SUPPORTING INFORMATION

Synthesis of 4-(Organoselenyl) Oxazolones via Cyclization of N-Alkynyl Ethylcarbamates Promoted by Organoselenium

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Materials and Methods

Proton nuclear magnetic resonance spectra (¹H NMR) were obtained on a NMR spectrometer at 400 MHz. Spectra were recorded in CDCl₃ solutions. Chemical shifts are reported in ppm, referenced to the solvent peak of CDCl₃ or tetramethylsilane (TMS) as the external reference. Data are reported as follows: chemical shift (δ), multiplicity, coupling constant (J) in Hertz and integrated intensity. Carbon-13 nuclear magnetic resonance spectra (¹³C NMR) were obtained on a 400 NMR spectrometer at 100 MHz. Spectra were recorded in CDCI₃ solutions. Chemical shifts are reported in ppm, referenced to the solvent peak of CDCl₃. Abbreviations to denote the multiplicity of a particular signal are s (singlet), d (doublet), t (triplet), quart (quartet), quint (quintet), sex (sextet), dd (double doublet) and m (multiplet). The ⁷⁷Se NMR experiment was carried out using capillary tube with diphenyl diselenide as internal reference. High resolution mass spectra were recorded on a mass spectrometer using electrospray ionization (ESI). Column chromatography was performed using Silica Gel (230-400 mesh). Thin layer chromatography (TLC) was performed using Gel GF254, 0.25 mm thickness. For visualization, TLC plates were either placed under ultraviolet light, or stained with iodine vapor, or acidic vanillin. Most reactions were monitored by TLC for disappearance of starting material. The following solvents were dried and purified by distillation from the reagents indicated: tetrahydrofuran from sodium with a benzophenone ketyl indicator. All other solvents were ACS or HPLC grade unless otherwise noted. Air and moisture-sensitive reactions were conducted in flame-dried or oven dried glassware equipped with tightly fitted rubber septa and under a positive atmosphere of dry nitrogen or argon. Reagents and solvents were handled using standard syringe techniques.

X-ray diffraction analysis

Data were collected on a Bruker D8 Venture Photon 100 diffractometer equipped with an Incoatec IµS high brilliance Mo-Kα X-ray tube with two-dimensional Montel micro-focusing optics. The structure was solved by direct methods using SHELXS.¹ Subsequent Fourier-difference map analyses yielded the positions of the non-hydrogen atoms. Refinements were carried out with the SHELXL package.² All refinements were made by full-matrix least-squares on F2 with anisotropic displacement parameters for all non–hydrogen atoms. Hydrogen atoms were included in the refinement in calculated positions but the atoms (of hydrogens) that are commenting performing special bond were located in the Fourier map. Drawings were done using ORTEP 3.1 for Windows [Y] Crystal data and more details of the data collection and refinements of the compounds can are presented in Table T1.

Single crystal of **2e** was obtained by controlled evaporation of temperature (20 - 25 $^{\circ}$ C) over a period of three days. The mixture used for such recrystallization was CH₂Cl₂ / MeOH in a ratio of 25/75%. Single crystal was colorless and tabular habit.



Figure F1. Projection of the molecular structure of the compound **2e**. Thermal ellipsoids with 50% probability level.

Supplementary data

CCDC 2151577 contain the supplementary crystallographic data for molecule 2e.

These data can be obtained free of charge via http://www.ccdc.cam.ac.uk/conts/retrieving.html, or from the Cambridge Crystallographic Data Centre, 12 Union Road, Cambridge CB2 1EZ, UK; fax: (+44) 1223–336–033; or e-mail: deposit@ccdc.cam.ac.uk

Complex	Molecule 2e
Empirical formula	C ₂₁ H ₁₄ CINO ₂ Se
Formula weight	426.74
Temperature (K)	100(2)
Wavelength	0.71073
Crystal system	Monoclinic
Space group	P21/c
<i>a</i> (Å)	14.6927(6)
b (Å)	6.0979(2)
<i>c</i> (Å)	20.1721(8)
α (°)	90
β (°)	104.3330(10)
γ (°)	90
Volume (Å ³)	1751.06(12)
Z	4
Calculated density (mg.m ⁻³)	1.619
Absorption coefficient (nm ⁻¹)	2.312
F (000)	856
Crystal size (mm)	0.39 × 0.20 × 0.13
Theta range for data collection (°)	2.08 to 28.34
Limiting indices	$-19 \le h \le 19, -6 \le k \le 8, -26 \le l \le 26$
Reflections collected	59681
Reflections unique	4362
Completeness to theta	99.8%
Absorption correction	Semi-empirical from equivalents
Max./Min Transmission	0.7631 and 0.4758

 Table T1. Crystal data and structure refinement for the molecule 2e.

Data / restraints / parameters	4362 / 0 / 235
Goodness-of-fit on <i>F</i> ²	1.062
Índice <i>R</i> int	0.0226
Final R indices R_1 and $wR_2[I>2\sigma(I)]$	0.0178/0.0466
R indices (all data) R_1 and wR_2	0.0195/0.0479
Largest diff. peak (e ⁻ Å ⁻³) and hole	0.351 – 0.402

Characterization Data for the Compounds Prepared

General procedure for the preparation of 4-(organoselenyl) oxazolones 2a-ae: In a Schlenke flask, under air atmosphere, at room temperature *N*-alkynyl ethylcarbamates (0.25 mmol) was added to a solution of iodine (1.2 equiv) and diorganyl diselenides (0.55 equiv) in nitromethane (3 mL), which was prepared 30 min before. After that, the reaction was stirred at 80 °C until the starting material had been fully consumed (1.5 h to 7.5 h; monitored by TLC). The reaction was diluted with ethyl acetate (10 mL), washed with a saturated solution of Na₂S₂O₃ (10 mL). The organic phase was separated, dried over MgSO₄, and concentrated under a vacuum. The residue was purified by flash chromatography. **5-Phenyl-4-(phenylselanyl)-3-(***p***-tolyl)oxazol-2(3***H***)-one (2a):³ The product was isolated by column chromatography (hexane:ethyl acetate 95:5) as a white solid. Yield: 0.095 g (93%); mp 119-121 °C. ¹H NMR (CDCl₃, 400 MHz): \delta (ppm) 8.02 (d,** *J* **= 7.1 Hz, 2H), 7.42-7.34 (m, 3H), 7.15-7.10 (m, 7H), 6.99 (d,** *J* **= 8.3 Hz, 2H), 2.33 (s, 3H). ¹³C{¹H} NMR (CDCl₃. 100 MHz): \delta (ppm) 153.6, 143.8, 138.7, 130.9, 130.3, 129.5, 129.4, 129.2, 129.0, 128.5, 127.8, 127.6, 127.3, 125.9, 109.6, 21.1. MS (EI, 70 eV;** *m/z* **(relative intensity)): 408 ([M+1], 6), 407 (28), 194 (18), 165 (18), 105 (100), 77 (29).**

5-Phenyl-4-(phenylselanyl)-3-(*m***-tolyl)oxazol-2(3***H***)-one (2b): The product was isolated by column chromatography (hexane:ethyl acetate 95:5) as a yellow solid. Yield: 0.085 g (84%); mp 129-130 °C. ¹H NMR (CDCl₃, 400 MHz): δ (ppm) 8.05-8.02 (m, 2H), 7.43-7.35 (m, 3H), 7.23-7.12 (m, 7H), 6.93 (d, J = 7.8 Hz, 1H), 6.82 (s, 1H), 2.23 (s, 3H). ¹³C{¹H} NMR (CDCl₃. 100 MHz): δ (ppm) 153.5, 143.7, 138.9, 133.3, 130.6, 129.5, 129.4, 129.1, 129.0, 128.7, 128.6, 128.5, 127.7, 127.2, 125.9, 125.1, 109.6, 21.05. MS (EI, 70 eV;** *m/z* **(relative intensity)): 408 ([M+1], 5), 407 (19), 194 (11), 165 (09), 105 (100), 77 (39). HRMS calcd for C₂₂H₁₈NO₂Se (ESI-TOF, [M + H]⁺): 408.0503. Found: 408.0510.**

5-Phenyl-4-(phenylselanyl)-3-(*o***-tolyl)oxazol-2(3***H***)-one (2c): The product was isolated by column chromatography (hexane:ethyl acetate 95:5) as a yellow solid. Yield: 0.083 g (82%); mp 122-124 °C. ¹H NMR (CDCl₃, 400 MHz): δ (ppm) 8.10-8.08 (m, 2H), 7.45-7.41 (m, 2H), 7.38-7.34 (m, 1H), 7.29-7.06 (m, 8H), 6.92 (d, J = 6.5 Hz, 1H), 1.93 (s, 3H). ¹³C{¹H} NMR (CDCl₃. 100 MHz): δ (ppm) 152.8, 143.4, 137.3, 132.2, 131.7, 130.7, 129.5, 129.4, 129.3, 129.0, 128.5, 128.2, 128.0, 127.3, 126.3, 125.8, 110.2, 17.3. MS (EI, 70 eV;** *m/z* **(relative intensity)): 408 ([M+1], 3), 407 (14), 194 (07), 165 (07), 105 (100), 77 (40). HRMS calcd for C₂₂H₁₈NO₂Se (ESI-TOF, [M + H]⁺): 408.0503. Found: 408.0495.**

3-(4-Methoxyphenyl)-5-phenyl-4-(phenylselanyl)oxazol-2(3*H***)-one (2d):³ The product was isolated by column chromatography (hexane:ethyl acetate 90:10) as a white solid. Yield: 0.093 g (88%); mp 126-128 °C. ¹H NMR (CDCl₃, 400 MHz): \delta (ppm) 8.03-8.01 (m, 2H), 7.42-7.35 (m, 3H), 7.20-7.12 (m, 5H), 7.00 (d,** *J* **= 9.0 Hz, 2H), 6.82 (d,** *J* **= 8.9 Hz, 2H), 3.77 (s, 3H). ¹³C{¹H} NMR (CDCl₃. 100 MHz): \delta (ppm) 159.6, 153.7, 143.6, 130.4, 129.5, 129.3, 129.0, 129.0, 128.5, 127.7, 127.2, 126.1, 125.9, 114.1, 109.9, 55.4. MS (EI, 70 eV;** *m/z* **(relative intensity)): 424 ([M+1], 5), 423 (20), 207 (24), 165 (17), 105 (100), 77 (36).**

3-(4-Chlorophenyl)-5-phenyl-4-(phenylselanyl)oxazol-2(3*H***)-one (2e):³ The product was isolated by column chromatography (hexane:ethyl acetate 95:5) as a white solid. Yield: 0.074 g (70%); mp 161-163 °C. ¹H NMR (CDCl₃, 400 MHz): \delta (ppm) 8.03-8.00 (m, 2H), 7.43-7.37 (m, 3H), 7.29 (d,** *J* **= 8.8 Hz, 2H), 7.23-7.12 (m, 5H), 7.06 (d,** *J* **= 8.7 Hz, 2H). ¹³C{¹H} NMR**

(CDCl₃. 100 MHz): δ (ppm) 153.2, 144.2, 134.6, 132.0, 130.5, 129.6, 129.3, 129.1, 128.7, 128.6, 127.9, 127.0, 126.1. ⁷⁷Se NMR (77 MHz, in CDCl₃ with diphenyl diselenide as external reference) δ (ppm) 271.0. MS (EI, 70 eV; *m/z* (relative intensity)): 429 ([M+2], 7), 427 (16), 207 (38), 165 (18), 105 (100), 77 (38).

5-Phenyl-4-(phenylselanyl)-3-(3-(trifluoromethyl)phenyl)oxazol-2(3*H***)-one (2f):³ The product was isolated by column chromatography (hexane:ethyl acetate 95:5) as a white solid. Yield: 0.094 g (82%); mp 117-119 °C. ¹H NMR (CDCl₃, 400 MHz): δ (ppm) 8.05-8.00 (m, 2H), 7.58 (d, J = 7.8 Hz, 1H), 7.44-7.36 (m, 6H), 7.24-7.07 (m, 5H). ¹³C{¹H} NMR (CDCl₃. 100 MHz): δ (ppm) 153.1, 144.2, 134.0, 131.4 (q, J = 33.2 Hz), 131.3, 130.7, 129.6, 129.5, 129.4, 128.6, 128.3, 128.1, 126.9, 126.1, 125.3 (q, J = 3.6 Hz), 125.10 (q, J = 3.9 Hz), 123.27 (q, J = 272.8 Hz), 109.0. ¹⁹F NMR (235 MHz, in CDCl₃): δ (ppm) -62.8. MS (EI, 70 eV;** *m/z* **(relative intensity)): 462 ([M+1], 6), 461 (25), 248 (20), 165 (17), 105 (100), 77 (33).**

3-Benzyl-5-phenyl-4-(phenylselanyl)oxazol-2(3*H***)-one (2g): The product was isolated by column chromatography (hexane:ethyl acetate 95:5) as a white solid. Yield: 0.081 g (80%); mp 100-102 °C. ¹H NMR (CDCl₃, 400 MHz): \delta (ppm) 7.95-7.93 (m, 2H), 7.38-7.30 (m, 3H), 7.27-7.16 (m, 10H), 4.82 (s, 2H). ¹³C{¹H} NMR (CDCl₃. 100 MHz): \delta (ppm) 154.6, 144.2, 135.9, 129.8, 129.3, 129.0, 128.9, 128.5, 128.4, 127.8, 127.7, 127.4, 127.2, 125.8, 107.8, 46.3. MS (EI, 70 eV;** *m/z* **(relative intensity)): 408 ([M+1], 7), 407 (30), 315 (12), 157 (14), 105 (100), 77 (59). HRMS calcd for C₂₂H₁₈NO₂Se (ESI-TOF, [M + H]⁺): 408.0503. Found: 408.0507.**

5-Phenyl-3-(*p***-tolyl)-4-**(*o***-tolylselanyl)oxazol-2(3***H***)-one (2h):** The product was isolated by column chromatography (hexane:ethyl acetate 95:05) as a white solid. Yield: 0.069 g (66%); mp 135-137 °C. ¹H NMR (CDCl₃, 400 MHz): δ (ppm) 8.00-7.98 (m, 2H), 7.42-7.32 (m, 3H), 7.13-7.02 (m, 5H), 7.02-6.95 (m, 3H), 2.33 (s, 3H), 2.08 (s, 3H). ¹³C{¹H} NMR (CDCl₃. 100 MHz): δ (ppm) 153.7, 144.1, 138.7, 137.8, 130.8, 130.4, 129.9, 129.8, 129.5, 129.0, 128.5, 127.6, 127.5, 127.2, 127.0, 125.8, 109.1, 21.3, 21.1. MS (EI, 70 eV; *m/z* (relative intensity)): 422 ([M+1], 3), 421 (15), 251 (12), 207 (22), 105 (100), 77 (41). HRMS calcd for C₂₃H₂₀NO₂Se (ESI-TOF, [M + H]⁺): 422.0659. Found: 422.0665.

5-Phenyl-3-(*p***-tolyl)-4-(***p***-tolylselanyl)oxazol-2(3***H***)-one (2i):³ The product was isolated by column chromatography (hexane:ethyl acetate 95:05) as a white solid. Yield: 0.067 g (64%); mp 157-159 °C. ¹H NMR (CDCl₃, 400 MHz): δ (ppm) 8.05-8.03 (m, 2H), 7.43-7.33 (m, 3H), 7.14 (d,** *J* **= 8.6 Hz, 2H), 7.03-6.96 (m, 6H), 2.36 (s, 3H), 2.27 (s, 3H). ¹³C{¹H} NMR (CDCl₃. 100 MHz): δ (ppm) 153.6, 143.5, 138.7, 137.8, 130.9, 130.6, 130.2, 129.5, 129.0, 128.5, 127.8, 127.3, 125.9, 125.4, 109.9, 21.2, 21.0. MS (EI, 70 eV;** *m/z* **(relative intensity)): 422 ([M+1], 5), 421 (22), 208 (23), 179 (11), 105 (100), 77 (25).**

4-((4-Methoxyphenyl)selanyl)-5-phenyl-3-(*p***-tolyl)oxazol-2(3***H***)-one (2j):³ The product was isolated by column chromatography (hexane:ethyl acetate 91:9) as a yellow solid. Yield: 0.062 g (57%); mp 131-133 °C. ¹H NMR (CDCl₃, 400 MHz): δ (ppm) 8.07-8.04 (m, 2H), 7.45-7.40 (m, 2H), 7.38-7.34 (m, 1H), 7.16 (d,** *J* **= 7.9 Hz, 2H), 7.01 (d,** *J* **= 9.1 Hz, 4H), 6.67 (d,** *J* **= 8.9 Hz, 2H), 3.73 (s, 3H), 2.37 (s, 3H). ¹³C{¹H} NMR (CDCl3. 100 MHz): δ (ppm) 159.7, 153.6, 142.9, 138.7, 133.3, 131.0, 129.5, 128.9, 128.5, 127.9, 127.4, 125.9, 118.7, 115.0, 110.7, 55.2, 21.1. MS (EI, 70 eV;** *m/z* **(relative intensity)): 438 ([M+2], 4), 437 (15), 357 (15), 224 (29), 105 (100), 77 (35).**

4-((4-Chlorophenyl)selanyl)-5-phenyl-3-(*p***-tolyl)oxazol-2(3***H***)-one (2k):³ The product was isolated by column chromatography (hexane:ethyl acetate 93:7) as a white solid. Yield: 0.041 g (37%); mp 179-181 °C. ¹H NMR (CDCl₃, 400 MHz): δ (ppm) 8.01-7.99 (m, 2H), 7.44-7.37 (m, 3H), 7.17-7.13 (m, 4H), 7.06-7.04 (m, 2H), 7.00 (d,** *J* **= 8.3 Hz, 2H), 2.37 (s, 3H). ¹³C{¹H} NMR (CDCl₃. 100 MHz): δ (ppm) 153.5, 144.0, 139.0, 134.1, 131.8, 130.8, 129.6, 129.3, 128.6, 127.8, 127.2, 127.1, 126.0, 109.2, 21.2. MS (EI, 70 eV;** *m/z* **(relative intensity)): 443 ([M+2], 12), 441 (27), 438 (13), 228 (12), 105 (100), 77 (29).**

4-((4-Fluorophenyl)selanyl)-5-phenyl-3-(*p***-tolyl)oxazol-2(3***H***)-one (2l)**:³ The product was isolated by column chromatography (hexane:ethyl acetate 94:6) as a white solid. Yield: 0.065 g (61%); mp 162-164 °C. ¹H NMR (CDCl₃, 400 MHz): δ (ppm) 8.03-8.01 (m, 2H), 7.45-7.37 (m, 3H), 7.16 (d, *J* = 7.9 Hz, 2H), 7.09-7.05 (m, 2H), 7.00 (d, *J* = 8.3 Hz, 2H), 6.85 (t, *J* = 8.7 Hz, 2H), 2.37 (s, 3H). ¹³C{¹H} NMR (CDCl₃. 100 MHz): δ (ppm) 162.6 (d, *J* = 248.7 Hz), 153.5, 143.4, 138.9, 133.2 (d, *J* = 8.0 Hz), 130.8, 129.6, 129.1, 128.6, 127.8, 127.1, 126.0, 123.3 (d, *J* = 3.4 Hz), 116.6 (d, *J* = 21.9 Hz), 109.9, 21.1. ¹⁹F NMR (235 MHz, in CDCl₃): δ (ppm) -113.0. MS (EI, 70 eV; *m/z* (relative intensity)): 426 ([M+2], 4), 425 (17), 207 (20), 105 (100), 89 (17), 77 (28).

5-Phenyl-3-(*p*-tolyl)-4-((3-(trifluoromethyl)phenyl)selanyl)oxazol-2(3*H*)-one (2m): The product was isolated by column chromatography (hexane:ethyl acetate 93:7) as a white solid. Yield: 0.084 g (71%); mp 151-153 °C. ¹H NMR (CDCl₃, 400 MHz): δ (ppm) 8.00-7.97 (m, 2H), 7.46-7.36 (m, 5H), 7.30-7.24 (m, 2H), 7.12 (d, *J* = 7.8 Hz, 2H), 6.97 (d, *J* = 8.4 Hz, 2H), 2.34 (s, 3H). ¹³C{¹H} NMR (CDCl₃. 100 MHz): δ (ppm) 153.4, 143.9, 139.1, 134.3, 131.5 (q, *J* = 32.4 Hz), 130.5, 129.8, 129.7, 129.6, 129.3, 128.6, 127.8 (q, *J* = 3.8 Hz), 127.7, 126.9, 126.0, 124.7 (q, *J* = 3.7 Hz), 123.2 (q, *J* = 272.8 Hz), 109.1, 21.0. ¹⁹F NMR (235 MHz, in CDCl₃): δ (ppm) - 62.9. MS (EI, 70 eV; *m/z* (relative intensity)): 476 ([M+1], 4), 475 (16), 262 (06), 207 (16), 105 (100), 77 (31). HRMS calcd for C₂₃H₁₇F₃NO₂Se (ESI-TOF, [M + H]⁺): 476.0377. Found: 476.0381.

4-(ButyIseIanyI)-5-phenyI-3-(*p***-tolyI)oxazol-2(3***H***)-one (2n):³ The product was isolated by column chromatography (hexane:ethyl acetate 95:5) as a yellow solid. Yield: 0.059 g (61%); mp 69-71 °C. ¹H NMR (CDCl₃, 400 MHz): δ (ppm) 8.03-8.00 (m, 2H), 7.43-7.39 (m, 2H), 7.35-7.31 (m, 1H), 7.29 (s, 4H), 2.44-2.40 (m, 5H), 1.40 (quint,** *J* **= 7.3 Hz, 2H), 1.17 (sext,** *J* **= 7.3 Hz, 2H), 0.72 (t,** *J* **= 7.3 Hz, 3H). ¹³C{¹H} NMR (CDCl3. 100 MHz): δ (ppm) 153.8, 142.7, 138.8, 131.2, 129.7, 128.6, 128.4, 127.7, 127.6, 125.9, 109.0, 31.4, 29.3, 22.3, 21.1, 13.2. MS (EI, 70 eV;** *m/z* **(relative intensity)): 389 ([M+2], 5), 387 (25), 331 (11), 251 (11), 207 (23), 105 (100).**

5-(4-Methoxyphenyl)-4-(phenylselanyl)-3-(*p***-tolyl)oxazol-2(3***H***)-one (20):³ The product was isolated by column chromatography (hexane:ethyl acetate 90:10) as a yellow solid. Yield: 0.032 g (30%); mp 155-157 °C. ¹H NMR (CDCl₃, 400 MHz): \delta (ppm) 7.96 (d,** *J* **= 9.0 Hz, 2H), 7.20-7.12 (m, 7H), 7.00 (d,** *J* **= 8.3 Hz, 2H), 6.94 (d,** *J* **= 9.0 Hz, 2H), 3.83 (s, 3H), 2.34 (s, 3H). ¹³C{¹H} NMR (CDCl₃. 100 MHz): \delta (ppm) 160.3, 153.7, 144.3, 138.7, 131.0, 130.1, 129.6, 129.5, 129.4, 127.8, 127.6, 127.5, 119.8, 114.0, 107.6, 55.3, 21.1. MS (EI, 70 eV;** *m/z* **(relative intensity)): 438 ([M+1], 4), 437 (15), 357 (10), 194 (18), 135 (100), 77 (16).**

5-(4-Chlorophenyl)-4-(phenylselanyl)-3-(*p***-tolyl)oxazol-2(3***H***)-one (2p): The product was isolated by column chromatography (hexane:ethyl acetate 95:5) as a white solid. Yield: 0.067 g (61%); mp 189-191 °C. ¹H NMR (CDCl₃, 400 MHz): \delta (ppm) 7.98 (d,** *J* **= 8.7 Hz, 2H), 7.39**

(d, J = 8.7 Hz, 2H), 7.25-7.13 (m, 7H), 6.99 (d, J = 8.3 Hz, 2H), 2.36 (s, 3H). ¹³C{¹H} NMR (CDCl₃. 100 MHz): δ (ppm) 153.4, 142.8, 138.9, 135.0, 130.8, 130.4, 129.6, 128.9, 127.9, 127.8, 127.1, 125.8, 110.2, 21.2. MS (EI, 70 eV; *m/z* (relative intensity)): 443 ([M+2], 8), 441 (18), 194 (15), 139 (100), 11 (28), 77 (12). HRMS calcd for C₂₂H₁₇CINO₂Se (ESI-TOF, [M + H]⁺): 442.0113. Found: 442.0119.

5-Phenyl-3-(o-tolyl)-4-(o-tolylselanyl)oxazol-2(3*H***)-one (2t): The product was isolated by column chromatography (hexane:ethyl acetate 95:5) as a yellow solid. Yield: 0.086 g (82%); mp 111-113 °C. ¹H NMR (CDCl₃, 400 MHz): δ (ppm) 8.08-8.06 (m, 2H), 7.46-7.32 (m, 3H), 7.28-7.22 (m, 1H), 7.18-6.99 (m, 5H), 6.97-6.90 (m, 1H), 6.86 (dd, J = 7.8, 1.4 Hz, 1H), 1.93 (m, 6H). ¹³C{¹H} NMR (CDCl₃. 100 MHz): δ (ppm) 152.9, 143.6, 139.2, 137.3, 132.1, 131.8, 130.7, 130.2, 129.4, 129.2, 128.9, 128.9, 128.5, 128.1, 127.2, 126.8, 126.3, 125.6, 109.9, 21.5, 17.3. MS (EI, 70 eV;** *m/z* **(relative intensity)): 422 ([M+1], 6), 421 (24), 251 (11), 207 (23), 105 (100), 77 (41). HRMS calcd for C₂₃H₂₀NO₂Se (ESI-TOF, [M + H]⁺): 422.0659. Found: 422.0670.**

4-((4-Fluorophenyl)selanyl)-5-phenyl-3-(o-tolyl)oxazol-2(3*H***)-one (2u): The product was isolated by column chromatography (hexane:ethyl acetate 95:5) as a yellow solid. Yield: 0.069 g (65%); mp 119-121 °C. ¹H NMR (CDCl₃, 400 MHz): \delta (ppm) 8.09-8.07 (m, 2H), 7.47-7.36 (m, 3H), 7.32-7.28 (m, 1H), 7.19-7.15 (m, 2H), 7.03-6.95 (m, 3H), 6.81 (t,** *J* **= 8.7 Hz, 2H), 1.91 (s, 3H). ¹³C{¹H} NMR (CDCl₃. 100 MHz): \delta (ppm) 162.8 (d,** *J* **= 248.9 Hz), 152.7, 143.0, 137.3, 134.5 (d,** *J* **= 8.1 Hz), 132.1, 130.8, 129.5, 129.4, 129.1, 128.6, 127.2, 126.3, 125.8, 122.4 (d,** *J* **= 3.2 Hz), 116.45 (d,** *J* **= 21.8 Hz), 110.3, 17.3. ¹⁹F NMR (235 MHz, in CDCl₃): \delta (ppm) -62.9. MS (EI, 70 eV;** *m/z* **(relative intensity)): 426 ([M+1], 4), 425 (16), 207 (11), 183 (05), 105 (100), 77 (37). HRMS calcd for C₂₂H₁₇FNO₂Se (ESI-TOF, [M + H]⁺): 426.0409. Found: 426.0415.**

5-Phenyl-3-(o-tolyl)-4-((3-(trifluoromethyl)phenyl)selanyl)oxazol-2(3*H***)-one (2v): The product was isolated by column chromatography (hexane:ethyl acetate 95:5) as a yellow solid. Yield: 0.038 g (32%); mp 101-103 °C. ¹H NMR (CDCl₃, 400 MHz): \delta (ppm) 8.07-8.04 (m, 2H), 7.49-7.13 (m, 10H), 6.94 (d,** *J* **= 7.3 Hz, 1H), 1.93 (s, 3H). ¹³C{¹H} NMR (CDCl₃. 100 MHz): \delta (ppm) 152.7, 143.8, 137.1, 135.3, 131.9, 131.5 (q,** *J* **= 32.7 Hz), 130.9, 129.8, 129.7, 129.3, 129.2, 129.1, 128.7, 127.8 (q,** *J* **= 3.8 Hz), 127.0, 126.4, 125.9, 125.1 (q,** *J* **= 3.7 Hz), 123.2 (q,** *J* **= 272.9 Hz), 109.4, 17.4. ¹⁹F NMR (235 MHz, in CDCl₃): \delta (ppm) -62.9. MS (EI, 70 eV;** *m/z* **(relative intensity)): 476 ([M+1], 4), 475 (17), 281 (06), 207 (19), 105 (100), 77 (31). HRMS calcd for C₂₃H₁₇F₃NO₂Se (ESI-TOF, [M + H]⁺): 476.0377. Found: 476.0383.**

3-(4-Methoxyphenyl)-5-phenyl-4-(o-tolyIselanyl)oxazol-2(3H)-one (2w): The product was isolated by column chromatography (hexane:ethyl acetate 91:09) as a yellow solid. Yield: 0.097 g (89%); mp 97-99 °C. ¹H NMR (CDCl₃, 400 MHz): δ (ppm) 8.01-7.98 (m, 2H), 7.42-7.32 (m, 3H), 7.13-6.97 (m, 6H), 6.79 (d, J = 9.0 Hz, 2H), 3.76 (s, 3H), 2.08 (s, 3H). ¹³C{¹H} NMR (CDCl₃. 100 MHz): δ (ppm) 159.6, 153.8, 143.9, 137.9, 130.4, 130.0, 129.8, 129.1, 129.0, 128.5, 127.6, 127.2, 127.0, 126.1, 125.8, 114.1, 109.5, 55.4, 21.3. MS (EI, 70 eV; *m/z* (relative intensity)): 438 ([M+1], 8), 437 (31), 267 (13), 223 (23), 105 (100), 77 (40). HRMS calcd for C₂₃H₂₀NO₃Se (ESI-TOF, [M + H]⁺): 438.0608. Found: 438.0617.

3-(4-Methoxyphenyl)-4-((4-methoxyphenyl)selanyl)-5-phenyloxazol-2(3H)-one (2x): The product was isolated by column chromatography (hexane:ethyl acetate 88:12) as a yellow solid. Yield: 0.052 g (46%); mp 115-117 °C. ¹H NMR (CDCl₃, 400 MHz): δ (ppm) 8.07-8.04 (m, 2H), 7.45-7.35 (m, 3H), 7.03-7.00 (m, 4H), 6.86 (d, J = 9.1 Hz, 2H), 6.68 (d, J = 8.9 Hz, 2H),

3.81 (s, 3H), 3.74 (s, 3H). ¹³C{¹H} NMR (CDCl₃. 100 MHz): δ (ppm) 159.7, 159.6, 153.8, 142.7, 133.4, 129.4, 128.9, 128.5, 127.4, 126.2, 125.9, 118.6, 115.0, 114.1, 111.0, 55.5, 55.2. MS (EI, 70 eV; *m/z* (relative intensity)): 453 (10), 373 (07), 240 (26), 105 (100), 89 (23), 77 (48). HRMS calcd for C₂₃H₂₀NO₄Se (ESI-TOF, [M + H]⁺): 454.0558. Found: 454.0555.

4-((4-Fluorophenyl)selanyl)-3-(4-methoxyphenyl)-5-phenyloxazol-2(3H)-one (2y): The product was isolated by column chromatography (hexane:ethyl acetate 90:10) as a white solid. Yield: 0.085 g (77%); mp 146-148 °C. ¹H NMR (CDCl₃, 400 MHz): δ (ppm) 8.03-8.01 (m, 2H), 7.45-7.35 (m, 3H), 7.09-7.00 (m, 4H), 6.87-6.84 (m, 4H), 3.80 (s, 3H). ¹³C{¹H} NMR (CDCl₃. 100 MHz): δ (ppm) 162.5 (d, J = 248.7 Hz), 159.6, 153.6, 143.2, 133.2 (d, J = 8.0 Hz), 129.3, 129.1, 128.5, 127.1, 126.0, 125.9, 123.2 (d, J = 3.6 Hz), 116.6 (d, J = 22.0 Hz), 114.1, 110.2, 55.4. ⁷⁷Se NMR (77 MHz, in CDCl₃): δ (ppm) -112.9. MS (EI, 70 eV; *m/z* (relative intensity)): 442 ([M+1], 5), 441 (22), 228 (12), 207 (08), 105 (100), 77 (40). HRMS calcd for C₂₂H₁₇FNO₃Se (ESI-TOF, [M + H]⁺): 442.0358. Found: 442.0364.

3-(4-Chlorophenyl)-5-phenyl-4-(o-tolylselanyl)oxazol-2(3H)-one (2z): The product was isolated by column chromatography (hexane:ethyl acetate 94:06) as a yellow solid. Yield: 0.081 g (74%); mp 147-149 °C. ¹H NMR (CDCl₃, 400 MHz): δ (ppm) 7.99-7.97 (m, 2H), 7.44-7.36 (m, 3H), 7.27-7.25 (m, 2H), 7.14-7.02 (m, 6H), 2.10 (s, 3H). ¹³C{¹H} NMR (CDCl₃. 100 MHz): δ (ppm) 153.3, 144.5, 137.9, 134.5, 131.9, 130.6, 129.9, 129.5, 129.3, 129.1, 129.0, 128.6, 127.8, 127.1, 126.9, 125.9, 108.6, 21.3. ⁷⁷Se NMR (77 MHz, in CDCl₃ with diphenyl diselenide as external reference) δ (ppm) 238.6. MS (EI, 70 eV; *m/z* (relative intensity)): 443 ([M+1], 9), 442 (05), 271 (16), 227 (19), 105 (100), 77 (42). HRMS calcd for C₂₂H₁₇CINO₂Se (ESI-TOF, [M + H]⁺): 442.0113. Found: 442. 0117.

3-(4-Chlorophenyl)-4-((4-methoxyphenyl)selanyl)-5-phenyloxazol-2(3*H***)-one (2aa): The product was isolated by column chromatography (hexane:ethyl acetate 90:10) as a yellow solid. Yield: 0.074 g (65%); mp 106-108 °C. ¹H NMR (CDCl₃, 400 MHz): \delta (ppm) 8.05-8.02 (m, 2H), 7.44-7.38 (m, 3H), 7.32 (d,** *J* **= 8.7 Hz, 2H), 7.07 (d,** *J* **= 8.7 Hz, 2H), 6.99 (d,** *J* **= 8.9 Hz, 2H), 6.67 (d,** *J* **= 8.9 Hz, 2H), 3.73 (s, 3H). ¹³C{¹H} NMR (CDCl₃. 100 MHz): \delta (ppm) 159.8, 153.2, 143.1, 134.4, 133.4, 132.0, 129.3, 129.1, 129.0, 128.5, 127.1, 126.0, 118.2, 115.1, 110.1, 55.2. ⁷⁷Se NMR (77 MHz, in CDCl₃ with diphenyl diselenide as external reference) \delta (ppm) 260.9. MS (EI, 70 eV;** *m/z* **(relative intensity)): 459 ([M+2], 8), 457 (17), 377 (12), 244 (28), 105 (100), 77 (52). HRMS calcd for C₂₂H₁₇CINO₃Se (ESI-TOF, [M + H]⁺): 458.0062. Found: 458.0065.**

3-(4-Chlorophenyl)-4-((4-fluorophenyl)selanyl)-5-phenyloxazol-2(3*H***)-one (2ab): The product was isolated by column chromatography (hexane:ethyl acetate 94:06) as a white solid. Yield: 0.085 g (77%); mp 147-149 °C. ¹H NMR (CDCl₃, 400 MHz): \delta (ppm) 8.02-7.99 (m, 2H), 7.45-7.39 (m, 3H), 7.32 (d,** *J* **= 8.8 Hz, 2H), 7.08-7.05 (m, 4H), 6.86 (t,** *J* **= 8.7 Hz, 2H). ¹³C{¹H} NMR (CDCl₃. 100 MHz): \delta (ppm) 162.6 (d,** *J* **= 249.3 Hz), 153.1, 143.8, 134.6, 133.2 (d,** *J* **= 8.0 Hz), 131.9, 129.4, 129.3, 129.1, 128.6, 126.8, 126.0, 122.9 (d,** *J* **= 3.3 Hz), 116.8 (d,** *J* **= 21.5 Hz), 109.4. ⁷⁷Se NMR (77 MHz, in CDCl₃): \delta (ppm) -117.6. MS (EI, 70 eV;** *m/z* **(relative intensity)): 447 ([M+2], 7), 445 (17), 232 (11), 183 (10), 105 (100), 77 (42). HRMS calcd for C₂₁H₁₄CIFNO₂Se (ESI-TOF, [M + H]⁺): 445.9862. Found: 445.9870.**

5-Phenyl-4-(o-tolylselanyl)-3-(3-(trifluoromethyl)phenyl)oxazol-2(3*H***)-one (2ac): The product was isolated by column chromatography (hexane:ethyl acetate 95:5) as a white solid. Yield: 0.069 g (58%); mp 139-141 °C. ¹H NMR (CDCl₃, 400 MHz): \delta (ppm) 8.02-7.99 (m, 2H), 7.56 (d,** *J* **= 7.7 Hz, 1H), 7.45-7.32 (m, 6H), 7.11-6.97 (m, 4H), 2.05 (s, 3H). ¹³C{¹H} NMR (CDCl₃. 100 MHz): \delta (ppm) 153.2, 144.7, 138.1, 134.0, 131.3 (d,** *J* **= 33.7 Hz), 131.1, 130.6, 130.1, 129.5, 129.4, 129.0, 128.6, 128.0, 127.1, 126.8, 126.0, 125.3 (q,** *J* **= 3.7 Hz), 124.8 (q,** *J* **= 3.8 Hz), 123.2 (q,** *J* **= 272.8 Hz), 108.5, 21.2. ¹⁹F NMR (235 MHz, in CDCl₃): \delta (ppm) -62.8. MS (EI, 70 eV;** *m/z* **(relative intensity)): 475 (10), 305 (08), 261 (15), 105 (100), 89 (18), 77 (47). HRMS calcd for C₂₃H₁₇F₃NO₂Se (ESI-TOF, [M + H]⁺): 476.0377. Found: 476.0386.**

4-((2-Methoxyphenyl)selanyl)-5-phenyl-3-(3-(trifluoromethyl)phenyl)oxazol-2(3*H***)-one (2ad)**: The product was isolated by column chromatography (hexane:ethyl acetate 92:8) as a yellow solid. Yield: 0.050 g (41%); mp 119-121 °C. ¹H NMR (CDCl₃, 400 MHz): $\bar{0}$ (ppm) 8.01-7.98 (m, 2H), 7.57-7.55 (m, 1H), 7.46-7.36 (m, 6H), 7.24-7.18 (m, 1H), 7.04 (dd, *J* = 7.7, 1.6 Hz, 1H), 6.83 (td, *J* = 7.5, 1.2 Hz, 1H), 6.77 (dd, *J* = 8.2, 1.2 Hz, 1H), 3.69 (s, 3H). ¹³C{¹H} NMR (CDCl₃. 100 MHz): $\bar{0}$ (ppm) 156.7, 153.3, 145.4, 134.0, 131.2 (q, *J* = 33.2 Hz), 131.0, 129.5, 129.3, 129.2, 128.8, 128.5, 126.9, 126.1, 125.1 (q, *J* = 3.7 Hz), 124.7 (q, *J* = 3.8 Hz), 123.3 (q, *J* = 272.5 Hz), 122.0, 55.6. ¹⁹F NMR (235 MHz, in CDCl₃): $\bar{0}$ (ppm) -62.9. MS (EI, 70 eV; *m/z* (relative intensity)): 492 ([M+1], 6), 491 (22), 278 (08), 207 (12), 105 (100), 77 (46). HRMS calcd for C₂₃H₁₇F₃NO₃Se (ESI-TOF, [M + H]⁺): 492.0326. Found: 492.0338.

4-((4-Fluorophenyl)selanyl)-5-phenyl-3-(3-(trifluoromethyl)phenyl)oxazol-2(3H)-one

(2ae): The product was isolated by column chromatography (hexane:ethyl acetate 92:08) as a white solid. Yield: 0.088 g (74%); mp 131-133 °C. ¹H NMR (CDCl₃, 400 MHz): δ (ppm) 8.03-8.01 (m, 2H), 7.63-7.61 (m, 1H), 7.52-7.38 (m, 6H), 7.05-7.02 (m, 2H), 6.84 (t, *J* = 8.7 Hz, 2H). ¹³C{¹H} NMR (CDCl₃. 100 MHz): δ (ppm) 162.7 (d, *J* = 249.9 Hz), 153.0, 144.0, 134.0, 133.4 (d, *J* = 8.1 Hz), 131.5 (q, *J* = 33.7 Hz), 131.3, 129.6, 129.5, 128.7, 126.8, 126.1, 125.4 (q, *J* = 3.7 Hz), 125.1 (q, *J* = 3.8 Hz), 123.2 (q, *J* = 272.7 Hz), 122.6 (d, *J* = 3.1 Hz), 116.9 (d, *J* = 22.0 Hz), 109.2. ¹⁹F NMR (235 MHz, in CDCl₃): δ (ppm) -62.8, -112.2. MS (EI, 70 eV; *m/z* (relative intensity)): 480 ([M+1], 5), 479 (22), 266 (17), 183 (09), 105 (100), 77 (42). HRMS calcd for C₂₂H₁₄F₄NO₂Se (ESI-TOF, [M + H]⁺): 480.0126. Found: 480. 0129.

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994.



SPECTRA















 $^{19}\mathsf{F}$ NMR (235 MHz, in CDCl₃) for **2f.**





S22











 $^{19}\mathsf{F}$ NMR (235 MHz, in CDCl3) for **21.**



S28



 $^{19}\mathsf{F}$ NMR (235 MHz, in CDCl₃) for **2m.**













 $^{19}\mathsf{F}$ NMR (235 MHz, in CDCl_3) for 2u.





 $^{19}\mathsf{F}$ NMR (235 MHz, in CDCl_3) for 2v.









 $^{19}\mathsf{F}$ NMR (235 MHz, in CDCl₃) for **2y.**



S42



700 680 660 640 620 600 580 560 540 520 500 480 460 440 420 400 380 360 340 320 300 280 260 240 220 200 180 160 140







 ^{77}Se NMR (77 MHz, in CDCl3 with diphenyl diselenide as external reference) for **2aa**.



S46



 $^{19}\mathsf{F}$ NMR (235 MHz, in CDCl₃) for **2ab.**



S48



 $^{19}\mathsf{F}$ NMR (235 MHz, in CDCl₃) for **2ac.**





 $^{19}\mathsf{F}$ NMR (235 MHz, in CDCl₃) for **2ad.**





 $^{19}\mathsf{F}$ NMR (235 MHz, in CDCl₃) for **2ae.**

Scheme S1. Tested substrates that did not work

