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# **Supporting Information**

## Regioselective *peri*-C–H Selenylation of Aromatic Compounds with Weakly Coordinating Ketone Groups

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## General information and materials:

Unless otherwise noted, all commercially available compounds were used as provided without further purification. Solvents for chromatography were technical grade. Column chromatography was performed using silica gel Merck 60 (particle size 0.040-0.063 mm). Solvent mixtures are understood as volume/volume.

<sup>1</sup>H-NMR and<sup>13</sup>C-NMRwere recorded on a *Bruker DRX400 (400 MHz)*, *DRX500 (500 MHz)* and *DRX600* (600 MHz) spectrometer in CDCl<sub>3</sub> ( $\delta$  = 7.26 ppm for <sup>1</sup>H,  $\delta$  = 77.00 ppm for <sup>13</sup>C) and in DMSO-*d*<sub>6</sub> ( $\delta$  = 2.50 ppm for <sup>1</sup>H,  $\delta$  = 39.43 ppm for <sup>13</sup>C). Data are reported in the following order: chemical shift ( $\delta$ ) in ppm; multiplicities are indicated s (singlet), d (doublet), t (triplet), q (quartet), m (multiplet); coupling constants (*J*)are given in Hertz (Hz). High resolution mass spectra were recorded on a LTQ Orbitrap massspectrometer coupled to an *Acceka HPLC-System* (HPLC column: *Hypersyl GOLD*, 50 mm ×1 mm, 1.9 µm). Chemical yields refer to isolated pure substances.

## General procedures for synthesis

## 1. General procedure for the synthesis of products 3:

A mixture of chromones **1** (0.2 mmol), diselenides **2** (0.24 mmol),  $[Ru(p-cymene)Cl_2]_2$  (10 mol%), AgNTf<sub>2</sub> (40 mol%), Cu(OAc)<sub>2</sub> (50 mol%), CuCl (2 equiv), and chlorobenzene (2 mL), was added in a 5 mL glass tube, which was stirred at 120 °C for 24–72 h in air. The reaction was stopped, and it was mixed with water and ethyl acetate. The reaction mixture was extracted three times with ethyl acetate. The combined organic layer was dried over anhydrous magnesium sulfate, and filtered. The filtrate was evaporated under a vacuum, and the residue was purified by flash column chromatography on silica gel (eluting with petroleum ether-ethyl acetate) to provide the desired product **3**.

## 2. General procedure for the synthesis of products 6:

A mixture of heteroarenes **1** (0.2 mmol), diselenides **2** (0.4 mmol),  $[Ru(p-cymene)Cl_2]_2$  (10 mol%), AgNTf<sub>2</sub> (40 mol%), Cu(OAc)<sub>2</sub> (50 mol%), CuCl (2 equiv), and chlorobenzene (2 mL), was added in a 5 mL glass tube, which was stirred at 120 °C for 24–45 h in air. The reaction was stopped, and it was mixed with water and ethyl acetate. The reaction mixture was extracted three times with ethyl acetate. The combined organic layer was dried over anhydrous magnesium sulfate, and filtered. The filtrate was evaporated under a vacuum, and the residue was purified by flash column chromatography on silica gel (eluting with petroleum ether-ethyl acetate) to provide the desired product **6**.

#### 3. Procedure for the synthesis of product 7:

A mixture of 3a (0.2 mmol), diphenyl diselenide 2a (1.5 equiv) and PIFA (1 equiv.) in DCM (2

mL) was added in a 5 mL glass tube, which was stirred at room temperature for 0.5 h. When the reaction was completed, it was mixed with water and ethyl acetate. The reaction mixture was extracted three times with ethyl acetate. The combined organic layer was dried over anhydrous magnesium sulfate and filtered. The filtrate was evaporated under vacuum and the residue was purified by flash column chromatography on silica gel (eluting with petroleum ether-ethyl acetate) to provide the desired products **7**.

#### **Optimization of reaction conditions**

#### Table S1. Optimization of solvents and additives<sup>a</sup>



Entry	Selvent	٨	Yield (%) <sup>b</sup>	
Entry	Solvent	Additive	3a	<b>4</b> a
1	DMF	$Cu(OAc)_2 (50 \text{ mol}\%) + CuCl (2 \text{ equiv})$	-	75
2	Toluene	$Cu(OAc)_2 (50 \text{ mol}\%) + CuCl (2 \text{ equiv})$	25	-
3	TFE	$Cu(OAc)_2$ (50 mol%) + $CuCl$ (2 equiv)	trace	45
4	1,4-Dioxane	$Cu(OAc)_2$ (50 mol%) + $CuCl$ (2 equiv)	trace	34
5	MeCN	$Cu(OAc)_2$ (50 mol%) + $CuCl$ (2 equiv)	-	-
6	t-AmOH	$Cu(OAc)_2$ (50 mol%) + $CuCl$ (2 equiv)	-	-
7	DMSO	$Cu(OAc)_2$ (50 mol%) + $CuCl$ (2 equiv)	-	trace
8	DCE	$Cu(OAc)_2 (50 \text{ mol}\%) + CuCl (2 \text{ equiv})$	66	-
9	Chlorobenzene	Cu(OAc) <sub>2</sub> (50 mol%) + CuCl (2 equiv)	70	-
10	Chlorobenzene	PivOH (50 mol%) + CuCl (2 equiv)	-	50
11	Chlorobenzene	$Ag_2CO_3 (50 \text{ mol}\%) + CuCl (2 \text{ equiv})$	trace	6
12	Chlorobenzene	$Cu(OTf)_2 (50 \text{ mol}\%) + CuCl (2 \text{ equiv})$	-	60
13	Chlorobenzene	CuO (50 mol%) + CuCl (2 equiv)	-	34
14	Chlorobenzene	KOAc (50 mol%) + CuCl (2 equiv)	trace	-
15	Chlorobenzene	$Cu(OAc)_2 (50 \text{ mol}\%) + CuBr (2 \text{ equiv})$	55	-
16	Chlorobenzene	-	_	trace
17	Chlorobenzene	Cu(OAc) <sub>2</sub> (50 mol%)	63	_
18	Chlorobenzene	CuCl (2 equiv)	_	40
19 <sup>c</sup>	Chlorobenzene	$Cu(OAc)_2 (50 \text{ mol}\%) + CuCl (2 \text{ equiv})$	-	47

<sup>*a*</sup>Reaction conditions: **1a** (0.2 mmol), **2a** (1.2 equiv),  $[Ru(p-cymene)Cl_2]_2$  (10 mol%), AgNTf<sub>2</sub> (40 mol%), additive in solvent (2 mL), at 120 °C in air. <sup>*b*</sup>Yield refers to isolated products after column chromatograph. <sup>*c*</sup> $[Ru(p-cymene)Cl_2]_2$  was replaced with  $[Cp*IrCl_2]_2$ .

## Table S2. Optimization of amounts of catalyst, additives and temperature<sup>a</sup>



Entry	Amount of Cu(OAc) <sub>2</sub> (equiv)	Amount of CuCl (equiv)	T (°C)	Yield (%) <sup>b</sup>
1	0.5	2	120	70
2	1	2	120	58
3	0.5	1	120	55
4	0.5	3	120	69
5	0.5	2	100	64
6 <sup>c</sup>	0.5	2	120	60
7 <sup>d</sup>	0.5	2	120	51

<sup>a</sup>Reaction conditions: **1a** (0.2 mmol), **2a** (1.2 equiv),  $[Ru(p-cymene)Cl_2]_2$  (10 mol%), AgNTf<sub>2</sub> (40 mol%), Cu(OAc)<sub>2</sub> (mol%), CuCl ( equiv), in chlorobenzene (2 mL) at T <sup>o</sup>C in air. <sup>b</sup>Yield refers to isolated products after column chromatography. <sup>c</sup> $[Ru(p-cymene)Cl_2]_2$  (7.5 mol%) and AgNTf<sub>2</sub> (30 mol%) were used. <sup>d</sup>The reaction was performed in nitrogen.

## Study on reaction mechanism

## 1. Radical trapping experiments



Entry	Additive (4 equiv)	Recovered 1a	Yield of <b>3a</b>	
1	-	8%	70%	
2	TEMPO	92%	-	
3	BHT	94%	-	
4	1,1-diphenylethylene	90%	-	PhSePh Ph <b>8</b> , 60%

## 2. Deuterium labeling experiments



A mixture of chromone **1a** (0.2 mmol),  $[Ru(p-cymene)Cl_2]_2$  (10 mol%), AgNTf<sub>2</sub> (40 mol%), Cu(OAc)<sub>2</sub> (50 mol%), CuCl (2 equiv), D<sub>2</sub>O (2 equiv.) and chlorobenzene (2 mL), was added in a 5 mL glass tube, which was stirred at 120 °C for 24 h in air. The reaction was stopped, and it was mixed with water and ethyl acetate. The reaction mixture was extracted three times with ethyl acetate. The combined organic layer was dried over anhydrous magnesium sulfate, and filtered. The filtrate was evaporated under a vacuum, and the residue was purified by flash column chromatography on silica gel (eluting with petroleum ether-ethyl acetate) to afford the recovered starting material **1aa** in 95% yield. The analysis by <sup>1</sup>H NMR showed deuterium incorporation at the C5-position of **1aa**.





A mixture of chromone **1a** (0.2 mmol), diphenyl diselenide **2a** (1.2 equiv),  $[\operatorname{Ru}(p-\operatorname{cymene})\operatorname{Cl}_2]_2$  (10 mol%), AgNTf<sub>2</sub> (40 mol%), Cu(OAc)<sub>2</sub> (50 mol%), CuCl (2 equiv), D<sub>2</sub>O (2 equiv.) and chlorobenzene (2 mL), was added in a 5 mL glass tube, which was stirred at 120 °C for 24 h in air. The reaction was stopped, and it was mixed with water and ethyl acetate. The reaction mixture was extracted three times with ethyl acetate. The combined organic layer was dried over anhydrous magnesium sulfate, and filtered. The filtrate was evaporated under a vacuum, and the residue was purified by flash column chromatography on silica gel (eluting with petroleum ether-ethyl acetate) to afford the recovered starting material **1aa'** and the product **3a** in 8% and 62% yields, respectively. The analysis by <sup>1</sup>H NMR showed deuterium incorporation at the C5-position of **1aa'**. The analysis by <sup>1</sup>H NMR showed no deuterium incorporation on the ring of **3a**.





## 3. Kinetic isotope experiment:

## (a) Parallel reaction



Diphenyl diselenide **2a** with chromone **1a** or chromone-*d*2 **1a'** respectively were performed to determine the KIE value. **1a** (0.2 mmol) or **1a'** (0.2 mmol), **2a** (0.24 mmol),  $[Ru(p-cymene)Cl_2]_2$  (10 mol%), AgNTf<sub>2</sub> (40 mol%), Cu(OAc)<sub>2</sub> (50 mol%), CuCl (2 equiv) and chlorobenzene (2 mL) were added in a 10 mL glass tube, which was stirred at 120 °C for 0.5 h, 1.5 h, 2.5 h, 3.5 h, 4.5 h in air, respectively. Then the reaction mass in two tubes was combined and was mixed with water and dichloromethane. The reaction mixturewas extracted three times with dichloromethane. The

combined organic layer waswashed two times with a little amount of water, dried over anhydrous magnesium sulfate and filtered. The filtrate was evaporated under vacuum and the residue was purified by flash column chromatography on silica gel (elutig with petroleum ether-ethyl acetate). The yields of **3a** and **3a'** were obtained by <sup>1</sup>H NMR analysis of the mixture. The KIE was determined as  $k_{\mu}/k_{p} = 9.03$ .

<b>t</b> [h]	0.5	1.5	2.5	3.5	4.5
<b>3a</b> [%]	30.2	33.4	37.9	40.8	43.2
<b>3a'</b> [%]	2.6	3.7	4.3	4.0	4.3



#### (b) Competition reaction



A mixture of chromone **1a** (0.2 mmol), chromone-*d*2 **1a'** (0.2 mmol), diphenyl diselenide **2a** (0.48 mmol), [Ru(*p*-cymene)Cl<sub>2</sub>]<sub>2</sub> (10 mol%), AgNTf<sub>2</sub> (40 mol%), Cu(OAc)<sub>2</sub> (50 mol%), CuCl (2 equiv) and chlorobenzene (4 mL), was added in a 10 mL glass tube, which was stirred at 120 °C for 12 h in air. The reaction was stopped, and it was mixed with water and ethyl acetate. The reaction mixture was extracted three times with ethyl acetate. The combined organic layer was dried over anhydrous magnesium sulfate, and filtered. The filtrate was evaporated under a vacuum, and the residue was purified by flash column chromatography on silica gel (eluting with petroleum ether-ethyl acetate). KIE ( $k_H/k_D = 9.00$ ) was determined from <sup>1</sup>H NMR.



X-ray structure of 3a





Figure S1. Single crystal structure of 3a

Table S3. X-ray crystallographic data of 3a

Bond precision:	C-C = 0.0070 A	Wavelength=0.71073	
Cell:	a=7.9033(5)	b=11.9615(7)	c=14.6472(9)
	alpha=73.300(5)	alpha=73.300(5)	gamma=74.420(5)
Temperature:	293 K		
	Calculated	Reported	
Volume	1276.68(14)	1276.68(14)	
Space group	P -1	P -1	
Hall group	-P 1	-P 1	
Moiety formula	$C_{15} H_{10} O_2 Se$	$C_{15}H_{10}O_2Se$	
Sum formula	$C_{15} H_{10} O_2 Se$	$C_{15}H_{10}O_2Se$	

Mr	301.19	301.19		
Dx,g cm- 3	1.567	1.567		
Z	4	4		
Mu (mm-1)	2.931	2.931		
F000	600.0	600.0		
F000′	599.88			
h,k, lmax	10,16,20	10,16,19		
Nref	6819	5792		
Tmin, Tmax	0.362,0.380	0.787,1.000		
Tmin′	0.335			
Correction method	Correction method= # Reported T Limits: Tmin=0.787 Tmax=1.000			
AbsCorr = MULTI-SCAN				
Data completeness= $0.849$ Theta (max)= 29.059				
R (reflections)= 0.0476(3696) wR2 (reflections)=0.1093(5792)				
<b>S</b> = 1.044	Npar= 325			

## Information of preparation of single crystal 3a:

**3a** (25 mg) with 1.2 mL *N*,*N*-dimethylformamide in a bottle and with 0.8 mL hexane on the upper layer of *N*,*N*-dimethylformamide. Subsequently, seal with sealing film. Place the bottle at room temperature to give the single crystal **3a** in 3 days.

## X-ray structure of 6h

Se 0 Ν̈́ Η 0

6h (CCDC 2205235 )



Figure S2. Single crystal structure of 6h

Table S4. X-ray crystallographic data of 6h

Bond precision:	C-C = 0.0030 A	Wavelength=0.7107	73
Cell:	a=8.0338(3)	b=8.4987(4)	c=13.3369(5)
	alpha=74.087(4)	alpha=74.630(3)	gamma=81.377(4)
Temperature:	200 K		
	Calculated	Reported	
Volume	841.45(6)	841.45(6)	
Space group	P -1	P -1	
Hall group	-P 1	-P 1	
Moiety formula	$C_{20} H_{19} N O_2 Se$	$C_{20}H_{19}NO_2Se$	
Sum formula	C <sub>20</sub> H <sub>19</sub> N O <sub>2</sub> Se	C <sub>20</sub> H <sub>19</sub> N O <sub>2</sub> Se	
Mr	384.32	384.32	
Dx,g cm- 3	1.517	1.517	
Z	2	2	
Mu (mm-1)	2.243	2.243	
F000	392.0	392.0	
F000′	391.96		

h,k, lmax	10, 11, 18	10, 11, 18	
Nref	4508	3985	
Tmin, Tmax	0.450, 0.488	0.962, 1.000	
Tmin'	0.442		
Correction method= # Reported T Limits: Tmin=0.962 Tmax=1.000 AbsCorr = MULTI-SCAN			
Data completeness	s= 0.884	Theta (max)= 29.101	
R (reflections)= 0.	0312( 3500) wR2 (reflections)=0	.0708( 3985)	
S = 1.078	Npar= 219		

## Information of preparation of single crystal 6h:

**6h** (25mg) with 1.2 mL *N*,*N*-dimethylformamide in a bottle and with 0.8 mL hexane on the upper layer of *N*,*N*-dimethylformamide. Subsequently, seal with sealing film. Place the bottle at  $4^{\circ}$ C to give the single crystal **6h** in 3 days.



## 5-(Phenylselanyl)-4*H*-chromen-4-one (3a)

Faint Yellow solid; mp 107.1-108.2 °C;  $R_f = 0.3$  (20% EtOAc in petroleum ether); <sup>1</sup>H NMR (600 MHz, CDCl<sub>3</sub>)  $\delta$  7.80 (d, J = 4.9 Hz, 1H), 7.74 (d, J = 7.2 Hz, 2H), 7.50 – 7.44 (m, 3H), 7.28 – 7.25 (m, 1H), 7.17 – 7.16 (m, 1H), 6.75 (d, J = 7.9 Hz, 1H), 6.37 (d, J = 5.3 Hz, 1H) ppm; <sup>13</sup>C NMR (151 MHz, CDCl<sub>3</sub>)  $\delta$  178.82, 158.05, 154.44, 140.07, 137.55, 132.69, 129.83, 129.23, 128.92, 124.36, 122.50, 113.91, 112.88 ppm; HRMS: calc.for C<sub>15</sub>H<sub>11</sub>O<sub>2</sub>Se<sup>+</sup> [M+H]<sup>+</sup>: 302.9924, found: 302.9917.



#### 2-Methyl-5-(phenylselanyl)-4H-chromen-4-one (3b)

Faint Yellow solid; mp 142.2-142.7 °C;  $R_f = 0.3$  (20% EtOAc in petroleum ether); <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)  $\delta$  7.73 – 7.71 (m, 2H), 7.48 – 7.40 (m, 3H), 7.22 (t, J = 8.1 Hz, 1H), 7.10 (d, J = 8.2 Hz, 1H), 6.69 (d, J = 7.9 Hz, 1H), 6.17 (s, 1H), 2.35 (s, 3H) ppm; <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>)  $\delta$  179.46, 165.28, 158.00, 139.72, 137.61, 132.43, 129.79, 129.16, 129.13, 124.07, 121.22, 113.61, 110.44, 20.26 ppm; HRMS: calc.for C<sub>16</sub>H<sub>13</sub>O<sub>2</sub>Se<sup>+</sup> [M+H]<sup>+</sup>: 317.0081, found: 317.0074.



## 2-Phenyl-5-(phenylselanyl)-4*H*-chromen-4-one (3c)

Faint Yellow solid; mp 157.4-158.1 °C;  $R_f = 0.5$  (20% EtOAc in petroleum ether); <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)  $\delta$  7.92 – 7.90 (m, 2H), 7.75 – 7.74 (m, 2H), 7.53 – 7.48 (m, 3H), 7.46 – 7.42 (m, 3H), 7.30 – 7.24 (m, 2H), 6.82 (s, 1H), 6.74 (dd, J = 6.6, 2.2 Hz, 1H) ppm; <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>)  $\delta$  179.50, 162.40, 157.68, 139.84, 137.54, 132.65, 131.57, 131.28, 129.77, 129.15, 128.99,

128.95, 126.15, 124.23, 121.54, 113.77, 107.27 ppm; HRMS: calc.for  $C_{21}H_{15}O_2Se^+$  [M+H]<sup>+</sup>: 379.0237, found: 379.0231.



#### 5-(Phenylselanyl)-2-(o-tolyl)-4H-chromen-4-one (3d)

Faint Yellow solid; mp 158.9-159.7 °C;  $R_f = 0.3$  (20% EtOAc in petroleum ether); <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)  $\delta$  7.76 – 7.74 (m, 2H), 7.55 – 7.53 (m, 1H), 7.49 – 7.41 (m, 4H), 7.34 – 7.26 (m, 3H), 7.19 (d, J = 7.9 Hz, 1H), 6.76 (d, J = 7.8 Hz, 1H), 6.50 (s, 1H), 2.49 (s, 3H) ppm; <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>)  $\delta$  179.47, 165.16, 158.02, 140.03, 137.61, 136.81, 132.73, 132.25, 131.27, 130.77, 129.83, 129.21, 129.14, 129.07, 126.21, 124.33, 121.47, 113.78, 111.79, 20.55 ppm; HRMS: calc.for C<sub>22</sub>H<sub>17</sub>O<sub>2</sub>Se<sup>+</sup> [M+H]<sup>+</sup>: 393.0394, found: 393.0386.



#### 2-(2-Methoxyphenyl)-5-(phenylselanyl)-4*H*-chromen-4-one (3e)

Faint Yellow solid; mp 139.1-140.1 °C;  $R_f = 0.3$  (20% EtOAc in petroleum ether); <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)  $\delta$  7.89 (dd, J = 7.8, 1.6 Hz, 1H), 7.75 (dd, J = 7.5, 1.5 Hz, 2H), 7.50 – 7.42 (m, 4H), 7.28 – 7.20 (m, 2H), 7.15 (s, 1H), 7.10 (t, J = 7.6 Hz, 1H), 7.04 (d, J = 8.4 Hz, 1H), 6.72 (dd, J = 7.5, 0.9 Hz, 1H), 3.94 (s, 3H) ppm; <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>)  $\delta$  180.02, 159.89, 158.06, 157.95, 139.69, 137.62, 132.50, 132.42, 129.77, 129.25, 129.14, 129.12, 123.94, 121.50, 120.69, 120.44, 113.75, 112.48, 111.74, 55.67 ppm; HRMS: calc.for C<sub>22</sub>H<sub>17</sub>O<sub>3</sub>Se<sup>+</sup> [M+H]<sup>+</sup>: 409.0343, found: 409.0336.



#### 2-(2-Fluorophenyl)-5-(phenylselanyl)-4H-chromen-4-one (3f)

Yellow solid; mp 115.2-116.3 °C;  $R_f = 0.3$  (20% EtOAc in petroleum ether); <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)  $\delta$  7.92 (td, J = 7.7, 1.7 Hz, 1H), 7.74 (dd, J = 7.7, 1.6 Hz, 2H), 7.54 – 7.42 (m, 4H), 7.34 – 7.20 (m, 4H), 6.94 (s, 1H), 6.75 (dd, J = 7.6, 1.1 Hz, 1H) ppm; <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>)  $\delta$  179.50, 160.54 (d, J = 257.55), 157.85, 157.82, 140.04, 137.59, 132.90 (d, J = 9.09), 132.79, 129.82, 129.21, 128.99, 128.93, 124.59 (d, J = 3.6 Hz), 124.32, 121.47, 119.94 (d, J = 10.0 Hz), 116.93 (d, J = 23.23 Hz), 113.73, 112.20 (d, J = 11.8 Hz) ppm; HRMS: calc.for C<sub>21</sub>H<sub>14</sub>FO<sub>2</sub>Se<sup>+</sup> [M+H]<sup>+</sup>: 397.0143, found: 397.0136.



## 5-(Phenylselanyl)-2-(m-tolyl)-4H-chromen-4-one (3g)

Faint Yellow solid; mp 135.2-136.1 °C;  $R_f = 0.3$  (20% EtOAc in petroleum ether); <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)  $\delta$  7.76 – 7.71 (m, 4H), 7.48 – 7.41 (m, 4H), 7.35 (d, J = 7.5 Hz, 1H), 7.27 (dd, J = 6.2, 3.0 Hz, 2H), 6.81 (s, 1H), 6.74 (dd, J = 5.7, 3.2 Hz, 1H), 2.46 (s, 3H) ppm; <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>)  $\delta$  179.60, 162.70, 157.78, 139.87, 138.82, 137.61, 132.65, 132.43, 131.32, 129.81, 129.19, 129.09, 128.90, 126.76, 124.25, 123.43, 121.64, 113.82, 107.31, 21.48 ppm; HRMS: calc.for  $C_{22}H_{17}O_2Se^+$  [M+H]<sup>+</sup>: 393.0394, found: 393.0386.



## 2-(3-Methoxyphenyl)-5-(phenylselanyl)-4H-chromen-4-one (3h)

Faint Yellow solid; mp 130.4-131.2 °C;  $R_f = 0.3$  (20% EtOAc in petroleum ether); <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)  $\delta$  7.75 (d, J = 7.4 Hz, 2H), 7.52 – 7.42 (m, 6H), 7.32 – 7.26 (m, 2H), 7.09 (d, J = 8.0 Hz, 1H), 6.82 (s, 1H), 6.75 (d, J = 6.5 Hz, 1H), 3.91 (s, 3H) ppm; <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>)  $\delta$  179.60, 162.25, 159.90, 157.69, 139.85, 137.58, 132.73, 132.64, 130.09, 129.82, 129.21, 128.93, 124.27, 121.56, 118.63, 117.13, 113.83, 111.63, 107.55, 55.47 ppm; HRMS: calc.for C<sub>22</sub>H<sub>17</sub>O<sub>3</sub>Se<sup>+</sup> [M+H]<sup>+</sup>: 409.0343, found: 409.0336.



### 2-(3-Chlorophenyl)-5-(phenylselanyl)-4*H*-chromen-4-one (3i)

Faint Yellow solid; mp 105.3-106.7 °C;  $R_f = 0.3$  (20% EtOAc in petroleum ether); <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)  $\delta$  7.91 (t, J = 1.6 Hz, 1H), 7.79 – 7.77 (m, 1H), 7.74 (dd, J = 7.7, 1.5 Hz, 2H), 7.52 – 7.42 (m, 5H), 7.32 – 7.25 (m, 2H), 6.80 (s, 1H), 6.75 (dd, J = 7.1, 1.7 Hz, 1H) ppm; <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>)  $\delta$  179.35, 160.87, 157.69, 140.14, 137.59, 135.24, 133.18, 132.89, 131.53, 130.30, 129.86, 129.26, 128.90, 126.26, 124.50, 124.32, 121.58, 113.79, 107.95 ppm; HRMS: calc.for C<sub>21</sub>H<sub>14</sub>ClO<sub>2</sub>Se<sup>+</sup> [M+H]<sup>+</sup>: 412.9848, found: 412.9838.



## 2-(4-Methoxyphenyl)-5-(phenylselanyl)-4H-chromen-4-one (3j)

Faint Yellow solid; mp 137.2-138.1 °C;  $R_f = 0.3$  (20% EtOAc in petroleum ether); <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)  $\delta$  7.87 (d, J = 8.9 Hz, 2H), 7.75 (dd, J = 7.6, 1.5 Hz, 2H), 7.49 – 7.40 (m, 3H), 7.28 – 7.22 (m, 2H), 7.02 (d, J = 8.9 Hz, 2H), 6.73 – 6.71 (m, 2H), 3.89 (s, 3H) ppm; <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>)  $\delta$  179.53, 162.50, 162.41, 157.66, 139.75, 137.62, 132.51, 129.79, 129.16, 127.94, 124.17, 123.61, 121.56, 114.43, 113.73, 105.94, 55.50 ppm; HRMS: calc.for C<sub>22</sub>H<sub>17</sub>O<sub>3</sub>Se<sup>+</sup> [M+H]<sup>+</sup>: 409.0343, found: 409.0336.



## 3-Methyl-5-(phenylselanyl)-4H-chromen-4-one (3k)

Faint Yellow solid; mp 161.3-162.2 °C;  $R_f = 0.3$  (10% EtOAc in petroleum ether); <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)  $\delta$  7.73 (d, J = 4.3 Hz, 3H), 7.47 – 7.41 (m, 3H), 7.22 (t, J = 8.1 Hz, 1H), 7.11 (d, J = 8.2 Hz, 1H), 6.71 (d, J = 7.8 Hz, 1H), 2.05 (s, 3H) ppm; <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>)  $\delta$  179.59,

158.18, 150.94, 139.85, 137.58, 132.32, 129.79, 129.18, 129.12, 123.92, 121.24, 120.56, 113.82, 11.00 ppm; HRMS: calc.for  $C_{16}H_{13}O_2Se^+$  [M+H]<sup>+</sup>: 317.0081, found: 317.0075.



3-Phenyl-5-(phenylselanyl)-4H-chromen-4-one (3l)

Faint Yellow solid; mp 147.6-148.1 °C;  $R_f = 0.3$  (10% EtOAc in petroleum ether); <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)  $\delta$  7.96 (s, 1H), 7.75 – 7.73 (m, 2H), 7.59 (d, J = 7.2 Hz, 2H), 7.50 – 7.40 (m, 6H), 7.28 (t, J = 8.0 Hz, 1H), 7.19 (d, J = 8.2 Hz, 1H), 6.78 (d, J = 7.8 Hz, 1H) ppm; <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>)  $\delta$  177.61, 157.85, 152.23, 140.82, 137.60, 132.61, 131.38, 129.85, 129.24, 128.99, 128.49, 128.27, 125.33, 124.47, 122.17, 113.83 ppm; HRMS: calc.for C<sub>21</sub>H<sub>15</sub>O<sub>2</sub>Se<sup>+</sup> [M+H]<sup>+</sup>: 379.0237, found: 379.0230.



#### 5-(Phenylselanyl)-3-(o-tolyl)-4H-chromen-4-one (3m)

Faint Yellow solid; mp 69.8-70.6 °C;  $R_f = 0.3$  (10% EtOAc in petroleum ether); <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)  $\delta$  7.83 (s, 1H), 7.75 – 7.73 (m, 2H), 7.48 – 7.42 (m, 3H), 7.34 – 7.20 (m, 6H), 6.79 (d, J = 7.8 Hz, 1H), 2.32 (s, 3H) ppm; <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>)  $\delta$  177.40, 158.03, 152.65, 140.79, 137.96, 137.57, 132.59, 131.04, 130.59, 130.21, 129.82, 129.24, 129.19, 128.68, 126.17, 125.78, 124.38, 121.98, 113.82, 20.15 ppm; HRMS: calc.for C<sub>22</sub>H<sub>17</sub>O<sub>2</sub>Se<sup>+</sup> [M+H]<sup>+</sup>: 393.0394, found: 393.0386.



3-(2-Fluorophenyl)-5-(phenylselanyl)-4*H*-chromen-4-one (3n)

Faint Yellow solid; mp 134.7-135.2 °C;  $R_f = 0.3$  (10% EtOAc in petroleum ether); <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)  $\delta$  7.99 (d, J = 1.0 Hz, 1H), 7.74 (dd, J = 7.5, 1.4 Hz, 2H), 7.55 (td, J = 7.5, 1.6 Hz, 1H), 7.50 – 7.36 (m, 4H), 7.31 – 7.16 (m, 4H), 6.78 (d, J = 7.8 Hz, 1H) ppm; <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>)  $\delta$  176.95, 160.20 (d, J = 248.26 Hz), 158.97, 157.85, 153.79 (d, J = 3.0 Hz), 140.86,

137.60, 132.73, 132.12 (d, J = 2.7 Hz), 130.18 (d, J = 8.2 Hz), 129.85, 129.25, 129.14, 124.58, 124.05 (d, J = 3.5 Hz), 122.01, 119.90, 118.95 (d, J = 14.9 Hz), 115.83 (d, J = 22.22 Hz), 113.85.ppm; HRMS: calc.for C<sub>21</sub>H<sub>14</sub>FO<sub>2</sub>Se<sup>+</sup> [M+H]<sup>+</sup>: 397.0143, found: 397.0137.



5-(Phenylselanyl)-3-(m-tolyl)-4H-chromen-4-one (30)

Faint Yellow solid; mp 154.2-155.3 °C;  $R_f = 0.3$  (10% EtOAc in petroleum ether); <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)  $\delta$  7.93 (s, 1H), 7.74 (dd, J = 7.5, 1.4 Hz, 2H), 7.48 – 7.43 (m, 4H), 7.37 – 7.32 (m, 2H), 7.27 (t, J = 8.0, 1H), 7.21 (d, J = 6.6 Hz, 1H), 7.18 (d, J = 8.2 Hz, 1H), 6.77 (dd, J = 7.8, 0.5 Hz, 1H), 2.42 (s, 3H) ppm; <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>)  $\delta$  177.64, 157.80, 152.19, 140.73, 138.07, 137.58, 132.54, 131.26, 129.82, 129.69, 129.26, 129.20, 129.05, 128.38, 125.99, 125.41, 124.39, 122.14, 113.80, 21.47 ppm; HRMS: calc.for C<sub>22</sub>H<sub>17</sub>O<sub>2</sub>Se<sup>+</sup> [M+H]<sup>+</sup>: 393.0394, found: 393.0386.



#### **3-(3-Methoxyphenyl)-5-(phenylselanyl)-4***H***-chromen-4-one (3p)**

Faint Yellow solid; mp 178.2-179.5 °C;  $R_f = 0.3$  (10% EtOAc in petroleum ether); <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)  $\delta$  8.28 (dd, J = 8.0, 1.4 Hz, 1H), 7.80 (s, 1H), 7.70 – 7.66 (m, 1H), 7.56 (d, J = 8.6 Hz, 1H), 7.47 – 7.40 (m, 2H), 7.25 – 7.22 (m, 2H), 7.16 – 7.12 (m, 3H), 6.93 (d, J = 2.8 Hz, 1H), 6.88 (dd, J = 8.6, 2.9 Hz, 1H), 3.82 (s, 3H) ppm; <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>)  $\delta$  176.02, 159.77, 156.26, 153.56, 137.40, 136.98, 133.59, 133.40, 131.45, 129.06, 126.55, 126.47, 126.33, 125.18, 124.41, 122.69, 118.04, 116.93, 115.44, 55.40 ppm; HRMS: calc.for C<sub>22</sub>H<sub>17</sub>O<sub>3</sub>Se<sup>+</sup> [M+H]<sup>+</sup>: 409.0343, found: 409.0338.



3-(4-Methoxyphenyl)-5-(phenylselanyl)-4H-chromen-4-one (3q)

Faint Yellow solid; mp 184.2-185.1 °C;  $R_f = 0.3$  (10% EtOAc in petroleum ether); <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)  $\delta$  7.92 (s, 1H), 7.74 (d, J = 6.9 Hz, 2H), 7.53 (d, J = 8.3 Hz, 2H), 7.48 – 7.42 (m, 3H), 7.26 (t, J = 8.0 Hz, 1H), 7.17 (d, J = 8.2 Hz, 1H), 6.99 (d, J = 8.3 Hz, 2H), 6.76 (d, J = 7.8 Hz, 1H), 3.85 (s, 3H) ppm; <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>)  $\delta$  177.83, 159.66, 157.82, 151.68, 140.69, 137.59, 132.49, 130.15, 129.82, 129.30, 129.20, 124.89, 124.34, 123.65, 122.10, 113.98, 113.81, 55.32 ppm; HRMS: calc.for C<sub>22</sub>H<sub>17</sub>O<sub>3</sub>Se<sup>+</sup> [M+H]<sup>+</sup>: 409.0343, found: 409.0335.



3-(4-Bromophenyl)-5-(phenylselanyl)-4H-chromen-4-one (3r)

Faint Yellow solid; mp 134.7-135.2 °C;  $R_f = 0.3$  (10% EtOAc in petroleum ether); <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)  $\delta$  7.95 (s, 1H), 7.73 (d, J = 6.4 Hz, 2H), 7.58 (d, J = 8.4 Hz, 2H), 7.49 – 7.42 (m, 5H), 7.28 (t, J = 8.0 Hz, 1H), 7.18 (d, J = 8.1 Hz, 1H), 6.78 (d, J = 7.8 Hz, 1H) ppm; <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>)  $\delta$  177.29, 157.84, 152.17, 140.90, 137.58, 132.76, 131.67, 130.54, 130.33, 129.89, 129.31, 129.09, 124.64, 124.29, 122.53, 122.04, 113.85 ppm; HRMS: calc.for  $C_{21}H_{14}BrO_2Se^+$  [M+H]<sup>+</sup>: 456.9342, found: 456.9333.



7-Methyl-5-(phenylselanyl)-4H-chromen-4-one (3s)

Faint Yellow solid; mp 140.2-141.3 °C;  $R_f = 0.3$  (20% EtOAc in petroleum ether); <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)  $\delta$  7.73 – 7.71 (m, 3H), 7.47 – 7.41 (m, 3H), 6.94 (s, 1H), 6.52 (s, 1H), 6.30 (d, J = 5.9 Hz, 1H), 2.19 (s, 3H) ppm; <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>)  $\delta$  178.57, 158.03, 154.16, 144.01, 139.58, 137.50, 129.75, 129.17, 128.95, 125.41, 120.38, 114.15, 112.77, 21.74 ppm; HRMS: calc.for  $C_{16}H_{13}O_2Se^+$  [M+H]<sup>+</sup>: 317.0081, found: 317.0075.



7-Methoxy-5-(phenylselanyl)-4H-chromen-4-one (3t)

Faint Yellow solid; mp 161.1-162.9 °C;  $R_f = 0.3$  (20% EtOAc in petroleum ether); <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)  $\delta$  7.72 – 7.67 (m, 3H), 7.46 – 7.43 (m, 3H), 6.57 (s, 1H), 6.27 (d, J = 2.2 Hz, 2H), 3.64 (s, 3H) ppm; <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>)  $\delta$  177.96, 162.91, 159.44, 153.92, 141.62, 137.55, 129.84, 129.33, 128.90, 116.83, 112.82, 112.76, 97.39, 55.39 ppm; HRMS: calc.for C<sub>16</sub>H<sub>13</sub>O<sub>3</sub>Se<sup>+</sup> [M+H]<sup>+</sup>: 333.0030, found: 333.0022.



## 8-Methyl-5-(phenylselanyl)-4H-chromen-4-one (3u)

Faint Yellow solid; mp 98.2-99.1 °C;  $R_f = 0.3$  (20% EtOAc in petroleum ether); <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)  $\delta$  7.83 (d, J = 5.9 Hz, 1H), 7.72 – 7.70 (m, 2H), 7.47 – 7.39 (m, 3H), 7.10 (d, J = 8.0 Hz, 1H), 6.61 (d, J = 8.0 Hz, 1H), 6.34 (d, J = 5.9 Hz, 1H), 2.32 (s, 3H) ppm; <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>)  $\delta$  179.07, 156.34, 154.29, 137.54, 136.37, 134.01, 129.72, 129.15, 129.06, 123.77, 123.08, 122.38, 112.67, 15.25 ppm; HRMS: calc.for C<sub>16</sub>H<sub>13</sub>O<sub>2</sub>Se<sup>+</sup> [M+H]<sup>+</sup>: 317.0081, found: 317.0074.



#### 8-Chloro-5-(phenylselanyl)-4*H*-chromen-4-one (3v)

Faint Yellow solid; mp 102.1-103.1 °C;  $R_f = 0.3$  (20% EtOAc in petroleum ether); <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)  $\delta$  7.87 (d, J = 5.9 Hz, 1H), 7.70 (d, J = 6.9 Hz, 2H), 7.50 – 7.42 (m, 3H), 7.31 (d, J = 8.6 Hz, 1H), 6.66 (d, J = 8.6 Hz, 1H), 6.41 (d, J = 5.9 Hz, 1H) ppm; <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>)  $\delta$  178.22, 154.36, 153.38, 138.98, 137.50, 132.97, 129.98, 129.47, 128.53, 124.34, 123.47, 118.63, 113.15 ppm; HRMS: calc.for C<sub>15</sub>H<sub>10</sub>ClO<sub>2</sub>Se<sup>+</sup> [M+H]<sup>+</sup>: 336.9535, found: 336.9527.



#### 5-(Phenylselanyl)-4*H*-benzo[*h*]chromen-4-one (3w)

Faint Yellow solid; mp 137.4-138 °C;  $R_f = 0.3$  (20% EtOAc in petroleum ether); <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)  $\delta$  8.33 (d, J = 7.7 Hz, 1H), 8.00 (d, J = 5.8 Hz, 1H), 7.79 – 7.78 (m, 2H), 7.56 – 7.41 (m, 6H), 7.02 (s, 1H), 6.54 (d, J = 5.8 Hz, 1H) ppm; <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>)  $\delta$  178.66, 155.22, 153.83, 137.71, 135.30, 133.01, 129.85, 129.73, 129.35, 129.21, 126.83, 125.94, 123.07, 122.30, 121.61, 120.00, 114.39 ppm; HRMS: calc.for C<sub>19</sub>H<sub>13</sub>O<sub>2</sub>Se<sup>+</sup> [M+H]<sup>+</sup>: 353.0081, found: 353.0074.



## 5-(O-Tolylselanyl)-4*H*-chromen-4-one (3x)

Faint Yellow solid; mp 109.3-110.4 °C;  $R_f = 0.3$  (20% EtOAc in petroleum ether); <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)  $\delta$  7.78 (d, J = 5.9 Hz, 1H), 7.75 (d, J = 7.5 Hz, 1H), 7.40 – 7.38 (m, 2H), 7.25 – 7.21 (m, 2H), 7.14 (dd, J = 8.2, 0.7 Hz, 1H), 6.59 (d, J = 7.8 Hz, 1H), 6.36 (d, J = 5.9 Hz, 1H), 2.44 (s, 3H) ppm; <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>)  $\delta$  178.83, 158.19, 154.39, 143.76, 139.18, 138.71, 132.80, 130.45, 130.06, 129.67, 127.24, 123.71, 122.69, 113.90, 112.99, 22.54 ppm; HRMS: calc.for  $C_{16}H_{13}O_2Se^+$  [M+H]<sup>+</sup>: 317.0081, found: 317.0075.



#### 5-((2-Fluorophenyl)selanyl)-4*H*-chromen-4-one (3y)

Faint Yellow solid; mp 113.2-114.9 °C;  $R_f = 0.3$  (20% EtOAc in petroleum ether); <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)  $\delta$  7.78 (d, J = 5.8 Hz, 1H), 7.73 (t, J = 6.7 Hz, 1H), 7.49 (dd, J = 12.7, 6.5 Hz, 1H), 7.28 (t, J = 8.0 Hz, 1H), 7.23 – 7.16 (m, 3H), 6.70 (d, J = 7.7 Hz, 1H), 6.36 (d, J = 5.8 Hz, 1H) ppm; <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>)  $\delta$  178.76, 163.61 (d, J = 246.3 Hz), 158.04, 154.64, 139.34 (d, J = 1.8 Hz), 138.09, 132.89, 132.12 (d, J = 7.8 Hz), 125.42 (d, J = 3.6 Hz), 124.08, 122.64, 116.01 (d, J = 24.3 Hz), 113.50 (d, J = 148.0 Hz) ppm; HRMS: calc.for C<sub>15</sub>H<sub>10</sub>FO<sub>2</sub>Se<sup>+</sup> [M+H]<sup>+</sup>: 320.9830, found: 320.9823.



## 5-((2-Chlorophenyl)selanyl)-4*H*-chromen-4-one (3z)

Faint Yellow solid; mp 147.2-148.1 °C;  $R_f = 0.3$  (20% EtOAc in petroleum ether); <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)  $\delta$  7.86 (dd, J = 7.6, 1.6 Hz, 1H), 7.79 (d, J = 5.9 Hz, 1H), 7.59 (dd, J = 8.0, 1.2 Hz, 1H), 7.43 (td, J = 7.7, 1.6 Hz, 1H), 7.32 – 7.27 (m, 2H), 7.18 (dd, J = 8.3, 0.8 Hz, 1H), 6.62 (dd, J = 7.9, 0.6 Hz, 1H), 6.37 (d, J = 5.9 Hz, 1H) ppm; <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>)  $\delta$  178.83, 158.07, 154.61, 141.11, 139.77, 138.16, 132.93, 131.21, 130.10, 129.47, 127.89, 123.95, 122.53, 114.20, 112.82 ppm; HRMS: calc.for C<sub>15</sub>H<sub>10</sub>ClO<sub>2</sub>Se<sup>+</sup> [M+H]<sup>+</sup>: 336.9535, found: 336.9527.



## 5-((3-Fluorophenyl)selanyl)-4*H*-chromen-4-one (3aa)

Faint Yellow solid; mp 118.3-119.5 °C;  $R_f = 0.3$  (20% EtOAc in petroleum ether); <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)  $\delta$  7.78 (d, J = 5.9 Hz, 1H), 7.50 (d, J = 7.5 Hz, 1H), 7.45 – 7.38 (m, 2H), 7.28 (t, J = 8.0, 1H), 7.17 – 7.13 (m, 2H), 6.72 (d, J = 7.9 Hz, 1H), 6.35 (d, J = 5.9 Hz, 1H) ppm; <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>)  $\delta$  178.76, 162.94 (d, J = 250.8 Hz), 158.02, 154.57, 139.33, 133.19 (d, J = 3.0 Hz), 132.85, 131.17 (d, J = 7.7 Hz), 130.62 (d, J = 6.0 Hz), 124.25, 124.18 (d, J = 21.21 Hz), 122.46, 116.45 (d, J = 21.0 Hz), 114.20, 112.80 ppm; HRMS: calc.for C<sub>15</sub>H<sub>10</sub>FO<sub>2</sub>Se<sup>+</sup> [M+H]<sup>+</sup>: 320.9830, found: 320.9823.



## 5-((3-Bromophenyl)selanyl)-4H-chromen-4-one (3ab)

Faint Yellow solid; mp 133.1-134.2 °C;  $R_f = 0.3$  (20% EtOAc in petroleum ether); <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)  $\delta$  7.88 (s, 1H), 7.79 (d, J = 5.9 Hz, 1H), 7.65 (d, J = 7.6 Hz, 1H), 7.60 (d, J = 8.1 Hz, 1H), 7.33 – 7.28 (m, 2H), 7.17 (d, J = 8.2 Hz, 1H), 6.71 (d, J = 7.8 Hz, 1H), 6.35 (d, J = 5.9 Hz,

1H) ppm; <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>)  $\delta$  178.75, 158.02, 154.59, 139.89, 139.29, 136.06, 132.91, 132.38, 131.25, 131.01, 124.32, 123.36, 122.45, 114.24, 112.82 ppm; HRMS: calc.for C<sub>15</sub>H<sub>10</sub>BrO<sub>2</sub>Se<sup>+</sup> [M+H]<sup>+</sup>: 380.9029, found: 380.9019.



#### 5-((4-Bromophenyl)selanyl)-4*H*-chromen-4-one (3ac)

Faint Yellow solid; mp 188.1-189.1 °C;  $R_f = 0.3$  (20% EtOAc in petroleum ether); <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)  $\delta$  7.78 (d, J = 5.9 Hz, 1H), 7.59 – 7.54 (m, 4H), 7.28 (t, J = 8.0 Hz, 1H), 7.17 (d, J = 8.2 Hz, 1H), 6.70 (d, J = 7.8 Hz, 1H), 6.35 (d, J = 5.9 Hz, 1H) ppm; <sup>13</sup>C NMR (101 MHz,CDCl<sub>3</sub>)  $\delta$  178.75, 158.03, 154.56, 139.43, 139.18, 133.07, 132.82, 127.87, 124.24, 124.09, 122.49, 114.18, 112.84 ppm; HRMS: calc.for C<sub>15</sub>H<sub>10</sub>BrO<sub>2</sub>Se<sup>+</sup> [M+H]<sup>+</sup>: 380.9029, found: 380.9020.



## 5-((4-Fluorophenyl)selanyl)-4*H*-chromen-4-one (3ad)

Faint Yellow solid; mp 153.1-154.4 °C;  $R_f = 0.3$  (20% EtOAc in petroleum ether); <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)  $\delta$  7.78 (d, J = 5.9 Hz, 1H), 7.70 – 7.66 (m, 2H), 7.27 (t, J = 8.0 Hz, 1H), 7.17 – 7.11 (m, 3H), 6.68 (d, J = 7.9 Hz, 1H), 6.35 (d, J = 5.9 Hz, 1H) ppm; <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>)  $\delta$  178.81, 163.58 (d, J = 249.7 Hz), 158.07, 154.52, 140.00, 139.64 (d, J = 8.1 Hz), 132.77, 124.16, 123.92 (d, J = 3.5 Hz), 122.51, 117.16 (d, J = 21.3 Hz), 114.08, 112.87 ppm; HRMS: calc.for  $C_{15}H_{10}FO_2Se^+$  [M+H]<sup>+</sup>: 320.9830, found: 320.9823.



## 5-((4-Chlorophenyl)selanyl)-4H-chromen-4-one (3ae)

Faint Yellow solid; mp 127.1-128.3 °C;  $R_f = 0.3$  (20% EtOAc in petroleum ether); <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)  $\delta$  7.79 (d, J = 5.9 Hz, 1H), 7.65 – 7.63 (m, 2H), 7.42 – 7.40 (m, 2H), 7.28 (t, J = 11.2, 4.9 Hz, 1H), 7.17 (dd, J = 8.3, 0.8 Hz, 1H), 6.70 (dd, J = 7.9, 0.6 Hz, 1H), 6.36 (d, J = 5.9

Hz, 1H) ppm; <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>)  $\delta$  178.76, 158.05, 154.55, 139.57, 138.93, 135.76, 132.81, 130.13, 127.23, 124.22, 122.50, 114.17, 112.85 ppm; HRMS: calc.for C<sub>15</sub>H<sub>10</sub>ClO<sub>2</sub>Se<sup>+</sup> [M+H]<sup>+</sup>: 336.9535, found: 336.9527.



5-((2-Fluorophenyl)selanyl)-2-phenyl-4H-chromen-4-one (3af)

Faint Yellow solid; mp 140.1-141.2 °C;  $R_f = 0.3$  (20% EtOAc in petroleum ether); <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)  $\delta$  7.92 (d, J = 6.4 Hz, 2H), 7.76 (t, J = 6.7 Hz, 1H), 7.54 – 7.47 (m, 4H), 7.34 – 7.28 (m, 2H), 7.22 (t, J = 7.7 Hz, 2H), 6.83 (s, 1H), 6.72 (d, J = 6.7 Hz, 1H) ppm; <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>)  $\delta$  179.55, 163.65 (d, J = 246.44 Hz), 162.73, 157.74, 139.39 (d, J = 2.0 Hz), 137.93, 132.90, 132.07 (d, J = 7.8 Hz), 131.68, 131.31, 129.02, 126.23, 125.40 (d, J = 3.7 Hz), 124.01, 121.78, 116.11 (d, J = 24.24 Hz), 116.01 (d, J = 24.24 Hz), 114.12, 107.22 ppm; HRMS: calc.for C<sub>21</sub>H<sub>14</sub>FO<sub>2</sub>Se<sup>+</sup> [M+H]<sup>+</sup>: 397.0143, found: 397.0139.



## 2-Phenyl-5-(*m*-tolylselanyl)-4*H*-chromen-4-one (3ag)

Faint Yellow solid; mp 136.1-137.2 °C;  $R_f = 0.3$  (20% EtOAc in petroleum ether); <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)  $\delta$  7.94 – 7.92 (m, 2H), 7.59 (s, 1H), 7.56 – 7.53 (m, 4H), 7.35 (t, J = 7.5 Hz, 1H), 7.29 (d, J = 7.5 Hz, 3H), 6.83 (s, 1H), 6.78 (d, J = 6.3 Hz, 1H), 2.41 (s, 3H) ppm; <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>)  $\delta$  179.56, 162.43, 157.75, 140.09, 139.65, 138.10, 134.54, 132.68, 131.60, 131.39, 129.99, 129.60, 129.00, 128.76, 126.21, 124.36, 121.61, 113.72, 107.37, 21.29 ppm; HRMS: calc.for C<sub>22</sub>H<sub>17</sub>O<sub>2</sub>Se<sup>+</sup> [M+H]<sup>+</sup>: 393.0394, found: 393.0386.



#### 5-((3-Fluorophenyl)selanyl)-2-phenyl-4H-chromen-4-one (3ah)

Faint Yellow solid; mp 131.2-132.1 °C;  $R_f = 0.3$  (20% EtOAc in petroleum ether); <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)  $\delta$  7.92 (d, J = 6.1 Hz, 2H), 7.53 (d, J = 6.6 Hz, 4H), 7.54 – 7.40 (m, 2H), 7.34 – 7.28 (m, 2H), 7.17 (t, J = 7.8 Hz, 1H), 6.83 (s, 1H), 6.74 (d, J = 6.7 Hz, 1H) ppm; <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>)  $\delta$  179.58, 162.96 (d, J = 252.5 Hz), 162.70, 157.74, 139.18, 133.24 (d, J = 2.9 Hz), 132.88, 131.71, 131.30, 131.15 (d, J = 7.8 Hz), 130.74 (d, J = 6.0 Hz), 129.04, 126.25, 124.24 (d, J = 20.2 Hz), 124.20, 121.59, 116.43 (d, J = 21.0 Hz), 114.10, 107.28 ppm; HRMS: calc.for C<sub>21</sub>H<sub>14</sub>FO<sub>2</sub>Se<sup>+</sup> [M+H]<sup>+</sup>: 397.0143, found: 397.0137.



## 1-(Phenylselanyl)-9H-xanthen-9-one (6a)

Yellow solid; mp 156.5-157.3 °C;  $R_f = 0.3$  (4% EtOAc in petroleum ether); <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)  $\delta$  8.34 (dd, J = 8.0, 1.6 Hz, 1H), 7.76 (dd, J = 7.6, 1.5 Hz, 2H), 7.73 – 7.69 (m, 1H), 7.51 – 7.43 (m, 4H), 7.39 – 7.35 (m, 1H), 7.30 (t, J = 8.1 Hz, 1H), 7.19 (dd, J = 8.2, 0.5 Hz, 1H), 6.73 (dd, J = 7.8, 0.5 Hz, 1H) ppm; <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>)  $\delta$  178.13, 157.78, 155.39, 141.53, 137.60, 134.82, 133.56, 129.82, 129.26, 129.07, 126.74, 124.00, 123.28, 121.59, 119.49, 117.53, 113.76 ppm; HRMS: calc.for C<sub>19</sub>H<sub>13</sub>O<sub>2</sub>Se<sup>+</sup> [M+H]<sup>+</sup>: 353.0081, found: 353.0074.



## 1-(Phenylselanyl)acridin-9(10H)-one (6b)

Yellow solid; mp 139.1-140.5 °C;  $R_f = 0.3$  (50% DCM in petroleum ether); <sup>1</sup>H NMR (400 MHz, DMSO)  $\delta$  11.78 (brs, 1H), 8.21 (d, J = 7.7 Hz, 1H), 7.75 – 7.69 (m, 3H), 7.53 – 7.47 (m, 4H), 7.36 (t, J = 8.0 Hz, 1H), 7.29 – 7.24 (m, 2H), 6.43 (d, J = 7.6 Hz, 1H) ppm; <sup>13</sup>C NMR (101 MHz, DMSO)  $\delta$  177.84, 142.77, 140.27, 139.74, 137.26, 133.69, 132.70, 130.01, 129.69, 129.22, 125.97, 121.33, 120.32, 119.51, 118.22, 117.03, 113.35 ppm; HRMS: calc.for C<sub>19</sub>H<sub>14</sub>NOSe<sup>+</sup> [M+H]<sup>+</sup>: 352.0241, found: 352.0234.



## 10-Methyl-1-(phenylselanyl)acridin-9(10H)-one (6c)

Yellow solid; mp 190.1-191.1 °C;  $R_f = 0.3$  (50% DCM in petroleum ether); <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)  $\delta$  8.55 (dd, J = 8.0, 1.3 Hz, 1H), 7.77 (dd, J = 7.3, 1.7 Hz, 2H), 7.73 – 7.69 (m, 1H), 7.50 – 7.42 (m, 4H), 7.32 – 7.27 (m, 2H), 7.20 (d, J = 8.5 Hz, 1H), 6.69 (d, J = 7.7 Hz, 1H), 3.85 (s, 3H) ppm; <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>)  $\delta$  178.92, 144.65, 142.94, 142.02, 137.63, 133.83, 132.49, 130.86, 129.69, 128.94, 127.87, 122.46, 121.49, 121.16, 120.28, 114.51, 110.68, 34.34 ppm; HRMS: calc.for C<sub>20</sub>H<sub>16</sub>NOSe<sup>+</sup> [M+H]<sup>+</sup>: 366.0397, found: 366.0391.



## 1,8-Bis(phenylselanyl)-9H-xanthen-9-one (6d)

Faint Yellow solid; mp 230.2-230.1 °C;  $R_f = 0.3$  (30% DCM in petroleum ether); <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)  $\delta$  7.77 (d, J = 6.3 Hz, 4H), 7.49 –7.44 (m, 6H), 7.29 (t, J = 8.1 Hz, 2H), 7.15 (d, J = 8.1 Hz, 2H), 6.73 (d, J = 7.9 Hz, 2H) ppm; <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>)  $\delta$  179.12, 157.08, 141.73, 137.62, 133.56, 129.83, 129.24, 129.17, 123.37, 119.43, 113.31 ppm; HRMS: calc.for  $C_{25}H_{16}O_2Se_2^+$  [M+H]<sup>+</sup>: 508.9559, found: 508.9562.



## 1,8-Bis(phenylselanyl)acridin-9(10H)-one (6e)

Yellow solid; mp 228.2-228.5 °C;  $R_f = 0.3$  (50% DCM in petroleum ether); <sup>1</sup>H NMR (400 MHz, DMSO)  $\delta$  11.81 (brs, 1H), 7.76 – 7.66 (m, 4H), 7.58 – 7.48 (m, 6H), 7.36 (t, J = 8.0 Hz, 2H), 7.22 (d, J = 8.0 Hz, 2H), 6.45 (d, J = 7.6 Hz, 2H) ppm; <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>)  $\delta$  180.31, 142.02, 141.54, 137.66, 132.54, 130.15, 129.69, 128.95, 121.13, 119.38, 111.88 ppm; HRMS: calc.for C<sub>25</sub>H<sub>17</sub>ONSe<sub>2</sub><sup>+</sup> [M+H]<sup>+</sup>: 507.9719, found: 507.9718.



## 10-Methyl-1,8-bis(phenylselanyl)acridin-9(10*H*)-one (6f)

Yellow solid; mp 280.2-281.1 °C;  $R_f = 0.5$  (50% DCM in petroleum ether); <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)  $\delta$  7.78 – 7.76 (m, 4H), 7.46 – 7.42 (m, 6H), 7.26 (t, *J* = 8.1 Hz, 2H), 7.14 (d, *J* = 8.5 Hz, 2H), 6.67 (d, *J* = 7.8 Hz, 2H), 3.79 (s, 3H) ppm; <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>)  $\delta$  179.79, 144.11, 143.01, 137.61, 132.44, 130.86, 129.68, 128.90, 121.30, 120.36, 110.44, 35.14 ppm; HRMS: calc.for C<sub>26</sub>H<sub>19</sub>NOSe<sub>2</sub><sup>+</sup> [M+H]<sup>+</sup>: 521.9875, found: 521.9859.



## 1-Methyl-5-(phenylselanyl)quinolin-4(1*H*)-one (6g)

White solid; mp 195.4-196.1 °C;  $R_f = 0.4$  (4% MeOH in dichloromethane ether); <sup>1</sup>H NMR (400 MHz, DMSO)  $\delta$  7.94 (d, J = 7.6 Hz, 1H), 7.66 – 7.64 (m, 2H), 7.47 (d, J = 6.6 Hz, 3H), 7.37 – 7.30 (m, 2H), 6.59 (d, J = 7.3 Hz, 1H), 6.07 (d, J = 7.6 Hz, 1H), 3.75 (s, 3H) ppm; <sup>13</sup>C NMR (101 MHz, DMSO)  $\delta$  178.05, 144.79, 142.47, 139.07, 137.26, 131.49, 130.50, 130.15, 129.24, 123.99, 122.18, 112.81, 108.62, 40.82 ppm; HRMS: calc.for C<sub>16</sub>H<sub>14</sub>NOSe<sup>+</sup> [M+H]<sup>+</sup>: 316.0241, found: 316.0234.



2-Methyl-5-(phenylselanyl)-3-(propylamino)naphthalene-1,4-dione (6h)

Red solid; mp 185.2-186.7 °C;  $R_f = 0.3$  (10% EtOAc in petroleum ether); <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)  $\delta$  7.83 (dd, J = 7.3, 0.8 Hz, 1H), 7.73 – 7.71 (m, 2H), 7.49 – 7.40 (m, 3H), 7.21 (t, J = 7.8 Hz, 1H), 7.14 – 7.12 (m, 1H), 5.68 (brs, 1H), 3.51 (m, 2H), 2.29 (s, 3H), 1.71 – 1.62 (m, 2H), 1.00 (t, J = 7.4 Hz, 3H) ppm; <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>)  $\delta$  184.92, 182.21, 145.45, 140.05, 137.57,

134.59, 131.89, 130.84, 129.78, 129.68, 129.19, 129.05, 124.04, 112.44, 47.19, 24.13, 11.24, 11.17 ppm; HRMS: calc.for  $C_{20}H_{20}NO_2Se^+$  [M+H]<sup>+</sup>: 386.0659, found: 386.0653.



3-(Phenylamino)-8-(phenylselanyl)naphthalene-1,4-dione (6i)

Red brown solid; mp 173.7-174.5 °C;  $R_f = 0.3$  (10% EtOAc in petroleum ether); <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)  $\delta$  8.13 (dd, J = 13.1, 7.5 Hz, 2H), 7.82 (brs, 1H), 7.73 (t, J = 7.4 Hz, 1H), 7.67 (t, J = 7.4 Hz, 1H), 7.17 (t, J = 7.7 Hz, 2H), 7.12 – 7.05 (m, 2H), 7.01 (t, J = 7.6 Hz, 2H), 6.90 (d, J = 7.4 Hz, 2H), 6.69 (d, J = 7.8 Hz, 2H) ppm; <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>)  $\delta$  181.62, 180.33, 143.43, 136.65, 134.66, 133.25, 132.80, 131.36, 130.45, 129.57, 128.52, 127.97, 127.06, 126.82, 126.66, 124.19, 122.29, 114.21 ppm; HRMS: calc.for C<sub>22</sub>H<sub>14</sub>NO<sub>2</sub>Se<sup>+</sup> [M+H]<sup>+</sup>: 406.03463, found: 406.0341.



#### 4,8-Bis(phenylselanyl)isoquinolin-1(2H)-one (6j)

White solid; mp 260.5-261.1 °C;  $R_f = 0.3$  (25% EtOAc in petroleum ether); <sup>1</sup>H NMR (400 MHz, DMSO)  $\delta$  11.84 (d, J = 5.7 Hz, 1H), 7.74 (d, J = 6.0 Hz, 1H), 7.67 (d, J = 6.3 Hz, 2H), 7.55 (d, J = 8.0 Hz, 1H), 7.52 – 7.47 (m, 3H), 7.33 (t, J = 8.0 Hz, 1H), 7.27 – 7.14 (m, 5H), 6.69 (d, J = 7.8 Hz, 1H) ppm; <sup>13</sup>C NMR (101 MHz, DMSO)  $\delta$  162.80, 140.31, 140.15, 138.15, 137.26, 132.49, 131.77, 130.14, 129.42, 128.73, 126.33, 125.79, 123.47, 123.43, 102.15 ppm; HRMS: calc.for C<sub>21</sub>H<sub>15</sub>NOSe<sub>2</sub><sup>+</sup> [M+H]<sup>+</sup>: 457.9562, found: 457.9555.



## **3,5-Bis(phenylselanyl)-4***H***-chromen-4-one** (7)

Faint Yellow solid; mp 126.2-127.3 °C;  $R_f = 0.5$  (10% EtOAc in petroleum ether); <sup>1</sup>H NMR (400 MHz, CDCl3)  $\delta$  7.73 (s, 1H), 7.72 (dd, J = 7.7, 1.5 Hz, 2H), 7.62 (dd, J = 6.5, 3.0 Hz, 2H), 7.47 – 7.41 (m, 3H), 7.34 – 7.31 (m, 3H), 7.24 (t, J = 8.0 Hz, 1H), 7.11 (dd, J = 8.2, 0.6 Hz, 1H), 6.76 – 6.74 (m, 1H) ppm; <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>)  $\delta$  176.40, 157.93, 154.66, 140.83, 137.47, 134.02, 132.70, 129.86, 129.58, 129.27, 128.93, 128.18, 127.85, 124.64, 120.68, 117.84, 113.75 ppm; HRMS: calc.for C<sub>21</sub>H<sub>15</sub>O<sub>2</sub>Se<sub>2</sub><sup>+</sup> [M+H]<sup>+</sup>: 458.9403, found: 458.9398.

Copies of <sup>1</sup>H and <sup>13</sup>C NMR spectra of products 3, 6 and 7





























<sup>13</sup>C NMR




<sup>1</sup>H NMR 11 1.00 ₽ 1.91 1.92 1.00 1.02 1.032 .5 4.5 f1 (ppm) 7.5 9.0 8.5 8.0 7.0 6.5 6.0 5.5 5.0 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0

<sup>13</sup>C NMR















<sup>13</sup>C NMR









<sup>1</sup>H NMR

















<sup>13</sup>C NMR









150 140 130 120 110 100 90 80 70 60 f1 (ppm)















<sup>13</sup>C NMR







<sup>13</sup>C NMR





100 90 f1 (ppm) 180 170 



Se





<sup>1</sup>H NMR



<sup>13</sup>C NMR







<sup>13</sup>C NMR







190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 f1 (ppm)



<sup>1</sup>H NMR







<sup>13</sup>C NMR









<sup>13</sup>C NMR









<sup>13</sup>C NMR





<sup>1</sup>H NMR





140 130 120 110 100 90 f1 (ppm)

190 180 170 160 150







<sup>13</sup>C NMR







<sup>13</sup>C NMR







<sup>13</sup>C NMR











100 90 f1 (ppm) 

H



















<sup>13</sup>C NMR






<sup>1</sup>H NMR



<sup>13</sup>C NMR





<sup>1</sup>H NMR









<sup>13</sup>C NMR

