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Supporting information for

Aerobic copper-mediated domino process for the synthesis of

3-(trifluoromethylseleno)indoles

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General information

¹H NMR, ¹⁹F NMR and ¹³C NMR spectra were recorded using Bruker AVIII 400 spectrometer. ¹H NMR and ¹³C NMR chemical shifts were reported in parts per million (ppm) downfield from tetramethylsilane and ¹⁹F NMR chemical shifts were determined relative to CFCl₃ as the external standard and low field is positive. Coupling constants (*J*) are reported in Hertz (Hz). The residual solvent peak was used as an internal reference: ¹H NMR (CDCl₃ δ 7.26), ¹³C NMR (CDCl₃ δ 77.0), The following abbreviations were used to explain the multiplicities: s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet, br = broad. [(bpy)CuSeCF₃]₂ (1)¹ and *N*-Ts 2-alkynylaniline derivatives^{2, 3} were prepared according to the published procedures. Solvents were freshly dried and degassed according to the published procedures prior to use.

General procedure for the synthesis of 3-((trifluoromethyl)selanyl)-1H-indole (3)



N-Ts 2-alkynylaniline derivatives **2** (0.20 mmol), $[(bpy)Cu(SeCF_3)]_2$ **1** (103.0 mg, 0.28 mmol based on Cu, 1.4 equiv), MeCN (2 mL) were added to a reaction tube equipped with a stir bar. The reaction mixture was stirred in air at 25 °C for 10 hours, then filtered through a pad of celite. The filtrate was concentrated by rotary evaporation and the residue was purified by column chromatography on silica gel with petroleum ether/ ethyl acetate.

Procedure for gram scale reaction for synthesis of 2-phenyl-1-tosyl-3-((trifluoromethyl)selanyl)-1*H*-indole (3a)



N-Ts 2-alkynylaniline **2a** (1.38 g, 4.00 mmol), $[(bpy)Cu(SeCF_3)]_2$ **1** (2.06 g, 5.60 mmol based on Cu, 1.4 equiv), MeCN (25 mL) were added to a round-bottomed flask equipped with a stir bar. The reaction mixture was stirred in air at 25 °C for 10 hours, then filtered through a pad of celite. The filtrate was concentrated by rotary evaporation and the residue was purified by column chromatography on silica gel with petroleum ether/ethyl acetate.

Procedures for derivatization of 3a

(a)



To a solution of **3a** (99.0 mg, 0.20 mmol) in MeOH (2 mL) was added KOH (336.0 mg, 6.00 mmol), and the mixture was refluxed for 4 h. To the mixture was added HCl (3.0 M, 2 mL), and the organic compounds were extracted with AcOEt. Organic layers were washed with brine and dried over Na₂SO₄. The solvents were filtered and evaporated under reduced pressure. The obtained residue was purified by column chromatography (petroleum ether/ethyl acetate = 8:1) to give **3a-6** as a white solid (65 mg, 95%).



To a stirred solution of indole **3a-6** (68.2 mg, 0.20 mmol) in dry DMF (2.0 mL) was added NaH (12.0 mg, 60% suspension in mineral oil, 0.30 mmol) under nitrogen atmosphere at room temperature and the resulting reaction mixture was stirred at r.t. for 1 h. CH₃I (19 μ L, 0.30 mmol) was added and then the reaction mixture was stirred overnight. The reaction was quenched with water (5 mL) and the aqueous layer was extracted with AcOEt. The combined organic layers were washed with brine, dried over anhydrous Na₂SO₄ and concentrated under reduced pressure. The residue was purified by column chromatography on silica gel (petroleum ether/ethyl acetate = 10:1) to give compound **3a-4** as a white solid (68.9 mg, 97% yield). **Control experiments**



In a nitrogen-filled glovebox, *N*-Ts 2-alkynylaniline **2a** (34.7 mg, 0.10 mmol), $[(bpy)Cu(SeCF_3)]_2$ **1** (51.5 mg, 0.14 mmol based on Cu, 1.4 equiv), MeCN (1 mL) were added to a reaction tube equipped with a stir bar. The reaction mixture was stirred at 25 °C for 10 hours under N₂ atmosphere. The resulting solution was filtered through a layer of celite and the filtrate was transferred to an NMR tube. An ¹⁹F NMR spectrum was acquired. The desired product **3a** was not detected. Instead, the yield of the the background 3-*H* indole by-product **3a'** was calculated to be 17%.



2-Phenyl-1-tosyl-1*H*-indole **3a'** (34.7 mg, 0.10 mmol), $[(bpy)Cu(SeCF_3)]_2$ **1** (51.5 mg, 0.14 mmol based on Cu, 1.4 equiv), and MeCN (1 mL) were added to a reaction tube equipped with a stir bar. The reaction mixture was stirred in air at 25 °C for 10 hours under air atmosphere. The resulting solution was filtered through a layer of celite and the filtrate was transferred to an NMR tube. An ¹⁹F NMR spectrum was acquired, and the desired product **3a** was not detected.



N-Ts 2-alkynylaniline **2a** (34.7 mg, 0.10 mmol), $[(bpy)Cu(SeCF_3)]_2$ **1** (51.5 mg, 0.14 mmol based on Cu, 1.4 equiv), TEMPO (31.2 mg, 0.20 mmol) or BHT (44.1 mg, 0.20 mmol), and MeCN (1 mL) were added to a reaction tube equipped with a stir bar. The reaction mixture was stirred at 25 °C for 10 h under air atmosphere. The resulting solution was filtered through a layer of celite and the filtrate was transferred to an NMR tube. An ¹⁹F NMR spectrum was acquired, and the yields of the desired product **3a** was calculated to be 86% and 90%, respectively.

Data for compounds 3



2-phenyl-1-tosyl-3-((trifluoromethyl)selanyl)-1*H*-indole (3a)

Obtained as a white solid in 89% yield (88.0 mg). Mp: 148.0–150.1 °C. R_f (petroleum ether/ethyl acetate = 8:1) = 0.60. ¹H NMR (400 MHz, CDCl₃) δ 8.37 (d, J = 8.0 Hz, 1H), 7.71 (d, J = 8.0 Hz, 1H), 7.52 – 7.38 (m, 5H), 7.34 (d, J = 8.0 Hz, 2H), 7.26 (d, J = 7.8 Hz, 2H), 7.11 (d, J = 8.0 Hz, 2H), 2.33 (s, 3H). ¹⁹F NMR (376 MHz, CDCl₃) δ -35.2 (s, 3F). ¹³C NMR (101 MHz, CDCl₃) δ 147.1 (s), 145.4 (s), 136.9 (s), 135.5 (s), 131.9 (s), 131.6 (s), 130.2 (s), 129.7 (s), 129.6 (s), 127.4 (s), 127.0 (s), 126.1 (s), 124.8 (s), 121.1 (s), 122.0 (q, J = 335.9 Hz), 115.8 (s), 104.5 (d, J = 1.5 Hz), 21.7 (s). IR (ATR): v 3054, 1596, 1487, 1445, 1376, 1303, 1264, 1220, 1189, 1177, 1128, 1085, 1037, 919, 831, 734, 697, 660, 569, 542 cm⁻¹. HRMS (ESI) m/z: calcd. for C₂₂H₁₅F₃NO₂SSe [M-H]⁻: 493.9946; found: 493.9946.



6-methyl-2-phenyl-1-tosyl-3-((trifluoromethyl)selanyl)-1*H*-indole (3b)

Obtained as a white solid in 87% yield (88.0 mg). Mp: 172.1–174.2 °C. R_f (petroleum ether/ethyl acetate = 8:1) = 0.73. ¹H NMR (400 MHz, CDCl₃) δ 8.19 (s, 1H), 7.58 (d, J = 8.0 Hz, 1H), 7.50 – 7.44 (m, 1H), 7.39 (t, J = 7.5 Hz, 2H), 7.33 (d, J = 8.3 Hz, 2H), 7.25 – 7.21 (m, 3H), 7.09 (d, J = 8.1 Hz, 2H), 2.55 (s, 3H), 2.31 (s, 3H). ¹⁹F NMR (376 MHz, CDCl₃) δ -35.2 (s, 3F). ¹³C NMR (101 MHz, CDCl₃) δ 146.4 (s), 145.3 (s), 137.3 (s), 136.4 (s), 135.6 (s), 131.9 (s), 130.3 (s), 129.6 (s), 129.5 (s), 104.4 (d, J = 127.3 (s), 127.0 (s), 126.3 (s), 122.0 (q, J = 335.9 Hz), 120.6 (s), 115.8 (s), 104.4 (d, J

= 1.7 Hz), 22.2 (s), 21.7 (s). IR (ATR): v 2919, 1597, 1494, 1380, 1293, 1260, 1179, 1083, 1035, 1017, 963, 922, 874, 809, 772, 735, 695, 576, 544 cm⁻¹. HRMS (ESI) m/z: calcd. for $C_{23}H_{17}F_3NO_2SSe$ [M-H]⁻: 508.0103; found: 508.0101.



5-methyl-2-phenyl-1-tosyl-3-((trifluoromethyl)selanyl)-1*H*-indole (3c)

Obtained as a white solid in 89% yield (91.0 mg). Mp: 112.1–114.6 °C. R_f (petroleum ether/ethyl acetate = 8:1) = 0.73. ¹H NMR (400 MHz, CDCl₃) δ 8.23 (d, J = 8.0 Hz, 1H), 7.51 – 7.46 (m, 2H), 7.41 (t, J = 7.5 Hz, 2H), 7.33 (d, J = 8.4 Hz 2H), 7.28 – 7.26 (m, 3H), 7.09 (d, J = 8.0 Hz, 2H), 2.48 (s, 3H), 2.31 (s, 3H). ¹⁹F NMR (376 MHz, CDCl₃) δ -35.2 (s, 3F). ¹³C NMR (101 MHz, CDCl₃) δ 147.2 (s), 145.3 (s), 135.5 (s), 135.2 (s), 134.6 (s), 131.9 (s), 131.8 (s), 130.3 (s), 129.6 (s), 129.6 (s), 127.6 (s), 127.3 (s), 127.0 (s), 122.0 (q, J = 335.9 Hz), 120.8 (s), 115.5 (s), 104.3 (q, J = 1.7 Hz), 21.7 (s), 21.5 (s). IR (ATR): v 2922, 1597, 1376, 1291, 1220, 1178, 1120, 1083, 1039, 919, 857, 808, 771, 736, 656, 580, 544 cm⁻¹. HRMS (ESI) m/z: calcd. for C₂₃H₁₈F₃NNaO₂SSe [M+Na]⁺: 532.0068; found: 532.0068.



methyl 2-phenyl-1-tosyl-3-((trifluoromethyl)selanyl)-1*H*-indole-5-carboxylate (3d)

Obtained as a white solid in 86% yield (95.0 mg). Mp: 202.4–203.1 °C. R_f (petroleum ether/ethyl acetate = 8:1) = 0.49. ¹H NMR (400 MHz, CDCl₃) δ 8.44 – 8.42 (m, 2H), 8.17 – 8.15 (m, 1H), 7.52 (t, J = 7.5 Hz, 1H), 7.43 (t, J = 7.5 Hz, 2H), 7.33 (d, J = 8.4

Hz, 2H), 7.25 (d, J = 6.8 Hz, 2H), 7.12 (d, J = 8.2 Hz, 2H), 3.97 (s, 3H), 2.34 (s, 3H). ¹⁹F NMR (376 MHz, CDCl₃) δ -35.2 (s, 3F). ¹³C NMR (101 MHz, CDCl₃) δ 167.0 (s), 148.4 (s), 145.8 (s), 139.5 (s), 135.2 (s), 131.9 (s), 131.5 (s), 129.9 (s), 129.8 (s), 129.6 (s), 127.4 (s), 127.2 (s), 127.1 (s), 126.9 (s), 123.2 (s), 121.9 (q, J = 335.8 Hz), 115.6 (s), 104.6 (d, J = 1.8 Hz), 52.4 (s), 21.7 (s). IR (ATR): v 2957, 1719, 1616, 1548, 1486, 1374, 1307, 1241, 1175, 1079, 1041, 985, 921, 777, 669, 577, 544 cm⁻¹. HRMS (ESI) m/z: calcd. for C₂₄H₁₇F₃NO₄SSe [M-H]⁻: 552.0001; found: 552.0005.





Obtained as a white solid in 87% yield (91.0 mg). Mp: 149.4–151.7 °C. R_f (petroleum ether/ ethyl acetate = 8:1) = 0.65. ¹H NMR (400 MHz, CDCl₃) δ 8.25 (d, J = 9.1 Hz, 1H), 7.52 – 7.46 (m, 1H), 7.42 (t, J = 7.5 Hz, 2H), 7.33 – 7.25 (m, 4H), 7.09 (m, 4H), 3.87 (s, 3H), 2.31 (s, 3H). ¹⁹F NMR (376 MHz, CDCl₃) δ -35.2 (s, 3F). ¹³C NMR (101 MHz, CDCl₃) δ 157.6 (s), 147.8 (s), 145.3 (s), 135.3 (s), 132.9 (s), 131.9 (s), 131.4 (s), 130.2 (s), 129.7 (s), 129.6 (s), 127.3 (s), 126.9 (s), 122.0 (q, J = 336.0 Hz), 116.9 (s), 115.3 (s), 104.5 (d, J = 1.8 Hz), 102.9 (s), 55.8 (s), 21.7 (s). IR (ATR): v 2937, 1611, 1581, 1469, 1374, 1264, 1206, 1189, 1170, 1127, 1085, 1033, 960, 921, 864, 801, 770, 735, 696, 585, 543 cm⁻¹. HRMS (ESI) m/z: calcd. for C₂₃H₁₇F₃NO₃SSe [M-H]⁻: 524.0052; found: 524.0048.



5-fluoro-2-phenyl-1-tosyl-3-((trifluoromethyl)selanyl)-1*H*-indole (3f)

Obtained as a white solid in 81% yield (83.0 mg). Mp: 190.6–192.8 °C. R_f (petroleum ether/ethyl acetate = 8:1) = 0.55. ¹H NMR (400 MHz, CDCl₃) δ 8.33 (dd, J = 9.2, 4.3 Hz, 1H), 7.51 (t, J = 7.3 Hz, 1H), 7.42 (t, J = 7.6 Hz, 2H), 7.35 (dd, J = 8.4, 2.7 Hz, 1H), 7.31 (d, J = 8.2 Hz, 2H), 7.28 – 7.23 (m, 2H), 7.18 (td, J = 9.1, 2.7 Hz, 1H), 7.11 (d, J = 8.1 Hz, 2H), 2.33 (s, 3H). ¹⁹F NMR (376 MHz, CDCl₃) δ -35.2 (s, 3F), -117.4 - -117.5 (m, 1F). ¹³C NMR (101 MHz, CDCl₃) δ 160.5 (d, J = 242.5 Hz), 148.8 (s), 145.6 (s), 135.2 (s), 133.2 (s), 133.1 (s), 133.0 (s), 131.9 (s), 129.9 (s), 129.8 (s), 129.7 (s), 127.4 (s), 127.1 (s), 121.9 (q, J = 335.8 Hz), 117.2 (d, J = 9.0 Hz), 114.1 (d, J = 25.3 Hz), 106.7 (d, J = 24.9 Hz), 21.71 (s). IR (ATR): v 2917, 1596, 1493, 1460, 1385, 1248, 1190, 1179, 1088, 1037, 1016, 921, 858, 808, 774, 696, 655, 583, 545 cm⁻¹. HRMS (ESI) m/z: calcd. for C₂₂H₁₄F₄NO₂SSe [M-H]⁻: 511.9852; found: 511.9852.



5-chloro-2-phenyl-1-tosyl-3-((trifluoromethyl)selanyl)-1H-indole (3g)

Obtained as a white solid in 66% yield (70 mg). Mp: 157.2–159.0 °C. R_f (petroleum ether/ethyl acetate = 8:1) = 0.60. ¹H NMR (400 MHz, CDCl₃) δ 8.30 (d, J = 8.9 Hz, 1H), 7.67 (d, J = 2.1 Hz, 1H), 7.51 (t, J = 7.4 Hz, 1H), 7.44 – 7.38 (m, 3H), 7.31 (d, J = 8.2 Hz, 2H), 7.24 (d, J = 7.5 Hz, 2H), 7.12 (d, J = 8.1 Hz, 2H), 2.35 (s, 3H). ¹⁹F NMR (376 MHz, CDCl₃) δ -35.2 (s, 3F). ¹³C NMR (101 MHz, CDCl₃) δ 148.5 (s), 145.8 (s), 135.3 (s), 135.2 (s), 133.0 (s), 131.9 (s), 130.8 (s), 129.9 (s), 129.8 (s), 129.7 (s), 127.4 (s), 127.1 (s), 126.4 (s), 121.9 (q, J = 336.0 Hz), 120.7 (s), 117.0 (s), 103.6 (d, J = 2.0 Hz), 21.8 (s). IR (ATR): v 3083, 1596, 1493, 1378, 1252, 1220, 954, 870, 845, 809, 772, 737, 698, 664, 577, 543 cm⁻¹. HRMS (ESI) m/z: calcd. for C₂₂H₁₅ClF₃NO₂SSe [M+H]⁺: 529.9702; found: 529.9702.



6-chloro-2-phenyl-1-tosyl-3-((trifluoromethyl)selanyl)-1H-indole (3h)

Obtained as a white solid in 86% yield (91.0 mg). Mp: 222.4–224.8 °C. R_f (petroleum ether/ethyl acetate = 8:1) = 0.66. ¹H NMR (400 MHz, CDCl₃) δ 8.42 (d, J = 1.8 Hz, 1H), 7.62 (d, J = 8.4 Hz, 1H), 7.50 (t, J = 7.4 Hz, 1H), 7.44 – 7.36 (m, 3H), 7.32 (d, J = 8.2 Hz, 2H), 7.23 – 7.19 (m, 2H), 7.13 (d, J = 8.2 Hz, 2H), 2.35 (s, 3H). ¹⁹F NMR (376 MHz, CDCl₃) δ -35.2 (s, 3F). ¹³C NMR (101 MHz, CDCl₃) δ 147.5 (s), 145.7 (s), 137.1 (s), 135.2 (s), 131.9 (s), 131.8 (s), 129.9 (s), 129.8 (s), 129.7 (s), 129.6 (s), 127.3 (s), 127.1 (s), 125.3 (s), 121.8 (q, J = 335.8 Hz), 121.7 (s), 115.8 (s), 103.9 (d, J = 2.0 Hz), 21.6 (s). IR (ATR): v 2961, 1596, 1487, 1376, 1283, 1189, 1174, 1130, 1086, 1038, 952, 810, 773, 735, 697, 662, 604, 572, 543 cm⁻¹. HRMS (ESI) m/z: calcd. for C₂₂H₁₄ClF₃NO₂SSe [M-H]⁻: 527.9554; found: 527.9554.



6-bromo-2-phenyl-1-tosyl-3-((trifluoromethyl)selanyl)-1*H*-indole (3i)

Obtained as a white solid in 79% yield (90.0 mg). Mp: 202.4–204.3 °C. R_f (petroleum ether/ethyl acetate = 8:1) = 0.61. ¹H NMR (400 MHz, CDCl₃) δ 8.58 (d, J = 1.6 Hz, 1H), 7.57 (d, J = 8.4 Hz, 1H), 7.54 – 7.48 (m, 2H), 7.41 (t, J = 7.7 Hz, 2H), 7.31 (d, J = 8.5 Hz, 2H), 7.21 (m, 2H), 7.13 (d, J = 8.1 Hz, 2H), 2.35 (s, 3H). ¹⁹F NMR (376 MHz, CDCl₃) δ -35.2 (s, 3F). ¹³C NMR (101 MHz, CDCl₃) δ 147.4 (s), 145.7 (s), 137.4 (s), 135.2 (s), 131.8 (s), 130.4 (s), 129.8 (s), 129.7 (s), 129.5 (s), 128.0 (s), 127.3 (s), 127.1 (s), 122.1 (s), 121.8 (q, J = 335.8 Hz), 119.7 (s), 118.6 (s), 103.9 (d, J = 2.0 Hz), 21.7. IR (ATR): v 2961, 1596, 1486, 1444, 1376, 1284, 1188, 1174, 1130,

1085, 1038, 943, 810, 773, 736, 662, 572, 543 cm⁻¹. HRMS (ESI) m/z: calcd. for C₂₂H₁₄BrF₃NO₂SSe [M-H]⁻: 571.9051; found: 571.9050.



2-(p-tolyl)-1-tosyl-3-((trifluoromethyl)selanyl)-1H-indole (3j)

Obtained as a white solid in 87% yield (100.0 mg). Mp: 159.3–160.4 °C. R_f (petroleum ether/ ethyl acetate = 8:1) = 0.67. ¹H NMR (400 MHz, CDCl₃) δ 8.36 (d, J = 8.3 Hz, 1H), 7.69 (d, J = 7.7 Hz, 1H), 7.47 – 7.42 (m, 1H), 7.41 – 7.38 (m, 1H), 7.35 (d, J = 8.4 Hz, 2H), 7.23 (d, J = 7.9 Hz, 2H), 7.16 (d, J = 8.0 Hz, 2H), 7.10 (d, J = 8.1 Hz, 2H), 2.46 (s, 3H), 2.32 (s, 3H). ¹⁹F NMR (376 MHz, CDCl₃) δ -35.2 (s, 3F). ¹³C NMR (101 MHz, CDCl₃) δ 147.4 (s), 145.4 (s), 139.7 (s), 136.9 (s), 135.4 (s), 131.8 (s), 131.7 (s), 129.6 (s), 128.1 (s), 127.2 (s), 127.0 (s), 125.9 (s), 124.8 (s), 122.0 (q, J = 335.9 Hz), 121.0 (s), 115.8 (s), 104.4 (d, J = 1.8 Hz), 21.7 (s), 21.6 (s). IR (ATR): v 2920, 1595, 1495, 1446, 1374, 1303, 1264, 1189, 1177, 1128, 1085, 1019, 935, 860, 820, 734, 703, 661, 645, 571, 540 cm⁻¹. HRMS (ESI) m/z: calcd. for C₂₃H₁₇F₃NO₂SSe [M-H]⁻: 508.0103; found: 508.0101.



2-(4-ethylphenyl)-1-tosyl-3-((trifluoromethyl)selanyl)-1*H*-indole (3k)

Obtained as a white solid in 80% yield (84.0 mg). Mp: 161.2–161.8 °C. R_f (petroleum ether/ethyl acetate = 8:1) = 0.73. ¹H NMR (400 MHz, CDCl₃) δ 8.36 (d, J = 8.3 Hz, 1H), 7.70 (d, J = 7.7 Hz, 1H), 7.47 – 7.43 (m, 1H), 7.41 – 7.37 (m, 1H), 7.33 (d, J = 8.4 Hz, 2H), 7.24 (d, J = 8.2 Hz, 2H), 7.18 (d, J = 8.2 Hz, 2H), 7.09 (d, J = 8.1 Hz,

2H), 2.77 (q, J = 7.6 Hz, 2H), 2.32 (s, 3H), 1.33 (t, J = 7.6 Hz, 3H). ¹⁹F NMR (376 MHz, CDCl₃) δ -35.2 (s, 3F). ¹³C NMR (101 MHz, CDCl₃) δ 147.5 (s), 145.8 (s), 145.3 (s), 136.9 (s), 135.5 (s), 131.9 (s), 131.7 (s), 129.6 (s), 127.3 (s), 127.1 (s), 126.8 (s), 125.9 (s), 124.7 (s), 122.0 (q, J = 335.9 Hz), 121.0 (s), 115.8 (s), 104.4 (d, J = 1.9 Hz), 28.9 (s), 21.7 (s), 15.3 (s). IR (ATR): v 2966, 1596, 1494, 1376, 1303, 1189, 1176, 1129, 1023, 1012, 935, 833, 812, 736, 702, 661, 642, 570, 541 cm⁻¹. HRMS (ESI) m/z: calcd. for C₂₄H₁₉F₃NO₂SSe [M-H]⁻: 522.0259; found: 522.0257.





Obtained as a white solid in 45% yield (63.0 mg). Mp: 121.7–123.3 °C. R_f (petroleum ether/ ethyl acetate = 8:1) = 0.62. ¹H NMR (400 MHz, CDCl₃) δ 8.38 (d, J = 8.3 Hz, 1H), 7.75 – 7.69 (m, 3H), 7.66 (d, J = 8.2 Hz, 2H), 7.51 – 7.45 (m, 3H), 7.44 – 7.39 (m, 2H), 7.38 – 7.32 (m, 4H), 7.11 (d, J = 8.2 Hz, 2H), 2.33 (s, 3H). ¹⁹F NMR (376 MHz, CDCl₃) δ -35.1 (s, 3F). ¹³C NMR (101 MHz, CDCl₃) δ 146.9 (s), 145.4 (s), 142.3 (s), 140.4 (s), 137.1 (s), 135.5 (s), 132.4 (s), 131.8 (s), 129.7 (s), 129.1 (s), 129.0 (s), 127.9 (s), 127.4 (s), 127.1 (s), 126.2 (s), 125.9 (s), 124.8 (s), 122.0 (q, J = 335.7 Hz), 121.1 (s), 115.9 (s), 104.7 (d, J = 1.6 Hz), 21.7 (s). IR (ATR): v 3031, 1723, 1567, 1484, 1377, 1306, 1221, 1188, 1175, 1125, 1083, 1086, 1007, 939, 834, 811, 768, 736, 697, 662, 569, 541 cm⁻¹. HRMS (ESI) m/z: calcd. for C₂₈H₁₉F₃NO₂SSe [M-H]⁻: 570.0259; found: 570.0258.



4-(1-tosyl-3-((trifluoromethyl)selanyl)-1*H*-indol-2-yl)benzonitrile (3m)

Obtained as a white solid in 70% yield (73.0 mg). Mp: 229.7–231.1 °C. R_f (petroleum ether/ethyl acetate = 8:1) = 0.47. ¹H NMR (400 MHz, CDCl₃) δ 8.35 (d, J = 8.4 Hz, 1H), 7.74 – 7.71 (m, 3H), 7.55 – 7.48 (m, 1H), 7.45 – 7.41 (m, 3H), 7.34 (d, J = 8.1 Hz, 2H), 7.15 (d, J = 8.1 Hz, 2H), 2.34 (s, 3H). ¹⁹F NMR (376 MHz, CDCl₃) δ -35.0 (s, 3F). ¹³C NMR (101 MHz, CDCl₃) δ 145.9 (s), 144.6 (s), 136.9 (s), 135.0 (s), 134.9 (s), 132.5 (s), 131.5 (s), 131.1 (s), 129.9 (s), 126.8 (s), 125.2 (s), 121.8 (q, J = 335.8 Hz), 121.3 (s), 118.5 (s), 115.8 (s), 113.4 (s), 105.6 (d, J = 1.8 Hz), 21.7 (s). IR (ATR): v 3068, 2227, 1608, 1597, 1490, 1447, 1375, 1309, 1248, 1174, 1085, 1012, 937, 848, 822, 817, 757, 679, 660, 628, 570, 541 cm⁻¹. HRMS (ESI) m/z: calcd. for C₂₃H₁₄F₃N₂O₂SSe [M-H]⁻: 518.9899; found: 518.9897.



4-(1-tosyl-3-((trifluoromethyl)selanyl)-1*H*-indol-2-yl)benzaldehyde (3n)

Obtained as a white solid in 87% yield (91.0 mg). Mp: 214.4–215.4 °C. R_f (petroleum ether/ethyl acetate = 8:1) = 0.31. ¹H NMR (400 MHz, CDCl₃) δ 10.13 (s, 1H), 8.36 (d, J = 8.4 Hz, 1H), 7.96 (d, J = 7.9 Hz, 2H), 7.72 (d, J = 7.8 Hz, 1H), 7.54 – 7.48 (m, 3H), 7.43 (t, J = 7.5 Hz, 1H), 7.36 (d, J = 8.1 Hz, 2H), 7.14 (d, J = 8.1 Hz, 2H), 2.34 (s, 3H). ¹⁹F NMR (376 MHz, CDCl₃) δ -35.0 (s, 3F). ¹³C NMR (101 MHz, CDCl₃) δ 191.9 (s), 145.8 (s), 145.4 (s), 136.9 (s), 136.8 (s), 136.4 (s), 135.0 (s), 132.6 (s), 131.6 (s), 129.9 (s), 128.6 (s), 126.9 (s), 126.6 (s), 125.1 (s), 121.9 (q, J = 335.8 Hz), 121.3 (s), 115.8 (s), 105.3 (d, J = 1.5 Hz), 21.7 (s). IR (ATR): v 3049, 2841, 1696, 1608, 1544, 1448, 1378, 1307, 1264, 1180, 1128, 1083, 1031, 980, 940, 834, 811, 735, 703, 658, 626, 569, 542 cm⁻¹. HRMS (ESI) m/z: calcd. for C₂₃H₁₅F₃NO₃SSe [M-H]⁻: 521.9895; found: 521.9894.



methyl 4-(1-tosyl-3-((trifluoromethyl)selanyl)-1H-indol-2-yl)benzoate (30)

Obtained as a white solid in 29% yield (32.0 mg). Mp: 224.9–225.8 °C. R_f (petroleum ether/ethyl acetate = 8:1) = 0.44. ¹H NMR (400 MHz, CDCl₃) δ 8.36 (d, J = 8.4 Hz, 1H), 8.11 (d, J = 8.3 Hz, 2H), 7.72 (d, J = 7.7 Hz, 1H), 7.51 – 7.46 (m, 1H), 7.44 – 7.40 (m, 1H), 7.38 – 7.33 (m, 4H), 7.13 (d, J = 8.2 Hz, 2H), 3.98 (s, 3H), 2.34 (s, 3H). ¹⁹F NMR (376 MHz, CDCl₃) δ -35.1 (s, 3F). ¹³C NMR (101 MHz, CDCl₃) δ 166.7 (s), 145.7 (s), 145.6 (s), 136.9 (s), 135.2 (s), 134.8 (s), 131.9 (s), 131.5 (s), 131.0 (s), 129.7 (s), 128.5 (s), 126.9 (s), 126.4 (s), 124.9 (s), 121.8 (q, J = 335.8 Hz), 121.1 (s), 115.7 (s), 104.9 (d, J = 1.8 Hz), 52.3 (s), 21.6 (s). IR (ATR): v 2951, 1721, 1611, 1596, 1493, 1446, 1378, 1307, 1275, 1176, 1085, 1023, 939, 860, 777, 704, 661, 571, 543 cm⁻¹. HRMS (ESI) m/z: calcd. for C₂₄H₁₇F₃NO₄SSe [M-H]⁻: 552.0001; found: 552.0002.



2-(4-nitrophenyl)-1-tosyl-3-((trifluoromethyl)selanyl)-1*H*-indole (3p)

Obtained as a yellow solid in 60% yield (65.0 mg). Mp: 229.6–231.5 °C. R_f (petroleum ether/ethyl acetate = 8:1) = 0.58. ¹H NMR (400 MHz, CDCl₃) δ 8.36 (d, J = 8.5 Hz, 1H), 8.31 (d, J = 8.6 Hz, 2H), 7.73 (d, J = 7.8 Hz, 1H), 7.55 – 7.49 (m, 3H), 7.44 (t, J = 7.5 Hz, 1H), 7.36 (d, J = 8.2 Hz, 2H), 7.16 (d, J = 8.1 Hz, 2H), 2.35 (s, 3H). ¹⁹F NMR (376 MHz, CDCl₃) δ -34.9 (s, 3F). ¹³C NMR (101 MHz, CDCl₃) δ 148.5 (s), 146.0 (s), 144.3 (s), 137.1 (s), 136.9 (s), 134.9 (s), 132.9 (s), 131.6 (s), 129.9 (s), 126.9 (s), 126.8 (s), 125.3 (s), 122.6 (s), 121.8 (q, J = 335.8 Hz), 121.4 (s),

115.8 (s), 105.8 (s), 21.8 (s). IR (ATR): v 2961, 1601, 1520, 1492, 1446, 1375, 1345, 1307, 1084, 1028, 938, 857, 812, 761, 737, 700, 661, 570, 542 cm⁻¹. HRMS (ESI) m/z: calcd. for C₂₂H₁₄F₃N₂O₄SSe [M-H]⁻: 538.9797; found: 538.9797.



2-(2-methoxyphenyl)-1-tosyl-3-((trifluoromethyl)selanyl)-1H-indole (3q)

Obtained as a white solid in 78% yield (82.0 mg). Mp: 164.2–165.4 °C. R_f (petroleum ether/ethyl acetate = 8:1) = 0.51. ¹H NMR (400 MHz, CDCl₃) δ 8.30 (d, J = 8.2 Hz, 1H), 7.72 (d, J = 7.7, 1H), 7.51 – 7.46 (m, 1H), 7.45 – 7.35 (m, 4H), 7.17 – 7.06 (m, 3H), 7.04 – 7.01 (m, 1H), 6.90 (d, J = 8.3 Hz, 1H), 3.59 (s, 3H), 2.32 (s, 3H). ¹⁹F NMR (376 MHz, CDCl₃) δ -35.0 (s, 3F). ¹³C NMR (101 MHz, CDCl₃) δ 158.5 (s), 144.9 (s), 143.6 (s), 136.7, 135.8 (s), 133.1 (s), 131.5 (s), 131.4 (s), 129.5 (s), 127.2 (s), 125.6 (s), 124.2 (s), 122.1 (q, J = 335.8 Hz), 120.8 (s), 119.5 (s), 119.4 (s), 115.1 (s), 110.2 (s), 104.1 (q, J = 1.7 Hz), 55.1 (s), 21.6 (s). IR (ATR): v 2941, 1596, 1546, 1485, 1444, 1376, 1306, 1256, 1176, 1128, 1083, 1048, 1024, 936, 811, 753, 736, 704, 658, 570, 543 cm⁻¹. HRMS (ESI) m/z: calcd. for C₂₃H₁₉F₃NO₃SSe [M+H]⁺: 526.0197; found: 526.0200.



2-(4-methoxyphenyl)-1-tosyl-3-((trifluoromethyl)selanyl)-1H-indole (3r)

Obtained as a yellow solid in 82% yield (86.0 mg). Mp: 186.6–188.7 °C. $R_{\rm f}$ (petroleum ether/ethyl acetate = 8:1) = 0.55. ¹H NMR (400 MHz, CDCl₃) δ 8.37 (d, J = 8.3 Hz, 1H), 7.69 (d, J = 7.7 Hz, 1H), 7.47 – 7.44 (m, 1H), 7.40 – 7.36 (m, 1H),

7.33 (d, J = 8.4 Hz, 2H), 7.19 (d, J = 8.7 Hz, 2H), 7.09 (d, J = 8.1 Hz, 2H), 6.94 (d, J = 8.8 Hz, 2H), 3.89 (s, 3H), 2.31 (s, 3H). ¹⁹F NMR (376 MHz, CDCl₃) δ -35.2 (s, 3F). ¹³C NMR (101 MHz, CDCl₃) δ 160.7 (s), 147.2 (s), 145.3 (s), 136.9 (s), 135.5 (s), 133.4 (s), 131.7 (s), 129.6 (s), 127.0 (s), 125.9 (s), 124.8 (s), 122.2 (s), 122.0 (q, J = 335.9 Hz), 120.9 (s), 115.9 (s), 112.8 (s), 104.4 (d, J = 1.6 Hz), 55.4 (s), 21.7 (s). IR (ATR): v 2963, 1612, 1554, 1446, 1376, 1305, 1244, 1188, 1176, 1126, 1084, 1024, 1007, 937, 833, 813, 735, 706, 659, 570, 541 cm⁻¹. HRMS (ESI) m/z: calcd. for C₂₃H₁₇F₃NO₃SSe [M-H]⁻: 524.0052; found: 524.0052.



2-(2-fluorophenyl)-1-tosyl-3-((trifluoromethyl)selanyl)-1*H*-indole (3s)

Obtained as a white solid in 88% yield (90.0 mg). Mp: 116.1–118.3 °C. R_f (petroleum ether/ethyl acetate = 8:1) = 0.57. ¹H NMR (400 MHz, CDCl₃) δ 8.32 (d, J = 8.3 Hz, 1H), 7.73 (d, J = 7.8 Hz, 1H), 7.54 – 7.35 (m, 5H), 7.27 – 7.22 (m, 2H), 7.17 – 7.12 (m, 3H), 2.32 (s, 3H). ¹⁹F NMR (376 MHz, CDCl₃) δ -35.0 (d, J = 2.9 Hz, 3F), -110.2 – -110.26 (m, 1F). ¹³C NMR (101 MHz, CDCl₃) δ 161.1 (d, J = 249.4 Hz), 145.6 (s), 140.6 (s), 136.1 (d, J = 148.3 Hz), 133.6 (s), 132.1 (d, J = 8.4 Hz), 131.4 (s), 129.8 (s), 127.1 (s), 126.3 (s), 124.7 (s), 123.3 (d, J = 3.6 Hz), 122.0 (q, J = 335.7 Hz), 121.1 (s), 118.8 (d, J = 15.2 Hz), 115.5 (s), 115.3 (s), 115.2 (s), 105.5 (s), 21.7 (s). IR (ATR): v 2962, 1595, 1482, 1376, 1309, 1250, 1177, 1127, 1084, 1035, 936, 809, 755, 659, 572, 545 cm⁻¹. HRMS (ESI) m/z: calcd. for C₂₂H₁₄F₄NO₂SSe [M-H]⁻: 511.9852; found: 511.9854.



2-(3-fluorophenyl)-1-tosyl-3-((trifluoromethyl)selanyl)-1H-indole (3t)

Obtained as a white solid in 83% yield (85.0 mg). Mp: 147.5–149.2 °C. R_f (petroleum ether/ethyl acetate = 8:1) = 0.72. ¹H NMR (400 MHz, CDCl₃) δ 8.36 (d, J = 8.4 Hz, 1H), 7.75 – 7.68 (m, 1H), 7.50 – 7.46 (m, 1H), 7.43 – 7.34 (m, 4H), 7.22 – 7.17 (m, 1H), 7.13 (d, J = 8.2 Hz, 2H), 7.10 – 7.08 (m, 1H), 6.95 – 6.92 (m, 1H), 2.34 (s, 3H). ¹⁹F NMR (376 MHz, CDCl₃) δ -35.1 (s, 3F), -113.5 – -113.6 (m, 1F). ¹³C NMR (101 MHz, CDCl₃) δ 161.7 (d, J = 246.6 Hz), 145.7 (s), 145.4 (s), 136.9 (s), 135.3 (s), 132.1 (d, J = 8.5 Hz), 131.4 (s), 129.8 (s), 128.9 (d, J = 8.3 Hz), 127.9 (d, J = 3.0 Hz), 127.0 (s), 126.4 (s), 124.9 (s), 121.9 (q, J = 335.8 Hz), 121.2 (s), 118.9 (d, J = 22.8 Hz), 116.7 (d, J = 20.9 Hz), 115.8 (s), 104.8 (d, J = 1.5 Hz), 21.7 (s). IR (ATR): v 2965, 1615, 1586, 1481, 1446, 1378, 1307, 1264, 1176, 1125, 1085, 1033, 912, 876, 790, 736, 701, 660, 570, 540 cm⁻¹. HRMS (ESI) m/z: calcd. for C₂₂H₁₄F₄NO₂SSe [M-H]⁻: 511.9852; found: 511.9850.



2-(4-fluorophenyl)-1-tosyl-3-((trifluoromethyl)selanyl)-1*H*-indole (3u)

Obtained as a white solid in 81% yield (83.0 mg). Mp: 199.6–201.2 °C. R_f (petroleum ether/ethyl acetate = 8:1) = 0.69. ¹H NMR (400 MHz, CDCl₃) δ 8.37 (d, J = 8.3 Hz, 1H), 7.71 (d, J = 7.8 Hz, 1H), 7.49 – 7.45 (m, 1H), 7.43 – 7.38 (m, 1H), 7.33 (d, J = 8.1 Hz, 2H), 7.26 – 7.21 (m, 2H), 7.15 – 7.07 (m, 4H), 2.33 (s, 3H). ¹⁹F NMR (376 MHz, CDCl₃) δ -35.2 (s, 3F), -110.7 – -110.8 (m, 1F). ¹³C NMR (101 MHz, CDCl₃) δ 163.6 (d, J = 250.0 Hz), 145.9 (s), 145.6 (s), 136.9 (s), 135.5 (s), 133.8 (d, J = 8.5 Hz),

131.5 (s), 129.8 (s), 126.9 (s), 126.3 (s), 126.1 (d, J = 3.5 Hz), 124.9 (s), 121.9 (q, J = 335.7 Hz), 121.1 (s), 115.8 (s), 114.6 (d, J = 21.9 Hz), 104.8 (s), 21.7 (s). IR (ATR): v 2961, 1606, 1554, 1497, 1445, 1374, 1302, 1264, 1223, 1177, 1085, 1002, 934, 840, 759, 736, 702, 663, 570, 540 cm⁻¹. HRMS (ESI) m/z: calcd. for C₂₂H₁₄F₄NO₂SSe [M-H]⁻: 511.9852; found: 511.9852.



2-(4-chlorophenyl)-1-tosyl-3-((trifluoromethyl)selanyl)-1*H*-indole (3v)

Obtained as a white solid in 80% yield (85.0 mg). Mp: 169.4–171.2 °C. R_f (petroleum ether/ethyl acetate = 8:1) = 0.64. ¹H NMR (400 MHz, CDCl₃) δ 8.36 (d, J = 8.5 Hz, 1H), 7.71 (d, J = 7.8 Hz, 1H), 7.50 – 7.45 (m, 1H), 7.43 – 7.38 (m, 3H), 7.34 (d, J = 8.4 Hz, 2H), 7.23 – 7.19 (m, 2H), 7.12 (d, J = 8.2 Hz, 2H), 2.33 (s, 3H). ¹⁹F NMR (376 MHz, CDCl₃) δ -35.1 (s, 3F). ¹³C NMR (101 MHz, CDCl₃) δ 145.8 (d, J = 1.5 Hz), 145.7 (s), 136.9 (s), 135.9 (s), 135.4 (s), 133.2 (s), 131.6 (s), 129.8 (s), 128.6 (s), 127.8 (s), 126.9 (s), 126.4 (s), 124.9 (s), 121.9 (q, J = 335.8 Hz), 121.2 (s), 115.8 (s), 104.9 (q, J = 1.6 Hz), 21.7 (s). IR (ATR): v 2924, 1596, 1483, 1445, 1373, 1304, 1264, 1174, 1120, 1081, 1012, 936, 831, 736, 721, 660, 568, 541 cm⁻¹. HRMS (ESI) m/z: calcd. for C₂₂H₁₄ClF₃NO₂SSe [M-H]⁻: 527.9557; found: 527.9556.



2-(4-bromophenyl)-1-tosyl-3-((trifluoromethyl)selanyl)-1H-indole (3w)

Obtained as a white solid in 82% yield (94.0 mg). Mp: 170.0–171.8 °C. R_f (petroleum ether/ethyl acetate = 8:1) = 0.64. ¹H NMR (400 MHz, CDCl₃) δ 8.36 (d, J = 8.3 Hz,

1H), 7.70 (d, J = 7.8 Hz, 1H), 7.56 (d, J = 8.4 Hz, 2H), 7.50 – 7.45 (m, 1H), 7.43 – 7.39 (m, 1H), 7.34 (d, J = 8.4 Hz, 2H), 7.16 – 7.11 (m, 4H), 2.33 (s, 3H). ¹⁹F NMR (376 MHz, CDCl₃) δ -35.1 (s, 3F). ¹³C NMR (101 MHz, CDCl₃) δ 145.8 (s), 145.7 (s), 136.9 (s), 135.3 (s), 133.4 (s), 131.6 (s), 130.7 (s), 129.8 (s), 129.1 (s), 126.9 (s), 126.4 (s), 124.9 (s), 121.9 (q, J = 335.9 Hz), 121.2 (s), 115.8 (s), 104.9 (s), 21.7 (s). IR (ATR): v 2951, 1596, 1482, 1377, 1306, 1250, 1189, 1175, 1125, 1083, 1067, 1009, 938, 828, 750, 736, 660, 568, 541 cm⁻¹. HRMS (ESI) m/z: calcd. for C₂₂H₁₄BrF₃NO₂SSe [M-H]⁻: 571.9051; found: 571.9049.



2-(pyridin-2-yl)-1-tosyl-3-((trifluoromethyl)selanyl)-1*H*-indole (3x)

Obtained as a white solid in 84% yield (83.0 mg). Mp: 182.7–183.5 °C. R_f (petroleum ether/ethyl acetate = 3:1) = 0.54. ¹H NMR (400 MHz, CDCl₃) δ 8.73 (d, J = 4.5 Hz, 1H), 8.18 (d, J = 8.3 Hz, 1H), 7.87 – 7.82 (m, 1H), 7.79 (d, J = 8.1 Hz, 2H), 7.72 (d, J = 7.8 Hz, 1H), 7.60 (d, J = 7.7 Hz, 1H), 7.47 – 7.29 (m, 3H), 7.19 (d, J = 8.1 Hz, 2H), 2.31 (s, 3H). ¹⁹F NMR (376 MHz, CDCl₃) δ -34.9 (s, 3F). ¹³C NMR (101 MHz, CDCl₃) δ 150.3 (s), 148.7 (s), 145.5 (s), 145.1 (s), 136.0 (s), 135.8 (s), 135.0 (s), 131.4 (s), 129.8 (s), 127.6 (s), 127.5 (s), 126.3 (s), 124.7 (s), 124.1 (s), 122.1 (q, J = 335.8 Hz), 121.3 (s), 115.1 (s), 104.5 (s), 21.7 (s). IR (ATR): v 3052, 1594, 1447, 1264, 1178, 1126, 1086, 1052, 940, 813, 795, 733, 703, 658, 571, 543 cm⁻¹. HRMS (ESI) m/z: calcd. for C₂₁H₁₄F₃N₂O₂SSe [M-H]⁻: 494.9898; found: 494.9898.



2-(pyridin-3-yl)-1-tosyl-3-((trifluoromethyl)selanyl)-1*H*-indole (3y)

Obtained as a white solid in 72% yield (71.0 mg). Mp: 166.5–168.9 °C. R_f (petroleum ether/ethyl acetate = 3:1) = 0.36. ¹H NMR (400 MHz, CDCl₃) δ 8.73 (d, J = 5.0 Hz, 1H), 8.39 – 8.37 (m, 2H), 7.77 (d, J =7.8, 1H), 7.73 (d, J = 7.8 Hz, 1H), 7.51 (t, J = 7.4 Hz, 1H), 7.45 – 7.41 (m, 2H), 7.32 (d, J = 8.2 Hz, 2H), 7.14 (d, J = 8.1 Hz, 2H), 2.33 (s, 3H). ¹⁹F NMR (376 MHz, CDCl₃) δ -35.2 (s, 3F). ¹³C NMR (101 MHz, CDCl₃) δ 151.0 (s), 150.3 (s), 145.9 (s), 143.2 (s), 139.9 (s), 137.1 (s), 135.2 (s), 131.4 (s), 129.9 (s), 126.9 (s), 126.8 (s), 126.7 (s), 125.1 (s), 122.5 (s), 121.8 (q, J = 335.8 Hz), 121.3 (s), 115.7 (s), 105.8 (d, J = 1.7 Hz), 21.7 (s). IR (ATR): v 3034, 1596, 1445, 1379, 1307, 1264, 1177, 1085, 1064, 937, 882, 812, 753, 706, 660, 569, 542 cm⁻¹. HRMS (ESI) m/z: calcd. for C₂₁H₁₄F₃N₂O₂SSe [M-H]⁻: 494.9899; found: 494.9899.



2-(thiophen-2-yl)-1-tosyl-3-((trifluoromethyl)selanyl)-1*H*-indole (3z)

Obtained as a yellow solid in 76% yield (76.0 mg). Mp: 144.4–146.6 °C. R_f (petroleum ether/ethyl acetate = 8:1) = 0.71. ¹H NMR (400 MHz, CDCl₃) δ 8.36 (d, J = 8.5 Hz, 1H), 7.70 (d, J = 7.7 Hz, 1H), 7.55 (dd, J = 4.9, 1.5 Hz, 1H), 7.49 – 7.45 (m, 1H), 7.43 – 7.37 (m, 3H), 7.16 – 7.09 (m, 4H), 2.33 (s, 3H). ¹⁹F NMR (376 MHz, CDCl₃) δ -35.1 (s, 3F). ¹³C NMR (101 MHz, CDCl₃) δ 145.5 (s), 139.5 (s), 137.3 (s), 135.3 (s), 133.0 (s), 131.4 (s), 129.7 (s), 129.5 (s), 129.3 (s), 127.1 (s), 126.5 (s), 126.5 (s), 124.8 (s), 121.9 (q, J = 335.9 Hz), 121.2 (s), 115.8 (s), 107.1 (d, J = 1.9 Hz), 21.7 (s). IR (ATR): v 3051, 1596, 1568, 1445, 1375, 1307, 1264, 1175, 1116, 1085, 1043, 1021, 985, 933, 858, 808, 734, 701, 663, 570, 539 cm⁻¹. HRMS (ESI) m/z: calcd. for C₂₀H₁₃F₃NO₂S₂Se [M-H]⁻: 499.9510; found: 499.9510.



2-(thiophen-3-yl)-1-tosyl-3-((trifluoromethyl)selanyl)-1*H*-indole (3aa)

Obtained as a white solid in 86% yield (86.0 mg). Mp: 175.7–177.9 °C. R_f (petroleum ether/ethyl acetate = 8:1) = 0.71. ¹H NMR (400 MHz, CDCl₃) δ 8.37 (d, J = 8.3 Hz, 1H), 7.69 (d, J = 7.8 Hz, 1H), 7.50 – 7.43 (m, 1H), 7.41 – 7.31 (m, 4H), 7.23 (d, J = 3.5 Hz, 1H), 7.14 – 7.07 (m, 3H), 2.32 (s, 3H). ¹⁹F NMR (376 MHz, CDCl₃) δ -35.3 (s, 3F). ¹³C NMR (101 MHz, CDCl₃) δ 145.4 (s), 142.2 (s), 137.1 (s), 135.4 (s), 131.5 (s), 131.1 (s), 129.7 (s), 129.6 (s), 129.0 (s), 126.9 (s), 126.1 (s), 124.7 (s), 124.2 (s), 122.0 (q, J = 335.7 Hz), 121.0 (s), 115.7 (s), 104.9 (d, J = 1.8 Hz), 21.7 (s). IR (ATR): v 2925, 1595, 1571, 1445, 1371, 1306, 1264, 1174, 1087, 1021, 932, 910, 866, 790, 734, 719, 660, 645, 590, 566 cm⁻¹. HRMS (ESI) m/z: calcd. for C₂₀H₁₃F₃NO₂S₂Se [M-H]⁻: 499.9510; found: 499.9509.



2-(cyclohex-1-en-1-yl)-1-tosyl-3-((trifluoromethyl)selanyl)-1*H*-indole (3ab)

Obtained as a white solid in 44% yield (44.0 mg). Mp: 181.3–183.0 °C. R_f (petroleum ether/ethyl acetate = 8:1) = 0.70. ¹H NMR ¹H NMR (400 MHz, CDCl₃) δ 8.25 (d, J = 8.2 Hz, 1H), 7.66 – 7.58 (m, 3H), 7.40 – 7.30 (m, 2H), 7.15 (d, J = 8.2 Hz, 2H), 5.45 – 5.42 (m, 1H), 2.70 – 2.66 (m, 1H), 2.31 (s, 3H), 2.25 – 2.17 (m, 2H), 2.09 – 2.01 (m, 1H), 1.86 – 1.81 (m, 3H), 1.75 – 1.67 (m, 1H). ¹⁹F NMR (376 MHz, CDCl₃) δ -35.3 (s, 3F). ¹³C NMR (101 MHz, CDCl₃) δ 149.8 (s), 145.3 (s), 136.5 (s), 135.8 (s), 133.5 (s), 131.8 (s), 130.2 (s), 129.7 (s), 126.9 (s), 125.6 (s), 124.5 (s), 122.1 (q, J = 335.7 Hz), 121.0 (s), 115.3 (s), 102.5 (d, J = 1.7 Hz), 30.9 (s), 25.7 (s), 22.6 (s), 21.8 (s), 21.7 (s).

IR (ATR): v 2934, 1597, 1534, 1493, 1446, 1375, 1292, 1187, 1173, 1082, 1046, 1023, 941, 858, 811, 747, 703, 660, 570, 543 cm⁻¹. HRMS (ESI) m/z: calcd. for $C_{22}H_{19}F_3NO_2SSe [M-H]^-$: 498.0259; found: 498.0259.



2-cyclopropyl-1-tosyl-3-((trifluoromethyl)selanyl)-1H-indole (3ac)

Obtained as a white solid in 68% yield (62.0 mg). Mp: 101.5–102.8 °C. R_f (petroleum ether/ethyl acetate = 8:1) = 0.63. ¹H NMR (400 MHz, CDCl₃) δ 8.23 (d, J = 8.2 Hz, 1H), 7.66 (d, J = 8.2 Hz, 2H), 7.62 (d, J = 7.8 Hz, 1H), 7.40 – 7.29 (m, 2H), 7.21 (d, J = 8.1 Hz, 2H), 2.36 (s, 3H), 2.21 – 2.14 (m, 1H), 1.16 – 1.11 (m, 2H), 1.01 – 0.96 (m, 2H). ¹⁹F NMR (376 MHz, CDCl₃) δ -35.5 (s, 3F). ¹³C NMR (101 MHz, CDCl₃) δ 147.6 (s), 145.3 (s), 136.9 (s), 136.4 (s), 131.7 (s), 129.9 (s), 126.6 (s), 125.7 (s), 124.3 (s), 122.2 (q, J = 336.9 Hz), 120.5 (s), 115.0 (s), 102.6 (d, J = 1.9 Hz), 21.7 (s), 9.9 (s), 9.6 (s). IR (ATR): v 3015, 1597, 1539, 1494, 1448, 1371, 1307, 1263, 1224, 1190, 1169, 1120, 1084, 1044, 900, 830, 810, 737, 658, 569, 541 cm⁻¹. HRMS (ESI) m/z: calcd. for C₁₉H₁₅F₃NO₂SSe [M-H]⁻: 457.9946; found: 457.9947.



2-(3-chloropropyl)-1-tosyl-3-((trifluoromethyl)selanyl)-1*H*-indole (3ad)

Obtained as a white solid in 33% yield (33.0 mg). Mp: 139.5–141.1 °C. R_f (petroleum ether/ ethyl acetate = 8:1) = 0.74. ¹H NMR (400 MHz, CDCl₃) δ 8.18 – 8.14 (m, 1H), 7.65 – 7.56 (m, 3H), 7.38 – 7.30 (m, 2H), 7.19 (d, J = 8.0 Hz, 2H), 3.64 (t, J = 6.3 Hz, 2H), 3.51 – 3.43 (m, 2H), 2.33 (s, 3H), 2.29 – 2.20 (m, 2H). ¹⁹F NMR (376 MHz,

CDCl₃) δ -35.5 (s, 3F). ¹³C NMR (101 MHz, CDCl₃) δ 147.5 (s), 145.6 (s), 136.8 (s), 135.6 (s), 131.6 (s), 130.2 (s), 126.4 (s), 125.7 (s), 124.7, 122.1 (q, *J* = 335.8 Hz), 120.7 (s), 115.2 (s), 103.8 (s), 44.6 (s), 33.6 (s), 26.3 (s), 21.7 (s). IR (ATR): v 2960, 1597, 1448, 1372, 1307, 1175, 1132, 1087, 1072, 1023, 973, 937, 809, 746, 703, 657, 598, 568 cm⁻¹. HRMS (ESI) m/z: calcd. for C₁₉H₁₈ClF₃NO₂SSe [M+H]⁺: 495.9859; found: 495.9860.



2-phenyl-3-((trifluoromethyl)selanyl)-1-((trifluoromethyl)sulfonyl)-1*H*-indole (3a-1)

Obtained as a white solid in 48% yield (45 mg). Mp: 134.4–136.6 °C. R_f (petroleum ether/ethyl acetate = 10:1) = 0.59. ¹H NMR (400 MHz, CDCl₃) δ 8.11 – 8.04 (m, 1H), 7.83 – 7.81 (m, 1H), 7.58 – 7.45 (m, 5H), 7.39 – 7.37 (m, 2H). ¹⁹F NMR (376 MHz, CDCl₃) δ -34.5 (s, 3F), -73.9 (s, 3F). ¹³C NMR (101 MHz, CDCl₃) δ 147.3 (s), 136.4 (s), 131.5 (s), 130.2 (s), 129.0 (s), 128.1 (s), 127.8 (s), 127.2 (s), 126.3 (s), 121.9 (q, *J* = 335.5 Hz), 121.8, 119.6 (q, *J* = 325.5 Hz), 115.4 (s), 107.9 (s). IR (ATR): v 1555, 1490, 1450, 1414, 1206, 1137, 1118, 1080, 943, 923, 829, 779, 766, 756, 695, 679, 631, 606, 575 cm⁻¹. HRMS (ESI) m/z: calcd. for C₁₆H₁₀F₆NO₂SSe [M+H]⁺: 473.9496; found: 473.9496.



1-((4-nitrophenyl)sulfonyl)-2-phenyl-3-((trifluoromethyl)selanyl)-1*H*-indole (3a-2)

Obtained as a yellow solid in 53% yield (56.0 mg). Mp: 235.1–235.7 °C. R_f (petroleum ether/ethyl acetate = 8:1) = 0.67. ¹H NMR (400 MHz, CDCl₃) δ 8.35 (d, J = 8.3 Hz, 1H), 8.16 (d, J = 7.9 Hz, 2H), 7.73 (d, J = 7.8 Hz, 1H), 7.61 (d, J = 8.1 Hz, 2H), 7.55 – 7.52 (m, 2H), 7.47 – 7.44 (m, 3H), 7.28 (d, J = 7.7 Hz, 2H). ¹⁹F NMR (376 MHz, CDCl₃) δ -34.9 (s, 3F). ¹³C NMR (101 MHz, CDCl₃) δ 150.7 (s), 146.6 (s), 143.2 (s), 136.7 (s), 131.8 (s), 131.7 (s), 130.0 (s), 129.4 (s), 128.3 (s), 127.6 (s),

126.7 (s), 125.5 (s), 124.2 (s), 121.8 (q, J = 335.7 Hz), 121.3 (s), 115.6 (s), 105.9 (s). IR (ATR): v 1606, 1528, 1487, 1444, 1390, 1347, 1317, 1300, 1260, 1185, 1140, 1112, 1085, 1033, 942, 907, 855, 790, 776, 742, 696, 679, 609, 562 cm⁻¹. HRMS (ESI) m/z: calcd. for C₂₁H₁₃F₃N₂NaO₄SSe [M+Na]⁺: 548.9606; found: 548.9606.



1-(methylsulfonyl)-2-phenyl-3-((trifluoromethyl)selanyl)-1H-indole (3a-3)

Obtained as a white solid in 68% yield (57.0 mg). Mp: 204.7–206.0 °C. $R_{\rm f}$ (petroleum ether/ethyl acetate = 8:1) = 0.45. ¹H NMR (400 MHz, CDCl₃) δ 8.22 – 8.19 (m, 1H), 7.90 – 7.84 (m, 1H), 7.58 – 7.47 (m, 7H), 3.03 (s, J = 2.1 Hz, 3H). ¹⁹F NMR (376 MHz, CDCl₃) δ -35.0 (s, 3F). ¹³C NMR (101 MHz, CDCl₃) δ 146.7 (s), 136.3 (s), 131.4 (s), 131.3 (s), 130.1 (s), 129.8 (s), 127.7 (s), 126.3 (s), 124.9 (s), 122.0 (q, J = 335.6 Hz), 121.3 (s), 114.9 (s), 104.2 (d, J = 1.9 Hz), 41.9 (s). IR (ATR): v 3010, 2930, 1445, 1362, 1323, 1244, 1217, 1173, 1087, 1070, 1026, 955, 924, 829, 770, 758, 737, 699, 676, 627, 586, 542 cm⁻¹. HRMS (ESI) m/z: calcd. for C₁₆H₁₂F₃NO₂SSe [M-H]⁻: 417.9633; found: 417.9630.



1-methyl-2-phenyl-3-((trifluoromethyl)selanyl)-1*H*-indole (3a-4)

Obtained as a white solid in 97% yield (69.0 mg). Mp: 116.1–118.1 °C. R_f (petroleum ether:ethyl acetate = 10:1) = 0.57. ¹H NMR (400 MHz, CDCl₃) δ 7.81 (d, J = 7.7 Hz, 1H), 7.56 – 7.48 (m, 3H), 7.44 – 7.38 (m, 3H), 7.38 – 7.28 (m, 2H), 3.67 (s, 3H). ¹⁹F NMR (376 MHz, CDCl₃) δ -37.2 (s, 3F). ¹³C NMR (101 MHz, CDCl₃) δ 147.8 (s),

137.5 (s), 131.1 (s), 130.9 (s), 130.7 (s), 129.3 (s), 128.4 (s), 123.2 (s), 122.5 (q, J = 336.6 Hz), 121.6 (s), 120.5 (s), 110.0 (s), 91.9 (d, J = 1.1 Hz), 31.9 (s). IR (ATR): v 3060, 2945, 1467, 1442, 1373, 1335, 1235, 1110, 1088, 1022, 1012, 952, 919, 826, 792, 740, 698, 613, 583, 547 cm⁻¹. HRMS (ESI) m/z: calcd. for C₁₆H₁₂F₃NNaSe [M+Na]⁺: 377.9979; found: 377.9980.



2-phenyl-3-((trifluoromethyl)selanyl)-1*H*-indole (3a-6)

Obtained as a white solid in 95% yield (65.0 mg). R_f (petroleum ether/ethyl acetate = 8:1) = 0.53. ¹H NMR (400 MHz, CDCl₃) δ 8.57 (br s, 1H), 7.85 – 7.77 (m, 1H), 7.75 – 7.65 (m, 2H), 7.53 – 7.38 (m, 4H), 7.33 – 7.25 (m, 2H). ¹⁹F NMR (376 MHz, CDCl₃) δ -36.6 (s, 3F). ¹³C NMR (101 MHz, CDCl₃) δ 144.2 (s), 135.9 (s), 132.3 (s), 131.5 (s), 129.3 (s), 129.2 (s), 128.8 (s), 123.8 (s), 122.6 (q, *J* = 336.5 Hz), 121.8 (s), 120.8 (s), 111.2 (s), 91.4 (d, *J* = 2.0 Hz).

Crystal structure analyses

The crystal samples of **3w** were prepared by slow volatilization in ethyl acetate. The suitable crystals of **3w** (CCDC 2084131) were mounted on quartz fibers and X-ray data collected on a Bruker AXS APEX diffractometer, equipped with a CCD detector at -50 °C, using CuK α radiation (λ 1.54178 Å). The data was corrected for Lorentz and polarisation effect with the **SMART** suite of programs and for absorption effects with SADABS. Structure solution and refinement were carried out with the SHELXTL suite of programs. The structure was solved by direct methods to locate the heavy atoms, followed by difference maps for the light non-hydrogen atoms.

Compound	3w (CCDC 2084131)
Empirical formula	C ₂₂ H ₁₅ BrF ₃ NO ₂ SSe
Formula weight	573.28
Temperature/K	296.15
Wavelength/Å	1.54178
Crystal system	Triclinic
a/Å	9.0368(4)
b/Å	9.7879(5)
c/Å	12.8089(6)
α/°	72.001(2)
β/°	83.060(2)
γ/°	79.877(2)
Volume/Å ³	1058.06(9)
Z	2
Density (calc.)/cm ³	1.799
Absorption coefficient /mm ⁻¹	5.960
F(000)	564.0
Crystal size/mm	$0.05 \times 0.04 \times 0.01$
Theta range for data collection / °	7.28~133.22
Reflections collected	21152
Reflections collected Independent reflections	21152 3696 [R(int) = 0.0301]
Reflections collected Independent reflections Data/restraints/parameters	21152 3696 [R(int) = 0.0301] 3969 / 0 / 282
Reflections collectedIndependent reflectionsData/restraints/parametersGoodness-of-fit on F2	21152 3696 [R(int) = 0.0301] 3969 / 0 / 282 1.090
Reflections collectedIndependent reflectionsData/restraints/parametersGoodness-of-fit on F²Final R indexes [I>=2σ (I)]	21152 3696 [R(int) = 0.0301] 3969 / 0 / 282 1.090 0.0248
Reflections collected Independent reflections Data/restraints/parameters Goodness-of-fit on F ² Final R indexes [I>=2σ (I)] Final R indexes [all data]	21152 3696 [R(int) = 0.0301] 3969 / 0 / 282 1.090 0.0248 0.0258

Table S1. Crystal data and structure refinement for compounds

ORTEP diagrams



Figure S1. ORTEP diagram of 3w with thermal ellipsoids at the 40% probability level

References

- C. Chen, L. Ouyang, Q. Lin, Y. Liu, C. Hou, Y. Yuan and Z. Weng, *Chem.-Eur. J.*, 2014, **20**, 657-661.
- 2. J. Liu, X. Xie and Y. Liu, *Chem. Commun.*, 2013, **49**, 11794-11796.
- C. M. Le, T. Sperger, R. Fu, X. Hou, Y. H. Lim, F. Schoenebeck and M. Lautens, *J. Am. Chem. Soc.*, 2016, **138**, 14441-14448.

Copies of ¹H NMR, ¹⁹FNMR and ¹³C NMR spectra







10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150

¹³C NMR spectra of **3a** in CDCl₃







¹³C NMR spectra of **3b** in CDCl₃

4	6	8	4	6	86	8	8	33	4	21	8	8	58	60	6	35	2	82	4	42
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5	5	Σ.	Σ.	Σ,	Σ.	Σ,	Σ,	Σ,	Σ.	Σ.	2	7	7	5	5	7	7	5	5	5





22.22 21.68
¹H NMR spectra of **3c** in CDCl₃













-21.74

¹H NMR spectra of **3e** in CDCl₃



¹⁹F NMR spectra of **3e** in CDCl₃

 $MeO_{t} \leftarrow f_{t} \leftarrow f_{t} \leftarrow f_{t}$

¹³C NMR spectra of **3e** in CDCl₃



¹H NMR spectra of **3f** in CDCl₃



^{19}F NMR spectra of **3f** in CDCl₃



¹³C NMR spectra of **3f** in CDCl₃

~161.76 ~159.35	148.81 145.67 135.20 135.20 135.20 133.19 133.19 133.16 127.05 127.05 127.05 127.05 127.05 127.05 112.28 112.58 111.58 112.58 112.58 11	-21.72
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¹H NMR spectra of **3g** in CDCl₃



¹⁹F NMR spectra of **3g** in CDCl₃

---35.15









10	0	-10	-20	-30	-40	-50	-60	-70	-80	-90	-100	-110	-120	-130	-140	-150	-16



¹H NMR spectra of **3i** in CDCl₃





¹⁹F NMR spectra of **3i** in CDCl₃



---35.19



¹H NMR spectra of **3j** in CDCl₃







¹H NMR spectra of **3k** in CDCl₃



¹⁹F NMR spectra of **3k** in CDCl₃



¹H NMR spectra of **3l** in CDCl₃

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¹H NMR spectra of **3m** in CDCl₃



¹⁹F NMR spectra of **3m** in CDCl₃

---35.00







¹H NMR spectra of **3n** in CDCl₃

10.13 8.37 7.95 7.73 7.73 7.74 7.44 7.44 7.44 7.44 7.44	2.34



^{19}F NMR spectra of **3n** in CDCl₃



SeCF3 ССНО



-21.72

¹³C NMR spectra of **3n** in CDCl₃

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စ	4	4	<u></u>	<u></u>	<u></u>	<u></u>	<u></u>	<u></u>	2	2	2		2	2	2	2	2			0	0
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¹⁹F NMR spectra of **30** in CDCl₃

---35.11



¹³C NMR spectra of **30** in CDCl₃



¹H NMR spectra of **3p** in CDCl₃

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19 F NMR spectra of **3p** in CDCl₃







-21.77

¹³C NMR spectra of **3p** in CDCl₃

148.52 146.04 144.31 137.07 136.99 134.98 132.87 132.87 131.55 123.95	126.94 126.94 126.94 125.30 125.30 125.30 125.30 125.30 125.30 125.31 120.18 116.28 116.28





¹H NMR spectra of **3q** in CDCl₃



 ^{19}F NMR spectra of **3q** in CDCl₃

---35.01



¹³C NMR spectra of **3q** in CDCl₃









60.67	45.33	36.96	35.49	33.35	31.70	29.63	27.03	26.70	25.96	24.75	23.70	22.15	20.95	20.36	17.03	15.87	12.83	04.42	04.41	5.38	
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-21.69



10 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10

¹H NMR spectra of **3s** in CDCl₃





¹³C NMR spectra of **3s** in CDCl₃









¹³C NMR spectra of **3t** in CDCl₃

23 8	$\begin{array}{c} 7.1\\ 2.5\\ 2.5\\ 2.5\\ 2.5\\ 2.5\\ 2.5\\ 2.5\\ 2.5$	2
62. 60.	$\begin{array}{c} 4.5, \\ 4.5, \\ 3.3, \\ 3.3, \\ 3.4, \\ 3.$	1.7
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57		

¹H NMR spectra of 3u in CDCl₃

¹³C NMR spectra of **3u** in CDCl₃

¹H NMR spectra of 3w in CDCl₃

 ^{19}F NMR spectra of 3w in CDCl₃

--35.12

^{13}C NMR spectra of 3w in CDCl₃

-21.74

200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10

¹H NMR spectra of 3y in CDCl₃

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80888777777777777777777777777777	Ņ

¹³C NMR spectra of **3y** in CDCl₃

¹H NMR spectra of **3z** in CDCl₃

13.5 12.5 11.5 10.5 9.5 8.5 7.5 6.5 5.5 4.5 3.5 2.5 1.5 0.5 -0.5 -1.

¹H NMR spectra of **3aa** in CDCl₃







10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150









-21.70

210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10

¹H NMR spectra of **3ab** in CDCl₃







¹H NMR spectra of **3ac** in CDCl₃

88 7.2332 7.2333 7.233 7.2	222 2222 2222 2222 2223 2223 2223 2223	0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000000
SeCF3		
7.7 7.6		







10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150





¹H NMR spectra of **3ad** in CDCl₃

115 115 115 117 117 117 117 117 117 117	35 35 35 35 35 35 35 35 35 35 35 35 35 3	2 2 3 3 3 3 3 4 4 4 4 4 4 4 4 4 4 4 4 4 4	335 4 4 4 8 8 6 6 6 6 6 6 6 6 6 6 6 6 6 6 6	22222225228
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¹H NMR spectra of **3a-1** in CDCl₃



¹³C NMR spectra of **3a-1** in CDCl₃







¹³C NMR spectra of **3a-2** in CDCl₃

105. 105. 105. 105. 105. 105. 105. 105.
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¹H NMR spectra of **3a-3** in CDCl₃



10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150









¹³C NMR spectra of **3a-4** in CDCl₃





¹H NMR spectra of **3a-6** in CDCl₃

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¹⁹F NMR spectra of **3a-6** in CDCl₃



¹³C NMR spectra of **3a-6** in CDCl₃

26 89 26	50 23 23 23 23 23 23 23 23 23 23 23 23 23	0 2 8 8 2 V	0 0 22
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210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10