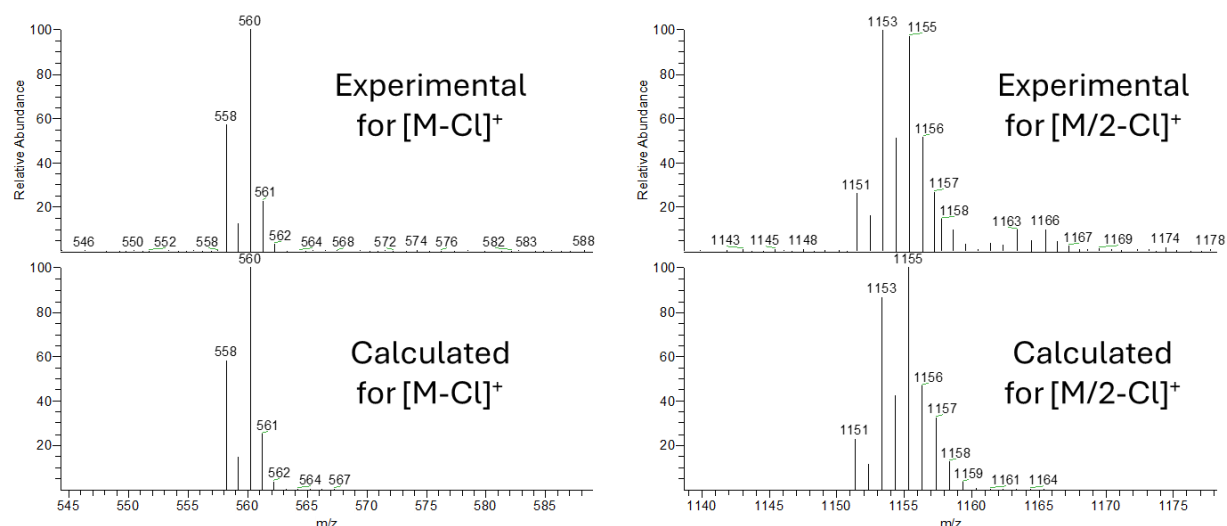


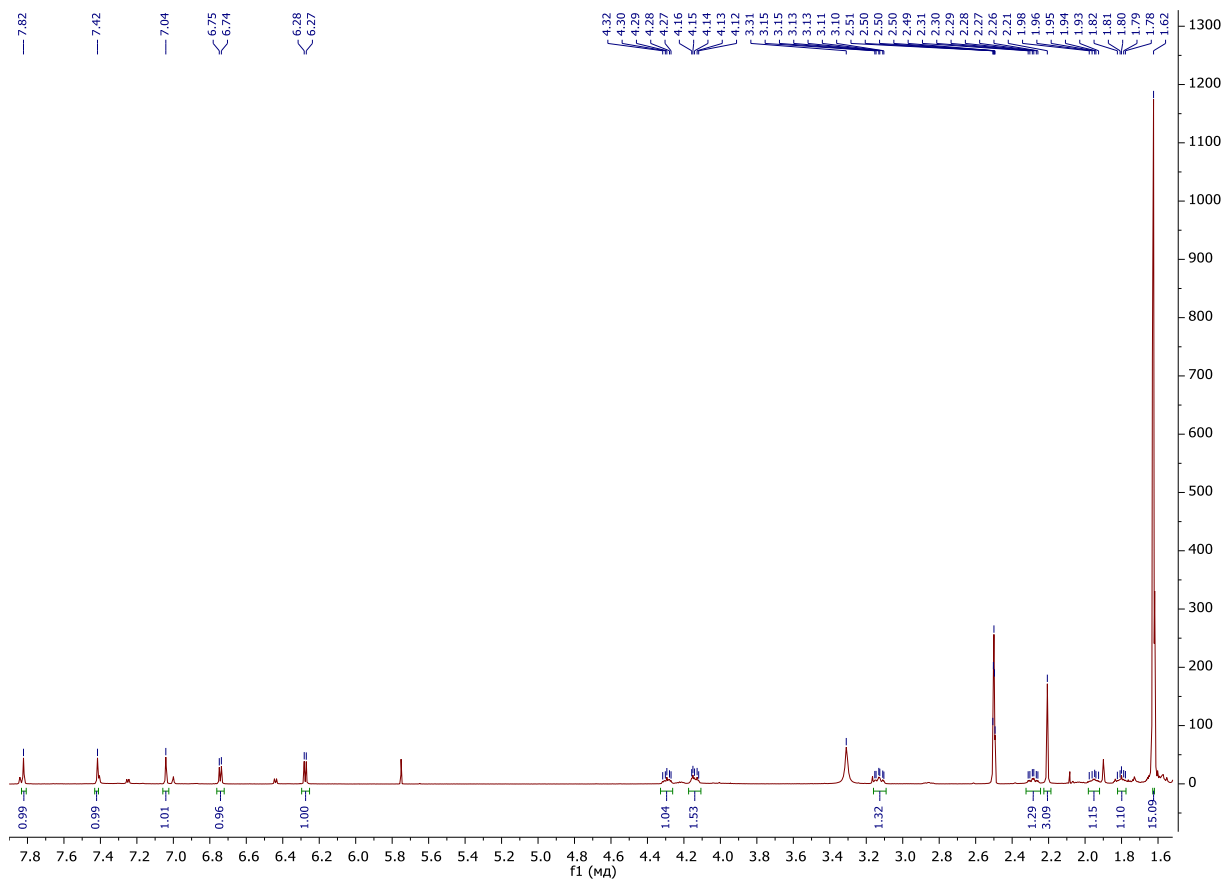
## Supplementary Materials

# Di- $\mu$ -(1-(3-(1*H*-imidazol-1-yl)propyl)-2-methyl-4-oxo-1,4-dihydropyridin-3-olate)-bis[( $\eta^5$ -pentamethylcyclopentadienyl)iridium(III)] chloride

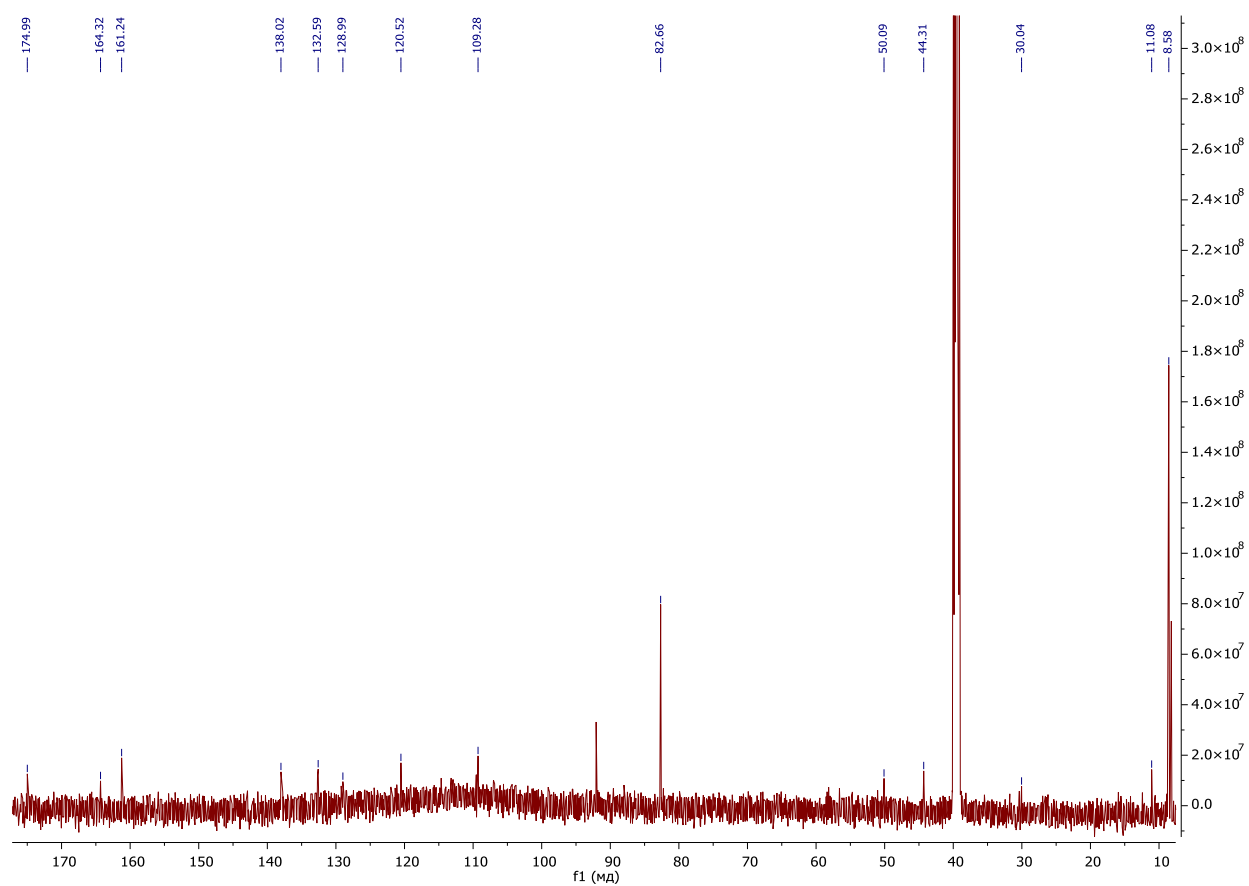
Ilya A. Shutkov, Nikolai A. Melnichuk, Konstantin A. Lyssenko, Nataliya E. Borisova, Olga N. Kovaleva, and Alexey A. Nazarov



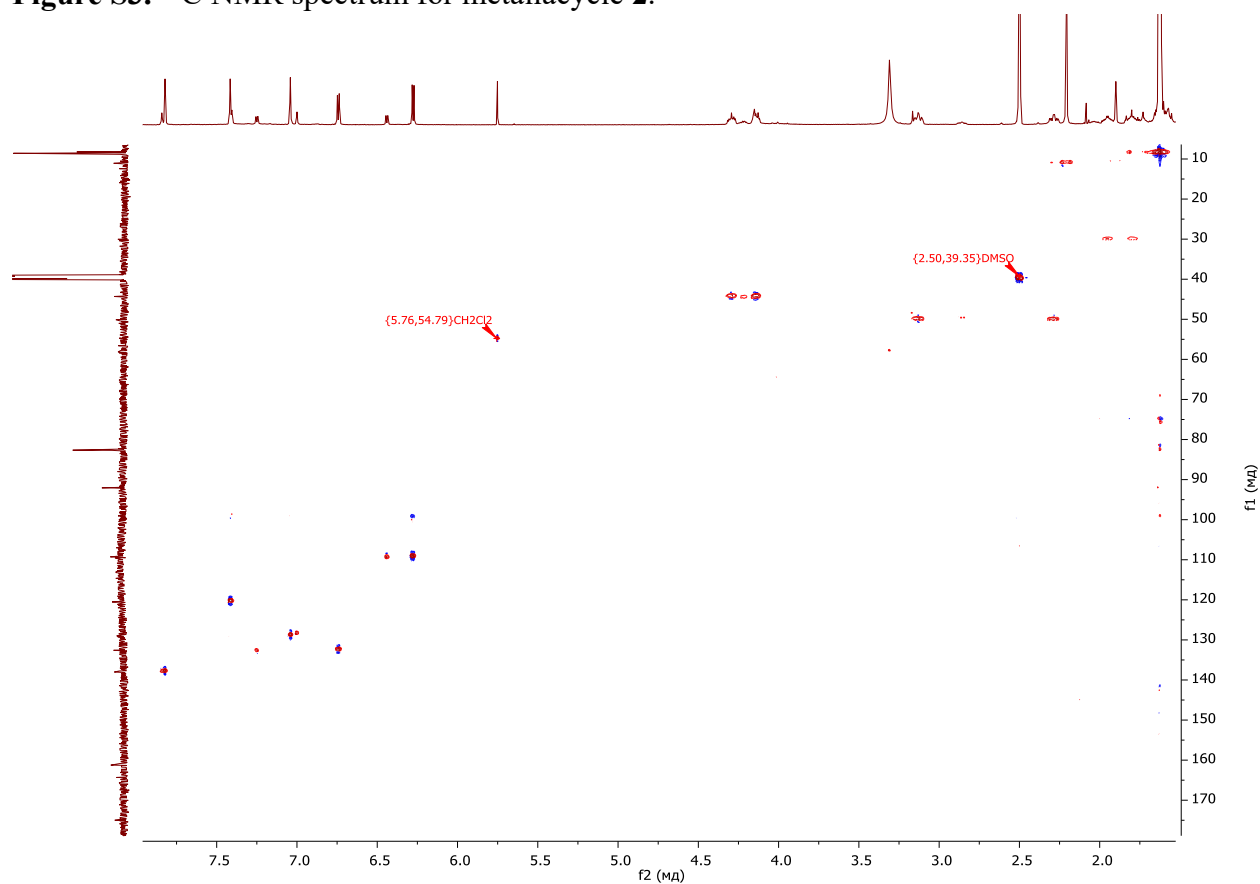
**Figure S1.** ESI mass-spectra of compound **2** in the mode of recording positively charged ions.



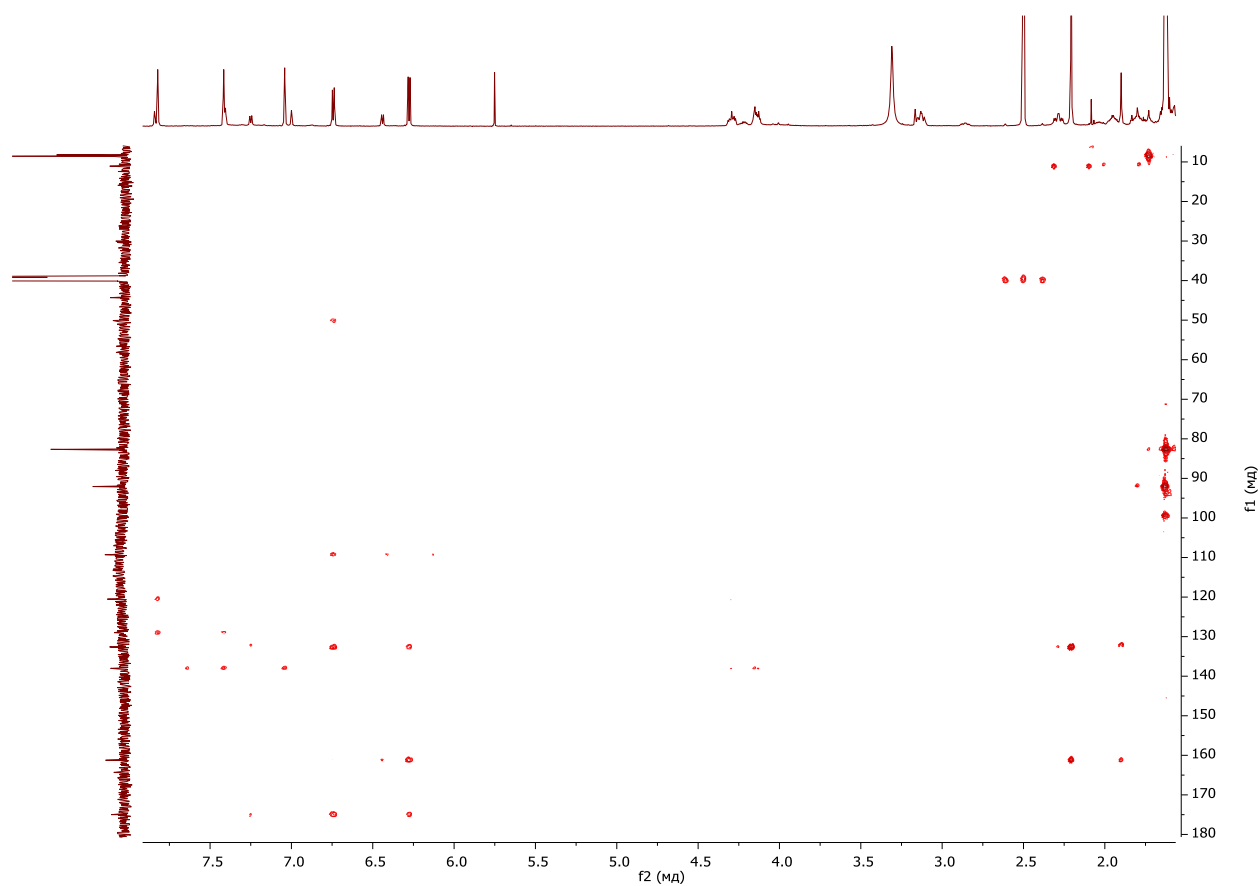
**Figure S2.**  $^1H$  NMR spectrum for metallacycle **2**.



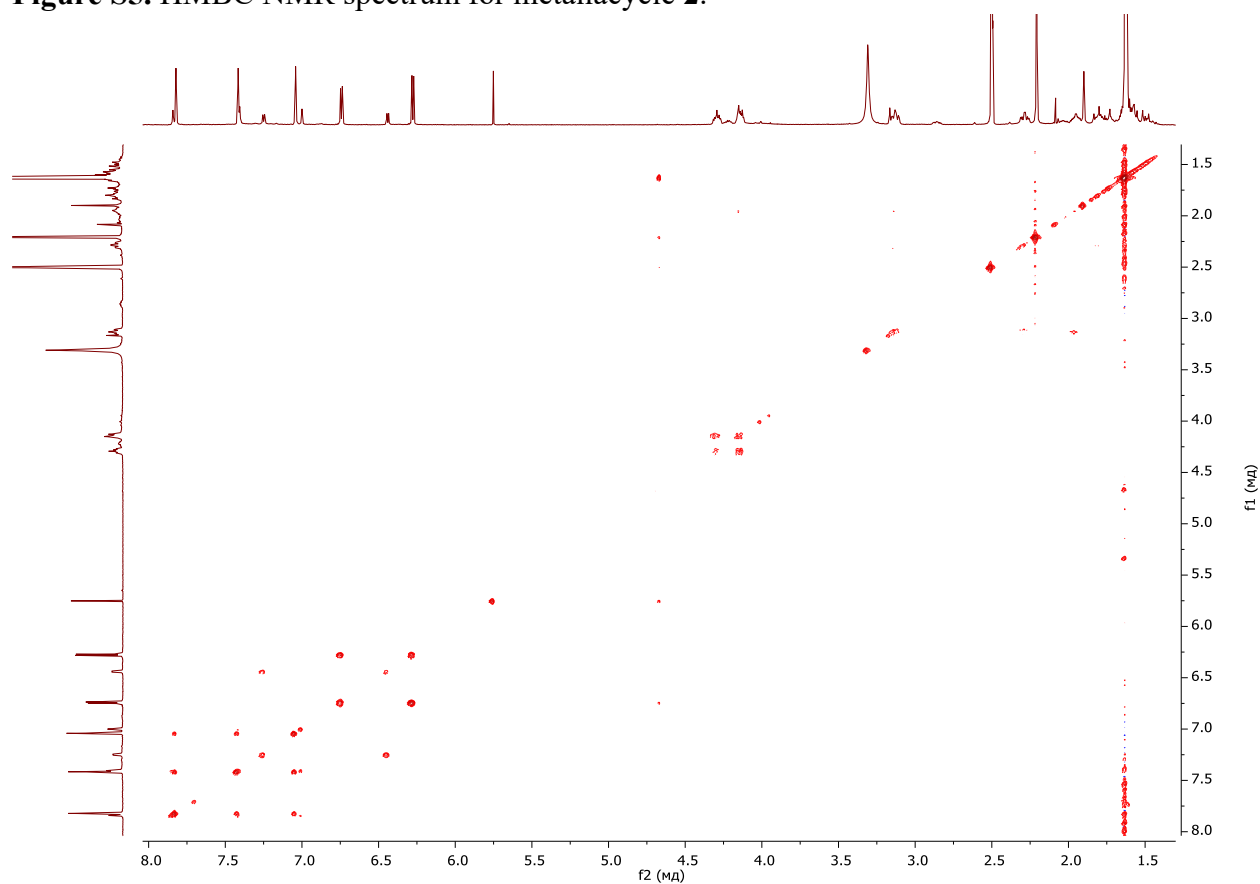
**Figure S3.**  $^{13}\text{C}$  NMR spectrum for metallacycle **2**.



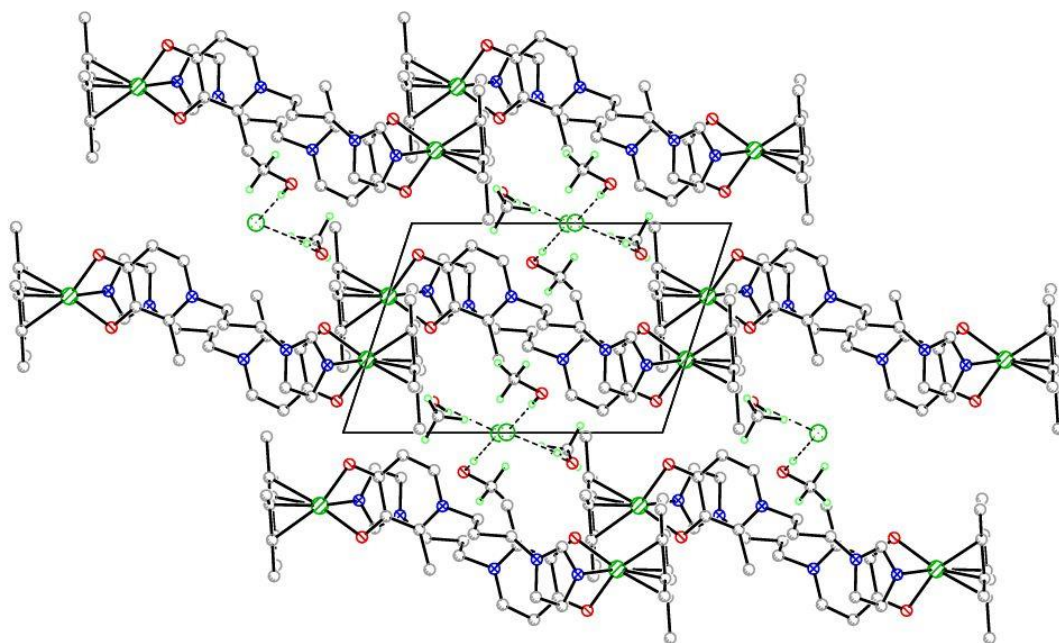
**Figure S4.** HSQC NMR spectrum for metallacycle **2**.



**Figure S5.** HMBC NMR spectrum for metallacycle **2**.



**Figure S6.** COSY NMR spectrum for metallacycle **2**.



**Figure S7. Molecular packing of 2**

**Table S1.** Selected crystallographic data and refinement parameters for **2** from single crystal X-ray diffraction.

Chemical formula	C <sub>48</sub> H <sub>74</sub> Cl <sub>2</sub> Ir <sub>2</sub> N <sub>6</sub> O <sub>8</sub>
Formula mass, g mol <sup>-1</sup>	1318.43
Crystal system	Triclinic
Space group	<i>P</i> -1
<i>a</i> , Å	7.9907(12)
<i>b</i> , Å	12.7188(18)
<i>c</i> , Å	14.746(2)
$\alpha$	114.437(4)
$\beta$	92.482(5)
$\gamma$	105.428(5)
<i>V</i> , Å <sup>3</sup>	1295.0(3)
<i>Z</i> ( <i>Z'</i> )	1(0.5)
<i>T</i> , K	110(2)
<i>d</i> <sub>calcd.</sub> , g cm <sup>3</sup>	1.691
$\mu$ , mm <sup>-1</sup>	52.92
$\theta$ range, °	3.846 < $\theta$ < 26.987
Collected reflections	21037
Independent reflections	7562
<i>R</i> <sub>σ</sub> / <i>R</i> <sub>int</sub>	0.0596/0.0679
Reflections with <i>I</i> > 2σ( <i>I</i> )	6505
Refined parameters	338
Largest difference peak/hole, e Å <sup>-3</sup>	2.965/-2.892
<i>R</i> <sub>1</sub> [ <i>I</i> > 2σ( <i>I</i> )] / <i>R</i> <sub>1</sub> [all data]	0.0379/0.0478
<i>wR</i> <sub>2</sub> [ <i>I</i> > 2σ( <i>I</i> )] / <i>wR</i> <sub>2</sub> [all data]	0.0789/0.0823
<i>GoF</i>	1.025