

## Supplementary Materials

# Design and Synthesis in Silico Drug-Like Prediction and Pharmacological Evaluation of Cyclopolymethylenic Homologous of LASSBio-1514.

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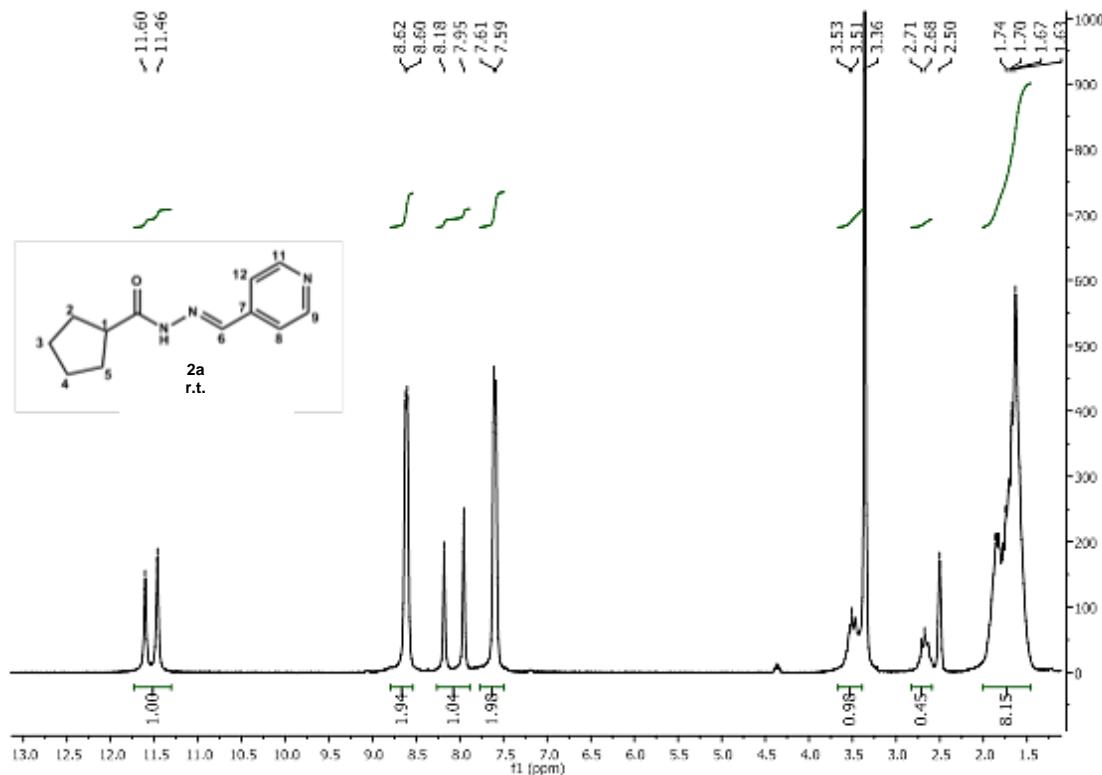
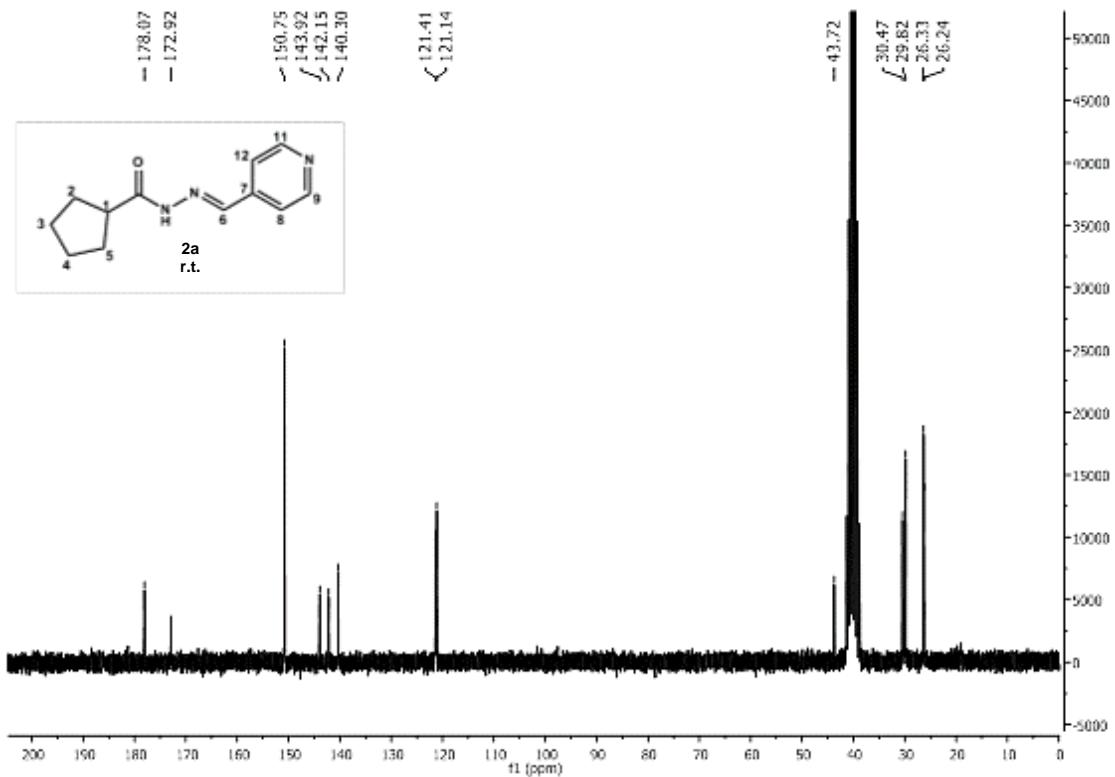
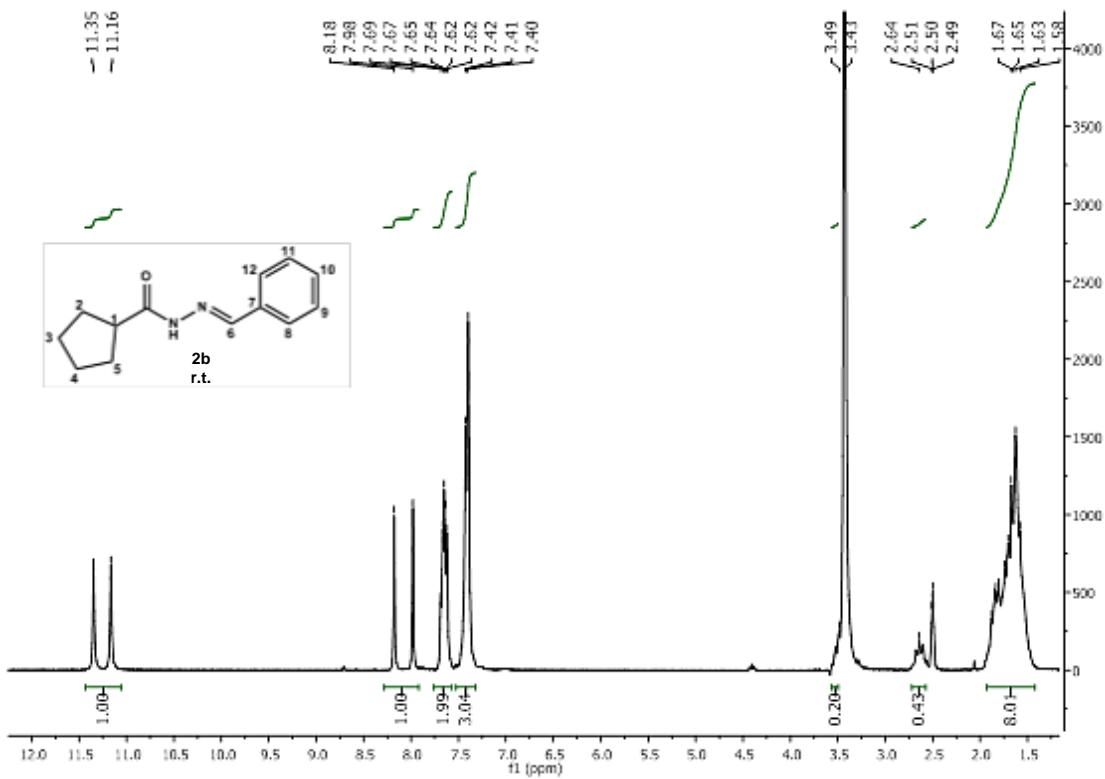


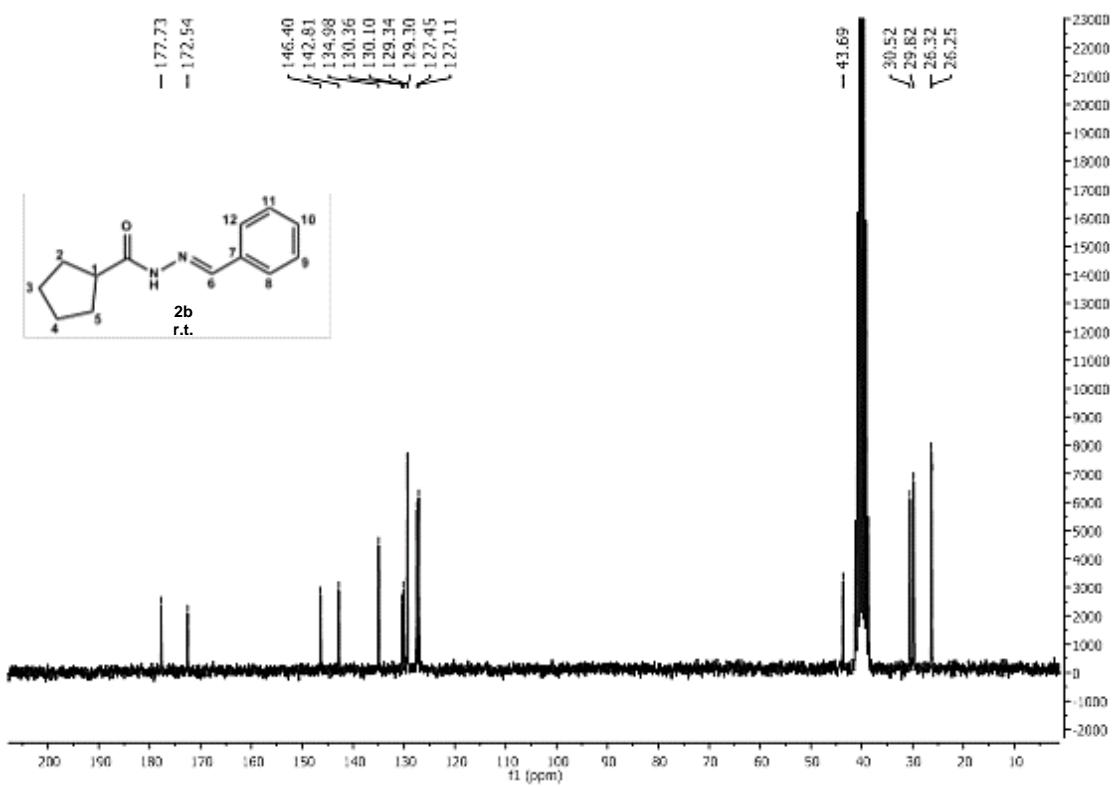
Figure S1. <sup>1</sup>H NMR spectrum of **2a** (DMSO-d<sub>6</sub>, 200 MHz).



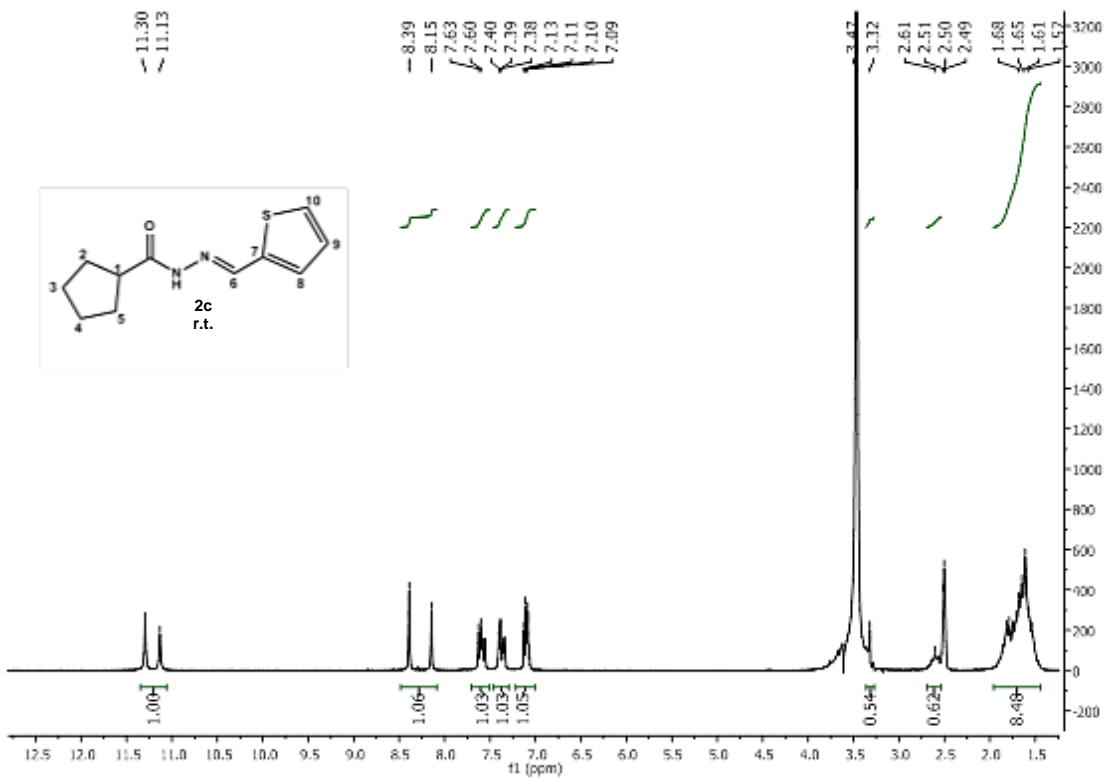
**Figure S2.**  $^{13}\text{C}$  NMR spectrum of **2a** (DMSO-d<sub>6</sub>, 50 MHz).



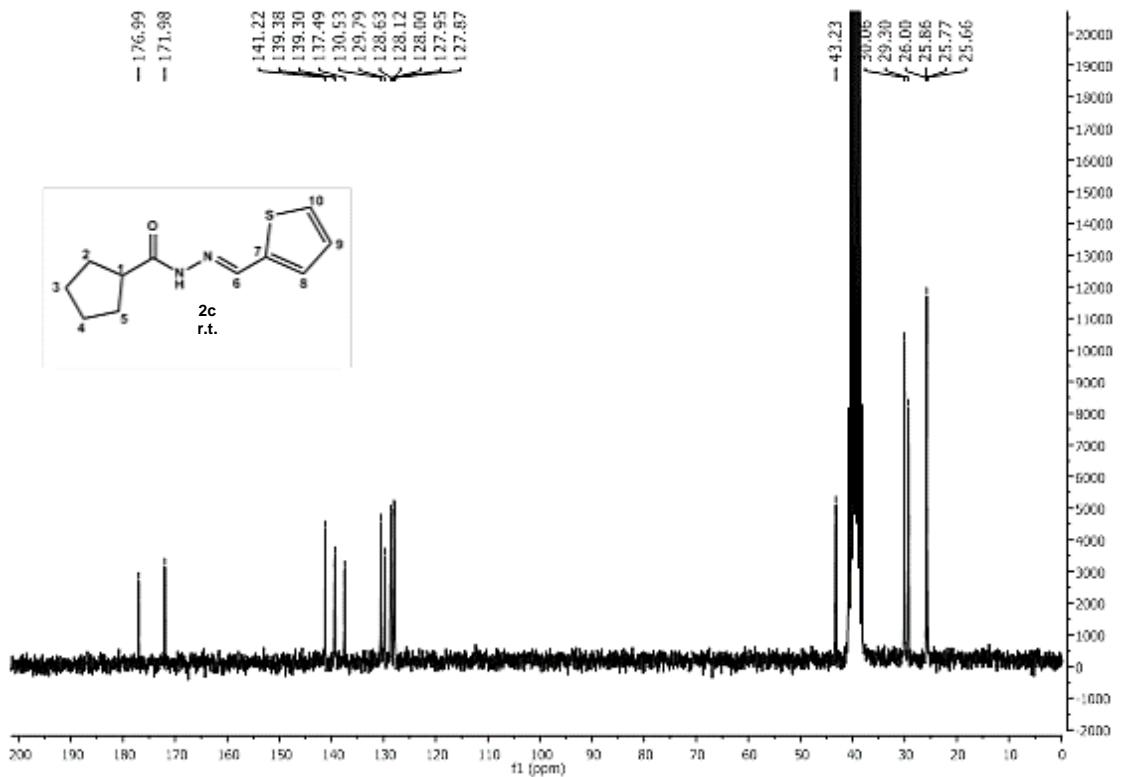
**Figure S3.**  $^1\text{H}$  NMR spectrum of **2b** (DMSO-d<sub>6</sub>, 200 MHz).



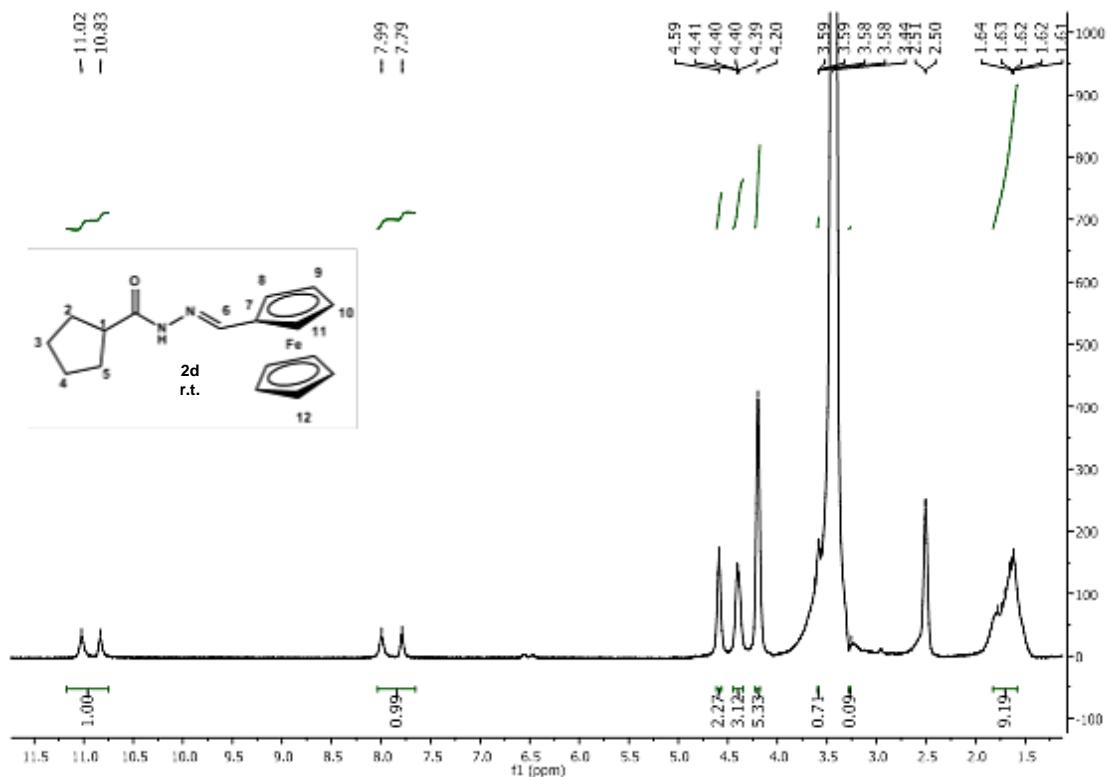
**Figure S4.**  $^{13}\text{C}$  NMR spectrum of **2b** (DMSO-d<sub>6</sub>, 50 MHz).



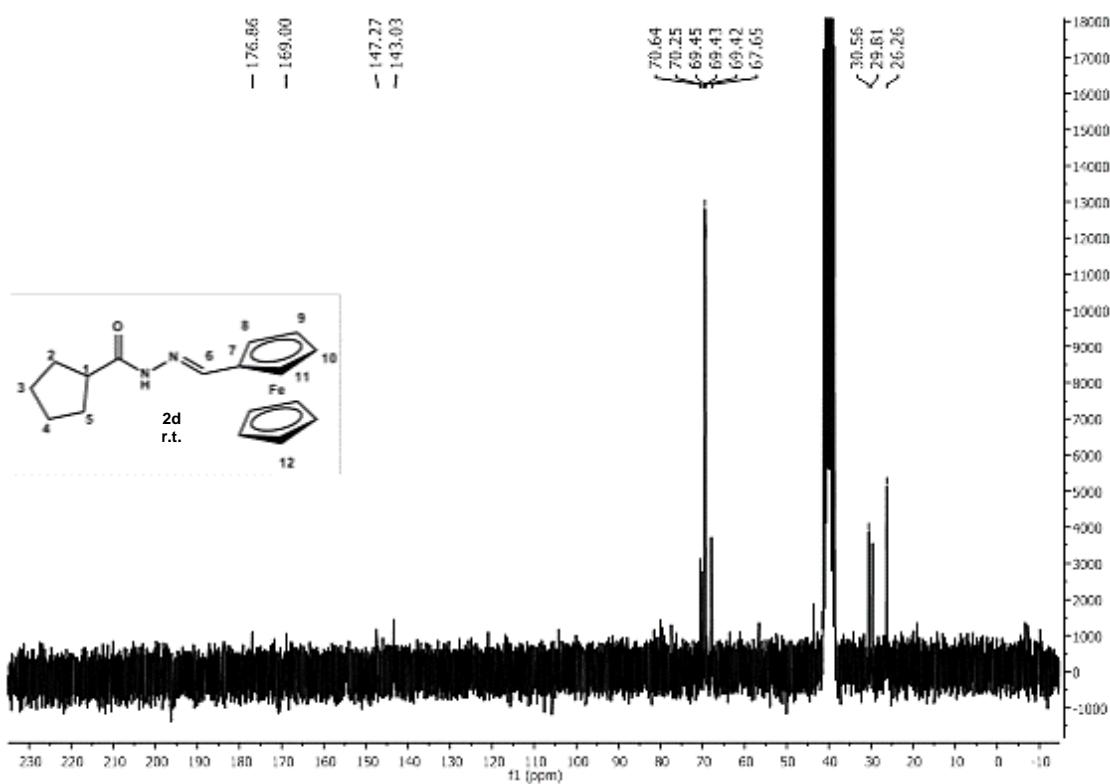
**Figure S5.**  $^1\text{H}$  NMR spectrum of **2c** (DMSO-d<sub>6</sub>, 200 MHz).



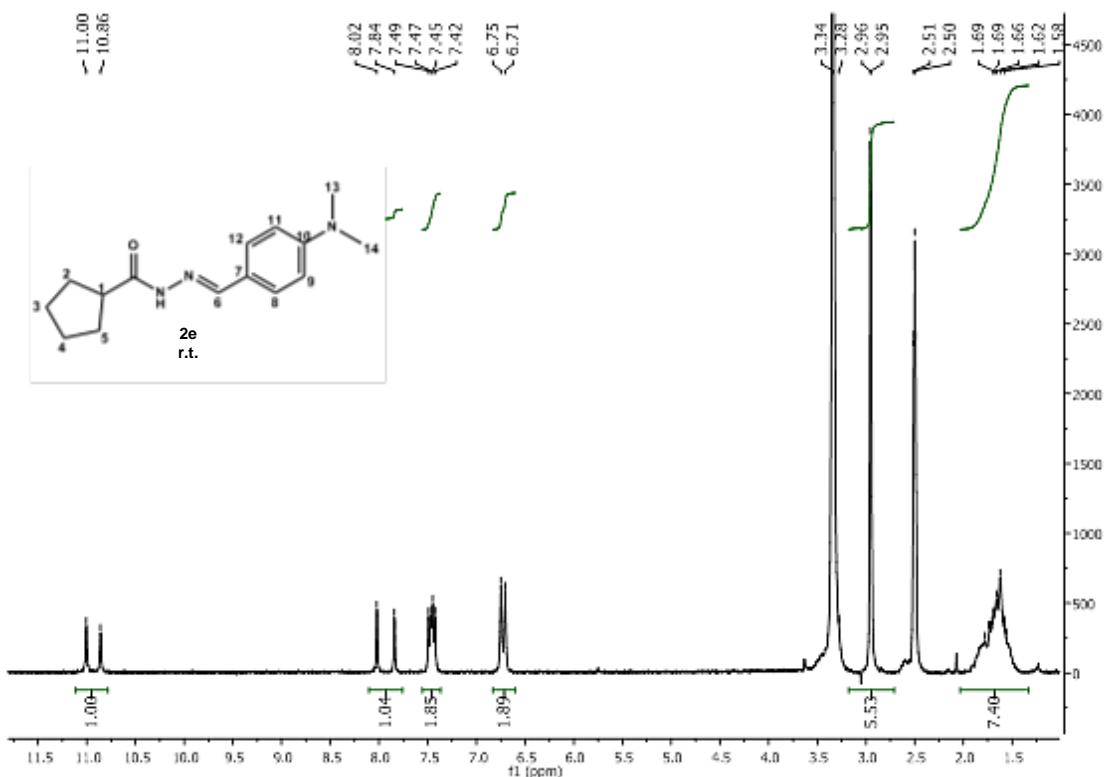
**Figure S6.**  $^{13}\text{C}$  NMR spectrum of **2c** (DMSO-d<sub>6</sub>, 50 MHz).



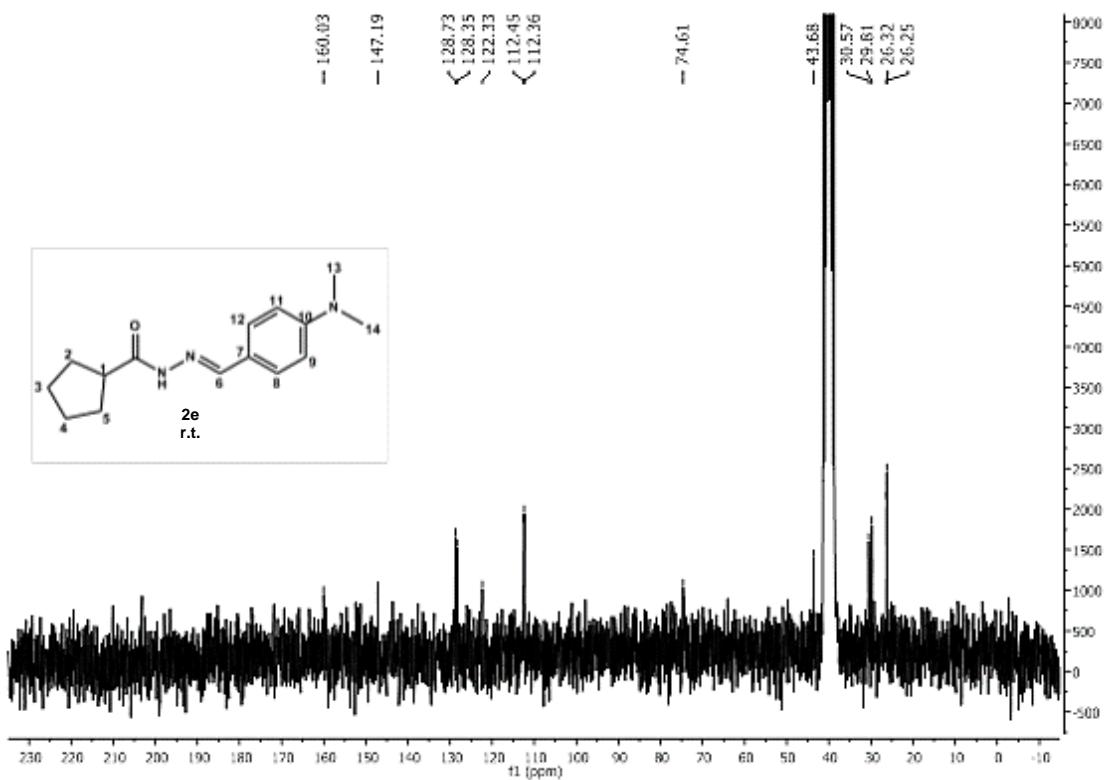
**Figure S7.**  $^1\text{H}$  NMR spectrum of **2d** (DMSO- $\text{d}_6$ , 200 MHz).



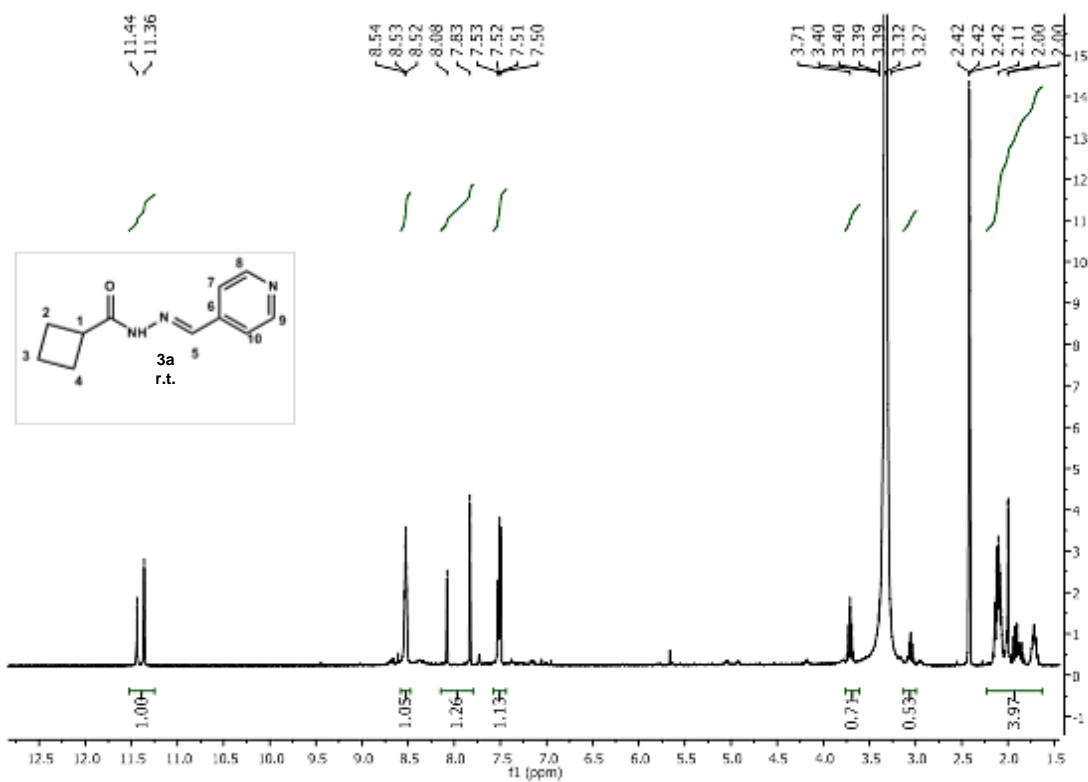
**Figure S8.** <sup>13</sup>C NMR spectrum of **2d** (DMSO-d<sub>6</sub>, 50 MHz).



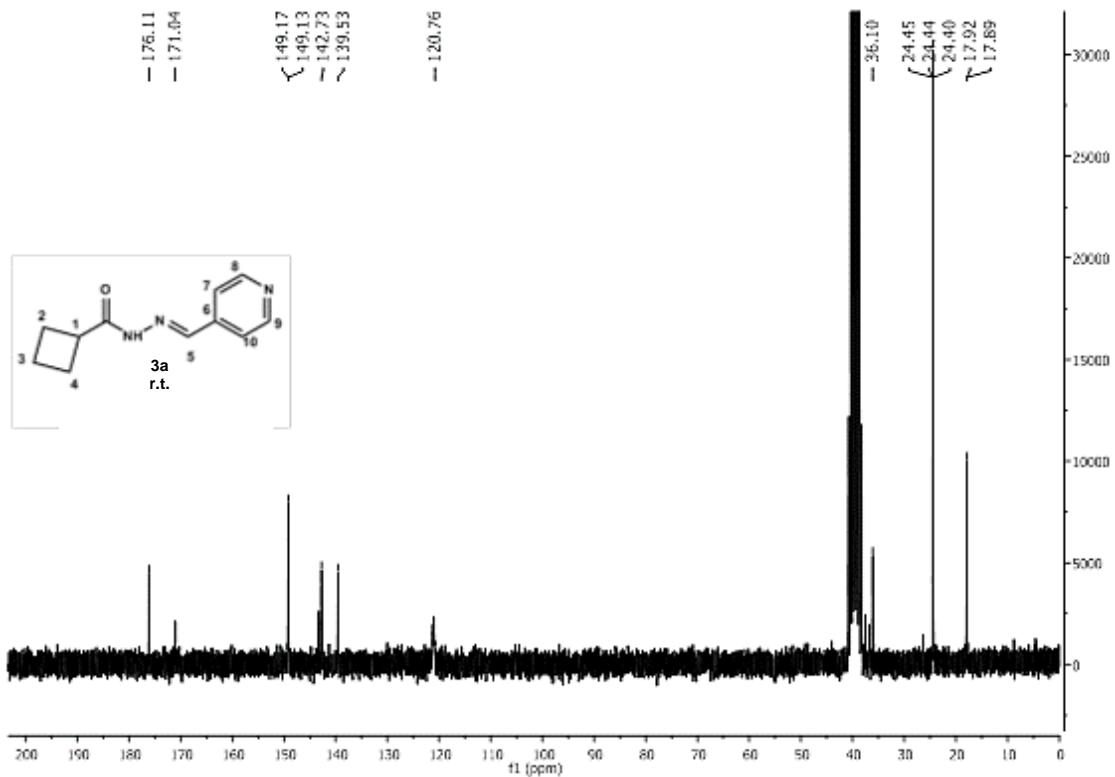
**Figure S9.** <sup>1</sup>H NMR spectrum of **2e** (DMSO-d<sub>6</sub>, 200 MHz).



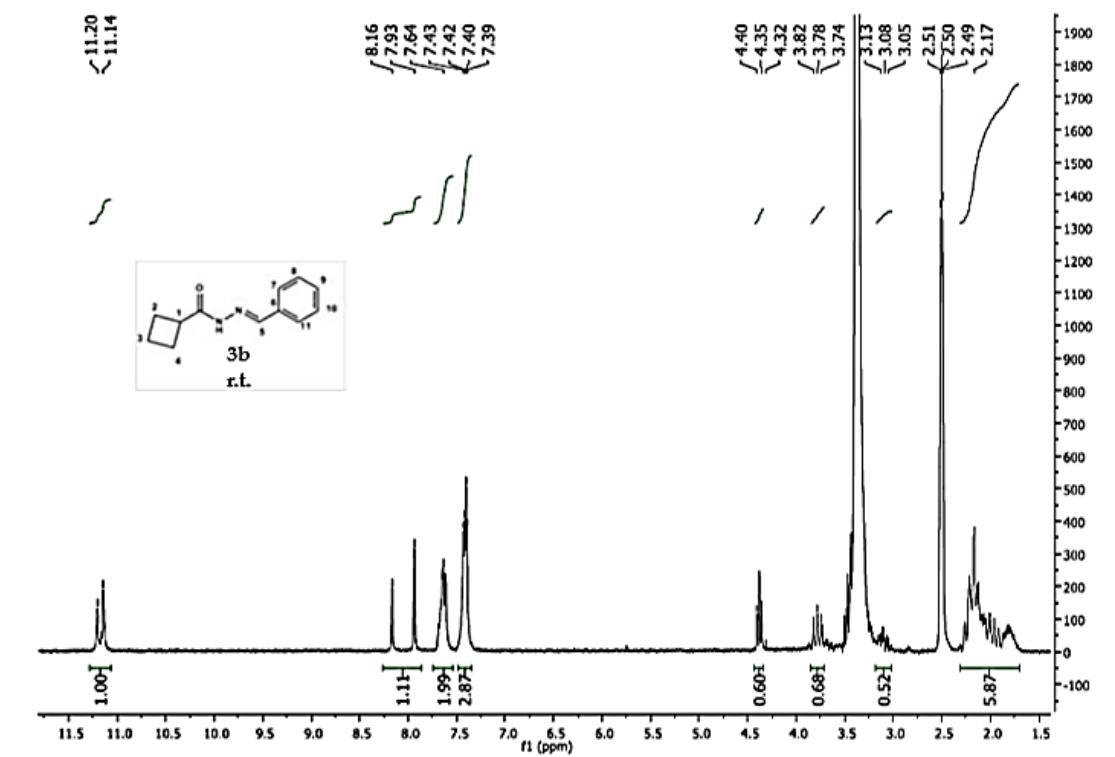
**Figure S10.**  $^{13}\text{C}$  NMR spectrum of **2e** ( $\text{CDCl}_3$ , 50 MHz).



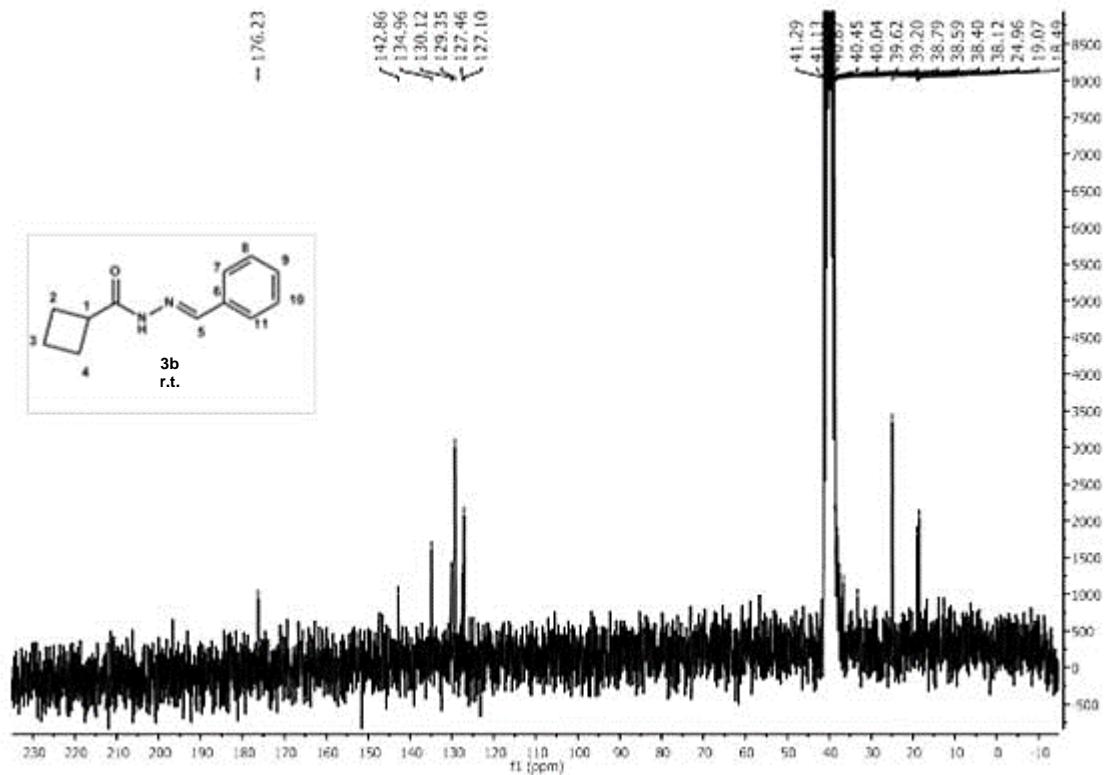
**Figure S11.**  $^1\text{H}$  NMR spectrum of **3a** (DMSO-d<sub>6</sub>, 200 MHz).



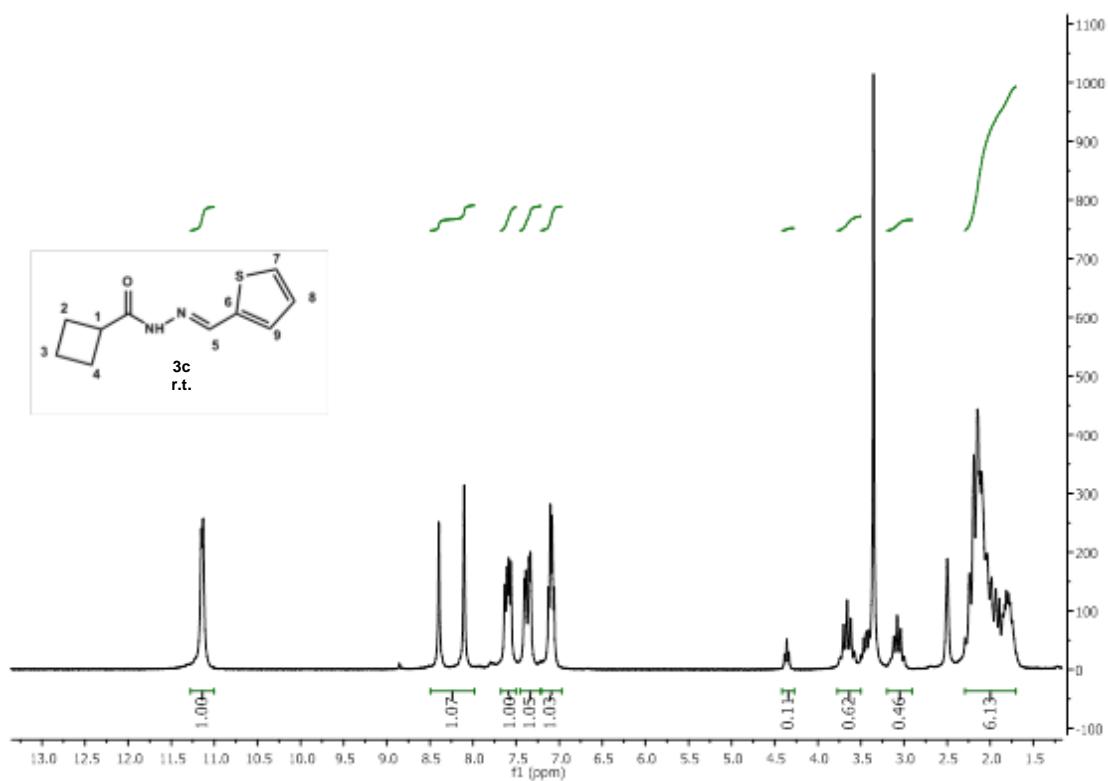
**Figure S12.**  $^{13}\text{C}$  NMR spectrum of **3a** (DMSO-d<sub>6</sub>, 50 MHz).



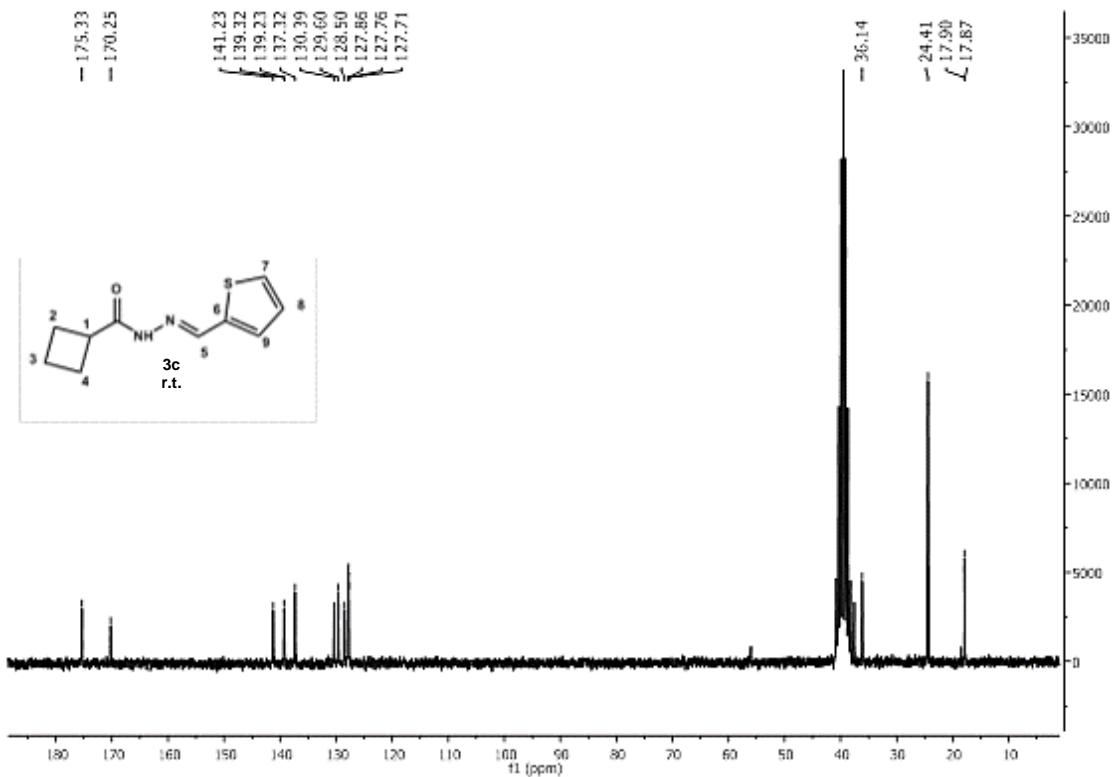
**Figure S13.**  $^1\text{H}$  NMR spectrum of **3b** (DMSO-d<sub>6</sub>, 400 MHz).



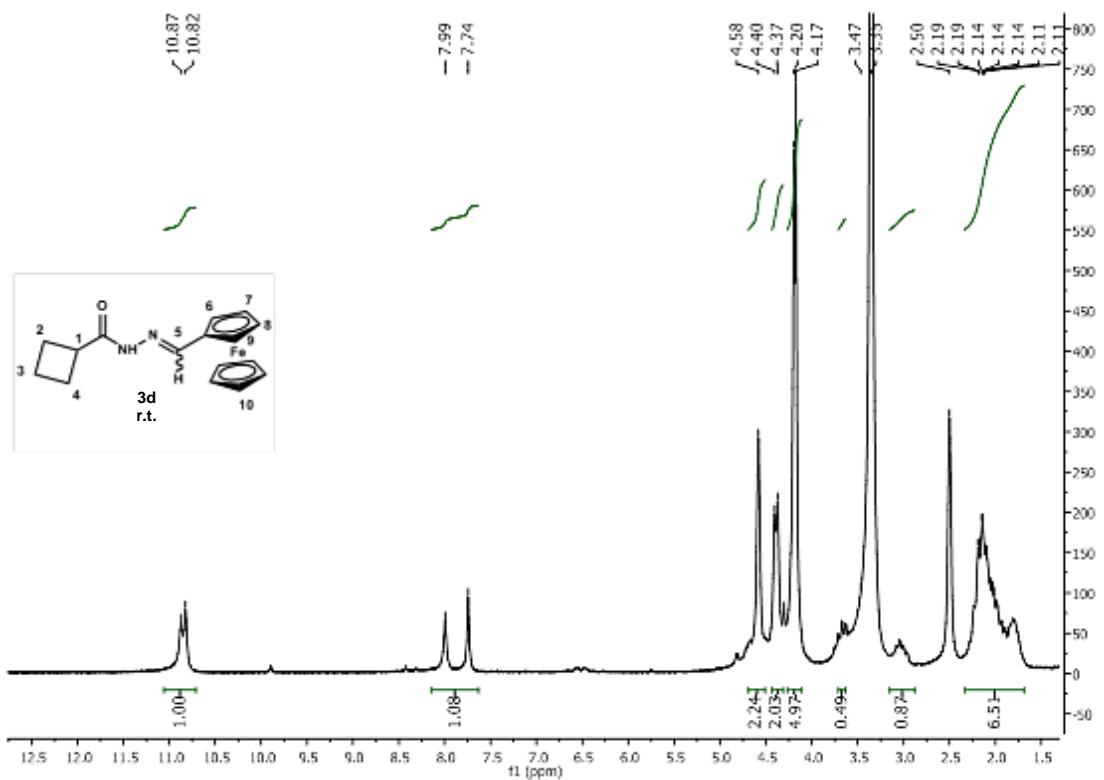
**Figure S14.**  $^{13}\text{C}$  NMR spectrum of **3b** (DMSO-d<sub>6</sub>, 50 MHz).



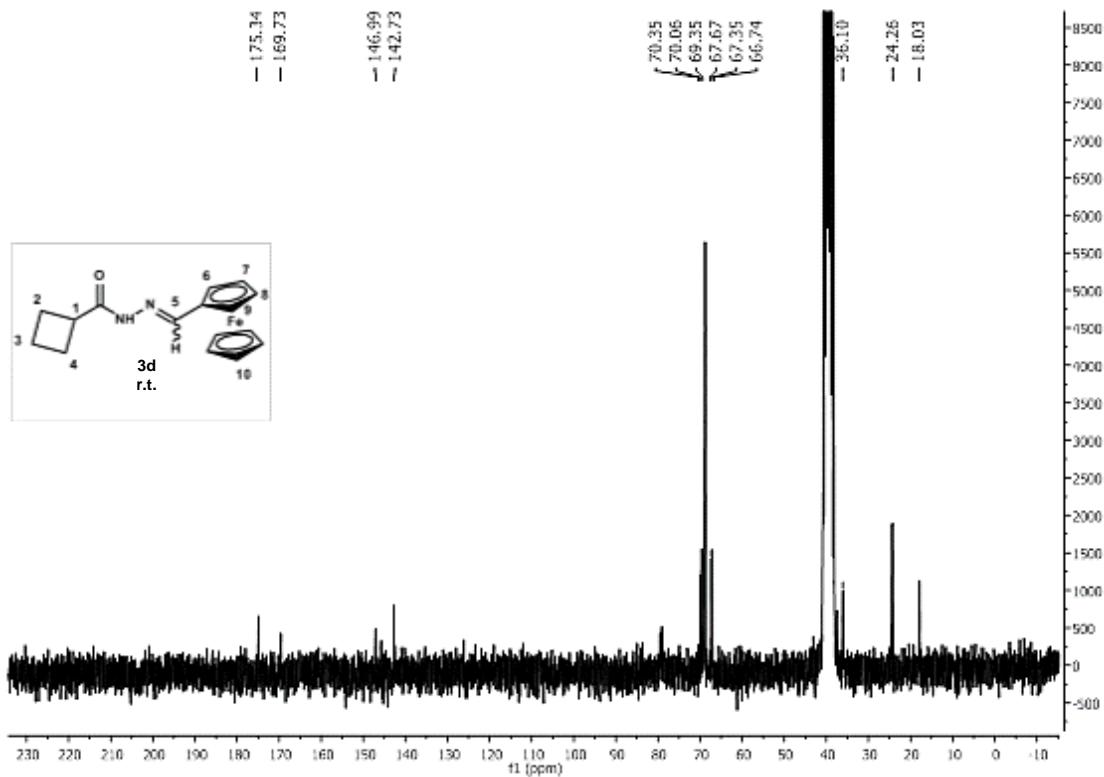
**Figure S15.**  $^1\text{H}$  NMR spectrum of **3c** (DMSO-d<sub>6</sub>, 200 MHz).



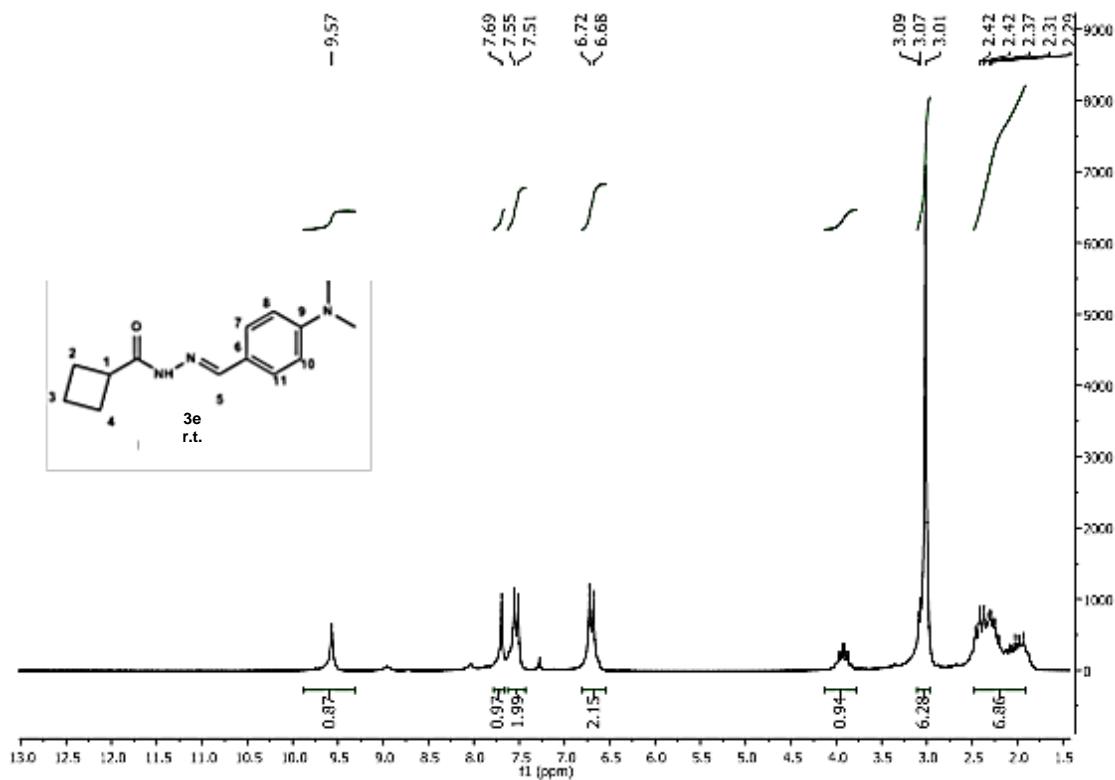
**Figure S16.**  $^{13}\text{C}$  NMR spectrum of **3c** (DMSO-d<sub>6</sub>, 50 MHz).



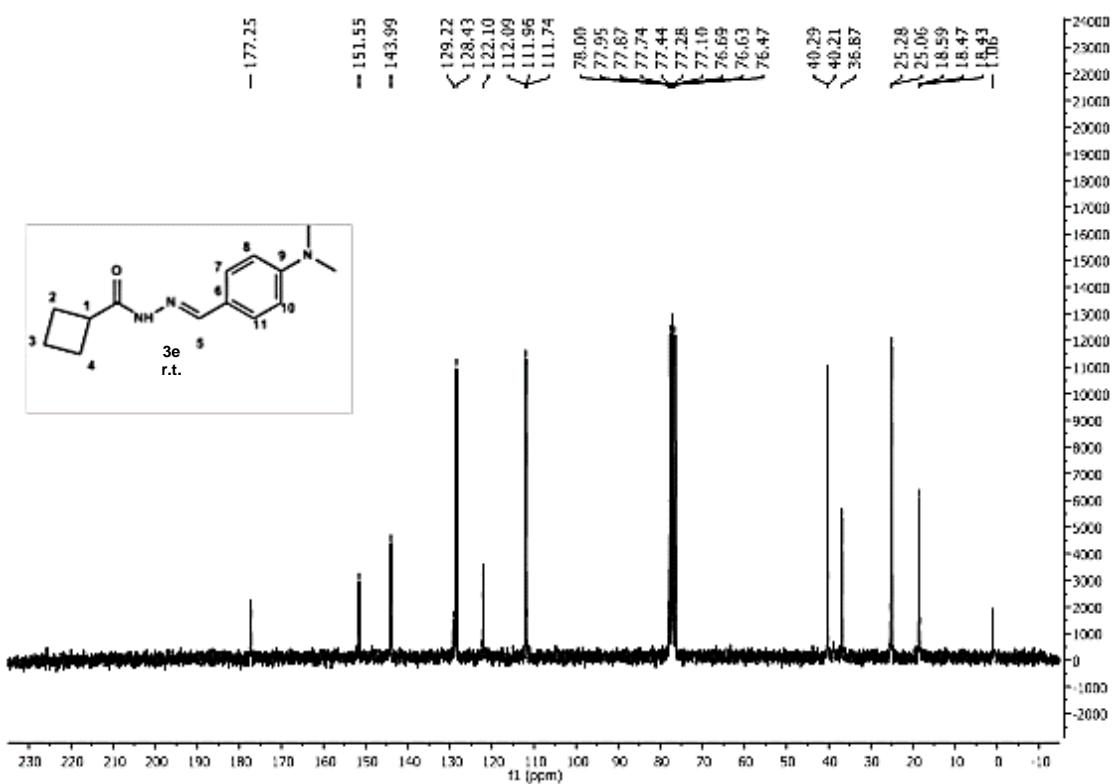
**Figure S17.**  $^1\text{H}$  NMR spectrum of **3d** (DMSO-d<sub>6</sub>, 200 MHz).



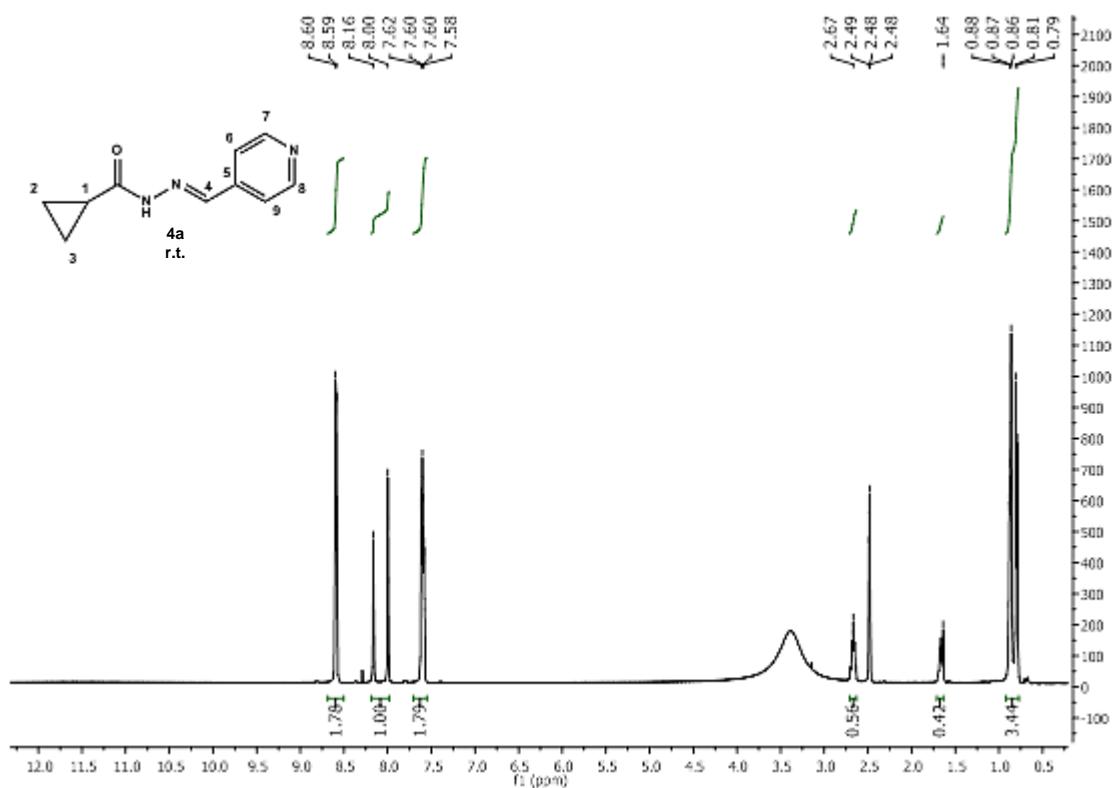
**Figure S18.**  $^{13}\text{C}$  NMR spectrum of **3d** (DMSO-d<sub>6</sub>, 50 MHz).



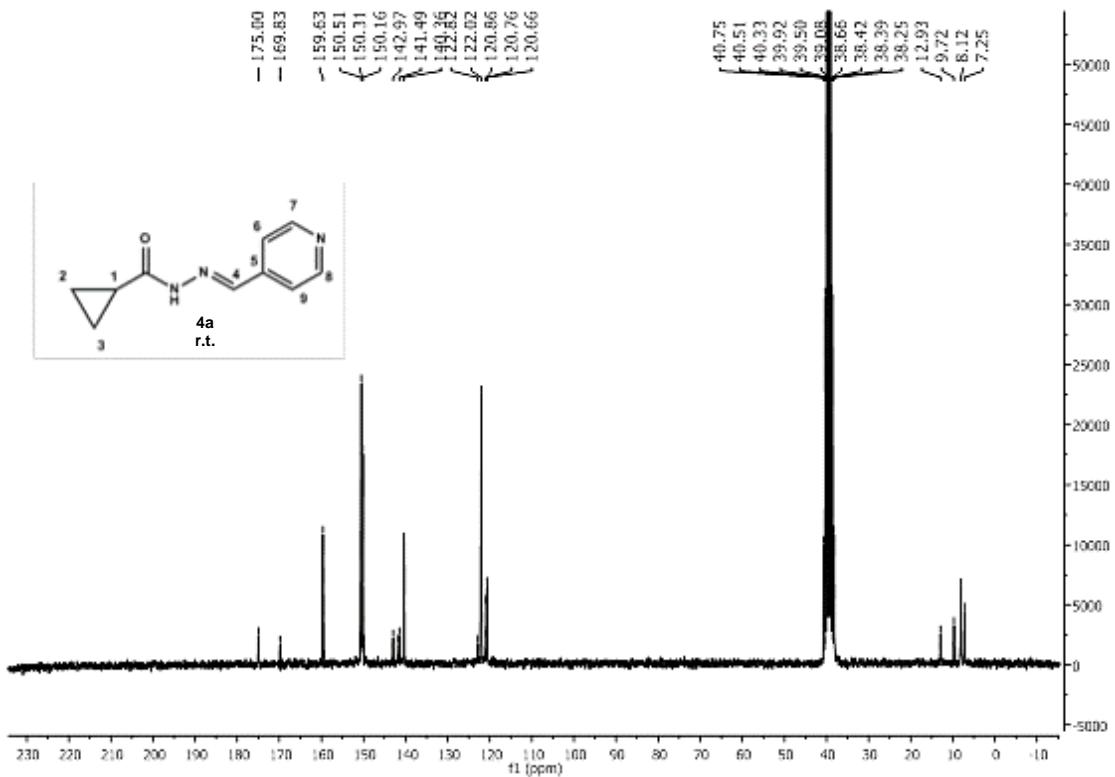
**Figure S19.**  $^1\text{H}$  NMR spectrum of **3e** ( $\text{CDCl}_3$ , 200 MHz).



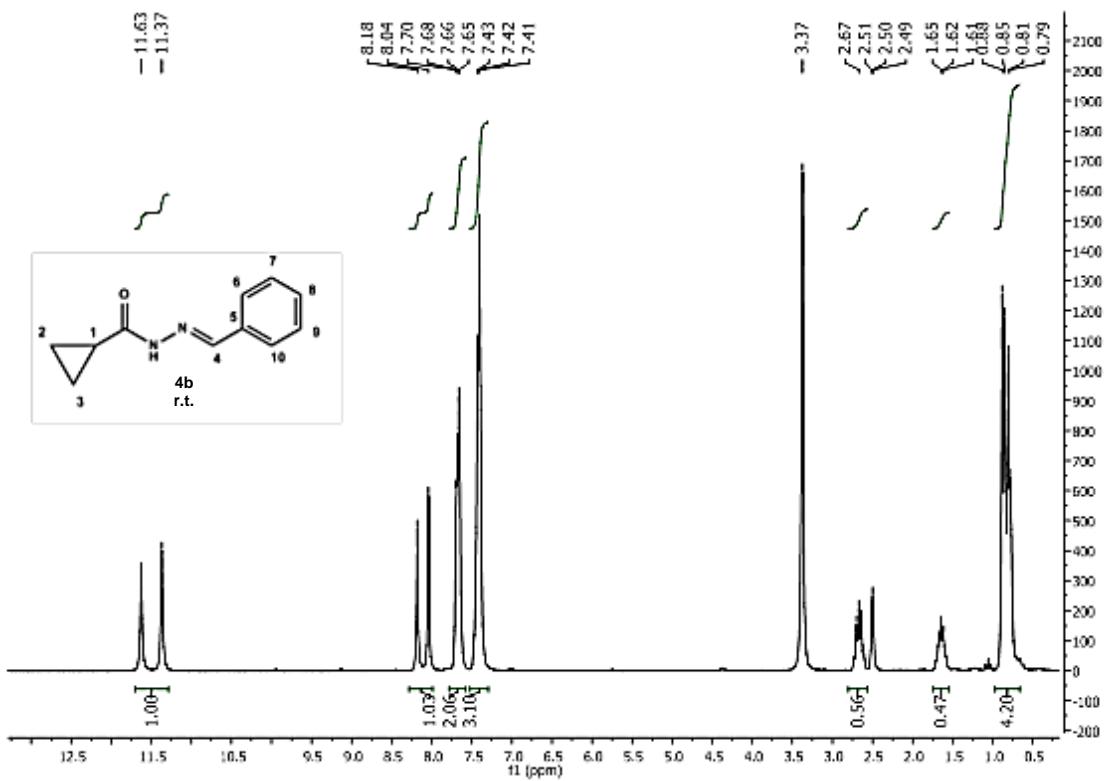
**Figure S20.**  $^{13}\text{C}$  NMR spectrum of **3e** ( $\text{CDCl}_3$ , 50 MHz).



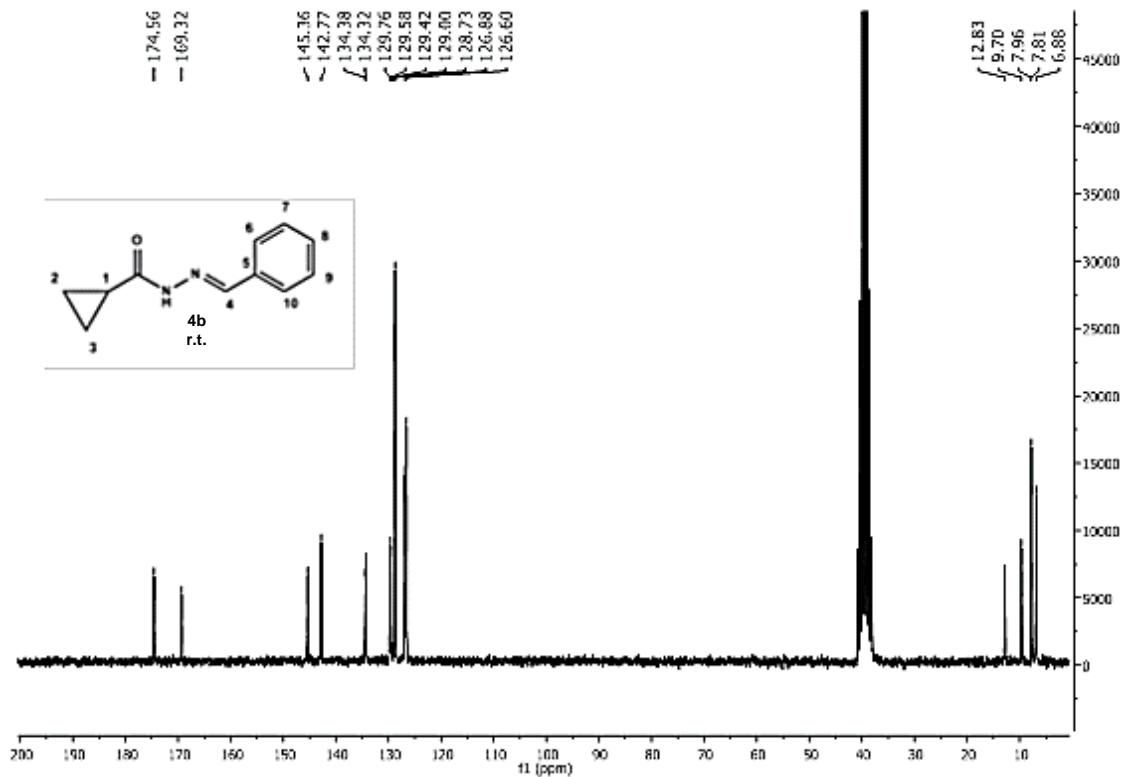
**Figure S21.**  $^1\text{H}$  NMR spectrum of **4a** ( $\text{DMSO-d}_6$ , 200 MHz).



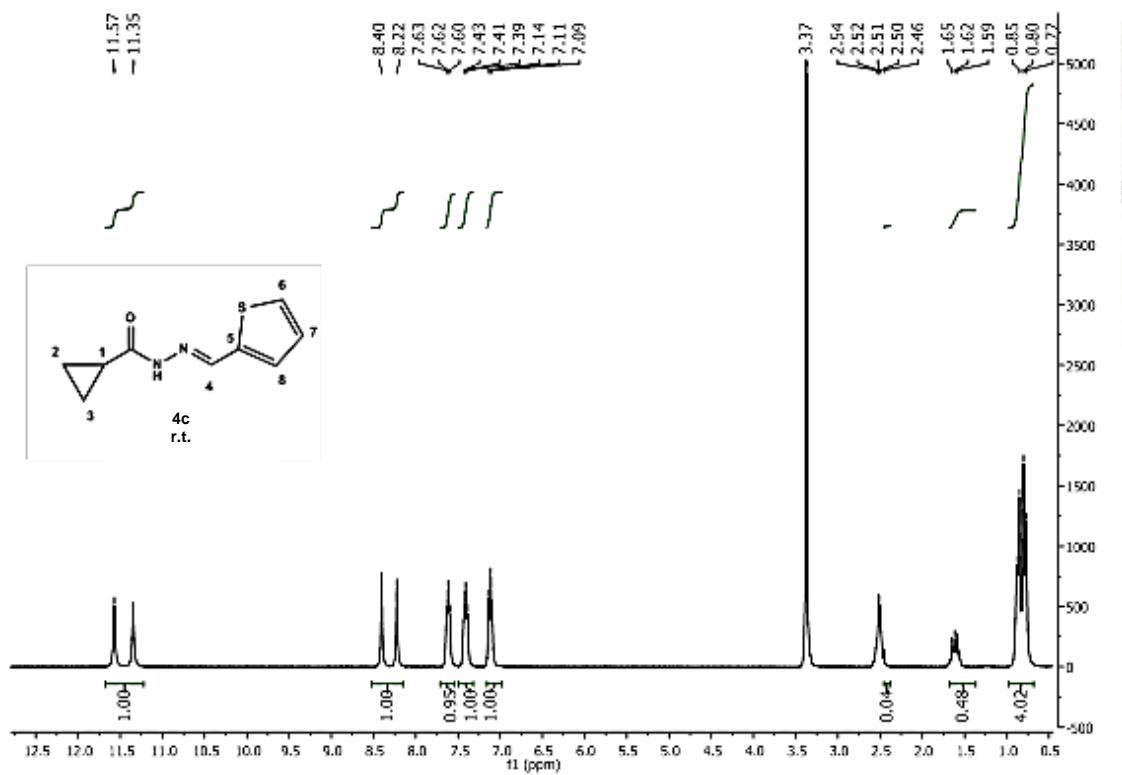
**Figure S22.**  $^{13}\text{C}$  NMR spectrum of **4a** (DMSO-d<sub>6</sub>, 50 MHz).



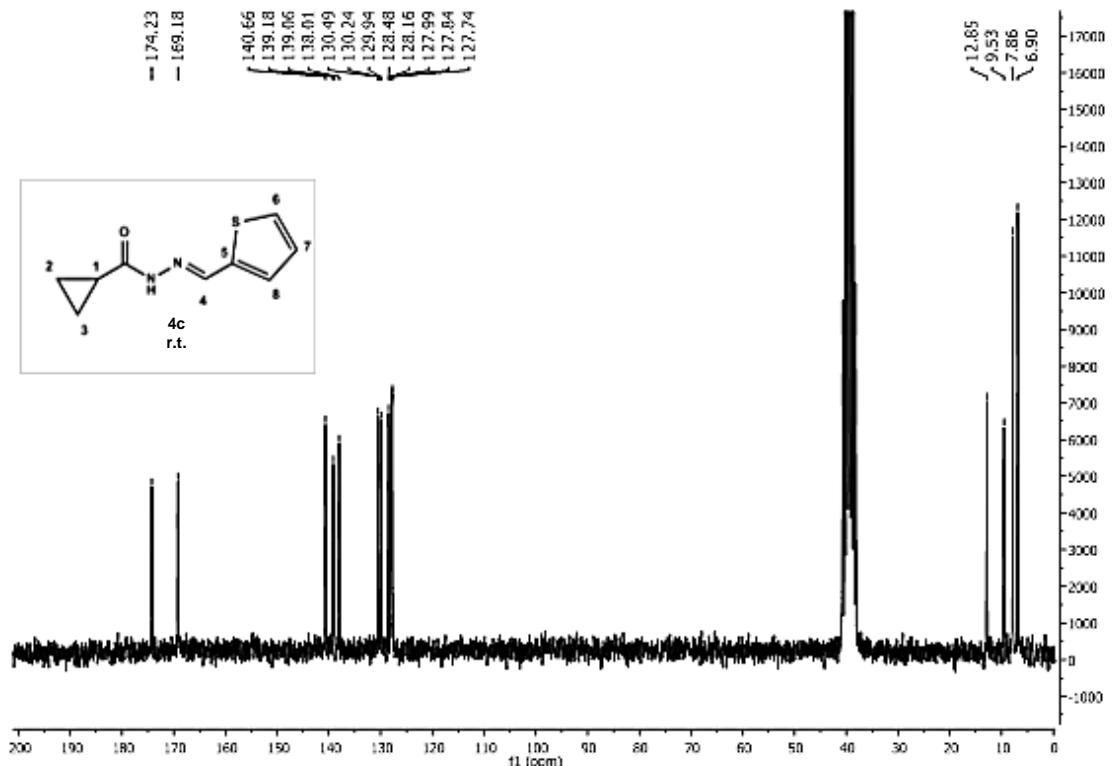
**Figure S23.**  $^1\text{H}$  NMR spectrum of **4b** (DMSO-d<sub>6</sub>, 200 MHz).



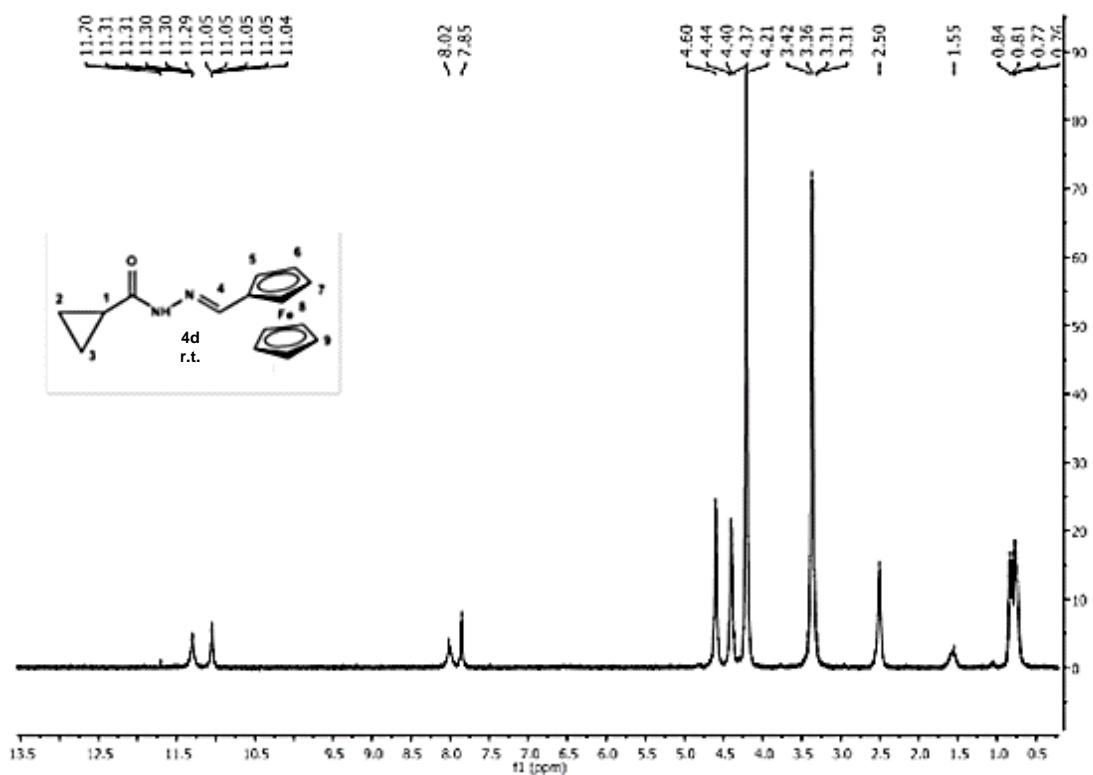
**Figure S24.**  $^{13}\text{C}$  NMR spectrum of **4b** (DMSO-d<sub>6</sub>, 50 MHz).



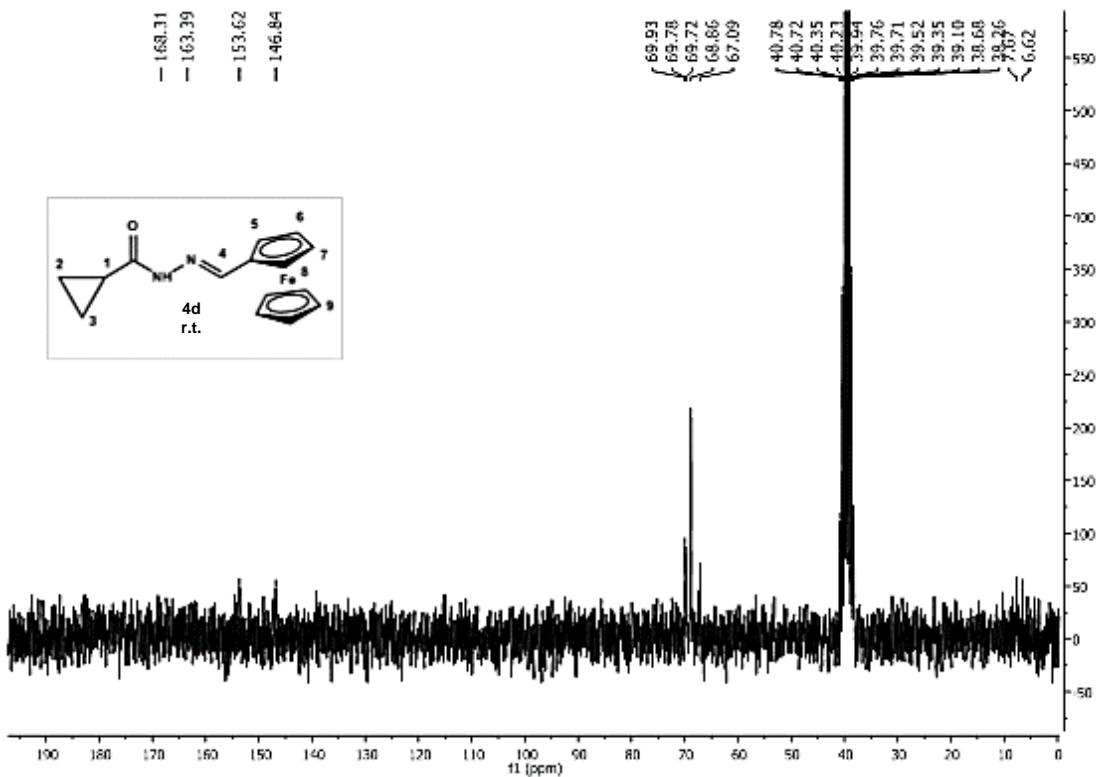
**Figure S25.**  $^1\text{H}$  NMR spectrum of **4c** (DMSO-d<sub>6</sub>, 200 MHz).



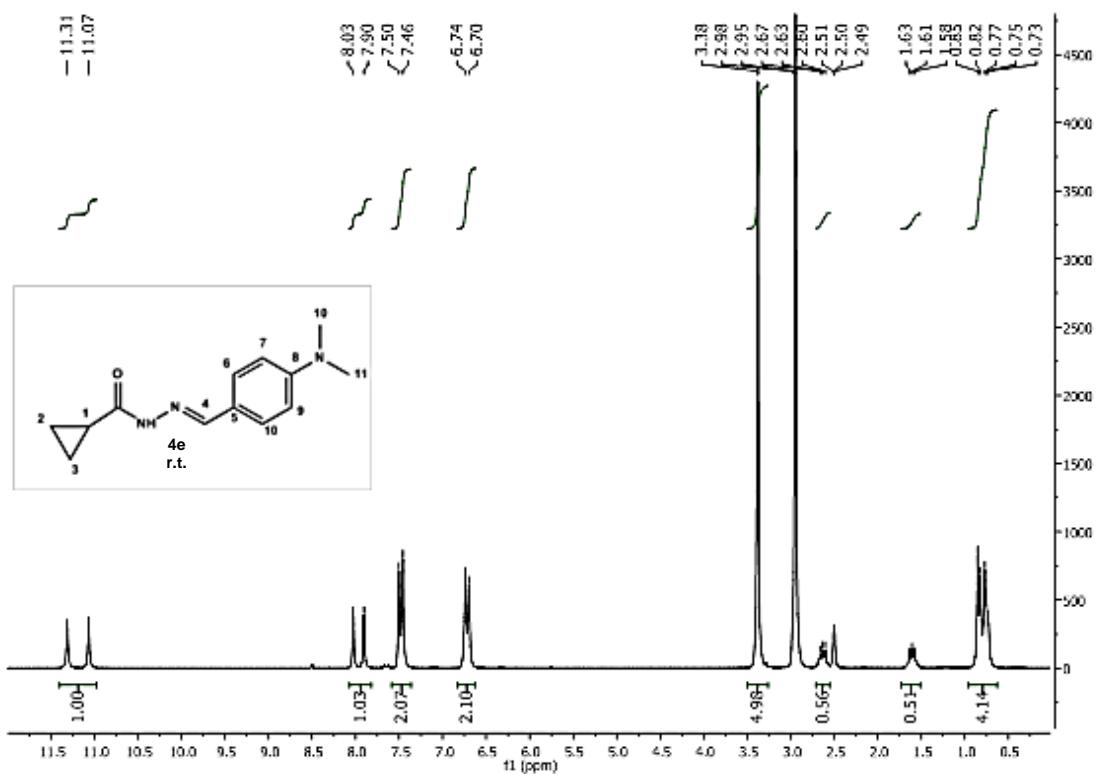
**Figure S26.**  $^{13}\text{C}$  NMR spectrum of **4c** (DMSO-d<sub>6</sub>, 50 MHz).



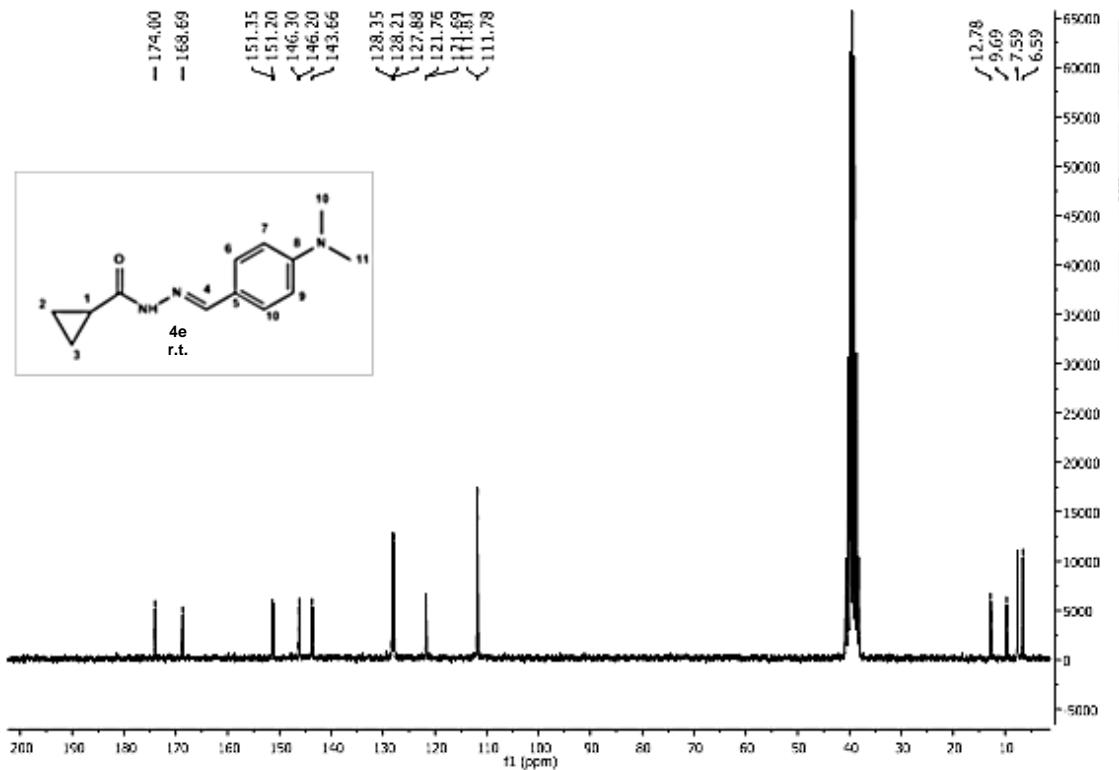
**Figure S27.**  $^1\text{H}$  NMR spectrum of **4d** (DMSO-d<sub>6</sub>, 200 MHz).



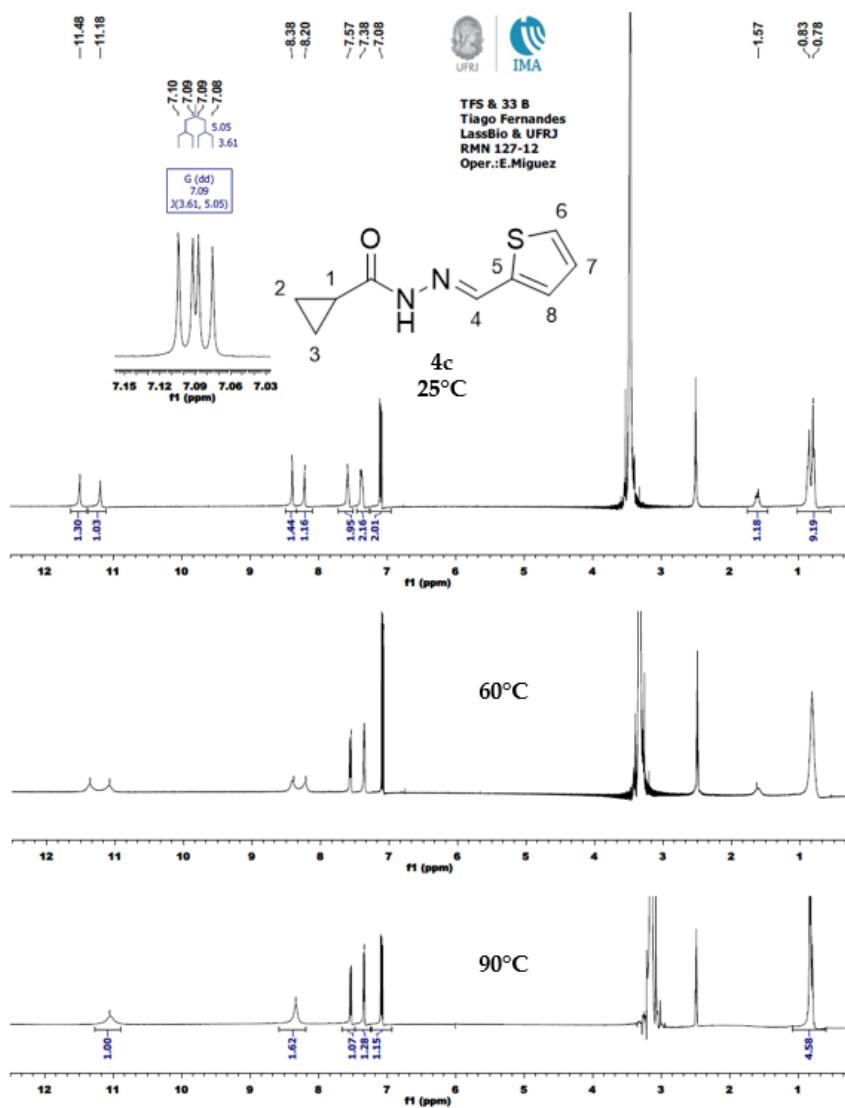
**Figure S28.**  $^{13}\text{C}$  NMR spectrum of **4d** (DMSO-d<sub>6</sub>, 50 MHz).



**Figure S29.**  $^1\text{H}$  NMR spectrum of **4e** (DMSO-d<sub>6</sub>, 200 MHz).



**Figure S30.** <sup>13</sup>C NMR spectrum of **4e** (DMSO-d<sub>6</sub>, 50 MHz).



**Figure S31.**  $^1\text{H}$  NMR spectra of **4c** at different temperatures (DMSO-d<sub>6</sub>, 300 MHz).