

## Electronic Supplementary Information

### Synthesis and Characterization of Chromium Complexes 2- $\text{Me}_4\text{CpC}_6\text{H}_4\text{CH}_2(\text{R})\text{NHCrCl}_2$ and Their Catalytic Properties in Ethylene Homo- and Co-polymerization

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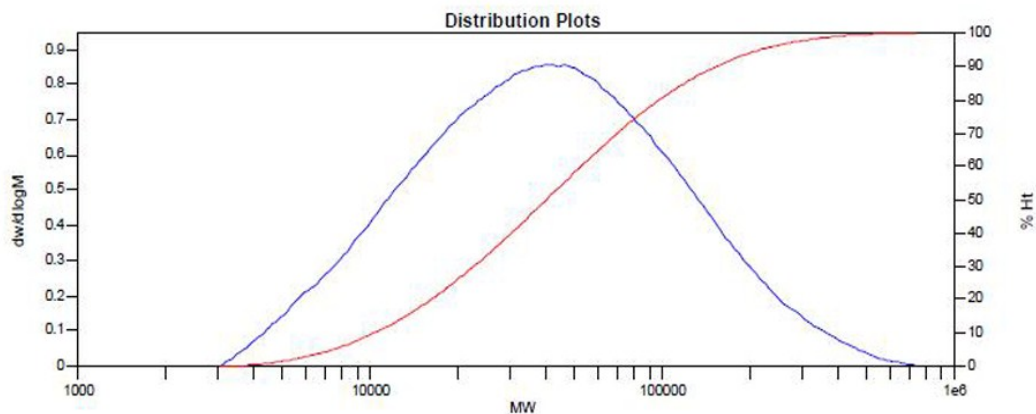
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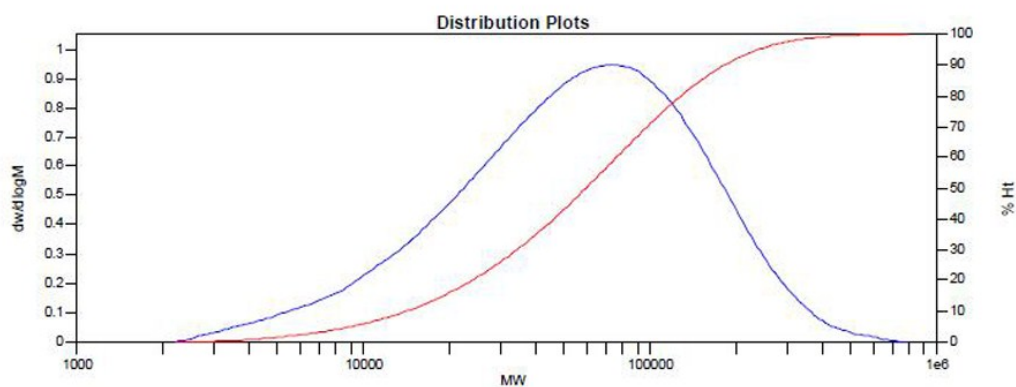
**Table S1** Crystal Data and Structure Refinements of Complexes **1**, **5** and **6**

	<b>1</b>	<b>5</b>	<b>6</b>
empirical formula	C <sub>19</sub> H <sub>25</sub> Cl <sub>2</sub> CrN	C <sub>24</sub> H <sub>27</sub> Cl <sub>2</sub> CrN	C <sub>26</sub> H <sub>31</sub> Cl <sub>2</sub> CrN
<i>M<sub>w</sub></i>	390.30	452.37	480.42
crystal system	Monoclinic	Monoclinic	Orthorhombic
space group	C2/c	P2(1)/c	Pna2(1)
<i>a</i> (Å)	25.969(2)	10.4590(8)	15.3969(7)
<i>b</i> (Å)	9.2271(8)	26.893(2)	18.3161(9)
<i>c</i> (Å)	16.7645(14)	8.5983(6)	8.5618(4)
<i>α</i> (deg)	90	90	90
<i>β</i> (deg)	110.1890(10)	113.7230(10)	90
<i>γ</i> (deg)	90	90	90
<i>V</i> (Å <sup>3</sup> )	3770.3(6)	2214.1(3)	2414.5(2)
<i>Z</i>	8	4	4
<i>D</i> <sub>calcd</sub> (mg m <sup>-3</sup> )	1.375	1.357	1.322
abs. coeff. (mm <sup>-1</sup> )	0.889	0.768	0.708
2θ mas (deg)	1.67-26.39	2.13-26.39	1.73-26.39
transmission range	0.8782-0.8493	0.8936-0.8679	0.9012-0.8772
reflections collected	10485	12593	12947
independent reflections	3838 [ <i>R</i> (int) = 0.0386]	4521 [ <i>R</i> (int) = 0.0367]	4864 [ <i>R</i> (int) = 0.0353]
<i>R</i> <sub>1</sub> <sup><i>a</i></sup> ( <i>wR</i> <sub>2</sub> ) <sup><i>b</i></sup> [ <i>I</i> > 2σ( <i>I</i> )]	0.0452 0.1077	0.0457 0.1043	0.0455 0.1128
GOF ( <i>F</i> <sup>2</sup> )	1.054	1.049	0.999
largest diff. peak and hole/e Å <sup>-3</sup>	0.693 -0.273	0.709 -0.265	0.407 -0.296

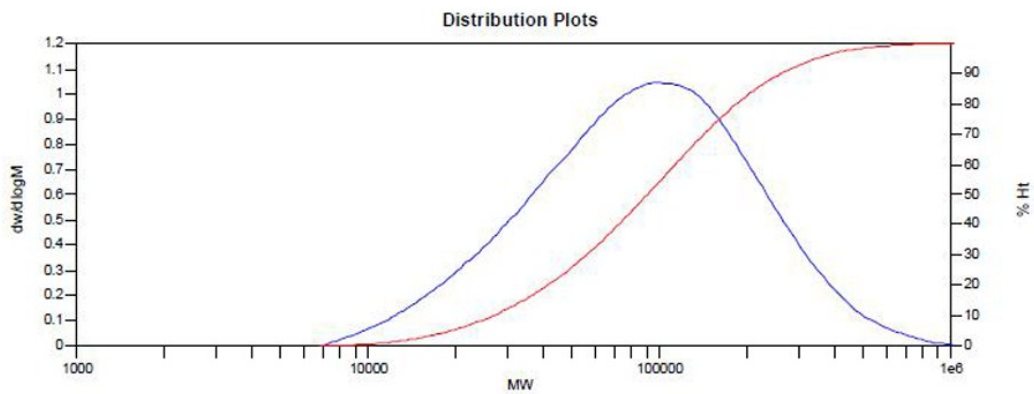
<sup>*a*</sup>  $R_1 = \sum ||F_o| - |F_c|| / \sum |F_o|$ .    <sup>*b*</sup>  $wR_2 = [\sum [w (F_o^2 - F_c^2)^2] / \sum [w (F_o^2)^2]]^{1/2}$



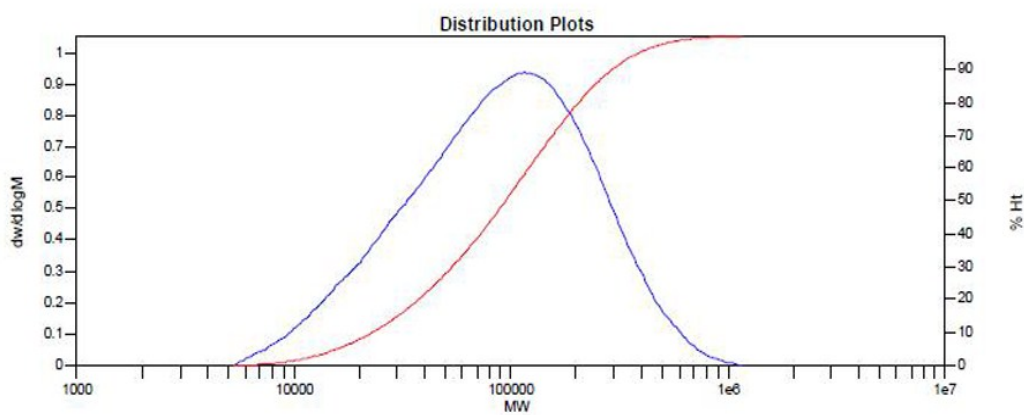
**Figure S1** GPC trace for poly(ethylene-co-1-hexene) sample (entry 18, Table 3,  $M_w = 6.48 \times 10^4$  g/mol,  $M_w/M_n = 2.68$ ).



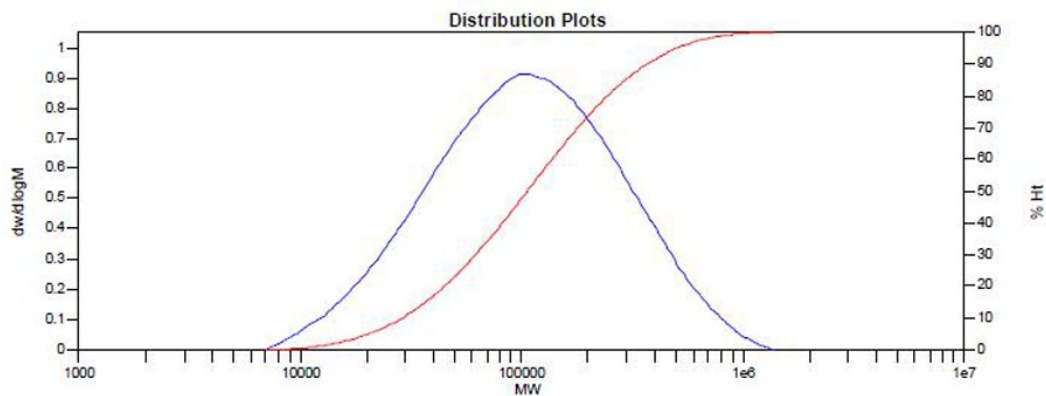
**Figure S2** GPC trace for poly(ethylene-co-1-hexene) sample (entry 21, Table 3,  $M_w = 8.20 \times 10^4$  g/mol,  $M_w/M_n = 2.62$ ).



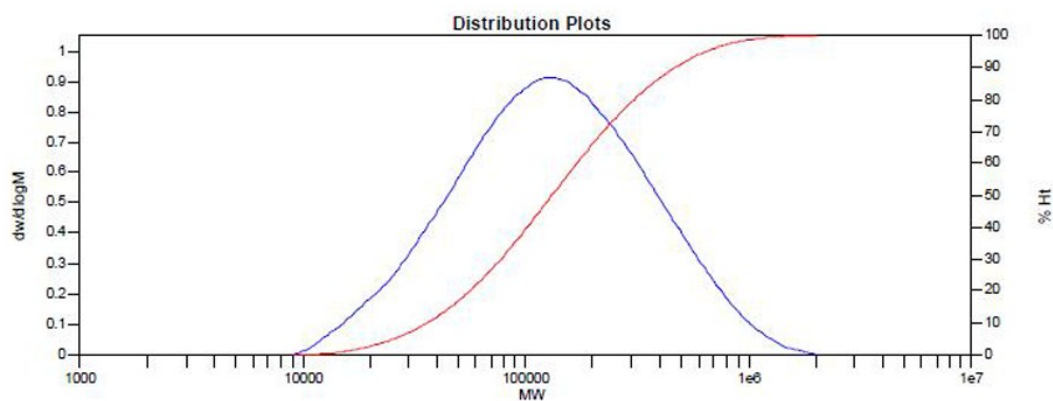
**Figure S3** GPC trace for poly(ethylene-co-1-hexene) sample (entry 24, Table 3,  $M_w = 12.22 \times 10^4$  g/mol,  $M_w/M_n = 2.08$ ).



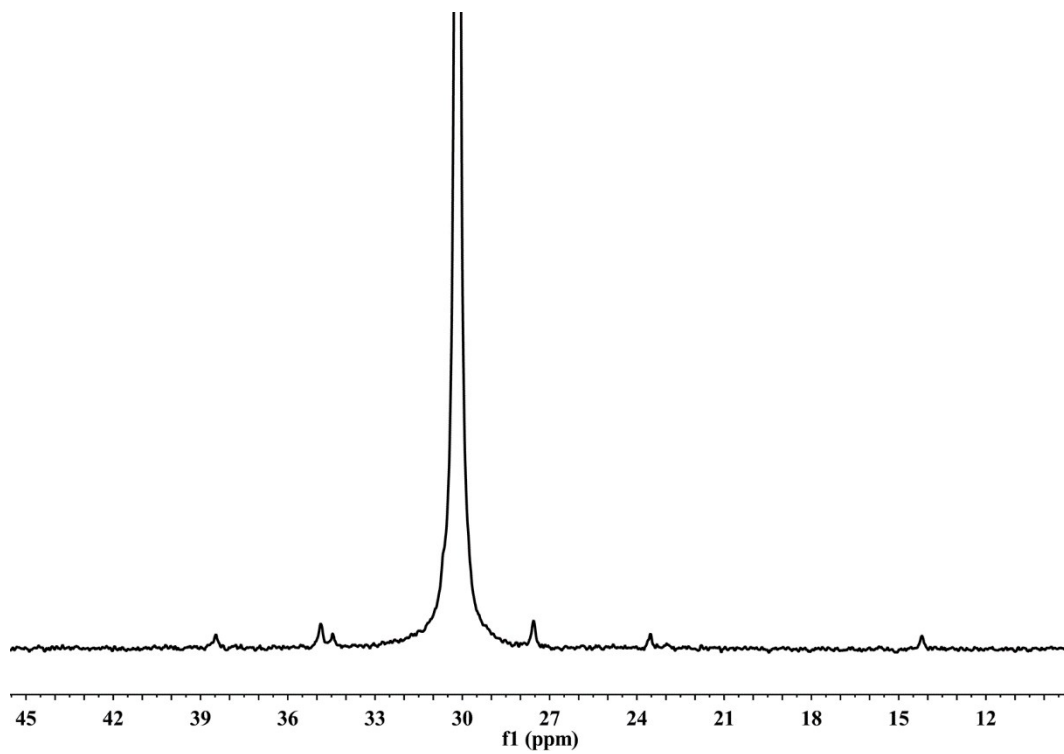
**Figure S4** GPC trace for poly(ethylene-co-1-hexene) sample (entry 27, Table 3,  $M_w = 13.18 \times 10^4$  g/mol,  $M_w/M_n = 2.47$ ).



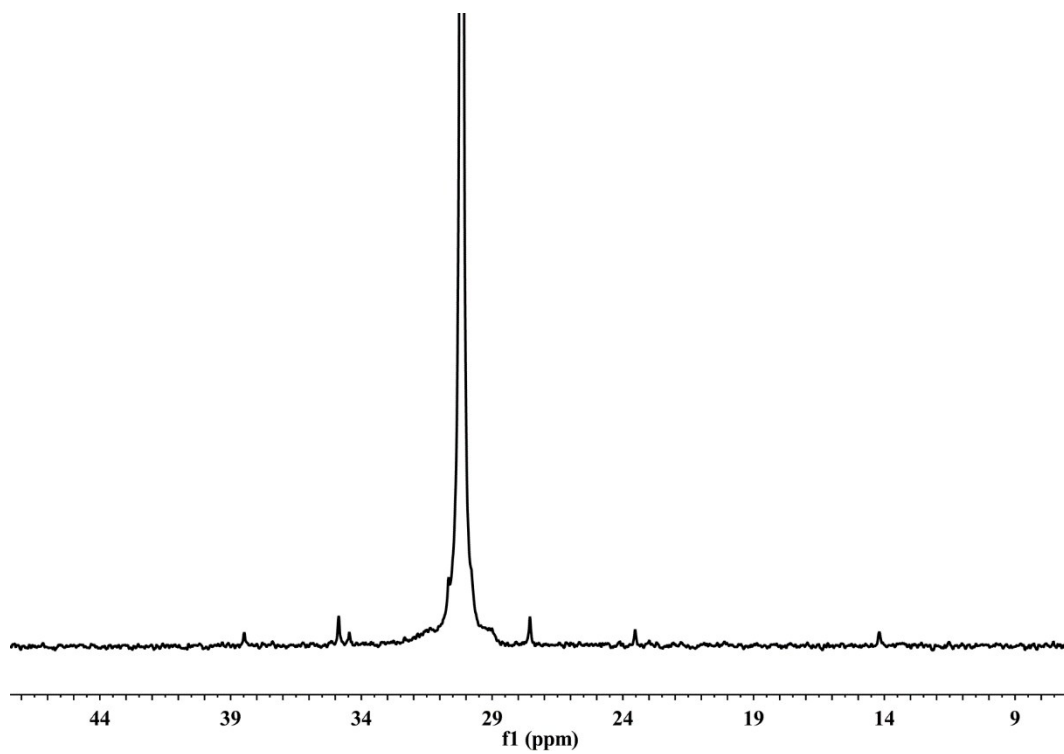
**Figure S5** GPC trace for poly(ethylene-co-1-hexene) sample (entry 30, Table 3,  $M_w = 16.02 \times 10^4$  g/mol,  $M_w/M_n = 2.45$ ).



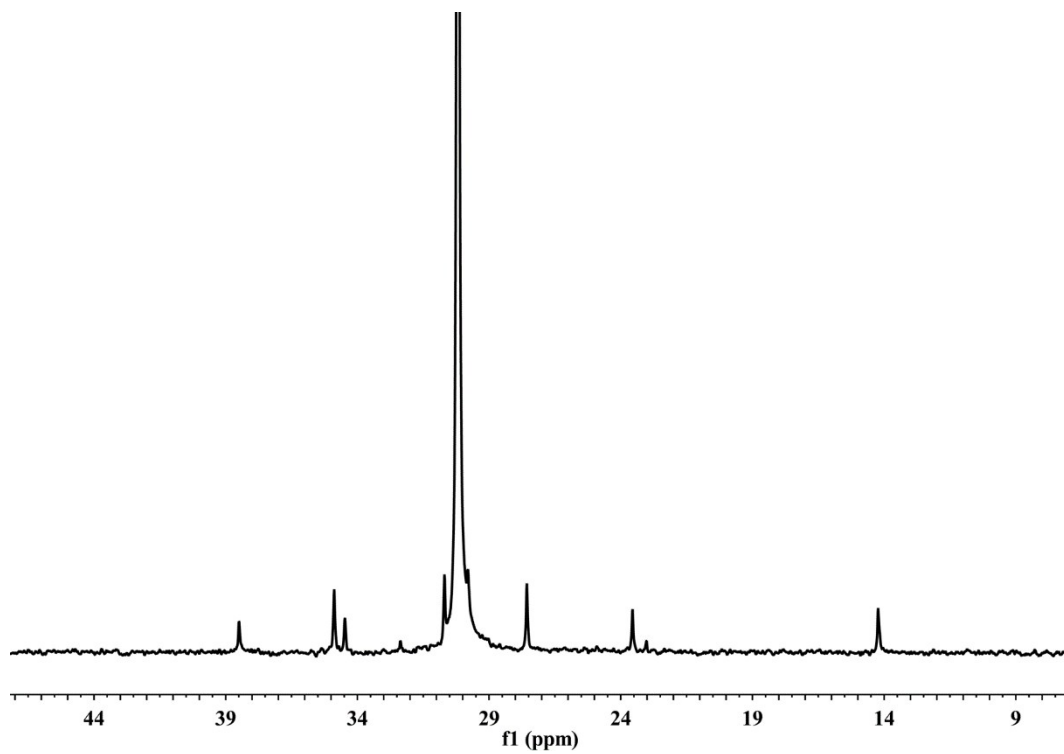
**Figure S6** GPC trace for poly(ethylene-co-1-hexene) sample (entry 33, Table 3,  $M_w = 20.31 \times 10^4$  g/mol,  $M_w/M_n = 2.48$ ).



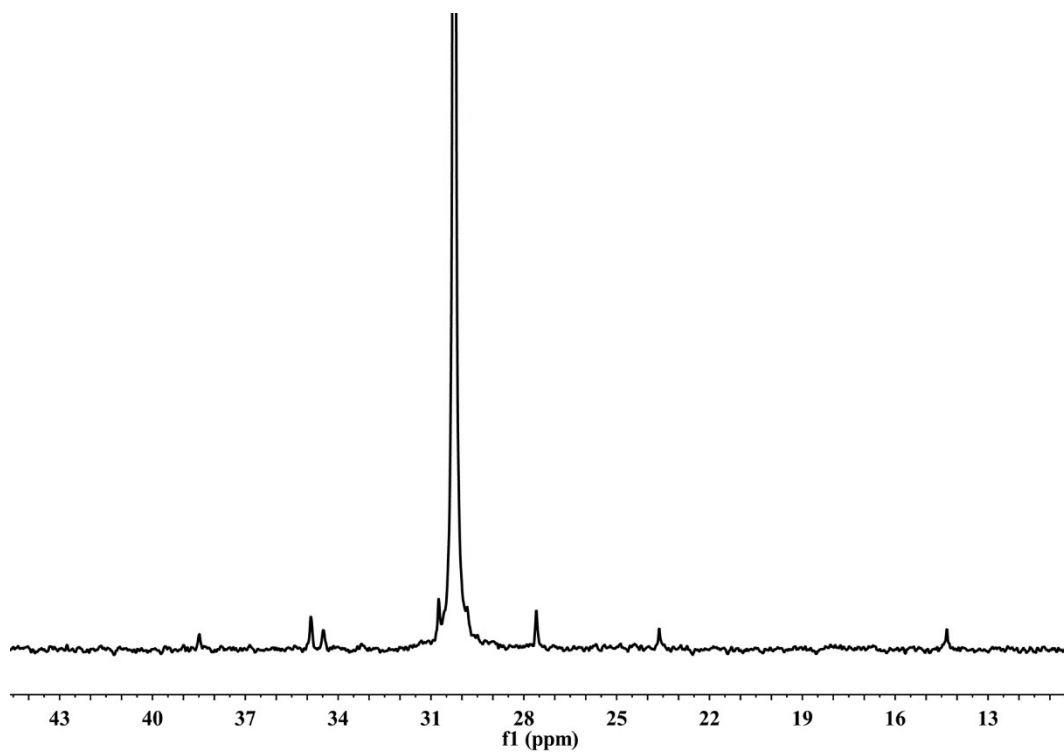
**Figure S7**  $^{13}\text{C}$  NMR spectra for poly(ethylene-co-1-hexene) sample (entry 21, Table 3).



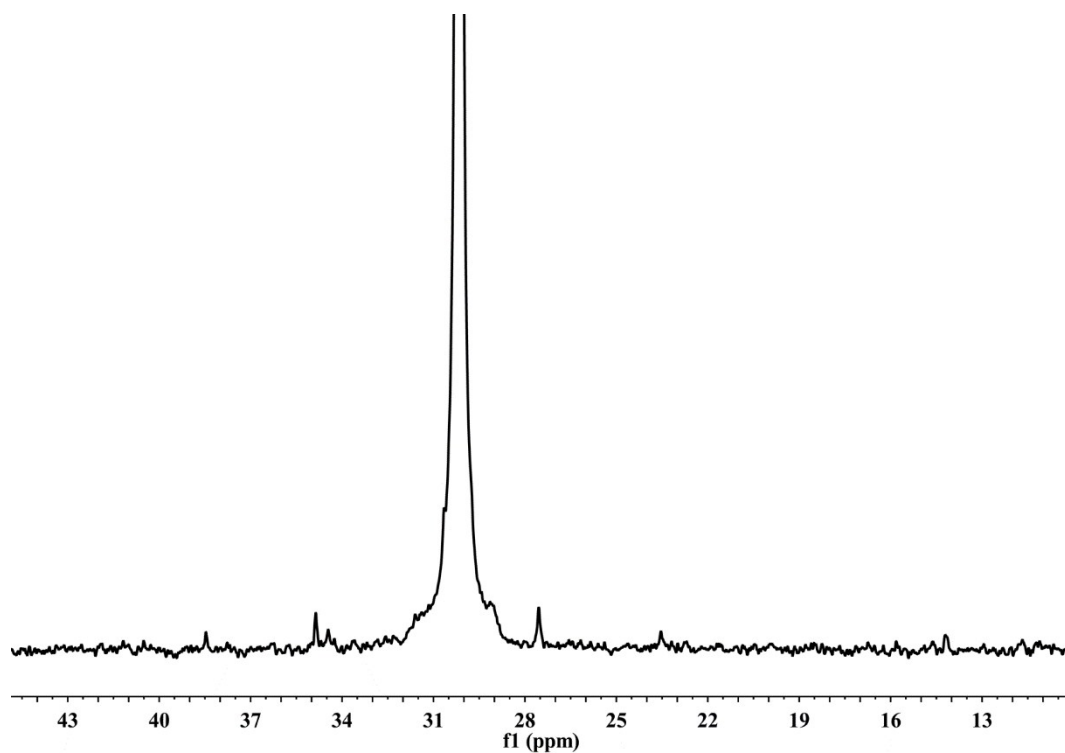
**Figure S8**  $^{13}\text{C}$  NMR spectra for poly(ethylene-co-1-hexene) sample (entry 24, Table 3).



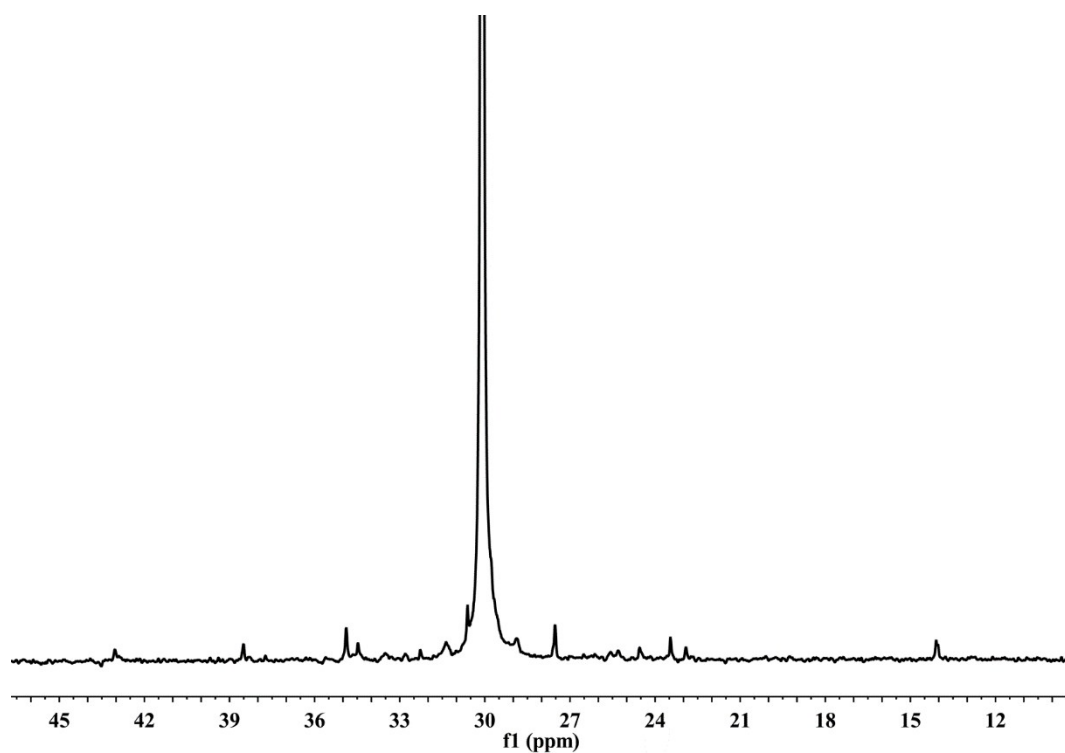
**Figure S9**  $^{13}\text{C}$  NMR spectra for poly(ethylene-co-1-hexene) sample (entry 27, Table 3).



**Figure S10**  $^{13}\text{C}$  NMR spectra for poly(ethylene-co-1-hexene) sample (entry 30, Table 3).

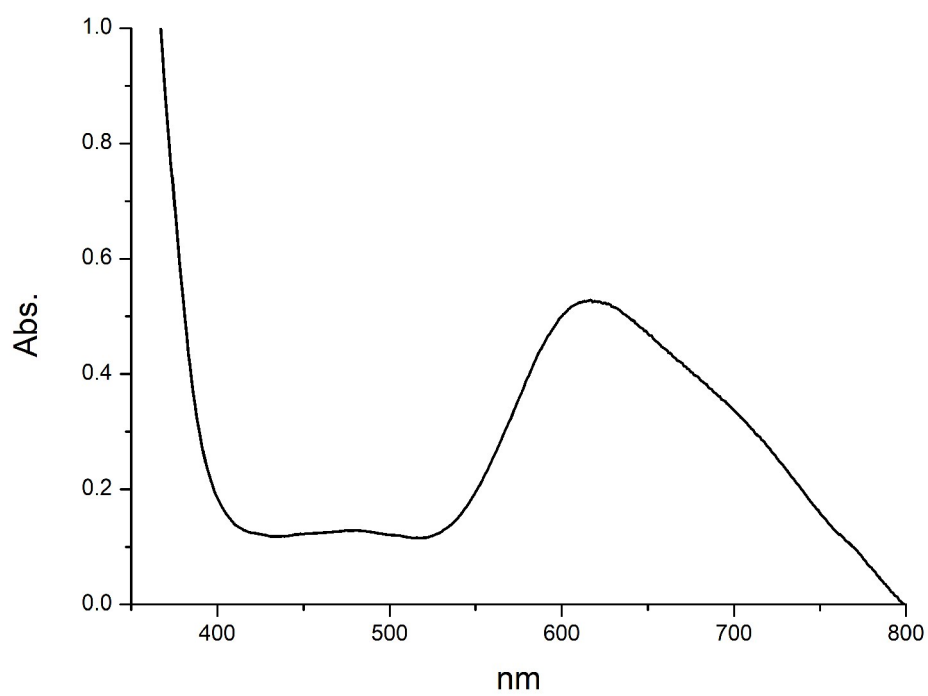


**Figure S11**  $^{13}\text{C}$  NMR spectra for poly(ethylene-co-1-hexene) sample (entry 33, Table 3).

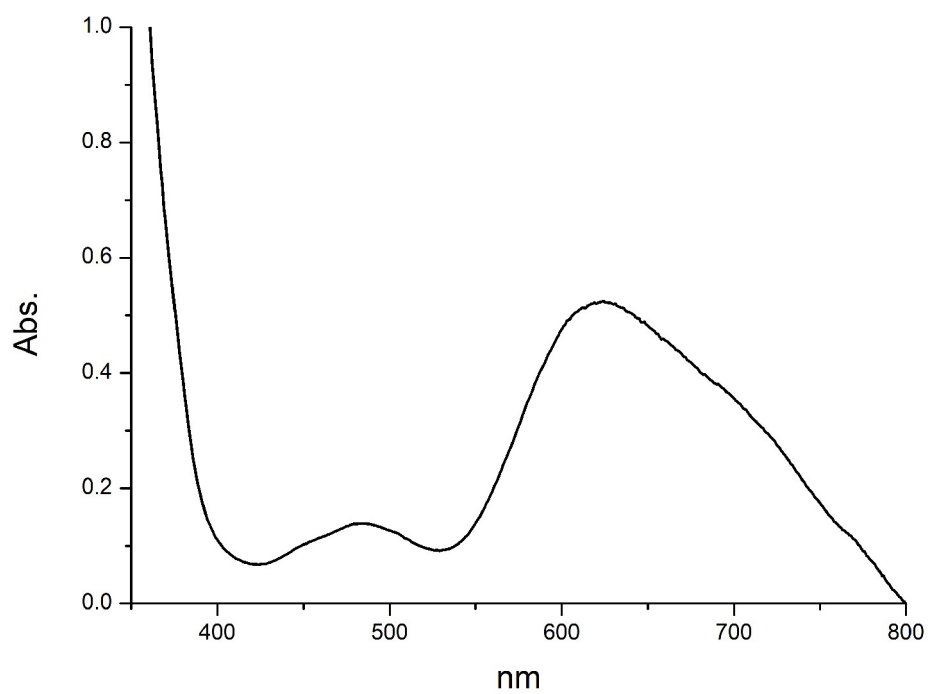


**Figure S12**  $^{13}\text{C}$  NMR spectra for poly(ethylene-co-1-hexene) sample (entry 36, Table 3).

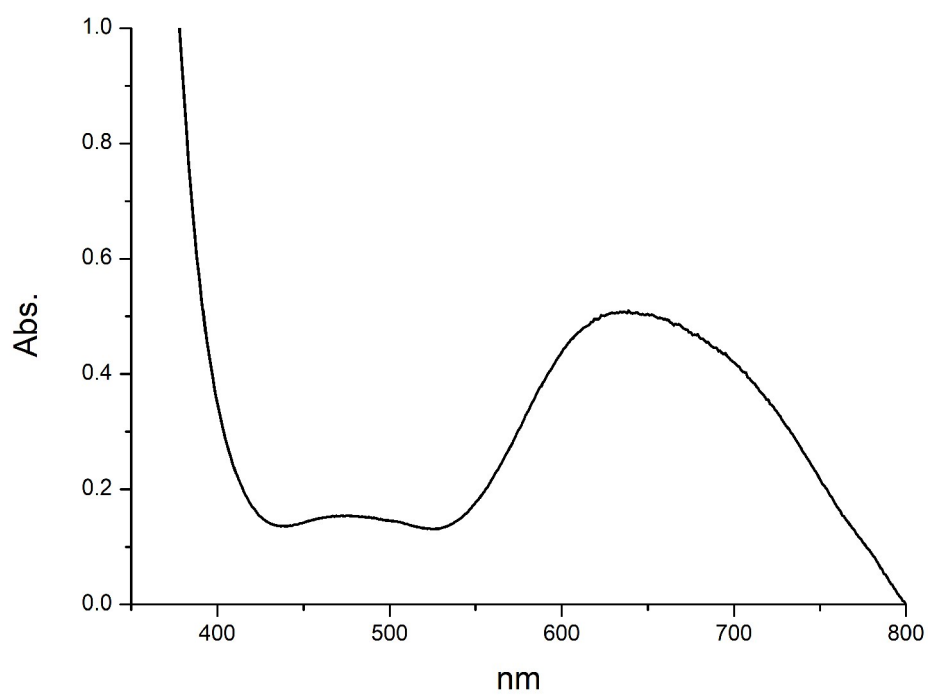




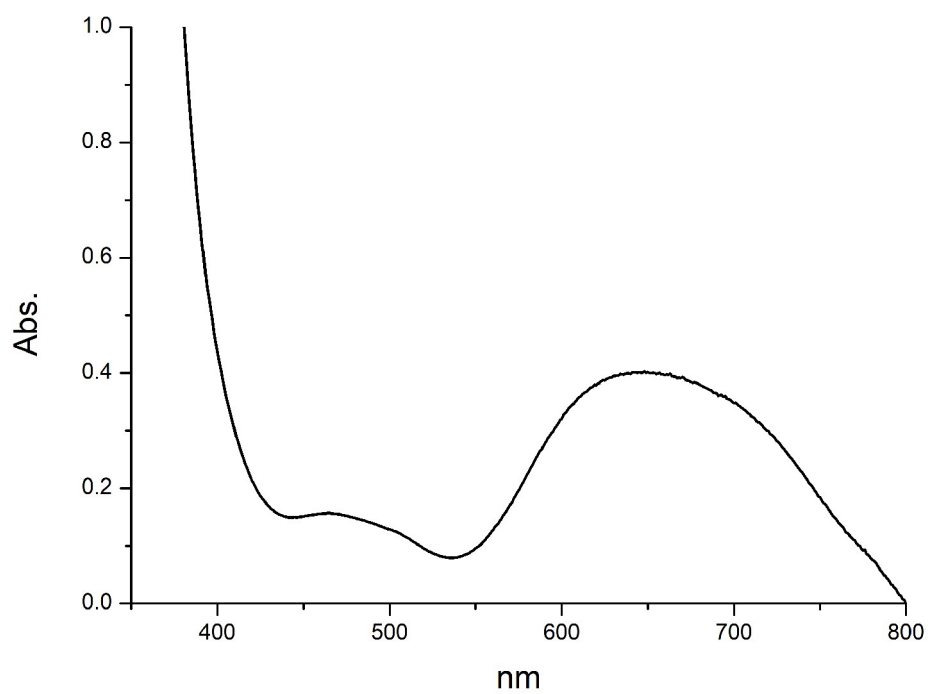
**Figure S13** UV/Vis spectra of complex 1.



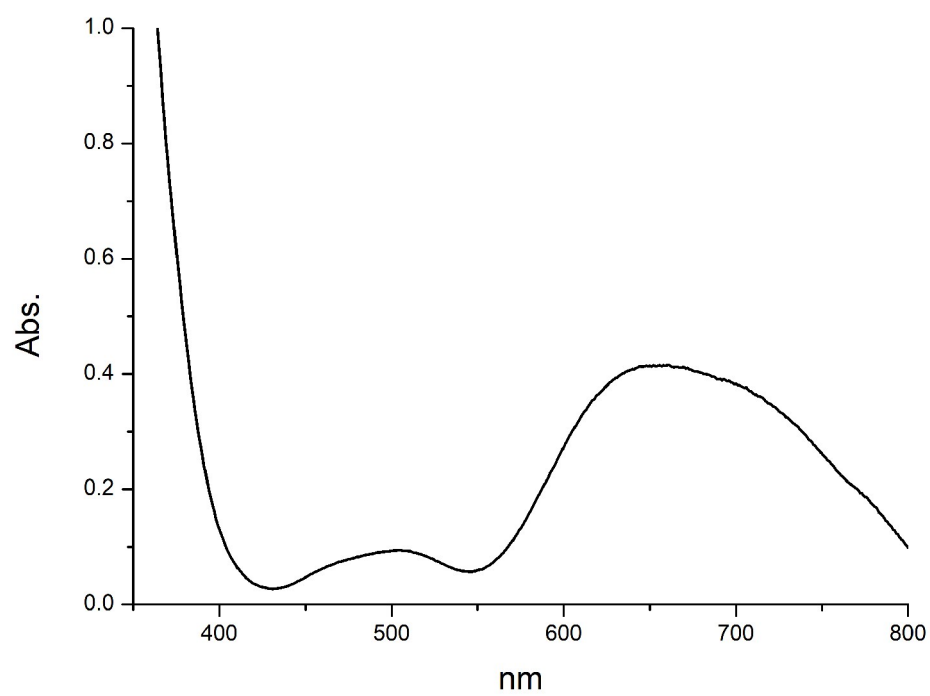
**Figure S14** UV/Vis spectra of complex 2.



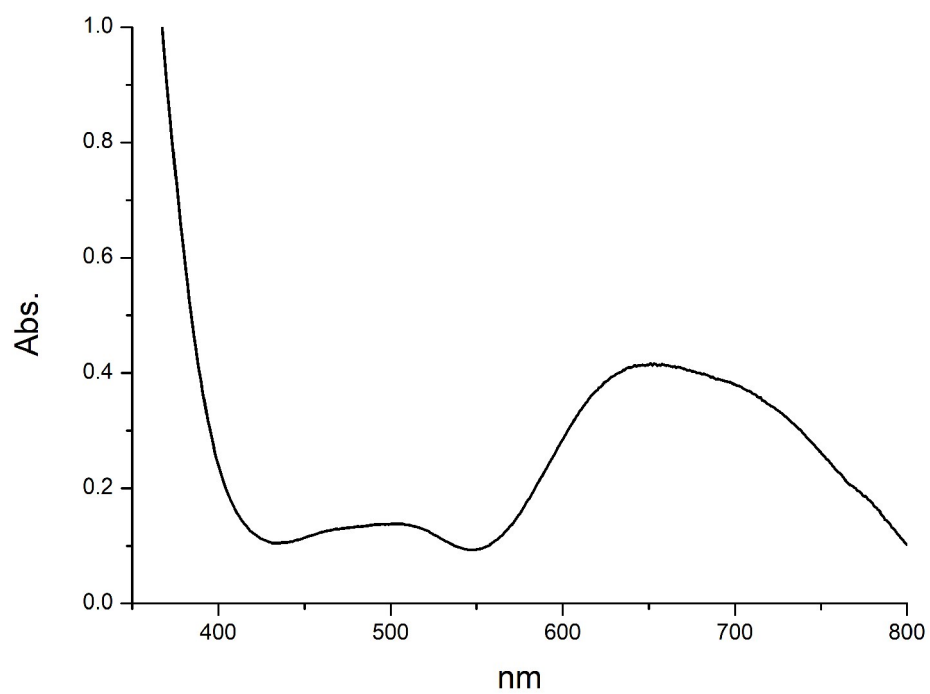
**Figure S15** UV/Vis spectra of complex **3**.



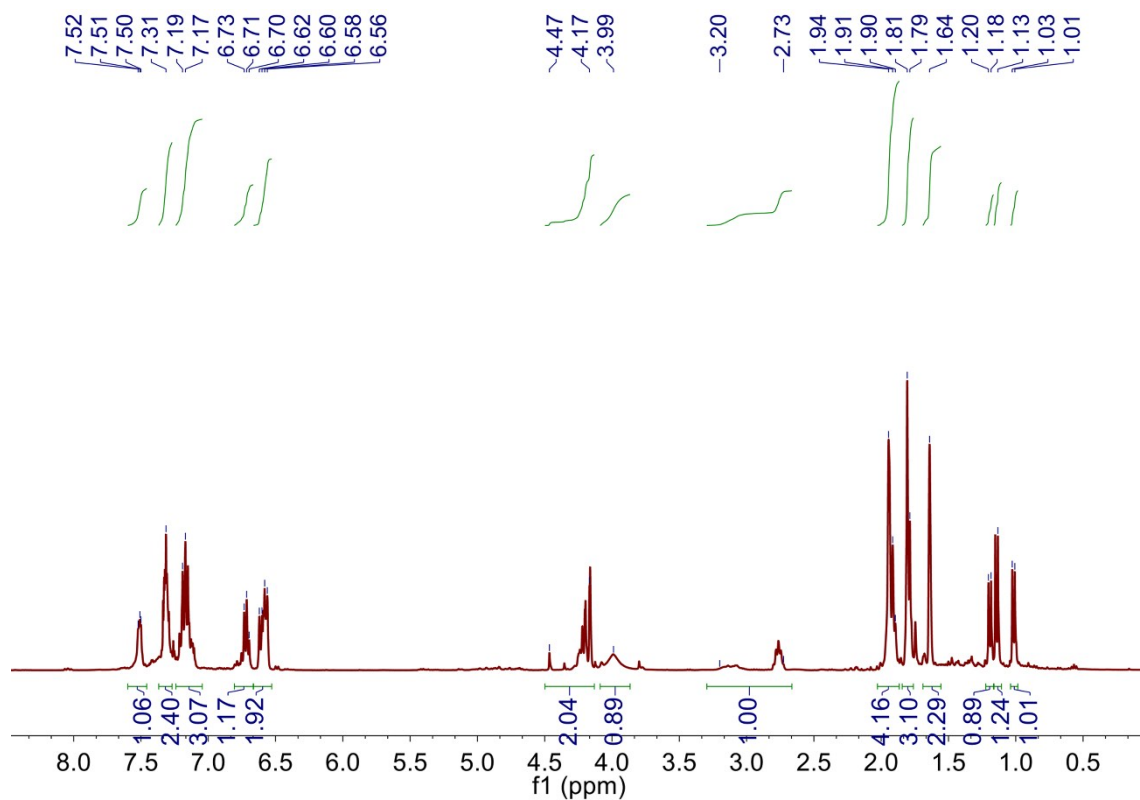
**Figure S16** UV/Vis spectra of complex **4**.



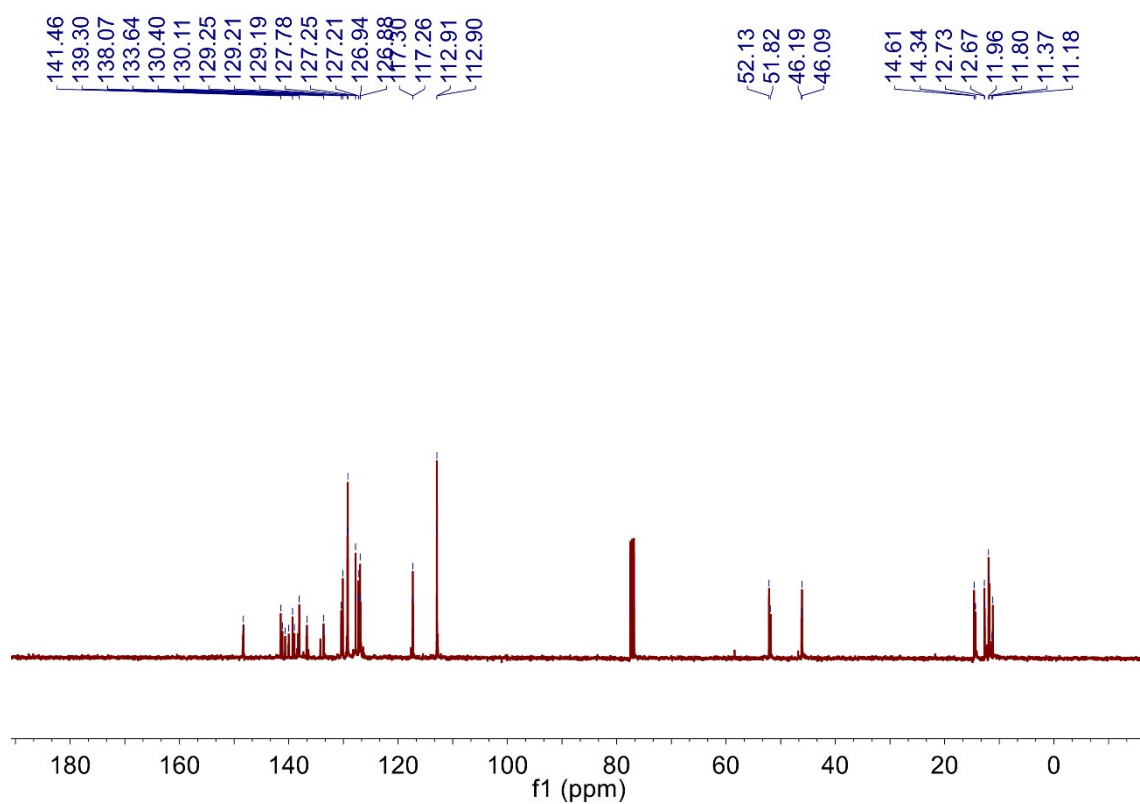
**Figure S17** UV/Vis spectra of complex 5.



**Figure S18** UV/Vis spectra of complex 6.



**Figure S19**  $^1\text{H}$  NMR spectrum of  $\text{H}_2\text{L3}$  (400 MHz,  $\text{CDCl}_3$ , 25 °C).



**Figure S20**  $^{13}\text{C}$   $\{^1\text{H}\}$  NMR spectrum of  $\text{H}_2\text{L3}$  (100 MHz,  $\text{CDCl}_3$ , 25 °C).

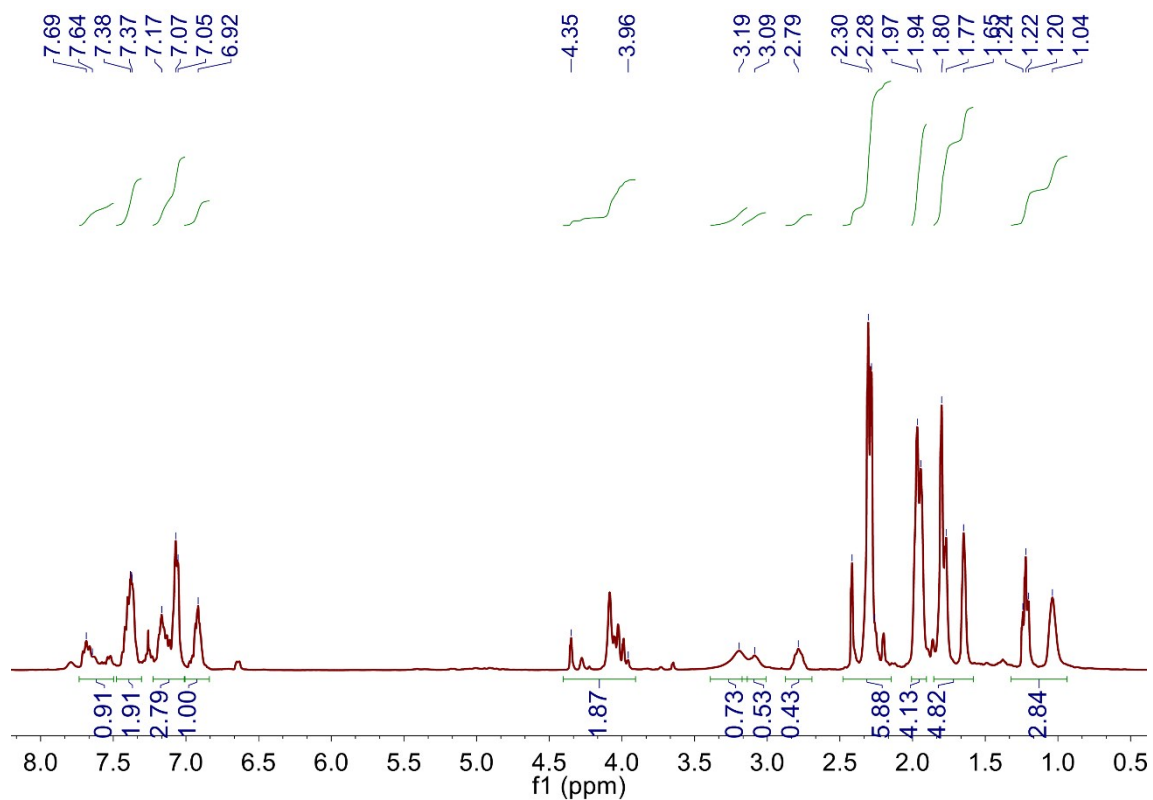


Figure S21  $^1\text{H}$  NMR spectrum of  $\text{H}_2\text{L5}$  (400 MHz,  $\text{CDCl}_3$ , 25  $^\circ\text{C}$ ).

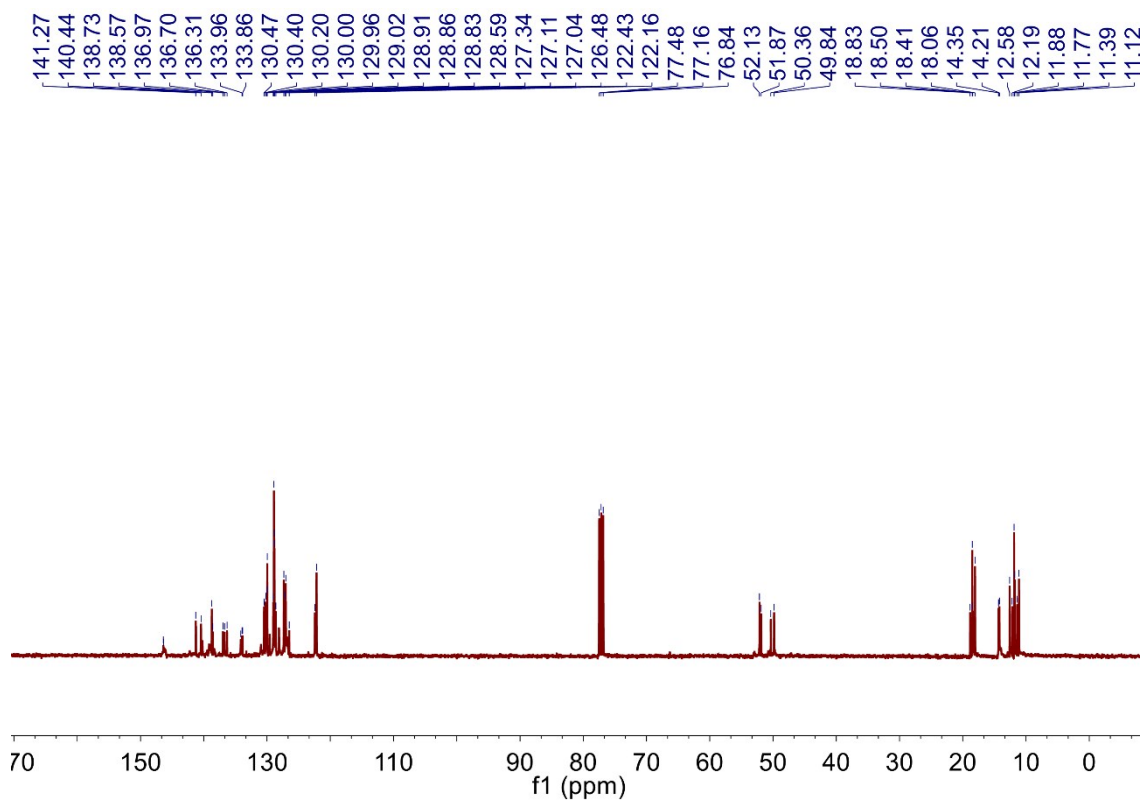
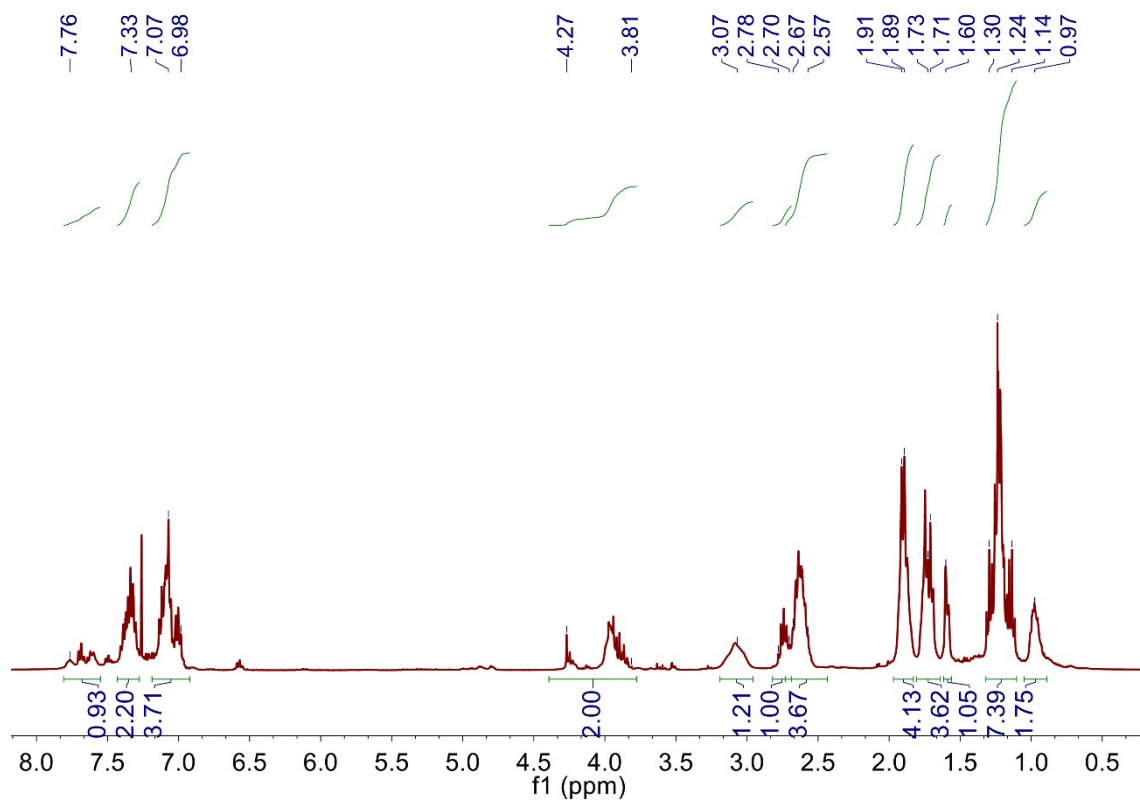
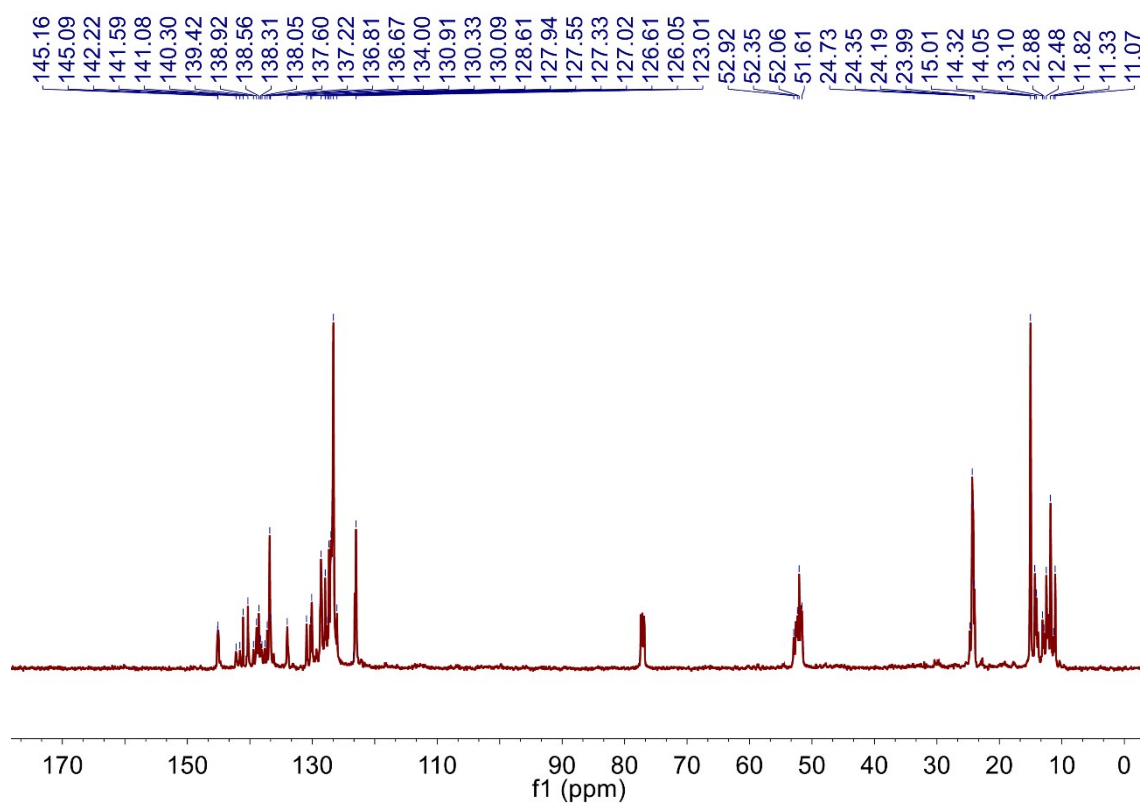


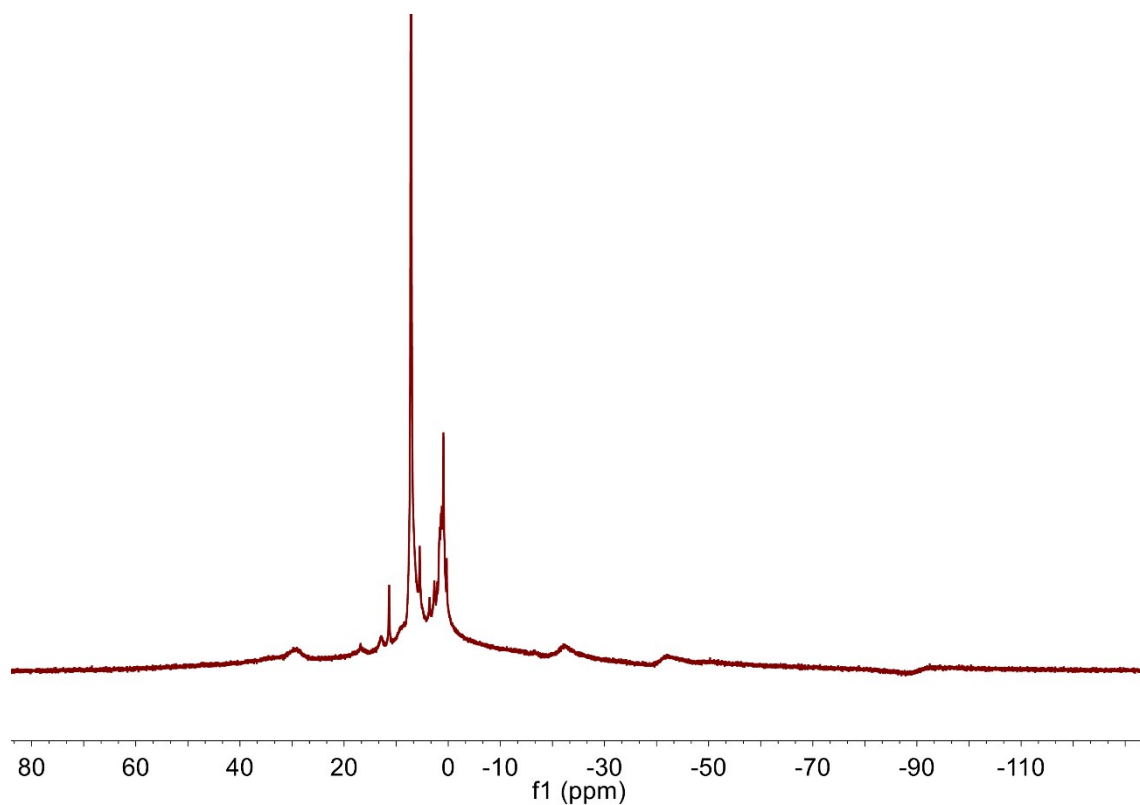
Figure S22  $^{13}\text{C}$   $\{^1\text{H}\}$  NMR spectrum of  $\text{H}_2\text{L5}$  (100 MHz,  $\text{CDCl}_3$ , 25  $^\circ\text{C}$ ).



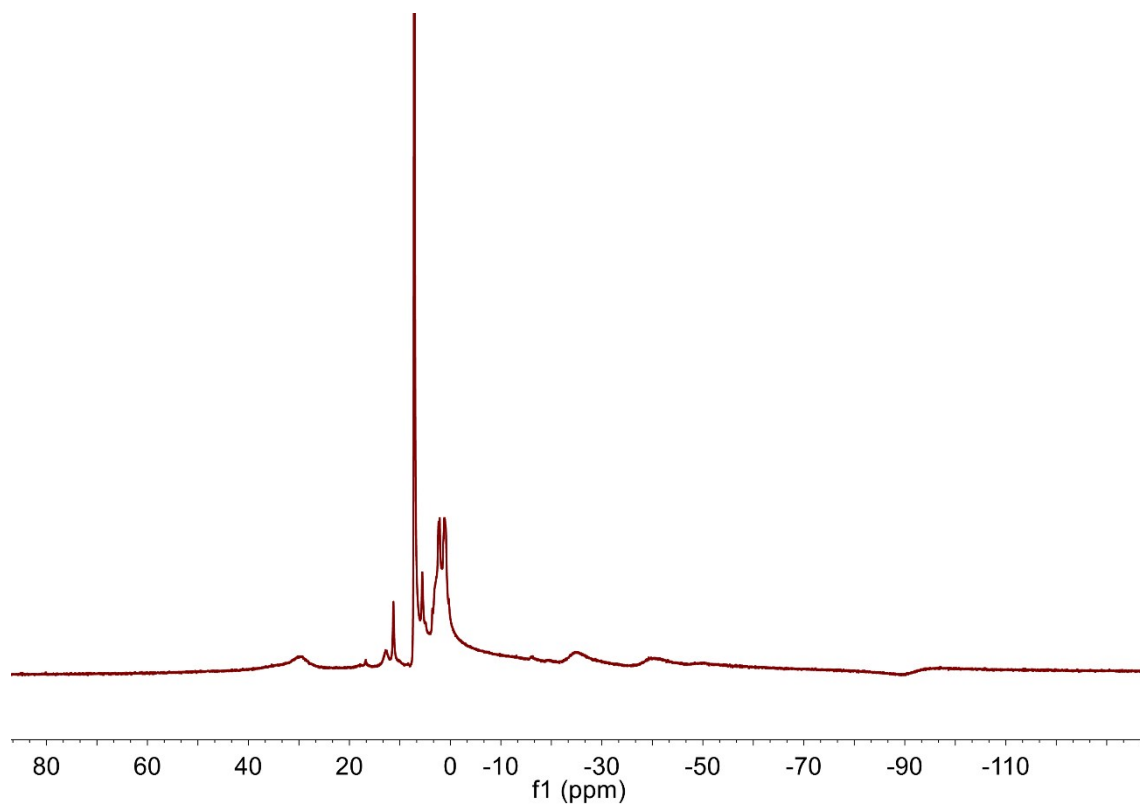
**Figure S23**  $^1\text{H}$  NMR spectrum of  $\text{H}_2\text{L6}$  (400 MHz,  $\text{CDCl}_3$ , 25 °C).



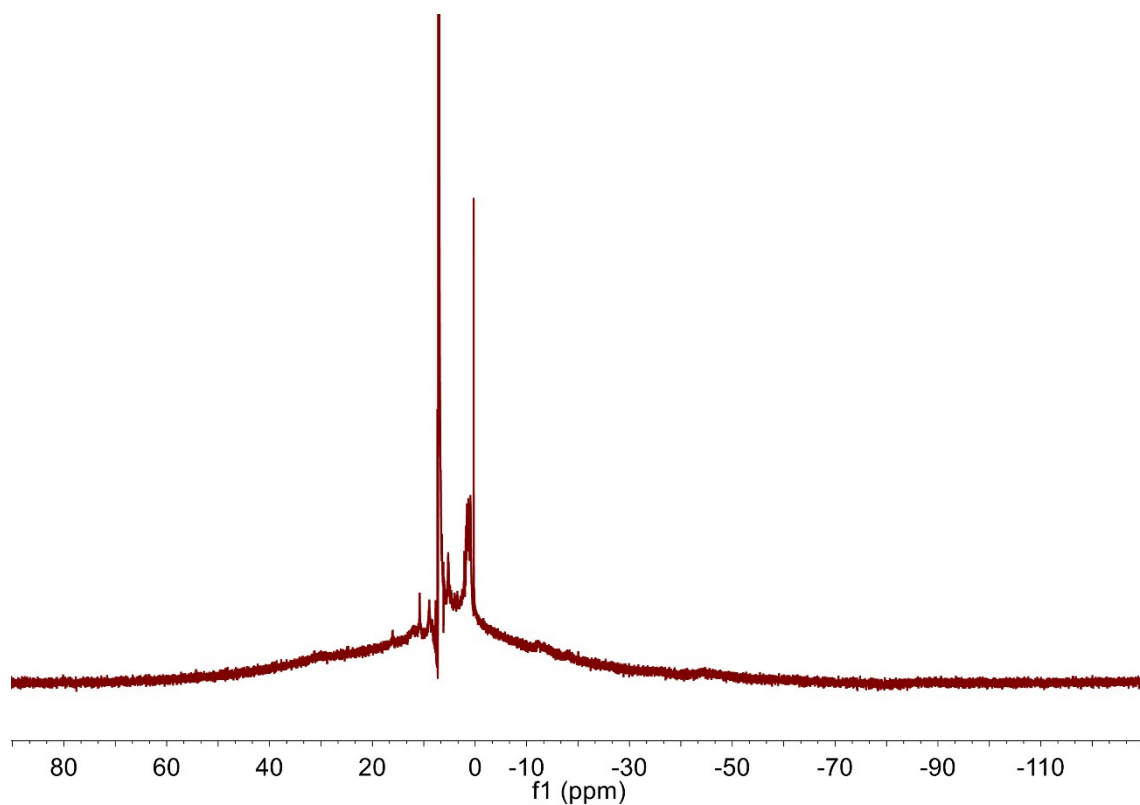
**Figure S24**  $^{13}\text{C}$   $\{^1\text{H}\}$  NMR spectrum of  $\text{H}_2\text{L6}$  (100 MHz,  $\text{CDCl}_3$ , 25 °C).



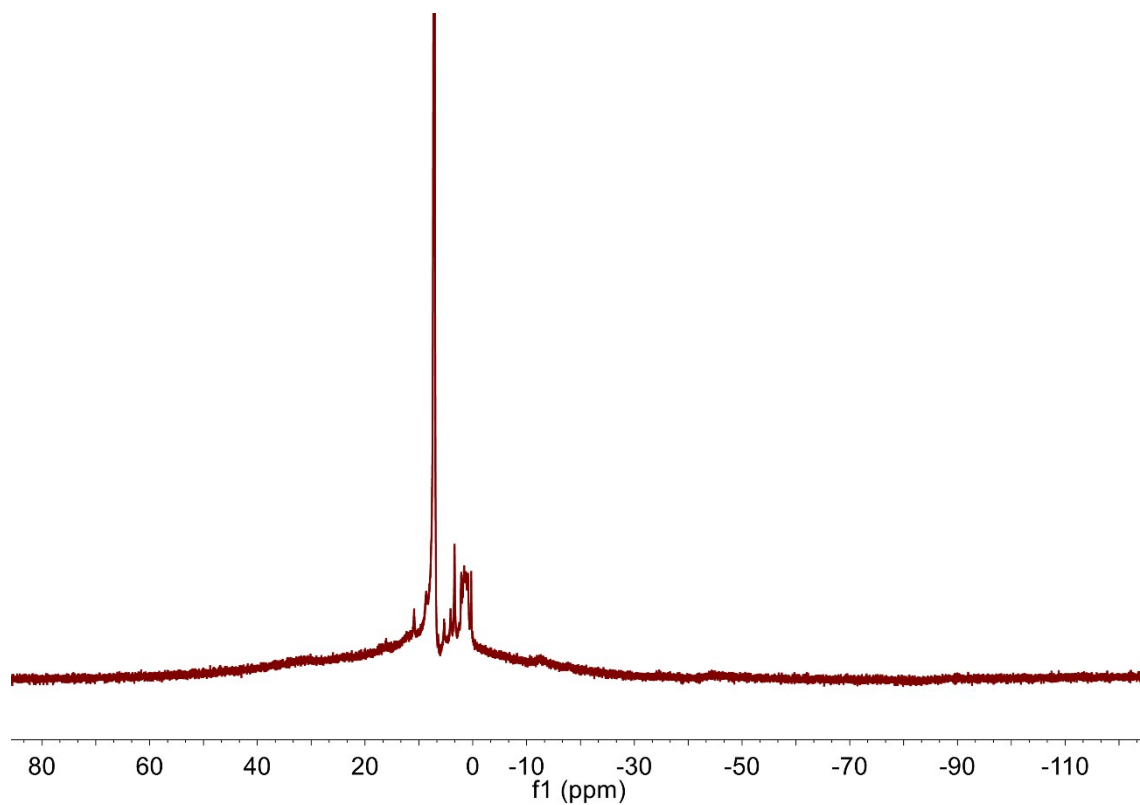
**Figure S25**  $^1\text{H}$  NMR spectrum of complex **1** (400 MHz,  $\text{C}_6\text{D}_6$ , 25  $^\circ\text{C}$ ).



**Figure S26**  $^1\text{H}$  NMR spectrum of complex **2** (400 MHz,  $\text{C}_6\text{D}_6$ , 25  $^\circ\text{C}$ ).

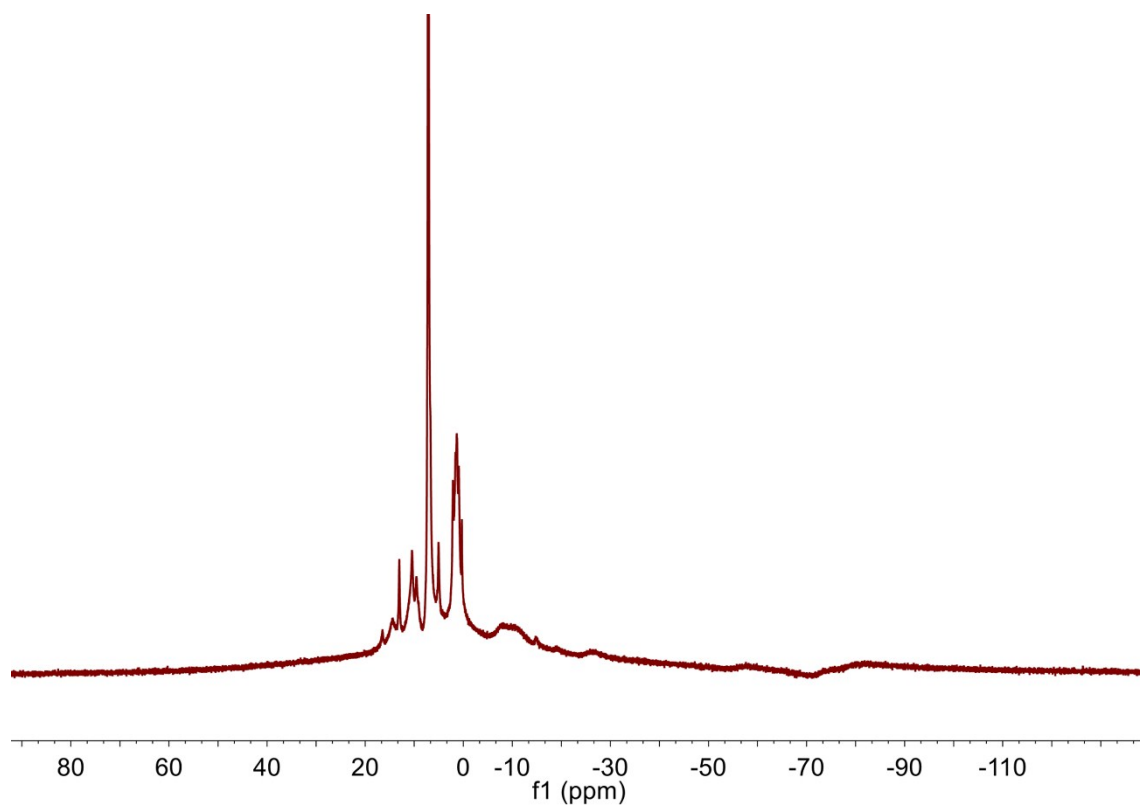


**Figure S27** <sup>1</sup>H NMR spectrum of complex **3** (400 MHz, C<sub>6</sub>D<sub>6</sub>, 25 °C).

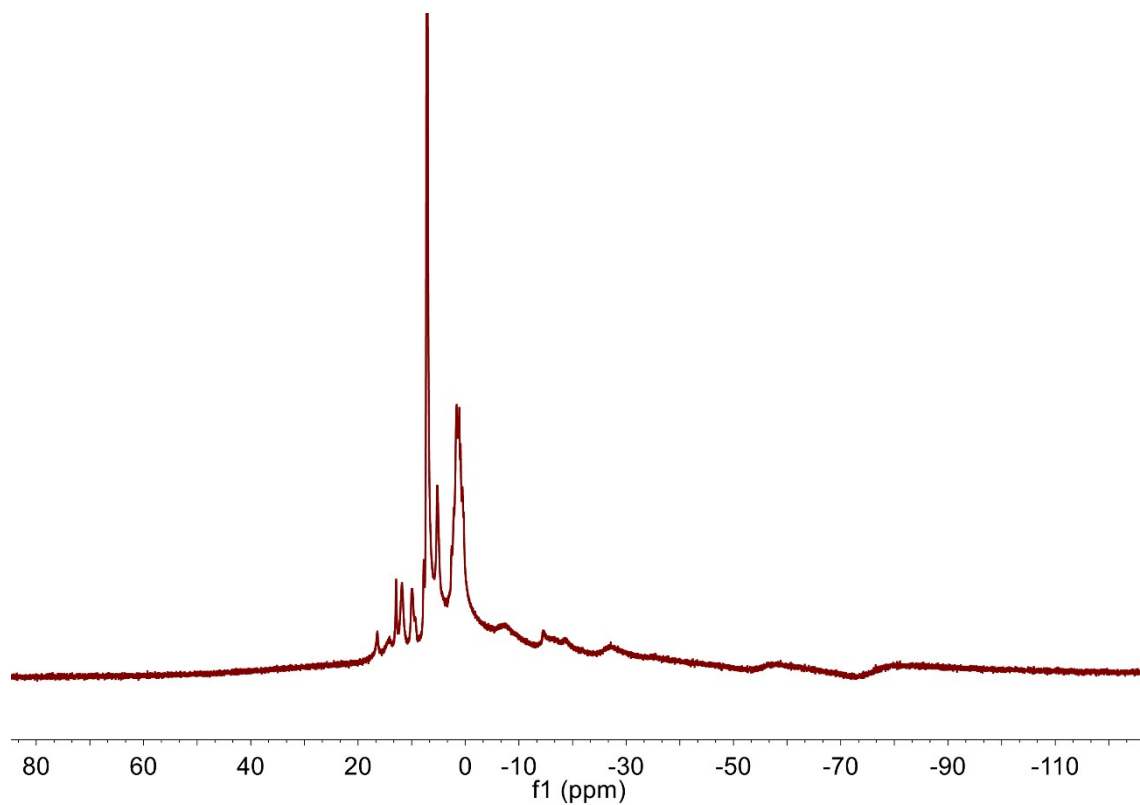


**Figure S28** <sup>1</sup>H NMR spectrum of complex **4** (400 MHz, C<sub>6</sub>D<sub>6</sub>, 25 °C).





**Figure S29** <sup>1</sup>H NMR spectrum of complex **5** (400 MHz, C<sub>6</sub>D<sub>6</sub>, 25 °C).



**Figure S30** <sup>1</sup>H NMR spectrum of complex **6** (400 MHz, C<sub>6</sub>D<sub>6</sub>, 25 °C).