

## **New spiro-linked indolinone pyrrolidine selenoxoimidazolones**

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$^1\text{H}$  and  $^{13}\text{C}$  NMR spectra were recorded on a Bruker Avance instrument with an operating frequency of 400 MHz for  $^1\text{H}$  NMR, 101 MHz for  $^{13}\text{C}$  NMR. Chemical shifts are given in parts per million on a scale of  $\delta$  relative to hexamethyldisiloxane as an internal standard.

High-resolution mass spectra were recorded on an Orbitrap Elite mass spectrometer (Thermo Scientific) with IREP. To enter solutions with a concentration of 0.1–9  $\mu\text{g ml}^{-1}$  (in 1% formic acid in acetonitrile), direct injection into the ion source using a syringe pump (5  $\mu\text{l min}^{-1}$ ) was used. Spray voltage  $\pm$  3.5 kV, capillary temperature 275  $^\circ\text{C}$ .

### **Synthesis**

**1. Ethyl 2-[3-(4-ethoxyphenyl)selenoureido]acetate (1).** Ethyl 2-isoselenocyanatoacetate (0.26 g, 1.3 mmol) was dissolved in diethyl ether, then added in portions to 4-ethoxyaniline solution (0.18 g, 1.3 mmol) in  $\text{Et}_2\text{O}$  (5 ml), after which 1 mol% DMAP was added. The mixture was stirred for 6 hours. The precipitate formed is filtered off and washed with diethyl ether. Yield: 0.36 g (85%), white powder.

$^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ,  $\delta$ , ppm): 8.21 (s, 1H, NH), 7.19 (d,  $J=8.8$  Hz, 2H, Ar), 6.95 (d,  $J=8.8$  Hz, 2H, Ar), 6.68 (s, 1H, NH), 4.50 (d,  $J=4.7$  Hz, 2H,  $\text{CH}_2$ ), 4.21 (q,  $J=7.2$  Hz, 2H,  $\text{C(O)OCH}_2\text{CH}_3$ ), 4.04 (q,  $J=7.0$  Hz, 2H,  $\text{ArOCH}_2\text{CH}_3$ ), 1.43 (t,  $J=7.0$  Hz, 3H,  $\text{ArOCH}_2\text{CH}_3$ ), 1.28 (t,  $J=7.2$  Hz, 3H,  $\text{C(O)OCH}_2\text{CH}_3$ ).

**2. 5-Indolinylidene-2-selenoxohydantoins 2a-c (general procedure).** A 2% solution of KOH in ethanol (1 eq. KOH) was added to compound **1** (1 eq.), then isatin (1 eq.) was added to the solution. The reaction mixture was stirred for 1 hour. Then, a dilute hydrochloric acid solution ( $\text{H}_2\text{O}$ : HCl conc = 9: 1) was added. The precipitate formed was filtered off, washed with water and diethyl ether. If the precipitate has not precipitated, the product is isolated by column chromatography.

**2.1. (Z)-3-(4-Ethoxyphenyl)-5-(2-oxoindolinylidene)-2-selenoxoimidazolidin-4-one (2a)** was obtained from compound **1** (0.13 g, 0.4 mmol) in ethanol (15 ml) and isatin (0.06 g, 0.4 mmol); yield: 0.13 g (81%), red powder. M.p.>260°C.

<sup>1</sup>H NMR (400 MHz, DMSO-d<sub>6</sub>, δ, ppm): 12.07-11.66 (m, 1H, NH), 11.21 (bs, 1H, NH), 8.53 (d, J=7.7 Hz, 1H, isatin), 7.39-7.33 (m, 1H, isatin), 7.35 (d, J=8.9 Hz, 2H, Ar), 7.06 (d, J=8.9 Hz, 2H, Ar), 7.02 (t, J=8.2 Hz, 1H, isatin), 6.94 (d, J=7.8 Hz, 1H, isatin), 4.09 (q, J=6.9 Hz, 2H, ArOCH<sub>2</sub>CH<sub>3</sub>), 1.36 (t, J=6.9 Hz, 3H, ArOCH<sub>2</sub>CH<sub>3</sub>).

**2.2. (Z)-5-(5-Chloro-2-oxoindolinylidene)-3-(4-ethoxyphenyl)-2-selenoxoimidazolidin-4-one (2b)** was obtained from compound **1** (0.13 g, 0.4 mmol) in ethanol (15 ml) and 5-chloroisatin (0.07 g, 0.4 mmol); yield: 0.14 g (84%), red powder. M.p.>260°C.

<sup>1</sup>H NMR (400 MHz, DMSO-d<sub>6</sub>, δ, ppm): 11.95 (bs, 1H, NH), 11.28 (s, 1H, NH), 8.57 (d, J=1.9 Hz, 1H, isatin), 7.40 (dd, J<sub>1</sub>=2.0 Hz, J<sub>2</sub>=8.3 Hz, 1H, isatin), 7.34 (d, J=8.8 Hz, 2H, Ar), 7.07 (d, J=8.8 Hz, 2H, Ar), 6.94 (d, J=8.4 Hz, 1H, isatin), 4.10 (q, J=6.9 Hz, 2H, ArOCH<sub>2</sub>CH<sub>3</sub>), 1.37 (t, J=6.9 Hz, 3H, ArOCH<sub>2</sub>CH<sub>3</sub>).

**2.3. (Z)-5-(5-Bromo-2-oxoindolinylidene)-3-(4-ethoxyphenyl)-2-selenoxoimidazolidin-4-one (2c)** was obtained from compound **1** (0.16 g, 0.5 mmol) in ethanol (15 ml) and 5-bromoisatin (0.11 g, 0.5 mmol); yield: 0.18 g (79%), red powder. M.p.>260°C.

<sup>1</sup>H NMR (400 MHz, DMSO-d<sub>6</sub>, δ, ppm): 11.96 (s, 1H, NH), 11.30 (s, 1H, NH), 8.71 (d, J=1.9 Hz, 1H, isatin), 7.53 (dd, J<sub>1</sub>=2.0 Hz, J<sub>2</sub>=8.4 Hz, 1H, isatin), 7.34 (d, J=8.9 Hz, 2H, Ar), 7.07 (d, J=9.9 Hz, 2H, Ar), 6.90 (d, J=8.3, 1H, isatin), 4.10 (q, J=7.0 Hz, 2H, ArOCH<sub>2</sub>CH<sub>3</sub>), 1.37 (t, J=7.0 Hz, 3H, ArOCH<sub>2</sub>CH<sub>3</sub>).

**3. 2-Selenoxodispiro[imidazolidine-5,3'-pyrrolidine-4',3''-indoline]-2'',4-diones 3a-c (general procedure).** Toluene was added to 5-indolinylidene-2-selenoxohydantoin (1 eq.) and sarcosine (8 eq.), and the mixture was brought to boiling. Paraformaldehyde (8 eq.) was then added. The mixture was refluxed for 6 hours, evaporated, and the residue was purified by silica gel column chromatography in the MeOH/CHCl<sub>3</sub> = 1: 50 mixture as the eluent.

**3.1. rac-(5R,4'S)-3-(4-Ethoxyphenyl)-1'-methyl-2-selenoxodispiro[imidazolidin-5,3'-pyrrolidin-4',3''-indoline]-2'',4-dione (3a)** was obtained from compound **2a** (0.11 g, 0.3 mmol), sarcosine (0.19 g, 2.2 mmol) and paraformaldehyde (0.07 g, 2.2 mmol) in toluene (15 ml); yield: 0.07 g (56%), light pink powder. M.p. 258-259°C.

<sup>1</sup>H NMR (400 MHz, DMSO-d<sub>6</sub>, δ, ppm): 11.27 (s, 1H, NH), 10.63 (s, 1H, NH), 7.27 (t, J=7.8 Hz, H, isatin), 7.13 (d, J=7.5 Hz, H, isatin), 6.95-6.92 (m, 1H, isatin), 6.93 (d, J=8.6 Hz, 2H, Ar), 6.86 (d, J=7.6 Hz, 1H, isatin), 6.73 (d, J=8.6 Hz, 2H, Ar), 4.03 (q, J=7.0 Hz, 2H, ArOCH<sub>2</sub>CH<sub>3</sub>), 3.50 (d, J=10.0 Hz, 1H, pyrrolidine), 3.34 (m, H, pyrrolidine), 3.33-3.29 (m, 1H,

pyrrolidine), 3.08 (d, J=10.2 Hz, 1H, pyrrolidine), 2.48 (s, 3H, NCH<sub>3</sub>), 1.32 (t, J=6.9 Hz, 3H, ArOCH<sub>2</sub>CH<sub>3</sub>).

<sup>13</sup>C NMR (101 MHz, DMSO-d<sub>6</sub>, δ, ppm): 183.5, 176.6, 172.7, 158.6, 143.1, 129.9, 129.5, 126.0, 125.0, 124.9, 121.4, 114.3, 109.6, 74.5, 63.3, 60.3, 58.8, 57.6, 42.0, 14.6.

HRMS (ESI, m/z): calculated (C<sub>22</sub>H<sub>22</sub>N<sub>4</sub>O<sub>3</sub>Se, M+H): 471.0930, found (M+H): 471.0923.

**3.2. *rac*-(5*R*,4'*S*)-5''-Chloro-3-(4-ethoxyphenyl)-1'-methyl-2-selenoxodispiro-[imidazolidine-5,3'-pyrrolidine-4',3''-indoline]-2'',4-dione (3b)** was obtained from compound **2b** (0.13 g, 0.3 mmol), sarcosine (0.21 g, 2.3 mmol) and paraformaldehyde (0.07 g, 2.2 mmol) in toluene (15 ml); yield: 0.10 g (66%), beige powder. M.p. >260°C.

<sup>1</sup>H NMR (400 MHz, DMSO-d<sub>6</sub>, δ, ppm): 11.39 (s, 1H, NH), 10.78 (s, 1H, NH), 7.33 (dd, J<sub>1</sub>=2.0 Hz, J<sub>2</sub>=8.3 Hz, 1H, isatin), 7.13 (d, J=1.8 Hz, 1H, isatin), 6.94 (d, J=8.8 Hz, 2H, Ar), 6.87 (d, J=8.3 Hz, 1H, isatin), 6.76 (d, J=8.6 Hz, 2H, Ar), 4.04 (q, J=6.9 Hz, 2H, ArOCH<sub>2</sub>CH<sub>3</sub>), 3.42 (d, J=11.7 Hz, 1H, pyrrolidine), 3.39 (d, J=10.7 Hz, 1H, pyrrolidine), 3.29 (m, 1H, pyrrolidine), 3.10 (d, J=10.1 Hz, 1H, pyrrolidine), 2.48 (s, 3H, NCH<sub>3</sub>), 1.33 (t, J=6.9 Hz, 3H, ArOCH<sub>2</sub>CH<sub>3</sub>).

<sup>13</sup>C NMR (101 MHz, DMSO-d<sub>6</sub>, δ, ppm): 183.3, 175.8, 172.5, 158.7, 141.8, 129.8, 129.2, 127.4, 126.0, 125.4, 125.0, 114.4, 111.0, 74.5, 63.4, 60.1, 59.1, 57.6, 41.8, 14.6.

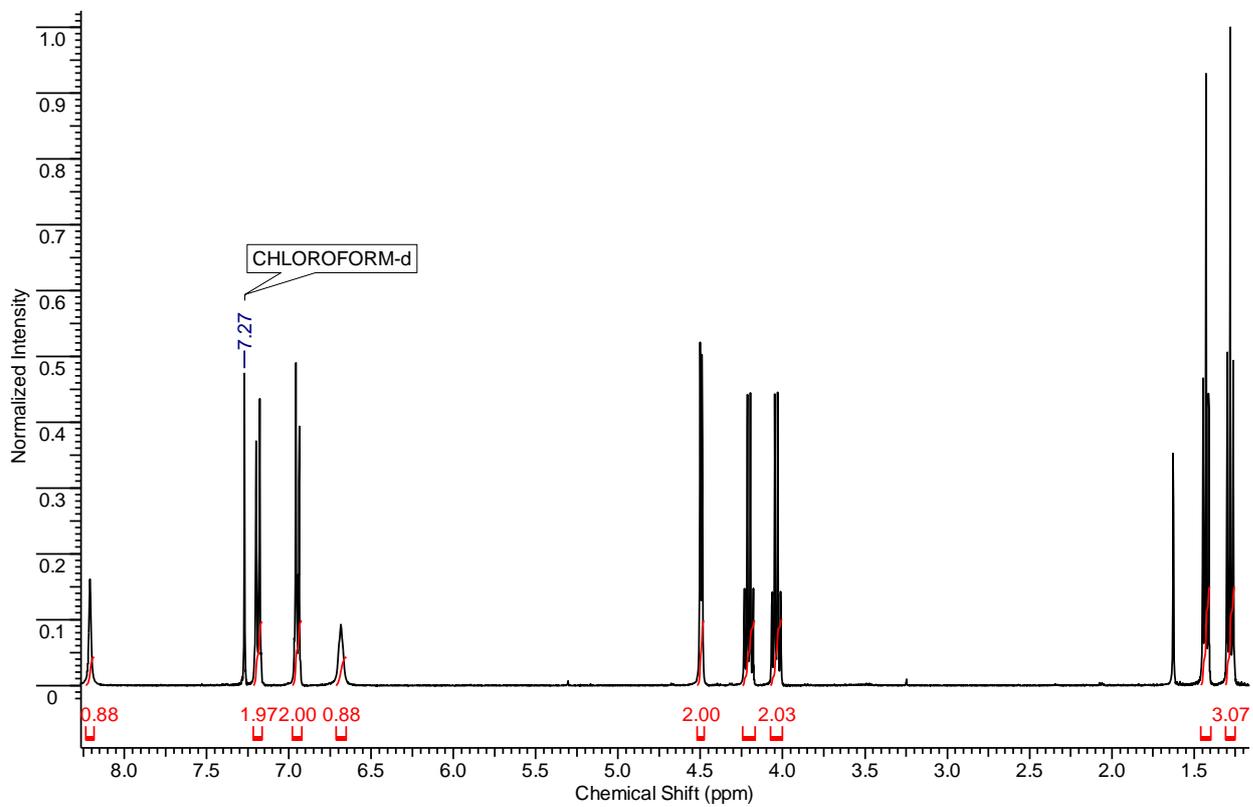
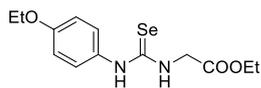
HRMS (ESI, m/z): calculated (C<sub>22</sub>H<sub>21</sub>ClN<sub>4</sub>O<sub>3</sub>Se, M+H): 505.0540, found (M+H): 505.0547.

**3.3. *rac*-(5*R*,4'*S*)-5''-Bromo-3-(4-ethoxyphenyl)-1'-methyl-2-selenoxodispiro-[imidazolidine-5,3'-pyrrolidine-4',3''-indoline]-2'',4-dione (3c)** was obtained from compound **2c** (0.13 g, 0.3 mmol), sarcosine (0.21 g, 2.3 mmol) and paraformaldehyde (0.07 g, 2.2 mmol) in toluene (15 ml); yield: 0.07 g (46%), red powder. M.p. >260°C.

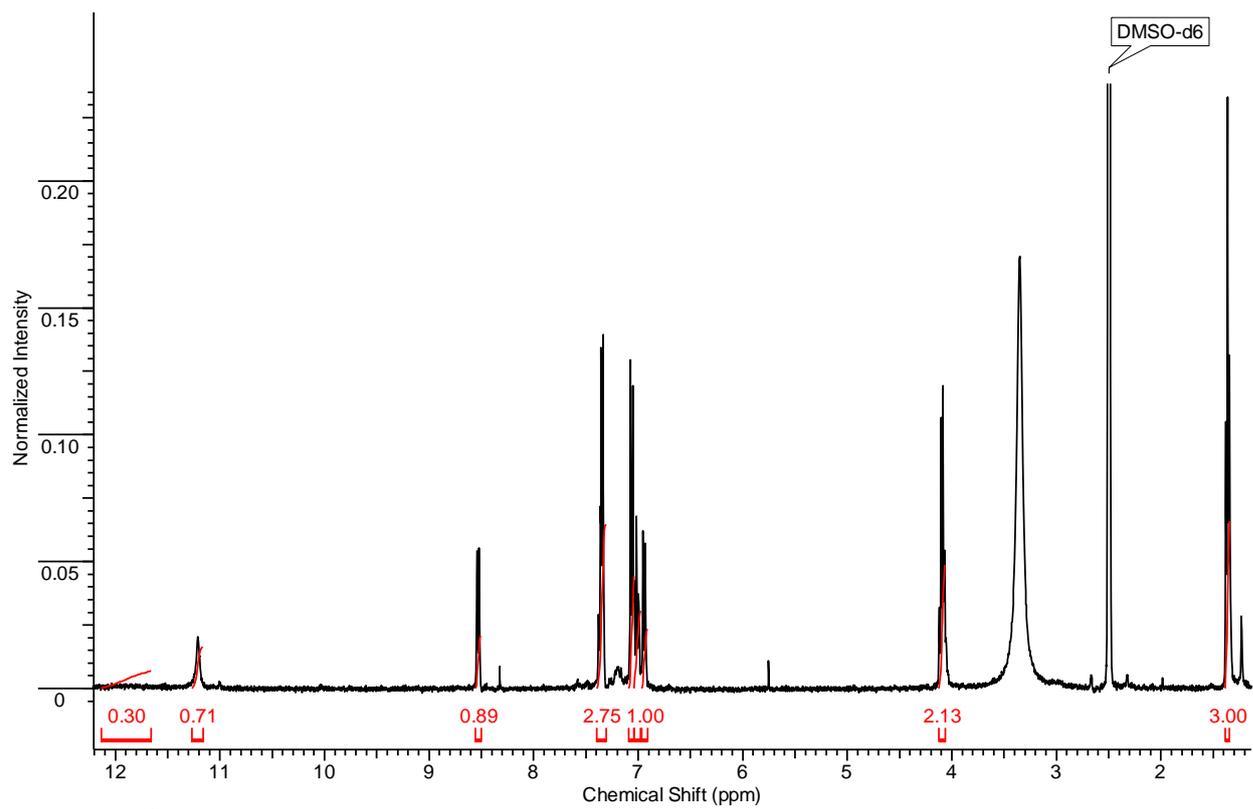
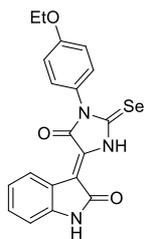
<sup>1</sup>H NMR (400 MHz, DMSO-d<sub>6</sub>, δ, ppm): 11.42 (s, 1H, NH), 10.81 (s, 1H, NH), 7.46 (dd, J<sub>1</sub>=1.4 Hz, J<sub>2</sub>=8.3 Hz, 1H, isatin), 7.24 (s, 1H, isatin), 6.94 (d, J=8.6 Hz, 2H, Ar), 6.83 (d, J=8.3 Hz, 1H, isatin), 6.77 (d, J=8.4 Hz, 2H, Ar), 4.04 (q, J=6.9 Hz, 2H, ArOCH<sub>2</sub>CH<sub>3</sub>), 3.43 (d, J=10.3 Hz, 1H, pyrrolidine), 3.39 (d, J=10.5 Hz, 1H, pyrrolidine), 3.32 (m, 1H, pyrrolidine), 3.10 (d, J=10.1 Hz, 1H, pyrrolidine), 2.48 (s, 3H, NCH<sub>3</sub>), 1.33 (t, J=6.9 Hz, 3H, ArOCH<sub>2</sub>CH<sub>3</sub>).

<sup>13</sup>C NMR (101 MHz, DMSO-d<sub>6</sub>, δ, ppm): 206.9, 183.3, 175.7, 172.5, 158.7, 142.3, 142.2, 132.0, 129.8, 127.7, 125.9, 114.4, 113.1, 111.5, 74.4, 63.3, 60.0, 59.0, 57.5, 41.9, 14.6.

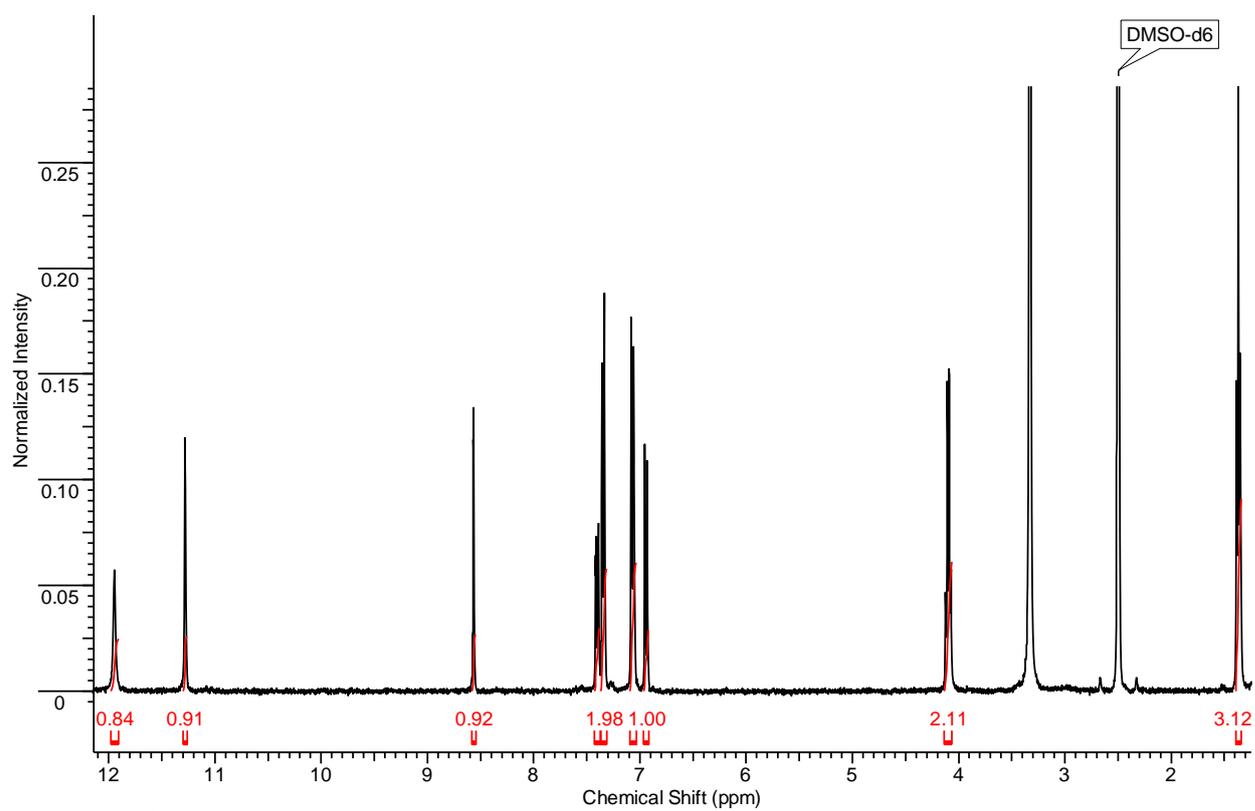
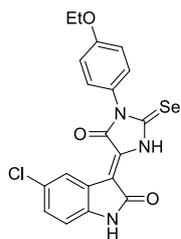
HRMS (ESI, m/z): calculated (C<sub>22</sub>H<sub>21</sub>BrN<sub>4</sub>O<sub>3</sub>Se, M+H): 549.0035, found (M+H): 549.0037.



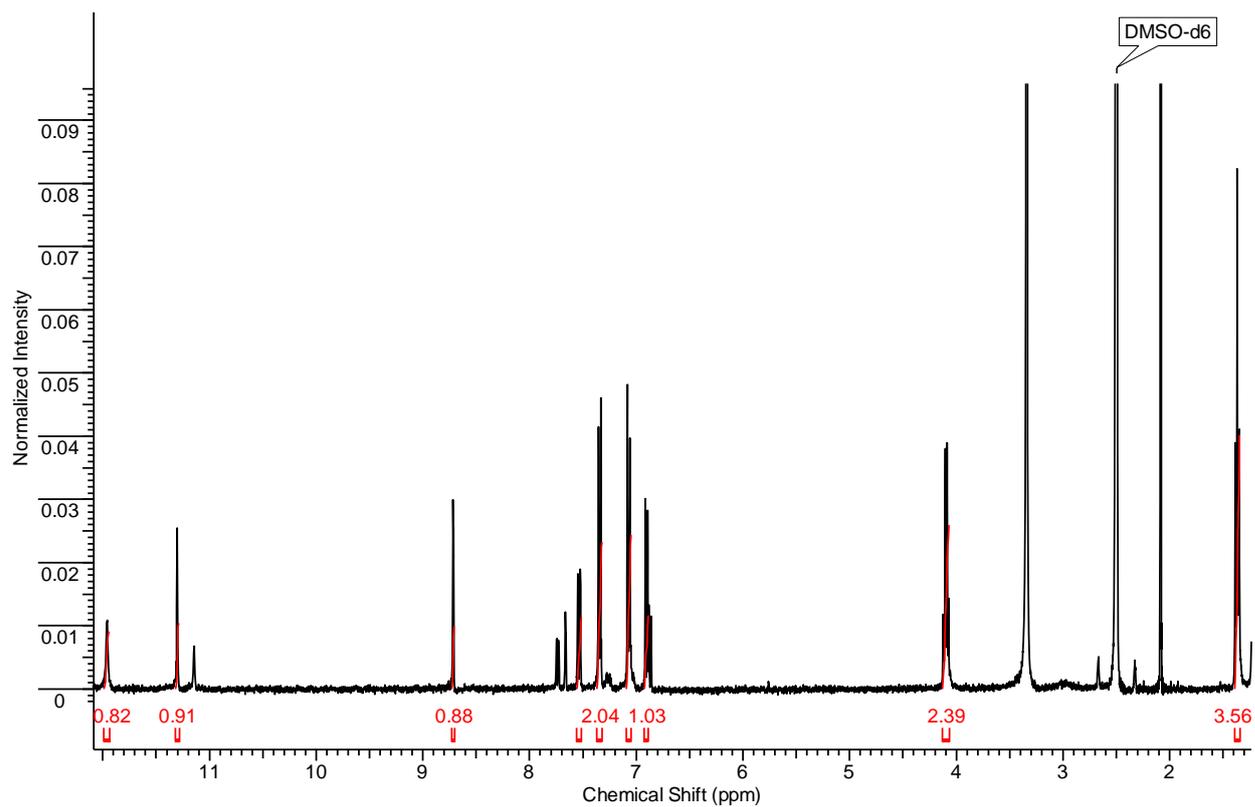
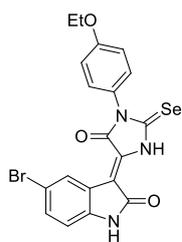
**Figure S1**  $^1\text{H}$  NMR spectrum of ethyl 2-[3-(4-ethoxyphenyl)selenoureido]acetate (**1**)



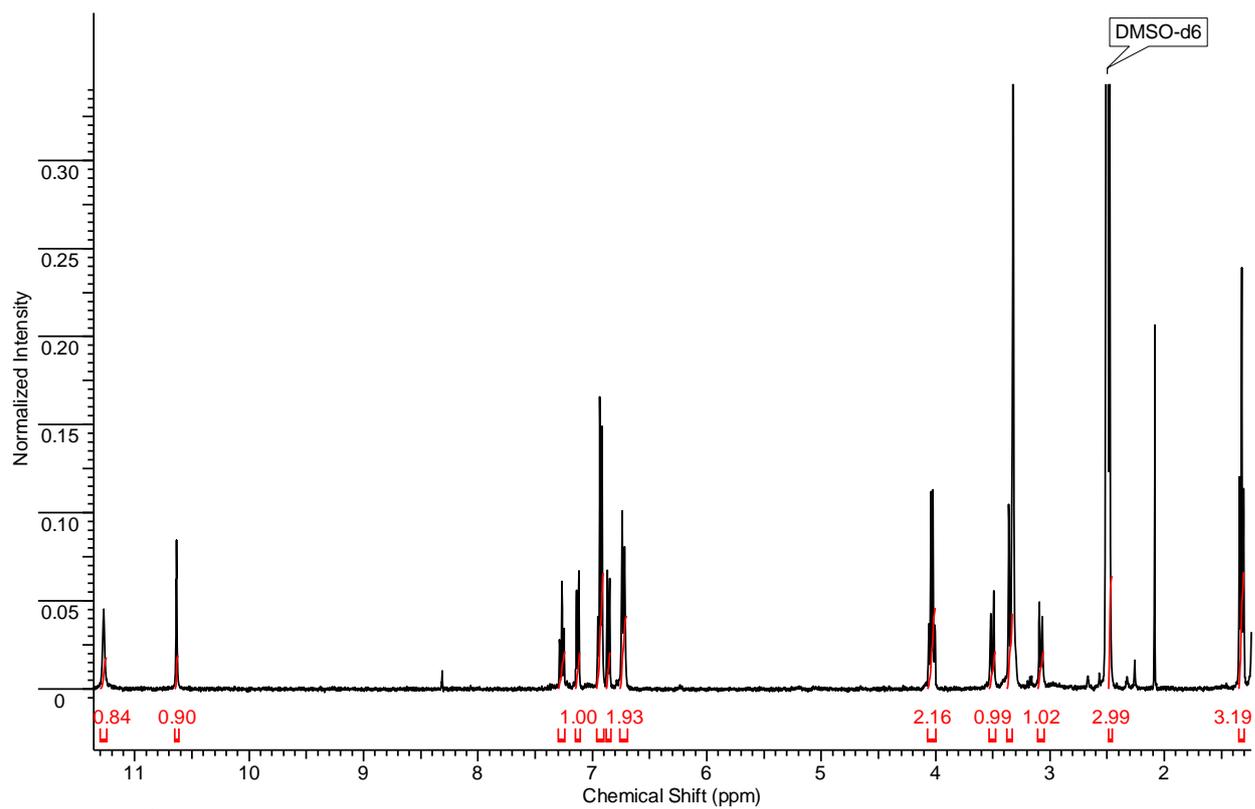
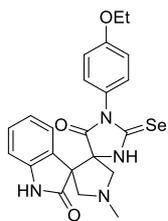
**Figure S2**  $^1\text{H}$  NMR spectrum of (*Z*)-3-(4-ethoxyphenyl)-5-(2-oxoindolinylidene)-2-selenoxoimidazolidin-4-one (**2a**)



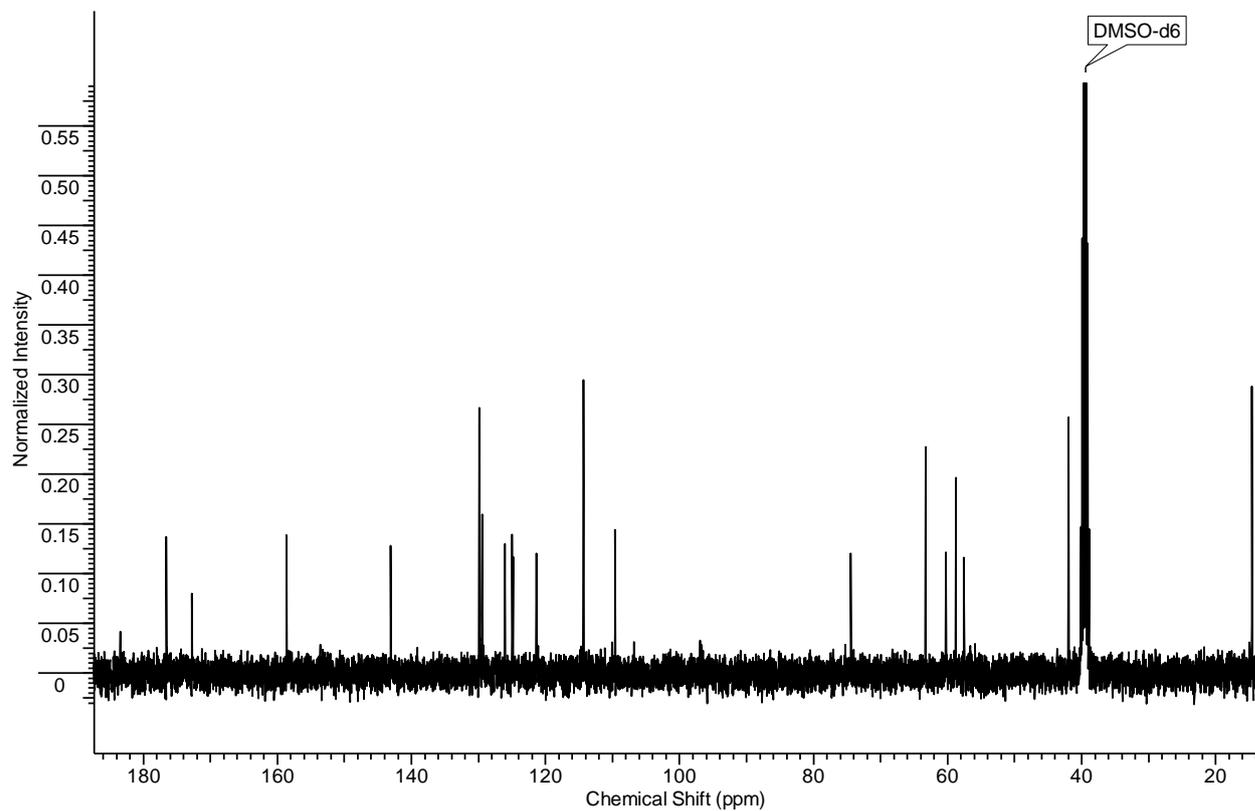
**Figure S3**  $^1\text{H}$  NMR spectrum of (*Z*)-5-(5-chloro-2-oxoindolinylidene)-3-(4-ethoxyphenyl)-2-selenoimidazolidin-4-one (**2b**)



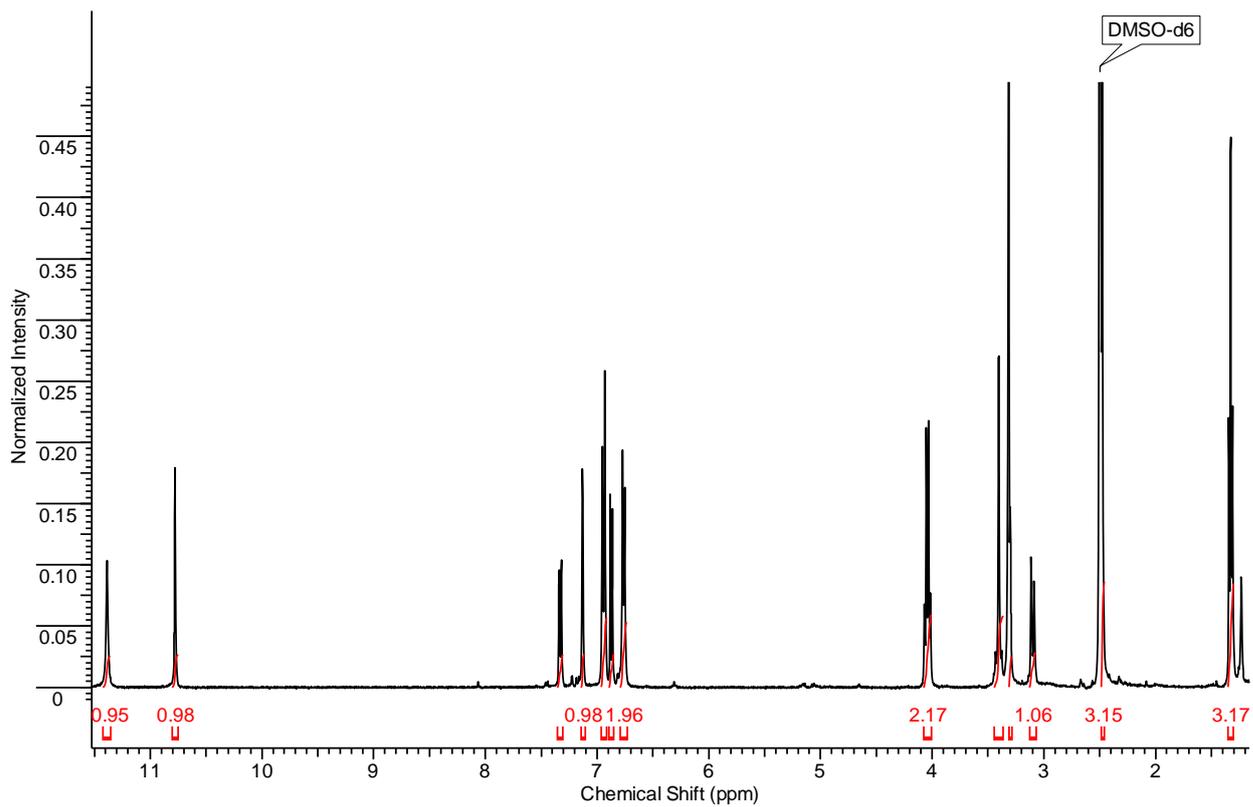
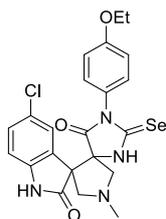
**Figure S4**  $^1\text{H}$  NMR spectrum of (*Z*)-5-(5-bromo-2-oxindolinylidene)-3-(4-ethoxyphenyl)-2-selenoimidazolidin-4-one (**2c**)



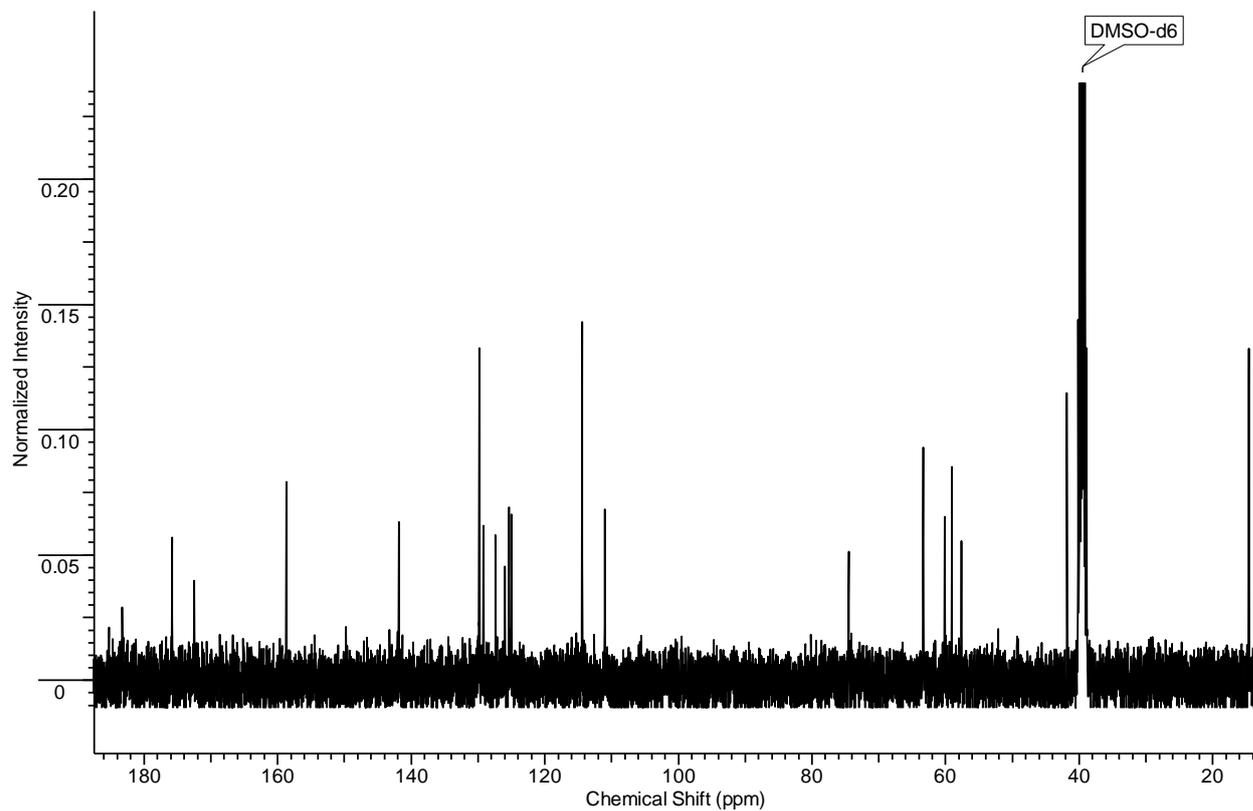
**Figure S5**  $^1\text{H}$  NMR spectrum of 3-(4-ethoxyphenyl)-1'-methyl-2-selenoxodispiro[imidazolidin-5,3'-pyrrolidin-4',3''-indoline]-2'',4-dione (**3a**)



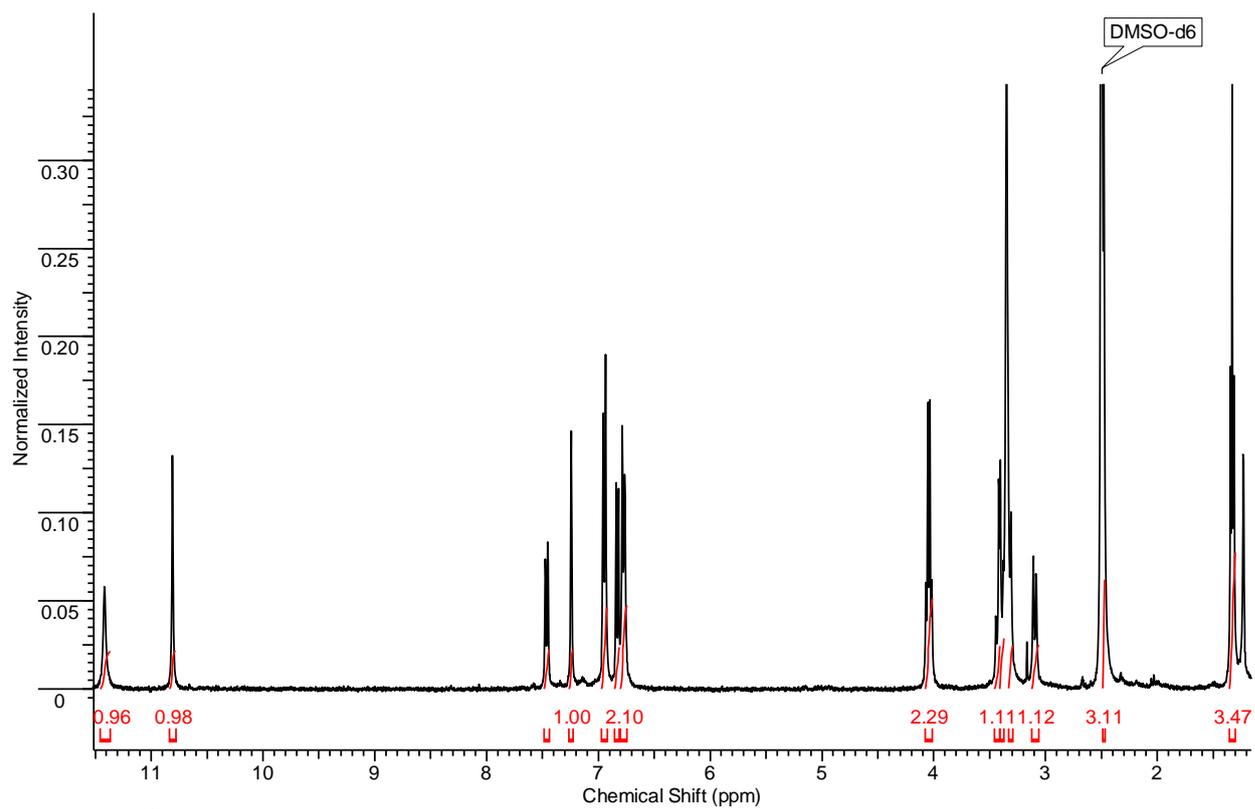
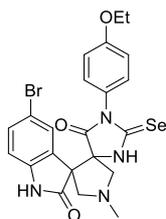
**Figure S6**  $^{13}\text{C}$  NMR spectrum of 3-(4-ethoxyphenyl)-1'-methyl-2-selenoxodispiro[imidazolidin-5,3'-pyrrolidin-4',3''-indoline]-2'',4-dione (**3a**)



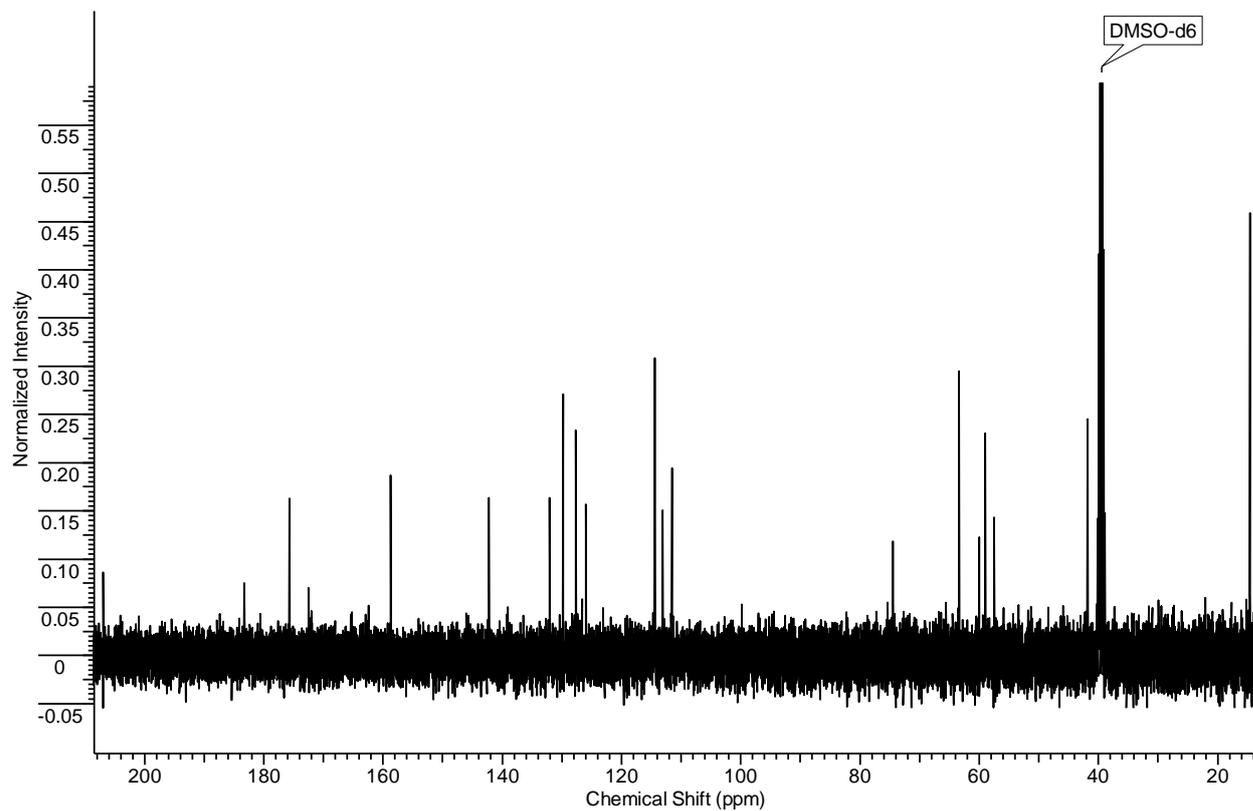
**Figure S7** <sup>1</sup>H NMR spectrum of 5''-chloro-3-(4-ethoxyphenyl)-1'-methyl-2-selenoxodispiro[imidazolidine-5,3'-pyrrolidine-4',3''-indoline]-2'',4-dione (**3b**)



**Figure S8**  $^{13}\text{C}$  NMR spectrum of 5"-chloro-3-(4-ethoxyphenyl)-1'-methyl-2-selenoxodispiro[imidazolidine-5,3'-pyrrolidine-4',3"-indoline]-2",4-dione (**3b**)



**Figure S9**  $^1\text{H}$  NMR spectrum of 5''-bromo-3-(4-ethoxyphenyl)-1'-methyl-2-selenoxodispiro[imidazolidine-5,3'-pyrrolidine-4',3''-indoline]-2'',4-dione (**3c**)



**Figure S10** <sup>13</sup>C NMR spectrum of 5''-bromo-3-(4-ethoxyphenyl)-1'-methyl-2-selenoxodispiro[imidazolidine-5,3'-pyrrolidine-4',3''-indoline]-2'',4-dione (**3c**)

## X-Ray for 3b

**Table S1.** Bond lengths [Å] and angles [°].

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Se(1A)-C(15A)	1.792(7)
Cl(1A)-C(6A)	1.729(8)
O(1A)-C(2A)	1.219(8)
O(2A)-C(14A)	1.226(7)
O(3A)-C(19A)	1.374(8)
O(3A)-C(22A)	1.433(8)
N(1A)-C(2A)	1.337(9)
N(1A)-C(9A)	1.393(9)
N(1A)-H(1A)	0.92(7)
N(2A)-C(12A)	1.453(8)
N(2A)-C(11A)	1.458(8)
N(2A)-C(24A)	1.483(8)
N(3A)-C(15A)	1.325(8)
N(3A)-C(13A)	1.449(7)
N(3A)-H(3A)	0.89(6)
N(4A)-C(14A)	1.376(8)
N(4A)-C(15A)	1.402(7)
N(4A)-C(16A)	1.451(8)
C(2A)-C(3A)	1.552(8)
C(3A)-C(10A)	1.486(9)
C(3A)-C(11A)	1.543(8)
C(3A)-C(13A)	1.570(8)
C(5A)-C(6A)	1.370(10)
C(5A)-C(10A)	1.388(8)
C(5A)-H(5A)	0.9300
C(6A)-C(7A)	1.358(11)
C(7A)-C(8A)	1.382(10)
C(7A)-H(7A)	0.9300
C(8A)-C(9A)	1.364(10)
C(8A)-H(8A)	0.9300
C(9A)-C(10A)	1.402(8)
C(11A)-H(11A)	0.9700
C(11A)-H(11B)	0.9700
C(12A)-C(13A)	1.515(9)
C(12A)-H(12A)	0.9700
C(12A)-H(12B)	0.9700
C(13A)-C(14A)	1.516(8)
C(16A)-C(21A)	1.355(9)
C(16A)-C(17A)	1.369(8)
C(17A)-C(18A)	1.413(9)
C(17A)-H(17A)	0.9300
C(18A)-C(19A)	1.371(10)
C(18A)-H(18A)	0.9300
C(19A)-C(20A)	1.393(9)
C(20A)-C(21A)	1.365(9)
C(20A)-H(20A)	0.9300
C(21A)-H(21A)	0.9300
C(22A)-C(23A)	1.488(11)
C(22A)-H(22A)	0.9700
C(22A)-H(22B)	0.9700
C(23A)-H(23A)	0.9600
C(23A)-H(23B)	0.9600
C(23A)-H(23C)	0.9600
C(24A)-H(24A)	0.9600
C(24A)-H(24B)	0.9600
C(24A)-H(24C)	0.9600
C(25A)-O(5A)	1.310(8)
C(25A)-H(25A)	0.9600

C(25A)-H(25B)	0.9600
C(25A)-H(25C)	0.9600
O(5A)-H(5A1)	0.8200
Se(1B)-C(15B)	1.800(6)
Cl(1B)-C(6B)	1.739(7)
O(1B)-C(2B)	1.217(7)
O(2B)-C(14B)	1.223(7)
O(3B)-C(19B)	1.370(7)
O(3B)-C(22B)	1.448(7)
N(1B)-C(2B)	1.359(8)
N(1B)-C(9B)	1.397(8)
N(1B)-H(1B)	1.04(11)
N(2B)-C(11B)	1.473(7)
N(2B)-C(24B)	1.473(7)
N(2B)-C(12B)	1.485(7)
N(3B)-C(15B)	1.326(7)
N(3B)-C(13B)	1.452(7)
N(3B)-H(3B)	1.00(7)
N(4B)-C(14B)	1.378(7)
N(4B)-C(15B)	1.409(7)
N(4B)-C(16B)	1.435(7)
C(2B)-C(3B)	1.534(8)
C(3B)-C(10B)	1.497(8)
C(3B)-C(11B)	1.528(7)
C(3B)-C(13B)	1.568(7)
C(5B)-C(10B)	1.378(8)
C(5B)-C(6B)	1.381(8)
C(5B)-H(5B)	0.9300
C(6B)-C(7B)	1.378(9)
C(7B)-C(8B)	1.383(8)
C(7B)-H(7B)	0.9300
C(8B)-C(9B)	1.367(8)
C(8B)-H(8B)	0.9300
C(9B)-C(10B)	1.407(8)
C(11B)-H(11C)	0.9700
C(11B)-H(11D)	0.9700
C(12B)-C(13B)	1.521(8)
C(12B)-H(12C)	0.9700
C(12B)-H(12D)	0.9700
C(13B)-C(14B)	1.504(7)
C(16B)-C(21B)	1.349(8)
C(16B)-C(17B)	1.388(8)
C(17B)-C(18B)	1.391(8)
C(17B)-H(17B)	0.9300
C(18B)-C(19B)	1.375(9)
C(18B)-H(18B)	0.9300
C(19B)-C(20B)	1.392(9)
C(20B)-C(21B)	1.363(8)
C(20B)-H(20B)	0.9300
C(21B)-H(21B)	0.9300
C(22B)-C(23B)	1.502(10)
C(22B)-H(22C)	0.9700
C(22B)-H(22D)	0.9700
C(23B)-H(23D)	0.9600
C(23B)-H(23E)	0.9600
C(23B)-H(23F)	0.9600
C(24B)-H(24D)	0.9600
C(24B)-H(24E)	0.9600
C(24B)-H(24F)	0.9600
C(25B)-O(5B)	1.375(8)
C(25B)-H(25D)	0.9600
C(25B)-H(25E)	0.9600

C(25B)-H(25F)	0.9600
O(5B)-H(5B1)	0.8200
C(19A)-O(3A)-C(22A)	117.1(7)
C(2A)-N(1A)-C(9A)	112.5(6)
C(2A)-N(1A)-H(1A)	118(5)
C(9A)-N(1A)-H(1A)	130(4)
C(12A)-N(2A)-C(11A)	109.0(5)
C(12A)-N(2A)-C(24A)	114.7(6)
C(11A)-N(2A)-C(24A)	112.2(6)
C(15A)-N(3A)-C(13A)	113.5(6)
C(15A)-N(3A)-H(3A)	127(4)
C(13A)-N(3A)-H(3A)	118(4)
C(14A)-N(4A)-C(15A)	110.4(6)
C(14A)-N(4A)-C(16A)	122.8(5)
C(15A)-N(4A)-C(16A)	126.8(5)
O(1A)-C(2A)-N(1A)	127.0(7)
O(1A)-C(2A)-C(3A)	125.5(7)
N(1A)-C(2A)-C(3A)	107.4(7)
C(10A)-C(3A)-C(11A)	118.4(5)
C(10A)-C(3A)-C(2A)	102.5(5)
C(11A)-C(3A)-C(2A)	110.4(5)
C(10A)-C(3A)-C(13A)	116.5(5)
C(11A)-C(3A)-C(13A)	100.2(5)
C(2A)-C(3A)-C(13A)	108.8(5)
C(6A)-C(5A)-C(10A)	118.1(7)
C(6A)-C(5A)-H(5A)	121.0
C(10A)-C(5A)-H(5A)	121.0
C(7A)-C(6A)-C(5A)	122.1(8)
C(7A)-C(6A)-Cl(1A)	119.4(8)
C(5A)-C(6A)-Cl(1A)	118.4(7)
C(6A)-C(7A)-C(8A)	120.6(9)
C(6A)-C(7A)-H(7A)	119.7
C(8A)-C(7A)-H(7A)	119.7
C(9A)-C(8A)-C(7A)	118.4(8)
C(9A)-C(8A)-H(8A)	120.8
C(7A)-C(8A)-H(8A)	120.8
C(8A)-C(9A)-N(1A)	129.7(7)
C(8A)-C(9A)-C(10A)	121.1(8)
N(1A)-C(9A)-C(10A)	109.2(7)
C(5A)-C(10A)-C(9A)	119.5(7)
C(5A)-C(10A)-C(3A)	132.1(6)
C(9A)-C(10A)-C(3A)	108.4(7)
N(2A)-C(11A)-C(3A)	105.4(5)
N(2A)-C(11A)-H(11A)	110.7
C(3A)-C(11A)-H(11A)	110.7
N(2A)-C(11A)-H(11B)	110.7
C(3A)-C(11A)-H(11B)	110.7
H(11A)-C(11A)-H(11B)	108.8
N(2A)-C(12A)-C(13A)	107.7(5)
N(2A)-C(12A)-H(12A)	110.2
C(13A)-C(12A)-H(12A)	110.2
N(2A)-C(12A)-H(12B)	110.2
C(13A)-C(12A)-H(12B)	110.2
H(12A)-C(12A)-H(12B)	108.5
N(3A)-C(13A)-C(12A)	117.5(6)
N(3A)-C(13A)-C(14A)	100.9(5)
C(12A)-C(13A)-C(14A)	111.3(5)
N(3A)-C(13A)-C(3A)	114.1(4)
C(12A)-C(13A)-C(3A)	103.2(5)
C(14A)-C(13A)-C(3A)	109.8(5)
O(2A)-C(14A)-N(4A)	126.0(6)

O(2A)-C(14A)-C(13A)	126.8(6)
N(4A)-C(14A)-C(13A)	107.2(5)
N(3A)-C(15A)-N(4A)	107.8(6)
N(3A)-C(15A)-Se(1A)	128.0(5)
N(4A)-C(15A)-Se(1A)	124.2(5)
C(21A)-C(16A)-C(17A)	123.0(7)
C(21A)-C(16A)-N(4A)	118.3(6)
C(17A)-C(16A)-N(4A)	118.5(7)
C(16A)-C(17A)-C(18A)	117.6(7)
C(16A)-C(17A)-H(17A)	121.2
C(18A)-C(17A)-H(17A)	121.2
C(19A)-C(18A)-C(17A)	120.2(7)
C(19A)-C(18A)-H(18A)	119.9
C(17A)-C(18A)-H(18A)	119.9
C(18A)-C(19A)-O(3A)	125.2(7)
C(18A)-C(19A)-C(20A)	119.4(8)
O(3A)-C(19A)-C(20A)	115.4(8)
C(21A)-C(20A)-C(19A)	120.7(8)
C(21A)-C(20A)-H(20A)	119.6
C(19A)-C(20A)-H(20A)	119.6
C(16A)-C(21A)-C(20A)	119.0(7)
C(16A)-C(21A)-H(21A)	120.5
C(20A)-C(21A)-H(21A)	120.5
O(3A)-C(22A)-C(23A)	106.9(8)
O(3A)-C(22A)-H(22A)	110.3
C(23A)-C(22A)-H(22A)	110.3
O(3A)-C(22A)-H(22B)	110.3
C(23A)-C(22A)-H(22B)	110.3
H(22A)-C(22A)-H(22B)	108.6
C(22A)-C(23A)-H(23A)	109.5
C(22A)-C(23A)-H(23B)	109.5
H(23A)-C(23A)-H(23B)	109.5
C(22A)-C(23A)-H(23C)	109.5
H(23A)-C(23A)-H(23C)	109.5
H(23B)-C(23A)-H(23C)	109.5
N(2A)-C(24A)-H(24A)	109.5
N(2A)-C(24A)-H(24B)	109.5
H(24A)-C(24A)-H(24B)	109.5
N(2A)-C(24A)-H(24C)	109.5
H(24A)-C(24A)-H(24C)	109.5
H(24B)-C(24A)-H(24C)	109.5
O(5A)-C(25A)-H(25A)	109.5
O(5A)-C(25A)-H(25B)	109.5
H(25A)-C(25A)-H(25B)	109.5
O(5A)-C(25A)-H(25C)	109.5
H(25A)-C(25A)-H(25C)	109.5
H(25B)-C(25A)-H(25C)	109.5
C(25A)-O(5A)-H(5A1)	109.5
C(19B)-O(3B)-C(22B)	116.3(6)
C(2B)-N(1B)-C(9B)	112.0(5)
C(2B)-N(1B)-H(1B)	128(6)
C(9B)-N(1B)-H(1B)	119(6)
C(11B)-N(2B)-C(24B)	114.0(5)
C(11B)-N(2B)-C(12B)	107.9(4)
C(24B)-N(2B)-C(12B)	114.2(5)
C(15B)-N(3B)-C(13B)	113.5(5)
C(15B)-N(3B)-H(3B)	118(3)
C(13B)-N(3B)-H(3B)	128(3)
C(14B)-N(4B)-C(15B)	110.2(5)
C(14B)-N(4B)-C(16B)	123.3(5)
C(15B)-N(4B)-C(16B)	126.3(5)
O(1B)-C(2B)-N(1B)	125.2(6)

O(1B)-C(2B)-C(3B)	127.4(6)
N(1B)-C(2B)-C(3B)	107.4(6)
C(10B)-C(3B)-C(11B)	118.6(5)
C(10B)-C(3B)-C(2B)	103.2(5)
C(11B)-C(3B)-C(2B)	110.7(5)
C(10B)-C(3B)-C(13B)	115.5(5)
C(11B)-C(3B)-C(13B)	100.1(4)
C(2B)-C(3B)-C(13B)	108.8(4)
C(10B)-C(5B)-C(6B)	118.5(6)
C(10B)-C(5B)-H(5B)	120.7
C(6B)-C(5B)-H(5B)	120.7
C(7B)-C(6B)-C(5B)	122.0(7)
C(7B)-C(6B)-Cl(1B)	119.9(6)
C(5B)-C(6B)-Cl(1B)	118.0(5)
C(6B)-C(7B)-C(8B)	120.1(6)
C(6B)-C(7B)-H(7B)	119.9
C(8B)-C(7B)-H(7B)	119.9
C(9B)-C(8B)-C(7B)	118.0(6)
C(9B)-C(8B)-H(8B)	121.0
C(7B)-C(8B)-H(8B)	121.0
C(8B)-C(9B)-N(1B)	128.1(6)
C(8B)-C(9B)-C(10B)	122.5(7)
N(1B)-C(9B)-C(10B)	109.4(6)
C(5B)-C(10B)-C(9B)	118.8(6)
C(5B)-C(10B)-C(3B)	133.4(5)
C(9B)-C(10B)-C(3B)	107.9(6)
N(2B)-C(11B)-C(3B)	106.1(5)
N(2B)-C(11B)-H(11C)	110.5
C(3B)-C(11B)-H(11C)	110.5
N(2B)-C(11B)-H(11D)	110.5
C(3B)-C(11B)-H(11D)	110.5
H(11C)-C(11B)-H(11D)	108.7
N(2B)-C(12B)-C(13B)	106.7(5)
N(2B)-C(12B)-H(12C)	110.4
C(13B)-C(12B)-H(12C)	110.4
N(2B)-C(12B)-H(12D)	110.4
C(13B)-C(12B)-H(12D)	110.4
H(12C)-C(12B)-H(12D)	108.6
N(3B)-C(13B)-C(14B)	101.1(5)
N(3B)-C(13B)-C(12B)	115.8(5)
C(14B)-C(13B)-C(12B)	110.8(5)
N(3B)-C(13B)-C(3B)	115.4(4)
C(14B)-C(13B)-C(3B)	110.3(4)
C(12B)-C(13B)-C(3B)	103.6(4)
O(2B)-C(14B)-N(4B)	124.6(6)
O(2B)-C(14B)-C(13B)	127.8(6)
N(4B)-C(14B)-C(13B)	107.7(5)
N(3B)-C(15B)-N(4B)	107.4(5)
N(3B)-C(15B)-Se(1B)	128.6(5)
N(4B)-C(15B)-Se(1B)	124.0(4)
C(21B)-C(16B)-C(17B)	120.9(6)
C(21B)-C(16B)-N(4B)	119.8(5)
C(17B)-C(16B)-N(4B)	119.0(6)
C(16B)-C(17B)-C(18B)	118.7(6)
C(16B)-C(17B)-H(17B)	120.6
C(18B)-C(17B)-H(17B)	120.6
C(19B)-C(18B)-C(17B)	119.9(6)
C(19B)-C(18B)-H(18B)	120.1
C(17B)-C(18B)-H(18B)	120.1
O(3B)-C(19B)-C(18B)	125.7(6)
O(3B)-C(19B)-C(20B)	114.3(7)
C(18B)-C(19B)-C(20B)	120.0(7)

C(21B)-C(20B)-C(19B)	119.5(7)
C(21B)-C(20B)-H(20B)	120.2
C(19B)-C(20B)-H(20B)	120.2
C(16B)-C(21B)-C(20B)	121.0(6)
C(16B)-C(21B)-H(21B)	119.5
C(20B)-C(21B)-H(21B)	119.5
O(3B)-C(22B)-C(23B)	105.7(6)
O(3B)-C(22B)-H(22C)	110.6
C(23B)-C(22B)-H(22C)	110.6
O(3B)-C(22B)-H(22D)	110.6
C(23B)-C(22B)-H(22D)	110.6
H(22C)-C(22B)-H(22D)	108.7
C(22B)-C(23B)-H(23D)	109.5
C(22B)-C(23B)-H(23E)	109.5
H(23D)-C(23B)-H(23E)	109.5
C(22B)-C(23B)-H(23F)	109.5
H(23D)-C(23B)-H(23F)	109.5
H(23E)-C(23B)-H(23F)	109.5
N(2B)-C(24B)-H(24D)	109.5
N(2B)-C(24B)-H(24E)	109.5
H(24D)-C(24B)-H(24E)	109.5
N(2B)-C(24B)-H(24F)	109.5
H(24D)-C(24B)-H(24F)	109.5
H(24E)-C(24B)-H(24F)	109.5
O(5B)-C(25B)-H(25D)	109.5
O(5B)-C(25B)-H(25E)	109.5
H(25D)-C(25B)-H(25E)	109.5
O(5B)-C(25B)-H(25F)	109.5
H(25D)-C(25B)-H(25F)	109.5
H(25E)-C(25B)-H(25F)	109.5
C(25B)-O(5B)-H(5B1)	109.5

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Symmetry transformations used to generate equivalent atoms:

**Table S2.** Torsion angles [°].

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C(9A)-N(1A)-C(2A)-O(1A)	-179.1(6)
C(9A)-N(1A)-C(2A)-C(3A)	-1.6(6)
O(1A)-C(2A)-C(3A)-C(10A)	177.2(6)
N(1A)-C(2A)-C(3A)-C(10A)	-0.3(6)
O(1A)-C(2A)-C(3A)-C(11A)	50.2(8)
N(1A)-C(2A)-C(3A)-C(11A)	-127.4(6)
O(1A)-C(2A)-C(3A)-C(13A)	-58.9(8)
N(1A)-C(2A)-C(3A)-C(13A)	123.6(6)
C(10A)-C(5A)-C(6A)-C(7A)	0.1(10)
C(10A)-C(5A)-C(6A)-Cl(1A)	177.2(4)
C(5A)-C(6A)-C(7A)-C(8A)	-2.7(11)
Cl(1A)-C(6A)-C(7A)-C(8A)	-179.8(5)
C(6A)-C(7A)-C(8A)-C(9A)	3.4(11)
C(7A)-C(8A)-C(9A)-N(1A)	178.5(6)
C(7A)-C(8A)-C(9A)-C(10A)	-1.6(10)
C(2A)-N(1A)-C(9A)-C(8A)	-177.1(6)
C(2A)-N(1A)-C(9A)-C(10A)	3.1(7)
C(6A)-C(5A)-C(10A)-C(9A)	1.7(8)
C(6A)-C(5A)-C(10A)-C(3A)	-175.6(6)
C(8A)-C(9A)-C(10A)-C(5A)	-1.0(9)
N(1A)-C(9A)-C(10A)-C(5A)	178.9(5)
C(8A)-C(9A)-C(10A)-C(3A)	177.0(6)
N(1A)-C(9A)-C(10A)-C(3A)	-3.1(6)
C(11A)-C(3A)-C(10A)-C(5A)	-58.6(9)
C(2A)-C(3A)-C(10A)-C(5A)	179.7(6)
C(13A)-C(3A)-C(10A)-C(5A)	61.1(8)
C(11A)-C(3A)-C(10A)-C(9A)	123.8(5)
C(2A)-C(3A)-C(10A)-C(9A)	2.1(6)
C(13A)-C(3A)-C(10A)-C(9A)	-116.5(5)
C(12A)-N(2A)-C(11A)-C(3A)	-23.9(6)
C(24A)-N(2A)-C(11A)-C(3A)	-152.0(6)
C(10A)-C(3A)-C(11A)-N(2A)	164.1(5)
C(2A)-C(3A)-C(11A)-N(2A)	-78.3(6)
C(13A)-C(3A)-C(11A)-N(2A)	36.3(6)
C(11A)-N(2A)-C(12A)-C(13A)	0.3(7)
C(24A)-N(2A)-C(12A)-C(13A)	127.1(6)
C(15A)-N(3A)-C(13A)-C(12A)	123.2(6)
C(15A)-N(3A)-C(13A)-C(14A)	1.9(6)
C(15A)-N(3A)-C(13A)-C(3A)	-115.8(6)
N(2A)-C(12A)-C(13A)-N(3A)	149.2(5)
N(2A)-C(12A)-C(13A)-C(14A)	-95.1(6)
N(2A)-C(12A)-C(13A)-C(3A)	22.7(6)
C(10A)-C(3A)-C(13A)-N(3A)	66.9(7)
C(11A)-C(3A)-C(13A)-N(3A)	-164.0(6)
C(2A)-C(3A)-C(13A)-N(3A)	-48.1(8)
C(10A)-C(3A)-C(13A)-C(12A)	-164.3(5)
C(11A)-C(3A)-C(13A)-C(12A)	-35.3(6)
C(2A)-C(3A)-C(13A)-C(12A)	80.6(6)
C(10A)-C(3A)-C(13A)-C(14A)	-45.5(6)
C(11A)-C(3A)-C(13A)-C(14A)	83.5(6)
C(2A)-C(3A)-C(13A)-C(14A)	-160.6(5)
C(15A)-N(4A)-C(14A)-O(2A)	-175.2(6)
C(16A)-N(4A)-C(14A)-O(2A)	6.0(10)
C(15A)-N(4A)-C(14A)-C(13A)	4.4(6)
C(16A)-N(4A)-C(14A)-C(13A)	-174.5(5)
N(3A)-C(13A)-C(14A)-O(2A)	175.8(6)
C(12A)-C(13A)-C(14A)-O(2A)	50.3(8)
C(3A)-C(13A)-C(14A)-O(2A)	-63.3(8)
N(3A)-C(13A)-C(14A)-N(4A)	-3.7(6)
C(12A)-C(13A)-C(14A)-N(4A)	-129.2(5)

C(3A)-C(13A)-C(14A)-N(4A)	117.1(5)
C(13A)-N(3A)-C(15A)-N(4A)	0.6(7)
C(13A)-N(3A)-C(15A)-Se(1A)	-179.5(5)
C(14A)-N(4A)-C(15A)-N(3A)	-3.2(7)
C(16A)-N(4A)-C(15A)-N(3A)	175.6(6)
C(14A)-N(4A)-C(15A)-Se(1A)	176.9(4)
C(16A)-N(4A)-C(15A)-Se(1A)	-4.3(8)
C(14A)-N(4A)-C(16A)-C(21A)	93.0(7)
C(15A)-N(4A)-C(16A)-C(21A)	-85.7(8)
C(14A)-N(4A)-C(16A)-C(17A)	-83.0(7)
C(15A)-N(4A)-C(16A)-C(17A)	98.3(7)
C(21A)-C(16A)-C(17A)-C(18A)	0.4(9)
N(4A)-C(16A)-C(17A)-C(18A)	176.2(5)
C(16A)-C(17A)-C(18A)-C(19A)	-1.6(9)
C(17A)-C(18A)-C(19A)-O(3A)	-177.7(6)
C(17A)-C(18A)-C(19A)-C(20A)	3.3(9)
C(22A)-O(3A)-C(19A)-C(18A)	7.2(9)
C(22A)-O(3A)-C(19A)-C(20A)	-173.8(6)
C(18A)-C(19A)-C(20A)-C(21A)	-3.8(10)
O(3A)-C(19A)-C(20A)-C(21A)	177.1(6)
C(17A)-C(16A)-C(21A)-C(20A)	-0.9(10)
N(4A)-C(16A)-C(21A)-C(20A)	-176.7(6)
C(19A)-C(20A)-C(21A)-C(16A)	2.6(10)
C(19A)-O(3A)-C(22A)-C(23A)	176.3(6)
C(9B)-N(1B)-C(2B)-O(1B)	-177.5(5)
C(9B)-N(1B)-C(2B)-C(3B)	1.9(6)
O(1B)-C(2B)-C(3B)-C(10B)	176.3(6)
N(1B)-C(2B)-C(3B)-C(10B)	-3.1(5)
O(1B)-C(2B)-C(3B)-C(11B)	48.5(7)
N(1B)-C(2B)-C(3B)-C(11B)	-130.9(5)
O(1B)-C(2B)-C(3B)-C(13B)	-60.6(8)
N(1B)-C(2B)-C(3B)-C(13B)	120.0(5)
C(10B)-C(5B)-C(6B)-C(7B)	-2.5(9)
C(10B)-C(5B)-C(6B)-Cl(1B)	177.7(4)
C(5B)-C(6B)-C(7B)-C(8B)	1.1(9)
Cl(1B)-C(6B)-C(7B)-C(8B)	-179.1(5)
C(6B)-C(7B)-C(8B)-C(9B)	-0.5(9)
C(7B)-C(8B)-C(9B)-N(1B)	179.6(5)
C(7B)-C(8B)-C(9B)-C(10B)	1.3(8)
C(2B)-N(1B)-C(9B)-C(8B)	-178.2(5)
C(2B)-N(1B)-C(9B)-C(10B)	0.2(6)
C(6B)-C(5B)-C(10B)-C(9B)	3.3(8)
C(6B)-C(5B)-C(10B)-C(3B)	-175.5(6)
C(8B)-C(9B)-C(10B)-C(5B)	-2.8(8)
N(1B)-C(9B)-C(10B)-C(5B)	178.7(5)
C(8B)-C(9B)-C(10B)-C(3B)	176.2(5)
N(1B)-C(9B)-C(10B)-C(3B)	-2.3(6)
C(11B)-C(3B)-C(10B)-C(5B)	-55.2(8)
C(2B)-C(3B)-C(10B)-C(5B)	-177.9(6)
C(13B)-C(3B)-C(10B)-C(5B)	63.6(8)
C(11B)-C(3B)-C(10B)-C(9B)	126.0(5)
C(2B)-C(3B)-C(10B)-C(9B)	3.2(5)
C(13B)-C(3B)-C(10B)-C(9B)	-115.3(5)
C(24B)-N(2B)-C(11B)-C(3B)	-151.8(5)
C(12B)-N(2B)-C(11B)-C(3B)	-23.9(6)
C(10B)-C(3B)-C(11B)-N(2B)	164.0(5)
C(2B)-C(3B)-C(11B)-N(2B)	-77.1(5)
C(13B)-C(3B)-C(11B)-N(2B)	37.5(5)
C(11B)-N(2B)-C(12B)-C(13B)	-0.8(6)
C(24B)-N(2B)-C(12B)-C(13B)	127.0(6)
C(15B)-N(3B)-C(13B)-C(14B)	0.9(6)
C(15B)-N(3B)-C(13B)-C(12B)	120.6(5)

C(15B)-N(3B)-C(13B)-C(3B)	-118.1(5)
N(2B)-C(12B)-C(13B)-N(3B)	151.6(4)
N(2B)-C(12B)-C(13B)-C(14B)	-94.1(5)
N(2B)-C(12B)-C(13B)-C(3B)	24.2(6)
C(10B)-C(3B)-C(13B)-N(3B)	66.7(7)
C(11B)-C(3B)-C(13B)-N(3B)	-164.8(5)
C(2B)-C(3B)-C(13B)-N(3B)	-48.7(7)
C(10B)-C(3B)-C(13B)-C(14B)	-47.1(6)
C(11B)-C(3B)-C(13B)-C(14B)	81.5(6)
C(2B)-C(3B)-C(13B)-C(14B)	-162.5(5)
C(10B)-C(3B)-C(13B)-C(12B)	-165.7(5)
C(11B)-C(3B)-C(13B)-C(12B)	-37.1(5)
C(2B)-C(3B)-C(13B)-C(12B)	78.9(6)
C(15B)-N(4B)-C(14B)-O(2B)	-175.4(5)
C(16B)-N(4B)-C(14B)-O(2B)	9.1(9)
C(15B)-N(4B)-C(14B)-C(13B)	3.2(6)
C(16B)-N(4B)-C(14B)-C(13B)	-172.3(5)
N(3B)-C(13B)-C(14B)-O(2B)	176.1(6)
C(12B)-C(13B)-C(14B)-O(2B)	52.8(7)
C(3B)-C(13B)-C(14B)-O(2B)	-61.3(7)
N(3B)-C(13B)-C(14B)-N(4B)	-2.5(5)
C(12B)-C(13B)-C(14B)-N(4B)	-125.7(5)
C(3B)-C(13B)-C(14B)-N(4B)	120.2(5)
C(13B)-N(3B)-C(15B)-N(4B)	1.0(6)
C(13B)-N(3B)-C(15B)-Se(1B)	-178.1(4)
C(14B)-N(4B)-C(15B)-N(3B)	-2.7(6)
C(16B)-N(4B)-C(15B)-N(3B)	172.7(5)
C(14B)-N(4B)-C(15B)-Se(1B)	176.5(4)
C(16B)-N(4B)-C(15B)-Se(1B)	-8.1(8)
C(14B)-N(4B)-C(16B)-C(21B)	92.3(7)
C(15B)-N(4B)-C(16B)-C(21B)	-82.5(7)
C(14B)-N(4B)-C(16B)-C(17B)	-82.4(7)
C(15B)-N(4B)-C(16B)-C(17B)	102.8(6)
C(21B)-C(16B)-C(17B)-C(18B)	0.3(9)
N(4B)-C(16B)-C(17B)-C(18B)	174.9(5)
C(16B)-C(17B)-C(18B)-C(19B)	-1.0(8)
C(22B)-O(3B)-C(19B)-C(18B)	6.5(9)
C(22B)-O(3B)-C(19B)-C(20B)	-172.0(6)
C(17B)-C(18B)-C(19B)-O(3B)	-177.0(5)
C(17B)-C(18B)-C(19B)-C(20B)	1.5(9)
O(3B)-C(19B)-C(20B)-C(21B)	177.5(5)
C(18B)-C(19B)-C(20B)-C(21B)	-1.1(9)
C(17B)-C(16B)-C(21B)-C(20B)	0.1(9)
N(4B)-C(16B)-C(21B)-C(20B)	-174.5(5)
C(19B)-C(20B)-C(21B)-C(16B)	0.4(9)
C(19B)-O(3B)-C(22B)-C(23B)	171.1(6)

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Symmetry transformations used to generate equivalent atoms:

**Table S3.** Hydrogen bonds [ $\text{\AA}$  and  $^\circ$ ].

D-H...A	d(D-H)	d(H...A)	d(D...A)	$\angle(\text{DHA})$
C(5A)-H(5A)...O(2A)	0.93	2.55	3.211(9)	128.6
C(11A)-H(11B)...O(2A)	0.97	2.60	3.099(7)	112.2
C(12A)-H(12B)...O(1A)#1	0.97	2.61	3.578(9)	175.9
C(18A)-H(18A)...Se(1A)#2	0.93	3.10	4.032(7)	175.4
C(25A)-H(25A)...Se(1A)	0.96	3.03	3.759(16)	134.3
O(5A)-H(5A1)...N(2A)#1	0.82	2.26	2.990(8)	148.2
C(5B)-H(5B)...O(2B)	0.93	2.61	3.246(7)	126.3
C(11B)-H(11C)...O(3A)#3	0.97	2.54	3.432(7)	152.5
C(11B)-H(11D)...O(2B)	0.97	2.54	3.063(7)	113.5
C(12B)-H(12D)...O(1B)#4	0.97	2.37	3.333(8)	171.0
C(18B)-H(18B)...Se(1B)#5	0.93	3.17	4.096(6)	176.1
C(23B)-H(23E)...Cl(1B)#6	0.96	2.89	3.428(9)	116.2
C(25B)-H(25E)...Se(1B)	0.96	3.13	3.833(9)	131.0
O(5B)-H(5B1)...O(1B)#4	0.82	2.63	3.161(7)	123.7
O(5B)-H(5B1)...N(2B)#4	0.82	2.17	2.930(7)	153.6
N(1A)-H(1A)...O(2A)#5	0.92(7)	1.98(7)	2.897(8)	174(6)
N(3A)-H(3A)...O(5A)	0.89(6)	1.90(6)	2.761(8)	162(6)
N(3B)-H(3B)...O(5B)	1.00(7)	1.75(7)	2.747(7)	174(5)
N(1B)-H(1B)...O(2B)#2	1.04(11)	1.88(11)	2.905(6)	169(9)

Symmetry transformations used to generate equivalent atoms:

#1  $-x+1, -y+1, -z$  #2  $x+1, y, z$  #3  $x-1, y+1, z$  #4  $-x+1, -y+2, -z+1$

#5  $x-1, y, z$  #6  $-x-1, -y+2, -z$