Supporting Information for

Efficient synthesis of polymethoxyselenoflavones via regioselective direct C-H arylation of selenochromones

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General Information

In preparation of selenochromones, all reactions were performed in oven-dried glassware with magnetic stirring under an inert atmosphere of dry nitrogen. All palladium coupling reactions were carried out in dried reaction vessels with sealed Teflon screw caps under dry nitrogen, unless otherwise specified. CH₂Cl₂ and THF used for the reaction were Liquid Chromatography grade reagents and were redistilled from calcium hydride and sodium benzophenone ketyl, respectively. The commercially available reagents were used as received without additional purification. Reactions were monitored by analytical thin-layer chromatography on 0.25 mm silica plate (F-254). Visualization was accomplished under UV light at 254 nm. Flash chromatography was performed on silica gel (40-63 mesh) by standard technique. NMR spectra (¹H and ¹³C) were obtained on 400 MHz NMR spectrometer systems using CDCl₃ solvents. Chemical shifts (δ) are reported in parts per million (ppm) from tetramethylsilane with the residual solvent resonance as the internal standard (CDCl₃ δ: 7.260). ¹H data is reported as follows: chemical shift (δ ppm), [integration, multiplicity (s = singlet, d = doublet, dd = doublet of doublet, t = triplet, q = quartet, m = multiplet), and coupling constants (J) are quoted in Hertz (Hz)]. HRMS data were determined on Q-TOF LC/MS analyzer with electrospray ionization (ESI). The major signals are quoted in m/z with the relative intensity in parentheses.
Experimental Procedures

General Procedure for Rieche Formylation (7)

A magnetically stirred solution of dichloromethyl methyl ether (40 mmol) and TiCl₄ (48 mmol) in anhyd CH₂Cl₂ (75 mL) was treated with a solution of commercially available aryl bromide (20 mmol) in anhyd CH₂Cl₂ (25 mL) at 0 °C. The reaction mixture was stirred at r.t for 4 h. After the addition of cold 5% aq HCl (20 mL) at 0 °C, the stirring was continued for 15 min. The organic layer was then separated and the aqueous solution extracted with CH₂Cl₂ (3 × 20 mL). The combined extracts were washed with 5% aq NaHCO₃ (80 mL) and brine (80 mL), dried (MgSO₄), and concentrated under reduced pressure to get bromobenzaldehydes 7.

General Procedure for Grignard Reaction (8)

A magnetically stirred solution of aldehyde 7 (18 mmol) in dry tetrahydrofuran (THF, 90 mL) was treated with a solution of ethynylmagnesium bromide in THF (0.5 M solution, 23.4 mmol) at 0 °C. The solution was stirred at 0 °C for 0.5 h and then warmed to r.t. and stirred for another 4 h. Saturated aqueous ammonium chloride solution (50 mL) was added, and the mixture was evaporated in vacuo and separated between ethyl acetate (100 mL) and saturated ammonium chloride solution. The organic layer was washed with brine, dried over MgSO₄, and evaporated in vacuo to get pure compounds 8 and were used for next without further purification.

General Procedure for TEMPO Oxidation (9)

To a stirred solution of NaBr (18 mmol), NaHCO₃ (36 mmol), TEMPO (0.9 mmol), and secondary alcohol 8 (18 mmol) in CH₂Cl₂ (90 mL) was added the solution of NaOCl (12%, 54mmol) at 0 °C. The reaction mixture was vigorously stirred at 0 °C and monitored by
TLC. After the oxidation was completed, the organic layer was separated and the aqueous solution extracted with CH$_2$Cl$_2$ (3 x 30 mL). The combined extracts were washed with brine (90 mL), dried (MgSO$_4$), and concentrated under vacuum. The residue was purified by flash column chromatography on silica gel to give the product 9.

General Procedure for Selenochromones (1)

\[
\begin{align*}
&\text{To a stirred solution of NaHSe (1.2 mmol) which was prepared from} \\
&\text{selenium powder (1.1 mmol) and NaBH}_4 \text{ (1.2 mmol) in anhyd DMF (10 mL) at 135 °C for 1 h, a} \\
&\text{solution of 9 (1.0 mmol) in anhyd DMF (10 mL) was added in one portion and the mixture was stirred} \\
&\text{for another 1 h. After the addition of water (10 mL), the mixture was filtered to remove remained} \\
&\text{selenium. The filtrate was extracted with ethyl acetate (3 x 10 mL). The combined organic extracts} \\
&\text{were washed with water (5 x 20 mL) and brine (20 mL), dried (MgSO}_4\text{), and concentrated. The} \\
&\text{resulting residue was purified by flash chromatography to give selenochromones 1.}
\end{align*}
\]

General Procedure for Palladium-Catalyzed Direct C-H Arylation of Selenochromones with Aryl Bromides (4-6).

\[
\begin{align*}
&\text{To a dried reaction vessel were added Pd(OAc)$_2$ (20 mol %), XPhos} \\
&(40 \text{ mol %), tri-} \text{-} \text{tert-butylphosphonium hydrogen tetrafluoroborate (40 mol %), pivalic acid (0.15 mmol),} \\
&\text{Cs}_2\text{CO}_3 \text{ (0.3 mmol), corresponding aryl halide 3 (0.2 mmol), selenochromone 1 (0.1 mmol), and DMA} \\
&(0.1 \text{ M). The flask was placed in a heating block and heated to 135 °C with constant stirring over 15h.} \\
&\text{After completion of the reaction, the resulting mixture was cooled to room temperature, diluted with} \\
&\text{EtOAc, washed with saturated brine and water, dried over MgSO}_4\text{, and concentrated. The residue} \\
&\text{obtained was purified by flash column chromatography over silica gel to give the final products 4-6.}
\end{align*}
\]
Characterization Data

2-bromo-4,5-dimethoxybenzaldehyde (7b)

The title compound was prepared from commercially available aryl bromide (4g, 18.43 mmol). The precipitated solid was filtered off, washed with hexane and dried under vacuum to get a white solid 7b (4.4g, 17.95 mmol, 97% yield), mp 148-150 °C. The compound was used for the next step without further purification. 1H NMR (400 MHz, CDCl3) δ 10.19 (s, 1H), 7.41 (s, 1H), 7.06 (s, 1H), 3.96 (s, 1H), 3.92 (s, 1H); 13C NMR (100 MHz, CDCl3) δ 190.8, 154.5, 148.9, 126.5, 120.4, 115.5, 110.4, 56.5, 56.2; HRMS (ESI-QTOF) calcd for C9H9BrO3 244.9813 ([M + H]+), found 244.9812.

2-bromo-4,6-dimethoxybenzaldehyde (7c)

The title compound was prepared from commercially available aryl bromide (4g, 18.43 mmol). The precipitated solid was filtered off, washed with hexane and dried under vacuum to get white solids 7c and 7ci. (4.4g, 17.95 mmol, 97% conversion yield, 85(7c):15(7ci) regioselectivity). The compounds were used for the next step without further purification. Regioisomeric compounds were separated on flash chromatography after Grignard reaction.

6-bromo-2,3,4-trimethoxybenzaldehyde (7d)

The title compound was prepared from commercially available aryl bromide (5g, 20.23 mmol). Flash chromatography (Hexane/EtOAc = 5:1) on silica gel gave 7d as a yellow solid (5.5g, 20 mmol, 99% yield), mp 51-52 °C. 1H NMR (400 MHz, CDCl3) δ 10.24 (s, 1H), 6.97 (s, 1H), 3.96 (s, 3H), 3.94 (s, 3H), 3.87 (s, 3H); 13C NMR (100 MHz, CDCl3) δ 189.4, 157.8, 156.9, 141.9, 121.5, 119.6, 113.4, 62.4, 61.0, 56.4; HRMS (ESI-QTOF) calcd for C10H11BrO4 296.9739 ([M + Na]+), found 296.9739.
found 296.9738.

1-(2-bromophenyl)prop-2-yn-1-ol (8a)

The title compound was prepared from commercially available bromobenzaldehyde 7a (4g, 21.6mmol). The yellow liquid compound 8a was used for the next step without further purification. 

$^1$H NMR (400 MHz, CDCl$_3$) $\delta$ 7.72 (d, $J = 7.6$ Hz, 1H), 7.50 (d, $J = 8.0$ Hz, 1H), 7.30 (t, $J = 7.6$ Hz, 1H), 7.14 (t, $J = 7.6$ Hz, 1H), 5.74 (s, 1H), 3.46 (d, $J = 3.6$ Hz, 1H), 2.62 (s, 1H); $^{13}$C NMR (100 MHz, CDCl$_3$) $\delta$ 138.9, 133.0, 130.1, 128.5, 127.9, 122.7, 82.4, 75.0, 63.9; HRMS (ESI-QTOF) calcd for C$_9$H$_7$BrO 210.9759 ([M + H]$^+$), found 192.9649 ([M – OH]$^+$).

1-(2-bromo-4,5-dimethoxyphenyl)prop-2-yn-1-ol (8b)

The title compound was prepared from bromobenzaldehyde 7b (4.4g, 17.95mmol). The precipitated solid was filtered off, washed with hexane and dried under vacuum to get a white solid 8b, mp 105-106 °C. The compound was used for the next step without further purification. $^1$H NMR (400 MHz, CDCl$_3$) $\delta$ 7.30 (s, 1H), 7.01 (s, 1H), 5.76 (s, 1H), 3.91 (s, 3H), 3.88 (s, 3H), 2.67 (s, 1H), 2.50 (d, $J = 3.2$ Hz, 1H); $^{13}$C NMR (100 MHz, CDCl$_3$) $\delta$ 149.8, 148.8, 131.2, 115.5, 112.8, 111.0, 82.9, 74.9, 63.9, 56.4, 56.2; HRMS (ESI-QTOF) calcd for C$_{15}$H$_{13}$O$_2$Br 314.0435 ([M + H]$^+$), found 314.0366 ([M + H]$^+$).

1-(2-bromo-4,6-dimethoxyphenyl)prop-2-yn-1-ol (8c)

The title compound was prepared from crude bromobenzaldehyde 7c (4.4g, 17.95mmol). Flash chromatography (Hexane/EtOAc/CH$_2$Cl$_2$ = 10:1:2) on silica gel gave 8c as an off-white solid (4.14g, 15.27mmol, 85% yield), mp 84-85 °C. $^1$H NMR (400 MHz, CDCl$_3$) $\delta$ 6.70 (s, 1H), 6.46 (s, 1H), 5.86 (d, $J = 11.2$ Hz, 1H), 3.93 (s, 1H), 3.89 (s, 3H), 3.77 (s, 3H), 2.50 (s, 1H); $^{13}$C NMR (100 MHz, CDCl$_3$) $\delta$ 160.5, 159.0, 123.0, 121.0, 109.5, 99.4, 83.5, 72.2, 62.4, 56.1, 55.6; HRMS (ESI-
QTOF) calcd for C$_{11}$H$_{11}$BrO$_3$ 270.9970 ([M + H]$^+$), found 252.9866 ([M - OH]$^+$).

1-(6-bromo-2,3,4-trimethoxyphenyl)prop-2-yn-1-ol (8d)

The title compound was prepared from bromobenzaldehyde 7d (5.5g, 20mmol). The yellow liquid compound 8d was used for the next step without further purification. $^1$H NMR (400 MHz, CDCl$_3$) δ 6.86 (s, 1H), 5.74 (dd, $J = 10.8$, 2.0 Hz, 1H), 4.10 (s, 1H), 4.07 (s, 3H), 3.85 (d, $J = 2.0$ Hz, 6H), 2.61 (d, $J = 2.4$ Hz, 1H); $^{13}$C NMR (100 MHz, CDCl$_3$) δ 153.9, 152.7, 142.0, 126.6, 115.5, 111.7, 84.2, 72.9, 62.9, 61.7, 60.7, 56.2; HRMS (ESI-QTOF) calcd for C$_{12}$H$_{13}$BrO$_3$ 301.0075 ([M + H]$^+$), found 282.9966 ([M - OH]$^+$).

1-(2-bromo-4-methylphenyl)prop-2-yn-1-ol (8e)

The title compound was prepared from commercially available bromobenzaldehyde (1g, 5.0mmol). The yellow liquid compound 8e was used for the next step without further purification. $^1$H NMR (400 MHz, CDCl$_3$) δ 7.62 (d, $J = 7.9$ Hz, 1H), 7.36 (s, 1H), 7.13 (d, $J = 7.8$ Hz, 1H), 5.72 (d, $J = 3.5$ Hz, 1H), 2.96 (d, $J = 5.4$ Hz, 1H), 2.62 (s, 1H), 2.30 (s, 3H); $^{13}$C NMR (100 MHz, CDCl$_3$) δ 140.3, 135.9, 133.3, 128.6, 128.2, 122.3, 82.6, 74.8, 63.6, 20.7; HRMS (ESI-QTOF) calcd for C$_{10}$H$_9$BrO 224.9915 ([M + H]$^+$), found 206.9808 ([M - OH]$^+$).

1-(2-bromo-5-fluorophenyl)prop-2-yn-1-ol (8f)

The title compound was prepared from commercially available bromobenzaldehyde (2g, 9.85mmol). The yellow liquid compound 8f was used for the next step without further purification. $^1$H NMR (400 MHz, CDCl$_3$) δ 7.50 (dd, $J = 8.5$, 4.6 Hz, 2H), 6.93 (td, $J = 8.5$, 3.0 Hz, 1H), 5.71 (dd, $J = 5.1$, 2.0 Hz, 1H), 2.97 (d, $J = 5.2$ Hz, 1H), 2.67 (d, $J = 2.2$ Hz, 1H); $^{13}$C NMR (100 MHz, CDCl$_3$) δ 162.1 (d, $J = 247.7$ Hz), 141.0 (d, $J = 7.1$ Hz), 134.2 (d, $J = 7.9$ Hz), 117.2 (d, $J = 22.6$ Hz), 116.4 (d, $J = 3.3$ Hz), 115.7 (d, $J = 24.5$ Hz), 81.8, 75.3, 63.5; HRMS (ESI-QTOF) calcd for C$_9$H$_8$BrFO 228.9664
(\([M + H]^+\)), found 210.9559 (\([M - OH]^+\)).

1-(2-bromo-5-(trifluoromethyl)phenyl)prop-2-yn-1-ol (8g)

The title compound was prepared from commercially available bromobenzaldehyde (1g, 3.95mmol). The white solid compound 8g was used for the next step without further purification.

\[^{1}H\text{ NMR (400 MHz, CDCl}_{3}\text{ ) }\delta 8.05\text{ (s, 1H), 7.70\text{ (d, }J = 8.3\text{ Hz, 1H), 7.46\text{ (d, }J = 8.3\text{ Hz, 1H), 5.80\text{ (dd, }J = 5.1, 2.1\text{ Hz, 1H), 2.72-2.69\text{ (m, 2H); }^{13}C\text{ NMR (100 MHz, CDCl}_{3}\text{ ) }\delta 140.0, 133.6, 130.4\text{ (q, }J = 33.2\text{ Hz), 126.6\text{ (q, }J = 3.7\text{ Hz), 126.4\text{ (q, }J = 1.4\text{ Hz), 125.3\text{ (q, }J = 3.8\text{ Hz), 123.6\text{ (q, }J = 272.5\text{ Hz), 81.5, 75.7, 63.5; HRMS (ESI-QTOF) calcd for C}_{10}H_{6}BrF_{3}O 278.9632\text{ ([M + H]}^+\text{), found 260.9529 ([M - OH]}^+\text{).}}

1-(2-bromophenyl)prop-2-yn-1-one (9a)

The title compound was prepared from crude 8a (4.56g, 21.6mmol). Flash chromatography (Hexane/EtOAc/CH_{2}Cl_{2} = 20:1:2) on silica gel gave 9a as a yellow solid (4.07g, 19.47mmol, 90% yield (2 steps)), mp 49-50 °C. \(^{1}H\text{ NMR (400 MHz, CDCl}_{3}\text{ ) }\delta 8.11\text{ (d, }J = 7.2\text{ Hz, 1H), 7.70\text{ (d, }J = 7.6\text{ Hz, 1H), 7.50-7.35\text{ (m, 2H), 3.49\text{ (s, 1H); }^{13}C\text{ NMR (100 MHz, CDCl}_{3}\text{ ) }\delta 176.4, 136.0, 135.2, 133.8, 133.6, 127.4, 121.4, 81.5, 80.8; HRMS (ESI-QTOF) calcd for C}_{9}H_{5}BrO 208.9602\text{ ([M + H]}^+\text{), found 208.9604.}

1-(2-bromo-4,5-dimethoxyphenyl)prop-2-yn-1-one (9b)

The title compound was prepared from crude 8b (4.87g, 17.95mmol). Flash chromatography (Hexane/EtOAc/CH_{2}Cl_{2} = 5:1:2) on silica gel gave 9b as a white solid (4.39g, 16.16mmol, 90% yield (2 steps)), mp 164-165 °C. \(^{1}H\text{ NMR (400 MHz, CDCl}_{3}\text{ ) }\delta 7.68\text{ (s, 1H), 7.13\text{ (s, 1H), 3.95\text{ (d, }J = 5.6\text{ Hz, 1H), 3.46\text{ (s, 1H); }^{13}C\text{ NMR (100 MHz, CDCl}_{3}\text{ ) }\delta 174.9, 153.2, 147.9, 127.8, 117.6, 116.1, 114.5, 81.2, 81.0, 56.5, 56.2; HRMS (ESI-QTOF) calcd for C}_{11}H_{9}BrO_{3} 268.9813\text{ ([M + H]}^+\text{), found 268.9808.)}}
1-(2-bromo-4,6-dimethoxyphenyl)prop-2-yn-1-one (9c)

The title compound was prepared from 8c (4.14g, 15.27mmol). Flash chromatography (Hexane/EtOAc/CH2Cl2 = 10:1:2) on silica gel gave 9c as an off-white solid (2.88g, 10.70mmol, 70% yield), mp 55-56 °C. 1H NMR (400 MHz, CDCl3) δ 6.70 (s, 1H), 6.43 (s, 1H), 3.82 (s, 6H), 3.41 (s, 1H); 13C NMR (100 MHz, CDCl3) δ 177.4, 162.4, 159.5, 122.9, 120.5, 110.0, 98.2, 82.3, 79.8, 56.1, 55.8; HRMS (ESI-QTOF)(calcd for C11H9BrO3 268.9813 ([M + H]+), found 268.9810.

1-(6-bromo-2,3,4-trimethoxyphenyl)prop-2-yn-1-one (9d)

The title compound was prepared from crude 8d (6.02g, 20mmol). Flash chromatography (Hexane/EtOAc/CH2Cl2 = 10:1:2) on silica gel gave 9d as a yellow liquid (5.38g, 18mmol, 90% yield (2 steps)). 1H NMR (400 MHz, CDCl3) δ 6.88 (s, 1H), 3.96 (s, 3H), 3.87 (d, J = 13.2 Hz, 6H), 3.45 (s, 1H); 13C NMR (100 MHz, CDCl3) δ 177.0, 155.8, 152.7, 141.5, 127.8, 113.1, 112.3, 82.3, 80.2, 61.9, 60.9, 56.4; HRMS (ESI-QTOF) calcd for C12H11BrO4 298.9919 ([M + H]+), found 298.9917.

1-(2-bromo-4-methylphenyl)prop-2-yn-1-one (9e)

The title compound was prepared from crude 8e (1.12g, 5.0mmol). Flash chromatography (Hexane/EtOAc = 5:1) on silica gel gave 9e as a pale-yellow solid (1.0g, 4.5mmol, 90% yield (2 steps)), mp 69 °C. 1H NMR (400 MHz, CDCl3) δ 8.05 (d, J = 7.9 Hz, 1H), 7.51 (s, 1H), 7.24 (d, J = 7.9 Hz, 1H), 3.46 (s, 1H), 2.39 (s, 3H); 13C NMR (100 MHz, CDCl3) δ 175.8, 145.4, 135.9, 134.2, 132.9, 128.1, 121.5, 81.0, 80.8, 21.2; HRMS (ESI-QTOF) calcd for C10H7BrO 277.9759 ([M + H]+), found 277.9757.

1-(2-bromo-5-fluorophenyl)prop-2-yn-1-one (9f)
The title compound was prepared from crude 8f (2.25g, 9.85mmol). Flash chromatography (Hexane/EtOAc/CH$_2$Cl$_2$ = 10:1:2) on silica gel gave 9f as a pale-yellow solid (2.12g, 9.36mmol, 95% yield (2 steps)), mp 71 °C. $^1$H NMR (400 MHz, CDCl$_3$) δ 7.81 (dd, J = 8.6, 3.0 Hz, 1H), 7.67 (dd, J = 8.8, 5.0 Hz, 1H), 7.15 (td, J = 8.6, 3.0 Hz, 1H), 3.54 (s, 1H); $^{13}$C NMR (100 MHz, CDCl$_3$) δ 175.1 (d, J = 1.9 Hz), 161.3 (d, J = 249.8 Hz), 137.2 (d, J = 6.2 Hz), 136.6 (d, J = 7.2 Hz), 121.1, 120.3 (d, J = 24.4 Hz), 115.6 (d, J = 3.5 Hz), 82.2, 80.4.

1-(2-bromo-5-(trifluoromethyl)phenyl)prop-2-yn-1-one (9g)

The title compound was prepared from crude 8g (1.1g, 3.95mmol). Flash chromatography (Hexane/EtOAc/CH$_2$Cl$_2$ = 10:1:2) on silica gel gave 9g as a pale-yellow liquid (1.04g, 3.75mmol, 95% yield (2 steps)). Volatile under vacuum.

4H-selenochromen-4-one (1a)

The title compound was prepared from 9a (0.21g, 1.0mmol). Flash chromatography (Hexane/EtOAc/CH$_2$Cl$_2$ = 3:1:2) on silica gel gave 1a as a pale-yellow solid (83.6mg, 0.4mmol, 40% yield), mp 91-92 °C. $^1$H NMR (400 MHz, CDCl$_3$) δ 8.62 (d, J = 5.6 Hz, 1H), 8.24 (d, J = 10.8 Hz, 1H), 7.66 (d, J = 5.6 Hz, 1H), 7.58-7.48 (m, 2H), 7.22 (d, J = 10.4 Hz, 1H); $^{13}$C NMR (100 MHz, CDCl$_3$) δ 181.4, 137.8, 136.5, 133.2, 131.4, 130.2, 128.8, 128.4, 127.9; HRMS (ESI-QTOF) calcd for C$_9$H$_6$OSe 210.9662 ([M + H]$^+$), found 210.9658.

6,7-dimethoxy-4H-selenochromen-4-one (1b)

The title compound was prepared from 9b (0.27g, 1.0mmol). Flash chromatography (Hexane/EtOAc/CH$_2$Cl$_2$ = 2:1:2) on silica gel gave 1b as a pale-yellow solid (80.7mg, 0.3mmol, 30% yield), mp 138-140 °C. $^1$H NMR (400 MHz, CDCl$_3$) δ 8.19 (d, J = 10.8 Hz, 1H), 8.07 (s, 1H), 7.20 (d, J
= 10.4 Hz, 1H), 7.03 (s, 1H), 3.99 (d, J = 7.2 Hz, 6H); 13C NMR (100 MHz, CDCl₃) δ 180.5, 152.4, 149.6, 136.6, 130.1, 127.7, 127.2, 110.3, 109.2, 56.3, 56.2; HRMS (ESI-QTOF) calcd for C₁₁H₁₀O₃Se 270.9873 ([M + H⁺], found 270.9871.

5,7-dimethoxy-4H-selenochromen-4-one (1c)

The title compound was prepared from 9c (0.27g, 1.0mmol). Flash chromatography (Hexane/EtOAc/CH₂Cl₂ = 2:1:2) on silica gel gave 1c as a pale-yellow solid (80.7mg, 0.3mmol, 30% yield), mp 154-155 °C. 1H NMR (400 MHz, CDCl₃) δ 7.85 (d, J = 10.8 Hz, 1H), 7.03 (d, J = 10.8 Hz, 1H), 6.67 (s, 1H), 6.50 (s, 1H), 3.90 (d, J = 22.4 Hz, 6H); 13C NMR (100 MHz, CDCl₃) δ 181.5, 163.8, 161.8, 141.0, 132.1, 130.9, 117.7, 103.2, 99.3, 56.3, 55.6; HRMS (ESI-QTOF) calcd for C₁₁H₁₀O₃Se 270.9873 ([M + H⁺], found 270.9874.

5,6,7-trimethoxy-4H-selenochromen-4-one (1d)

The title compound was prepared from 9d (0.30g, 1.0mmol). Flash chromatography (Hexane/EtOAc/CH₂Cl₂ = 2:1:2) on silica gel gave 1d as a pale-yellow solid (53.85mg, 0.18mmol, 18% yield), mp 86-87 °C. 1H NMR (400 MHz, CDCl₃) δ 7.94 (d, J = 10.8 Hz, 1H), 7.05 (d, J = 10.4 Hz, 1H), 6.88 (s, 1H), 3.93 (d, J = 14.0 Hz, 9H); 13C NMR (100 MHz, CDCl₃) δ 181.2, 156.7, 156.0, 143.1, 133.7, 133.0, 129.8, 122.3, 106.1, 61.9, 61.3, 56.2; HRMS (ESI-QTOF) calcd for C₁₂H₁₂O₄Se 300.9979 ([M + H⁺], found 300.9984.

7-methyl-4H-selenochromen-4-one (1e)

The title compound was prepared from 9e (0.22g, 1.0mmol). Flash chromatography (Hexane/EtOAc/CH₂Cl₂ = 5:1:2) on silica gel gave 1e as a pale-yellow solid (12.94mg, 0.26mmol, 26% yield), mp 90 °C. 1H NMR (400 MHz, CDCl₃) δ 8.50 (d, J = 8.3 Hz, 1H), 8.19 (d, J = 10.6 Hz, 1H), 7.45 (s, 1H), 7.32 (d, J = 8.3 Hz, 1H), 7.19 (d, J = 10.6 Hz, 1H), 2.44 (s, 3H); 13C NMR (100 MHz, CDCl₃) δ
6-fluoro-4H-selenochromen-4-one (1f)

The title compound was prepared from 9f (0.23g, 1.0mmol). Flash chromatography (Hexane/EtOAc/CH₂Cl₂ = 5:1:2) on silica gel gave 1f as a pale-yellow solid (22.7mg, 0.1mmol, 10% yield), mp 130 °C. ¹H NMR (400 MHz, CDCl₃) δ 8.34-8.25 (m, 2H), 7.67 (dd, J = 8.7, 5.0 Hz, 1H), 7.33 (td, J = 8.6, 2.9 Hz, 1H), 7.23 (d, J = 10.6 Hz, 1H); ¹³C NMR (100 MHz, CDCl₃) δ 180.5 (d, J = 2.3 Hz), 162.4 (d, J = 249.0 Hz), 138.0, 134.9 (d, J = 6.5 Hz), 131.2 (d, J = 2.8 Hz), 130.6 (d, J = 7.3 Hz), 127.5, 120.1 (d, J = 23.7 Hz), 115.9 (d, J = 22.7 Hz); HRMS (ESI-QTOF) calcd for C₉H₅FOSe 228.9568 ([M + H]+), found 228.9562.

6-(trifluoromethyl)-4H-chromen-4-one (1g)

The title compound was prepared from 9g (0.28g, 1.0mmol). Flash chromatography (Hexane/EtOAc/CH₂Cl₂ = 5:1:2) on silica gel gave 1g as a pale-yellow solid (27.7mg, 0.1mmol, 10% yield), mp 96-97 °C. ¹H NMR (400 MHz, CDCl₃) δ 8.89 (s, 1H), 8.26 (d, J = 10.6 Hz, 1H), 7.80 (d, J = 8.4 Hz, 1H), 7.75 (d, J = 8.4 Hz, 1H), 7.26 (d, J = 10.6 Hz, 1H); ¹³C NMR (100 MHz, CDCl₃) δ 180.4, 140.3, 137.8, 133.2, 130.4 (q, J = 33.6 Hz), 130.0, 128.5, 127.4 (q, J = 4.0 Hz), 127.2 (q, J = 3.4 Hz), 123.5 (q, J = 272.4 Hz); HRMS (ESI-QTOF) calcd for C₁₀H₅F₃OSe 300.9355 ([M + Na]+), found 300.9351.

2-(3,4-dimethoxyphenyl)-4H-selenochromen-4-one (4a)

The title compound was prepared from 1a (21mg, 0.1mmol). Flash chromatography (Hexane/EtOAc/CH₂Cl₂ = 3:1:2) on silica gel gave 4a as a pale-yellow solid (20.71mg, 0.06mmol, 60% yield), mp 149-151 °C. ¹H NMR (400 MHz, CDCl₃) δ 8.60 (d, J = 6.0 Hz, 1H), 7.68 (d, J = 6.0 Hz, 1H), 7.58-7.48 (m, 2H), 7.35 (s, 1H), 7.25 (d, J = 8.4 Hz, 1H), 7.15 (s, 1H), 6.95 (d, J = 8.0 Hz, 1H), 3.95 (d, J = 7.3 Hz), 3.85 (s, 3H), 3.75 (s, 3H).
$J = 2.8 \text{ Hz, } 6\text{H}); \ ^{13}\text{C NMR (100 MHz, CDCl}_3\hspace{1cm}\delta \hspace{1cm} 182.9, 153.9, 151.4, 149.6, 136.8, 131.8, 131.6, 130.8, 130.1, 128.3, 127.8, 124.5, 120.1, 111.4, 109.5, 56.1; \ \text{HRMS (ESI-QTOF) calcd for C}_{17}\text{H}_{12}\text{O}_3\text{Se} 347.0186 ([M + H]^\ast), \ \text{found 347.0187.}$

2-(3,4,5-trimethoxyphenyl)-4H-selenochromen-4-one (4b)

The title compound was prepared from 1a (21mg, 0.1mmol). Flash chromatography (Hexane/EtOAc/CH$_2$Cl$_2 = 3:1:2$) on silica gel gave 4b as a pale-yellow solid (20.64mg, 0.055mmol, 55% yield), mp 91-92 °C. $^1$H NMR (400 MHz, cdcl$_3$) $\delta$ 8.61 (d, $J = 6.8 \text{ Hz, } 1\text{H}$), 7.69 (d, $J = 6.8 \text{ Hz, } 1\text{H}$), 7.58-7.49 (m, 2H), 7.35 (s, 1H), 6.86 (s, 2H), 3.93 (d, $J = 7.6 \text{ Hz, } 9\text{H}$); $^{13}\text{C NMR (100 MHz, CDCl}_3\hspace{1cm}\delta \hspace{1cm} 182.9, 154.2, 153.8, 140.2, 136.8, 133.7, 131.8, 131.7, 130.1, 128.3, 127.9, 125.3, 104.2, 61.0, 56.4; \ \text{HRMS (ESI-QTOF) calcd for C}_{18}\text{H}_{16}\text{O}_4\text{Se} 377.0292 ([M + H]^\ast), \ \text{found 377.0286.}$

2-(3,5-dimethoxyphenyl)-4H-selenochromen-4-one (4c)

The title compound was prepared from 1a (21mg, 0.1mmol). Flash chromatography (Hexane/EtOAc/CH$_2$Cl$_2 = 3:1:2$) on silica gel gave 4c as a pale-yellow solid (22.44mg, 0.065mmol, 65% yield), mp 105-106 °C. $^1$H NMR (400 MHz, cdcl$_3$) $\delta$ 8.61 (d, $J = 6.8 \text{ Hz, } 1\text{H}$), 7.69 (d, $J = 6.8 \text{ Hz, } 1\text{H}$), 7.58-7.48 (m, 2H), 7.38 (s, 1H), 6.77 (s, 2H), 6.58 (s, 1H), 3.85 (s, 6H); $^{13}\text{C NMR (100 MHz, CDCl}_3\hspace{1cm}\delta \hspace{1cm} 182.8, 161.3, 154.1, 140.1, 137.0, 131.9, 131.6, 130.1, 128.3, 127.9, 125.7, 105.0, 102.6, 55.6; \ \text{HRMS (ESI-QTOF) calcd for C}_{17}\text{H}_{14}\text{O}_3\text{Se} 347.0186 ([M + H]^\ast), \ \text{found 347.0183.}$

2-(4-methoxyphenyl)-4H-selenochromen-4-one (4d)

The title compound was prepared from 1a (21mg, 0.1mmol). Flash chromatography (Hexane/EtOAc/CH$_2$Cl$_2 = 3:1:2$) on silica gel gave 4d as a pale-yellow solid (17.65mg, 0.056mmol, 56% yield), mp 91-92 °C. $^1$H NMR (400 MHz, cdcl$_3$) $\delta$ 8.61 (d, $J = 6.8 \text{ Hz, } 1\text{H}$), 7.69 (d, $J = 6.8 \text{ Hz, } 1\text{H}$), 7.58-7.49 (m, 2H), 7.35 (s, 1H), 6.86 (s, 2H), 3.93 (d, $J = 7.6 \text{ Hz, } 9\text{H}$); $^{13}\text{C NMR (100 MHz, CDCl}_3\hspace{1cm}\delta \hspace{1cm} 182.9, 154.2, 153.8, 140.2, 136.8, 133.7, 131.8, 131.7, 130.1, 128.3, 127.9, 125.3, 104.2, 61.0, 56.4; \ \text{HRMS (ESI-QTOF) calcd for C}_{18}\text{H}_{16}\text{O}_4\text{Se} 377.0292 ([M + H]^\ast), \ \text{found 377.0286.}$
yield), mp 150-152 °C. ^1^H NMR (400 MHz, CDCl\textsubscript{3}) δ 8.60 (d, J = 6.8 Hz, 1H), 7.68 (d, J = 7.2 Hz, 1H), 7.60 (d, J = 8.4 Hz, 2H), 7.56-7.48 (m, 2H), 7.33 (s, 1H), 7.00 (d, J = 8.8 Hz, 2H), 3.87 (s, 3H); ^13^C NMR (100 MHz, CDCl\textsubscript{3}) δ 183.0, 161.9, 153.9, 136.9, 131.9, 131.6, 130.6, 130.2, 128.4, 127.9, 124.5, 114.8, 55.6; HRMS (ESI-QTOF) calcd for C\textsubscript{16}H\textsubscript{12}O\textsubscript{2}Se 317.0081 ([M + H]^+), found 317.0078.

2-(3-methoxyphenyl)-4H-selenochromen-4-one (4e)

![Chemical structure of 4e](image)

The title compound was prepared from 1a (21mg, 0.1mmol). Flash chromatography (Hexane/EtOAc/CH\textsubscript{2}Cl\textsubscript{2} = 3:1:2) on silica gel gave 4e as a pale-yellow solid (21.12mg, 0.067mmol, 67% yield), mp 123-124 °C. ^1^H NMR (400 MHz, CDCl\textsubscript{3}) δ 8.62 (d, J = 7.6 Hz, 1H), 7.70 (d, J = 7.2 Hz, 1H), 7.60-7.48 (m, 2H), 7.43-7.37 (m, 2H), 7.22 (d, J = 7.6 Hz, 1H), 7.16 (s, 1H), 7.04 (d, J = 8.0 Hz, 1H), 3.87 (s, 3H); ^13^C NMR (100 MHz, CDCl\textsubscript{3}) δ 182.8, 160.2, 154.0, 139.5, 136.9, 131.8, 131.6, 130.4, 130.1, 128.3, 127.9, 125.7, 119.3, 116.4, 112.2, 55.5; HRMS (ESI-QTOF) calcd for C\textsubscript{16}H\textsubscript{12}O\textsubscript{2}Se 317.0081 ([M + H]^+), found 317.0078.

2-(2-methoxyphenyl)-4H-selenochromen-4-one (4f)

![Chemical structure of 4f](image)

The title compound was prepared from 1a (21mg, 0.1mmol). Flash chromatography (Hexane/EtOAc/CH\textsubscript{2}Cl\textsubscript{2} = 3:1:2) on silica gel gave 4f as a pale-yellow solid (11.03mg, 0.035mmol, 35% yield), mp 99-100 °C. ^1^H NMR (400 MHz, CDCl\textsubscript{3}) δ 8.62 (d, J = 6.8 Hz, 1H), 7.67 (d, J = 6.4 Hz, 1H), 7.58-7.38 (m, 4H), 7.32 (s, 1H), 7.03 (m, 2H), 3.88 (s, 3H); ^13^C NMR (100 MHz, CDCl\textsubscript{3}) δ 182.8, 156.2, 150.8, 138.2, 131.4, 131.3, 129.94, 129.85, 128.4, 128.1, 127.5, 126.9, 121.1, 111.7, 55.7; HRMS (ESI-QTOF) calcd for C\textsubscript{16}H\textsubscript{12}O\textsubscript{2}Se 317.0081 ([M + H]^+), found 317.0078.

2-(p-tolyl)-4H-selenochromen-4-one (4g)

![Chemical structure of 4g](image)

The title compound was prepared from 1a (21mg, 0.1mmol). Flash chromatography (Hexane/EtOAc/CH\textsubscript{2}Cl\textsubcript{2} = 3:1:2) on silica gel gave 4g as a pale-yellow solid (21.12mg, 0.067mmol, 67% yield), mp 150-152 °C. ^1^H NMR (400 MHz, CDCl\textsubscript{3}) δ 8.60 (d, J = 6.8 Hz, 1H), 7.68 (d, J = 7.2 Hz, 1H), 7.60 (d, J = 8.4 Hz, 2H), 7.56-7.48 (m, 2H), 7.33 (s, 1H), 7.00 (d, J = 8.8 Hz, 2H), 3.87 (s, 3H); ^13^C NMR (100 MHz, CDCl\textsubscript{3}) δ 183.0, 161.9, 153.9, 136.9, 131.9, 131.6, 130.6, 130.2, 128.4, 127.9, 124.5, 114.8, 55.6; HRMS (ESI-QTOF) calcd for C\textsubscript{16}H\textsubscript{12}O\textsubscript{2}Se 317.0081 ([M + H]^+), found 317.0078.
(Hexane/EtOAc/CH$_2$Cl$_2$ = 10:1:2) on silica gel gave 4g as a pale-yellow solid (22.14mg, 0.074mmol, 74% yield), mp 141-142 °C.  $^1$H NMR (400 MHz, CDCl$_3$) δ 8.61 (d, $J = 6.8$ Hz, 1H), 7.68 (d, $J = 7.2$ Hz, 1H), 7.56-7.48 (m, 4H), 7.36 (s, 1H), 7.28 (d, $J = 7.2$ Hz, 2H), 2.41 (s, 3H); $^{13}$C NMR (100 MHz, CDCl$_3$) δ 182.9, 154.1, 141.2, 136.9, 135.3, 131.8, 131.5, 130.04, 130.00, 128.3, 127.8, 126.7, 125.0, 21.4; HRMS (ESI-QTOF) calcd for C$_{16}$H$_{12}$OSe 301.0131 ([M + H]$^+$), found 301.0134.

2-(4-(tert-butyl)phenyl)-4H-selenochromen-4-one (4h)

The title compound was prepared from 1a (21mg, 0.1mmol). Flash chromatography (Hexane/EtOAc/CH$_2$Cl$_2$ = 10:1:2) on silica gel gave 4h as a pale-yellow solid (20.48mg, 0.060mmol, 60% yield), mp 105-106 °C.  $^1$H NMR (400 MHz, CDCl$_3$) δ 8.61 (d, $J = 6.8$ Hz, 1H), 7.69 (d, $J = 6.0$ Hz, 1H), 7.59 (d, $J = 8.0$ Hz, 2H), 7.55-7.48 (m, 4H), 7.38 (s, 1H), 1.36 (s, 9H); $^{13}$C NMR (100 MHz, CDCl$_3$) δ 182.9, 154.3, 154.1, 136.9, 135.2, 131.8, 131.5, 130.1, 128.3, 127.8, 126.6, 126.3, 125.1, 34.9, 31.2; HRMS (ESI-QTOF) calcd for C$_{19}$H$_{18}$OSe 343.0601 ([M + H]$^+$), found 343.0598.

2-(4-chlorophenyl)-4H-selenochromen-4-one (4i)

The title compound was prepared from 1a (21mg, 0.1mmol). Flash chromatography (Hexane/EtOAc/CH$_2$Cl$_2$ = 10:1:2) on silica gel gave 4i as a pale-yellow solid (16.62mg, 0.052mmol, 52% yield), mp 128-130 °C.  $^1$H NMR (400 MHz, CDCl$_3$) δ 8.61 (d, $J = 4.8$ Hz, 1H), 7.70 (d, $J = 4.3$ Hz, 1H), 7.60-7.52 (m, 4H), 7.48 (d, $J = 8.2$ Hz, 2H), 7.34 (s, 1H); $^{13}$C NMR (100 MHz, CDCl$_3$) δ 182.7, 152.4, 136.9, 136.60, 136.55, 131.7, 131.6, 130.2, 129.6, 128.3, 127.8, 126.0, 125.9; HRMS (ESI-QTOF) calcd for C$_{15}$H$_{9}$ClOSe 320.9585 ([M + H]$^+$), found 320.9580.

2-(4-fluorophenyl)-4H-selenochromen-4-one (4j)
The title compound was prepared from 1a (21mg, 0.1mmol). Flash chromatography (Hexane/EtOAc/CH₂Cl₂ = 10:1:2) on silica gel gave 4j as a pale-yellow solid (17.58mg, 0.058mmol, 58% yield), mp 141-143 °C. ¹H NMR (400 MHz, CDCl₃) δ 8.61 (d, J = 8.1 Hz, 1H), 7.68 (d, J = 7.5 Hz, 1H), 7.65-7.59 (m, 2H), 7.58-7.49 (m, 2H), 7.31 (s, 1H), 7.18 (t, J = 8.5 Hz, 2H); ¹³C NMR (100 MHz, CDCl₃) δ 182.7, 164.2 (d, J = 250.6 Hz), 152.7, 136.6, 134.3 (d, J = 3.3 Hz), 131.7, 131.6, 130.1, 128.9 (d, J = 8.6 Hz), 128.3, 128.0, 125.7, 116.5 (d, J = 21.8 Hz); HRMS (ESI-QTOF) calcd for C₁₅H₁₀FOSe 304.9881 ([M + H]+), found 304.9878.

2-(4-(trifluoromethyl)phenyl)-4H-selenochromen-4-one (4k)

The title compound was prepared from 1a (21mg, 0.1mmol). Flash chromatography (Hexane/EtOAc/CH₂Cl₂ = 10:1:2) on silica gel gave 4k as a pale-yellow solid (21.55mg, 0.061mmol, 61% yield), mp 173-174 °C. ¹H NMR (400 MHz, CDCl₃) δ 8.62 (d, J = 7.4 Hz, 1H), 7.76 (s, 4H), 7.71 (d, J = 8.16 Hz, 1H), 7.62-7.52 (m, 2H), 7.38 (s, 1H); ¹³C NMR (100 MHz, CDCl₃) δ 182.6, 151.9, 141.6, 136.5, 132.1 (q, J = 32.94 Hz), 131.9, 131.6, 130.2, 128.4, 128.2, 127.4, 126.8, 126.33 (q, J = 3.72 Hz), 126.27 (q, J = 270.76 Hz); HRMS (ESI-QTOF) calcd for C₁₆H₉F₃OSe 354.9851 ([M + H]+), found 354.9851.

2-(4-nitrophenyl)-4H-selenochromen-4-one (4l)

The title compound was prepared from 1a (21mg, 0.1mmol). Flash chromatography (Hexane/EtOAc/CH₂Cl₂ = 10:1:2) on silica gel gave 4l as a pale-yellow solid (15.85mg, 0.048mmol, 48% yield), mp 172-173 °C. ¹H NMR (400 MHz, CDCl₃) δ 8.63 (d, J = 7.6 Hz, 1H), 8.36 (d, J = 8.7 Hz, 2H), 7.81 (d, J = 8.7 Hz, 2H), 7.73 (d, J = 7.4 Hz, 1H), 7.65-7.54 (m, 2H), 7.40 (s, 1H); ¹³C NMR (100 MHz, CDCl₃) δ 182.4, 150.6, 148.9, 144.2, 136.2, 132.1, 131.5, 130.3, 128.4, 128.0, 127.4, 124.5, 123.6; HRMS (ESI-QTOF) calcd for C₁₅H₉NO₃Se 331.9826 ([M + H]+), found 331.9829.
4-(4-oxo-4H-selenochromen-2-yl)benzonitrile (4m)

The title compound was prepared from 1a (21mg, 0.1mmol). Flash chromatography (Hexane/EtOAc/CH₂Cl₂ = 10:1:2) on silica gel gave 4m as a pale-yellow solid (12.10mg, 0.039mmol, 39% yield), mp 194-195 °C. ¹H NMR (400 MHz, CDCl₃) δ 8.63 (d, J = 7.6 Hz, 1H), 7.81 (d, J = 8.3 Hz, 2H), 7.76-7.70 (m, 3H), 7.63-7.53 (m, 2H), 7.37 (s, 1H); ¹³C NMR (100 MHz, CDCl₃) δ 182.5, 151.2, 142.4, 136.3, 133.1, 132.0, 131.5, 130.3, 128.4, 128.3, 127.7, 127.0, 117.9, 114.3; HRMS (ESI-QTOF) calcd for C₁₆H₉NOSe 311.9928 ([M + H]⁺), found 311.9928.

2-(pyridin-3-yl)-4H-selenochromen-4-one (4n)

The title compound was prepared from 1a (21mg, 0.1mmol). Flash chromatography (Hexane/EtOAc/CH₂Cl₂ = 3:1:2) on silica gel gave 4n as a pale-yellow solid (18.03mg, 0.063mmol, 63% yield), mp 153-154 °C. ¹H NMR (400 MHz, CDCl₃) δ 8.75 (d, J = 2.96 Hz, 1H), 8.63 (d, J = 7.92 Hz, 1H), 7.93 (d, J = 7.8 Hz, 1H), 7.72 (d, J = 7.08 Hz, 1H), 7.62-7.52 (m, 2H), 7.45 (t, J = 5.56 Hz, 1H), 7.37 (s, 1H); ¹³C NMR (100 MHz, CDCl₃) δ 182.4, 151.6, 150.0, 147.7, 136.4, 134.3, 134.2, 131.9, 131.6, 130.3, 128.4, 128.2, 126.7, 123.9; HRMS (ESI-QTOF) calcd for C₁₄H₉NOSe 287.9928 ([M + H]⁺), found 287.9928.

2-(thiophen-2-yl)-4H-selenochromen-4-one (4o)

The title compound was prepared from 1a (21mg, 0.1mmol). Flash chromatography (Hexane/EtOAc/CH₂Cl₂ = 10:1:2) on silica gel gave 4o as a yellow solid (9.45mg, 0.045mmol, 45% yield), mp 142 °C. ¹H NMR (400 MHz, CDCl₃) δ 8.55 (d, J = 7.8 Hz, 1H), 7.62 (d, J = 7.3 Hz, 1H), 7.55-7.43 (m, 4H), 7.35 (s, 1H), 7.13 (dd, J = 5.0, 3.8 Hz, 1H); ¹³C NMR (100 MHz, CDCl₃) δ 182.6, 145.0, 140.8, 135.9, 131.9, 131.8, 130.1, 129.1, 128.5, 128.1, 127.9, 127.3, 123.6; HRMS (ESI-QTOF) calcd for C₁₃H₈OSSe 292.9539 ([M + H]⁺), found 292.9536.
2-(thiophen-3-yl)-4H-selenochromen-4-one (4p)

The title compound was prepared from 1a (21mg, 0.1mmol). Flash chromatography (Hexane/EtOAc/CH$_2$Cl$_2$ = 10:1:2) on silica gel gave 4p as a yellow solid (7.14mg, 0.034mmol, 34% yield), mp 146 ºC. $^1$H NMR (400 MHz, CDCl$_3$) δ 8.57 (d, $J$ = 7.5 Hz, 1H), 7.70-7.62 (m, 2H), 7.54-7.47 (m, 2H), 7.47-7.43 (m, 1H), 7.41-7.35 (m, 2H); $^{13}$C NMR (100 MHz, CDCl$_3$) δ 183.0, 147.0, 139.4, 136.2, 131.9, 131.7, 130.1, 128.2, 127.8, 127.6, 125.3, 124.9, 124.3; HRMS (ESI-QTOF) calcd for C$_{13}$H$_8$OSSe 292.9539 ([M + H]$^+$), found 292.9537.

2-phenyl-4H-selenochromen-4-one (5a)

The title compound was prepared from 1a (21mg, 0.1mmol). Flash chromatography (Hexane/EtOAc/CH$_2$Cl$_2$ = 10:1:2) on silica gel gave 5a as a pale-yellow solid (22.82mg, 0.080mmol, 80% yield), mp 127-128 ºC. $^1$H NMR (400 MHz, CDCl$_3$) δ 8.62 (d, $J$ = 7.2 Hz, 1H), 7.70 (d, $J$ = 7.2 Hz, 1H), 7.64 (d, $J$ = 3.2 Hz, 2H), 7.60-7.45 (m, 5H), 7.38 (s, 1H); $^{13}$C NMR (100 MHz, CDCl$_3$) δ 182.8, 154.1, 138.2, 136.9, 131.8, 131.6, 130.7, 130.1, 129.3, 128.3, 127.9, 126.9, 125.7; HRMS (ESI-QTOF) calcd for C$_{15}$H$_{10}$OSe 286.9975 ([M + H]$^+$), found 286.9973.

6,7-dimethoxy-2-phenyl-4H-selenochromen-4-one (5b)

The title compound was prepared from 1b (26.9mg, 0.1mmol). Flash chromatography (Hexane/EtOAc/CH$_2$Cl$_2$ = 5:1:2) on silica gel gave 5b as a pale-yellow solid (14.0mg, 0.052mmol, 52% yield), mp 176 ºC. $^1$H NMR (400 MHz, CDCl$_3$) δ 8.08 (s, 1H), 7.63 (dd, $J$ = 6.6, 2.9 Hz, 2H), 7.51-7.47 (m, 3H), 7.37 (s, 1H), 7.08 (s, 1H), 4.01 (d, $J$ = 5.1 Hz, 6H); $^{13}$C NMR (100 MHz, CDCl$_3$) δ 181.8, 153.0, 152.6, 149.6, 138.2, 130.5, 129.3, 126.9, 125.8, 125.1, 110.3, 108.8, 56.3, 56.2; HRMS (ESI-QTOF) calcd for C$_{17}$H$_{16}$O$_3$Se 347.0186 ([M + H]$^+$), found 347.0184.
7-methyl-2-phenyl-4H-selenochromen-4-one (5c)

The title compound was prepared from 1e (22.3mg, 0.1mmol). Flash chromatography (Hexane/EtOAc/CH₂Cl₂ = 5:1:2) on silica gel gave 5c as a pale-yellow solid (16.7mg, 0.075mmol, 75% yield), mp 90 °C. ¹H NMR (400 MHz, CDCl₃) δ 8.50 (d, J = 8.2 Hz, 1H), 7.65-7.61 (m, 2H), 7.51-7.46 (m, 4H), 7.36-7.30 (m, 2H), 2.46 (s, 3H); ¹³C NMR (100 MHz, CDCl₃) δ 182.7, 153.6, 142.5, 138.2, 137.0, 130.6, 129.9, 129.5, 129.32, 129.28, 128.2, 126.9, 125.7, 21.5; HRMS (ESI-QTOF) calcd for C₁₆H₁₂OSe 301.0132 ([M + H]+), found 301.0136.

6-fluoro-2-phenyl-4H-selenochromen-4-one (5d)

The title compound was prepared from 1f (22.7mg, 0.1mmol). Flash chromatography (Hexane/EtOAc/CH₂Cl₂ = 5:1:2) on silica gel gave 5d as a pale-yellow solid (9.5mg, 0.042mmol, 42% yield), mp 155°C. ¹H NMR (400 MHz, CDCl₃) δ 8.32 (dd, J = 9.8, 2.9 Hz, 1H), 7.71 (dd, J = 8.7, 5.0 Hz, 1H), 7.66-7.62 (m, 2H), 7.53-7.49 (m, 3H), 7.34 (s, 1H), 7.38 (td, J = 8.5, 2.9 Hz, 1H); ¹³C NMR (100 MHz, CDCl₃) δ 181.9 (d, J = 2.3 Hz), 162.4 (d, J = 248.7 Hz), 154.6, 137.9, 133.6 (d, J = 6.6 Hz), 131.6 (d, J = 2.7 Hz), 130.9, 130.2 (d, J = 7.3 Hz), 129.4, 126.9, 124.9, 120.2 (d, J = 23.7 Hz), 115.8 (d, J = 22.8 Hz); HRMS (ESI-QTOF) calcd for C₁₅H₁₀FOSe 326.9700 ([M + Na]+), found 326.9736.

2-phenyl-6-(trifluoromethyl)-4H-selenochromen-4-one (5e)

The title compound was prepared from 1g (27.7mg, 0.1mmol). Flash chromatography (Hexane/EtOAc/CH₂Cl₂ = 5:1:2) on silica gel gave 5e as a pale-yellow solid (15.2mg, 0.055mmol, 55% yield), mp 175°C. ¹H NMR (400 MHz, CDCl₃) δ 8.89 (s, 1H), 7.84 (d, J = 8.3 Hz, 1H), 7.76 (d, J = 8.2 Hz, 1H), 7.66-7.62 (m, 2H), 7.54-7.50 (m, 3H), 7.40 (s, 1H); ¹³C NMR (100 MHz, CDCl₃) δ 181.7, 154.3, 140.7, 137.6, 131.9, 131.1, 130.3 (q, J = 33.5 Hz), 129.5, 129.3, 127.5 (q, J = 3.4 Hz), 127.4 (q, J = 4.1 Hz), 126.9, 125.6, 123.6 (q, J = 272.6 Hz); HRMS (ESI-QTOF) calcd for
The title compound was prepared from 1b (26.9mg, 0.1mmol). Flash chromatography (Hexane/EtOAc/CH₂Cl₂ = 2:1:2) on silica gel gave 6a as a pale-yellow solid (24.32mg, 0.060mmol, 60% yield), mp 205-206 °C. ¹H NMR (400 MHz, CDCl₃) δ 8.06 (s, 1H), 7.33 (s, 1H), 7.22 (d, J = 8.3 Hz, 1H), 7.15 (s, 1H), 7.06 (s, 1H), 6.95 (d, J = 8.4 Hz, 1H), 4.00 (d, J = 6.8 Hz, 6H), 3.95 (d, J = 6.3 Hz, 6H); ¹³C NMR (100 MHz, CDCl₃) δ 182.0, 152.9, 152.6, 151.2, 149.6, 149.5, 130.9, 130.4, 125.9, 124.0, 119.9, 111.4, 110.3, 109.5, 108.8, 56.3, 56.2, 56.1; HRMS (ESI-QTOF) calcd for C₁₉H₁₉O₅Se 407.0397 ([M + H]⁺), found 407.0391.

2-(3,4-dimethoxyphenyl)-5,7-dimethoxy-4H-selenochromen-4-one (6b)

The title compound was prepared from 1c (26.9mg, 0.1mmol). Flash chromatography (Hexane/EtOAc/CH₂Cl₂ = 2:1:2) on silica gel gave 6b as a pale-yellow solid (15.40mg, 0.038mmol, 38% yield), mp 178-180 °C. ¹H NMR (400 MHz, CDCl₃) δ 7.22-7.16 (m, 2H), 7.13 (s, 1H), 6.93 (d, J = 8.4 Hz, 1H), 6.72 (s, 1H), 6.51 (s, 1H), 3.96 (s, 6H), 3.94 (s, 3H), 3.89 (s, 3H); ¹³C NMR (100 MHz, CDCl₃) δ 183.3, 163.7, 162.0, 151.1, 149.4, 147.8, 141.3, 130.1, 126.6, 120.0, 116.5, 111.3, 109.4, 102.9, 99.2, 56.3, 56.1, 56.1, 55.7; HRMS (ESI-QTOF) calcd for C₁₉H₁₉O₅Se 407.0397 ([M + H]⁺), found 407.0400.

2-(3,4-dimethoxyphenyl)-5,6,7-trimethoxy-4H-selenochromen-4-one (6c)

The title compound was prepared from 1d (30mg, 0.1mmol). Flash chromatography (Hexane/EtOAc/CH₂Cl₂ = 2:1:2) on silica gel gave 6c as a yellow liquid (17.41mg, 0.040mmol, 40% yield). ¹H NMR (400 MHz, CDCl₃) δ 7.21 (d, J = 11.8 Hz, 2H), 7.13 (s, 1H), 6.94 (d,
$J = 11.8$ Hz, 2H), 3.97 (d, $J = 2.0$ Hz, 6H), 3.96 (s, 3H), 3.94 (d, $J = 1.6$ Hz, 6H); $\textsuperscript{13}$C NMR (100 MHz, CDCl$_3$) $\delta$ 182.9, 156.6, 156.1, 151.1, 149.5, 148.9, 143.0, 134.0, 130.2, 125.8, 120.9, 119.9, 111.3, 109.4, 105.7, 62.0, 61.4, 59.2, 56.1, 56.1; HRMS (ESI-QTOF) calcd for C$_{20}$H$_{20}$O$_6$Se 437.0503 ([M + H]$^+$), found 437.0502.

5,6,7-trimethoxy-2-(3,4,5-trimethoxyphenyl)-4H-selenochromen-4-one (6d)

The title compound was prepared from 1d (30mg, 0.1mmol). Flash chromatography (Hexane/EtOAc/CH$_2$Cl$_2$ = 2:1:2) on silica gel gave 6d as a pale-yellow solid (13.96mg, 0.030mmol, 30% yield), mp 195-197 °C. $\textsuperscript{1}$H NMR (400 MHz, CDCl$_3$) $\delta$ 7.19 (s, 1H), 6.93 (s, 1H), 6.83 (s, 2H), 3.97 (d, $J = 3.3$ Hz, 6H), 3.93 (s, 9H), 3.91 (s, 3H); $\textsuperscript{13}$C NMR (100 MHz, CDCl$_3$) $\delta$ 182.9, 156.7, 156.2, 153.7, 149.1, 143.1, 140.0, 134.0, 133.2, 126.5, 120.9, 105.7, 104.2, 62.0, 61.4, 61.0, 56.3, 56.2; HRMS (ESI-QTOF) calcd for C$_{21}$H$_{22}$O$_7$Se 467.0609 ([M + H]$^+$), found 467.0605.

**NMR Spectra**

2-bromo-4,5-dimethoxybenzaldehyde (7b)
6-bromo-2,3,4-trimethoxybenzaldehyde (7d)
1-(2-bromophenyl)prop-2-yn-1-ol (8a)

S23
1-(2-bromo-4,5-dimethoxyphenyl)prop-2-yn-1-ol (8b)
1-(2-bromo-4,6-dimethoxyphenyl)prop-2-yn-1-ol (8c)
1-(6-bromo-2,3,4-trimethoxyphenyl)prop-2-yn-1-ol (8d)
1-(2-bromo-4-methylphenyl)prop-2-yn-1-ol (8e)
S27
1-(2-bromo-5-fluorophenyl)prop-2-yn-1-ol (8f)

S28
1-(2-bromo-5-(trifluoromethyl)phenyl)prop-2-yn-1-ol (8g)

S29
1-(2-bromophenyl)prop-2-yn-1-one (9a)

S30
1-(2-bromo-4,5-dimethoxyphenyl)prop-2-yn-1-one (9b)

S31
1-(6-bromo-2,3,4-trimethoxyphenyl)prop-2-yn-1-one (9d)

S33
1-(2-bromo-4-methylphenyl)prop-2-yn-1-one (9e)

S34
1-(2-bromo-5-fluorophenyl)prop-2-yn-1-one (9f)
S35
4H-selenochromen-4-one (1a)
S36
6,7-dimethoxy-4H-selenochromen-4-one (1b)

S37
6,7-dimethoxy-4H-selenochromen-4-one (1b)

5,7-dimethoxy-4H-selenochromen-4-one (1c)

S38
5,6,7-trimethoxy-4H-selenochromen-4-one (1d)

S39
7-methyl-4H-selenochromen-4-one (1e)

S40
1a
7-methyl-4H-selenochromen-4-one

H₂C—\text{Se}—\text{H}²

1b
7-methyl-4H-selenochromen-4-one

H₂C—\text{Se}—\text{H}²

6-fluoro-4H-selenochromen-4-one (1f)

S41
6-(trifluoromethyl)-4H-chromen-4-one ($1g$)
2-(3,4-dimethoxyphenyl)-4H-selenochromen-4-one (4a)

S43
2-(3,5-dimethoxyphenyl)-4H-selenochromen-4-one (4c)
2-(3-methoxyphenyl)-4H-selenochromen-4-one (4e)

S47
2-(p-tolyl)-4H-selenochromen-4-one (4g)

S49
2-(4-(tert-butyl)phenyl)-4H-selenochromen-4-one (4h)

S50
2-(4-chlorophenyl)-4H-selenochromen-4-one (4i)

SS1
2-(4-fluorophenyl)-4H-selenochromen-4-one (4j)

S52
2-(4-(trifluoromethyl)phenyl)-4H-selenochromen-4-one (4k)
2-(4-nitrophenyl)-4H-selenochromen-4-one (4l)
4-(4-oxo-4H-selenochromen-2-yl)benzonitrile (4m)

S55
2-(pyrid-3-yl)-4H-selenochromen-4-one (4n)
2-(thiophen-2-yl)-4H-selenochromen-4-one (4o)
2-(thiophen-2-yl)-4H-selenochromen-4-one (4p)

S58
2-phenyl-4H-selenochromen-4-one (5a)
S59
6,7-dimethoxy-2-phenyl-4H-selenochromen-4-one (5b)

S60
7-methyl-2-phenyl-4H-selenochromen-4-one (5c)

S61
6-fluoro-2-phenyl-4H-selenochromen-4-one (5d)
S62
2-phenyl-6-(trifluoromethyl)-4H-selenchromen-4-one (5e)

S63
2-(3,4-dimethoxyphenyl)-6,7-dimethoxy-4H-selenochromen-4-one (6a)
S64
2-(3,4-dimethoxyphenyl)-5,7-dimethoxy-4H-selenochromen-4-one (6b)

S65
2-(3,4-dimethoxyphenyl)-5,6,7-trimethoxy-4H-selenochromen-4-one (6c)
5,6,7-trimethoxy-2-(3,4,5-trimethoxyphenyl)-4H-selenochromen-4-one (6d)
5,6,7-trimethoxy-2-(3,4,5-trimethoxyphenyl)-4H-selenochromen-4-one