

## *Supporting Information*

# **N-Heterocyclic Carbene Copper (I) Complexes Incorporating Pyrene Chromophore: Synthesis, Crystal Structure, and Luminescent Properties**

Yaping Cheng <sup>1</sup>, Geoffrey Gontard <sup>1</sup>, Abderrahim Khatyr <sup>2</sup>, Michael Knorr <sup>2</sup> and Hani Amouri <sup>1,\*</sup>

<sup>1</sup> Institut Parisien de Chimie Moléculaire (IPCM), UMR CNRS 8232, Sorbonne Université-Campus Pierre et Marie Curie, 4 Place Jussieu, CEDEX 05, 75252 Paris, France;

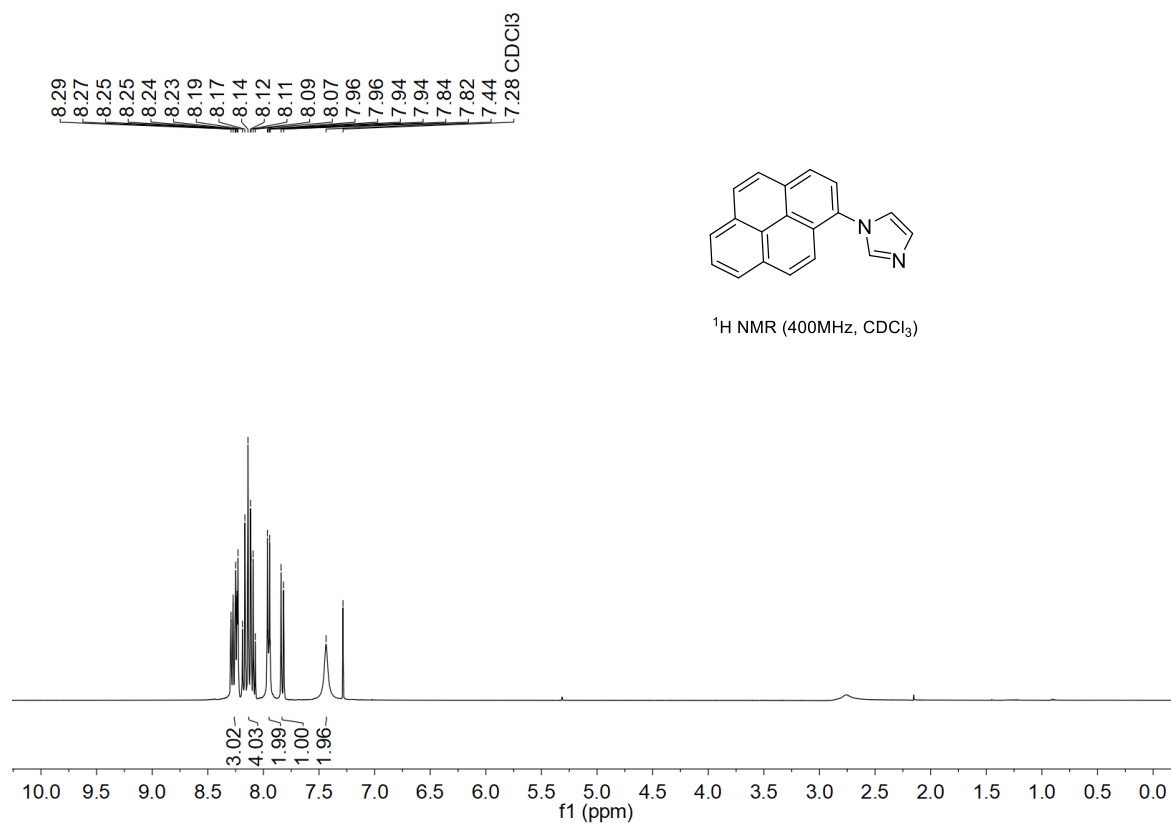
yaping.cheng@sorbonne-universite.fr (Y.C.); geoffrey.gontard@sorbonne-universite.fr (G.G.)

<sup>2</sup> Institut UTINAM, UMR CNRS 6213, Université de Franche-Comté, 16 Route de Gray, 25030 Besançon, France; abderrahim.khatyr@univ-fcomte.fr (A.K.); michael.knorr@univ-fcomte.fr (M.K.)

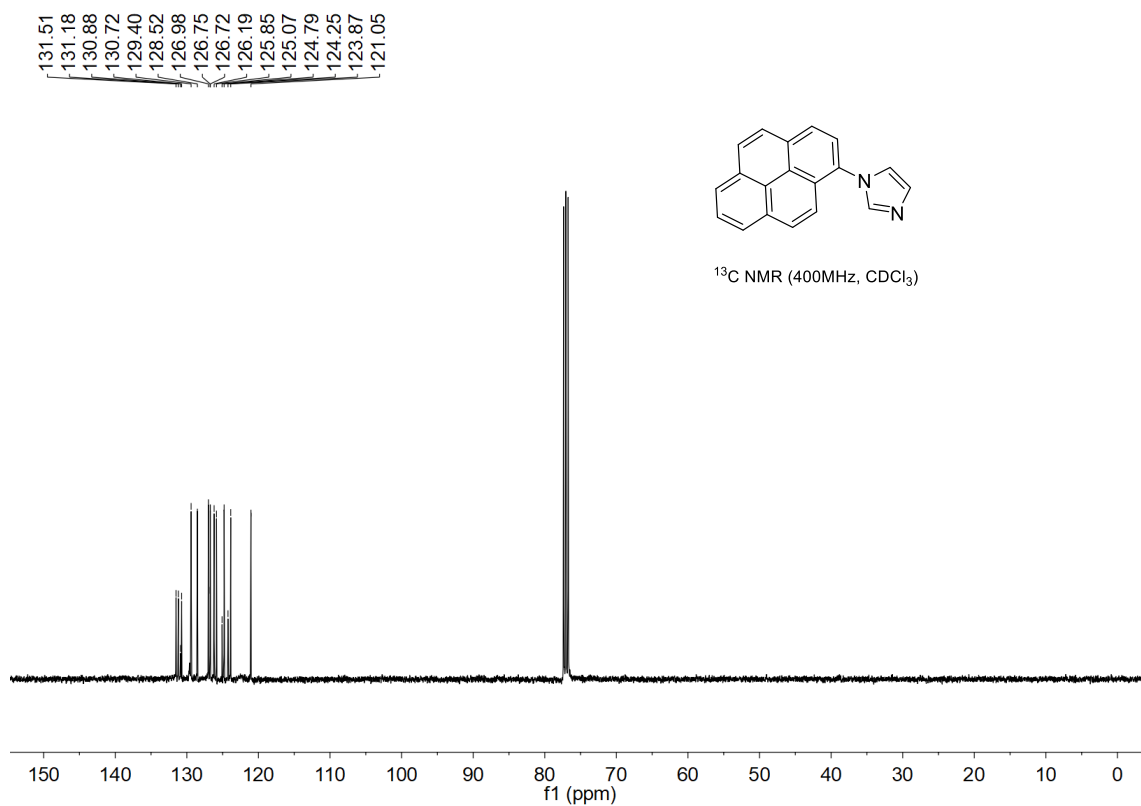
\* Correspondence: hani.amouri@sorbonne-universite.fr

## **TABLE OF CONTENTS**

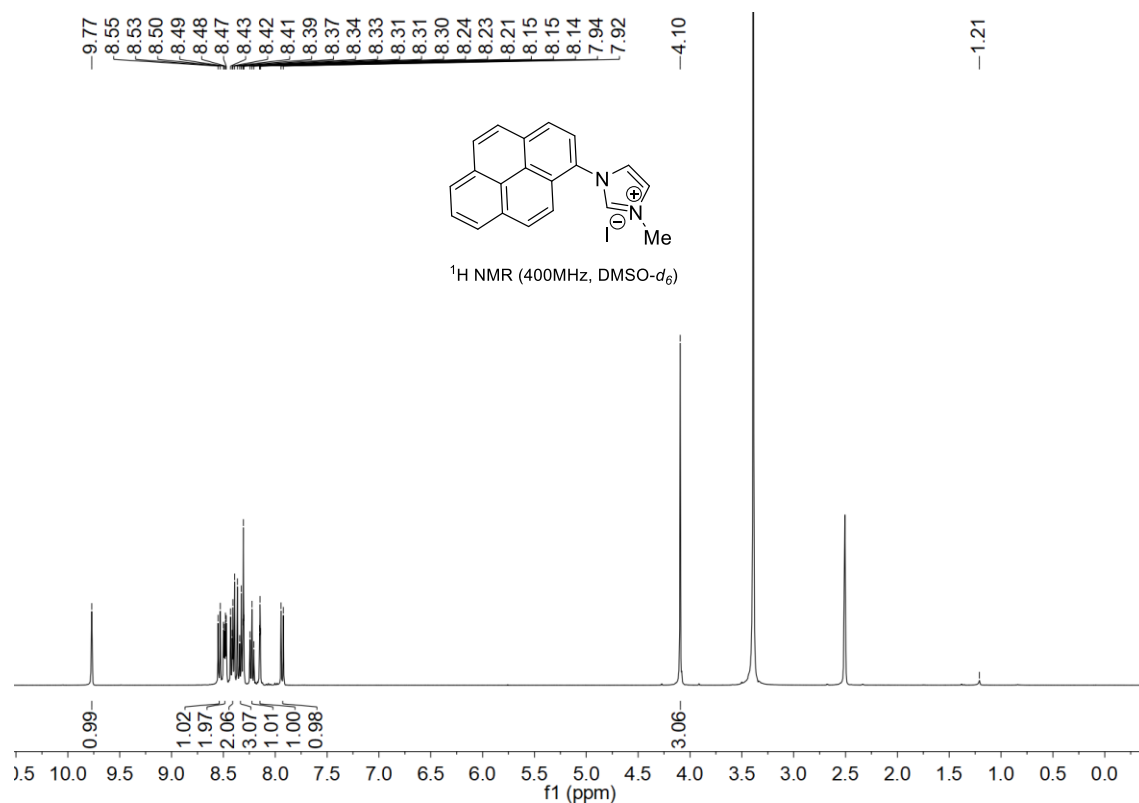
<b>Figures S1–S10</b>	( <sup>1</sup> H, <sup>13</sup> C) -NMR spectra of compounds ( <b>1</b> , <b>2a</b> , <b>2b</b> , <b>3</b> and <b>4</b> ).
<b>Figure S11</b>	Normalized emission spectra of ligand <b>1</b> and complexes <b>3-4</b> in solid-state at rt.
<b>Figures S12–S14</b>	Emission decay of compounds <b>1</b> , <b>3</b> and <b>4</b> in CH <sub>2</sub> Cl <sub>2</sub> at rt.
<b>Figures S15–S17</b>	Emission decay of compounds <b>1</b> , <b>3</b> and <b>4</b> in solid-state at rt.



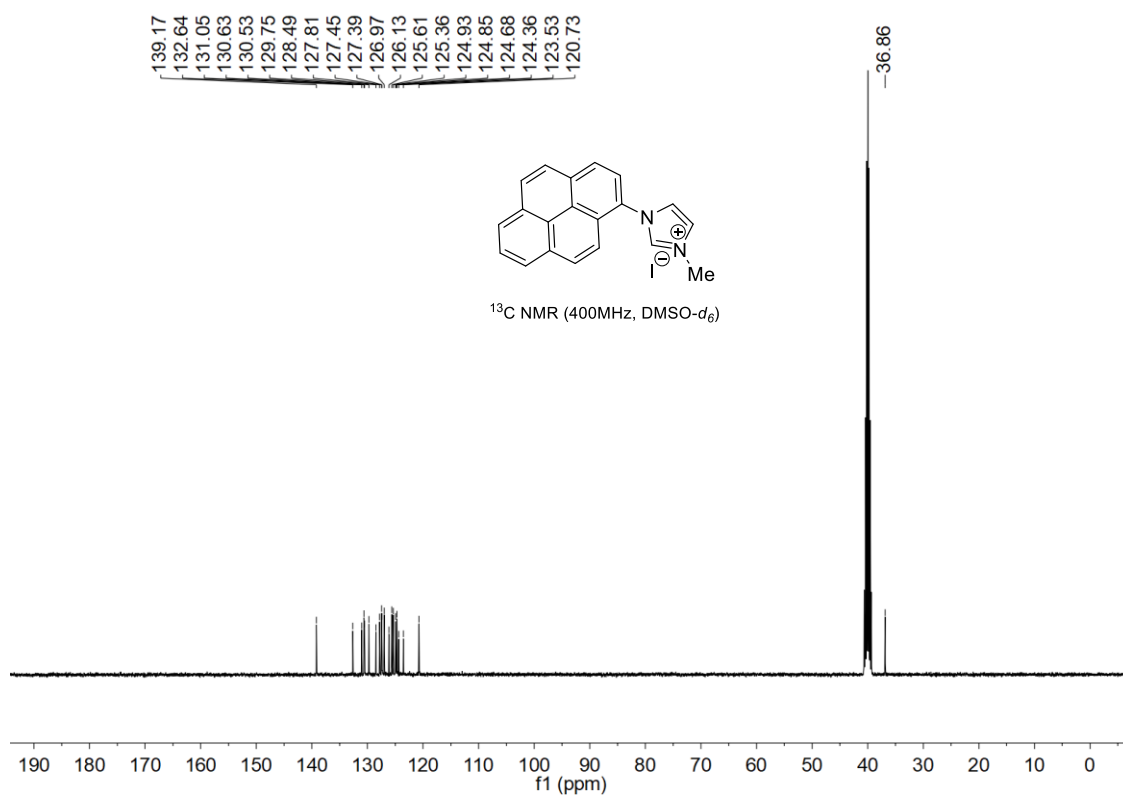
**Figure S1.** <sup>1</sup>H NMR of compound **1** in CDCl<sub>3</sub>



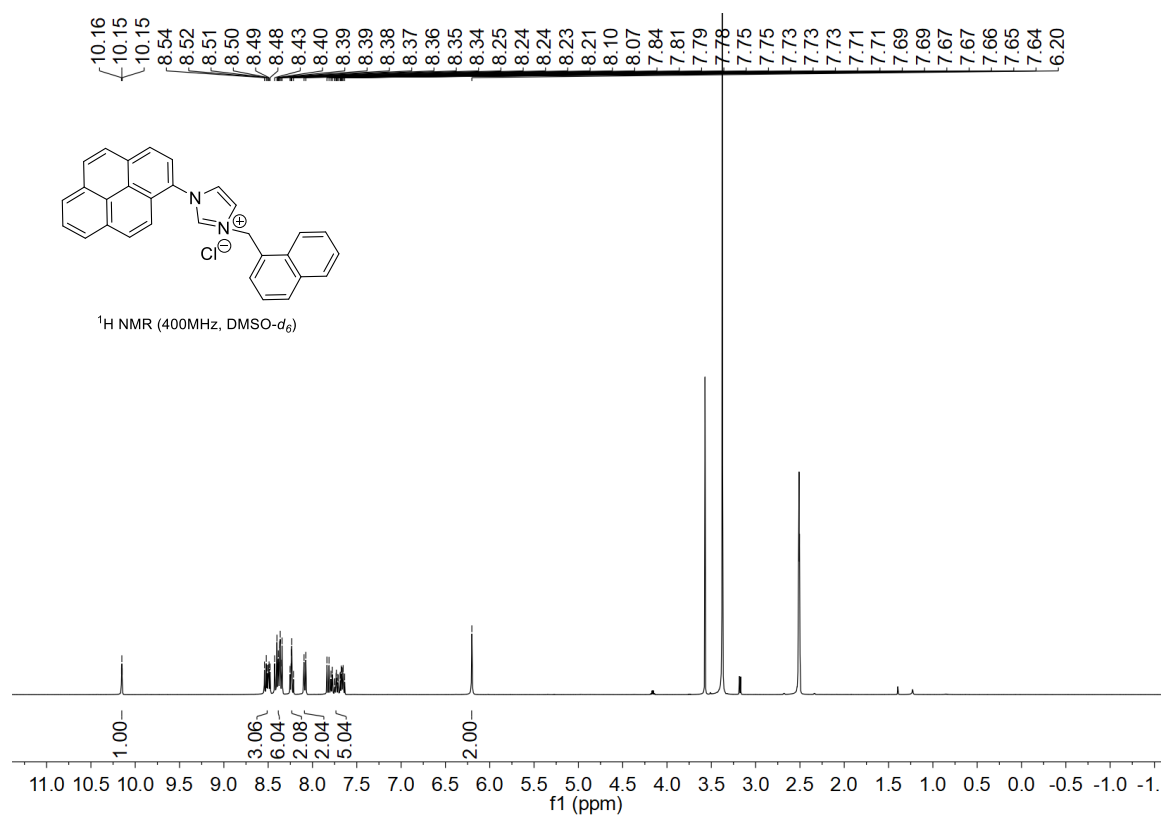
**Figure S2.** <sup>13</sup>C NMR of compound **1** in CDCl<sub>3</sub>



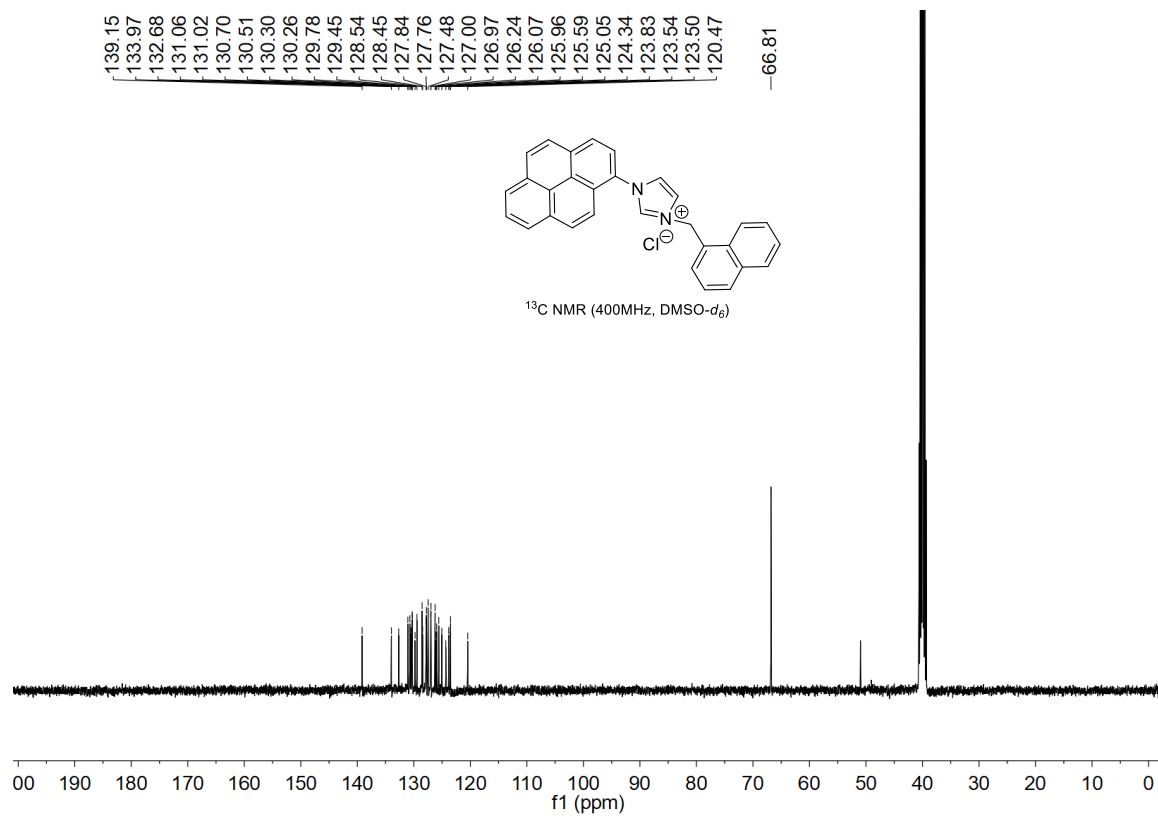
**Figure S3.** <sup>1</sup>H NMR of compound 2a in DMSO



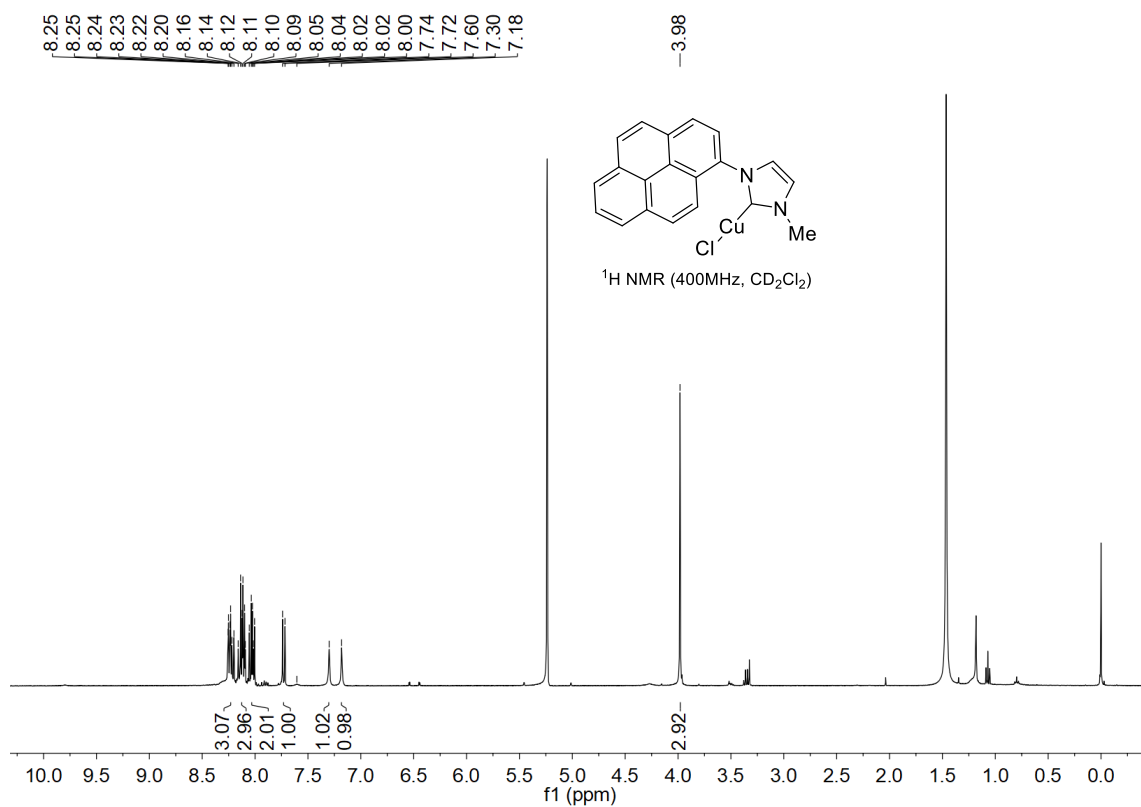
**Figure S4.** <sup>13</sup>C NMR of compound 2a in DMSO



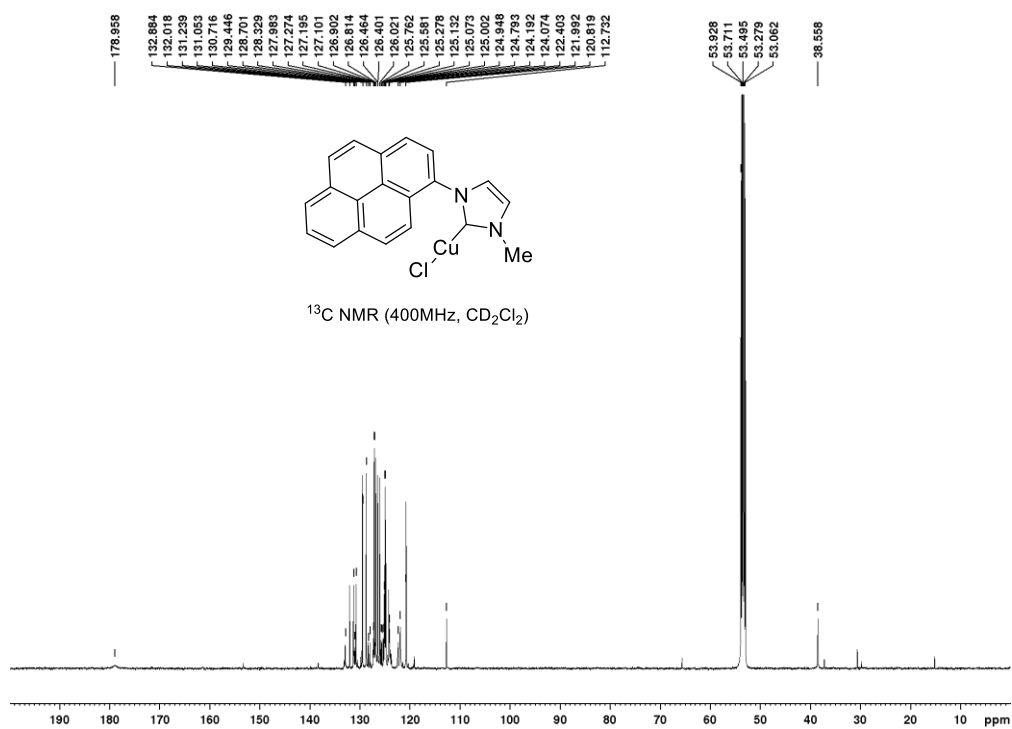
**Figure S5.** <sup>1</sup>H NMR of compound **2b** in DMSO



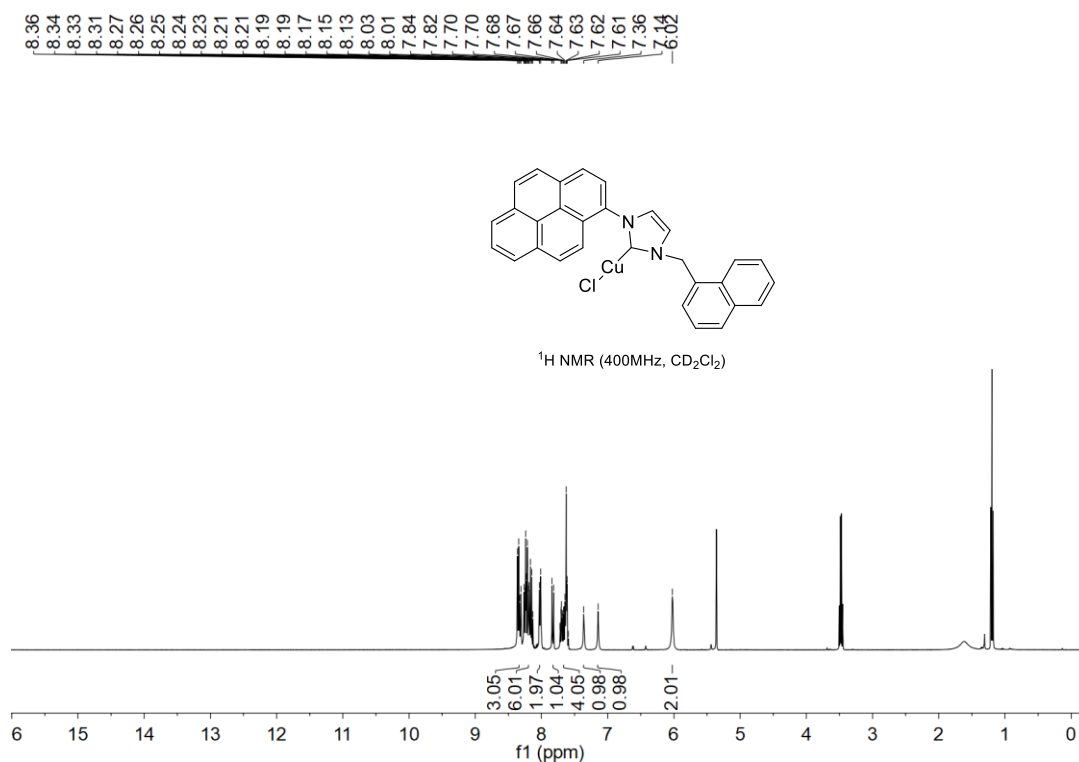
**Figure S6.** <sup>13</sup>C NMR of compound **2b** in DMSO



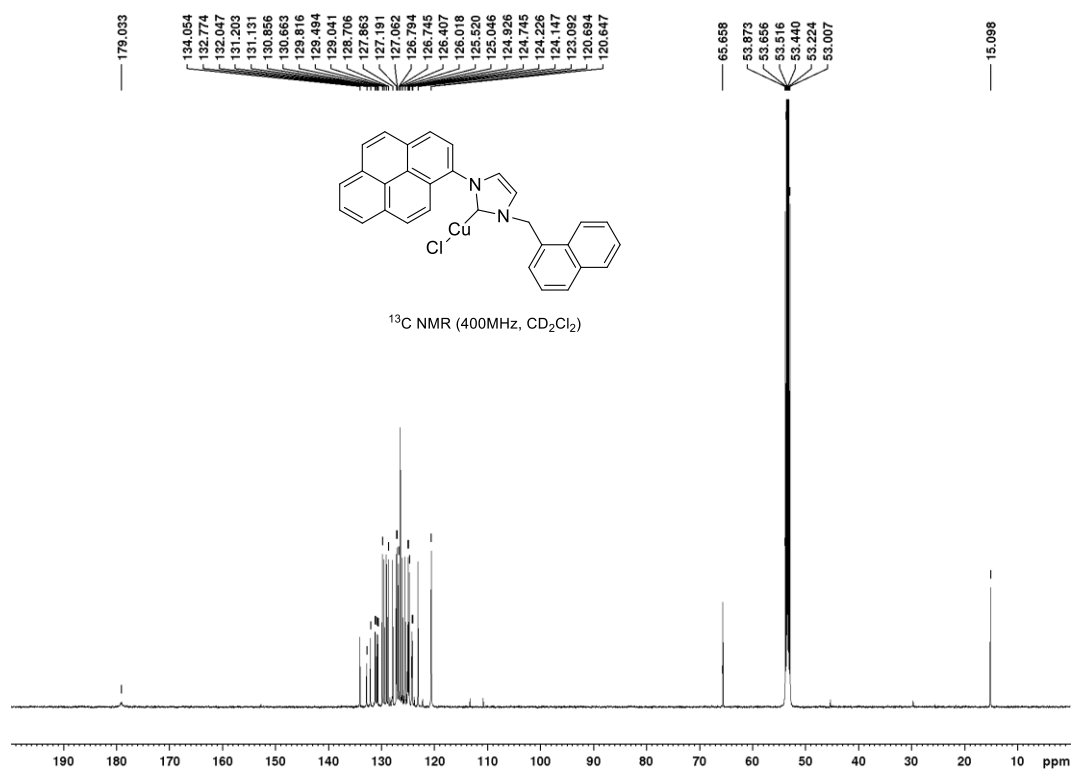
**Figure S7.**  $^1\text{H}$  NMR of complex 3 in  $\text{CD}_2\text{Cl}_2$



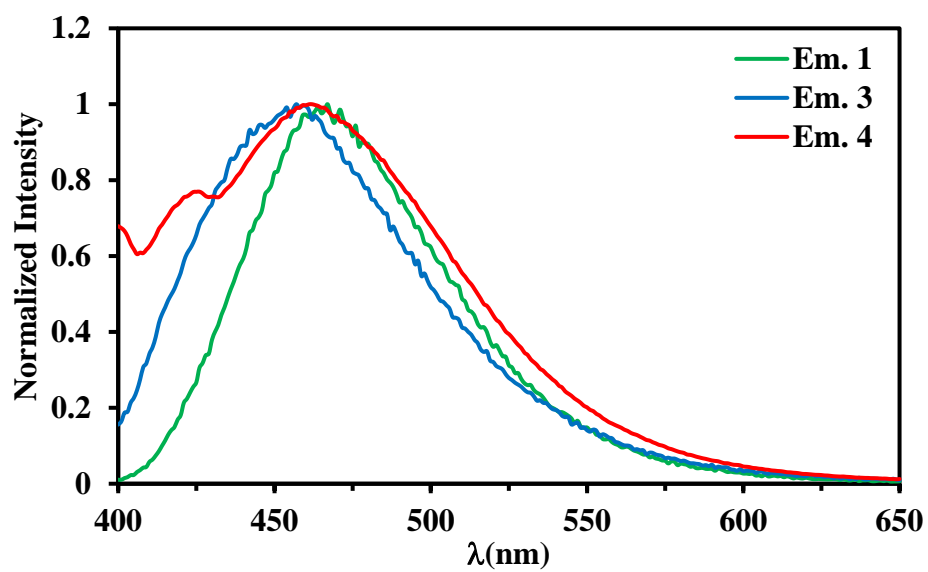
**Figure S8.**  $^{13}\text{C}$  NMR of complex 3 in  $\text{CD}_2\text{Cl}_2$



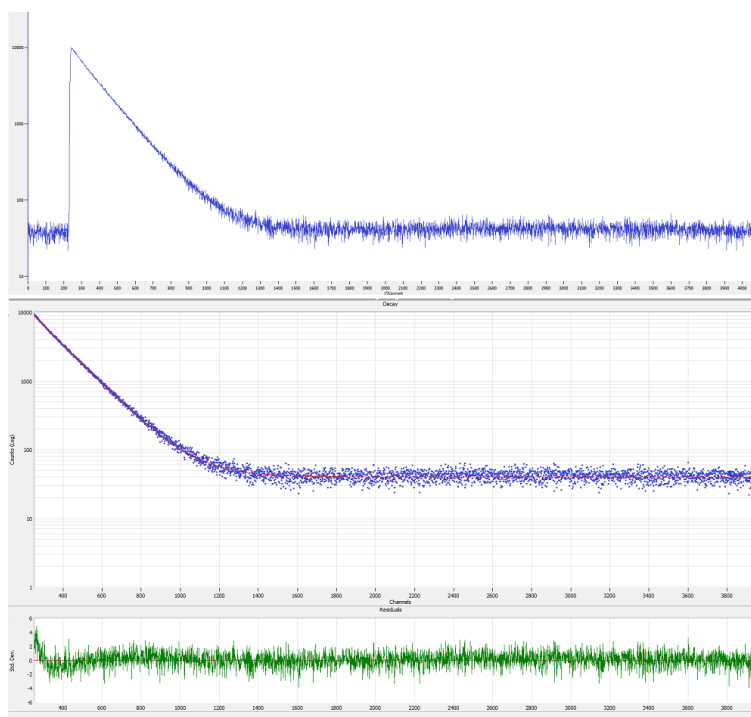
**Figure S9.** <sup>1</sup>H NMR of complex 4 in CD<sub>2</sub>Cl<sub>2</sub>



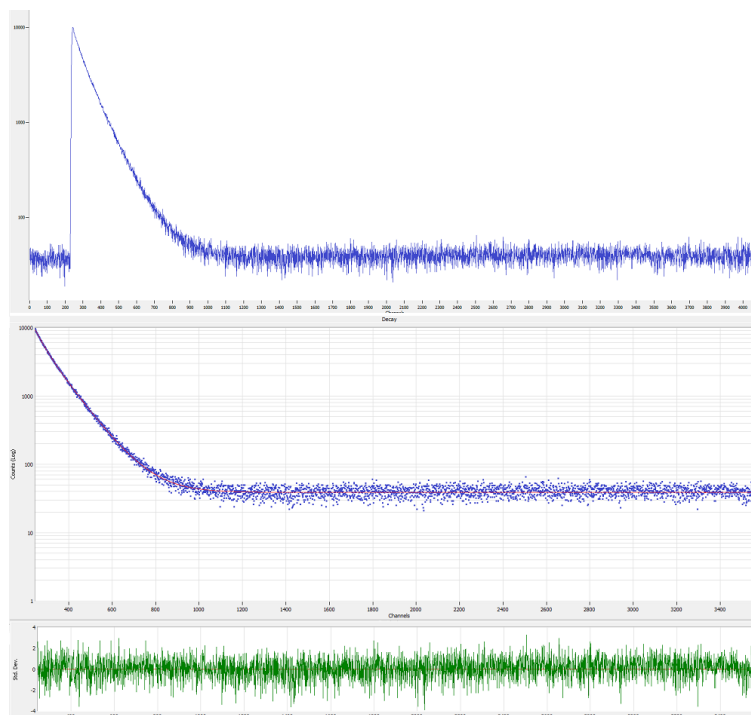
**Figure S10.** <sup>13</sup>C NMR of complex 4 in CD<sub>2</sub>Cl<sub>2</sub>



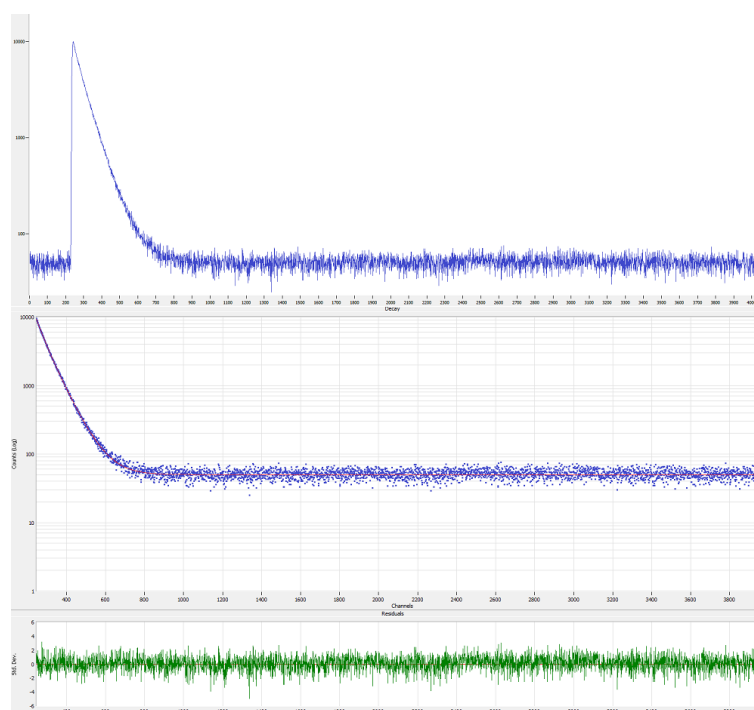
**Figure S11.** Normalized emission spectra of ligand **1** and complexes **3-4** in solid-state at rt.



**Figure S12.** Emission decay (blue), best fit (red) and residuals (green) of **1** in  $\text{CH}_2\text{Cl}_2$  at rt;  $\chi^2 = 1.123$ .

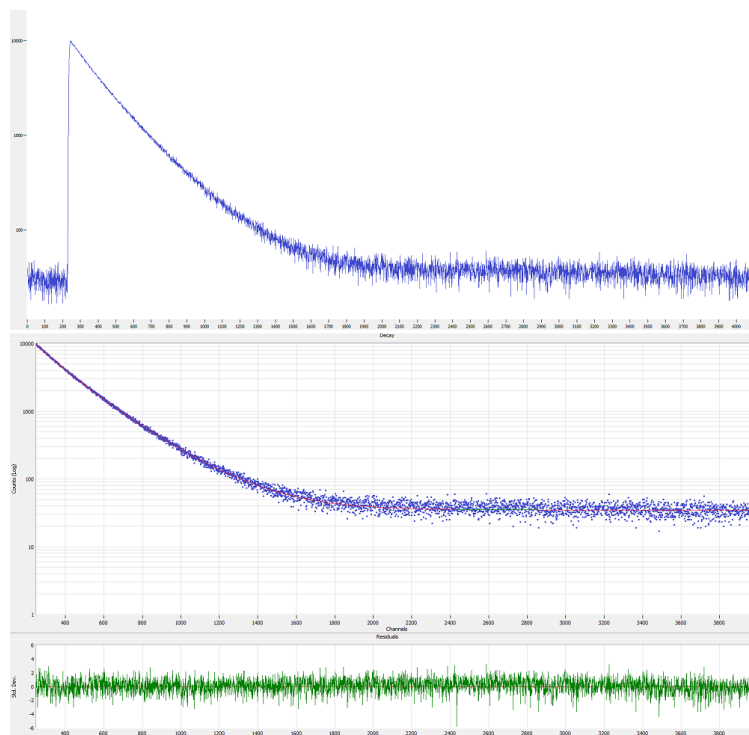


**Figure S13.** Emission decay (blue), best fit (red) and residuals (green) of **3** in CH<sub>2</sub>Cl<sub>2</sub> at rt;  $\chi^2 = 1.050$ .

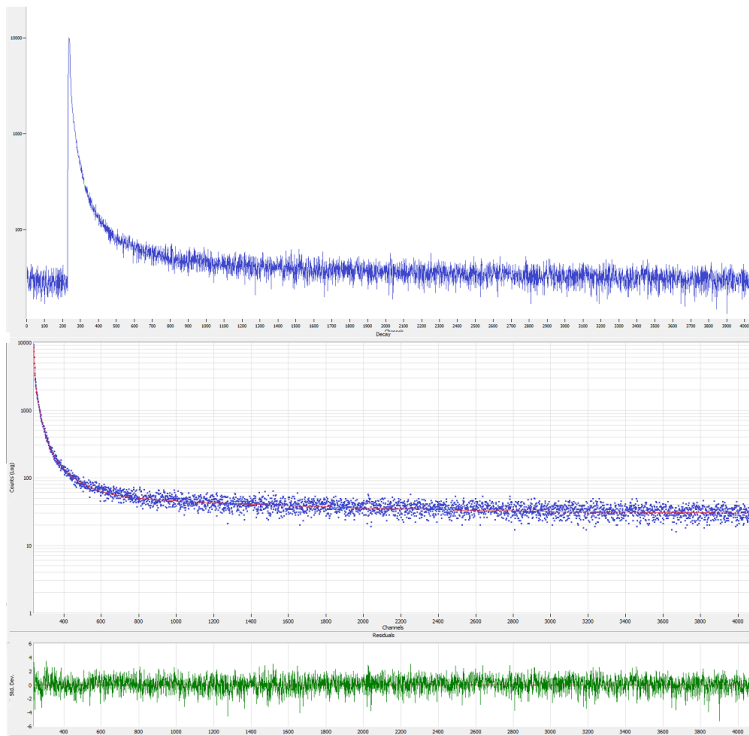


**Figure S14.** Emission decay (blue), best fit (red) and residuals (green) of **4** in CH<sub>2</sub>Cl<sub>2</sub> at rt;  $\chi^2 = 1.056$ .

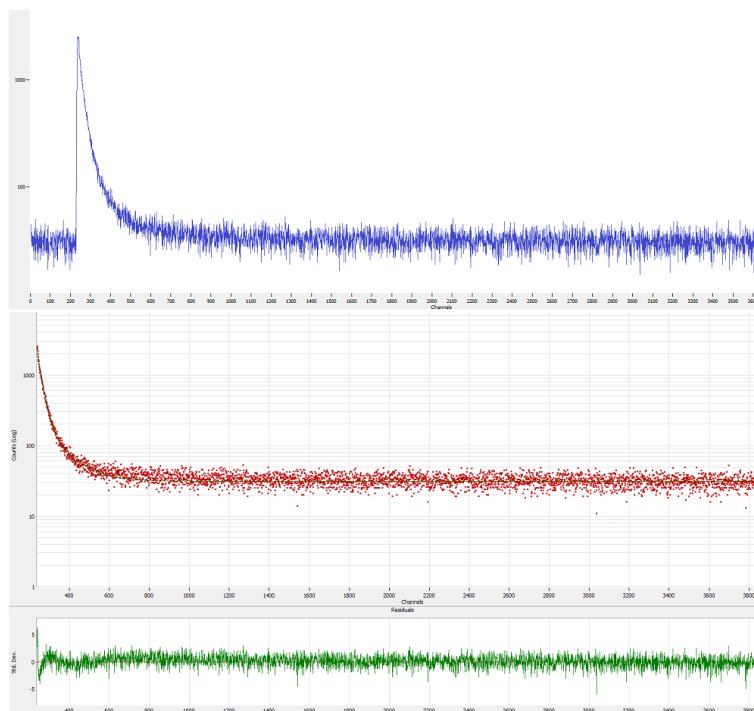




**Figure S15.** Emission decay (blue), best fit (red) and residuals (green) of **1** in solid-state at rt;  $\chi^2 = 1.084$ .



**Figure S16.** Emission decay (blue), best fit (red) and residuals (green) of **3** in solid-state at rt;  $\chi^2 = 1.061$ .



**Figure S17.** Emission decay (blue), best fit (red) and residuals (green) of **4** in solid-state at rt;  $\chi^2 = 1.150$ .