

## “Supporting Information”

### Ligand Design Controls Biomolecule Binding and Cytotoxicity in Platinum(II) Complexes with ONS-Type Tridentate Ligands

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**Table S1. Important spectroscopic signals of the ligands and their platinum complexes.**

	IR spectroscopy (cm <sup>-1</sup> )		<sup>1</sup> H NMR		<sup>13</sup> C NMR	
	$\nu(\text{CH}=\text{N})$	H—C=N (Schiff base)	SCH <sub>3</sub>	R groups	H—C=N (Schiff base)	C-S
<b>L1</b>	1610	8.60	2.42	3.90	161.7	125.3
<b>L2</b>	1602	8.52	2.47	3.84	166.9	127.1
<b>L3</b>	1616	8.52	2.40	3.73	161.5	125.0
<b>L4</b>	1609	8.63	2.47	4.18 / 1.52	161.9	135.2
<b>L5</b>	1607	8.46	2.46	-	159.3	133.5
<b>L6</b>	1609	8.47	2.46	-	160.2	128.0
<b>L7</b>	1608	8.60	-	3.96	162.9	-
<b>L8</b>	1632	8.37	2.15	3.91	165.9	35.1
<b>L9</b>	1615	8.25	2.16	3.83	165.0	35.2
<b>Pt1</b>	1608	9.62	2.90	3.82	154.7	129.7
<b>Pt2</b>	1611	9.32	2.78	3.73	167.2	131.9
<b>Pt3</b>	1626	9.53	2.79	3.67	159.0	132.5
<b>Pt4</b>	1604	9.62	2.90	4.11 / 1.33	155.2	129.7
<b>Pt5</b>	1586	9.63	2.82	-	159.0	132.5
<b>Pt6</b>	1596	9.69	2.91	-	159.0	132.1
<b>Pt7</b>	1598	9.38	-	3.84	153.6	-
<b>Pt8</b>	1602	8.69	2.55	3.74	161.4	38.1
<b>Pt9</b>	1602	8.51	2.53	3.81	165.2	38.3

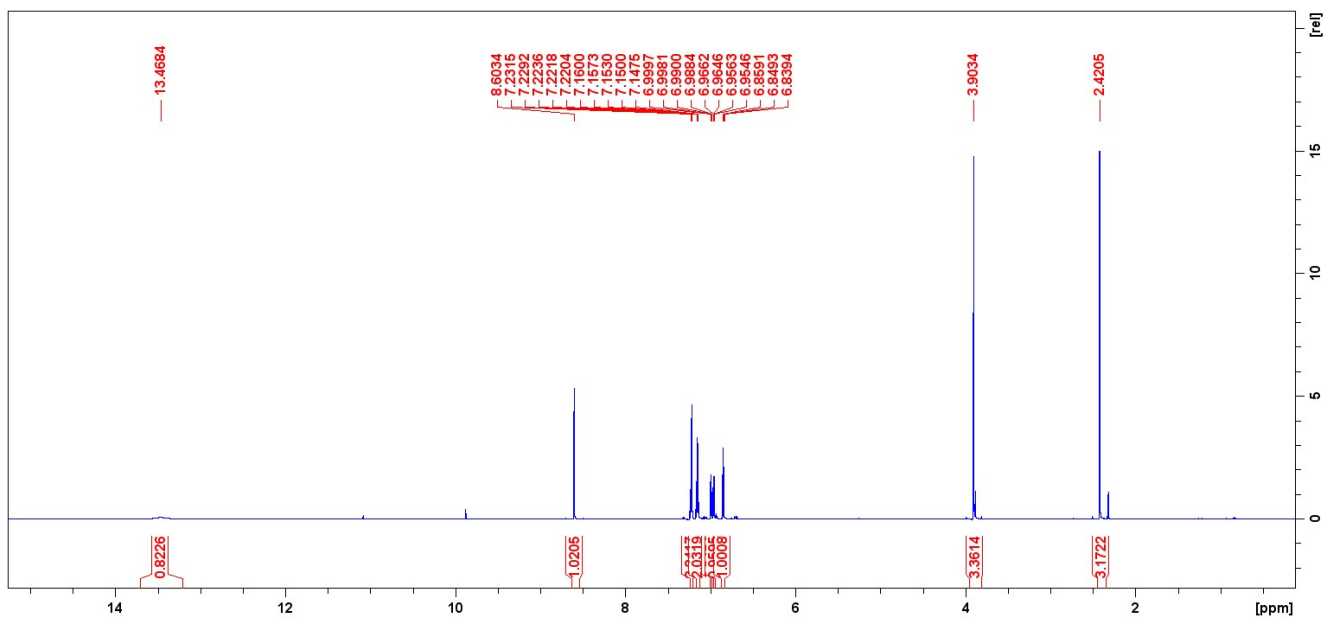


Figure S1.  $^1\text{H}$  NMR spectrum of L1 in  $\text{CDCl}_3$

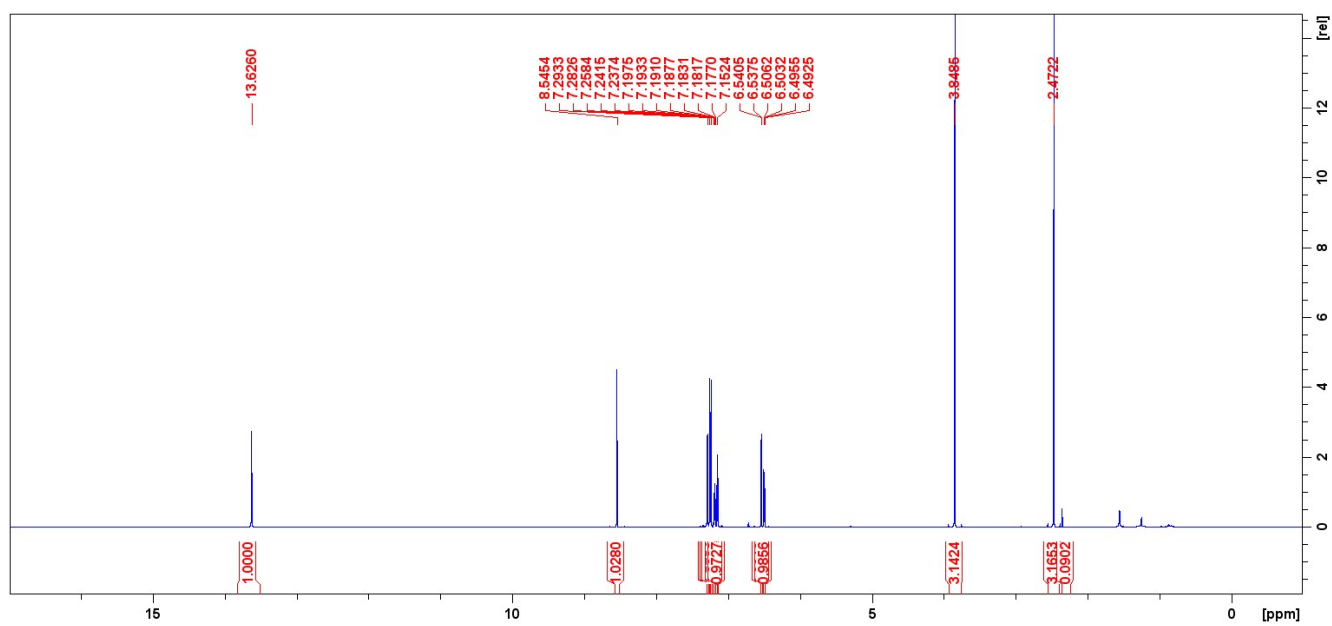


Figure S2.  $^1\text{H}$  NMR spectrum of L2 in  $\text{CDCl}_3$

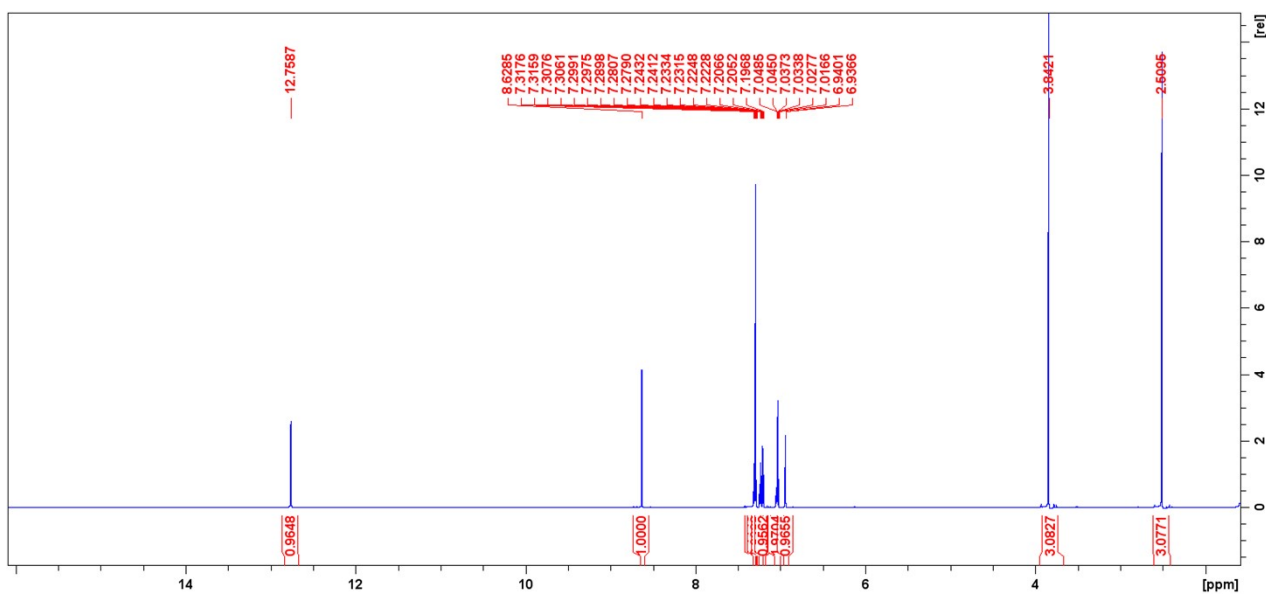


Figure S3.  $^1\text{H}$  NMR spectrum of L3 in  $\text{CDCl}_3$

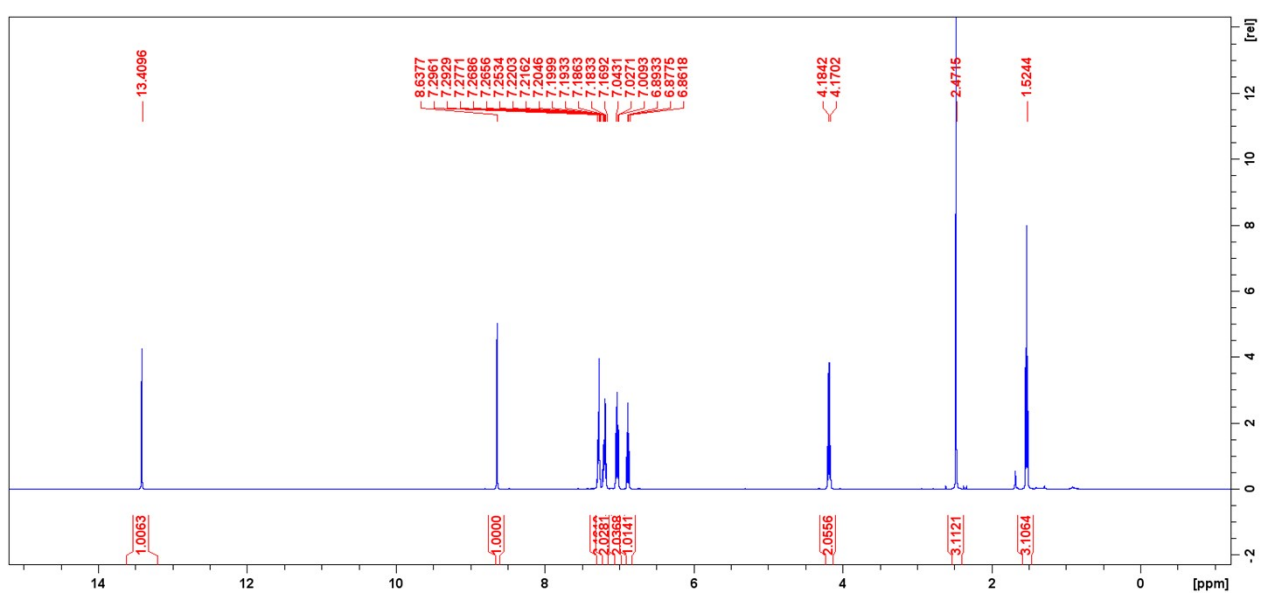


Figure S4.  $^1\text{H}$  NMR spectrum of L4 in  $\text{CDCl}_3$

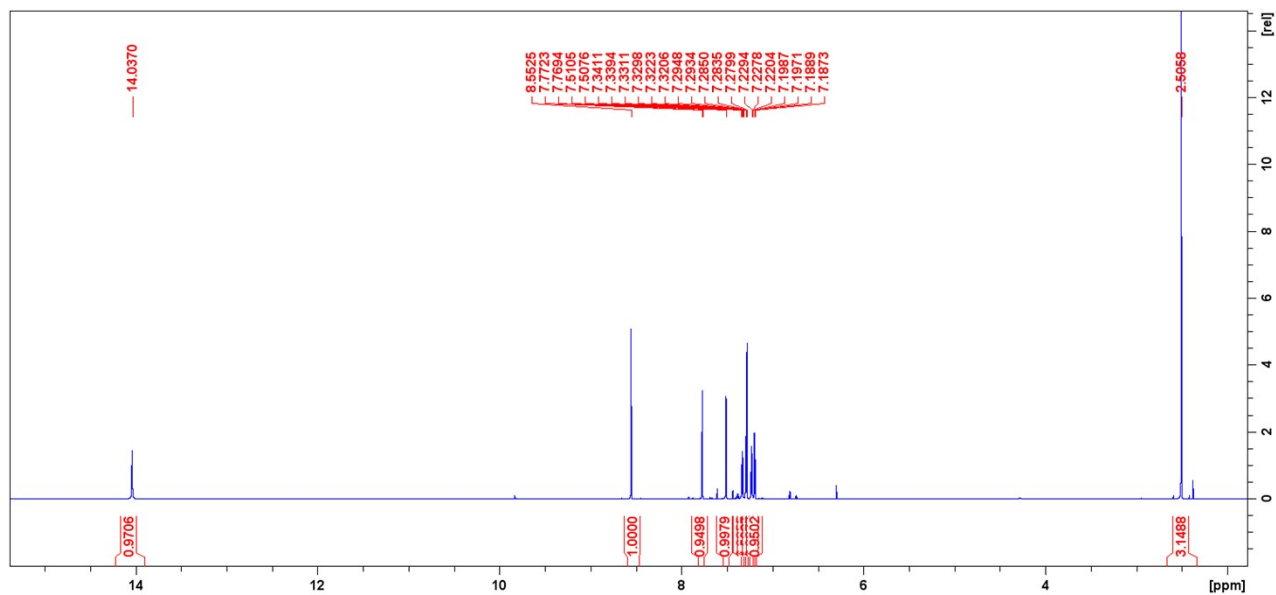


Figure S5.  $^1\text{H}$  NMR spectrum of L5 in  $\text{CDCl}_3$

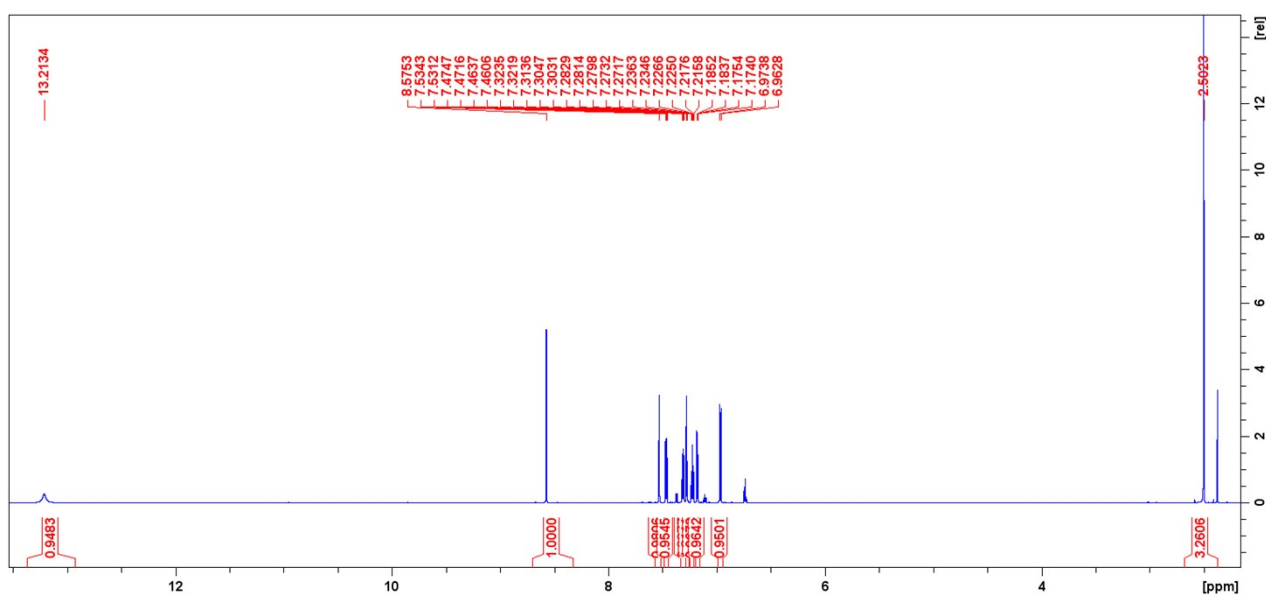


Figure S6.  $^1\text{H}$  NMR spectrum of L6 in  $\text{CDCl}_3$

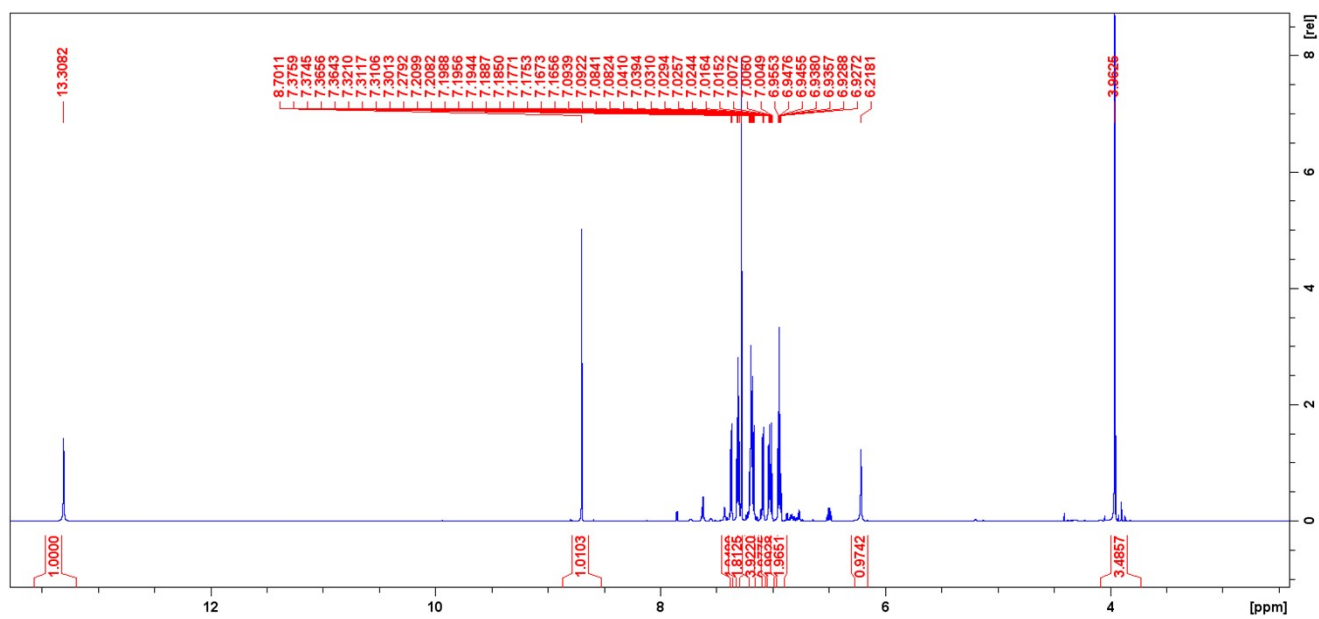


Figure S7.  $^1\text{H}$  NMR spectrum of L7 in  $\text{CDCl}_3$

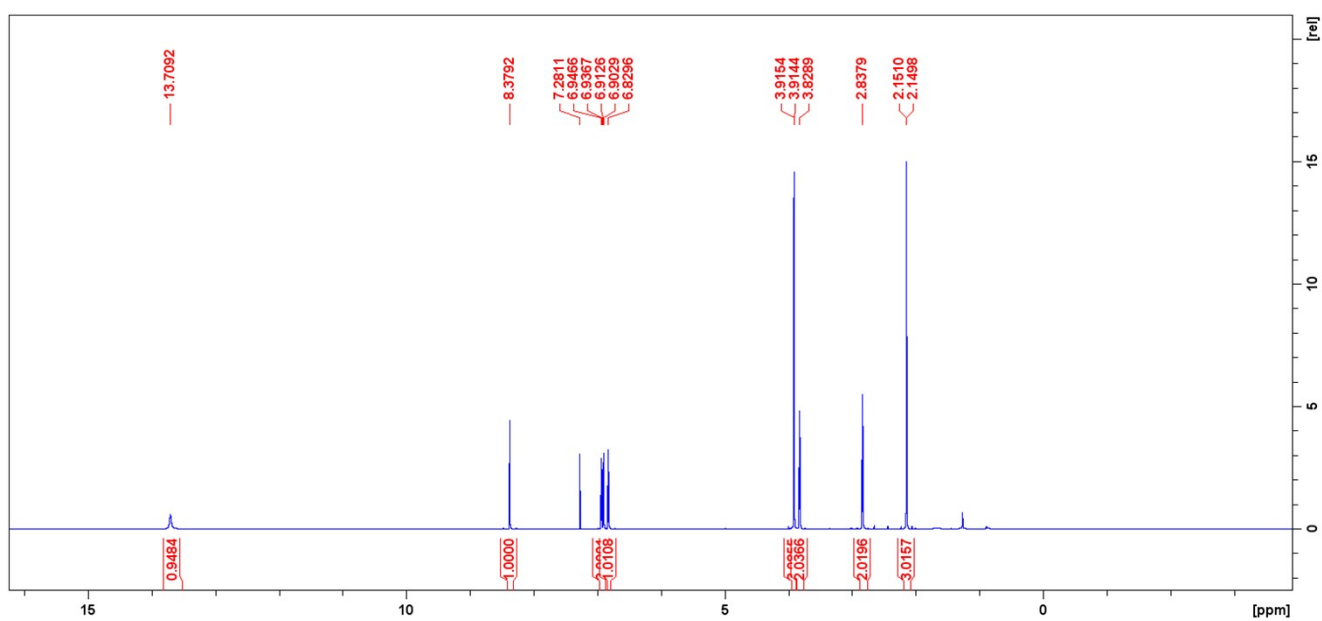


Figure S8.  $^1\text{H}$  NMR spectrum of L8 in  $\text{CDCl}_3$

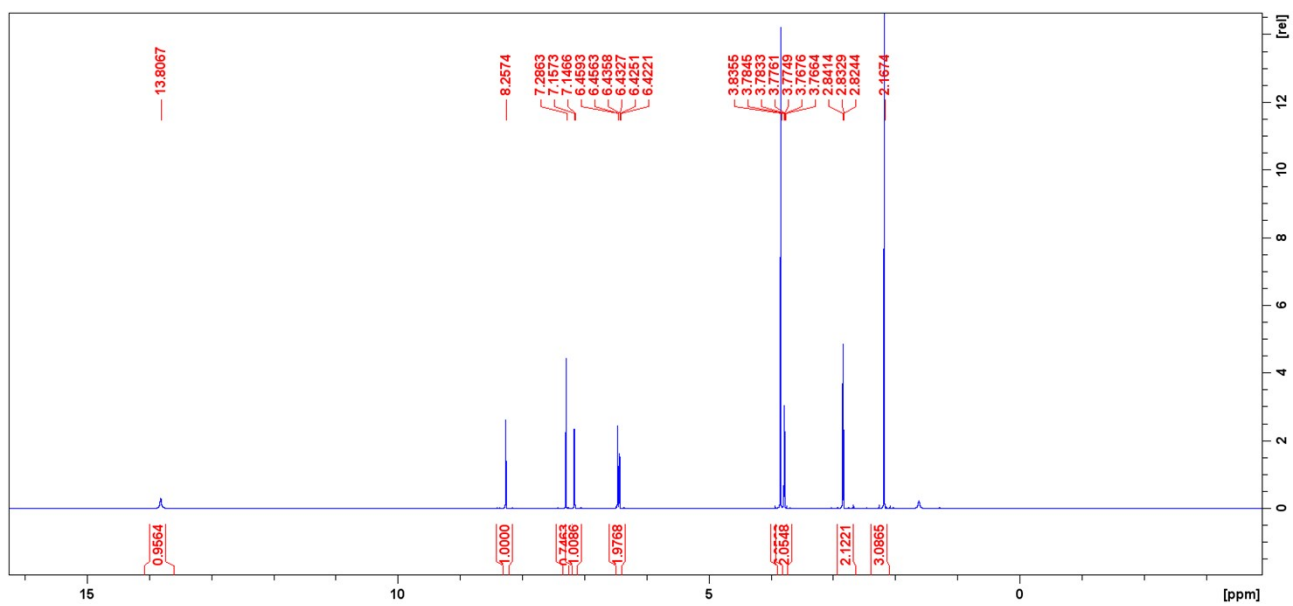


Figure S9.  $^1\text{H}$  NMR spectrum of L9 in  $\text{CDCl}_3$

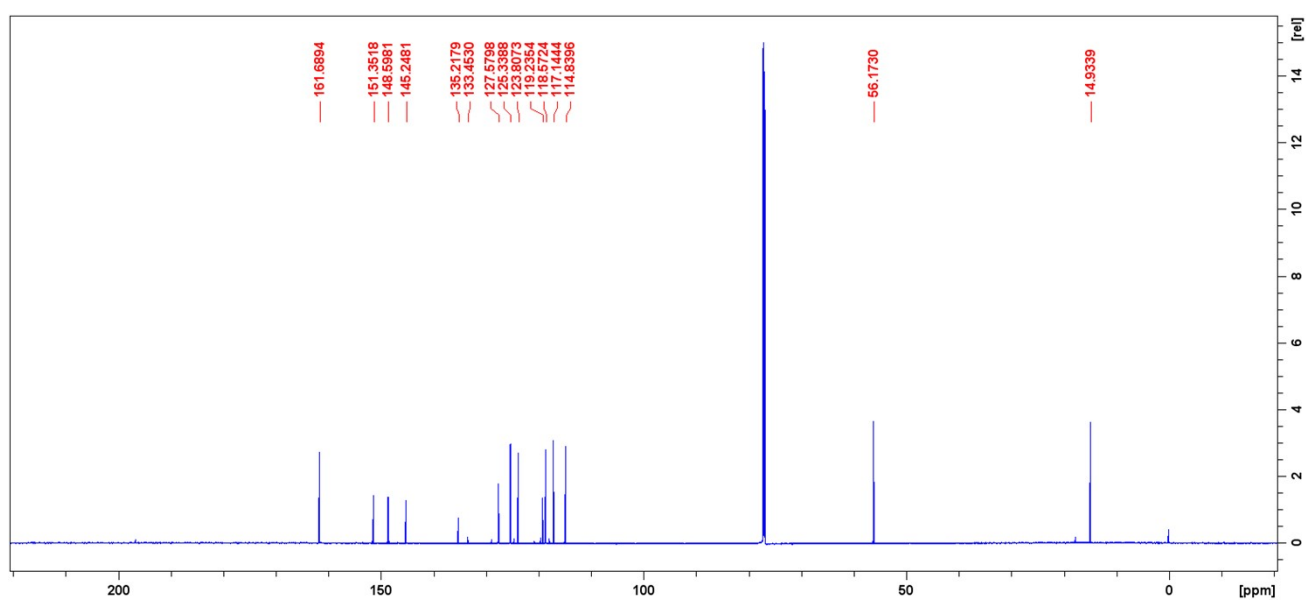


Figure S10.  $^{13}\text{C}$  NMR spectrum of L1 in  $\text{CDCl}_3$

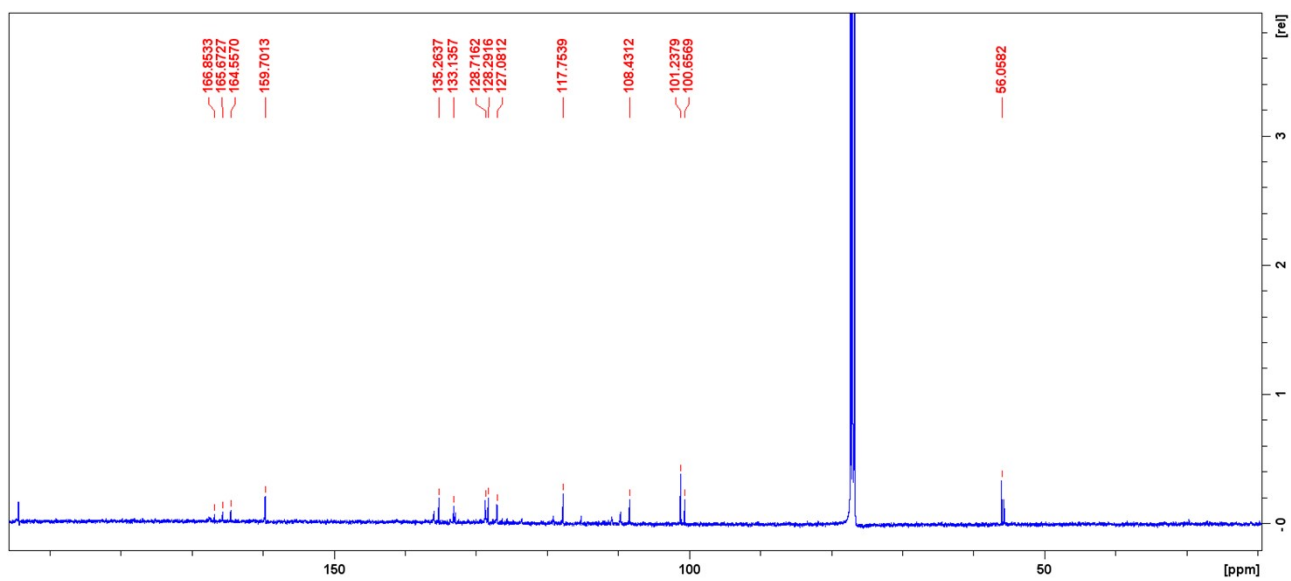


Figure S11.  $^{13}\text{C}$  NMR spectrum of L2 in  $\text{CDCl}_3$

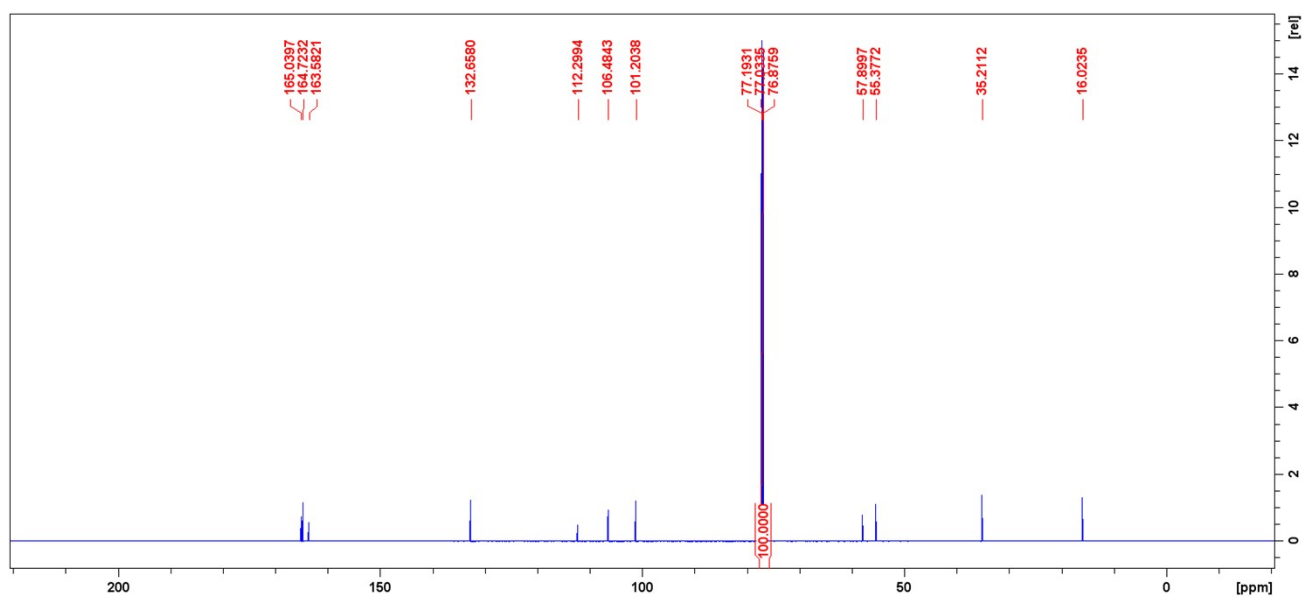


Figure S12.  $^{13}\text{C}$  NMR spectrum of L3 in  $\text{CDCl}_3$

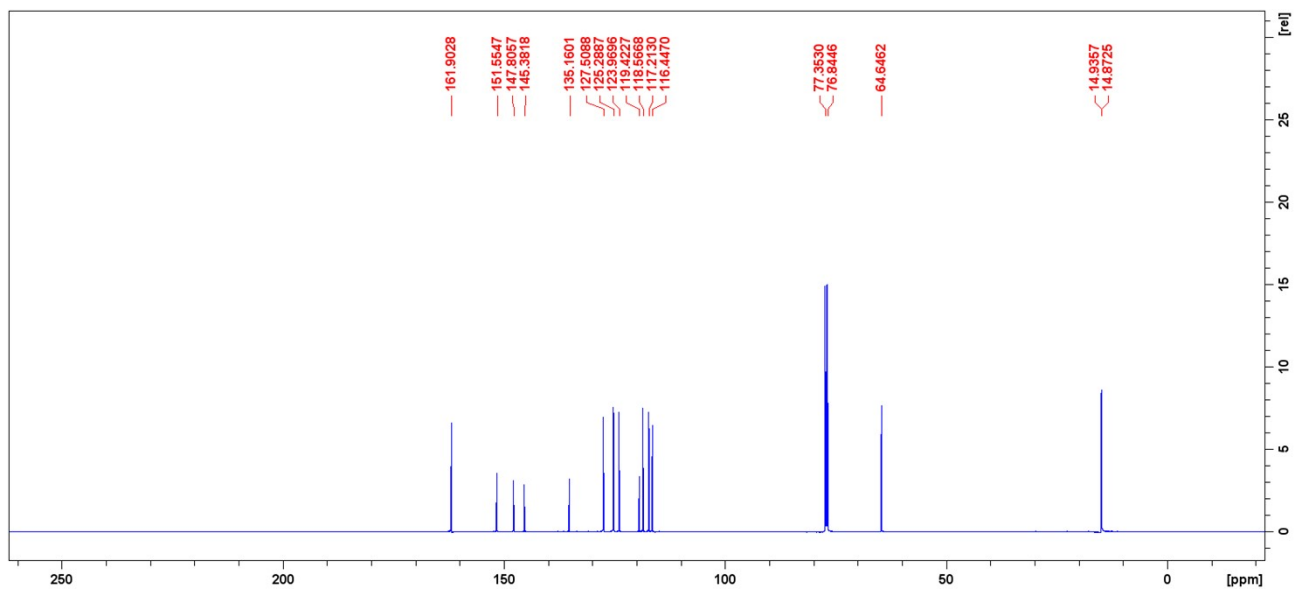


Figure S13.  $^{13}\text{C}$  NMR spectrum of L4 in  $\text{CDCl}_3$

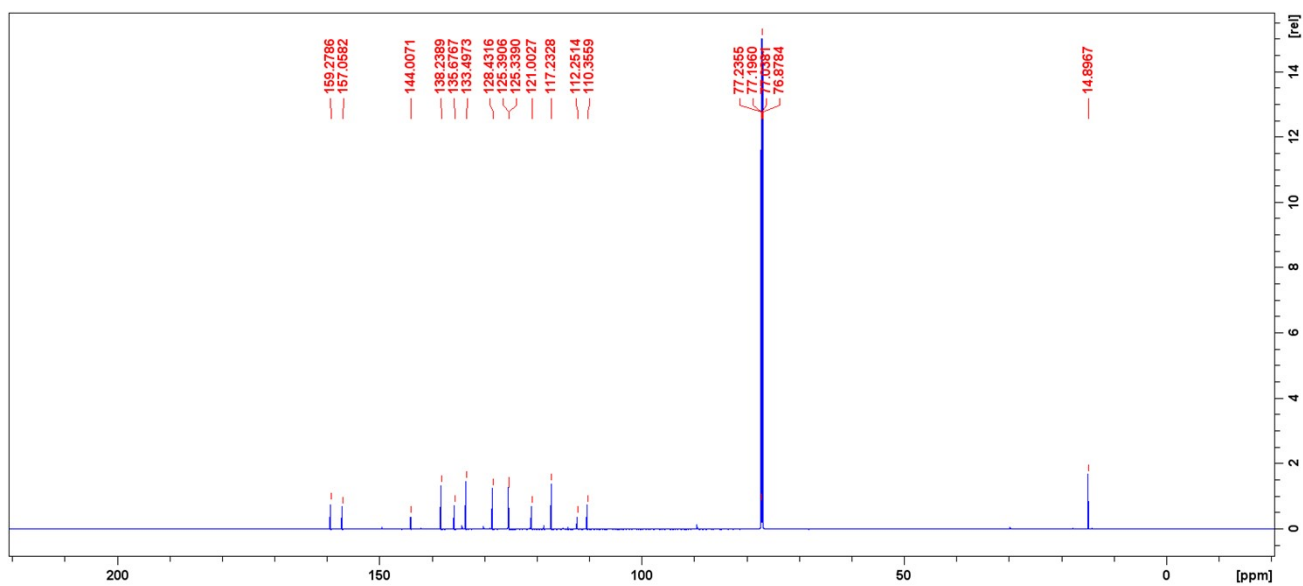


Figure S14.  $^{13}\text{C}$  NMR spectrum of L5 in  $\text{CDCl}_3$

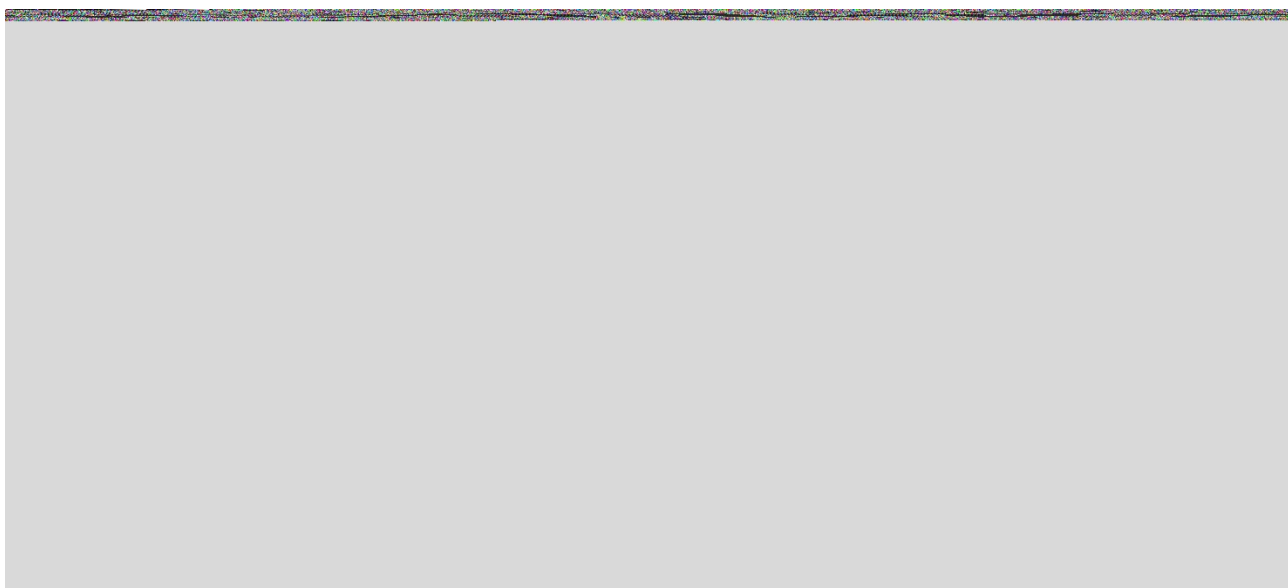


Figure S15.  $^{13}\text{C}$  NMR spectrum of L6 in  $\text{CDCl}_3$

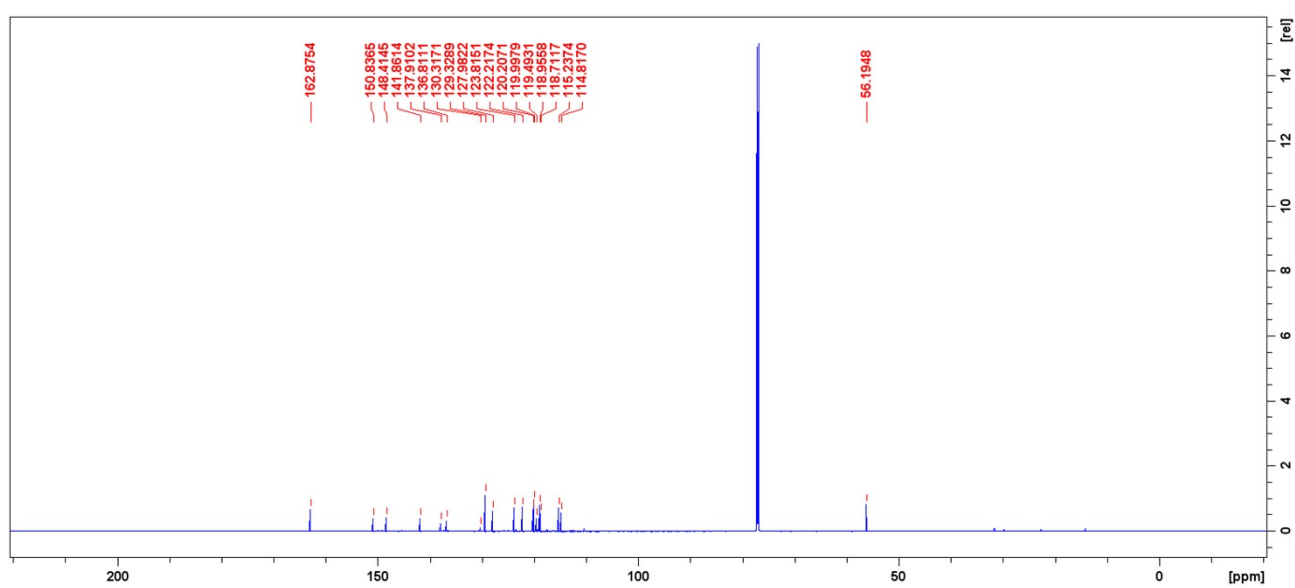


Figure S16.  $^{13}\text{C}$  NMR spectrum of L7 in  $\text{CDCl}_3$

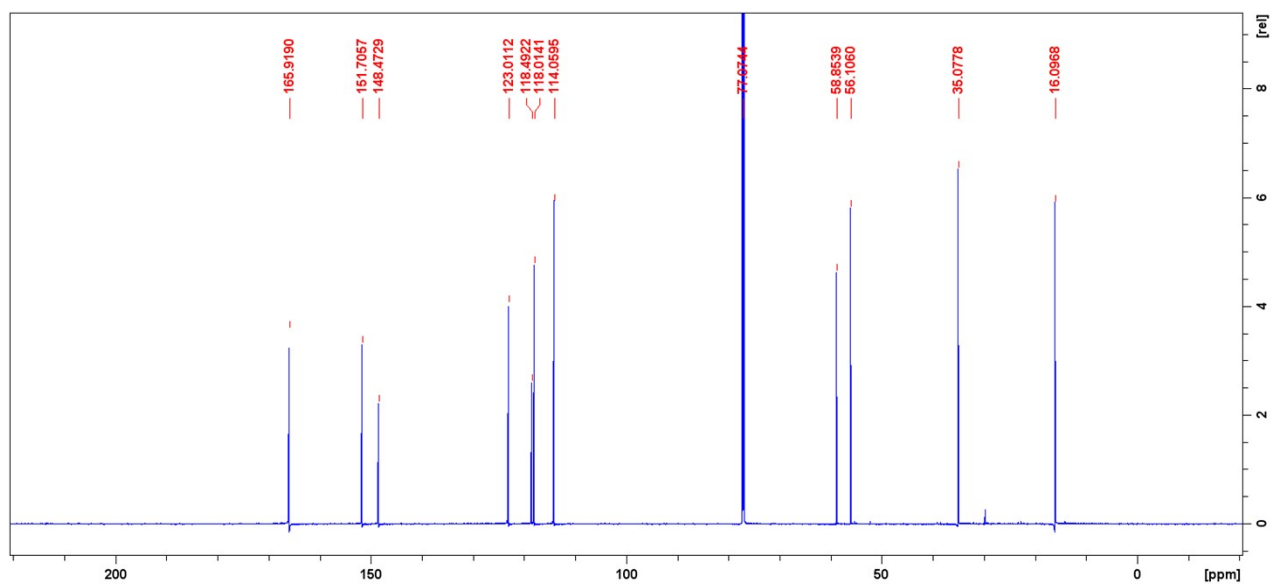


Figure S17.  $^{13}\text{C}$  NMR spectrum of L8 in  $\text{CDCl}_3$

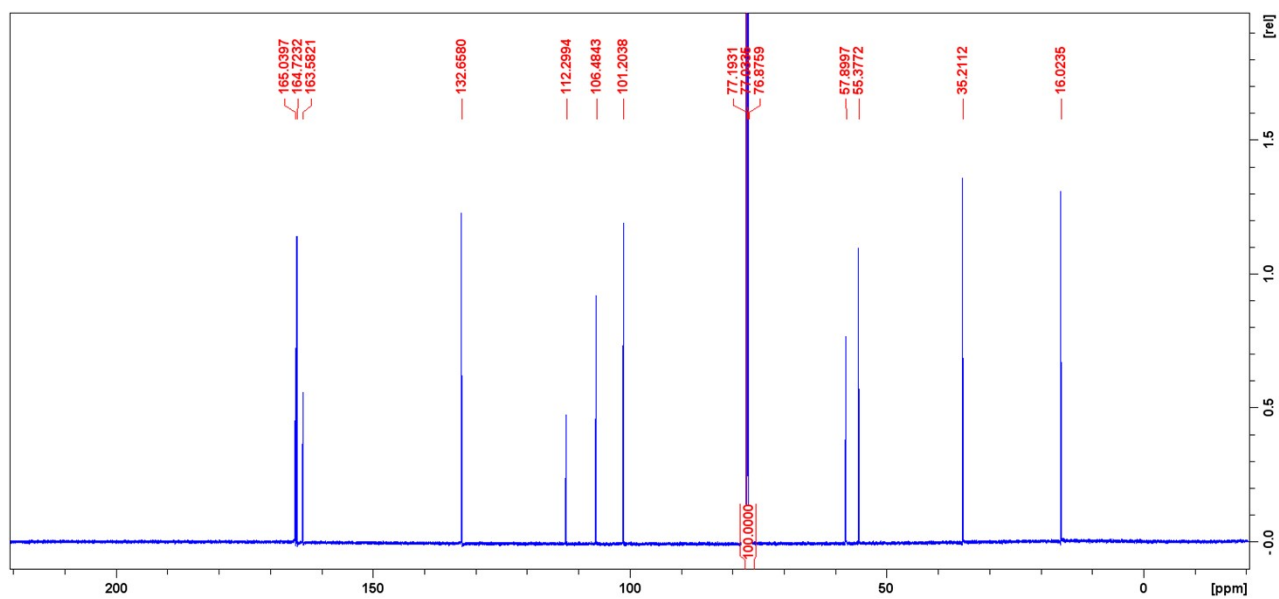


Figure S18.  $^{13}\text{C}$  NMR spectrum of L9 in  $\text{CDCl}_3$

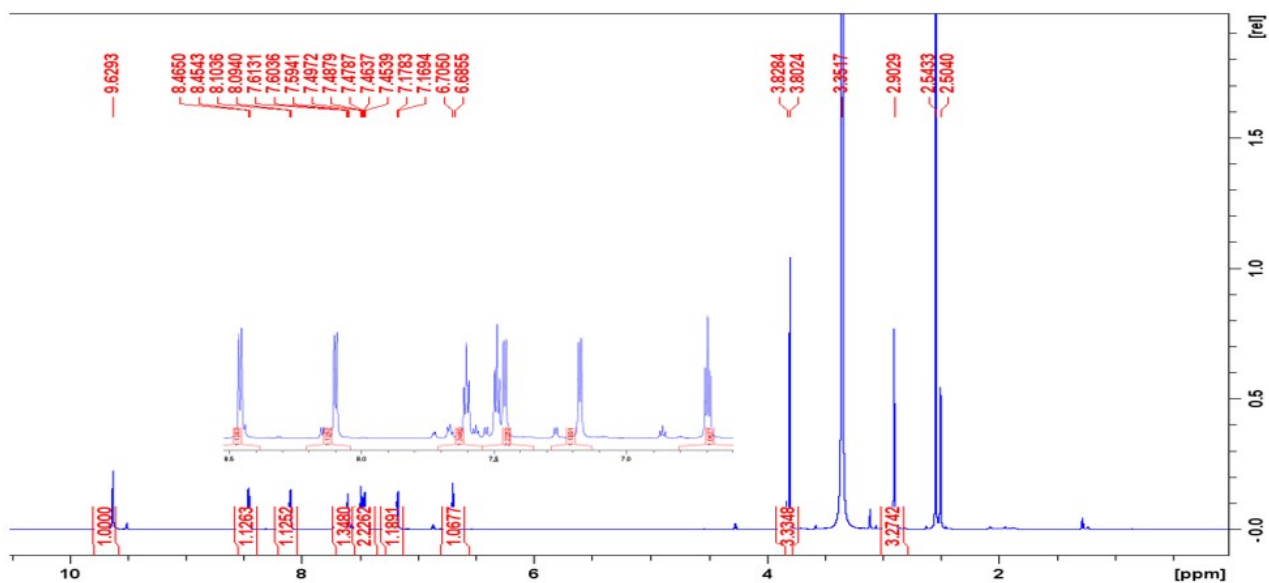


Figure S19.  $^1\text{H}$  NMR spectrum of Pt1 in  $\text{DMSO-}d_6$ .

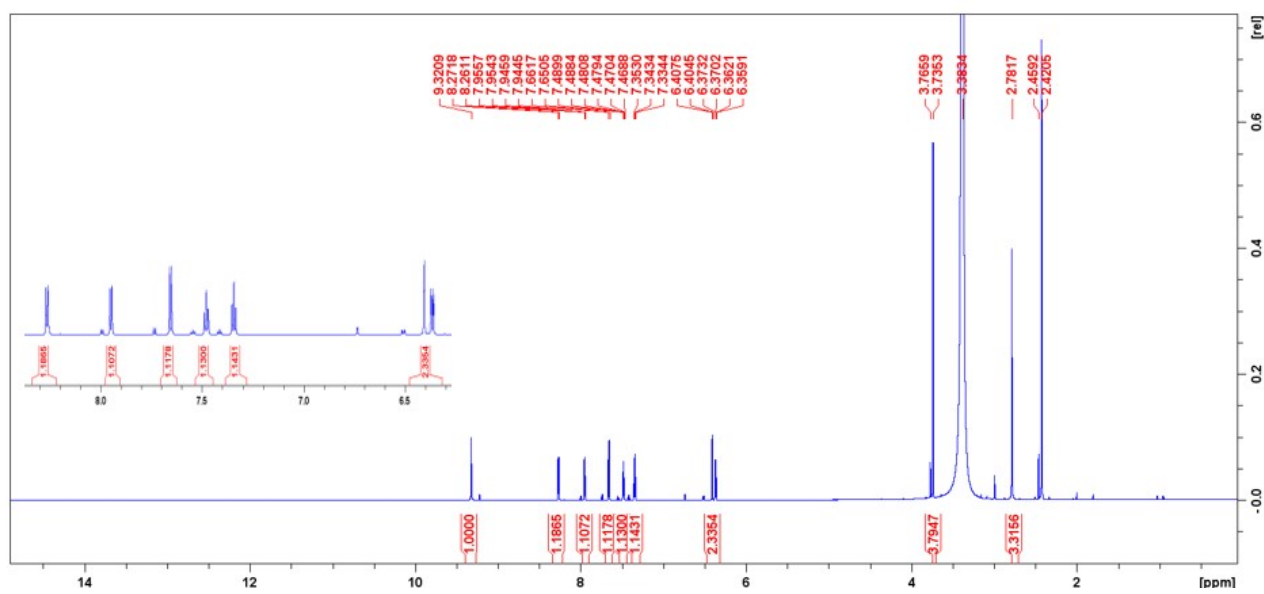


Figure S20.  $^1\text{H}$  NMR spectrum of Pt2 in  $\text{DMSO-}d_6$ .

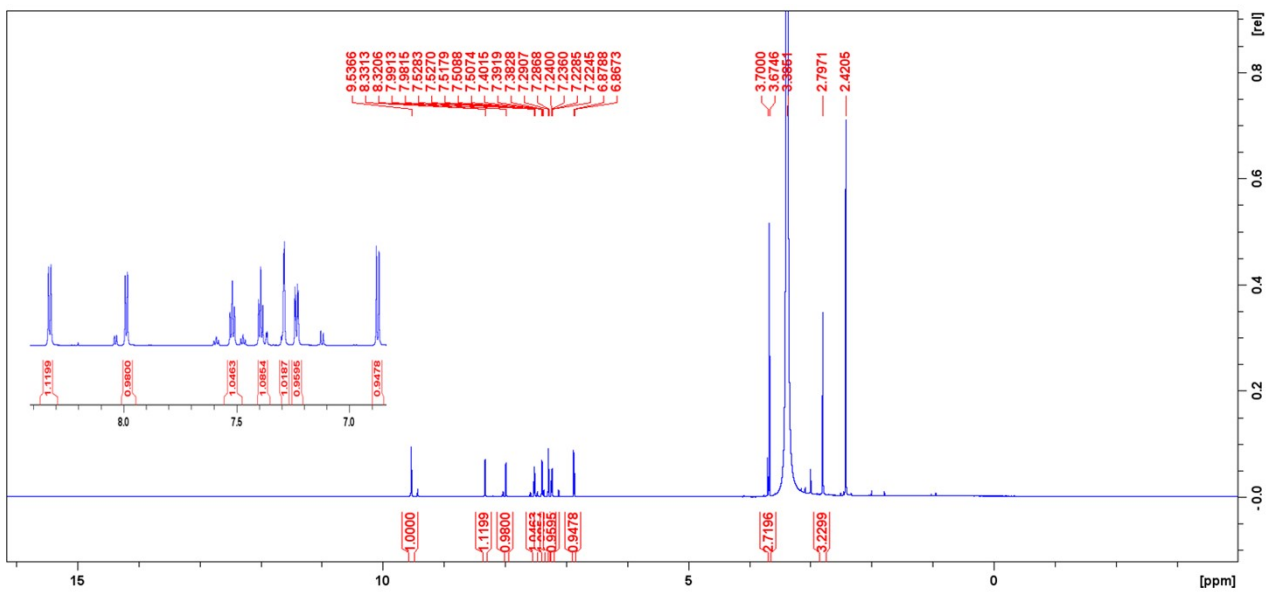


Figure S21.  $^1\text{H}$  NMR spectrum of Pt3 in  $\text{DMSO-}d^6$ .

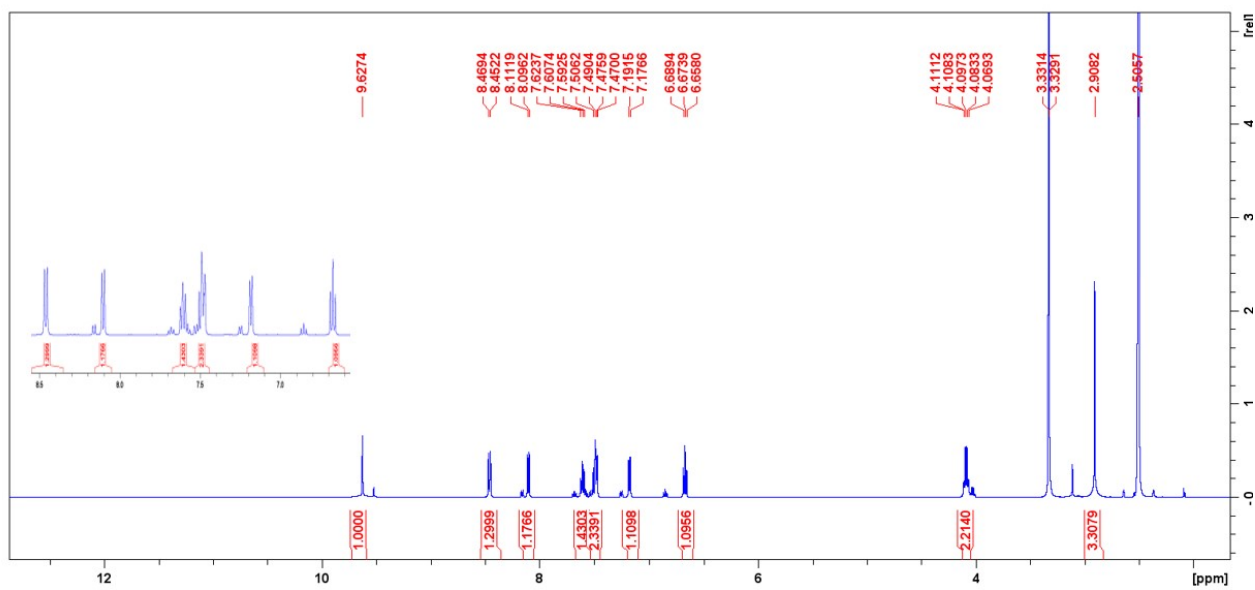


Figure S22.  $^1\text{H}$  NMR spectrum of Pt4 in  $\text{DMSO-}d^6$ .

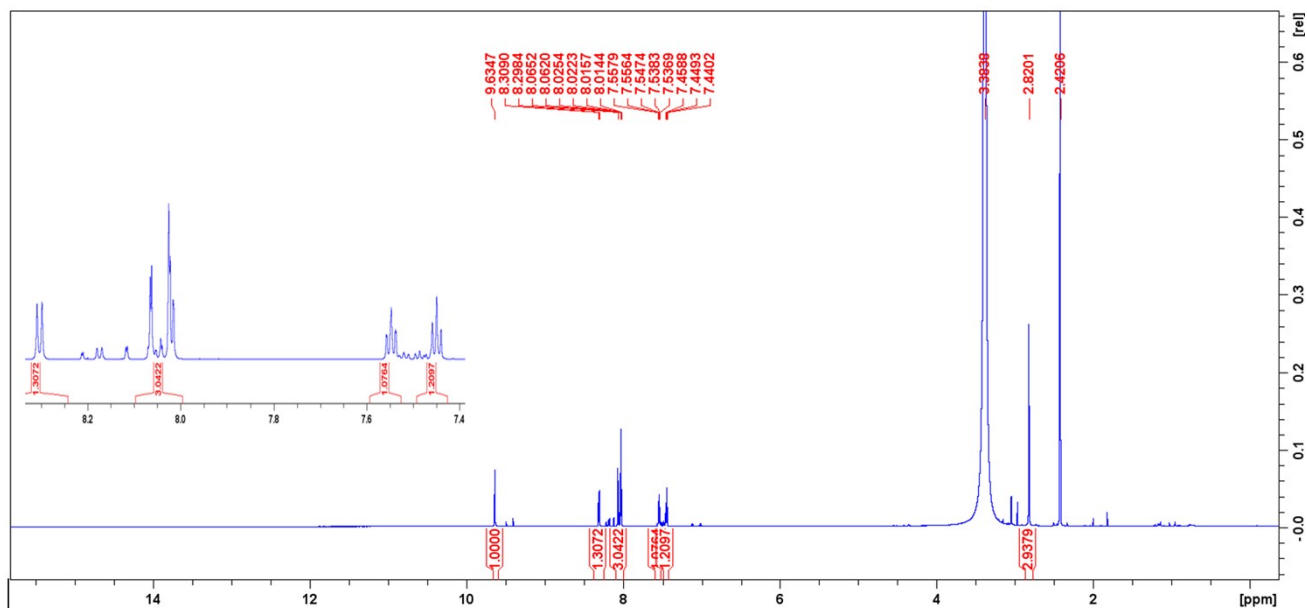


Figure 23.  $^1\text{H}$  NMR spectrum of Pt5 in  $\text{DMSO-}d^6$ .

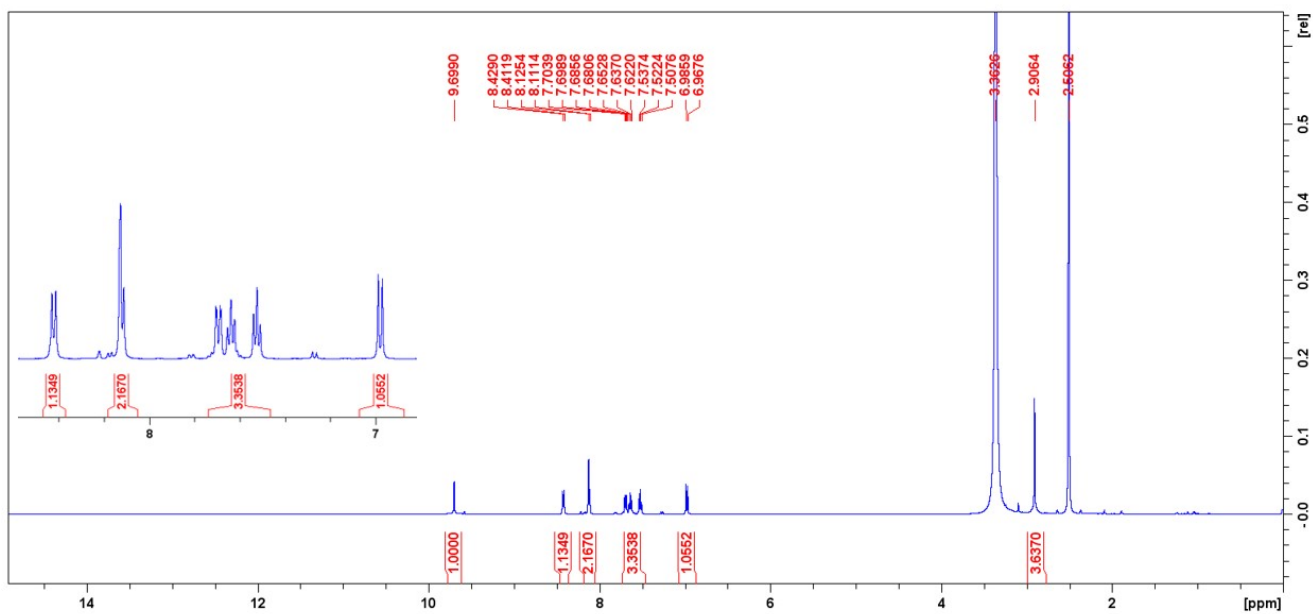


Figure 24.  $^1\text{H}$  NMR spectrum of Pt6 in  $\text{DMSO-}d^6$ .

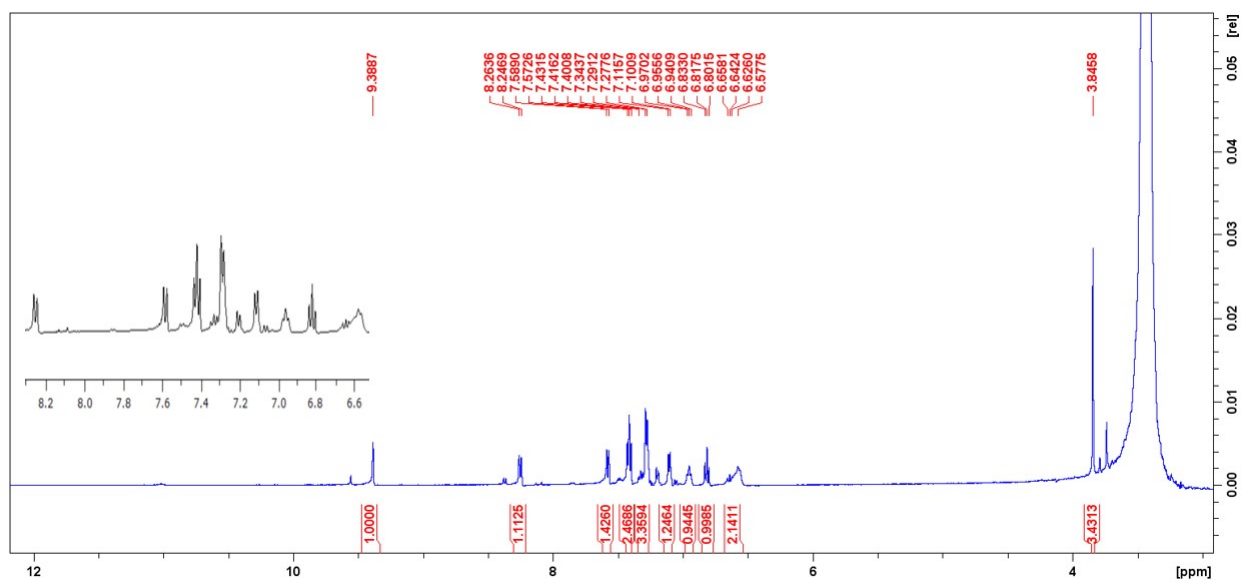


Figure 25.  $^1\text{H}$  NMR spectrum of Pt7 in  $\text{DMSO-}d^6$ .

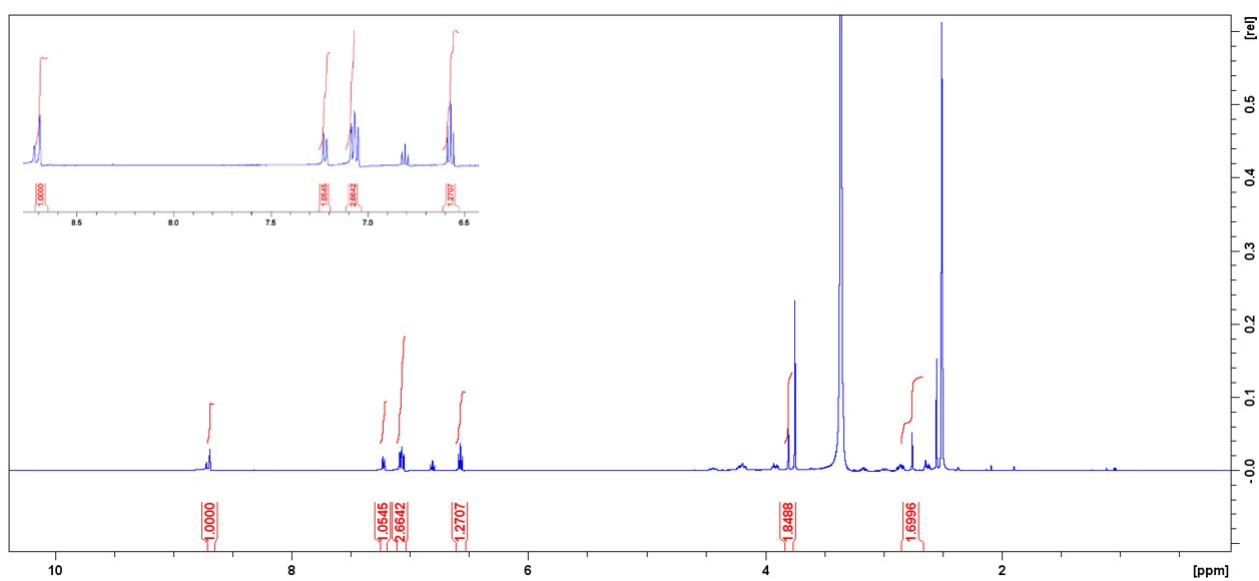


Figure 26.  $^1\text{H}$  NMR spectrum of Pt8 and  $\text{DMSO-adduct}$  in  $\text{DMSO-}d^6$ .

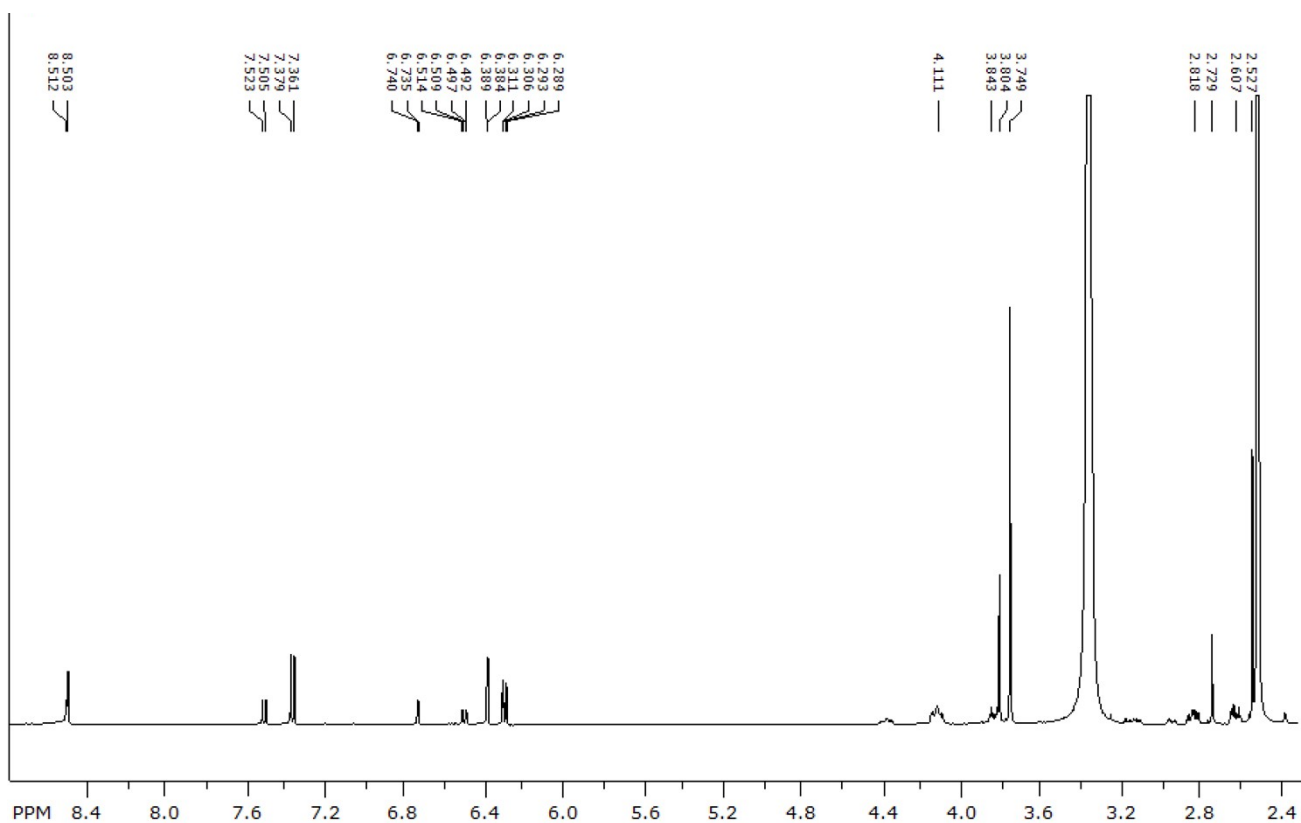


Figure 27.  $^1\text{H}$  NMR spectrum of Pt9 and DMSO-adduct in  $\text{DMSO-}d_6$ .

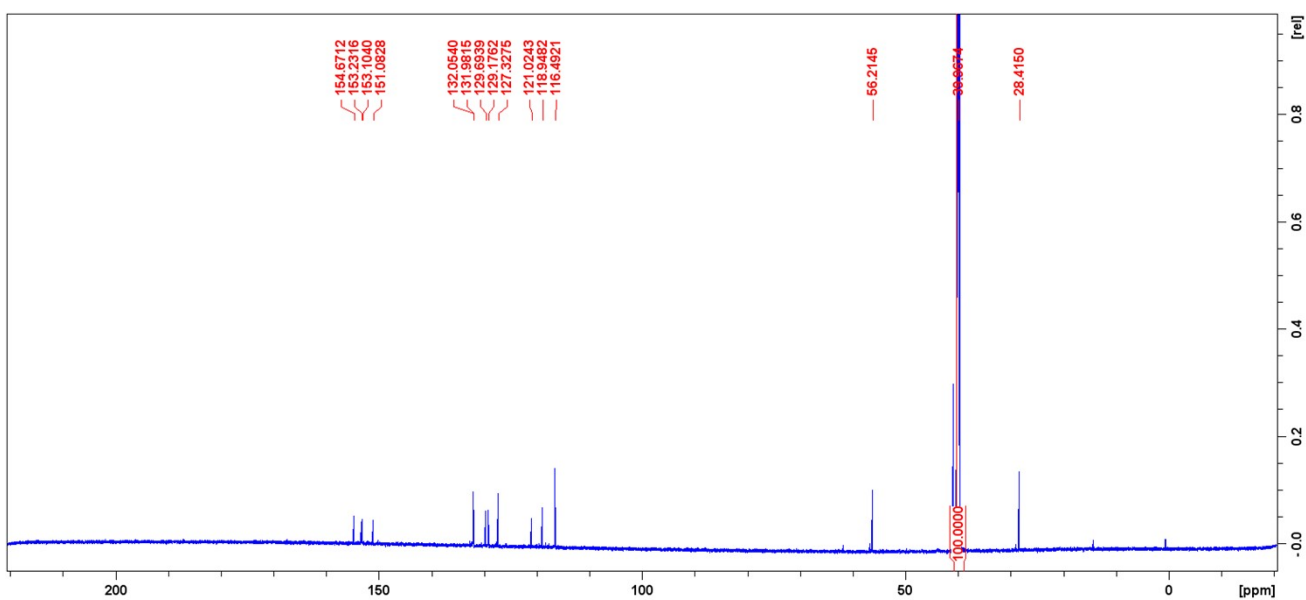


Figure 28.  $^{13}\text{C}$  NMR spectrum of Pt1 in  $\text{DMSO-}d_6$ .

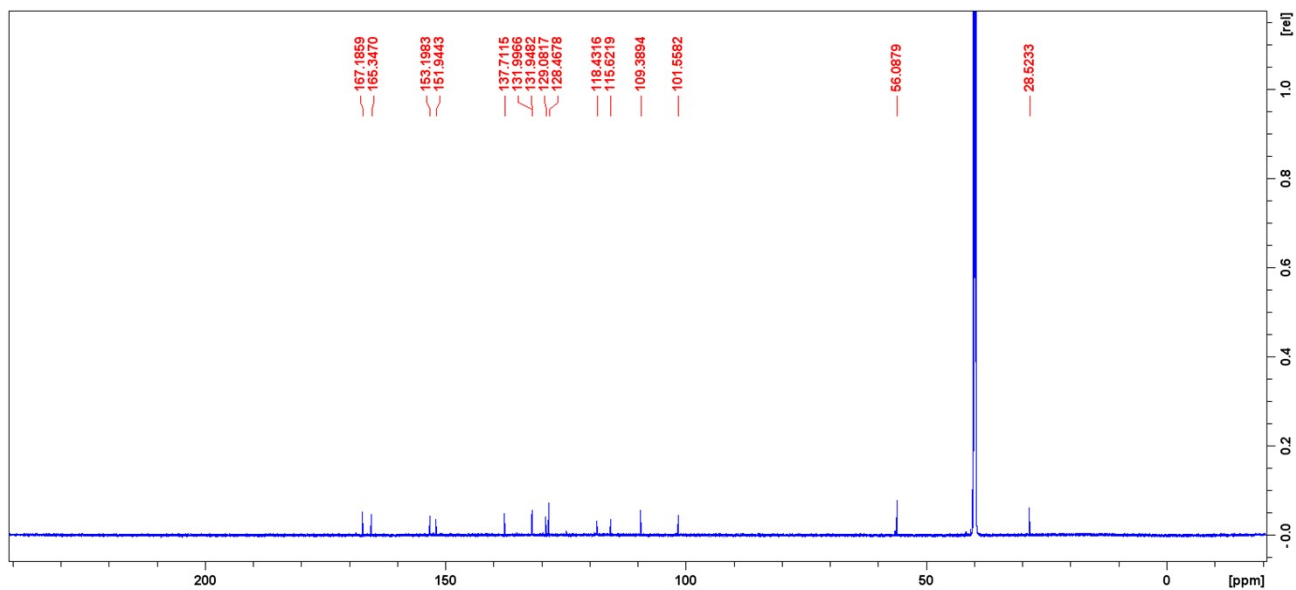


Figure 29.  $^{13}\text{C}$  NMR spectrum of Pt2 in DMSO- $d_6$ .

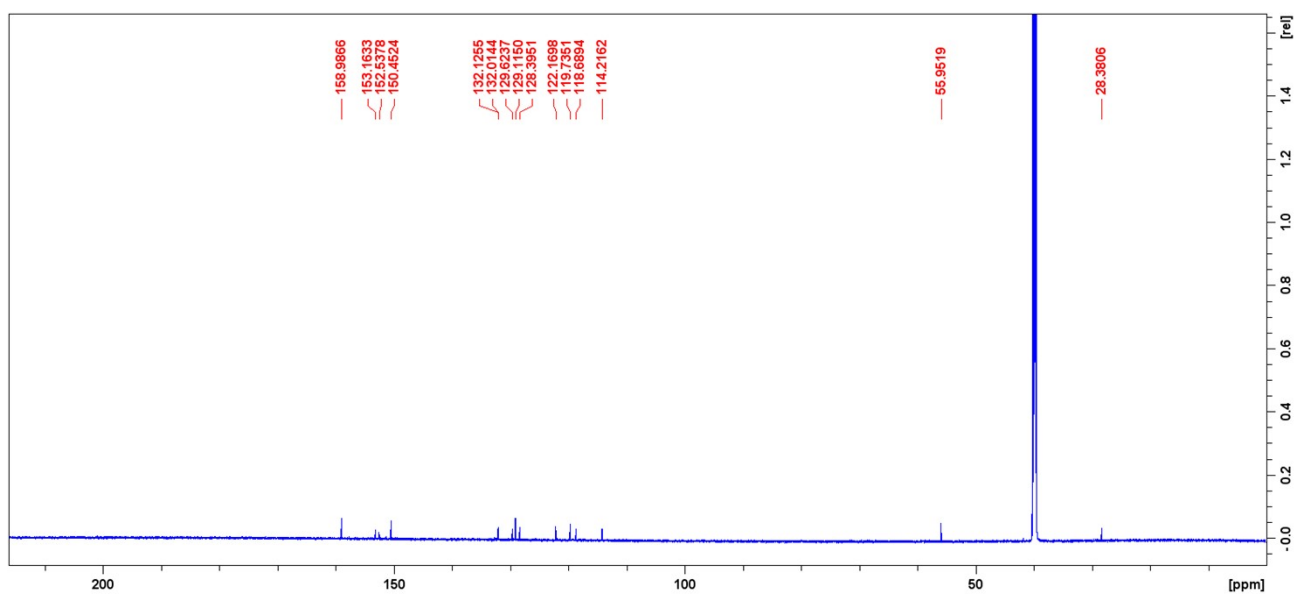


Figure 30.  $^{13}\text{C}$  NMR spectrum of Pt3 in DMSO- $d_6$ .

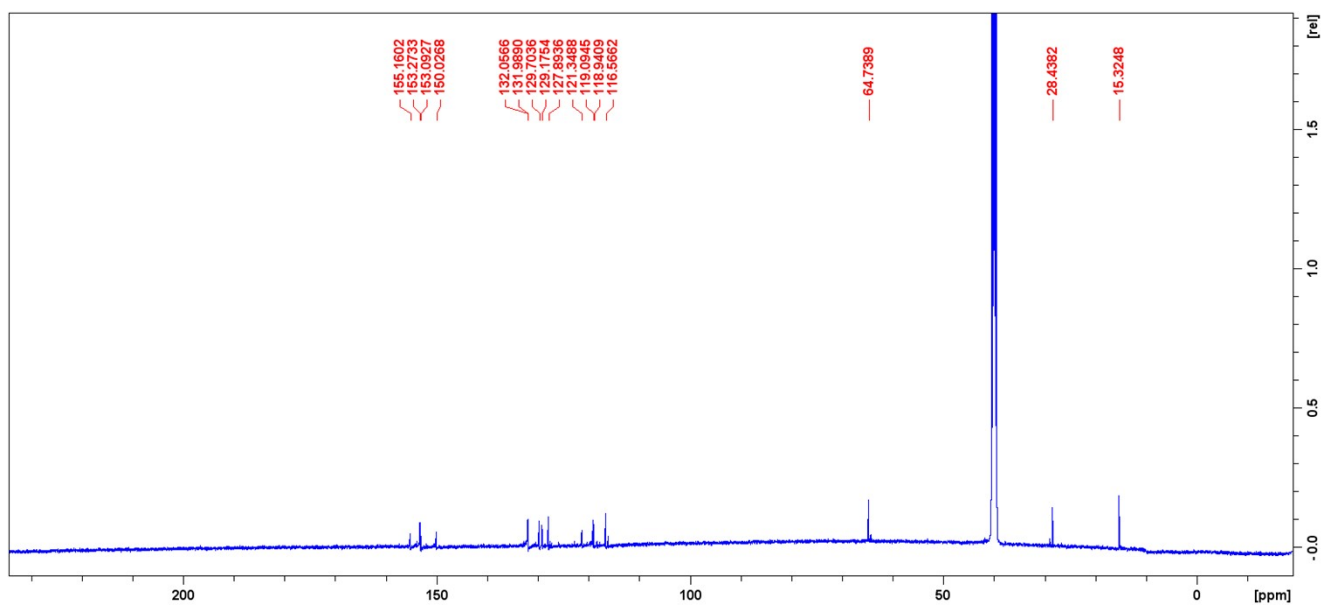


Figure 31.  $^{13}\text{C}$  NMR spectrum of Pt4 in  $\text{DMSO-}d^6$ .

pivot = 39.85 ppm Phase increment = 0.20 ph0 = -1.61 ph1 = 0.80

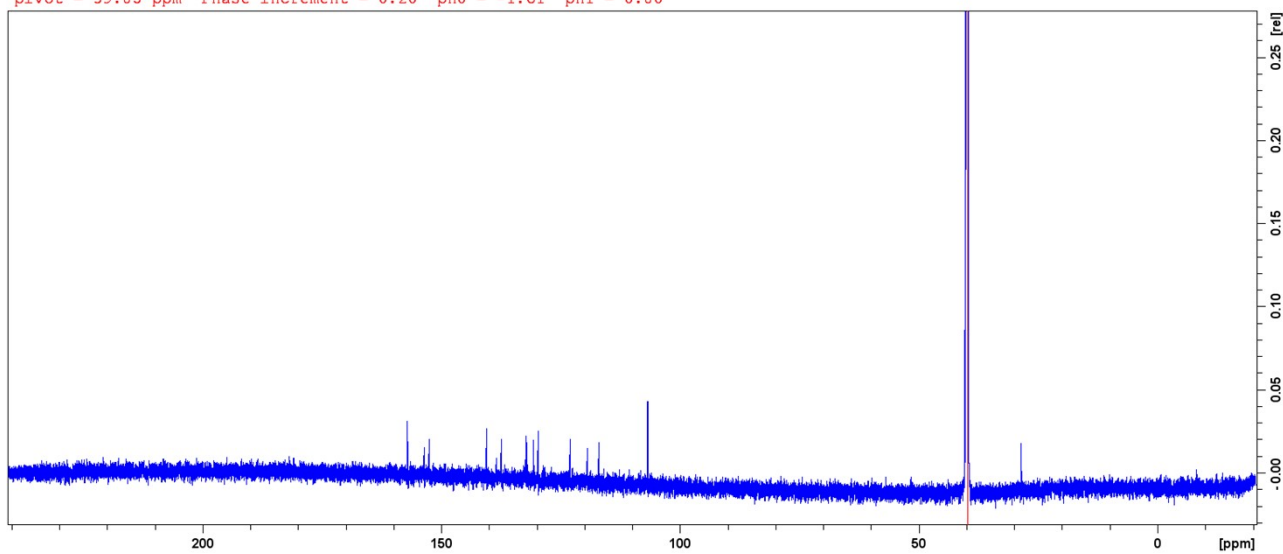


Figure 32.  $^{13}\text{C}$  NMR spectrum of Pt5 in  $\text{DMSO-}d^6$ .

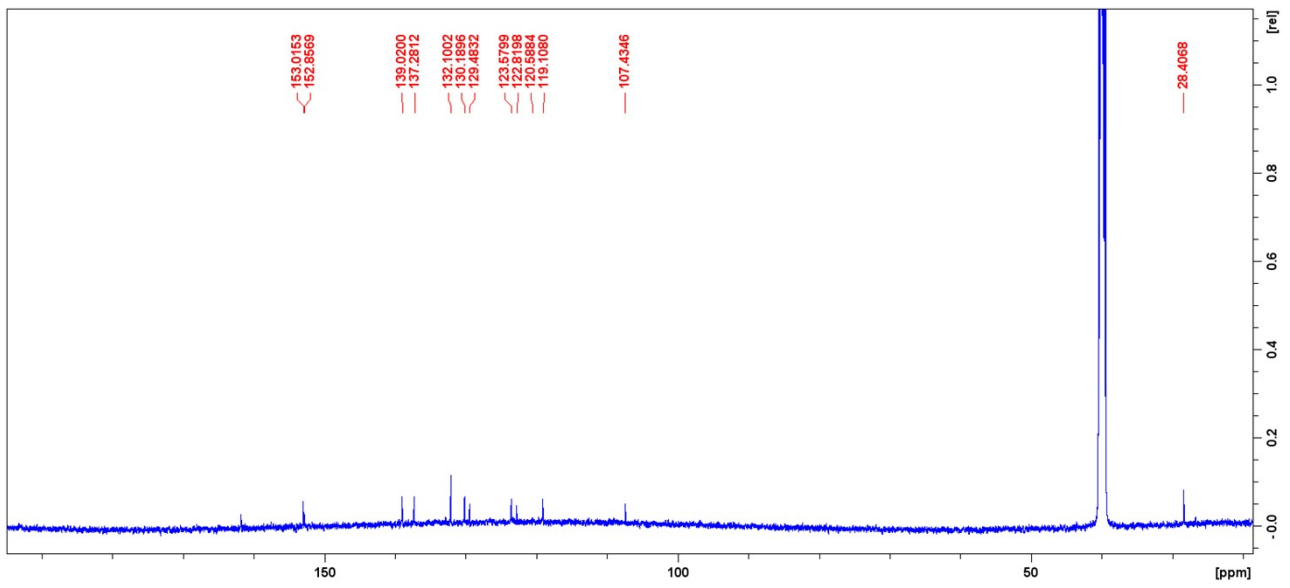


Figure 33.  $^{13}\text{C}$  NMR spectrum of Pt6 in  $\text{DMSO-}d_6$ .

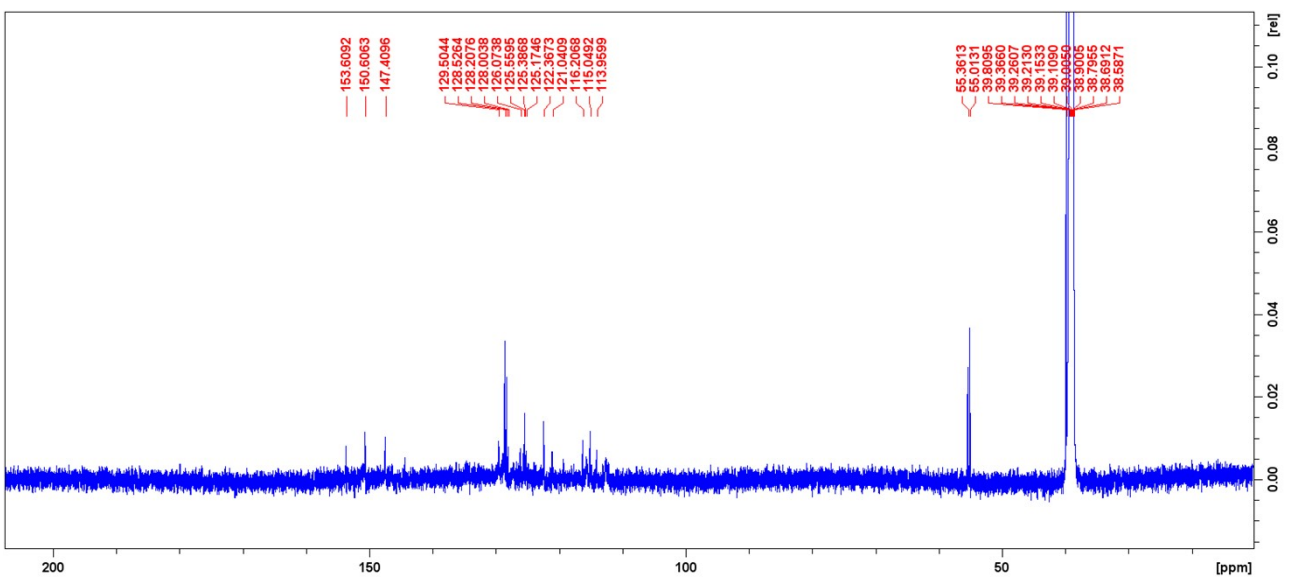


Figure 34.  $^{13}\text{C}$  NMR spectrum of Pt7 in  $\text{DMSO-}d_6$ .

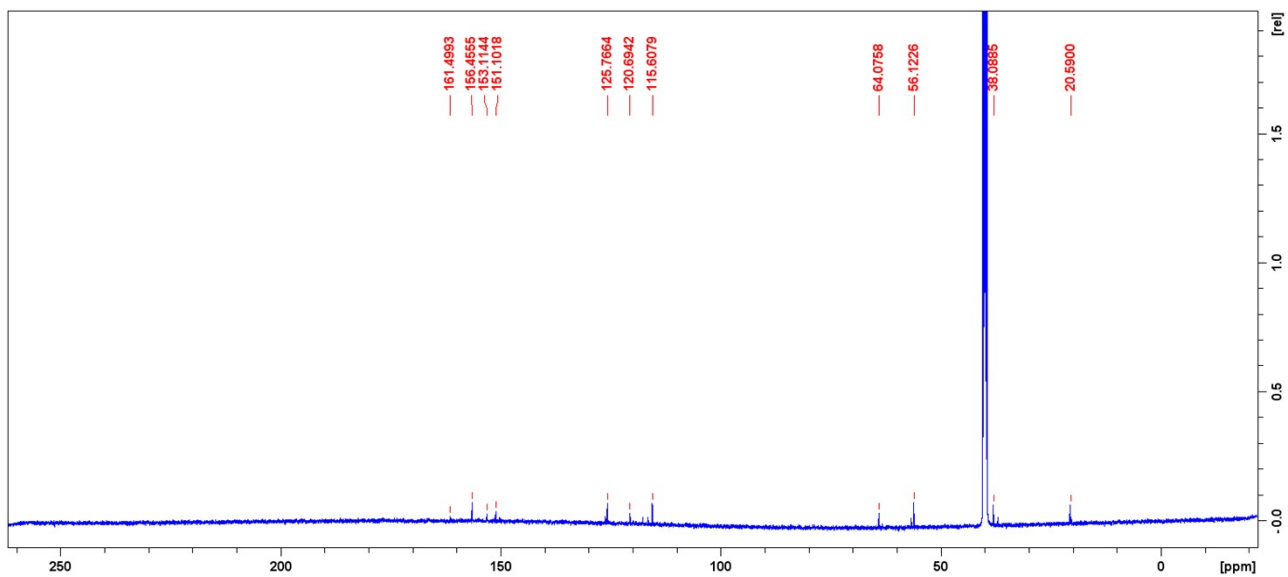


Figure 35.  $^{13}\text{C}$  NMR spectrum of Pt8 in  $\text{DMSO-}d_6$ .

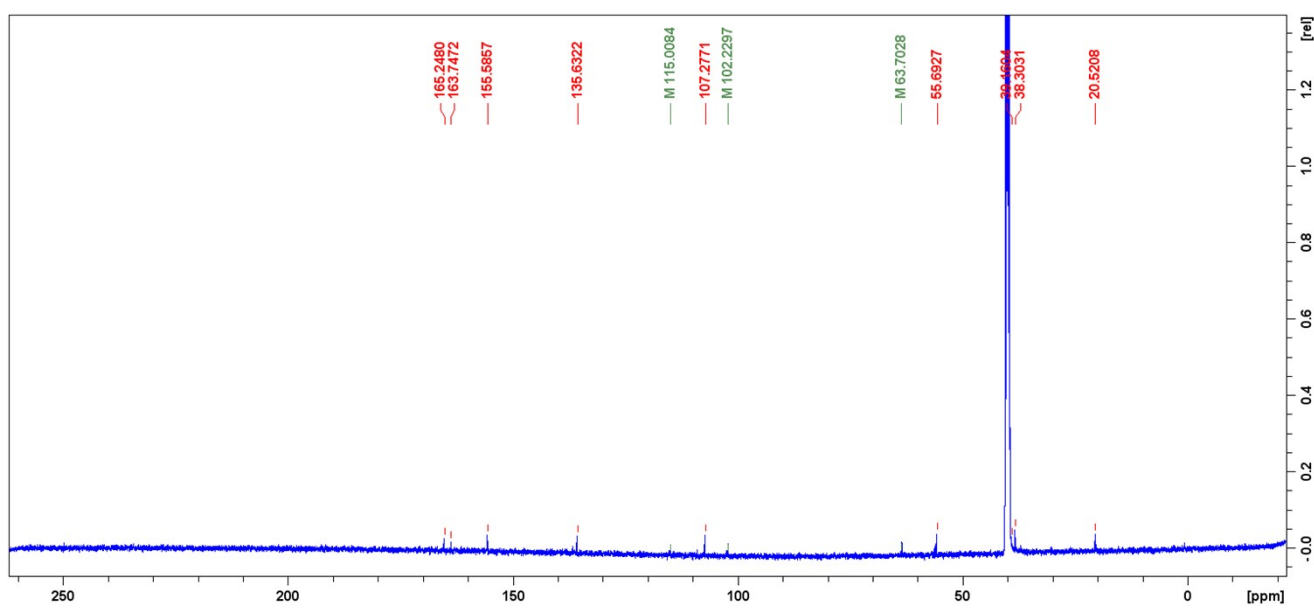
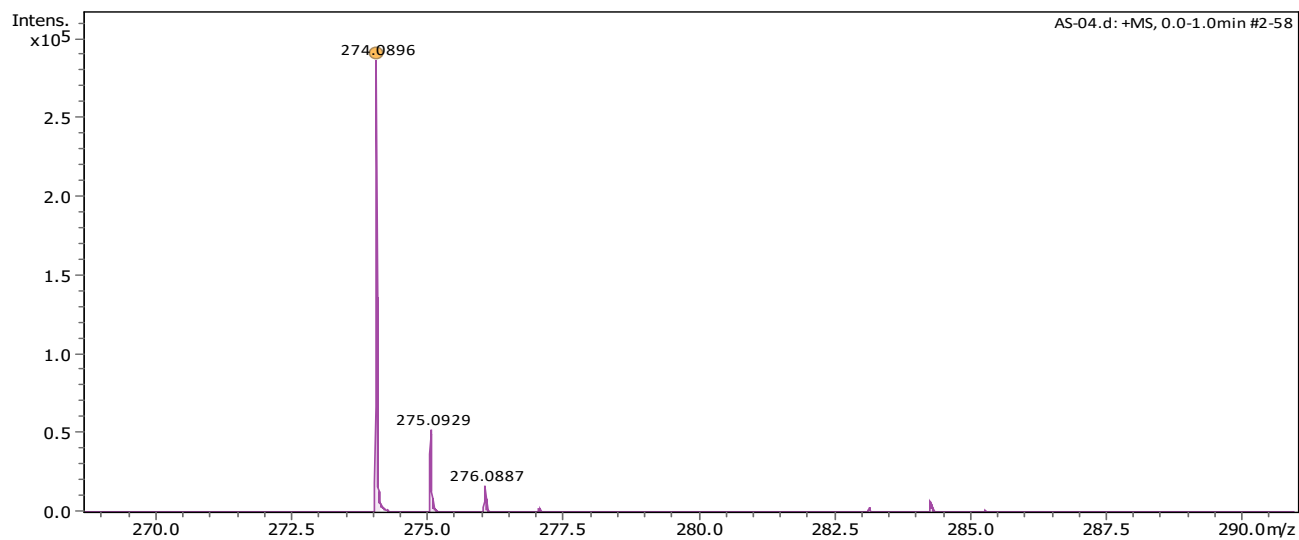
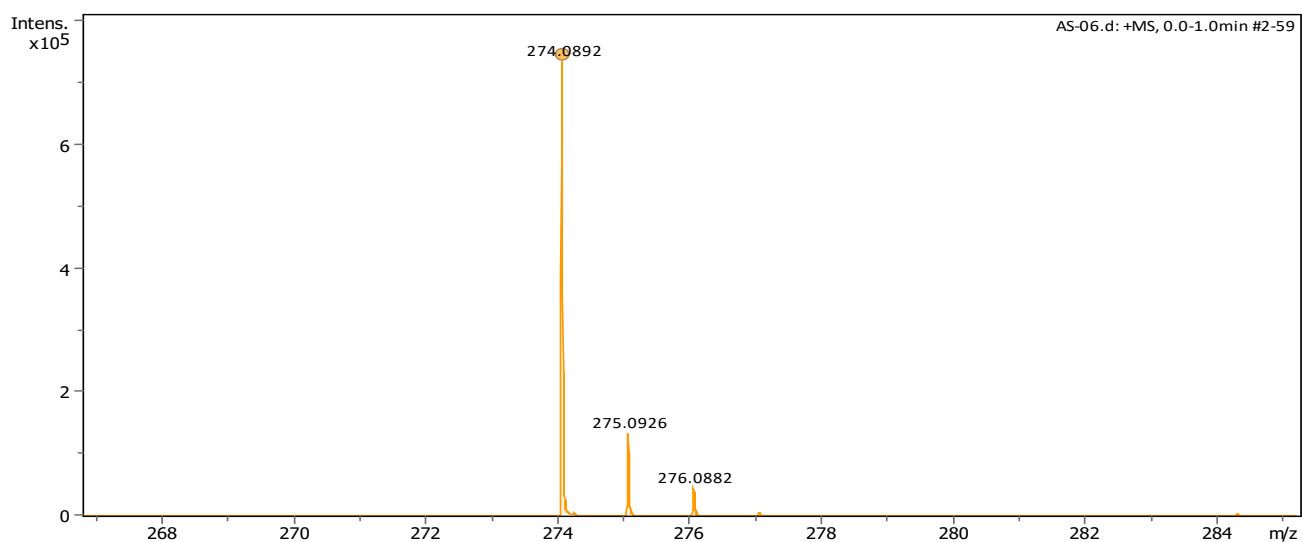


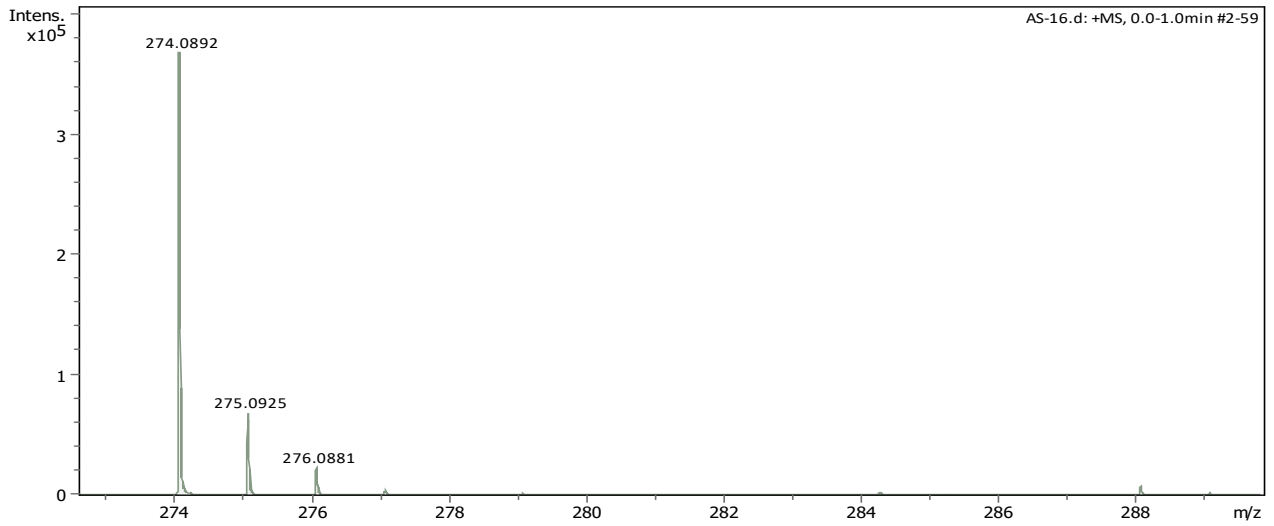
Figure 36.  $^{13}\text{C}$  NMR spectrum of Pt9 in  $\text{DMSO-}d_6$ .



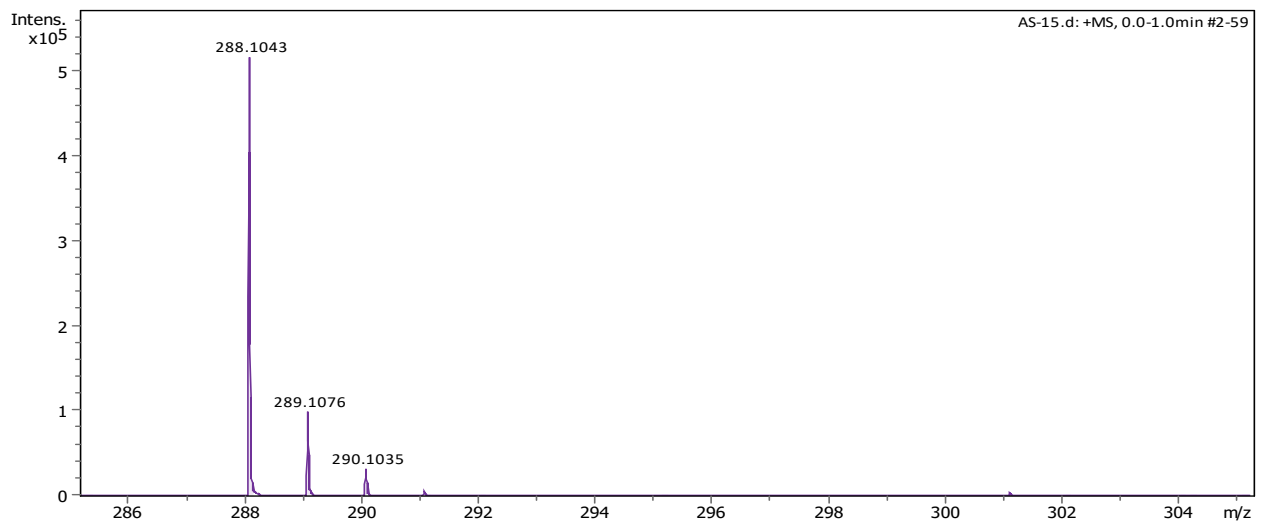
**Figure 37. Mass spectrum of L1**



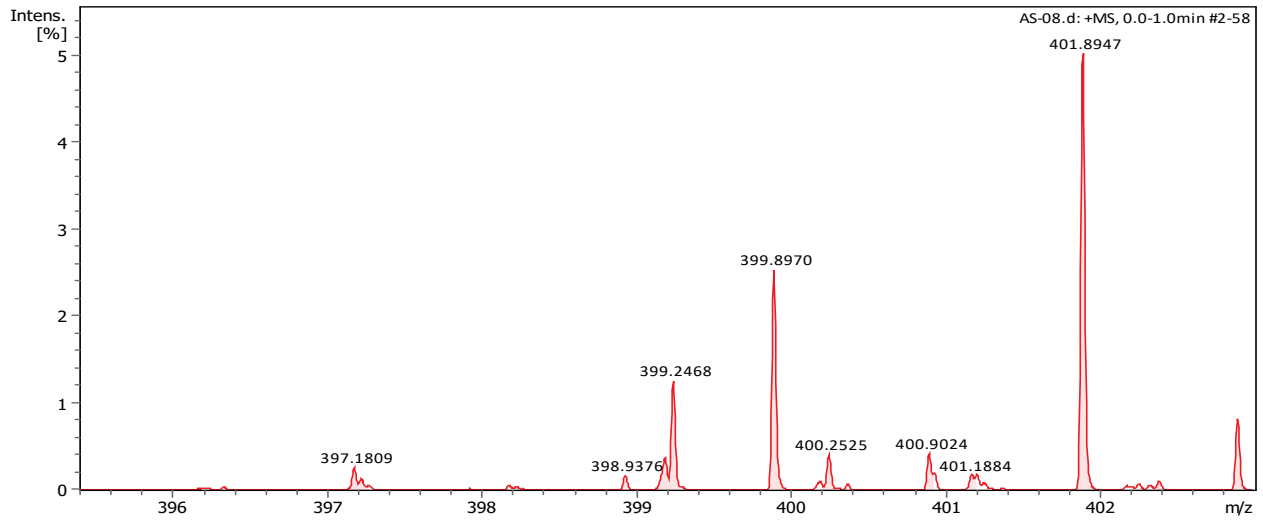
**Figure 37. Mass spectrum of L2**



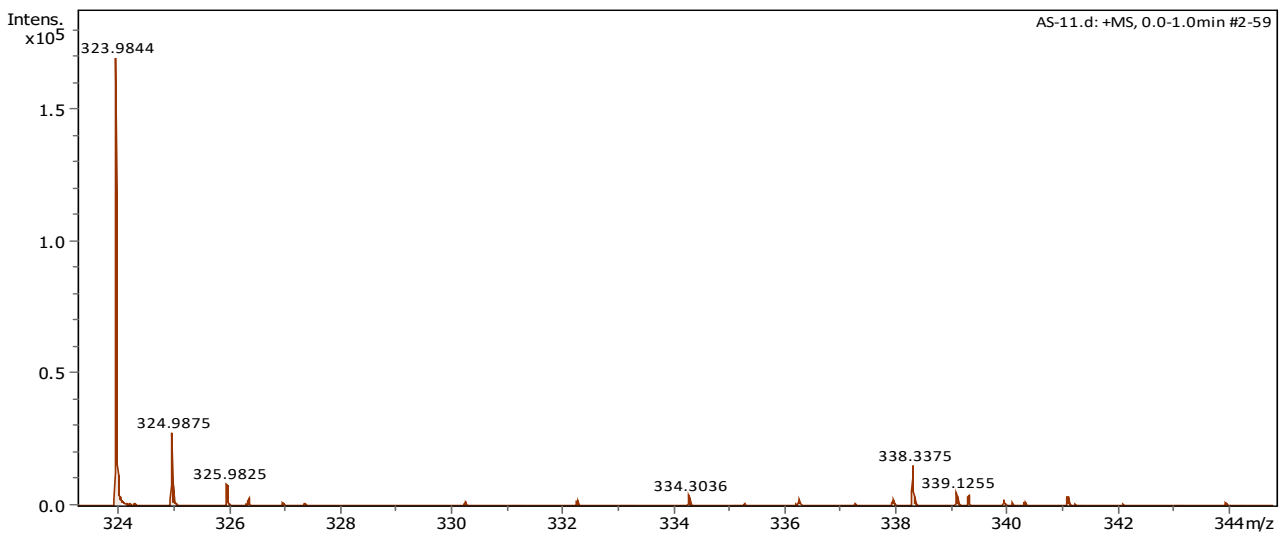
**Figure 39. Mass spectrum of L3**



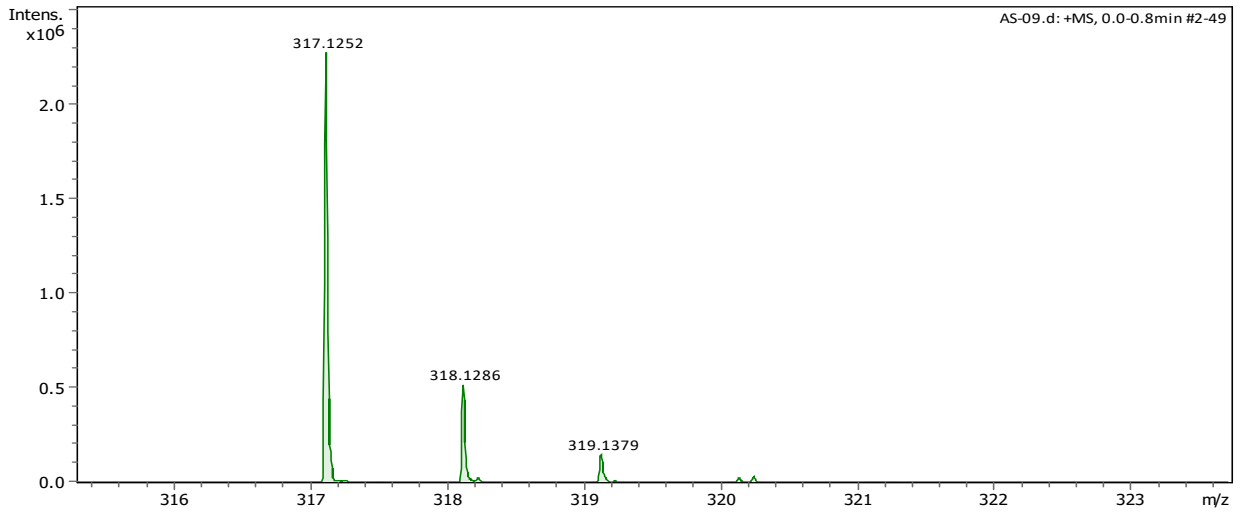
**Figure 40. Mass spectrum of L4**



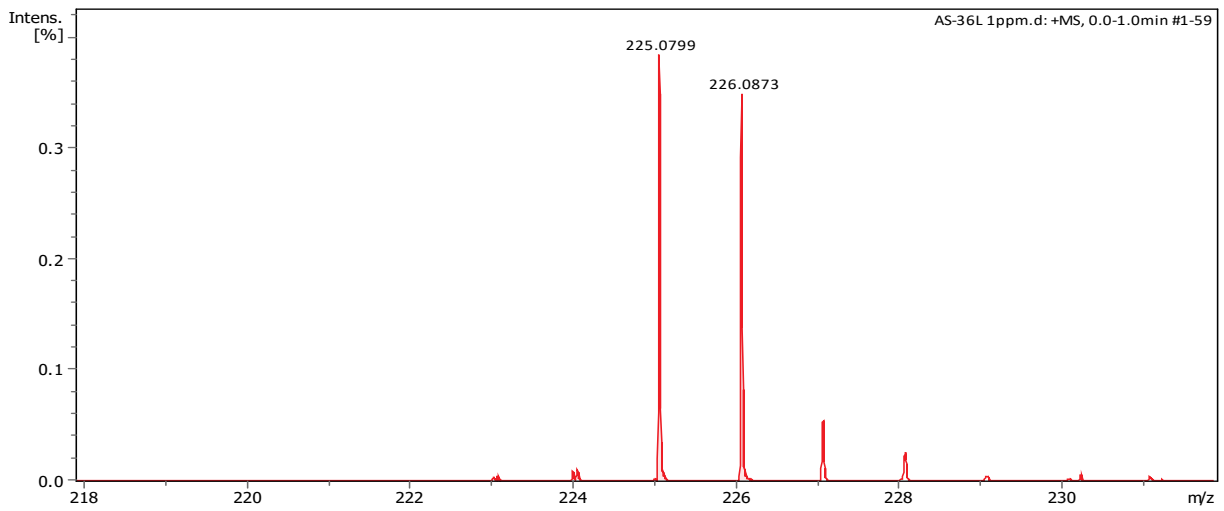
**Figure 41. Mass spectrum of L5**



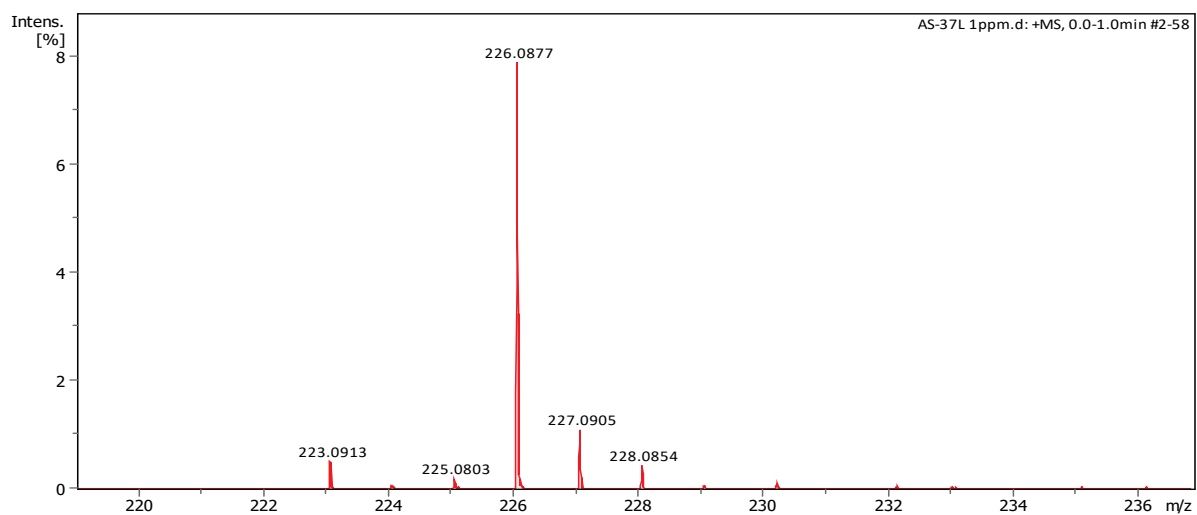
**Figure 42. Mass spectrum of L6**



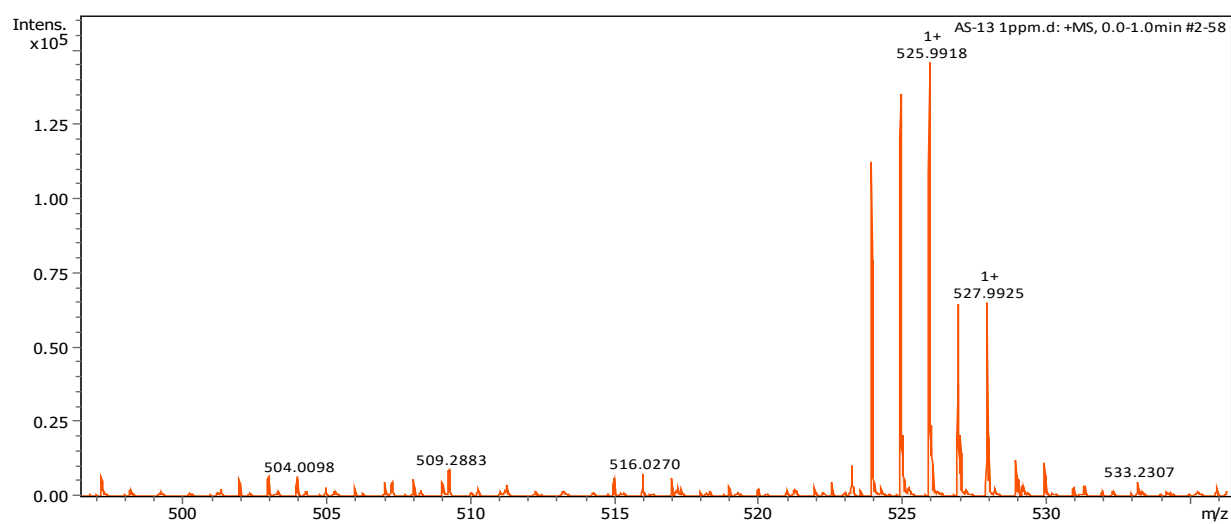
**Figure 43. Mass spectrum of L7**



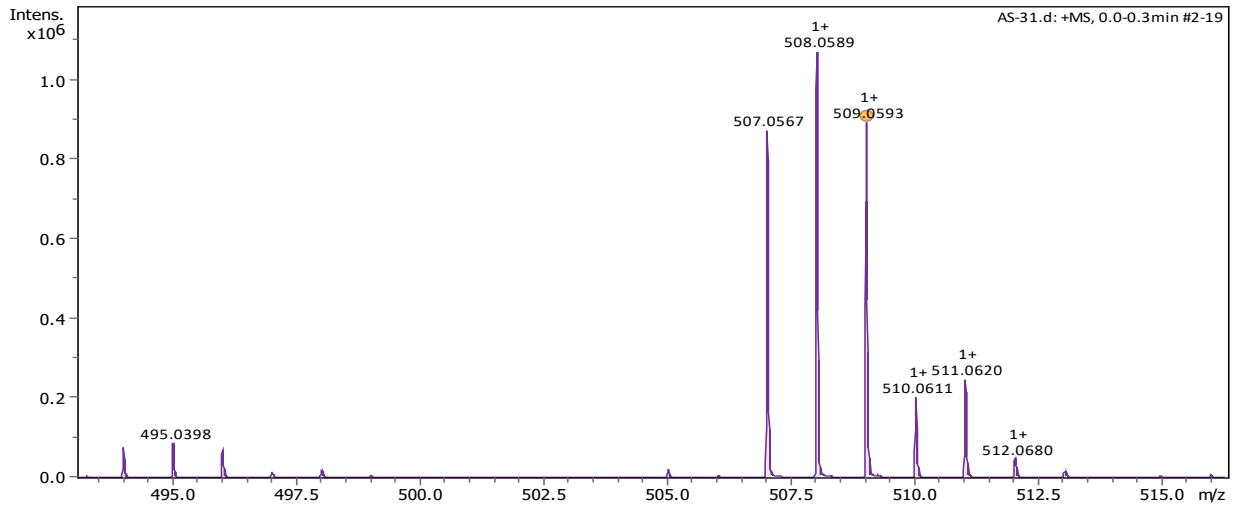
**Figure 44. Mass spectrum of L8**



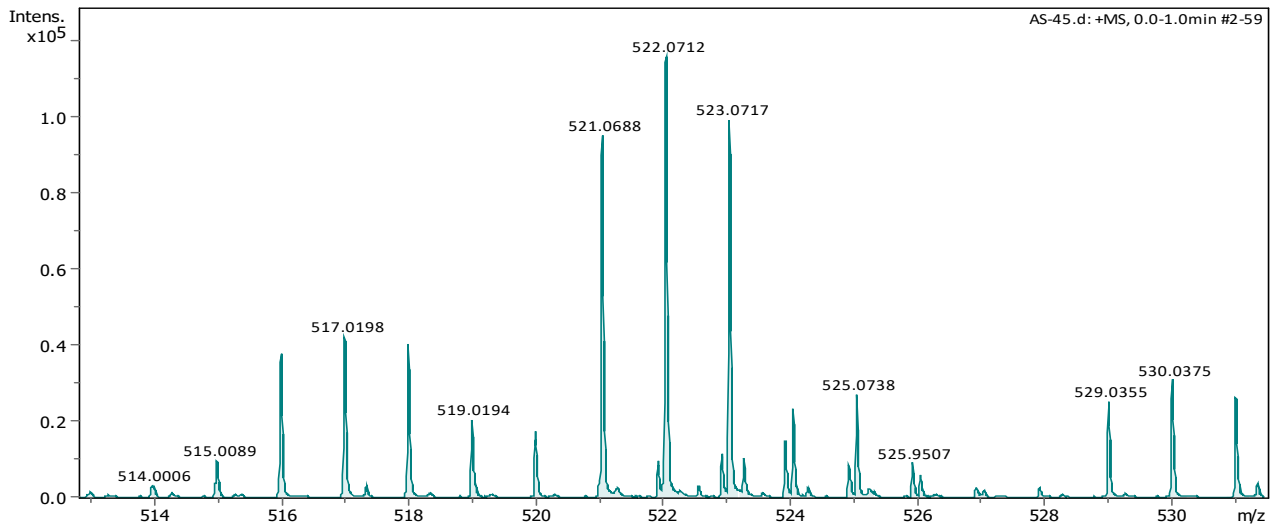
**Figure 45. Mass spectrum of L9**



**Figure 46. Mass spectrum of Pt1**



**Figure 47. Mass spectrum of Pt2**



**Figure 48. Mass spectrum of Pt4**

**F**

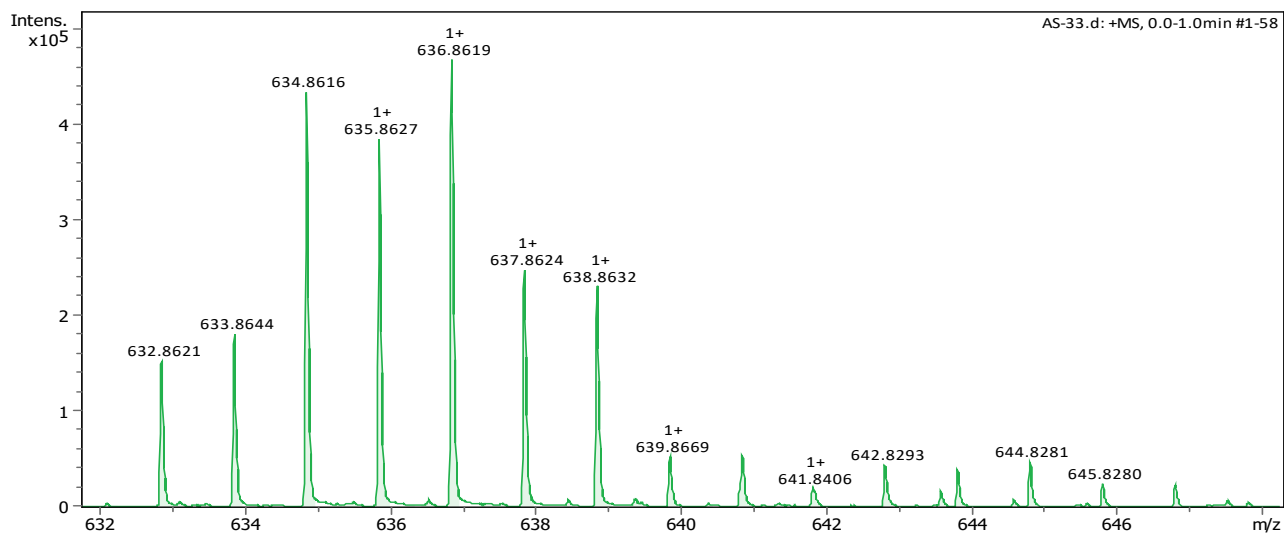


Figure 49. Mass spectrum of Pt5

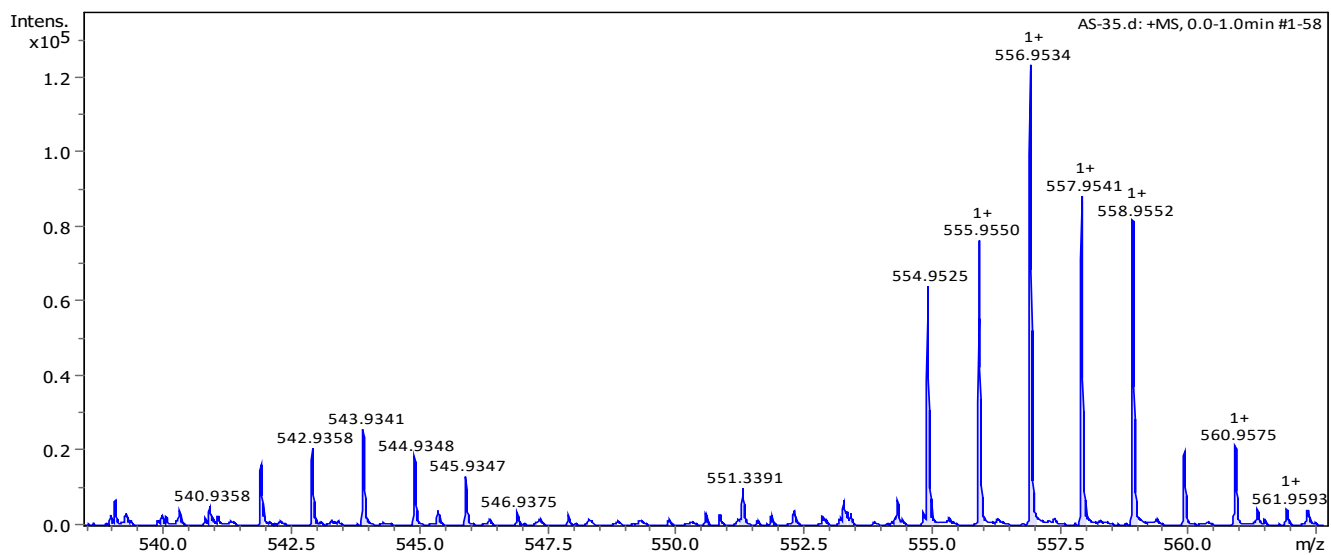
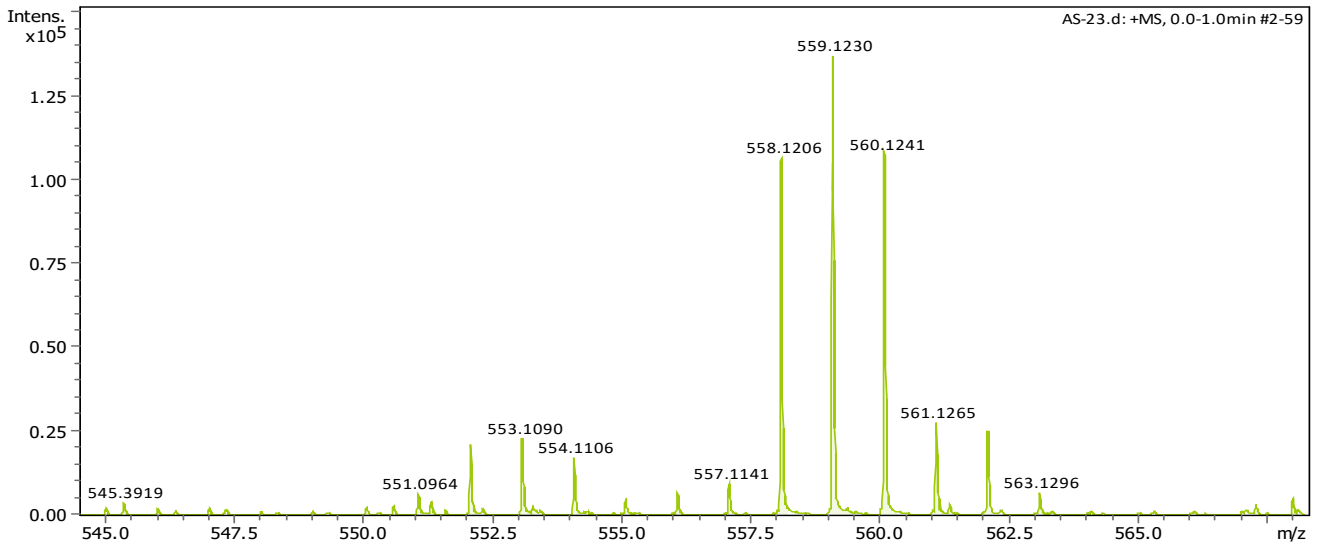
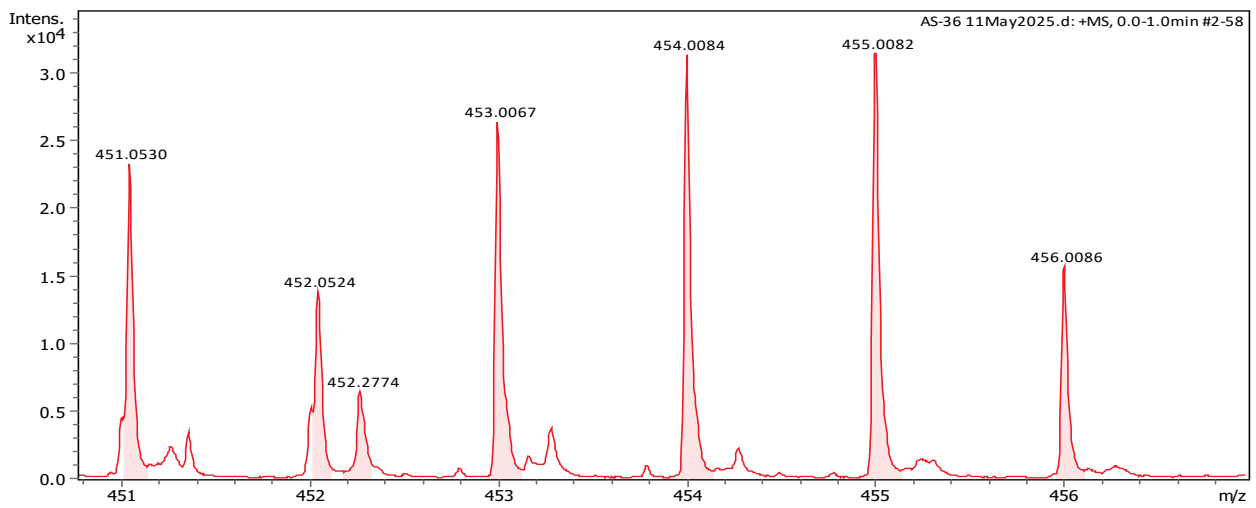


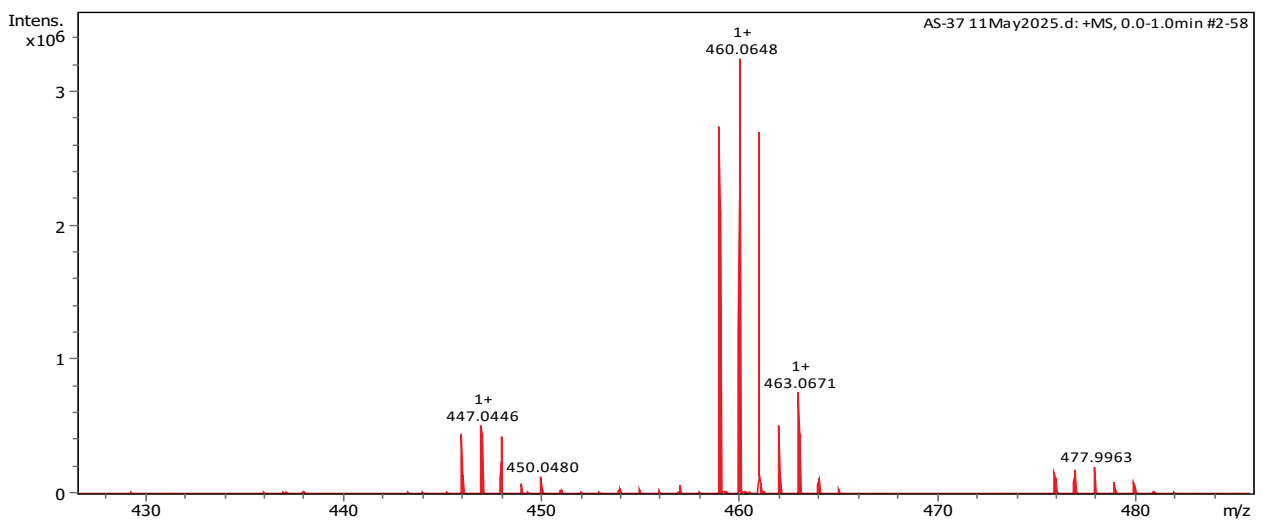
Figure 50. Mass spectrum of Pt6



**Figure 51. Mass spectrum of Pt7**



**Figure 52. Mass spectrum of Pt8**



**Figure 53. Mass spectrum of Pt9**