

## New Journal of Chemistry

### *Supporting Information*

#### **Coordination compounds containing 2-pyridylselenium ligands: synthesis, structural characterization, and antibacterial evaluation**

Rodrigo Cervo,<sup>a</sup> Thaísa R. R. Lopes,<sup>b</sup> Adriana R. de Vasconcelos,<sup>b</sup> Juliana F. Cargnelutti,<sup>b</sup> Ricardo F. Schumacher,<sup>b</sup> Bárbara Tirloni,<sup>a</sup> Sailer S. dos Santos,<sup>a</sup> Ulrich Abram,<sup>c</sup> Ernesto S. Lang<sup>a</sup> and Roberta Cargnelutti<sup>a\*</sup>

<sup>a</sup> Departamento de Química, CCNE, Universidade Federal de Santa Maria – UFSM, Santa Maria, 97105-900, RS, Brazil.

<sup>b</sup> Laboratório de Bacteriologia (LABAC), Departamento de Medicina Veterinária Preventiva – CCR/UFSM, Santa Maria, 97105-900, RS, Brazil.

<sup>c</sup> Institute of Chemistry and Biochemistry, Freie Universität Berlin, Fabeckstr. 34-36, D-14195, Berlin, Germany.

\* Corresponding author: [roberta.cargnelutti@ufsm.br](mailto:roberta.cargnelutti@ufsm.br)

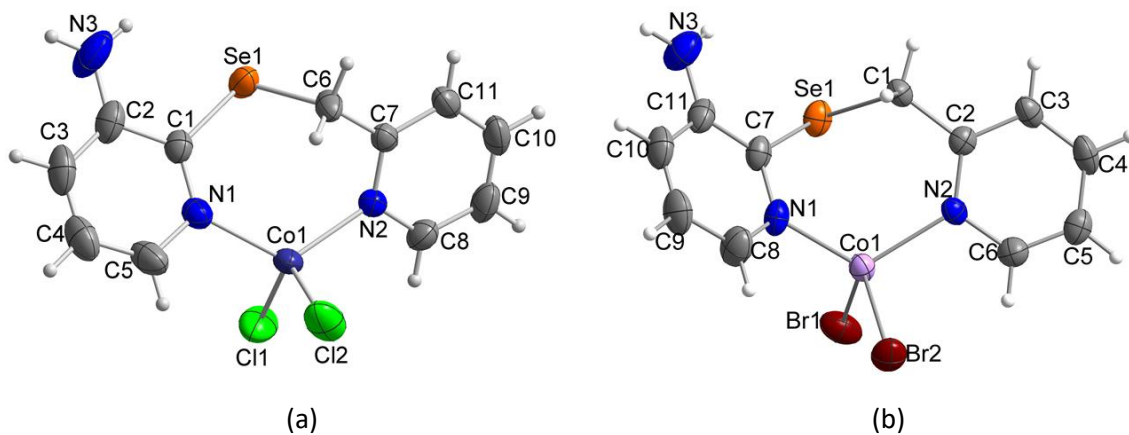
## Table of Contents

<b>Table S1.</b> Crystallographic and structure refinement data for complexes <b>1</b> , <b>2</b> , <b>3</b> , <b>5</b> and <b>6</b> .....	03
<b>Figure S1.</b> Ellipsoid representations (50% probability) of [CoCl <sub>2</sub> (L)] ( <b>1</b> ) (a) and [CoBr <sub>2</sub> (L)] ( <b>2</b> ) (b).....	04
<b>Figure S2.</b> Ellipsoid representations (50% probability) of [CuCl <sub>2</sub> (L)] ( <b>3</b> ) and ZnCl <sub>2</sub> (L)] ( <b>5</b> ).....	04
<b>Figure S3.</b> Ellipsoid representations (50% probability) of [ReO(apySe) <sub>2</sub> ]Cl·DMF ( <b>6</b> ).....	04
<b>Figure S4.</b> <sup>77</sup> Se NMR (76 MHz, CDCl <sub>3</sub> ) spectrum of Ligand L.....	05
<b>Figure S5.</b> <sup>1</sup> H NMR (400 MHz, DMSO- <i>d</i> <sub>6</sub> ) spectrum of complex <b>5</b> .....	05
<b>Figure S6.</b> <sup>13</sup> C NMR (100 MHz, DMSO- <i>d</i> <sub>6</sub> ) spectrum of complex <b>5</b> .....	06
<b>Figure S7.</b> <sup>77</sup> Se NMR (76 MHz, DMSO- <i>d</i> <sub>6</sub> ) spectrum of complex <b>5</b> .....	06
<b>Figure S8.</b> 2D COSY NMR spectrum of complex <b>5</b> (DMSO- <i>d</i> <sub>6</sub> ).....	07
<b>Figure S9.</b> 2D COSY expansion spectrum of complex <b>5</b> (DMSO- <i>d</i> <sub>6</sub> ).....	07
<b>Figure S10.</b> 2D HMQC NMR spectrum of complex <b>5</b> (DMSO- <i>d</i> <sub>6</sub> ).....	08
<b>Figure S11.</b> 2D HSQC expansion spectrum of complex <b>5</b> (DMSO- <i>d</i> <sub>6</sub> ).....	08
<b>Figure S12.</b> <sup>1</sup> H NMR (400 MHz, DMSO- <i>d</i> <sub>6</sub> ) spectrum of (apySe) <sub>2</sub> .....	09
<b>Figure S13.</b> <sup>77</sup> Se NMR (76 MHz, DMSO- <i>d</i> <sub>6</sub> ) spectrum of (apySe) <sub>2</sub> .....	09
<b>Figure S14.</b> <sup>1</sup> H NMR (400 MHz, DMSO- <i>d</i> <sub>6</sub> ) spectrum of complex <b>6</b> .....	10
<b>Figure S15.</b> <sup>13</sup> C NMR (100 MHz, DMSO- <i>d</i> <sub>6</sub> ) spectrum of complex <b>6</b> .....	10
<b>Figure S16.</b> <sup>77</sup> Se NMR (76 MHz, DMSO- <i>d</i> <sub>6</sub> ) spectrum of complex <b>6</b> .....	11
<b>Figure S17.</b> 2D COSY NMR spectrum of complex <b>6</b> (DMSO- <i>d</i> <sub>6</sub> ).....	11
<b>Figure S18.</b> 2D COSY expansion spectrum of complex <b>6</b> (DMSO- <i>d</i> <sub>6</sub> ).....	12
<b>Figure S19.</b> 2D HSQC NMR spectrum of complex <b>6</b> (DMSO- <i>d</i> <sub>6</sub> ).....	12
<b>Figure S20.</b> 2D HSQC expansion spectrum of complex <b>6</b> (DMSO- <i>d</i> <sub>6</sub> ).....	13
<b>Figure S21.</b> Electronic UV–Vis spectra for L in H <sub>2</sub> O/DMSO (4:1, v/v) solution, measured every 1 hour (total 5 hours); [ ] = 1x10 <sup>-4</sup> M.....	13
<b>Figure S22.</b> Electronic UV–Vis spectra for <b>1</b> in H <sub>2</sub> O/DMSO (4:1, v/v) solution, measured every 1 hour (total 5 hours); [ ] = 1x10 <sup>-4</sup> M. ....	14
<b>Figure S23.</b> Electronic UV–Vis spectra for <b>2</b> in H <sub>2</sub> O/DMSO (4:1, v/v) solution, measured every 1 hour (total 5 hours); [ ] = 1x10 <sup>-4</sup> M.....	14
<b>Figure S24.</b> Electronic UV–Vis spectra for <b>3</b> in H <sub>2</sub> O/DMSO (4:1, v/v) solution, measured every 1 hour (total 5 hours); [ ] = 1x10 <sup>-4</sup> M.....	15
<b>Figure S25.</b> Electronic UV–Vis spectra for <b>4</b> in H <sub>2</sub> O/DMSO (4:1, v/v) solution, measured every 1 hour (total 5 hours); [ ] = 1x10 <sup>-4</sup> M.....	15
<b>Figure S26.</b> Electronic UV–Vis spectra for <b>5</b> in H <sub>2</sub> O/DMSO (4:1, v/v) solution, measured every 1 hour (total 5 hours); [ ] = 1x10 <sup>-4</sup> M.....	16
<b>Figure S27.</b> Electronic UV–Vis spectra for <b>6</b> in H <sub>2</sub> O/DMSO (4:1, v/v) solution, measured every 1 hour (total 5 hours); [ ] = 1x10 <sup>-4</sup> M.....	16

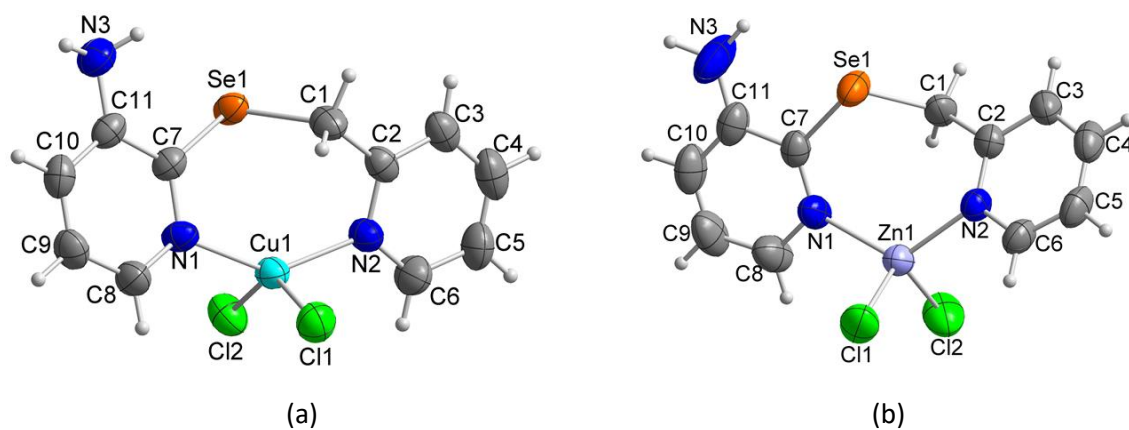
**Table S1.** Crystallographic and structure refinement data for complexes **1**, **2**, **3**, **5** and **6**.

Complex	<b>1</b>	<b>2</b>	<b>3</b>	<b>5</b>	<b>6</b>
Formula	C <sub>11</sub> H <sub>11</sub> Cl <sub>2</sub> CoN <sub>3</sub> Se	C <sub>11</sub> H <sub>11</sub> Br <sub>2</sub> CoN <sub>3</sub> Se	C <sub>11</sub> H <sub>11</sub> Cl <sub>2</sub> CuN <sub>3</sub> Se	C <sub>11</sub> H <sub>11</sub> Cl <sub>2</sub> N <sub>3</sub> SeZn	C <sub>10</sub> H <sub>10</sub> N <sub>4</sub> OReSe <sub>2</sub> Cl <sub>2</sub> C <sub>3</sub> H <sub>7</sub> NO
CCDC n°	2075668	2075669	2075670	2075671	2075672
F.W. (g·mol <sup>-1</sup> )	394.02	482.94	398.63	400.46	654.89
Crystal system	Triclinic	Monoclinic	Orthorhombic	Triclinic	Orthorhombic
Space group	<i>P</i> -1	<i>P</i> 2 <sub>1</sub> / <i>n</i>	<i>Pna</i> 2 <sub>1</sub>	<i>P</i> -1	<i>Pbca</i>
<i>a</i> (Å)	7.6910(4)	8.3309(6)	13.8873(8)	7.6948(8)	7.0855(16)
<i>b</i> (Å)	7.7691(4)	12.1666(9)	12.4918(7)	7.7787(8)	16.597(5)
<i>c</i> (Å)	12.7167(6)	14.2649(12)	7.9670(4)	12.7007(14)	31.064(9)
<i>α</i> (°)	97.9940(10)	90	90	98.027(3)	90
<i>β</i> (°)	91.522(2)	93.019(3)	90	91.224(3)	90
<i>γ</i> (°)	112.2890(10)	90	90	112.402(3)	90
T (K)	296(2)	296(2)	295(2)	296(2)	100(2)
V (Å <sup>3</sup> )	693.63(6)	1443.87(19)	1382.09(13)	693.64(13)	3653.2(17)
Z	2	4	4	2	8
<i>r</i> <sub>calc.</sub> (g·cm <sup>-3</sup> )	1.887	2.222	1.916	1.920	2.381
<i>μ</i> (mm <sup>-1</sup> )	2.219	4.907	2.413	2.507	10.801
<i>F</i> (000)	386	916	780	392	2448
Collected reflections	55879	19972	41077	10908	44575
Independent reflections [ <i>R</i> <sub>int</sub> ]	4225 [0.0427]	4433 [0.1132]	4120 [0.0578]	2690 [0.0475]	9869 [0.0361]
<i>R</i> <sub>1</sub> [ <i>I</i> > 2σ( <i>I</i> )]	0.0394	0.0491	0.0361	0.0493	0.0189
<i>wR</i> <sub>2</sub> [ <i>I</i> > 2σ( <i>I</i> )]	0.0937	0.0746	0.0815	0.1082	0.0374
<i>R</i> <sub>1</sub> (all data) <sup>[a]</sup>	0.0499	0.1199	0.0505	0.0588	0.0241
<i>wR</i> <sub>2</sub> (all data) <sup>[b]</sup>	0.0980	0.0898	0.0872	0.1146	0.0400
GOOF on <i>F</i> <sup>2</sup>	1.174	0.998	1.045	1.086	1.166
Largest diff. peak and hole (e·Å <sup>-3</sup> )	0.703 and -0.565	0.535 and -0.579	0.403 and -0.451	0.590 and -0.382	0.538 and -0.917

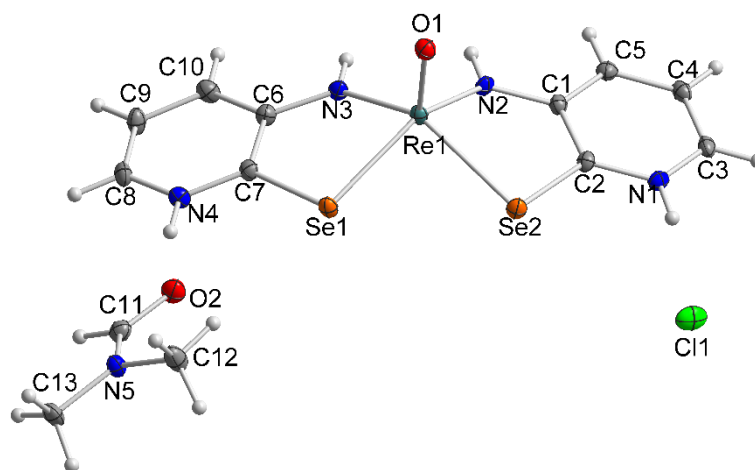
$$^{[a]}R_1 = \sum ||F_o| - |F_c|| / \sum |F_o|; \quad ^{[b]}wR_2 = \{\sum w(F_o^2 - F_c^2)^2 / \sum w(F_o^2)^2\}^{1/2}$$



**Figure S1.** Ellipsoid representations (50% probability) of [CoCl<sub>2</sub>(L)] (**1**) (a) and [CoBr<sub>2</sub>(L)] (**2**) (b).



**Figure S2.** Ellipsoid representations (50% probability) of [CuCl<sub>2</sub>(L)] (**3**) (a) and [ZnCl<sub>2</sub>(L)] (**5**) (b).



**Figure S3.** Ellipsoid representations (50% probability) of [ReO(apySe)<sub>2</sub>]Cl·DMF (**6**).

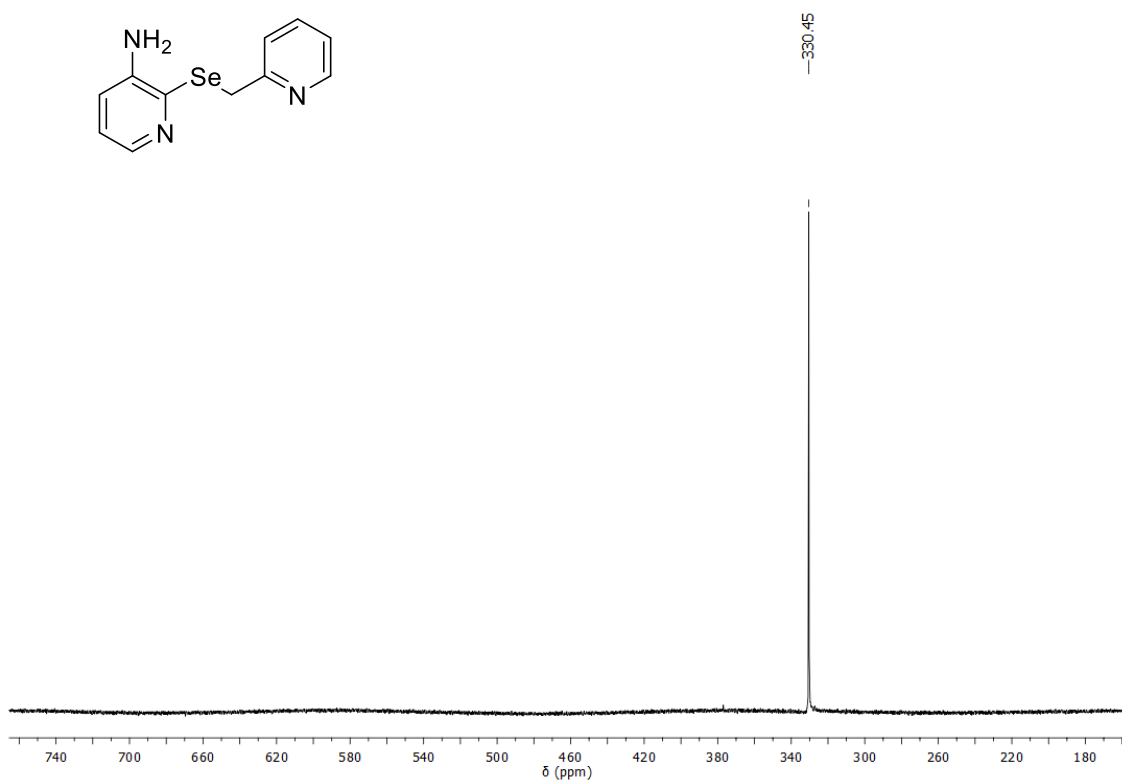


Figure S4.  $^{77}\text{Se}$  NMR (76 MHz,  $\text{CDCl}_3$ ) spectrum of Ligand L.

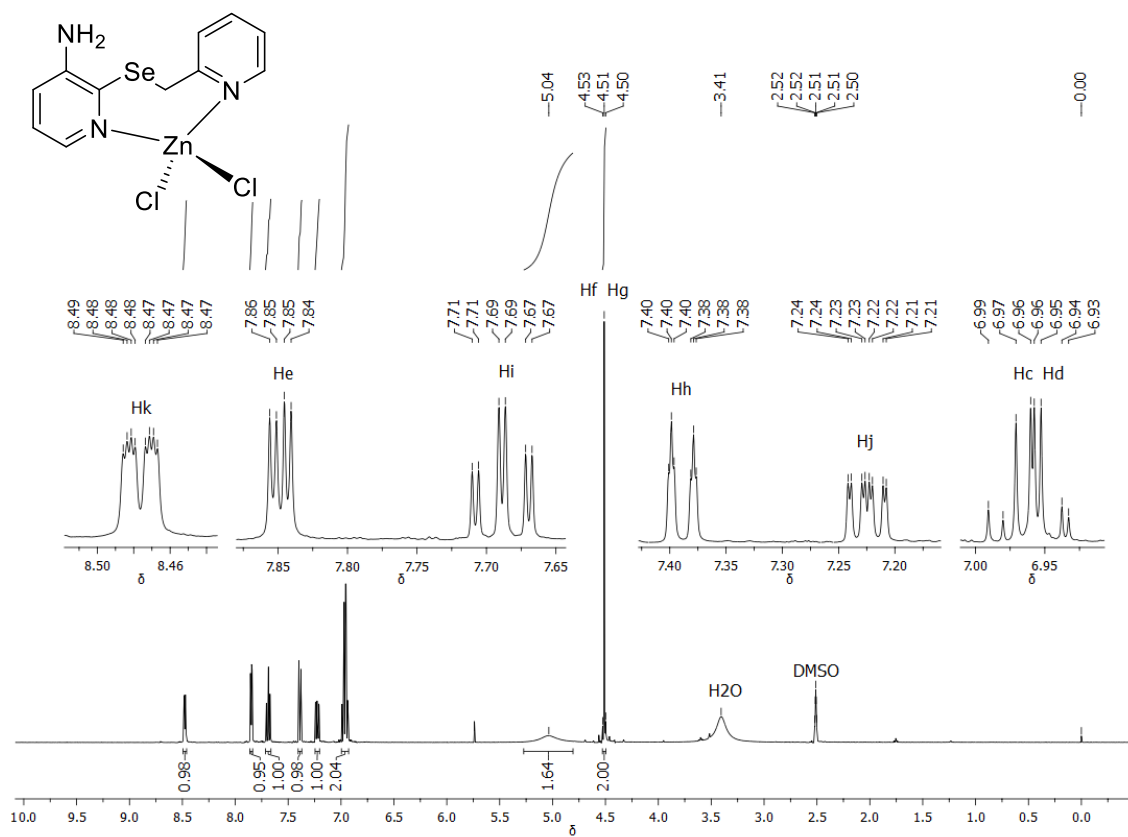


Figure S5.  $^1\text{H}$  NMR (400 MHz,  $\text{DMSO-}d_6$ ) spectrum of complex 5.

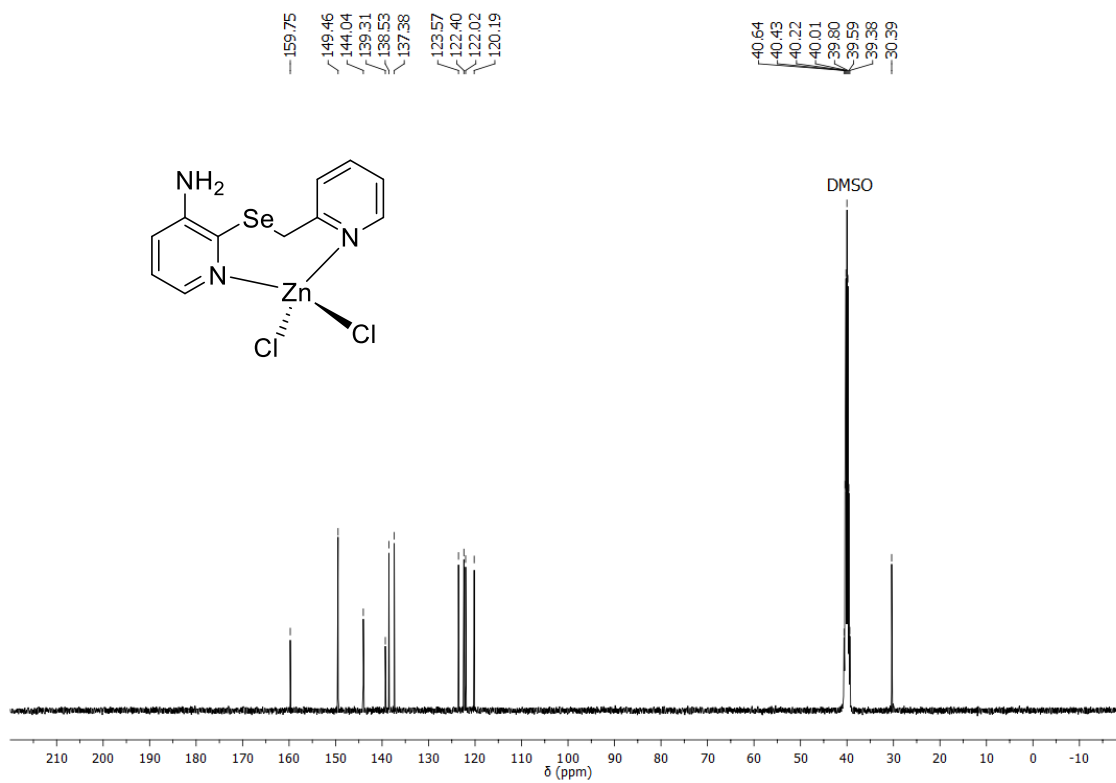


Figure S6.  $^{13}\text{C}$  NMR (100 MHz,  $\text{DMSO-}d_6$ ) spectrum of complex 5.

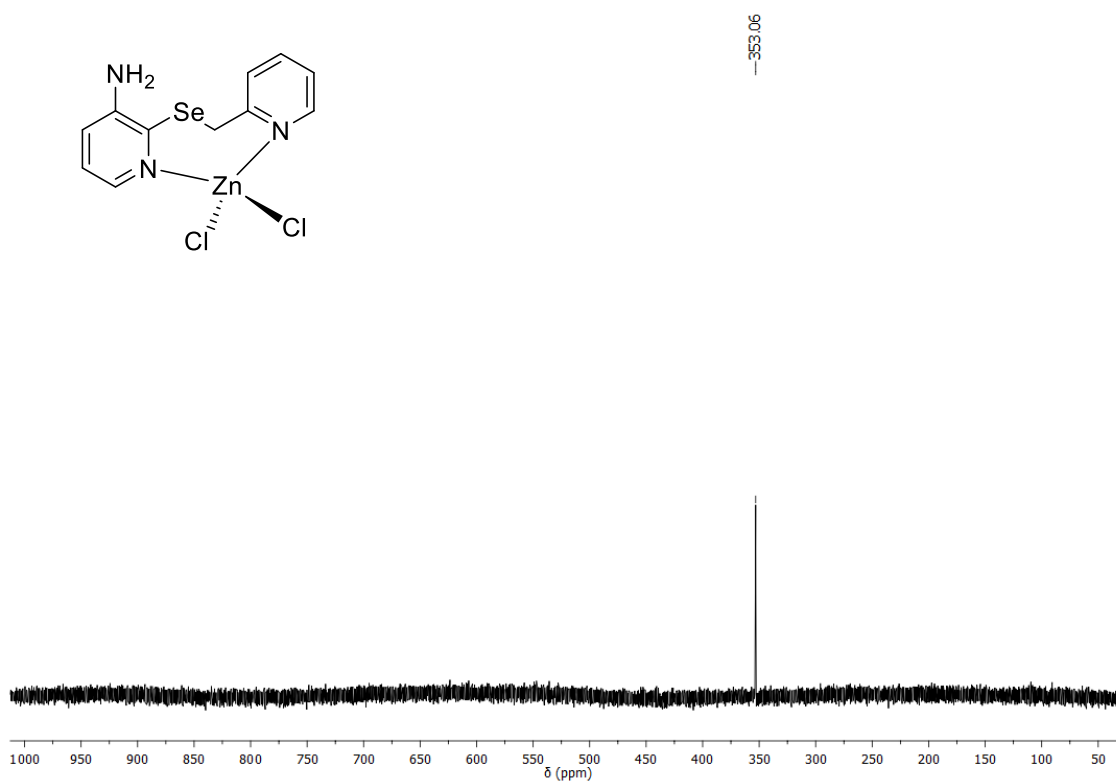
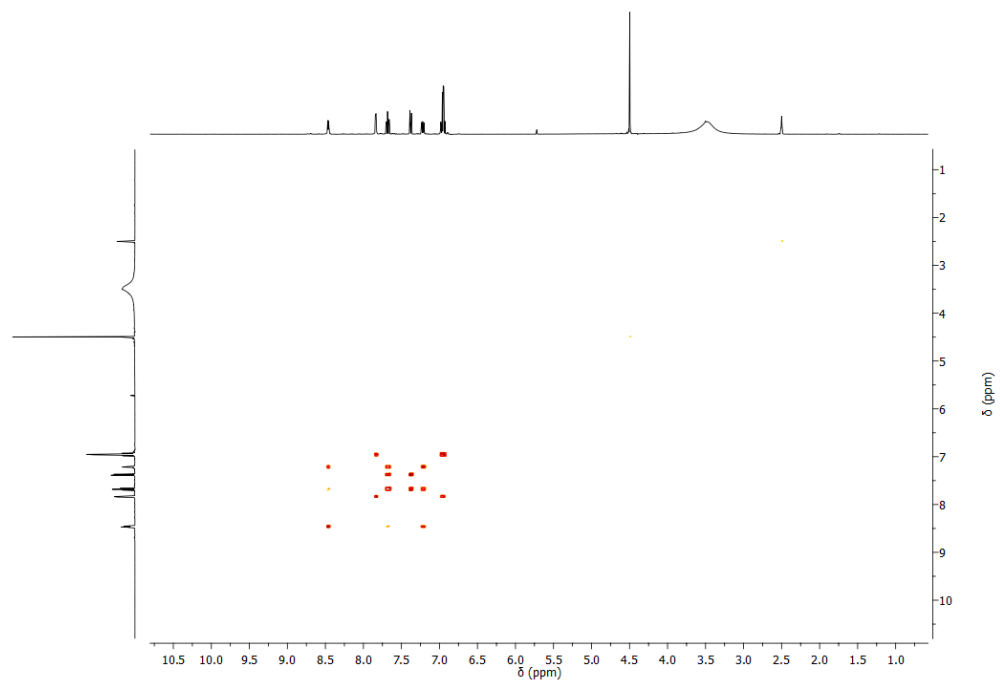
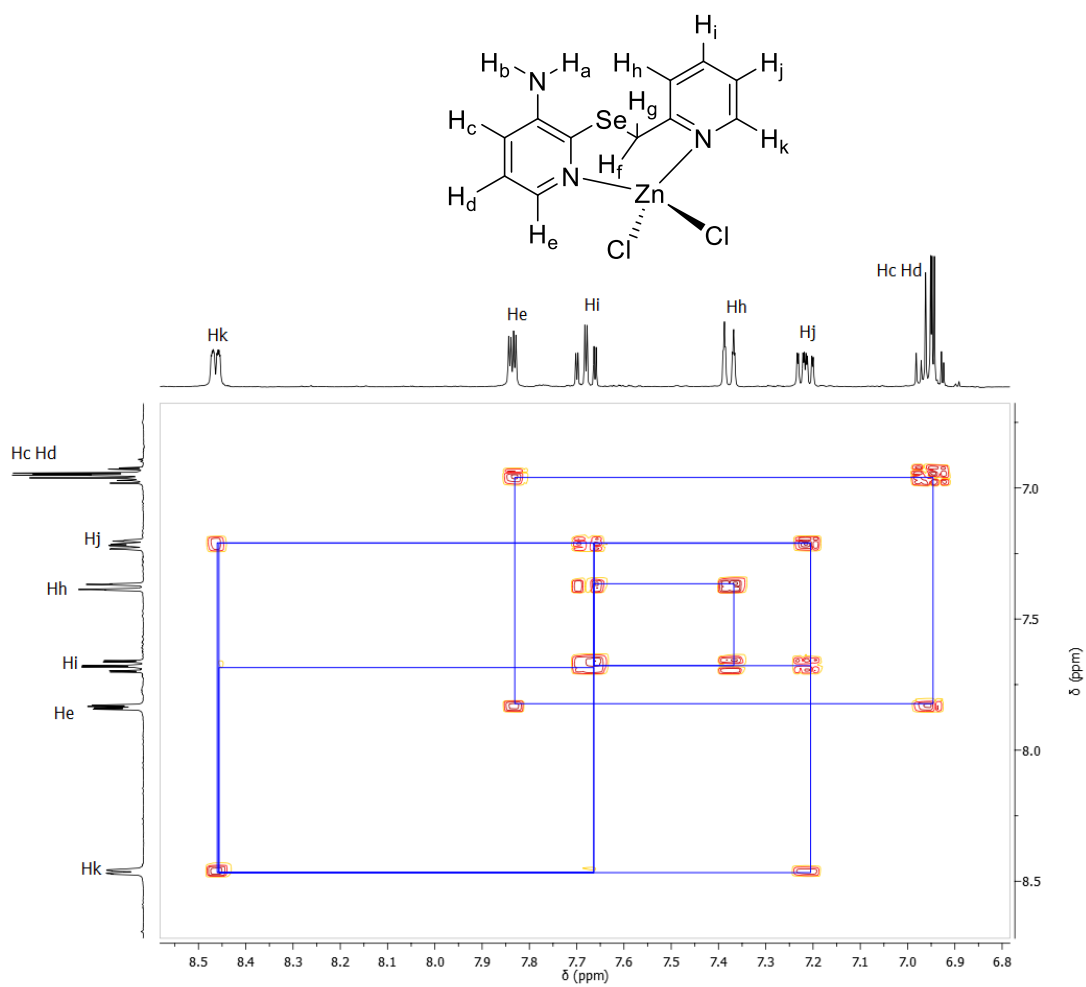


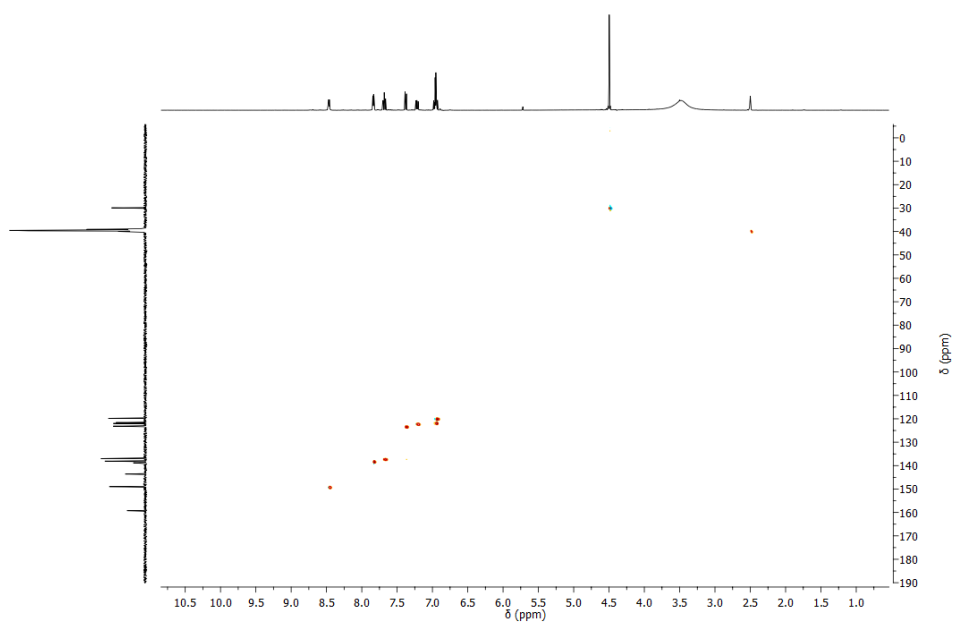
Figure S7.  $^{77}\text{Se}$  NMR (76 MHz,  $\text{DMSO-}d_6$ ) spectrum of complex 5.



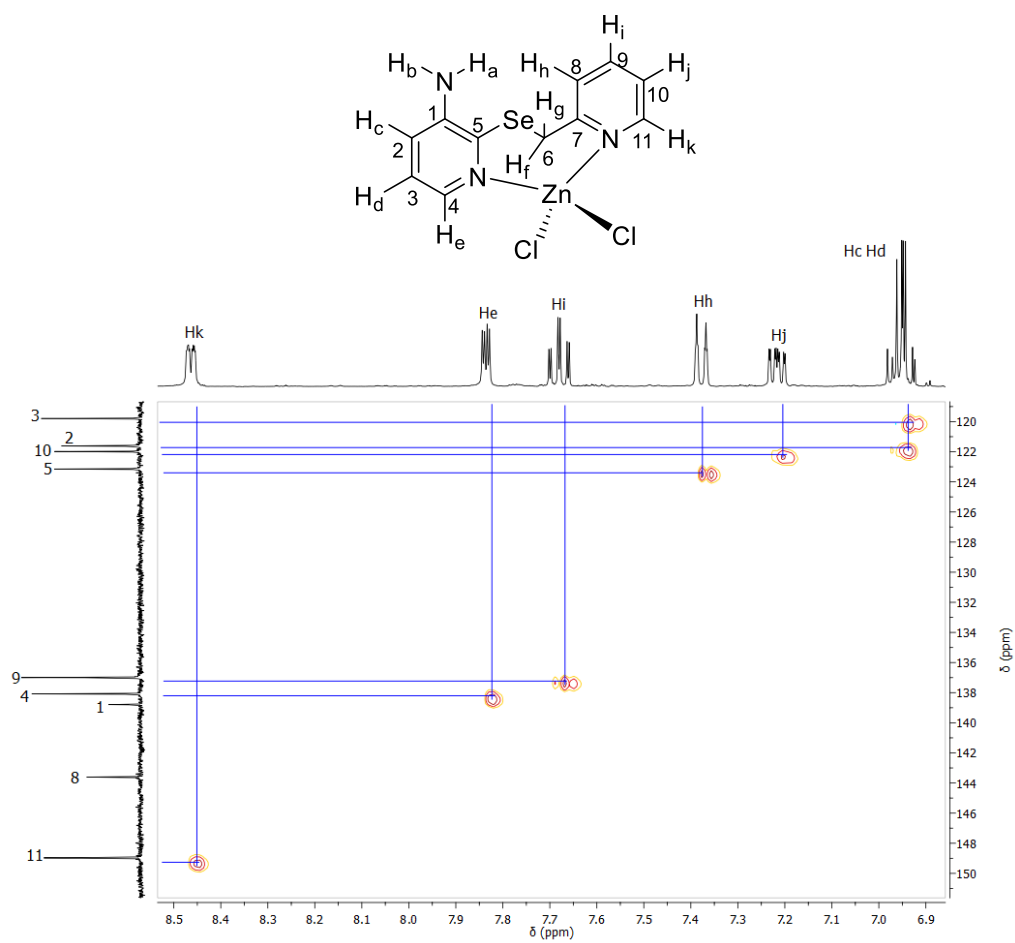
**Figure S8.** 2D COSY NMR spectrum of complex **5** (DMSO- $d_6$ ).



**Figure S9.** 2D COSY expansion spectrum of complex **5** (DMSO- $d_6$ ).



**Figure S10.** 2D HMQC NMR spectrum of complex **5** (DMSO- $d_6$ ).



**Figure S11.** 2D HMQC expansion spectrum of complex **5** (DMSO- $d_6$ ).



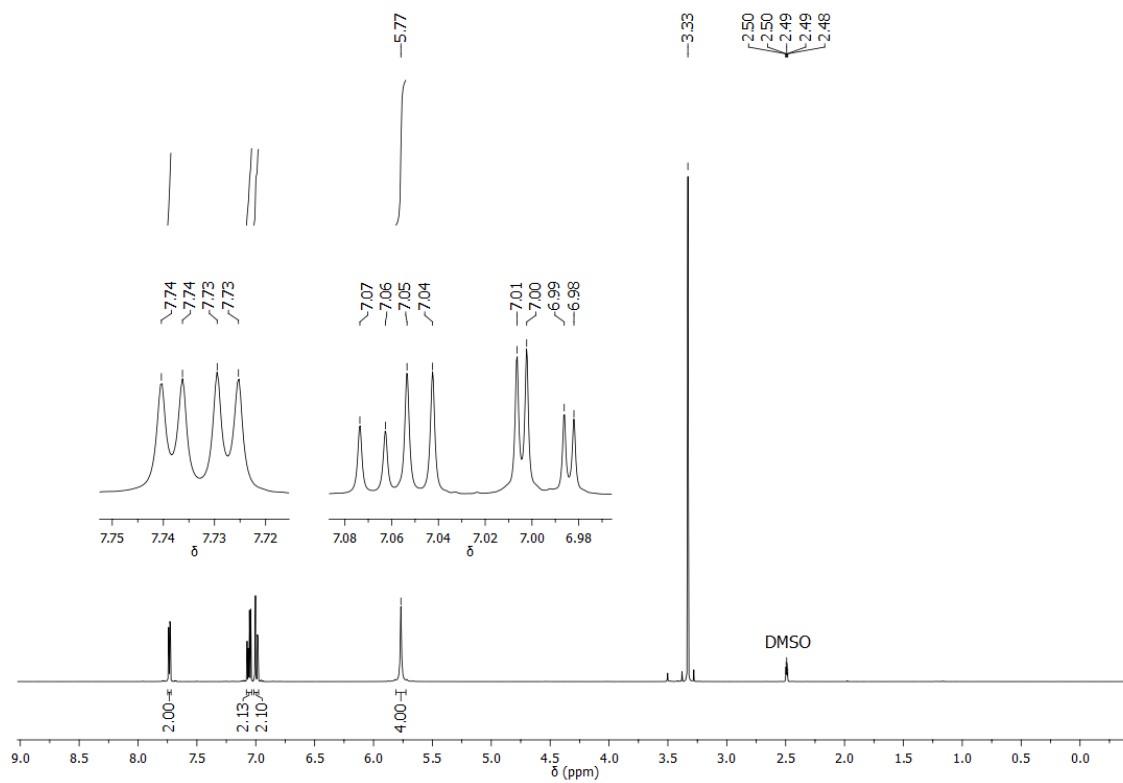


Figure S12. <sup>1</sup>H NMR (400 MHz, DMSO-*d*<sub>6</sub>) spectrum of (apySe)<sub>2</sub>.

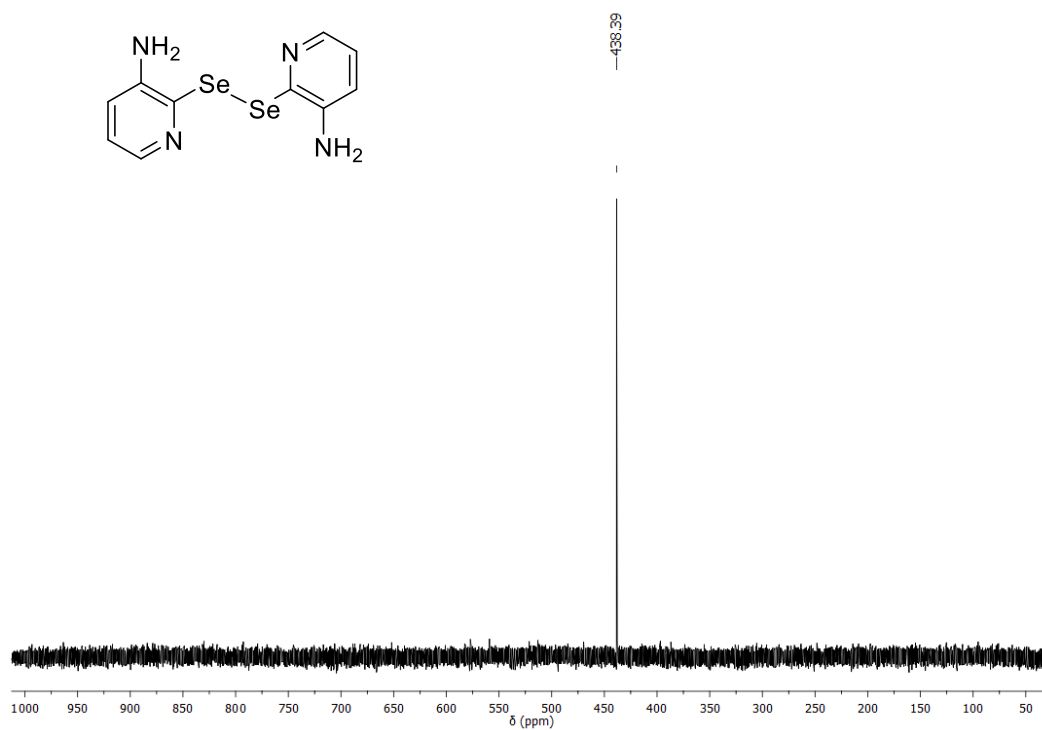


Figure S13. <sup>77</sup>Se NMR (76 MHz, DMSO-*d*<sub>6</sub>) spectrum of (apySe)<sub>2</sub>.

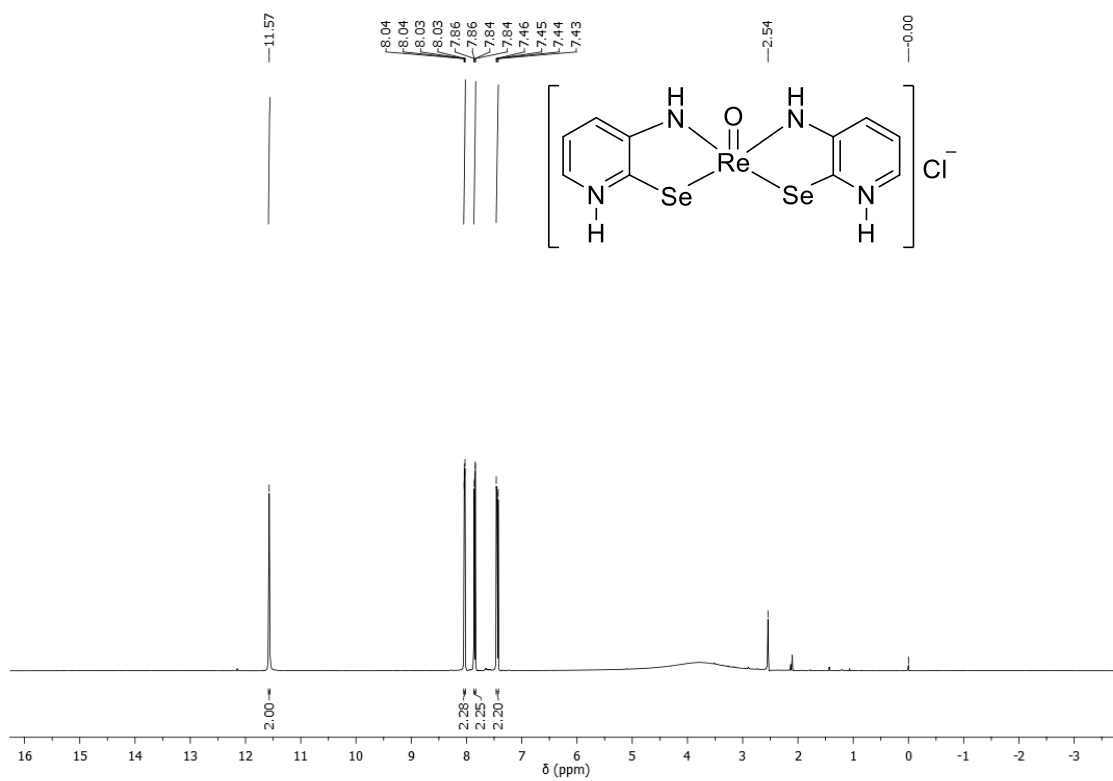


Figure S14.  $^1\text{H NMR}$  (400 MHz,  $\text{DMSO-}d_6$ ) spectrum of complex 6.

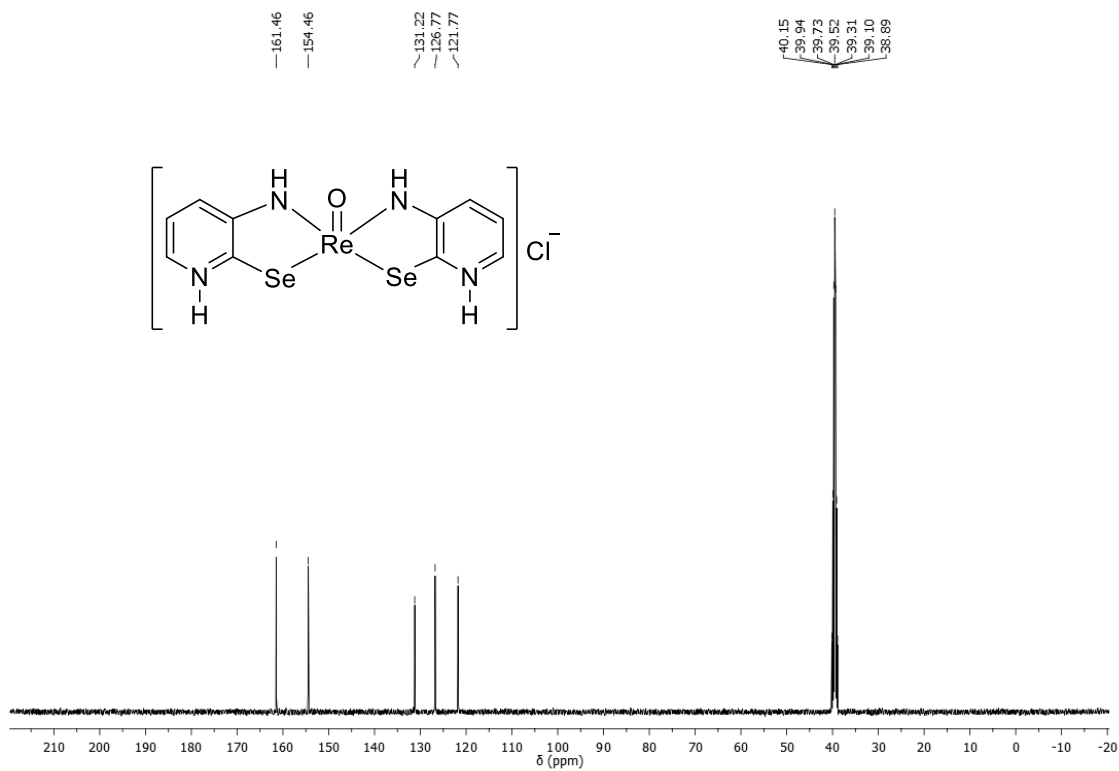


Figure S15.  $^{13}\text{C NMR}$  (100 MHz,  $\text{DMSO-}d_6$ ) spectrum of complex 6.

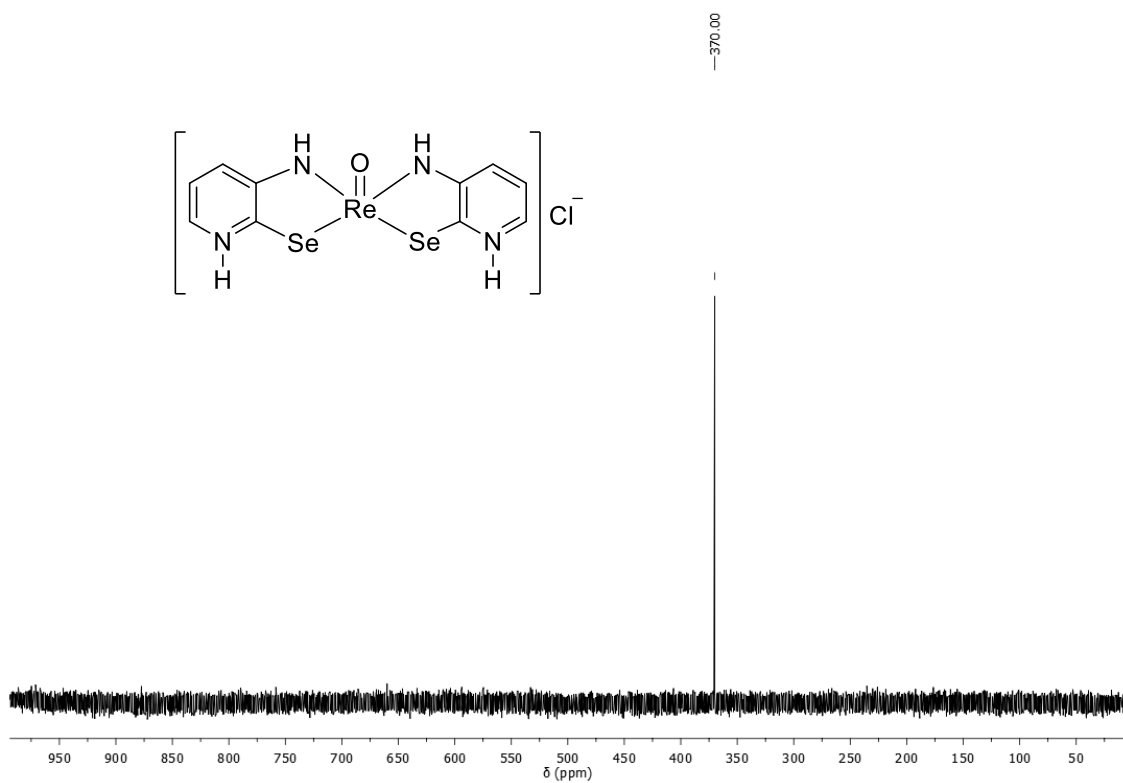


Figure S16.  $^{77}\text{Se}$  NMR (76 MHz,  $\text{DMSO-}d_6$ ) spectrum of complex 6.

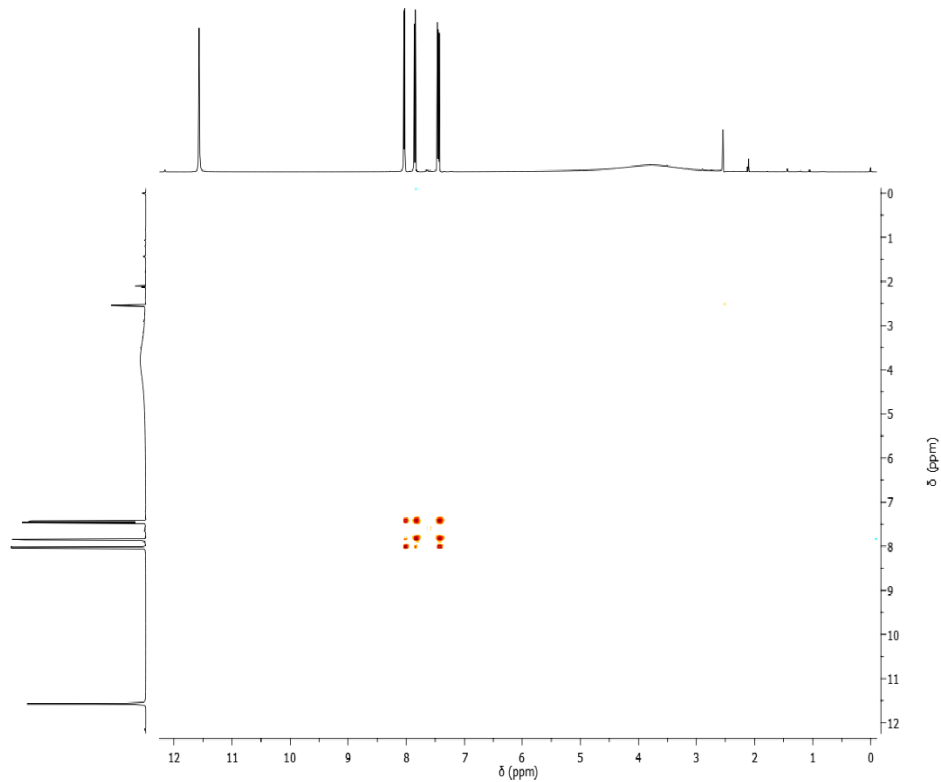
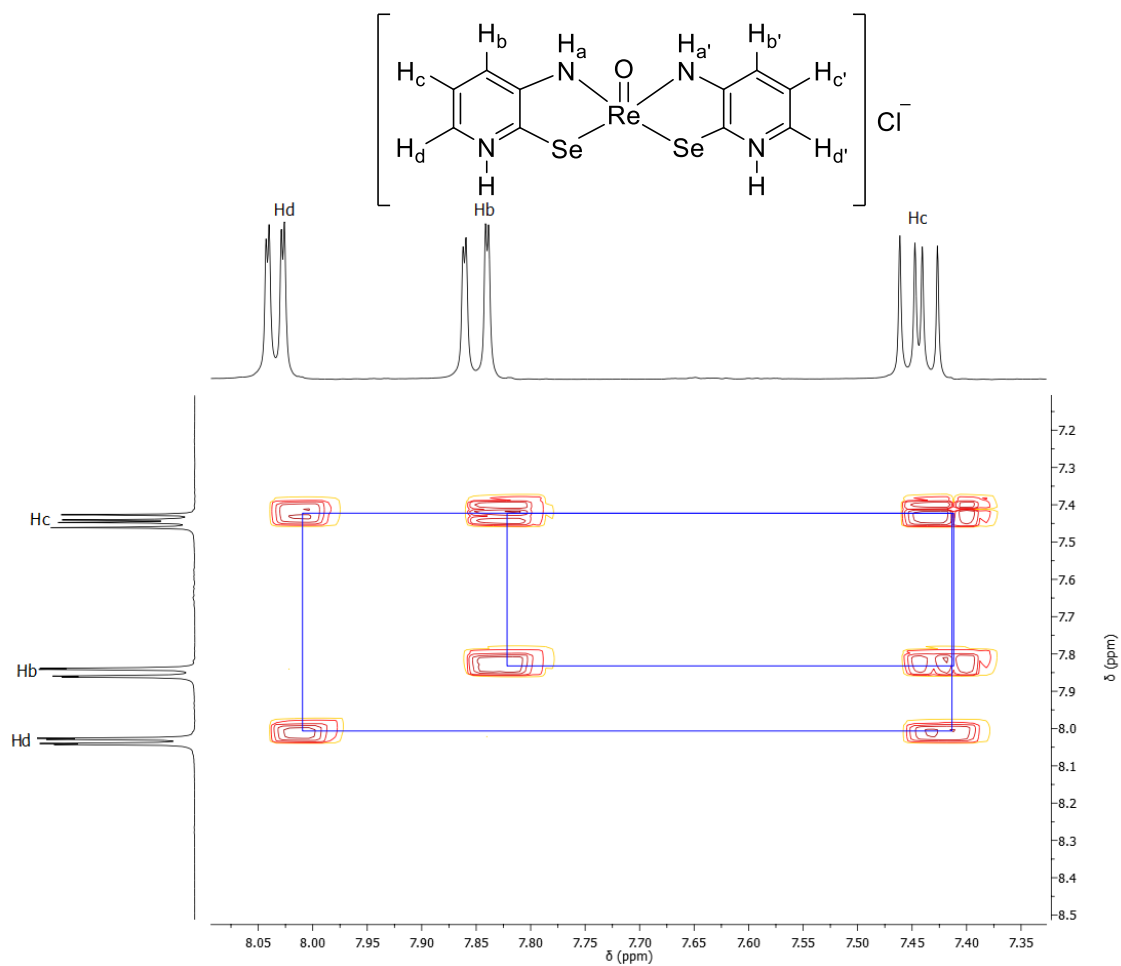
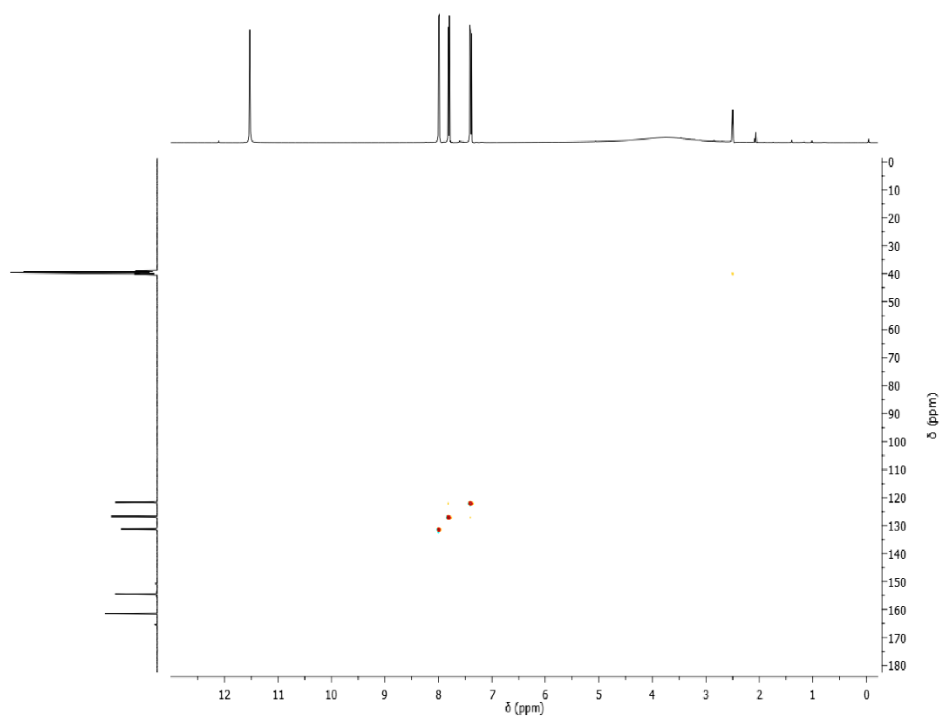


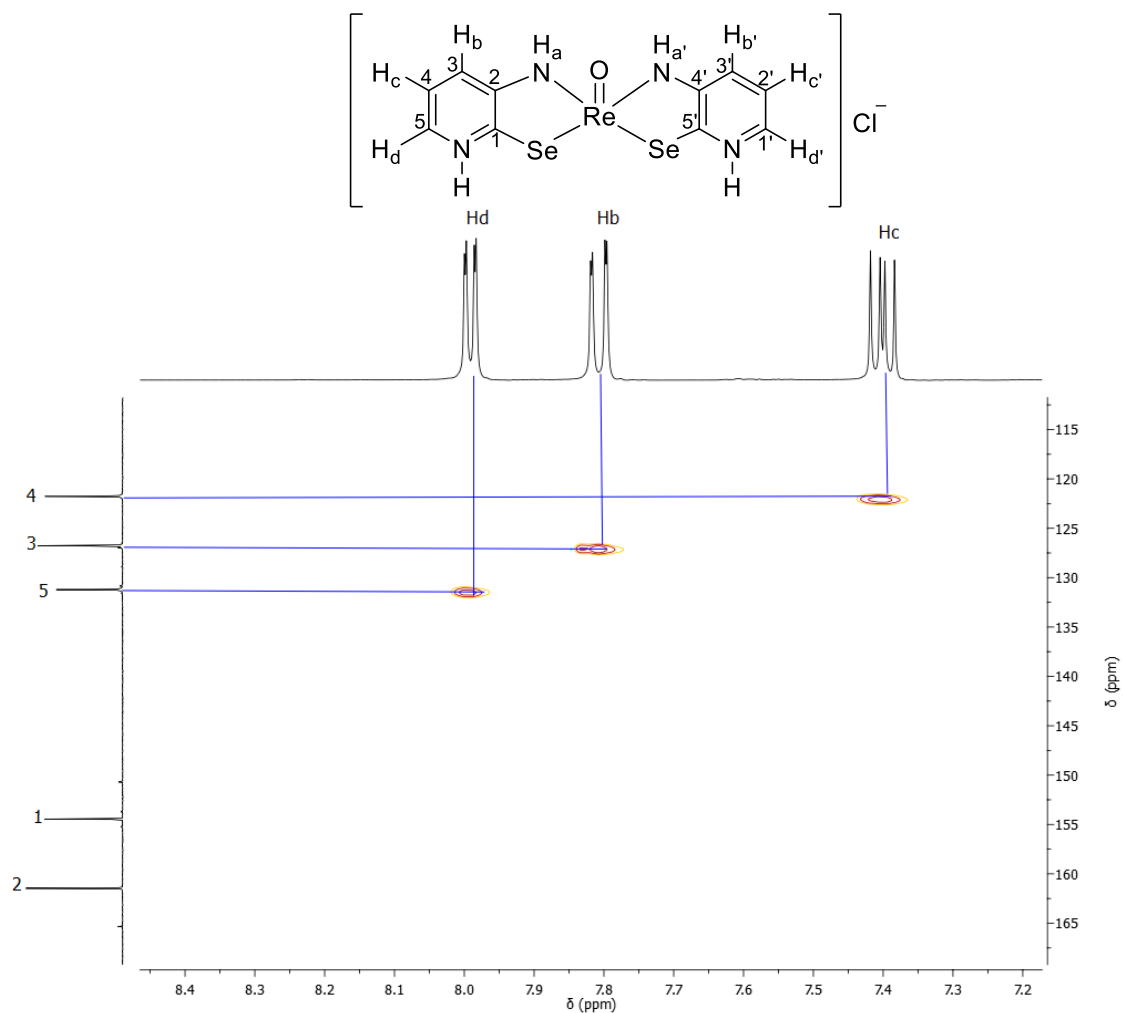
Figure S17. 2D COSY NMR spectrum of complex 6 ( $\text{DMSO-}d_6$ ).



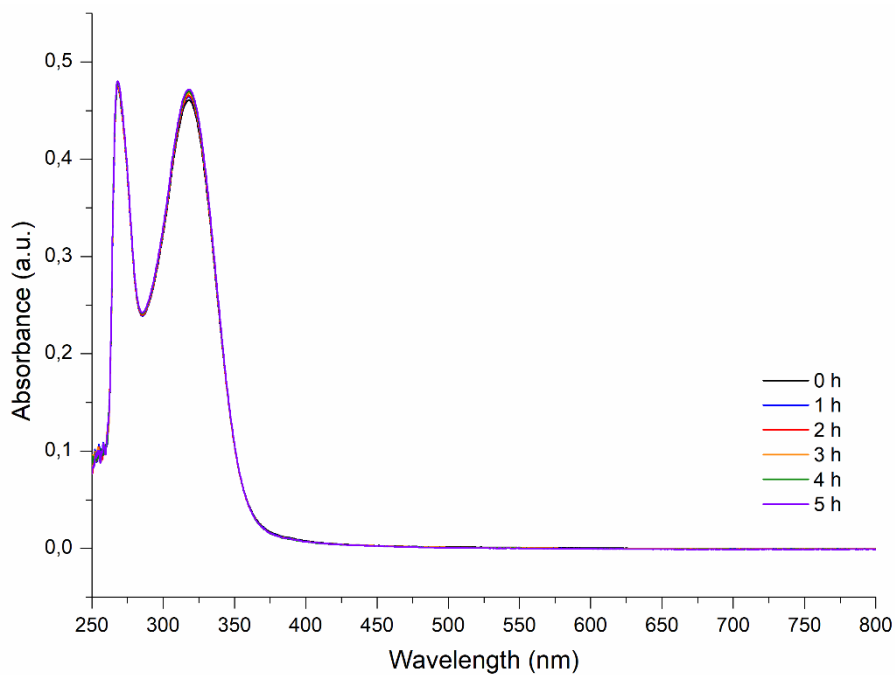
**Figure S18.** 2D COSY expansion spectrum of complex 6 (DMSO- $d_6$ ).



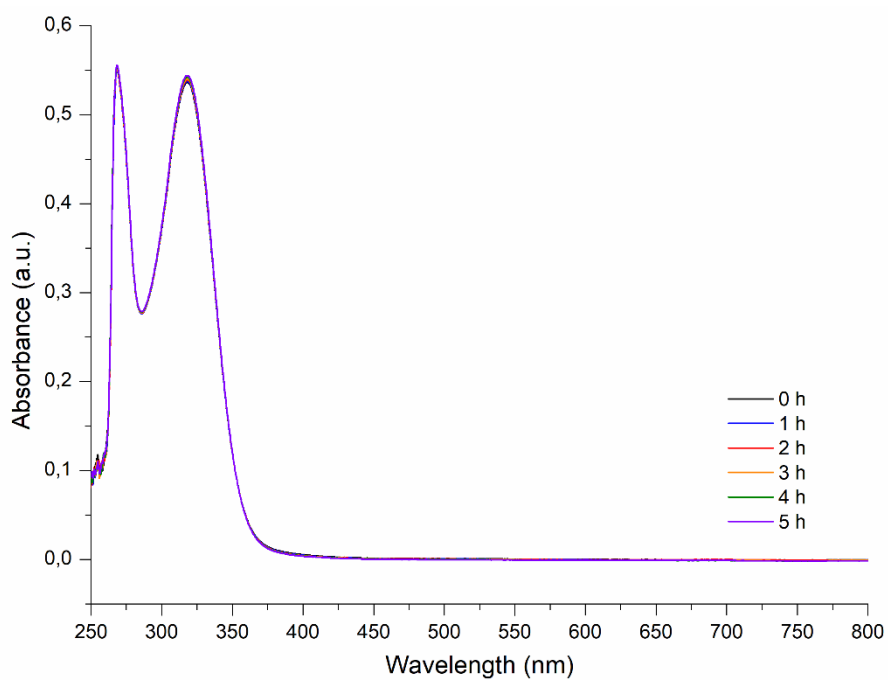
**Figure S19.** 2D HSQC NMR spectrum of complex 6 (DMSO- $d_6$ ).



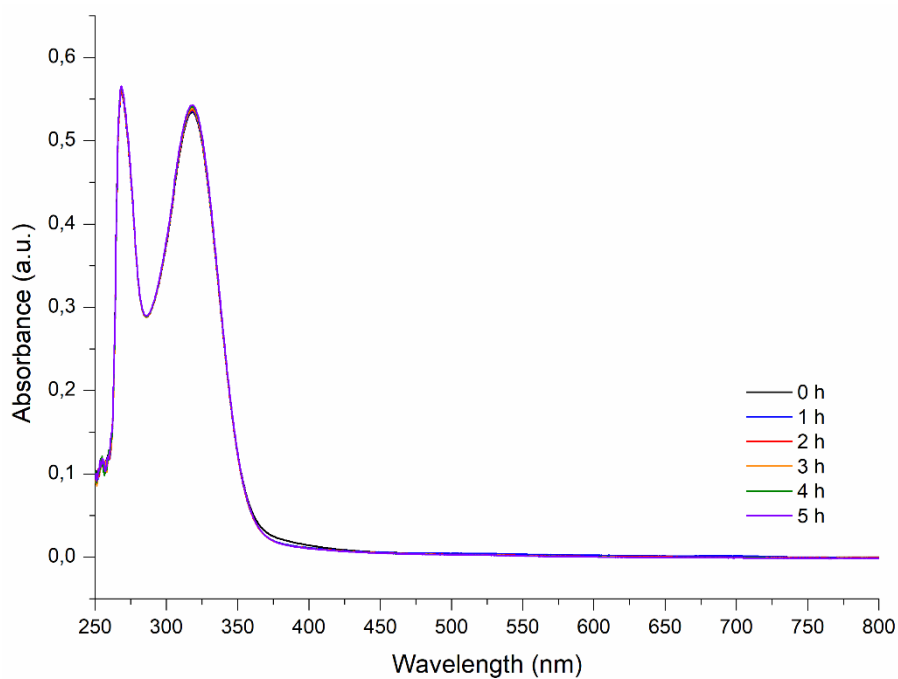
**Figure S20.** 2D HSQC expansion spectrum of complex **6** (DMSO- $d_6$ ).



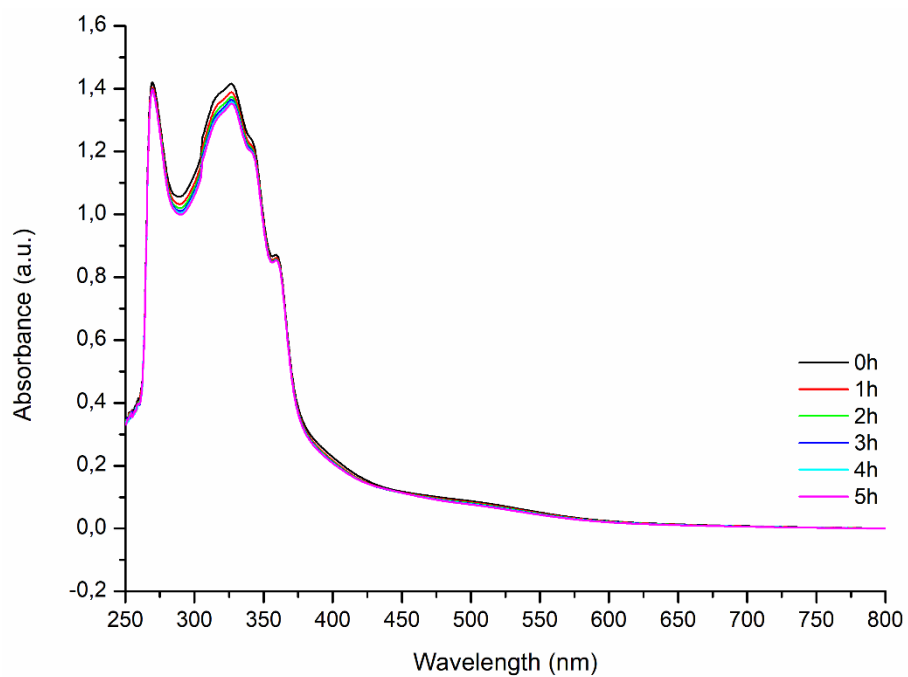
**Figure S21.** Electronic UV-Vis spectra for **L** in H<sub>2</sub>O/DMSO (4:1, v/v) solution, measured every 1 hour (total 5 hours); [ ] =  $1 \times 10^{-4}$  M.



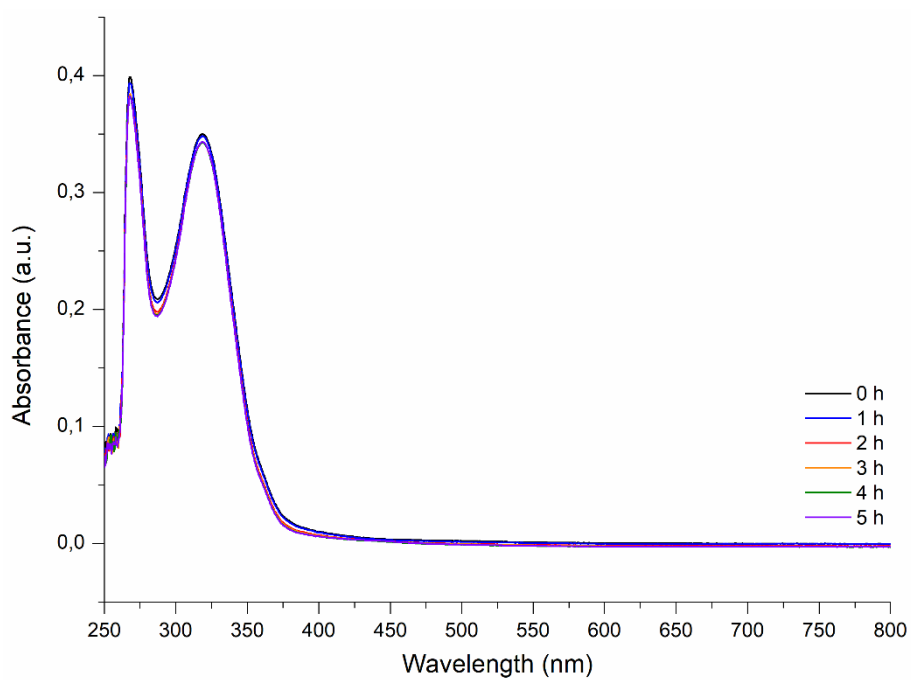
**Figure S22.** Electronic UV-Vis spectra for **1** in H<sub>2</sub>O/DMSO (4:1, v/v) solution, measured every 1 hour (total 5 hours); [ ] =  $1 \times 10^{-4}$  M.



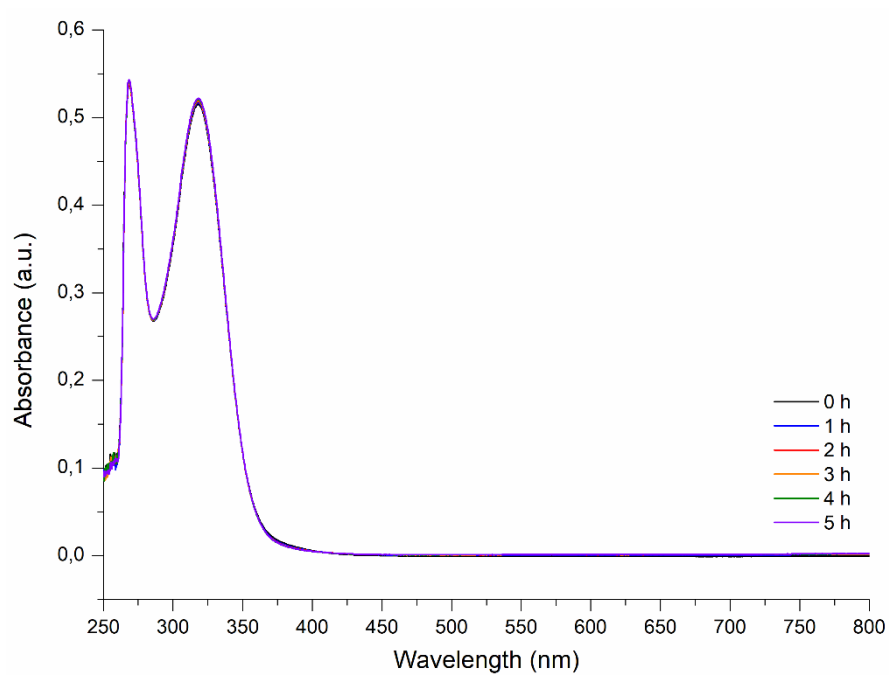
**Figure S23.** Electronic UV-Vis spectra for **2** in H<sub>2</sub>O/DMSO (4:1, v/v) solution, measured every 1 hour (total 5 hours); [ ] =  $1 \times 10^{-4}$  M.



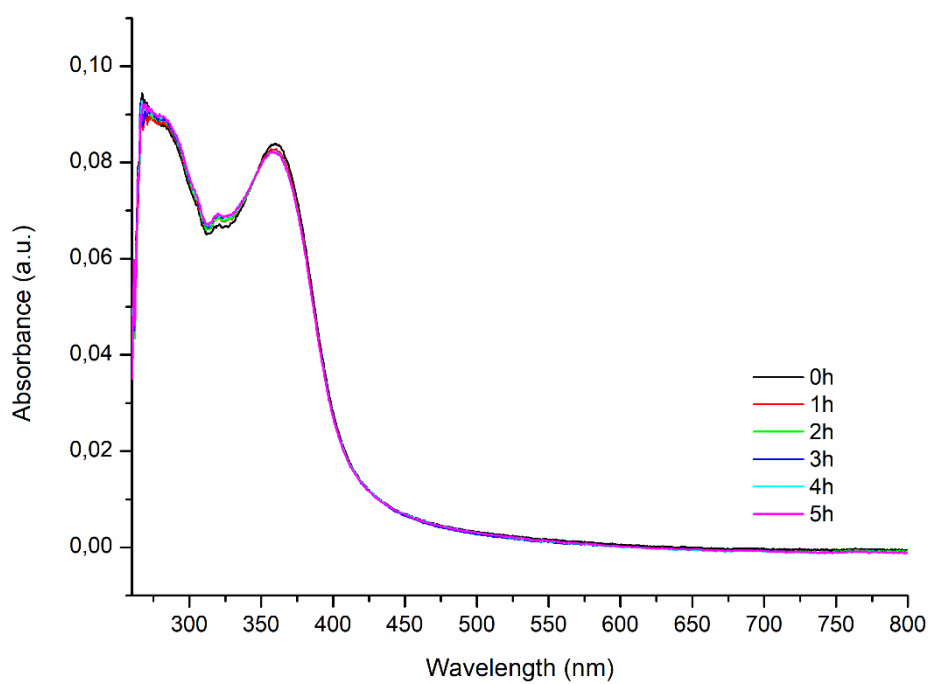
**Figure S24.** Electronic UV-Vis spectra for **3** in H<sub>2</sub>O/DMSO (4:1, v/v) solution, measured every 1 hour (total 5 hours); [ ] =  $1 \times 10^{-4}$  M.



**Figure S25.** Electronic UV-Vis spectra for **4** in H<sub>2</sub>O/DMSO (4:1, v/v) solution, measured every 1 hour (total 5 hours); [ ] =  $1 \times 10^{-4}$  M.



**Figure S26.** Electronic UV-Vis spectra for **5** in H<sub>2</sub>O/DMSO (4:1, v/v) solution, measured every 1 hour (total 5 hours); [ ] =  $1 \times 10^{-4}$  M.



**Figure S27.** Electronic UV-Vis spectra for **6** in H<sub>2</sub>O/DMSO (4:1, v/v) solution, measured every 1 hour (total 5 hours); [ ] =  $1 \times 10^{-4}$  M.