

Supplementary Data

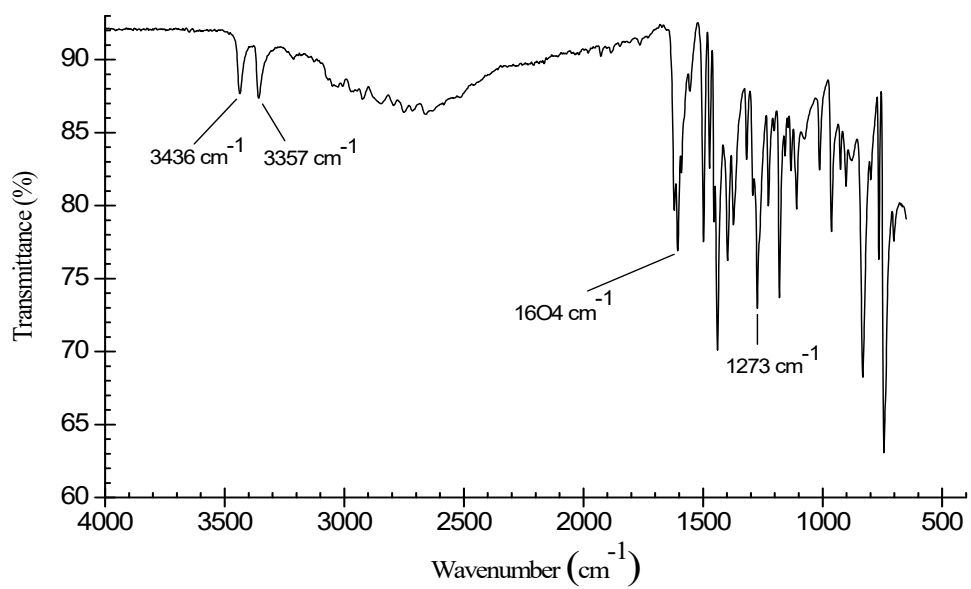


Figure S1. Infrared spectrum of A-1

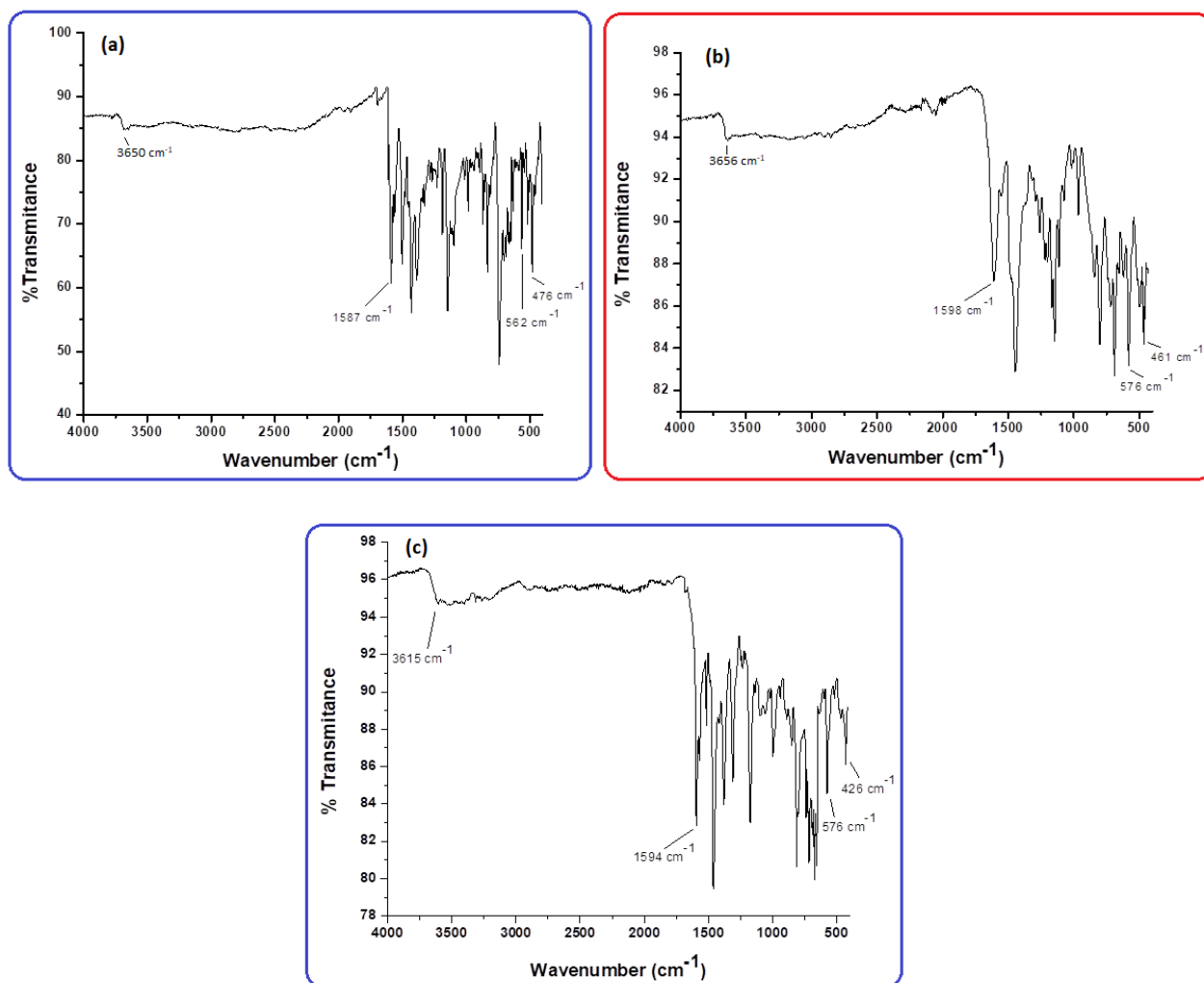


Figure S2. Infrared spectra of Complexes 2 (a), 3 (b) and 4 (c)

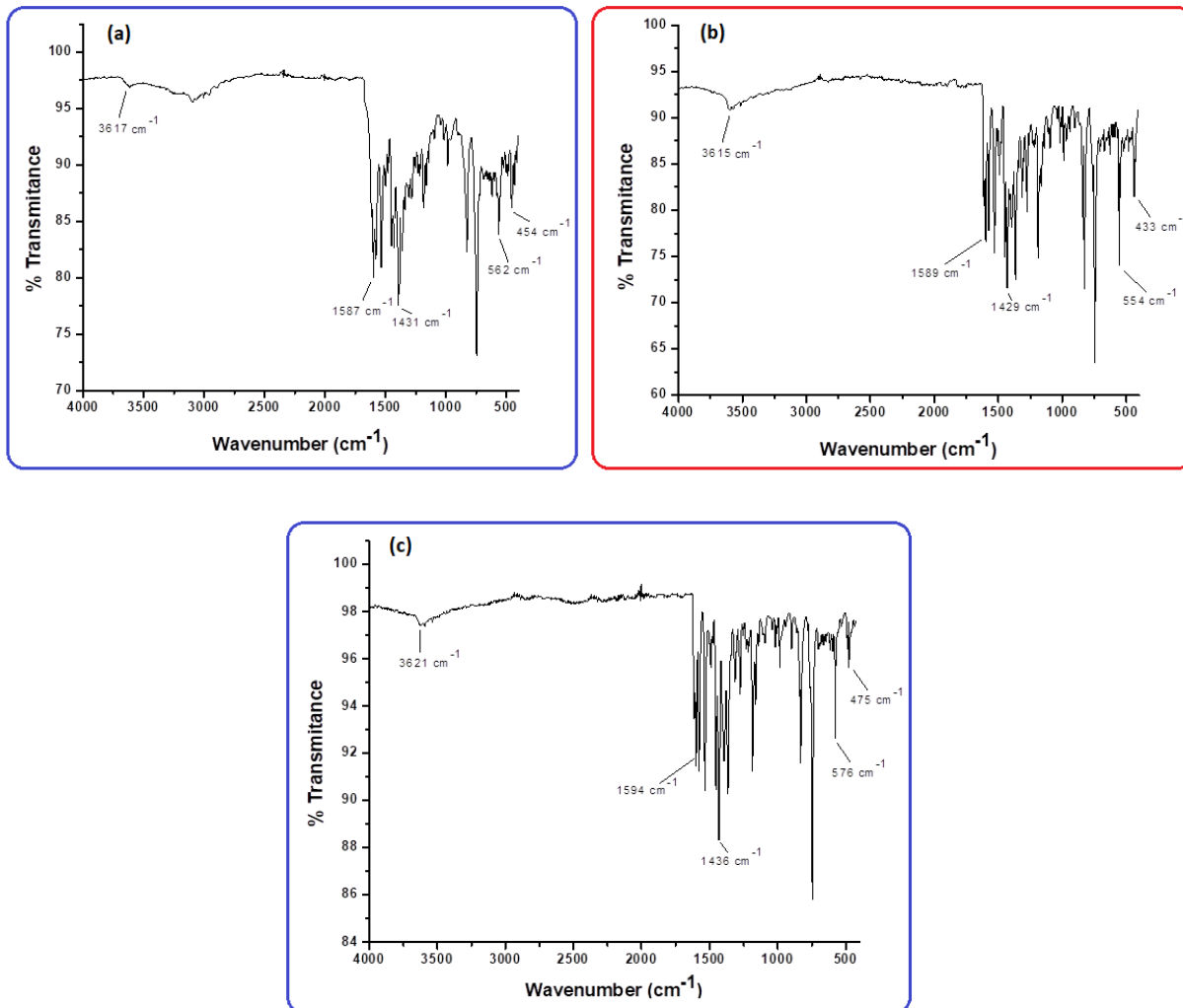


Figure S3. Infrared spectra of Complexes 6 (a), 7 (b) and 8 (c)

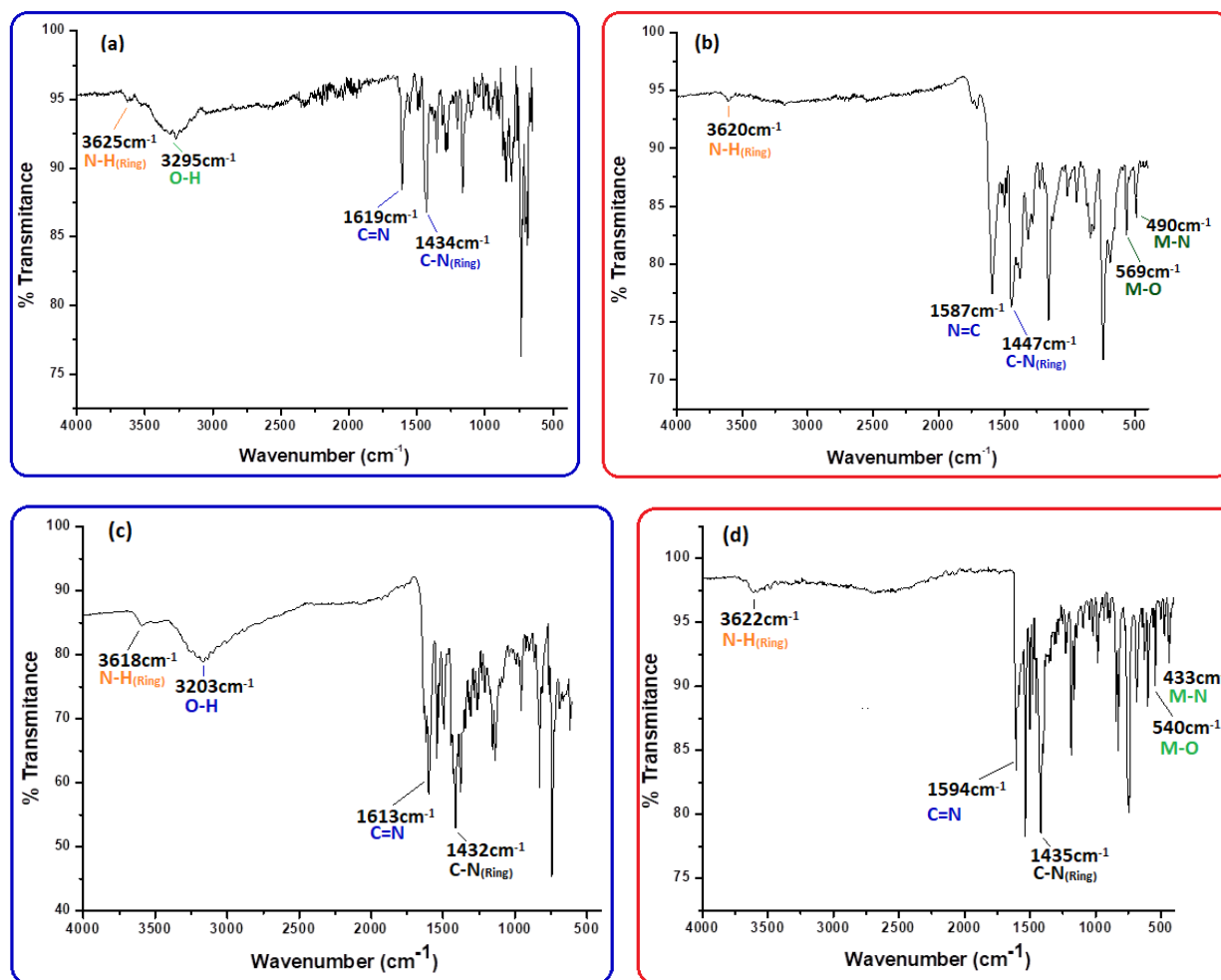


Fig. S4. Representative FT-IR spectra of ligands  $L_1$  (a),  $L_2$  (c) and Cu(II) complexes (1) (b), 5 (d).

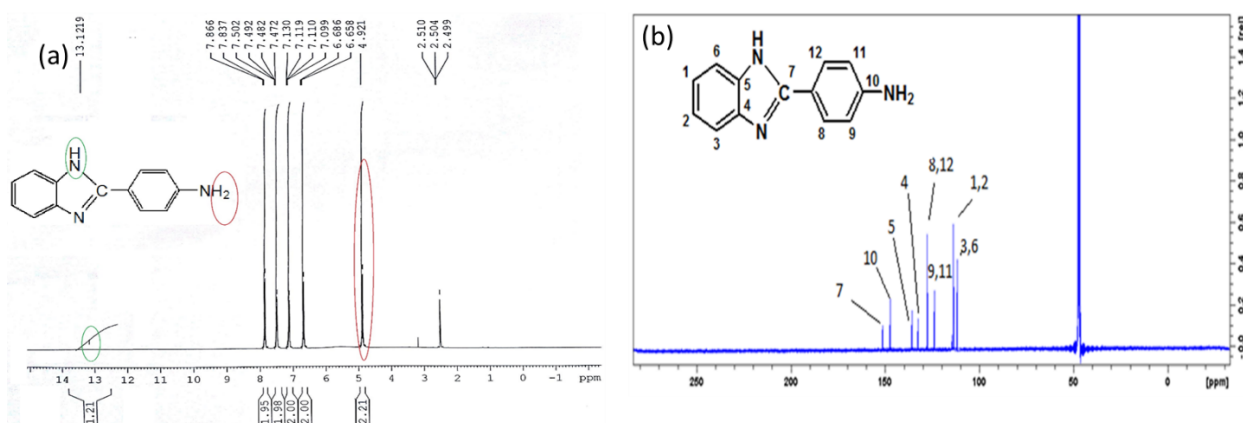


Figure S5.  $^1\text{H}$  NMR (a) and  $^{13}\text{C}$  NMR (b) spectra of A-1 in  $\text{DMSO-d}_6$

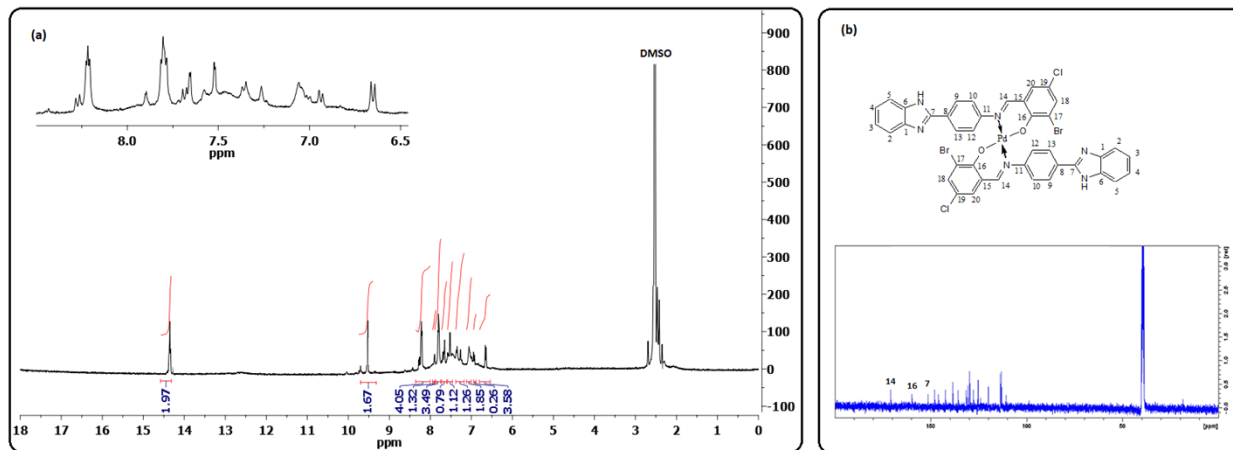


Figure S6.  $^1\text{H}$  NMR (a) and  $^{13}\text{C}$  NMR (b) spectra of Ni(II) complex **2** in DMSO- $d_6$

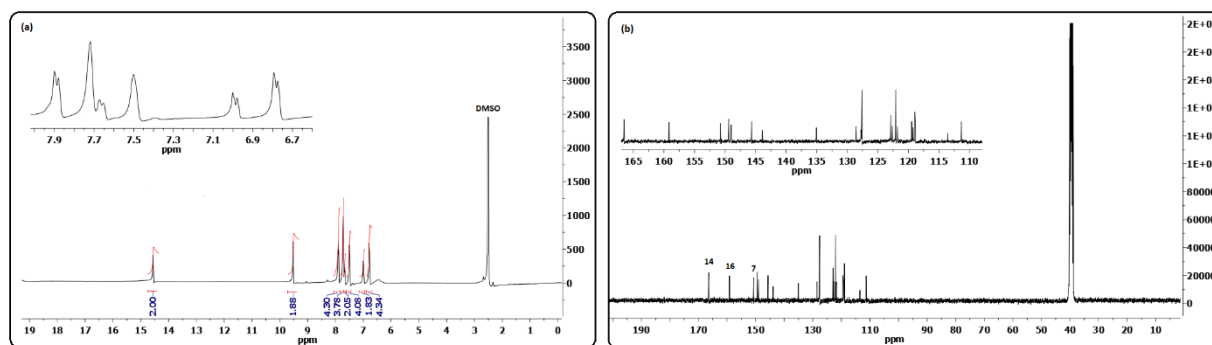


Figure S7.  $^1\text{H}$  NMR (a) and  $^{13}\text{C}$  NMR (b) spectra of Pd(II) complex **3** in DMSO- $d_6$

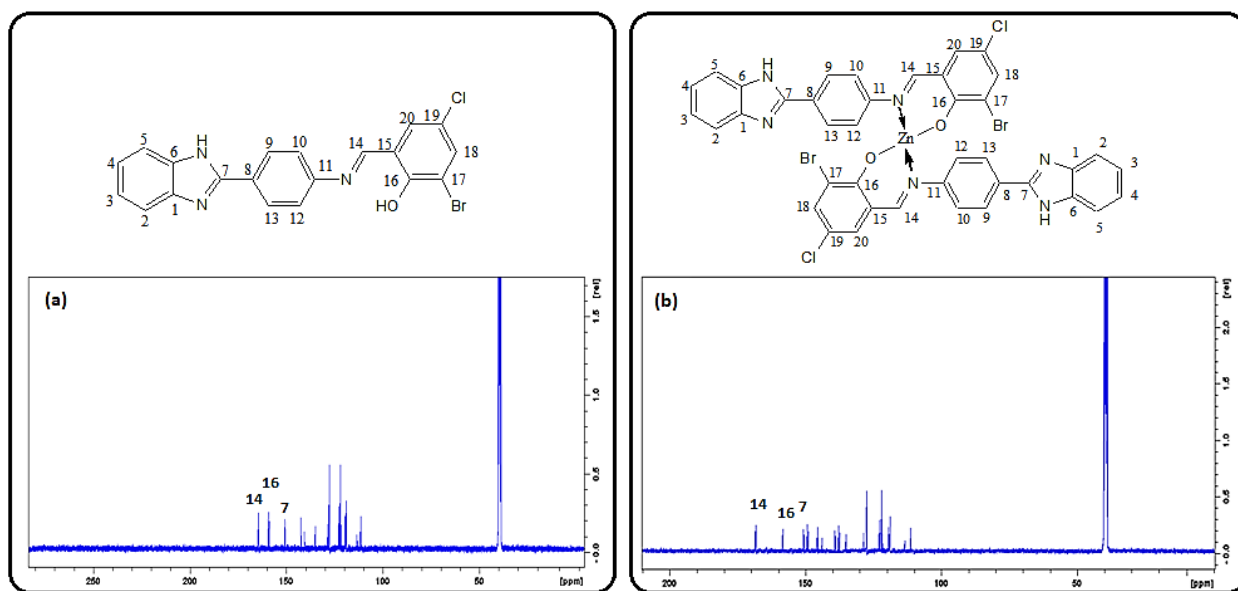


Figure S8.  $^{13}\text{C}$  NMR spectrum of ligand  $L_1$  (a) and Zn(II) complex **4** (b) in DMSO- $d_6$

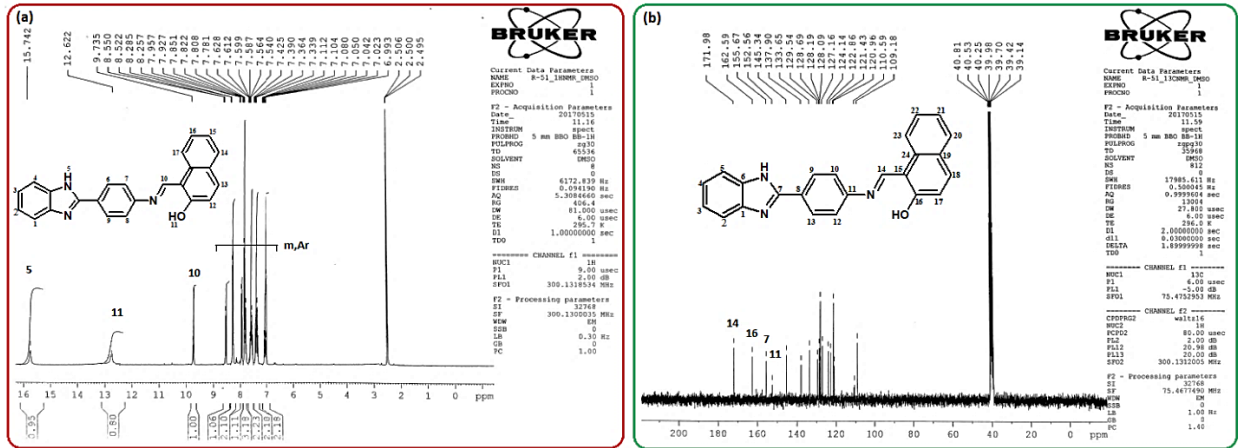


Figure S9. <sup>1</sup>H NMR (a) and <sup>13</sup>C NMR (b) spectra of ligand L<sub>2</sub> in DMSO-d<sub>6</sub>

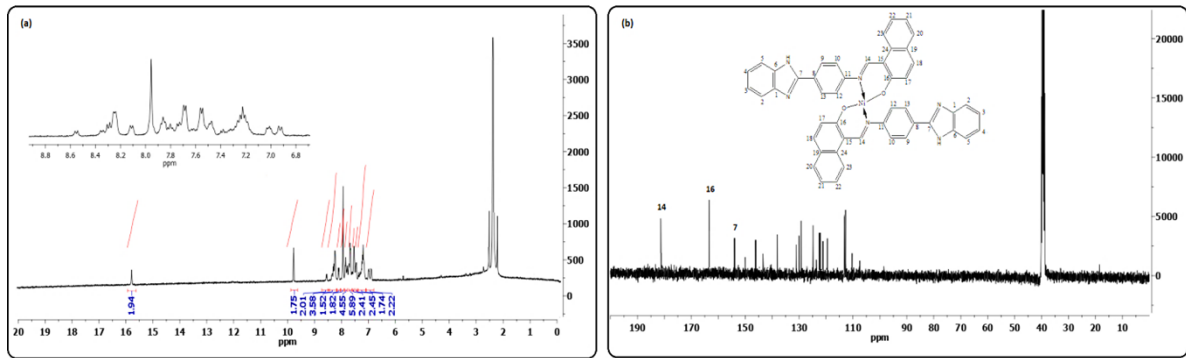


Figure S10. <sup>1</sup>H NMR (a) and <sup>13</sup>C NMR (b) spectra of Zn(II) complex 6 in DMSO-d<sub>6</sub>

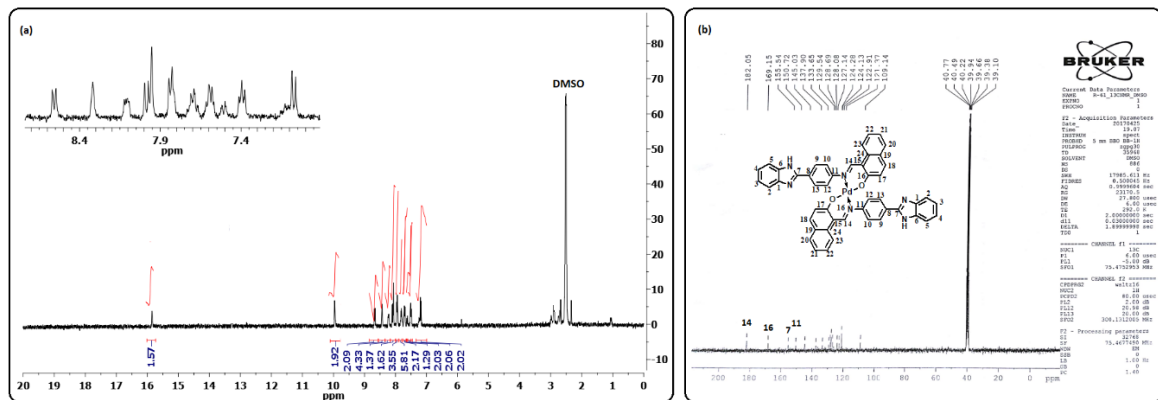


Figure S11. <sup>1</sup>H NMR (a) and <sup>13</sup>C NMR (b) spectra of Pd(II) complex 7 in DMSO-d<sub>6</sub>

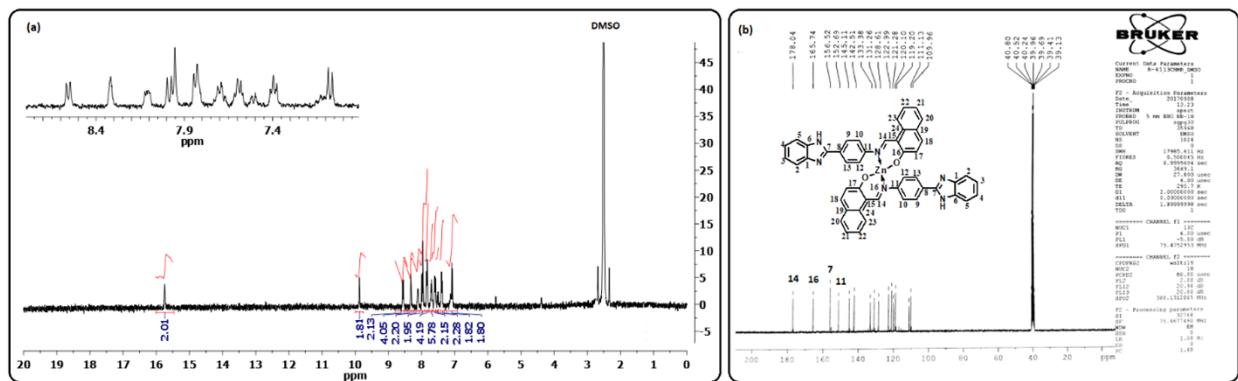
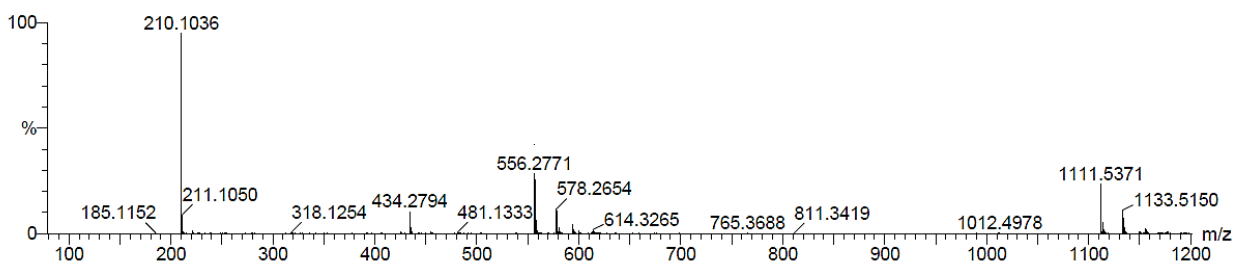
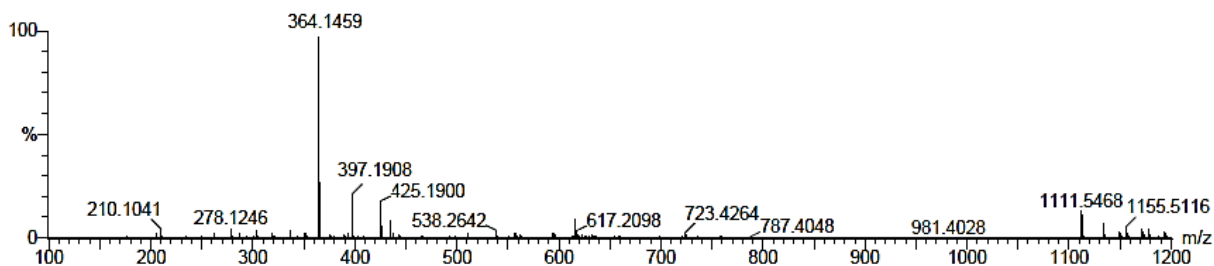


Figure S12.  $^1\text{H}$  NMR (a) and  $^{13}\text{C}$  NMR (b) spectra of Zn(II) complex **8** in DMSO- $d_6$



Minimum:				0.5		
Maximum:		5.0	10.0	100.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
210.1036	210.1031	0.5	2.4	9.5	201.6	C13 H12 N3

Figure S13. High resolution mass spectrum of A-1



Minimum:				0.5		
Maximum:		5.0	10.0	200.0		
Mass	Calc. Mass	mDa	PPM	DBE	1-FIT	Formula
364.1459	364.1450	0.9	2.5	17.5	3.5	C24 H18 N3 O

Figure S14. High Resolution Mass spectrum of L<sub>2</sub>

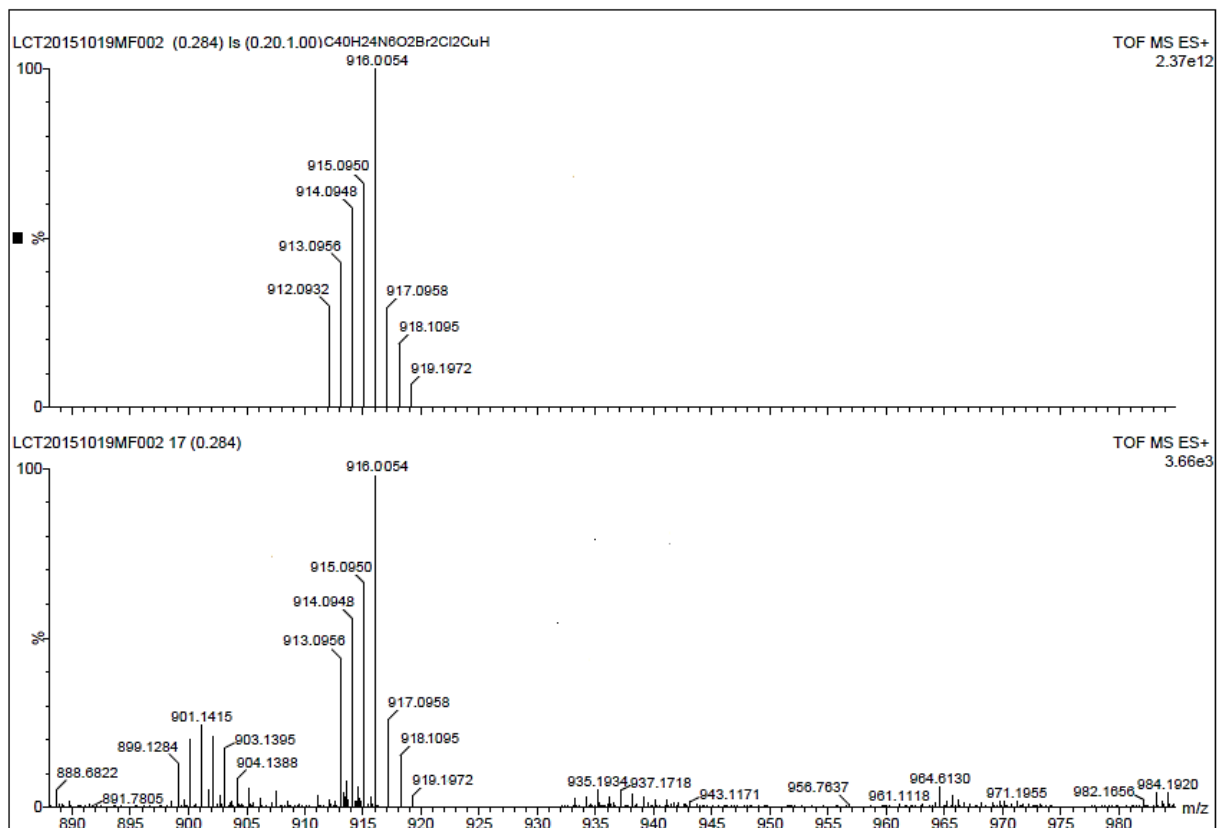


Figure S15. High Resolution Mass spectrum of complex 1

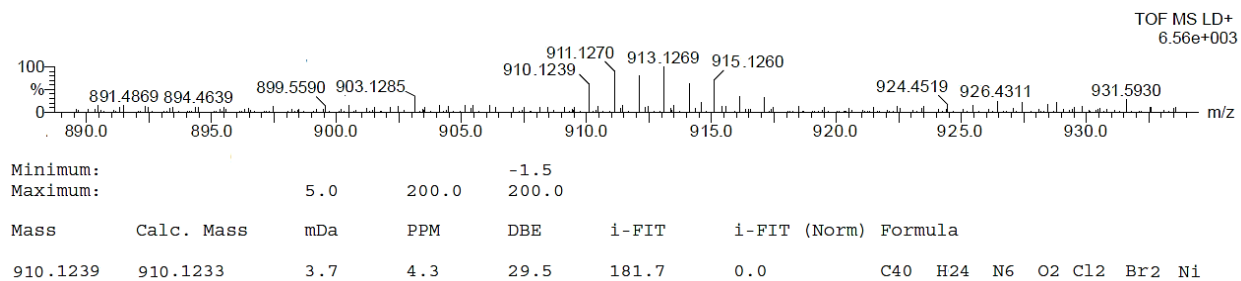


Figure S16. High Resolution Mass spectrum of complex 2



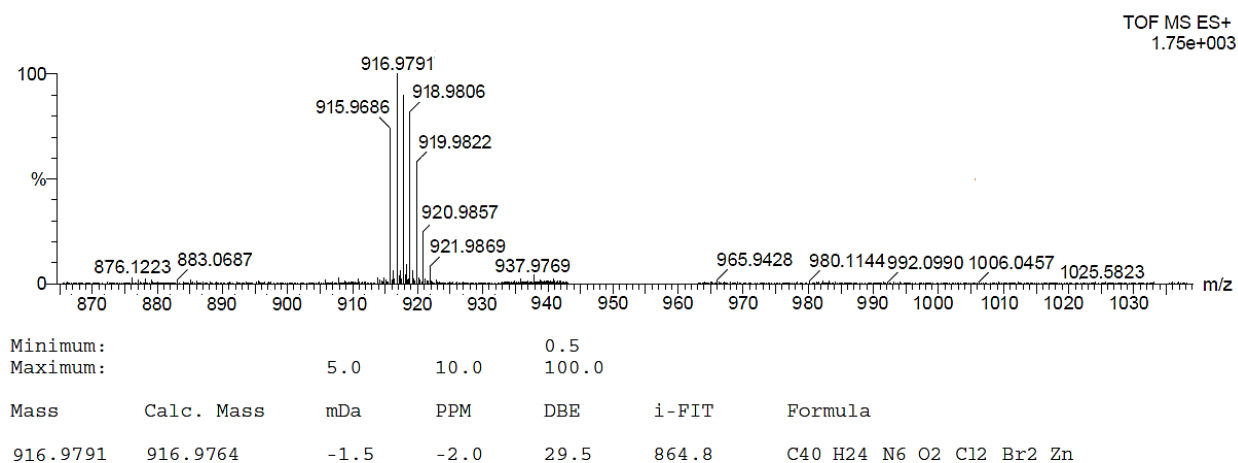


Figure S17. High Resolution Mass spectrum of complex 4

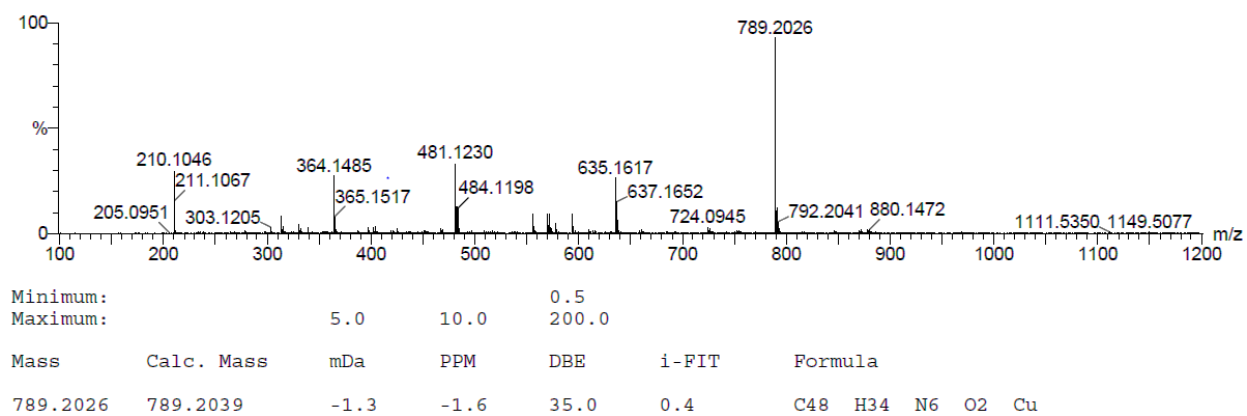
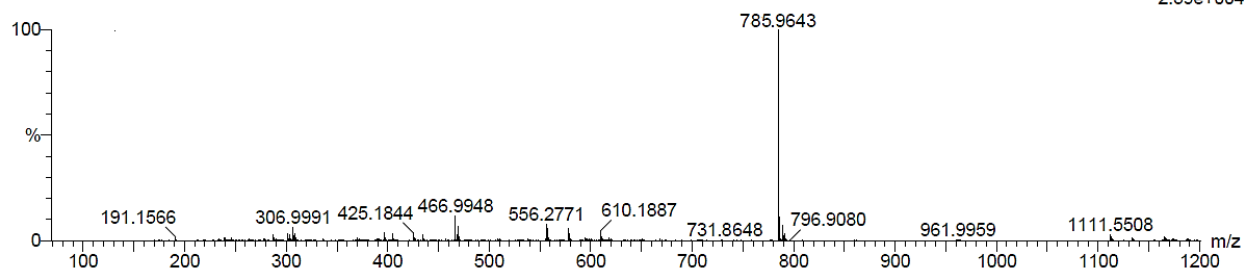


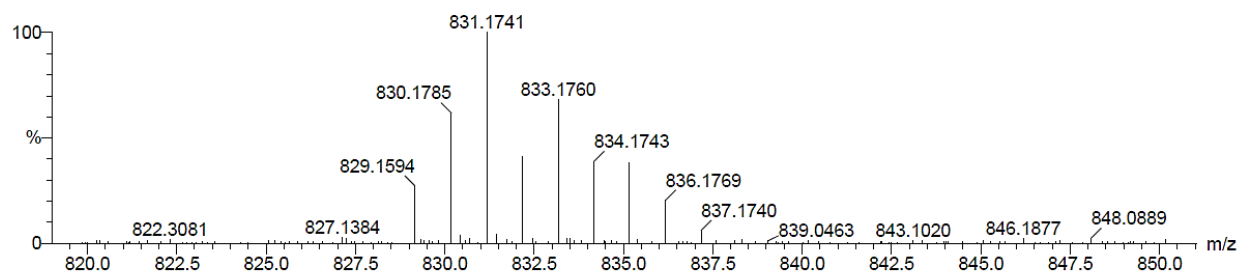
Figure S18. High Resolution Mass spectrum of complex 5

LCT20151126MF014 43 (0.717)

TOF MS ES+  
2.59e+004

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
785.9643	785.9635	-0.1	-0.2	16.0	1.0	C48 H33 N6 O2 Ni

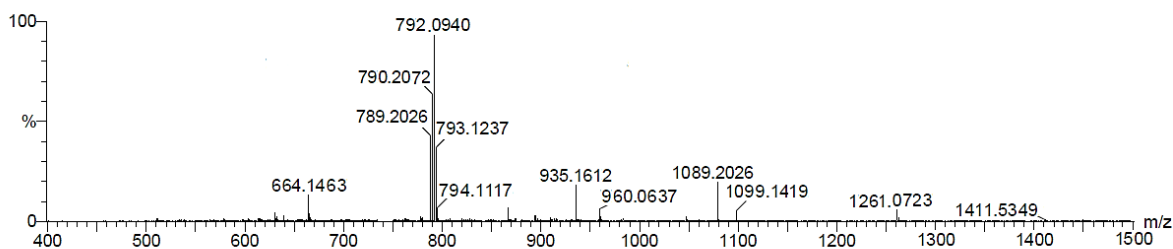
Figure S19. High Resolution Mass spectrum of complex 6



Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
831.1741	831.1700	4.1	4.9	35.5	1.5	C48 H33 N6 O2 Pd

Figure S20. High Resolution Mass spectrum of complex 7

LCT20151117MF020 23 (0.383)

TOF MS ES+  
7.08e+003

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
792.0940	792.0961	-0.5	-1.5	25.0	0.6	C48 H33 N6 O2 Zn

Figure S21. High Resolution Mass spectrum of complex 8

**Table S1:** Determination of minimum inhibitory concentration (MIC  $\mu\text{g}/\text{mL}$ ) of test compounds

Compounds	<i>M. luteus</i>						<i>S. aureus</i>						<i>E. coli</i>						<i>E. aerogenes</i>					
	a	b	c	d	e	f	a	b	c	d	e	f	a	b	c	d	e	f	a	b	c	d	e	f
L1	-	-	+	+	+	+	+	+	+	+	+	+	-	-	-	+	+	+	-	-	-	+	+	+
L2	+	+	+	+	+	+	+	+	+	+	+	+	-	-	+	+	+	+	-	-	-	+	+	+
1	+	+	+	+	+	+	-	-	+	+	+	+	-	-	-	+	+	+	-	-	+	+	+	+
2	-	-	-	-	+	+	-	-	-	-	+	+	-	-	-	-	-	+	-	-	-	+	+	+
3	-	-	+	+	+	+	+	+	+	+	+	+	+	+	+	+	+	+	+	+	+	+	+	+
4	-	+	+	+	+	+	+	+	+	+	+	+	-	-	-	+	+	+	-	-	-	+	+	+
5	+	+	+	+	+	+	+	+	+	+	+	+	+	+	+	+	+	+	+	+	+	+	+	+
6	-	-	-	+	+	+	-	-	+	+	+	+	-	-	-	-	+	+	-	-	+	+	+	+
7	-	-	+	+	+	+	-	-	+	+	+	+	+	+	+	+	+	+	+	+	+	+	+	+
8	-	-	+	+	+	+	+	+	+	+	+	+	-	-	-	+	+	+	+	+	+	+	+	+

$a=200 \mu\text{g}/\text{mL}$ ,  $b=100 \mu\text{g}/\text{mL}$ ,  $c=50 \mu\text{g}/\text{mL}$ ,  $d=25 \mu\text{g}/\text{mL}$ ,  $e=12.5 \mu\text{g}/\text{mL}$ ,  $f=6.25 \mu\text{g}/\text{mL}$

Minus (-) indicate the absence of growth, Plus (+) indicate the presence of growth

**Table S2:** Results of DPPH free radical scavenging assay

Compounds	Percentage Scavenging					IC <sub>50</sub> $\mu\text{g}/\text{mL}^{-1}$
	200 $\mu\text{g}/\text{mL}^{-1}$	66.6 $\mu\text{g}/\text{mL}^{-1}$	22.2 $\mu\text{g}/\text{mL}^{-1}$	7.4 $\mu\text{g}/\text{mL}^{-1}$	2.46 $\mu\text{g}/\text{mL}^{-1}$	
<b>L1</b>	52.88	50.23	48.47	45.56	14.38	60.25
<b>L2</b>	52.67	50.94	47.35	42.88	32.39	61.45
<b>1</b>	65.57	53.58	49.44	21.66	11.15	26.47
<b>2</b>	62.39	57.17	51.63	41.01	20.3	19.25
<b>3</b>	78.52	62.11	53.64	23.97	19.71	17.34
<b>4</b>	51.11	50.74	45.2	31.41	12	60.15
<b>5</b>	68.42	59.39	45.32	31.66	28.15	51.21
<b>6</b>	85	67.17	65.63	51.01	40.3	7.1
<b>7</b>	73.8	62.6	62.44	52.34	49.71	3.32
<b>8</b>	50.05	49.32	46.56	38.17	12.81	88.98
<b>Ascorbic acid</b>	82.43	66.59	61.74	55.41	40.31	4.23

Table S3: Results of brine shrimp cytotoxicity assay

Comp.	Percentage mortality after 24 hours			LD <sub>50</sub> µg/ml
	200µg/ml	66.6µg/ml	22.2µg/ml	
L <sub>1</sub>	70	20	20	127.61
L <sub>2</sub>	30	10	10	>200
1	40	30	10	>200
2	30	20	10	>200
3	20	10	10	>200
4	-	-	-	-
5	-	-	-	-
6	30	20	10	>200
7	60	40	10	125
8	-	-	-	-
Doxorubicin	95	90	70	3.22