

## Supporting Information

# Polymer-Supported Oxidovanadium(IV) Complexes and Their Catalytic Applications in One-Pot Multicomponent Reactions Producing Biologically Active 2,4,5-Trisubstituted-1*H*-imidazoles

Mannar R. Maurya <sup>1,\*</sup>, Monojit Nandi <sup>1</sup>, Akhil Patter <sup>2</sup>, Fernando Avecilla <sup>2</sup> and Kaushik Ghosh <sup>1</sup>

<sup>1</sup> Department of Chemistry, Indian Institute of Technology Roorkee, Roorkee 247667, India

<sup>2</sup> Grupo NanoToxGen, Centro Interdisciplinar de Química y Biología (CICA), Departamento de Química, Facultade de Ciencias, Campus de A Coruña, Universidade da Coruña, 15071 A Coruña, Spain

\* Correspondence: m.maurya@cy.iitr.ac.in

**Table S1.** Selected bond lengths [Å] and angles [°] for the for the HL<sub>1</sub> (**I**).

Bond lengths		Bond angles	
C(1)–N(1)	1.285(2)	N(2)–N(1)–C(1)	121.39(15)
N(1)–N(2)	1.361(2)	C(8)–N(2)–N(1)	117.45(14)
C(8)–N(2)	1.405(2)	C(14)–N(2)–N(1)	120.85(14)
C(14)–N(2)	1.447(2)	C(14)–N(2)–C(8)	121.67(15)

**Table S2.** Selected bond lengths [Å] and angles [°] for complex **1**.

Bond lengths		Bond angles	
V(1)–N(1)	2.1042(12)	O(1)–V(1)–N(1)	95.70(6)
V(1)–N(3)	2.0995(13)	O(2)–V(1)–N(1)	88.83(5)
V(1)–O(1)	1.6002(15)	O(2)–V(1)–O(1)	99.35(8)
V(1)–O(2)	1.9553(13)	N(3)–V(1)–N(1)	87.75(5)

V(1)–O(3A)	2.1303(14)	N(3)–V(1)–O(1)	91.09(6)
V(1)–O(4A)	1.9997(13)	N(3)–V(1)–O(2)	169.29(7)
		O(3A)–V(1)–N(1)	85.01(5)
		O(3A)–V(1)–O(1)	173.12(6)
		O(3A)–V(1)–O(2)	87.51(6)
		O(3A)–V(1)–N(3)	82.09(5)
		O(4A)–V(1)–N(1)	168.01(7)
		O(4A)–V(1)–O(1)	96.28(8)
		O(4A)–V(1)–O(2)	88.74(6)
		O(4A)–V(1)–N(3)	92.51(6)
		O(4A)–V(1)–O(3A)	83.15(7)

---

### Analytical and spectral data of ligands

**Data for HL<sub>1</sub> (I):** Yield 1.14 g (67.0 %). Greyish-white powder. C<sub>21</sub>H<sub>18</sub>N<sub>4</sub>O (342.40). Calcd C, 73.6; H, 5.25; N, 16.35. Found C, 73.54; H, 5.21; N, 16.27%. <sup>1</sup>H NMR (500 MHz, DMSO-d<sub>6</sub>, δ/ppm): 12.38 (s, 1H, N–H), 10.46 (s, 1H, O–H), 8.00 (s, 1H, HC=N–), 7.54 – 7.50 (m, 2H, aromatic, 7.43–7.39 (m, 2H, aromatic, 7.37 – 7.31 (m, 4H, aromatic, 7.11 (m, 3H, aromatic, 6.93 (tt, 1H, *J* = 6.9, 1.3 Hz), 6.84 – 6.79 (m, 2H, aromatic, 5.43 (s, 2H, CH<sub>2</sub>). <sup>13</sup>C NMR (126 MHz, DMSO-d<sub>6</sub>, δ/ppm): 156.09, 150.36, 147.31, 134.29, 129.81, 128.01, 121.43, 119.91, 116.48, 115.34, 45.09, 40.03.

**Data for H<sub>2</sub>L<sub>2</sub> (II):** Yield 1.39 g (61.0 %). White powder. C<sub>29</sub>H<sub>34</sub>N<sub>4</sub>O (454.62). Calcd C, 71.39; H, 7.48; N, 12.32. Found C, 71.35; H, 7.41; N, 12.29%. <sup>1</sup>H NMR (500 MHz, DMSO-d<sub>6</sub>, δ/ppm): 12.46 (s, 1H, N–H), 11.84 (s, 1H, O–H), 8.19 (s, 1H, HC=N–), 7.56 (d, 1H, aromatic, *J* = 7.6 Hz), 7.46 (d, 1H, aromatic, *J* = 8.0 Hz), 7.40 (m, 2H, aromatic, 7.28 (d, 2H, aromatic, *J* = 7.9 Hz), 7.20 (d, 1H, aromatic, *J* = 2.4 Hz), 7.18 (d, 1H, aromatic, *J* = 2.3 Hz), 7.15 (ddd, 2H, aromatic, *J* = 9.1, 7.5, 1.2 Hz), 6.99 (t, 1H, aromatic, *J* = 7.3 Hz), 5.54 (s, 2H, CH<sub>2</sub>), 1.43 (s, 9H, <sup>t</sup>but), 1.24 (s, 9H, <sup>t</sup>but). <sup>13</sup>C NMR (126 MHz, DMSO-d<sub>6</sub>, δ/ppm): 153.42, 150.17, 146.69, 143.79, 140.95, 140.36,

135.69, 134.90, 130.00, 125.54, 124.20, 122.59, 121.75, 119.06, 115.01, 111.94, 44.54, 35.15, 34.39, 31.86, 29.91.

### Spectral data of isolated compounds (MCR products)

**Data for 1(a):** Molecular Formula:  $C_{21}H_{16}N_2$ . Mol. Wt.= 296.37 g/mol. Solid white powder.  $^1H$  NMR (500 MHz, DMSO- $d_6$ ,  $\delta$ /ppm): 12.65 (s, 1H, N-H), Aromatic= 8.05 (dt, 2H,  $J$  = 8.2, 1.5 Hz), 7.51 (dt, 2H,  $J$  = 8.1, 1.6 Hz), 7.48 – 7.39 (m, 6H), 7.36 – 7.32 (m, 2H), 7.29 – 7.24 (m, 2H), 7.21 – 7.16 (m, 1H).  $^{13}C$  NMR (126 MHz, DMSO- $d_6$ ,  $\delta$ /ppm): 195.37, 146.03, 137.63, 136.09, 135.70, 131.62, 130.88, 130.14, 130.05, 129.22, 129.19, 128.99, 128.78, 128.72, 128.31, 127.60, 127.04, 125.72.

**Data for 1(b):** Molecular Formula:  $C_{21}H_{15}ClN_2$ . Mol. Wt.= 330.82 g/mol. Solid white powder.  $^1H$  NMR (500 MHz, DMSO- $d_6$ ,  $\delta$ /ppm): 12.79 (s, 1H, N-H), Aromatic= 8.13 – 8.09 (m, 2H), 7.57 – 7.54 (m, 4H), 7.53 – 7.49 (m, 2H), 7.45 (t, 2H,  $J$  = 7.5 Hz), 7.39 (t, 1H,  $J$  = 7.3 Hz), 7.31 (t, 2H,  $J$  = 7.5 Hz), 7.23 (t, 1H,  $J$  = 7.3 Hz).  $^{13}C$  NMR (126 MHz, DMSO- $d_6$ ,  $\delta$ /ppm): 195.36, 144.95, 137.83, 136.09, 135.52, 133.28, 131.44, 130.14, 130.05, 129.72, 129.31, 129.21, 129.10, 128.96, 128.74, 128.41, 127.60, 127.37, 127.15.

**Data for 1(c):** Molecular Formula:  $C_{21}H_{15}BrN_2$ . Mol. Wt.= 375.27 g/mol. Solid white powder.  $^1H$  NMR (500 MHz, DMSO- $d_6$ ,  $\delta$ /ppm): 12.79 (s, 1H, N-H), Aromatic= 8.06 – 8.02 (m), 7.71 – 7.67 (m, 2H), 7.53 (br., 4H), 7.48 – 7.36 (br., 3H), 7.31 (br., 2H), 7.24 (br., 1H).  $^{13}C$  NMR (126 MHz, DMSO- $d_6$ ,  $\delta$ /ppm): 194.86, 144.45, 137.32, 135.59, 135.02, 132.78, 130.94, 129.63, 129.54, 129.22, 128.81, 128.71, 128.59, 128.45, 128.24, 127.91, 127.10, 126.87, 126.64.

**Data for 1(d):** Molecular Formula:  $C_{21}H_{15}N_3O_2$ . Mol. Wt.= 341.37 g/mol. Solid orange powder.  $^1H$  NMR (500 MHz, DMSO- $d_6$ ,  $\delta$ /ppm): 13.14 (s, N-H), Aromatic= 8.34 (q, 4H,  $J$  = 2.2 Hz), 7.84–7.80 (m, 2H), 7.58 – 7.55 (m, 2H), 7.54 – 7.52 (m, 2H), 7.49 – 7.46 (m, 2H), 7.33 (t, 2H,  $J$  = 7.5 Hz).  $^{13}C$  NMR (126 MHz, DMSO- $d_6$ ,  $\delta$ /ppm): 195.35, 147.06, 143.92, 138.99, 136.63, 135.14, 131.04, 130.60, 130.13, 130.04, 129.27, 129.06, 128.81, 127.67, 126.26, 127.79.

**Data for 1(e):** Molecular Formula:  $C_{22}H_{18}N_2O$ . Mol. Wt.= 326.40 g/mol. Solid white powder.  $^1H$  NMR (500 MHz, DMSO- $d_6$ ,  $\delta$ /ppm): 12.52 (s, N-H), Aromatic= 8.05 – 8.01 (m, 2H), 7.56 (d, 2H,  $J$  = 7.1 Hz), 7.50 (d, 2H,  $J$  = 7.1 Hz), 7.44 (t, 2H,  $J$  = 7.6 Hz), 7.36 (t, 1H,  $J$  = 7.3 Hz), 7.30 (t, 2H,  $J$  = 7.5 Hz), 7.22 (t, 1H,  $J$  = 7.3 Hz), 7.08 – 7.03 (m, 2H), 3.82 (s, 1H, -OMe).  $^{13}C$  NMR

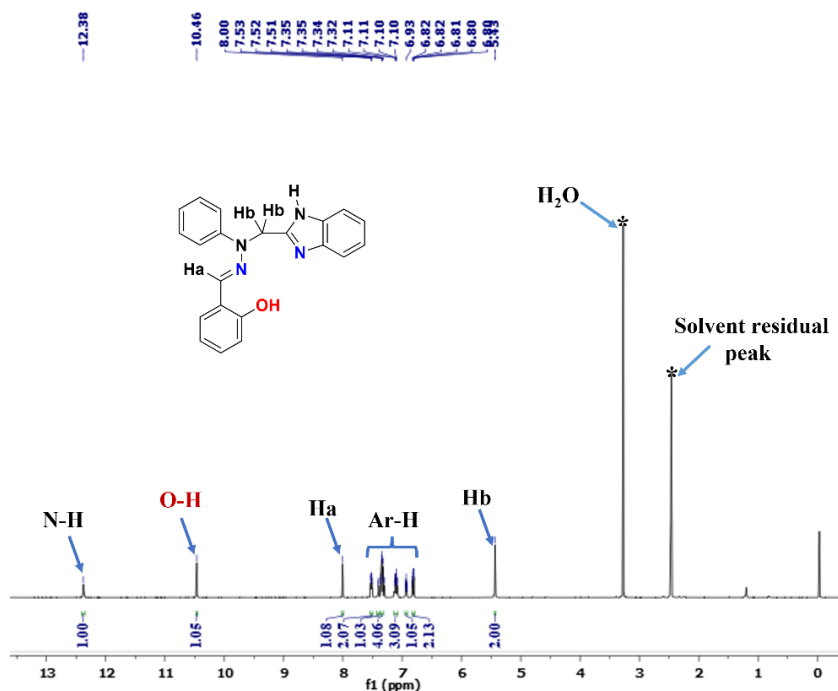
(126 MHz, DMSO-d<sub>6</sub>, δ/ppm): 195.36, 159.95, 146.16, 137.29, 129.16, 128.89, 128.68, 128.18, 127.58, 127.23, 123.67, 114.62, 55.73.

**Data for 1(f):** Molecular Formula: C<sub>22</sub>H<sub>18</sub>N<sub>2</sub>. Mol. Wt.= 310.40 g/mol. Solid white powder. <sup>1</sup>H NMR (500 MHz, DMSO-d<sub>6</sub>, δ/ppm): 12.59 (s, N-H), 8.00 – 7.97 (m, 2H), 7.55 (dt, 2H, *J* = 8.1, 1.6 Hz), 7.50 (dt, 2H, *J* = 8.0, 1.7 Hz), 7.44 (t, 2H, *J* = 7.5 Hz), 7.37 (t, 1H, *J* = 7.3 Hz), 7.32 – 7.27 (m, 4H), 7.22 (t, 1H, *J* = 7.3 Hz), 2.35 (s, 3H, -Me). <sup>13</sup>C NMR (126 MHz, DMSO-d<sub>6</sub>, δ/ppm): 195.36, 146.20, 138.20, 137.46, 136.08, 135.80, 132.78, 131.72, 130.13, 130.05, 129.77, 129.16, 128.94, 128.69, 128.46, 128.23, 128.21, 127.59, 126.98, 125.70, 21.42.

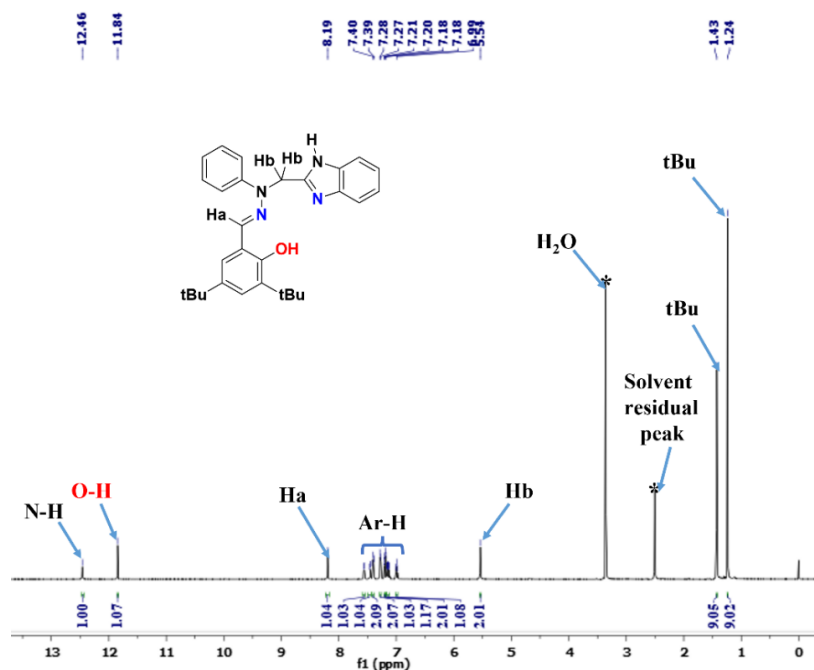
**Data for 1(g):** Molecular Formula: C<sub>21</sub>H<sub>15</sub>N<sub>3</sub>O<sub>2</sub>. Mol. Wt.= 341.37 g/mol. Solid yellow powder. <sup>1</sup>H NMR (500 MHz, DMSO-d<sub>6</sub>, δ/ppm): 12.96 (s, N-H), Aromatic= 8.00 (d, 1H, *J* = 7.8 Hz), 7.93 (d, 1H, *J* = 8.1 Hz), 7.79 (t, 1H, *J* = 7.6 Hz), 7.67 – 7.61 (m, 1H), 7.48 (dt, 6H, *J* = 21.3, 7.4 Hz), 7.39 (t, 1H, *J* = 7.3 Hz), 7.31 (t, 2H, *J* = 7.5 Hz), 7.23 (t, 1H, *J* = 7.3 Hz). <sup>13</sup>C NMR (126 MHz, DMSO-d<sub>6</sub>, δ/ppm): 148.87, 141.56, 138.06, 135.25, 132.64, 131.18, 130.30, 130.06, 129.29, 129.25, 128.82, 128.77, 128.56, 127.52, 127.27, 124.55, 123.94.

**Data for 1(h):** Molecular Formula: C<sub>36</sub>H<sub>24</sub>N<sub>4</sub>. Mol. Wt.= 514.63 g/mol. Solid yellow powder. <sup>1</sup>H NMR (500 MHz, DMSO-d<sub>6</sub>, δ/ppm): 10.02 (s, N-H, 2H), 8.29 (d, 4H, *J* = 8.3 Hz), 8.03 – 8.00 (m, 4H), 7.55 – 7.52 (m, 10H), 7.33 (m, 6H). <sup>13</sup>C NMR (126 MHz, DMSO-d<sub>6</sub>, δ/ppm): 193.09, 144.78, 135.87, 135.86, 130.66, 130.12, 130.07, 129.05, 129.02, 128.32, 125.97.

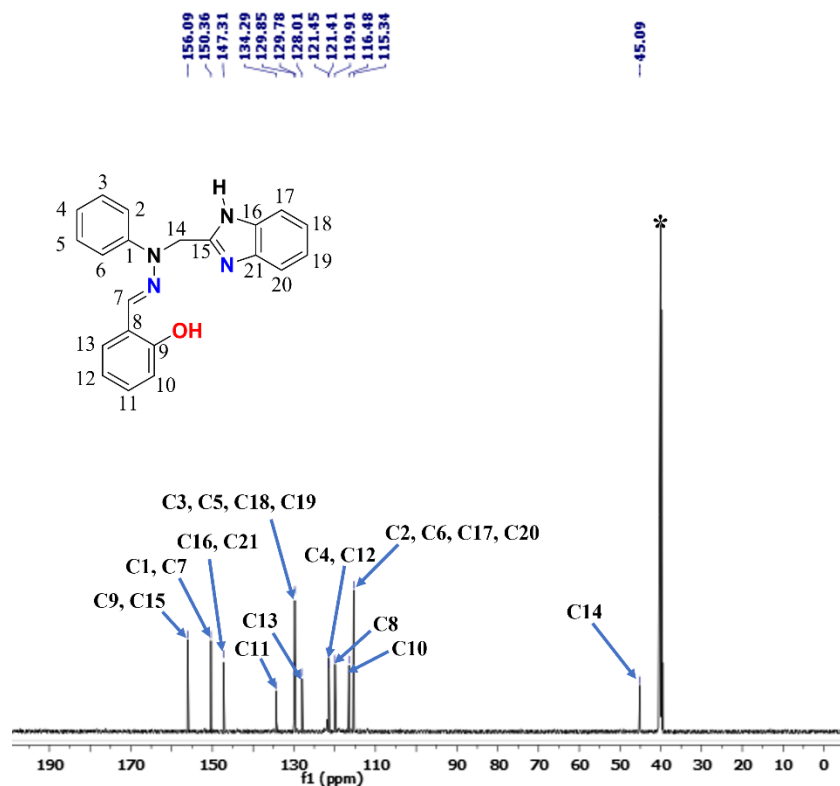
**Data for 1(i):** Molecular Formula: C<sub>15</sub>H<sub>12</sub>N<sub>2</sub>. Mol. Wt.= 220.28 g/mol. Solid white powder. <sup>1</sup>H NMR (500 MHz, DMSO-d<sub>6</sub>, δ/ppm): 12.49 (s, N-H), 7.79 (s, -N=C-H, 1H), 7.46 (d, 4H, *J* = 7.2 Hz), 7.34 (s, br, 4H), 7.27 (s, br, 2H). <sup>13</sup>C NMR (126 MHz, DMSO-d<sub>6</sub>, δ/ppm): 136.15, 128.95, 127.99, 127.39.



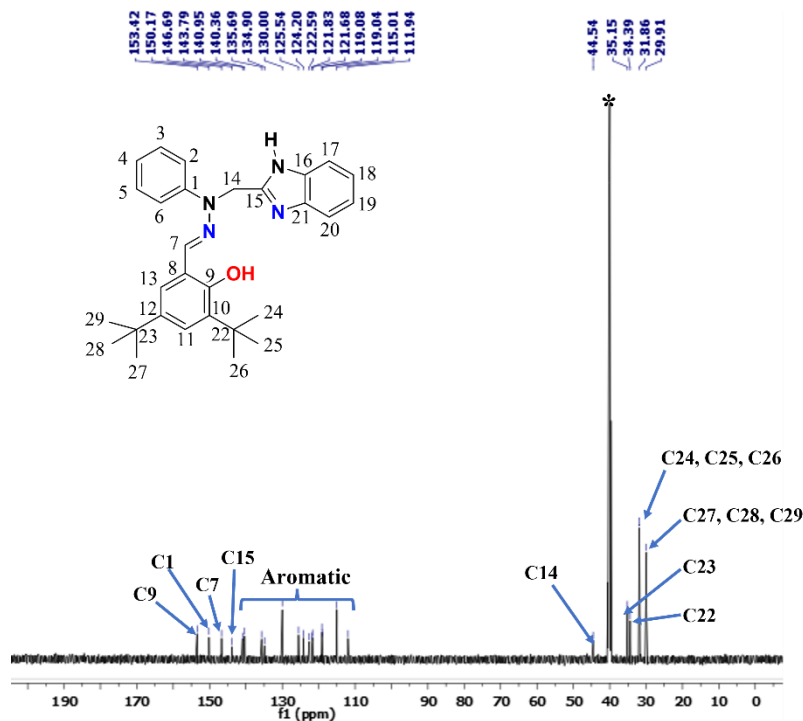
**Figure S1.** <sup>1</sup>H-NMR spectra of ligand **HL1** (**I**) recorded in DMSO-d<sub>6</sub>. \* Indicates the solvent residual peak at  $\delta = 2.5$  ppm and that of moisture at  $\delta = 3.33$  ppm.



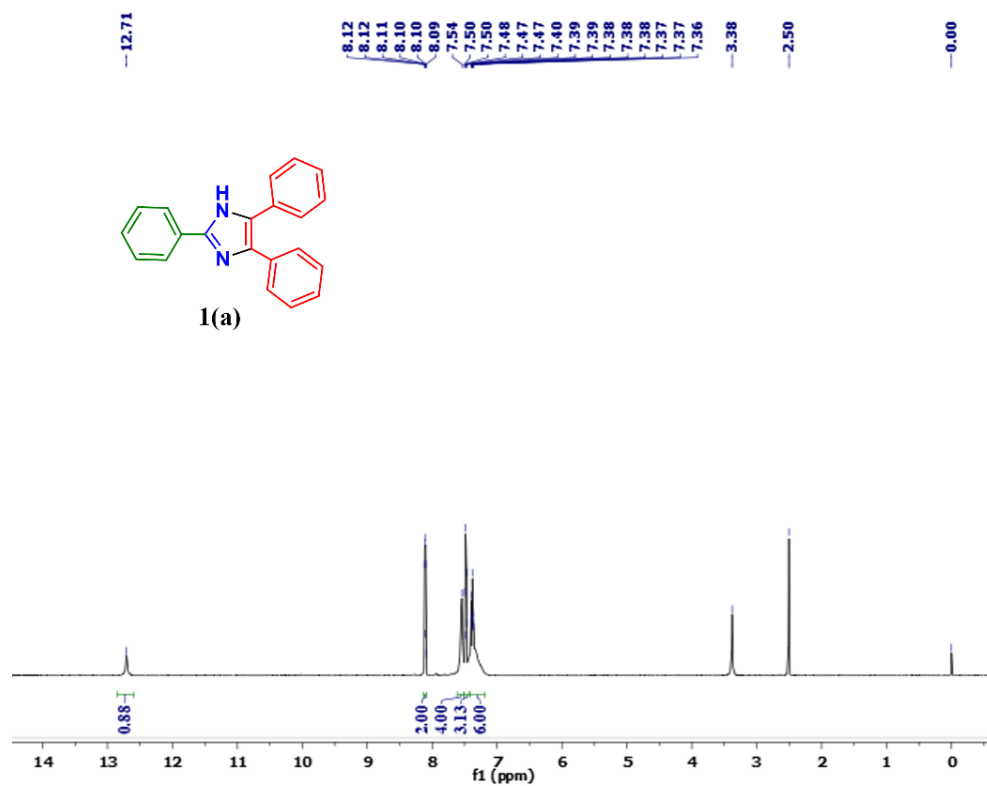
**Figure S2.** <sup>1</sup>H-NMR spectra of ligand **HL2** (**II**) recorded in DMSO-d<sub>6</sub>. \* Indicates the solvent residual peak at  $\delta = 2.5$  ppm and that of moisture at  $\delta = 3.33$  ppm.



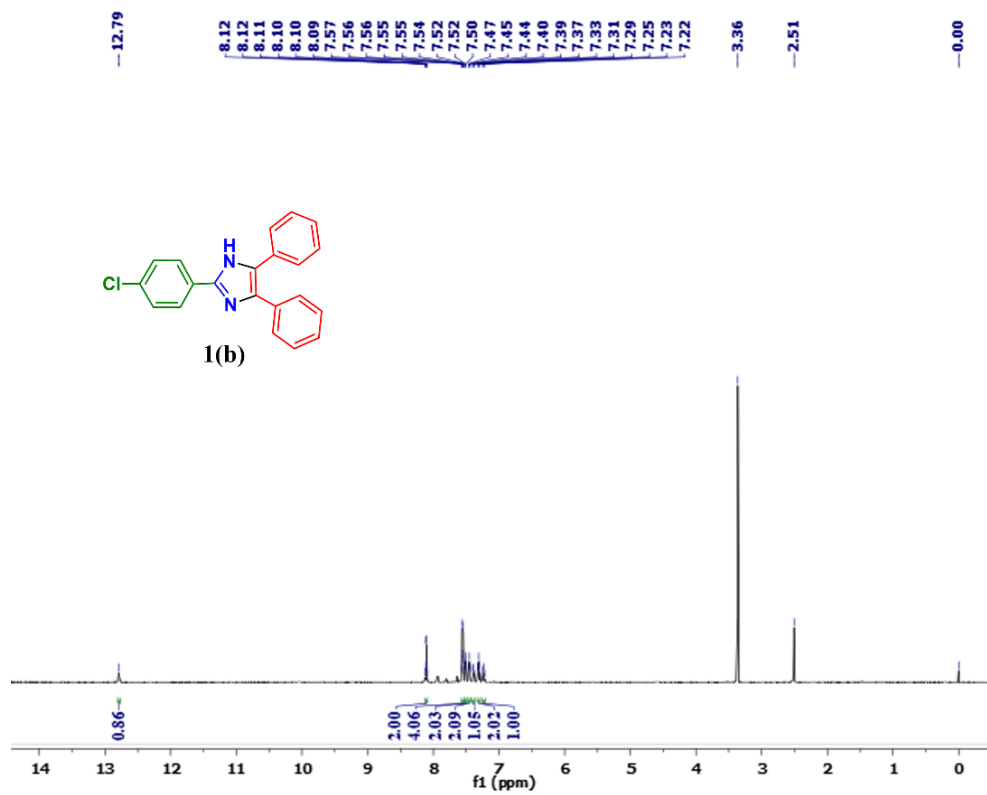
**Figure S3.**  $^{13}\text{C}$ -NMR spectra of ligand **HL1** (I) recorded in  $\text{DMSO-d}_6$ . \* Indicates the solvent residual peak at  $\delta = 40$  ppm.



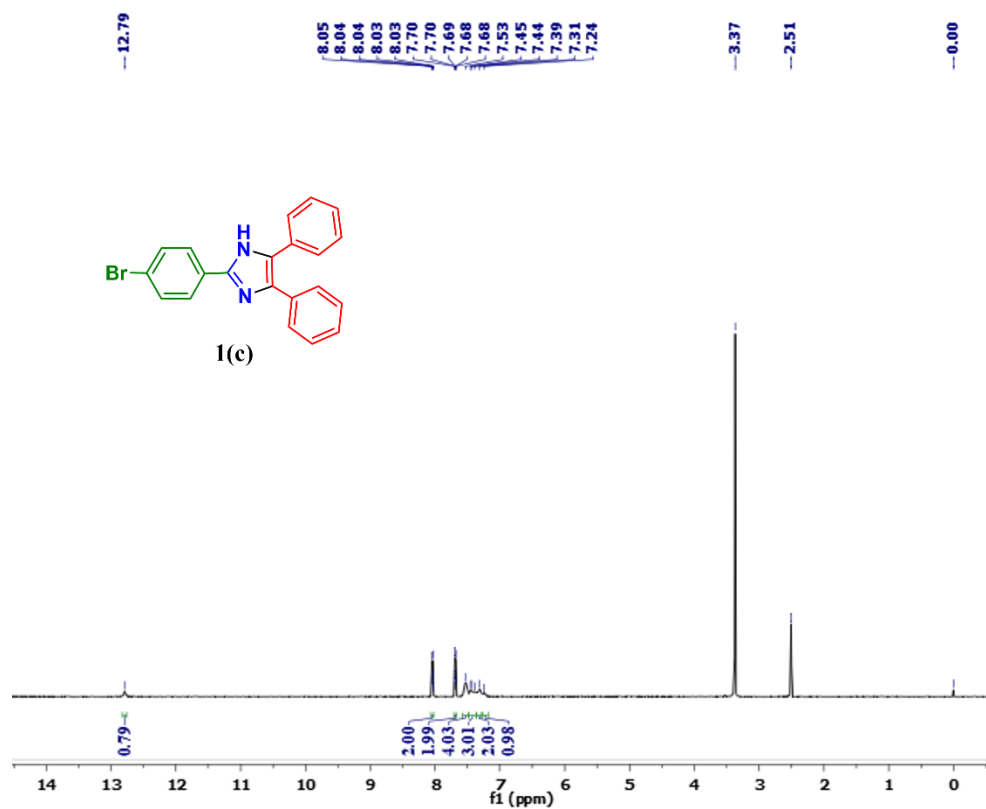
**Figure S4.**  $^{13}\text{C}$ -NMR spectra of ligand **HL2** (II) recorded in  $\text{DMSO-d}_6$ . \* Indicates the solvent residual peak at  $\delta = 40$  ppm.



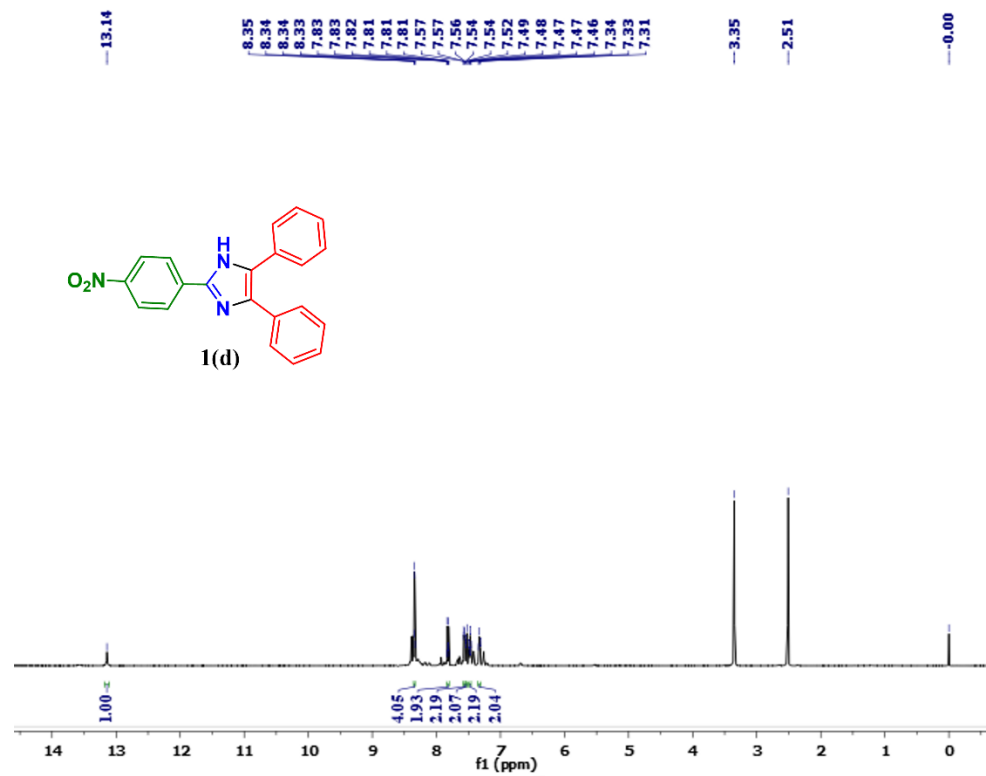
**Figure S5.** <sup>1</sup>H-NMR spectra of **1(a)** recorded in DMSO-d<sub>6</sub>.



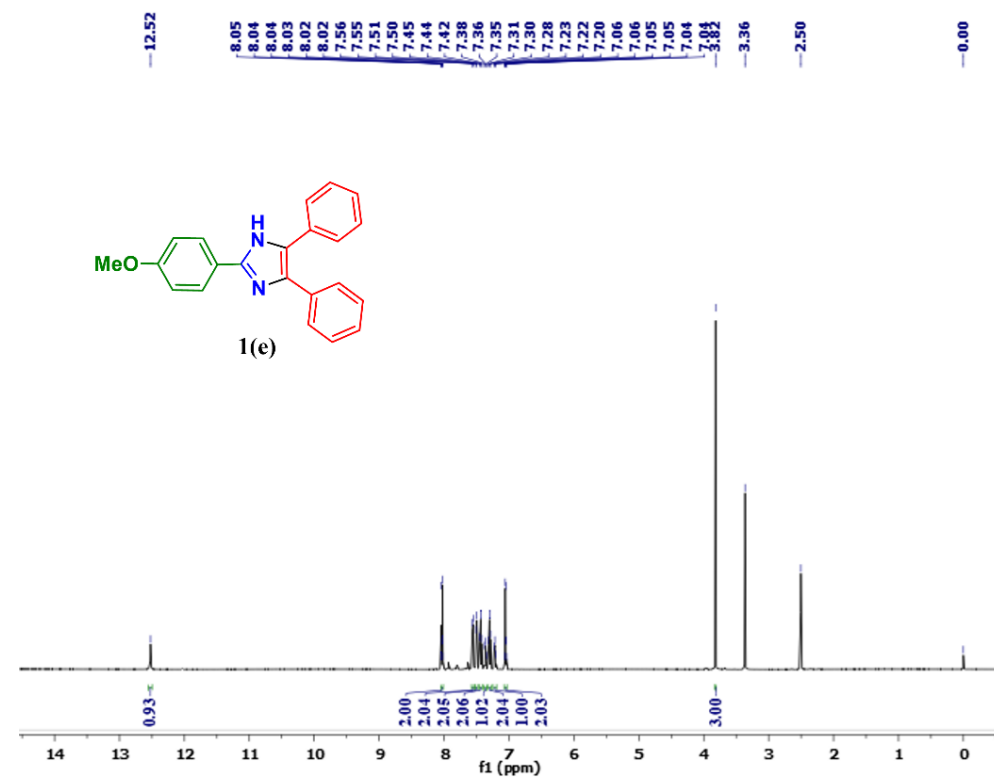
**Figure S6.** <sup>1</sup>H-NMR spectra of **1(b)** recorded in DMSO-d<sub>6</sub>.



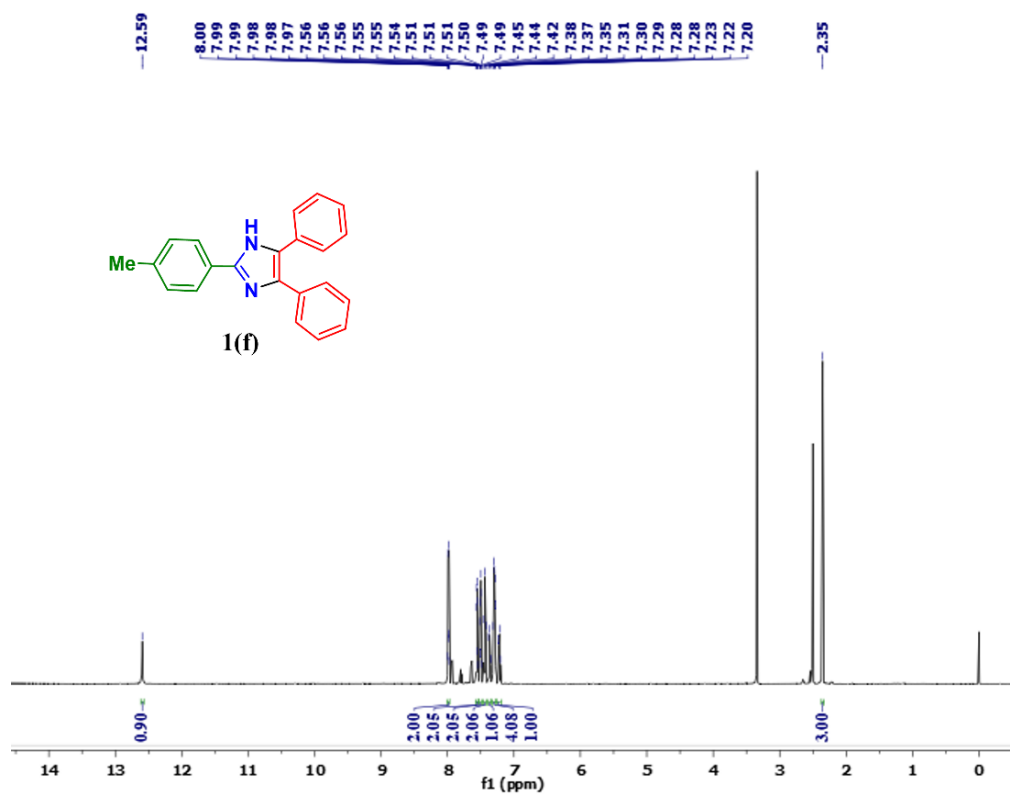
**Figure S7.** <sup>1</sup>H-NMR spectra of **1(c)** recorded in DMSO-d<sub>6</sub>.



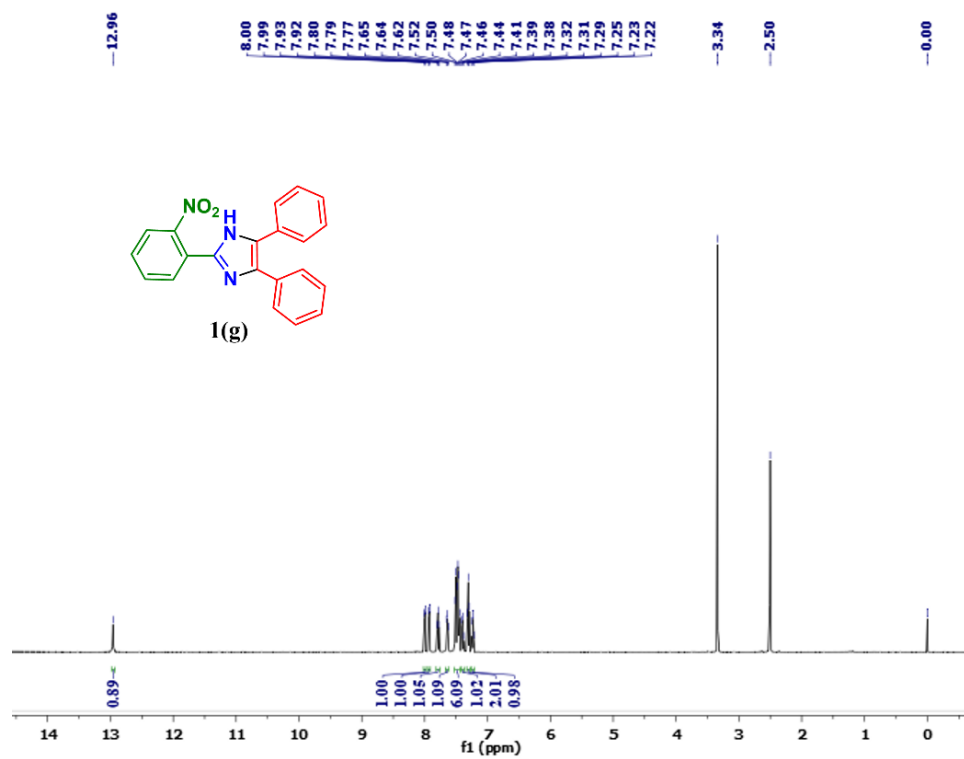
**Figure S8.** <sup>1</sup>H-NMR spectra of **1(d)** recorded in DMSO-d<sub>6</sub>.



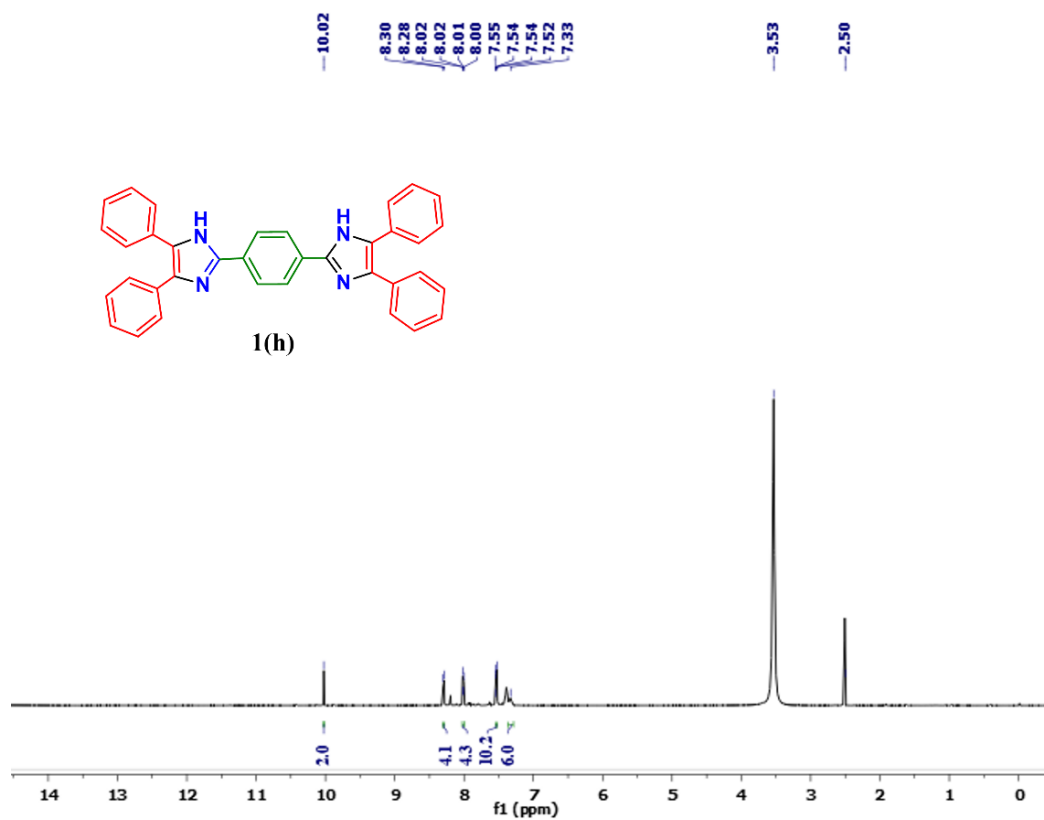
**Figure S9.** <sup>1</sup>H-NMR spectra of **1(e)** recorded in DMSO-d<sub>6</sub>.



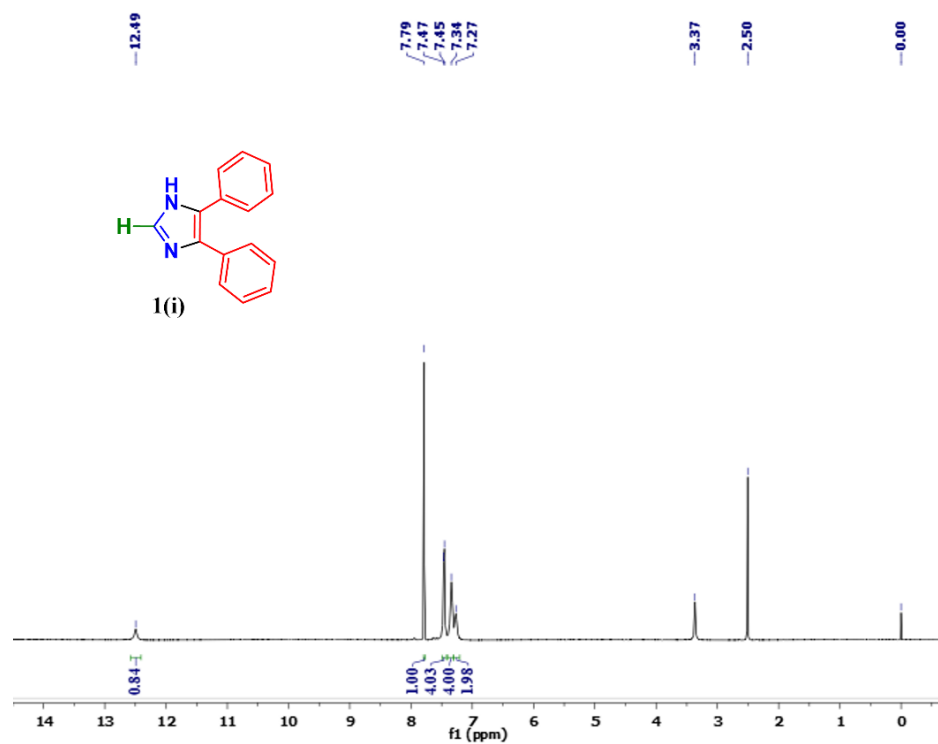
**Figure S10.** <sup>1</sup>H-NMR spectra of **1(f)** recorded in DMSO-d<sub>6</sub>.



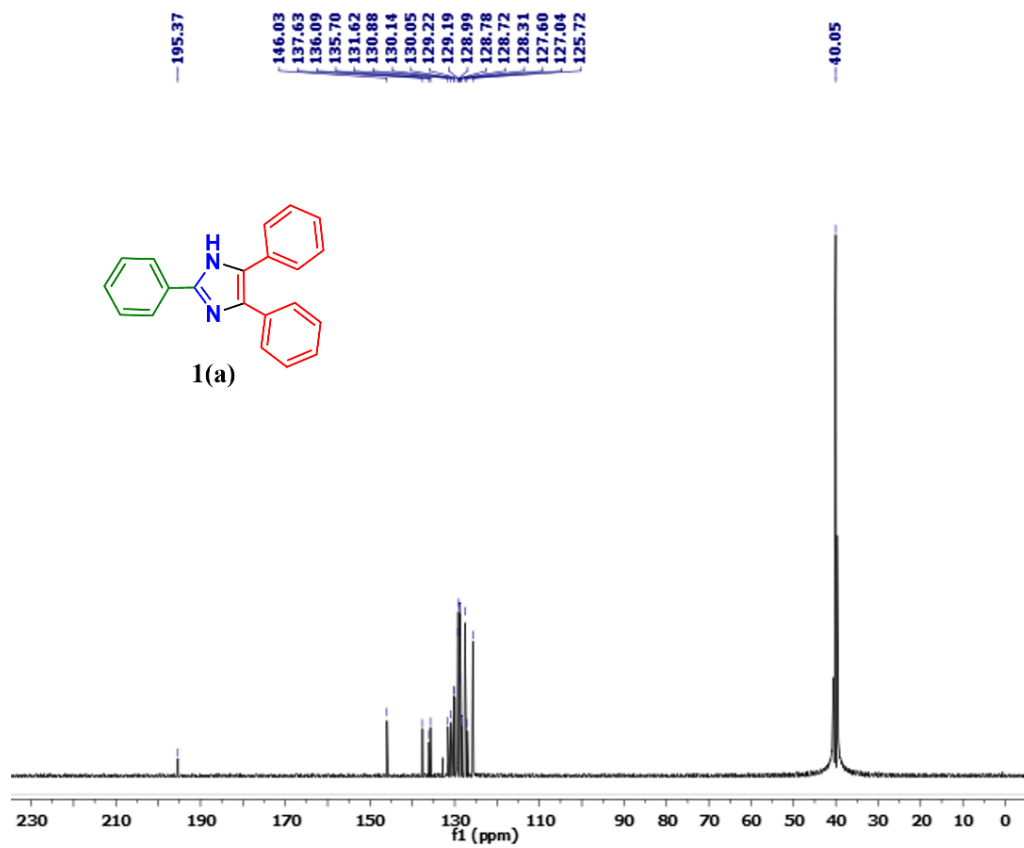
**Figure S11.** <sup>1</sup>H-NMR spectra of **1(g)** recorded in DMSO-d<sub>6</sub>.



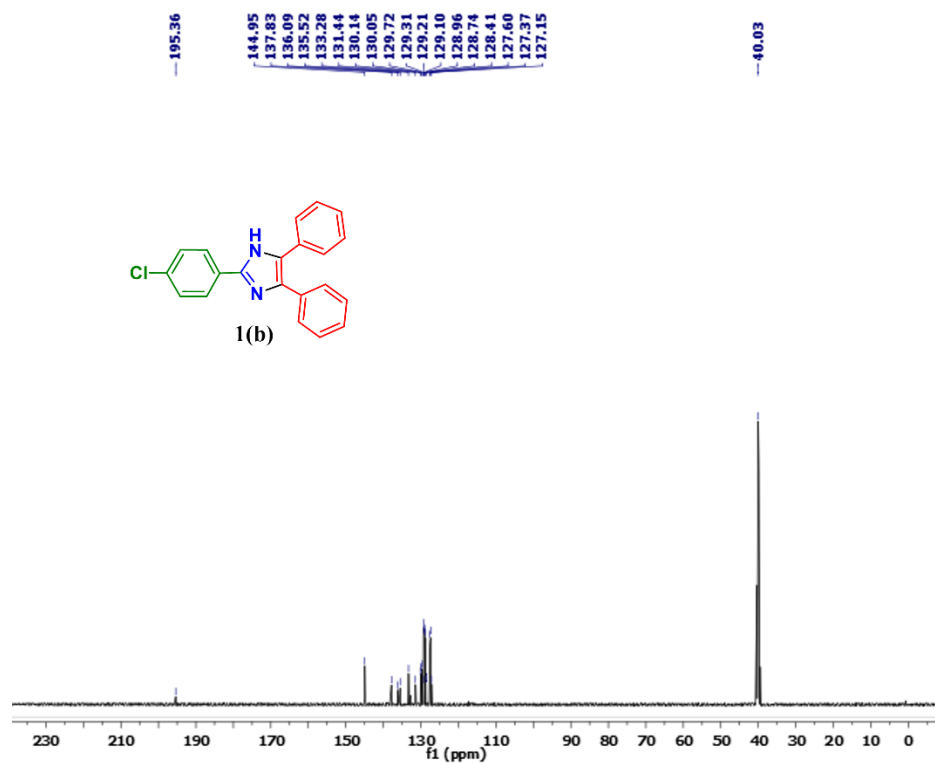
**Figure S12.** <sup>1</sup>H-NMR spectra of **1(h)** recorded in DMSO-d<sub>6</sub>.



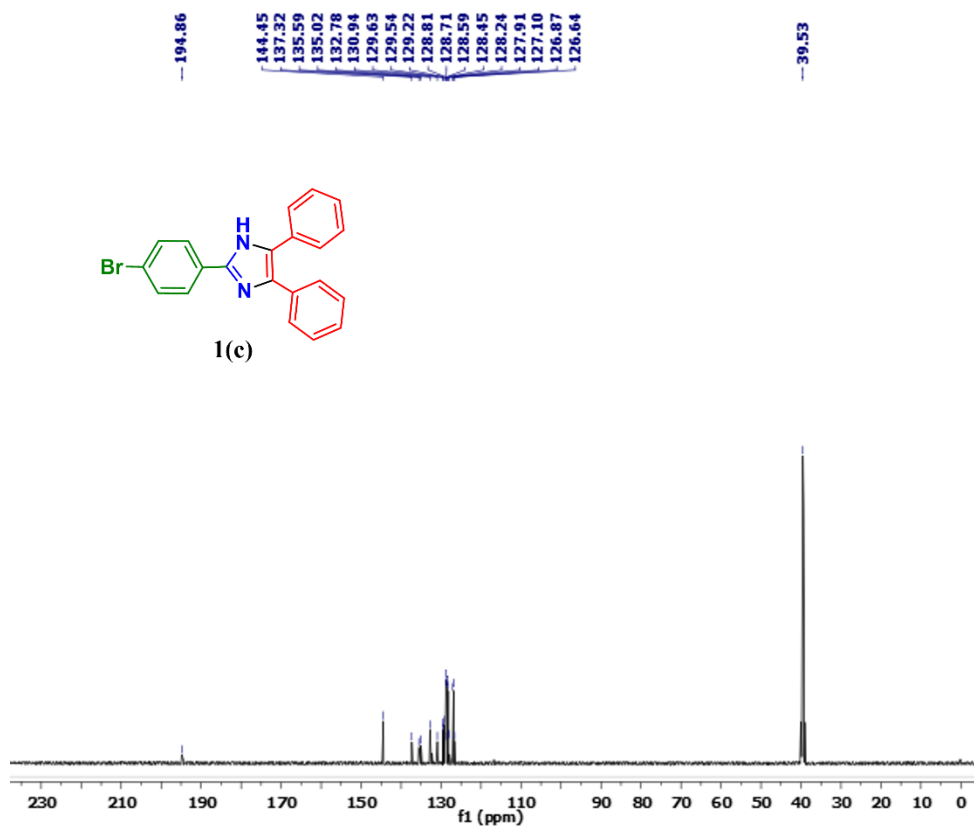
**Figure S13.** <sup>1</sup>H-NMR spectra of **1(i)** recorded in DMSO-d<sub>6</sub>.



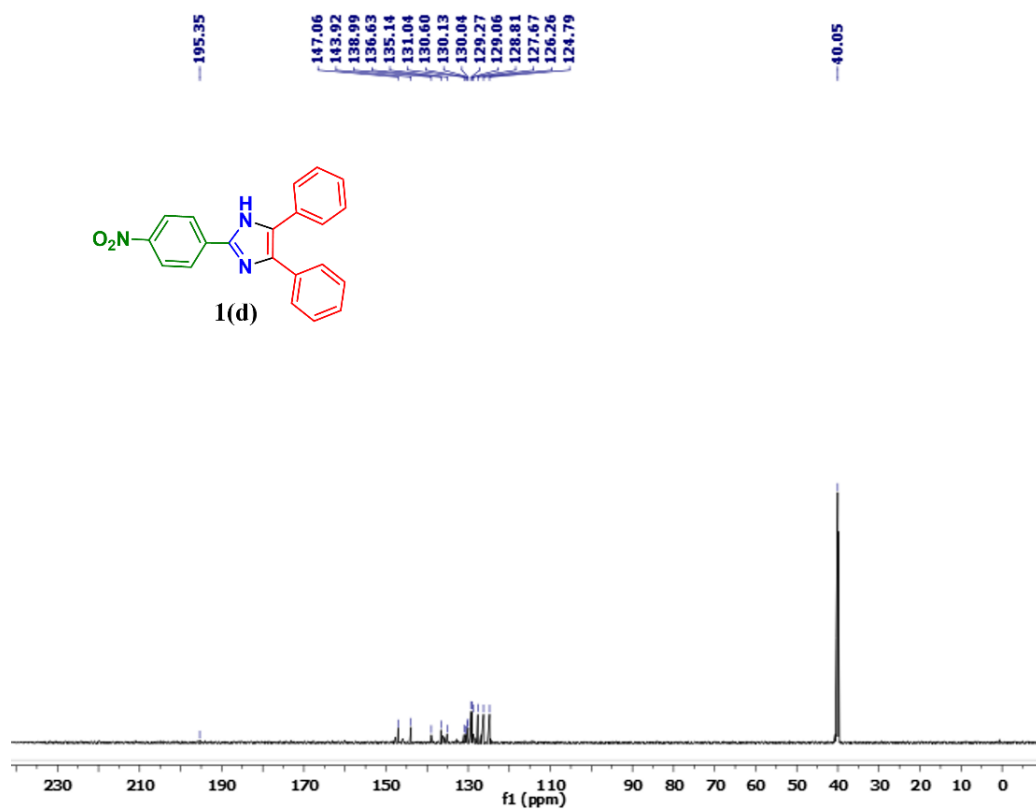
**Figure S14.** <sup>13</sup>C-NMR spectra of **1(a)** recorded in DMSO-d<sub>6</sub>.



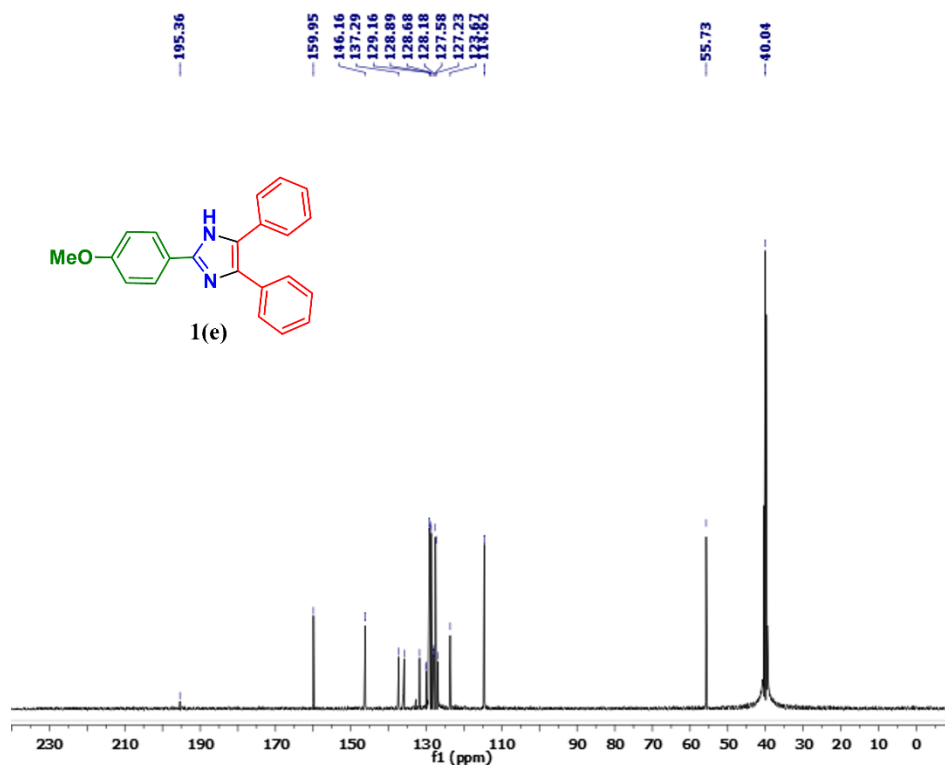
**Figure S15.** <sup>13</sup>C-NMR spectra of **1(b)** recorded in DMSO-d<sub>6</sub>.



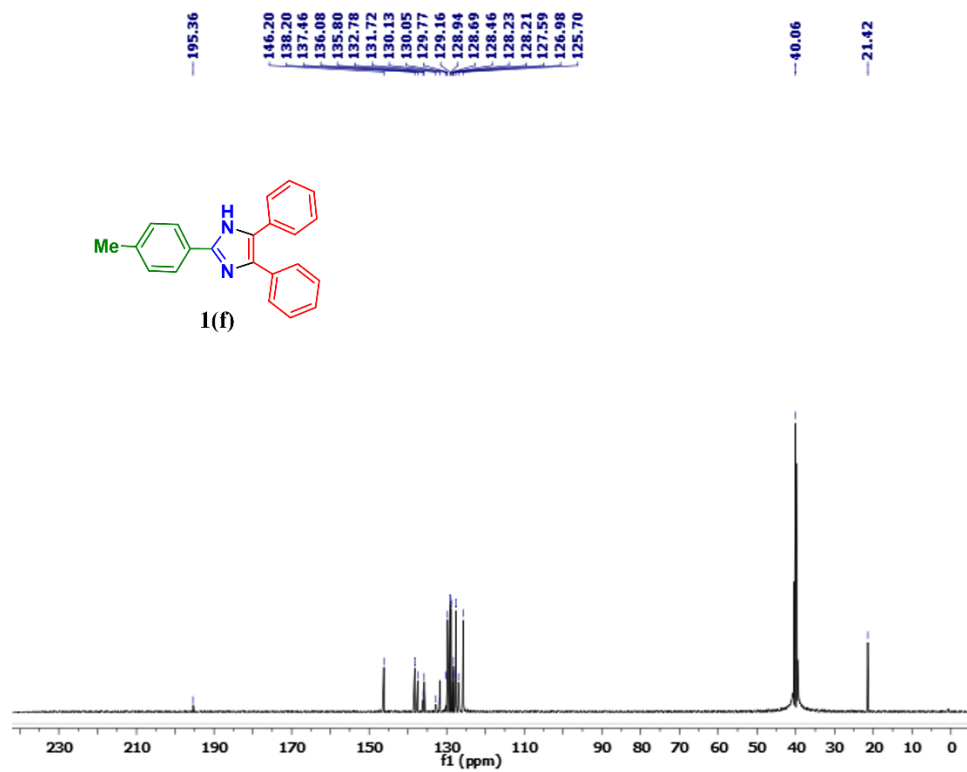
**Figure S16.** <sup>13</sup>C-NMR spectra of **1(c)** recorded in DMSO-d<sub>6</sub>.



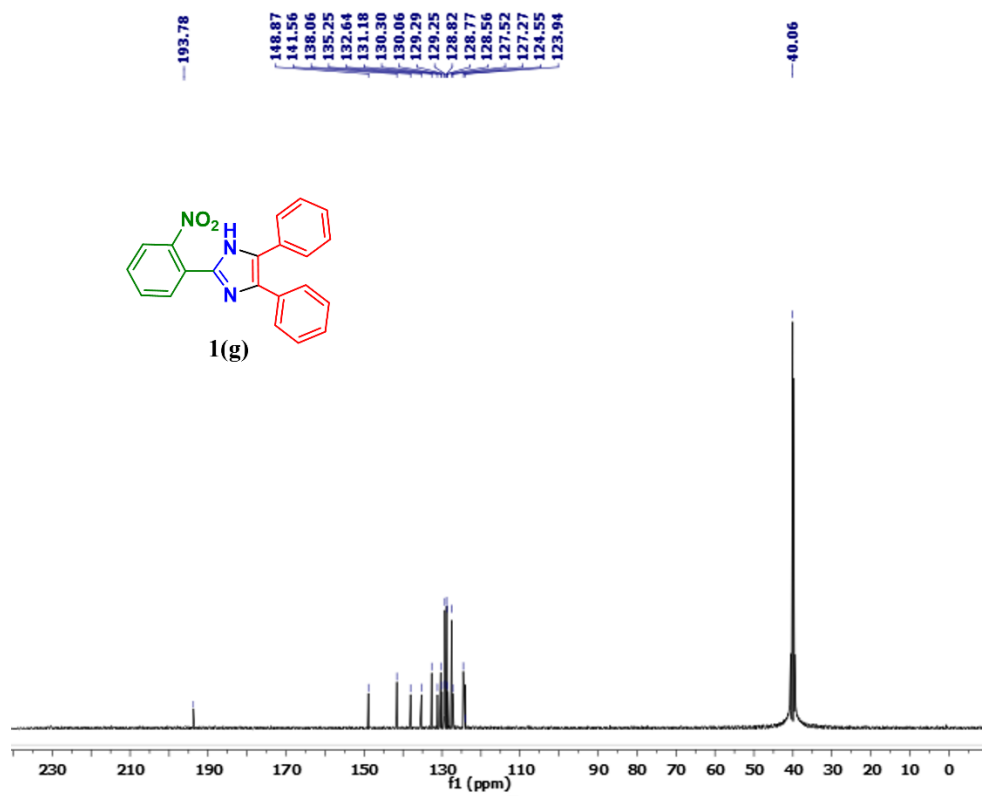
**Figure S17.** <sup>13</sup>C-NMR spectra of **1(d)** recorded in DMSO-d<sub>6</sub>.



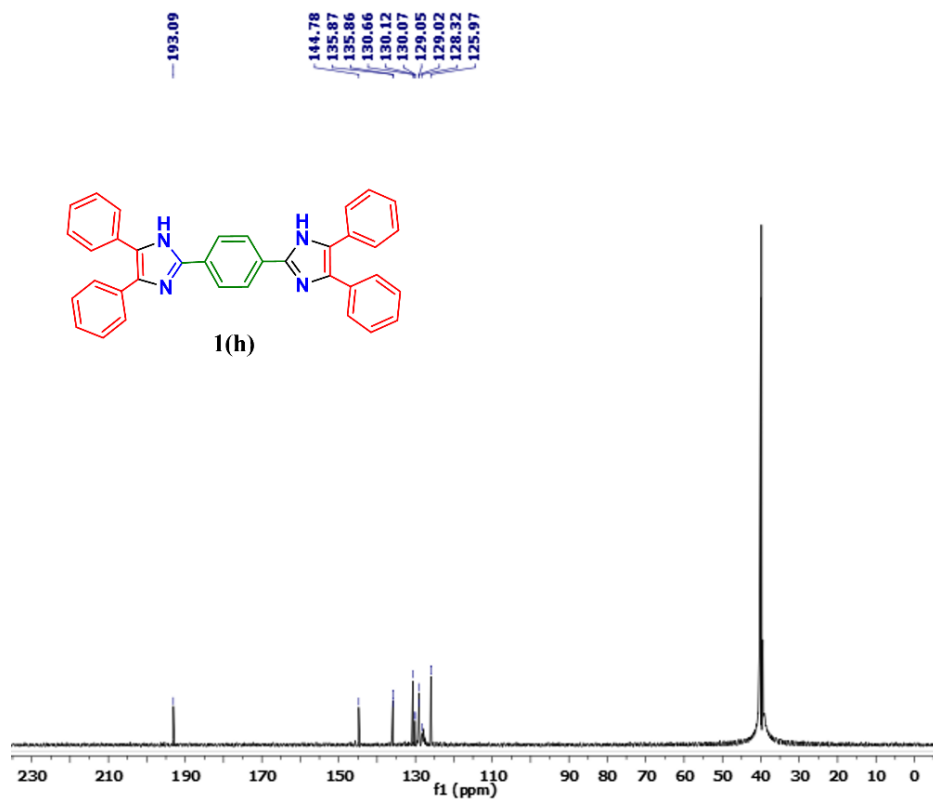
**Figure S18.** <sup>13</sup>C-NMR spectra of **1(e)** recorded in DMSO-d<sub>6</sub>.



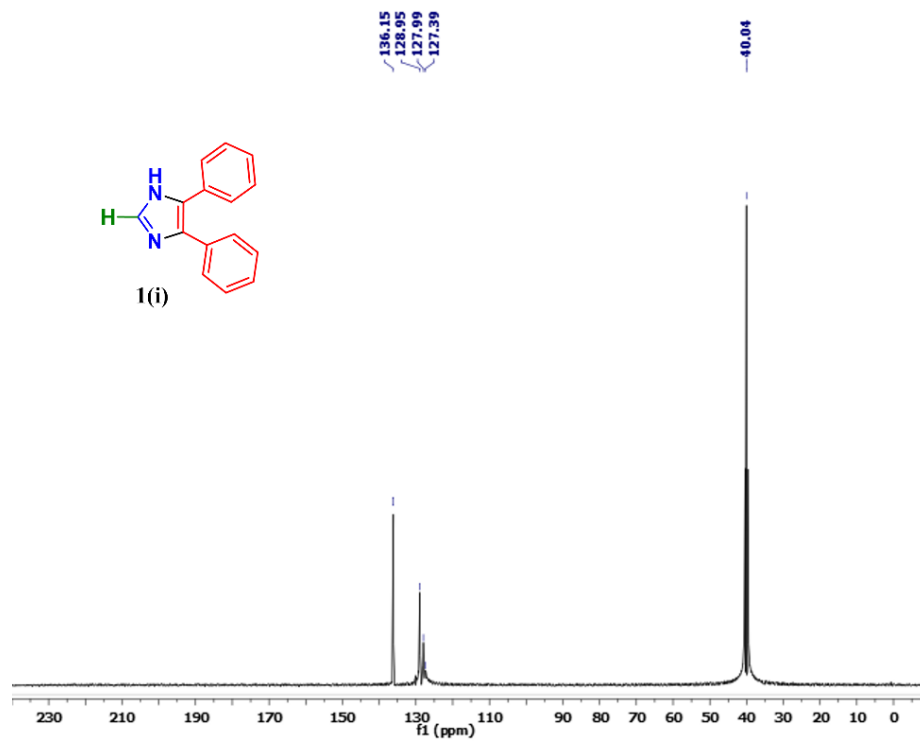
**Figure S19.** <sup>13</sup>C-NMR spectra of **1(f)** recorded in DMSO-d<sub>6</sub>.



**Figure S20.** <sup>13</sup>C-NMR spectra of **1(g)** recorded in DMSO-d<sub>6</sub>.



**Figure S21.** <sup>13</sup>C-NMR spectra of **1(h)** recorded in DMSO-d<sub>6</sub>.



**Figure S22.** <sup>13</sup>C-NMR spectra of **1(i)** recorded in DMSO-d<sub>6</sub>.