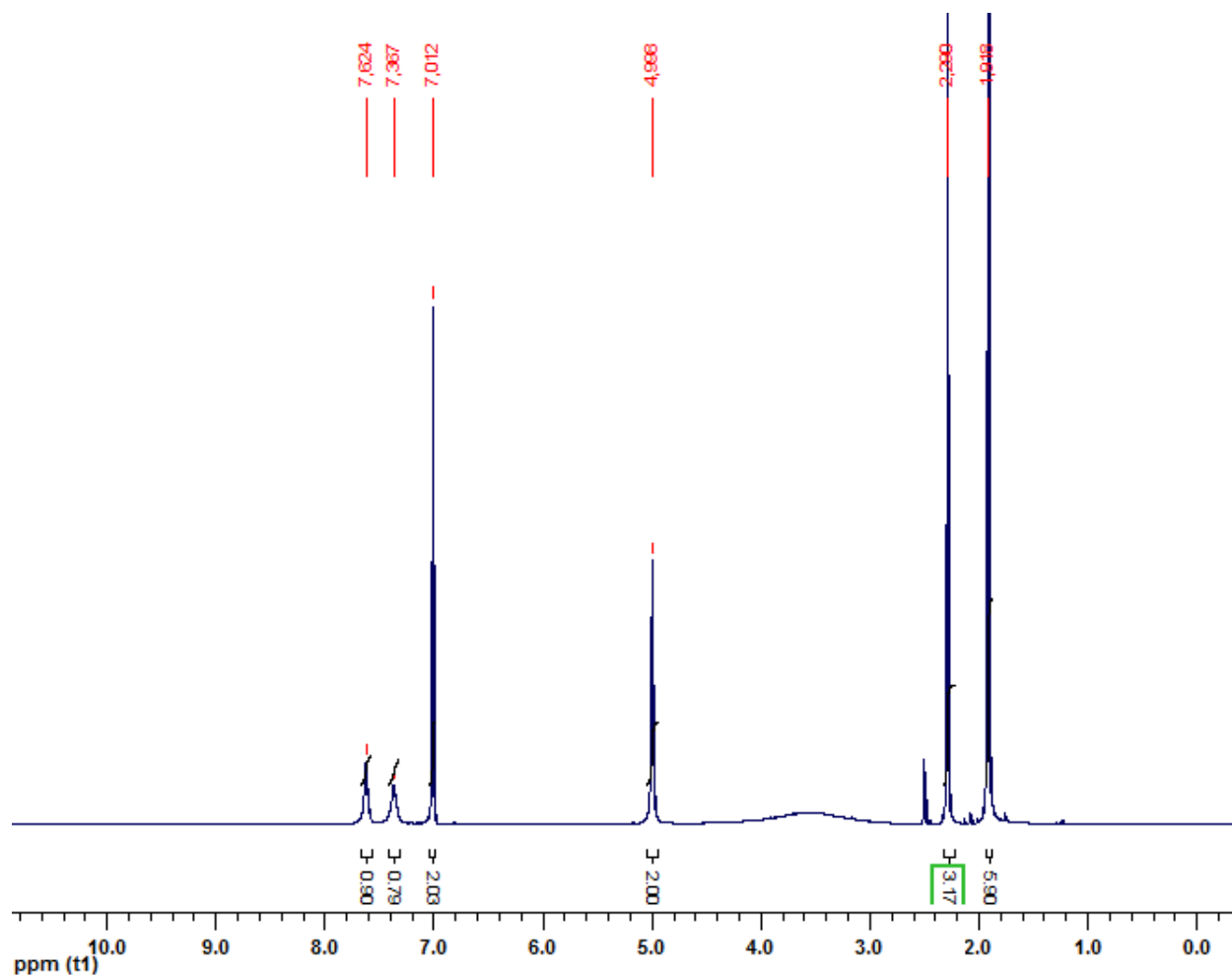
Chatla Naga Babu, Katam Srinivas and Ganesan Prabusankar\*

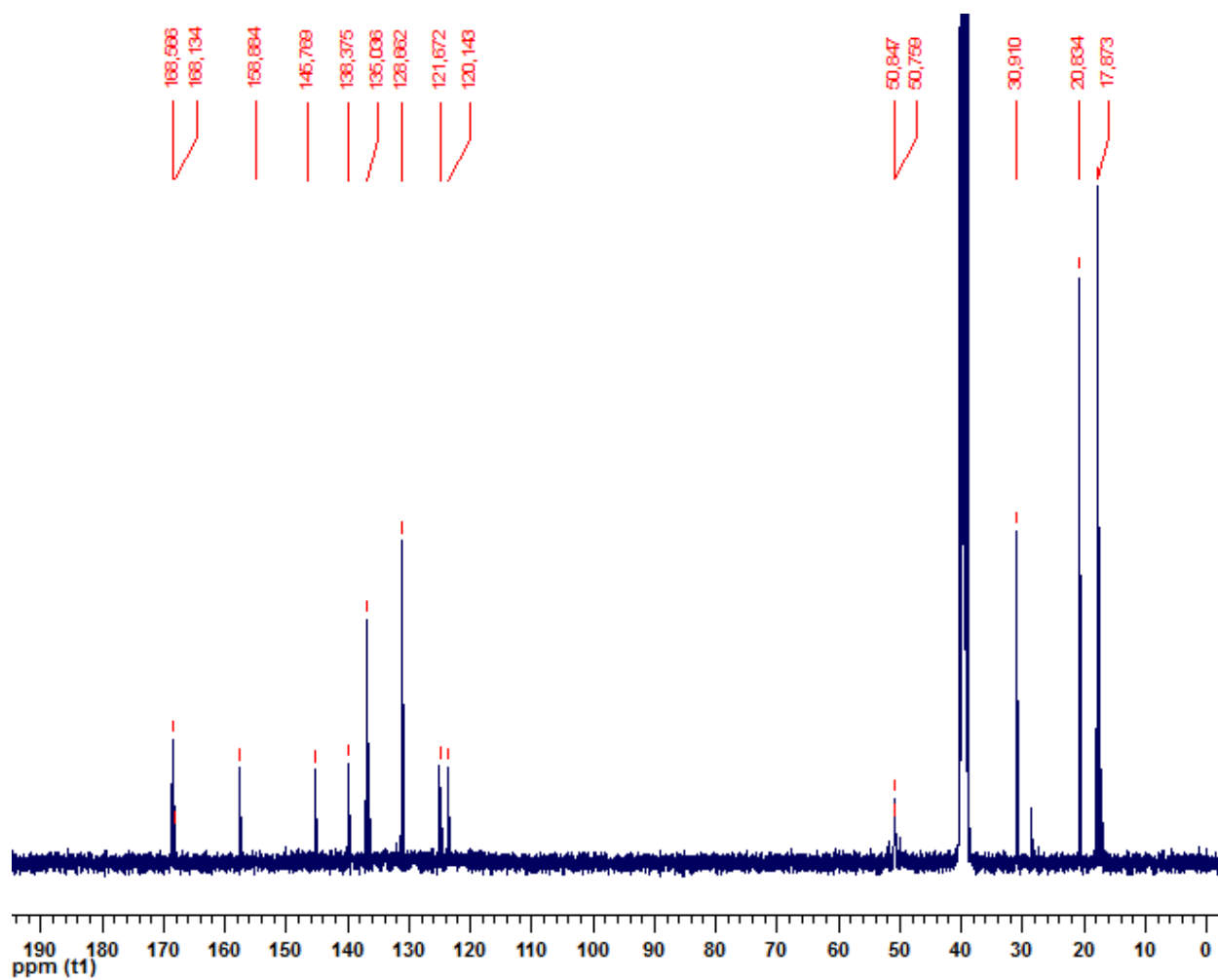
*a*. Department of Chemistry, Indian Institute of Technology Hyderabad, Kandi, Medak, TS, INDIA-502 285. Fax: +91 40 2301 6032; Tel: +91 40 2301 6089; E-mail: prabu@iith.ac.in.

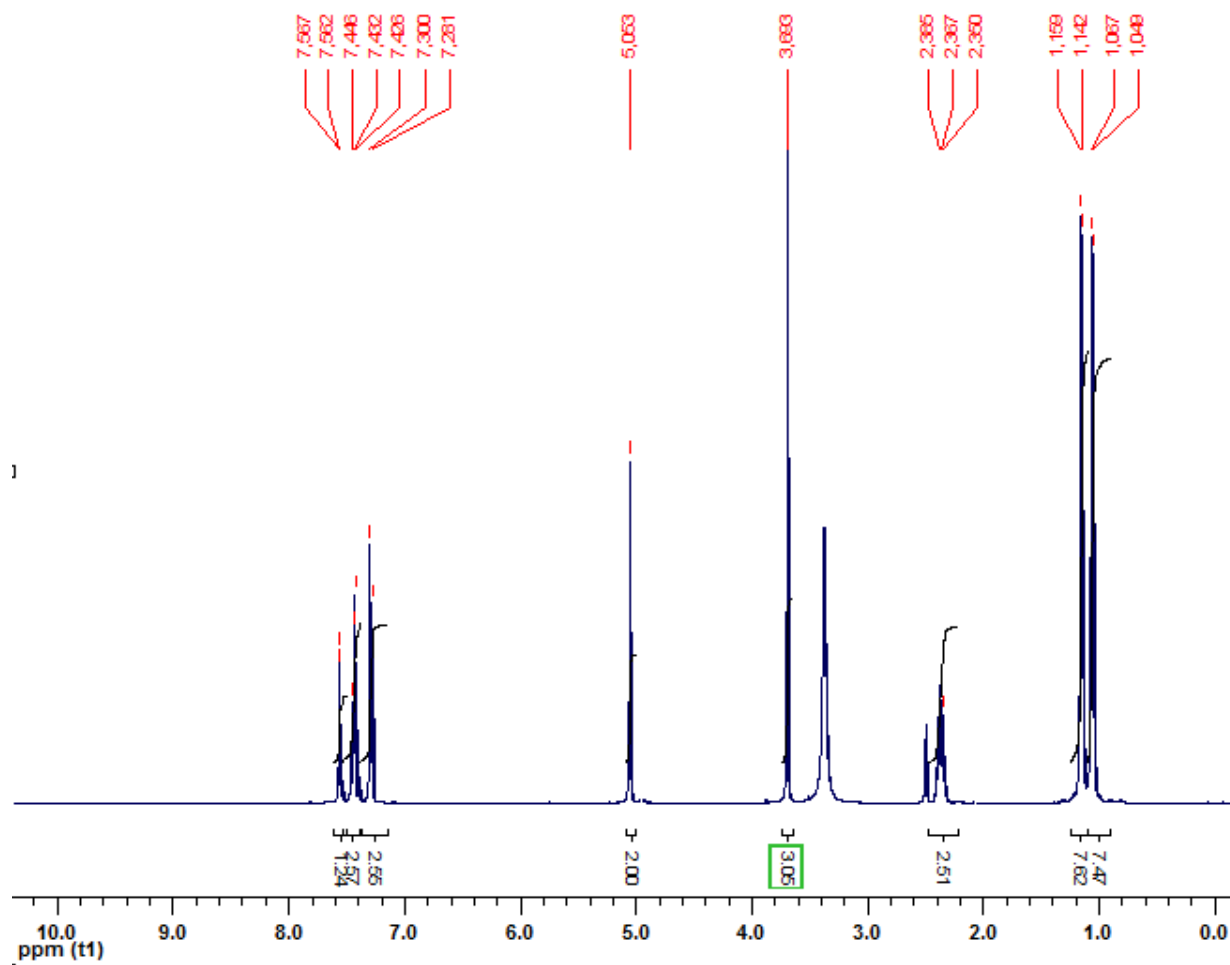
**Figure S1.**  $^1\text{H}$  NMR spectrum of compound **L1** in  $\text{DMSO-d}_6$  at RT.

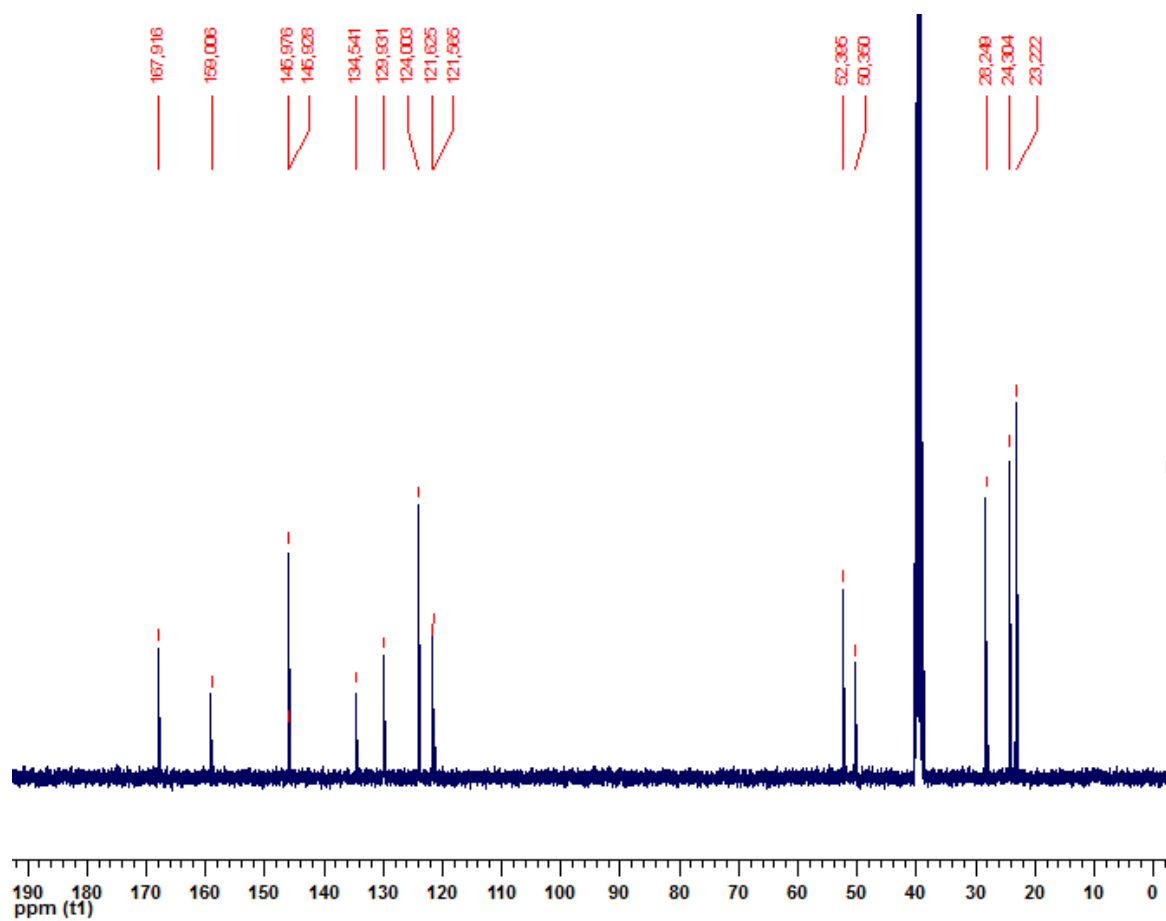


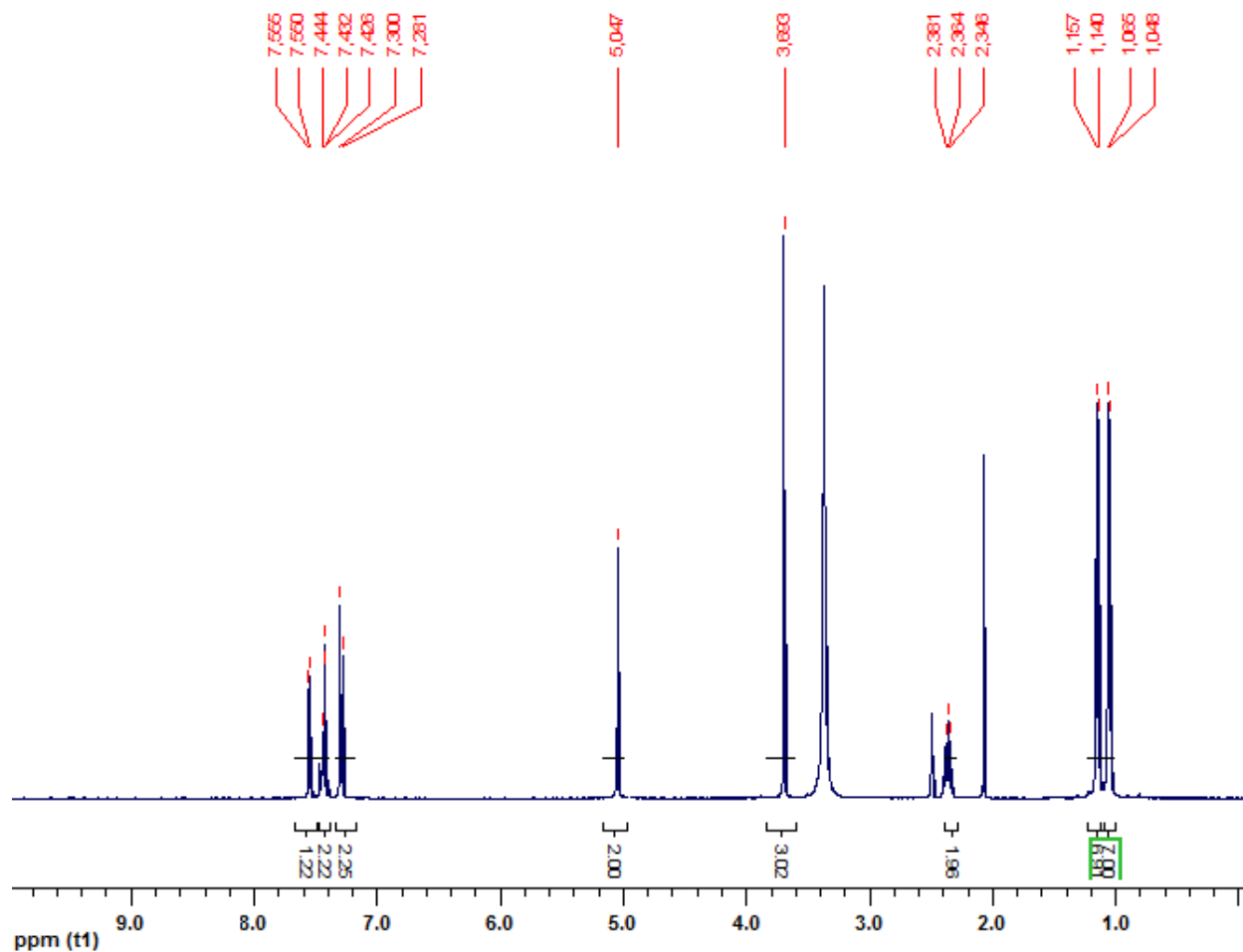
**Figure S2.**  $^{13}\text{C}$  NMR spectrum of compound **L1** in  $\text{DMSO-d}_6$  at RT.

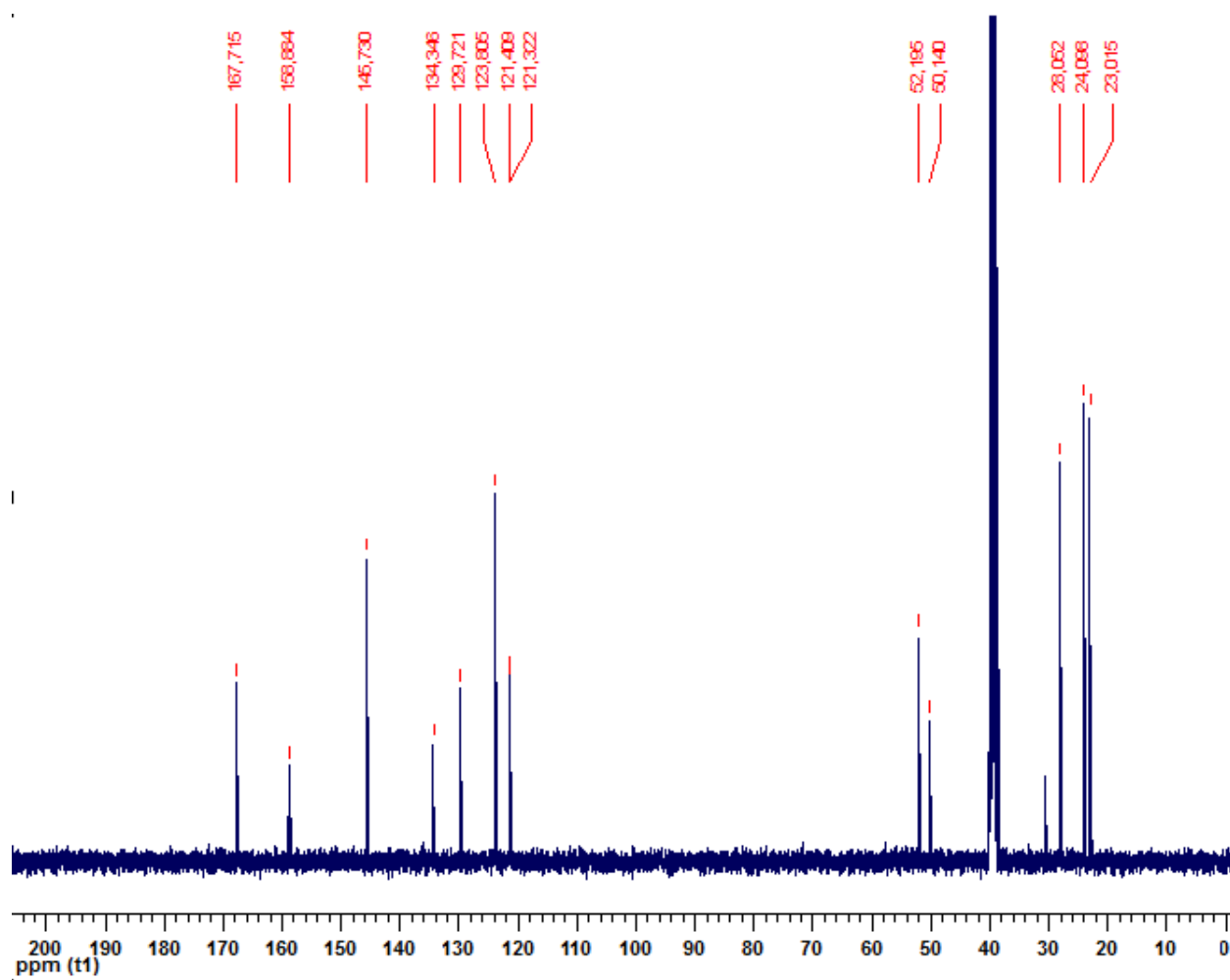
**Figure S3.**  $^1\text{H}$  NMR spectrum of compound **L2** in  $\text{DMSO-d}_6$  at RT.

**Figure S4.**  $^{13}\text{C}$  NMR spectrum of compound **L2** in  $\text{DMSO-d}_6$  at RT.

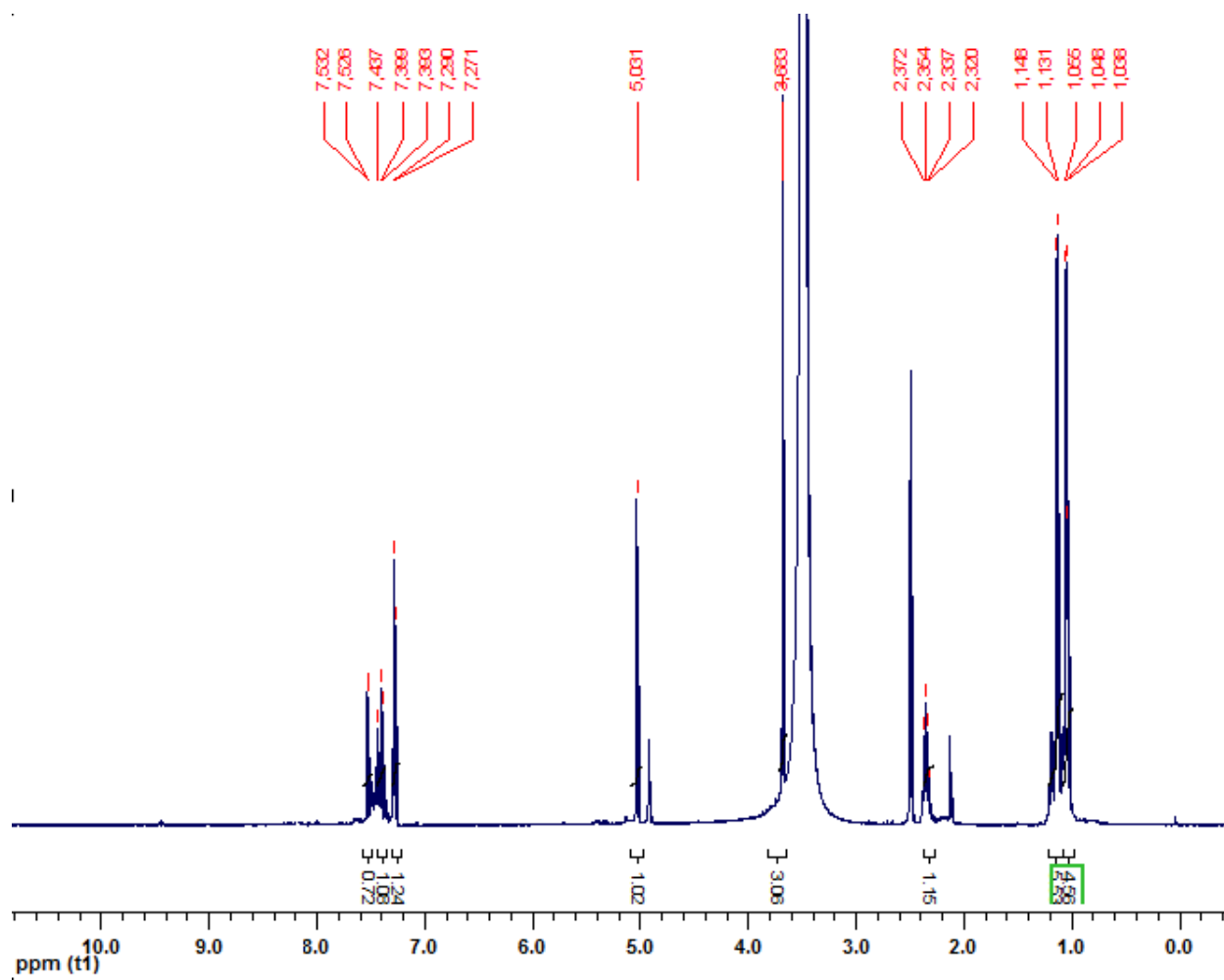
**Figure S5.**  $^1\text{H}$  NMR spectrum of compound **1** in  $\text{DMSO-d}_6$  at RT.

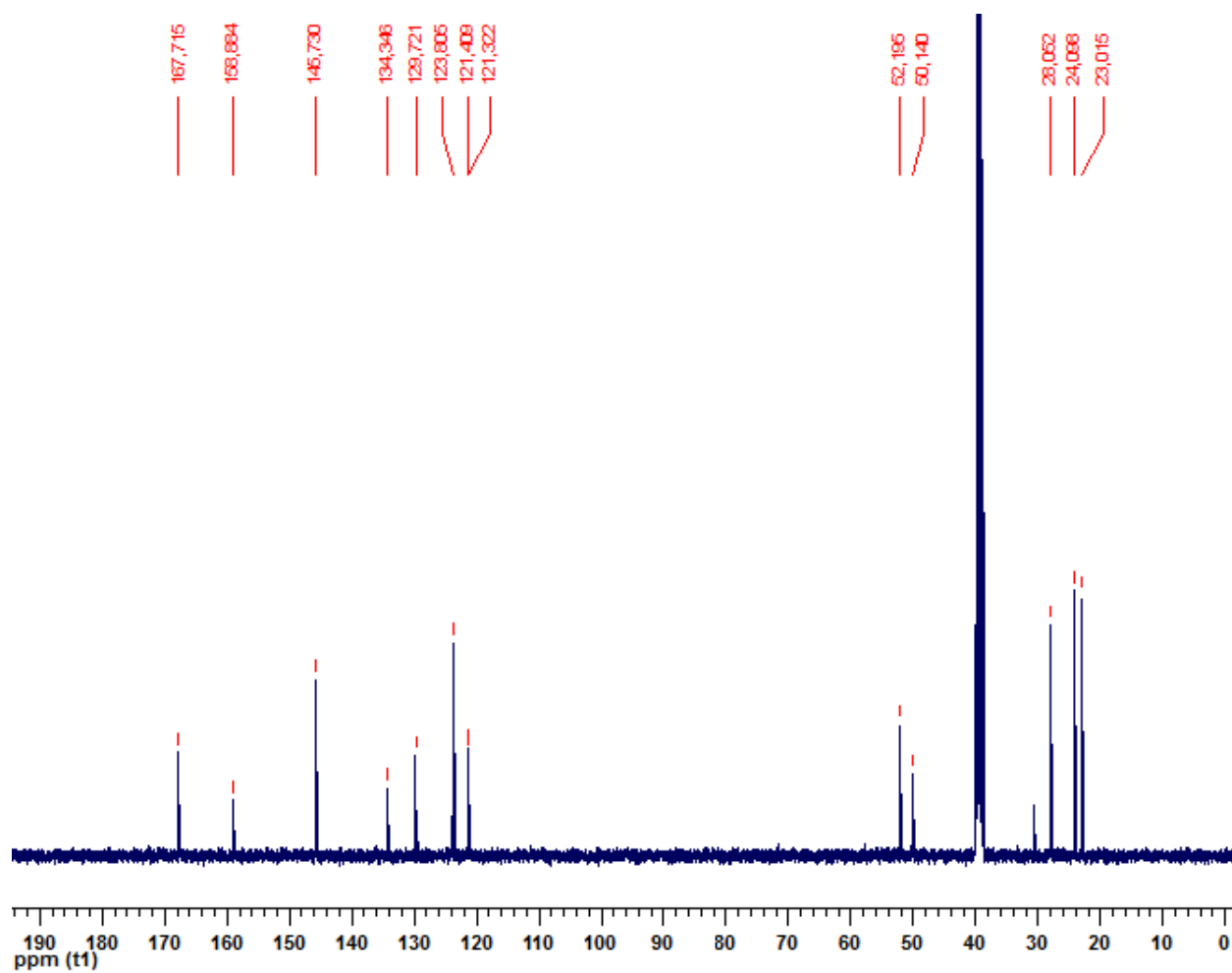
**Figure S6.**  $^{13}\text{C}$  NMR spectrum of compound **1** in DMSO- $d_6$  at RT.

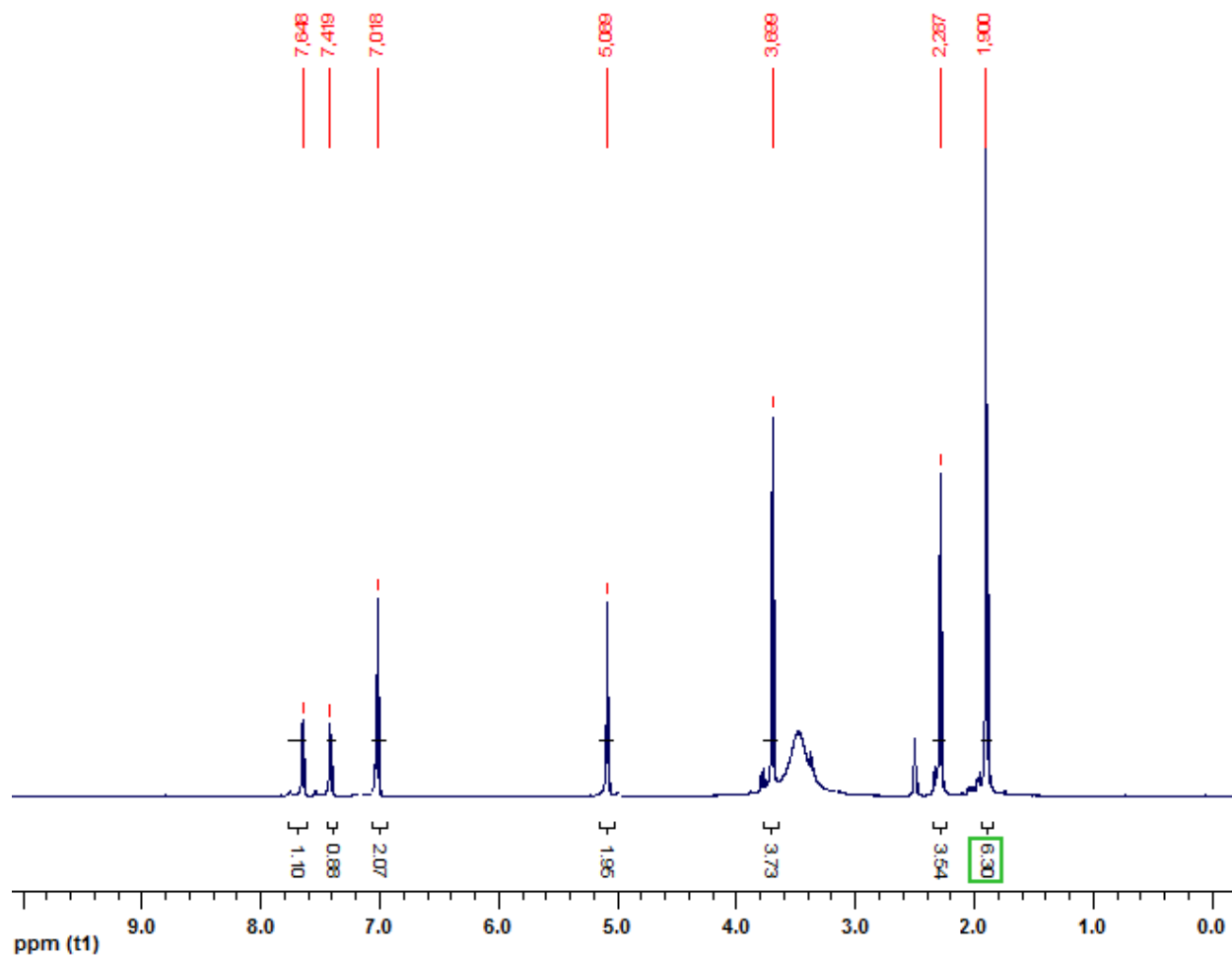
**Figure S7.**  $^1\text{H}$ NMR spectrum of compound **2** in  $\text{DMSO-d}_6$  at RT.

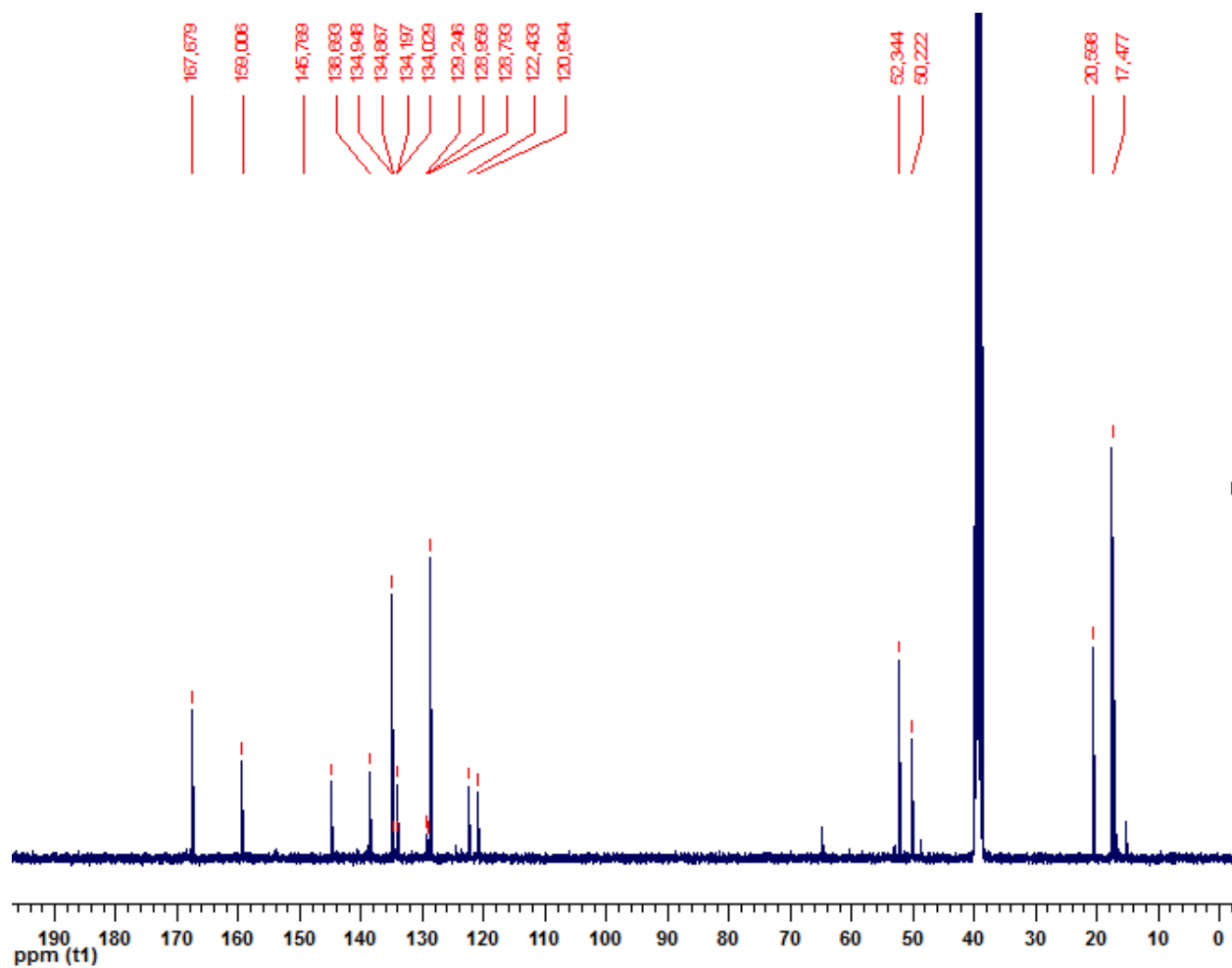
**Figure S8.**  $^{13}\text{C}$  NMR spectrum of compound **2** in  $\text{DMSO-d}_6$  at RT.

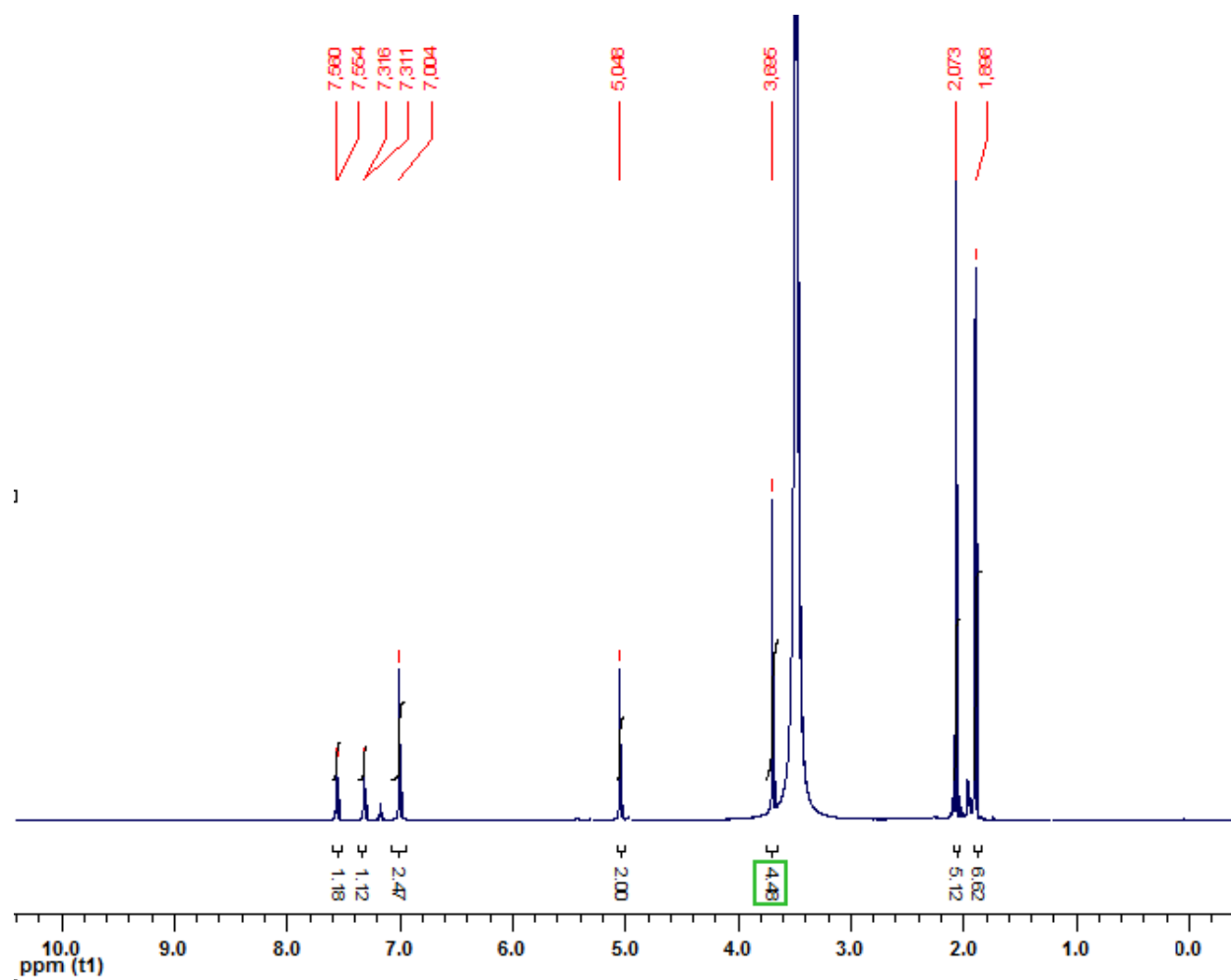


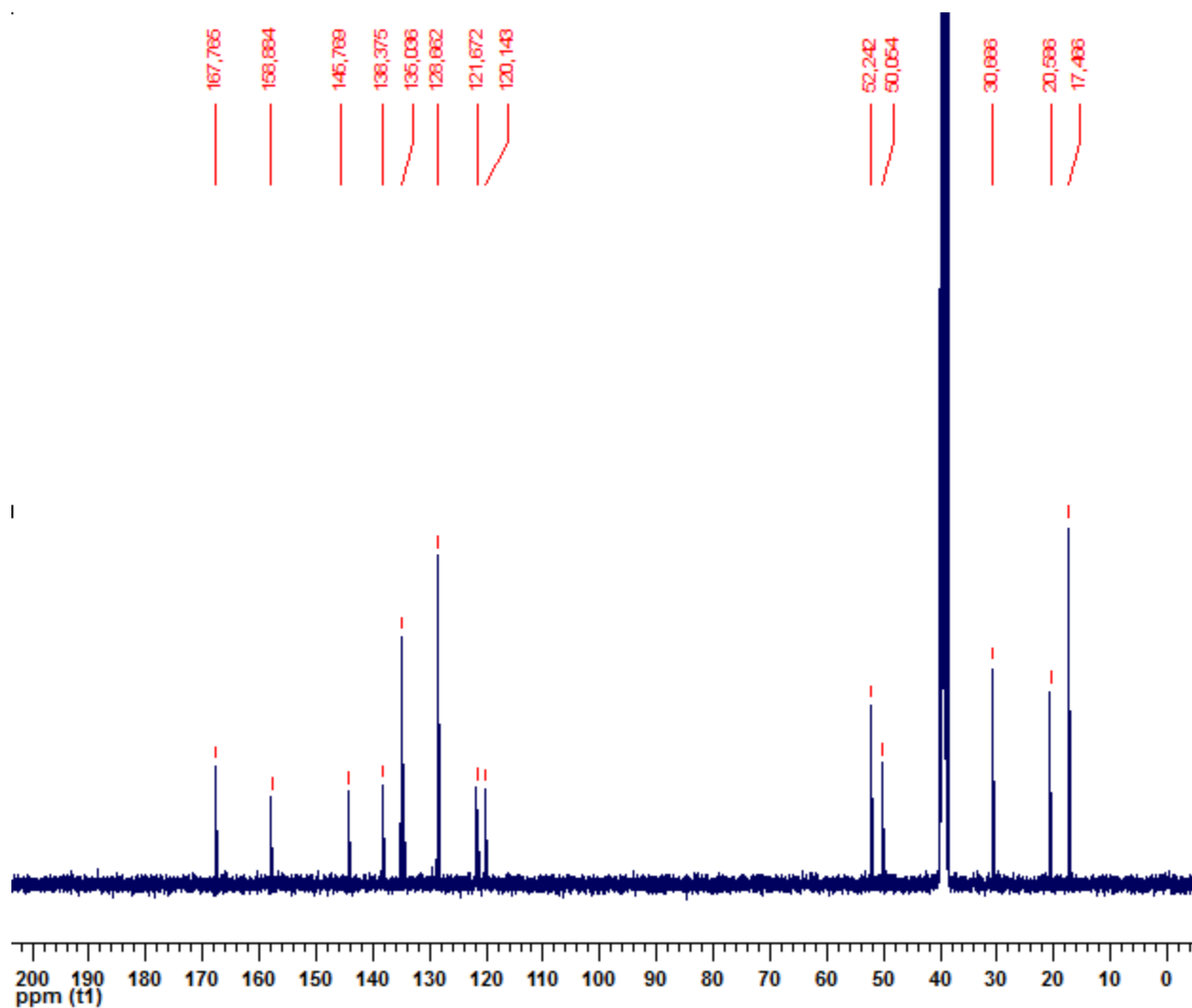
**Figure S9.**  $^1\text{H}$ NMR spectrum of compound **3** in  $\text{DMSO-d}_6$  at RT.

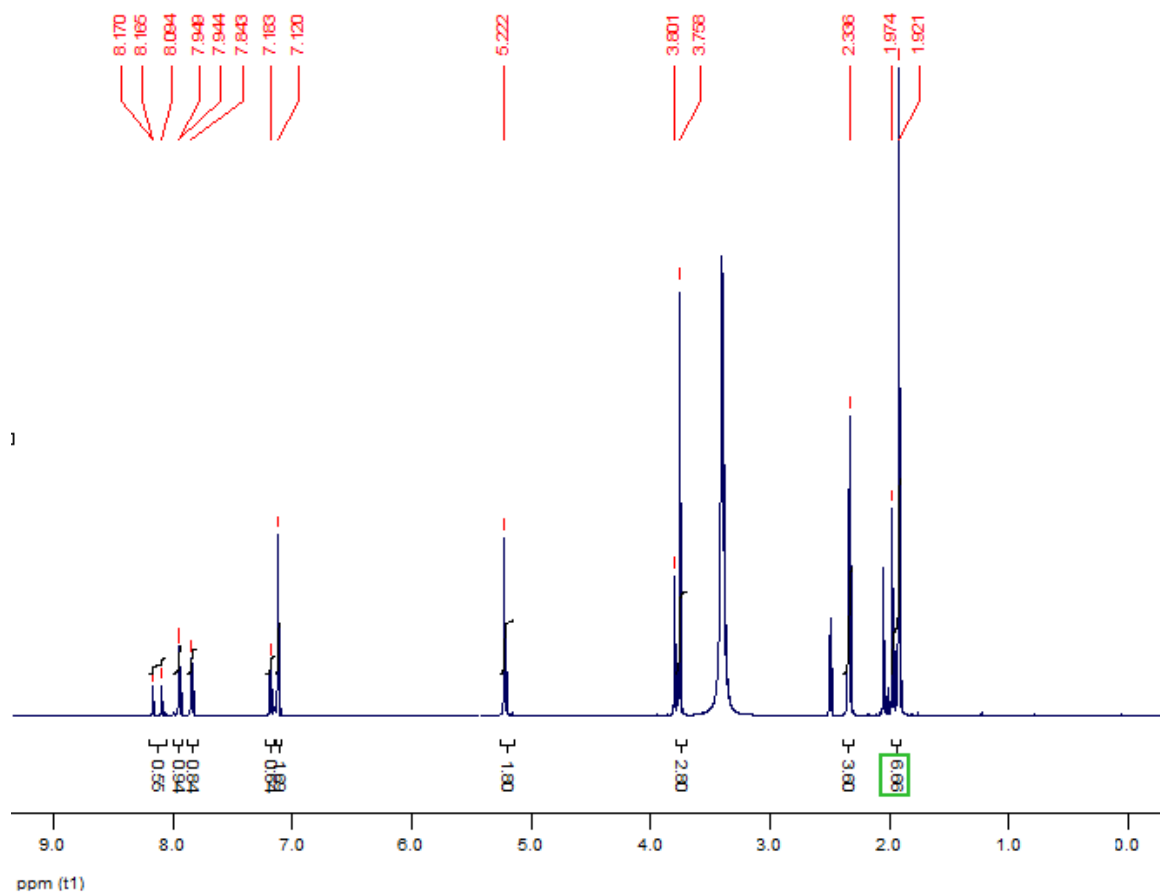
**Figure S10.**  $^{13}\text{C}$  NMR spectrum of compound **3** in  $\text{DMSO-d}_6$  at RT.

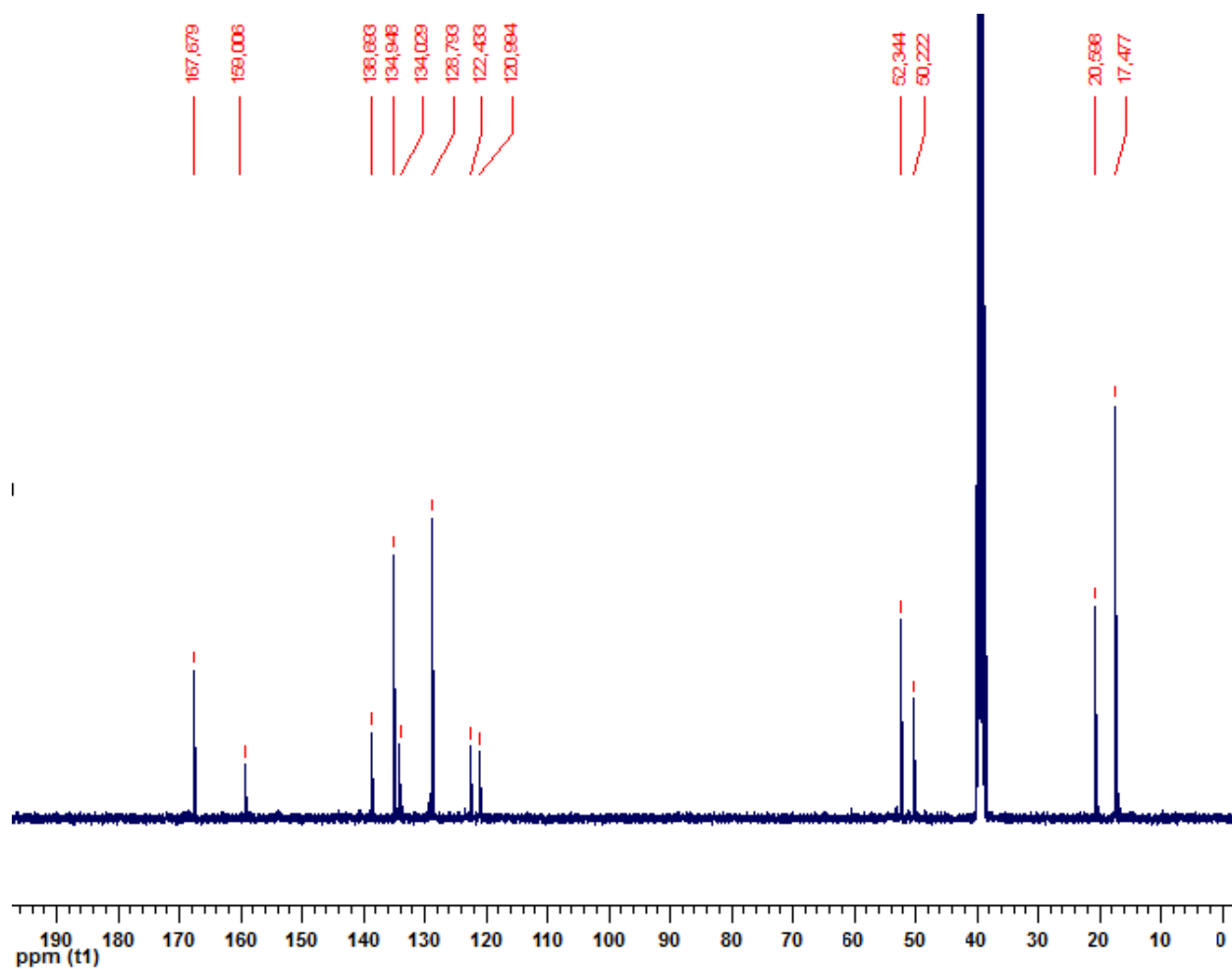
**Figure S11.**  $^1\text{H}$ NMR spectrum of compound **4** in DMSO- $d_6$  at RT.

**Figure S12.**  $^{13}\text{C}$ NMR spectrum of compound **4** in DMSO- $d_6$  at RT.

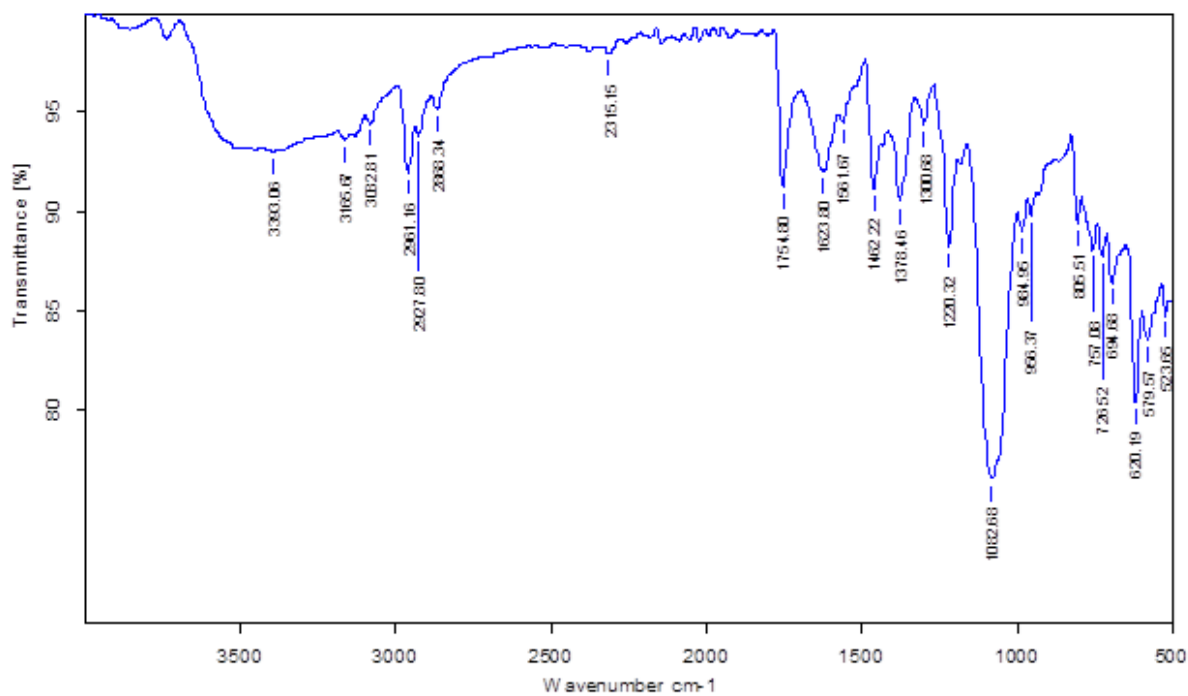
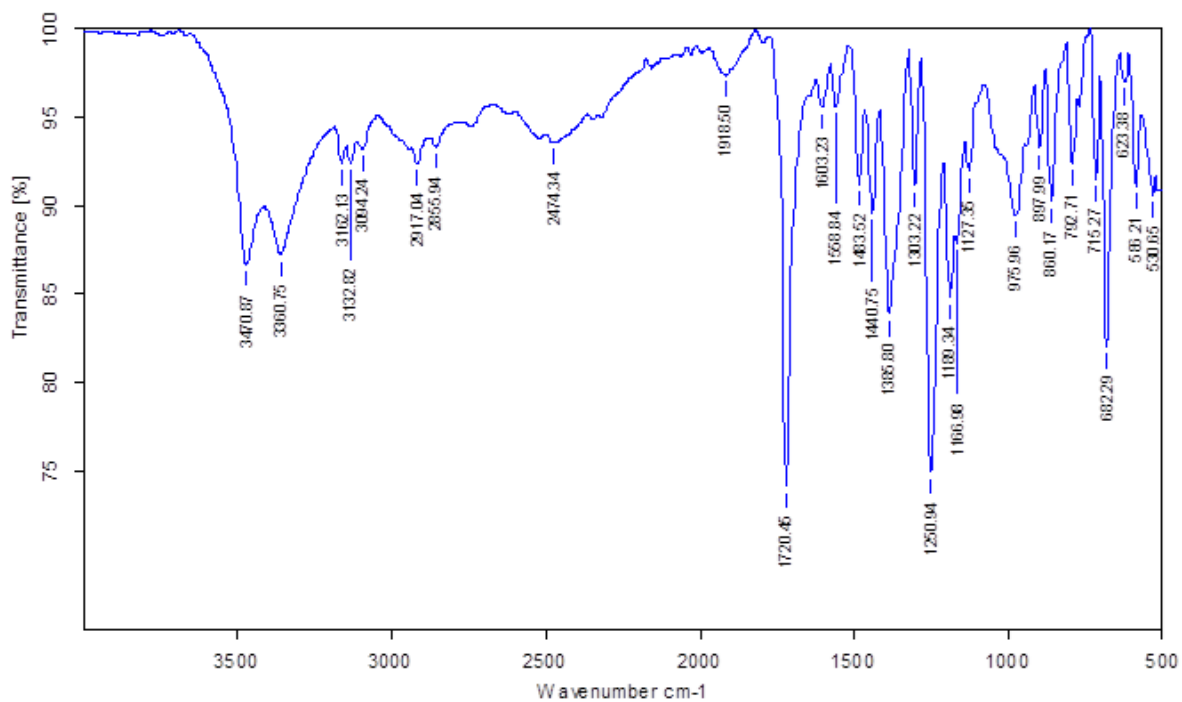
**Figure S13.**  $^1\text{H}$ NMR spectrum of compound **5** in  $\text{DMSO-d}_6$  at RT.

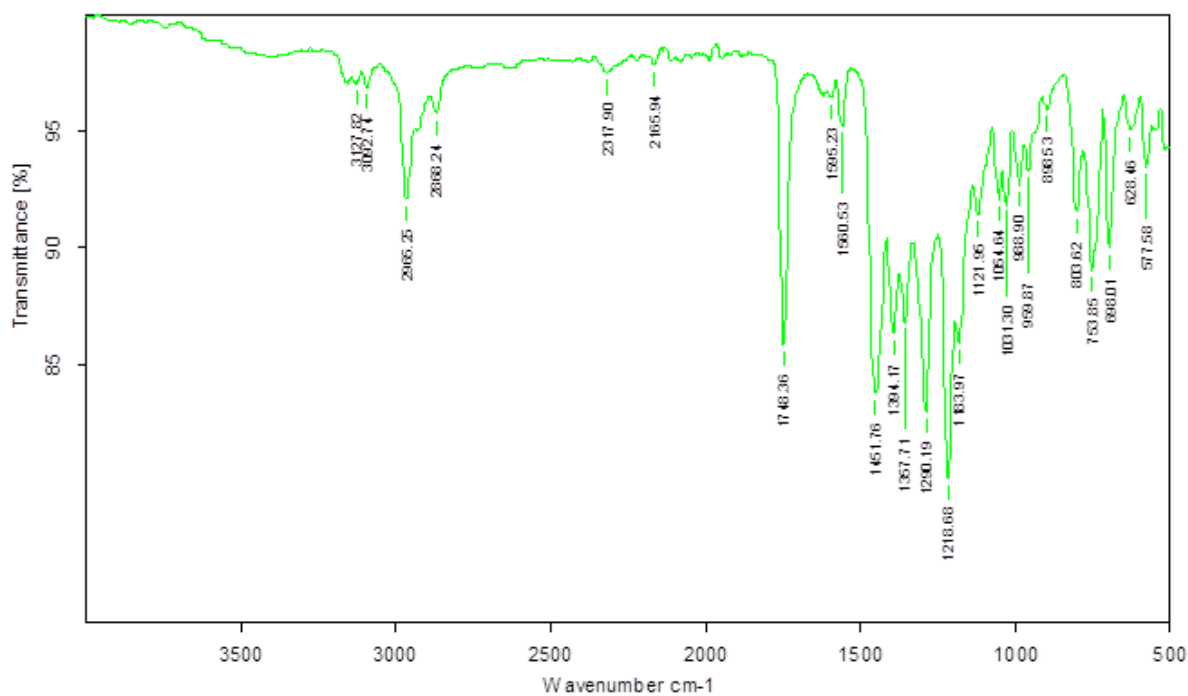
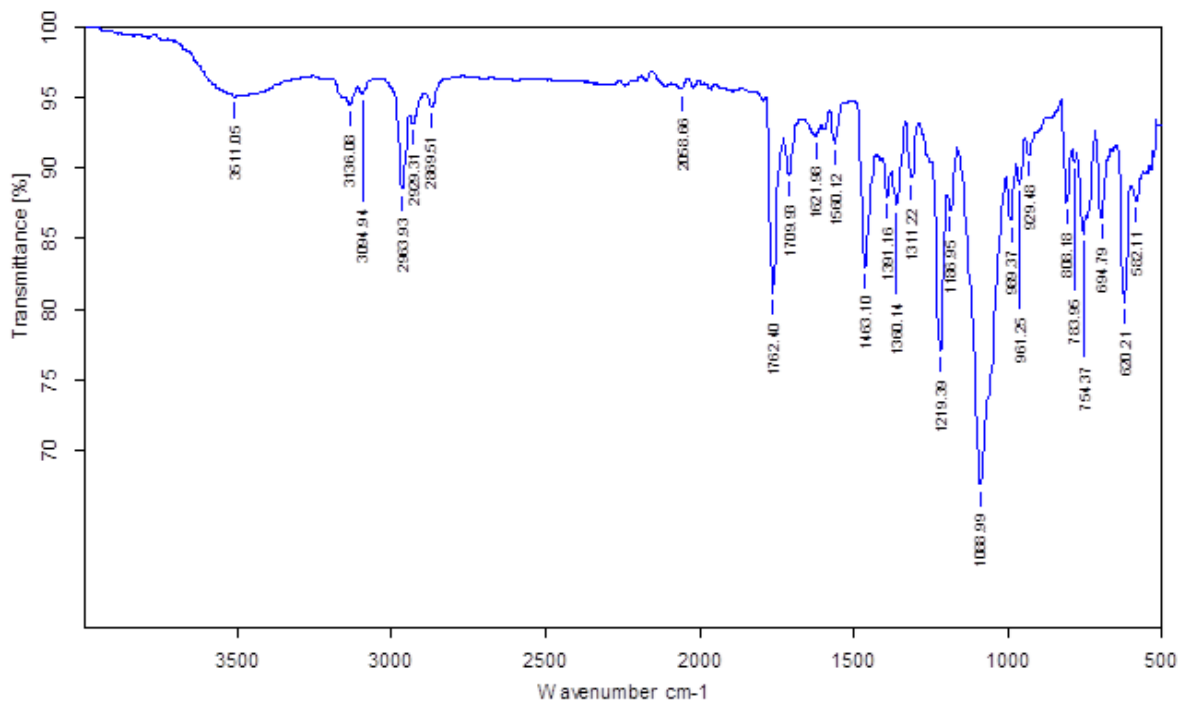
**Figure S14.**  $^{13}\text{C}$ NMR spectrum of compound **5** in  $\text{DMSO-d}_6$  at RT.

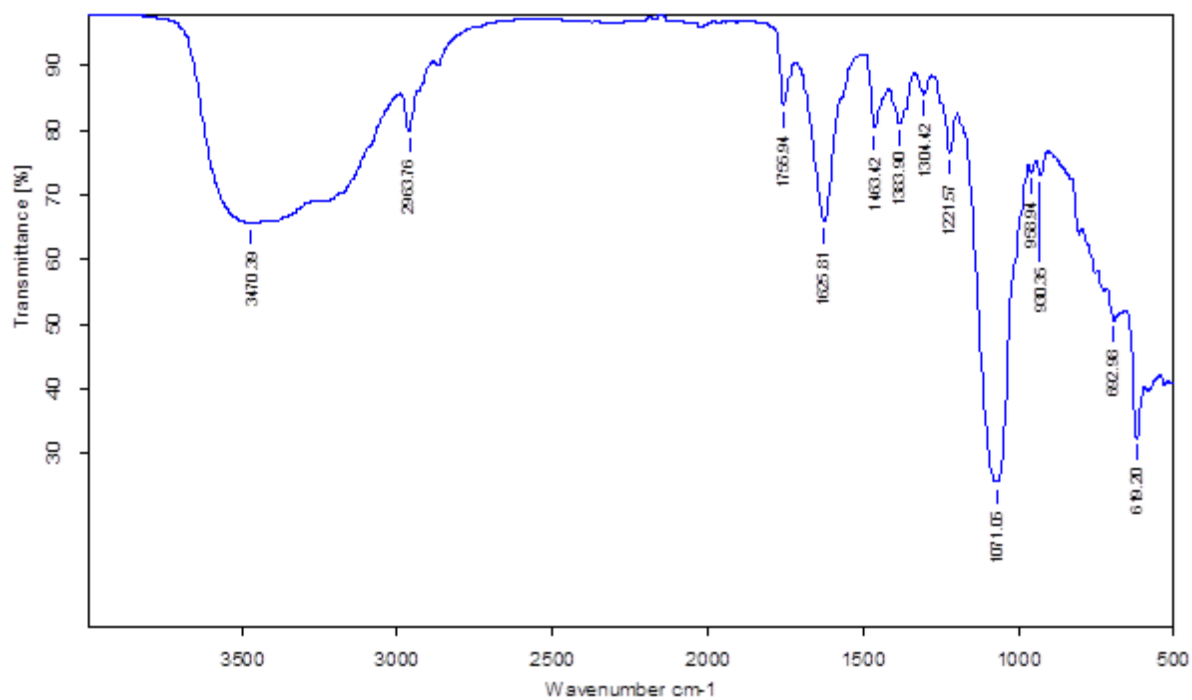
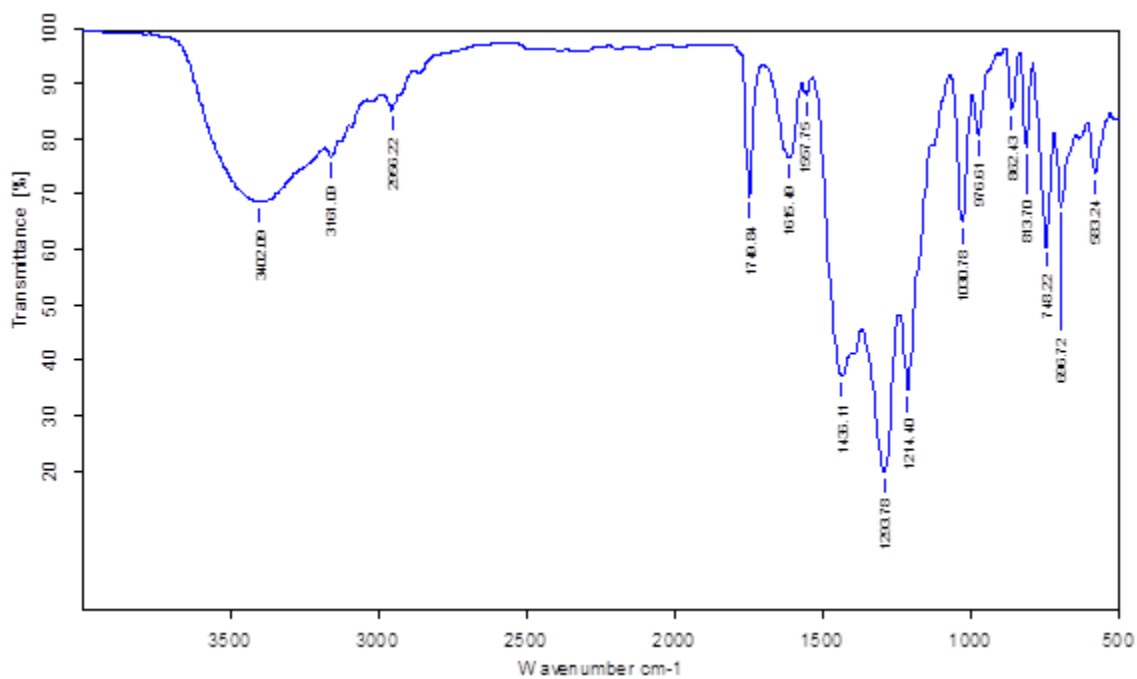
**Figure S15.**  $^1\text{H}$ NMR spectrum of compound **6** in  $\text{DMSO-d}_6$  at RT.

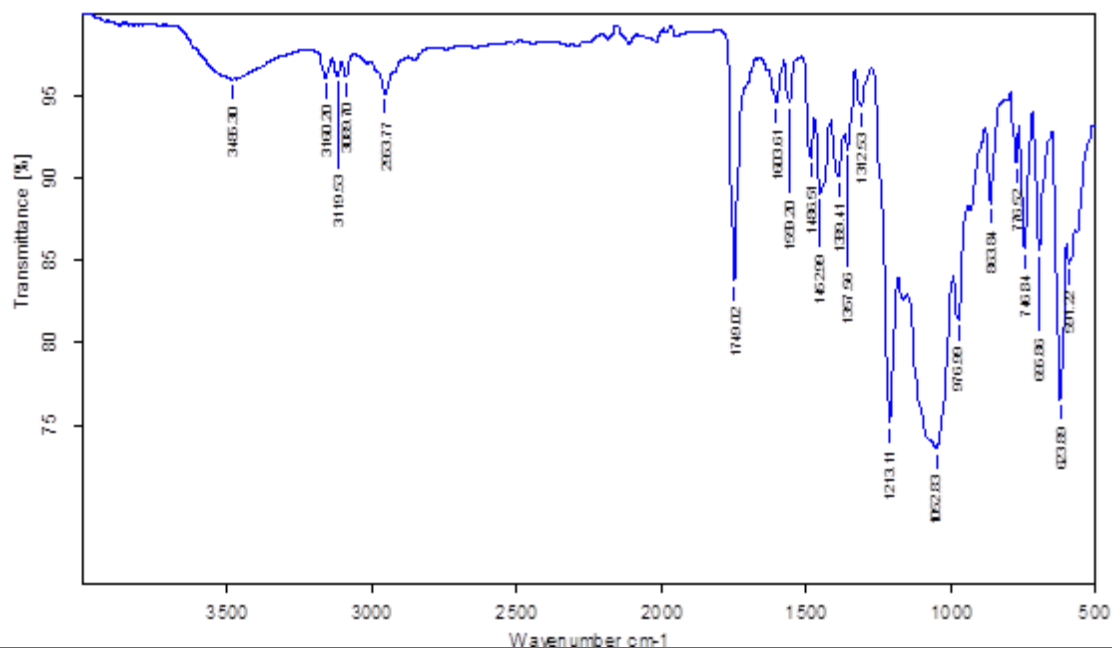
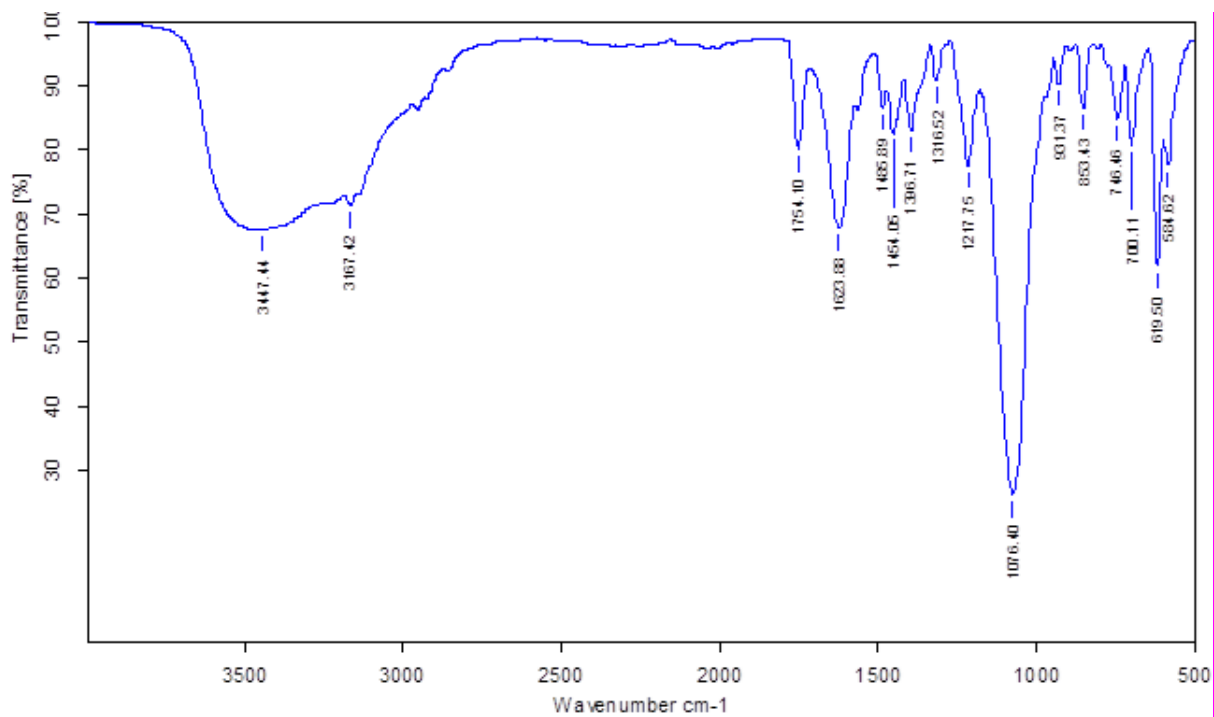
**Figure S16.**  $^{13}\text{C}$  NMR spectrum of compound **6** in  $\text{DMSO-d}_6$  at RT.



**Figure S17.** FT-IR spectrum of L1.**Figure S18.** FT-IR spectrum of L2.

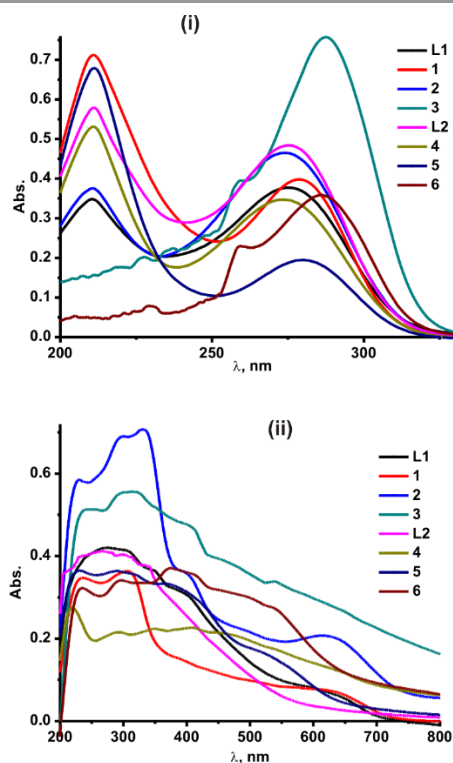
**Figure S19.** FT-IR spectrum of **1**.**Figure S20.** FT-IR spectrum of **2**.

**Figure S21.** FT-IR spectrum of **3**.**Figure S22.** FT-IR spectrum of **4**.

**Figure S23.** FT-IR spectrum of **5**.**Figure S24.** FT-IR spectrum of **6**.

## UV-vis absorption studies of L1, L2 and 1-6.

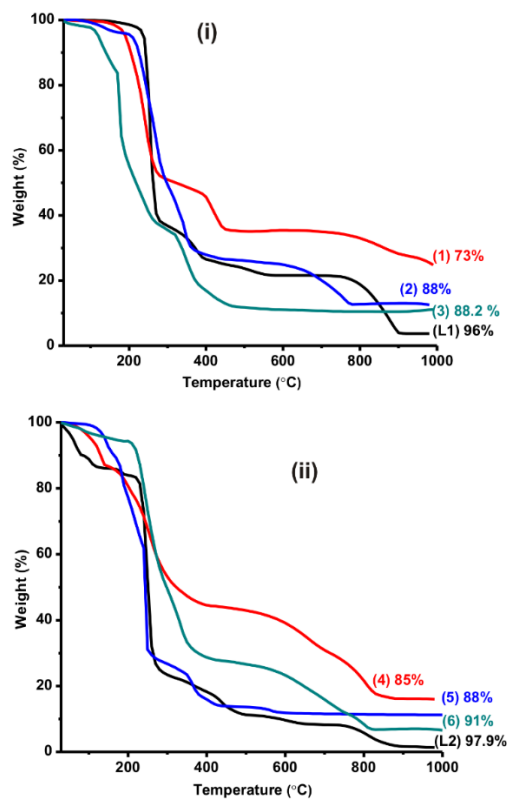
The solution state UV-vis absorption spectra of **1-6** were recorded in DMSO at room temperature (Fig. 7(i)). In solution state, the UV-vis absorption spectra of **L1**, **L2**, and **1-6** showed nearly comparable absorption patterns. The absorption band observed between 211-218 nm can be attributed to the  $\pi \rightarrow \pi^*$  transition, while the absorption band observed around 270-290 nm can be assigned to the  $n \rightarrow \pi^*$  transition. The solid state UV-vis absorption spectra of **1-6** are not comparable with solution state absorption spectra of **1-6**. In the case of solid state absorption spectra (Fig. 7(ii)), the  $\pi \rightarrow \pi^*$  and  $n \rightarrow \pi^*$  transitions are merged together to give a broad absorption band. In addition, a broad absorption peak from 300 to 650 nm is observed for **1-6** in the solid-state UV-visible absorption study.



**Figure S25.** (i) Solution state UV-vis spectra of **L1**, **L2** and **1-6** in DMSO at 25 °C ( $3.64 \times 10^{-5}$  M); (ii) Solid state UV-vis spectra of **L1**, **L2** and **1-6** at 25 °C.

### Thermogravimetric analysis of 1-6.

The thermal stability of molecule **1-6** is analyzed by TGA. The figure 8 reveals the thermal breakdown pathway of **1-6** based on thermal investigation under a flowing nitrogen atmosphere ( $10\text{ }^{\circ}\text{C min}^{-1}$ , 30-1000  $^{\circ}\text{C}$ ). A small weight loss about 2–8% was observed for **1-6** in the initial stage ( $<80\text{ }^{\circ}\text{C}$ ), can be attributable to the loss of moisture. Complexes **1-6** and compounds **L1** and **L2** showed a sudden weight loss in single step from 200 to 320  $^{\circ}\text{C}$  range, which can be validated for the decomposition of organic moieties. Subsequently, a gradual weight loss was observed till 1000  $^{\circ}\text{C}$  with 9-25% residue for the metal chalcogenides. Whereas, complexes **1** and **4** displayed an extreme thermal stability till 250-280  $^{\circ}\text{C}$  and showed a gradual weight loss till 1000  $^{\circ}\text{C}$ . Compounds **2** and **6** showed enough stability till 220-240  $^{\circ}\text{C}$  range then showed a sudden weight loss of about 70% till 400  $^{\circ}\text{C}$ . Subsequently, **2** and **6** showed the gradual weight loss till 800  $^{\circ}\text{C}$  with 9-12% residual weights. Complex **3** shows gradual weight loss till 420  $^{\circ}\text{C}$  then remains unchanged till 1000  $^{\circ}\text{C}$ . Similarly complex **5** loses 70% weight around 250  $^{\circ}\text{C}$  then showed the gradual weight loss till 590  $^{\circ}\text{C}$  and remains unchanged till 1000  $^{\circ}\text{C}$ . The ligands **L1** and **L2** loses the major weight within 250  $^{\circ}\text{C}$  then loses almost the rest within 900  $^{\circ}\text{C}$ . The black residue obtained from **1-6** were in accord with the calculated values for the respective metal selenide.



**Figure S26.** (i) TGA curve of L1 and 1-3; (ii) L2 and 4-6 from 30 to 1000 °C under a nitrogen atmosphere with a heating rate of 10 °C min

**Table S1** Crystal data and structure refinement for **L1**

Empirical formula	C <sub>10</sub> H <sub>19</sub> N <sub>2</sub> O <sub>4</sub> Se
Formula weight	228.77
Temperature/K	298
Crystal system	orthorhombic
Space group	P2 <sub>1</sub> 2 <sub>1</sub> 2 <sub>1</sub>
a/Å	16.2382(8)
b/Å	7.0046(4)
c/Å	15.8492(9)
α/°	90
β/°	90
γ/°	90
Volume/Å <sup>3</sup>	1802.71(16)
Z	6
ρ <sub>calc</sub> /g/cm <sup>3</sup>	1.2643
μ/mm <sup>-1</sup>	2.881
F(000)	662.7
Crystal size/mm <sup>3</sup>	0.07 × 0.05 × 0.05
Radiation	Cu Kα (λ = 1.54184)
2θ range for data collection/°	7.8 to 142.42
Index ranges	-19 ≤ h ≤ 13, -6 ≤ k ≤ 8, -19 ≤ l ≤ 18
Reflections collected	3951
Independent reflections	2883 [R <sub>int</sub> = 0.0128, R <sub>sigma</sub> = 0.0281]
Data/restraints/parameters	2883/0/183
Goodness-of-fit on F <sup>2</sup>	1.649
Final R indexes [I ≥ 2σ (I)]	R <sub>1</sub> = 0.1277, wR <sub>2</sub> = 0.3537
Final R indexes [all data]	R <sub>1</sub> = 0.1433, wR <sub>2</sub> = 0.3852
Largest diff. peak/hole / e Å <sup>-3</sup>	2.27/-0.95
Flack parameter	0.8(3)

**Table S2** Fractional Atomic Coordinates (×10<sup>4</sup>) and Equivalent Isotropic Displacement Parameters (Å<sup>2</sup>×10<sup>3</sup>) for **L1**. U<sub>eq</sub> is defined as 1/3 of the trace of the orthogonalised U<sub>ij</sub> tensor.



Atom	x	y	z	U(eq)
Se1	1445.8(6)	2577.8(18)	8685.9(8)	67.4(5)
N1	1865(8)	6686(16)	8541(7)	71(3)
N2	2856(6)	4899(15)	8234(6)	65(2)
C1	2063(9)	4787(17)	8492(7)	67(3)
C4	1006(8)	7390(20)	8730(8)	74(3)
C5	486(7)	7630(20)	7919(8)	72(3)
O1	749(7)	7190(40)	7233(7)	197(12)
C7	3890(5)	2620(17)	8695(5)	51(2)
C11	3412(6)	2510(19)	7229(5)	53(2)
C6	3391(6)	3304(17)	8060(7)	57(2)
C8	4458(10)	1190(30)	8466(14)	108(7)
C9	4498(9)	450(30)	7688(16)	105(6)
C10	3985(12)	1150(60)	7091(15)	176(14)
O2	-260(7)	7760(20)	8062(8)	108(4)
C3	2490(8)	7750(20)	8333(10)	83(4)
C2	3090(11)	6810(20)	8149(12)	89(4)
C12	3834(9)	2960(50)	9572(8)	134(11)
C13	4484(12)	4610(30)	9844(16)	118(7)
C15	2806(10)	3200(70)	6581(9)	230(20)
C14	3630(30)	2810(70)	10310(40)	240(20)
C0aa	2451(18)	3140(40)	6036(18)	137(8)
C1aa	3380(15)	4710(40)	5952(14)	125(7)

**Table S3** Anisotropic Displacement Parameters ( $\text{\AA}^2 \times 10^3$ ) for **L1**. The Anisotropic displacement factor exponent takes the form:  $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\dots]$ .

Atom	U <sub>11</sub>	U <sub>22</sub>	U <sub>33</sub>	U <sub>12</sub>	U <sub>13</sub>	U <sub>23</sub>
Se1	41.3(7)	72.5(8)	88.5(9)	-3.4(5)	11.1(4)	2.4(7)
N1	76(7)	64(5)	74(6)	6(5)	2(5)	-2(5)
N2	57(6)	73(6)	65(5)	-1(5)	14(5)	7(5)
C1	83(8)	68(6)	51(5)	13(6)	8(5)	9(5)
C4	48(6)	97(9)	76(7)	5(7)	12(4)	-25(9)
C5	57(6)	85(8)	74(6)	-19(7)	5(5)	10(8)
O1	79(7)	450(40)	64(6)	93(15)	11(5)	45(12)
C7	34(4)	69(5)	51(4)	3(5)	4(3)	-8(6)
C11	37(4)	75(6)	48(4)	13(5)	-2(3)	0(5)
C6	38(5)	67(5)	66(6)	12(4)	1(4)	6(5)

C8	61(9)	131(14)	133(15)	38(10)	26(10)	60(12)
C9	36(7)	129(14)	150(17)	9(8)	32(9)	14(13)
C10	70(11)	330(40)	132(17)	-21(18)	52(12)	-120(20)
O2	68(6)	150(11)	105(7)	48(7)	-12(5)	-23(8)
C3	45(6)	96(10)	109(10)	-1(7)	10(6)	-1(9)
C2	77(9)	82(8)	107(11)	-3(8)	-1(9)	17(8)
C12	61(7)	290(30)	49(6)	-20(16)	0(5)	3(12)
C13	71(11)	119(14)	163(19)	-14(10)	-39(12)	-24(14)
C15	66(9)	580(70)	51(7)	-140(20)	-31(6)	83(18)

**Table S4** Bond Lengths for **L1**.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
Se1	C1	1.869(13)	C7	C12	1.413(16)
N1	C1	1.371(16)	C11	C6	1.429(15)
N1	C4	1.508(18)	C11	C10	1.35(3)
N1	C3	1.300(19)	C11	C15	1.50(2)
N2	C1	1.353(16)	C8	C9	1.34(3)
N2	C6	1.442(14)	C9	C10	1.35(4)
N2	C2	1.399(19)	C3	C2	1.21(2)
C4	C5	1.546(18)	C12	C13	1.63(3)
C5	O1	1.206(18)	C12	C14	1.22(6)
C5	O2	1.237(16)	C15	C0aa	1.04(3)
C7	C6	1.378(14)	C15	C1aa	1.73(3)
C7	C8	1.41(2)	C0aa	C1aa	1.87(4)

**Table S5** Bond Angles for **L1**.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
C4	N1	C1	123.0(12)	C15	C11	C10	124.6(19)
C3	N1	C1	110.9(13)	C7	C6	N2	118.9(10)
C3	N1	C4	125.9(12)	C11	C6	N2	119.5(9)
C6	N2	C1	125.9(10)	C11	C6	C7	121.6(10)
C2	N2	C1	110.1(11)	C9	C8	C7	123.1(15)
C2	N2	C6	124.0(12)	C10	C9	C8	118.2(18)
N1	C1	Se1	131.9(11)	C9	C10	C11	124.6(17)
N2	C1	Se1	127.4(9)	C2	C3	N1	112.4(16)

N2	C1	N1	100.6(11)	C3	C2	N2	106.0(15)
C5	C4	N1	112.0(9)	C13	C12	C7	109.8(17)
O1	C5	C4	121.9(12)	C14	C12	C7	161(3)
O2	C5	C4	113.0(11)	C14	C12	C13	89(3)
O2	C5	O1	122.0(13)	C0aa	C15	C11	157(5)
C8	C7	C6	116.3(11)	C1aa	C15	C11	103.8(12)
C12	C7	C6	128.5(13)	C1aa	C15	C0aa	81(2)
C12	C7	C8	114.5(16)	C1aa	C0aa	C15	66(2)
C10	C11	C6	116.2(13)	C0aa	C1aa	C15	33.3(11)
C15	C11	C6	119.2(17)				

**Table S6** Crystal data and structure refinement for **L2**.

Identification code	<b>L2</b>
Empirical formula	C <sub>14</sub> H <sub>18</sub> N <sub>2</sub> O <sub>3</sub> Se
Formula weight	341.27
Temperature/K	293(2)
Crystal system	monoclinic
Space group	P2 <sub>1</sub> /c
a/Å	7.6495(3)
b/Å	12.4690(5)
c/Å	16.5823(6)
α/°	90
β/°	92.492(3)
γ/°	90
Volume/Å <sup>3</sup>	1580.14(10)
Z	4
ρ <sub>calc</sub> /cm <sup>3</sup>	1.4344
μ/mm <sup>-1</sup>	3.298
F(000)	694.7
Crystal size/mm <sup>3</sup>	0.17 × 0.16 × 0.12
Radiation	Cu Kα (λ = 1.54184)
2θ range for data collection/°	8.88 to 141.58
Index ranges	-9 ≤ h ≤ 5, -15 ≤ k ≤ 14, -20 ≤ l ≤ 19
Reflections collected	6145
Independent reflections	2972 [R <sub>int</sub> = 0.0232, R <sub>sigma</sub> = 0.0306]
Data/restraints/parameters	2972/0/188
Goodness-of-fit on F <sup>2</sup>	1.069

Final R indexes [ $I \geq 2\sigma(I)$ ]  $R_1 = 0.0403$ ,  $wR_2 = 0.1088$

Final R indexes [all data]  $R_1 = 0.0514$ ,  $wR_2 = 0.1213$

Largest diff. peak/hole /  $e \text{ \AA}^{-3}$  0.61/-0.66

**Table S7** Fractional Atomic Coordinates ( $\times 10^4$ ) and Equivalent Isotropic Displacement Parameters ( $\text{\AA}^2 \times 10^3$ ) for **L2**.  $U_{eq}$  is defined as 1/3 of the trace of the orthogonalised  $U_{ij}$  tensor.

Atom	x	y	z	U(eq)
C1	2379(4)	6089(2)	2295.7(18)	54.8(7)
C2	2138(6)	4314(3)	2376(3)	94.0(13)
C3	3149(6)	4524(3)	1762(3)	92.6(13)
C4	762(4)	5414(3)	3450.4(19)	68.4(9)
C5	2048(4)	5475(3)	4157(2)	62.8(8)
C6	4286(4)	6188(2)	1128.8(17)	52.9(7)
C7	3537(4)	6423(3)	375.9(18)	57.5(7)
C8	4528(4)	6989(3)	-161.4(18)	58.9(7)
C9	6219(4)	7309(2)	35.4(19)	56.4(7)
C10	6938(4)	7030(3)	789(2)	62.4(8)
C11	6010(4)	6468(3)	1346.0(18)	60.0(7)
C12	6811(5)	6167(4)	2159(2)	98.6(14)
C13	7257(5)	7955(3)	-547(2)	77(1)
C14	1682(5)	6088(4)	135(3)	94.8(14)
N1	1654(3)	5273(2)	2702.3(16)	64.2(7)
N2	3281(3)	5627(2)	1705.3(15)	59.2(6)
O1	1364(3)	5904(2)	4790.2(14)	75.7(7)
O2	3529(4)	5174(3)	4142.0(17)	95.4(9)
O3	3274(3)	9209(2)	1094.2(16)	75.5(7)
Se1	2145.6(6)	7519.8(3)	2524.6(2)	72.4(2)

**Table S8** Anisotropic Displacement Parameters ( $\text{\AA}^2 \times 10^3$ ) for **L2**. The Anisotropic displacement factor exponent takes the form:  $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\dots]$ .

Atom	$U_{11}$	$U_{22}$	$U_{33}$	$U_{12}$	$U_{13}$	$U_{23}$
C1	54.3(15)	57.3(17)	53.7(15)	-3.3(13)	11.8(12)	-0.3(13)
C2	124(3)	59(2)	103(3)	-24(2)	50(3)	-4(2)

C3	127(3)	51.5(19)	103(3)	-17(2)	54(3)	-13.7(19)
C4	54.3(17)	89(2)	63.3(18)	-8.7(16)	20.4(14)	9.3(17)
C5	60.7(18)	58.4(18)	70.5(19)	1.6(15)	17.1(15)	10.3(15)
C6	54.1(16)	52.7(15)	53.3(15)	-5.2(13)	16.0(12)	-7.3(12)
C7	46.8(15)	66.9(18)	59.5(17)	-5.0(13)	9.3(13)	-13.2(14)
C8	60.8(17)	67.6(19)	48.9(15)	3.3(15)	8.0(13)	-3.8(14)
C9	56.5(17)	54.5(16)	59.8(17)	-2.5(13)	19.7(13)	-5.9(13)
C10	47.6(16)	72(2)	68.8(19)	-6.5(14)	10.0(14)	-4.3(16)
C11	54.6(16)	69.6(19)	56.0(16)	-3.1(14)	5.6(13)	-0.7(14)
C12	79(3)	142(4)	74(2)	-9(3)	-10(2)	25(3)
C13	89(3)	69(2)	75(2)	-14.1(19)	29.8(19)	1.7(18)
C14	59(2)	138(4)	87(3)	-20(2)	1.7(18)	-10(3)
N1	63.8(15)	65.9(16)	64.6(15)	-10.8(13)	22.7(12)	3.6(13)
N2	63.4(15)	52.0(13)	63.9(15)	-10.0(11)	21.9(12)	-6.6(11)
O1	62.5(13)	95.7(18)	70.0(14)	8.5(13)	13.8(11)	0.4(13)
O2	73.2(16)	124(2)	88.8(18)	38.0(16)	7.9(13)	-3.6(17)
O3	74.0(15)	75.4(16)	78.0(16)	-7.0(13)	13.1(12)	8.8(13)
Se1	92.7(3)	57.8(3)	68.8(3)	9.61(17)	26.6(2)	-0.05(16)

**Table S9** Bond Lengths for **L2**.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
C1	N1	1.352(4)	C6	C7	1.382(4)
C1	N2	1.351(4)	C6	C11	1.396(4)
C1	Se1	1.835(3)	C6	N2	1.435(3)
C2	C3	1.331(5)	C7	C8	1.388(4)
C2	N1	1.370(5)	C7	C14	1.516(5)
C3	N2	1.382(4)	C8	C9	1.379(4)
C4	C5	1.498(5)	C9	C10	1.388(5)
C4	N1	1.452(4)	C9	C13	1.509(4)
C5	O1	1.308(4)	C10	C11	1.380(4)
C5	O2	1.195(4)	C11	C12	1.504(5)

**Table S1-** Bond Angles for **L2**.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
N2	C1	N1	105.9(3)	C9	C8	C7	121.9(3)

Se1	C1	N1	125.6(2)	C10	C9	C8	118.1(3)
Se1	C1	N2	128.5(2)	C13	C9	C8	121.1(3)
N1	C2	C3	107.9(3)	C13	C9	C10	120.7(3)
N2	C3	C2	107.1(3)	C11	C10	C9	122.3(3)
N1	C4	C5	110.9(3)	C10	C11	C6	117.5(3)
O1	C5	C4	112.1(3)	C12	C11	C6	120.8(3)
O2	C5	C4	124.0(3)	C12	C11	C10	121.6(3)
O2	C5	O1	123.9(3)	C2	N1	C1	109.6(3)
C11	C6	C7	122.0(3)	C4	N1	C1	123.5(3)
N2	C6	C7	119.5(3)	C4	N1	C2	126.1(3)
N2	C6	C11	118.5(3)	C3	N2	C1	109.5(3)
C8	C7	C6	118.1(3)	C6	N2	C1	125.4(2)
C14	C7	C6	121.8(3)	C6	N2	C3	125.0(3)
C14	C7	C8	120.1(3)				

**Table S11** Hydrogen Atom Coordinates ( $\text{\AA}\times 10^4$ ) and Isotropic Displacement Parameters ( $\text{\AA}^2\times 10^3$ ) for **L2**.

Atom	<i>x</i>	<i>y</i>	<i>z</i>	U(eq)
H2	1817(6)	3637(3)	2552(3)	112.8(16)
H3	3668(6)	4023(3)	1432(3)	111.1(16)
H4a	-30(4)	4818(3)	3523.7(19)	82.1(11)
H4b	74(4)	6068(3)	3421.0(19)	82.1(11)
H8	4039(4)	7157(3)	-668.8(18)	70.7(9)
H10	8086(4)	7228(3)	924(2)	74.9(9)
H12a	6140(30)	6480(20)	2575(2)	148(2)
H12b	6820(40)	5400(4)	2213(9)	148(2)
H12c	7989(17)	6430(30)	2207(9)	148(2)
H13a	7840(30)	7478(3)	-901(12)	115.5(15)
H13b	6482(7)	8415(17)	-859(12)	115.5(15)
H13c	8110(30)	8382(18)	-251(2)	115.5(15)
H14a	1334(17)	6420(20)	-370(11)	142(2)
H14b	1631(11)	5322(5)	80(20)	142(2)
H14c	907(8)	6310(30)	542(11)	142(2)
H1	2060(30)	5850(40)	5180(8)	113.6(10)
H3a	3280(50)	8710(30)	1450(20)	113.3(10)
H3b	4313(18)	9430(30)	1040(20)	113.3(10)



**Table S12:** Structural parameters of **1-6** (CCDC: 1442188-1442193).

Parameters	1	2	3	4	5	6
Empirical formula	C <sub>36</sub> H <sub>48</sub> CdClN <sub>5</sub> O <sub>7</sub> Se <sub>2</sub>	C <sub>48</sub> H <sub>96</sub> O <sub>16</sub> Cl <sub>2</sub> Se <sub>4</sub> CdN <sub>8</sub>	C <sub>48</sub> H <sub>96</sub> N <sub>8</sub> O <sub>16</sub> ZnSe <sub>4</sub> Cl <sub>2</sub>	C <sub>15</sub> H <sub>18</sub> CdCl <sub>2</sub> N <sub>2</sub> O <sub>2</sub> Se	C <sub>7.5</sub> H <sub>9</sub> NO <sub>1.666667</sub> Cd <sub>0.166667</sub> Cl <sub>0.33333</sub> <sup>33</sup> Se <sub>0.5</sub>	C <sub>7.5</sub> H <sub>10.5</sub> NO <sub>3.75</sub> Zn <sub>0.25</sub> Se <sub>0.5</sub> Cl <sub>3</sub>
Formula weight	968.57	5386.84	5373.79	520.57	1259.16	990.87
Temperature	150	293	150.01	293	293	150
Crystal system	monoclinic	cubic	cubic	monoclinic	trigonal	tetragonal
Space group	P2 <sub>1</sub> /c	F-43c	F-43c	P2 <sub>1</sub> /c	R-3	P4 <sub>1</sub> 22
a/Å	15.4327(6)	39.4115(4)	38.8082(5)	7.3578(2)	14.6180(3)	11.82385(11)
b/Å	9.9492(4)	39.4115(4)	38.8082(5)	11.7976(3)	14.6180(3)	11.82385(11)
c/Å	26.6209(9)	39.4115(4)	38.8082(5)	21.8444(5)	45.0966(10)	28.5490(4)
α/°	90.00	90	90.00	90	90	90
β/°	91.820(3)	90	90.00	93.068(2)	90	90
γ/°	90.00	90	90.00	90	120	90
Volume/Å <sup>3</sup>	4085.4(2)	61216.6(19)	58448.3(14)	1893.47(8)	8345.5(3)	3991.24(8)
Z	4	8	8	4	6	4
ρ <sub>calc</sub> /cm <sup>3</sup>	1.575	1.113	1.134	1.826	1.503	1.6506
Absorption coefficient/mm <sup>-1</sup>	7.3430	4.103	2.852	14.110	6.732	4.785
F(000)	1952.6	20904.0	20472.0	1016.0	3780.5	2000.1
Data collected	14393	11660	10660	12418	19412	10355
Unique data	7737	3950	4783	3596	3558	3794
R <sub>int</sub>	0.0428	0.0294	0.0325	0.0413	0.0391	0.0262
GOF on F <sup>2</sup>	1.037	1.137	1.103	0.969	1.032	1.050
R <sub>1</sub> [I>=2σ(I)]	0.0690	0.0545	0.0666	0.0378	0.0417	0.0622
R <sub>1</sub> values (all data)	0.0760	0.0658	0.0721	0.0407	0.0449	0.0675
wR <sub>1</sub> values (all data)	0.2032	0.1662	0.1954	0.1225	0.1475	0.1849