

## Supplementary data

### Synthesis, structure and biological activity of indole-imidazole complexes with ZnCl<sub>2</sub>: can coordination enhance functionality of bioactive ligands?

Karolina Babijczuk<sup>1</sup>, Beata Warżajtis<sup>2</sup>, Justyna Starzyk<sup>3</sup>, Lucyna Mrówczyńska<sup>4</sup>, Beata Jasiewicz<sup>1\*</sup> and Urszula Rychlewska<sup>2\*</sup>

<sup>1</sup>Department of Bioactive Products, Faculty of Chemistry, Adam Mickiewicz University, Uniwersytetu Poznańskiego 8, 61-614 Poznań, Poland,

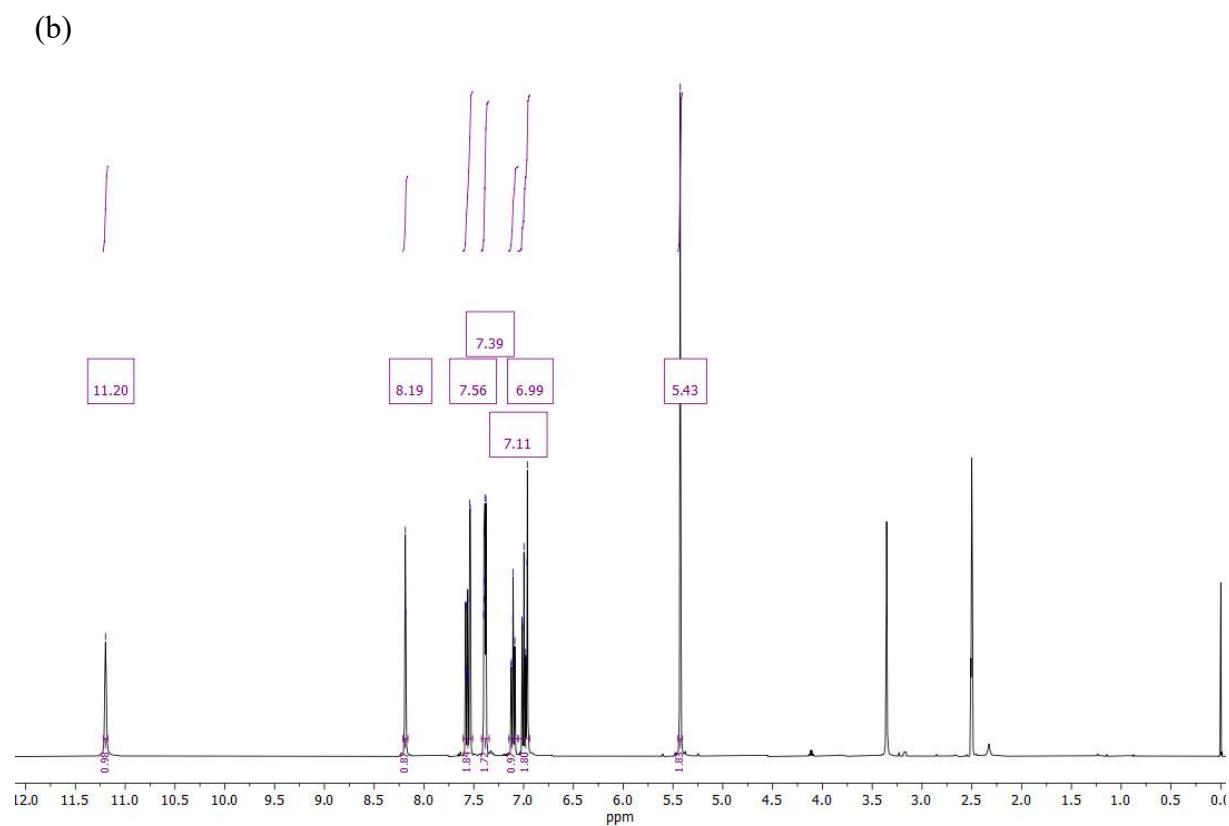
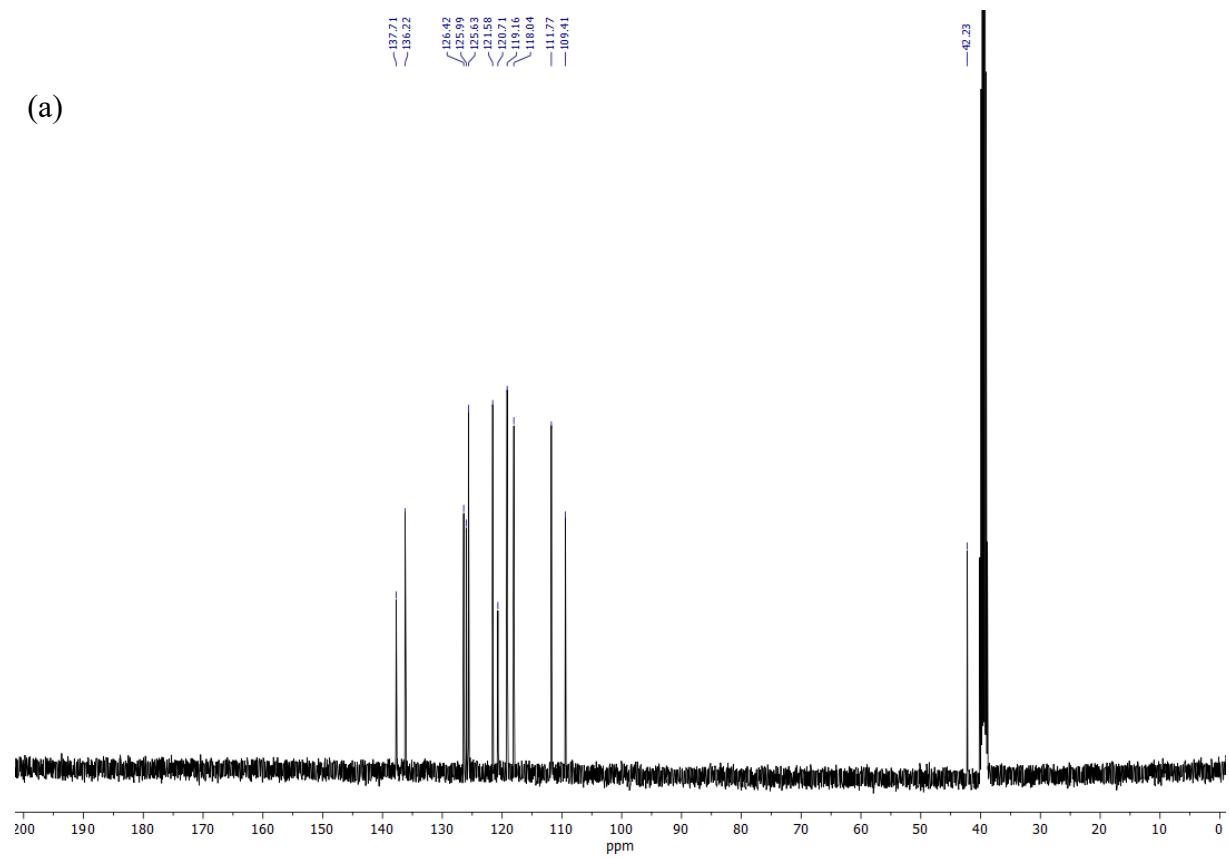
<sup>2</sup>Department of Crystallography, Faculty of Chemistry, Adam Mickiewicz University, Uniwersytetu Poznańskiego 8, 61-614 Poznań, Poland,

<sup>3</sup>Department of Soil Science and Microbiology, Faculty of Agronomy, Horticulture, and Bioengineering, University of Life Science, Szydłowska 50, 60-656 Poznań, Poland,

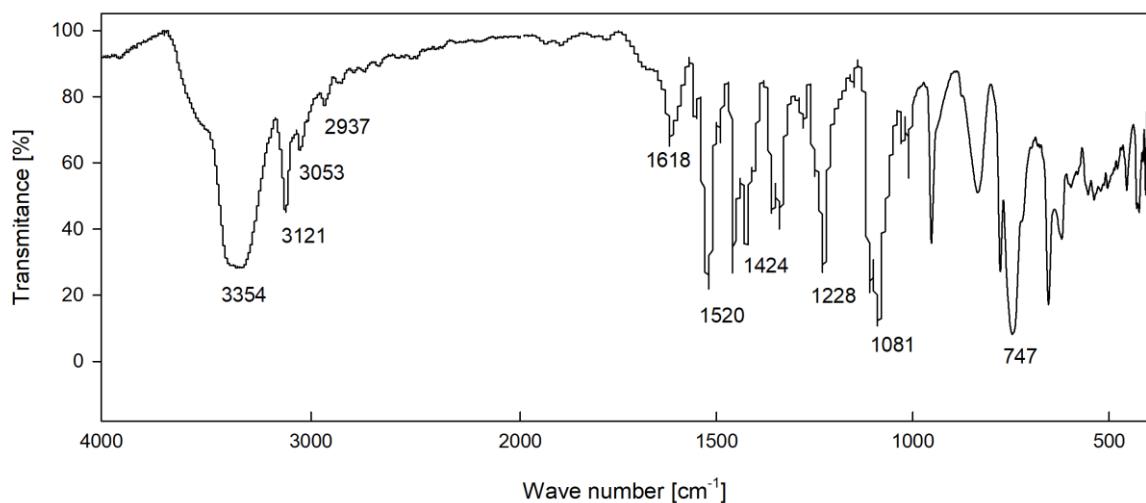
<sup>4</sup>Department of Cell Biology, Faculty of Biology, Adam Mickiewicz University, Uniwersytetu Poznańskiego 6, 61-614 Poznań, Poland,

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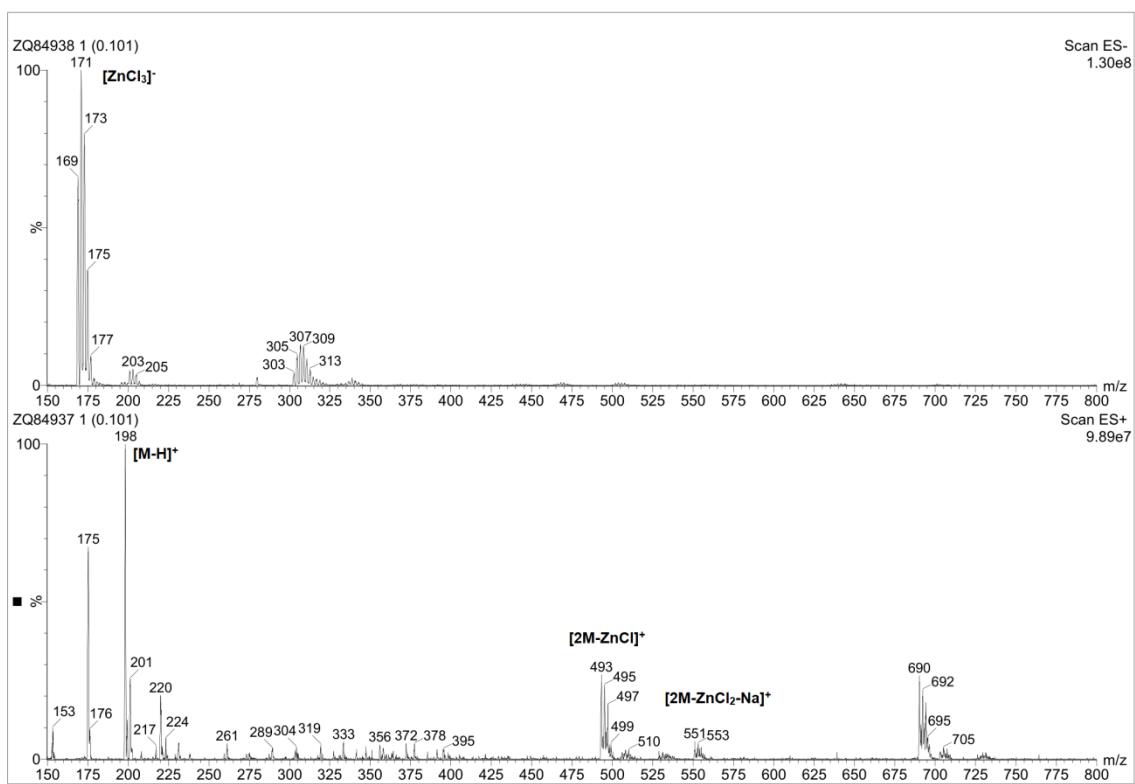
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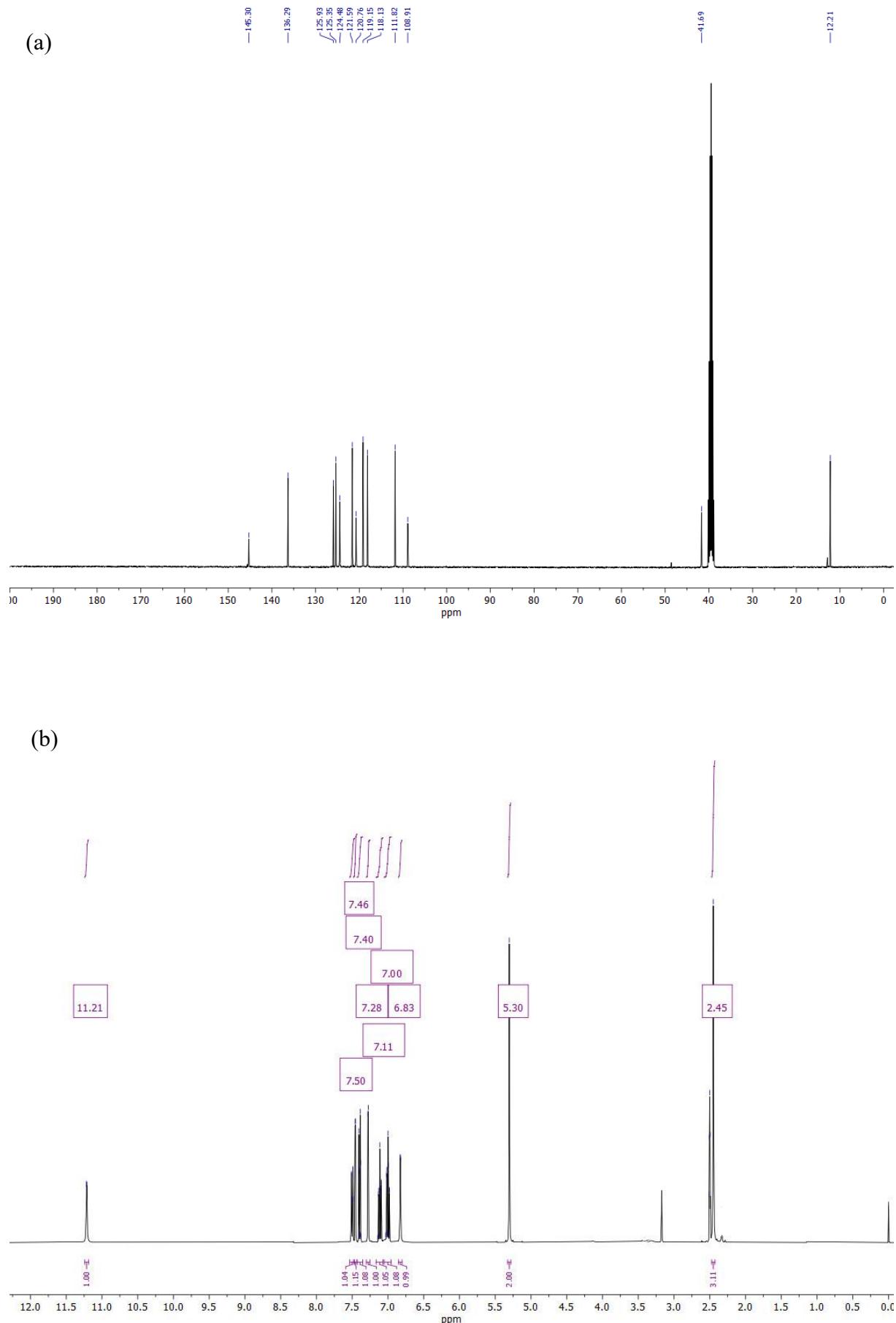
**Figure S1 (a)** <sup>13</sup>C NMR spectrum of complex **1** **(b)** <sup>1</sup>H NMR spectrum of complex **1**



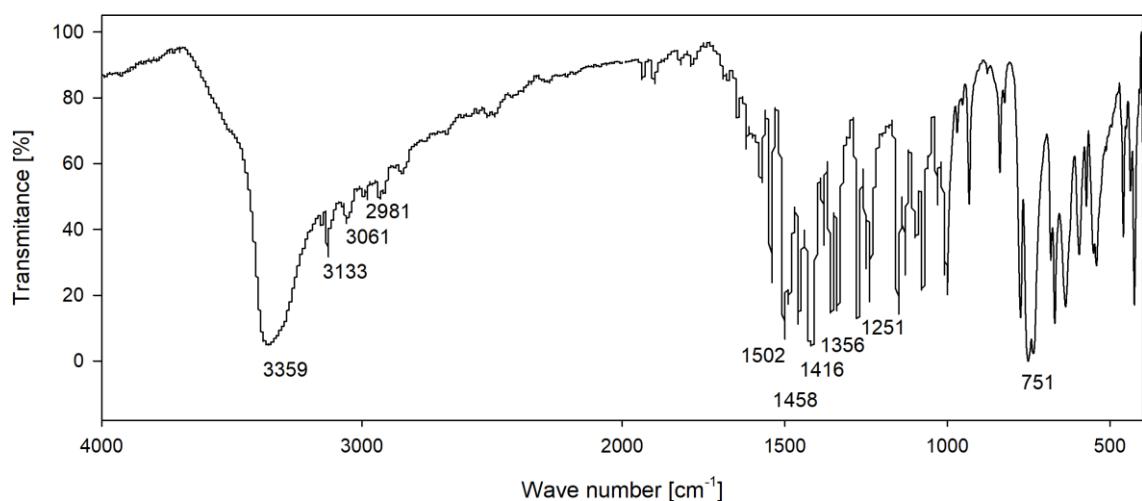
**Figure S2.** IR spectrum of complex **1**



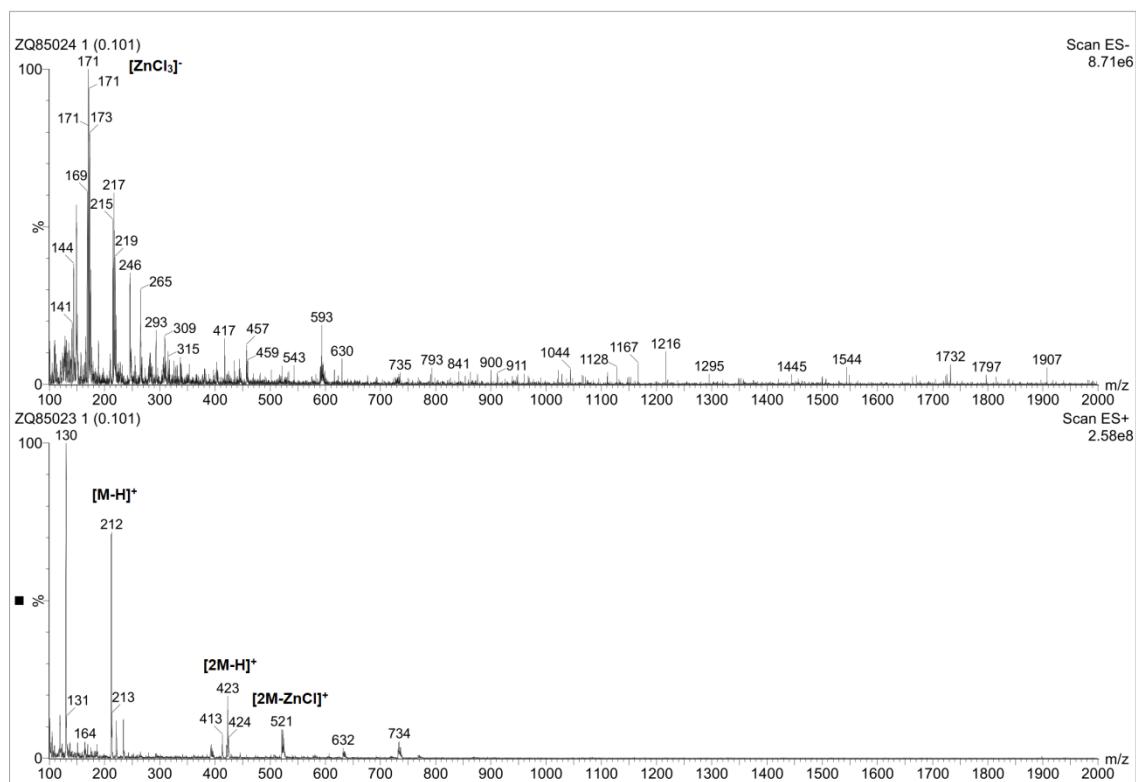
**Figure S3.** ESI-MS spectrum of complex **1**



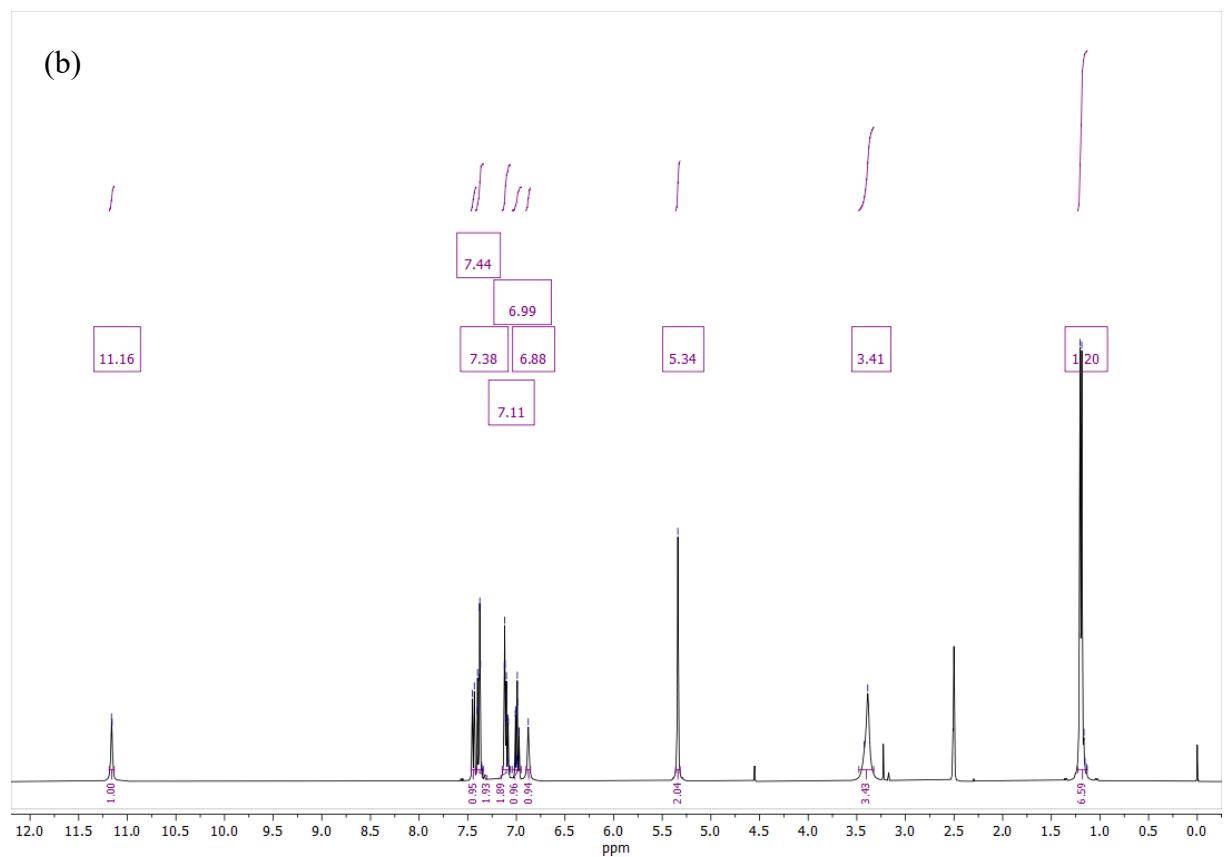
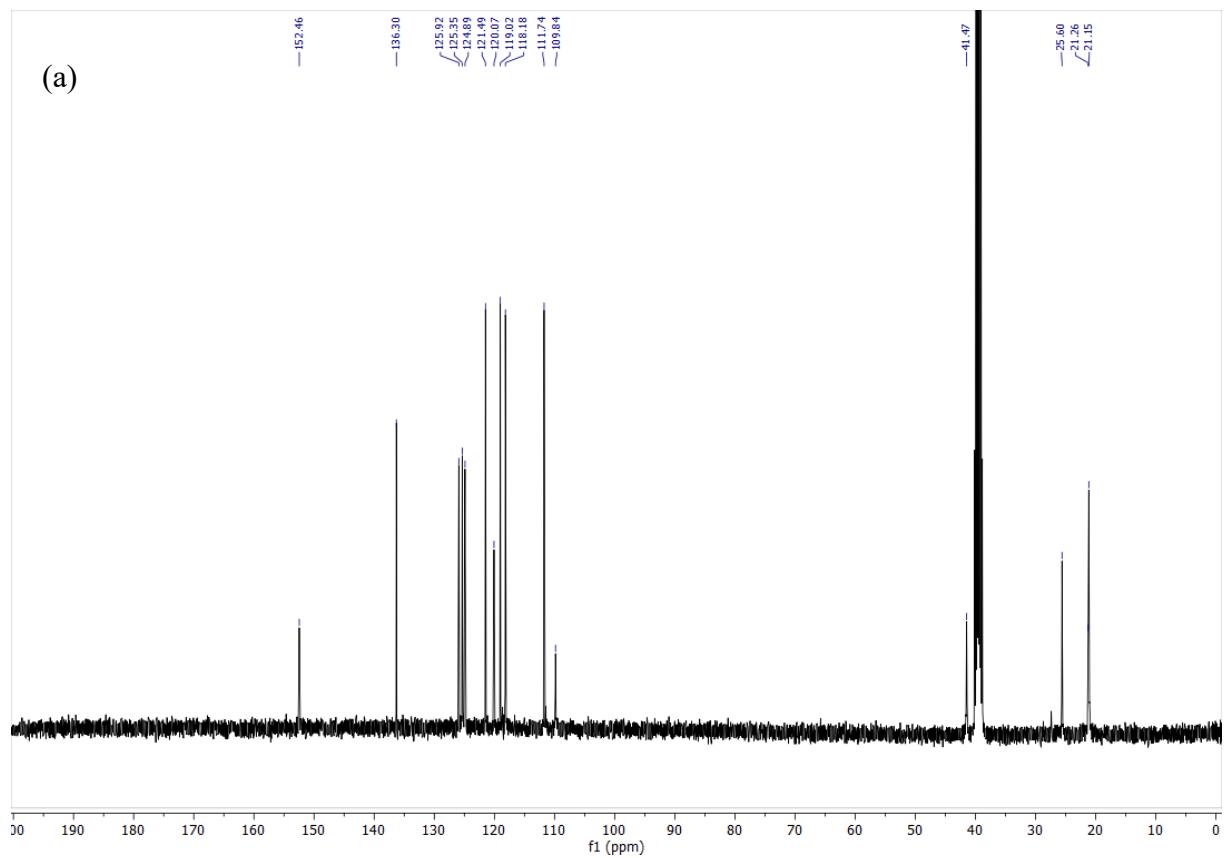
**Figure S4 (a)**  $^{13}\text{C}$  NMR spectrum of complex **2** **(b)**  $^1\text{H}$  NMR spectrum of complex **2**



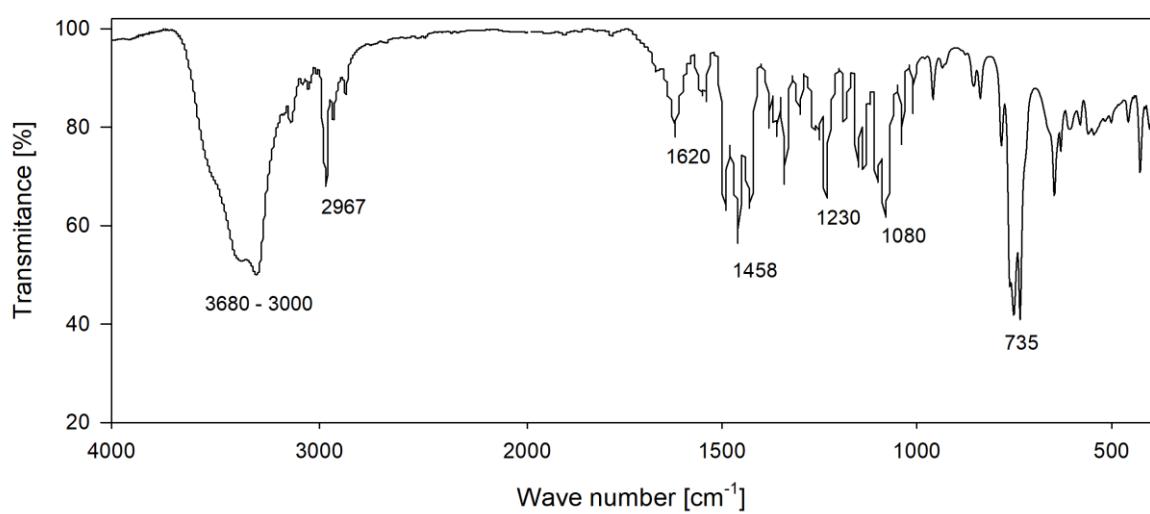
**Figure S5.** IR spectrum of complex 2



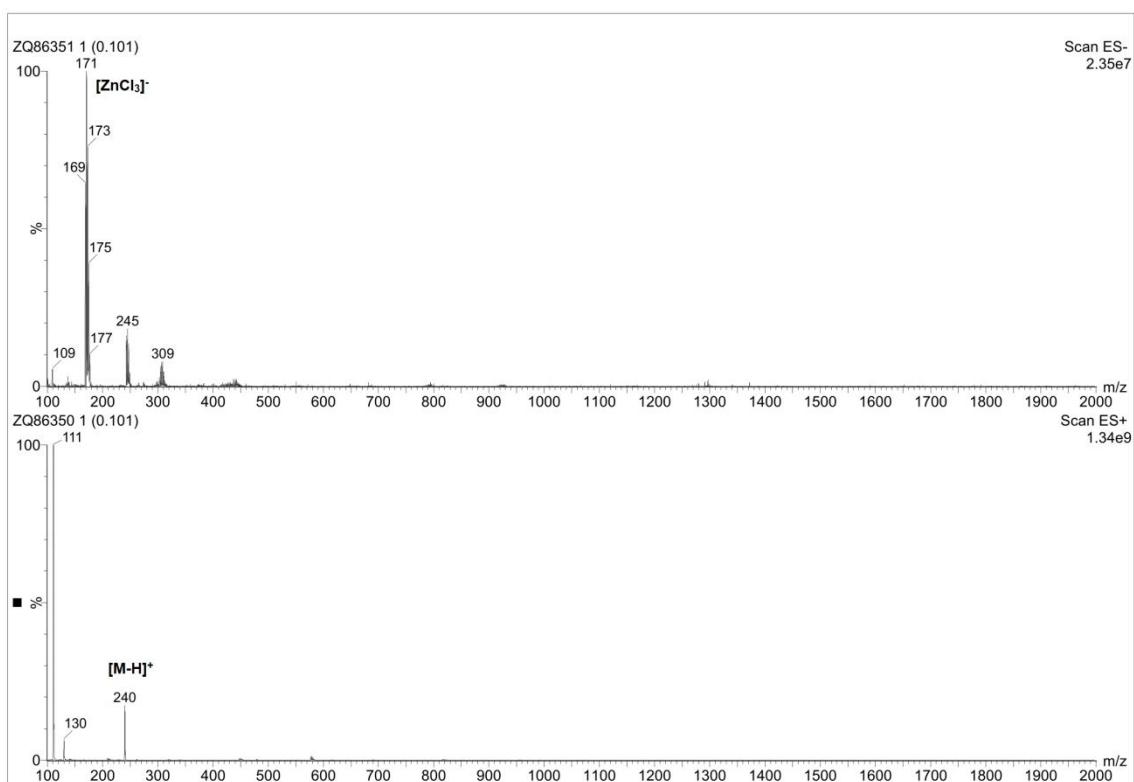
**Figure S6.** ESI-MS spectrum of complex 2



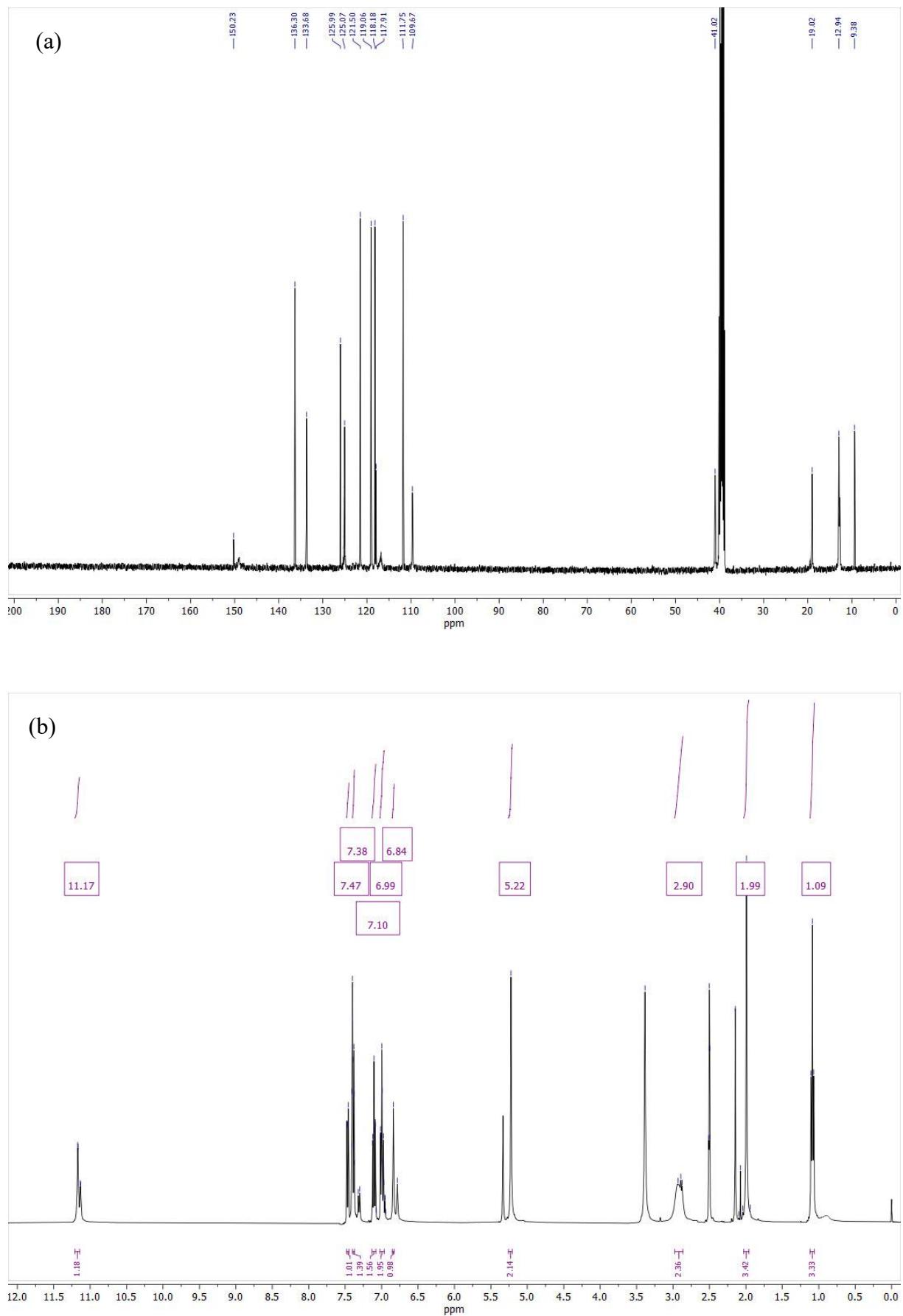
**Figure S7 (a)** <sup>13</sup>C NMR spectrum of complex 3 **(b)** <sup>1</sup>H NMR spectrum of complex 3



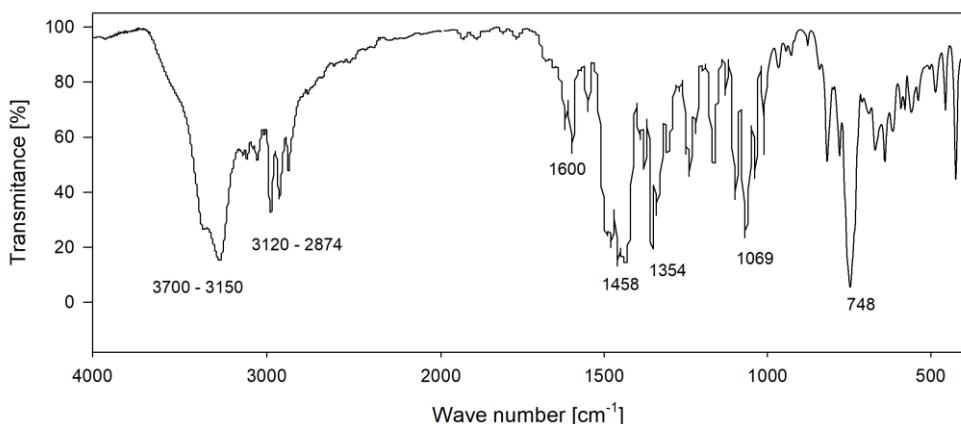
**Figure S8.** IR spectrum of complex 3



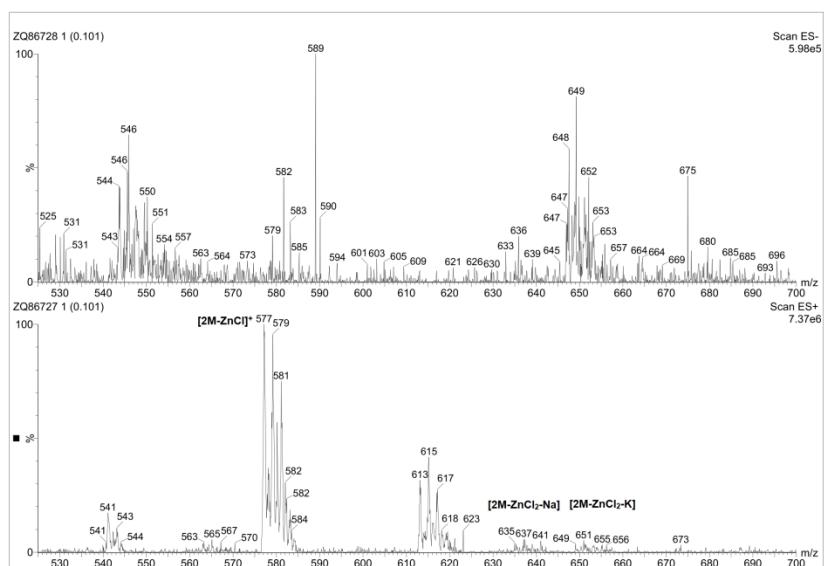
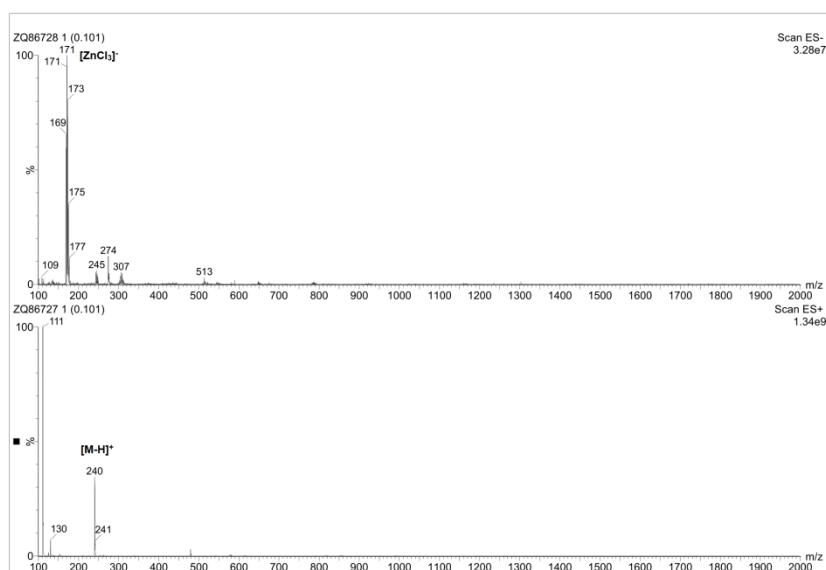
**Figure S9.** ESI-MS spectrum of complex 3



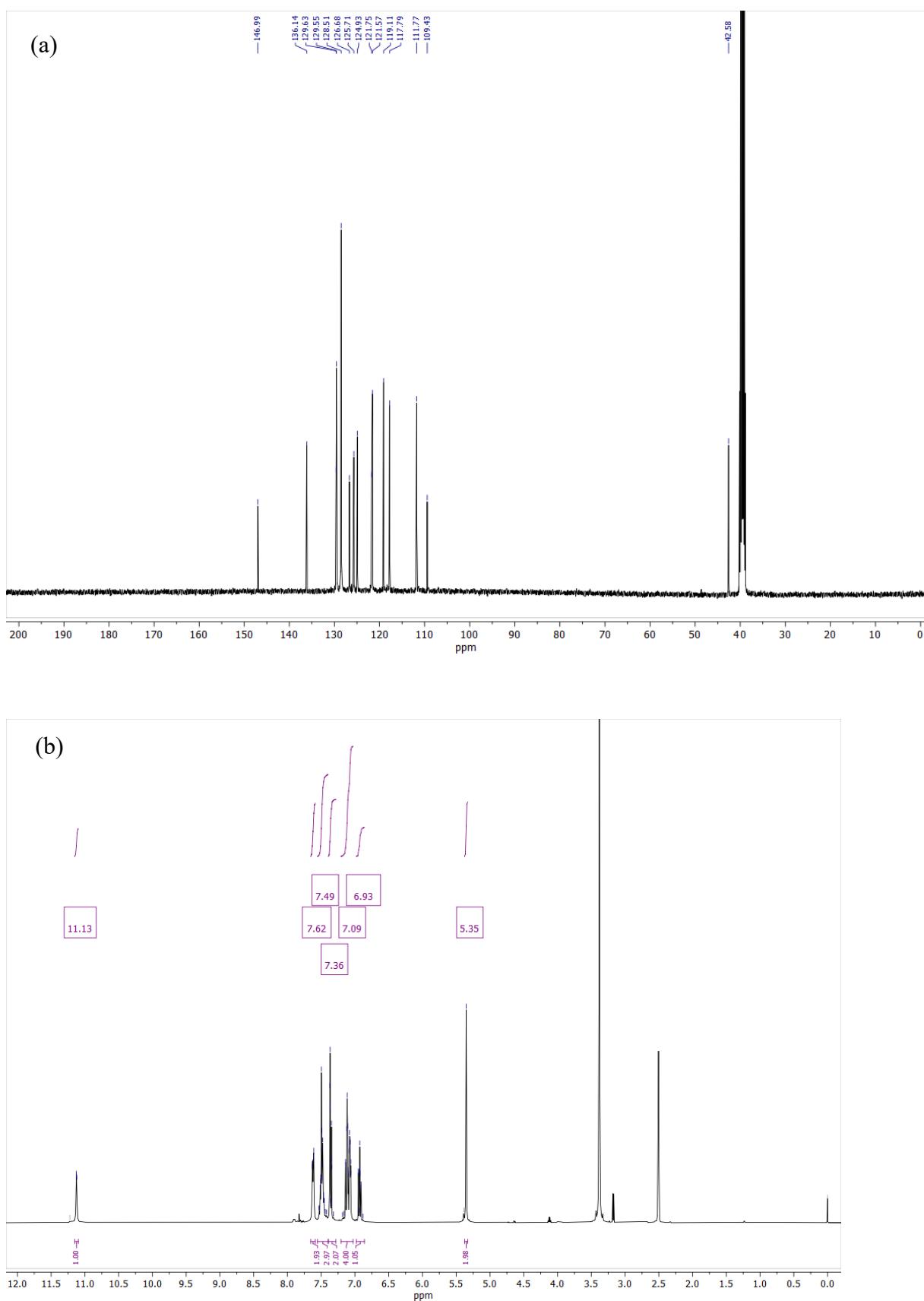
**Figure S10 (a)**  $^{13}\text{C}$  NMR spectrum of complex **4** **(b)**  $^1\text{H}$  NMR spectrum of complex **4**



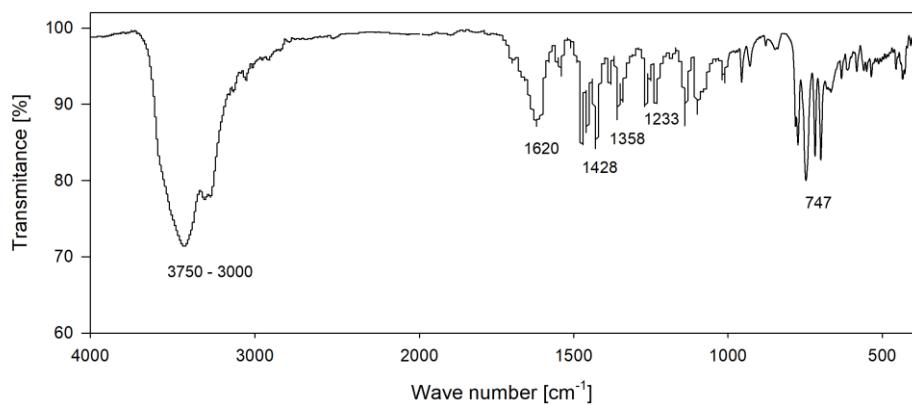
**Figure S11.** IR spectrum of complex 4



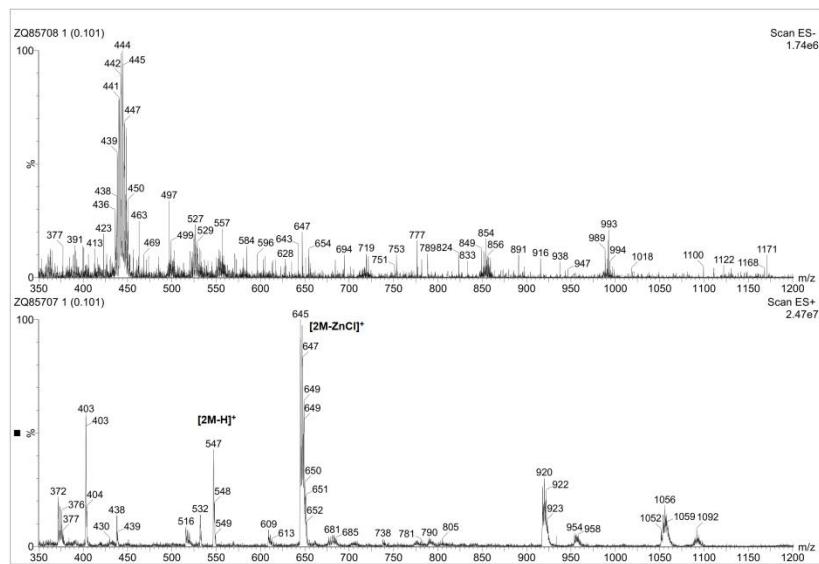
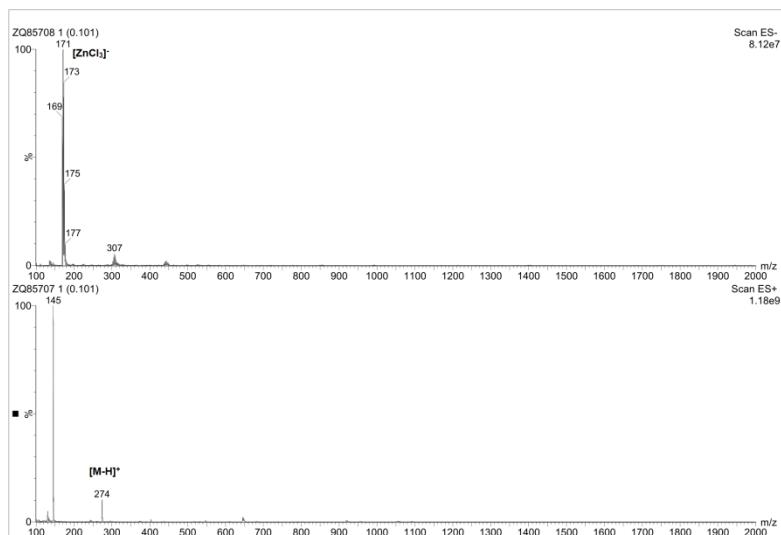
**Figure S12.** ESI-MS spectra of complex 4



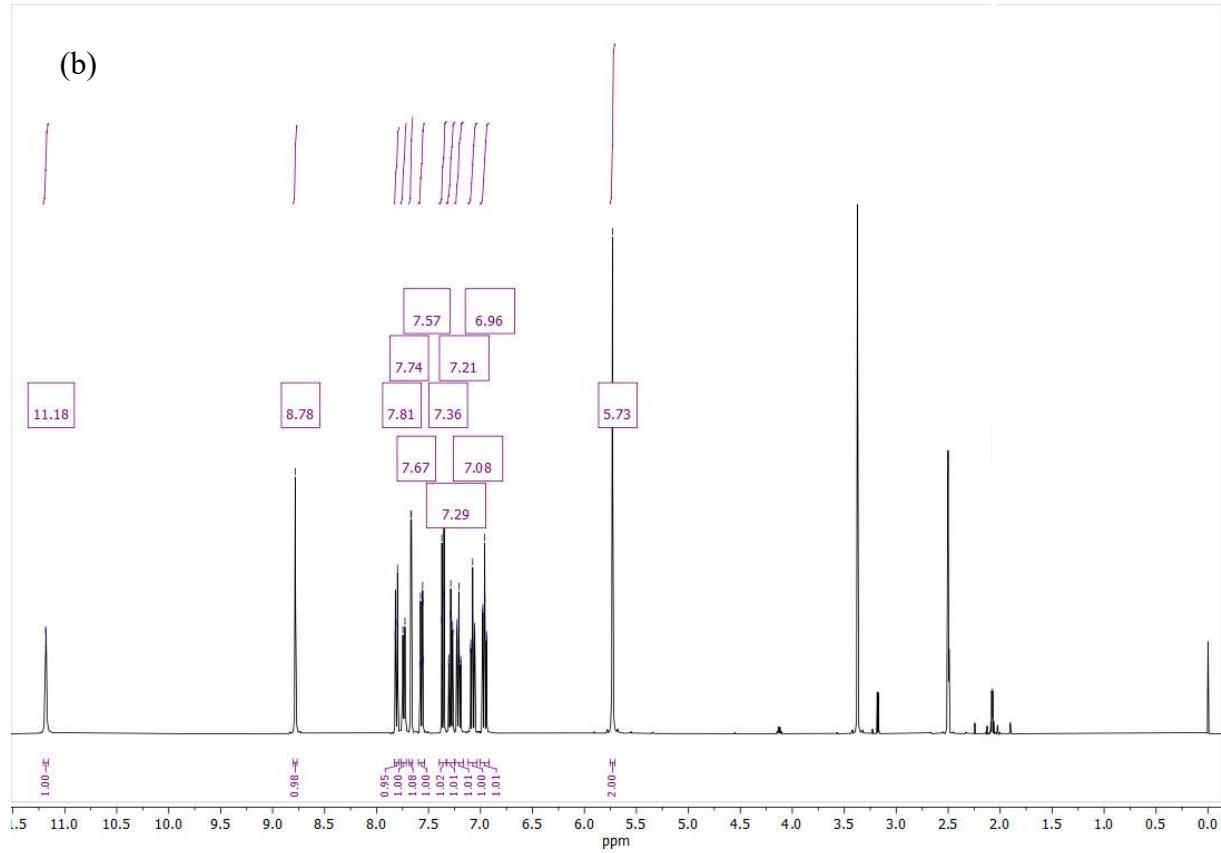
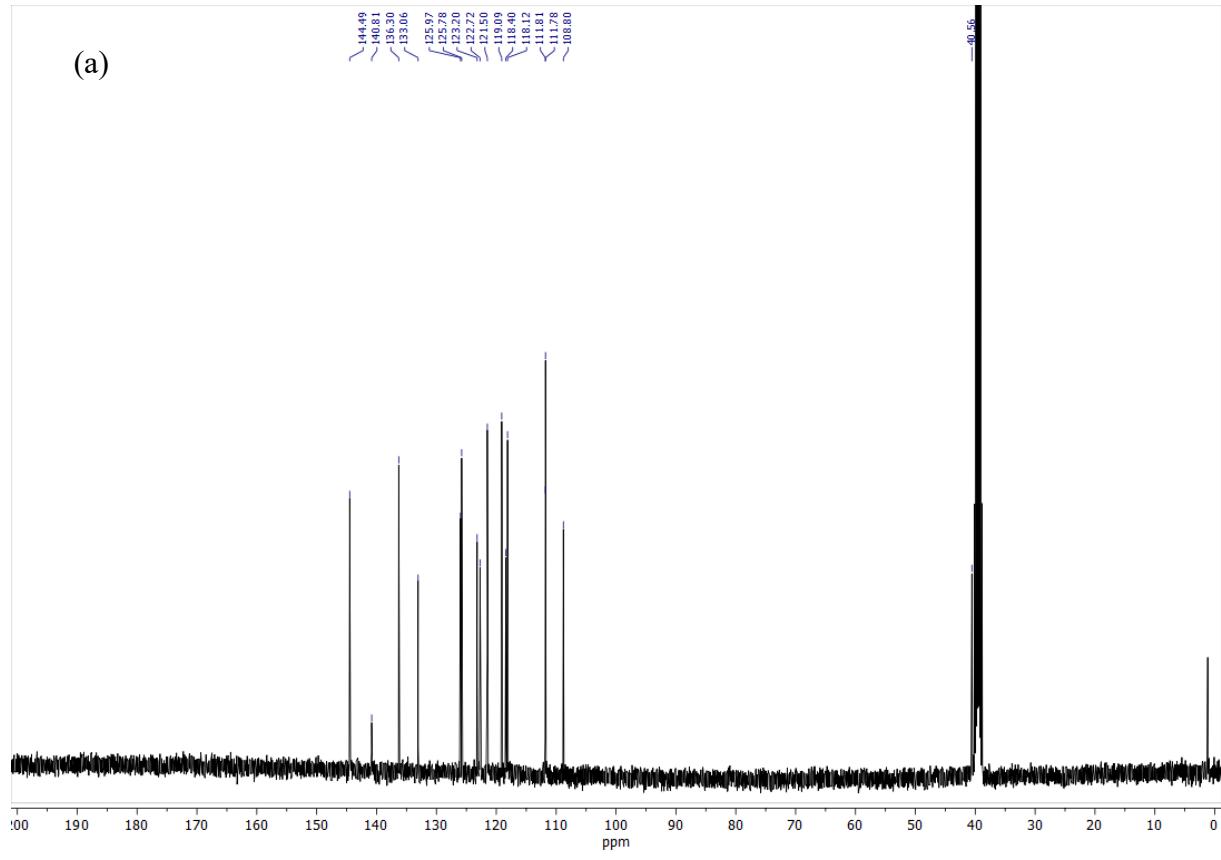
**Figure S13 (a)**  $^{13}\text{C}$  NMR spectrum of complex **5** **(b)**  $^1\text{H}$  NMR spectrum of complex **5**



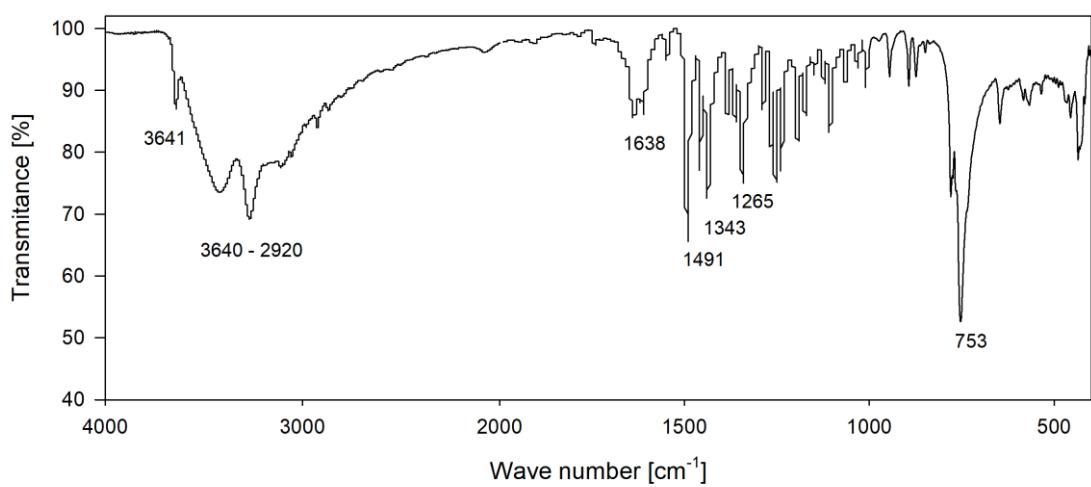
**Figure S14.** IR spectrum of complex 5



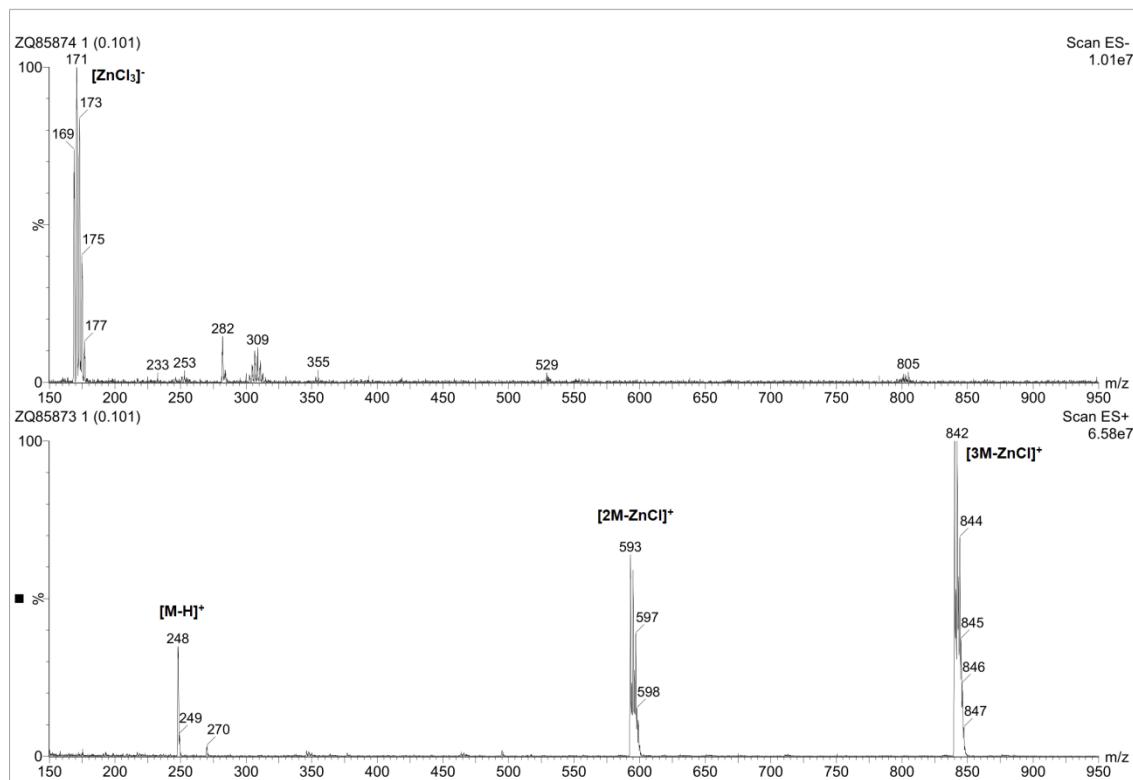
**Figure S15.** ESI-MS spectra of complex 5



**Figure S16 (a)**  $^{13}\text{C}$  NMR spectrum of complex **6** **(b)**  $^1\text{H}$  NMR spectrum of complex **6**



**Figure S17.** IR spectrum of complex 6



**Figure S18.** ESI-MS spectrum of complex 6

**Table S1.** Selected bond lengths ( $\text{\AA}$ ) and valence angles ( $^\circ$ ) for complexes **1-5**.

	<b>1</b>	<b>2</b>	<b>3</b>	<b>4</b>	<b>5</b>
Zn1—N3			2.020 (3)		2.000 (2)
Zn1—N23	2.007 (3)	2.0140 (19)	2.020 (3)	2.022 (4)	2.005 (3)
Zn1—Cl1			2.2257 (14)		2.2543 (12)
Zn1—Cl2	2.2458 (9)	2.2607 (7)	2.2348 (14)	2.2594 (15)	2.2508 (12)
N3—Zn1— N3 <sup>i</sup> (N23)	105.83 (14)	110.53 (11)	102.68 (12)	108.9 (2)	112.56 (11)
N3—Zn1—Cl1	111.16 (8)	112.31 (6)	110.05 (10)	106.37(11)	109.38 (9)
N23—Zn1—Cl2			110.27 (10)		110.49 (9)
N3—Zn1— Cl1 <sup>i</sup> (Cl2)	109.38 (8)	107.41 (6)	108.97 (11) 109.01 (11)	114.62(12)	109.69 (9) 106.88 (10)
Cl1—Zn1— Cl <sup>i</sup> (Cl2)	109.89 (5)	106.87 (4)	115.13 (6)	106.19 (10)	107.68 (5)

Symmetry code(s): (i)  $-x+1, -y+1, z$  (for complexes **1** and **2**);  $-x+1, y, -z+3/2$  (for complex 4).