Supporting information

Synthesis and Transformation of [Difluoro(phenylseleno)methyl]trimethylsilane (PhSeCF₂TMS)

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2,2-Difluoro-2-phenylseleno-1-phenylethanol (3b). The pure product **3b** (45 mg, 64%) was obtained by column chromatography [petroleum ether/EtOAc, 5/1 (v/v)] as a pale yellow liquid: ¹H NMR (300 MHz, CD₃COCD₃) δ 2.82 (1H, d, *J* = 9.9 Hz), 5.08-5.17 (1H, m), 7.33-7.65 (10H, m); ¹³C NMR (75 MHz, CD₃COCD₃) δ 76.7 (t, ²*J*_{CF} = 24 Hz), 124.3, 127.4 (t, ¹*J*_{CF} = 298 Hz), 127.8, 127.9, 128.5, 129.1, 129.2, 137.0, 137.1; ¹⁹F NMR (282 MHz, CD₃COCD₃) δ -77.1 (1F, dd, ²*J*_{FF} = 204 Hz, ³*J*_{FH} = 9.9 Hz), -81.4 (1F, dd, ²*J*_{FF} = 203 Hz, ³*J*_{FH} = 12.4 Hz); IR (neat) ν 3433, 1579, 1478, 1440, 1156, 1061 cm⁻¹; MS (EI) *m/z* = 314 (M⁺, 22), 208 (31), 107 (100), 77 (59); HRMS (MALDI) calcd for C₁₄H₁₂OF₂SeNa⁺ 336.9919, found 336.9914.

1,1-Difluoro-1-phenylseleno-2-amyl alcohol (3c). The pure product **3c** (49 mg, 78%) was obtained by column chromatography [petroleum ether/EtOAc, 10/1 (v/v)] as a pale yellow liquid: ¹H NMR (300 MHz, CDCl₃) δ 0.96 (3H, t, *J* = 7.0 Hz), 1.38-1.76 (4H, m), 2.21 (1H, br), 3.85 (1H, m), 7.33-7.74 (5H, m); ¹³C NMR (125MHz, CDCl₃) δ 13.8, 18.7, 32.6, 74.8 (t, ²*J*_{CF} = 24 Hz), 123.6, 128.0 (t, ¹*J*_{CF} = 298 Hz), 129.2, 129.4, 137.3; ¹⁹F NMR (282 MHz, CDCl₃) δ -79.3 (1F, dd, ²*J*_{FF} = 208 Hz, ³*J*_{FH} = 9.6 Hz), -84.1 (1F, dd, ²*J*_{FF} = 208 Hz, ³*J*_{FH} = 11.8 Hz); IR (neat) ν 3399, 2963, 1580, 1478, 1440, 1180, 1061 cm⁻¹; MS (EI) *m/z* = 280 (M⁺, 11), 158 (28), 127 (18), 77 (30), 57 (100), 43 (76); HRMS (EI) calcd for C₁₁H₁₄OF₂Se 280.0177, found 280.0186; Anal. Calcd for C₁₁H₁₄OF₂Se: C, 47.32; H, 5.05. found: C, 47.41; H, 5.22.

2,2-Difluoro-2-phenylseleno-1-(1',4'-chlorophenyl)ethanol (3d). The pure product **3d** (62 mg, 73%) was obtained by column chromatography [petroleum ether/EtOAc, 5/1 (v/v)] as a pale yellow liquid: ¹H NMR (300 MHz, CDCl₃) δ 2.80 (1H, br), 5.44 (1H, m), 7.25-7.68 (8H, m); ¹³C NMR (75 MHz, CDCl₃) δ 72.1 (t, ²*J*_{CF} = 25.1 Hz), 123.6, 127.4, 128.0, 129.3, 129.7, 130.1 (t, ¹*J*_{CF} = 300 Hz), 130.6, 131.7, 134.7, 135.5, 137.1; ¹⁹F NMR (282 MHz, CDCl₃) δ -79.9 (1F, dd, ²*J*_{FF} = 211 Hz, ³*J*_{FH} = 6.2 Hz), -85.4 (1F, dd, ²*J*_{FF} = 215 Hz, ³*J*_{FH} = 12.4 Hz); IR (neat) ν

3405, 1591, 1562, 1477, 1440, 1155, 1066 cm^{-1} ; MS (EI) m/z = 381 (M^+ , 5), 208 (26), 175 (100), 157 (17), 111 (31), 77 (22); HRMS (EI) calcd for $\text{C}_{14}\text{H}_{10}\text{OF}_2\text{Cl}_2\text{Se}$ 381.9241, found 381.9218; Anal. Calcd for $\text{C}_{14}\text{H}_{10}\text{OF}_2\text{Cl}_2\text{Se}$: C, 44.01; H, 2.64. Found: C, 44.48; H, 2.94.

1,1-Difluoro-1-phenylseleno-2-methyl-2-butyl alcohol (3e). The pure product **3e** (31 mg, 49%) was obtained by column chromatography [petroleum ether/EtOAc, 10/1 (v/v)] as a pale yellow liquid: ^1H NMR (300 MHz, CDCl_3) δ 1.02 (3H, t, J = 7.5 Hz), 1.37 (3H, s), 1.70-1.85 (2H, m), 1.93 (1H, br), 7.33-7.45 (3H, m), 7.71-7.74 (2H, m); ^{19}F NMR (282 MHz, CDCl_3) δ -81.1 (1F, d, $^2J_{\text{FF}}$ = 204 Hz), -81.5 (1F, d, $^2J_{\text{FF}}$ = 200 Hz); IR (neat) ν 3450, 2981, 2945, 2886, 1580, 1478, 1440, 1092, 1063 cm^{-1} ; MS (MALDI) m/z 303.0 ($\text{M} + \text{Na}^+$), 298.1 ($\text{M} + \text{NH}_4^+$); Anal. Calcd for $\text{C}_{11}\text{H}_{14}\text{OF}_2\text{Se}$: C, 47.32; H, 5.05. Found: C, 47.13; H, 5.07.

1-Difluoro(phenylseleno)methylcyclohexanol (3f). The pure product **3f** (25 mg, 37%) was obtained by column chromatography [petroleum ether/EtOAc, 10/1 (v/v)] as a pale yellow liquid: ^1H NMR (300 MHz, CDCl_3) δ 1.59-1.86 (11H, m), 7.31-7.41 (3H, m), 7.70-7.72 (2H, m); ^{13}C NMR (100 MHz, CDCl_3) δ 20.9, 25.4, 29.7, 31.1, 124.0, 129.0, 129.2, 130.8 (t, $^1J_{\text{CF}}$ = 302 Hz), 137.5; ^{19}F NMR (282 MHz, CDCl_3) δ -83.51 (2F, s); IR (neat) ν 3437, 2938, 2860, 1580, 1477, 1440, 1187, 1080 cm^{-1} ; MS (EI) m/z = 306 (M^+ , 11), 208 (32), 158 (33), 99 (94), 81 (100), 77 (29); HRMS (EI) calcd for $\text{C}_{13}\text{H}_{16}\text{OF}_2\text{Se}$ 306.0334, Found 306.0327.

Compound 1:

PhSeCF₂Br

¹H-NMR

Compound 1:

PhSeCF2Br

^{13}C -NMR

PhSeCF₂TMSPhSeCF₂TMS¹H-NMR

Compound 2:

PhSeCF₂TMS

¹³C-NMR

N#Cc1ccc(cc1)C(O)C(F)(F)FSc2ccccc2

¹H NMR spectrum of compound 10 in CDCl₃. The spectrum shows peaks from 0 to 8 ppm. Key features include a triplet at ~0.9 ppm (3H, integration 3.00), a multiplet at ~1.5 ppm (3H, integration 3.03), a multiplet at ~4.5 ppm (2H, integration 2.00), and a multiplet at ~7.5 ppm (2H, integration 2.00). Solvent peaks for CDCl₃ are visible at ~7.26 ppm. Integration values are shown below the baseline.

Compound 3a:

¹³C-NMR

Compound 3b:

¹H-NMR

Compound 3b:

^{13}C -NMR

Compound 3c:

¹H-NMR

Compound 3c:

^{13}C -NMR

Compound 3d

¹H-NMR

Compound 3d

^{13}C -NMR

Compound 3e

¹H-NMR

Compound 3f

¹H-NMR

Compound 3f

¹³C-NMR

Compound 4

¹H-NMR

Compound 4

^{13}C -NMR