Electronic Supplementary Material (ESI) for Organic Chemistry Frontiers.

Supporting Information

(1S)-(-)-*N*-Trifluoromethylthio-2,10-camphorsultam and its Derivatives: Easily Available, Optically Pure Reagents for Asymmetric Trifluoromethylthiolation

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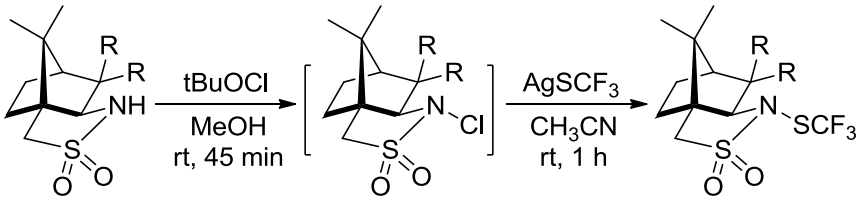
General information. All solvents were purified by standard method. ^{1}H , ^{13}C and ^{19}F NMR spectra were acquired on 400 MHz, 125 MHz, 100 MHz, 375 MHz spectrometer (400 MHz for ^{1}H ; 100 MHz or 125 MHz for ^{13}C; 375 MHz for ^{19}F). ^{1}H NMR and ^{13}C NMR chemical shifts were determined relative to internal standard TMS at δ 0.0 ppm and ^{19}F NMR chemical shifts were determined relative to $CFCl_3$ as inter standard. Chemical shifts (δ) are reported in ppm, and coupling constants (*J*) are in hertz (Hz). The following abbreviations were used to explain the multiplicities: s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet, br = broad. All reactions were monitored by TLC or ^{19}F NMR. Flash column chromatograph was carried out using 300-400 mesh silica gel at medium pressure.

Materials. All reagents were received from commercial sources. Solvents were freshly dried and degassed according to the purification handbook Purification of Laboratory Chemicals before using.

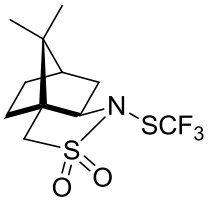
General procedure for the preparation of optically active electrophilic trifluoromethylthiolating reagents 1a-f



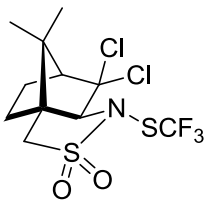
R = H, **1a**, 68%
Cl, **1b**, 73%
OMe, **1c**, 79%

Preparation of (1S)-(-)-*N*-chloro-2,10-camphorsultam.[1] To a solution of (1S)-(-)-2,10-camphorsultam (2.15 g, 10.0 mmol) in methanol (15.0 mL), and in a 50 mL round-bottom flask covered with aluminum foil was added *tert*-butylhypochlorite (2.71g, 25.0 mmol) under an argon atmosphere. The solution was then stirred at room temperature for 45 min. The solution was evaporated at reduce pressure to give (1S)-(-)-*N*-chloro-2,10-camphorsultam quantitatively, which was used directly without further purification.

Preparation of (1S)-(-)-*N*-trifluoromethylthio-2,10-camphorsultam.[2-3] To an oven dried 500 mL Schlenk flask equipped with a stir bar was added dry (1S)-(-)-*N*-chloro-2,10-camphorsultam (2.50 g, 10.0 mmol). The flask was fitted with a glass stopper and evacuated and refilled with Ar for three times. Under Ar pressure, dry MeCN (30.0 mL) was injected into the flask, then $AgSCF_3$ (2.49 g, 12.0 mmol) was added. The mixture was stirred vigorously at room temperature for 1 h. The CH_3CN was then evaporated under reduced pressure. And the residue was extracted with CH_2Cl_2 (3 × 30.0 mL). The solution was combined, dried over anhydrous Na_2SO_4. The solvent was evaporated under vacuum and the residue was purified by recrystallization from a solution of THF and petroleum ether to give (1S)-(-)-*N*-trifluoromethylthio-2,10-camphorsultam as a white solid (2.14 g, 68.0% yield).

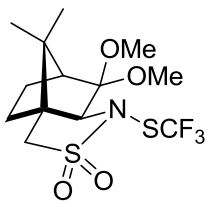


(3aR,6R,7aR)-8,8-Dimethyl-1-((trifluoromethyl)thio)hexahydro-1*H*-3a,6-methanobenzo[c]isothiazole 2,2-dioxide 1a. Yield 68%, white solid. Mp：86.0 – 88.0 ^{o}C. ^{1}H NMR (400 MHz, $CDCl_3$, 298 K) δ 3.48 (br, 1 H), 3.30 – 3.20 (m, 2 H), 2.18 (d, *J* = 12.4 Hz, 1 H), 2.06 – 1.67 (m, 4 H), 1.46 – 1.39 (m, 1 H), 1.32 – 1.25 (m, 1 H), 1.15 – 0.70 (br, 6 H); ^{1}H NMR (400 MHz, $CDCl_3$, 213 K) δ 3.70 – 3.15 (m, 3 H), 2.15 (t, *J* = 12.4 Hz, 1 H), 2.03 – 1.72 (m, 4 H), 1.48 – 1.21 (m, 2 H), 1.00 – 0.78 (m, 6 H); ^{1}H NMR (400 MHz, $CDCl_3$, 323 K) δ 3.62 – 3.12 (m, 3 H), 2.20 (d, *J* = 12.1 Hz, 1 H), 2.03 – 1.84 (m, 3 H), 1.81 – 1.74 (m, 1 H), 1.50 – 1.21 (m, 2 H), 0.95 – 0.90 (m, 6 H); ^{13}C NMR (101 MHz, $CDCl_3$, 298 K) δ 133.19 – 123.72 (br), 68.25 (br), 51.12 (br), 49.00 (br), 47.82, 44.21, 34.19 (br), 32.06 (br), 27.00, 19.88 (2 C); ^{13}C NMR (101 MHz, $CDCl_3$, 213 K) δ 128.58 (q, *J* = 322.2 Hz), 128.00 (q, *J* = 313.1 Hz), 69.30, 66.73, 52.19, 50.45, 49.24, 48.47, 48.14, 48.09, 43.83, 43.53, 34.65, 33.60, 32.24, 31.36, 27.14, 20.27, 20.15, 20.04, 19.72; ^{13}C NMR (101 MHz, $CDCl_3$, 323 K) δ 128.50 (q, *J* = 317.0 Hz), 68.37 (br), 51.18 (br), 49.03, 47.79, 44.37, 34.20, 32.13, 26.98, 19.86 (2 C); ^{19}F NMR (376 MHz, $CDCl_3$, 298 K) δ -46.67 (s, 3 F), -48.09 (s, 3 F); ^{19}F NMR (376 MHz, $CDCl_3$, 213 K) δ -46.27 (s, 3 F), -48.03 (s, 3 F); ^{19}F NMR (376 MHz, $CDCl_3$, 323 K) δ -46.95 (s, 3 F), -47.69 (s, 3 F) ppm. IR (KBr): ν = 3019, 2964, 2884, 1485, 1464, 1412, 1393, 1378, 1332, 1173, 1147, 1115, 958, 920, 854, 831, 774, 757, 653, 533 cm^{-1}. MS (EI): 150 (100), 315 (23); HRMS (EI) for $C_{11}H_{16}O_2NF_3S_2$ Calcd: 315.0575, Found: 315.0574. Elemental Aanlysis for $C_{11}H_{16}O_2NF_3S_2$ Calcd: C, 41.89; H, 5.11; N, 4.44; S, 20.33; F, 18.07; Found: C, 41.92; H, 5.00; N, 4.46; S, 20.46; F, 18.34.



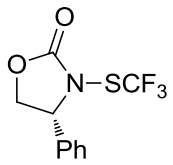
(3aR,6S,7aS)-7,7-Dichloro-8,8-dimethyl-1-((trifluoromethyl)thio)hexahydro-1*H*-3

a,6-methanobenzo[c]isothiazole 2,2-dioxide 1b. Yield 73%, white solid. Mp： 133.0 – 135.0 ^{o}C. ^{1}H NMR (400 MHz, $CDCl_3$, 298 K) δ 4.05 (br, 1 H), 3.39 (s, 2 H), 2.56 (d, *J* = 4.6 Hz, 1 H), 2.31 (ddd, *J* = 13.4, 9.1, 4.0 Hz, 1 H), 2.05 (tt, *J* = 14.2, 4.3 Hz, 1 H), 1.94 (td, *J* = 12.2, 3.9 Hz, 1 H), 1.58 (ddd, *J* = 12.8, 9.3, 3.9 Hz, 1 H), 1.37 (s, 3 H), 1.05 (s, 3 H); ^{1}H NMR (400 MHz, $CDCl_3$, 213 K) δ 4.09 – 3.73 (m, 1 H), 3.60 – 3.20 (m, 2 H), 2.58 (d, *J* = 4.0 Hz, 1 H), 2.27 – 2.22 (m, 1 H), 2.06 (t, *J* = 12.5 Hz, 1 H), 2.02 – 1.80 (m, 1 H), 1.59 (t, *J* = 8.8 Hz, 1 H), 1.38 – 1.31 (d, 3 H), 1.03 (s, 3 H); ^{1}H NMR (400 MHz, $CDCl_3$, 323 K) δ 4.02 – 3.97 (m, 1 H), 3.37 – 3.32 (m, 2 H), 2.57 – 2.51 (m, 1 H), 2.40 – 2.22 (m, 1 H), 2.13 – 2.00 (m, 1 H), 1.99 – 1.84 (m, 1 H), 1.62 – 1.50 (m, 1 H), 1.39 – 1.34 (m, 3 H), 1.07 – 1.01 (m, 3 H); ^{13}C NMR (101 MHz, $CDCl_3$, 298 K) δ 129.10 (br), 92.79, 81.22, 62.21, 52.44, 49.74, 48.48, 31.78, 25.32, 23.53, 22.98; ^{13}C NMR (101 MHz, $CDCl_3$, 213 K) δ 129.37 (q, *J* = 324.0 Hz), 93.11, 80.66, 61.58, 52.52, 49.75, 48.56, 31.46, 25.44, 23.73, 23.20; ^{13}C NMR (101 MHz, $CDCl_3$, 323 K) δ 129.04 (q, *J* = 323.2 Hz), 92.79, 81.39, 62.38, 52.51, 49.75, 48.49, 31.84, 25.28, 23.48, 22.91; ^{19}F NMR (376 MHz, $CDCl_3$, 298 K) δ -42.30 (s, 3 F), -43.96 (s, 3 F); ^{19}F NMR (376 MHz, $CDCl_3$, 213 K) δ -41.86 (s, 3 F), -43.52 (s, 3 F); ^{19}F NMR (376 MHz, $CDCl_3$, 323 K) δ -42.73 (s, 3 F) ppm. IR (KBr): ν = 3019, 3003, 2991, 2945, 2885, 1478, 1417, 1347, 1259, 1225, 1167, 1101, 953, 906, 827, 751, 672, 659, 546, 522 cm^{-1}. MS (DART POS): 393.1 ($M+NH_4$); HRMS (DART POS): $C_{11}H_{18}O_2N_2Cl_2F_3S_2$ ($M+NH_4$) Calcd: 401.0133, Found: 401.0133. Elemental Aanlysis for $C_{11}H_{14}O_2NCl_2F_3S_2$ Calcd: C, 34.38; H, 3.67; N, 3.65; S, 16.69; F, 14.83; Cl, 18.45 Found: C, 34.46; H, 3.68; N, 3.66; S, 16.45; F, 15.05; Cl, 18.78.



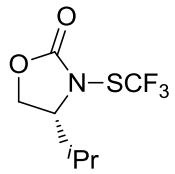
(3aR,6S,7aS)-7,7-Dimethoxy-8,8-dimethyl-1-((trifluoromethyl)thio)hexahydro-1*H*-3a,6-methanobenzo[c]isothiazole 2,2-dioxide 1c. Yield 79 %, white solid. Mp： 131.0 – 133.0 ^{o}C. ^{1}H NMR (400 MHz, $CDCl_3$, 298 K) δ 3.41 – 3.15 (m, 9 H), 2.23 (d, *J* = 4.4 Hz, 1 H), 1.96 (ddd, *J* = 13.1, 9.3, 3.9 Hz, 1 H), 1.84 (td, *J* = 11.9, 3.8 Hz, 1 H),

1.72 (ddd, *J* = 16.2, 10.1, 5.3 Hz, 1 H), 1.57 – 1.42 (m, 1 H), 1.29 (s, 3 H), 0.90 (s, 3 H); ^{1}H NMR (400 MHz, $CDCl_3$, 213 K) δ 3.55 – 3.15 (m, 9 H), 2.26 (dd, *J* = 11.2, 4.1 Hz, 1 H), 1.90 – 1.70 (m, 3 H), 1.47 (t, *J* = 12.6 Hz, 1 H), 1.28 – 1.23 (m, 3 H), 0.88 (s, 3 H); ^{1}H NMR (400 MHz, $CDCl_3$, 323 K) δ 3.44 – 3.14 (m, 9 H), 2.22 (br, 1 H), 2.00 (br, 1 H), 1.85 (br, 1 H), 1.77 – 1.67 (m, 1 H), 1.49 (br, 1 H), 1.30 (br, 3 H), 0.91 (br, 3 H); ^{13}C NMR (101 MHz, $CDCl_3$, 298 K) δ 108.83, 73.53, 51.04, 50.43, 49.23, 49.06 (2 C), 47.81, 32.37, 21.50, 20.56, 20.04 (br); ^{13}C NMR (101 MHz, $CDCl_3$, 213 K) δ 129.89 (q, *J* = 324.2 Hz) 127.99 (q, *J* = 316.1 Hz) 108.70, 108.20, 73.43, 72.71, 51.45, 51.01, 50.73, 50.58, 49.88, 49.28, 48.47, 48.38, 48.32, 48.15, 47.77, 47.48, 32.07, 21.75, 21.69, 20.66, 20.57, 19.64; ^{13}C NMR (101 MHz, $CDCl_3$, 323 K) δ 108.94, 73.65, 51.08, 50.34, 49.24, 49.15, 47.97, 47.79, 32.44, 21.45, 20.54, 20.03; ^{19}F NMR (376 MHz, $CDCl_3$, 298 K) δ -44.46 (s, 3 F), -46.86 (s, 3 F); ^{19}F NMR (376 MHz, $CDCl_3$, 213 K) δ -43.90 (s, 3 F), -46.40 (s, 3 F); ^{19}F NMR (376 MHz, $CDCl_3$, 323 K) δ -46.00 (s, 3 F) ppm. IR (KBr): ν = 2998,2963, 2911, 2836, 1733, 1463, 1334, 1313,1191, 1155, 1139, 1108, 1065, 1035, 919, 902, 803, 584, 566, 531, 515, 499 cm^{-1}. MS (DART POS): 393.1 ($M+NH_4$); HRMS (DART POS): $C_{13}H_{24}O_4N_2F_3S_2$ (M+H) Calcd: 393.1124, Found: 393.1120. Elemental Aanlysis for $C_{13}H_{20}F_3NO_4S_2$ Calcd: C, 41.59; H, 5.37; N, 3.73; S, 17.08; F, 15.18 Found: C, 41.57; H, 5.34; N, 3.71; S, 17.05; F, 15.43.

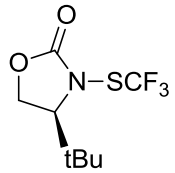


(R)-4-Phenyl-3-((trifluoromethyl)thio)oxazolidin-2-one 1d. Yield 76%, yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.46 – 7.41 (m, 3 H), 7.28 (dd, *J* = 7.2, 2.2 Hz, 2 H), 4.99 (t, *J* = 8.0 Hz, 1 H), 4.78 (td, *J* = 8.9, 1.5 Hz, 1 H), 4.39 – 4.32 (m, 1 H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 157.12, 136.26, 129.90, 129.53, 128.82 (q, *J* = 318.15 Hz), 127.49, 70.36, 63.53; ^{19}F NMR (376 MHz, $CDCl_3$) δ -48.88 (s, 3 F) ppm. IR (KBr): ν = 2968, 2881, 2364, 1785, 1487, 1467, 1390, 1375, 1300, 1193, 1113, 1059, 973, 754, 609 cm^{-1}. MS (EI): 91 (100), 263 (16); HRMS (EI) for $C_{10}H_8NO_2F_3S$ Calcd: 263.0228,

Found: 263.0231.

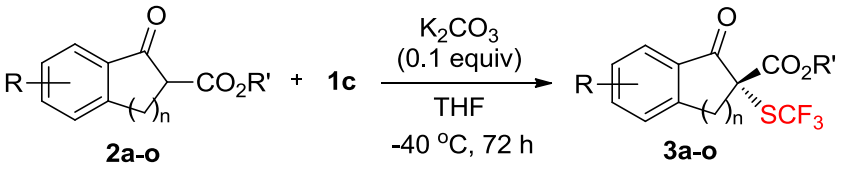


(R)-4-Isopropyl-3-((trifluoromethyl)thio)oxazolidin-2-one 1e. Yield 71%, colourless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 4.39 (t, *J* = 8.9 Hz, 1 H), 4.22 – 4.14 (m, 1 H), 3.96 – 3.88 (m, 1 H), 2.33 – 2.21 (m, 1 H), 0.95 (dd, *J* = 7.0, 3.0 Hz, 3 H), 0.84 (dd, *J* = 6.6, 2.9 Hz, 3 H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 157.58, 128.78 (q, *J* = 316.5 Hz), 64.08, 62.99, 28.16, 17.39, 14.08; ^{19}F NMR (376 MHz, $CDCl_3$) δ -49.51 (s, 3 F) ppm. IR (KBr): ν = 2968, 2881, 2364, 1785, 1487, 1467, 1390, 1375, 1300, 1193, 1113, 1059, 973, 754, 609 cm^{-1}. MS (EI): 142 (100), 229 (21); HRMS (EI) for $C_7H_{10}NO_2F_3S$ Calcd: 229.0384, Found: 229.0387.

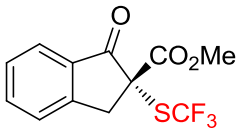


(S)-4-(*tert*-Butyl)-3-((trifluoromethyl)thio)oxazolidin-2-one 1f. Yield 82%, colourless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 4.42 – 4.34 (m, 1 H), 4.27 (ddd, *J* = 9.3, 3.7, 2.0 Hz, 1 H), 3.69 (dd, *J* = 8.3, 3.7 Hz, 1 H), 0.98 (d, *J* = 2.8 Hz, 9 H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 158.04, 129.05 (q, *J* = 317.1 Hz), 67.64, 65.48, 34.94, 25.31; ^{19}F NMR (376 MHz, $CDCl_3$) δ -50.21 (s, 3 F) ppm. IR (KBr): ν = 2968.1, 2361.6, 1789, 1480, 1404, 1388, 1371, 1317, 1185, 1112, 1063, 1030, 972, 761 cm^{-1}. MS (EI): 57 (100), 243 (9); HRMS (EI) for $C_8H_{12}NO_2F_3S$ Calcd: 243.0541, Found: 243.0535.

General procedure for asymmetric trifluoromethylthiolation of *β*-ketoester.

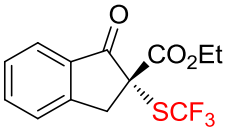


β-Ketoester **2a** (95.1 mg, 0.500 mmol, 1.0 equiv), potasium carbonate (7.90 mg, 0.0500 mmol, 0.1 equiv) and reagent **1c** (206 mg, 0.550 mmol, 1.1 equiv) were added into a flame-dried Schlenk tube. The tube was putted into liquid nitrogen, and dry tetrahydrofuran (2.5 mL) was added under argon atmosphere. The resulting solution was stirred at -40 ^{o}C for 72 h (or -25 ^{o}C for 32 h). After the reaction was completed as monitored by ^{19}F NMR spectroscopy, the reaction was quenched by addition of HCl (2 M). The mixture was extracted with Et_2O (3 × 10.0 mL). The organic phase was separated and dried over anhydrous Na_2SO_4. After filtration, the solvent was removed under vacuum. The residue was purified by flash chromatography to give the trifluoromethylthiolated product **3a** (R)-methyl-1-oxo-2-((trifluoromethyl)thio)-2,3-dihydro-1*H*-indene-2-carboxylate **3a** as a white solid (136 mg, 93.6% yield).



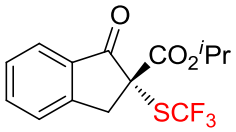
(R)-Methyl-1-oxo-2-((trifluoromethyl)thio)-2,3-dihydro-1*H*-indene-2-carboxylate 3a.[4] Yield 94%, white solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.83 (d, *J* = 7.7 Hz, 1 H), 7.71 (t, *J* = 7.9 Hz, 1 H), 7.52 (d, *J* = 7.7 Hz, 1 H), 7.46 (t, *J* = 7.5 Hz, 1 H), 4.20 (d, *J* = 17.7 Hz, 1 H), 3.79 (s, 3 H), 3.66 (d, *J* = 17.7 Hz, 1 H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 194.79, 167.29, 151.69, 136.62, 132.78, 129.79 (q, *J* = 310.1), 128.54, 126.28, 125.61, 63.38, 54.27, 40.35; ^{19}F NMR (376 MHz, $CDCl_3$) δ -37.76 (s, 3 F) ppm.

HPLC: (IE-3 (0.46 × 25 cm, 3 μm), Hexane/^{i}PrOH = 97/3, 0.7 mL/min, 214 nm), t_R (major) = 12.13 min, t_S (minor) = 12.93 min (88% ee); $[\alpha]_D^{25}$ = -99.2 (c = 0.110, $CHCl_3$, 88% ee).



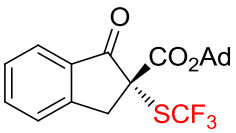
(R)-Ethyl-1-oxo-2-((trifluoromethyl)thio)-2,3-dihydro-1*H*-indene-2-carboxylate 3b.[4] Yield 90%, white solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.80 (d, *J* = 7.7 Hz, 1 H), 7.68 (td, *J* = 7.7, 1.1 Hz, 1 H), 7.50 (d, *J* = 7.8 Hz, 1 H), 7.43 (t, *J* = 7.5 Hz, 1 H), 4.29 – 4.13 (m, 3 H), 3.64 (d, *J* = 17.7 Hz, 1 H), 1.23 (t, *J* = 7.1 Hz, 3 H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 194.94, 166.76, 151.71, 136.49, 132.89, 129.85 (q, *J* = 310.1), 128.47, 126.23, 125.58, 63.65, 63.48, 40.38, 13.75; ^{19}F NMR (376 MHz, $CDCl_3$) δ -37.10 (s, F) ppm.

HPLC: (IF-3 (0.46 × 25 cm, 3 μm), Hexane/^{i}PrOH = 98/2, 0.7 mL/min, 214 nm), t_R (major) = 13.50 min, t_S (minor) = 14.74 min (90% ee); $[\alpha]_D^{25}$ = -81.9 (c = 0.145, $CHCl_3$, 90% ee).



(R)-Isopropyl-1-oxo-2-((trifluoromethyl)thio)-2,3-dihydro-1*H*-indene-2-carboxylate 3c.[4] Yield 95%, white solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.79 (d, *J* = 7.7 Hz, 1 H), 7.67 (td, *J* = 7.6, 1.1 Hz, 1 H), 7.50 (d, *J* = 7.8 Hz, 1 H), 7.45 – 7.40 (m, 1 H), 5.01 (hept, *J* = 6.3 Hz, 1 H), 4.13 (d, *J* = 17.7 Hz, 1 H), 3.63 (d, *J* = 17.7 Hz, 1 H), 1.20 (d, *J* = 6.3 Hz, 6 H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 195.05, 166.24, 151.72, 136.41, 132.95, 129.89 (q, *J* = 310.1), 128.41, 126.20, 125.50, 71.79, 63.58, 40.34, 21.30, 21.11; ^{19}F NMR (376 MHz, $CDCl_3$) δ -37.03 (s, 3 F) ppm.

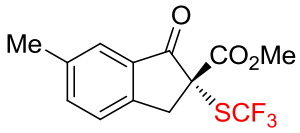
HPLC: (IE-3 (0.46 × 25 cm, 3 μm), Hexane/^{i}PrOH = 98/2, 0.7 mL/min, 214 nm), t_R (major) = 11.87 min, t_S (minor) = 12.93 min (89% ee); $[\alpha]_D^{25}$ = -83.9 (c = 0.125, $CHCl_3$, 89% ee).



(R)-Adamantan-1-yl-1-oxo-2-((trifluoromethyl)thio)-2,3-dihydro-1*H*-indene-2-carboxylate 3d.[5] Yield 93%, white solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.79 (d, *J* = 7.7

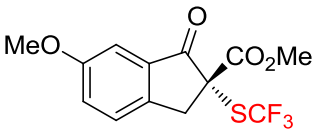
Hz, 1 H), 7.66 (td, *J* = 7.6, 1.1 Hz, 1 H), 7.48 (d, *J* = 7.7 Hz, 1 H), 7.41 (t, *J* = 7.5 Hz, 1 H), 4.05 (d, *J* = 17.7 Hz, 1 H), 3.61 (d, *J* = 17.7 Hz, 1 H), 2.11 (s, 3 H), 2.01 (d, *J* = 3.1 Hz, 6 H), 1.59 (t, *J* = 2.8 Hz, 6 H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 195.59, 165.21, 151.68, 136.17, 133.24, 129.95 (q, *J* = 309.2 Hz), 128.28, 126.10, 125.40, 84.82, 64.37, 40.72, 40.48 (d, *J* = 1.2 Hz), 35.87, 30.88; ^{19}F NMR (376 MHz, $CDCl_3$) δ -36.85 (s, 3 F) ppm.

HPLC: (IE-3 (0.46 × 25 cm, 3 μm), Hexane/^{i}PrOH = 95/5, 0.7 mL/min, 214 nm), t_R (major) = 10.95 min, t_S (minor) = 11.91 min (92% ee); $[\alpha]_D^{25}$ = -71.7 (c = 0.050, $CHCl_3$, 92% ee).



(R)-Methyl-6-methyl-1-oxo-2-((trifluoromethyl)thio)-2,3-dihydro-1*H*-indene-2-carboxylate 3e. Yield 93%, pale yellow solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.59 (s, 1 H), 7.50 (dd, *J* = 7.9, 1.1 Hz, 1 H), 7.39 (d, *J* = 7.9 Hz, 1 H), 4.12 (d, *J* = 17.6 Hz, 1 H), 3.75 (s, 3 H), 3.59 (d, *J* = 17.7 Hz, 1 H), 2.39 (s, 3 H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 194.72, 167.39, 149.09, 138.73, 137.88, 132.99, 129.82 (q, *J* = 309.2 Hz), 125.92, 125.39, 63.73 (d, *J* = 0.5 Hz), 54.15, 40.07 (d, *J* = 1.0 Hz), 20.95; ^{19}F NMR (376 MHz, $CDCl_3$) δ -37.31 (s, 3 F) ppm. IR (KBr): ν = 2958, 1745, 1724, 1618, 1585, 1495, 1435, 1384, 1281, 1252, 1223, 1154, 1112, 1027, 985, 925, 865, 819, 758, 687, 503 cm^{-1}. MS (EI): 171 (100), 304 (0.08); HRMS (EI) for $C_{13}H_{11}O_3F_3S$ Calcd: 304.0381, Found: 304.0376. Mp: 28.0 – 29.0 ^{o}C.

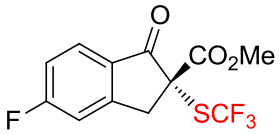
HPLC: (IE-3 (0.46 × 25 cm, 3 μm), Hexane/^{i}PrOH = 7/3, 0.7 mL/min, 214 nm), t_R (major) = 6.89 min, t_S (minor) = 7.21 min (91% ee); $[\alpha]_D^{25}$ = -96.5 (c = 0.100, $CHCl_3$, 91% ee).



(R)-Methyl-6-methoxy-1-oxo-2-((trifluoromethyl)thio)-2,3-dihydro-1*H*-indene-2-carboxylate 3f. Yield 77%, pale yellow solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.42 –

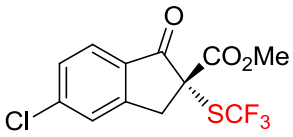
7.32 (m, 1 H), 7.27 (dd, *J* = 8.4, 2.6 Hz, 1 H), 7.20 (d, *J* = 2.5 Hz, 1 H), 4.07 (d, *J* = 17.4 Hz, 1 H), 3.81 (s, 3 H), 3.76 (s, 3 H), 3.56 (d, *J* = 17.4 Hz, 1 H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 194.69, 167.34, 160.16, 144.57, 134.05, 129.77 (q, *J* = 309.3 Hz), 126.95, 126.12, 106.43, 63.99, 55.65, 54.21, 39.77 (d, *J* = 1.0 Hz); ^{19}F NMR (376 MHz, $CDCl_3$) δ -37.25 (s, 3 F) ppm. IR (KBr): ν = 3010, 2958, 2842, 1724, 1653, 1617, 1587, 1495, 1435, 1342, 1280, 1251, 1108, 1027, 968, 858, 829, 759 cm^{-1}. MS (EI): 187 (100), 320 (0.42); HRMS (EI) for $C_{13}H_{11}O_4F_3S$ Calcd: 320.0330, Found: 320.0322. Mp: 35.5 – 36.5 ^{o}C.

HPLC: (IE-3 (0.46 × 25 cm, 3 μm), Hexane/^{i}PrOH = 95/5, 0.7 mL/min, 214 nm), t_R (major) = 13.41 min, t_S (minor) = 15.20 min (91% ee); $[\alpha]_D^{25}$ = -74.1 (c = 0.100, $CHCl_3$, 91% ee).



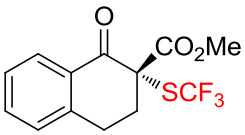
(R)-Methyl-5-fluoro-1-oxo-2-((trifluoromethyl)thio)-2,3-dihydro-1*H*-indene-2-carboxylate 3g.[4] Yield 81%, white solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.51 - 7.48 (m, 1 H), 7.45-7.39 (m, 2 H), 4.14 (d, *J* = 17.6 Hz, 1 H), 3.78 (s, 3 H), 3.61 (d, *J* = 17.4 Hz, 1 H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 193.99 (d, *J* = 2.8 Hz), 166.97, 162.72 (d, *J* = 250.3 Hz), 147.12, 134.58 (d, *J* = 8.0 Hz), 129.65 (q, *J* = 309.2 Hz), 127.79 (d, *J* = 8.1 Hz), 124.41 (d, *J* = 23.8 Hz), 111.35 (d, *J* = 22.6 Hz), 63.95, 54.39, 39.84; ^{19}F NMR (376 MHz, $CDCl_3$) δ -37.23 (s, 3 F), -112.34 (m, 1 F) ppm. IR (KBr): ν = 2960, 1731, 1615, 1489, 1437, 1290, 1268, 1224, 1155, 1112, 1028, 867, 830, 764, 526 cm^{-1}. MS (DART POS): 309.0 (M+H); HRMS (DART POS): $C_{12}H_{12}O_3NF_4S$ (M+NH_4) Calcd: 326.0469, Found: 326.0464. Mp：44.5 – 45.5 ^{o}C.

HPLC: (IE-3 (0.46 × 25 cm, 3 μm), Hexane/^{i}PrOH = 8/2, 0.7 mL/min, 214 nm), t_R (major) = 6.97 min, t_S (minor) = 7.45 min (86% ee); $[\alpha]_D^{25}$ = -49.4 (c = 0.100, $CHCl_3$, 86% ee).



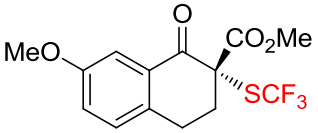
(R)-Methyl-5-chloro-1-oxo-2-((trifluoromethyl)thio)-2,3-dihydro-1*H*-indene-2-carboxylate 3h.[4] Yield 72%, colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.74 (d, *J* = 8.2 Hz, 1 H), 7.51 (s, 1 H), 7.45 – 7.40 (m, 1 H), 4.16 (d, *J* = 17.9 Hz, 1 H), 3.78 (s, 3 H), 3.63 (d, *J* = 17.9 Hz, 1 H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 193.35, 166.94, 153.02, 143.39, 131.27, 129.69 (q, *J* = 311.1 Hz), 129.44, 126.68, 126.52, 63.44, 54.40, 40.01; ^{19}F NMR (376 MHz, $CDCl_3$) δ -37.22 (s, 3 F) ppm.

HPLC: (IE-3 (0.46 × 25 cm, 3 μm), Hexane/^{i}PrOH = 8/2, 0.7 mL/min, 214 nm), t_R (major) = 7.09 min, t_S (minor) = 7.75 min (80% ee); $[\alpha]_D^{25}$ = -68.7 (c = 0.125, $CHCl_3$, 80% ee).



(R)-Methyl-1-oxo-2-((trifluoromethyl)thio)-1,2,3,4-tetrahydronaphthalene-2-carboxylate 3i.[4] Yield 82%, pale yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.99 (d, *J* = 7.9 Hz, 1 H), 7.51 (t, *J* = 7.5 Hz, 1 H), 7.31 (t, *J* = 7.6 Hz, 1 H), 7.23 (d, *J* = 7.9 Hz, 1 H), 3.74 (s, 3 H), 3.31 – 3.18 (m, 1 H), 3.12 – 3.03 (m, 2 H), 2.56 – 2.48 (m, 1 H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 188.94, 167.43, 142.64, 134.71, 130.33, 129.85 (q, *J* = 313.1 Hz), 128.88, 128.64, 127.21, 64.38, 53.77, 32.83, 26.23; ^{19}F NMR (376 MHz, $CDCl_3$) δ -36.20 (s, 3 F) ppm.

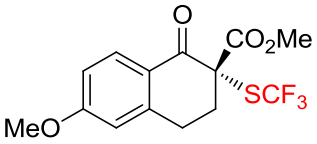
HPLC: (IE-3 (0.46 × 25 cm, 3 μm), Hexane/^{i}PrOH = 95/5, 0.7 mL/min, 214 nm), t_R (major) = 11.08 min, t_S (minor) = 9.77 min (98% ee); $[\alpha]_D^{25}$ = -7.7 (c = 0.110, $CHCl_3$, 98% ee).



(R)-Methyl-7-methoxy-1-oxo-2-((trifluoromethyl)thio)-1,2,3,4-tetrahydronaphthalene-2-carboxylate 3j. Yield 87%, yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.44 (d, *J* = 2.5 Hz, 1 H), 7.14 (d, *J* = 8.5 Hz, 1 H), 7.09 (dd, *J* = 8.5, 2.7 Hz, 1 H), 3.81 (s, 3 H), 3.75 (s, 3 H), 3.23 – 2.94 (m, 3 H), 2.58 – 2.46 (m, 1 H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 188.99, 167.42, 158.62, 135.22, 131.03, 130.11, 129.80 (q, *J* = 309.2 Hz),

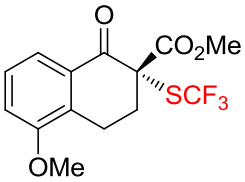
123.39, 110.13, 64.32, 55.49, 53.78, 33.09, 25.50; ^{19}F NMR (376 MHz, $CDCl_3$) δ -36.19 (s, 3 F) ppm. IR (KBr): ν = 3005, 2956, 2841, 1743, 1686, 1611, 1576, 1499, 1436, 1343, 1327, 1287, 1250, 1203, 1105, 1068, 1035, 992, 972, 913, 878, 830, 811, 758, 711, 627, 552 cm^{-1}. MS (EI): 233 (100), 334 (0.66); HRMS (EI) for $C_{14}H_{13}O_4F_3S$ Calcd: 334.0487, Found: 334.0486.

HPLC: (IE-3 (0.46 × 25 cm, 3 μm), Hexane/^{i}PrOH = 9/1, 0.7 mL/min, 214 nm), t_R (major) = 10.21 min, t_S (minor) = 9.12 min (95% ee); $[\alpha]_D^{25}$ = +18.38 (c = 0.100, $CHCl_3$, 95% ee).



(R)-Methyl-6-methoxy-1-oxo-2-((trifluoromethyl)thio)-1,2,3,4-tetrahydronaphthalene-2-carboxylate 3k. Yield 92%, white solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.97 (d, *J* = 8.8 Hz, 1 H), 6.84 (dd, *J* = 8.8, 2.5 Hz, 1 H), 6.67 (d, *J* = 2.4 Hz, 1 H), 3.85 (s, 3 H), 3.76 (s, 3 H), 3.37 – 3.19 (m, 1 H), 3.13 – 2.98 (m, 2 H), 2.56 – 2.49 (m, 1 H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 187.41, 167.64, 164.71, 145.41, 131.22, 129.94 (q, *J* = 311.1 Hz), 123.63, 114.24, 112.37, 64.25, 55.58, 53.72, 32.90, 26.65; ^{19}F NMR (376 MHz, $CDCl_3$) δ -36.33 (s, 3 F) ppm. IR (KBr): ν = 2955, 2844, 1740, 1679, 1601, 1572, 1497, 1435, 1353, 1262, 1226, 1108, 1069, 1037, 970, 889, 852, 756, 738, 687, 587 cm^{-1}. MS (DART POS): 335.1 (M+H); HRMS (DART POS): $C_{14}H_{14}O_4F_3S$ (M+H) Calcd: 335.0559, Found: 335.0558. Mp: 55.5 – 56.5 ^{o}C.

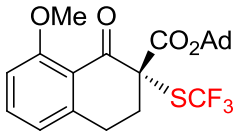
HPLC: (IE-3 (0.46 × 25 cm, 3 μm), Hexane/^{i}PrOH = 8/2, 0.7 mL/min, 214 nm), t_R (major) = 10.05 min, t_S (minor) = 9.53 min (94% ee); $[\alpha]_D^{25}$ = -7.4 (c = 0.100, $CHCl_3$, 94% ee).



(R)-Methyl-5-methoxy-1-oxo-2-((trifluoromethyl)thio)-1,2,3,4-tetrahydronaphthalene-2-carboxylate 3l. Yield 96%, yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.59 (d, *J* = 7.9 Hz, 1 H), 7.29 (t, *J* = 8.0 Hz, 1 H), 7.06 (d, *J* = 8.1 Hz, 1 H), 3.86 (s, 3 H),

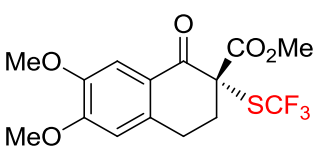
3.74 (s, 3 H), 3.17 – 2.95 (m, 3 H), 2.52 – 2.44 (m, 1 H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 189.29, 167.35, 156.66, 131.68, 131.18, 129.87 (q, *J* = 313.1 Hz), 127.58, 119.86, 115.21, 64.21, 55.69, 53.71, 32.07, 20.63; ^{19}F NMR (376 MHz, $CDCl_3$) δ -36.24 (s, 3 F) ppm. IR (KBr): ν = 2956, 2842, 1743, 1693, 1597, 1585, 1474, 1439, 1339, 1317, 1268, 1244, 1226, 1108, 1064, 1030, 993, 971, 886, 780, 758, 742 cm^{-1}. MS (EI): 233 (100), 334 (0.15); HRMS (EI) for $C_{14}H_{13}O_4F_3S$ Calcd: 334.0487, Found: 334.0481.

HPLC: (IE-3 (0.46 × 25 cm, 3 μm), Hexane/^{i}PrOH = 9/1, 0.7 mL/min, 214 nm), t_R (major) = 11.32 min, t_S (minor) = 9.80 min (96% ee); $[\alpha]_D^{25}$ = +1.8 (c = 0.100, $CHCl_3$, 96% ee).



(R)-Adamantan-1-yl-8-methoxy-1-oxo-2-((trifluoromethyl)thio)-1,2,3,4-tetrahydronaphthalene-2-carboxylate 3m.[4] Yield 90%, white solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.47 (d, *J* = 2.7 Hz, 1 H), 7.15 (d, *J* = 8.5 Hz, 1 H), 7.10 (dd, *J* = 8.5, 2.7 Hz, 1 H), 3.83 (s, 3 H), 3.21 – 3.11 (m, 1 H), 3.04 – 2.93 (m, 2 H), 2.52 – 2.44 (m, 1 H), 2.12 (s, 3 H), 2.01 (s, 6 H), 1.60 (s, 6 H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 189.60, 165.49, 158.58, 134.86, 131.69, 129.96 (q, *J* = 311.1 Hz), 129.92, 122.90, 109.99, 84.28, 65.37, 55.54, 40.71, 35.92, 33.16, 30.83, 25.71; ^{19}F NMR (376 MHz, $CDCl_3$) δ -35.48 (s, 3 F) ppm. IR (KBr): ν = 3063, 2940, 2231, 1728, 1612, 1492, 1473, 1407, 1368, 1346, 1260, 1107, 1086, 1022, 943, 845, 803, 757, 689, 556, 539 cm^{-1}. MS (DART POS): 477.1 (M+Na); HRMS (DART POS): $C_{23}H_{26}O_4F_3S$ (M+H) Calcd: 455.1498, Found: 455.1490.

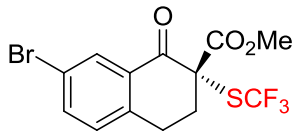
HPLC: (IE-3 (0.46 × 25 cm, 3 μm), Hexane/^{i}PrOH = 9/1, 0.7 mL/min, 214 nm), t_R (major) = 11.96 min, t_S (minor) = 9.53 min (98% ee); $[\alpha]_D^{25}$ = +37.1 (c = 0.100, $CHCl_3$, 98% ee).



(R)-Methyl-6,7-dimethoxy-1-oxo-2-((trifluoromethyl)thio)-1,2,3,4-tetrahydronap

hthalene-2-carboxylate 3n. Yield 95%, white solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.41 (s, 1 H), 6.62 (s, 1 H), 3.91 (s, 3 H), 3.87 (s, 3 H), 3.74 (s, 3 H), 3.18 (ddd, *J* = 16.5, 10.3, 4.6 Hz, 1 H), 3.11 – 3.03 (m, 1 H), 2.97 (dt, *J* = 17.3, 4.6 Hz, 1 H), 2.51 (ddd, *J* = 15.0, 10.3, 5.0 Hz, 1 H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 187.52, 167.58, 154.88, 148.44, 138.05, 129.91 (q, *J* = 309.1 Hz), 123.22, 110.00, 109.32, 64.00, 56.19, 56.01, 53.74, 33.18, 26.13; ^{19}F NMR (376 MHz, $CDCl_3$) δ -36.32 (s, 3 F) ppm. IR (KBr): ν = 3080, 3027, 2982, 2957, 2836, 1745, 1662, 1600, 1581, 1514, 1467, 1450, 1415, 1378, 1359, 1334, 1280, 1267, 1240, 1202, 1176, 1142, 1107, 1066, 1029, 995, 962, 909, 890, 870, 846, 793, 764, 757, 640, 586, 550 cm^{-1}. MS (EI): 150 (100), 364 (13); HRMS (EI) for $C_{15}H_{15}O_5F_3S$ Calcd: 364.0592, Found: 364.0590. Mp: 104.0 – 105.0 ^{o}C.

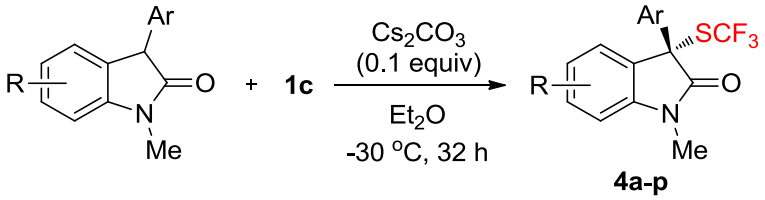
HPLC: (IE-3 (0.46 × 25 cm, 3 μm), Hexane/^{i}PrOH = 9/1, 0.7 mL/min, 214 nm), t_R (major) = 20.57 min, t_S (minor) = 19.05 min (95% ee); $[\alpha]_D^{25}$ = +8.3 (c = 0.100, $CHCl_3$, 95% ee).



(R)-Methyl-7-bromo-1-oxo-2-((trifluoromethyl)thio)-1,2,3,4-tetrahydronaphthalene-2-carboxylate 3o.[4] Yield 84%, white solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.13 – 8.06 (m, 1 H), 7.66 – 7.57 (m, 1 H), 7.14 (d, *J* = 8.2 Hz, 1 H), 3.76 (s, 3 H), 3.24 – 3.12 (m, 1 H), 3.12 – 2.99 (m, 2 H), 2.56 – 2.47 (m, *J* = 18.9, 1 H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 187.80, 167.11, 141.29, 137.47, 131.76, 131.17, 130.71, 128.10 (q, *J* = 310.7 Hz), 121.16, 63.98, 53.94, 32.59, 25.83; ^{19}F NMR (376 MHz, $CDCl_3$) δ -36.10 (s, 3 F) ppm.

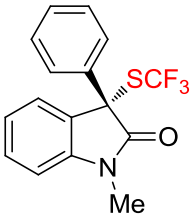
HPLC: (IE-3 (0.46 × 25 cm, 3 μm), Hexane/^{i}PrOH = 8/2, 0.7 mL/min, 214 nm), t_R (major) = 8.52 min, t_S (minor) = 7.47 min (96% ee); $[\alpha]_D^{25}$ = +8.00 (c = 0.100, $CHCl_3$, 96% ee).

General procedure for asymmetric trifluoromethylthiolation of oxindoles with reagent 1c.



4a-p

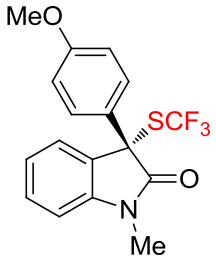
Oxindole (112 mg, 0.500 mmol, 1.0 equiv), cesium carbonate (16.3 mg, 0.0500 mmol, 0.1 equiv) and compound **1c** (206 mg, 0.550 mmol, 1.1 equiv) were added into a flame-dried Schlenk tube. The tube was putted into liquid nitrogen. Dry ethyl ether (2.5 mL) was added under argon atmosphere. The resulting solution was stirred at -30 ^{o}C for 32 h. After the reaction was completed as monitored by ^{19}F NMR spectroscopy, the reaction was quenched by HCl (2.0 M). The mixture was extracted with Et_2O (3 × 10.0 mL). The combined organic phase was separated and dried over anhydrous Na_2SO_4. After filtration, the solvent was removed under vacuum. The residue was purified by flash chromatography to (S)-1-methyl-3-phenyl-3-((trifluoromethyl)thio) indolin-2-one **4a** as a white solid (122 mg, 75.5% yield).



(S)-1-Methyl-3-phenyl-3-((trifluoromethyl)thio)indolin-2-one 4a. Yield 76%, white solid. Mp: 55.0 – 56.0 ^{o}C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.60 (m, 3 H), 7.42 (td, *J* = 7.8, 1.2 Hz, 1 H), 7.39 – 7.31 (m, 3 H), 7.22 (td, *J* = 7.6, 0.9 Hz, 1 H), 6.93 (d, *J* = 7.8 Hz, 1 H), 3.24 (s, 3 H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 174.21, 142.95, 134.21, 130.14, 129.16, 129.02, 128.69 (q, *J* = 310.6 Hz), 127.65, 127.47, 126.91, 123.11, 109.03, 58.85, 27.07; ^{19}F NMR (376 MHz, $CDCl_3$) δ -39.13 (s, 3 F) ppm. IR (KBr): ν = 3063, 2970, 2935, 1964, 1723, 1608, 1581, 1490, 1470, 1447, 1419, 1371, 1347, 1301, 1258, 1215, 1149, 1108, 1033, 1024, 1001, 949, 913, 885, 763, 756, 744, 709, 695, 657, 618, 605, 539, 511 cm^{-1}. MS (DART POS): 324.0 (M+H); HRMS (DART POS): $C_{16}H_{13}ONF_3S$ (M+H) Calcd: 324.0664, Found: 324.0661.

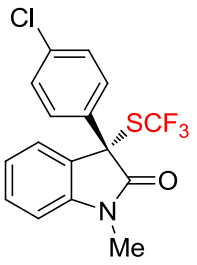
HPLC: (AD-H (0.46 × 25 cm, 5 μm), Hexane/^{i}PrOH = 95/5, 0.7 mL/min, 214 nm), t_S (major) = 9.83 min, t_R (minor) = 9.04 min (93% ee); $[\alpha]_D^{25}$ = +102.4 (c = 0.140, $CHCl_3$, 93% ee).

When compound **1b** was used as the electrophilic trifluoromethylthiolating reagent. Yield 69%. HPLC: (AD-H (0.46 × 25 cm, 5 μm), Hexane/^{i}PrOH = 95/5, 0.7 mL/min, 214 nm), t_S (major) = 9.57 min, t_R (minor) = 8.82 min (96% ee)^{b}; $[\alpha]_D^{25}$ = +127.1 (c = 0.100, $CHCl_3$, 96% ee).



(S)-3-(4-Methoxyphenyl)-1-methyl-3-((trifluoromethyl)thio)indolin-2-one 4b. Yield 86%, colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.62 – 7.52 (m, 3 H), 7.41 (td, *J* = 7.8, 1.1 Hz, 1 H), 7.21 (td, *J* = 7.6, 0.8 Hz, 1 H), 6.92 (d, *J* = 7.8 Hz, 1 H), 6.89 – 6.84 (m, 2 H), 3.76 (s, 3 H), 3.22 (s, 3 H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 174.40, 160.21, 142.90, 130.06, 129.11, 128.63 (q, *J* = 310.9 Hz), 127.61, 126.87, 125.63, 123.03, 114.36, 109.02, 58.37, 55.32, 27.00; ^{19}F NMR (376 MHz, $CDCl_3$) δ -39.43 (s, 3 F) ppm. IR (KBr): ν = 3059, 3004, 2937, 2839, 1728, 1611, 1578, 1509, 1492, 1472, 1419, 1369, 1344, 1304, 1256, 1185, 1108, 1086, 1033, 951, 937, 887, 839, 805, 756, 690, 580, 540 cm^{-1}. MS (DART POS): 354.0 (M+H); HRMS (DART POS): $C_{17}H_{15}O_2NF_3S$ (M+H) Calcd: 354.0770, Found: 354.0766.

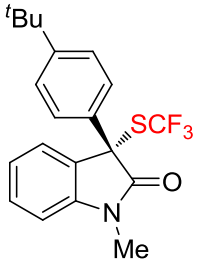
HPLC: (IE-3 (0.46 × 25 cm, 3 μm), Hexane/^{i}PrOH =75/3, 0.7 mL/min, 214 nm), t_S (major) = 8.26 min, t_R (minor) = 8.64 min (92% ee); $[\alpha]_D^{25}$ = +169.7 (c = 0.050, $CHCl_3$, 92% ee).



(S)-3-(4-Chlorophenyl)-1-methyl-3-((trifluoromethyl)thio)indolin-2-one 4c. Yield 72%, white solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.58 – 7.54 (m, 3 H), 7.43 (td, *J* = 7.8, 1.1 Hz, 1 H), 7.34 – 7.28 (m, 2 H), 7.23 (td, *J* = 7.6, 0.8 Hz, 1 H), 6.94 (d, *J* = 7.9 Hz, 1 H), 3.23 (s, 3 H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 173.76, 142.91, 135.46, 132.69, 130.40, 129.19, 129.15, 128.53 (q, *J* = 313.1 Hz), 126.96, 126.81, 123.27, 109.22, 58.27, 27.11; ^{19}F NMR (376 MHz, $CDCl_3$) δ -39.03 (s, 3 F) ppm. IR (KBr): ν = 3093, 3065, 1726, 1717, 1682, 1611, 1588, 1492, 1470, 1402, 1366, 1348, 1262, 1153, 1126, 1109, 1013, 942, 887, 837, 802, 754, 745, 689, 517 cm^{-1}. MS (DART POS): 358.0 (M+H); HRMS (DART POS): $C_{16}H_{12}ONClF_3S$ (M+H) Calcd: 358.0275, Found: 358.0273. Mp: 68.5 – 69.5 ^{o}C.

HPLC: (IE-3 (0.46 × 25 cm, 3 μm), Hexane/^{i}PrOH = 9/1, 0.7 mL/min, 214 nm), t_S (major) = 9.09 min, t_R (minor) = 9.47 min (88% ee); $[\alpha]_D^{25}$ = +107.6 (c = 0.150, $CHCl_3$, 88% ee).

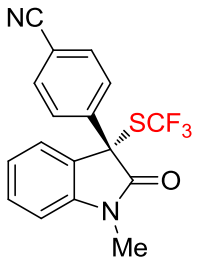
When compound **1b** was used as the electrophilic trifluoromethylthiolating reagent. Yield 95%. HPLC: (IE-3 (0.46 × 25 cm, 3 μm), Hexane/^{i}PrOH = 9/1, 0.7 mL/min, 214 nm), t_R (major) = 9.07 min, t_R (minor) = 9.42 min (93% ee)^{b}; $[\alpha]_D^{25}$ = +120.3 (c = 0.100, $CHCl_3$, 93% ee).



(S)-3-(4-(*tert*-Butyl)phenyl)-1-methyl-3-((trifluoromethyl)thio)indolin-2-one 4d. Yield 94%, colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.58 (m, 3 H), 7.47 – 7.35 (m, 3 H), 7.22 (td, *J* = 7.6, 0.9 Hz, 1 H), 6.93 (d, *J* = 7.9 Hz, 1 H), 3.23 (s, 3 H), 1.29 (s, 9 H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 174.36, 152.30, 142.97, 131.04, 130.07, 128.75 (q, *J* = 312.1 Hz), 127.66, 127.36, 126.90, 126.03, 123.04, 108.98, 58.66, 34.58, 31.16, 27.01; ^{19}F NMR (376 MHz, $CDCl_3$) δ -39.24 (s, 3 F) ppm. IR (KBr): ν = 3058, 2964, 1728, 1612, 1492, 1473, 1410, 1369, 1343, 1258, 1112, 1085, 1020, 942, 892, 836, 805, 756, 745, 690, 562, 540 cm^{-1}. MS (DART POS): 380.1 (M+H); HRMS (DART

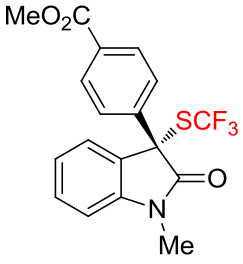
POS): $C_{20}H_{21}ONF_3S$ (M+H) Calcd: 380.1290, Found: 380.1288.

HPLC: (AD-H (0.46 × 25 cm, 5 μm), Hexane/^{i}PrOH = 95/5, 0.7 mL/min, 214 nm), t_S (major) = 8.00 min, t_R (minor) = 7.44 min (92% ee); $[\alpha]_D^{25}$ = +102.0 (c = 0.100, $CHCl_3$, 92% ee).



(S)-4-(1-Methyl-2-oxo-3-((trifluoromethyl)thio)indolin-3-yl)benzonitrile 4e. Yield 97%, colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.75 – 7.70 (m, 2 H), 7.64 – 7.60 (m, 2 H), 7.50 (d, *J* = 7.6 Hz, 1 H), 7.44 (td, *J* = 7.8, 1.2 Hz, 1 H), 7.22 (td, *J* = 7.6, 0.9 Hz, 1 H), 6.95 (d, *J* = 7.9 Hz, 1 H), 3.23 (s, 3 H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 173.04, 142.90, 139.48, 132.61, 130.77, 128.66, 128.44 (q, *J* = 312.1 Hz), 126.78, 126.27, 123.54, 118.04, 113.11, 109.46, 58.53, 27.23; ^{19}F NMR (376 MHz, $CDCl_3$) δ -38.61 (s, 3 F) ppm. IR (KBr): ν = 3060, 3000, 2953, 1717, 1611, 1572, 1492, 1473, 1436, 1407, 1368, 1343, 1281, 1191, 1108, 1020, 945, 894, 862, 827, 756, 700, 689, 540 cm^{-1}. MS (DART POS): 349.0 (M+H); HRMS (DART POS): $C_{17}H_{12}ON_2F_3S$ (M+H) Calcd: 349.0617, Found: 349.0616.

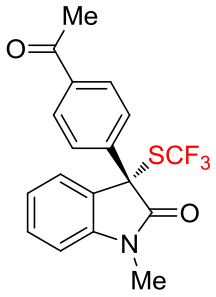
HPLC: (IC (0.46 × 25 cm, 5 μm), Hexane/^{i}PrOH = 8/2, 0.7 mL/min, 214 nm), t_S (major) = 16.37 min, t_R (minor) = 15.21 min (94% ee); $[\alpha]_D^{25}$ = +126.6 (c = 0.065, $CHCl_3$, 94% ee).



(S)-Methyl-4-(1-methyl-2-oxo-3-((trifluoromethyl)thio)indolin-3-yl)benzoate 4f. Yield 86%, colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.05 – 7.96 (m, 2 H), 7.71 – 7.64 (m, 2 H), 7.54 (d, *J* = 7.5 Hz, 1 H), 7.43 (td, *J* = 7.8, 1.1 Hz, 1 H), 7.22 (td, *J* =

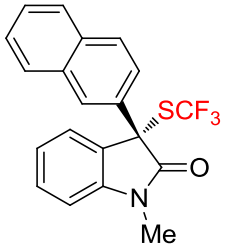
7.6, 0.8 Hz, 1 H), 6.94 (d, *J* = 7.8 Hz, 1 H), 3.88 (s, 3 H), 3.24 (s, 3 H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 173.54, 166.26, 142.90, 139.08, 130.77, 130.44, 130.10, 128.56 (q, *J* = 312.1 Hz), 127.77, 126.93, 126.81, 123.33, 109.23, 58.75, 52.26, 27.14; ^{19}F NMR (376 MHz, $CDCl_3$) δ -38.79 (s, 3 F) ppm. IR (KBr): ν = 2913, 2854, 1732, 1689, 1611, 1575, 1498, 1457, 1422, 1355, 1343, 1352, 1286, 1246, 1187, 1101, 1067, 1049, 964, 869, 834, 757, 731, 708, 628, 558 cm^{-1}. MS (DART POS): 382.0 (M+H); HRMS (DART POS): $C_{18}H_{15}O_3NF_3S$ (M+H) Calcd: 382.0719, Found: 382.0720.

HPLC: (IE-3 (0.46 × 25 cm, 3 μm), Hexane/^{i}PrOH = 8/2, 0.7 mL/min, 214 nm), t_S (major) = 15.62 min, t_R (minor) = 20.25 min (94% ee); $[\alpha]_D^{25}$ = +117.3 (c = 0.100, $CHCl_3$, 94% ee).



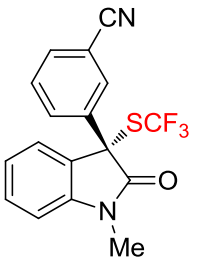
(S)-3-(4-Acetylphenyl)-1-methyl-3-((trifluoromethyl)thio)indolin-2-one 4g. Yield 95%, colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.91 (d, *J* = 8.4 Hz, 2 H), 7.69 (d, *J* = 8.4 Hz, 2 H), 7.53 (d, *J* = 7.5 Hz, 1 H), 7.43 (t, *J* = 7.8 Hz, 1 H), 7.22 (t, *J* = 7.6 Hz, 1 H), 6.95 (d, *J* = 7.9 Hz, 1 H), 3.24 (s, 3 H), 2.56 (s, 3 H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 197.29, 173.50, 142.88, 139.20, 137.35, 130.49, 128.54(q, *J* = 312.1 Hz), 128.81, 127.99, 126.87, 126.78, 123.37, 109.28, 58.75, 27.16, 26.66; ^{19}F NMR (376 MHz, $cdcl_3$) δ -38.79 (s, 3 F) ppm. IR (KBr): ν = 3061, 2940, 1729, 1686, 1611, 1568, 1492, 1473, 1421, 1406, 1367, 1346, 1267, 1191, 1108, 1087, 1019, 961, 944, 894, 845, 802, 756, 689, 595, 539 cm^{-1}. MS (DART POS): 366.1 (M+H); HRMS (DART POS): $C_{18}H_{15}O_2NF_3S$ (M+H) Calcd: 366.0770, Found: 366.0767.

HPLC: (IE-3 (0.46 × 25 cm, 3 μm), Hexane/^{i}PrOH = 8/2, 0.7 mL/min, 214 nm), t_S (major) = 18.47 min, t_R (minor) = 20.13 min (89% ee); $[\alpha]_D^{25}$ = +105.0 (c = 0.100, $CHCl_3$, 89% ee).



(S)-1-Methyl-3-(naphthalen-2-yl)-3-((trifluoromethyl)thio)indolin-2-one 4h. Yield 85%, white solid. Mp: 81.0 – 82.0 ^{o}C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.98 (s, 1 H), 7.84 (br, 2 H), 7.82 – 7.73 (m, 2 H), 7.65 (d, *J* = 7.5 Hz, 1 H), 7.53 – 7.40 (m, 3 H), 7.25 (td, *J* = 7.3, 1.0 Hz, 1 H), 6.94 (d, *J* = 7.4 Hz, 1 H), 3.25 (d, *J* = 1.8 Hz, 3 H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 174.03, 142.85, 133.10, 132.86, 131.30, 130.12, 128.89, 128.64 (q, *J* = 311.1 Hz), 128.34, 127.44, 127.41, 127.26, 127.03, 126.82, 126.54, 124.54, 123.08, 109.01, 59.05, 26.95; ^{19}F NMR (376 MHz, $CDCl_3$) δ -38.90 (d, *J* = 4.5 Hz, 3 F) ppm. IR (KBr): ν = 3420, 3057, 2965, 2936, 2886, 1961, 1720, 1608, 1491, 1472, 1418, 1373, 1350, 1261, 1144, 1125, 1027, 859, 825, 772, 759, 750, 691, 678, 539, 490 cm^{-1}. MS (DART POS): 374.0 (M+H); HRMS (DART POS): $C_{20}H_{15}ONF_3S$ (M+H) Calcd: 374.0821, Found: 374.0821.

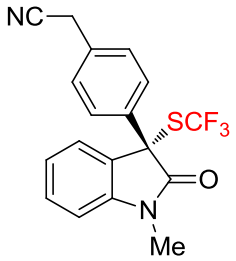
HPLC: (IE-3 (0.46 × 25 cm, 3 μm), Hexane/^{i}PrOH = 8/2, 0.7 mL/min, 214 nm), t_S (major) = 9.92 min, t_R (minor) = 10.42 min (95% ee); $[\alpha]_D^{25}$ = +88.9 (c = 0.100, $CHCl_3$, 95% ee).



(S)-3-(1-Methyl-2-oxo-3-((trifluoromethyl)thio)indolin-3-yl)benzonitrile 4i. Yield 88%, white solid. Mp: 117.0 – 119.0 ^{o}C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.96 (ddd, *J* = 8.1, 1.9, 1.1 Hz, 1 H), 7.80 (t, *J* = 1.3 Hz, 1 H), 7.62 (d, *J* = 7.7 Hz, 1 H), 7.55 – 7.42 (m, 3 H), 7.25 (t, *J* = 7.4 Hz, 1 H), 6.96 (d, *J* = 7.9 Hz, 1 H), 3.23 (s, 3 H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 173.12, 142.91, 136.12, 132.65, 132.48, 131.33, 130.82, 129.90, 128.42 (q, *J* = 312.1 Hz), 126.78, 126.13, 123.62, 118.07, 113.23, 109.49, 58.08, 27.21; ^{19}F NMR (376 MHz, $CDCl_3$) δ -38.73 (s, 3 F) ppm. IR (KBr): ν = 3072, 2969,

2938, 2229, 1728, 1688, 1579, 1494, 1474, 1417, 1370, 1350, 1304, 1261, 1155, 1112, 1022, 759, 687, 541 cm^{-1}. MS (DART POS): 349.0 (M+H); HRMS (DART POS): $C_{17}H_{12}ON_2F_3S$ (M+H) Calcd: 349.0617, Found: 349.0616.

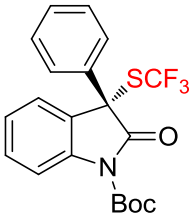
HPLC: (IE-3 (0.46 × 25 cm, 3 μm), Hexane/^{i}PrOH = 7/3, 0.7 mL/min, 214 nm), t_S (major) = 11.55 min, t_R (minor) = 13.17 min (93% ee); $[\alpha]_D^{25}$ = +84.6 (c = 0.100, $CHCl_3$, 93% ee).



(S)-2-(4-(1-Methyl-2-oxo-3-((trifluoromethyl)thio)indolin-3-yl)phenyl)acetonitrile 4j. Yield 87%, white solid. Mp: 105.0 – 106.0 ^{o}C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.62 (d, *J* = 8.5 Hz, 2 H), 7.54 (d, *J* = 7.5 Hz, 1 H), 7.43 (td, *J* = 7.8, 1.1 Hz, 1 H), 7.32 (d, *J* = 8.3 Hz, 2 H), 7.22 (td, *J* = 7.6, 0.8 Hz, 1 H), 6.95 (d, *J* = 7.9 Hz, 1 H), 3.72 (s, 2 H), 3.23 (s, 3 H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 173.83, 142.90, 134.36, 131.15, 130.39, 128.59, 128.58 (q, *J* = 311.1 Hz), 128.52, 127.07, 126.78, 123.29, 117.34, 109.22, 58.50, 27.11, 23.19; ^{19}F NMR (376 MHz, $CDCl_3$) δ -39.00 (s, 3 F) ppm. IR (KBr): ν = 3073, 2934, 2253, 1716, 1614, 1512, 1495, 1474, 1418, 1370, 1350, 1302, 1261, 1202, 1111, 1087, 1021, 946, 891, 836, 787, 762, 688, 541 cm^{-1}. MS (DART POS): 363.1 (M+H); HRMS (DART POS): $C_{17}H_{12}ON_2F_3S$ (M+H) Calcd: 363.0773, Found: 363.0771.

HPLC: (IE-3 (0.46 × 25 cm, 3 μm), Hexane/^{i}PrOH = 7/3, 0.7 mL/min, 214 nm), t_S (major) = 13.36 min, t_R (minor) = 14.52 min (57% ee); $[\alpha]_D^{25}$ = +72.4 (c = 0.110, $CHCl_3$, 57% ee).

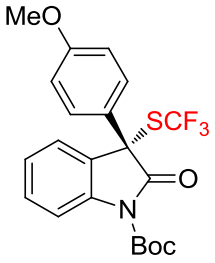
When compound **1b** was used as the electrophilic trifluoromethylthiolating reagent. Yield 97%. HPLC: (IE-3 (0.46 × 25 cm, 3 μm), Hexane/^{i}PrOH = 7/3, 0.7 mL/min, 214 nm), t_S (major) = 13.36 min, t_R (minor) = 14.52 min (94% ee)^{b}; $[\alpha]_D^{25}$ = +126.1 (c = 0.100, $CHCl_3$, 94% ee).



(S)-*tert*-Butyl-2-oxo-3-phenyl-3-((trifluoromethyl)thio)indoline-1-carboxylate 4k. Using reagent **1b** as the electrophilic trifluoromethylthiolating reagent. Yield 98%, yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.00 (d, *J* = 8.2 Hz, 1 H), 7.58 (dd, *J* = 7.6, 1.0 Hz, 1 H), 7.53 (m, 2 H), 7.47 (td, *J* = 8.2, 1.4 Hz, 1 H), 7.40 – 7.30 (m, 4 H), 1.63 (s, 9 H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 172.35, 148.93, 139.29, 134.10, 130.43, 129.43, 129.15, 128.62 (q, *J* = 312.1 Hz), 127.71, 126.95, 126.09, 124.86, 115.72, 85.04, 59.56, 28.00; ^{19}F NMR (376 MHz, $CDCl_3$) δ -38.81 (s, 3 F) ppm. IR (KBr): ν = 3062, 2941, 2231, 1728, 1612, 1493, 1473, 1408, 1368, 1345, 1260, 1136, 1108, 1086, 757, 689, 557, 539 cm^{-1}. MS (DART POS): 432.0 (M+Na); HRMS (DART POS): $C_{20}H_{22}O_3N_2F_3S$ (M+NH_4) Calcd: 427.1298, Found: 427.1295.

HPLC: (IE-3 (0.46 × 25 cm, 3 μm), Hexane/^{i}PrOH = 95/5, 0.7 mL/min, 214 nm), t_S (major) = 6.80 min, t_R (minor) = 7.28 min (93% ee); $[\alpha]_D^{25}$ = +56.4 (c = 0.100, $CHCl_3$, 93% ee).

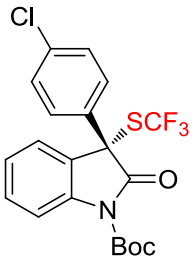
When compound **1b** was used as the electrophilic trifluoromethylthiolating reagent. Yield 92%. HPLC: (IE-3 (0.46 × 25 cm, 3 μm), Hexane/^{i}PrOH = 95/5, 0.7 mL/min, 214 nm), t_S (major) = 6.80 min, t_R (minor) = 7.28 min (91% ee)[b]; $[\alpha]_D^{25}$ = +47.6 (c = 0.175, $CHCl_3$, 91% ee).



(S)-*tert*-Butyl-3-(4-methoxyphenyl)-2-oxo-3-((trifluoromethyl)thio)indoline-1-carboxylate 4l. Using reagent **1b** as the electrophilic trifluoromethylthiolating reagent. Yield 94%, pale yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.97 (d, *J* = 8.2 Hz, 1 H), 7.58 (d, *J* = 7.5 Hz, 1 H), 7.45 (m, 3 H), 7.32 (t, *J* = 7.6 Hz, 1 H), 6.87 (d, *J* = 8.9 Hz,

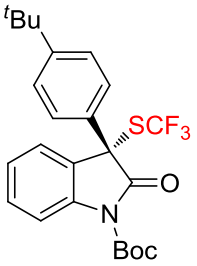
2 H), 3.76 (s, 3 H), 1.61 (s, 9 H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 172.52, 160.41, 148.97, 139.20, 130.32, 129.15, 128.54 (q, *J* = 312.1 Hz), 126.90, 126.27, 125.49, 124.77, 115.69, 114.48, 84.97, 59.11, 55.31, 27.99; ^{19}F NMR (376 MHz, $CDCl_3$) δ -39.08 (s, 3 F) ppm. IR (KBr): ν = 3079, 2982, 2935, 2840, 2561, 2258, 2053, 1774, 1735, 1605, 1579, 1508, 1479, 1467, 1418, 1395, 1371, 1341, 1289, 1255, 1146, 1033, 997, 866, 826, 756, 578, 530 cm^{-1}. MS (DART POS): 462.0 (M+Na); HRMS (DART POS): $C_{21}H_{24}O_4N_2F_3S$ (M+NH_4) Calcd: 457.1403, Found: 457.1398.

HPLC: (IE-3 (0.46 × 25 cm, 3 μm), Hexane/^{i}PrOH = 95/5, 0.7 mL/min, 214 nm), t_S (major) = 8.89 min, t_R (minor) = 11.49 min (93% ee); $[\alpha]_D^{25}$ = +46.5 (c = 0.125, $CHCl_3$, 93% ee).



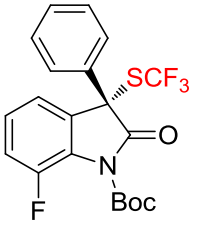
(S)-*tert*-Butyl-3-(4-chlorophenyl)-2-oxo-3-((trifluoromethyl)thio)indoline-1-carboxylate 4m. Using reagent **1b** as the electrophilic trifluoromethylthiolating reagent. Yield 99%, yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.98 (d, *J* = 8.2 Hz, 1 H), 7.54 (d, *J* = 7.5 Hz, 1 H), 7.50 – 7.44 (m, 3 H), 7.33 (m, 3 H), 1.62 (s, 9 H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 172.00, 148.79, 139.25, 135.83, 132.51, 130.67, 129.30, 129.20, 128.42 (q, *J* = 312.1 Hz), 126.81, 125.59, 124.99, 115.86, 85.25, 58.99, 27.98; ^{19}F NMR (376 MHz, $CDCl_3$) δ -38.77 (s, 3 F) ppm. IR (KBr): ν = 3078, 2983, 2934, 1771, 1739, 1606, 1589, 1489, 1479, 1467, 1401, 1371, 1340, 1289, 1251, 1110, 1046, 1015, 996, 868, 839, 819, 756, 729, 516 cm^{-1}. MS (DART POS): 466.0 (M+Na); HRMS (DART POS): $C_{20}H_{21}O_3N_2ClF_3S$ (M+NH_4) Calcd: 461.0908, Found: 461.0903.

HPLC: (IE-3 (0.46 × 25 cm, 3 μm), Hexane/^{i}PrOH = 95/5, 0.7 mL/min, 214 nm), t_S (major) = 6.43 min, t_R (minor) = 7.07 min (91% ee); $[\alpha]_D^{25}$ = +48.0 (c = 0.125, $CHCl_3$, 91% ee).



(S)-*tert*-Butyl-3-(4-(*tert*-butyl)phenyl)-2-oxo-3-((trifluoromethyl)thio)indoline-1-carboxylate 4n. Using reagent **1b** as the electrophilic trifluoromethylthiolating reagent. Yield 96%, colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.99 (d, *J* = 8.2 Hz, 1 H), 7.60 (d, *J* = 7.5 Hz, 1 H), 7.50 – 7.43 (m, 3 H), 7.39 (d, *J* = 8.6 Hz, 2 H), 7.33 (t, *J* = 7.6 Hz, 1 H), 1.63 (s, 9 H), 1.29 (s, 9 H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 172.49, 152.61, 148.98, 139.28, 130.92, 130.32, 128.65 (q, *J* = 312.1 Hz), 127.41, 126.95, 126.29, 126.16, 124.78, 115.68, 84.95, 59.35, 34.61, 31.13, 28.02; ^{19}F NMR (376 MHz, $CDCl_3$) δ -38.91 (s, 3 F) ppm. IR (KBr): ν = 2966, 2870, 1775, 1738, 1606, 1505, 1479, 1467, 1410, 1395, 1370, 1342, 1301, 1290, 1252, 1149, 1113, 1091, 1022, 825, 756, 562 cm^{-1}. MS (DART POS): 483.2 ($M+NH_4$); HRMS (DART POS): $C_{24}H_{30}O_3N_2F_3S$ ($M+NH_4$) Calcd: 483.1924, Found: 483.1919.

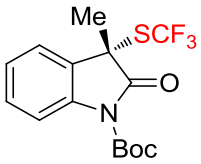
HPLC: (IE-3 (0.46 × 25 cm, 3 μm), Hexane/^{i}PrOH = 95/5, 0.7 mL/min, 214 nm), t_S (major) = 5.89 min, t_R (minor) = 6.65 min (93% ee); $[\alpha]_D^{25}$ = +63.9 (c = 0.050, $CHCl_3$, 93% ee).



(S)-*tert*-Butyl-7-fluoro-2-oxo-3-phenyl-3-((trifluoromethyl)thio)indoline-1-carboxylate 4o. Using reagent **1b** as the electrophilic trifluoromethylthiolating reagent. Yield 75%, colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.53 – 7.49 (m, 2 H), 7.37 (m, 4 H), 7.30 (td, *J* = 8.0, 4.4 Hz, 1 H), 7.24 – 7.18 (m, 1 H), 1.59 (s, 9 H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 172.07, 148.80 (d, *J* = 252.4 Hz), 147.06, 133.35, 129.64, 129.54, 129.28, 128.46 (q, *J* = 312.1), 127.52, 126.41 (d, *J* = 10.4 Hz), 125.80 (d, *J* = 6.9 Hz), 122.73 (d, *J* = 3.4 Hz), 118.43 (d, *J* = 20.4 Hz), 85.67, 59.66, 27.60; ^{19}F NMR (376

MHz, $CDCl_3$) δ -38.87 (s, 3 F), -118.76 (dd, *J* = 10.9, 4.2 Hz, 1 F) ppm. IR (KBr): ν = 3064, 2984, 2936, 1801, 1761, 1626, 1602, 1491, 1465, 1449, 1396, 1372, 1346, 1290, 1269, 1197, 1143, 1112, 1003, 844, 757, 746, 694, 586 cm^{-1}. MS (DART POS): 450.0 (M+Na); HRMS (DART POS): $C_{20}H_{21}O_3N_2F_4S$ (M+NH_4) Calcd: 445.1204, Found: 445.1198.

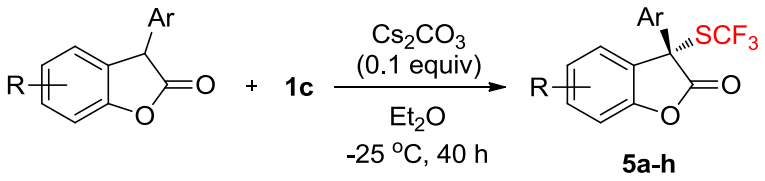
HPLC: (IE-3 (0.46 × 25 cm, 3 μm), Hexane/^{i}PrOH = 95/5, 0.7 mL/min, 214 nm), t_S (major) = 9.65 min, t_R (minor) = 11.05 min (88% ee); $[\alpha]_D^{25}$ = +49.2 (c = 0.125, $CHCl_3$, 88% ee).



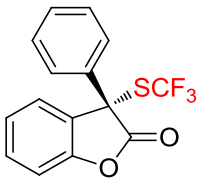
(S)-*tert*-Butyl 3-methyl-2-oxo-3-((trifluoromethyl)thio)indoline-1-carboxylate 4p. Yield 76%, colourless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.88 (d, *J* = 8.1 Hz, 1 H), 7.41 (d, *J* = 7.5 Hz, 1 H), 7.37 (td, *J* = 8.2, 1.1 Hz, 1 H), 7.22 (t, *J* = 7.5 Hz, 1 H), 1.72 (s, 3 H), 1.63 (s, 9 H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 173.87, 148.93, 138.46, 130.14, 128.83 (q, *J* = 311.1), 128.05, 125.03, 124.15, 115.51, 85.00, 52.76, 28.01, 24.06; ^{19}F NMR (376 MHz, $CDCl_3$) δ -38.41 (s, 3 F) ppm. IR (KBr): ν = 2983, 2932, 1801, 1777, 1736, 1607, 1541, 1480, 1468, 1396, 1372, 1344, 1304, 1290, 1251, 1151, 1115, 1101, 1074, 1005, 843, 776, 757, 704 cm^{-1}. MS (DART POS): 370.0 (M+Na); HRMS (DART POS): $C_{15}H_{20}O_3N_2F_3S$ (M+NH_4) Calcd: 365.1141, Found: 365.1139.

HPLC: (IE-3 (0.46 × 25 cm, 3 μm), Hexane/^{i}PrOH = 9/1, 0.7 mL/min, 214 nm), t_S (major) = 5.83 min, t_R (minor) = 6.22 min (79% ee); $[\alpha]_D^{25}$ = +71.9 (c = 0.150, $CHCl_3$, 79% ee).

General procedure for asymmetric trifluoromethylthiolation of benzofuranone with compound 1c

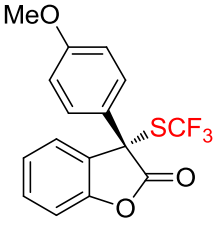


Benzofuranone (105 mg, 0.500 mmol, 1.0 equiv), cesium carbonate (16.3 mg , 0.0500 mmol, 0.1 equiv) and compound **1c** (206 mg, 0.550 mmol, 1.1 equiv) were added into a flame-dried Schlenk tube. The tube was putted into liquid nitrogen. Dry ethyl ether (2.5 mL) was added under argon atmosphere. The resulting solution was stirred at -25 ^{o}C for 40 h. After the reaction was completed as monitored by ^{19}F NMR spectroscopy, the reaction was quenched by HCl (2.0 M). The mixture was extracted using Et_2O (3 × 10.0 mL). The organic phase was separated and dried over anhydrous Na_2SO_4. After filtration, the solvent was removed under vacuum. The residue was purified by flash chromatography to give (S)-3-Phenyl-3-((trifluoromethyl)thio) benzofuran-2(3*H*)-one **5a** as a colorless oil (102 mg, 65.7% yield).



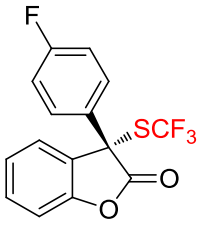
(S)-3-Phenyl-3-((trifluoromethyl)thio)benzofuran-2(3*H*)-one 5a. Yield 66%, colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.63 – 7.58 (m, 3 H), 7.47 (td, *J* = 8.0, 1.3 Hz, 1 H), 7.44 – 7.38 (m, 3 H), 7.35 (td, *J* = 7.6, 0.6 Hz, 1 H), 7.21 (d, *J* = 8.1 Hz, 1 H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 173.76, 152.42, 132.77, 131.17, 129.82, 129.40, 128.27 (q, *J* = 313.1), 127.47, 127.04, 125.64, 124.93, 111.68, 57.35; ^{19}F NMR (376 MHz, $CDCl_3$) δ -39.24 (s, 3 F) ppm. IR (KBr): ν = 2924, 1812, 1654, 1636, 1618, 1598, 1559, 1541, 1507, 1477, 1465, 1448, 1318, 1289, 1230, 1112, 1058, 948, 754, 694 cm^{-1}. MS (EI): 209 (100), 310 (0.72); HRMS (EI) for $C_{15}H_9O_2F_3S$ Calcd: 310.0275, Found: 310.0268.

HPLC: (IE-3 (0.46 × 25 cm, 3 μm), Hexane/^{i}PrOH = 98/2, 0.7 mL/min, 214 nm), t_S (major) = 8.25 min, t_R (minor) = 7.93 min (92% ee); $[\alpha]_D^{25}$ = +92.9 (c = 0.050, $CHCl_3$, 92% ee)



(S)-3-(4-Methoxyphenyl)-3-((trifluoromethyl)thio)benzofuran-2(3*H*)-one (5b): Yield 81%, yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.61 (dd, *J* = 7.6, 1.2 Hz, 1 H), 7.55 – 7.50 (m, 2 H), 7.46 (td, *J* = 7.9, 1.4 Hz, 1 H), 7.34 (td, *J* = 7.6, 1.0 Hz, 1 H), 7.20 (d, *J* = 8.1 Hz, 1 H), 6.94 – 6.88 (m, 2 H), 3.79 (s, 3 H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 173.94, 160.64, 152.38, 131.06, 128.96, 128.22 (q, *J* = 312.1), 127.00, 125.85, 124.86, 124.08, 114.72, 111.64, 56.89, 55.39; ^{19}F NMR (376 MHz, $CDCl_3$) δ -39.50 (s, 3 F) ppm. IR (KBr): ν = 2936, 2841, 1813, 1606, 1578, 1509, 1477, 1465, 1443, 1419, 1302, 1287, 1261, 1229, 1186, 1111, 1061, 1033, 951, 825, 756, 576 cm^{-1}. MS (DART POS): 363.0 (M+Na); HRMS (DART POS): $C_{16}H_{15}O_3NF_3S$ (M+NH_4) Calcd: 358.0719, Found: 358.0716.

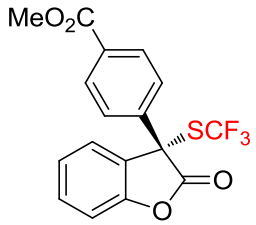
HPLC: (AD-H (0.46 × 25 cm, 5 μm), Hexane/^{i}PrOH = 9/1, 0.7 mL/min, 214 nm), t_S (major) = 7.95 min, t_R (minor) = 9.39 min (89% ee); $[\alpha]_D^{25}$ = +69.0 (c = 0.100, $CHCl_3$, 89% ee).



(S)-3-(4-Fluorophenyl)-3-((trifluoromethyl)thio)benzofuran-2(3*H*)-one 5c. Yield 90%, pink oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.64 – 7.59 (m, 3 H), 7.48 (td, *J* = 8.0, 1.4 Hz, 1 H), 7.36 (t, *J* = 7.6 Hz, 1 H), 7.22 (d, *J* = 8.1 Hz, 1 H), 7.13 – 7.05 (m, 2 H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 173.61, 163.38 (d, *J* = 251.4 Hz), 152.40, 131.37, 129.70 (d, *J* = 8.7 Hz), 128.43 (d, *J* = 3.0 Hz), 128.11 (q, *J* = 313.1), 126.96, 125.36, 125.07, 116.44 (d, *J* = 22.0 Hz), 111.81, 56.66; ^{19}F NMR (376 MHz, $CDCl_3$) δ -39.34

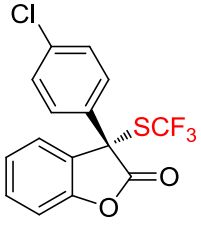
(s, 3 F), -110.70 (qd, *J* = 8.0, 5.2 Hz, 1 F) ppm. IR (KBr): ν = 3079, 1813, 1618, 1602, 1507, 1475, 1465, 1410, 1320, 1285, 1228, 1112, 1063, 1015, 953, 942, 827, 758, 684, 525 cm^{-1}. MS (DART POS): 351.0 (M+Na); HRMS (DART POS): $C_{15}H_{12}O_2NF_4S$ ($M+NH_4$) Calcd: 346.0519, Found: 346.0517.

HPLC: (AD-H (0.46 × 25 cm, 5 μm), Hexane/^{i}PrOH = 98/2, 0.7 mL/min, 214 nm), t_S (major) = 13.47 min, t_R (minor) = 16.35 min (64% ee); $[\alpha]_D^{25}$ = +71.0 (c = 0.100, $CHCl_3$, 64% ee).



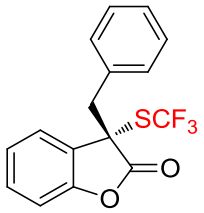
(S)-Methyl-4-(2-oxo-3-((trifluoromethyl)thio)-2,3-dihydrobenzofuran-3-yl)benzoate 5d. Yield 79%, yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.08 – 8.01 (m, 2 H), 7.67 (d, *J* = 8.6 Hz, 2 H), 7.59 (d, *J* = 7.6 Hz, 1 H), 7.47 (t, *J* = 7.9 Hz, 1 H), 7.34 (t, *J* = 7.6 Hz, 1 H), 7.21 (d, *J* = 8.1 Hz, 1 H), 3.90 (s, 3 H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 173.17, 165.98, 152.37, 137.39, 131.52, 131.44, 130.45, 128.13 (q, *J* = 313.1), 127.59, 126.94, 125.19, 125.06, 111.82, 57.19, 52.39; ^{19}F NMR (376 MHz, $CDCl_3$) δ -38.93 (d, *J* = 1.7 Hz, 3 F) ppm. IR (KBr): ν = 3002, 2955, 2848, 1816, 1728, 1618, 1599, 1573, 1507, 1476, 1465, 1434, 1408, 1319, 1282, 1229, 1192, 1108, 1061, 1020, 966, 926, 873, 845, 827, 757, 741, 724, 699, 684, 632 cm^{-1}. MS (DART POS): 369.0 (M+H); HRMS (DART POS): $C_{17}H_{12}O_4F_3S$ (M+H) Calcd: 369.0403, Found: 369.0400.

HPLC: (IE-3 (0.46 × 25 cm, 3 μm), Hexane/^{i}PrOH = 9/1, 0.7 mL/min, 214 nm), t_S (major) = 13.40 min, t_R (minor) = 16.24 min (81% ee); $[\alpha]_D^{25}$ = +61.1 (c = 0.100, $CHCl_3$, 81% ee).



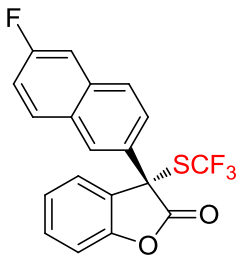
(S)-3-(4-Chlorophenyl)-3-((trifluoromethyl)thio)benzofuran-2(3*H*)-one 5e. Yield 88%, colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.59 (d, *J* = 7.6 Hz, 1 H), 7.55 (d, *J* = 8.7 Hz, 2 H), 7.48 (td, *J* = 7.9, 1.3 Hz, 1 H), 7.35 (m, 3 H), 7.22 (d, *J* = 8.1 Hz, 1 H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 173.40, 152.39, 136.25, 131.46, 131.20, 129.58, 128.97, 128.11 (q, *J* = 313.1 Hz), 126.93, 125.13, 111.83, 56.78; ^{19}F NMR (376 MHz, $CDCl_3$) δ -39.12 (s, 3 F) ppm. IR (KBr): ν = 2904, 1812, 1618, 1598, 1491, 1474, 1465, 1403, 1320, 1288, 1227, 1112, 1062, 1015, 954, 942, 921, 893, 870, 816, 757, 684, 513 cm^{-1}. MS (DART POS): 362.0 ($M+NH_4$); HRMS (DART POS): $C_{15}H_{12}O_2NClF_3S$ ($M+NH_4$) Calcd: 362.0221, Found: 362.0224.

HPLC: (AD-H (0.46 × 25 cm, 5 μm), Hexane/^{i}PrOH = 98/2, 0.7 mL/min, 214 nm), t_S (major) = 8.35 min, t_R (minor) = 9.55 min (86% ee); $[\alpha]_D^{25}$ = +68.3 (c = 0.075, $CHCl_3$, 86% ee).



(S)-3-Benzyl-3-((trifluoromethyl)thio)benzofuran-2(3*H*)-one 5f. Yield 76%, white solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.40 (d, *J* = 7.5 Hz, 1 H), 7.31 (td, *J* = 7.9, 1.4 Hz, 1 H), 7.23 (t, *J* = 7.6 Hz, 1 H), 7.20 – 7.11 (m, 3 H), 6.92 (d, *J* = 8.1 Hz, 1 H), 6.89 (d, *J* = 7.6 Hz, 2 H), 3.38 (m, 2 H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 174.40, 152.41, 131.70, 130.87, 130.33, 128.6 (q, *J* = 311.1 Hz), 128.39, 128.04, 125.38, 125.12, 124.59, 111.22, 55.96, 42.79; ^{19}F NMR (376 MHz, $CDCl_3$) δ -37.69 (s, 3 F) ppm. IR (KBr): ν = 3054, 3032, 2932, 1805, 1619, 1601, 1584, 1495, 1479, 1464, 1320, 1293, 1225, 1168, 1109, 1083, 1063, 1016, 975, 880, 772, 758, 750, 720, 700, 682, 623, 585, 521 cm^{-1}. MS (DART POS): 342.1 ($M+NH_4$); HRMS (DART POS): $C_{16}H_{15}O_2NF_3S$ ($M+NH_4$) Calcd: 342.0770, Found: 342.0767. Mp: 57.5 – 58.5 ^{o}C.

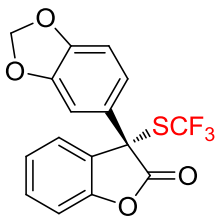
HPLC: (AD-H (0.46 × 25 cm, 5 μm), Hexane/^{i}PrOH = 98/2, 0.7 mL/min, 214 nm), t_S (major) = 8.18 min, t_R (minor) = 9.04 min (83% ee); $[\alpha]_D^{25}$ = +46.9 (c = 0.100, $CHCl_3$, 83% ee).



(S)-3-(6-Fluoronaphthalen-2-yl)-3-((trifluoromethyl)thio)benzofuran-2(3*H*)-one

5g. Yield 88%, pale yellow solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.98 (s, 1 H), 7.85 (d, *J* = 1.1 Hz, 2 H), 7.82 (dd, *J* = 9.0, 5.6 Hz, 1 H), 7.72 (d, *J* = 7.6 Hz, 1 H), 7.53 (td, *J* = 7.9, 1.4 Hz, 1 H), 7.46 (dd, *J* = 9.5, 2.5 Hz, 1 H), 7.42 (td, *J* = 7.6, 0.6 Hz, 1 H), 7.35 – 7.26 (m, 2 H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 173.65, 161.58 (d, *J* = 249.1 Hz), 152.47, 134.29 (d, *J* = 9.7 Hz), 131.35, 131.10 (d, *J* = 9.3 Hz), 129.92, 129.27, 128.89 (d, *J* = 5.4 Hz), 128.26 (q, *J* = 313.1), 127.54, 127.05, 125.57, 125.09, 125.06, 117.53 (d, *J* = 25.5 Hz), 111.82, 110.87 (d, *J* = 20.7 Hz), 57.49; ^{19}F NMR (376 MHz, $CDCl_3$) δ -38.98 (s, 3 F), -111.48 – -111.57 (m, 1 F) ppm. IR (KBr): ν = 3068, 2921, 2361, 1809, 1636, 1620, 1599, 1575, 1508, 1479, 1466, 1377, 1320, 1230, 1155, 1116, 1066, 1017, 981, 961, 945, 926, 867, 797, 753, 738, 686, 657 cm^{-1}. MS (DART POS): 396.1 ($M+NH_4$); HRMS (DART POS): $C_{19}H_{14}O_2NF_4S$ ($M+NH_4$) Calcd: 396.0676, Found: 396.0672. Mp: 79.5 – 80.5 ^{o}C.

HPLC: (IE-3 (0.46 × 25 cm, 3 μm), Hexane/^{i}PrOH = 95/5, 0.7 mL/min, 214 nm), t_S (major) = 9.02 min, t_R (minor) = 9.44 min (84% ee); $[\alpha]_D^{25}$ = +43.3 (c = 0.100, $CHCl_3$, 84% ee).



(S)-3-(Benzo[d][1,3]dioxol-5-yl)-3-((trifluoromethyl)thio)benzofuran-2(3*H*)-one

5h. Yield 83%, yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.59 (d, *J* = 7.6 Hz, 1 H), 7.46 (t, *J* = 7.9 Hz, 1 H), 7.34 (t, *J* = 7.6 Hz, 1 H), 7.19 (d, *J* = 8.1 Hz, 1 H), 7.15 (d, *J* = 1.9 Hz, 1 H), 7.01 (dd, *J* = 8.3, 1.9 Hz, 1 H), 6.77 (d, *J* = 8.3 Hz, 1 H), 5.97 (s, 2 H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 173.73, 152.35, 148.98, 148.64, 131.20, 128.17 (q, *J* =

312.1), 127.02, 125.83, 125.64, 124.93, 121.79, 111.66, 108.62, 108.04, 101.88, 57.08; ^{19}F NMR (376 MHz, $CDCl_3$) δ -39.40 (s, 3 F) ppm. IR (KBr): ν = 2904, 1812, 1618, 1599, 1505, 1489, 1465, 1439, 1352, 1320, 1290, 1253, 1236, 1111, 1062, 1040, 931, 812, 757, 685 cm^{-1}. MS (DART POS): 372.1 ($M+NH_4$); HRMS (DART POS): $C_{16}H_{13}O_4NF_3S$ ($M+NH_4$) Calcd: 372.0512, Found: 372.0509.

HPLC: (AD-H (0.46 × 25 cm, 5 μm), Hexane/^{i}PrOH = 8/2, 0.7 mL/min, 214 nm), t_S (major) = 6.61 min, t_R (minor) = 7.35 min (72% ee); $[\alpha]_D^{25}$ = +58.9 (c = 0.140, $CHCl_3$, 72% ee).

References

1. Duhamel. L.; Ple. G., Angibaud. P. *Synth. Commun.* **1993**, *23*, 2423.

2. Teverovskiy, G.; Surry, D. S.; Buchwald, S. L. *Angew. Chem. Int. Ed.* **2011**, *50*, 7312.

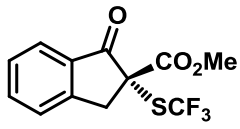
3. Xu, C.; Ma, B.; Shen, Q. *Angew. Chem. Int. Ed.* **2014**, *53*, 9316.

4. Shao, X.; Wang, X.; Yang, T.; Lu, L.; Shen, Q. *Angew. Chem. Int. Ed.* **2013**, *52*, 3457.

5. Wang, X.; Yang, T.; Cheng, X. *Angew. Chem. Int. Ed.* **2013**, *52*, 12860.

HPLC spectra of 3a-o, 4a-p and 5a-h

HPLC spectra for compound 3a



3a

HPLC: (IE (0.46 × 25 cm, 3 μm), Hexane/iPrOH = 97/3, 0.7 mL/min, 214 nm), t_R (major) = 12.13 min, t_R (minor) = 12.93 min (88% ee); $[\alpha]_D^{25}$ = -99.2 (c = 0.110, $CHCl_3$, 88% ee).

Operator:GC Timebase:U3000 Sequence:WXL-2

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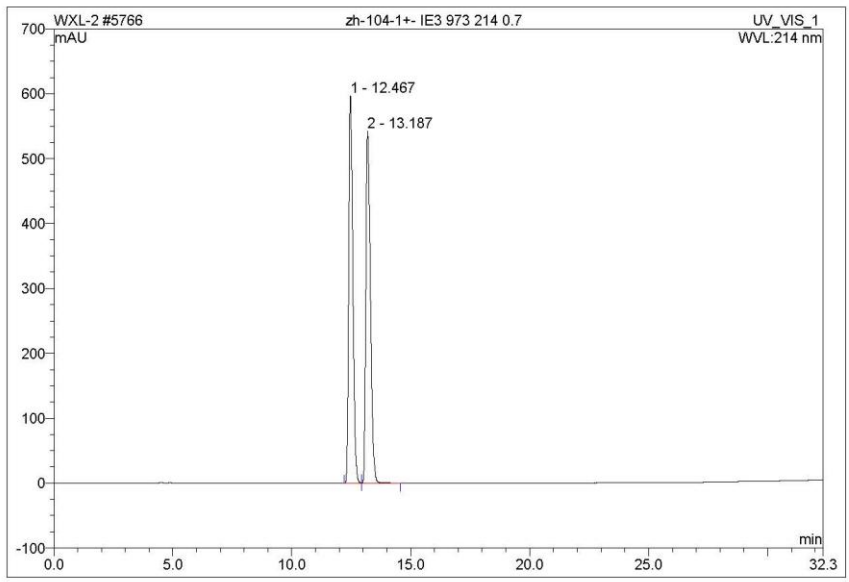
5766 zh-104-1+- IE3 973 214 0.7

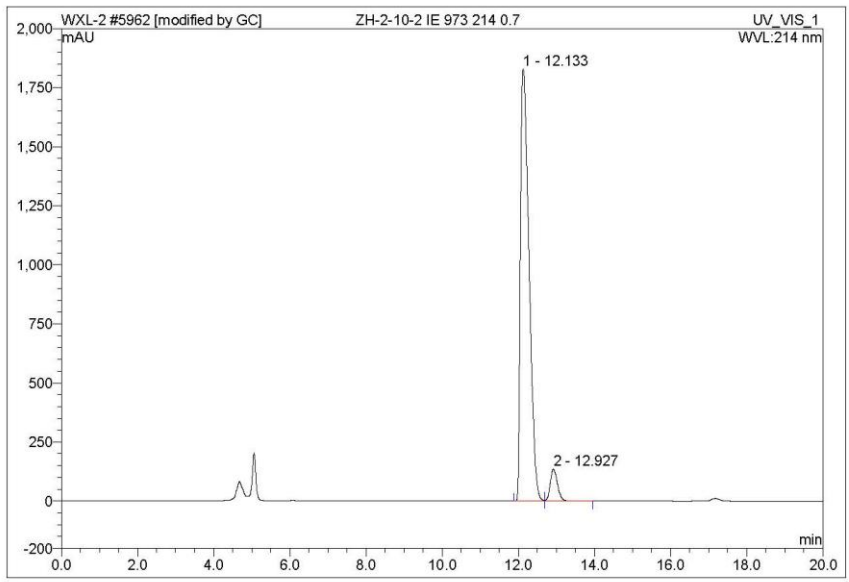
Sample Name:	**zh-104-1+- IE3 973 214 0.7**	*Injection Volume:*	**1.0**
Vial Number:	**RA2**	*Channel:*	**UV_VIS_1**
Sample Type:	**unknown**	*Wavelength:*	**214**
Control Program:	**WXL-2014**	*Bandwidth:*	**n.a.**
Quantif. Method:	**WXL**	*Dilution Factor:*	**1.0000**
Recording Time:	**2015/11/16 15:16**	*Sample Weight:*	**1.0000**
Run Time (min):	**32.33**	*Sample Amount:*	**1.0000**



No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	12.47	n.a.	597.042	119.942	49.69	n.a.	BM
2	13.19	n.a.	542.594	121.446	50.31	n.a.	MB
Total:			1139.637	241.388	100.00	0.000	

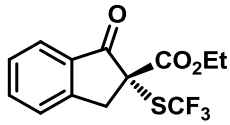
5962 ZH-2-10-2 IE 973 214 0.7

Sample Name:	**ZH-2-10-2 IE 973 214 0.7**	*Injection Volume:*	**2.0**
Vial Number:	**RE2**	*Channel:*	**UV_VIS_1**
Sample Type:	**unknown**	*Wavelength:*	**214**
Control Program:	**WXL-2014**	*Bandwidth:*	**n.a.**
Quantif. Method:	**WXL**	*Dilution Factor:*	**1.0000**
Recording Time:	**2015/12/14 17:54**	*Sample Weight:*	**1.0000**
Run Time (min):	**20.00**	*Sample Amount:*	**1.0000**



No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	12.13	n.a.	1828.604	479.317	94.10	n.a.	BM
2	12.93	n.a.	135.723	30.065	5.90	n.a.	MB
Total:			1964.327	509.382	100.00	0.000	

HPLC spectra for compound 3b



3b

HPLC: (IF-3 (0.46 × 25 cm, 3 μm), Hexane/^{i}PrOH = 98/2, 0.7 mL/min, 214 nm), t_R (major) = 13.50 min, t_R (minor) = 14.74 min (90% ee); $[\alpha]_D^{25}$ = -81.9 (c = 0.145, $CHCl_3$, 90% ee).

Operator:Administrator Timebase:HPLC Sequence:20151027-DAD

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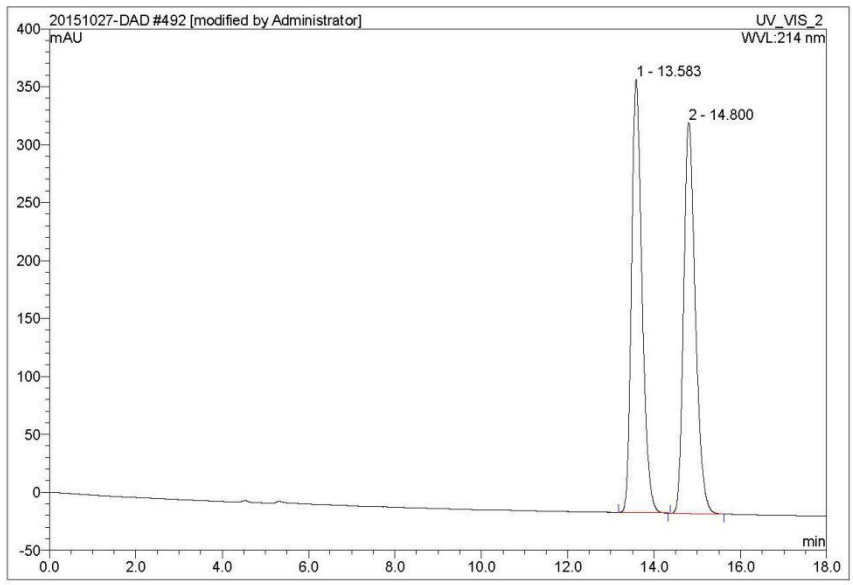
492 ZH-2-11-1+- IF3 982 214 0.7

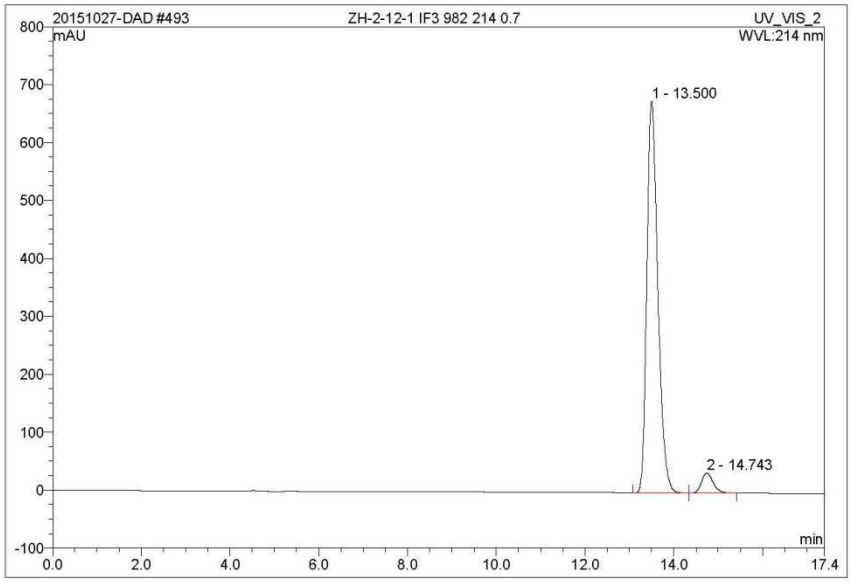
Sample Name:	**ZH-2-11-1+- IF3 982 214 0.7**	*Injection Volume:*	**1.0**
Vial Number:	**RB5**	*Channel:*	**UV_VIS_2**
Sample Type:	**unknown**	*Wavelength:*	**214.0**
Control Program:	**test-dad**	*Bandwidth:*	**4**
Quantif. Method:	**WXL**	*Dilution Factor:*	**1.0000**
Recording Time:	**2015-12-18 17:12**	*Sample Weight:*	**1.0000**
Run Time (min):	**17.98**	*Sample Amount:*	**1.0000**



No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	13.58	n.a.	373.797	105.165	49.83	n.a.	BM *
2	14.80	n.a.	337.334	105.893	50.17	n.a.	BMB
Total:			711.131	211.058	100.00	0.000	

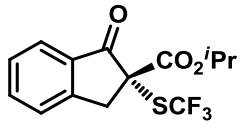
493 ZH-2-12-1 IF3 982 214 0.7

Sample Name:	**ZH-2-12-1 IF3 982 214 0.7**	*Injection Volume:*	**1.0**
Vial Number:	**RB4**	*Channel:*	**UV_VIS_2**
Sample Type:	**unknown**	*Wavelength:*	**214.0**
Control Program:	**test-dad**	*Bandwidth:*	**4**
Quantif. Method:	**WXL**	*Dilution Factor:*	**1.0000**
Recording Time:	**2015-12-18 17:31**	*Sample Weight:*	**1.0000**
Run Time (min):	**17.39**	*Sample Amount:*	**1.0000**



No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	13.50	n.a.	676.367	194.148	94.82	n.a.	BM
2	14.74	n.a.	34.708	10.603	5.18	n.a.	MB
Total:			711.075	204.751	100.00	0.000	

HPLC spectra for compound 3c



3c

HPLC: (IE-3 (0.46 × 25 cm, 3 μm), Hexane/^{i}PrOH = 98/2, 0.7 mL/min, 214 nm), t_R (major) = 11.87 min, t_R (minor) = 12.93 min (89% ee); $[\alpha]_D^{25}$ = -83.9 (c = 0.125, $CHCl_3$, 89% ee).

Operator:Administrator Timebase:HPLC Sequence:20151027-DAD

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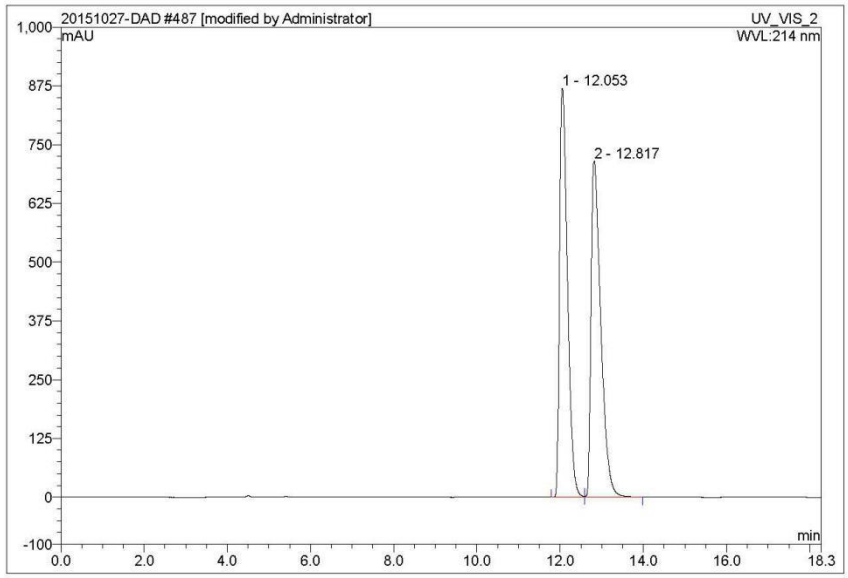
2016-7-22 8:04 下午

487 ZH-2-11-2+- IE3 982 214 0.7

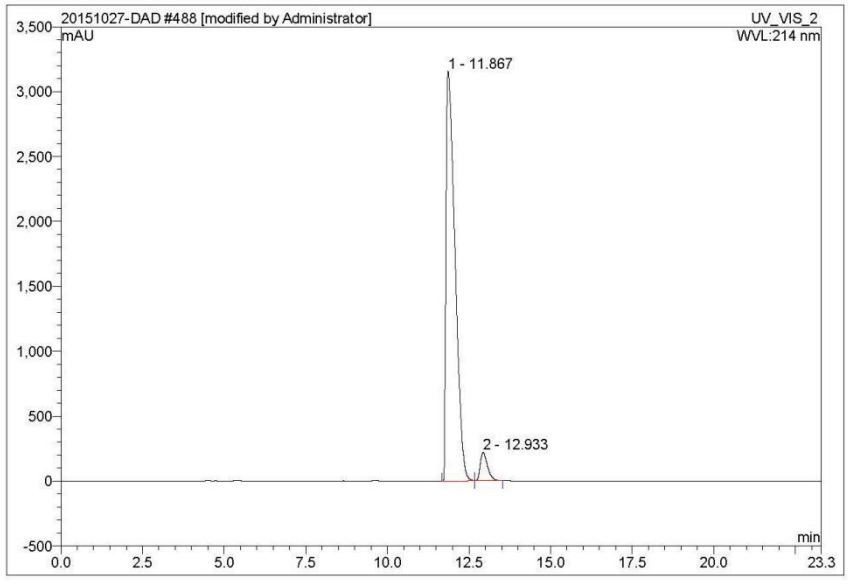
Sample Name:	**ZH-2-11-2+- IE3 982 214 0.7**	*Injection Volume:*	**2.0**
Vial Number:	**RC5**	*Channel:*	**UV_VIS_2**
Sample Type:	**unknown**	*Wavelength:*	**214.0**
Control Program:	**test-dad**	*Bandwidth:*	**4**
Quantif. Method:	**WXL**	*Dilution Factor:*	**1.0000**
Recording Time:	**2015-12-18 15:31**	*Sample Weight:*	**1.0000**
Run Time (min):	**18.27**	*Sample Amount:*	**1.0000**



No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	12.05	n.a.	869.901	191.246	49.60	n.a.	BM
2	12.82	n.a.	714.611	194.322	50.40	n.a.	MB
Total:			1584.512	385.569	100.00	0.000	

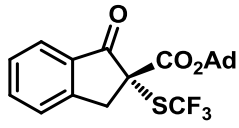
488 ZH-2-12-2 IE3 982 214 0.7

Sample Name:	**ZH-2-12-2 IE3 982 214 0.7**	*Injection Volume:*	**2.0**
Vial Number:	**RC4**	*Channel:*	**UV_VIS_2**
Sample Type:	**unknown**	*Wavelength:*	**214.0**
Control Program:	**test-dad**	*Bandwidth:*	**4**
Quantif. Method:	**WXL**	*Dilution Factor:*	**1.0000**
Recording Time:	**2015-12-18 15:51**	*Sample Weight:*	**1.0000**
Run Time (min):	**23.29**	*Sample Amount:*	**1.0000**



No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	11.87	n.a.	3155.627	1007.611	94.71	n.a.	BM
2	12.93	n.a.	218.063	56.259	5.29	n.a.	MB
Total:			3373.689	1063.870	100.00	0.000	

HPLC spectra for compound 3d



3d

HPLC: (IE-3 (0.46 × 25 cm, 3 μm), Hexane/^{i}PrOH = 95/5, 0.7 mL/min, 214 nm), t_R (major) = 10.95 min, t_R (minor) = 11.91 min (92% ee); $[\alpha]_D^{25}$ = -71.7 (c = 0.050, $CHCl_3$, 92% ee).

Operator:Administrator Timebase:HPLC Sequence:20151027-DAD

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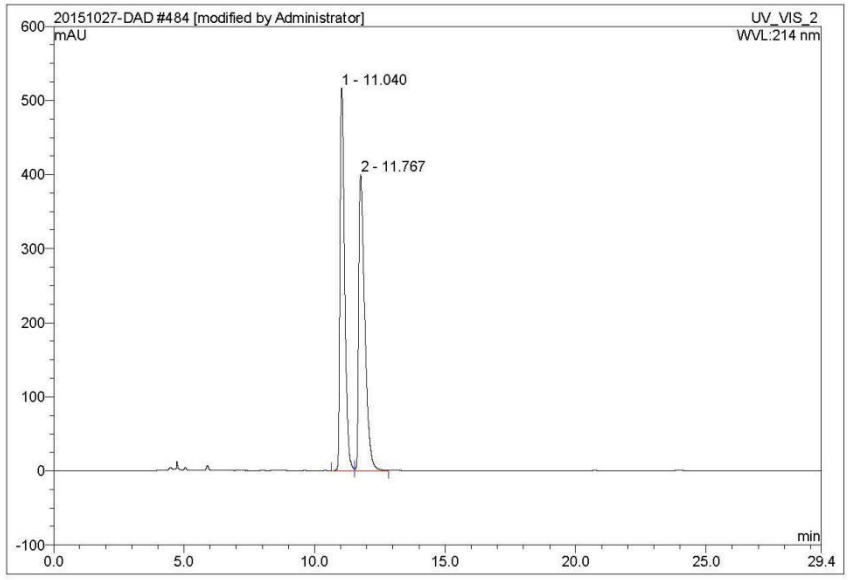
2016-7-22 8:05 下午

484 ZH-2-11-3+- IE3 955 214 0.7

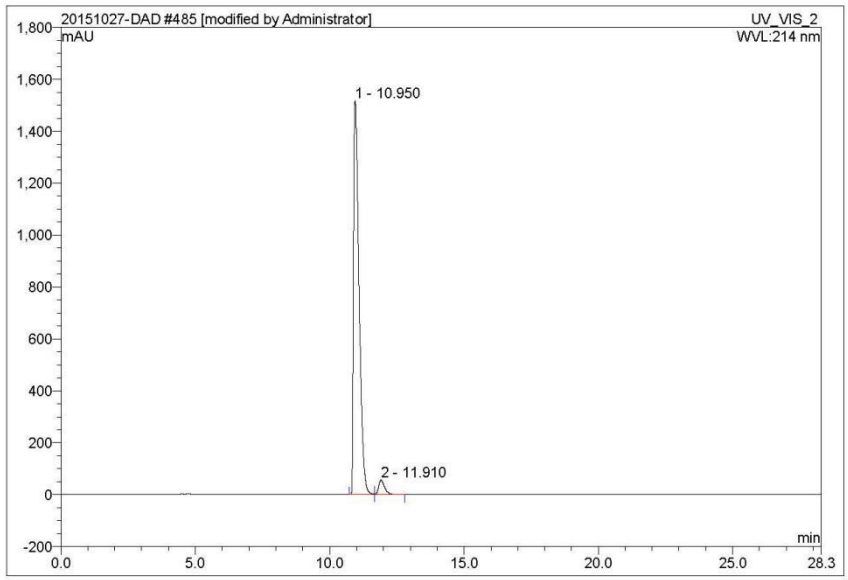
Sample Name:	**ZH-2-11-3+- IE3 955 214 0.7**	*Injection Volume:*	**2.0**
Vial Number:	**RD5**	*Channel:*	**UV_VIS_2**
Sample Type:	**unknown**	*Wavelength:*	**214.0**
Control Program:	**test-dad**	*Bandwidth:*	**4**
Quantif. Method:	**WXL**	*Dilution Factor:*	**1.0000**
Recording Time:	**2015-12-18 13:37**	*Sample Weight:*	**1.0000**
Run Time (min):	**29.40**	*Sample Amount:*	**1.0000**



No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	11.04	n.a.	516.637	107.335	49.80	n.a.	BM *
2	11.77	n.a.	399.604	108.215	50.20	n.a.	M *
Total:			916.242	215.550	100.00	0.000	

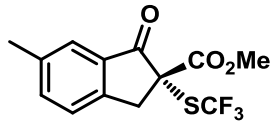
485 ZH-2-12-3 IE3 955 214 0.7

Sample Name:	**ZH-2-12-3 IE3 955 214 0.7**	*Injection Volume:*	**2.0**
Vial Number:	**RD4**	*Channel:*	**UV_VIS_2**
Sample Type:	**unknown**	*Wavelength:*	**214.0**
Control Program:	**test-dad**	*Bandwidth:*	**4**
Quantif. Method:	**WXL**	*Dilution Factor:*	**1.0000**
Recording Time:	**2015-12-18 14:08**	*Sample Weight:*	**1.0000**
Run Time (min):	**28.29**	*Sample Amount:*	**1.0000**



No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	10.95	n.a.	1518.122	361.300	96.10	n.a.	BM
2	11.91	n.a.	56.123	14.675	3.90	n.a.	MB
Total:			1574.244	375.975	100.00	0.000	

HPLC spectra for compound 3e



3e

HPLC: (IE-3 (0.46 ×25 cm, 3 μm), Hexane/^{i}PrOH = 7/3, 0.7 mL/min, 214 nm), t_R (major) = 6.89 min, t_R (minor) = 7.21 min (91% ee); $[\alpha]_D^{25}$ = -96.5 (c = 0.100, $CHCl_3$, 91% ee).

Operator:Administrator Timebase:HPLC Sequence:20151027-DAD

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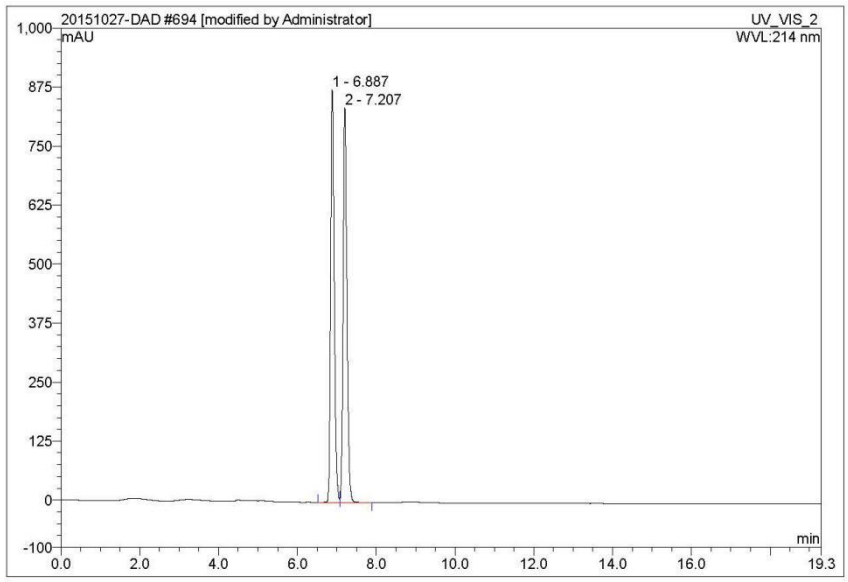
2016-7-22 8:01 下午

694 ZH-2-19-4 IE3 73 214 0.7

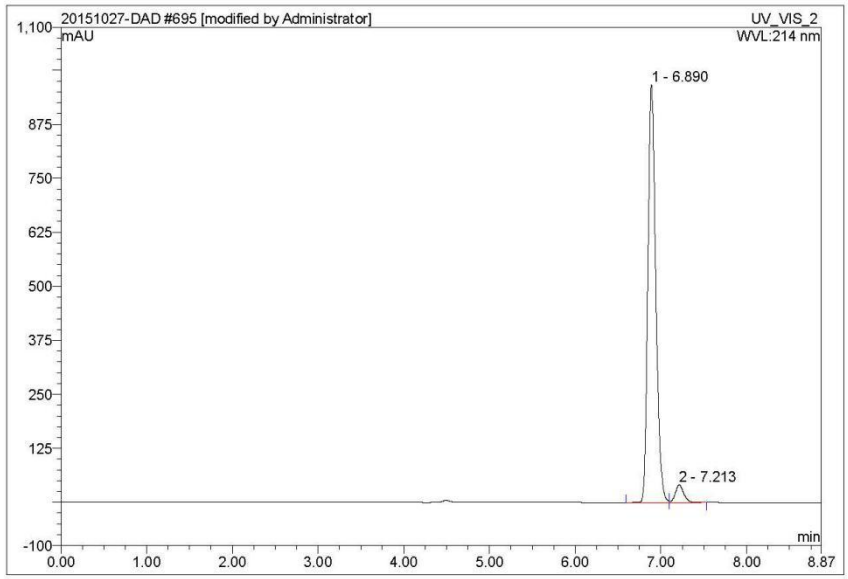
Sample Name:	**ZH-2-19-4 IE3 73 214 0.7**	*Injection Volume:*	**1.0**
Vial Number:	**RE5**	*Channel:*	**UV_VIS_2**
Sample Type:	**unknown**	*Wavelength:*	**214.0**
Control Program:	**test-dad2**	*Bandwidth:*	**4**
Quantif. Method:	**WXL**	*Dilution Factor:*	**1.0000**
Recording Time:	**2016-1-8 15:42**	*Sample Weight:*	**1.0000**
Run Time (min):	**19.29**	*Sample Amount:*	**1.0000**



No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	6.89	n.a.	874.646	93.349	49.76	n.a.	BM *
2	7.21	n.a.	836.328	94.239	50.24	n.a.	MB*
Total:			1710.974	187.587	100.00	0.000	

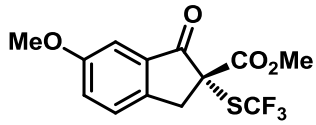
695 ZH-2-18-4 IE3 73 214 0.7

Sample Name:	**ZH-2-18-4 IE3 73 214 0.7**	*Injection Volume:*	**2.0**
Vial Number:	**RD5**	*Channel:*	**UV_VIS_2**
Sample Type:	**unknown**	*Wavelength:*	**214.0**
Control Program:	**test-dad2**	*Bandwidth:*	**4**
Quantif. Method:	**WXL**	*Dilution Factor:*	**1.0000**
Recording Time:	**2016-1-8 16:03**	*Sample Weight:*	**1.0000**
Run Time (min):	**8.87**	*Sample Amount:*	**1.0000**



No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	6.89	n.a.	967.686	103.083	95.69	n.a.	BM *
2	7.21	n.a.	41.137	4.642	4.31	n.a.	MB*
Total:			1008.823	107.725	100.00	0.000	

HPLC spectra for compound 3f



3f

HPLC: (IE-3 (0.46 × 25 cm, 3 μm), Hexane/^{i}PrOH = 95/5, 0.7 mL/min, 214 nm), t_R (major) = 13.41 min, t_R (minor) = 15.20 min (91% ee); $[\alpha]_D^{25}$ = -74.1 (c = 0.100, $CHCl_3$, 91% ee).

Operator:Administrator Timebase:HPLC Sequence:20151027-DAD

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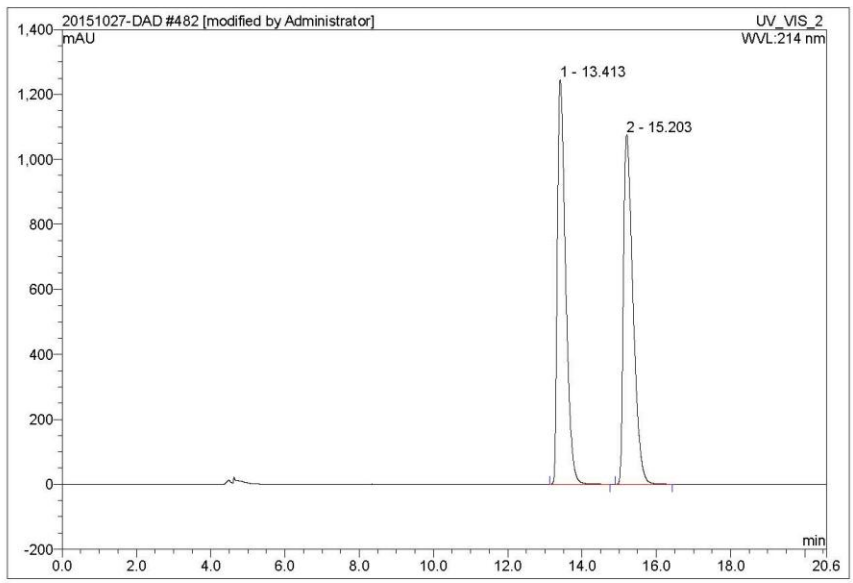
2016-12-29 11:08 下午

482 ZH-2-14-2+- IE3 955 214 0.7

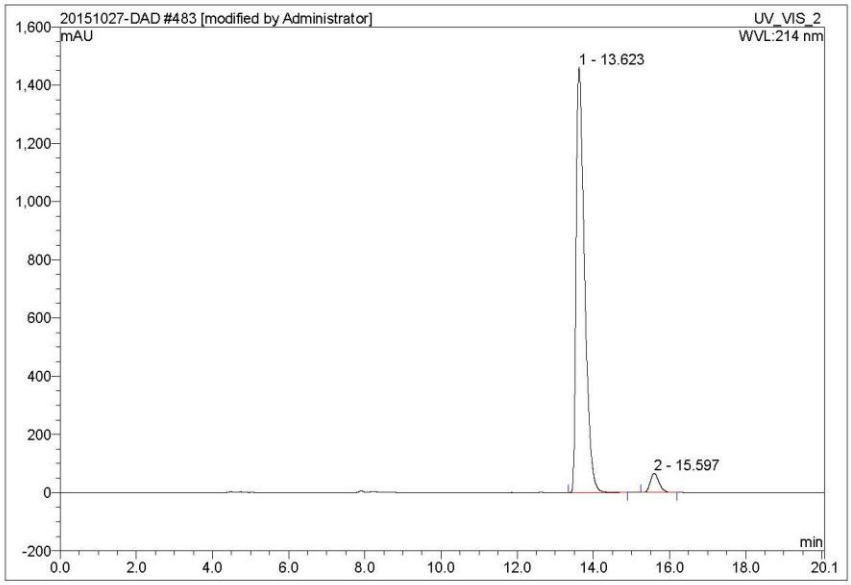
Sample Name:	**ZH-2-14-2+- IE3 955 214 0.7**	*Injection Volume:*	**3.0**
Vial Number:	**RE5**	*Channel:*	**UV_VIS_2**
Sample Type:	**unknown**	*Wavelength:*	**214.0**
Control Program:	**test-dad**	*Bandwidth:*	**4**
Quantif. Method:	**WXL**	*Dilution Factor:*	**1.0000**
Recording Time:	**2015-12-18 12:54**	*Sample Weight:*	**1.0000**
Run Time (min):	**20.58**	*Sample Amount:*	**1.0000**



No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	13.41	n.a.	1245.921	319.966	49.94	n.a.	BMB
2	15.20	n.a.	1075.455	320.683	50.06	n.a.	BMB
Total:			2321.377	640.649	100.00	0.000	

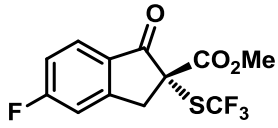
483 ZH-2-14-4 IE3 955 214 0.7

Sample Name:	**ZH-2-14-4 IE3 955 214 0.7**	*Injection Volume:*	**2.0**
Vial Number:	**RE4**	*Channel:*	**UV_VIS_2**
Sample Type:	**unknown**	*Wavelength:*	**214.0**
Control Program:	**test-dad**	*Bandwidth:*	**4**
Quantif. Method:	**WXL**	*Dilution Factor:*	**1.0000**
Recording Time:	**2015-12-18 13:15**	*Sample Weight:*	**1.0000**
Run Time (min):	**20.06**	*Sample Amount:*	**1.0000**



No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	13.62	n.a.	1461.436	373.620	95.46	n.a.	BMB
2	15.60	n.a.	66.602	17.763	4.54	n.a.	BMB
Total:			1528.038	391.383	100.00	0.000	

HPLC spectra for compound 3g



3g

HPLC: (IE-3 (0.46 × 25 cm, 3 μm), Hexane/^{i}PrOH = 8/2, 0.7 mL/min, 214 nm), t_R (major) = 6.97 min, t_R (minor) = 7.45 min (86% ee); $[\alpha]_D^{25}$ = -49.4 (c = 0.100, $CHCl_3$, 86% ee).

Operator:Administrator Timebase:HPLC Sequence:20151027-DAD

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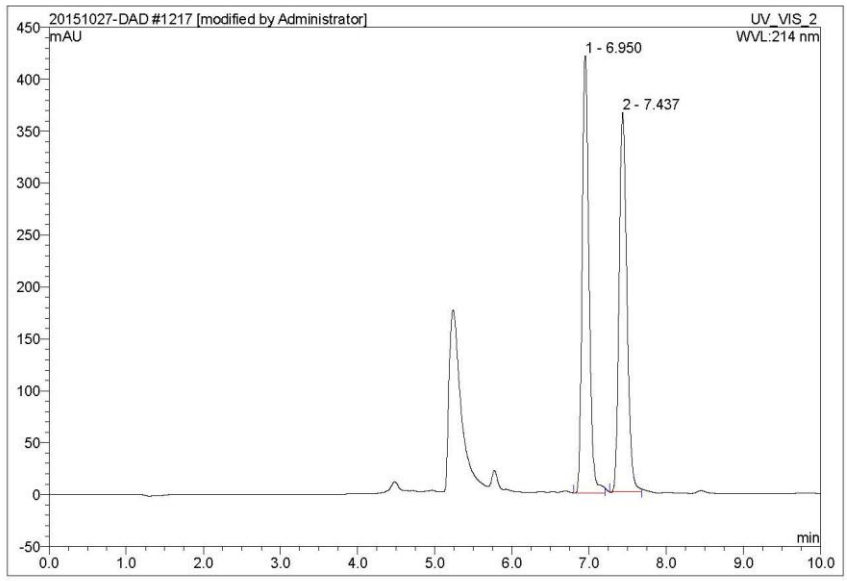
1217 ZH-2-57-3+- IE3 82 214 0.7

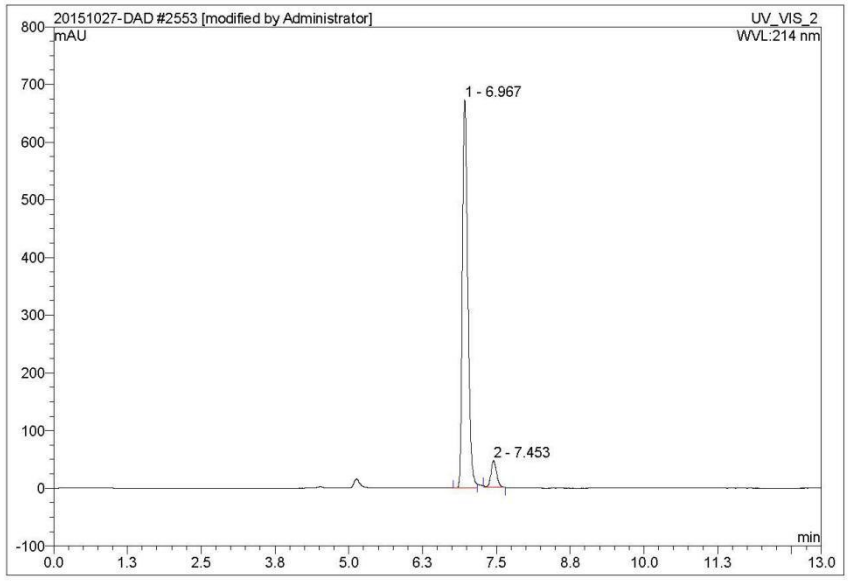
Sample Name:	**ZH-2-57-3+- IE3 82 214 0.7**	*Injection Volume:*	**4.0**
Vial Number:	**RB5**	*Channel:*	**UV_VIS_2**
Sample Type:	**unknown**	*Wavelength:*	**214.0**
Control Program:	**test-dad2**	*Bandwidth:*	**4**
Quantif. Method:	**WXL**	*Dilution Factor:*	**1.0000**
Recording Time:	**2016-3-21 13:59**	*Sample Weight:*	**1.0000**
Run Time (min):	**10.00**	*Sample Amount:*	**1.0000**



No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	6.95	n.a.	421.241	43.093	50.17	n.a.	BM *
2	7.44	n.a.	365.750	42.798	49.83	n.a.	BM *
Total:			786.991	85.891	100.00	0.000	

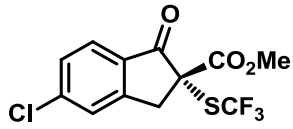
2553 ZH-2-86-1 IE3 82 214 0.7

Sample Name:	**ZH-2-86-1 IE3 82 214 0.7**	*Injection Volume:*	**1.0**
Vial Number:	**RC6**	*Channel:*	**UV_VIS_2**
Sample Type:	**unknown**	*Wavelength:*	**214.0**
Control Program:	**test-dad3**	*Bandwidth:*	**4**
Quantif. Method:	**WXL**	*Dilution Factor:*	**1.0000**
Recording Time:	**2016-7-15 19:12**	*Sample Weight:*	**1.0000**
Run Time (min):	**13.00**	*Sample Amount:*	**1.0000**



No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	6.97	n.a.	673.557	71.680	93.18	n.a.	BM *
2	7.45	n.a.	46.440	5.246	6.82	n.a.	MB*
Total:			719.997	76.926	100.00	0.000	

HPLC spectra for compound 3h



3h

HPLC: (IE-3 (0.46 × 25 cm, 3 μm), Hexane/^{i}PrOH = 8/2, 0.7 mL/min, 214 nm), t_R (major) = 7.09 min, t_R (minor) = 7.75 min (79% ee); $[\alpha]_D^{25}$ = -68.7 (c = 0.125, $CHCl_3$, 79% ee).

Operator:Administrator Timebase:HPLC Sequence:20151027-DAD

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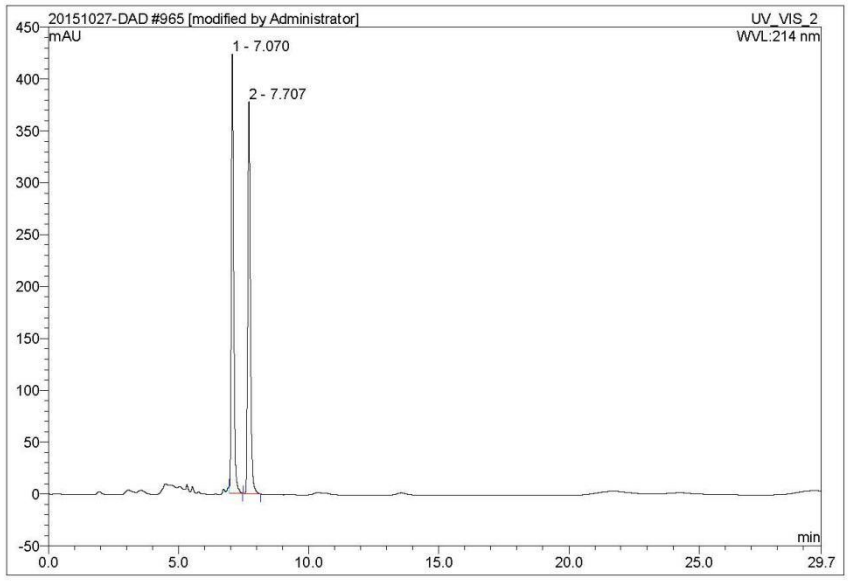
965 ZH-2-32-6+- IE3 82 214 0.7

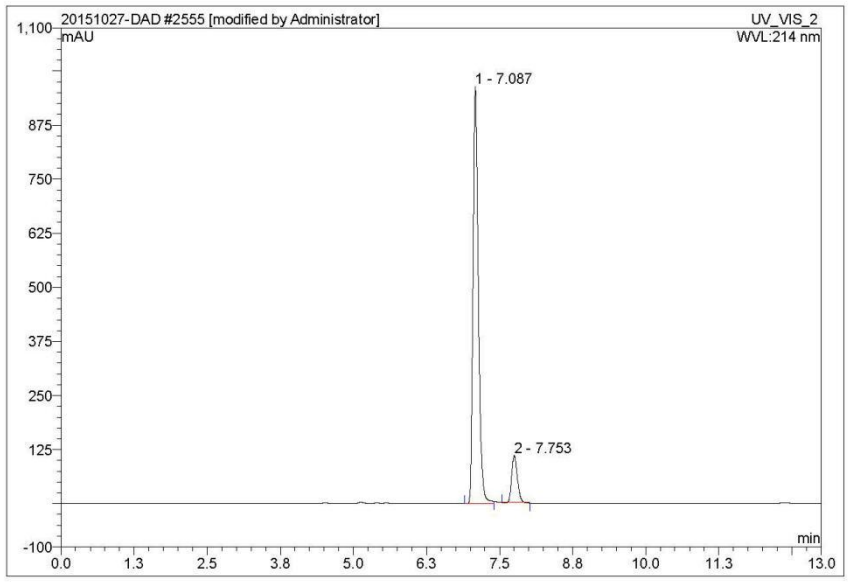
Sample Name:	**ZH-2-32-6+- IE3 82 214 0.7**	*Injection Volume:*	**1.0**
Vial Number:	**RD5**	*Channel:*	**UV_VIS_2**
Sample Type:	**unknown**	*Wavelength:*	**214.0**
Control Program:	**test-dad2**	*Bandwidth:*	**4**
Quantif. Method:	**WXL**	*Dilution Factor:*	**1.0000**
Recording Time:	**2016-2-19 11:51**	*Sample Weight:*	**1.0000**
Run Time (min):	**29.69**	*Sample Amount:*	**1.0000**



No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	7.07	n.a.	423.597	45.216	50.37	n.a.	MB*
2	7.71	n.a.	377.877	44.552	49.63	n.a.	BMB*
Total:			801.474	89.768	100.00	0.000	

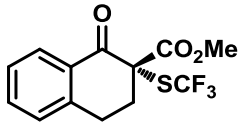
2555 ZH-2-68-1 IE3 82 214 0.7

Sample Name:	**ZH-2-68-1 IE3 82 214 0.7**	*Injection Volume:*	**0.5**
Vial Number:	**RD6**	*Channel:*	**UV_VIS_2**
Sample Type:	**unknown**	*Wavelength:*	**214.0**
Control Program:	**test-dad3**	*Bandwidth:*	**4**
Quantif. Method:	**WXL**	*Dilution Factor:*	**1.0000**
Recording Time:	**2016-7-15 19:38**	*Sample Weight:*	**1.0000**
Run Time (min):	**13.00**	*Sample Amount:*	**1.0000**



No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	7.09	n.a.	963.796	101.610	89.42	n.a.	BM *
2	7.75	n.a.	108.467	12.018	10.58	n.a.	BM *
Total:			1072.262	113.628	100.00	0.000	

HPLC spectra for compound 3i



3i

HPLC: (IE-3 (0.46 × 25 cm, 3 μm), Hexane/^{i}PrOH = 95/5, 0.7 mL/min, 214 nm), t_R (major) = 11.08 min, t_R (minor) = 9.77 min (98% ee); $[\alpha]_D^{25}$ = -7.7 (c = 0.110, $CHCl_3$, 98% ee).

Operator:Administrator Timebase:HPLC Sequence:20151027-DAD

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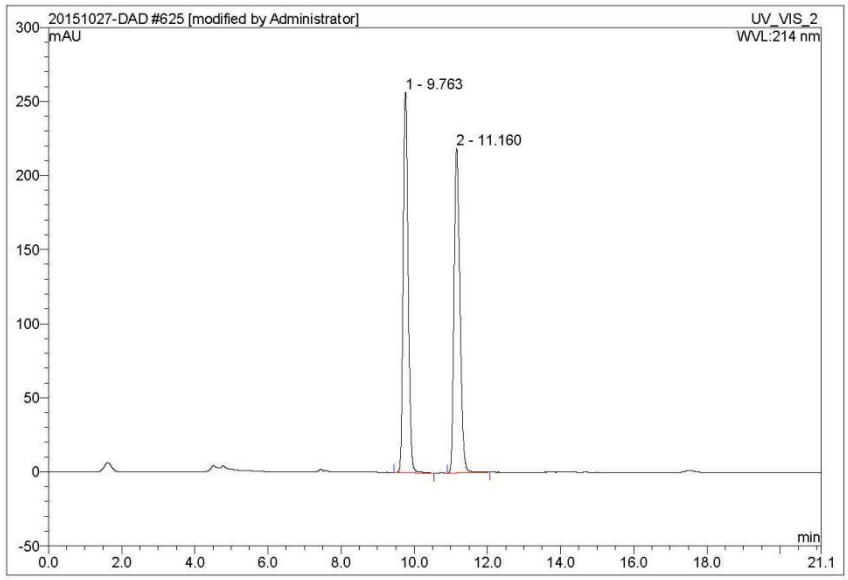
625 2-19-2+- IE3 955 214 0.7

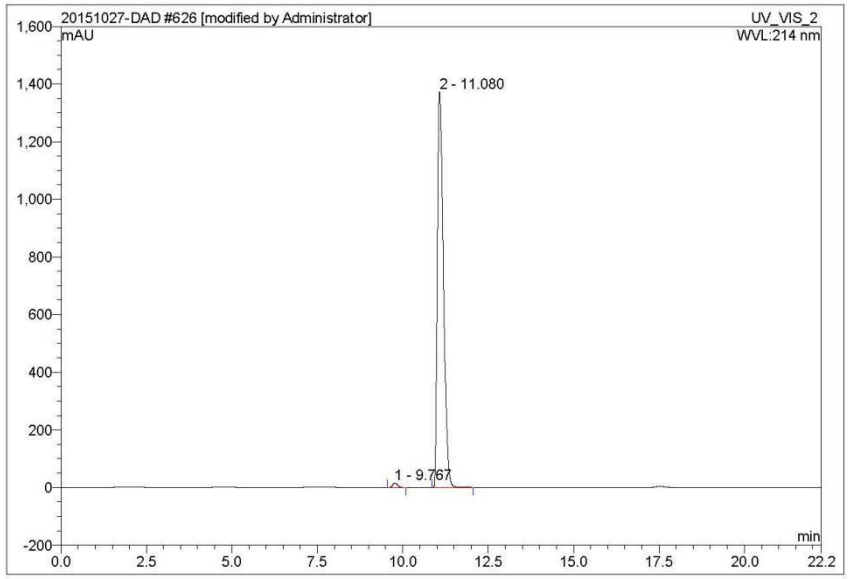
Sample Name:	**2-19-2+- IE3 955 214 0.7**	*Injection Volume:*	**1.0**
Vial Number:	**RB5**	*Channel:*	**UV_VIS_2**
Sample Type:	**unknown**	*Wavelength:*	**214.0**
Control Program:	**test-dad2**	*Bandwidth:*	**4**
Quantif. Method:	**WXL**	*Dilution Factor:*	**1.0000**
Recording Time:	**2015-12-30 14:04**	*Sample Weight:*	**1.0000**
Run Time (min):	**21.12**	*Sample Amount:*	**1.0000**



No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	9.76	n.a.	256.674	40.455	49.95	n.a.	BMB
2	11.16	n.a.	219.417	40.531	50.05	n.a.	BMB
Total:			476.091	80.985	100.00	0.000	

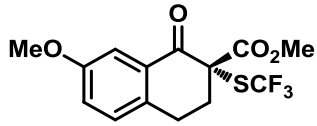
626 2-18-2 IE3 955 214 0.7

Sample Name:	**2-18-2 IE3 955 214 0.7**	*Injection Volume:*	**1.0**
Vial Number:	**RA5**	*Channel:*	**UV_VIS_2**
Sample Type:	**unknown**	*Wavelength:*	**214.0**
Control Program:	**test-dad2**	*Bandwidth:*	**4**
Quantif. Method:	**WXL**	*Dilution Factor:*	**1.0000**
Recording Time:	**2015-12-30 14:26**	*Sample Weight:*	**1.0000**
Run Time (min):	**22.24**	*Sample Amount:*	**1.0000**



No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	9.77	n.a.	16.166	2.504	0.88	n.a.	BMB
2	11.08	n.a.	1373.693	282.206	99.12	n.a.	BMB
Total:			1389.859	284.710	100.00	0.000	

HPLC spectra for compound 3j



3j

HPLC: (IE-3 (0.46 × 25 cm, 3 μm), Hexane/^{i}PrOH = 9/1, 0.7 mL/min, 214 nm), t_R (major) = 10.21 min, t_R (minor) = 9.12 min (95% ee); $[\alpha]_D^{25}$ = +18.38 (c = 0.100, $CHCl_3$, 95% ee).

Operator:Administrator Timebase:HPLC Sequence:20151027-DAD

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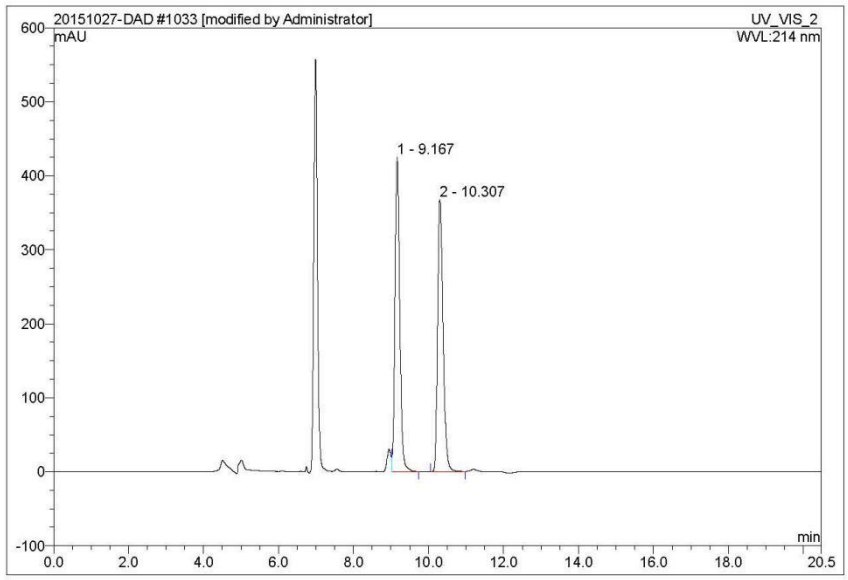
2016-7-22 7:56 下午

1033 ZH-2-48-1+- IE3 91 214 0.7

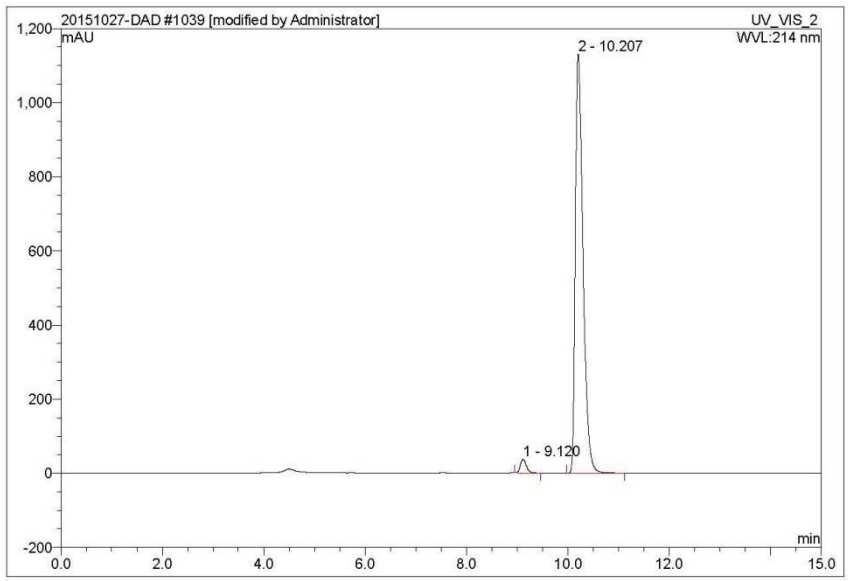
Sample Name:	**ZH-2-48-1+- IE3 91 214 0.7**	*Injection Volume:*	**2.0**
Vial Number:	**RE7**	*Channel:*	**UV_VIS_2**
Sample Type:	**unknown**	*Wavelength:*	**214.0**
Control Program:	**test-dad2**	*Bandwidth:*	**4**
Quantif. Method:	**WXL**	*Dilution Factor:*	**1.0000**
Recording Time:	**2016-2-29 16:22**	*Sample Weight:*	**1.0000**
Run Time (min):	**20.47**	*Sample Amount:*	**1.0000**



No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	9.17	n.a.	425.530	62.651	50.47	n.a.	MB*
2	10.31	n.a.	367.549	61.473	49.53	n.a.	BMB*
Total:			793.080	124.123	100.00	0.000	

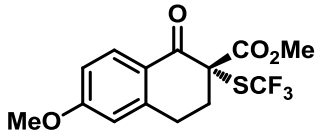
1039 ZH-2-47-1 IE3 91 214 0.7

Sample Name:	**ZH-2-47-1 IE3 91 214 0.7**	*Injection Volume:*	**2.0**
Vial Number:	**RE6**	*Channel:*	**UV_VIS_2**
Sample Type:	**unknown**	*Wavelength:*	**214.0**
Control Program:	**test-dad**	*Bandwidth:*	**4**
Quantif. Method:	**WXL**	*Dilution Factor:*	**1.0000**
Recording Time:	**2016-2-29 18:39**	*Sample Weight:*	**1.0000**
Run Time (min):	**15.00**	*Sample Amount:*	**1.0000**



No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	9.12	n.a.	36.537	5.063	2.49	n.a.	BMB
2	10.21	n.a.	1131.057	198.534	97.51	n.a.	BMB
Total:			1167.594	203.597	100.00	0.000	

HPLC spectra for compound 3k



3k

HPLC: (IE-3 (0.46 × 25 cm, 3 μm), Hexane/^{i}PrOH = 8/2, 0.7 mL/min, 214 nm), t_R (major) = 10.05 min, t_R (minor) = 9.53 min (94% ee); $[\alpha]_D^{25}$ = -7.4 (c = 0.100, $CHCl_3$, 94% ee).

Operator:Administrator Timebase:HPLC Sequence:20151027-DAD

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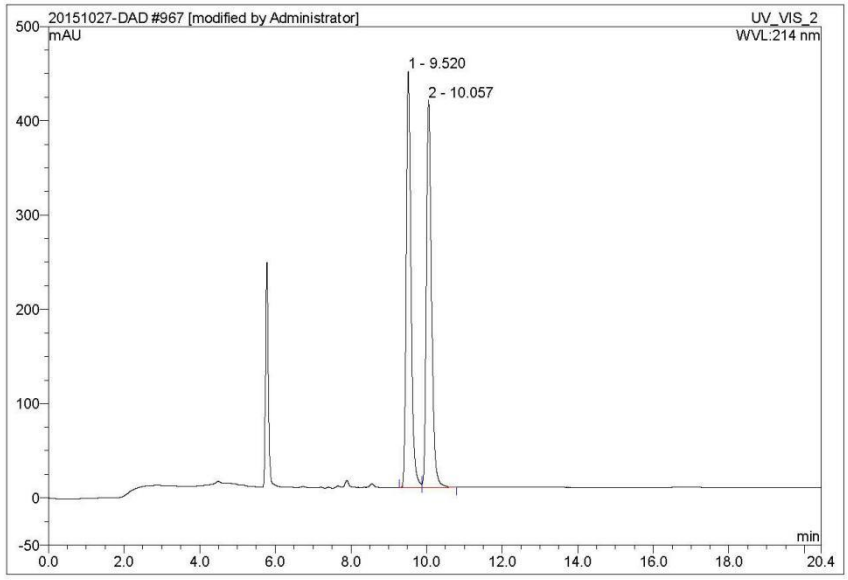
2016-7-22 7:57 下午

967 ZH-2-32-3+- IE3 82 214 0.7

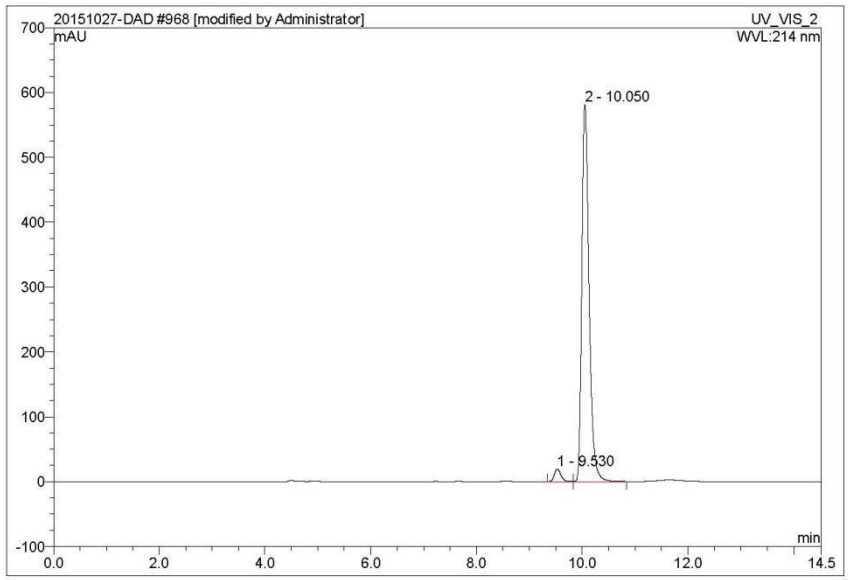
Sample Name:	**ZH-2-32-3+- IE3 82 214 0.7**	*Injection Volume:*	**1.0**
Vial Number:	**RB5**	*Channel:*	**UV_VIS_2**
Sample Type:	**unknown**	*Wavelength:*	**214.0**
Control Program:	**test-dad2**	*Bandwidth:*	**4**
Quantif. Method:	**WXL**	*Dilution Factor:*	**1.0000**
Recording Time:	**2016-2-19 12:39**	*Sample Weight:*	**1.0000**
Run Time (min):	**20.44**	*Sample Amount:*	**1.0000**



No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	9.52	n.a.	441.387	64.708	49.89	n.a.	BM
2	10.06	n.a.	410.577	65.002	50.11	n.a.	MB
Total:			851.963	129.711	100.00	0.000	

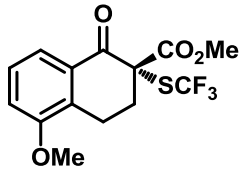
968 ZH-2-24-3 IE3 82 214 0.7

Sample Name:	**ZH-2-24-3 IE3 82 214 0.7**	*Injection Volume:*	**1.0**
Vial Number:	**RA5**	*Channel:*	**UV_VIS_2**
Sample Type:	**unknown**	*Wavelength:*	**214.0**
Control Program:	**test-dad2**	*Bandwidth:*	**4**
Quantif. Method:	**WXL**	*Dilution Factor:*	**1.0000**
Recording Time:	**2016-2-19 13:01**	*Sample Weight:*	**1.0000**
Run Time (min):	**14.52**	*Sample Amount:*	**1.0000**



No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	9.53	n.a.	19.146	2.767	2.92	n.a.	BM
2	10.05	n.a.	581.300	91.867	97.08	n.a.	MB
Total:			600.445	94.634	100.00	0.000	

HPLC spectra for compound 3l



3l

HPLC: (IE-3 (0.46 × 25 cm, 3 μm), Hexane/^{i}PrOH = 9/1, 0.7 mL/min, 214 nm), t_R (major) = 11.32 min, t_R (minor) = 9.80 min (96% ee); $[\alpha]_D^{25}$ = +1.8 (c = 0.100, $CHCl_3$, 96% ee).

Operator:Administrator Timebase:HPLC Sequence:20151027-DAD

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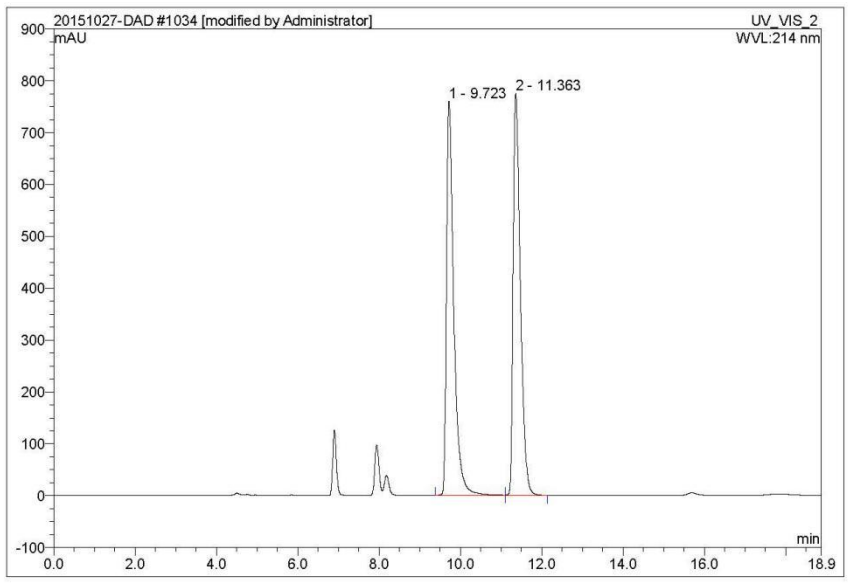
2016-7-22 7:55 下午

1034 ZH-2-48-2+- IE3 91 214 0.7

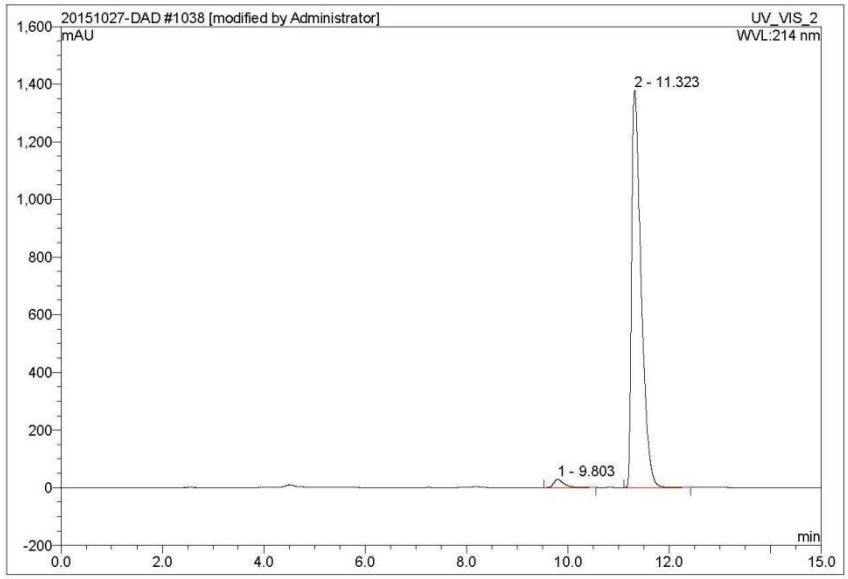
Sample Name:	**ZH-2-48-2+- IE3 91 214 0.7**	*Injection Volume:*	**2.0**
Vial Number:	**RD7**	*Channel:*	**UV_VIS_2**
Sample Type:	**unknown**	*Wavelength:*	**214.0**
Control Program:	**test-dad2**	*Bandwidth:*	**4**
Quantif. Method:	**WXL**	*Dilution Factor:*	**1.0000**
Recording Time:	**2016-2-29 16:44**	*Sample Weight:*	**1.0000**
Run Time (min):	**18.87**	*Sample Amount:*	**1.0000**



No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	9.72	n.a.	760.613	158.708	49.83	n.a.	BM
2	11.36	n.a.	776.143	159.788	50.17	n.a.	MB
Total:			1536.756	318.496	100.00	0.000	

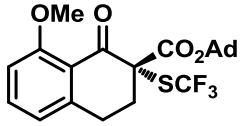
1038 ZH-2-47-2 IE3 91 214 0.7

Sample Name:	**ZH-2-47-2 IE3 91 214 0.7**	*Injection Volume:*	**2.0**
Vial Number:	**RD6**	*Channel:*	**UV_VIS_2**
Sample Type:	**unknown**	*Wavelength:*	**214.0**
Control Program:	**test-dad**	*Bandwidth:*	**4**
Quantif. Method:	**WXL**	*Dilution Factor:*	**1.0000**
Recording Time:	**2016-2-29 18:24**	*Sample Weight:*	**1.0000**
Run Time (min):	**15.00**	*Sample Amount:*	**1.0000**



No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	9.80	n.a.	28.691	6.963	2.26	n.a.	BMB
2	11.32	n.a.	1379.488	301.057	97.74	n.a.	BMB
Total:			1408.178	308.021	100.00	0.000	

HPLC spectra for compound 3m



3m

HPLC: (IE-3 (0.46 × 25 cm, 3 μm), Hexane/^{i}PrOH = 9/1, 0.7 mL/min, 214 nm), t_R (major) = 11.96 min, t_R (minor) = 9.53 min (98% ee); $[\alpha]_D^{25}$ = +37.1 (c = 0.100, $CHCl_3$, 98% ee).

Operator:Administrator Timebase:HPLC Sequence:20151027-DAD

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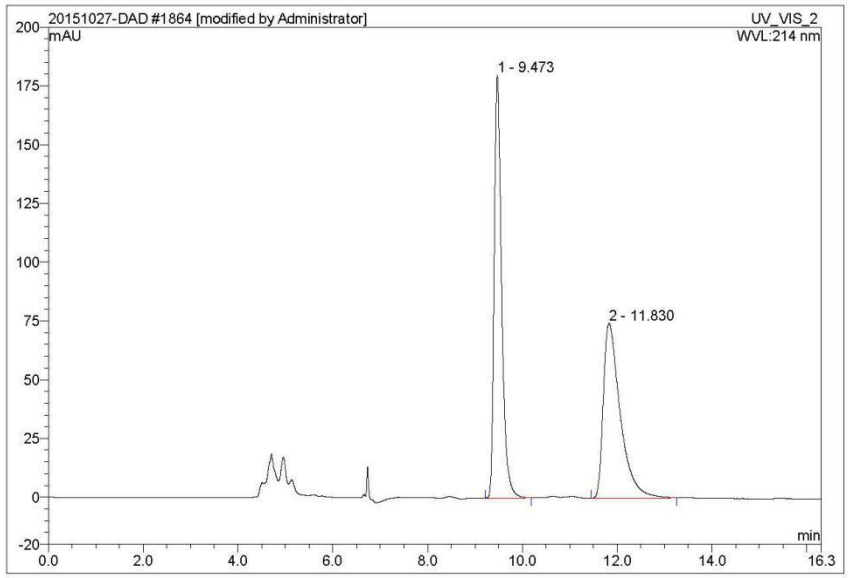
2016-7-22 7:38 下午

1864 ZH-2-94-1+- IE3 91 214 0.7

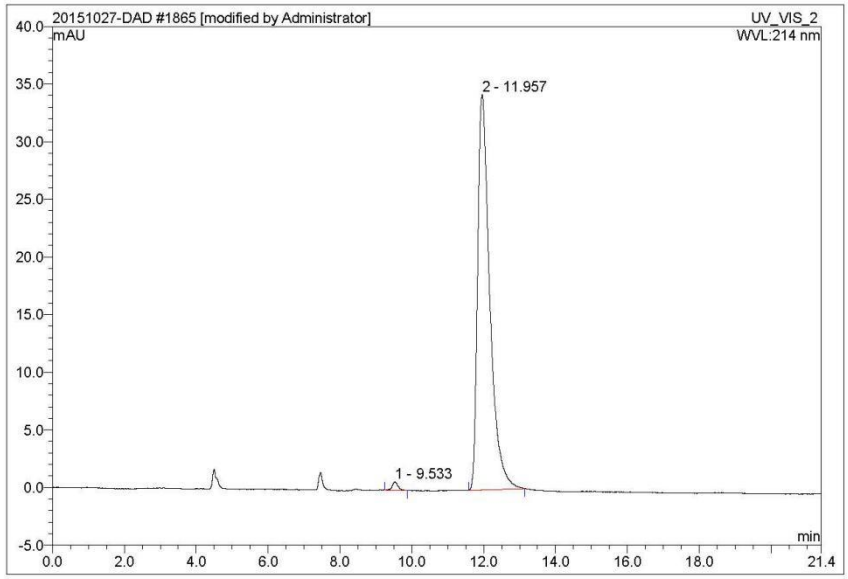
Sample Name:	**ZH-2-94-1+- IE3 91 214 0.7**	*Injection Volume:*	**1.0**
Vial Number:	**RE7**	*Channel:*	**UV_VIS_2**
Sample Type:	**unknown**	*Wavelength:*	**214.0**
Control Program:	**test-dad2**	*Bandwidth:*	**4**
Quantif. Method:	**WXL**	*Dilution Factor:*	**1.0000**
Recording Time:	**2016-5-16 9:54**	*Sample Weight:*	**1.0000**
Run Time (min):	**16.30**	*Sample Amount:*	**1.0000**



No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	9.47	n.a.	179.813	32.642	51.61	n.a.	BMB
2	11.83	n.a.	74.409	30.602	48.39	n.a.	BMB
Total:			254.222	63.244	100.00	0.000	

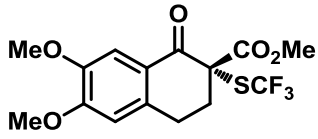
1865 ZH-2-96-1 IE3 91 214 0.7

Sample Name:	**ZH-2-96-1 IE3 91 214 0.7**	*Injection Volume:*	**1.0**
Vial Number:	**RD7**	*Channel:*	**UV_VIS_2**
Sample Type:	**unknown**	*Wavelength:*	**214.0**
Control Program:	**test-dad2**	*Bandwidth:*	**4**
Quantif. Method:	**WXL**	*Dilution Factor:*	**1.0000**
Recording Time:	**2016-5-16 10:12**	*Sample Weight:*	**1.0000**
Run Time (min):	**21.39**	*Sample Amount:*	**1.0000**



No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	9.53	n.a.	0.751	0.138	1.02	n.a.	BMB*
2	11.96	n.a.	34.283	13.414	98.98	n.a.	BMB
Total:			35.034	13.552	100.00	0.000	

HPLC spectra for compound 3n



3n

HPLC: (IE-3 (0.46 × 25 cm, 3 μm), Hexane/^{i}PrOH = 9/1, 0.7 mL/min, 214 nm), t_R (major) = 20.57 min, t_R (minor) = 19.05 min (95% ee); $[\alpha]_D^{25}$ = +8.3 (c = 0.100, $CHCl_3$, 95% ee).

Operator:Administrator Timebase:HPLC Sequence:20151027-DAD

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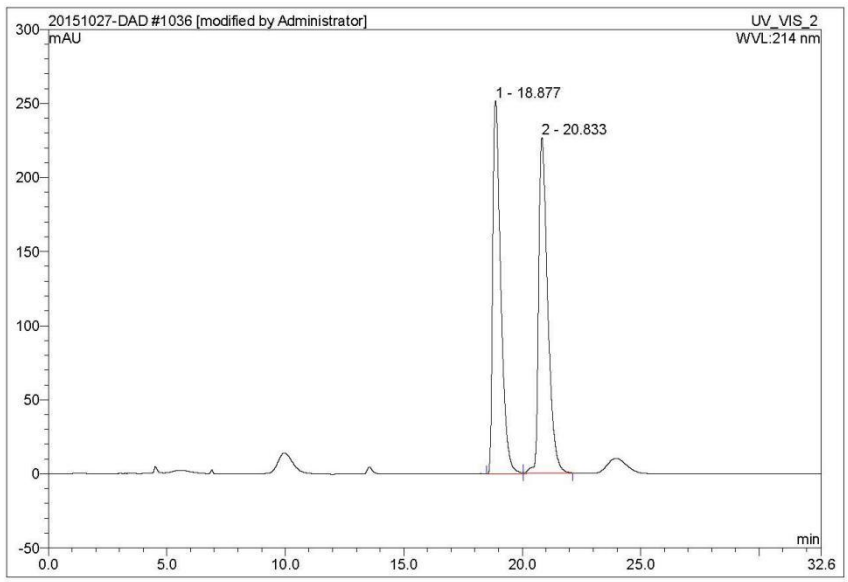
2016-7-22 7:55 下午

1036 ZH-2-48-3+- IE3 91 214 0.7

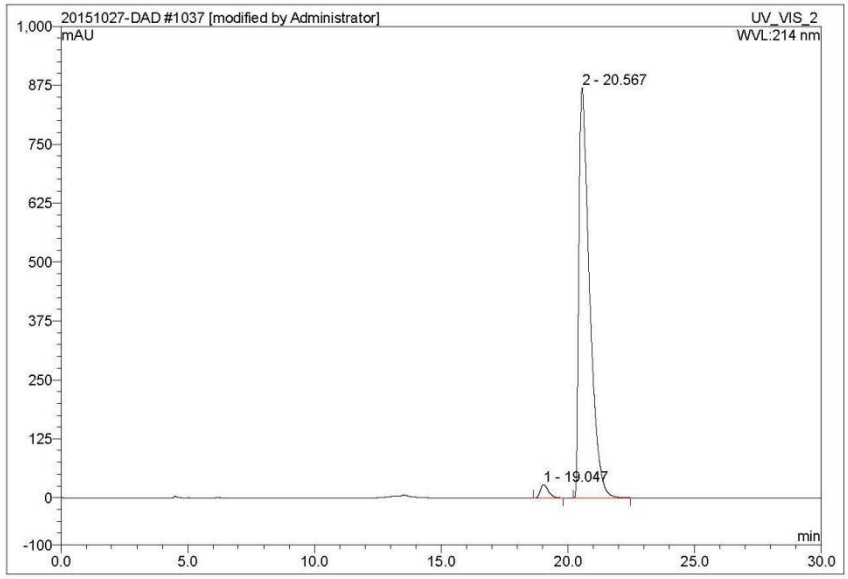
Sample Name:	**ZH-2-48-3+- IE3 91 214 0.7**	*Injection Volume:*	**2.0**
Vial Number:	**RB7**	*Channel:*	**UV_VIS_2**
Sample Type:	**unknown**	*Wavelength:*	**214.0**
Control Program:	**test-dad2**	*Bandwidth:*	**4**
Quantif. Method:	**WXL**	*Dilution Factor:*	**1.0000**
Recording Time:	**2016-2-29 17:18**	*Sample Weight:*	**1.0000**
Run Time (min):	**32.62**	*Sample Amount:*	**1.0000**



No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	18.88	n.a.	251.792	98.977	49.57	n.a.	BM
2	20.83	n.a.	226.767	100.709	50.43	n.a.	MB
Total:			478.560	199.686	100.00	0.000	

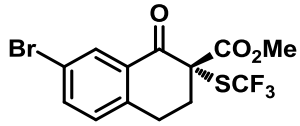
1037 ZH-2-47-3 IE3 91 214 0.7

Sample Name:	**ZH-2-47-3 IE3 91 214 0.7**	*Injection Volume:*	**2.0**
Vial Number:	**RB6**	*Channel:*	**UV_VIS_2**
Sample Type:	**unknown**	*Wavelength:*	**214.0**
Control Program:	**test-dad2**	*Bandwidth:*	**4**
Quantif. Method:	**WXL**	*Dilution Factor:*	**1.0000**
Recording Time:	**2016-2-29 17:53**	*Sample Weight:*	**1.0000**
Run Time (min):	**30.00**	*Sample Amount:*	**1.0000**



No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	19.05	n.a.	28.769	10.733	2.46	n.a.	BMB
2	20.57	n.a.	870.295	425.724	97.54	n.a.	BMB
Total:			899.065	436.458	100.00	0.000	

HPLC spectra for compound 3o



3o

HPLC: (IE-3 (0.46 × 25 cm, 3 μm), Hexane/^{i}PrOH = 8/2, 0.7 mL/min, 214 nm), t_R (major) = 8.52 min, t_R (minor) = 7.47 min (96% ee); $[\alpha]_D^{25}$ = +8.00 (c = 0.100, $CHCl_3$, 96% ee).

Operator:Administrator Timebase:HPLC Sequence:20151027-DAD

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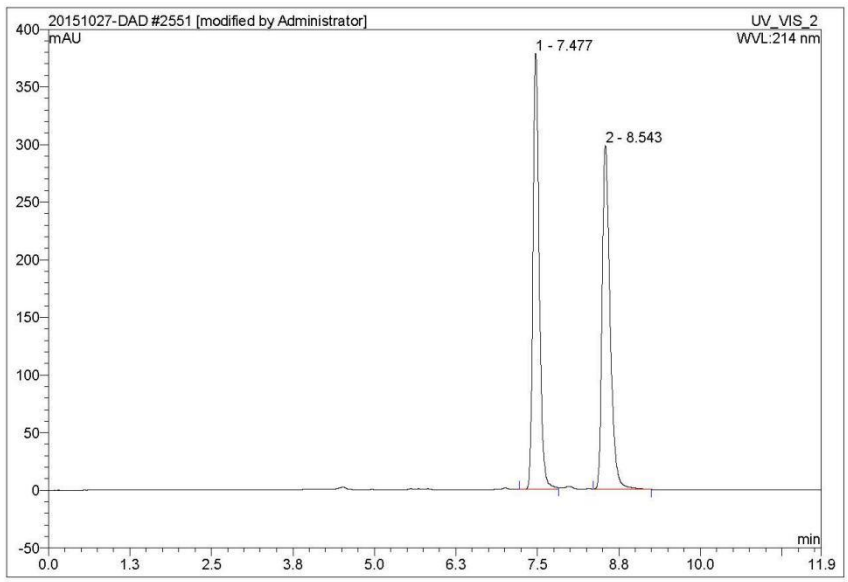
2016-7-22 7:16 下午

2551 ZH-2-87-3+- IE3 82 214 0.7

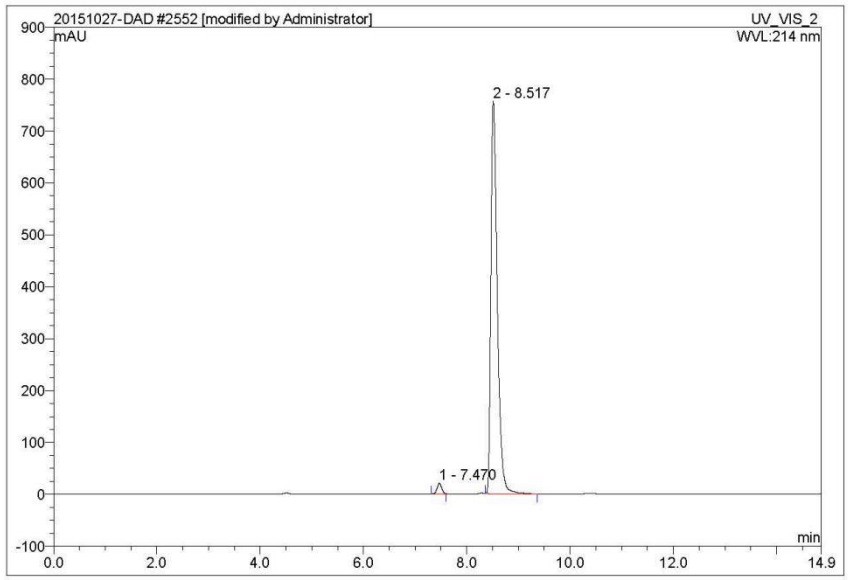
Sample Name:	**ZH-2-87-3+- IE3 82 214 0.7**	*Injection Volume:*	**1.0**
Vial Number:	**RD6**	*Channel:*	**UV_VIS_2**
Sample Type:	**unknown**	*Wavelength:*	**214.0**
Control Program:	**test-dad3**	*Bandwidth:*	**4**
Quantif. Method:	**WXL**	*Dilution Factor:*	**1.0000**
Recording Time:	**2016-7-15 18:41**	*Sample Weight:*	**1.0000**
Run Time (min):	**11.85**	*Sample Amount:*	**1.0000**



No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	7.48	n.a.	377.680	42.018	49.92	n.a.	BM *
2	8.54	n.a.	298.430	42.152	50.08	n.a.	BMB
Total:			676.109	84.170	100.00	0.000	

2552 ZH-2-86-3 IE3 82 214 0.7

Sample Name:	**ZH-2-86-3 IE3 82 214 0.7**	*Injection Volume:*	**1.0**
Vial Number:	**RC6**	*Channel:*	**UV_VIS_2**
Sample Type:	**unknown**	*Wavelength:*	**214.0**
Control Program:	**test-dad3**	*Bandwidth:*	**4**
Quantif. Method:	**WXL**	*Dilution Factor:*	**1.0000**
Recording Time:	**2016-7-15 18:55**	*Sample Weight:*	**1.0000**
Run Time (min):	**14.86**	*Sample Amount:*	**1.0000**



No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	7.47	n.a.	20.881	2.223	2.01	n.a.	BMB*
2	8.52	n.a.	757.097	108.212	97.99	n.a.	BMB
Total:			777.977	110.435	100.00	0.000	

HPLC spectra for compound 4a

4a

HPLC: (AD-H (0.46 × 25 cm, 5 μm), Hexane/^{i}PrOH = 95/5, 0.7 mL/min, 214 nm), t_R (major) = 9.83 min, t_R (minor) = 9.04 min (93% ee); $[\alpha]_D^{25}$ = +102.4 (c = 0.140, $CHCl_3$, 93% ee).

Operator:Administrator Timebase:HPLC Sequence:20151027-DAD

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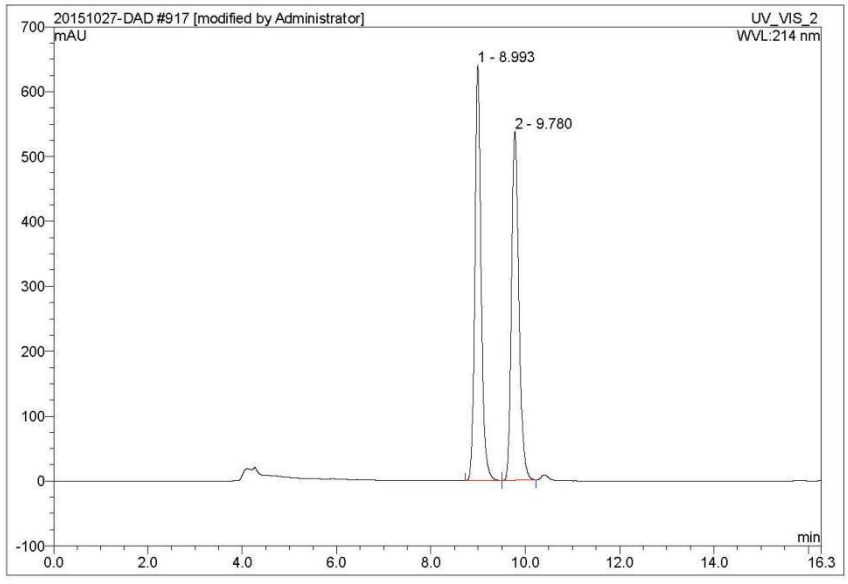
2016-7-22 8:55 下午

917 ZH-2-35-1+- ADH 955 214 0.7

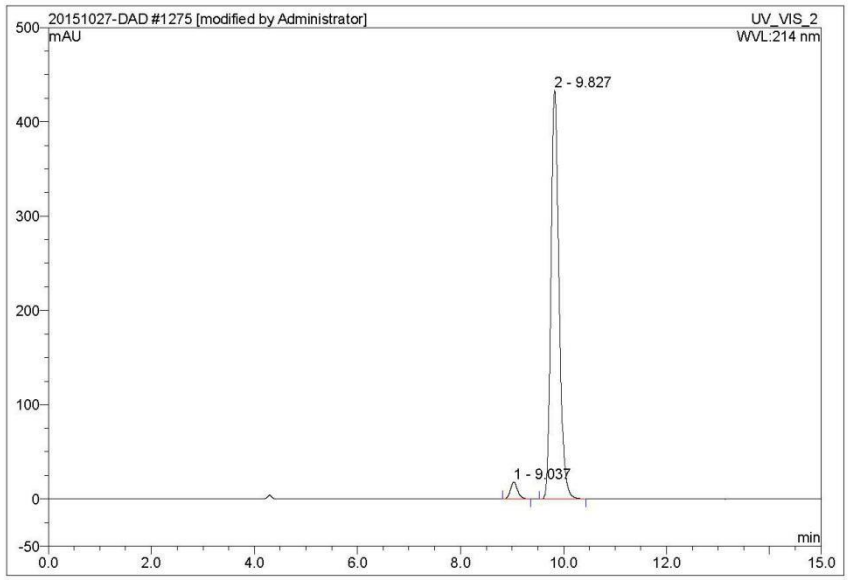
Sample Name:	**ZH-2-35-1+- ADH 955 214 0.7**	*Injection Volume:*	**1.0**
Vial Number:	**RD4**	*Channel:*	**UV_VIS_2**
Sample Type:	**unknown**	*Wavelength:*	**214.0**
Control Program:	**test-dad2**	*Bandwidth:*	**4**
Quantif. Method:	**WXL**	*Dilution Factor:*	**1.0000**
Recording Time:	**2016-1-29 12:47**	*Sample Weight:*	**1.0000**
Run Time (min):	**16.27**	*Sample Amount:*	**1.0000**



No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	8.99	n.a.	640.812	97.552	50.04	n.a.	BM *
2	9.78	n.a.	537.392	97.393	49.96	n.a.	MB*
Total:			1178.204	194.945	100.00	0.000	

1275 ZH-2-58-1 ADH 955 214 0.7

Sample Name:	**ZH-2-58-1 ADH 955 214 0.7**	*Injection Volume:*	**2.0**
Vial Number:	**RE7**	*Channel:*	**UV_VIS_2**
Sample Type:	**unknown**	*Wavelength:*	**214.0**
Control Program:	**test-dad4**	*Bandwidth:*	**4**
Quantif. Method:	**WXL**	*Dilution Factor:*	**1.0000**
Recording Time:	**2016-3-27 11:39**	*Sample Weight:*	**1.0000**
Run Time (min):	**15.00**	*Sample Amount:*	**1.0000**



No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	9.04	n.a.	17.828	2.939	3.60	n.a.	BMB
2	9.83	n.a.	433.148	78.712	96.40	n.a.	BMB
Total:			450.976	81.651	100.00	0.000	

Compound **4a** obtained using compound **1b** as the electrophilic trifluoromethylthiolating reagent. HPLC: (AD-H (0.46 × 25 cm, 5 μm), Hexane/^{i}PrOH = 95/5, 0.7 mL/min, 214 nm), t_R (major) = 9.57 min, t_R (minor) = 8.82 min (96% ee)[b]; $[\alpha]_D^{25}$ = +127.1 (c = 0.100, $CHCl_3$, 96% ee).

Operator:GC Timebase:U3000 Sequence:WXL-2

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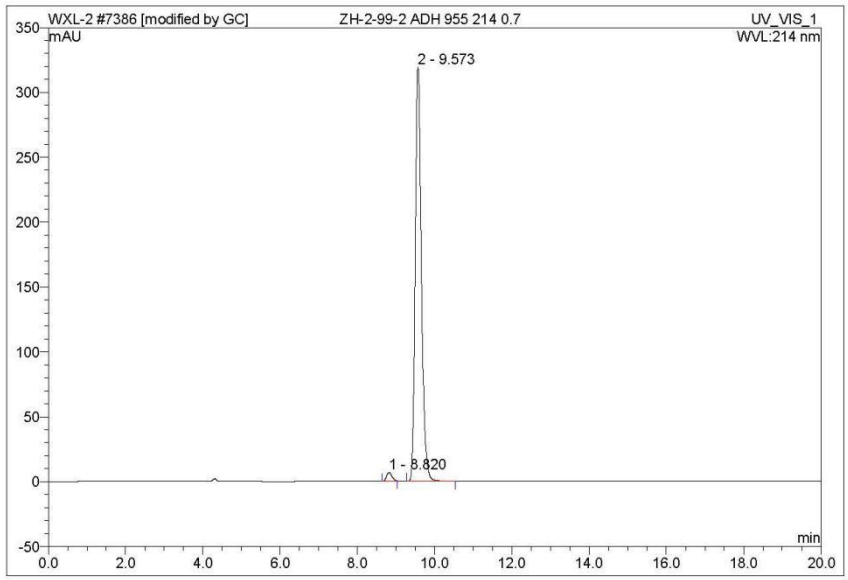
2016/7/22 8:33 下午

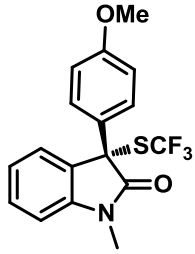
7386 ZH-2-99-2 ADH 955 214 0.7

Sample Name:	**ZH-2-99-2 ADH 955 214 0.7**	*Injection Volume:*	**1.0**
Vial Number:	**BE1**	*Channel:*	**UV_VIS_1**
Sample Type:	**unknown**	*Wavelength:*	**214**
Control Program:	**WXL-2014-1**	*Bandwidth:*	**n.a.**
Quantif. Method:	**WXL**	*Dilution Factor:*	**1.0000**
Recording Time:	**2016/5/27 18:09**	*Sample Weight:*	**1.0000**
Run Time (min):	**20.01**	*Sample Amount:*	**1.0000**



No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	8.82	n.a.	6.757	1.070	1.78	n.a.	BMB*
2	9.57	n.a.	319.051	58.862	98.22	n.a.	BMB
Total:			325.809	59.931	100.00	0.000	

HPLC spectra for compound 4b



4b

HPLC: (IE-3 (0.46 × 25 cm, 3 μm), Hexane/^{i}PrOH =75/3, 0.7 mL/min, 214 nm), t_R (major) = 8.26 min, t_R (minor) = 8.64 min (92% ee); $[\alpha]_D^{25}$ = +169.7 (c = 0.050, $CHCl_3$, 92% ee).

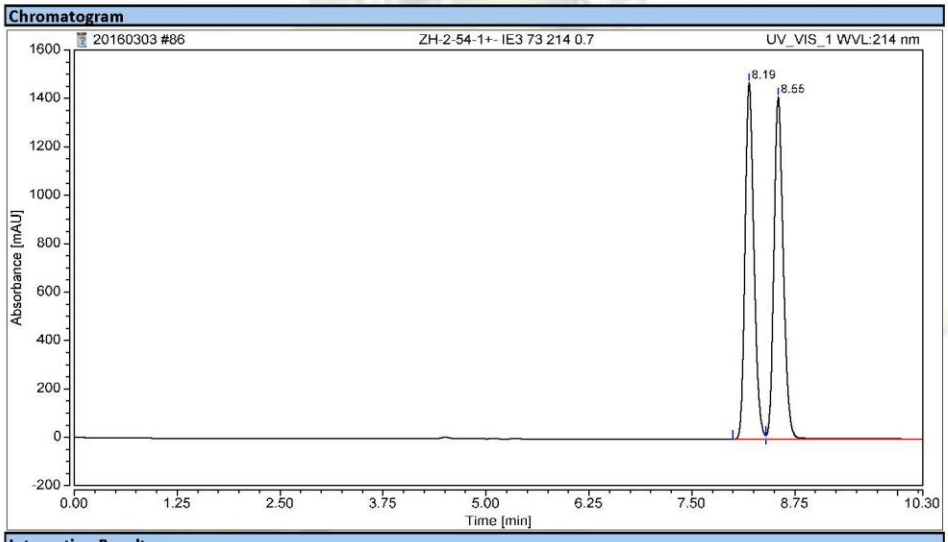
Instrument:U3000 Sequence:20160303 Page 1 of 1

Chromatogram and Results

Injection Details

Injection Name:	ZH-2-54-1+- IE3 73 214 0.7	*Run Time (min):*	10.30
Vial Number:	RB7	*Injection Volume:*	2.00
Injection Type:	Unknown	*Channel:*	UV_VIS_1
Calibration Level:		*Wavelength:*	214.0
Instrument Method:	20160223-DAD1	*Bandwidth:*	4
Processing Method:	20160223	*Dilution Factor:*	1.0000
Injection Date/Time:	16/三月/16 18:50	*Sample Weight:*	1.0000

Chromatogram

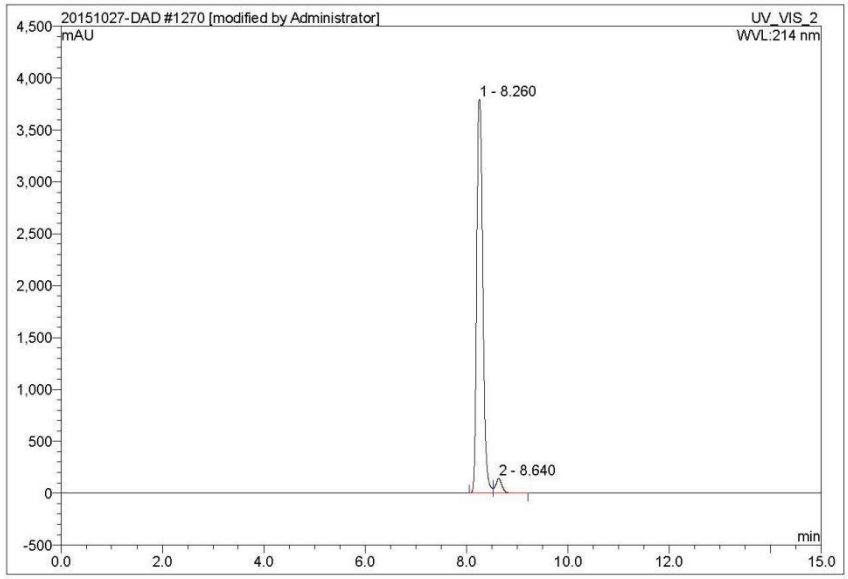


Integration Results

No.	Retention Time min	Area mAU*min	Height mAU	Relative Area %
1	8.193	183.116	1472.415	49.35
2	8.547	187.904	1413.228	50.65
Total:		**371.020**	**2885.642**	**100.00**

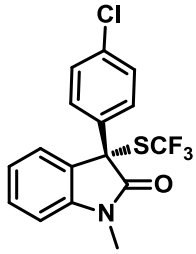
1270 zh-2-58-2 IE3 73 214 0.7

Sample Name:	**zh-2-58-2 IE3 73 214 0.7**	*Injection Volume:*	**2.0**
Vial Number:	**RE4**	*Channel:*	**UV_VIS_2**
Sample Type:	**unknown**	*Wavelength:*	**214.0**
Control Program:	**test-dad2**	*Bandwidth:*	**4**
Quantif. Method:	**WXL**	*Dilution Factor:*	**1.0000**
Recording Time:	**2016-3-25 20:56**	*Sample Weight:*	**1.0000**
Run Time (min):	**15.00**	*Sample Amount:*	**1.0000**



No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	8.26	n.a.	3797.399	527.055	96.11	n.a.	BM
2	8.64	n.a.	142.977	21.313	3.89	n.a.	MB
Total:			3940.376	548.368	100.00	0.000	

HPLC spectra for compound 4c



4c

HPLC: (IE-3 (0.46 × 25 cm, 3 μm), Hexane/^{i}PrOH = 9/1, 0.7 mL/min, 214 nm), t_R (major) = 9.09 min, t_R (minor) = 9.47 min (88% ee); $[\alpha]_D^{25}$ = +107.6 (c = 0.150, $CHCl_3$, 88% ee).

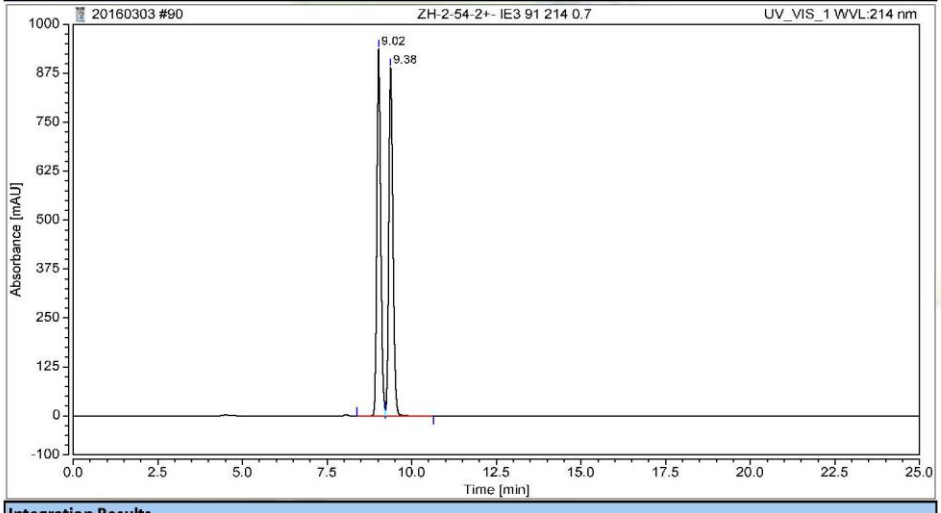
Instrument:U3000 Sequence:20160303 Page 1 of 1

Chromatogram and Results

Injection Details

Injection Name:	**ZH-2-54-2+- IE3 91 214 0.7**	*Run Time (min):*	**25.00**
Vial Number:	**RB5**	*Injection Volume:*	**2.00**
Injection Type:	**Unknown**	*Channel:*	**UV_VIS_1**
Calibration Level:		*Wavelength:*	**214.0**
Instrument Method:	**20160223-DAD2**	*Bandwidth:*	**4**
Processing Method:	**20160223**	*Dilution Factor:*	**1.0000**
Injection Date/Time:	**16/三月/16 21:06**	*Sample Weight:*	**1.0000**

Chromatogram

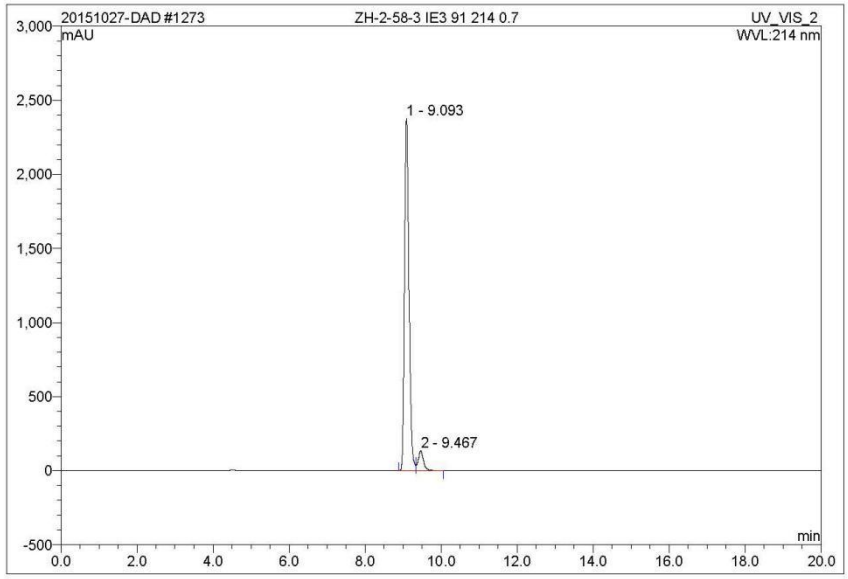


Integration Results

No.	Retention Time min	Area mAU*min	Height mAU	Relative Area %
1	9.023	123.868	938.075	49.73
2	9.377	125.219	890.117	50.27
Total:		**249.088**	**1828.192**	**100.00**

1273 ZH-2-58-3 IE3 91 214 0.7

Sample Name:	**ZH-2-58-3 IE3 91 214 0.7**	*Injection Volume:*	**2.0**
Vial Number:	**RC4**	*Channel:*	**UV_VIS_2**
Sample Type:	**unknown**	*Wavelength:*	**214.0**
Control Program:	**test-dad4**	*Bandwidth:*	**4**
Quantif. Method:	**WXL**	*Dilution Factor:*	**1.0000**
Recording Time:	**2016-3-25 21:48**	*Sample Weight:*	**1.0000**
Run Time (min):	**20.00**	*Sample Amount:*	**1.0000**



No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	9.09	n.a.	2377.513	324.807	93.86	n.a.	BM
2	9.47	n.a.	134.392	21.237	6.14	n.a.	MB
Total:			2511.905	346.043	100.00	0.000	

Compound **4c** obtained using compound **1b** as the electrophilic trifluoromethylthiolating reagent. HPLC: (IE-3 (0.46 × 25 cm, 3 μm), Hexane/^{i}PrOH = 9/1, 0.7 mL/min, 214 nm), t_R (major) = 9.07 min, t_R (minor) = 9.42 min (93% ee)[b]; $[\alpha]_D^{25}$ = +120.3 (c = 0.100, $CHCl_3$, 93% ee).

Operator:Administrator Timebase:HPLC Sequence:20151027-DAD

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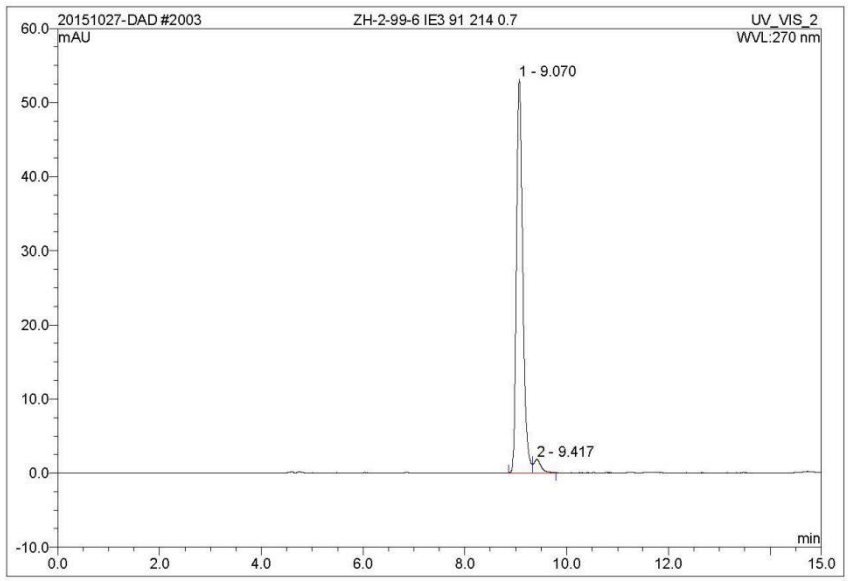
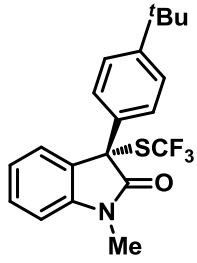
2003 ZH-2-99-6 IE3 91 214 0.7

Sample Name:	**ZH-2-99-6 IE3 91 214 0.7**	*Injection Volume:*	**1.0**
Vial Number:	**RA5**	*Channel:*	**UV_VIS_2**
Sample Type:	**unknown**	*Wavelength:*	**270.0**
Control Program:	**test-dad2**	*Bandwidth:*	**4**
Quantif. Method:	**WXL**	*Dilution Factor:*	**1.0000**
Recording Time:	**2016-5-27 18:37**	*Sample Weight:*	**1.0000**
Run Time (min):	**15.00**	*Sample Amount:*	**1.0000**



No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	9.07	n.a.	53.135	7.605	96.23	n.a.	BM
2	9.42	n.a.	1.812	0.298	3.77	n.a.	MB
Total:			54.947	7.903	100.00	0.000	

HPLC spectra for compound 4d



4d

HPLC: (AD-H (0.46 × 25 cm, 5 μm), Hexane/^{i}PrOH = 95/5, 0.7 mL/min, 214 nm), t_R (major) = 8.00 min, t_R (minor) = 7.44 min (92% ee); $[\alpha]_D^{25}$ = +102.0 (c = 0.100, $CHCl_3$, 92% ee).

Operator:GC Timebase:U3000 Sequence:WXL-2

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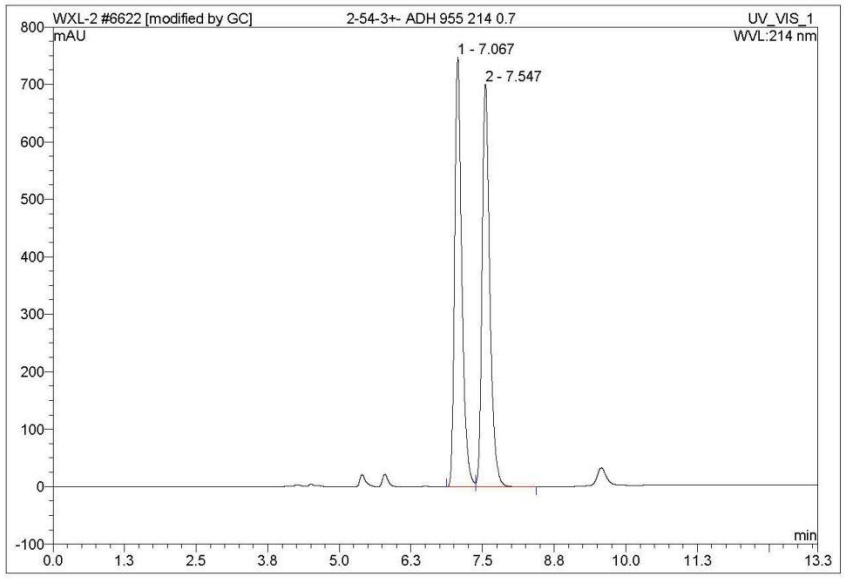
2016/7/22 8:43 下午

6622 2-54-3+- ADH 955 214 0.7

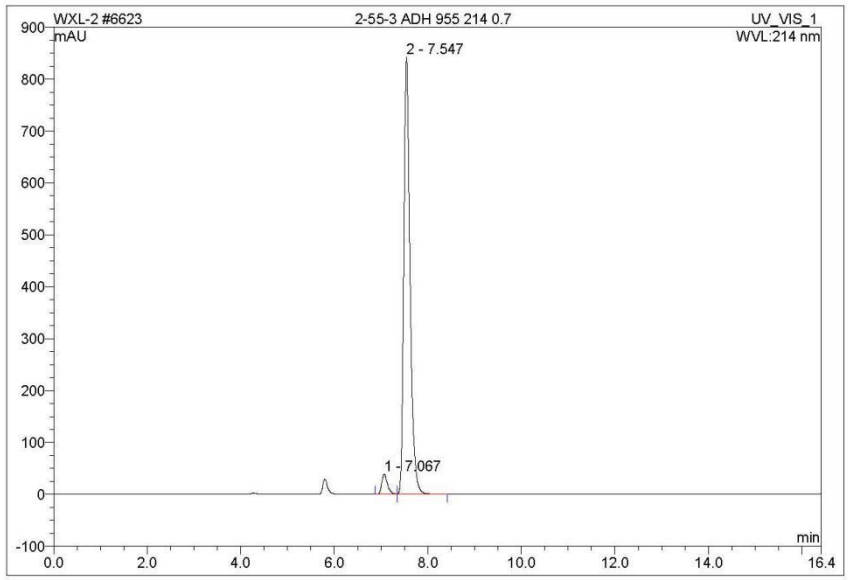
Sample Name:	**2-54-3+- ADH 955 214 0.7**	*Injection Volume:*	**0.8**
Vial Number:	**RB1**	*Channel:*	**UV_VIS_1**
Sample Type:	**unknown**	*Wavelength:*	**214**
Control Program:	**WXL-2014**	*Bandwidth:*	**n.a.**
Quantif. Method:	**WXL**	*Dilution Factor:*	**1.0000**
Recording Time:	**2016/3/17 18:51**	*Sample Weight:*	**1.0000**
Run Time (min):	**13.35**	*Sample Amount:*	**1.0000**



No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	7.07	n.a.	747.998	108.514	49.77	n.a.	BM
2	7.55	n.a.	700.894	109.501	50.23	n.a.	MB
Total:			1448.891	218.015	100.00	0.000	

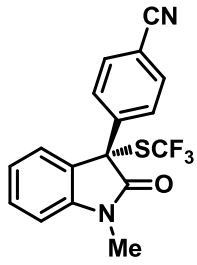
6623 2-55-3 ADH 955 214 0.7

Sample Name:	**2-55-3 ADH 955 214 0.7**	*Injection Volume:*	**0.8**
Vial Number:	**RB2**	*Channel:*	**UV_VIS_1**
Sample Type:	**unknown**	*Wavelength:*	**214**
Control Program:	**WXL-2014**	*Bandwidth:*	**n.a.**
Quantif. Method:	**WXL**	*Dilution Factor:*	**1.0000**
Recording Time:	**2016/3/17 19:05**	*Sample Weight:*	**1.0000**
Run Time (min):	**16.41**	*Sample Amount:*	**1.0000**



No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	7.07	n.a.	38.706	5.519	4.08	n.a.	BM
2	7.55	n.a.	843.142	129.882	95.92	n.a.	MB
Total:			881.848	135.401	100.00	0.000	

HPLC spectra for compound 4e



4e

HPLC: (IC, Hexane/^{i}PrOH = 8/2, 0.7 mL/min, 214 nm), t_R (major) = 16.37 min, t_R (minor) = 15.21 min (94% ee); $[\alpha]_D^{25}$ = +126.6 (c = 0.065, $CHCl_3$, 94% ee).

Operator:Administrator Timebase:HPLC Sequence:20151027-DAD

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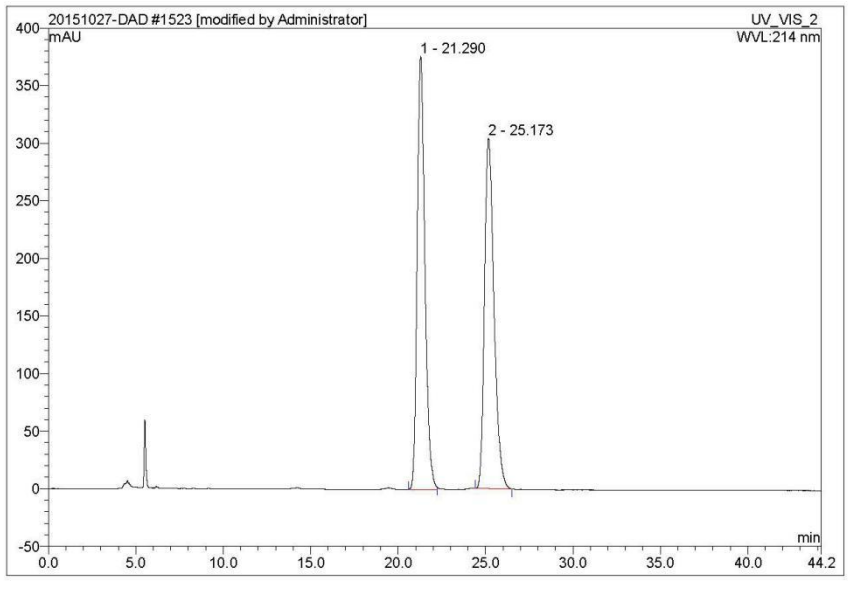
1523 ZH-2-66-1+- IC 82 214 0.7

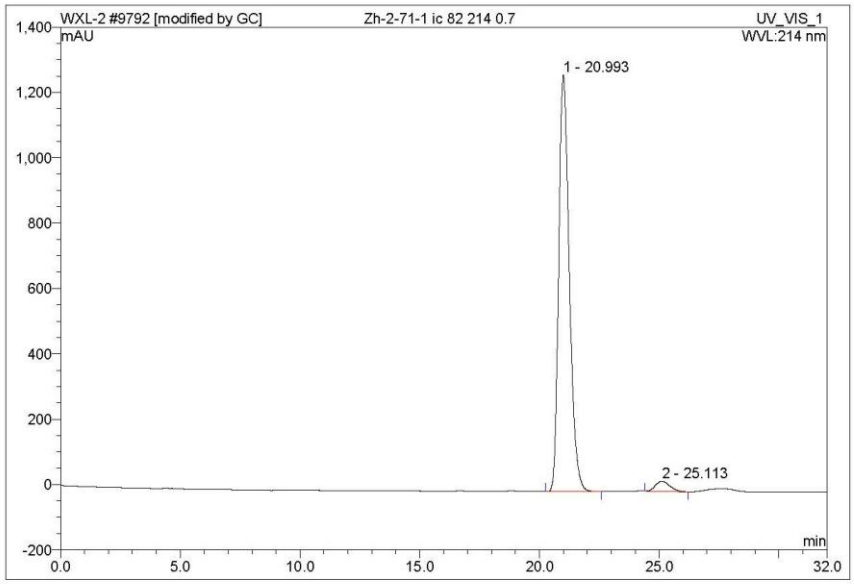
Sample Name:	**ZH-2-66-1+- IC 82 214 0.7**	*Injection Volume:*	**2.0**
Vial Number:	**RD7**	*Channel:*	**UV_VIS_2**
Sample Type:	**unknown**	*Wavelength:*	**214.0**
Control Program:	**test-dad4**	*Bandwidth:*	**4**
Quantif. Method:	**WXL**	*Dilution Factor:*	**1.0000**
Recording Time:	**2016-4-12 16:32**	*Sample Weight:*	**1.0000**
Run Time (min):	**44.19**	*Sample Amount:*	**1.0000**



No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	21.29	n.a.	376.249	192.736	50.14	n.a.	BM *
2	25.17	n.a.	304.455	191.656	49.86	n.a.	BMB
Total:			680.703	384.391	100.00	0.000	

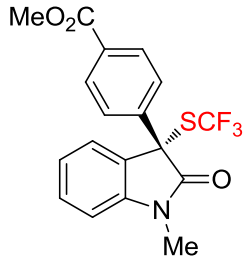
9792 Zh-2-71-1 ic 82 214 0.7

Sample Name:	**Zh-2-71-1 ic 82 214 0.7**	*Injection Volume:*	**1.0**
Vial Number:	**BA1**	*Channel:*	**UV_VIS_1**
Sample Type:	**unknown**	*Wavelength:*	**214**
Control Program:	**WXL-2014**	*Bandwidth:*	**n.a.**
Quantif. Method:	**WXL**	*Dilution Factor:*	**1.0000**
Recording Time:	**2017/1/3 10:25**	*Sample Weight:*	**1.0000**
Run Time (min):	**32.00**	*Sample Amount:*	**1.0000**



No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	20.99	n.a.	1274.501	651.584	96.77	n.a.	BMB
2	25.11	n.a.	31.411	21.777	3.23	n.a.	BMB
Total:			1305.912	673.362	100.00	0.000	

HPLC spectra for compound 4f



4f

HPLC: (IE-3 (0.46 × 25 cm, 3 μm), Hexane/^{i}PrOH = 8/2, 0.7 mL/min, 214 nm), t_R (major) = 15.62 min, t_R (minor) = 20.25 min (94% ee); $[\alpha]_D^{25}$ = +117.3 (c = 0.100, $CHCl_3$, 94% ee).

Operator:Administrator Timebase:HPLC Sequence:20151027-DAD

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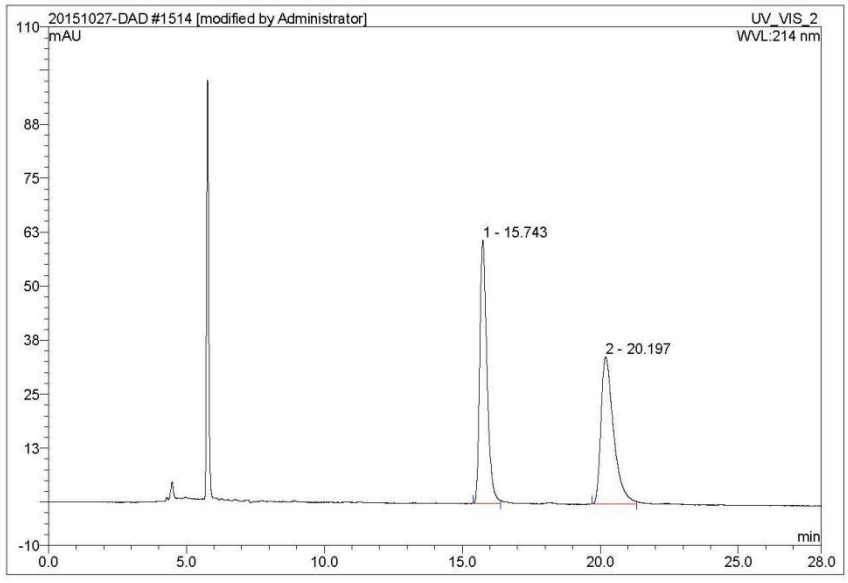
1514 ZH-2-66-4+- IE3 82 214 0.7

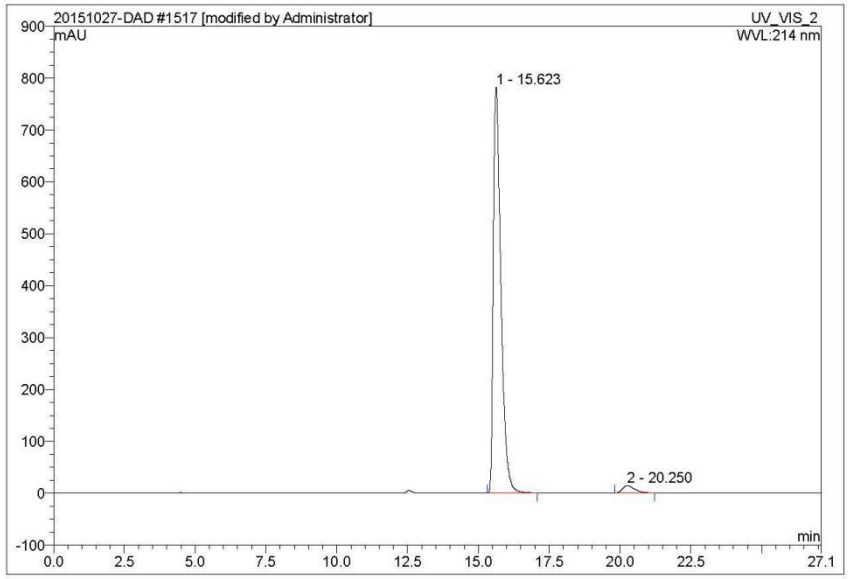
Sample Name:	**ZH-2-66-4+- IE3 82 214 0.7**	*Injection Volume:*	**2.0**
Vial Number:	**RB7**	*Channel:*	**UV_VIS_2**
Sample Type:	**unknown**	*Wavelength:*	**214.0**
Control Program:	**test-dad4**	*Bandwidth:*	**4**
Quantif. Method:	**WXL**	*Dilution Factor:*	**1.0000**
Recording Time:	**2016-4-11 19:21**	*Sample Weight:*	**1.0000**
Run Time (min):	**28.00**	*Sample Amount:*	**1.0000**



No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	15.74	n.a.	60.907	18.478	50.49	n.a.	BM *
2	20.20	n.a.	34.095	18.121	49.51	n.a.	BM *
Total:			95.002	36.599	100.00	0.000	

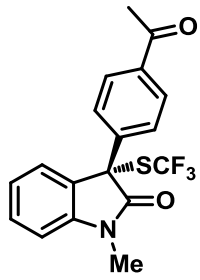
1517 ZH-2-67-4 IE3 82 214 0.7

Sample Name:	**ZH-2-67-4 IE3 82 214 0.7**	*Injection Volume:*	**0.2**
Vial Number:	**RB6**	*Channel:*	**UV_VIS_2**
Sample Type:	**unknown**	*Wavelength:*	**214.0**
Control Program:	**test-dad4**	*Bandwidth:*	**4**
Quantif. Method:	**WXL**	*Dilution Factor:*	**1.0000**
Recording Time:	**2016-4-11 20:43**	*Sample Weight:*	**1.0000**
Run Time (min):	**27.10**	*Sample Amount:*	**1.0000**



No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	15.62	n.a.	783.197	243.042	96.98	n.a.	BMB
2	20.25	n.a.	14.578	7.576	3.02	n.a.	BMB
Total:			797.776	250.618	100.00	0.000	

HPLC spectra for compound 4g



4g

HPLC: (IE-3 (0.46 ×25 cm, 3 μm), Hexane/^{i}PrOH = 8/2, 0.7 mL/min, 214 nm), t_R (major) = 18.47 min, t_R (minor) = 20.13 min (89% ee); $[\alpha]_D^{25}$ = +105.0 (c = 0.100, $CHCl_3$, 89% ee).

Operator:Administrator Timebase:HPLC Sequence:20151027-DAD

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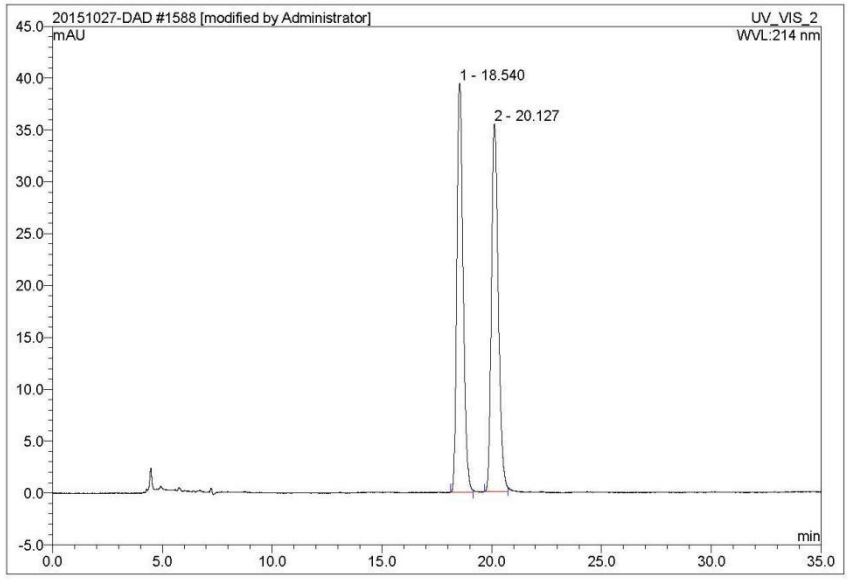
1588 2-75-1+- IE3 82 214 0.7

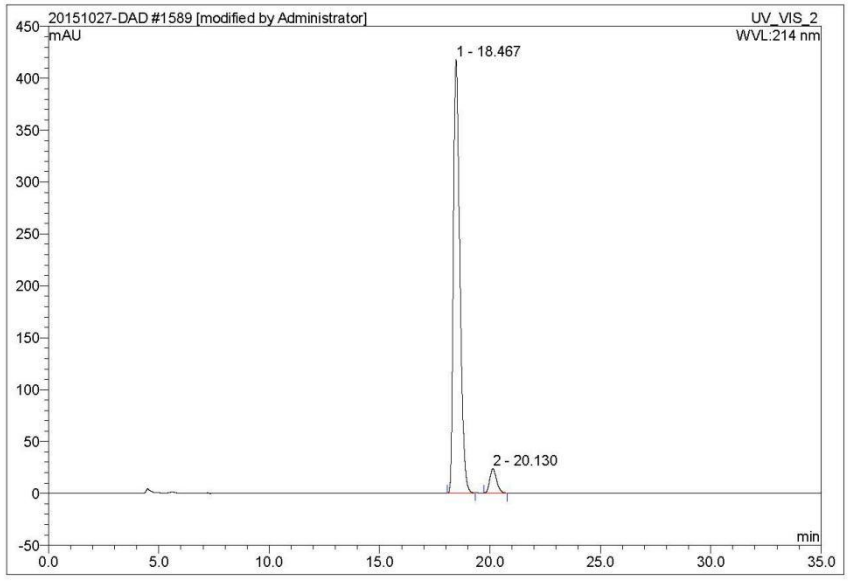
Sample Name:	**2-75-1+- IE3 82 214 0.7**	*Injection Volume:*	**1.0**
Vial Number:	**RA7**	*Channel:*	**UV_VIS_2**
Sample Type:	**unknown**	*Wavelength:*	**214.0**
Control Program:	**test-dad4**	*Bandwidth:*	**4**
Quantif. Method:	**WXL**	*Dilution Factor:*	**1.0000**
Recording Time:	**2016-4-18 21:56**	*Sample Weight:*	**1.0000**
Run Time (min):	**35.00**	*Sample Amount:*	**1.0000**



No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	18.54	n.a.	39.454	12.973	50.03	n.a.	BM *
2	20.13	n.a.	35.505	12.960	49.97	n.a.	BM *
Total:			74.959	25.934	100.00	0.000	

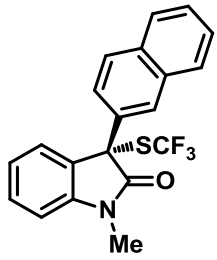
1589 2-75-2 IE3 82 214 0.7

Sample Name:	**2-75-2 IE3 82 214 0.7**	*Injection Volume:*	**1.0**
Vial Number:	**RE6**	*Channel:*	**UV_VIS_2**
Sample Type:	**unknown**	*Wavelength:*	**214.0**
Control Program:	**test-dad4**	*Bandwidth:*	**4**
Quantif. Method:	**WXL**	*Dilution Factor:*	**1.0000**
Recording Time:	**2016-4-18 22:32**	*Sample Weight:*	**1.0000**
Run Time (min):	**35.00**	*Sample Amount:*	**1.0000**



No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	18.47	n.a.	417.968	141.352	94.30	n.a.	BMB
2	20.13	n.a.	23.583	8.538	5.70	n.a.	BMB
Total:			441.551	149.889	100.00	0.000	

HPLC spectra for compound 4h



4h

HPLC: (IE-3 (0.46 × 25 cm, 3 μm), Hexane/^{i}PrOH = 8/2, 0.7 mL/min, 214 nm), t_R (major) = 9.92 min, t_R (minor) = 10.42 min (95% ee); $[\alpha]_D^{25}$ = +88.9 (c = 0.100, $CHCl_3$, 95% ee).

Operator:Administrator Timebase:HPLC Sequence:20151027-DAD

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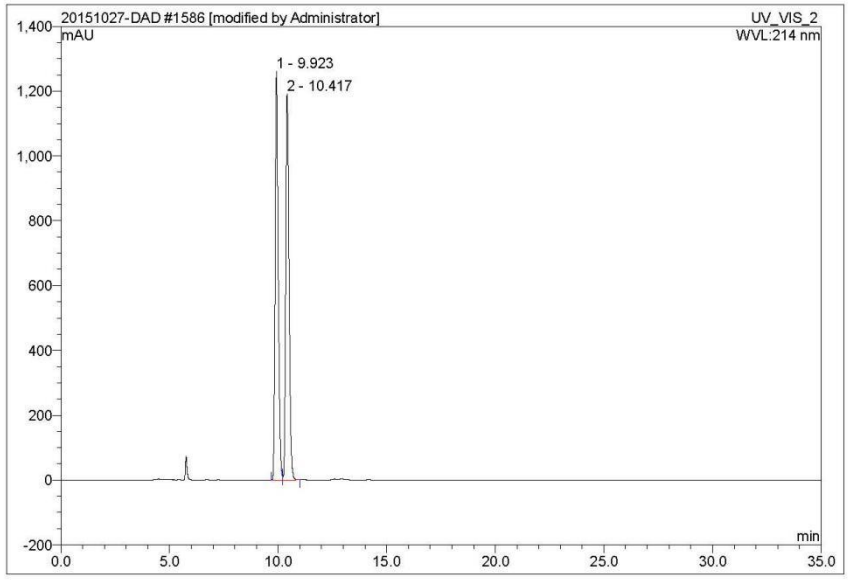
1586 2-75-2+- IE3 82 214 0.7

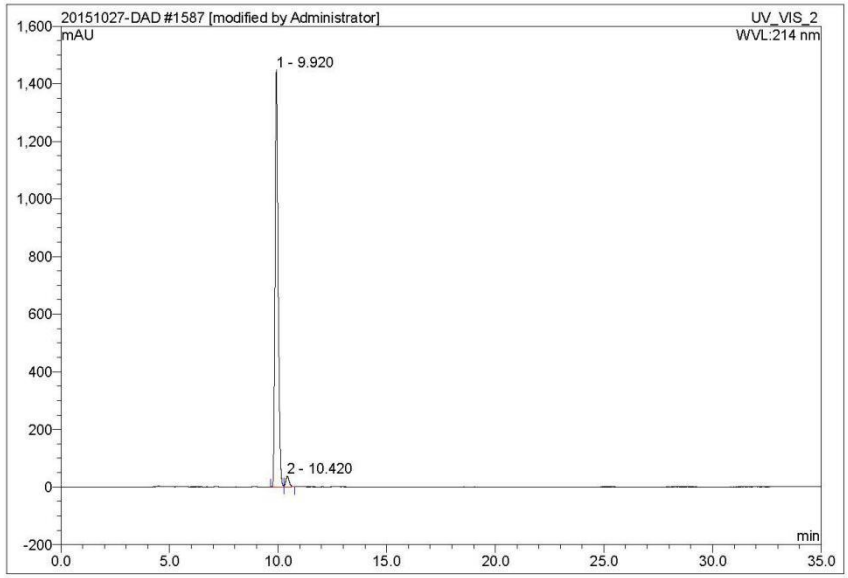
Sample Name:	**2-75-2+- IE3 82 214 0.7**	*Injection Volume:*	**1.0**
Vial Number:	**RC7**	*Channel:*	**UV_VIS_2**
Sample Type:	**unknown**	*Wavelength:*	**214.0**
Control Program:	**test-dad4**	*Bandwidth:*	**4**
Quantif. Method:	**WXL**	*Dilution Factor:*	**1.0000**
Recording Time:	**2016-4-18 20:44**	*Sample Weight:*	**1.0000**
Run Time (min):	**35.00**	*Sample Amount:*	**1.0000**



No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	9.92	n.a.	1261.836	208.720	49.84	n.a.	BM
2	10.42	n.a.	1191.789	210.061	50.16	n.a.	MB
Total:			2453.625	418.782	100.00	0.000	

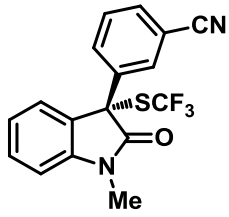
1587 2-74-2 IE3 82 214 0.7

Sample Name:	**2-74-2 IE3 82 214 0.7**	*Injection Volume:*	**1.0**
Vial Number:	**RB7**	*Channel:*	**UV_VIS_2**
Sample Type:	**unknown**	*Wavelength:*	**214.0**
Control Program:	**test-dad4**	*Bandwidth:*	**4**
Quantif. Method:	**WXL**	*Dilution Factor:*	**1.0000**
Recording Time:	**2016-4-18 21:20**	*Sample Weight:*	**1.0000**
Run Time (min):	**35.00**	*Sample Amount:*	**1.0000**



No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	9.92	n.a.	1447.560	239.485	97.29	n.a.	BM
2	10.42	n.a.	37.068	6.666	2.71	n.a.	MB
Total:			1484.628	246.151	100.00	0.000	

HPLC spectra for compound 4i



4i

HPLC: (IE-3 (0.46 × 25 cm, 3 μm), Hexane/^{i}PrOH = 7/3, 0.7 mL/min, 214 nm), t_R (major) = 11.55 min, t_R (minor) = 13.17 min (93% ee); $[\alpha]_D^{25}$ = +84.6 (c = 0.100, $CHCl_3$, 93% ee).

Operator:GC Timebase:U3000 Sequence:WXL-2

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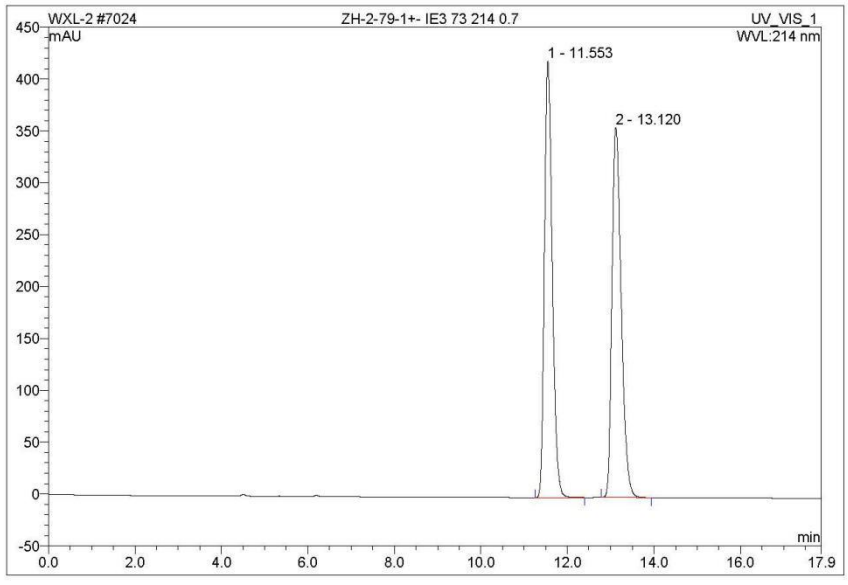
7024 ZH-2-79-1+- IE3 73 214 0.7

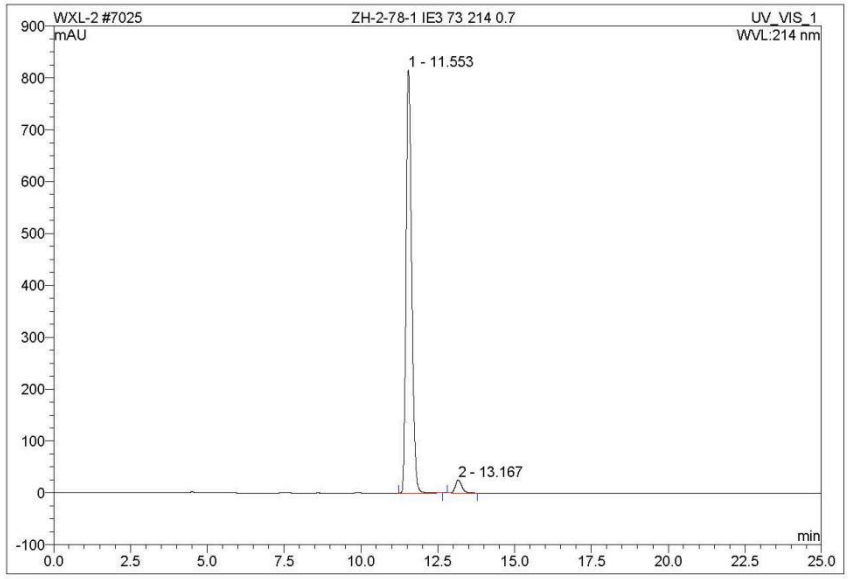
Sample Name:	**ZH-2-79-1+- IE3 73 214 0.7**	*Injection Volume:*	**1.0**
Vial Number:	**BC2**	*Channel:*	**UV_VIS_1**
Sample Type:	**unknown**	*Wavelength:*	**214**
Control Program:	**WXL-2014**	*Bandwidth:*	**n.a.**
Quantif. Method:	**WXL**	*Dilution Factor:*	**1.0000**
Recording Time:	**2016/4/20 9:54**	*Sample Weight:*	**1.0000**
Run Time (min):	**17.87**	*Sample Amount:*	**1.0000**



No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	11.55	n.a.	421.116	88.371	50.02	n.a.	BMB
2	13.12	n.a.	356.430	88.311	49.98	n.a.	BMB
Total:			777.546	176.682	100.00	0.000	

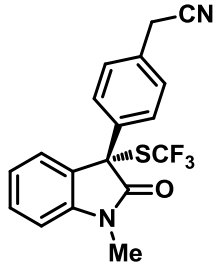
7025 ZH-2-78-1 IE3 73 214 0.7

Sample Name:	**ZH-2-78-1 IE3 73 214 0.7**	*Injection Volume:*	**1.0**
Vial Number:	**BC2**	*Channel:*	**UV_VIS_1**
Sample Type:	**unknown**	*Wavelength:*	**214**
Control Program:	**WXL-2014**	*Bandwidth:*	**n.a.**
Quantif. Method:	**WXL**	*Dilution Factor:*	**1.0000**
Recording Time:	**2016/4/20 10:22**	*Sample Weight:*	**1.0000**
Run Time (min):	**24.97**	*Sample Amount:*	**1.0000**



No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	11.55	n.a.	816.252	172.827	96.61	n.a.	BMB
2	13.17	n.a.	25.134	6.067	3.39	n.a.	BMB
Total:			841.386	178.894	100.00	0.000	

HPLC spectra for compound 4j



4j

HPLC: (IE-3 (0.46 ×25 cm, 3 μm), Hexane/^{i}PrOH = 7/3, 0.7 mL/min, 214 nm), t_R (major) = 13.36 min, t_R (minor) = 14.52 min (57% ee); $[\alpha]_D^{25}$ = +72.4 (c = 0.110, $CHCl_3$, 57% ee).

Operator:GC Timebase:U3000 Sequence:WXL-2

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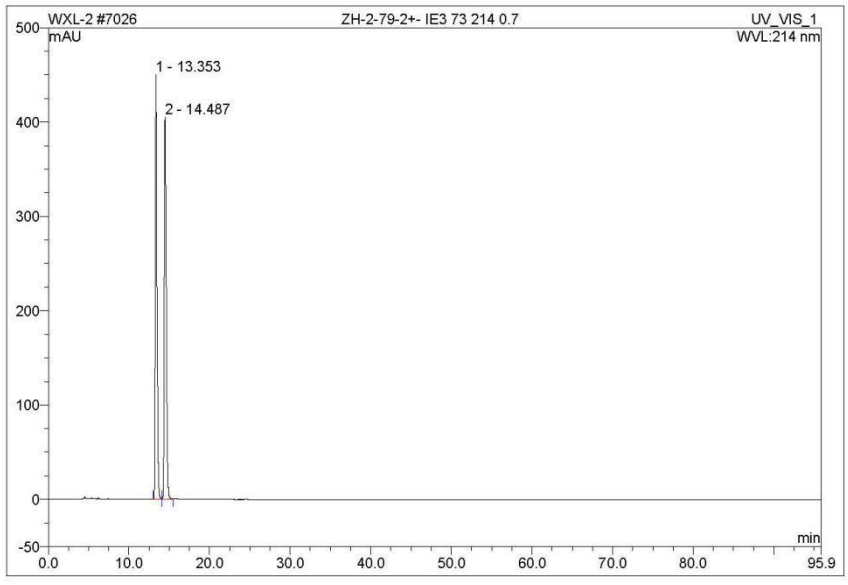
7026 ZH-2-79-2+- IE3 73 214 0.7

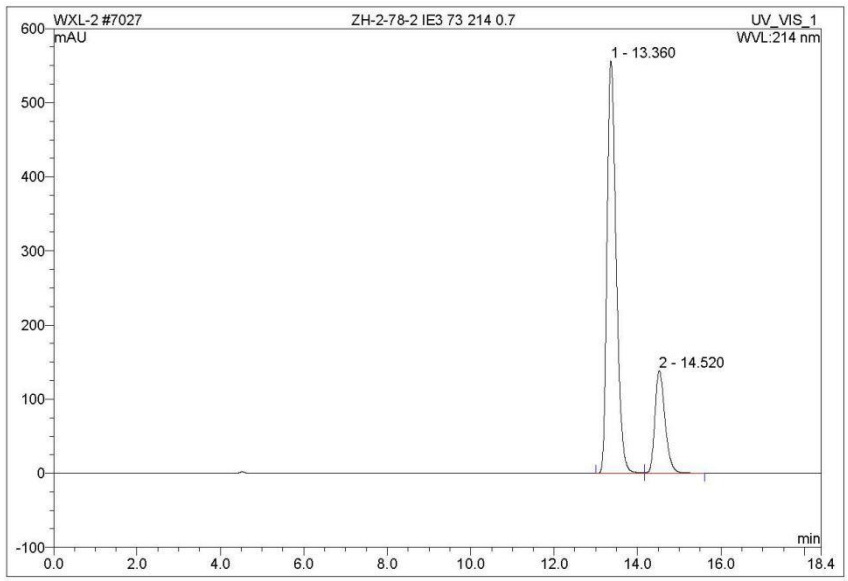
Sample Name:	**ZH-2-79-2+- IE3 73 214 0.7**	*Injection Volume:*	**1.0**
Vial Number:	**BC3**	*Channel:*	**UV_VIS_1**
Sample Type:	**unknown**	*Wavelength:*	**214**
Control Program:	**WXL-2014**	*Bandwidth:*	**n.a.**
Quantif. Method:	**WXL**	*Dilution Factor:*	**1.0000**
Recording Time:	**2016/4/20 10:52**	*Sample Weight:*	**1.0000**
Run Time (min):	**95.87**	*Sample Amount:*	**1.0000**



No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	13.35	n.a.	449.775	113.726	49.94	n.a.	BM
2	14.49	n.a.	404.726	114.018	50.06	n.a.	MB
Total:			854.501	227.744	100.00	0.000	

7027 ZH-2-78-2 IE3 73 214 0.7

Sample Name:	**ZH-2-78-2 IE3 73 214 0.7**	*Injection Volume:*	**1.0**
Vial Number:	**BC4**	*Channel:*	**UV_VIS_1**
Sample Type:	**unknown**	*Wavelength:*	**214**
Control Program:	**WXL-2014**	*Bandwidth:*	**n.a.**
Quantif. Method:	**WXL**	*Dilution Factor:*	**1.0000**
Recording Time:	**2016/4/20 12:31**	*Sample Weight:*	**1.0000**
Run Time (min):	**18.40**	*Sample Amount:*	**1.0000**



No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	13.36	n.a.	556.275	141.234	78.41	n.a.	BM
2	14.52	n.a.	138.422	38.881	21.59	n.a.	MB
Total:			694.697	180.115	100.00	0.000	

Compound **4j** obtained using compound **1b** as the electrophilic trifluoromethylthiolating reagent. HPLC: (IE-3 (0.46 × 25 cm, 3 μm), Hexane/^{i}PrOH = 7/3, 0.7 mL/min, 214 nm), t_R (major) = 13.36 min, t_R (minor) = 14.52 min (94% ee)[b]; $[\alpha]_D^{25}$ = +126.1 (c = 0.100, $CHCl_3$, 94% ee).

Operator:Administrator Timebase:HPLC Sequence:20151027-DAD

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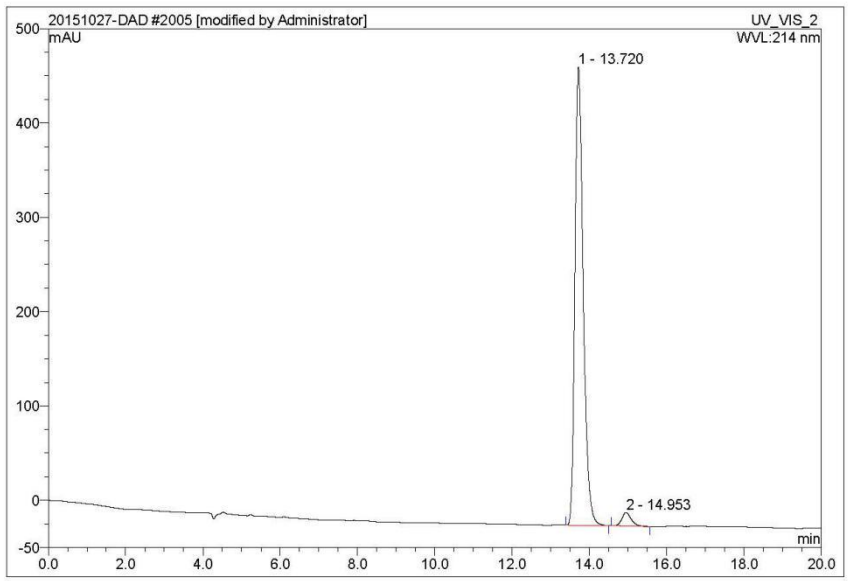
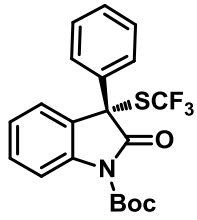
2005 ZH-2-99-5 IE3 73 214 0.7

Sample Name:	**ZH-2-99-5 IE3 73 214 0.7**	*Injection Volume:*	**1.0**
Vial Number:	**RB5**	*Channel:*	**UV_VIS_2**
Sample Type:	**unknown**	*Wavelength:*	**214.0**
Control Program:	**test-dad6**	*Bandwidth:*	**4**
Quantif. Method:	**WXL**	*Dilution Factor:*	**1.0000**
Recording Time:	**2016-5-27 19:14**	*Sample Weight:*	**1.0000**
Run Time (min):	**20.00**	*Sample Amount:*	**1.0000**



No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	13.72	n.a.	485.675	120.432	96.79	n.a.	BMB
2	14.95	n.a.	14.251	3.998	3.21	n.a.	BMB
Total:			499.926	124.430	100.00	0.000	

HPLC spectra for compound 4k



4k

HPLC: (IE-3 (0.46 × 25 cm, 3 μm), Hexane/^{i}PrOH = 95/5, 0.7 mL/min, 214 nm), t_R (major) = 6.83 min, t_R (minor) = 7.20 min (93% ee); $[\alpha]_D^{25}$ = +56.4 (c = 0.100, $CHCl_3$, 93% ee).

Operator:Administrator Timebase:HPLC Sequence:20151027-DAD

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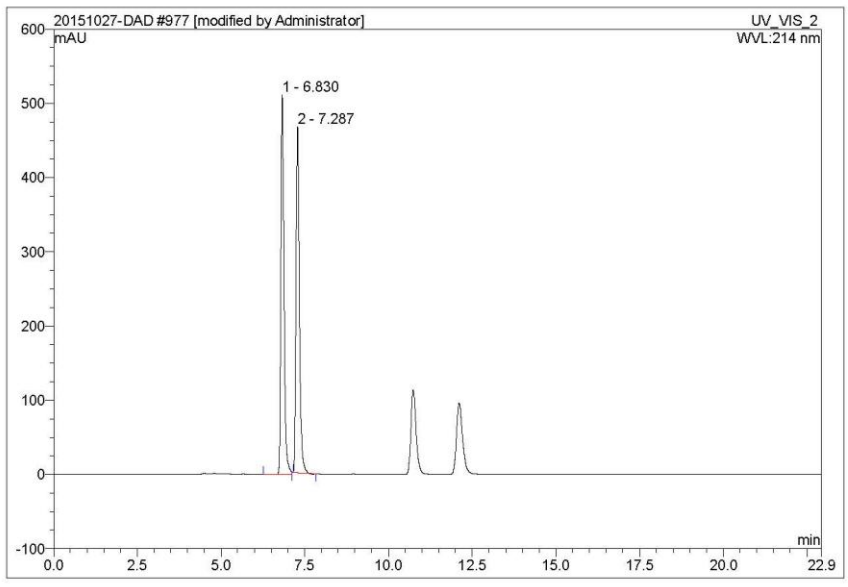
977 ZH-2-39-1+- IE3 955 214 0.7

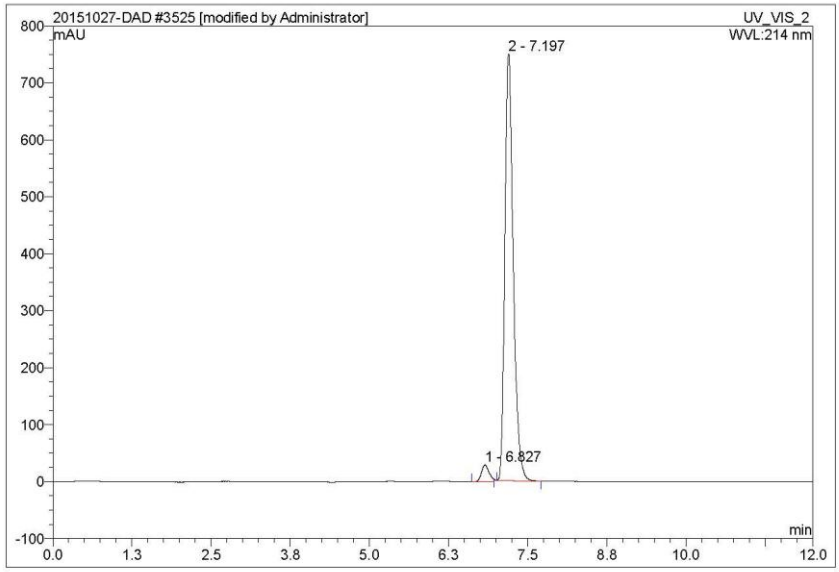
Sample Name:	**ZH-2-39-1+- IE3 955 214 0.7**	*Injection Volume:*	**1.0**
Vial Number:	**RD4**	*Channel:*	**UV_VIS_2**
Sample Type:	**unknown**	*Wavelength:*	**214.0**
Control Program:	**test-dad2**	*Bandwidth:*	**4**
Quantif. Method:	**WXL**	*Dilution Factor:*	**1.0000**
Recording Time:	**2016-2-22 13:41**	*Sample Weight:*	**1.0000**
Run Time (min):	**22.92**	*Sample Amount:*	**1.0000**



No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	6.83	n.a.	511.892	55.528	50.47	n.a.	BM *
2	7.29	n.a.	466.172	54.500	49.53	n.a.	BMB*
Total:			978.064	110.028	100.00	0.000	

3525 ZH-2-76-1-2 IC 982 214 0.7

Sample Name:	**ZH-2-76-1-2 IC 982 214 0.7**	*Injection Volume:*	**0.6**
Vial Number:	**RD6**	*Channel:*	**UV_VIS_2**
Sample Type:	**unknown**	*Wavelength:*	**214.0**
Control Program:	**test-dad3**	*Bandwidth:*	**4**
Quantif. Method:	**WXL**	*Dilution Factor:*	**1.0000**
Recording Time:	**2016-10-8 10:52**	*Sample Weight:*	**1.0000**
Run Time (min):	**12.00**	*Sample Amount:*	**1.0000**



No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	6.83	n.a.	29.314	4.066	3.41	n.a.	BM *
2	7.20	n.a.	749.494	115.191	96.59	n.a.	BMB*
Total:			778.808	119.257	100.00	0.000	

Compound **4k** obtained using compound **1b** as the electrophilic trifluoromethylthiolating reagent. HPLC: (IE-3 (0.46 × 25 cm, 3 μm), Hexane/^{i}PrOH = 95/5, 0.7 mL/min, 214 nm), t_R (major) = 6.80 min, t_R (minor) = 7.28 min (91% ee)[b]; $[\alpha]_D^{25}$ = +47.6 (c = 0.175, $CHCl_3$, 91% ee).

Operator:Administrator Timebase:HPLC Sequence:20151027-DAD

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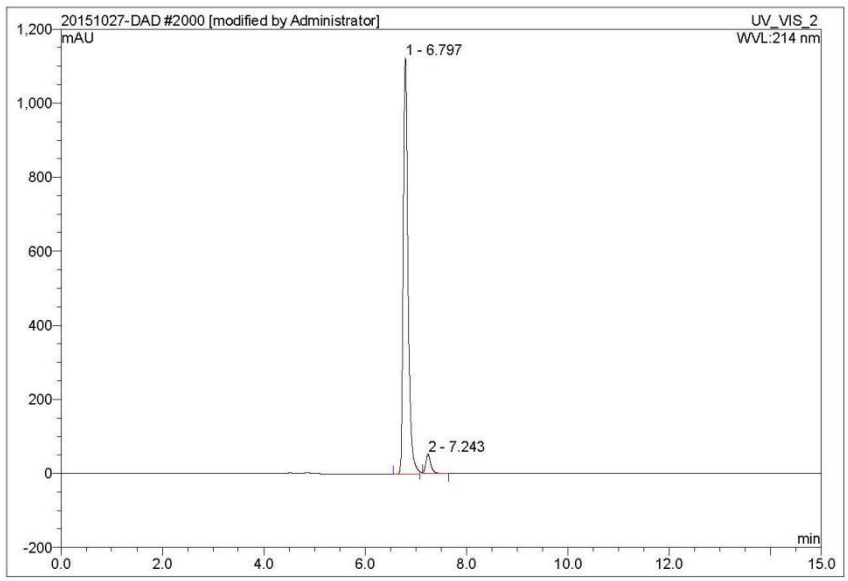
2000 ZH-2-99-1 IE3 955 214 0.7

Sample Name:	**ZH-2-99-1 IE3 955 214 0.7**	*Injection Volume:*	**1.0**
Vial Number:	**RE5**	*Channel:*	**UV_VIS_2**
Sample Type:	**unknown**	*Wavelength:*	**214.0**
Control Program:	**test-dad4**	*Bandwidth:*	**4**
Quantif. Method:	**WXL**	*Dilution Factor:*	**1.0000**
Recording Time:	**2016-5-27 17:49**	*Sample Weight:*	**1.0000**
Run Time (min):	**15.00**	*Sample Amount:*	**1.0000**



No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	6.80	n.a.	1123.887	122.536	95.29	n.a.	BM *
2	7.24	n.a.	51.983	6.060	4.71	n.a.	MB*
Total:			1175.870	128.596	100.00	0.000	

HPLC spectra for compound 4l

4l

HPLC: (IE-3 (0.46 × 25 cm, 3 μm), Hexane/^{i}PrOH = 95/5, 0.7 mL/min, 214 nm), t_R (major) = 8.89 min, t_R (minor) = 11.49 min (93% ee); $[\alpha]_D^{25}$ = +46.5 (c = 0.125, $CHCl_3$, 93% ee).

Operator:GC Timebase:U3000 Sequence:WXL-2

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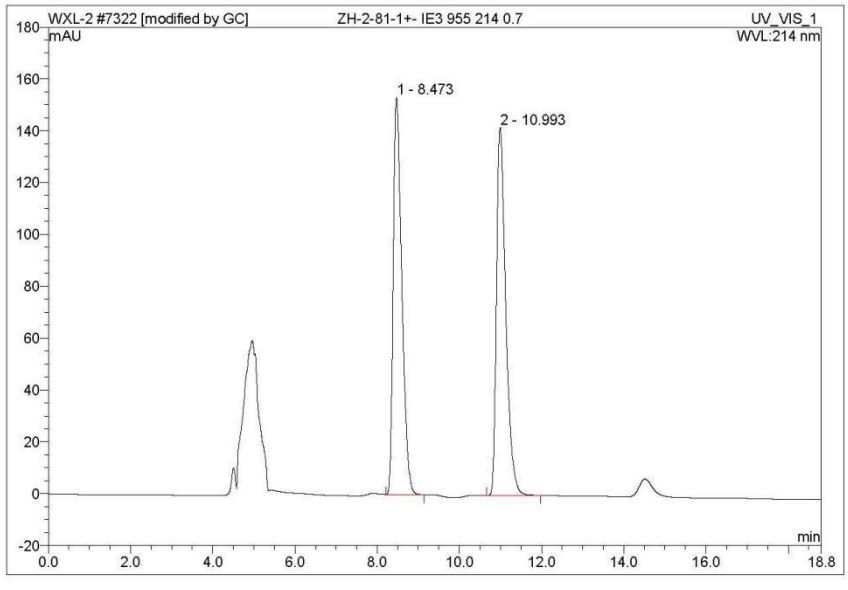
2016/7/22 8:37 下午

7322 ZH-2-81-1+- IE3 955 214 0.7

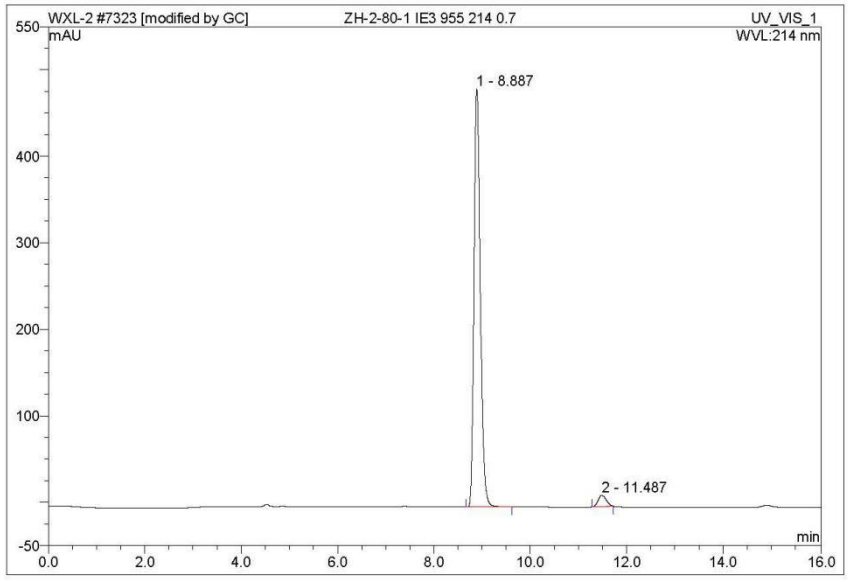
Sample Name:	**ZH-2-81-1+- IE3 955 214 0.7**	*Injection Volume:*	**1.0**
Vial Number:	**BE2**	*Channel:*	**UV_VIS_1**
Sample Type:	**unknown**	*Wavelength:*	**214**
Control Program:	**WXL-2014-1**	*Bandwidth:*	**n.a.**
Quantif. Method:	**WXL**	*Dilution Factor:*	**1.0000**
Recording Time:	**2016/5/23 11:41**	*Sample Weight:*	**1.0000**
Run Time (min):	**18.80**	*Sample Amount:*	**1.0000**



No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	8.47	n.a.	153.247	37.071	49.98	n.a.	BMB
2	10.99	n.a.	142.003	37.100	50.02	n.a.	BMB
Total:			295.249	74.171	100.00	0.000	

7323 ZH-2-80-1 IE3 955 214 0.7

Sample Name:	**ZH-2-80-1 IE3 955 214 0.7**	*Injection Volume:*	**1.0**
Vial Number:	**BE3**	*Channel:*	**UV_VIS_1**
Sample Type:	**unknown**	*Wavelength:*	**214**
Control Program:	**WXL-2014-1**	*Bandwidth:*	**n.a.**
Quantif. Method:	**WXL**	*Dilution Factor:*	**1.0000**
Recording Time:	**2016/5/23 12:01**	*Sample Weight:*	**1.0000**
Run Time (min):	**16.03**	*Sample Amount:*	**1.0000**



No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	8.89	n.a.	483.529	72.940	96.53	n.a.	BMB
2	11.49	n.a.	13.150	2.624	3.47	n.a.	BMB*
Total:			496.679	75.564	100.00	0.000	

HPLC spectra for compound 4m

4m

HPLC: (IE-3 (0.46 × 25 cm, 3 μm), Hexane/^{i}PrOH = 95/5, 0.7 mL/min, 214 nm), t_R (major) = 6.43 min, t_R (minor) = 7.07 min (91% ee); $[\alpha]_D^{25}$ = +48.0 (c = 0.125, $CHCl_3$, 91% ee).

Operator:GC Timebase:U3000 Sequence:WXL-2

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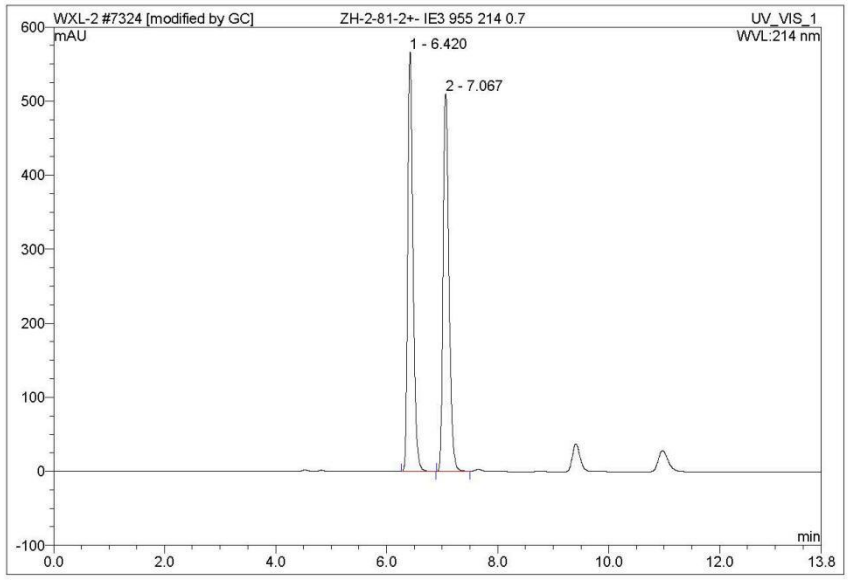
7324 ZH-2-81-2+- IE3 955 214 0.7

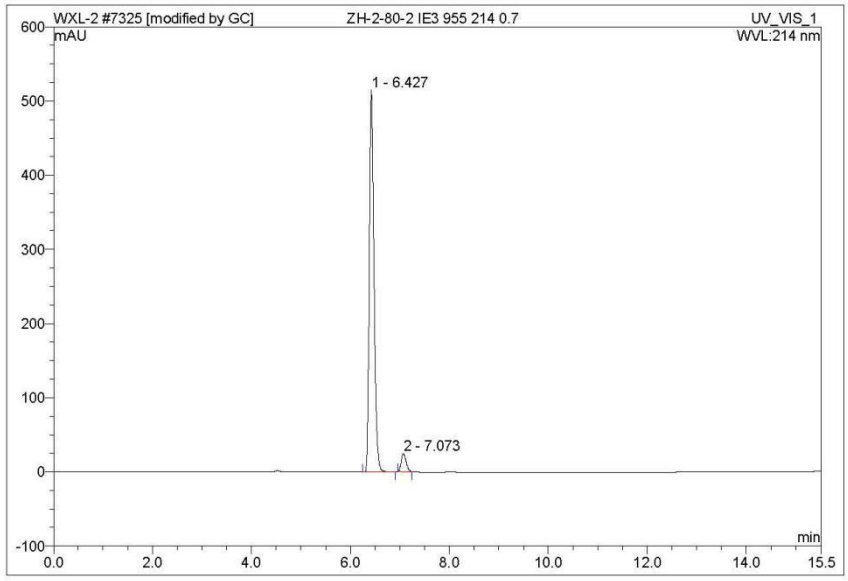
Sample Name:	**ZH-2-81-2+- IE3 955 214 0.7**	*Injection Volume:*	**1.0**
Vial Number:	**BE4**	*Channel:*	**UV_VIS_1**
Sample Type:	**unknown**	*Wavelength:*	**214**
Control Program:	**WXL-2014-1**	*Bandwidth:*	**n.a.**
Quantif. Method:	**WXL**	*Dilution Factor:*	**1.0000**
Recording Time:	**2016/5/23 12:18**	*Sample Weight:*	**1.0000**
Run Time (min):	**13.83**	*Sample Amount:*	**1.0000**



No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	6.42	n.a.	566.706	62.743	50.24	n.a.	BMB
2	7.07	n.a.	510.071	62.146	49.76	n.a.	BMB
Total:			1076.777	124.889	100.00	0.000	

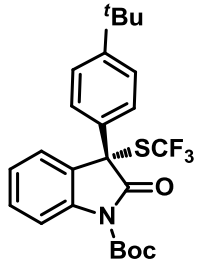
7325 ZH-2-80-2 IE3 955 214 0.7

Sample Name:	**ZH-2-80-2 IE3 955 214 0.7**	*Injection Volume:*	**1.0**
Vial Number:	**BE5**	*Channel:*	**UV_VIS_1**
Sample Type:	**unknown**	*Wavelength:*	**214**
Control Program:	**WXL-2014-1**	*Bandwidth:*	**n.a.**
Quantif. Method:	**WXL**	*Dilution Factor:*	**1.0000**
Recording Time:	**2016/5/23 12:33**	*Sample Weight:*	**1.0000**
Run Time (min):	**15.51**	*Sample Amount:*	**1.0000**



No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	6.43	n.a.	515.282	56.512	95.28	n.a.	BMB
2	7.07	n.a.	24.175	2.801	4.72	n.a.	BMB*
Total:			539.457	59.313	100.00	0.000	

HPLC spectra for compound 4n



4n

HPLC: (IE-3 (0.46 × 25 cm, 3 μm), Hexane/^{i}PrOH = 95/5, 0.7 mL/min, 214 nm), t_R (major) = 5.89 min, t_R (minor) = 6.65 min (93% ee); $[\alpha]_D^{25}$ = +63.9 (c = 0.050, $CHCl_3$, 93% ee).

Operator:GC Timebase:U3000 Sequence:WXL-2

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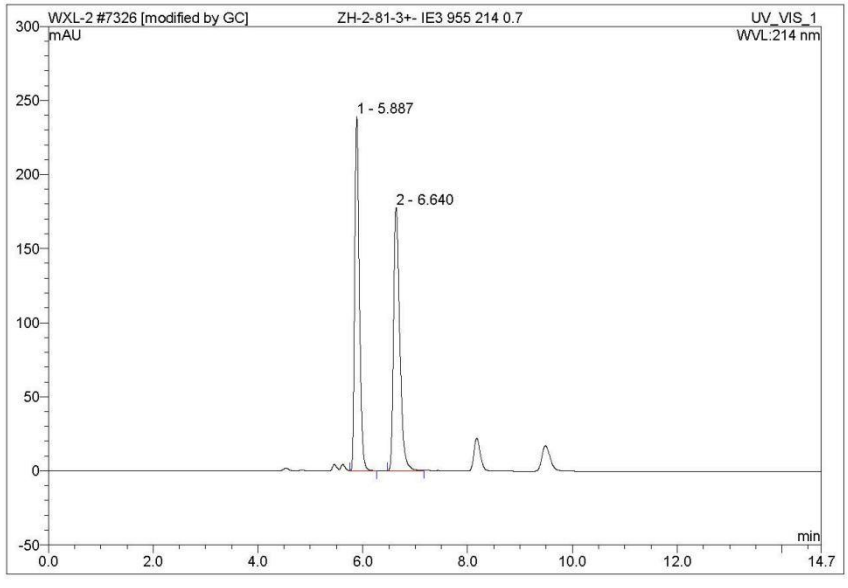
7326 ZH-2-81-3+- IE3 955 214 0.7

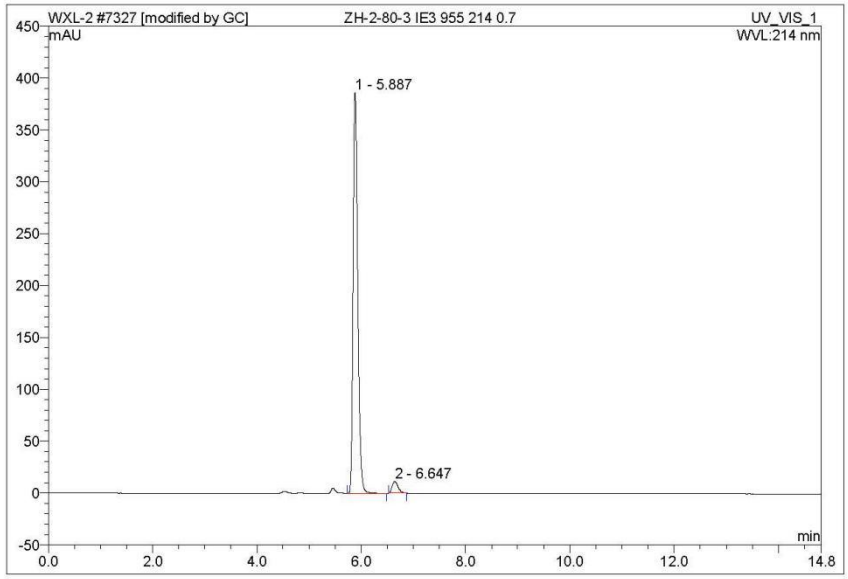
Sample Name:	**ZH-2-81-3+- IE3 955 214 0.7**	*Injection Volume:*	**1.0**
Vial Number:	**BE6**	*Channel:*	**UV_VIS_1**
Sample Type:	**unknown**	*Wavelength:*	**214**
Control Program:	**WXL-2014-1**	*Bandwidth:*	**n.a.**
Quantif. Method:	**WXL**	*Dilution Factor:*	**1.0000**
Recording Time:	**2016/5/23 12:52**	*Sample Weight:*	**1.0000**
Run Time (min):	**14.75**	*Sample Amount:*	**1.0000**



No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	5.89	n.a.	239.275	24.632	50.13	n.a.	BMB
2	6.64	n.a.	177.413	24.500	49.87	n.a.	BM *
Total:			416.688	49.132	100.00	0.000	

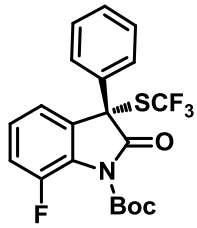
7327 ZH-2-80-3 IE3 955 214 0.7

Sample Name:	**ZH-2-80-3 IE3 955 214 0.7**	*Injection Volume:*	**1.0**
Vial Number:	**BE2**	*Channel:*	**UV_VIS_1**
Sample Type:	**unknown**	*Wavelength:*	**214**
Control Program:	**WXL-2014-1**	*Bandwidth:*	**n.a.**
Quantif. Method:	**WXL**	*Dilution Factor:*	**1.0000**
Recording Time:	**2016/5/23 13:07**	*Sample Weight:*	**1.0000**
Run Time (min):	**14.82**	*Sample Amount:*	**1.0000**



No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	5.89	n.a.	386.517	39.910	96.44	n.a.	BMB
2	6.65	n.a.	11.190	1.472	3.56	n.a.	BMB*
Total:			397.707	41.382	100.00	0.000	

HPLC spectra for compound 4o



4o

HPLC: (IE-3 (0.46 × 25 cm, 3 μm), Hexane/^{i}PrOH = 95/5, 0.7 mL/min, 214 nm), t_R (major) = 9.65 min, t_R (minor) = 11.05 min (88% ee); $[\alpha]_D^{25}$ = +49.2 (c = 0.125, $CHCl_3$, 88% ee).

Operator:GC Timebase:U3000 Sequence:WXL-2

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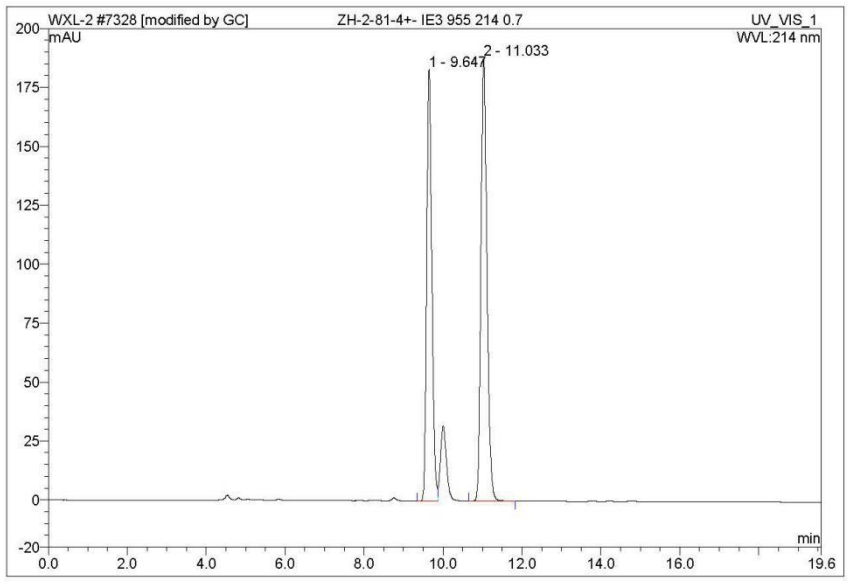
7328 ZH-2-81-4+- IE3 955 214 0.7

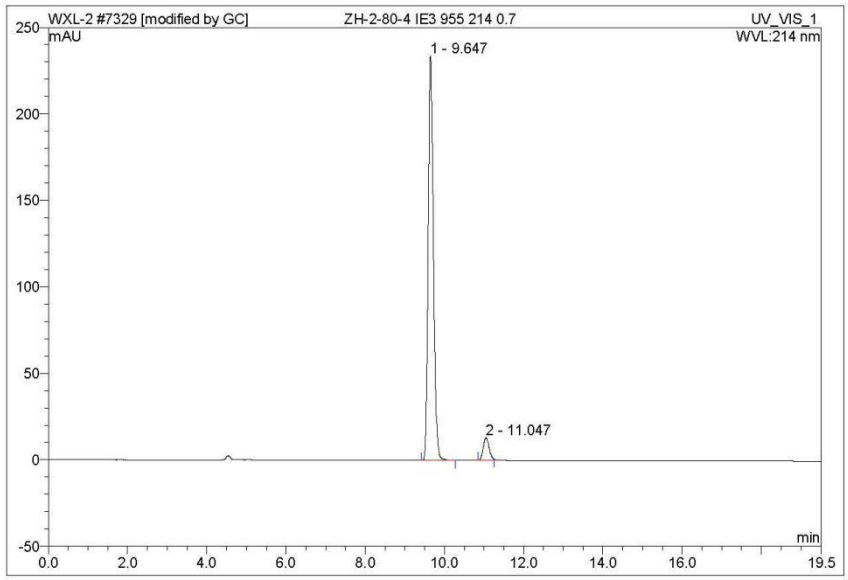
Sample Name:	**ZH-2-81-4+- IE3 955 214 0.7**	*Injection Volume:*	**1.0**
Vial Number:	**BE3**	*Channel:*	**UV_VIS_1**
Sample Type:	**unknown**	*Wavelength:*	**214**
Control Program:	**WXL-2014-1**	*Bandwidth:*	**n.a.**
Quantif. Method:	**WXL**	*Dilution Factor:*	**1.0000**
Recording Time:	**2016/5/23 13:24**	*Sample Weight:*	**1.0000**
Run Time (min):	**19.58**	*Sample Amount:*	**1.0000**



No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	9.65	n.a.	182.940	27.737	45.42	n.a.	BM *
2	11.03	n.a.	187.652	33.330	54.58	n.a.	BMB*
Total:			370.592	61.067	100.00	0.000	

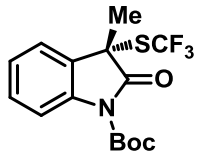
7329 ZH-2-80-4 IE3 955 214 0.7

Sample Name:	**ZH-2-80-4 IE3 955 214 0.7**	*Injection Volume:*	**1.0**
Vial Number:	**BE4**	*Channel:*	**UV_VIS_1**
Sample Type:	**unknown**	*Wavelength:*	**214**
Control Program:	**WXL-2014-1**	*Bandwidth:*	**n.a.**
Quantif. Method:	**WXL**	*Dilution Factor:*	**1.0000**
Recording Time:	**2016/5/23 13:47**	*Sample Weight:*	**1.0000**
Run Time (min):	**19.51**	*Sample Amount:*	**1.0000**



No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	9.65	n.a.	233.888	35.670	94.02	n.a.	BMB
2	11.05	n.a.	13.179	2.267	5.98	n.a.	BM *
Total:			247.067	37.936	100.00	0.000	

HPLC spectra for compound 4p



4p

HPLC: (IE-3 (0.46 × 25 cm, 3 μm), Hexane/^{i}PrOH = 9/1, 0.7 mL/min, 214 nm), t_R (major) = 5.83 min, t_R (minor) = 6.22 min (79% ee); $[\alpha]_D^{25}$ = +71.9 (c = 0.150, $CHCl_3$, 79% ee).

Operator:GC Timebase:U3000 Sequence:WXL-2

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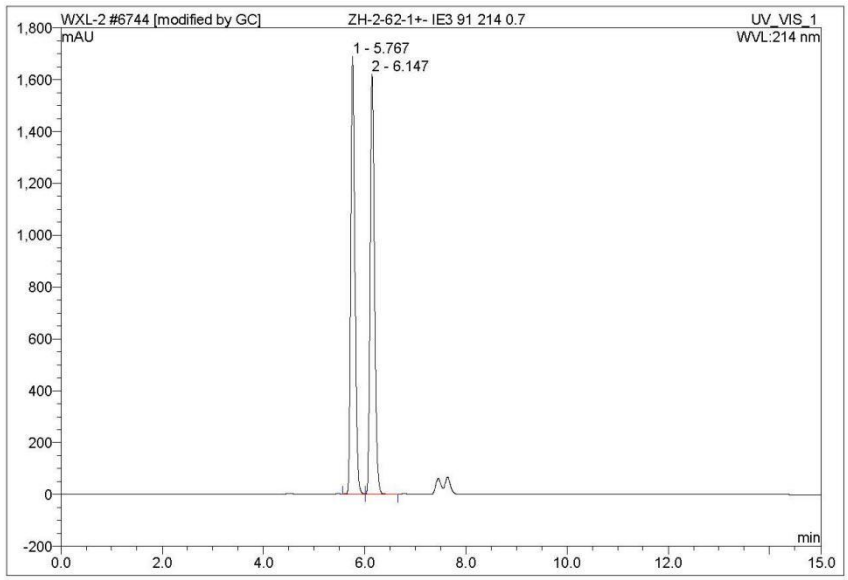
6744 ZH-2-62-1+- IE3 91 214 0.7

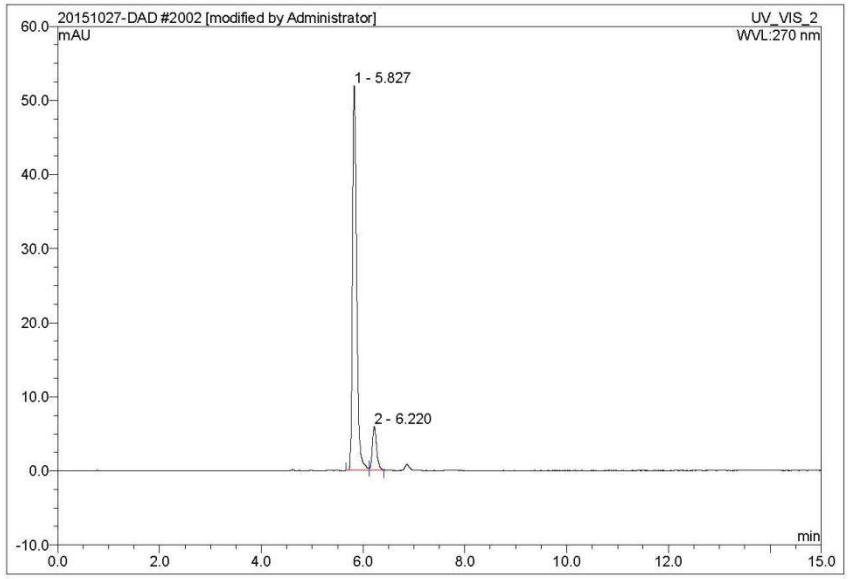
Sample Name:	**ZH-2-62-1+- IE3 91 214 0.7**	*Injection Volume:*	**2.0**
Vial Number:	**RB1**	*Channel:*	**UV_VIS_1**
Sample Type:	**unknown**	*Wavelength:*	**214**
Control Program:	**WXL-2014**	*Bandwidth:*	**n.a.**
Quantif. Method:	**WXL**	*Dilution Factor:*	**1.0000**
Recording Time:	**2016/3/29 16:49**	*Sample Weight:*	**1.0000**
Run Time (min):	**15.02**	*Sample Amount:*	**1.0000**



No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	5.77	n.a.	1689.596	162.226	49.81	n.a.	BM
2	6.15	n.a.	1620.134	163.444	50.19	n.a.	MB
Total:			3309.730	325.671	100.00	0.000	

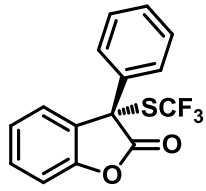
2002 ZH-2-99-3 IE3 91 214 0.7

Sample Name:	**ZH-2-99-3 IE3 91 214 0.7**	*Injection Volume:*	**1.0**
Vial Number:	**RD5**	*Channel:*	**UV_VIS_2**
Sample Type:	**unknown**	*Wavelength:*	**270.0**
Control Program:	**test-dad2**	*Bandwidth:*	**4**
Quantif. Method:	**WXL**	*Dilution Factor:*	**1.0000**
Recording Time:	**2016-5-27 18:21**	*Sample Weight:*	**1.0000**
Run Time (min):	**15.00**	*Sample Amount:*	**1.0000**



No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	5.83	n.a.	51.967	4.921	89.43	n.a.	BM *
2	6.22	n.a.	5.919	0.582	10.57	n.a.	MB*
Total:			57.887	5.503	100.00	0.000	

HPLC spectra for compound 5a



5a

HPLC: (IE-3 (0.46 × 25 cm, 3 μm), Hexane/^{i}PrOH = 98/2, 0.7 mL/min, 214 nm), t_R (major) = 8.25 min, t_R (minor) = 7.93 min (92% ee); $[\alpha]_D^{25}$ = +92.9 (c = 0.050, $CHCl_3$, 92% ee).

Operator:Administrator Timebase:HPLC Sequence:20151027-DAD

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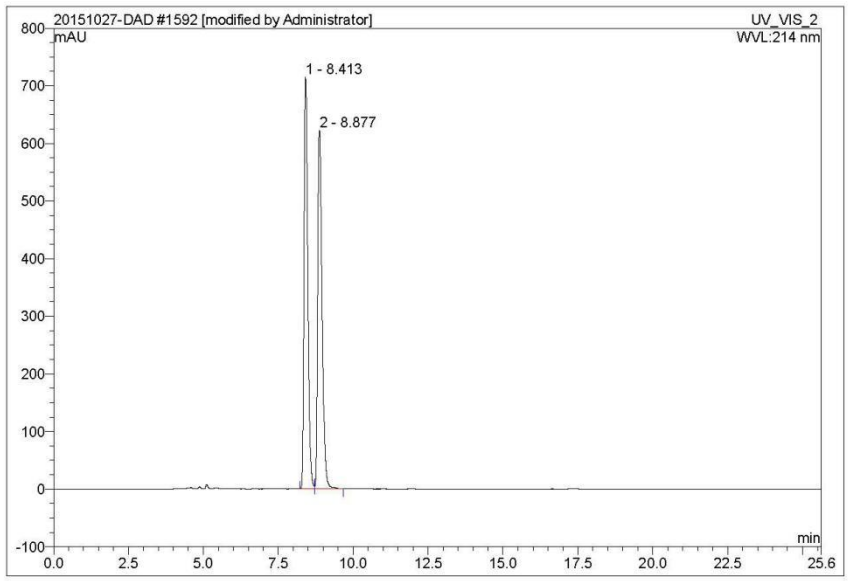
2016-7-22 8:52 下午

1592 2-75-3+- IE3 982 214 0.7

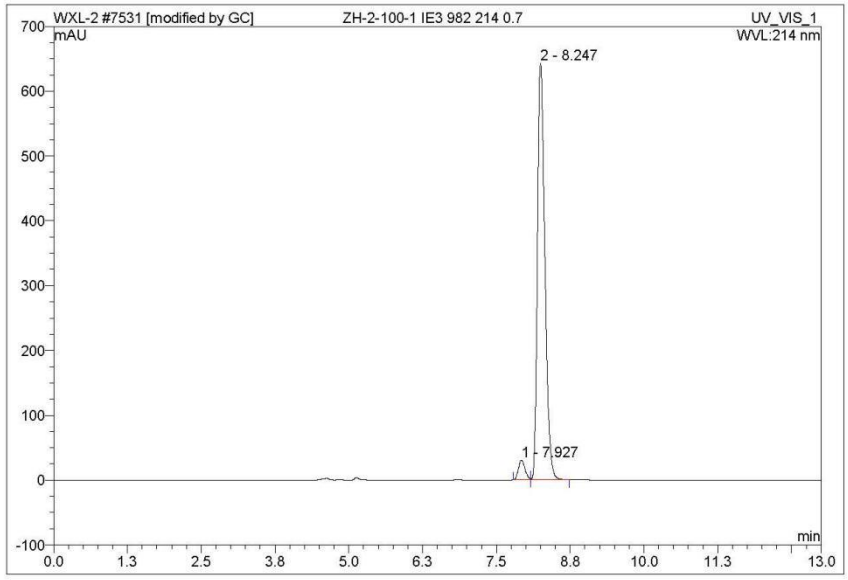
Sample Name:	**2-75-3+- IE3 982 214 0.7**	*Injection Volume:*	**1.0**
Vial Number:	**RD6**	*Channel:*	**UV_VIS_2**
Sample Type:	**unknown**	*Wavelength:*	**214.0**
Control Program:	**test-dad4**	*Bandwidth:*	**4**
Quantif. Method:	**WXL**	*Dilution Factor:*	**1.0000**
Recording Time:	**2016-4-19 10:23**	*Sample Weight:*	**1.0000**
Run Time (min):	**25.62**	*Sample Amount:*	**1.0000**



No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	8.41	n.a.	715.025	104.355	49.63	n.a.	BM
2	8.88	n.a.	622.735	105.924	50.37	n.a.	MB
Total:			1337.761	210.280	100.00	0.000	

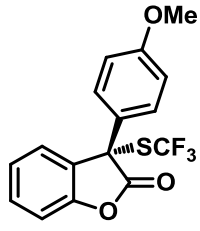
7531 ZH-2-100-1 IE3 982 214 0.7

Sample Name:	**ZH-2-100-1 IE3 982 214 0.7**	*Injection Volume:*	**1.0**
Vial Number:	**RE1**	*Channel:*	**UV_VIS_1**
Sample Type:	**unknown**	*Wavelength:*	**214**
Control Program:	**WXL-2014-1**	*Bandwidth:*	**n.a.**
Quantif. Method:	**WXL**	*Dilution Factor:*	**1.0000**
Recording Time:	**2016/6/7 18:05**	*Sample Weight:*	**1.0000**
Run Time (min):	**13.00**	*Sample Amount:*	**1.0000**



No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	7.93	n.a.	30.529	3.921	4.02	n.a.	BM *
2	8.25	n.a.	642.314	93.531	95.98	n.a.	MB*
Total:			672.843	97.452	100.00	0.000	

HPLC spectra for compound 5b



5b

HPLC: (AD-H (0.46 × 25 cm, 5 μm), Hexane/^{i}PrOH = 9/1, 0.7 mL/min, 214 nm), t_R (major) = 7.95 min, t_R (minor) = 9.39 min (89% ee); $[\alpha]_D^{25}$ = +69.0 (c = 0.100, $CHCl_3$, 89% ee).

Operator:GC Timebase:U3000 Sequence:WXL-2

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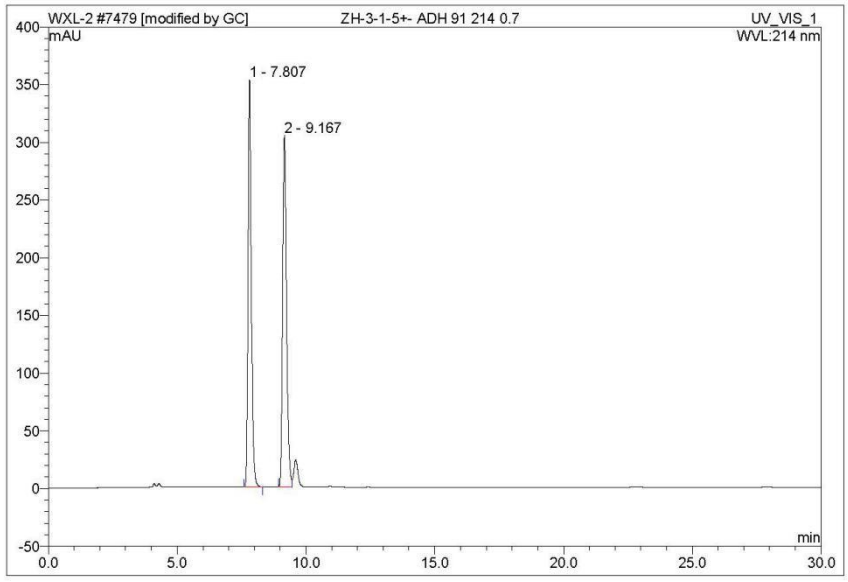
7479 ZH-3-1-5+- ADH 91 214 0.7

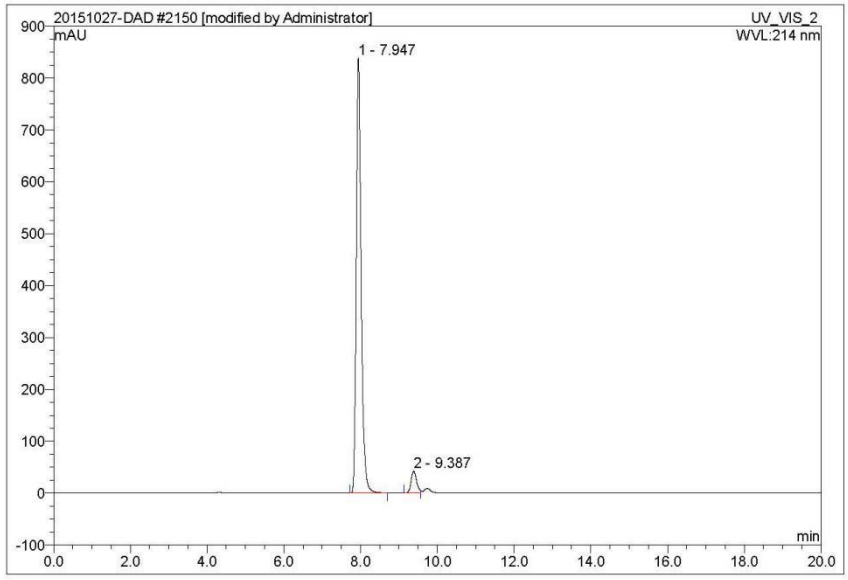
Sample Name:	**ZH-3-1-5+- ADH 91 214 0.7**	*Injection Volume:*	**2.0**
Vial Number:	**RD1**	*Channel:*	**UV_VIS_1**
Sample Type:	**unknown**	*Wavelength:*	**214**
Control Program:	**WXL-2014-1**	*Bandwidth:*	**n.a.**
Quantif. Method:	**WXL**	*Dilution Factor:*	**1.0000**
Recording Time:	**2016/6/3 20:53**	*Sample Weight:*	**1.0000**
Run Time (min):	**30.00**	*Sample Amount:*	**1.0000**



No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	7.81	n.a.	352.774	53.265	50.08	n.a.	BMB
2	9.17	n.a.	304.436	53.087	49.92	n.a.	BM *
Total:			657.210	106.352	100.00	0.000	

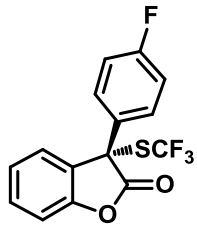
2150 ZH-3-4-1 ADH 91 214 0.7

Sample Name:	**ZH-3-4-1 ADH 91 214 0.7**	*Injection Volume:*	**1.0**
Vial Number:	**RD6**	*Channel:*	**UV_VIS_2**
Sample Type:	**unknown**	*Wavelength:*	**214.0**
Control Program:	**test-dad2**	*Bandwidth:*	**4**
Quantif. Method:	**WXL**	*Dilution Factor:*	**1.0000**
Recording Time:	**2016-6-7 20:32**	*Sample Weight:*	**1.0000**
Run Time (min):	**20.00**	*Sample Amount:*	**1.0000**



No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	7.95	n.a.	838.459	123.606	94.58	n.a.	BMB
2	9.39	n.a.	42.259	7.080	5.42	n.a.	BM *
Total:			880.718	130.686	100.00	0.000	

HPLC spectra for compound 5c



5c

HPLC: (AD-H (0.46 × 25 cm, 5 μm), Hexane/^{i}PrOH = 98/2, 0.7 mL/min, 214 nm), t_R (major) = 13.47 min, t_R (minor) = 16.35 min (64% ee); $[\alpha]_D^{25}$ = +71.0 (c = 0.100, $CHCl_3$, 64% ee).

Operator:Administrator Timebase:HPLC Sequence:20151027-DAD

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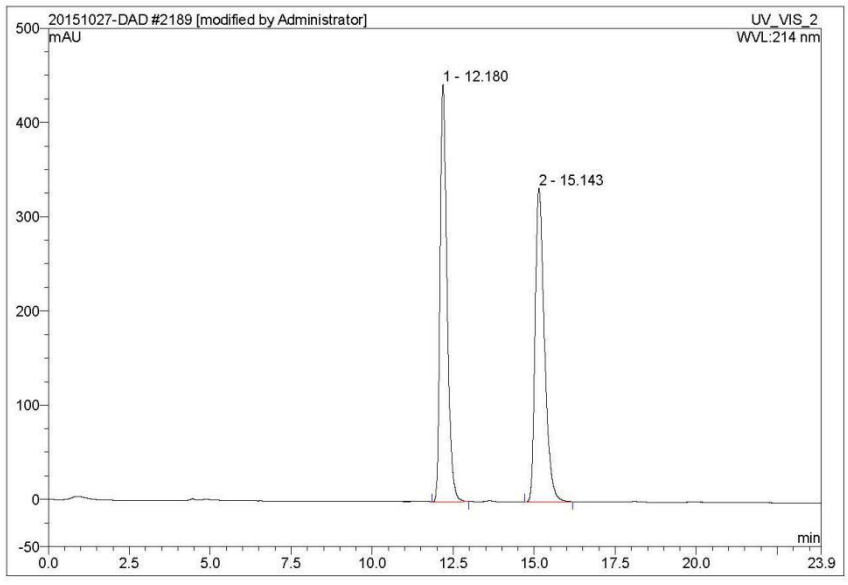
2189 zh-3-7-2+- ADH 982 214 0.7

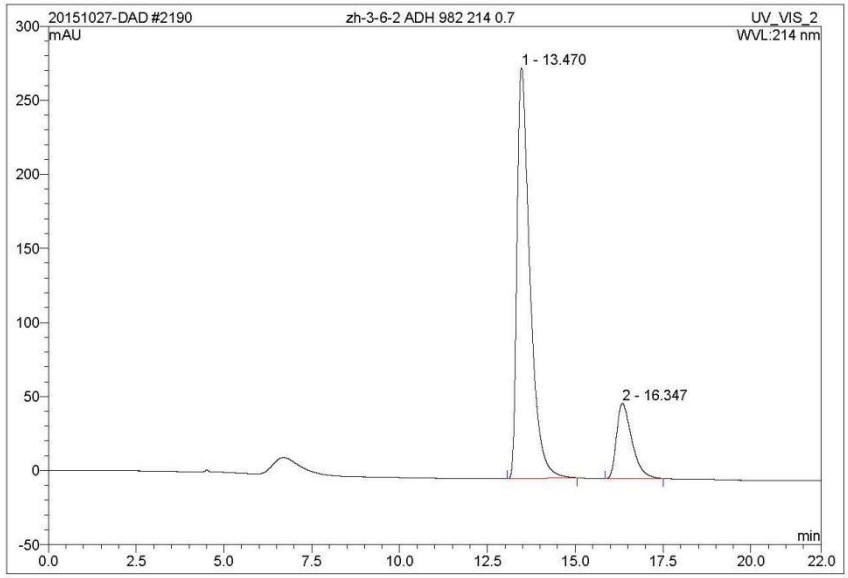
Sample Name:	**zh-3-7-2+- ADH 982 214 0.7**	*Injection Volume:*	**1.0**
Vial Number:	**RD6**	*Channel:*	**UV_VIS_2**
Sample Type:	**unknown**	*Wavelength:*	**214.0**
Control Program:	**test-dad4**	*Bandwidth:*	**4**
Quantif. Method:	**WXL**	*Dilution Factor:*	**1.0000**
Recording Time:	**2016-6-14 12:06**	*Sample Weight:*	**1.0000**
Run Time (min):	**23.85**	*Sample Amount:*	**1.0000**



No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	12.18	n.a.	442.420	110.411	49.90	n.a.	BMB
2	15.14	n.a.	332.724	110.843	50.10	n.a.	BMB
Total:			775.144	221.255	100.00	0.000	

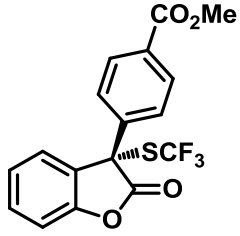
2190 zh-3-6-2 ADH 982 214 0.7

Sample Name:	**zh-3-6-2 ADH 982 214 0.7**	*Injection Volume:*	**1.0**
Vial Number:	**RB6**	*Channel:*	**UV_VIS_2**
Sample Type:	**unknown**	*Wavelength:*	**214.0**
Control Program:	**test-dad4**	*Bandwidth:*	**4**
Quantif. Method:	**WXL**	*Dilution Factor:*	**1.0000**
Recording Time:	**2016-6-14 12:31**	*Sample Weight:*	**1.0000**
Run Time (min):	**22.00**	*Sample Amount:*	**1.0000**



No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	13.47	n.a.	277.298	118.586	82.17	n.a.	BMB
2	16.35	n.a.	50.922	25.732	17.83	n.a.	BMB
Total:			328.220	144.318	100.00	0.000	

HPLC spectra for compound 5d



5d

HPLC: (IE-3 (0.46 × 25 cm, 3 μm), Hexane/^{i}PrOH = 9/1, 0.7 mL/min, 214 nm), t_R (major) = 13.40 min, t_R (minor) = 16.24 min (81% ee); $[\alpha]_D^{25}$ = +61.1 (c = 0.100, $CHCl_3$, 81% ee).

Operator:GC Timebase:U3000 Sequence:WXL-2

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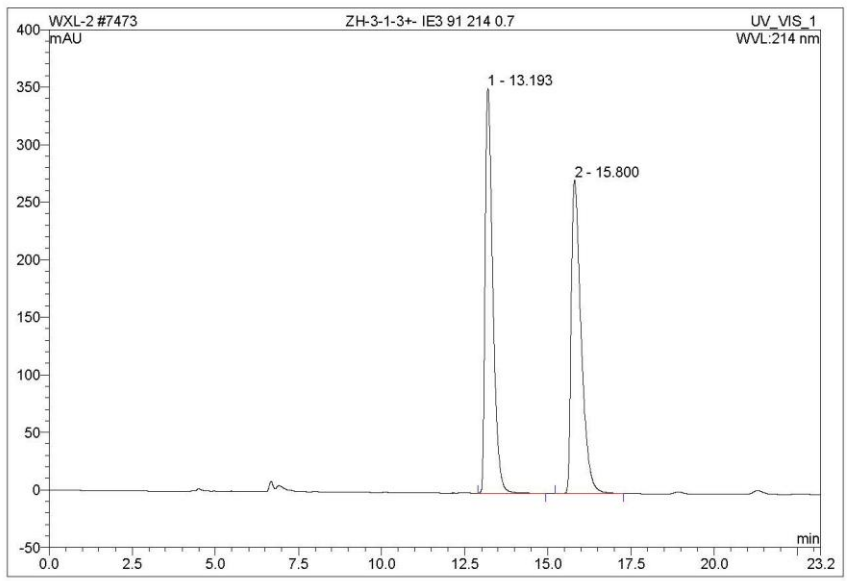
7473 ZH-3-1-3+- IE3 91 214 0.7

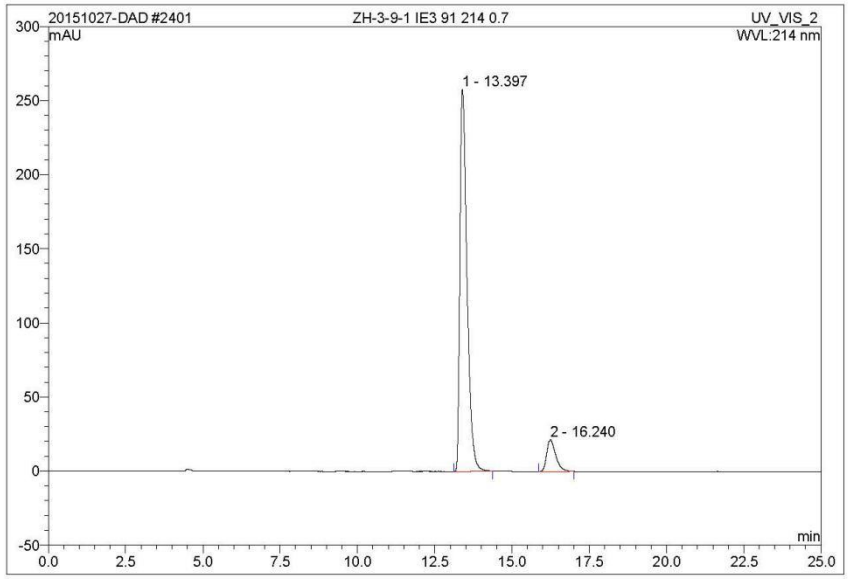
Sample Name:	**ZH-3-1-3+- IE3 91 214 0.7**	*Injection Volume:*	**1.0**
Vial Number:	**RD1**	*Channel:*	**UV_VIS_1**
Sample Type:	**unknown**	*Wavelength:*	**214**
Control Program:	**WXL-2014-1**	*Bandwidth:*	**n.a.**
Quantif. Method:	**WXL**	*Dilution Factor:*	**1.0000**
Recording Time:	**2016/6/3 16:14**	*Sample Weight:*	**1.0000**
Run Time (min):	**23.19**	*Sample Amount:*	**1.0000**



No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	13.19	n.a.	352.011	94.308	50.11	n.a.	BMB
2	15.80	n.a.	272.460	93.906	49.89	n.a.	BMB
Total:			624.472	188.214	100.00	0.000	

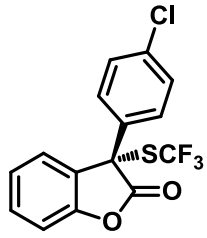
2401 ZH-3-9-1 IE3 91 214 0.7

Sample Name:	**ZH-3-9-1 IE3 91 214 0.7**	*Injection Volume:*	**1.0**
Vial Number:	**RE4**	*Channel:*	**UV_VIS_2**
Sample Type:	**unknown**	*Wavelength:*	**214.0**
Control Program:	**test-dad6**	*Bandwidth:*	**4**
Quantif. Method:	**WXL**	*Dilution Factor:*	**1.0000**
Recording Time:	**2016-7-5 2:27**	*Sample Weight:*	**1.0000**
Run Time (min):	**25.00**	*Sample Amount:*	**1.0000**



No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	13.40	n.a.	257.842	68.376	90.39	n.a.	BMB
2	16.24	n.a.	21.609	7.269	9.61	n.a.	BMB
Total:			279.451	75.644	100.00	0.000	

HPLC spectra for compound 5e



5e

HPLC: (AD-H (0.46 × 25 cm, 5 μm), Hexane/^{i}PrOH = 98/2, 0.7 mL/min, 214 nm), t_R (major) = 8.35 min, t_R (minor) = 9.55 min (86% ee); $[\alpha]_D^{25}$ = +68.3 (c = 0.075, $CHCl_3$, 86% ee).

Operator:GC Timebase:U3000 Sequence:WXL-2

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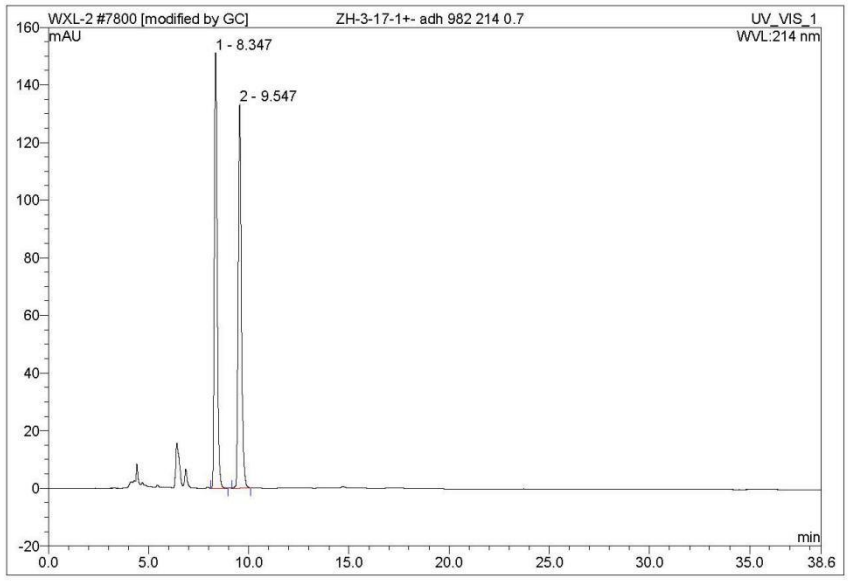
7800 ZH-3-17-1+- adh 982 214 0.7

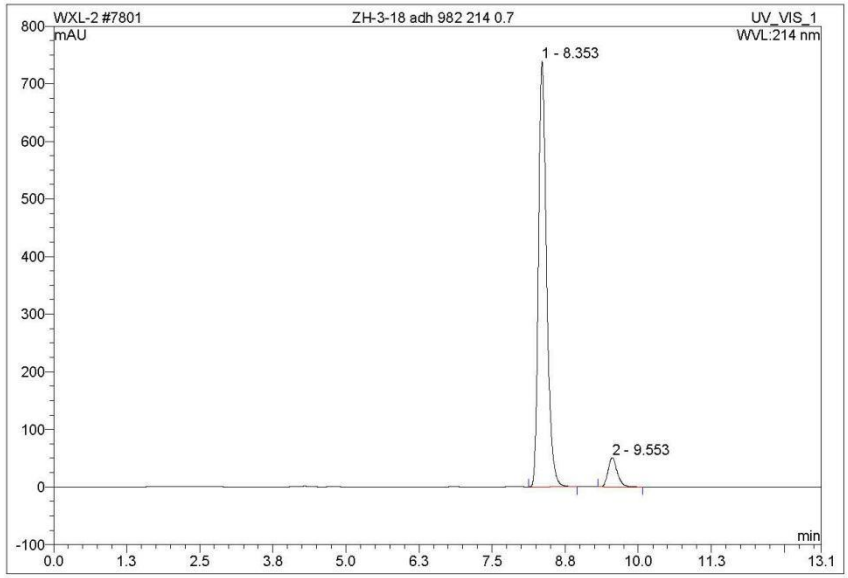
Sample Name:	**ZH-3-17-1+- adh 982 214 0.7**	*Injection Volume:*	**1.0**
Vial Number:	**GE3**	*Channel:*	**UV_VIS_1**
Sample Type:	**unknown**	*Wavelength:*	**214**
Control Program:	**WXL-2014-1**	*Bandwidth:*	**n.a.**
Quantif. Method:	**WXL**	*Dilution Factor:*	**1.0000**
Recording Time:	**2016/7/5 11:09**	*Sample Weight:*	**1.0000**
Run Time (min):	**38.57**	*Sample Amount:*	**1.0000**



No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	8.35	n.a.	151.252	24.287	49.88	n.a.	BM *
2	9.55	n.a.	133.209	24.403	50.12	n.a.	BMB
Total:			284.461	48.690	100.00	0.000	

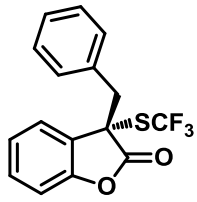
7801 ZH-3-18 adh 982 214 0.7

Sample Name:	**ZH-3-18 adh 982 214 0.7**	*Injection Volume:*	**1.0**
Vial Number:	**GE4**	*Channel:*	**UV_VIS_1**
Sample Type:	**unknown**	*Wavelength:*	**214**
Control Program:	**WXL-2014-1**	*Bandwidth:*	**n.a.**
Quantif. Method:	**WXL**	*Dilution Factor:*	**1.0000**
Recording Time:	**2016/7/5 11:49**	*Sample Weight:*	**1.0000**
Run Time (min):	**13.13**	*Sample Amount:*	**1.0000**



No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	8.35	n.a.	738.969	119.079	92.83	n.a.	BMB
2	9.55	n.a.	50.648	9.192	7.17	n.a.	BMB
Total:			789.617	128.271	100.00	0.000	

HPLC spectra for compound 5f



5f

HPLC: (AD-H (0.46 × 25 cm, 5 μm), Hexane/^{i}PrOH = 98/2, 0.7 mL/min, 214 nm), t_R (major) = 8.18 min, t_R (minor) = 9.04 min (83% ee); $[\alpha]_D^{25}$ = +46.9 (c = 0.100, $CHCl_3$, 83% ee).

Operator:GC Timebase:U3000 Sequence:WXL-2

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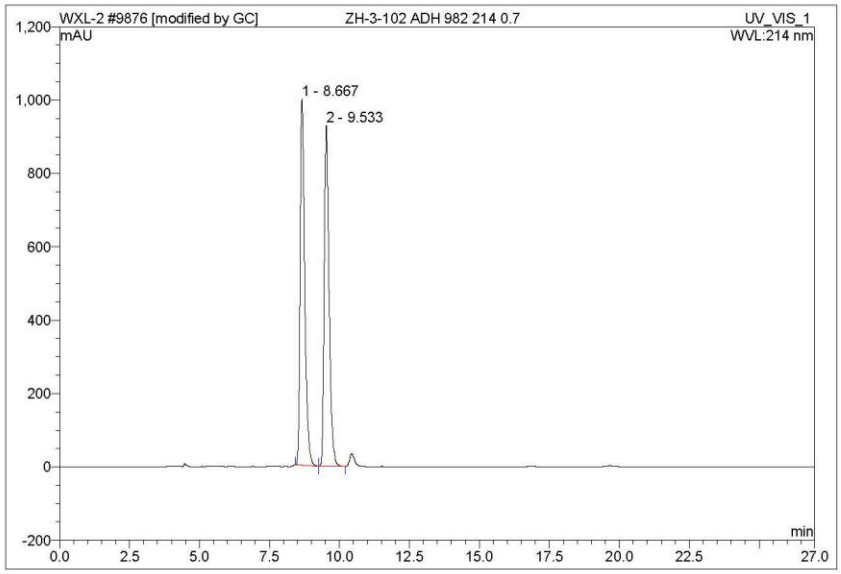
2017/1/6 2:24 下午

9876 ZH-3-102 ADH 982 214 0.7

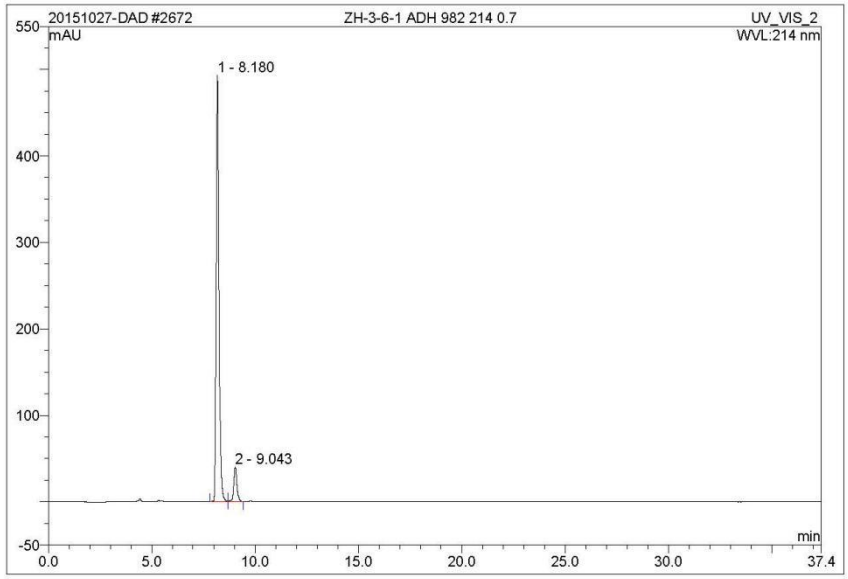
Sample Name:	**ZH-3-102 ADH 982 214 0.7**	*Injection Volume:*	**1.0**
Vial Number:	**BC1**	*Channel:*	**UV_VIS_1**
Sample Type:	**unknown**	*Wavelength:*	**214**
Control Program:	**WXL-2014**	*Bandwidth:*	**n.a.**
Quantif. Method:	**WXL**	*Dilution Factor:*	**1.0000**
Recording Time:	**2017/1/6 10:04**	*Sample Weight:*	**1.0000**
Run Time (min):	**26.97**	*Sample Amount:*	**1.0000**



No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	8.67	n.a.	998.852	190.861	50.59	n.a.	BMB
2	9.53	n.a.	929.418	186.388	49.41	n.a.	BMB
Total:			1928.271	377.249	100.00	0.000	

2672 ZH-3-6-1 ADH 982 214 0.7

Sample Name:	**ZH-3-6-1 ADH 982 214 0.7**	*Injection Volume:*	**1.0**
Vial Number:	**RD7**	*Channel:*	**UV_VIS_2**
Sample Type:	**unknown**	*Wavelength:*	**214.0**
Control Program:	**test-dad4**	*Bandwidth:*	**4**
Quantif. Method:	**WXL**	*Dilution Factor:*	**1.0000**
Recording Time:	**2016-7-22 17:01**	*Sample Weight:*	**1.0000**
Run Time (min):	**37.39**	*Sample Amount:*	**1.0000**



No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	8.18	n.a.	493.631	76.753	91.45	n.a.	BM
2	9.04	n.a.	40.042	7.179	8.55	n.a.	MB
Total:			533.673	83.931	100.00	0.000	

HPLC spectra for compound 5g

5g

HPLC: (IE-3 (0.46 × 25 cm, 3 μm), Hexane/^{i}PrOH = 95/5, 0.7 mL/min, 214 nm), t_R (major) = 9.02 min, t_R (minor) = 9.44 min (84% ee); $[\alpha]_D^{25}$ = +43.3 (c = 0.100, $CHCl_3$, 84% ee).

Operator:Administrator Timebase:HPLC Sequence:20151027-DAD

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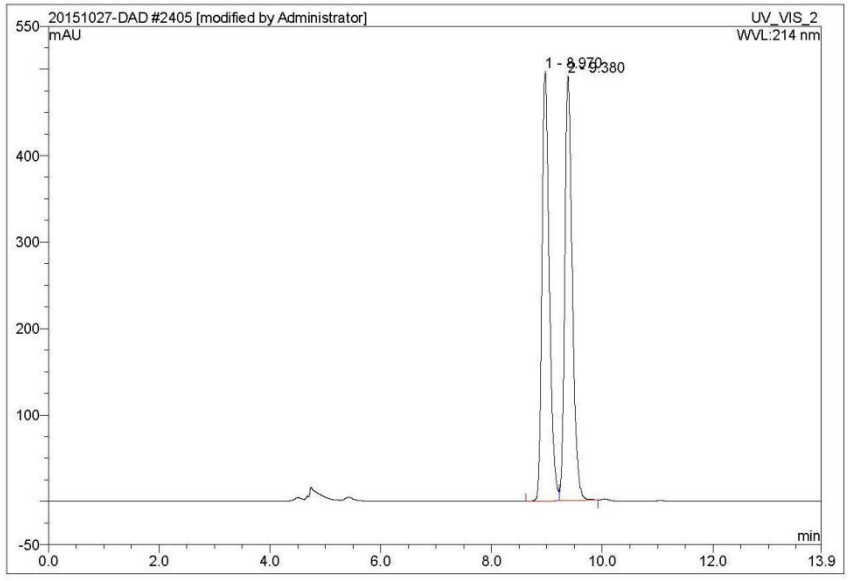
2405 ZH-3-17-3+- IE3 955 214 0.7

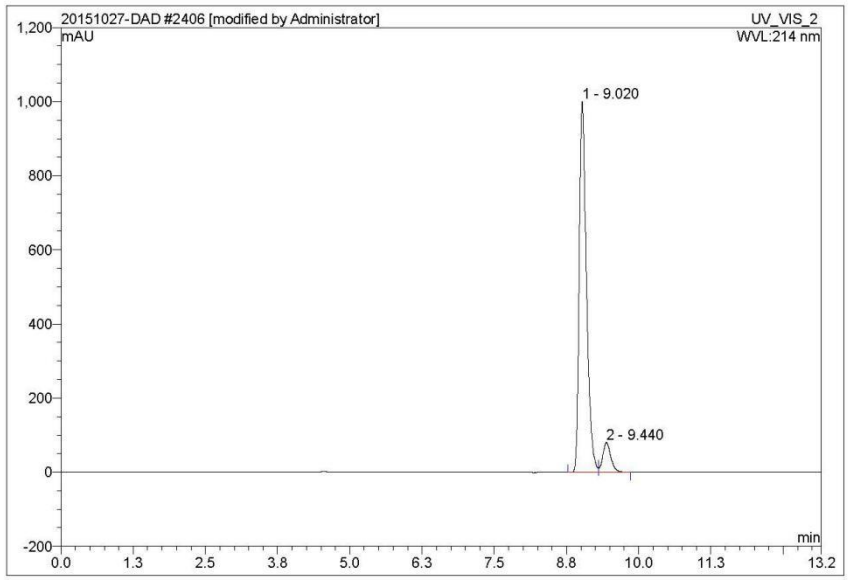
Sample Name:	**ZH-3-17-3+- IE3 955 214 0.7**	*Injection Volume:*	**1.0**
Vial Number:	**RB7**	*Channel:*	**UV_VIS_2**
Sample Type:	**unknown**	*Wavelength:*	**214.0**
Control Program:	**test-dad2**	*Bandwidth:*	**4**
Quantif. Method:	**WXL**	*Dilution Factor:*	**1.0000**
Recording Time:	**2016-7-5 9:30**	*Sample Weight:*	**1.0000**
Run Time (min):	**13.95**	*Sample Amount:*	**1.0000**



No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	8.97	n.a.	497.678	76.299	49.62	n.a.	BM *
2	9.38	n.a.	491.602	77.478	50.38	n.a.	MB*
Total:			989.280	153.776	100.00	0.000	

2406 ZH-3-19 IE3 955 214 0.7

Sample Name:	**ZH-3-19 IE3 955 214 0.7**	*Injection Volume:*	**1.0**
Vial Number:	**RE5**	*Channel:*	**UV_VIS_2**
Sample Type:	**unknown**	*Wavelength:*	**214.0**
Control Program:	**test-dad2**	*Bandwidth:*	**4**
Quantif. Method:	**WXL**	*Dilution Factor:*	**1.0000**
Recording Time:	**2016-7-5 9:46**	*Sample Weight:*	**1.0000**
Run Time (min):	**13.16**	*Sample Amount:*	**1.0000**



No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	9.02	n.a.	1000.175	145.491	91.73	n.a.	BM
2	9.44	n.a.	80.713	13.123	8.27	n.a.	MB
Total:			1080.888	158.613	100.00	0.000	

HPLC spectra for compound 5h

5h

HPLC: (AD-H (0.46 × 25 cm, 5 μm), Hexane/^{i}PrOH = 8/2, 0.7 mL/min, 214 nm), t_R (major) = 6.61 min, t_R (minor) = 7.35 min (72% ee); $[\alpha]_D^{25}$ = +58.9 (c = 0.140, $CHCl_3$, 72% ee).

Operator:GC Timebase:U3000 Sequence:WXL-2

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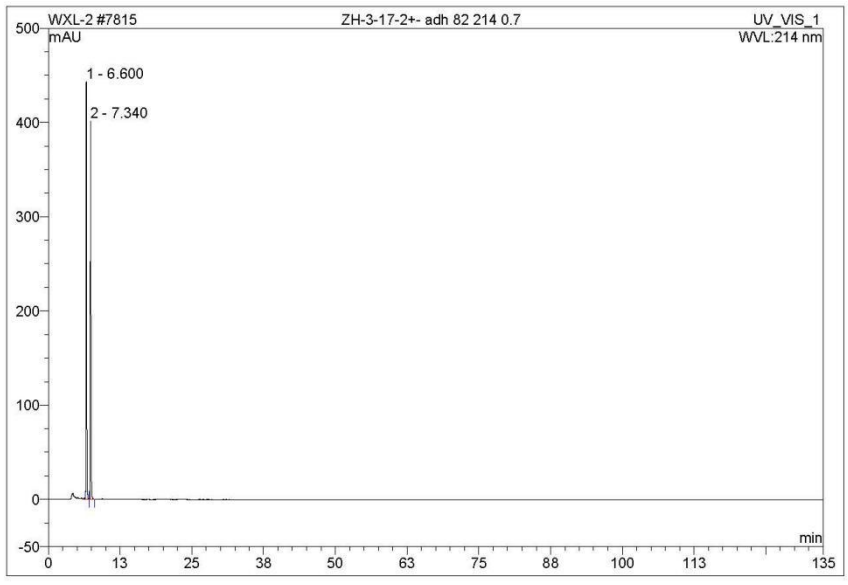
7815 ZH-3-17-2+- adh 82 214 0.7

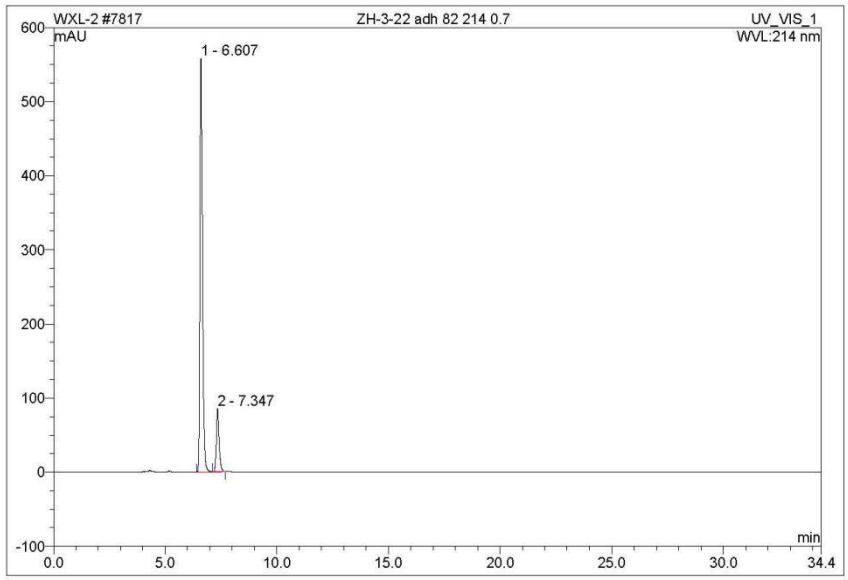
Sample Name:	**ZH-3-17-2+- adh 82 214 0.7**	*Injection Volume:*	**2.0**
Vial Number:	**GE1**	*Channel:*	**UV_VIS_1**
Sample Type:	**unknown**	*Wavelength:*	**214**
Control Program:	**WXL-2014-1**	*Bandwidth:*	**n.a.**
Quantif. Method:	**WXL**	*Dilution Factor:*	**1.0000**
Recording Time:	**2016/7/6 0:16**	*Sample Weight:*	**1.0000**
Run Time (min):	**135.00**	*Sample Amount:*	**1.0000**



No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	6.60	n.a.	442.634	57.789	49.88	n.a.	BMB
2	7.34	n.a.	401.339	58.058	50.12	n.a.	BMB
Total:			843.972	115.847	100.00	0.000	

7817 ZH-3-22 adh 82 214 0.7

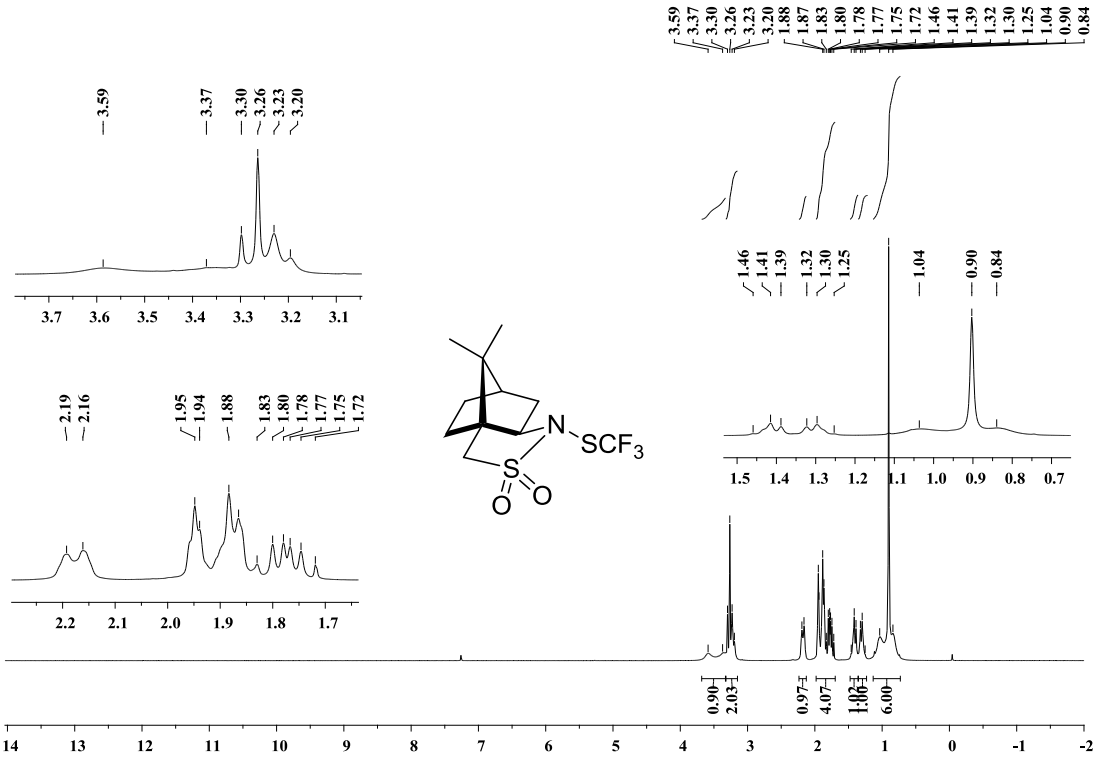
Sample Name:	**ZH-3-22 adh 82 214 0.7**	*Injection Volume:*	**1.0**
Vial Number:	**GE2**	*Channel:*	**UV_VIS_1**
Sample Type:	**unknown**	*Wavelength:*	**214**
Control Program:	**WXL-2014-1**	*Bandwidth:*	**n.a.**
Quantif. Method:	**WXL**	*Dilution Factor:*	**1.0000**
Recording Time:	**2016/7/6 10:27**	*Sample Weight:*	**1.0000**
Run Time (min):	**34.38**	*Sample Amount:*	**1.0000**



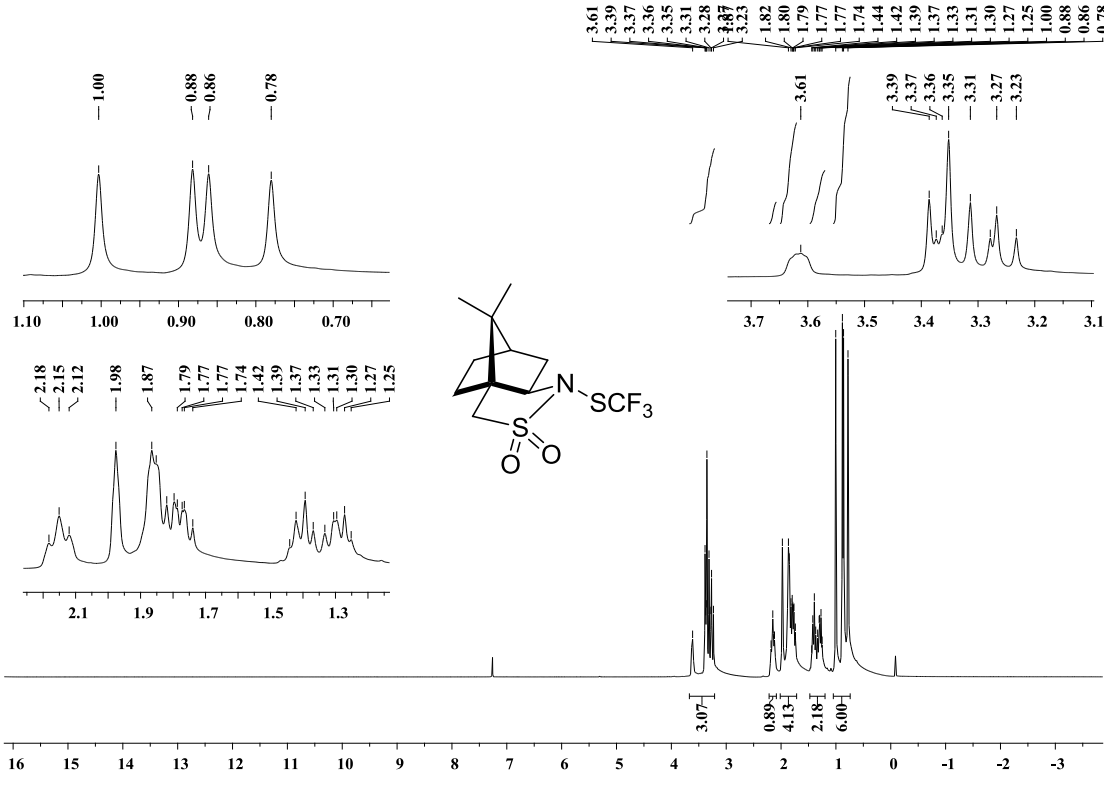
No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	6.61	n.a.	558.276	73.341	85.85	n.a.	BMB
2	7.35	n.a.	84.938	12.090	14.15	n.a.	Rd
Total:			643.214	85.432	100.00	0.000	

^{1}H, ^{13}C, ^{19}F NMR spectra 1a-f, 3a-o, 4a-p and 5a-h

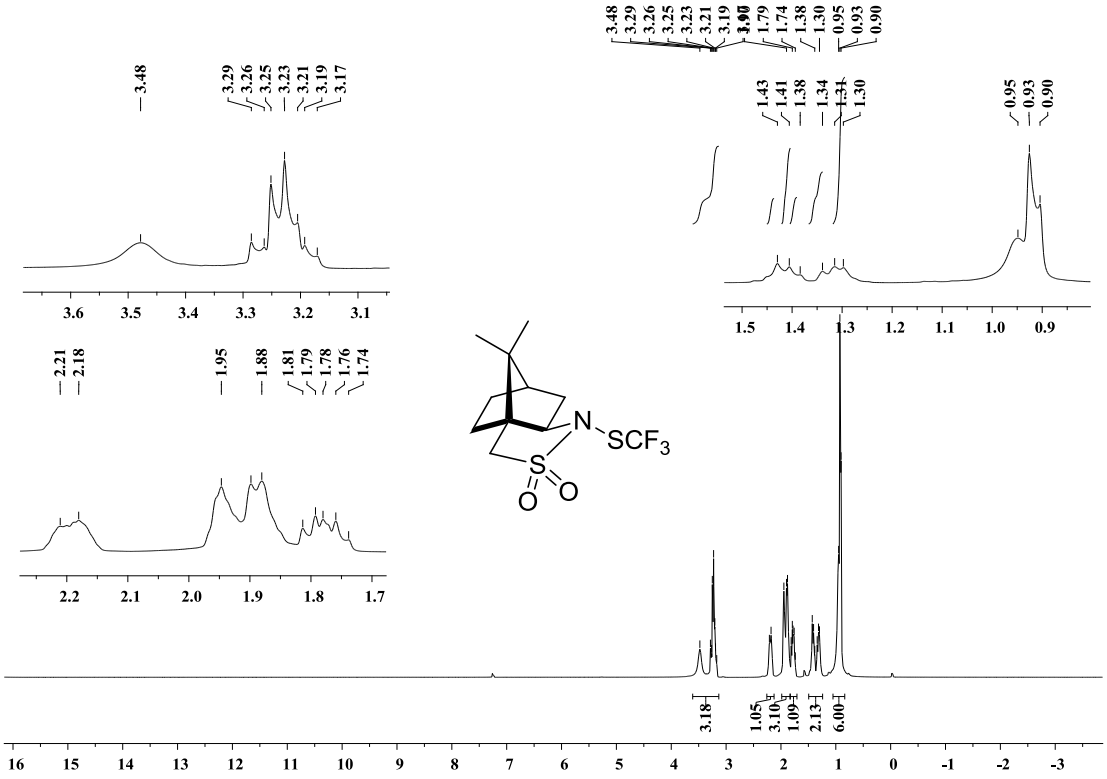
^{1}H NMR Spectrum for (3aS,6R,7aR)-8,8-Dimethyl-1-((trifluoromethyl)thio)hexahydro-1*H*-3a,6-methanobenzo[c]isothiazole 2,2-dioxide 1a at 298 K



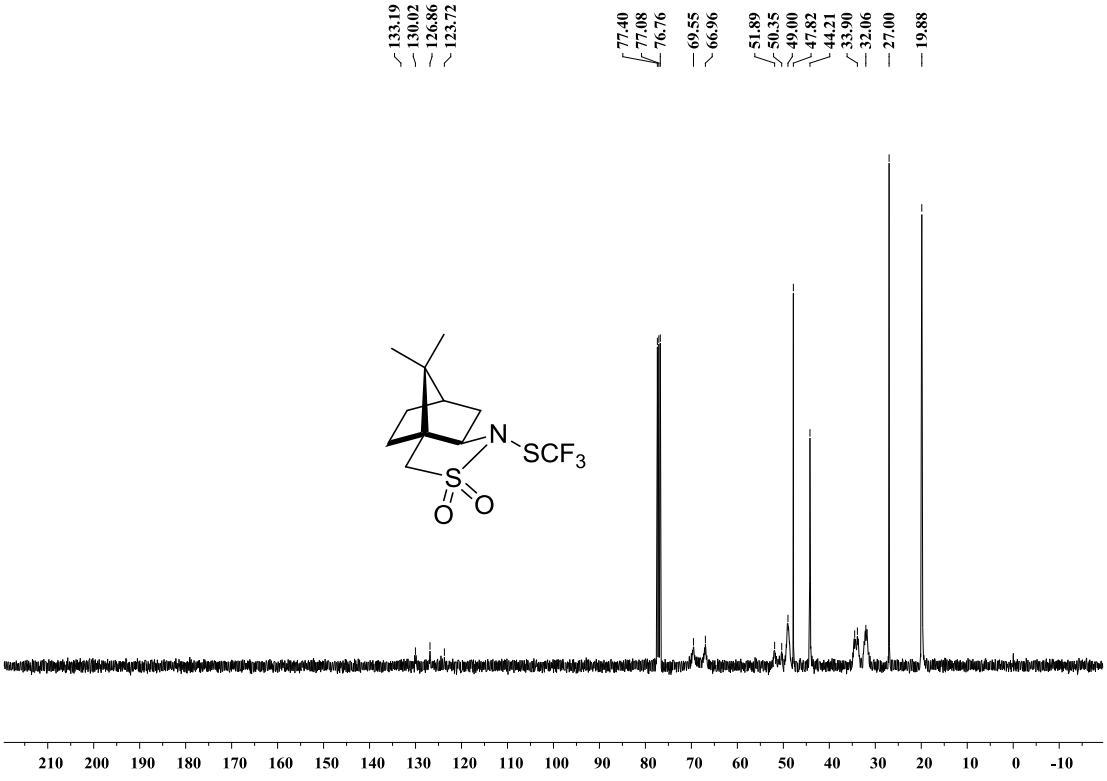
^{1}H NMR Spectrum for (3aS,6R,7aR)-8,8-Dimethyl-1-((trifluoromethyl)thio)hexahydro-1*H*-3a,6-methanobenzo[c]isothiazole 2,2-dioxide 1a at 213 K



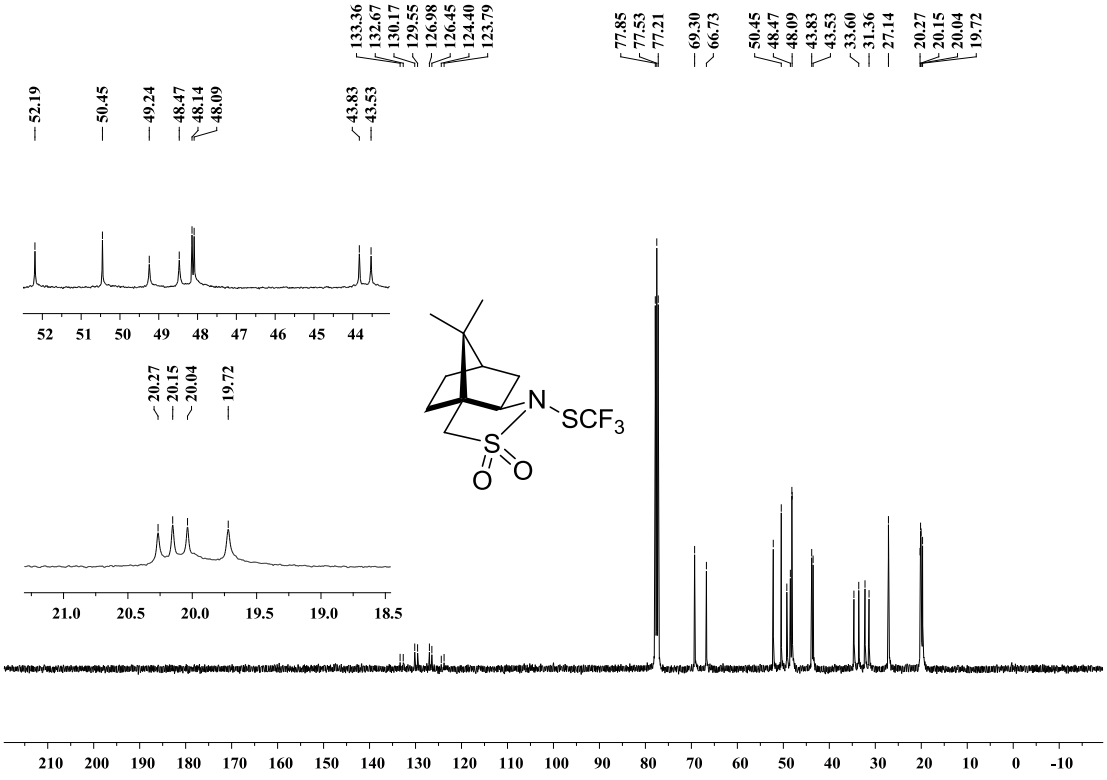
^{1}H NMR Spectrum for (3aS,6R,7aR)-8,8-Dimethyl-1-((trifluoromethyl)thio)hexahydro-1*H*-3a,6-methanobenzo[c]isothiazole 2,2-dioxide 1a at 323 K



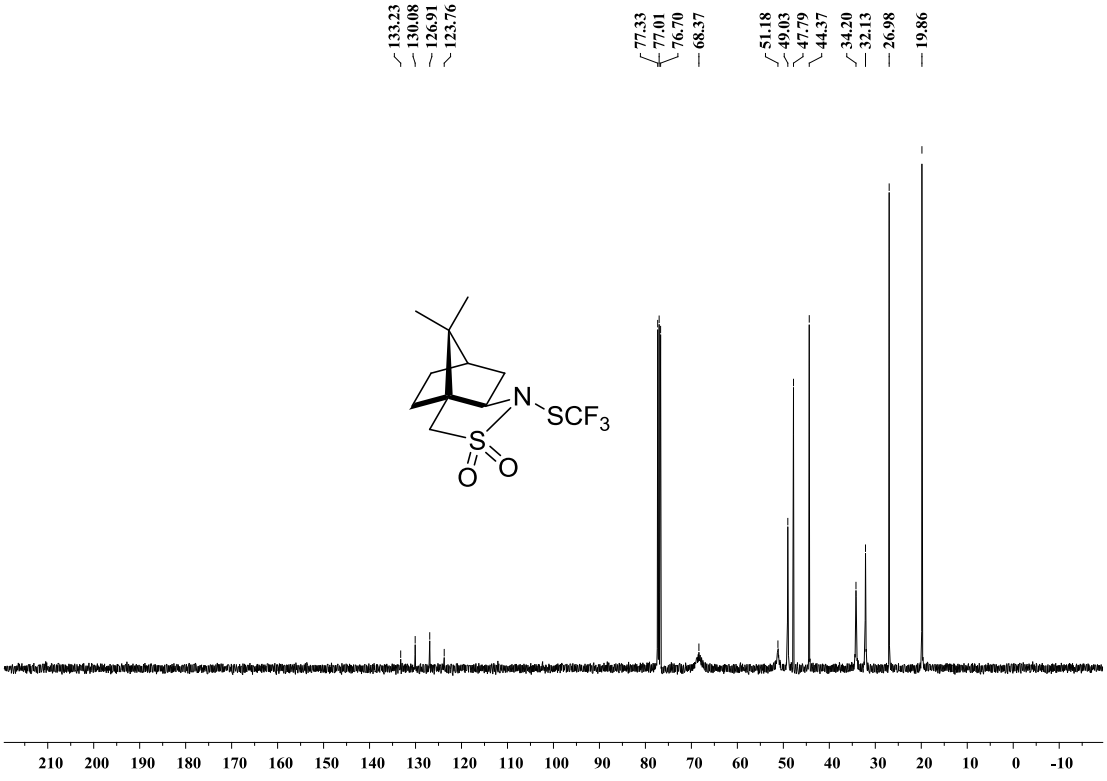
^{13}C NMR Spectrum for (3aS,6R,7aR)-8,8-Dimethyl-1-((trifluoromethyl)thio)hexahydro-1*H*-3a,6-methanobenzo[c]isothiazole 2,2-dioxide 1a at 298 K



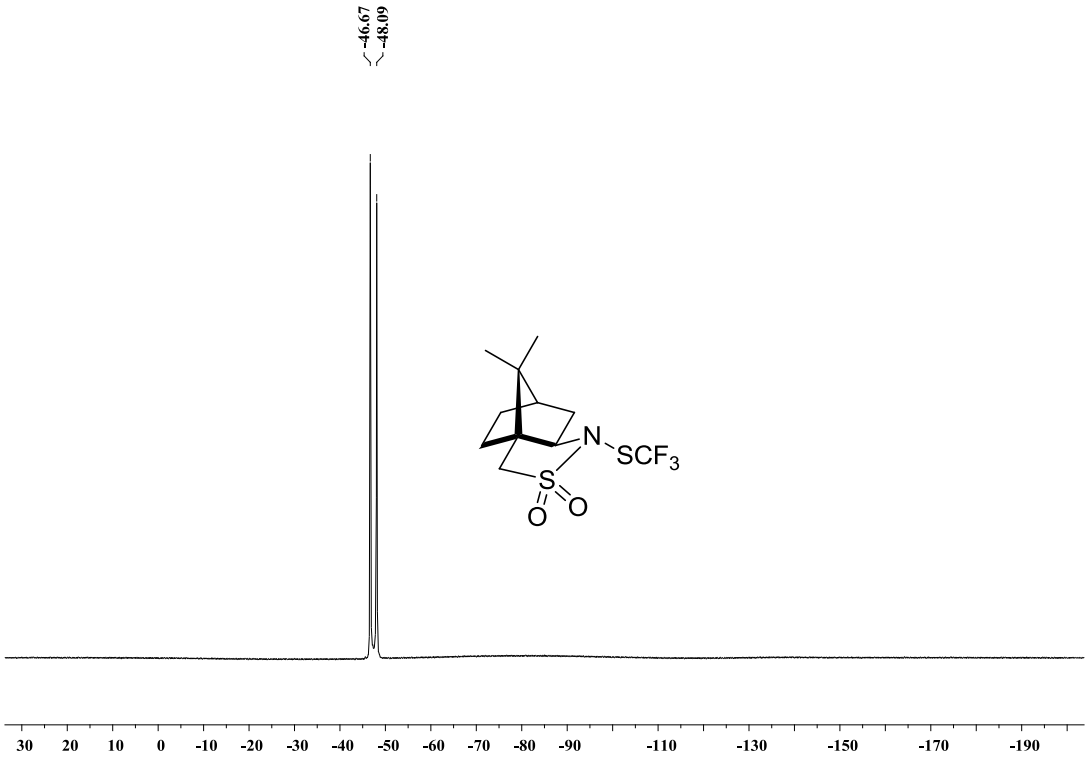
^{13}C NMR Spectrum for (3aS,6R,7aR)-8,8-Dimethyl-1-((trifluoromethyl)thio)hexahydro-1*H*-3a,6-methanobenzo[c]isothiazole 2,2-dioxide 1a at 213 K



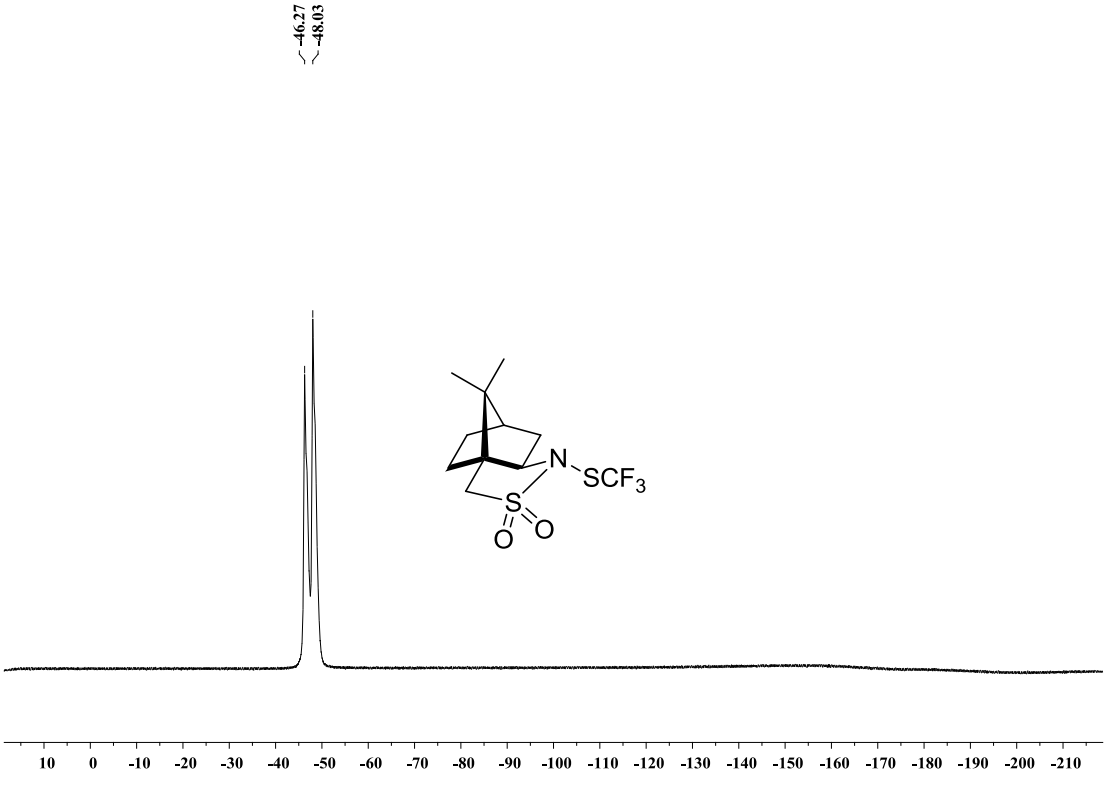
^{13}C NMR Spectrum for (3aS,6R,7aR)-8,8-Dimethyl-1-((trifluoromethyl)thio)hexahydro-1*H*-3a,6-methanobenzo[c]isothiazole 2,2-dioxide 1a at 323 K



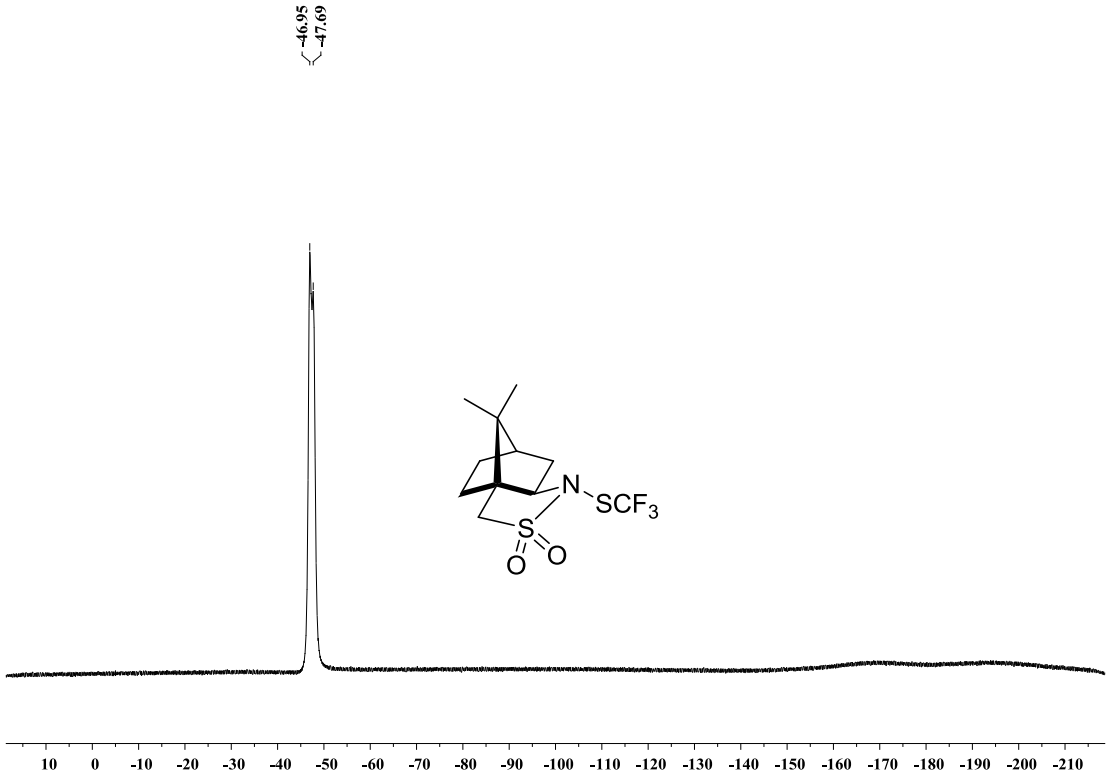
^{19}F NMR Spectrum for (3aS,6R,7aR)-8,8-Dimethyl-1-((trifluoromethyl)thio)hexahydro-1*H*-3a,6-methanobenzo[c]isothiazole 2,2-dioxide 1a at 298 K



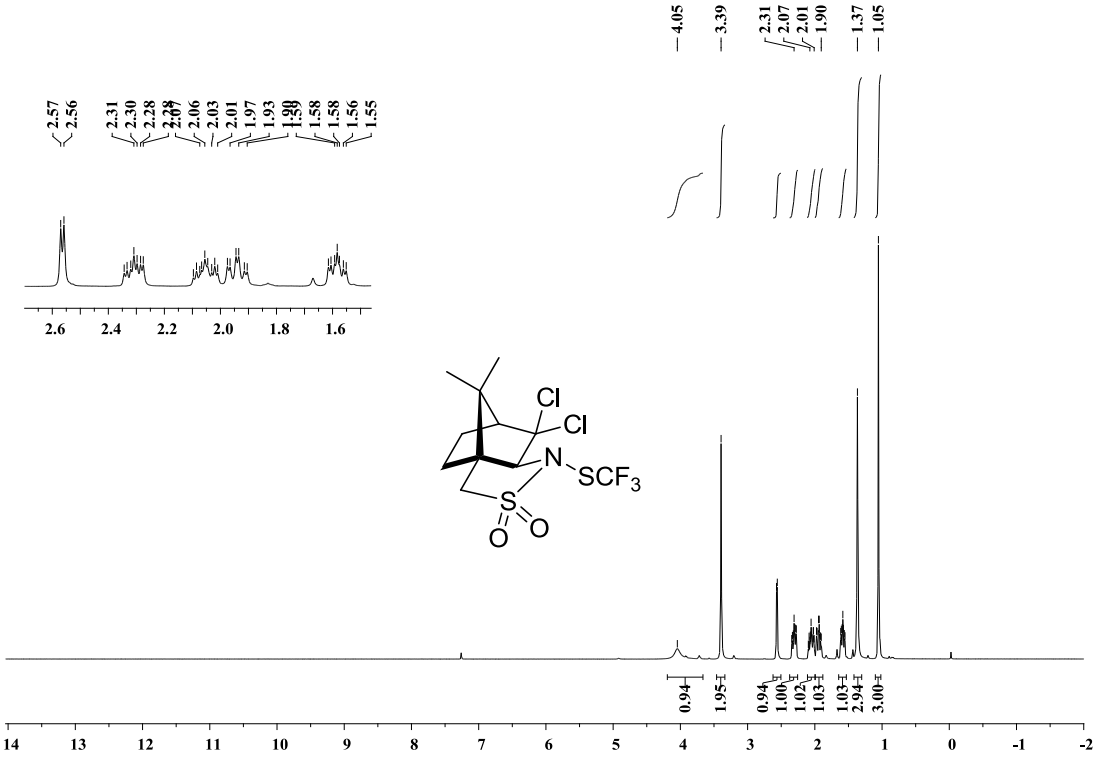
^{19}F NMR Spectrum for (3aS,6R,7aR)-8,8-Dimethyl-1-((trifluoromethyl)thio)hexahydro-1*H*-3a,6-methanobenzo[c]isothiazole 2,2-dioxide 1a at 213 K



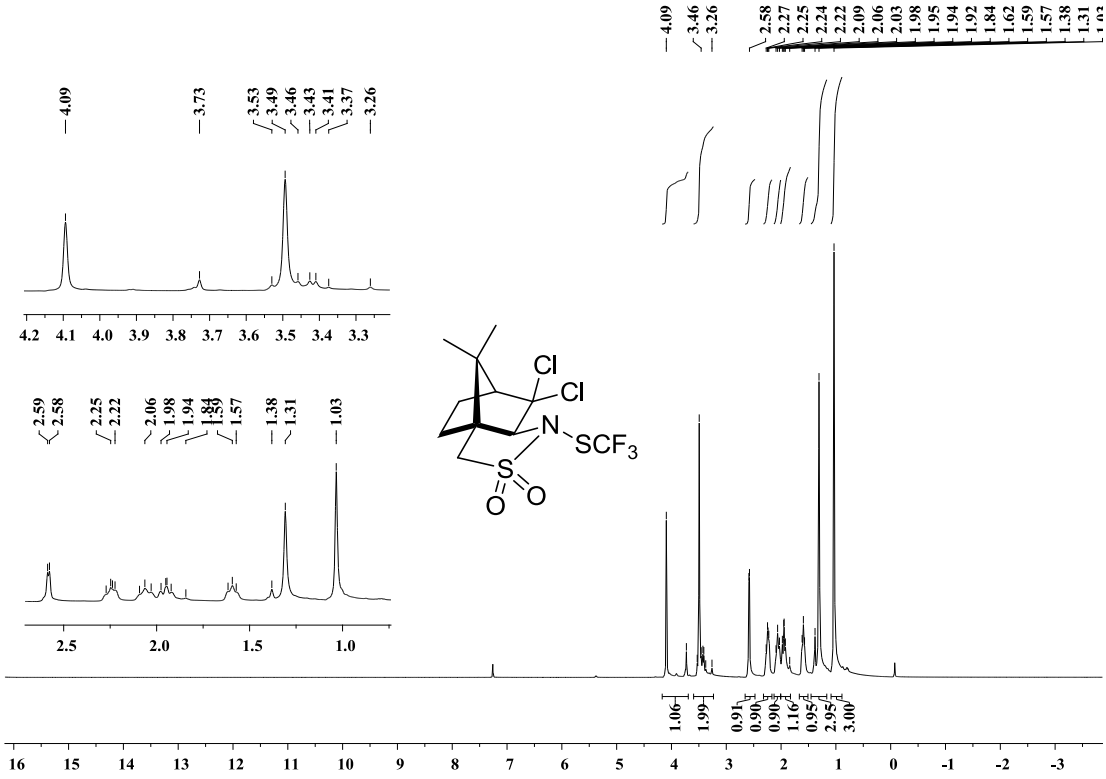
^{19}F NMR Spectrum for (3aS,6R,7aR)-8,8-Dimethyl-1-((trifluoromethyl)thio)hexahydro-1*H*-3a,6-methanobenzo[c]isothiazole 2,2-dioxide 1a at 323 K



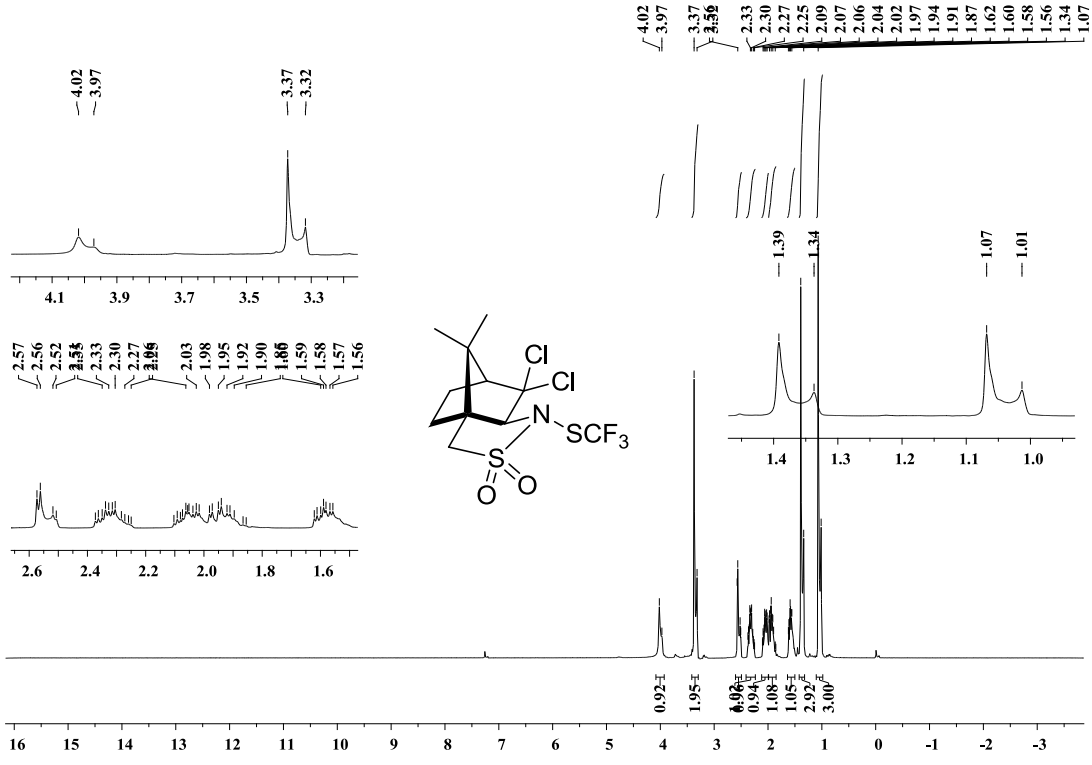
^{1}H NMR Spectrum for (3aS,6S,7aS)-7,7-Dichloro-8,8-dimethyl-1-((trifluoromethyl)thio)hexahydro-1*H*-3a,6-methanobenzo[c]isothiazole 2,2-dioxide 1b at 298 K



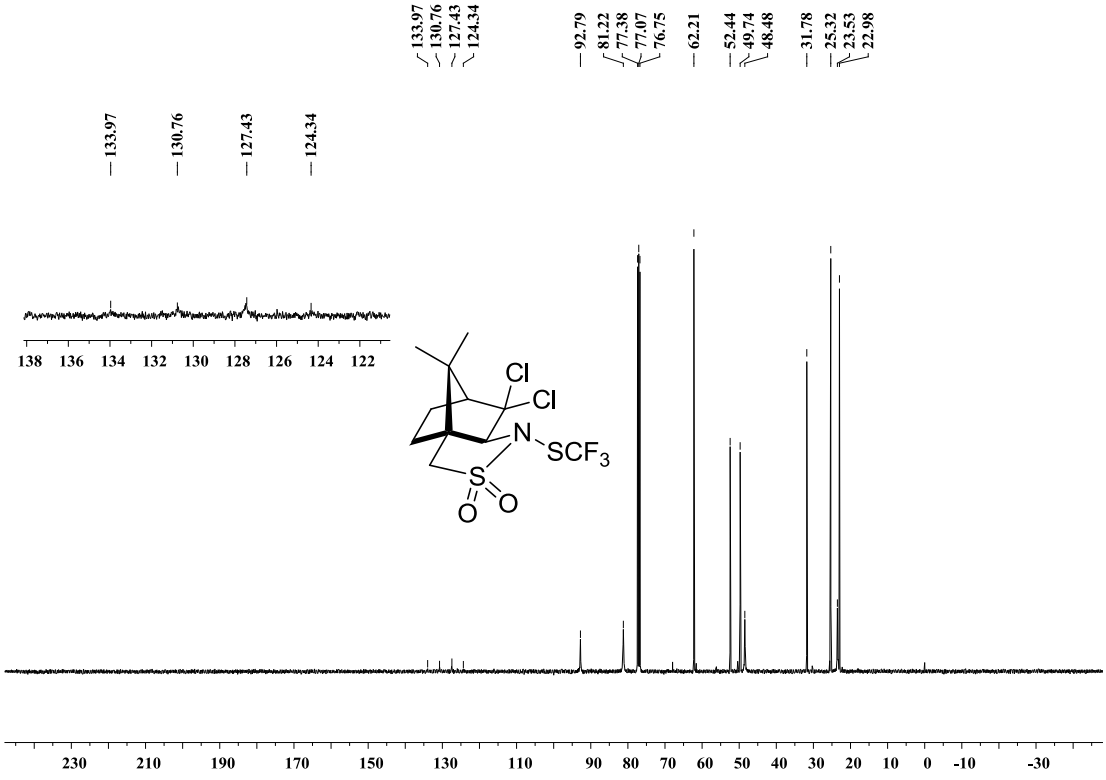
^{1}H NMR Spectrum for (3aS,6S,7aS)-7,7-Dichloro-8,8-dimethyl-1-((trifluoromethyl)thio)hexahydro-1*H*-3a,6-methanobenzo[c]isothiazole 2,2-dioxide 1b at 213 K



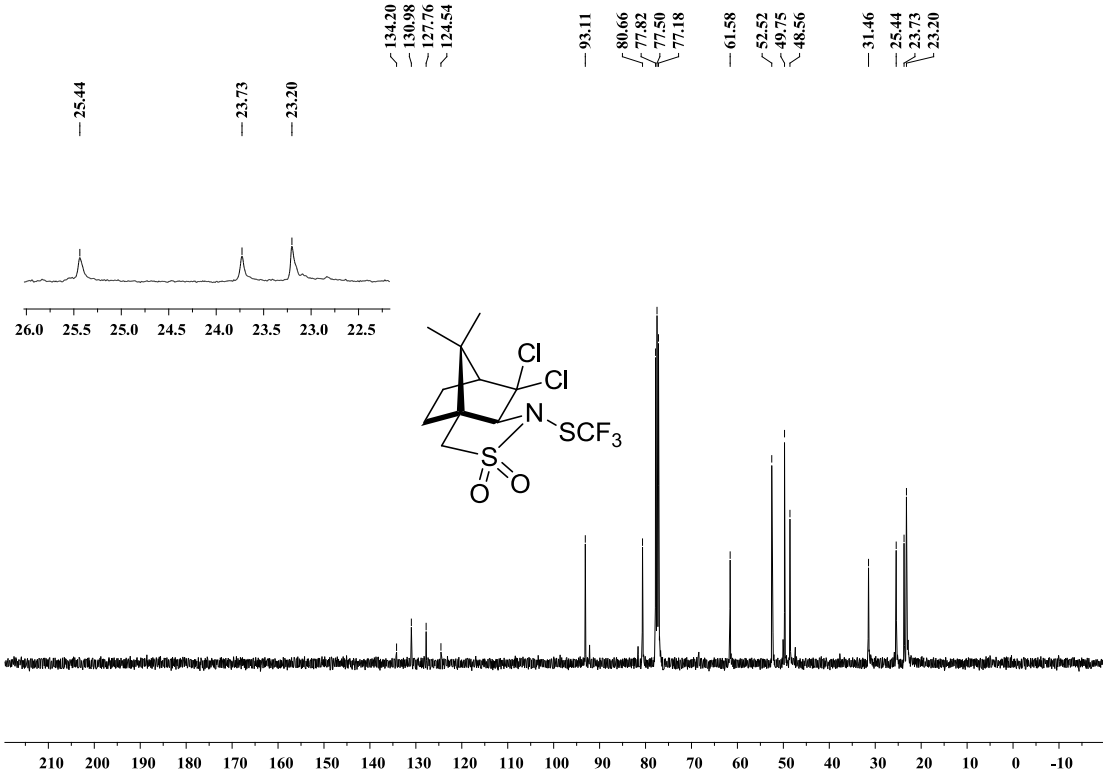
^{1}H NMR Spectrum for (3aS,6S,7aS)-7,7-Dichloro-8,8-dimethyl-1-((trifluoromethyl)thio)hexahydro-1*H*-3a,6-methanobenzo[c]isothiazole 2,2-dioxide 1b at 323 K



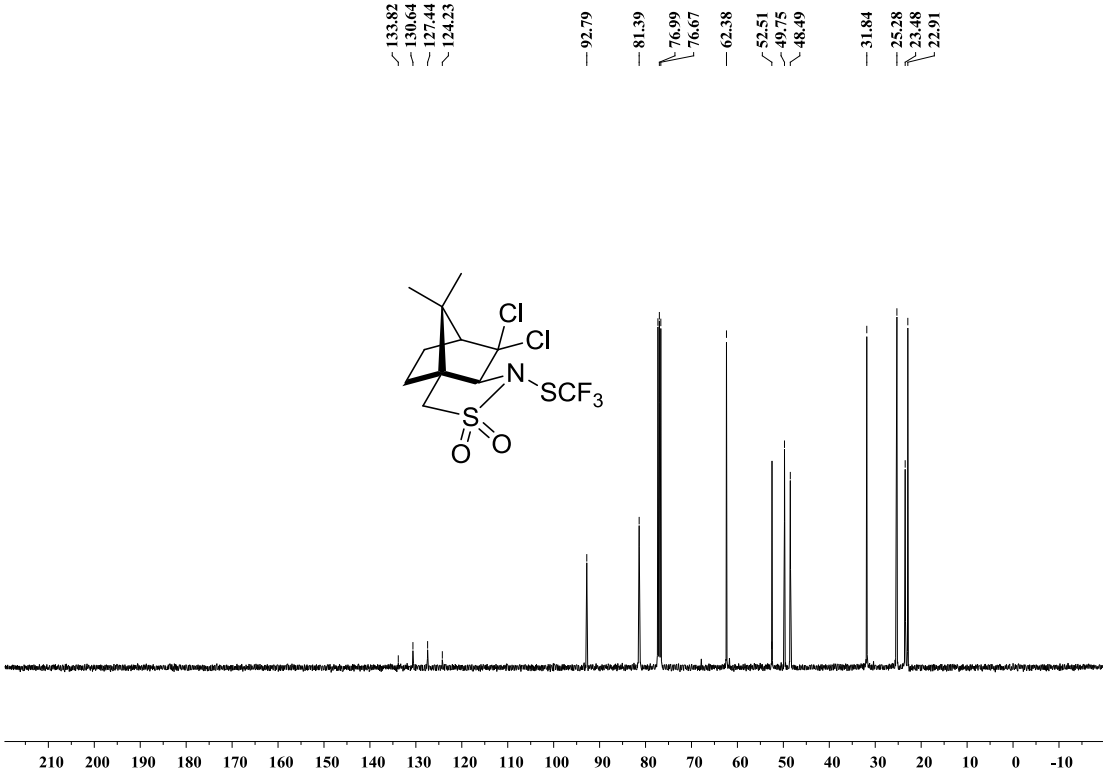
^{13}C NMR Spectrum for (3aS,6S,7aS)-7,7-Dichloro-8,8-dimethyl-1-((trifluoromethyl)thio)hexahydro-1*H*-3a,6-methanobenzo[c]isothiazole 2,2-dioxide 1b at 298 K



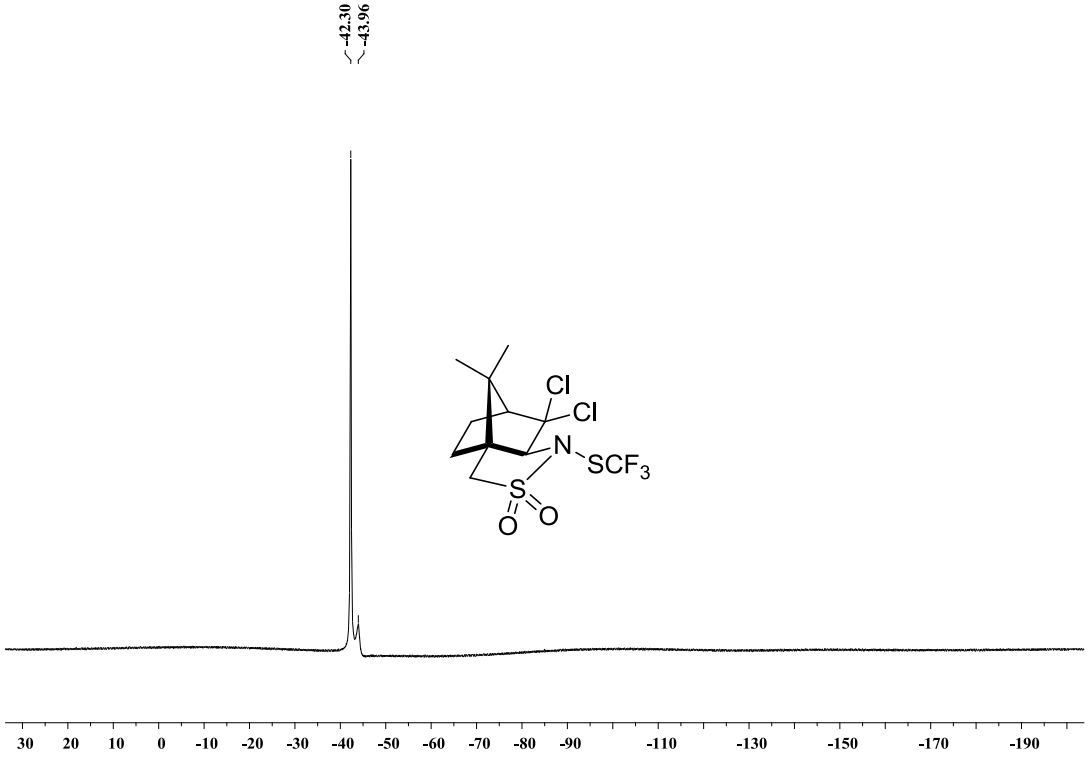
^{13}C NMR Spectrum for (3aS,6S,7aS)-7,7-Dichloro-8,8-dimethyl-1-((trifluoromethyl)thio)hexahydro-1*H*-3a,6-methanobenzo[c]isothiazole 2,2-dioxide 1b at 213 K



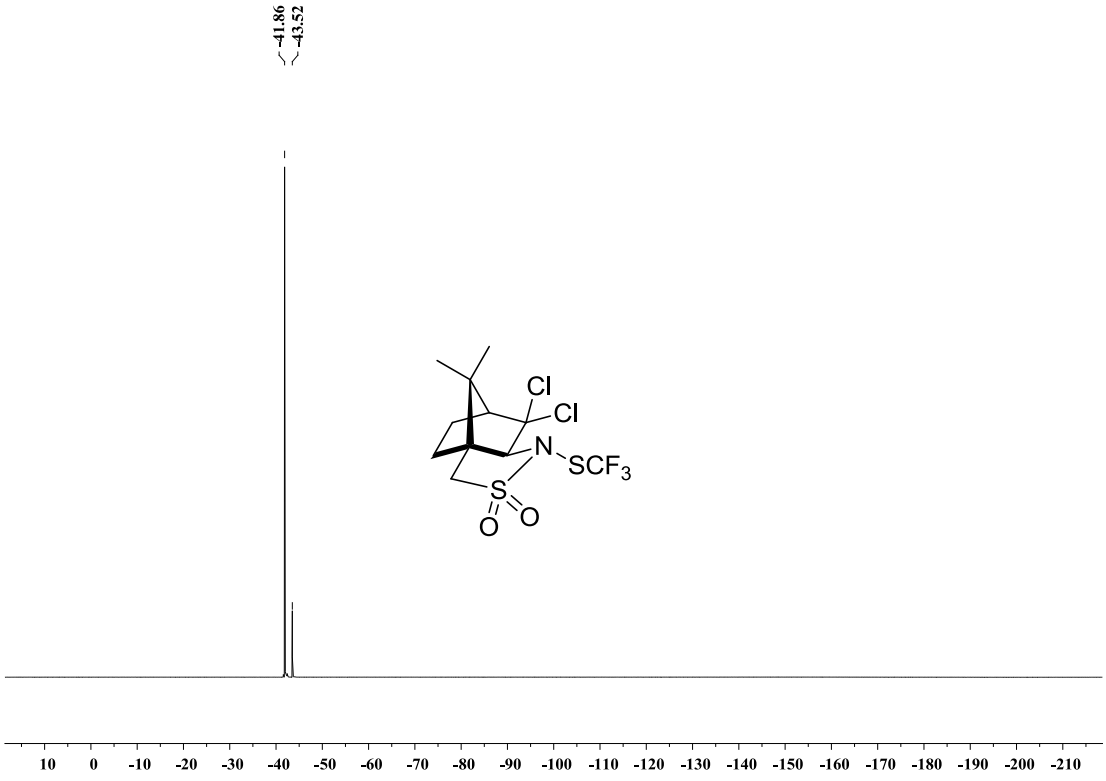
^{13}C NMR Spectrum for (3aS,6S,7aS)-7,7-Dichloro-8,8-dimethyl-1-((trifluoromethyl)thio)hexahydro-1*H*-3a,6-methanobenzo[c]isothiazole 2,2-dioxide 1b at 323 K



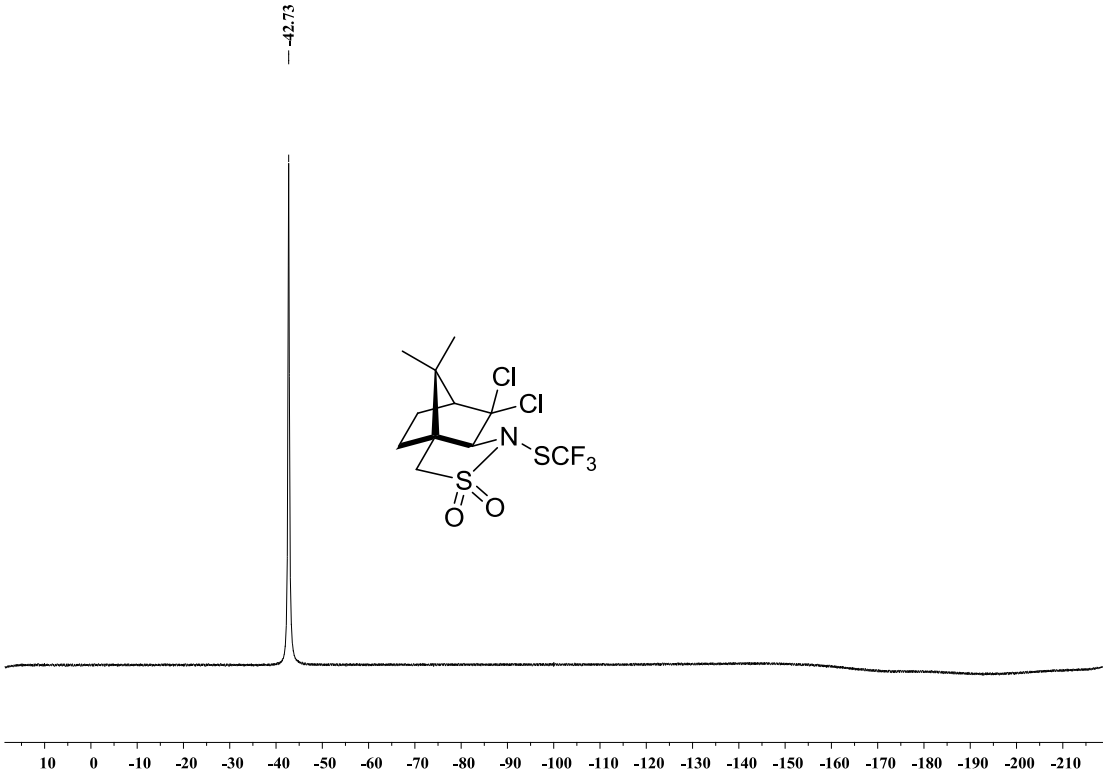
^{19}F NMR Spectrum for (3aS,6S,7aS)-7,7-Dichloro-8,8-dimethyl-1-((trifluoromethyl)thio)hexahydro-1*H*-3a,6-methanobenzo[c]isothiazole 2,2-dioxide 1b at 298 K



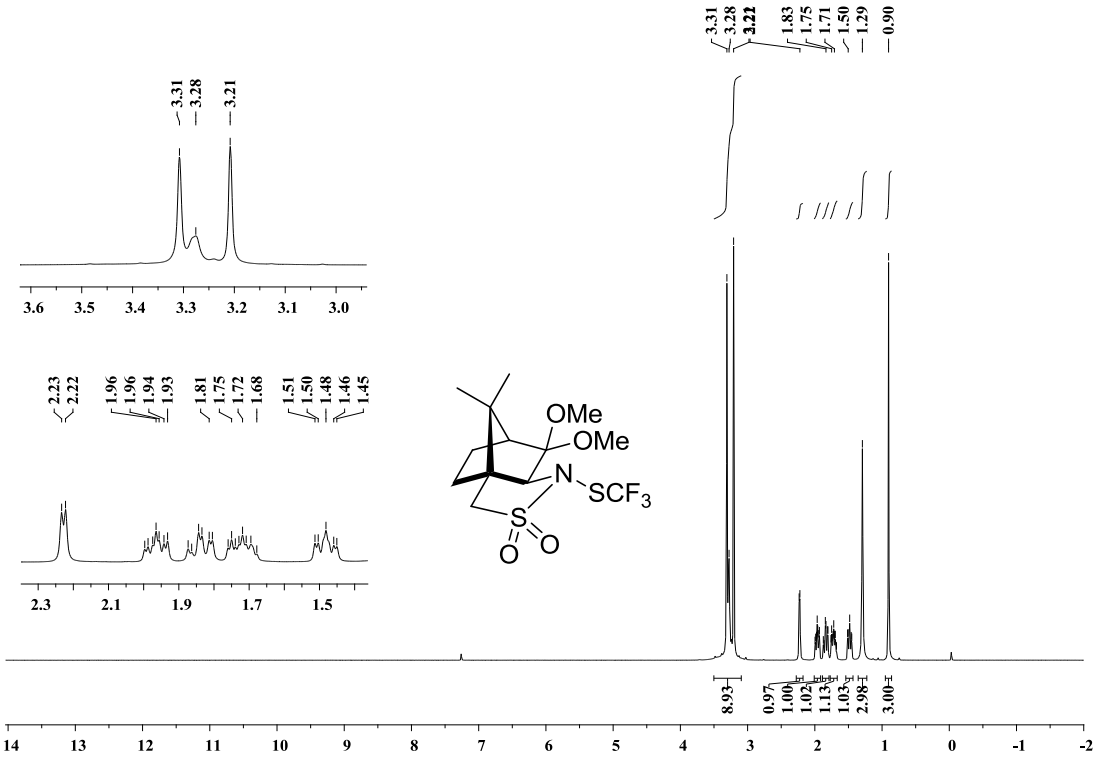
^{19}F NMR Spectrum for (3aS,6S,7aS)-7,7-Dichloro-8,8-dimethyl-1-((trifluoromethyl)thio)hexahydro-1*H*-3a,6-methanobenzo[c]isothiazole 2,2-dioxide 1b at 213 K



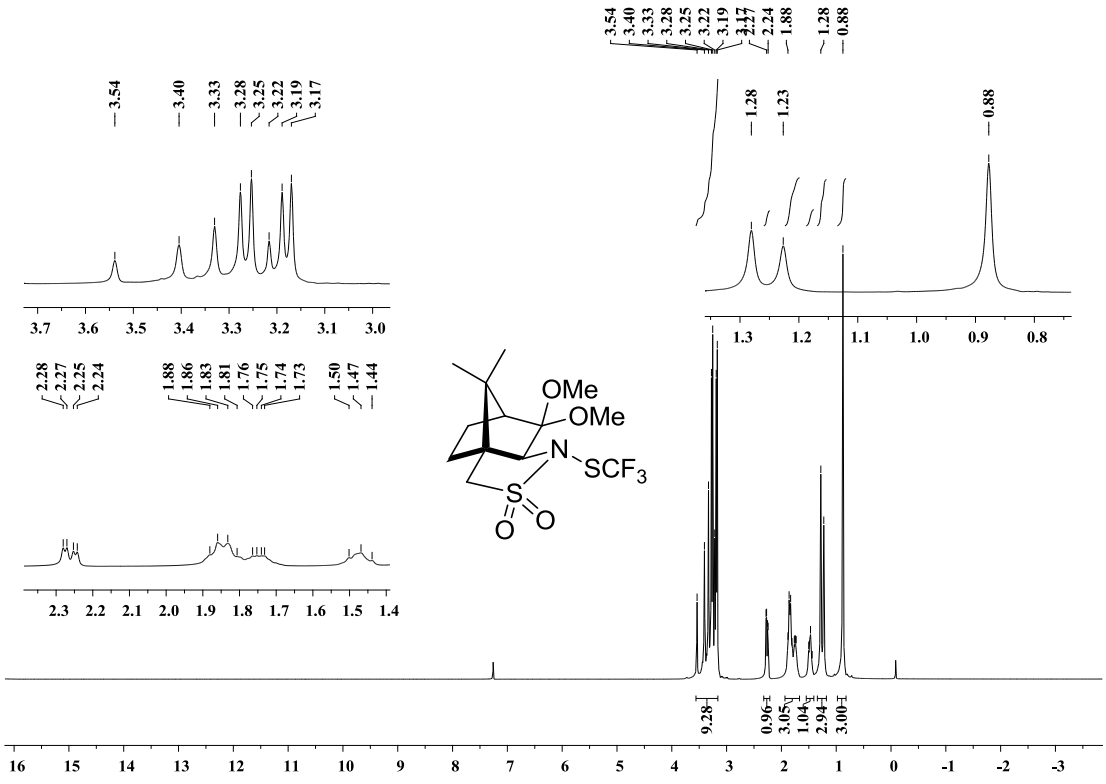
^{19}F NMR Spectrum for (3aS,6S,7aS)-7,7-Dichloro-8,8-dimethyl-1-((trifluoromethyl)thio)hexahydro-1*H*-3a,6-methanobenzo[c]isothiazole 2,2-dioxide 1b at 323 K



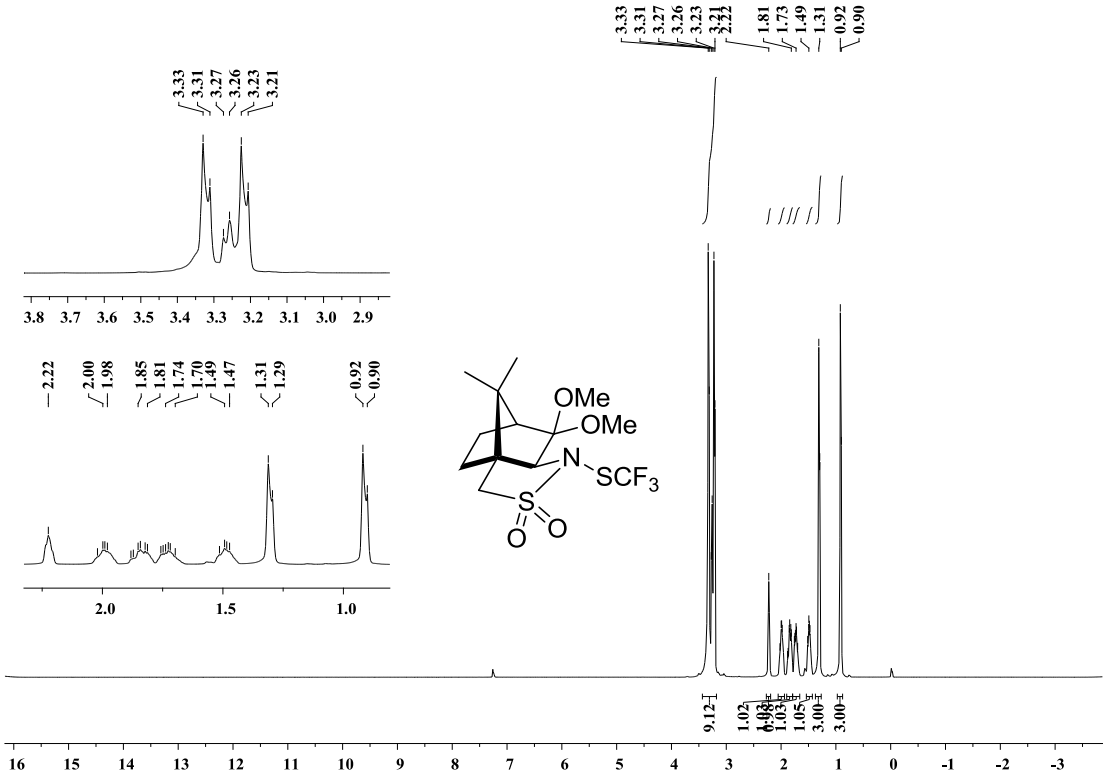
^{1}H NMR Spectrum for (3aS,6S,7aS)-7,7-Dimethoxy-8,8-dimethyl-1-((trifluoromethyl)thio)hexahydro-1*H*-3a,6-methanobenzo[c]isothiazole 2,2-dioxide 1c at 298 K



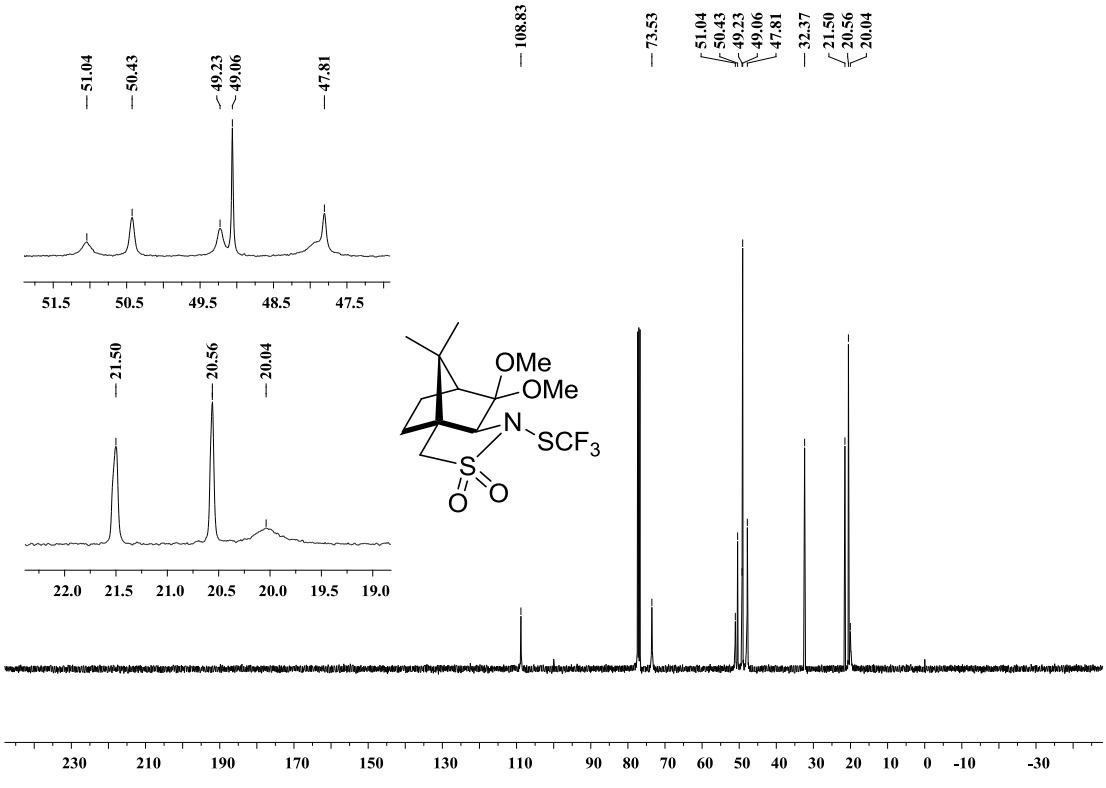
^{1}H NMR Spectrum for (3aS,6S,7aS)-7,7-Dimethoxy-8,8-dimethyl-1-((trifluoromethyl)thio)hexahydro-1*H*-3a,6-methanobenzo[c]isothiazole 2,2-dioxide 1c at 213 K



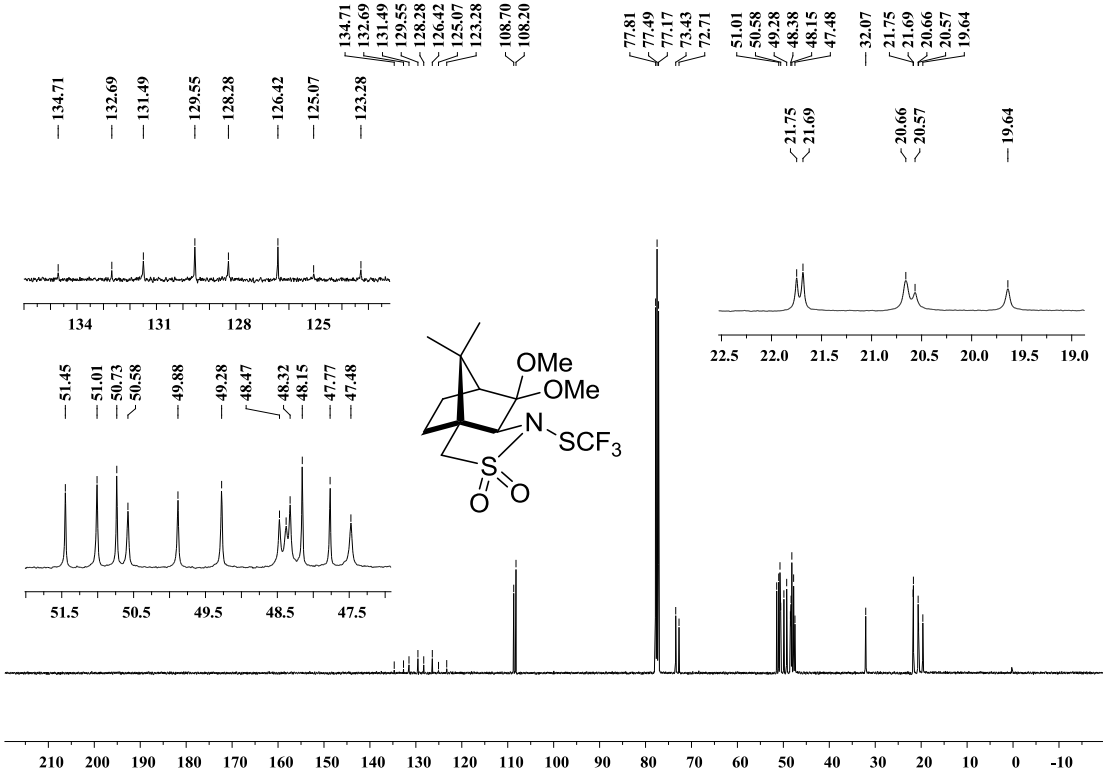
^{1}H NMR Spectrum for (3aS,6S,7aS)-7,7-Dimethoxy-8,8-dimethyl-1-((trifluoromethyl)thio)hexahydro-1*H*-3a,6-methanobenzo[c]isothiazole 2,2-dioxide 1c at 323 K



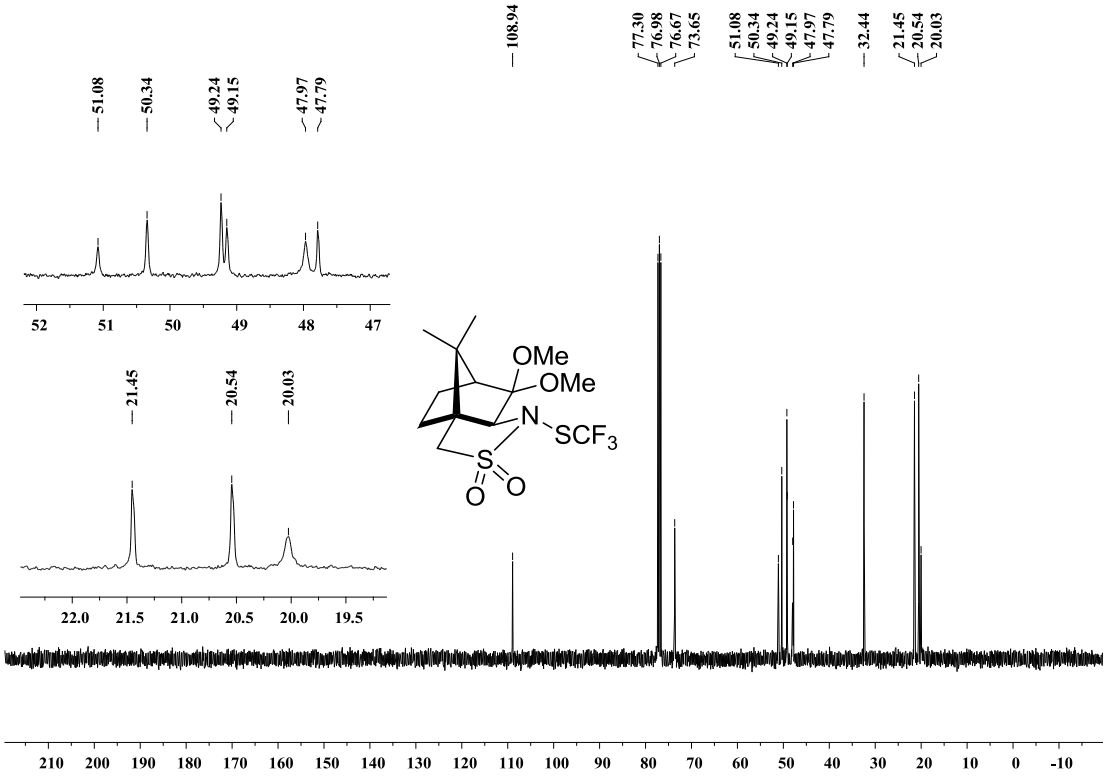
^{13}C NMR Spectrum for (3aS,6S,7aS)-7,7-Dimethoxy-8,8-dimethyl-1-((trifluoromethyl)thio)hexahydro-1*H*-3a,6-methanobenzo[c]isothiazole 2,2-dioxide 1c at 298 K



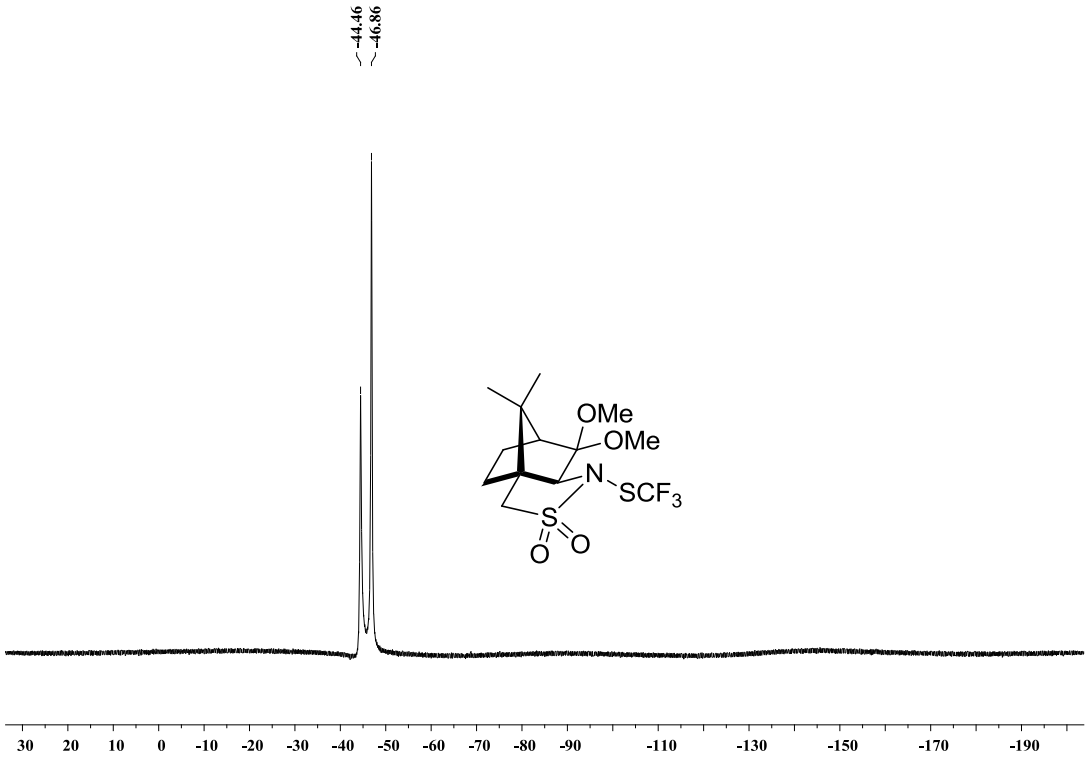
^{13}C NMR Spectrum for (3aS,6S,7aS)-7,7-Dimethoxy-8,8-dimethyl-1-((trifluoromethyl)thio)hexahydro-1*H*-3a,6-methanobenzo[c]isothiazole 2,2-dioxide 1c at 213 K



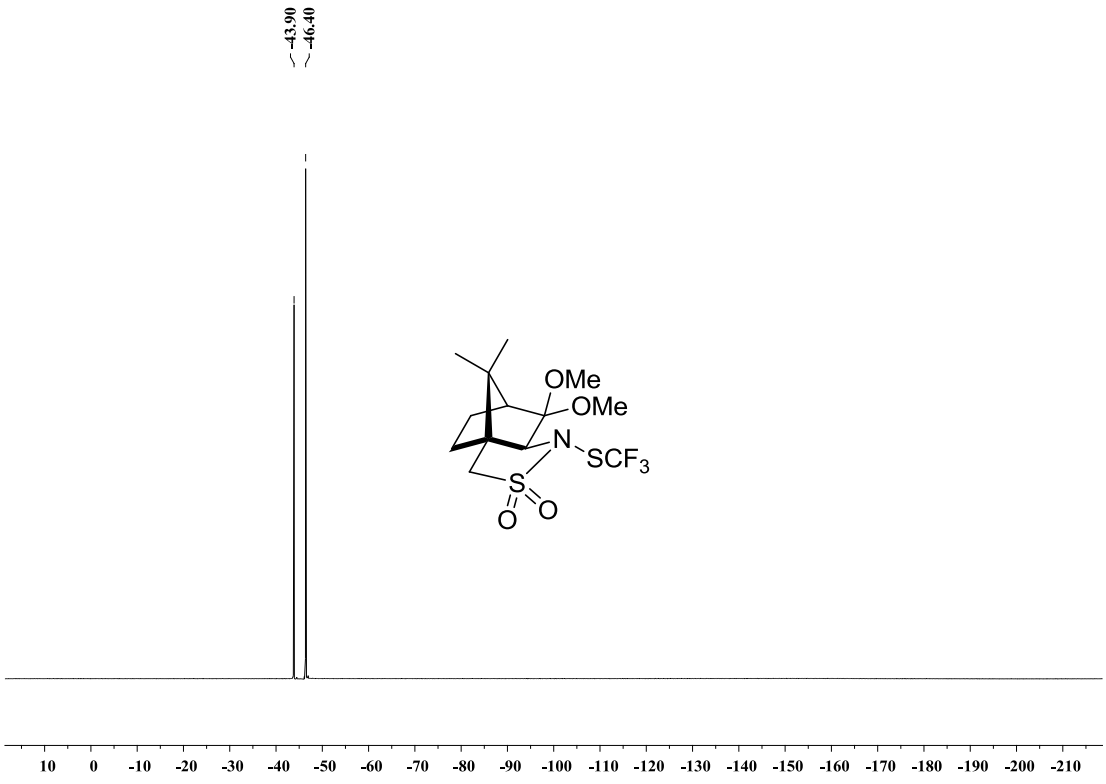
^{13}C NMR Spectrum for (3aS,6S,7aS)-7,7-Dimethoxy-8,8-dimethyl-1-((trifluoromethyl)thio)hexahydro-1*H*-3a,6-methanobenzo[c]isothiazole 2,2-dioxide 1c at 323 K



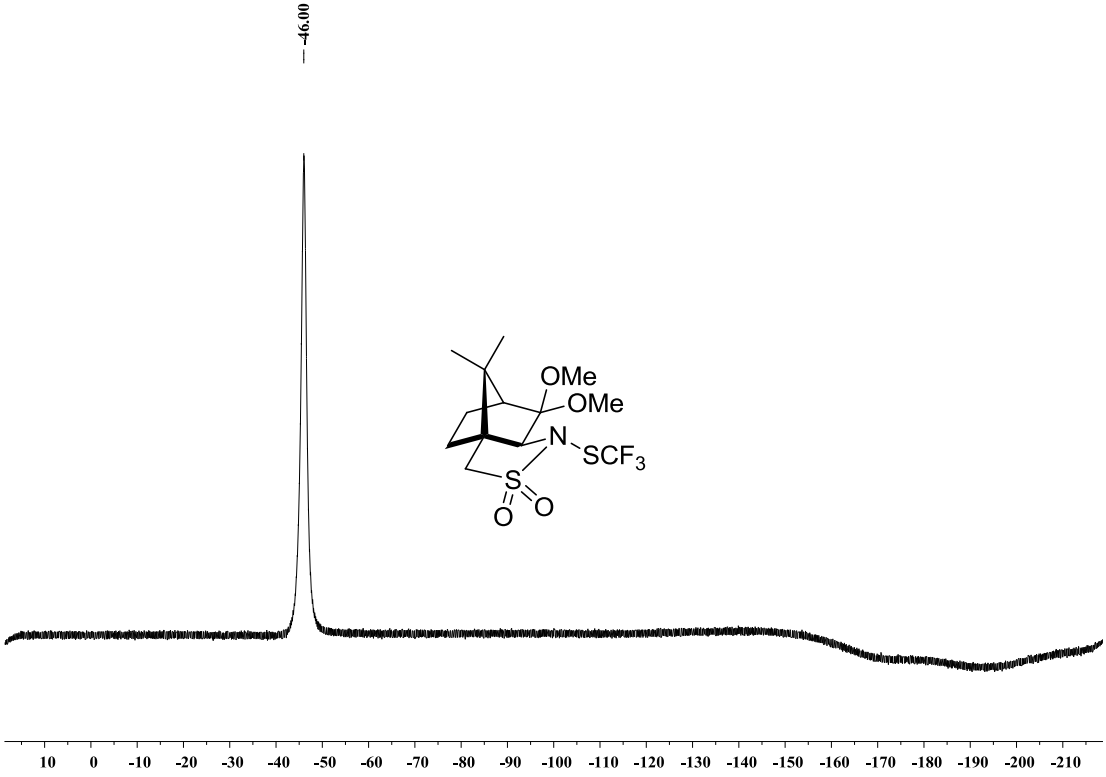
^{19}F NMR Spectrum for (3aS,6S,7aS)-7,7-Dimethoxy-8,8-dimethyl-1-((trifluoromethyl)thio)hexahydro-1*H*-3a,6-methanobenzo[c]isothiazole 2,2-dioxide 1c at 298 K



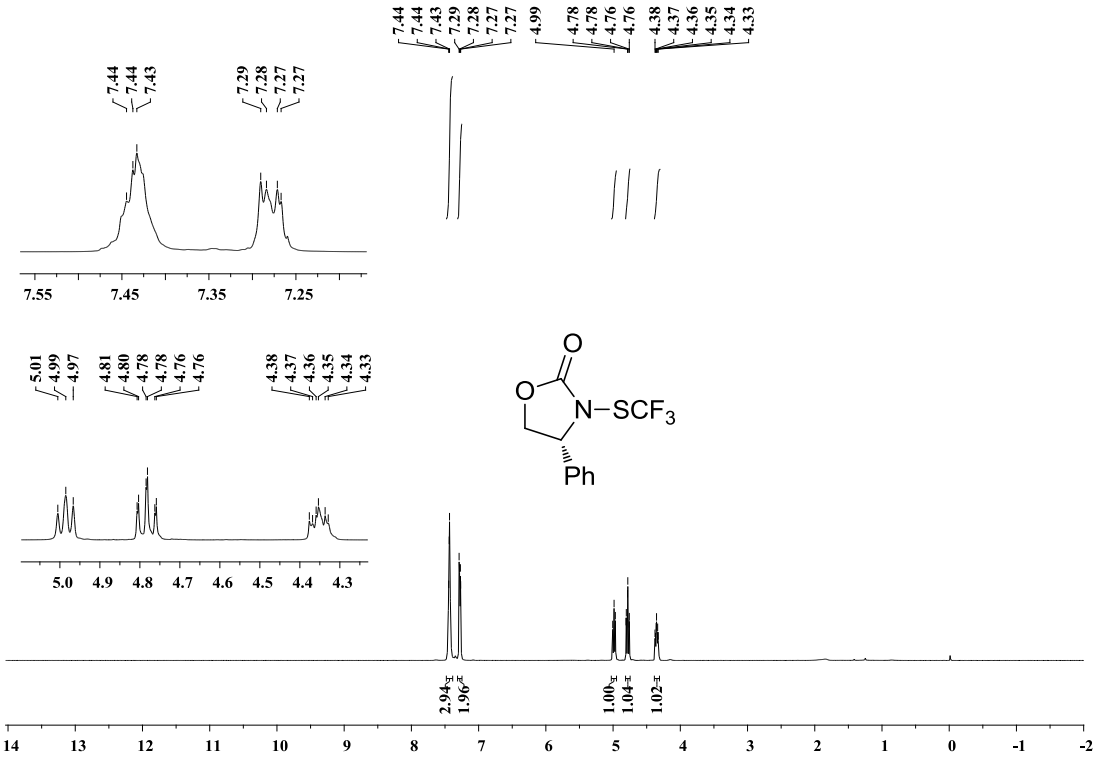
^{19}F NMR Spectrum for (3aS,6S,7aS)-7,7-Dimethoxy-8,8-dimethyl-1-((trifluoromethyl)thio)hexahydro-1*H*-3a,6-methanobenzo[c]isothiazole 2,2-dioxide 1c at 213 K



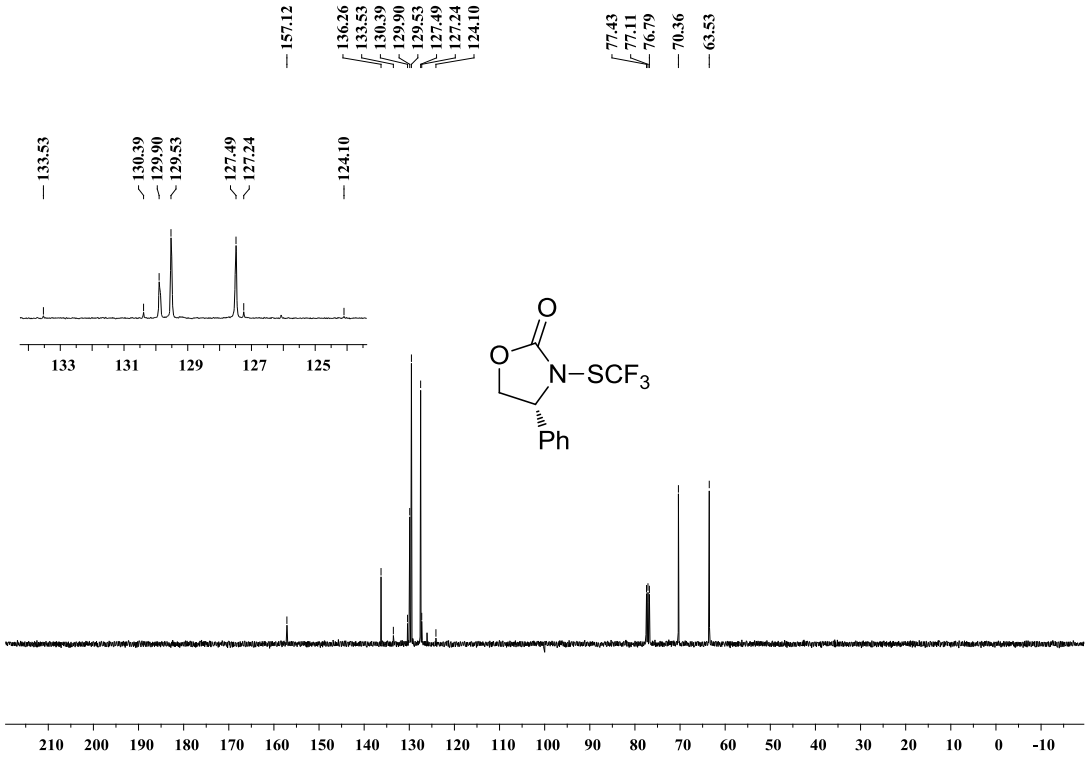
^{19}F NMR Spectrum for (3aS,6S,7aS)-7,7-Dimethoxy-8,8-dimethyl-1-((trifluoromethyl)thio)hexahydro-1*H*-3a,6-methanobenzo[c]isothiazole 2,2-dioxide 1c at 323 K



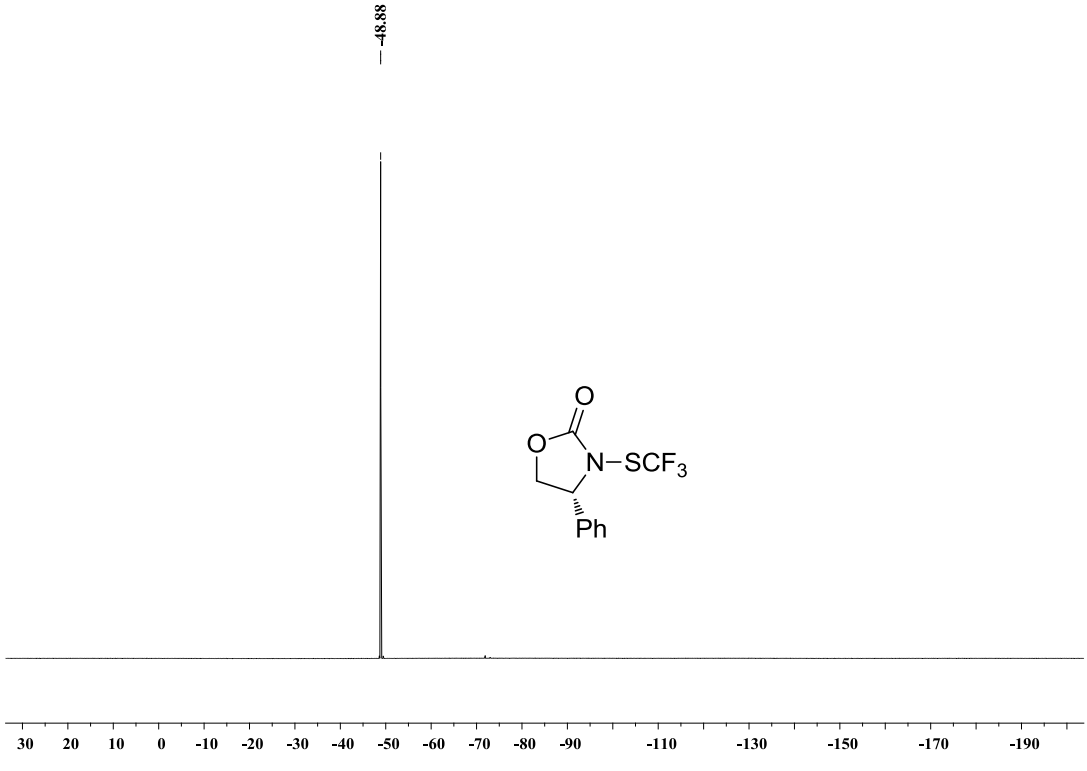
^{1}H NMR Spectrum for (R)-4-Phenyl-3-((trifluoromethyl)thio)oxazolidin-2-one 1d



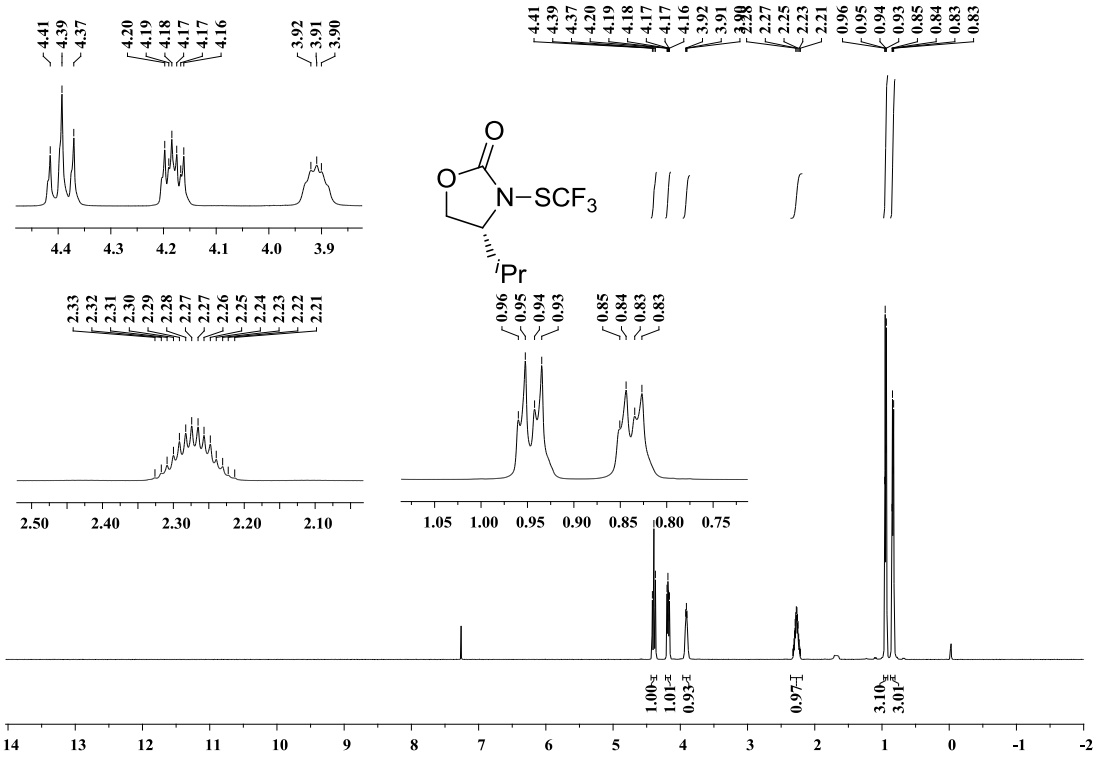
^{13}C NMR Spectrum for (R)-4-Phenyl-3-((trifluoromethyl)thio)oxazolidin-2-one 1d



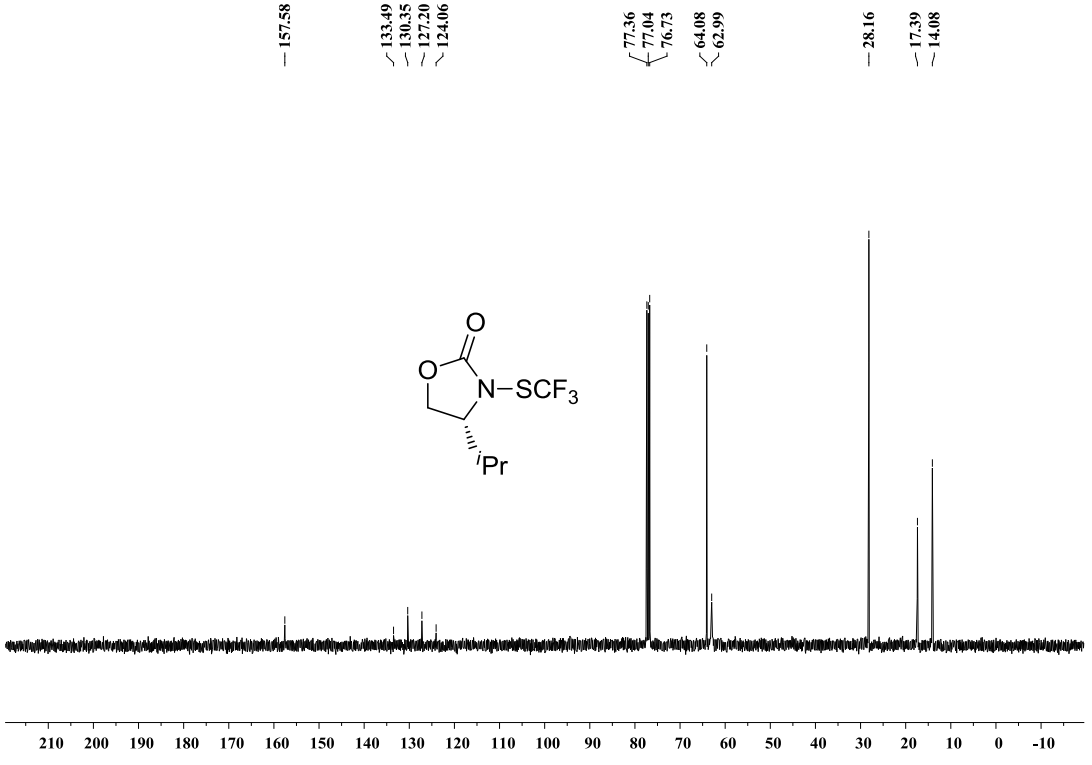
^{19}F NMR Spectrum for (R)-4-Phenyl-3-((trifluoromethyl)thio)oxazolidin-2-one 1d



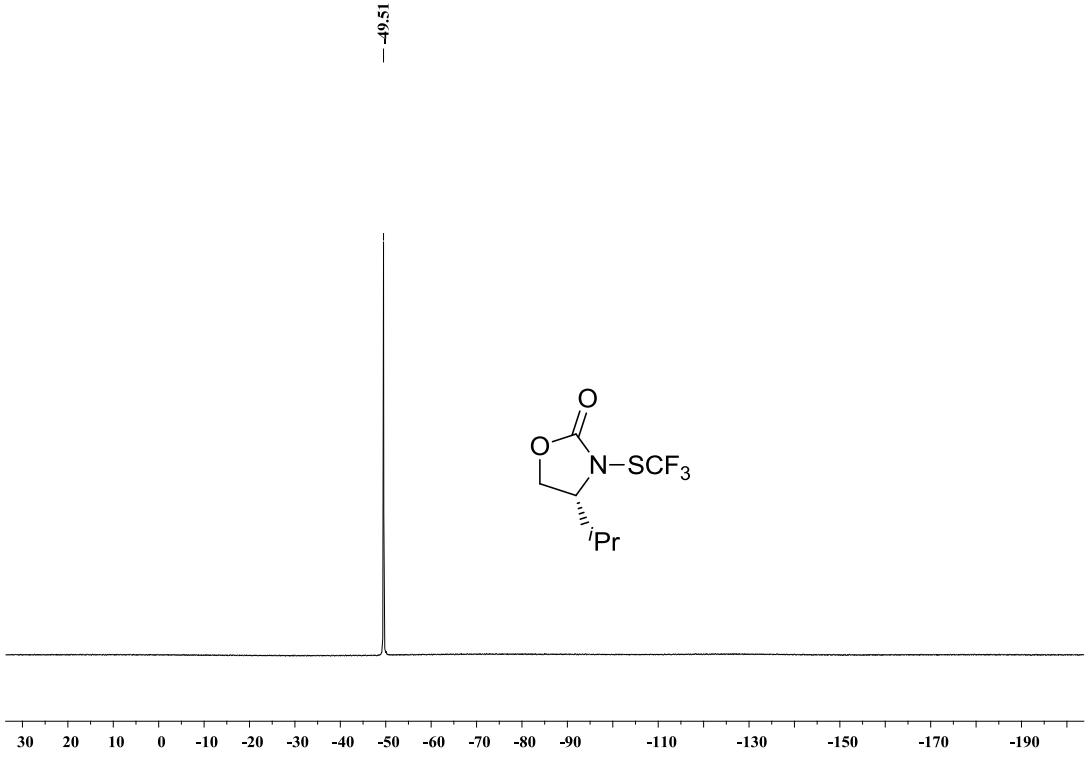
^{1}H NMR Spectrum for (R)-4-Isopropyl-3-((trifluoromethyl)thio)oxazolidin-2-one 1e



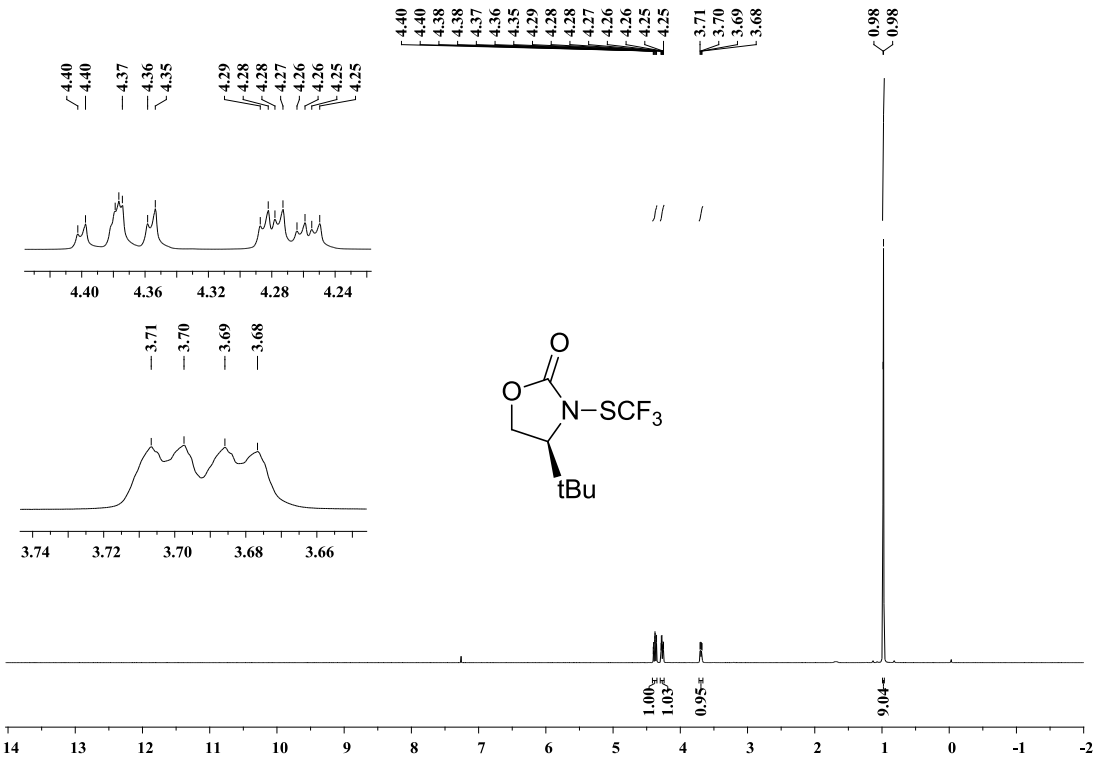
^{13}C NMR Spectrum for (R)-4-Isopropyl-3-((trifluoromethyl)thio)oxazolidin-2-one 1e



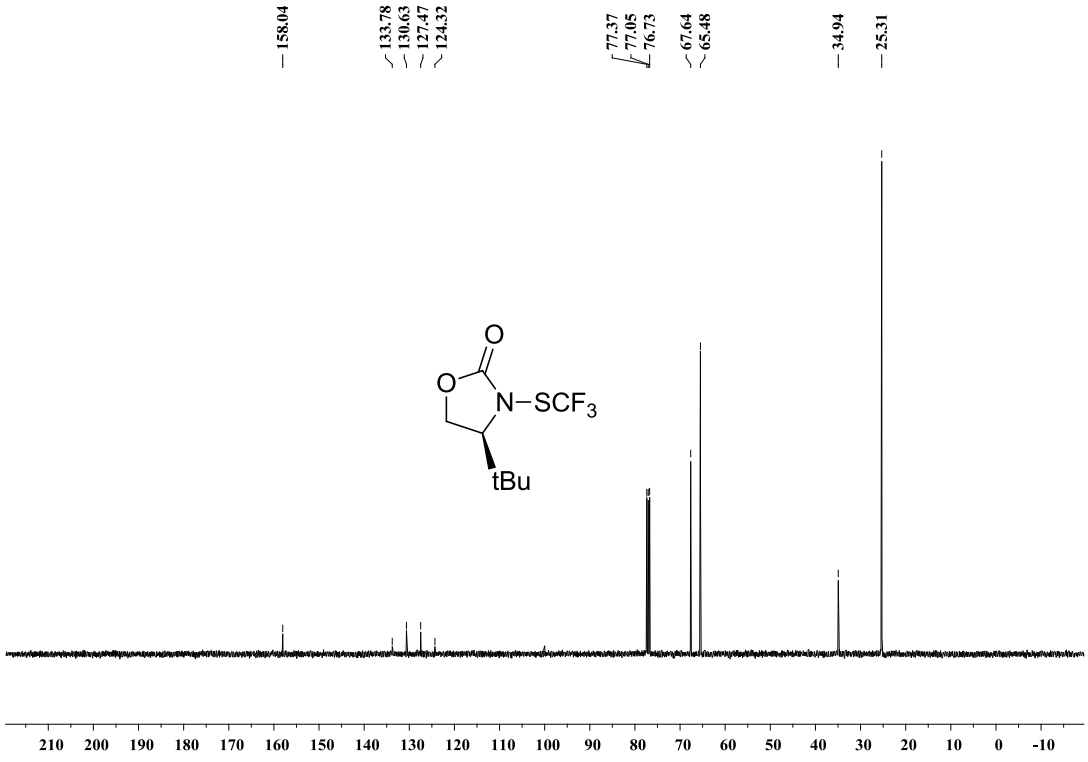
^{19}F NMR Spectrum for (R)-4-Isopropyl-3-((trifluoromethyl)thio)oxazolidin-2-one 1e



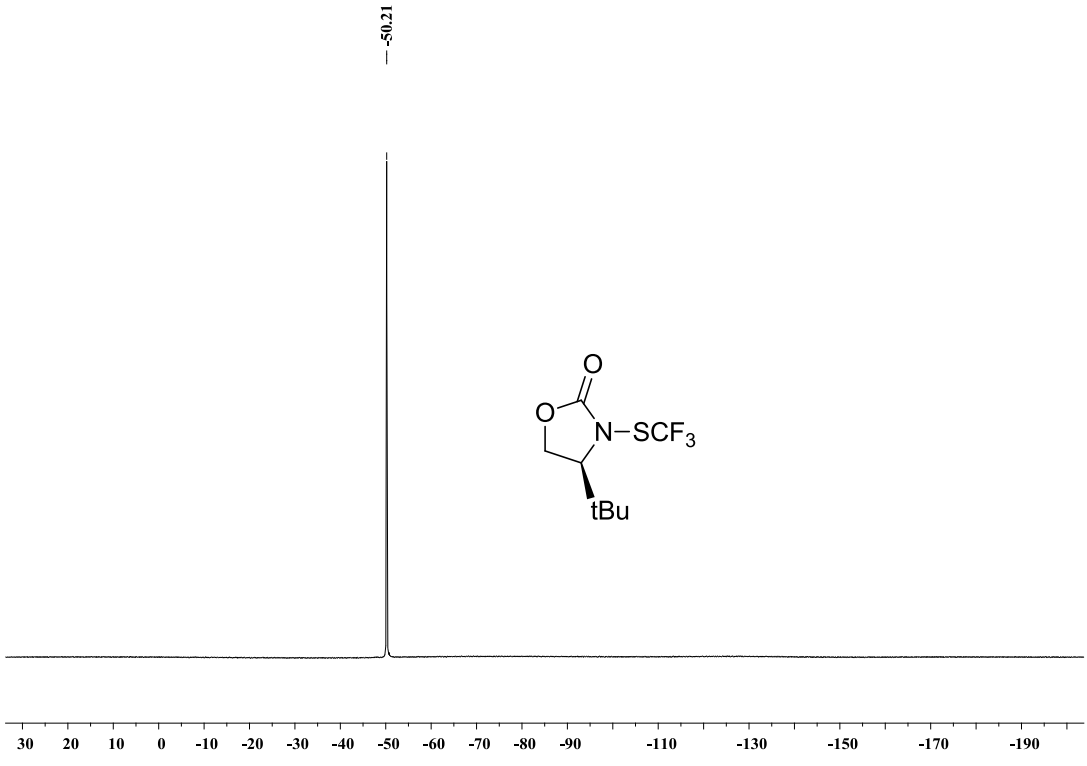
^{1}H NMR Spectrum for (S)-4-(*tert*-Butyl)-3-((trifluoromethyl)thio)oxazolidin-2-one 1f



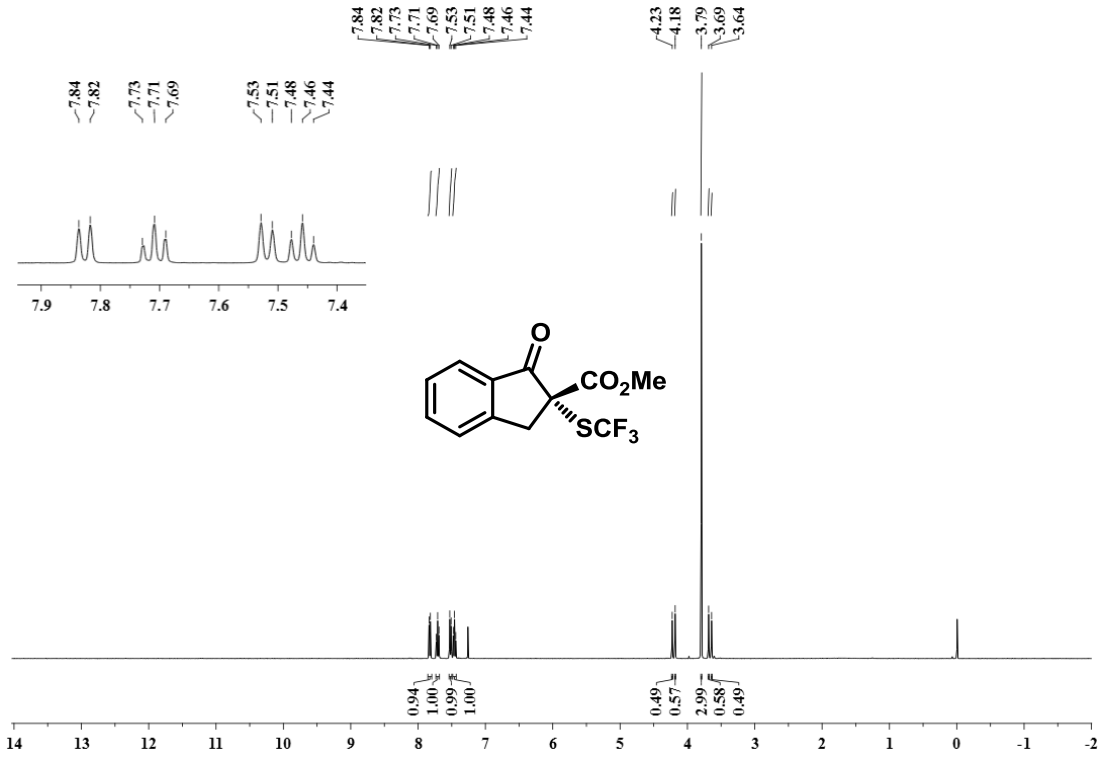
^{13}C NMR Spectrum for (S)-4-(*tert*-Butyl)-3-((trifluoromethyl)thio)oxazolidin-2-one 1f



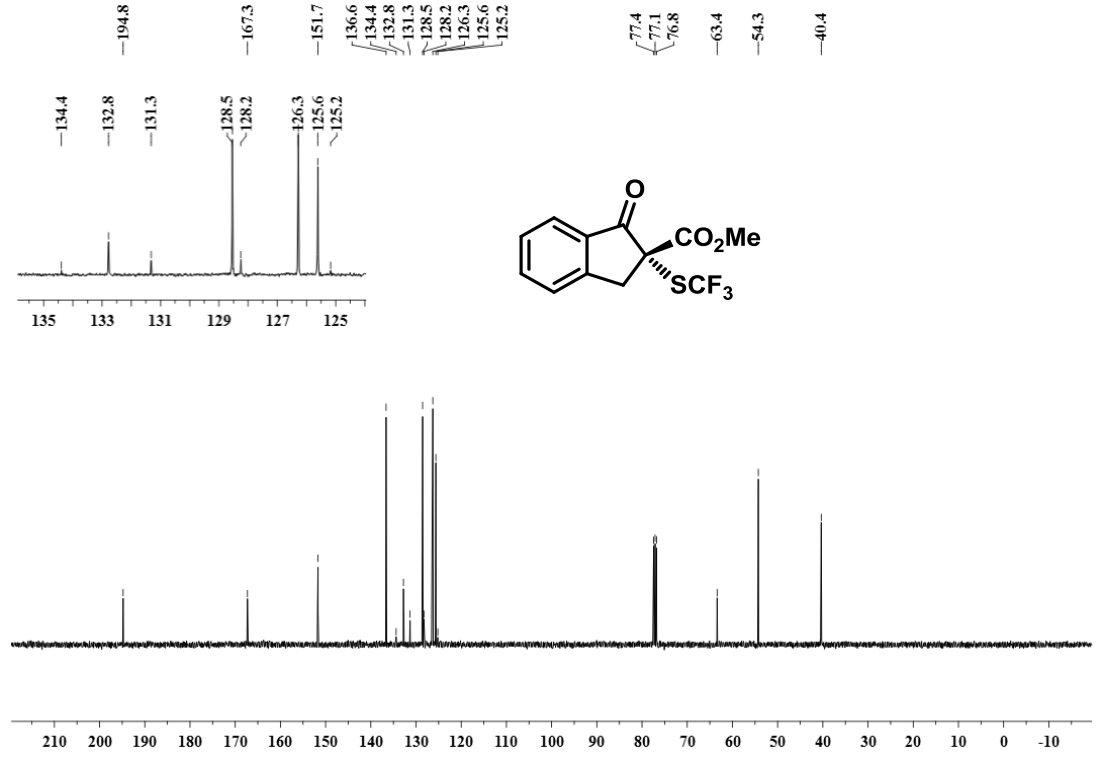
^{19}F NMR Spectrum for (S)-4-(*tert*-Butyl)-3-((trifluoromethyl)thio)oxazolidin-2-one 1f



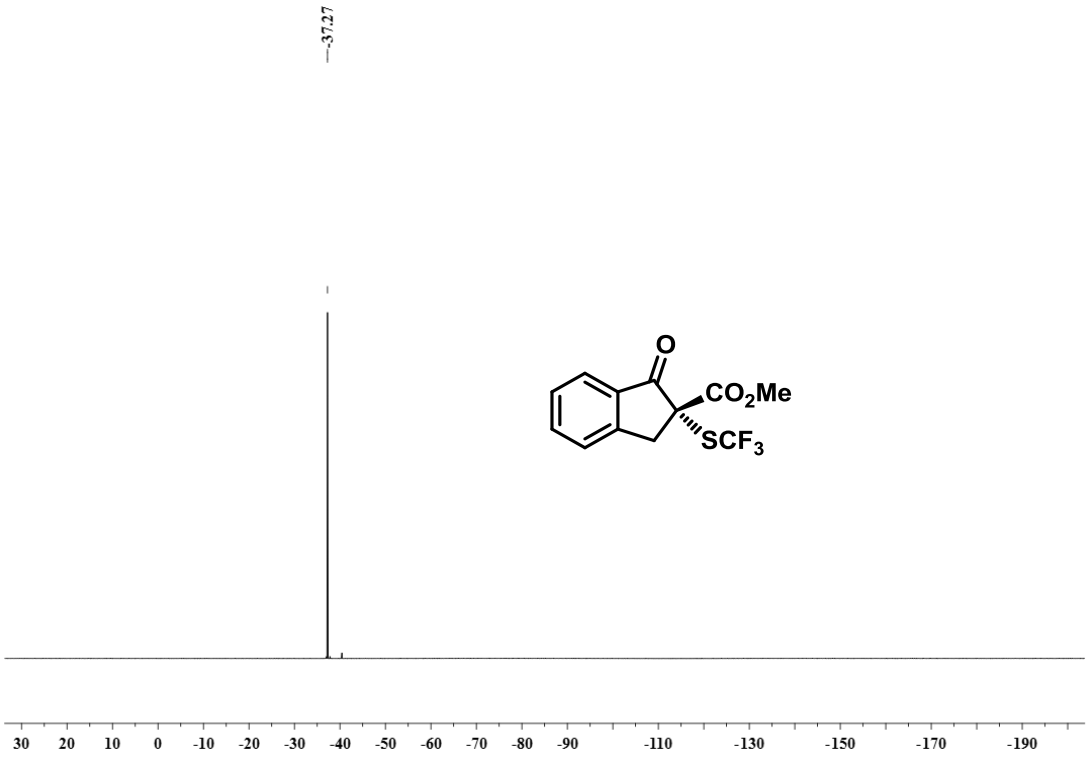
^{1}H NMR Spectrum for (R)-Methyl-1-oxo-2-((trifluoromethyl)thio)-2,3-dihydro-1*H*-indene-2-carboxylate 3a



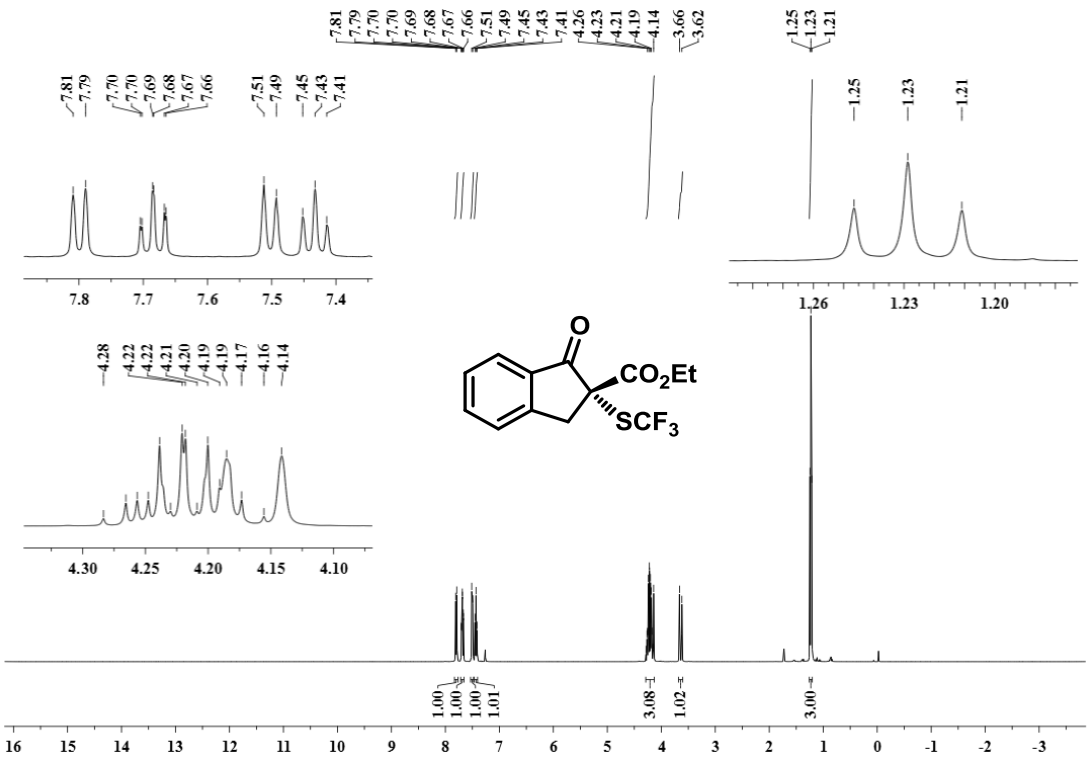
^{13}C NMR Spectrum for (R)-Methyl-1-oxo-2-((trifluoromethyl)thio)-2,3-dihydro-1*H*-indene-2-carboxylate 3a



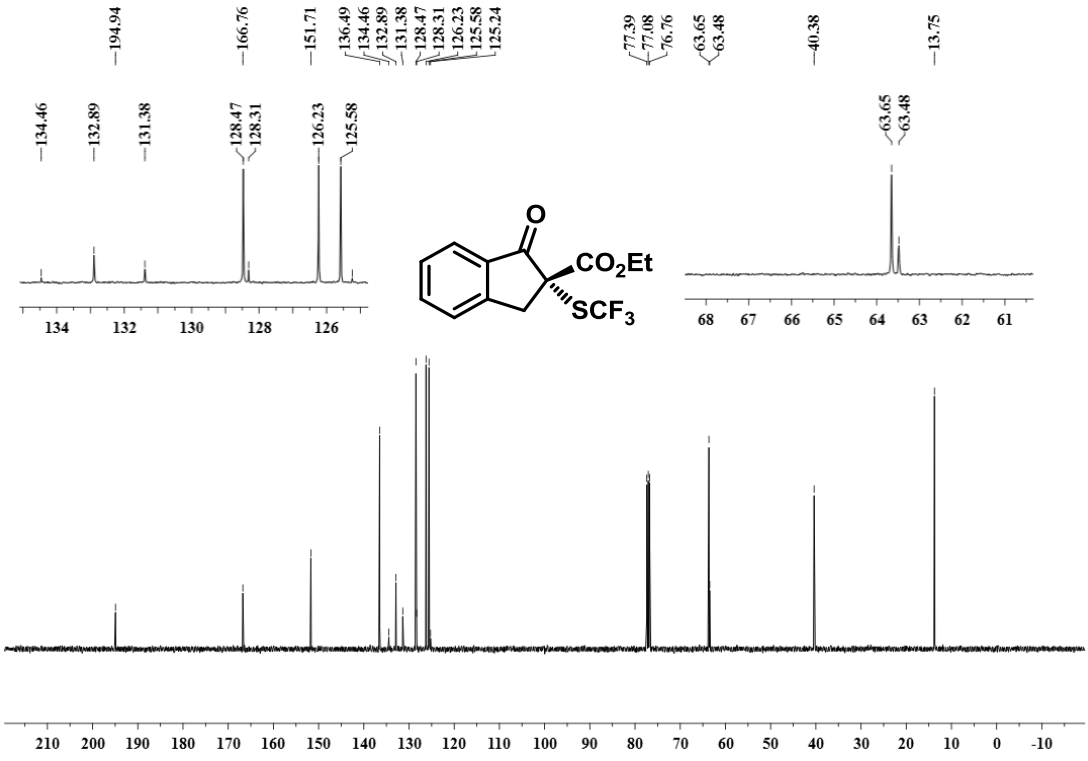
^{19}F NMR Spectrum for (R)-Methyl-1-oxo-2-((trifluoromethyl)thio)-2,3-dihydro-1*H*-indene-2-carboxylate 3a



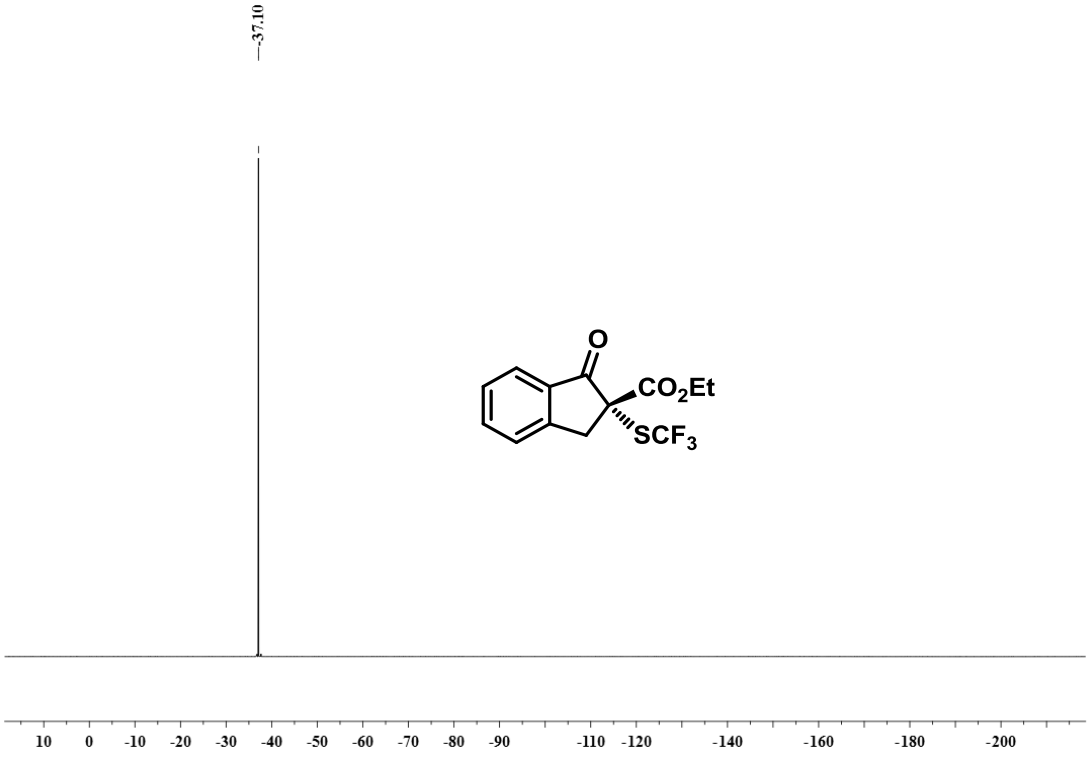
^{1}H NMR Spectrum for (R)-Ethyl-1-oxo-2-((trifluoromethyl)thio)-2,3-dihydro-1*H*-indene-2-carboxylate 3b



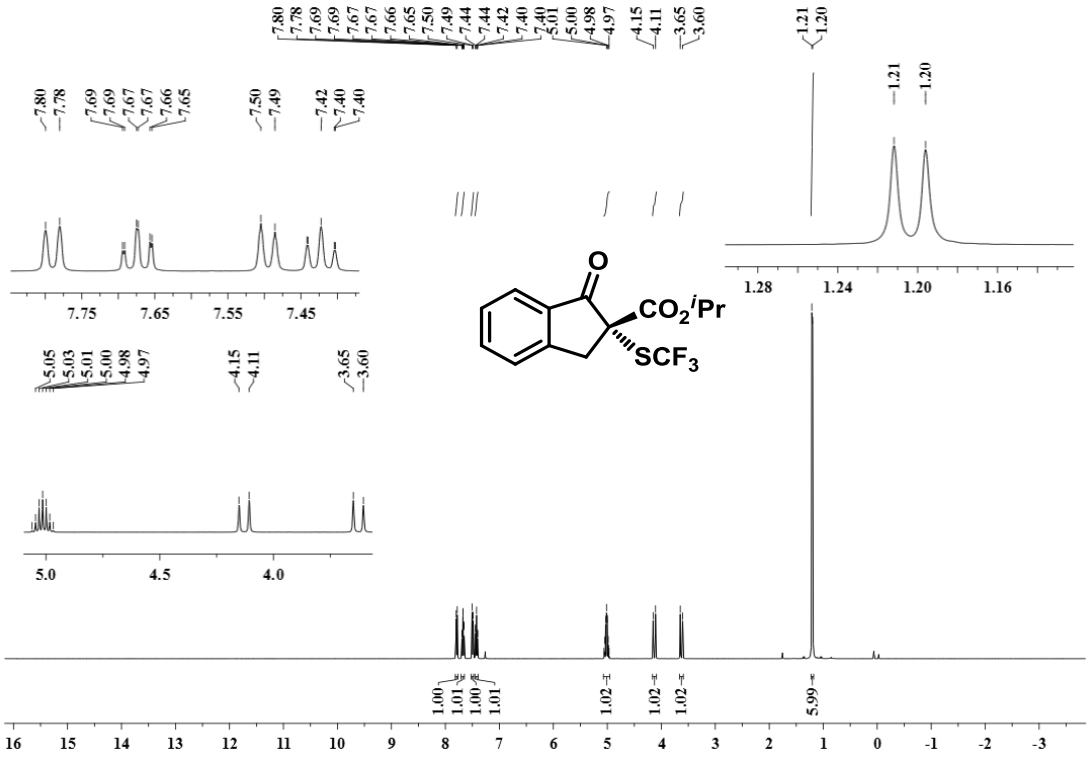
^{13}C NMR Spectrum for (R)-Ethyl-1-oxo-2-((trifluoromethyl)thio)-2,3-dihydro-1*H*-indene-2-carboxylate 3b



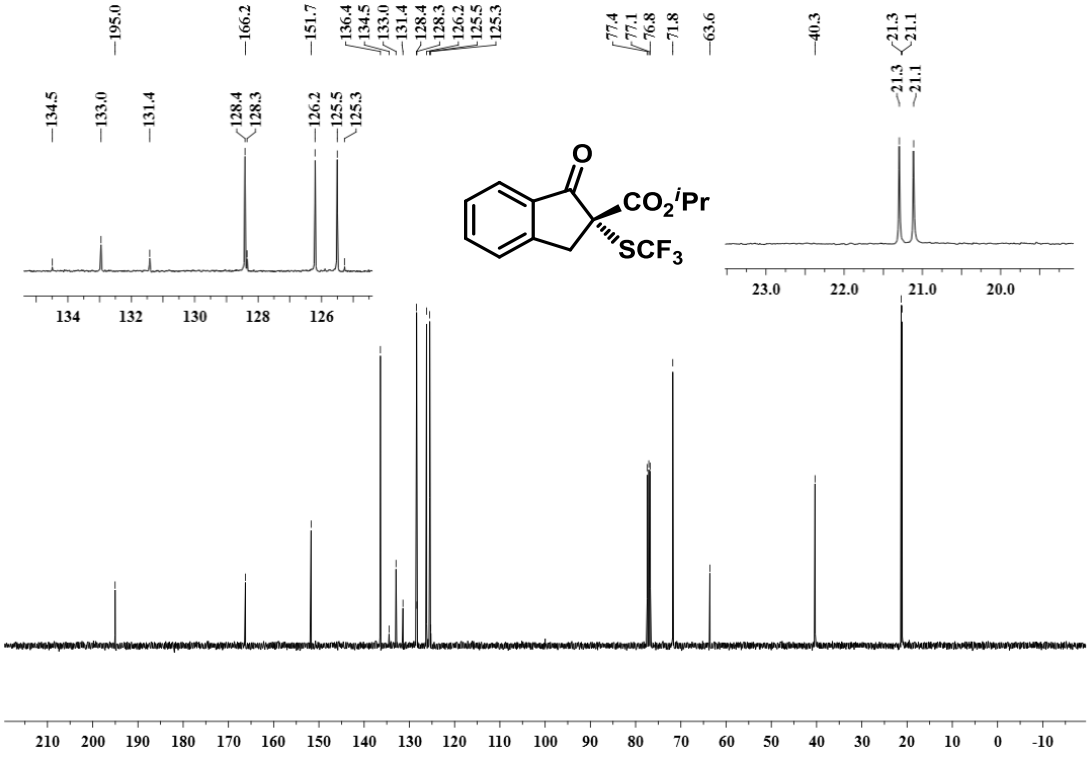
^{19}F NMR Spectrum for (R)-Ethyl-1-oxo-2-((trifluoromethyl)thio)-2,3-dihydro-1*H*-indene-2-carboxylate 3b



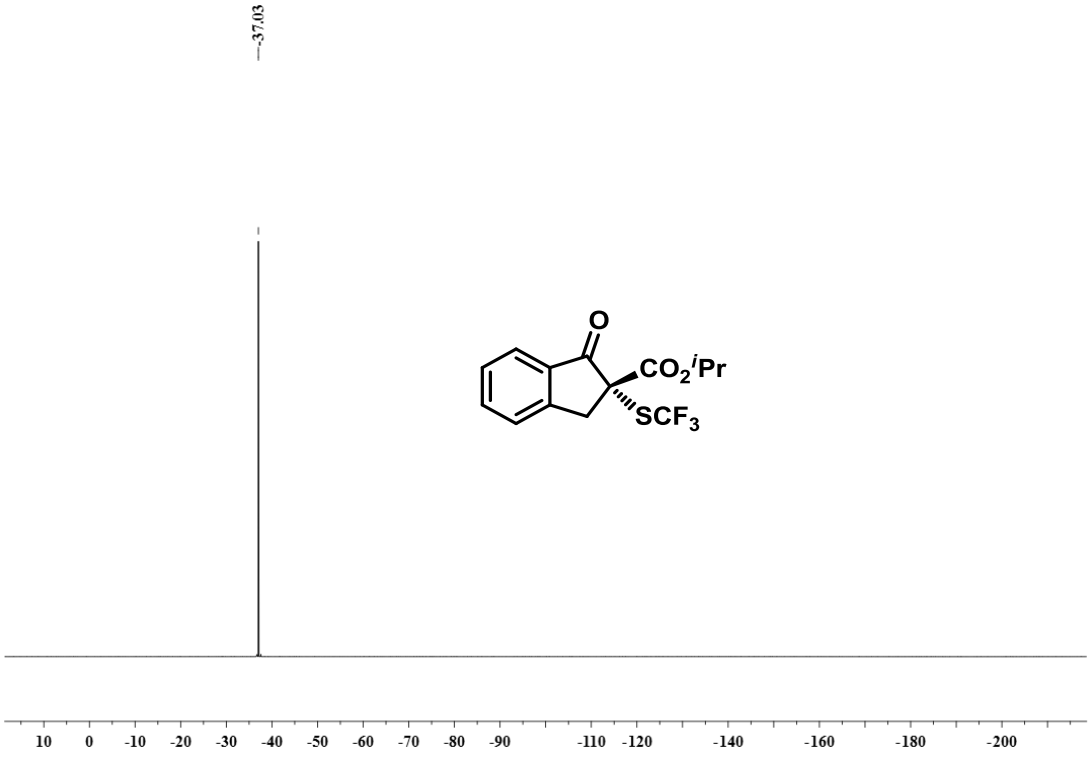
^{1}H NMR Spectrum for (R)-Isopropyl-1-oxo -2-((trifluoromethyl)thio)-2,3-dihydro-1*H*-indene-2-carboxylate 3c



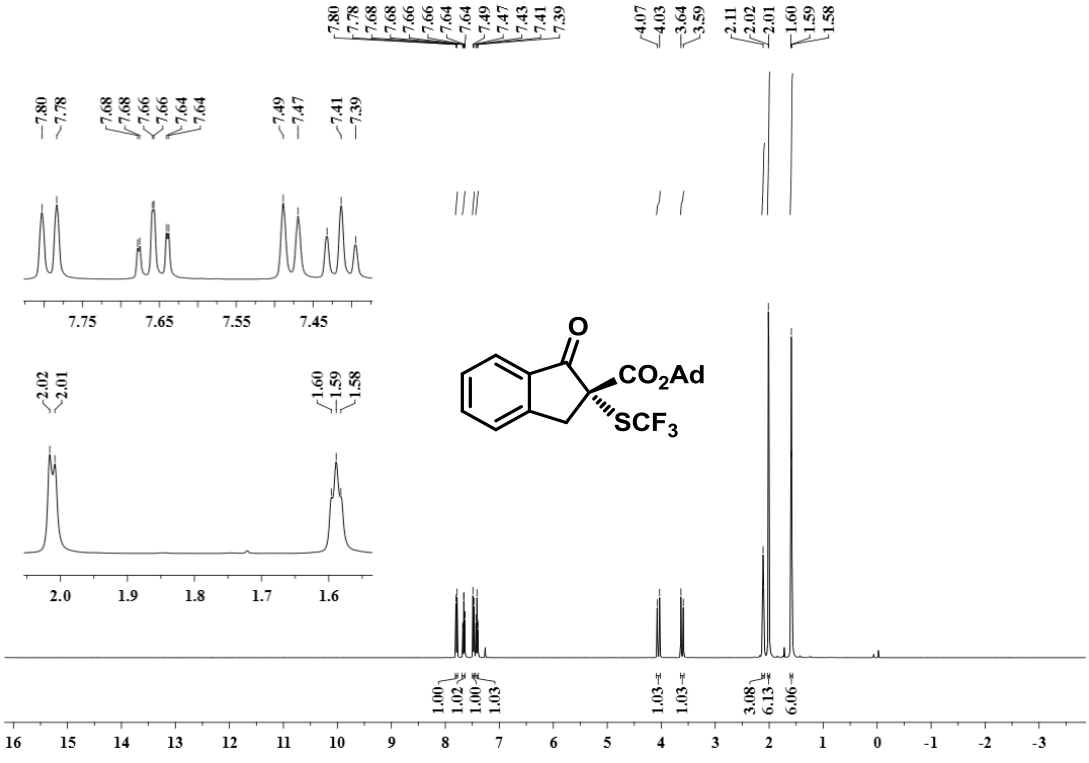
^{13}C NMR Spectrum for (R)-Isopropyl-1-oxo-2-((trifluoromethyl)thio)-2,3-dihydro-1*H*-indene-2-carboxylate 3c



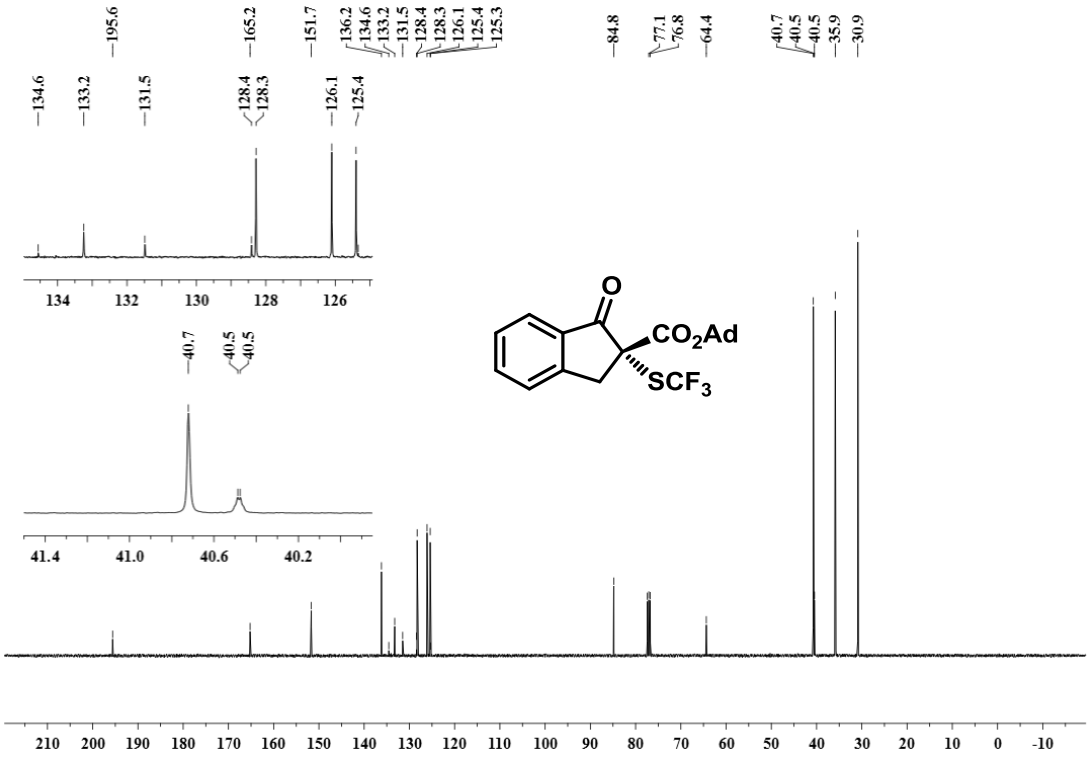
^{19}F NMR Spectrum for (R)-Isopropyl-1-oxo-2-((trifluoromethyl)thio)-2,3-dihydro-1*H*-indene-2-carboxylate 3c



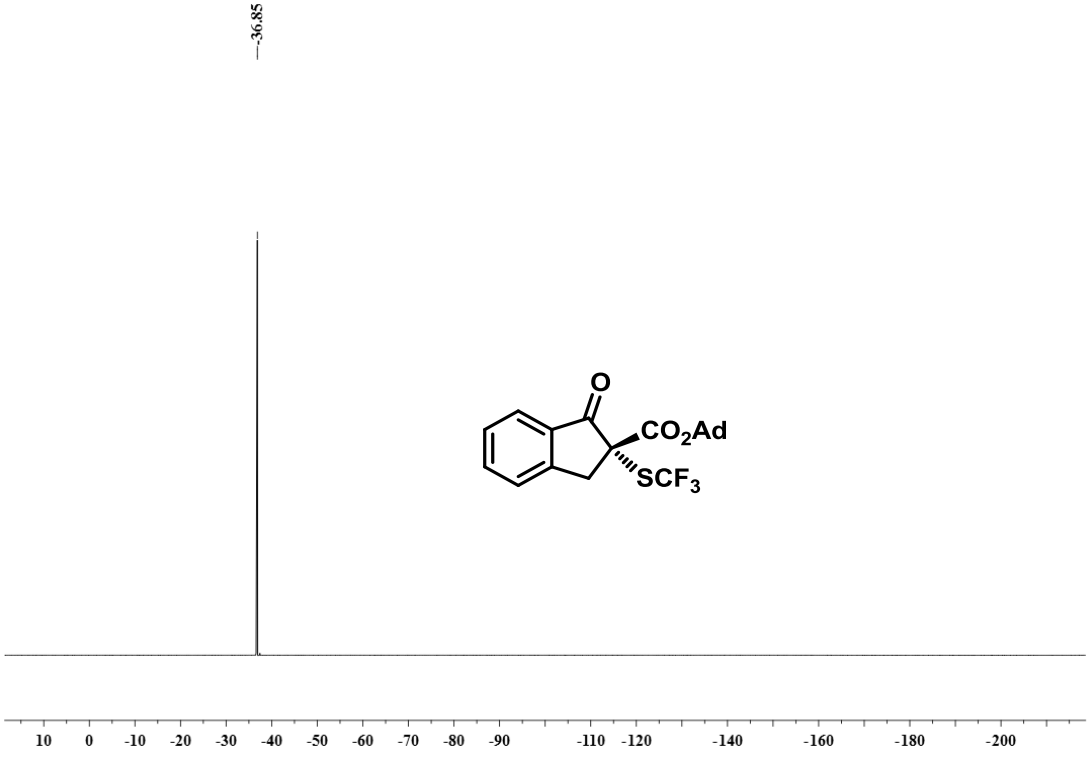
^{1}H NMR Spectrum for (R)-Adamantan-1-yl-1-oxo-2-((trifluoromethyl)thio)-2,3-dihydro-1*H*-indene-2-carboxylate 3d



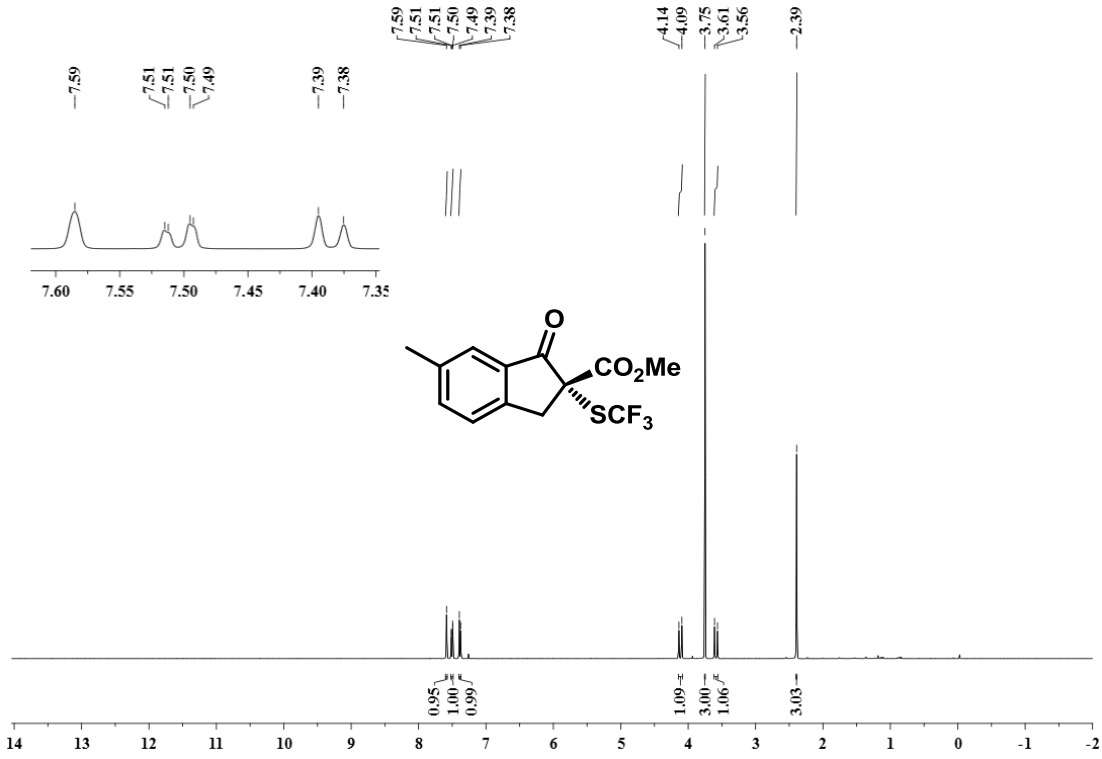
^{13}C NMR Spectrum for (R)-Adamantan-1-yl-1-oxo-2-((trifluoromethyl)thio)-2,3-dihydro-1*H*-indene-2-carboxylate 3d



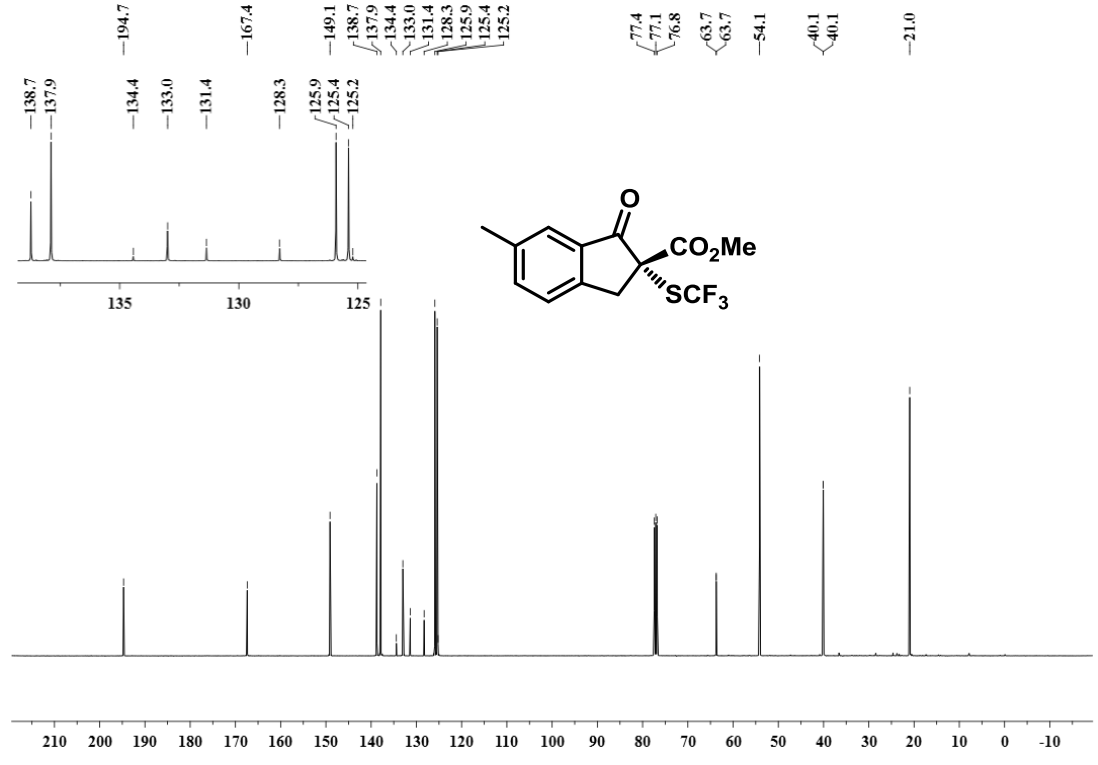
^{19}F NMR Spectrum for (R)-Adamantan-1-yl-1-oxo-2-((trifluoromethyl)thio)-2,3-dihydro-1*H*-indene-2-carboxylate 3d



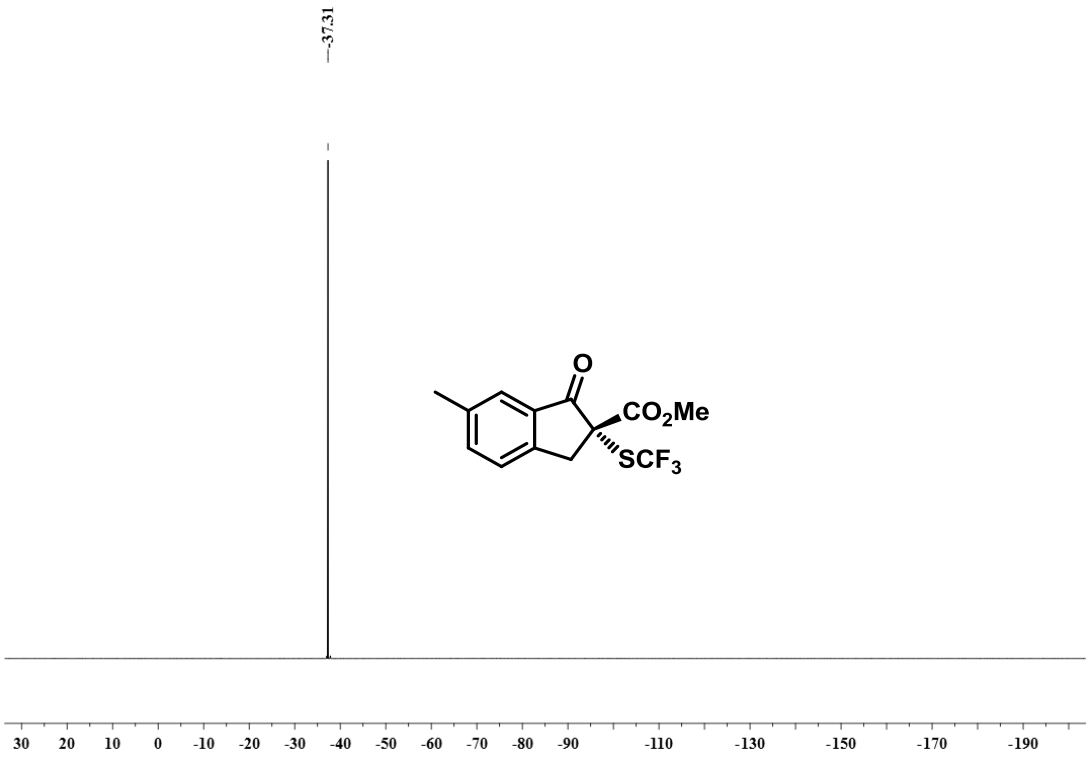
^{1}H NMR Spectrum for (R)-Methyl-6-methyl-1-oxo-2-((trifluoromethyl)thio)-2,3-dihydro-1*H*-indene-2-carboxylate 3e



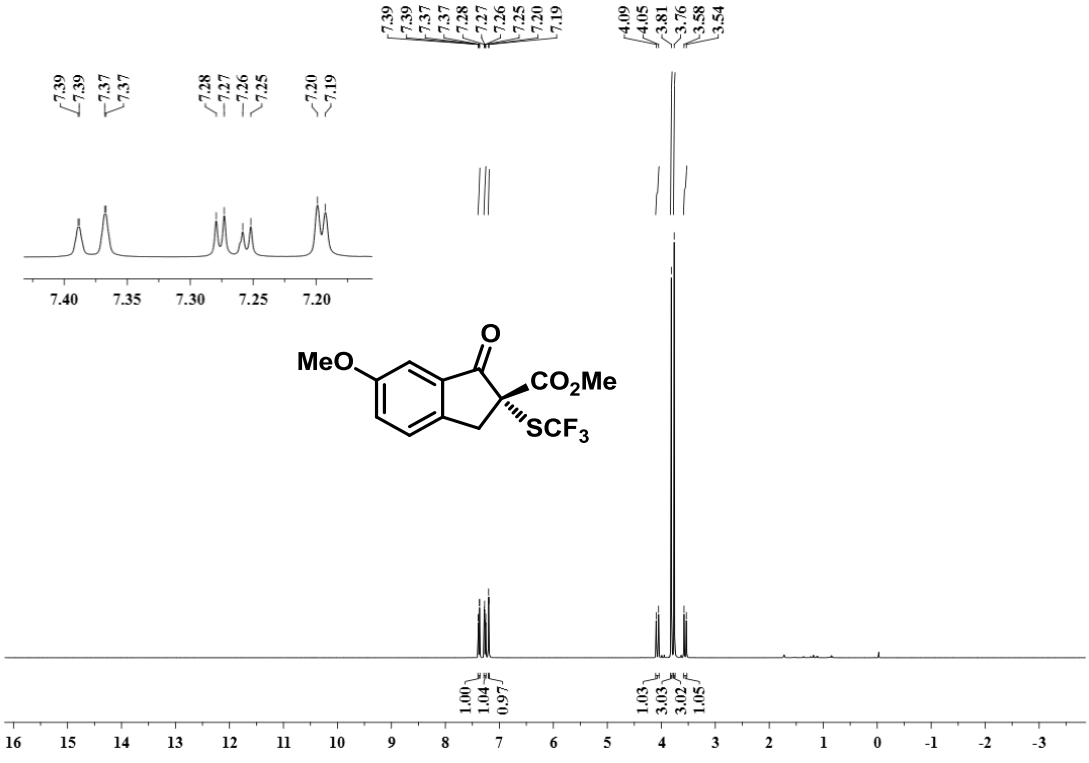
^{13}C NMR Spectrum for (R)-Methyl-6-methyl-1-oxo-2-((trifluoromethyl)thio)-2,3-dihydro-1*H*-indene-2-carboxylate 3e



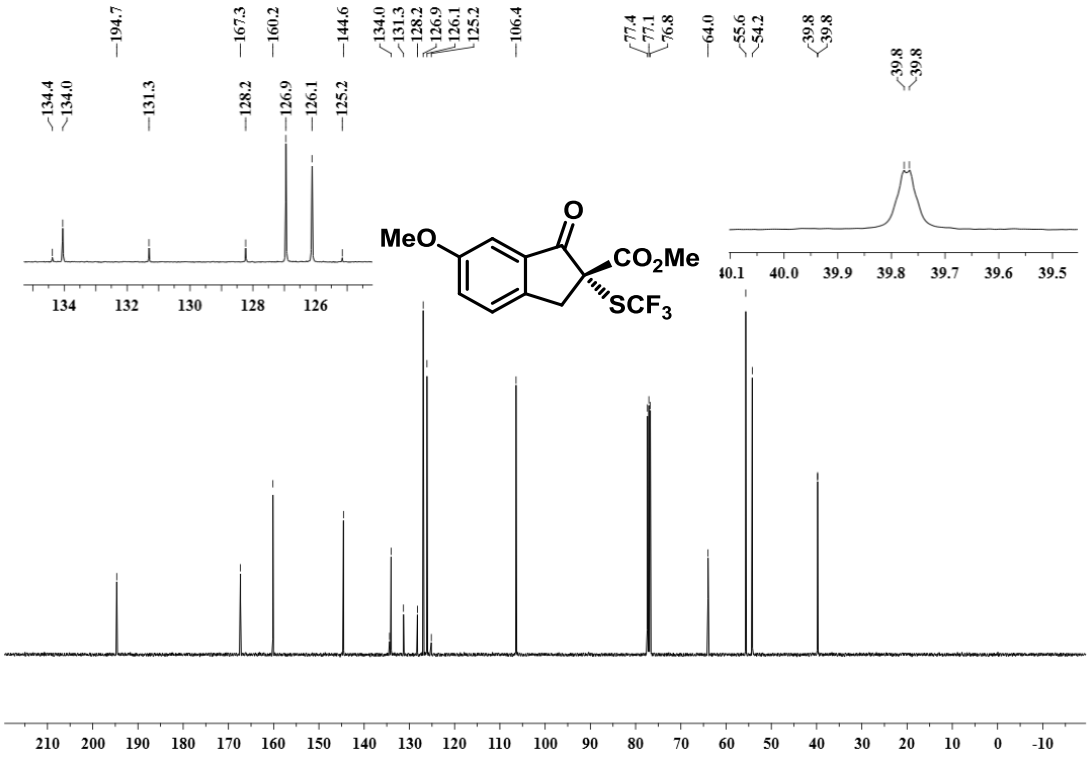
^{19}F NMR Spectrum for (R)-Methyl-6-methyl-1-oxo-2-((trifluoromethyl)thio)-2,3-dihydro-1*H*-indene-2-carboxylate 3e



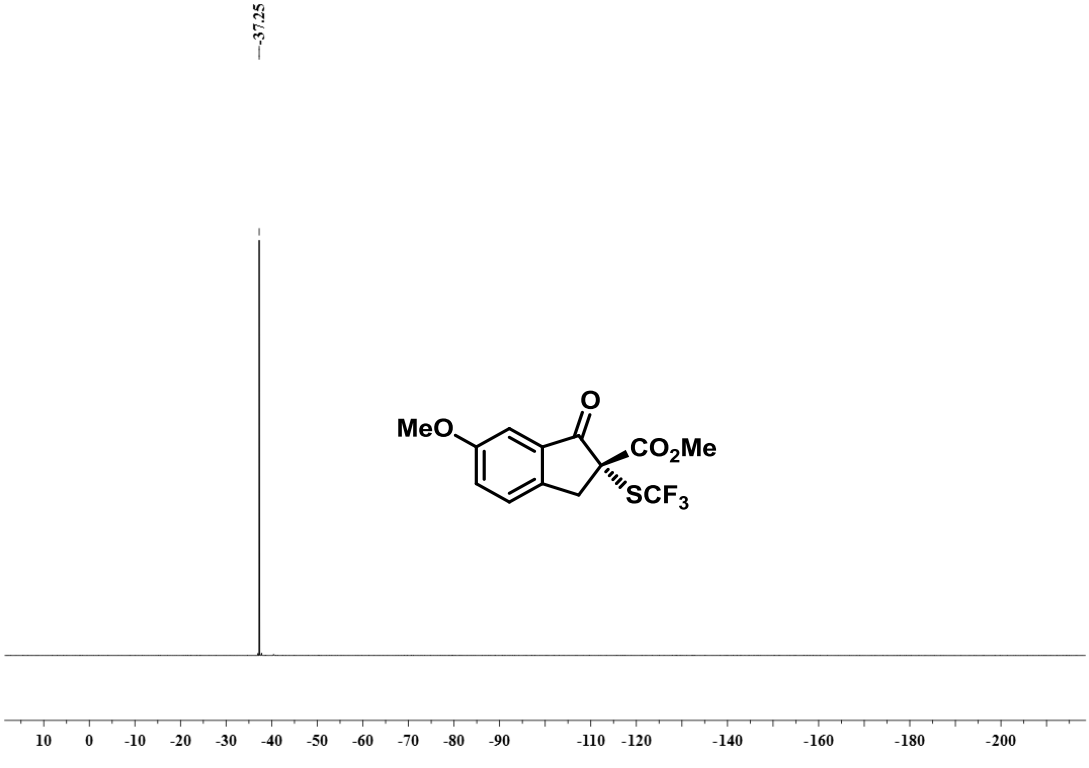
^{1}H NMR Spectrum for (R)-Methyl-6-methoxy-1-oxo-2-((trifluoromethyl)thio)-2,3-dihydro-1*H*-indene-2-carboxylate 3f



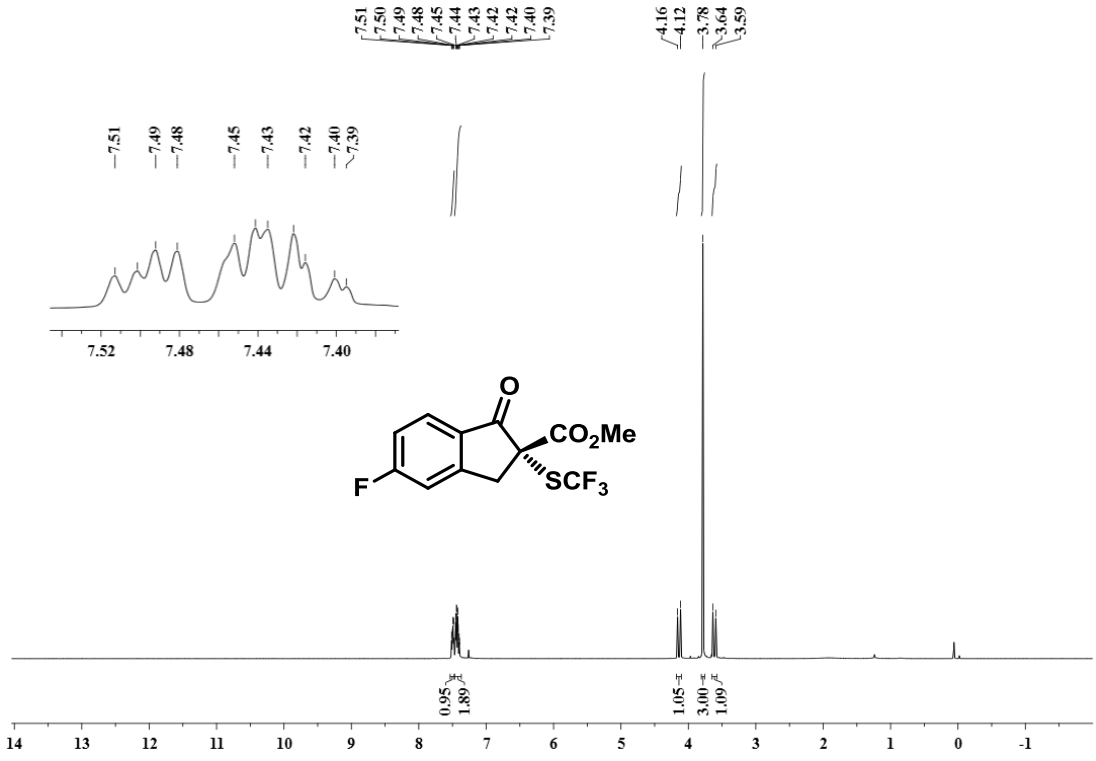
^{13}C NMR Spectrum for (R)-Methyl-6-methoxy-1-oxo-2-((trifluoromethyl)thio)-2,3-dihydro-1*H*-indene-2-carboxylate 3f



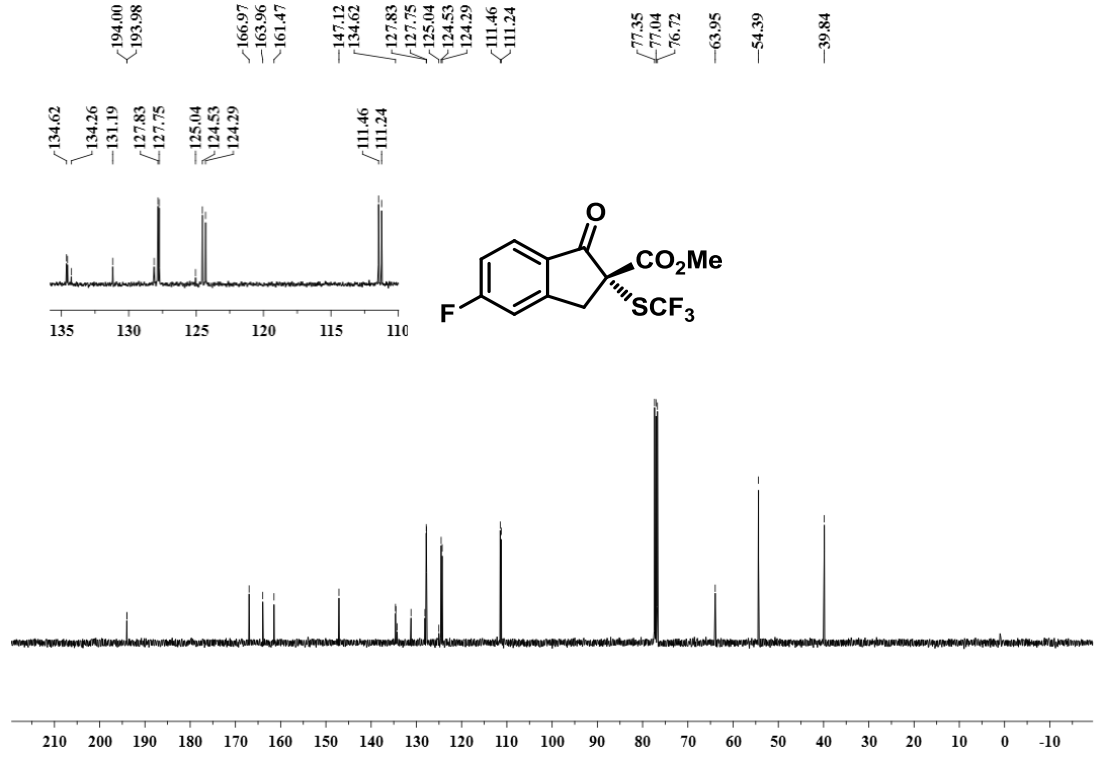
^{19}F NMR Spectrum for (R)-Methyl-6-methoxy-1-oxo-2-((trifluoromethyl)thio)-2,3-dihydro-1*H*-indene-2-carboxylate 3f



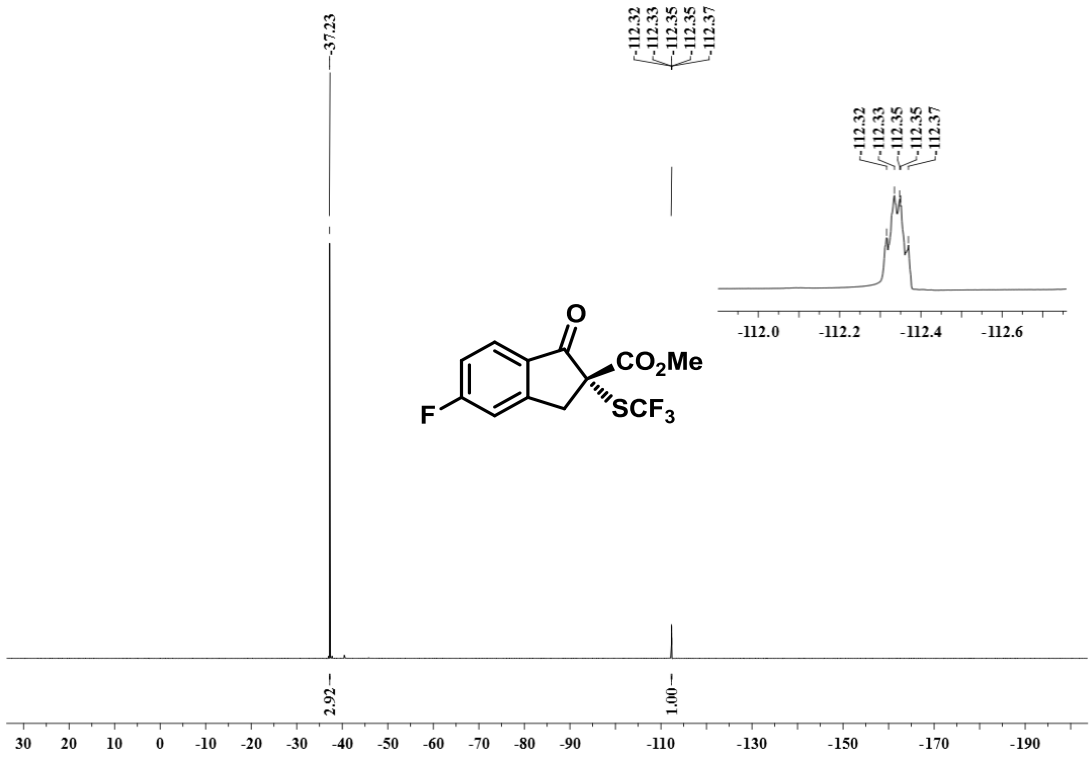
^{1}H NMR Spectrum for (R)-Methyl-5-fluoro-1-oxo-2-((trifluoromethyl)thio)-2,3-dihydro-1*H*-indene-2-carboxylate 3g



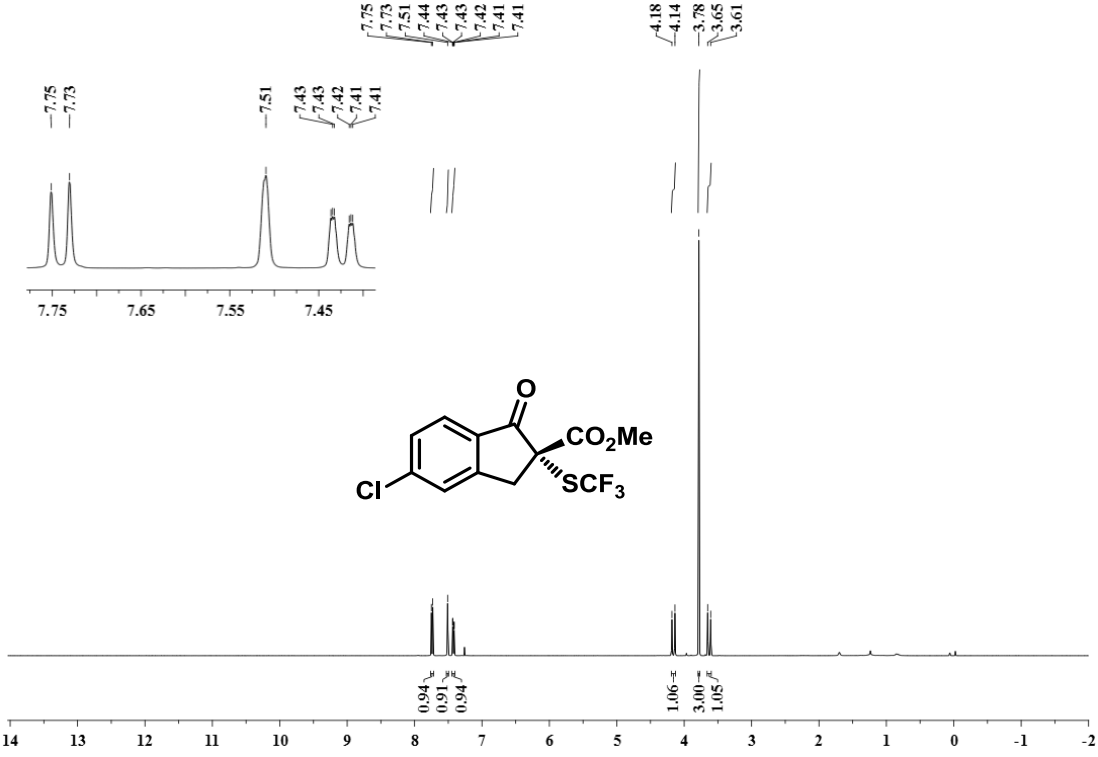
^{13}C NMR Spectrum for (R)-Methyl-5-fluoro-1-oxo-2-((trifluoromethyl)thio)-2,3-dihydro-1*H*-indene-2-carboxylate 3g



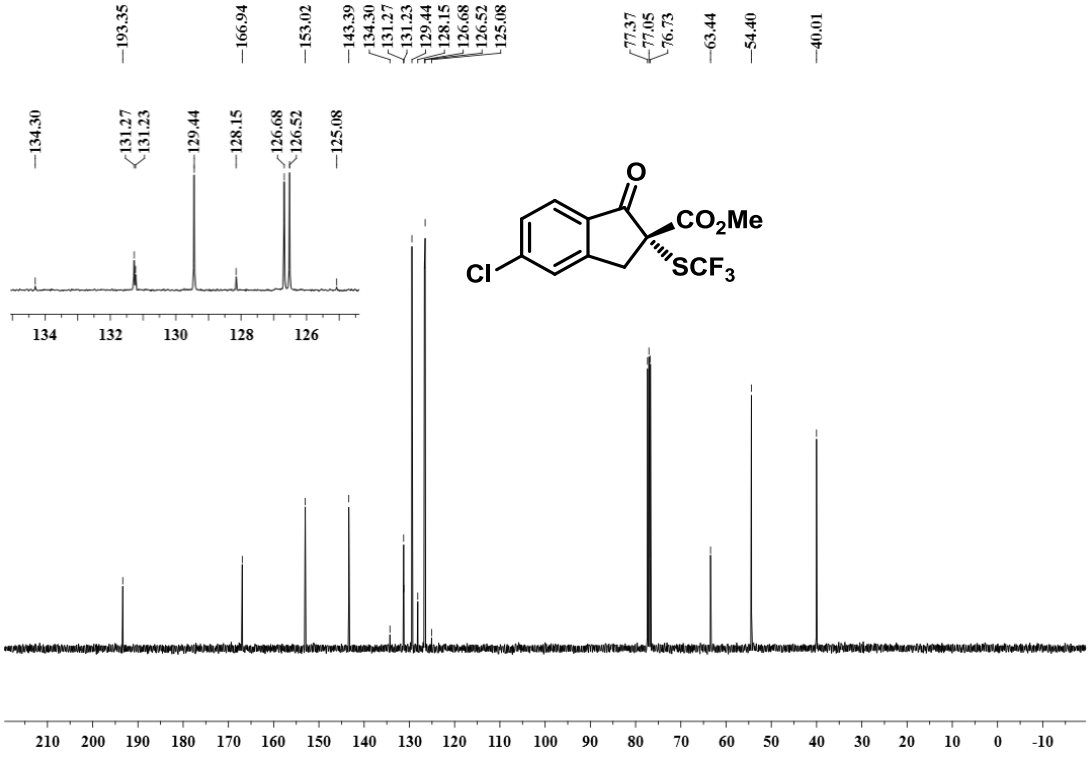
^{19}F NMR Spectrum for (R)-Methyl-5-fluoro-1-oxo-2-((trifluoromethyl)thio)-2,3-dihydro-1*H*-indene-2-carboxylate 3g



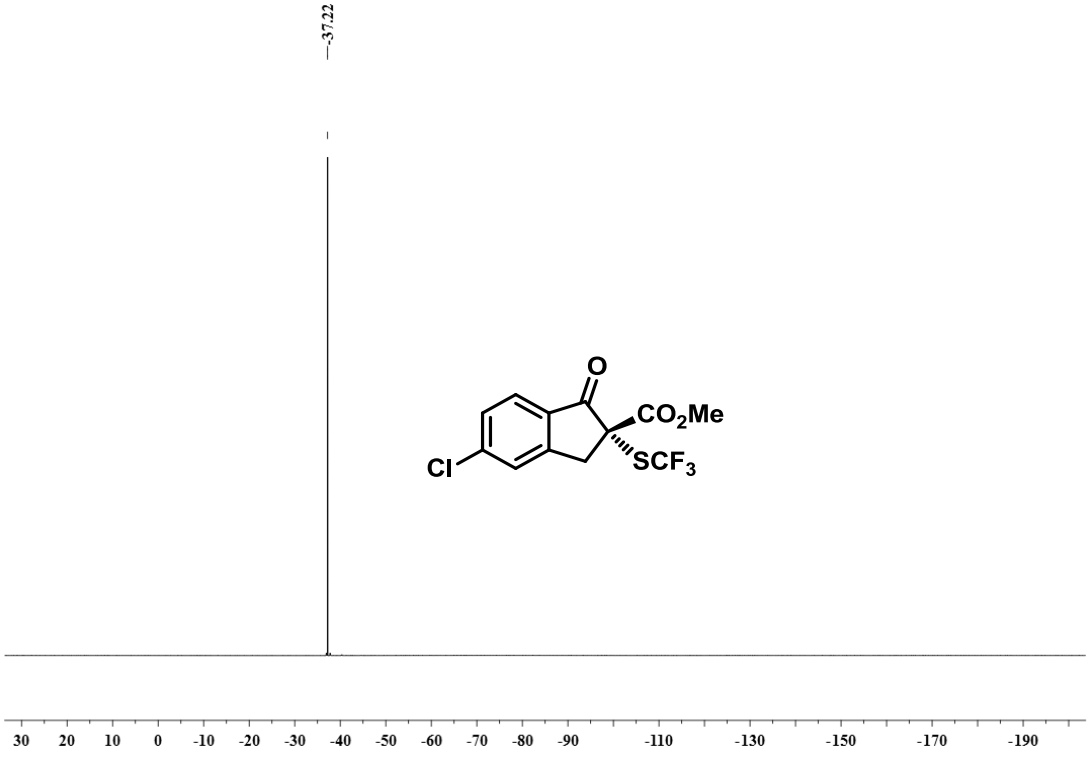
^{1}H NMR Spectrum for (R)-Methyl-5-chloro-1-oxo-2-((trifluoromethyl)thio)-2,3-dihydro-1*H*-indene-2-carboxylate 3h



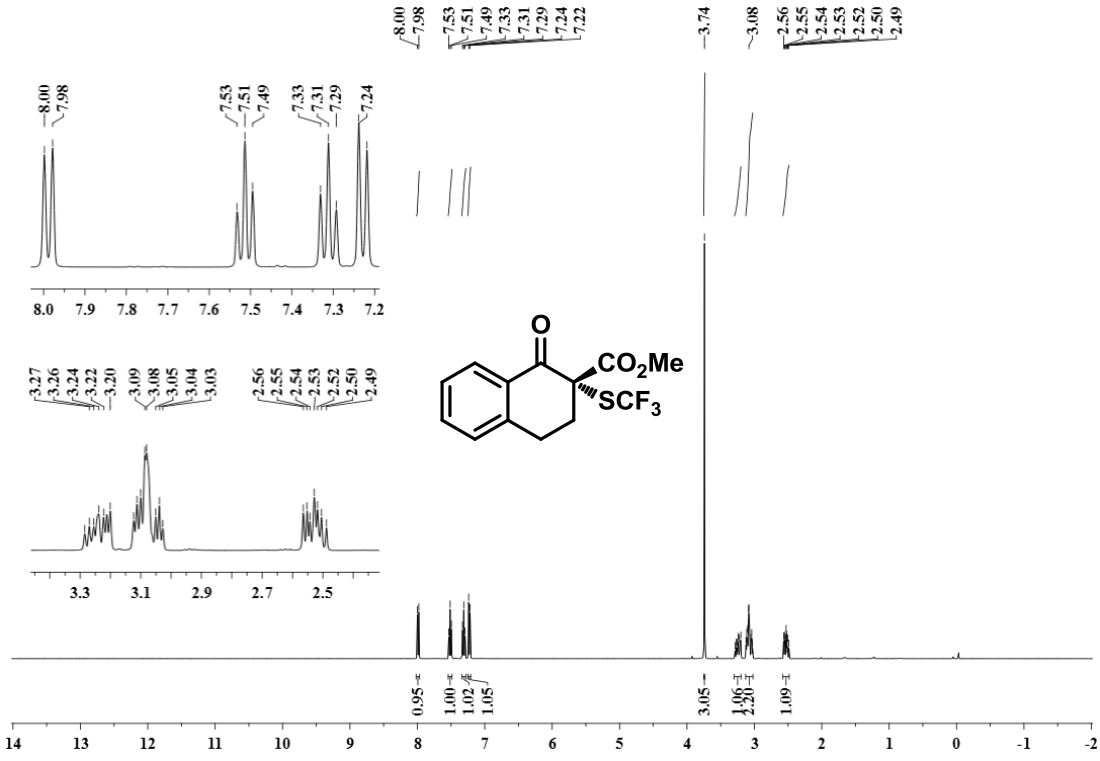
^{13}C NMR Spectrum for (R)-Methyl-5-chloro-1-oxo-2-((trifluoromethyl)thio)-2,3-dihydro-1*H*-indene-2-carboxylate 3h



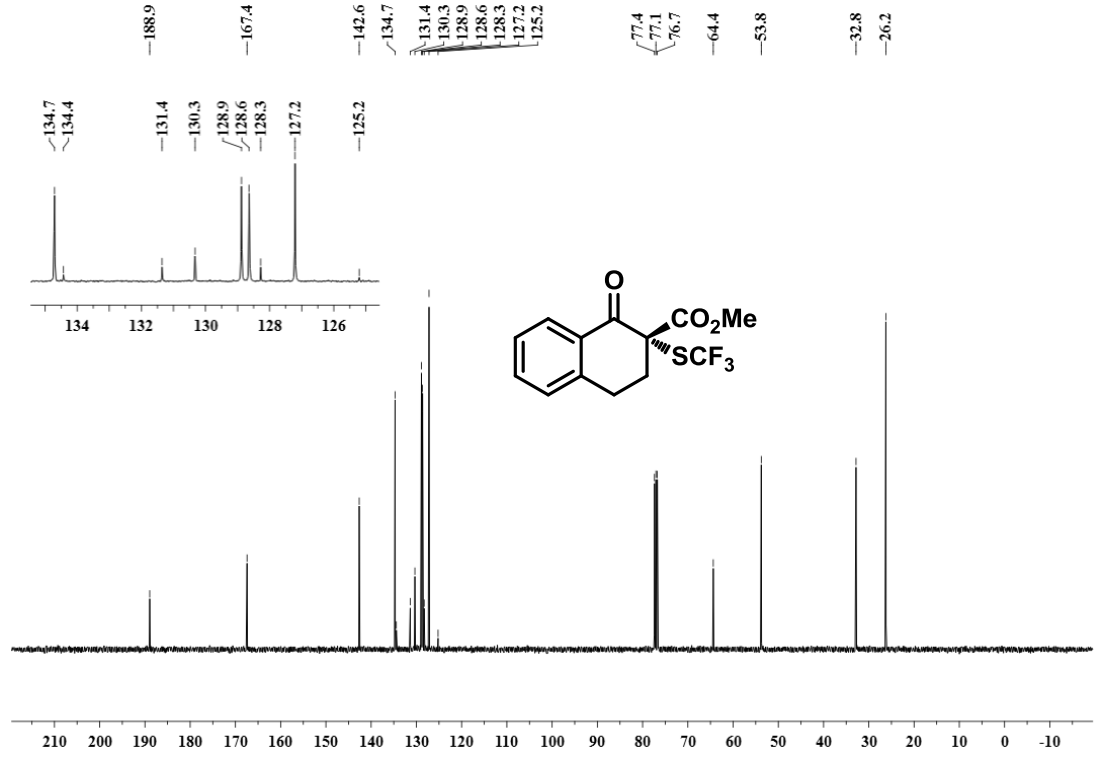
^{19}F NMR Spectrum for (R)-Methyl-5-chloro-1-oxo-2-((trifluoromethyl)thio)-2,3-dihydro-1*H*-indene-2-carboxylate 3h



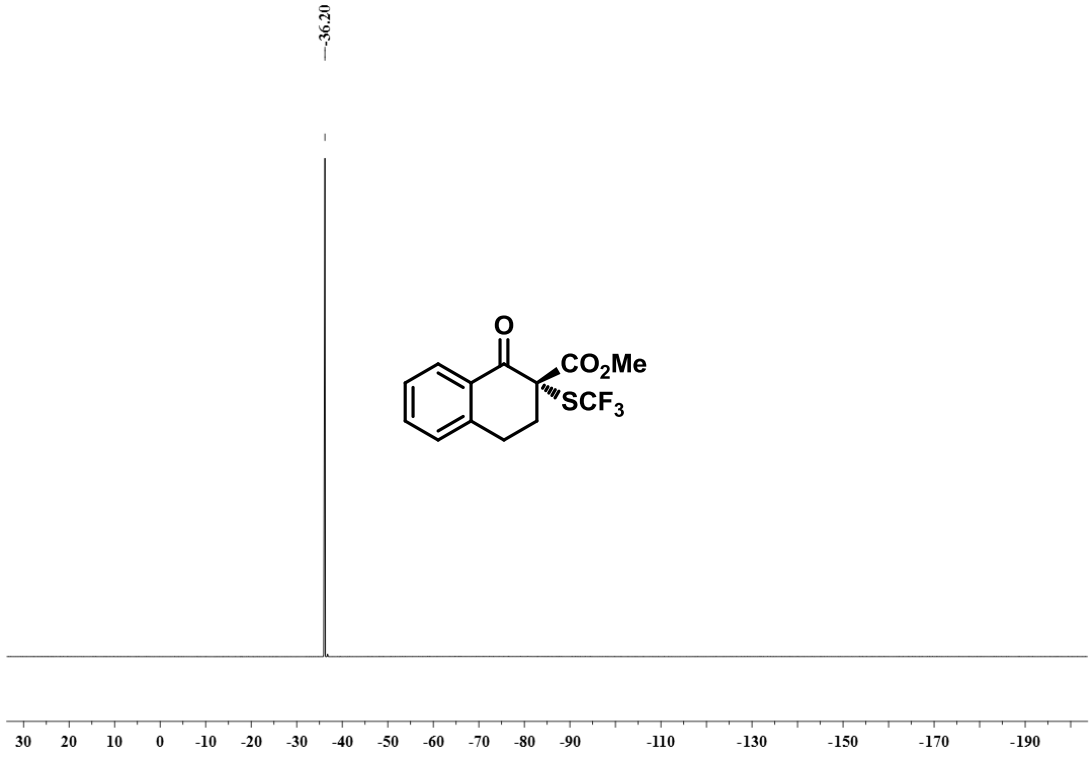
^{1}H NMR Spectrum for (R)-Methyl-1-oxo-2-((trifluoromethyl)thio)-1,2,3,4-tetrahydronaphthalene-2-carboxylate 3i



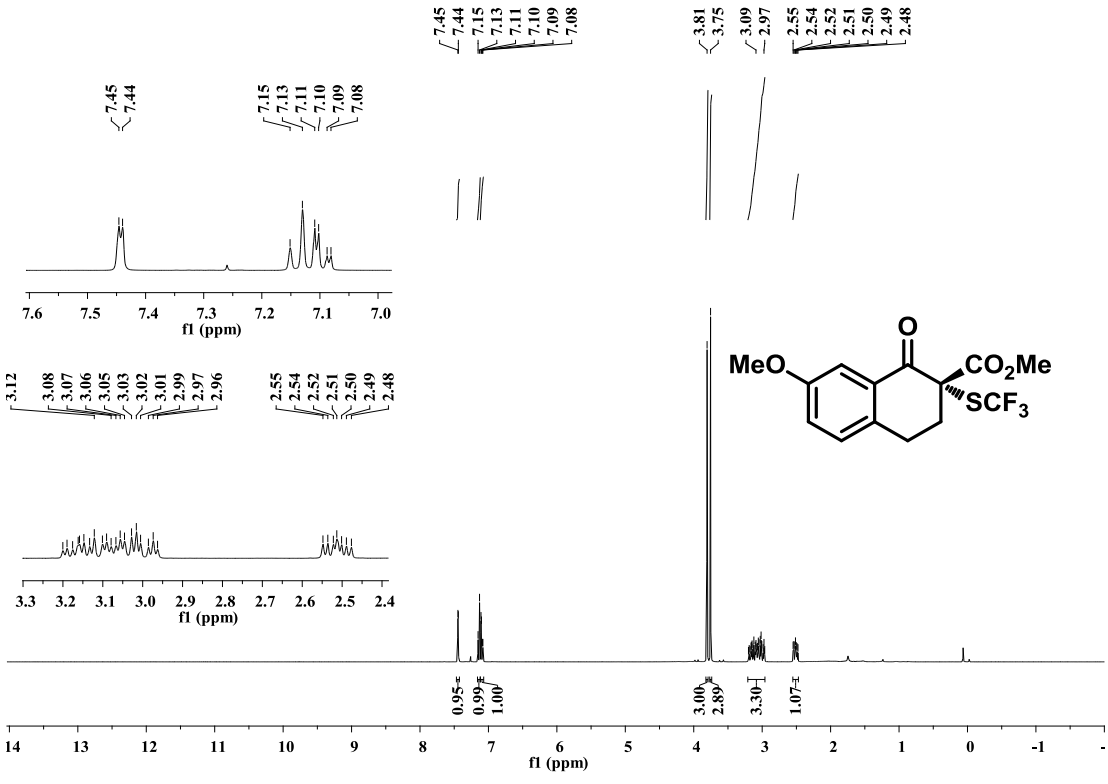
^{13}C NMR Spectrum for (R)-Methyl-1-oxo-2-((trifluoromethyl)thio)-1,2,3,4-tetrahydronaphthalene-2-carboxylate 3i



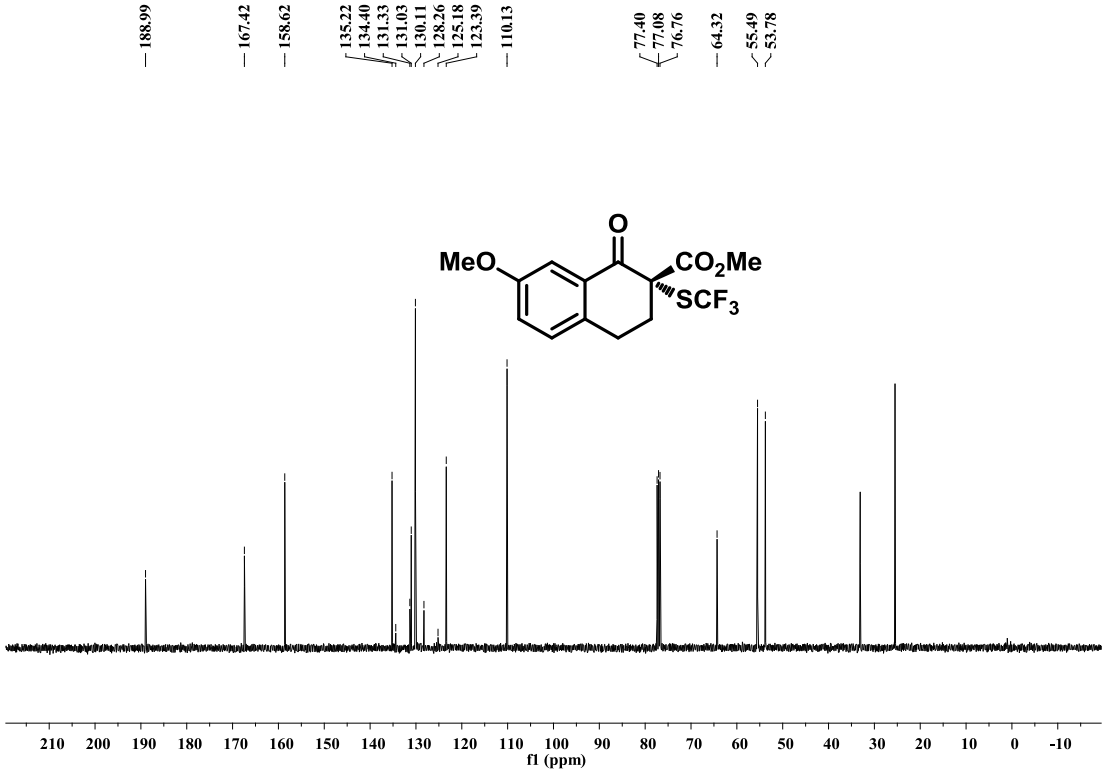
^{19}F NMR Spectrum for (R)-Methyl-1-oxo-2-((trifluoromethyl)thio)-1,2,3,4-tetrahydronaphthalene-2-carboxylate 3i



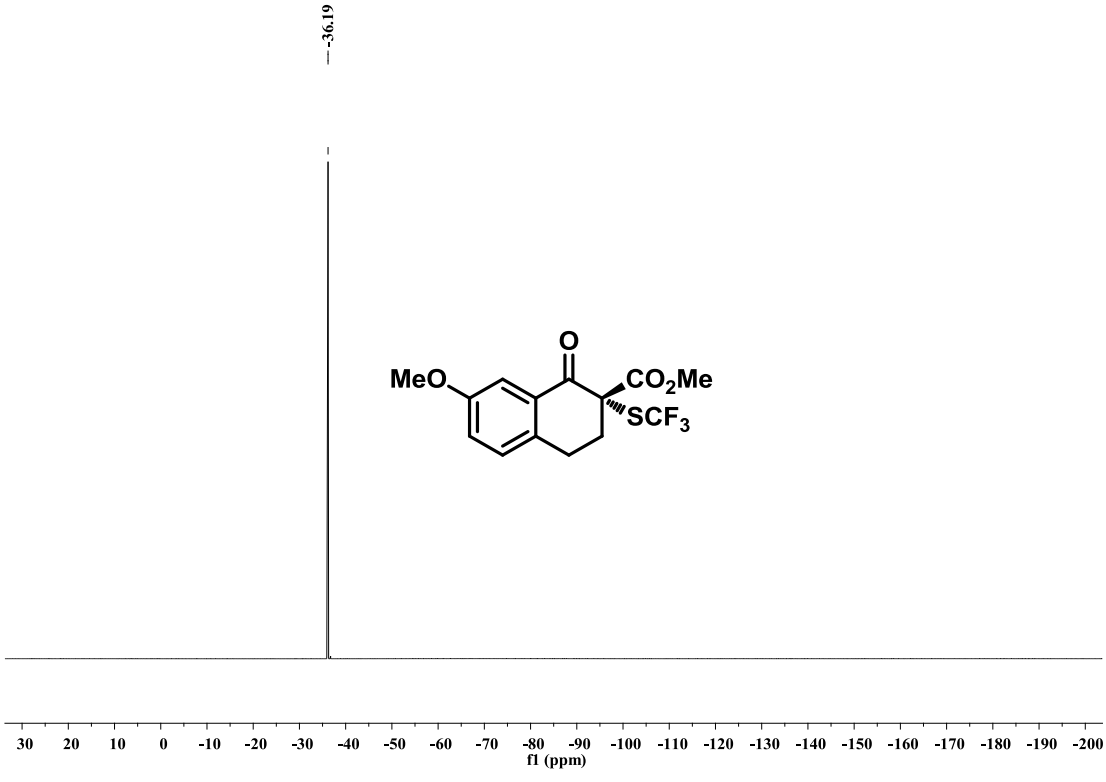
^{1}H NMR Spectrum for (R)-Methyl-7-methoxy-1-oxo-2-((trifluoromethyl)thio)-1,2,3,4-tetrahydronaphthalene-2-carboxylate 3j



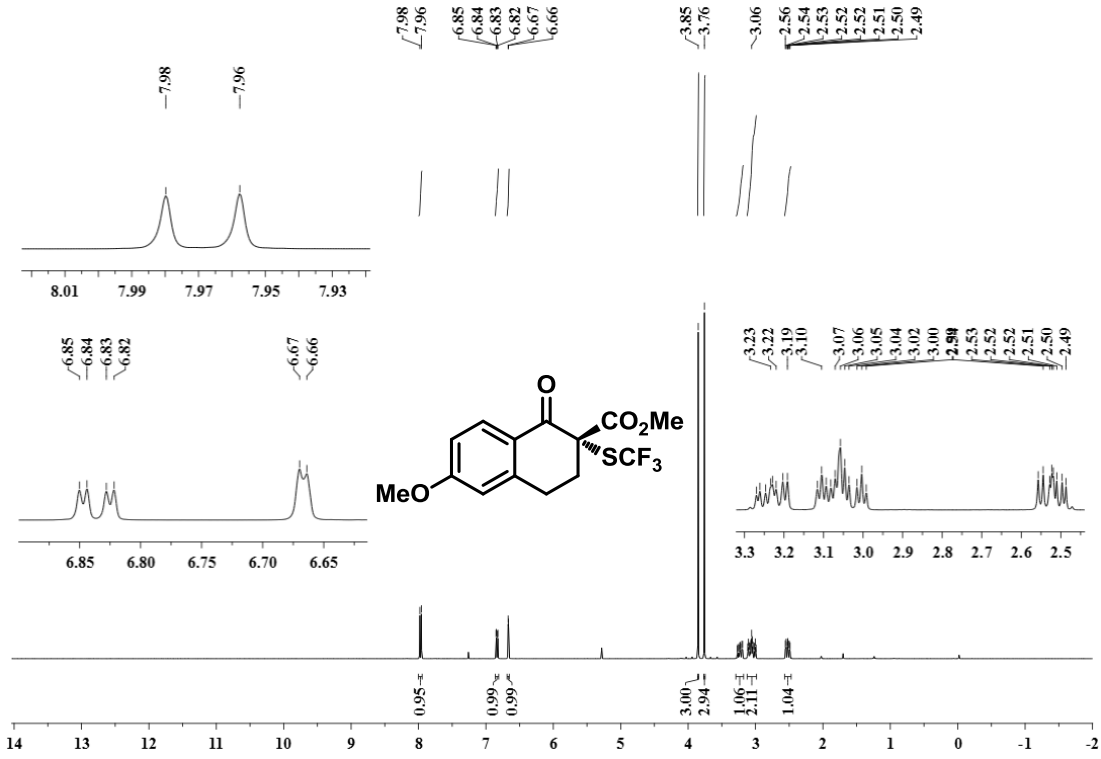
^{13}C NMR Spectrum for (R)-Methyl-7-methoxy-1-oxo-2-((trifluoromethyl)thio)-1,2,3,4-tetrahydronaphthalene-2-carboxylate 3j



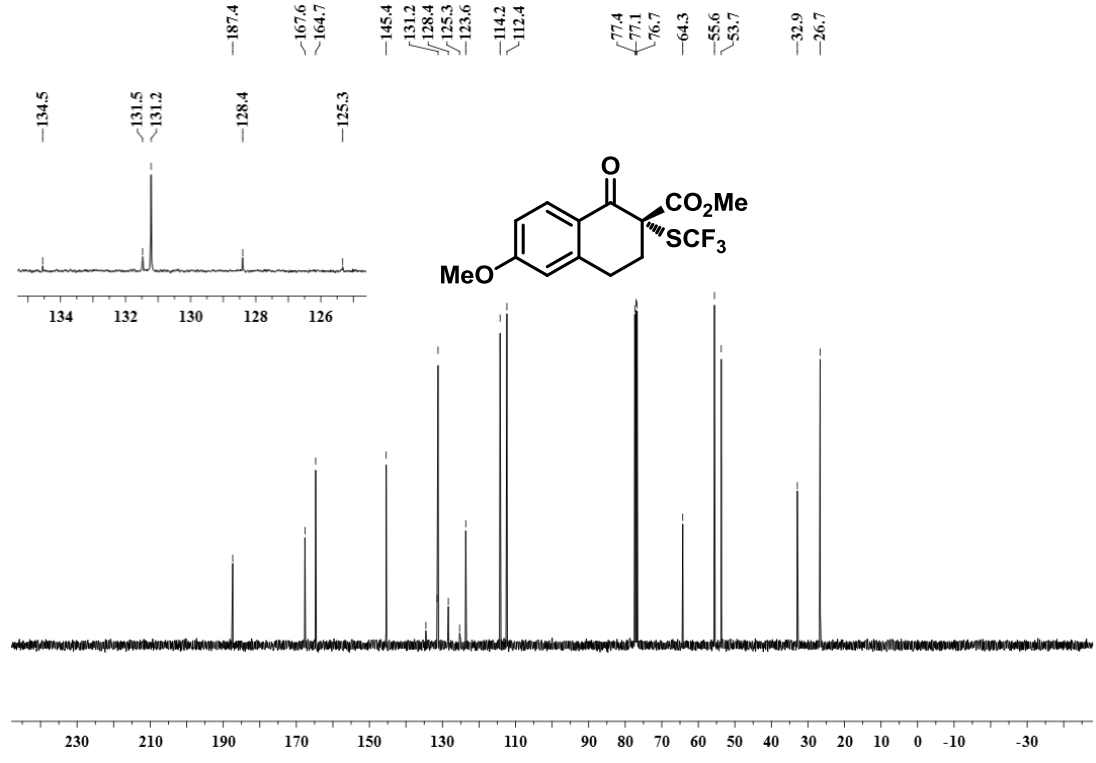
^{19}F NMR Spectrum for (R)-Methyl-7-methoxy-1-oxo-2-((trifluoromethyl)thio)-1,2,3,4-tetrahydronaphthalene-2-carboxylate 3j



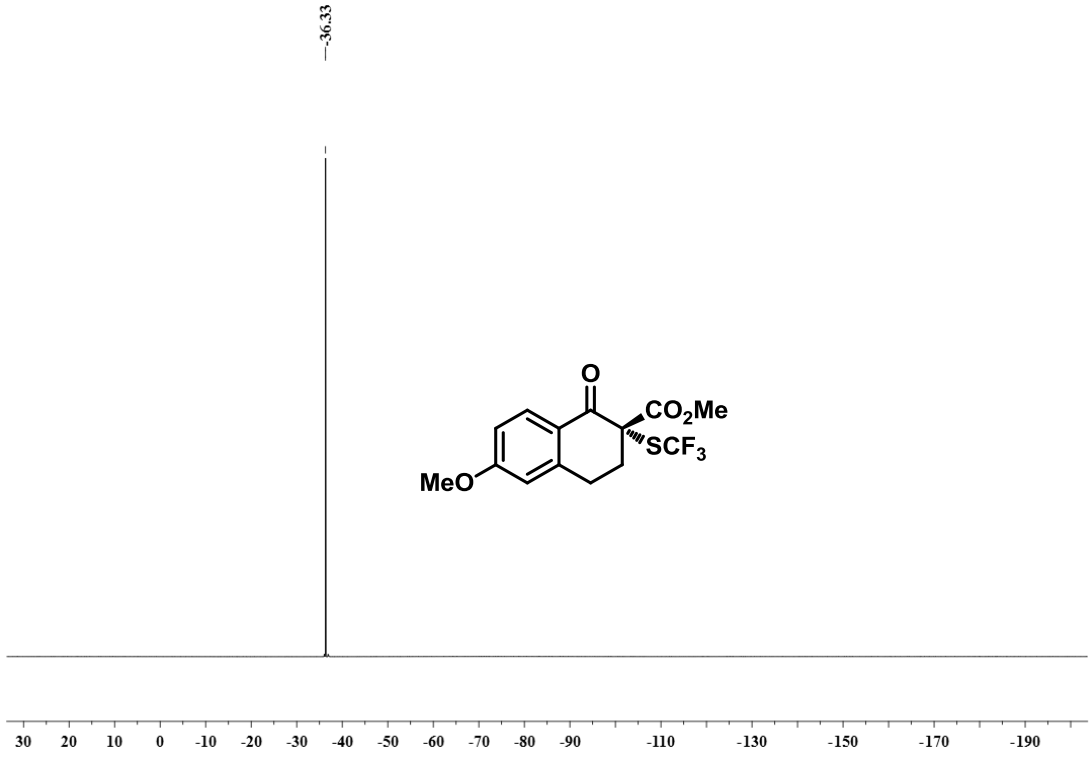
^{1}H NMR Spectrum for (R)-Methyl-6-methoxy-1-oxo-2-((trifluoromethyl)thio)-1,2,3,4-tetrahydronaphthalene-2-carboxylate 3k



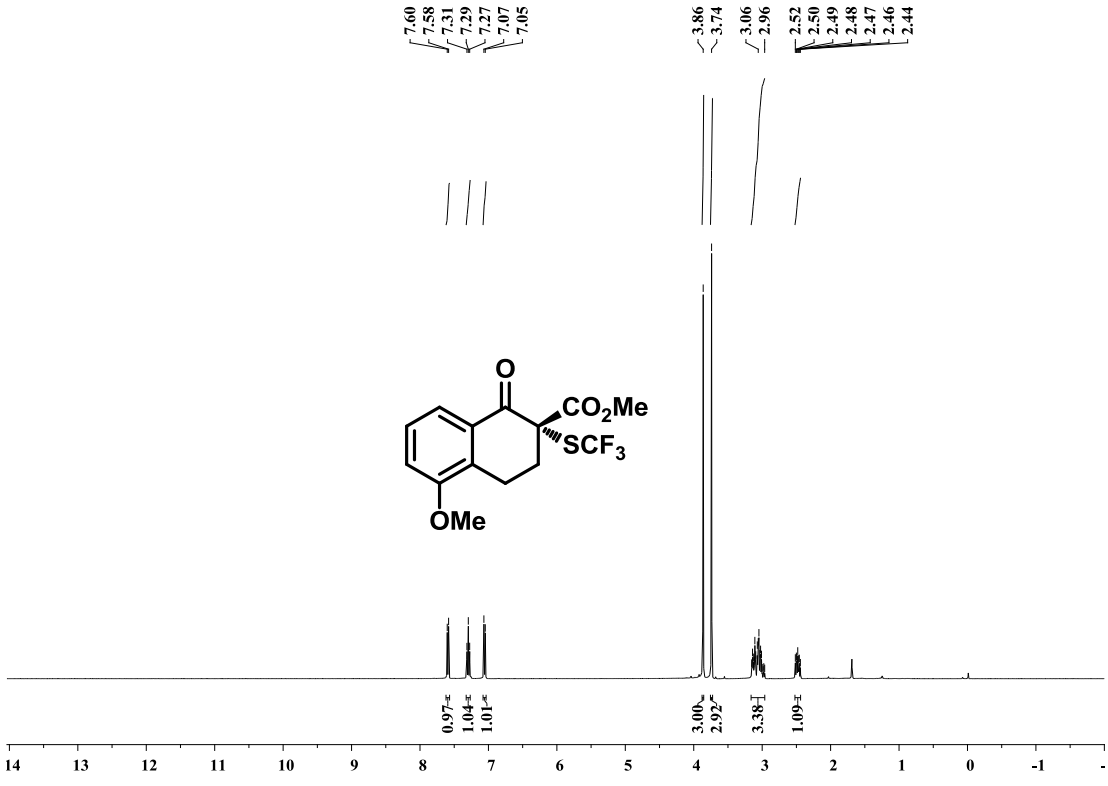
^{13}C NMR Spectrum for (R)-Methyl-6-methoxy-1-oxo-2-((trifluoromethyl)thio)-1,2,3,4-tetrahydronaphthalene-2-carboxylate 3k



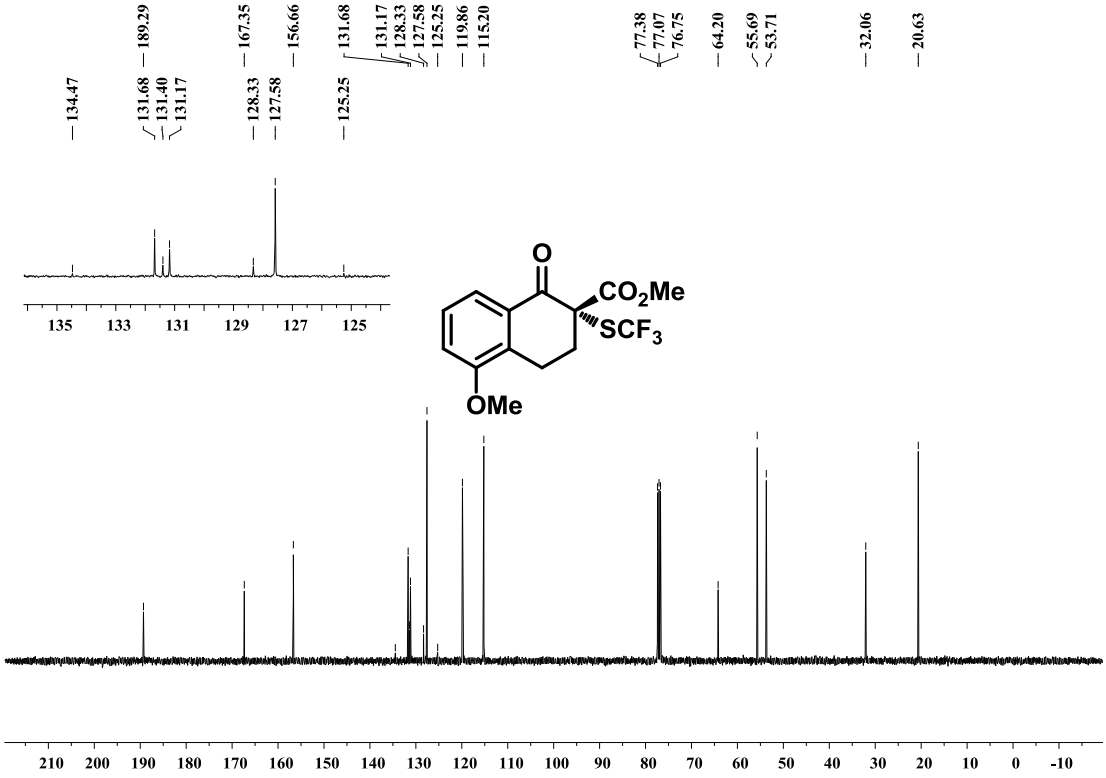
^{19}F NMR Spectrum for (R)-Methyl-6-methoxy-1-oxo-2-((trifluoromethyl)thio)-1,2,3,4-tetrahydronaphthalene-2-carboxylate 3k



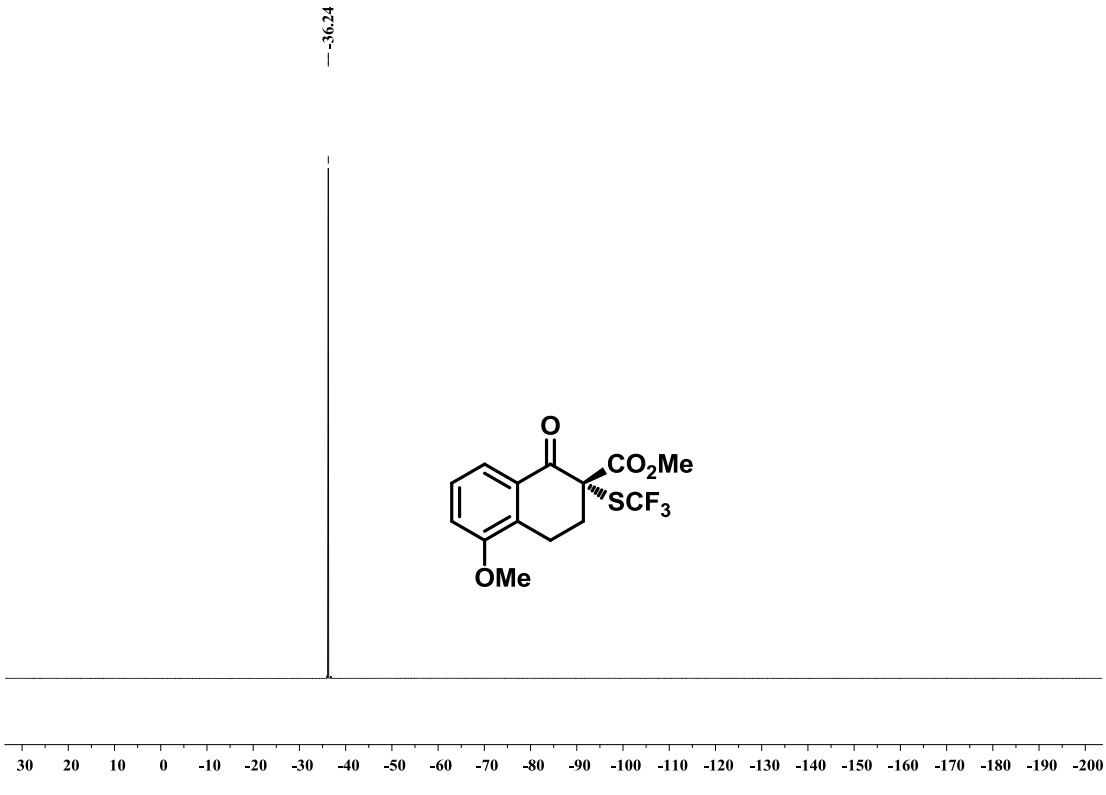
^{1}H NMR Spectrum for (R)-Methyl-5-methoxy-1-oxo-2-((trifluoromethyl)thio)-1,2,3,4-tetrahydronaphthalene-2-carboxylate 3l



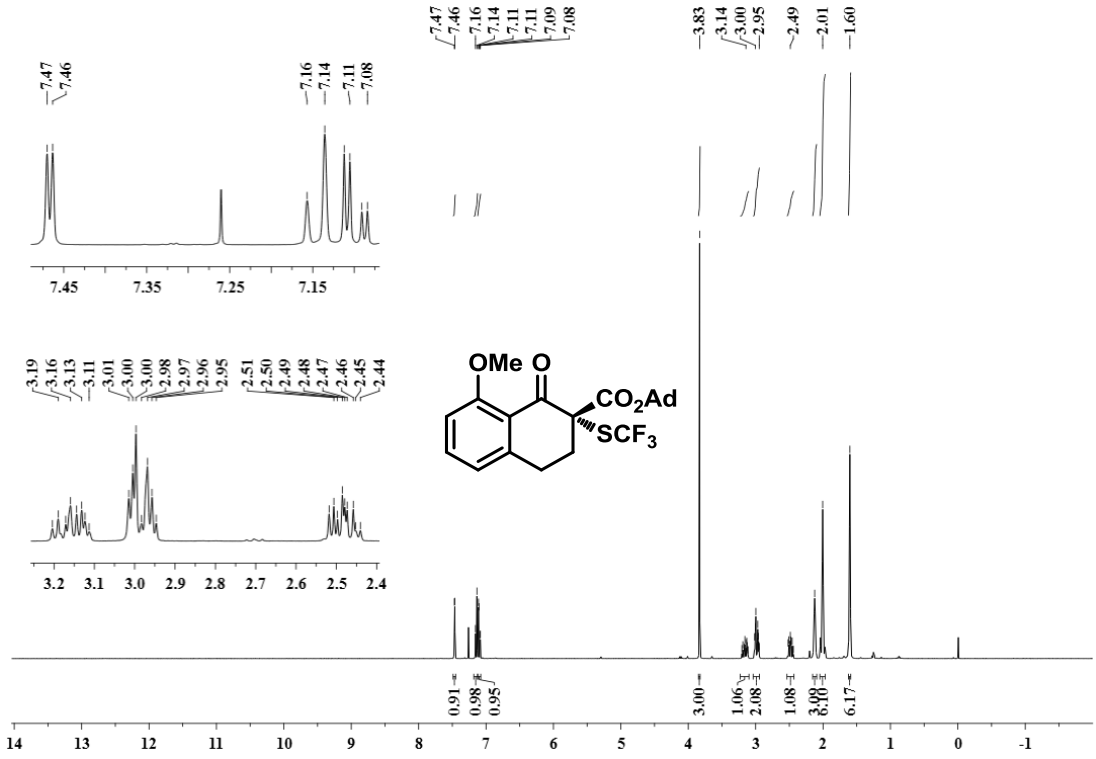
^{13}C NMR Spectrum for (R)-Methyl-5-methoxy-1-oxo-2-((trifluoromethyl)thio)-1,2,3,4-tetrahydronaphthalene-2-carboxylate 3l



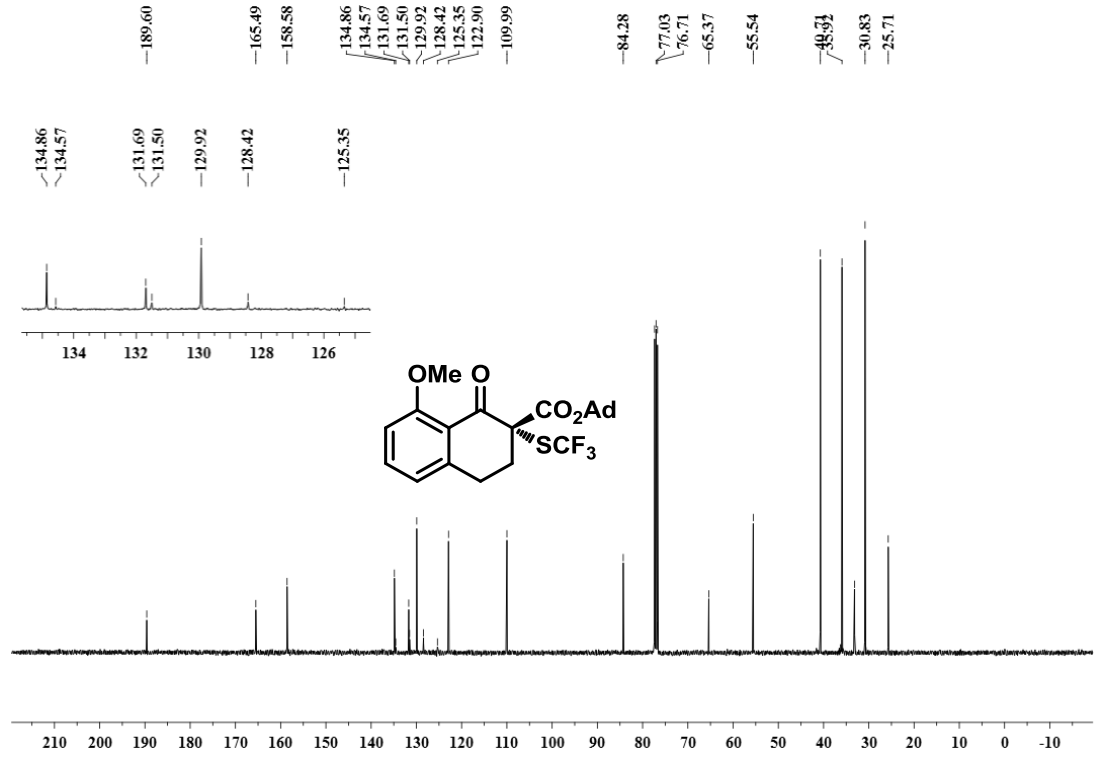
^{19}F NMR Spectrum for (R)-Methyl-5-methoxy-1-oxo-2-((trifluoromethyl)thio)-1,2,3,4-tetrahydronaphthalene-2-carboxylate 3l



^{1}H NMR Spectrum for (R)-Adamantan-1-yl-8-methoxy-1-oxo-2-((trifluoromethyl)thio)-1,2,3,4-tetrahydronaphthalene-2-carboxylate 3m

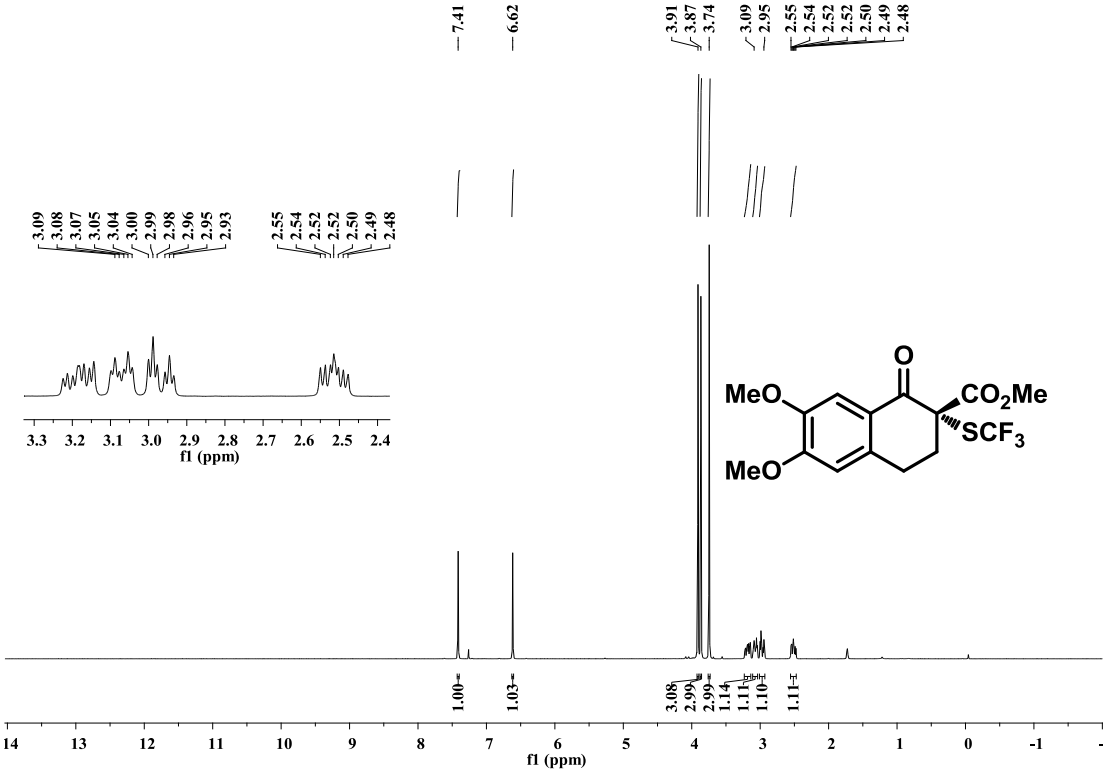


^{13}C NMR Spectrum for (R)-Adamantan-1-yl-8-methoxy-1-oxo-2-((trifluoromethyl)thio)-1,2,3,4-tetrahydronaphthalene-2-carboxylate 3m

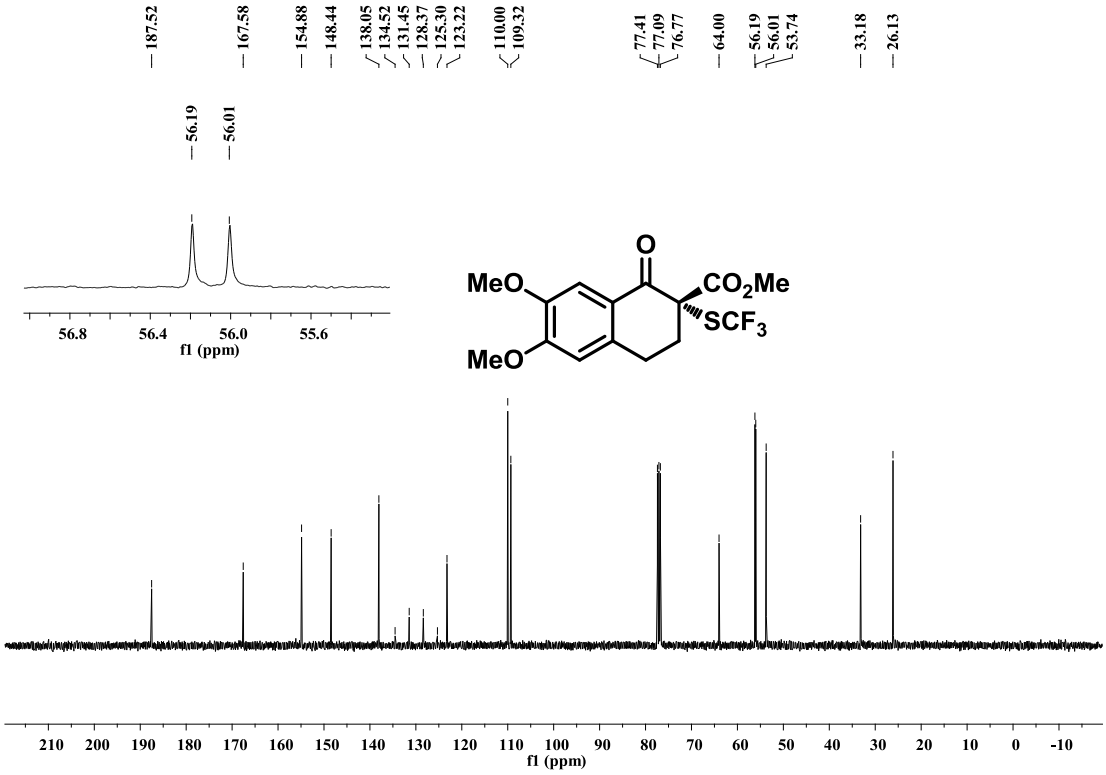


^{19}F NMR Spectrum for (R)-Adamantan-1-yl-8-methoxy-1-oxo-2-((trifluoromethyl)thio)-1,2,3,4-tetrahydronaphthalene-2-carboxylate 3m

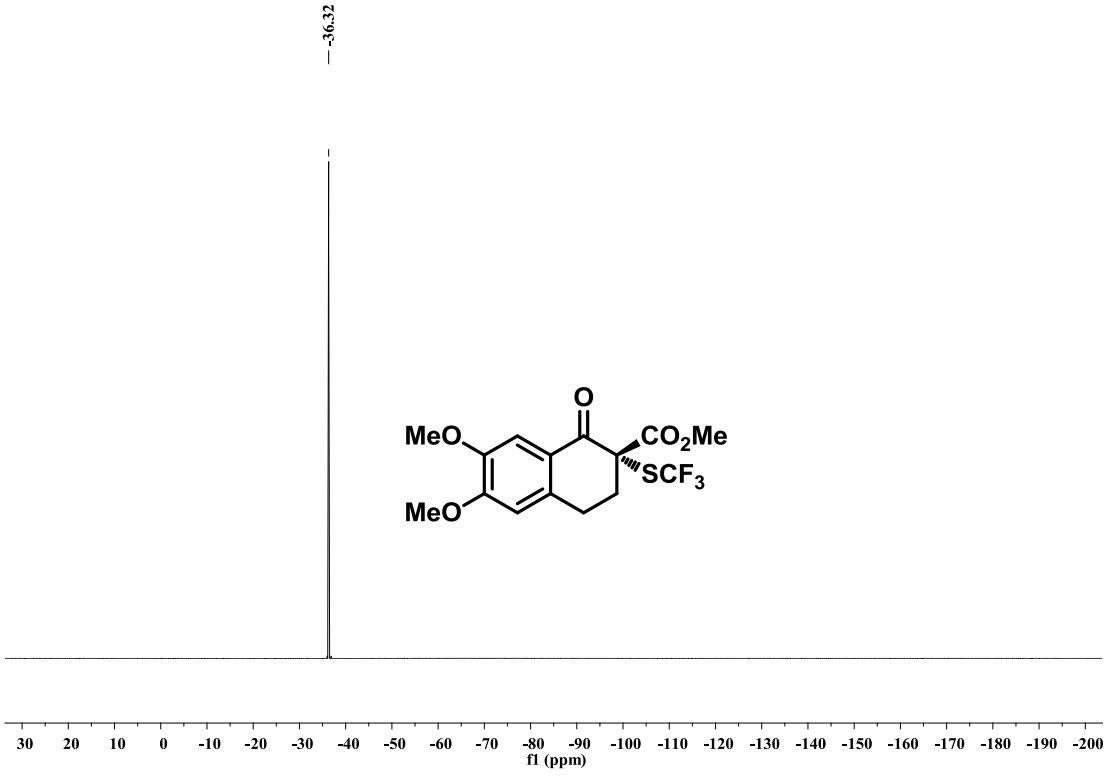
^{1}H NMR Spectrum for (R)-Methyl-6,7-dimethoxy-1-oxo-2-((trifluoromethyl)thio)-1,2,3,4-tetrahydronaphthalene-2-carboxylate 3n



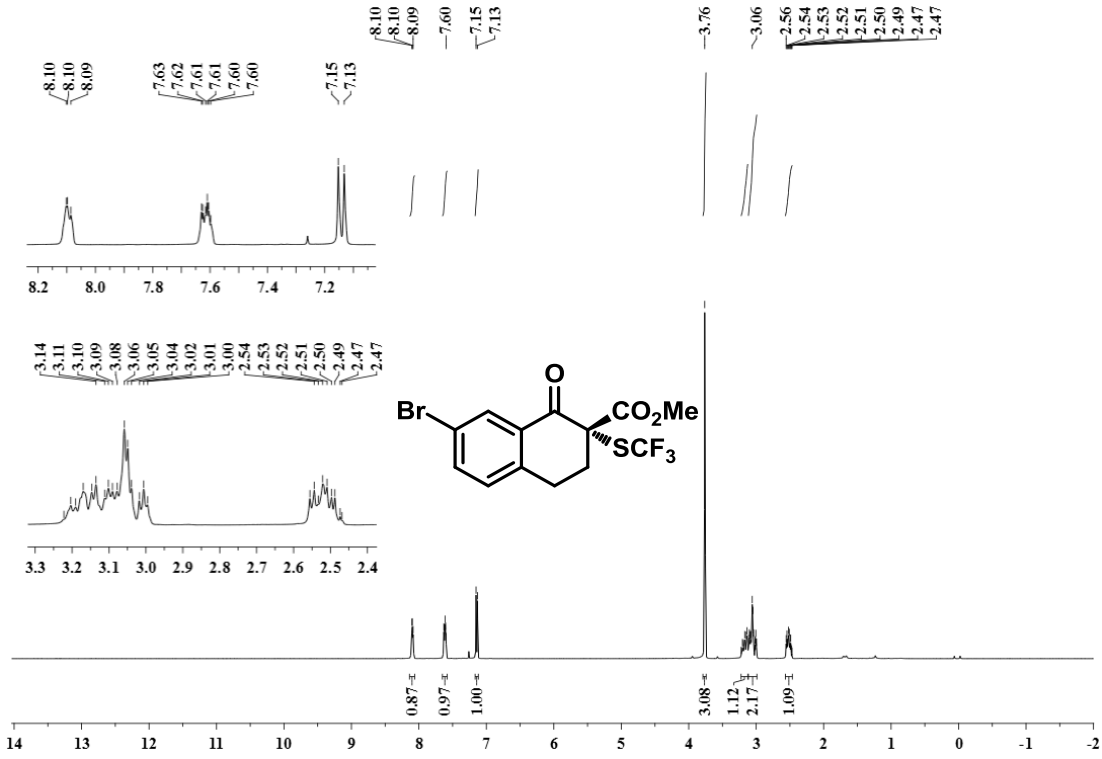
^{13}C NMR Spectrum for (R)-Methyl-6,7-dimethoxy-1-oxo-2-((trifluoromethyl)thio)-1,2,3,4-tetrahydronaphthalene-2-carboxylate 3n



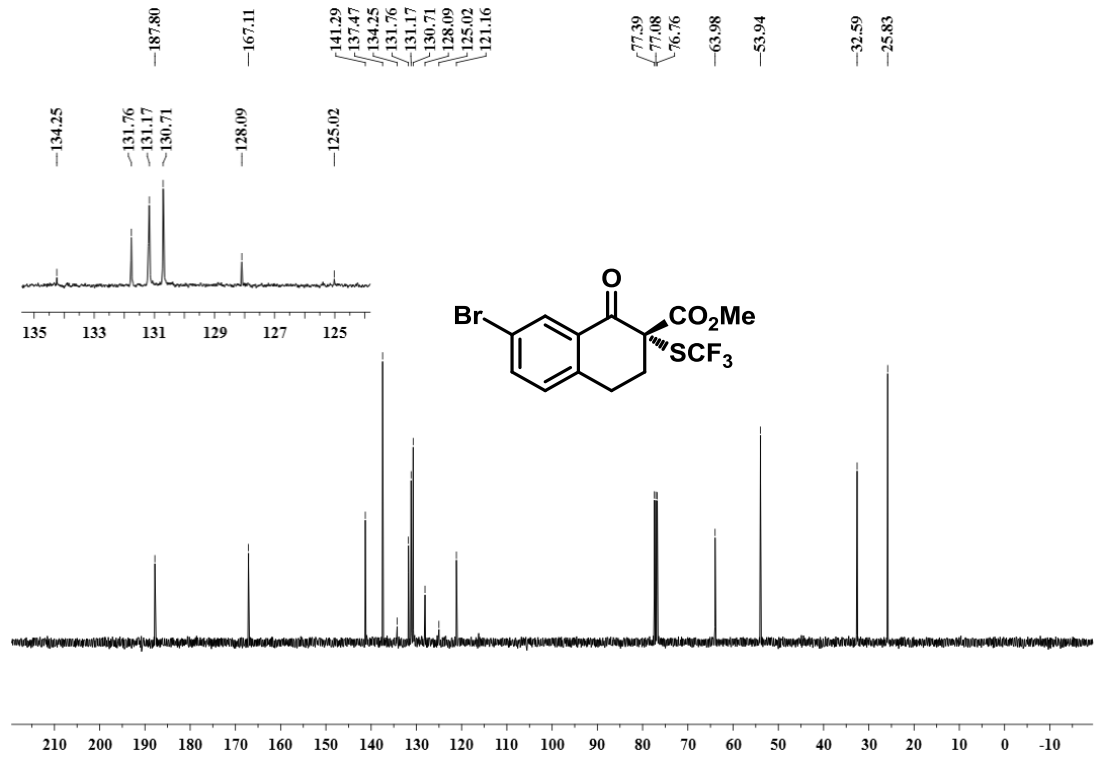
^{19}F NMR Spectrum for (R)-Methyl-6,7-dimethoxy-1-oxo-2-((trifluoromethyl)thio)-1,2,3,4-tetrahydronaphthalene-2-carboxylate 3n



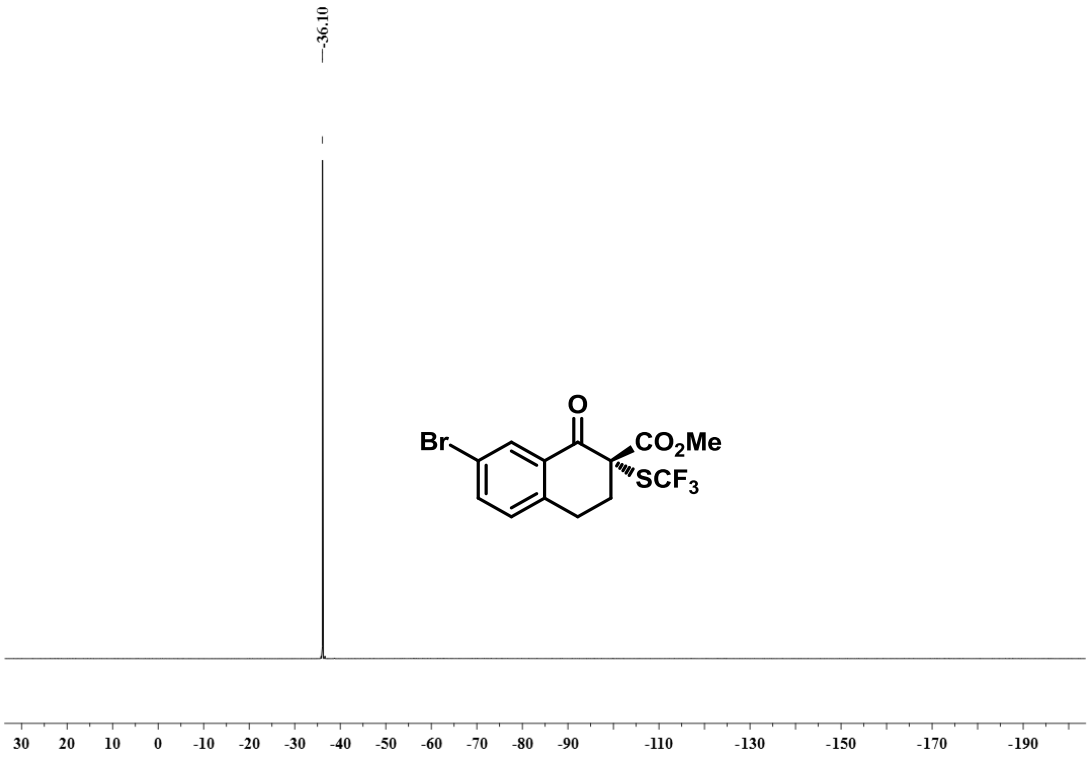
^{1}H NMR Spectrum for (R)-Methyl-7-bromo-1-oxo-2-((trifluoromethyl)thio)-1,2,3,4-tetrahydronaphthalene-2-carboxylate 3o



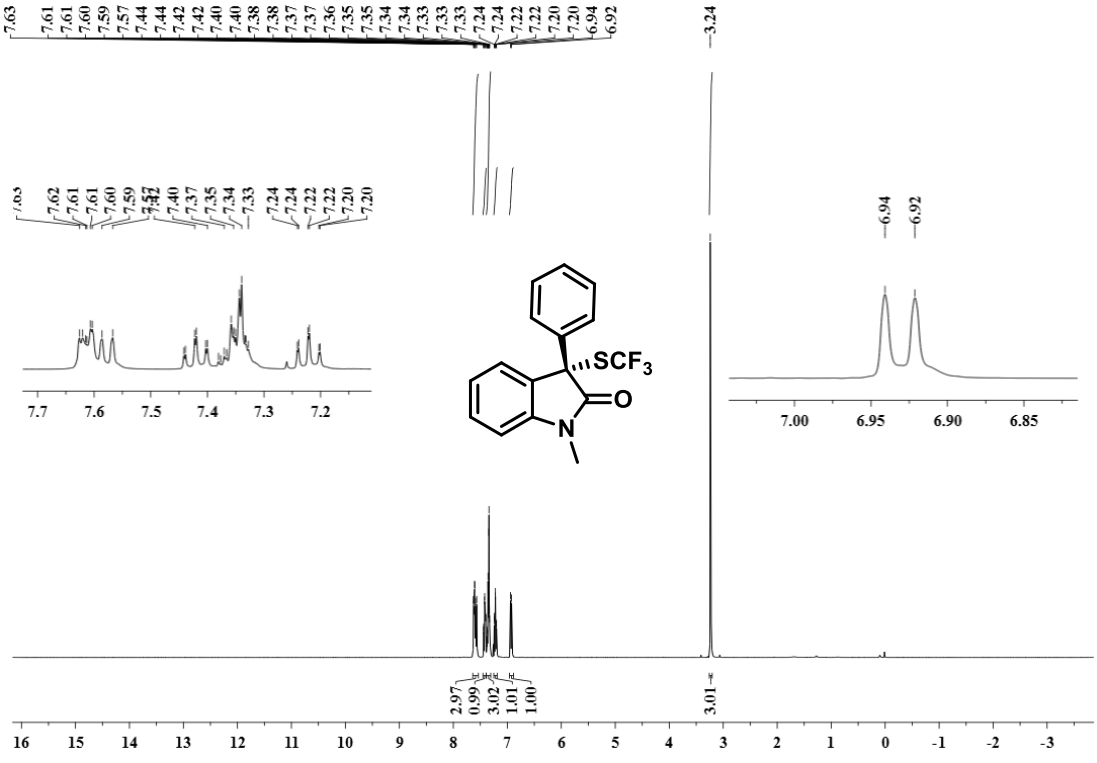
^{13}C NMR Spectrum for (R)-Methyl-7-bromo-1-oxo-2-((trifluoromethyl)thio)-1,2,3,4-tetrahydronaphthalene-2-carboxylate 3o



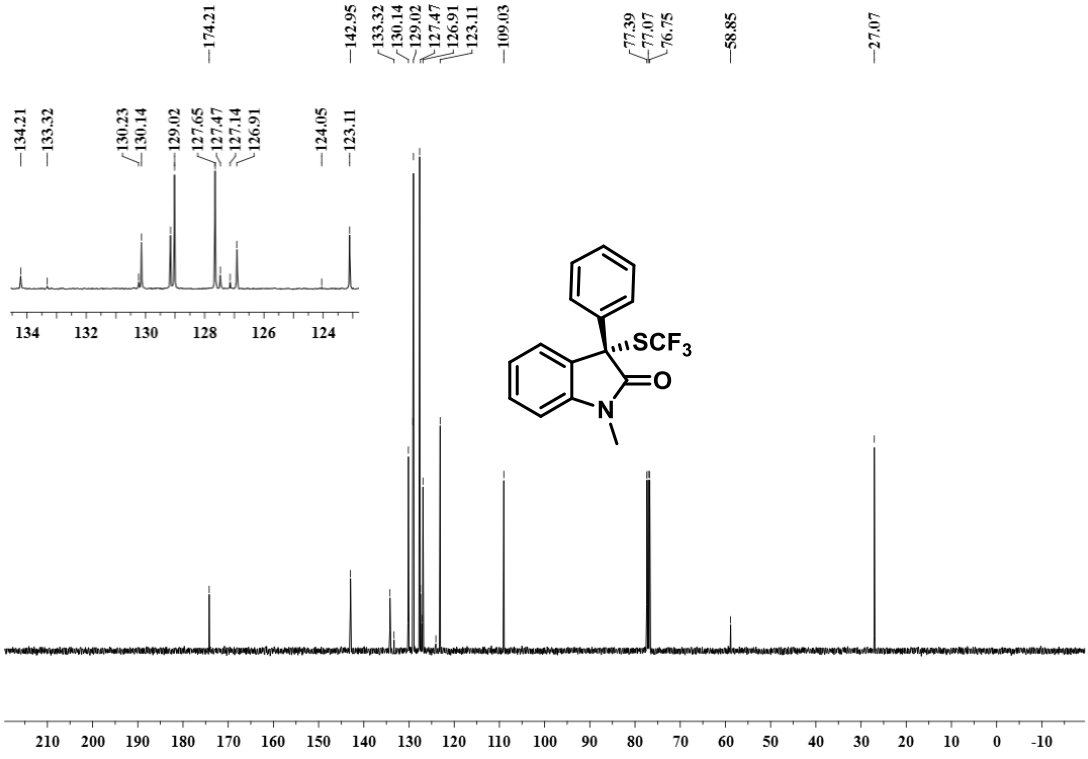
^{19}F NMR Spectrum for (R)-Methyl-7-bromo-1-oxo-2-((trifluoromethyl)thio)-1,2,3,4-tetrahydronaphthalene-2-carboxylate 3o



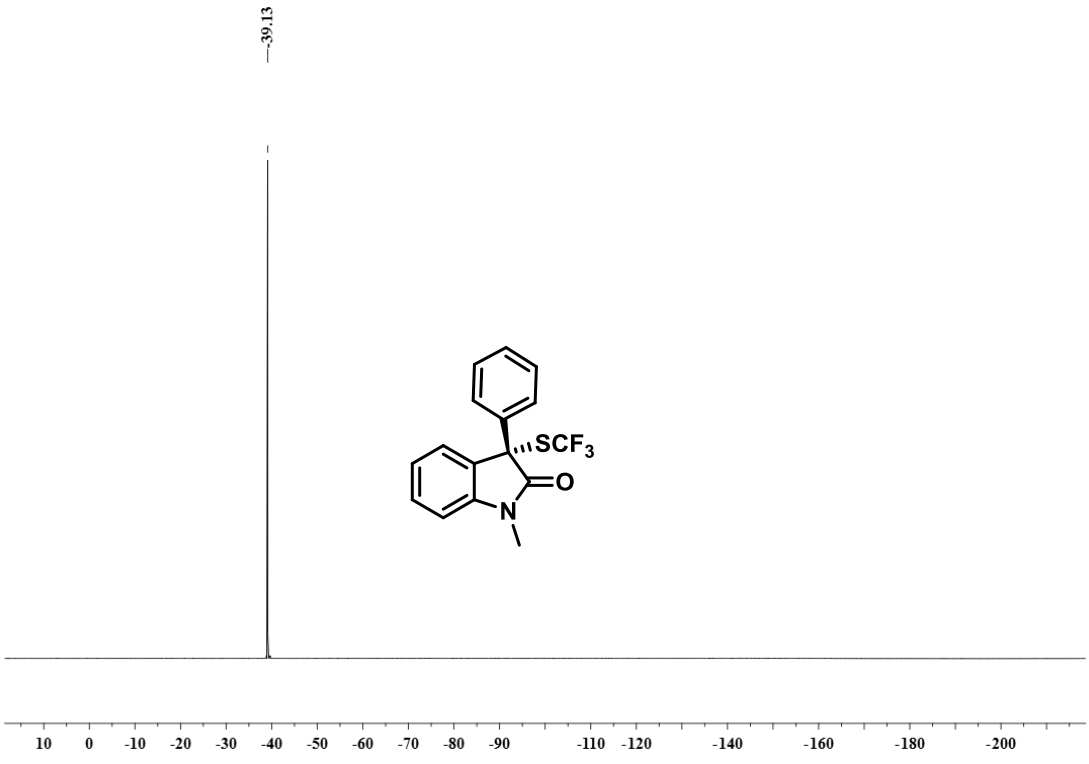
^{1}H NMR Spectrum for (S)-1-Methyl-3-phenyl-3-((trifluoromethyl)thio)indolin-2-one 4a



^{13}C NMR Spectrum for (S)-1-Methyl-3-phenyl-3-((trifluoromethyl)thio)indolin-2-one 4a

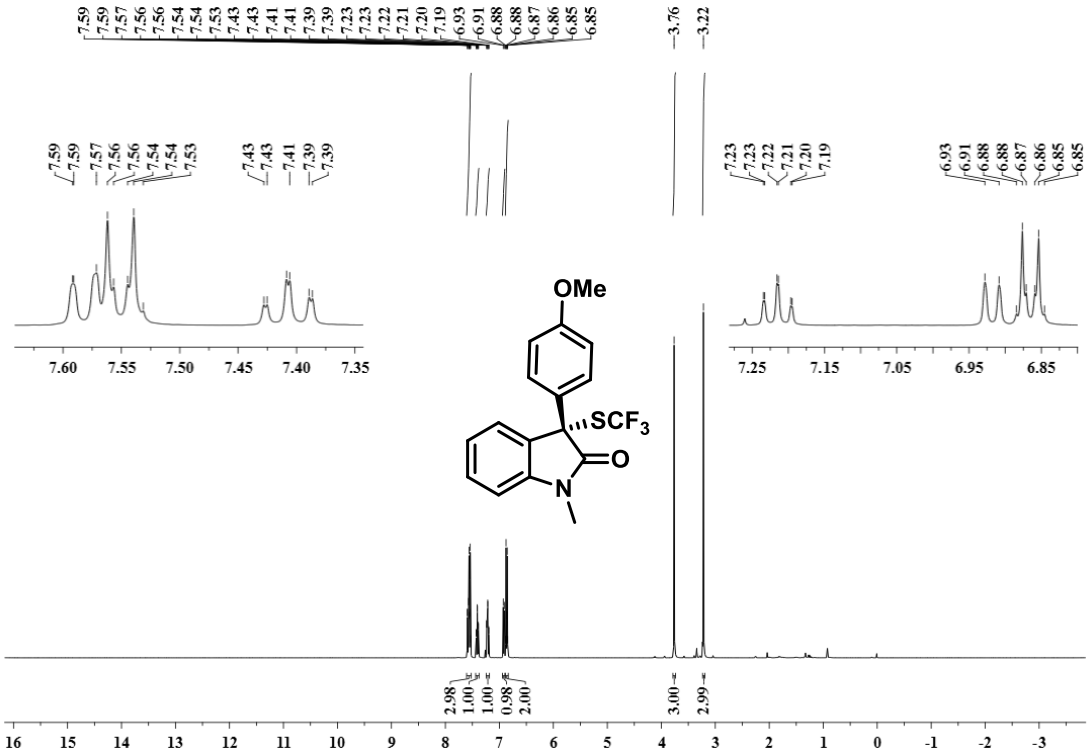


^{19}F NMR Spectrum for (S)-1-Methyl-3-phenyl-3-((trifluoromethyl)thio)indolin-2-one 4a



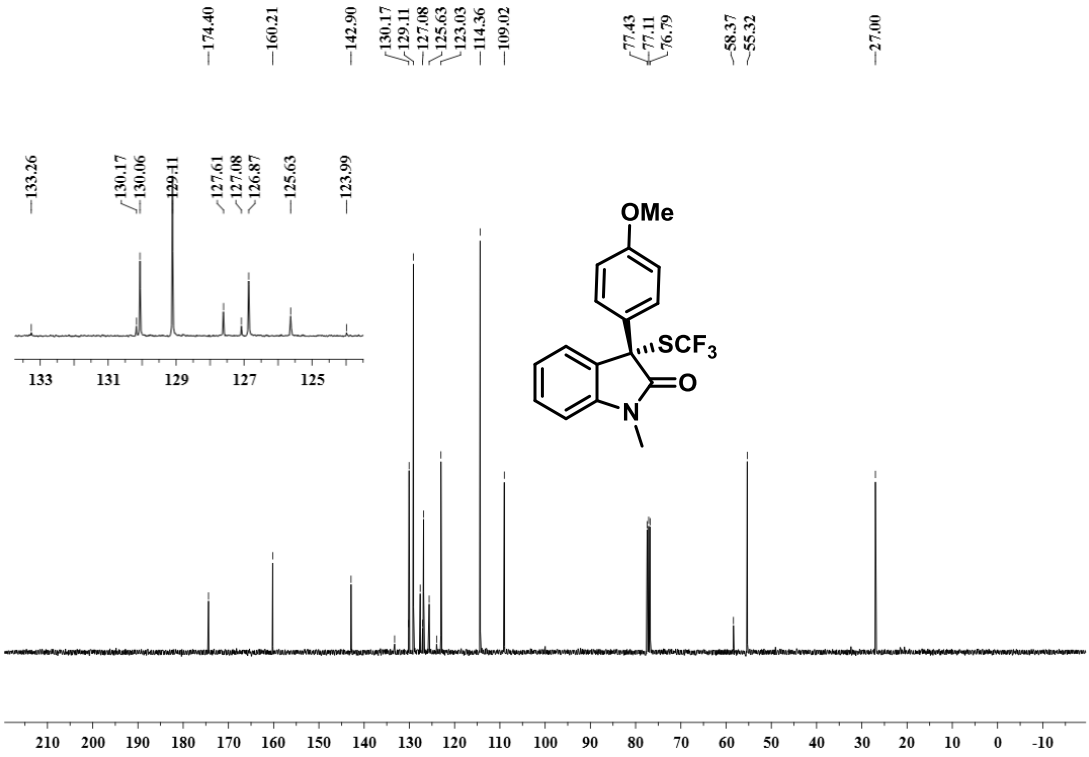
^{1}H NMR Spectrum for

(S)-3-(4-Methoxyphenyl)-1-methyl-3-((trifluoromethyl)thio)indolin-2-one 4b



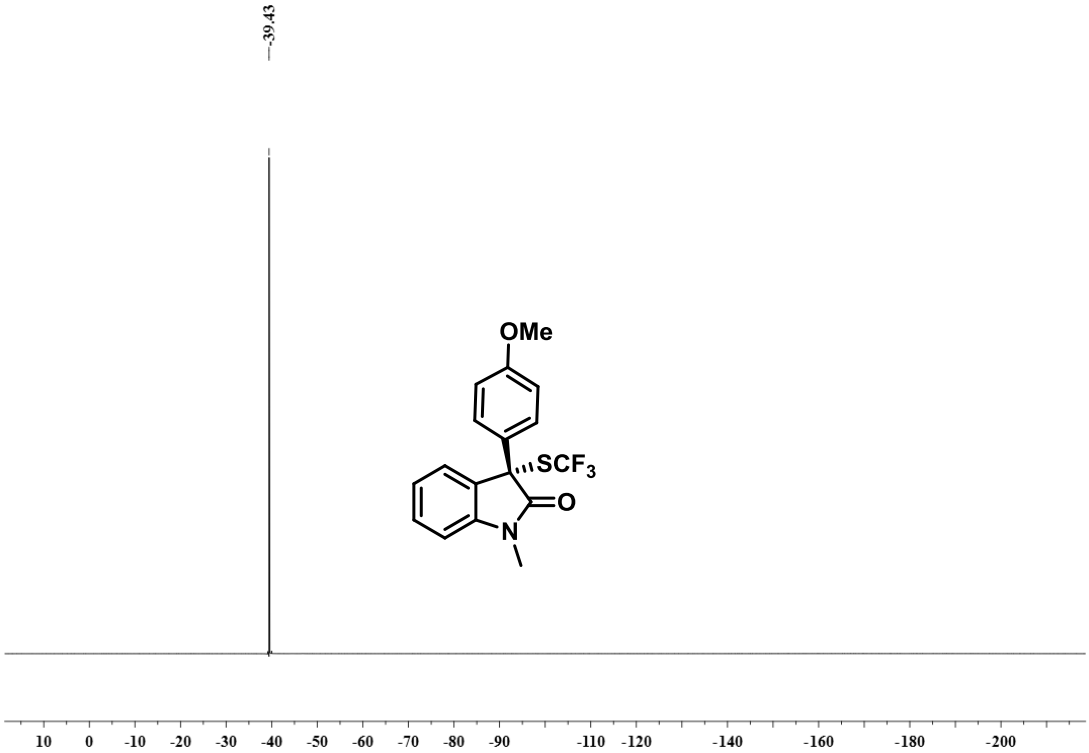
^{13}C NMR Spectrum for

(S)-3-(4-Methoxyphenyl)-1-methyl-3-((trifluoromethyl)thio)indolin-2-one 4b



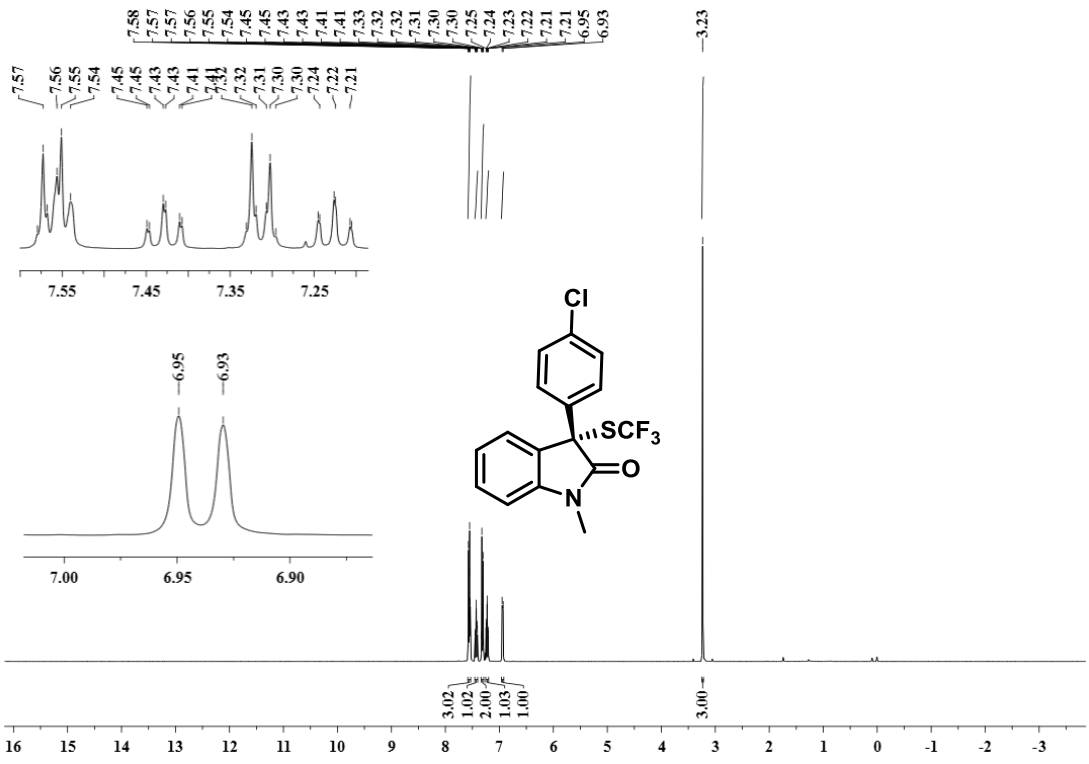
^{19}F NMR Spectrum for

(S)-3-(4-Methoxyphenyl)-1-methyl-3-((trifluoromethyl)thio)indolin-2-one 4b



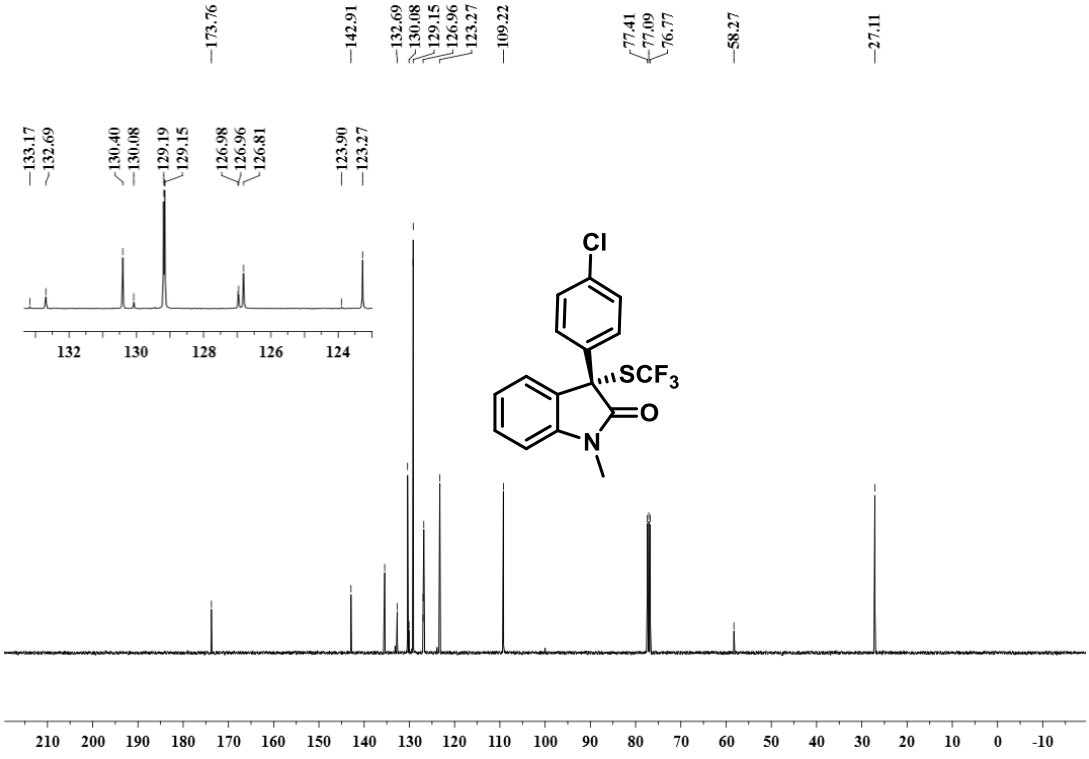
^{1}H NMR Spectrum for

(S)-3-(4-Chlorophenyl)-1-methyl-3-((trifluoromethyl)thio)indolin-2-one 4c



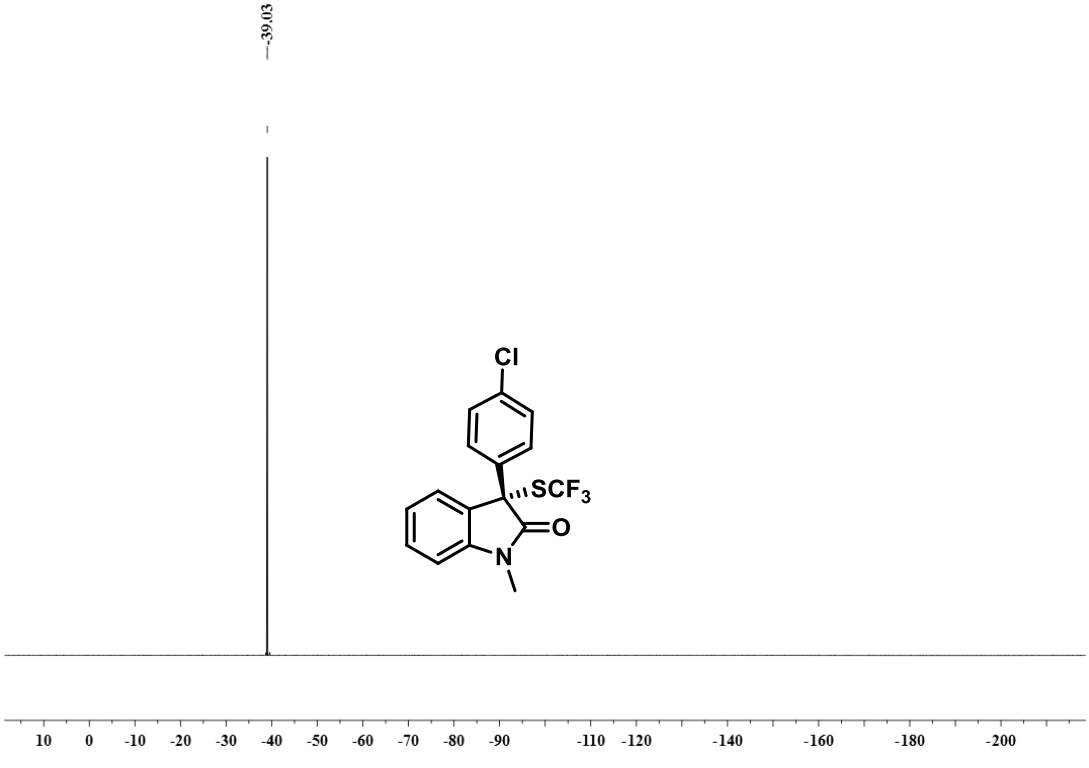
^{13}C NMR Spectrum for

(S)-3-(4-Chlorophenyl)-1-methyl-3-((trifluoromethyl)thio)indolin-2-one 4c



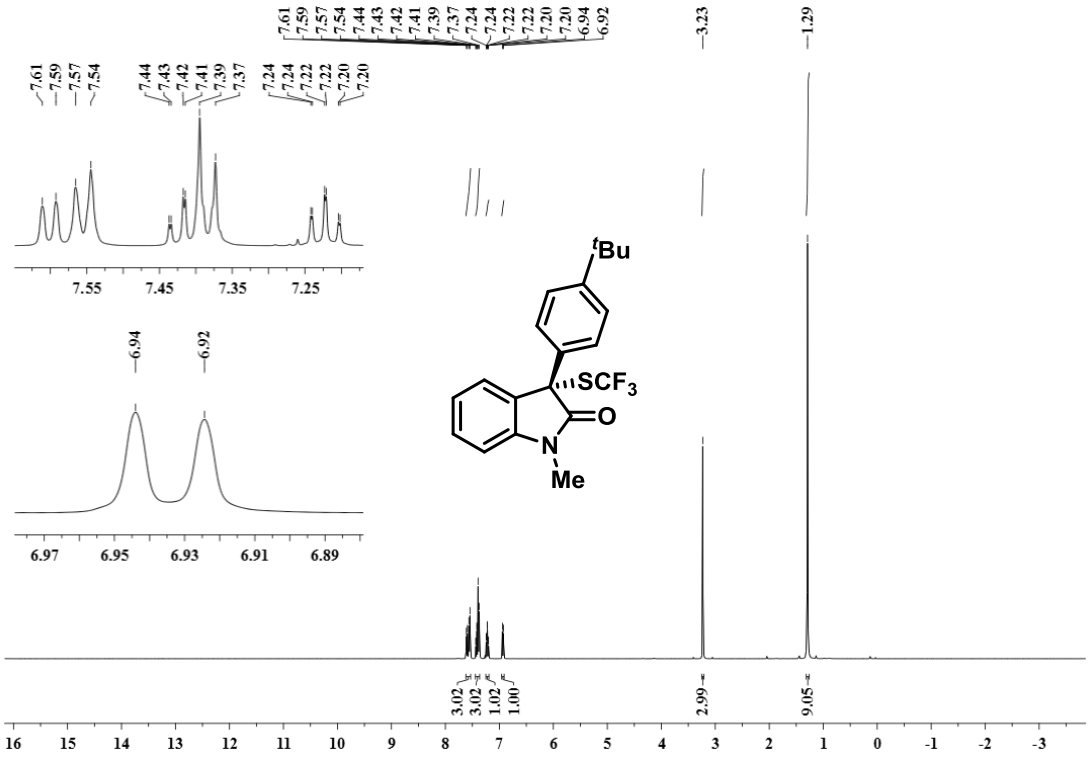
^{19}F NMR Spectrum for

(S)-3-(4-Chlorophenyl)-1-methyl-3-((trifluoromethyl)thio)indolin-2-one 4c



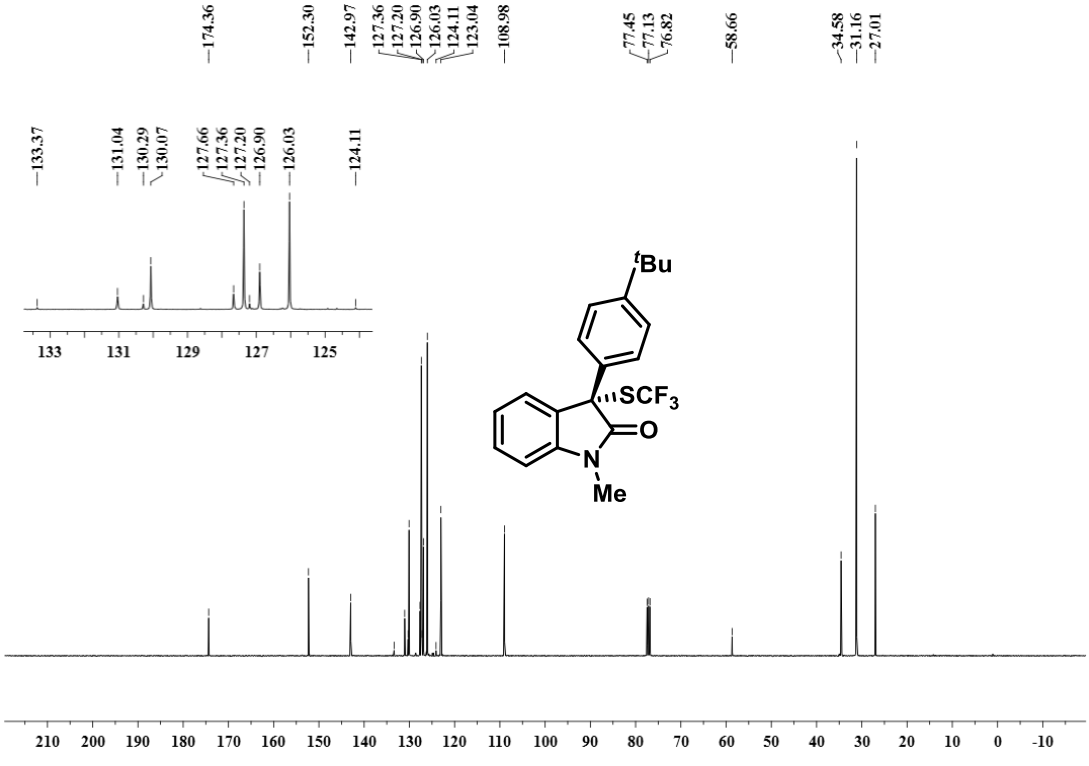
^{1}H NMR Spectrum for

(S)-3-(4-(*tert*-Butyl)phenyl)-1-methyl-3-((trifluoromethyl)thio)indolin-2-one 4d



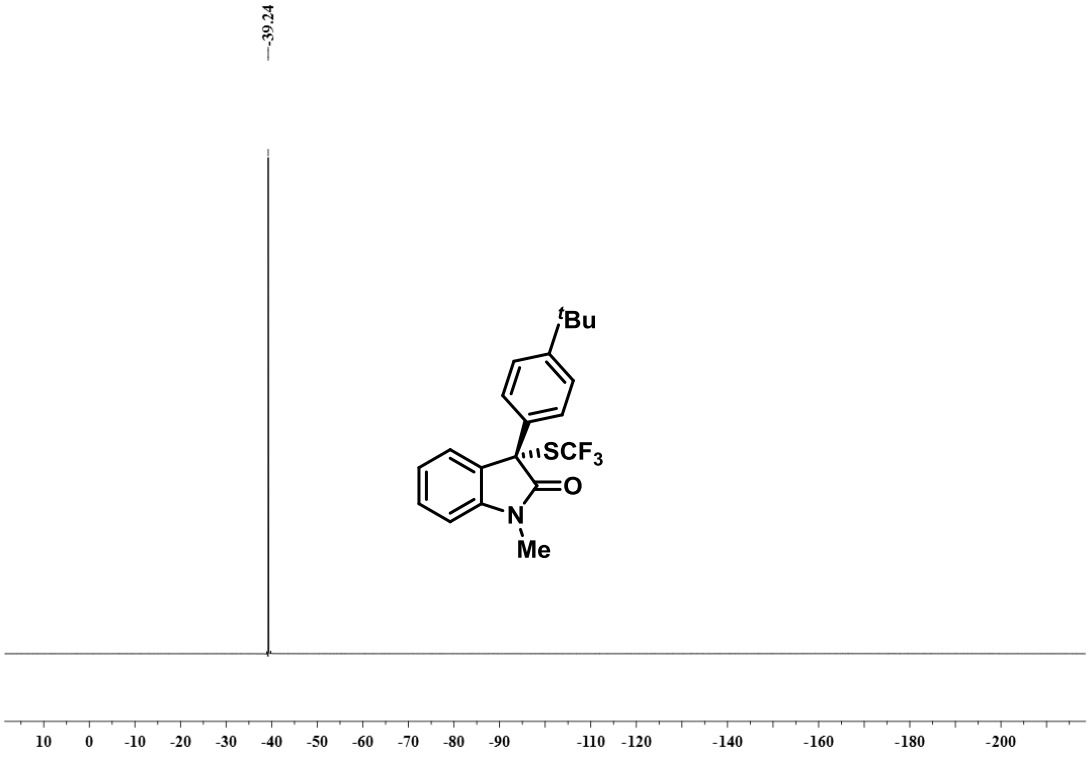
^{13}C NMR Spectrum for

(S)-3-(4-(*tert*-Butyl)phenyl)-1-methyl-3-((trifluoromethyl)thio)indolin-2-one 4d



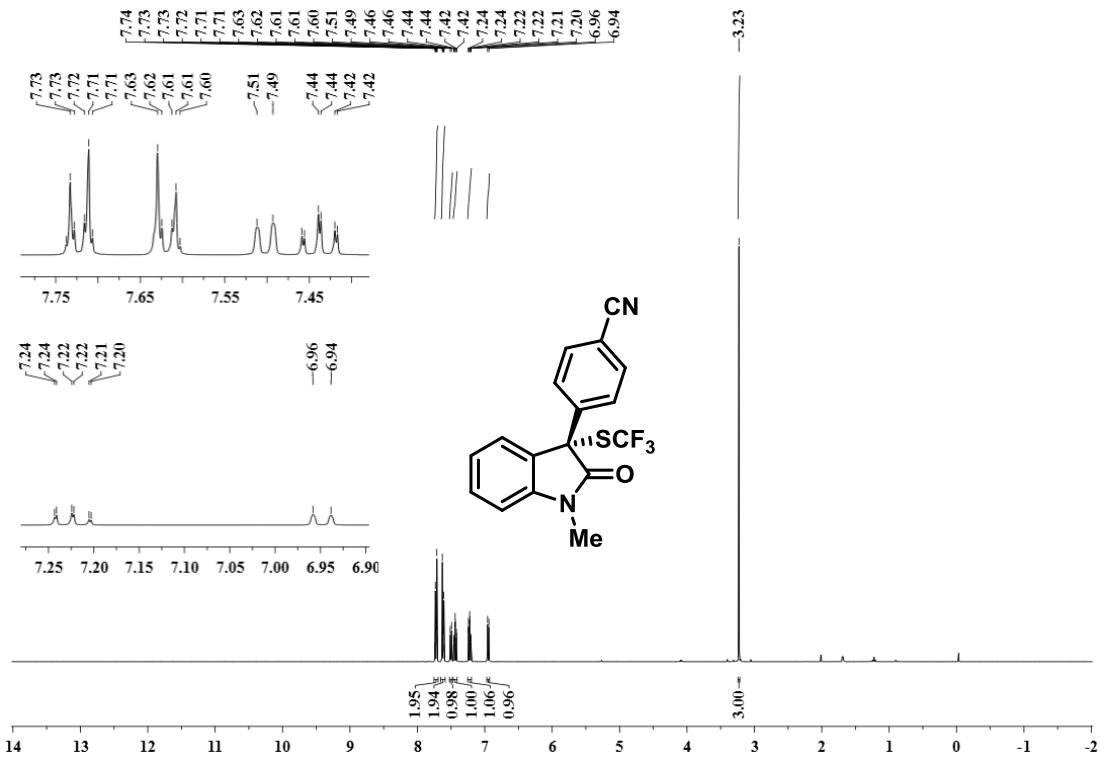
^{19}F NMR Spectrum for

(S)-3-(4-(*tert*-Butyl)phenyl)-1-methyl-3-((trifluoromethyl)thio)indolin-2-one 4d



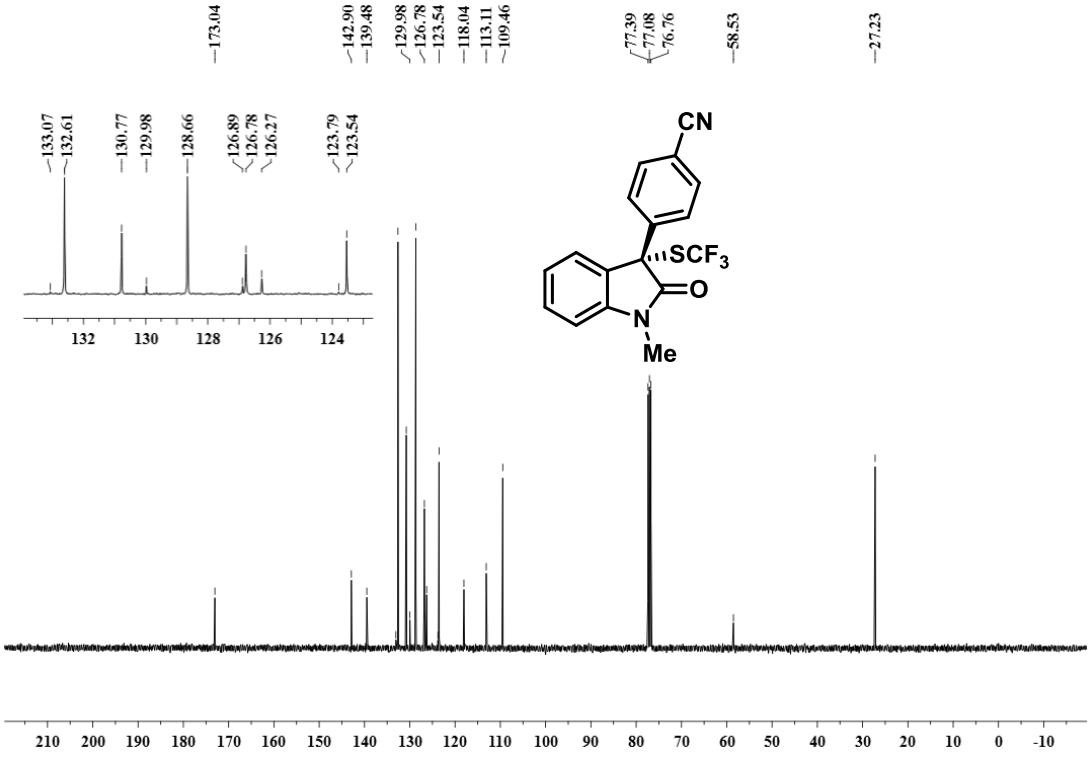
^{1}H NMR Spectrum for

(S)-4-(1-Methyl-2-oxo-3-((trifluoromethyl)thio)indolin-3-yl)benzonitrile 4e



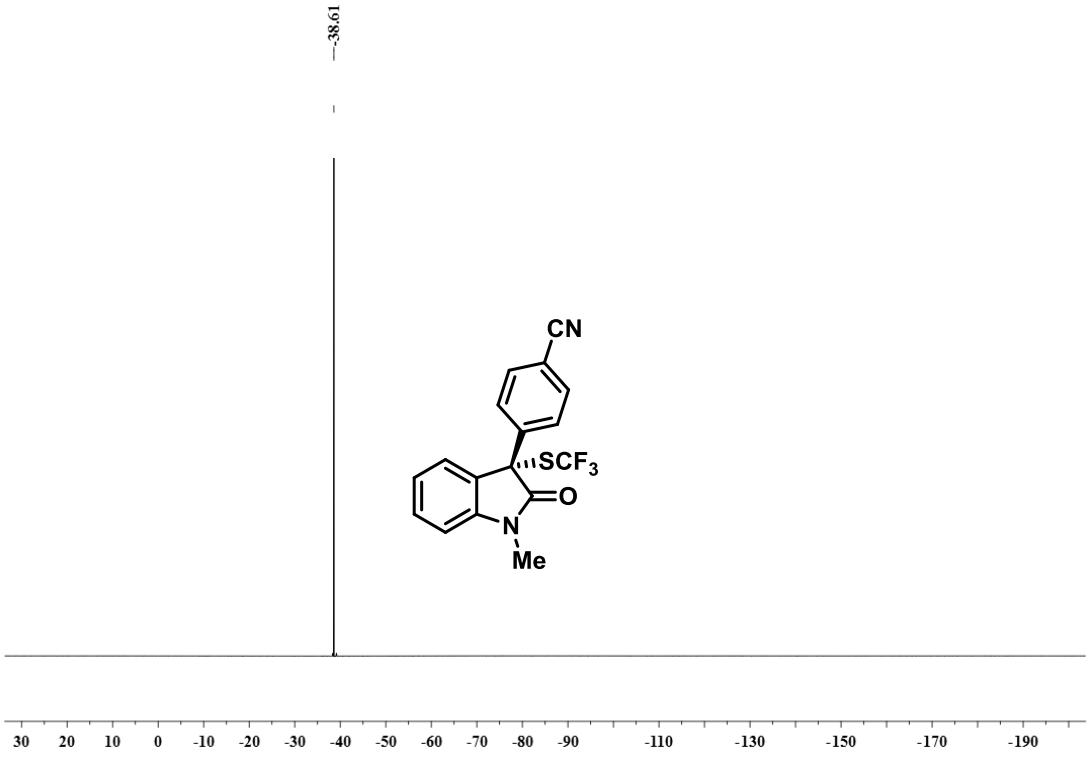
^{13}C NMR Spectrum for

(S)-4-(1-Methyl-2-oxo-3-((trifluoromethyl)thio)indolin-3-yl)benzonitrile 4e

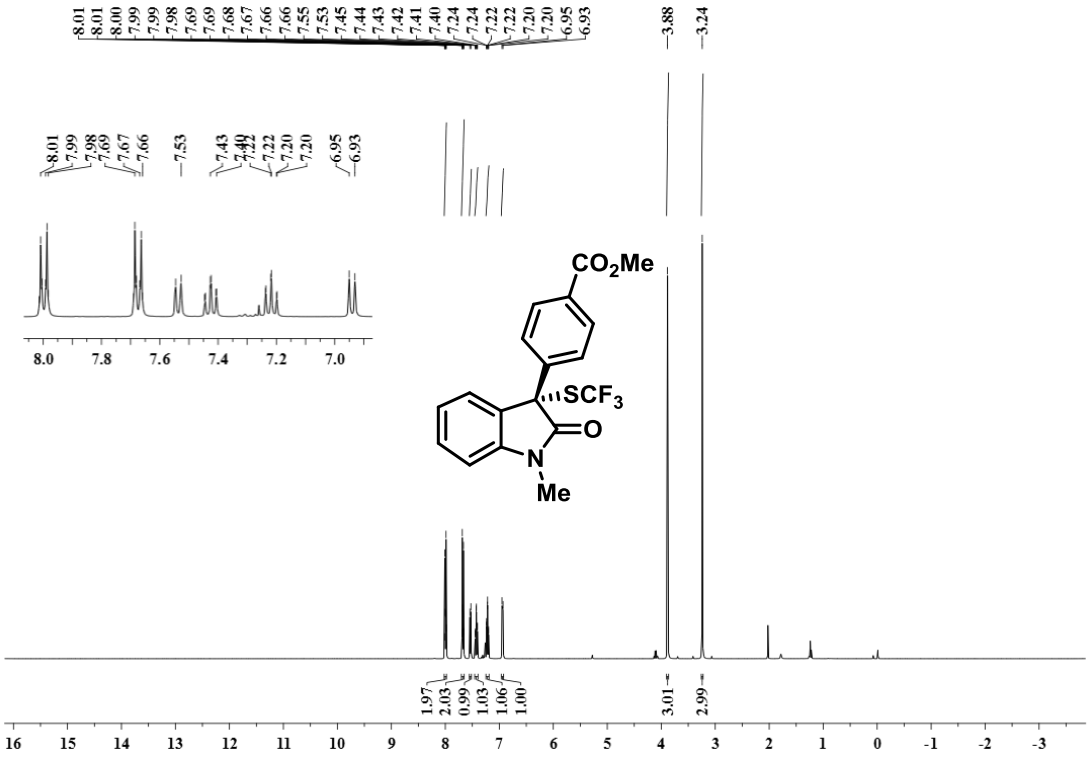


^{19}F NMR Spectrum for

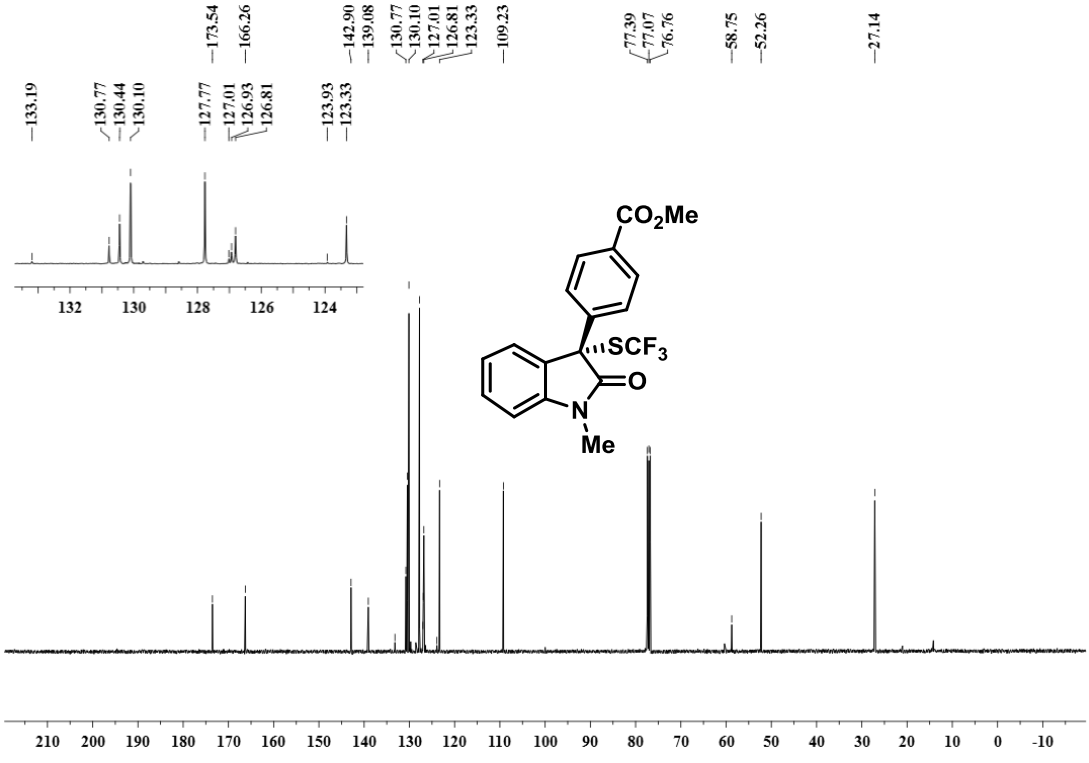
(S)-4-(1-Methyl-2-oxo-3-((trifluoromethyl)thio)indolin-3-yl)benzonitrile 4e



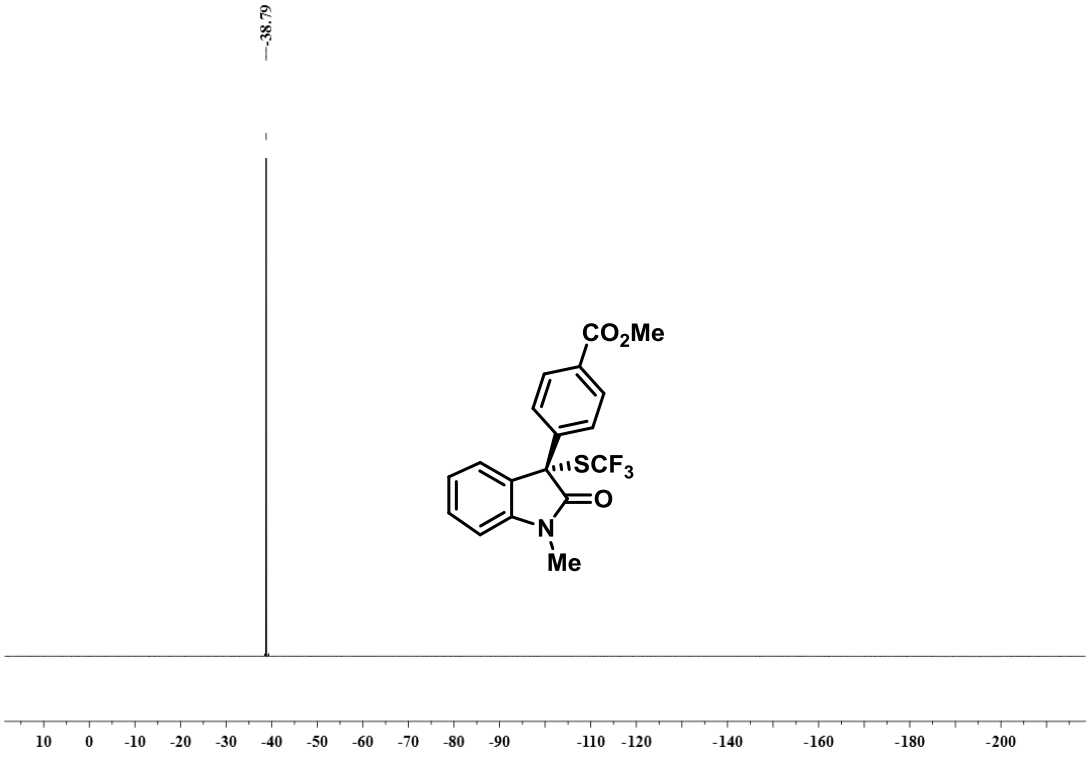
^{1}H NMR Spectrum for (S)-Methyl
4-(1-methyl-2-oxo-3-((trifluoromethyl)thio)indolin-3-yl)benzoate 4f



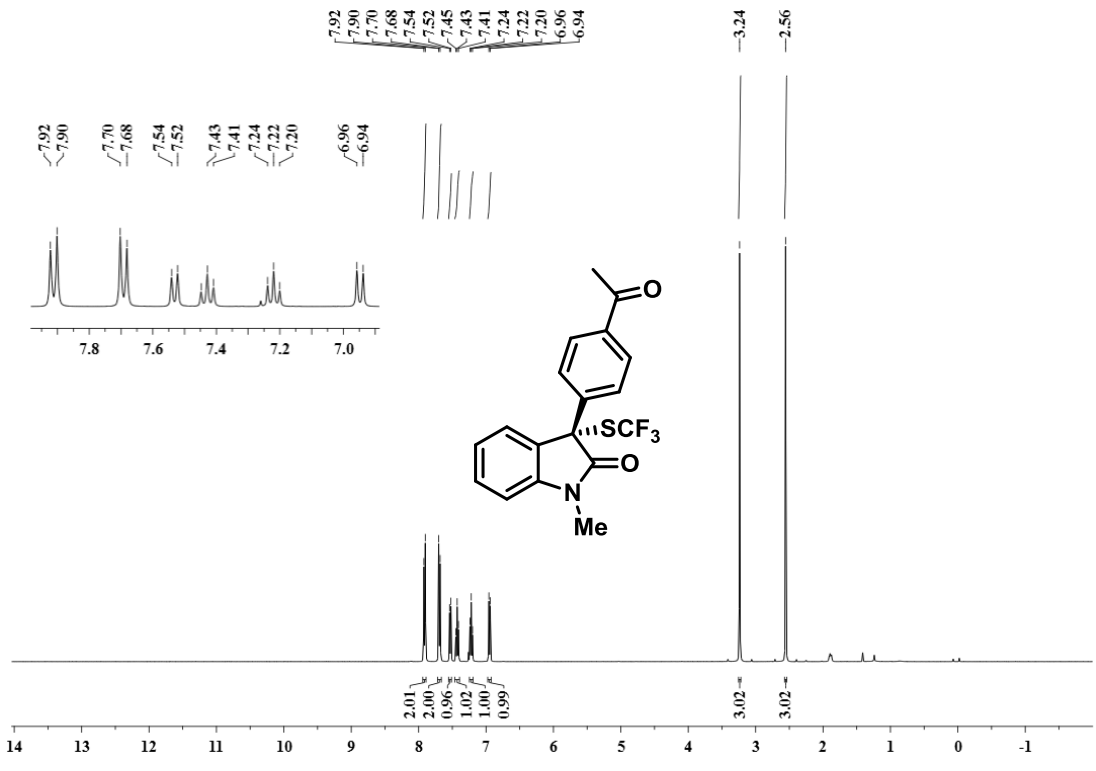
^{13}C NMR Spectrum for (S)-Methyl
4-(1-methyl-2-oxo-3-((trifluoromethyl)thio)indolin-3-yl)benzoate 4f



^{19}F NMR Spectrum for (S)-Methyl
4-(1-methyl-2-oxo-3-((trifluoromethyl)thio)indolin-3-yl)benzoate 4f

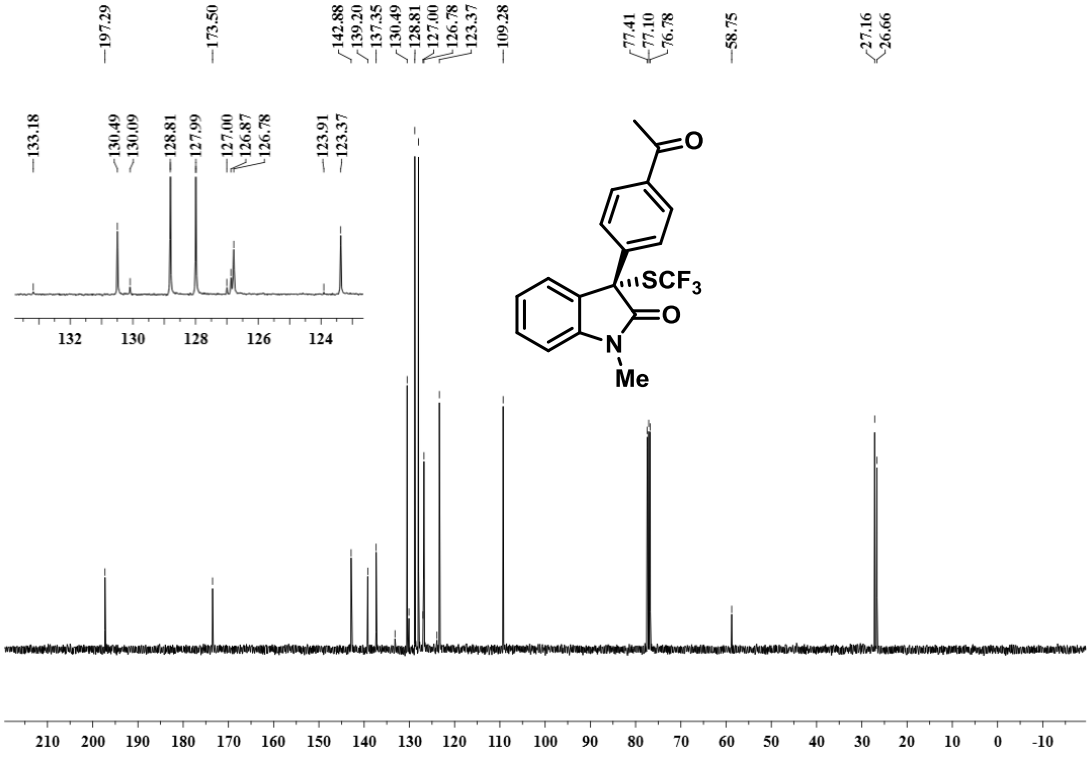


^{1}H NMR Spectrum for
(S)-3-(4-Acetylphenyl)-1-methyl-3-((trifluoromethyl)thio)indolin-2-one 4g



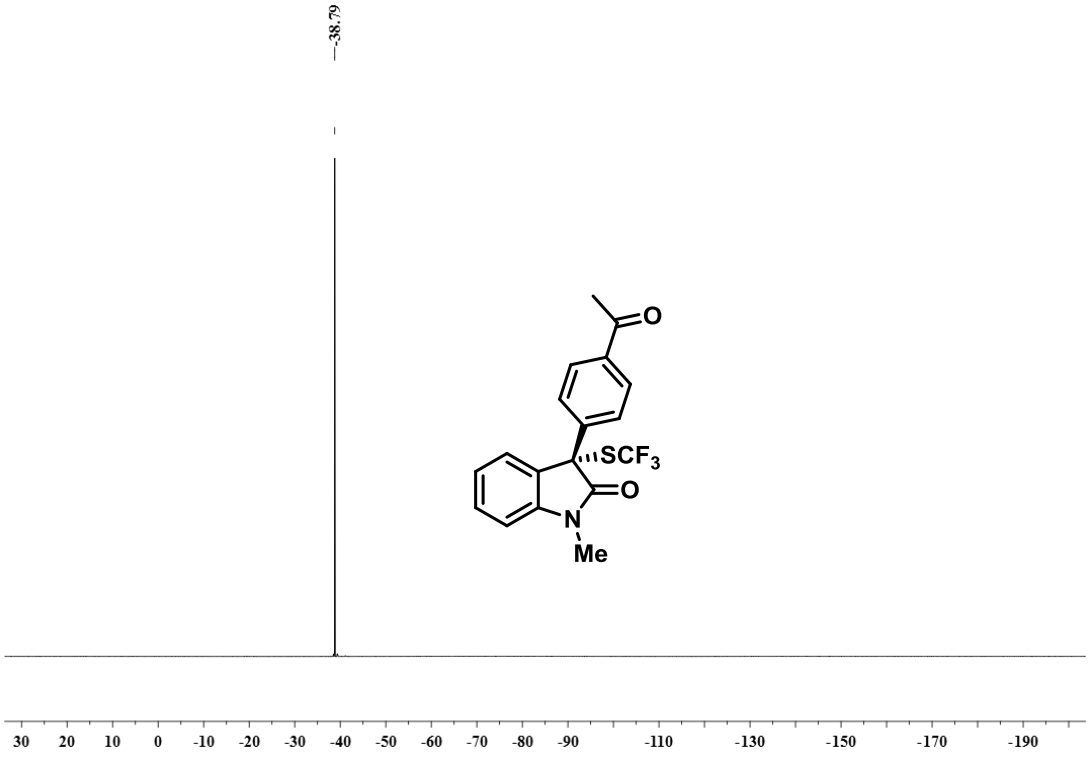
^{13}C NMR Spectrum for

(S)-3-(4-Acetylphenyl)-1-methyl-3-((trifluoromethyl)thio)indolin-2-one 4g



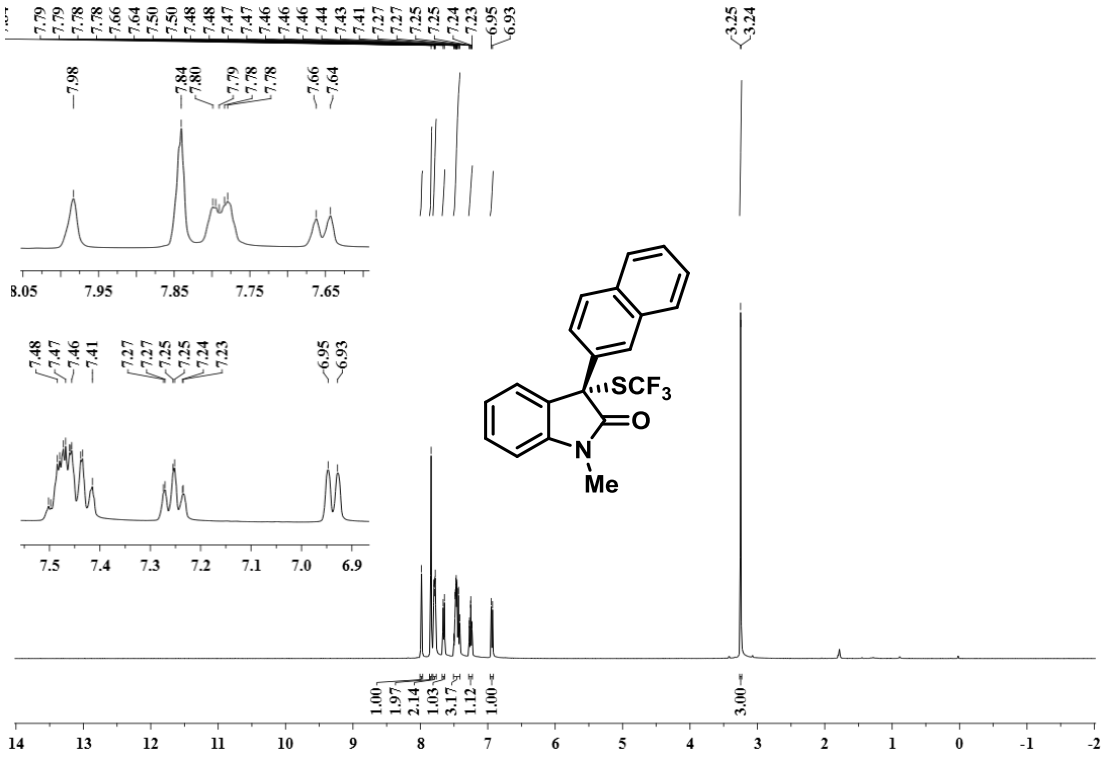
^{19}F NMR Spectrum for

(S)-3-(4-Acetylphenyl)-1-methyl-3-((trifluoromethyl)thio)indolin-2-one 4g



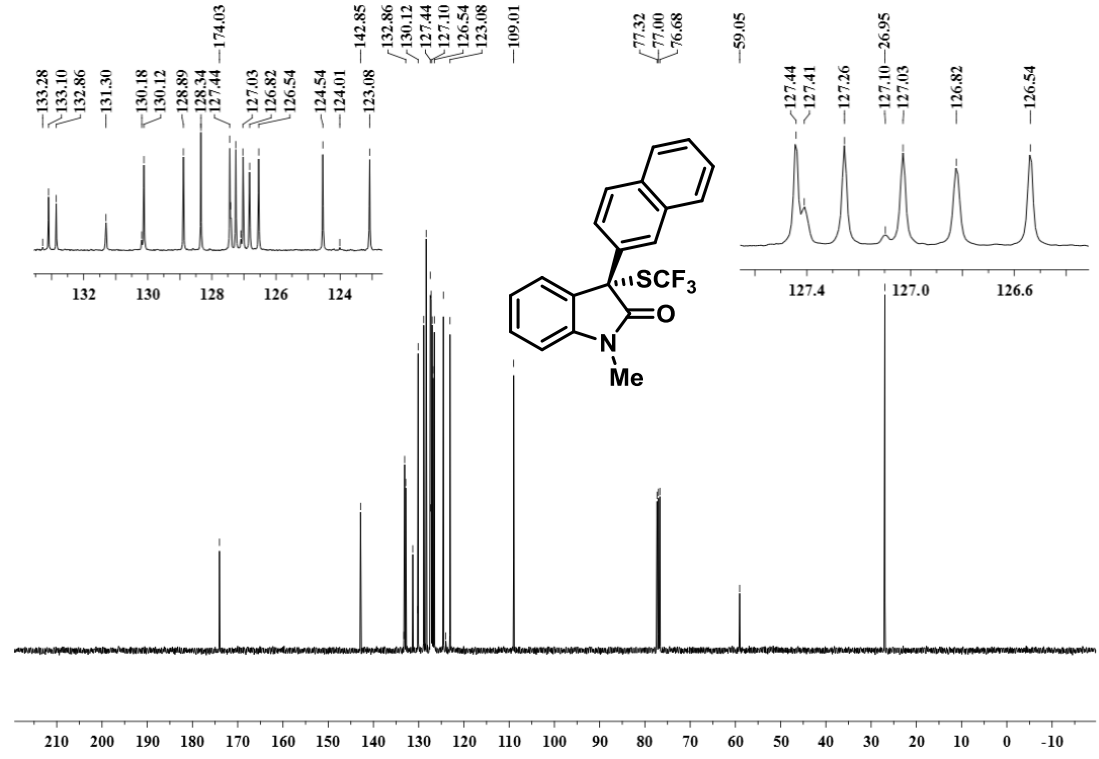
^{1}H NMR Spectrum for

(S)-1-Methyl-3-(naphthalen-2-yl)-3-((trifluoromethyl)thio)indolin-2-one 4h



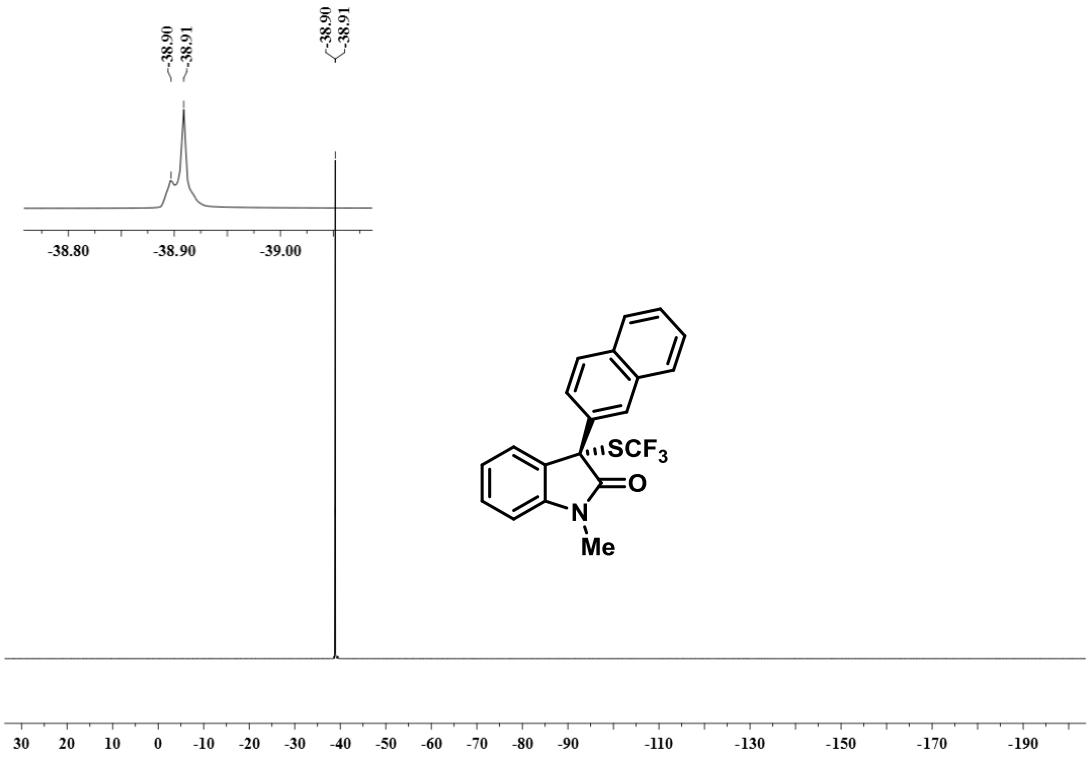
^{13}C NMR Spectrum for

(S)-1-Methyl-3-(naphthalen-2-yl)-3-((trifluoromethyl)thio)indolin-2-one 4h



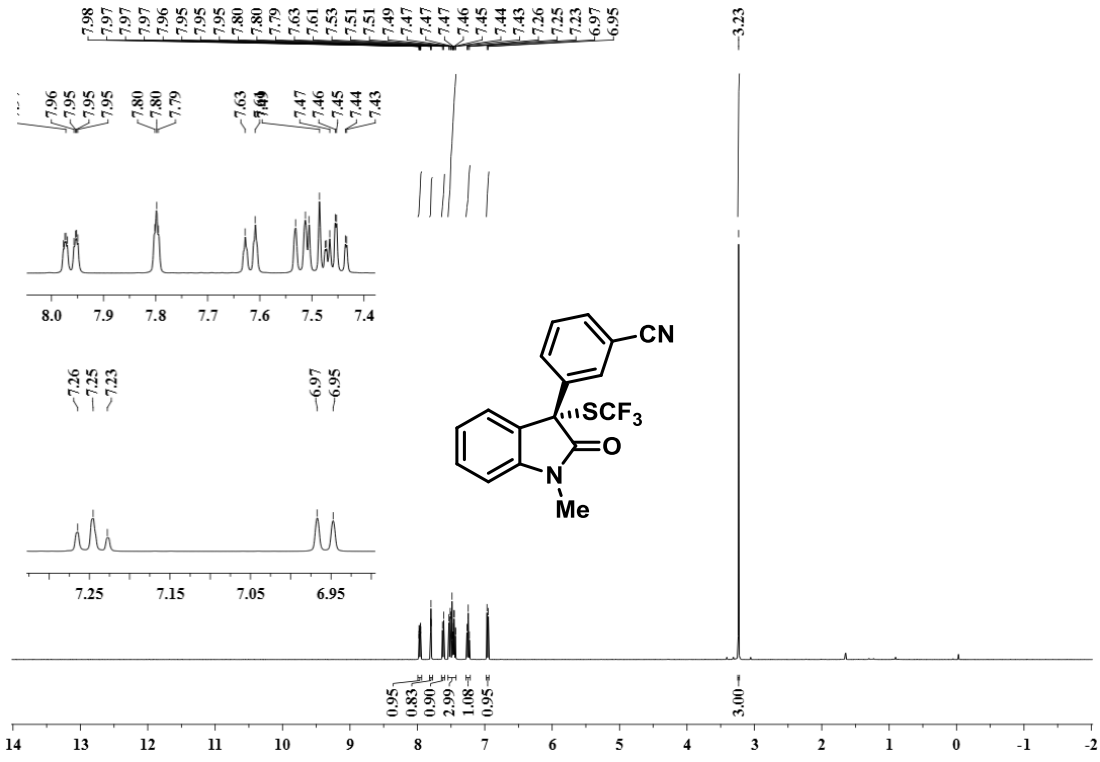
^{19}F NMR Spectrum for

(S)-1-Methyl-3-(naphthalen-2-yl)-3-((trifluoromethyl)thio)indolin-2-one 4h



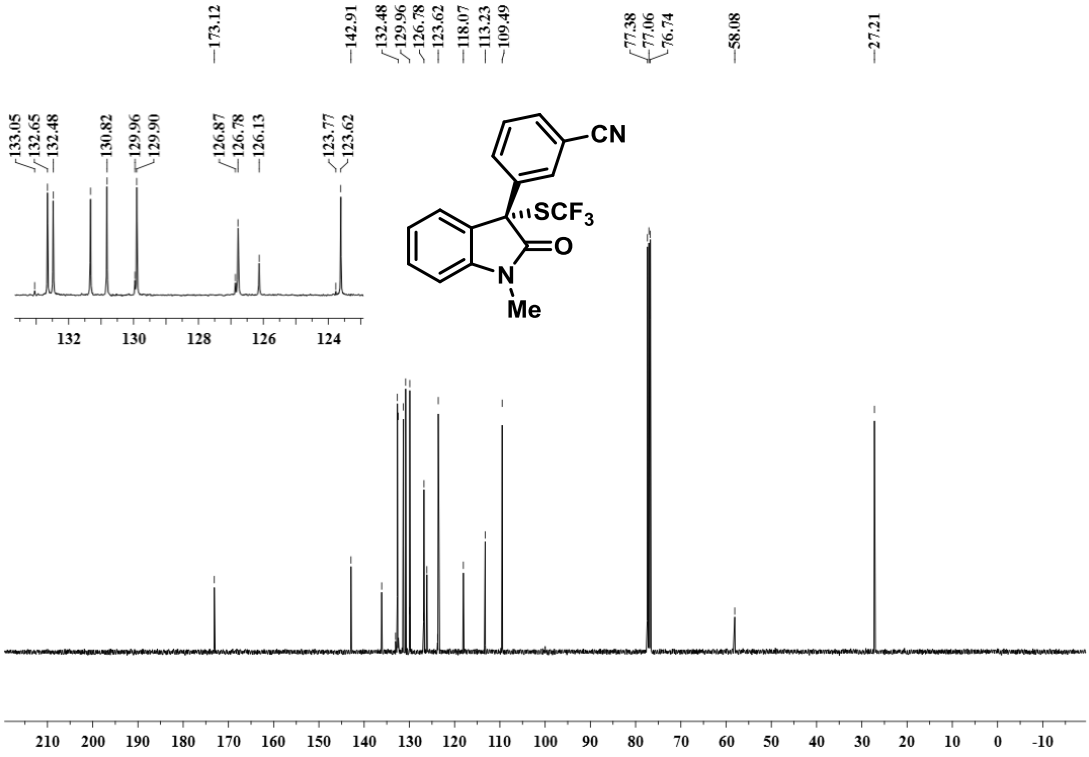
^{1}H NMR Spectrum for

(S)-3-(1-Methyl-2-oxo-3-((trifluoromethyl)thio)indolin-3-yl)benzonitrile 4i



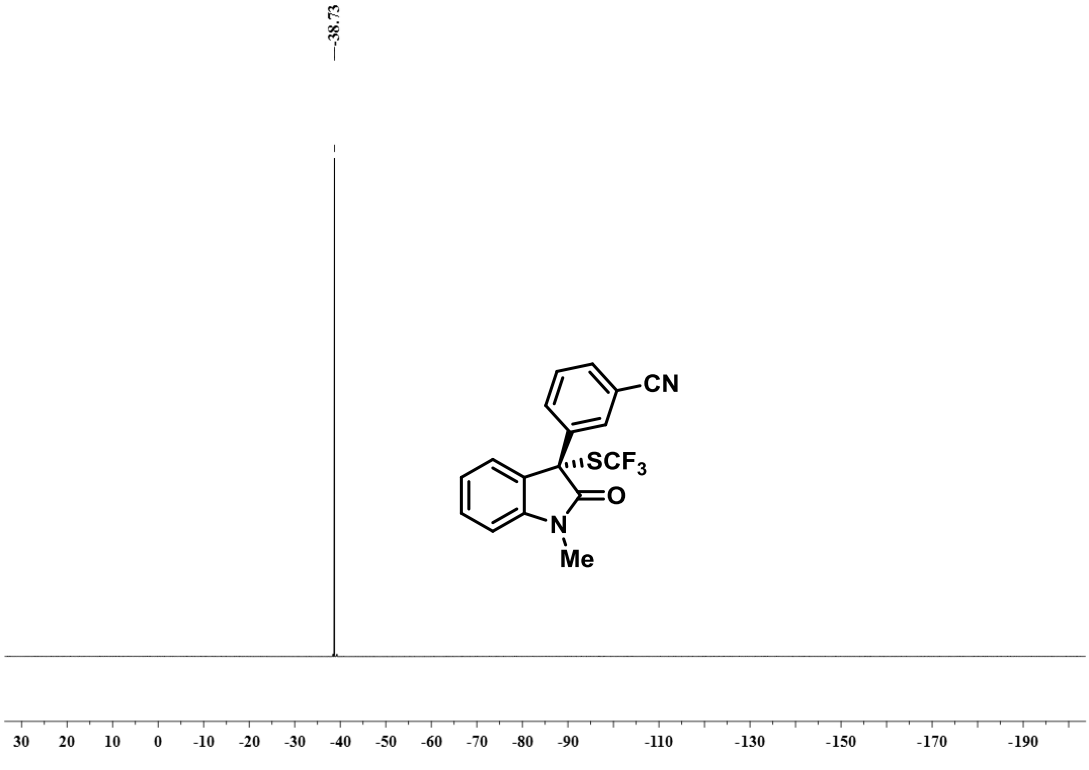
^{13}C NMR Spectrum for

(S)-3-(1-Methyl-2-oxo-3-((trifluoromethyl)thio)indolin-3-yl)benzonitrile 4i



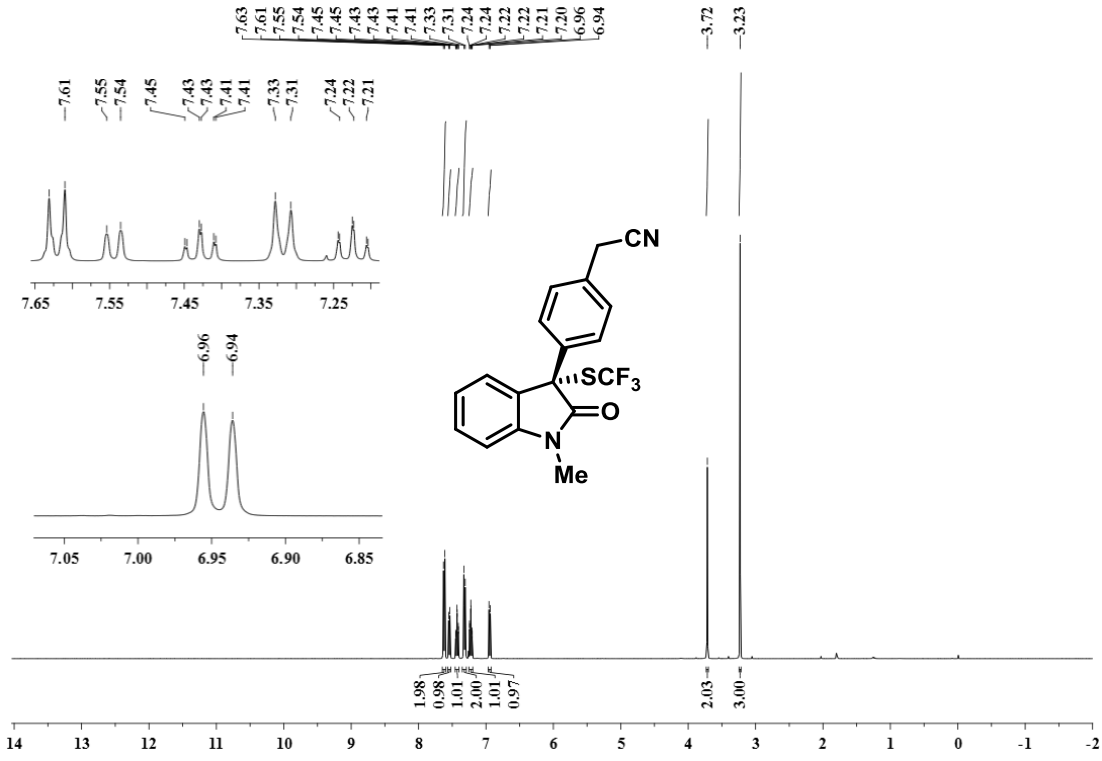
^{19}F NMR Spectrum for

(S)-3-(1-Methyl-2-oxo-3-((trifluoromethyl)thio)indolin-3-yl)benzonitrile 4i



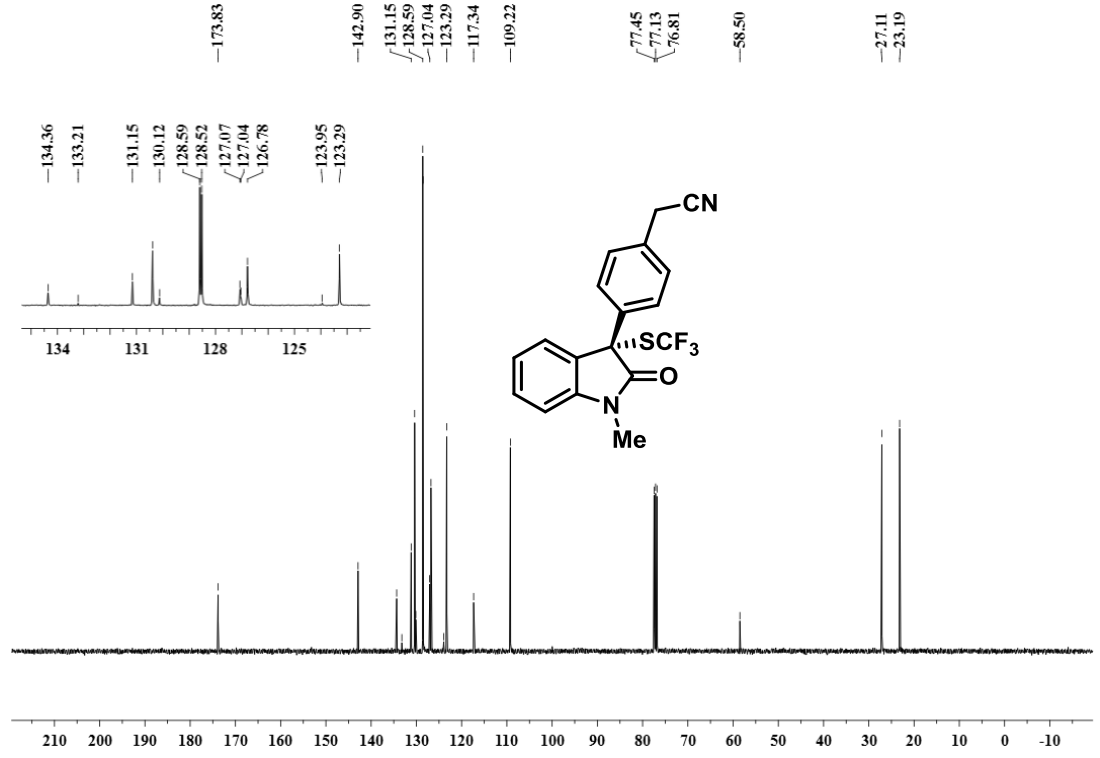
^{1}H NMR Spectrum for

(S)-2-(4-(1-Methyl-2-oxo-3-((trifluoromethyl)thio)indolin-3-yl)phenyl)acetonitrile 4j



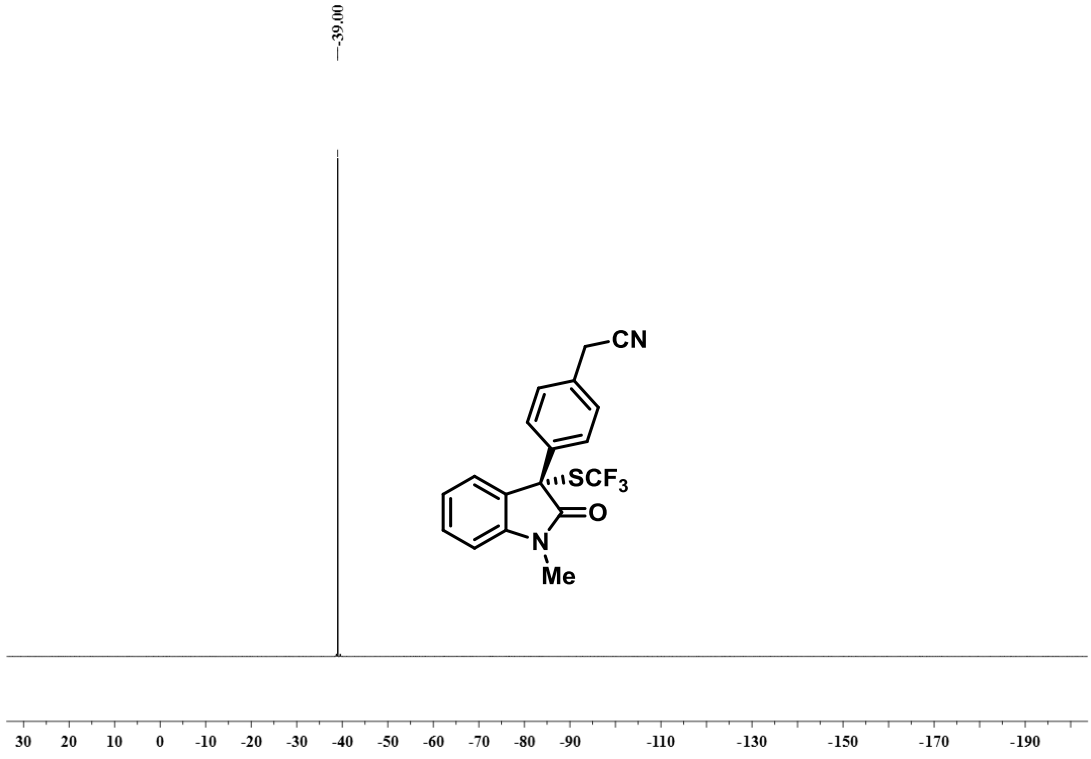
^{13}C NMR Spectrum for

(S)-2-(4-(1-Methyl-2-oxo-3-((trifluoromethyl)thio)indolin-3-yl)phenyl)acetonitrile 4j



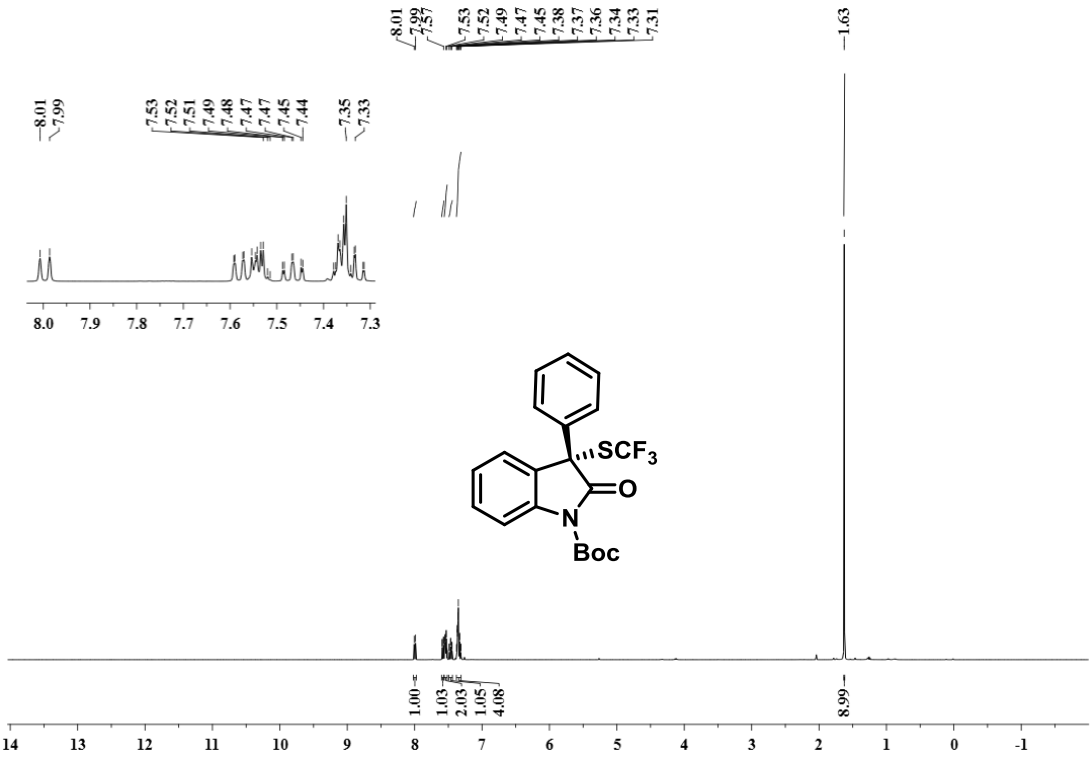
^{19}F NMR Spectrum for

(S)-2-(4-(1-Methyl-2-oxo-3-((trifluoromethyl)thio)indolin-3-yl)phenyl)acetonitrile 4j



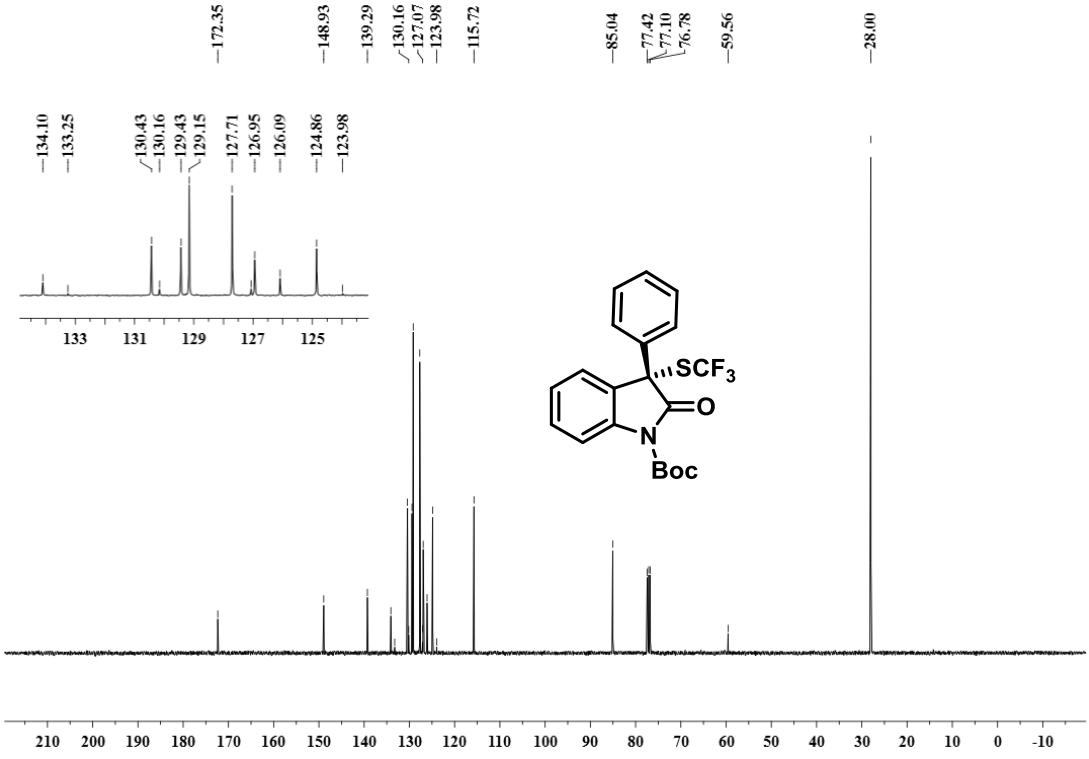
^{1}H NMR Spectrum for

(S)-*tert*-Butyl2-oxo-3-phenyl-3-((trifluoromethyl)thio)indoline-1-carboxylate 4k



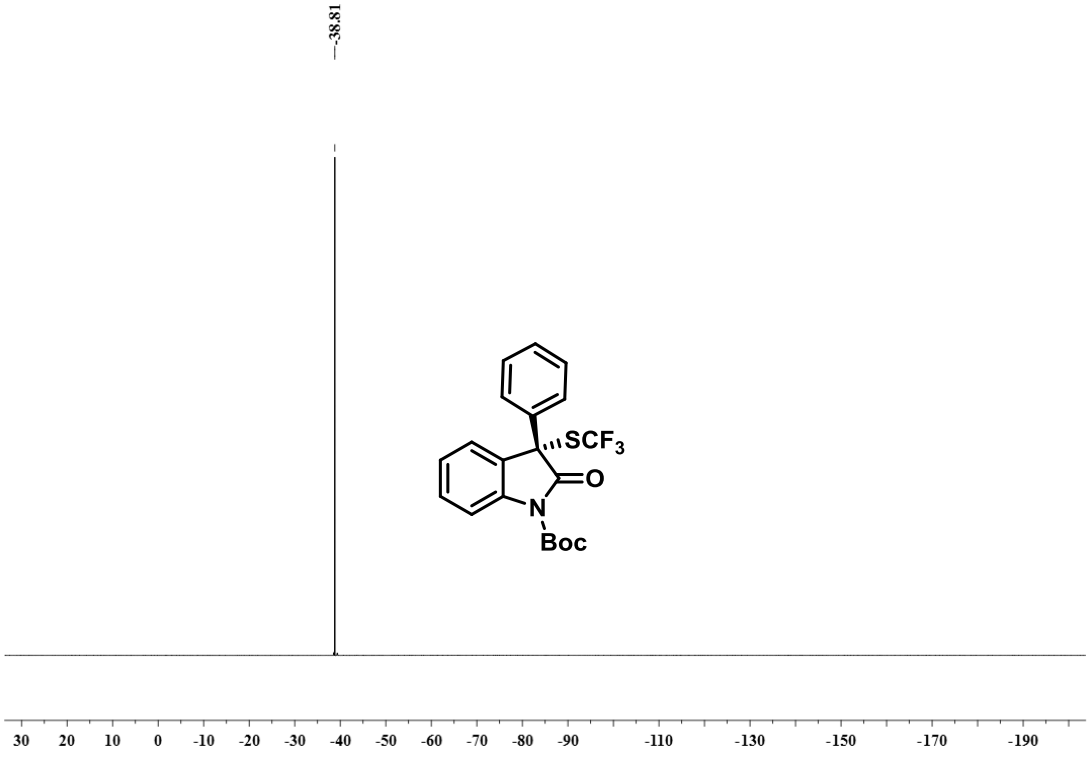
^{13}C NMR Spectrum for

(S)-*tert*-Butyl2-oxo-3-phenyl-3-((trifluoromethyl)thio)indoline-1-carboxylate 4k



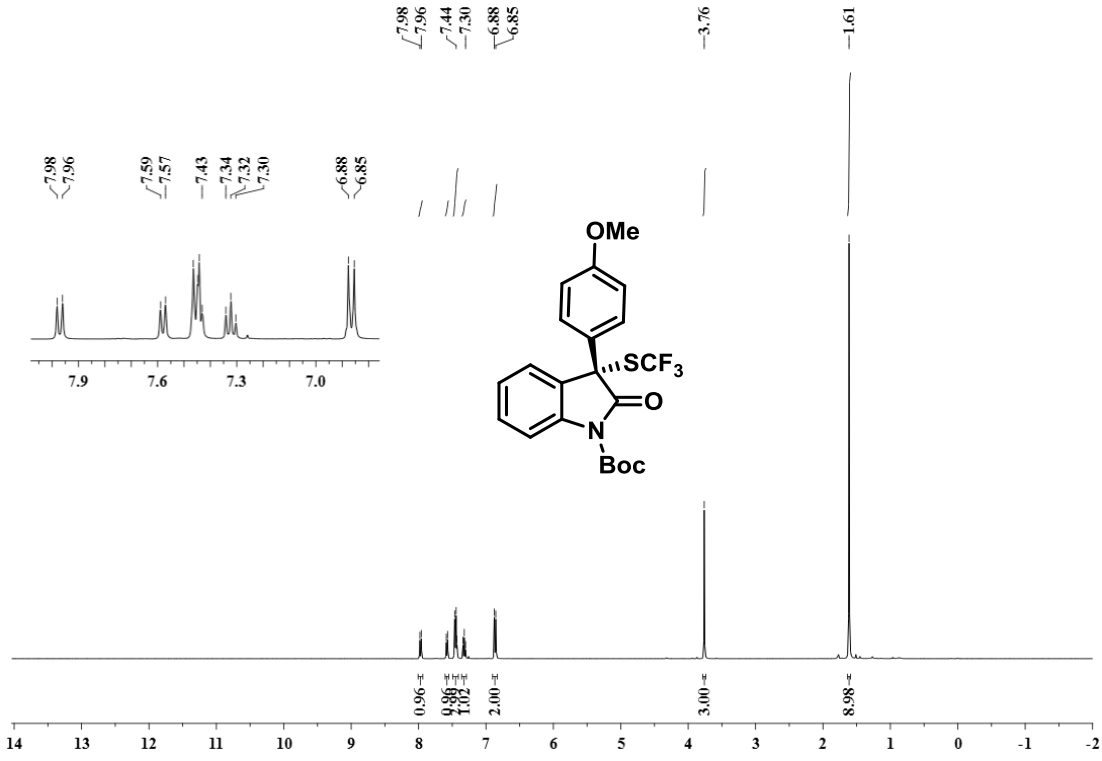
^{19}F NMR Spectrum for

(S)-*tert*-Butyl2-oxo-3-phenyl-3-((trifluoromethyl)thio)indoline-1-carboxylate 4k



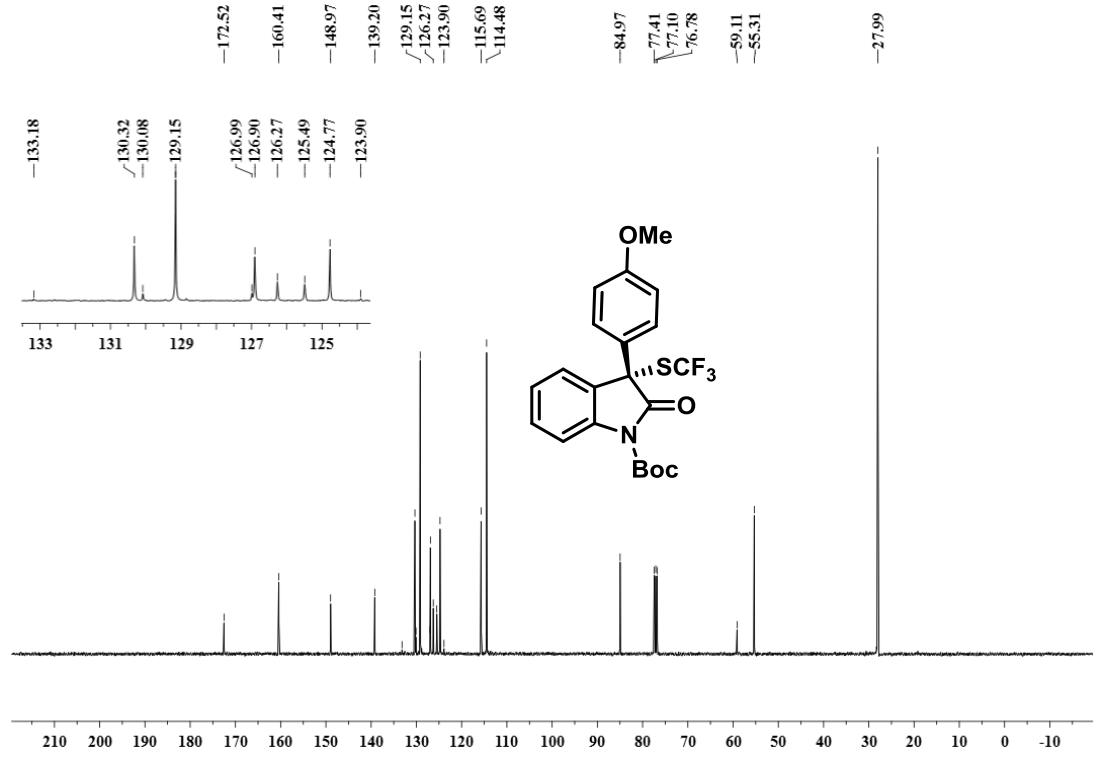
^{1}H NMR Spectrum for

(S)-*tert*-Butyl-3-(4-methoxyphenyl)-2-oxo-3-((trifluoromethyl)thio)indoline-1-carboxylate 4l



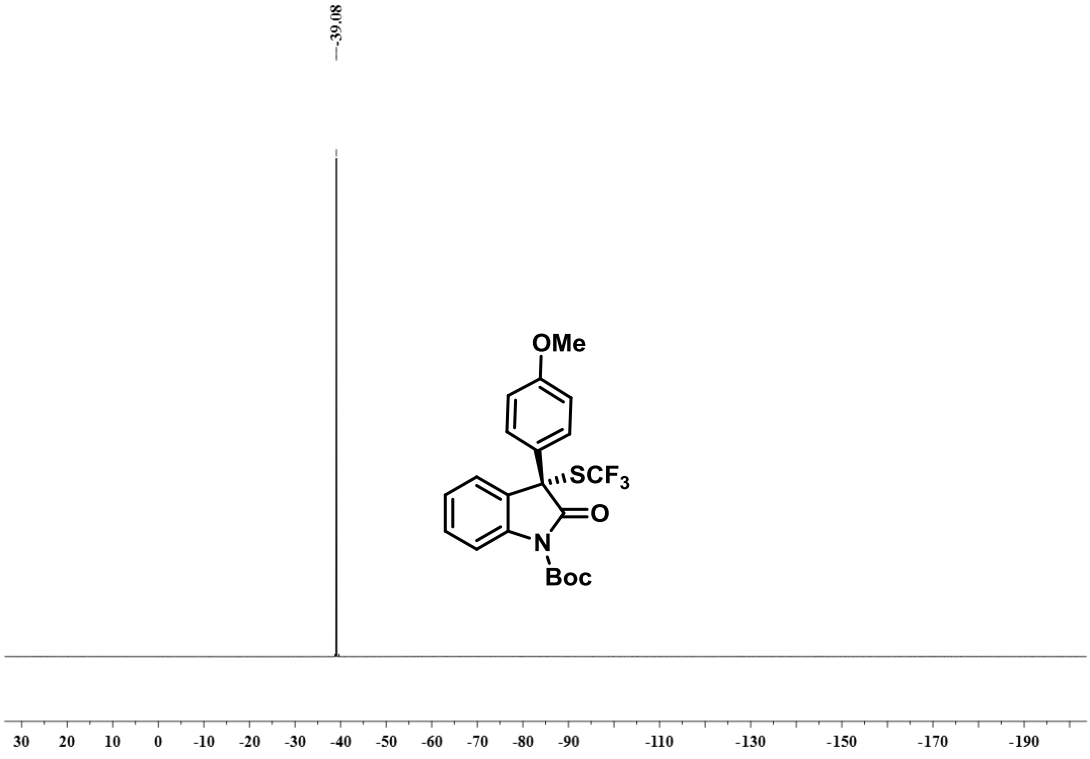
^{13}C NMR Spectrum for

(S)-*tert*-Butyl-3-(4-methoxyphenyl)-2-oxo-3-((trifluoromethyl)thio)indoline-1-carboxylate 4l



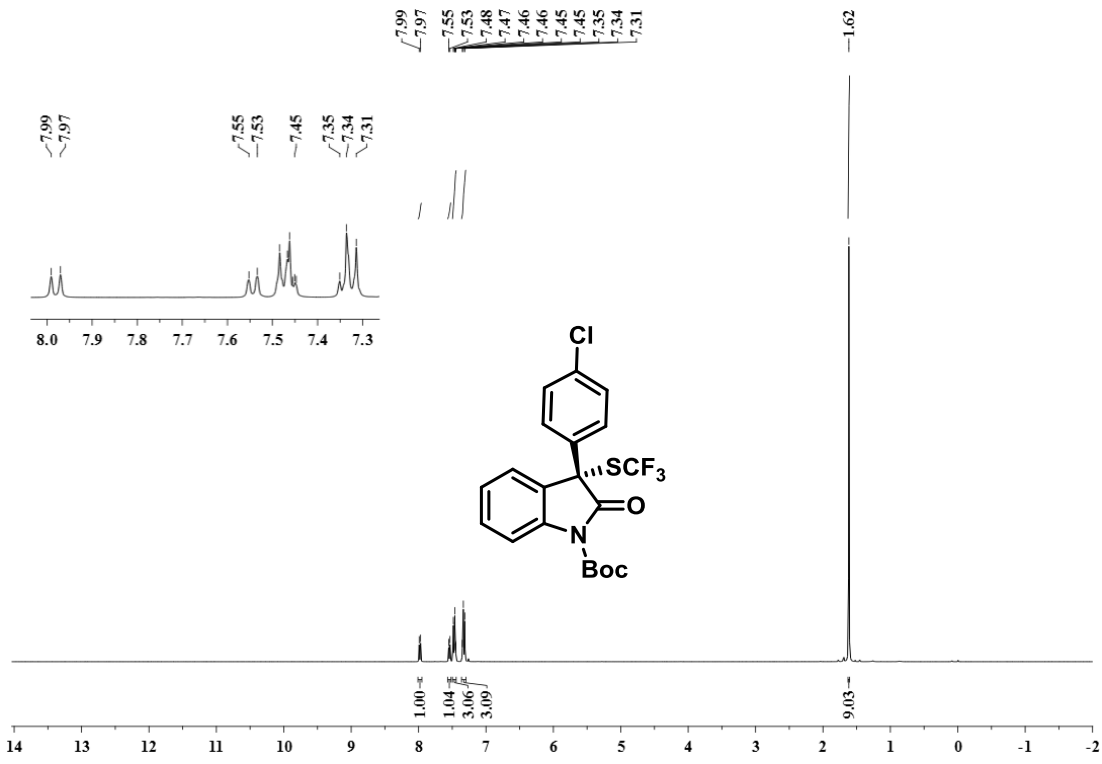
^{19}F NMR Spectrum for

(S)-*tert*-Butyl-3-(4-methoxyphenyl)-2-oxo-3-((trifluoromethyl)thio)indoline-1-carboxylate 4l



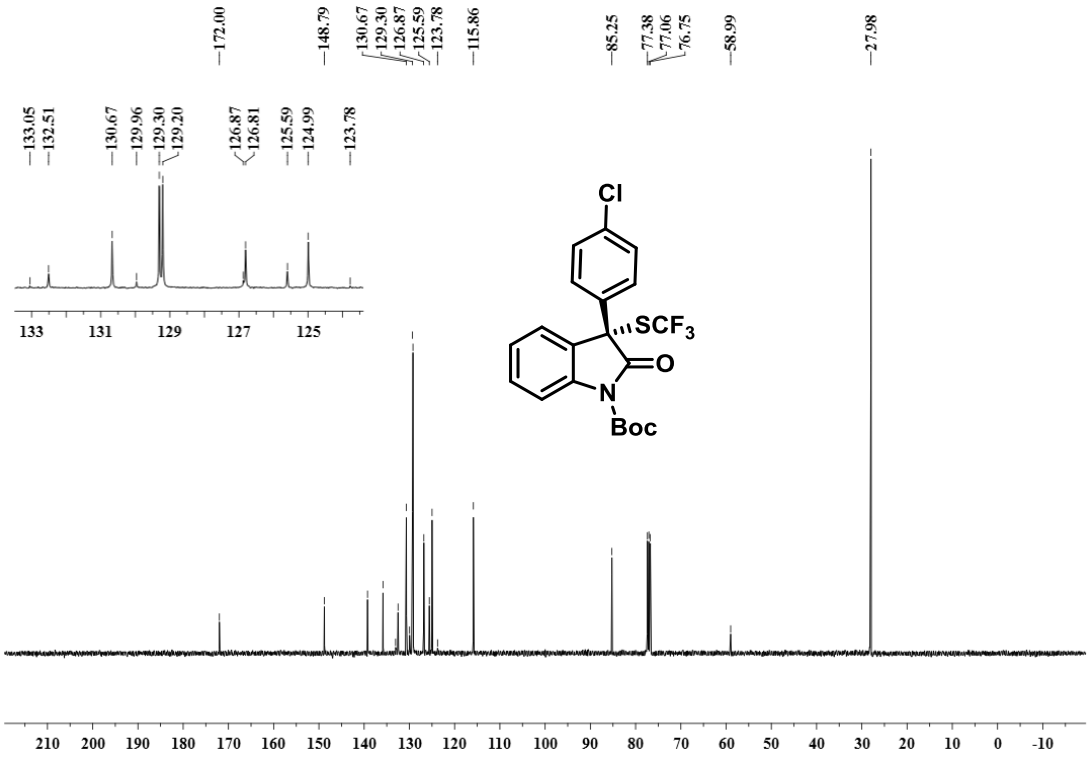
^{1}H NMR Spectrum for

(S)-*tert*-Butyl-3-(4-chlorophenyl)-2-oxo-3-((trifluoromethyl)thio)indoline-1-carboxylate 4m



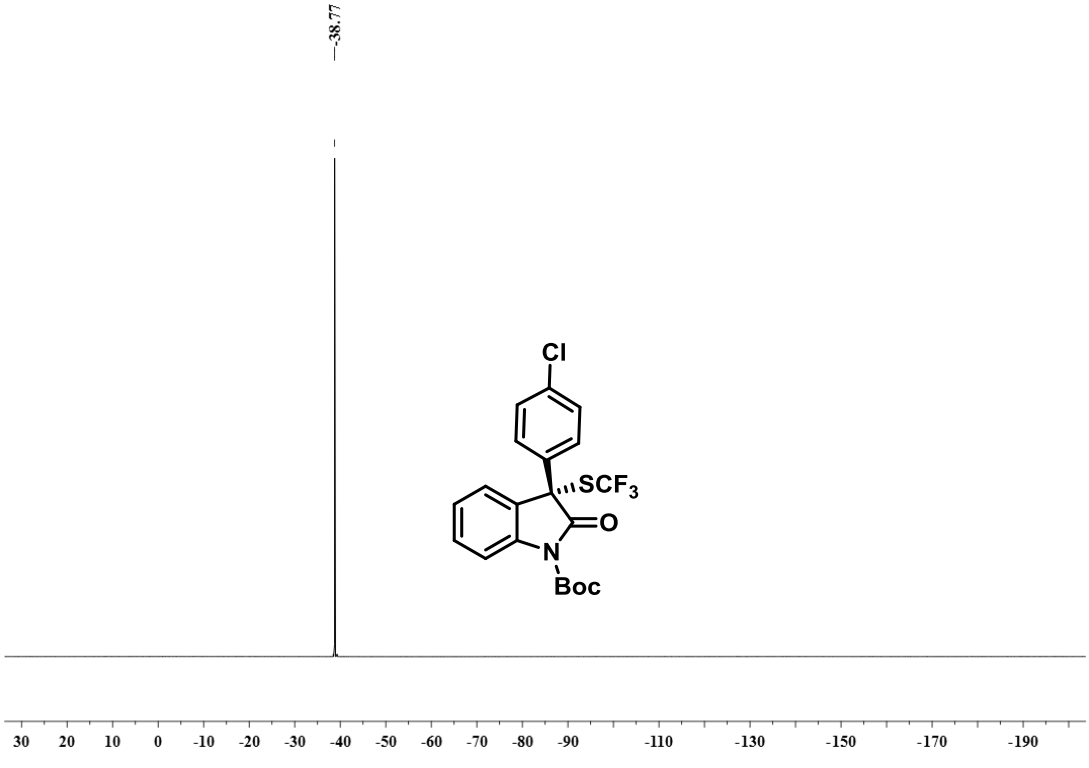
^{13}C NMR Spectrum for

(S)-*tert*-Butyl-3-(4-chlorophenyl)-2-oxo-3-((trifluoromethyl)thio)indoline-1-carboxylate 4m



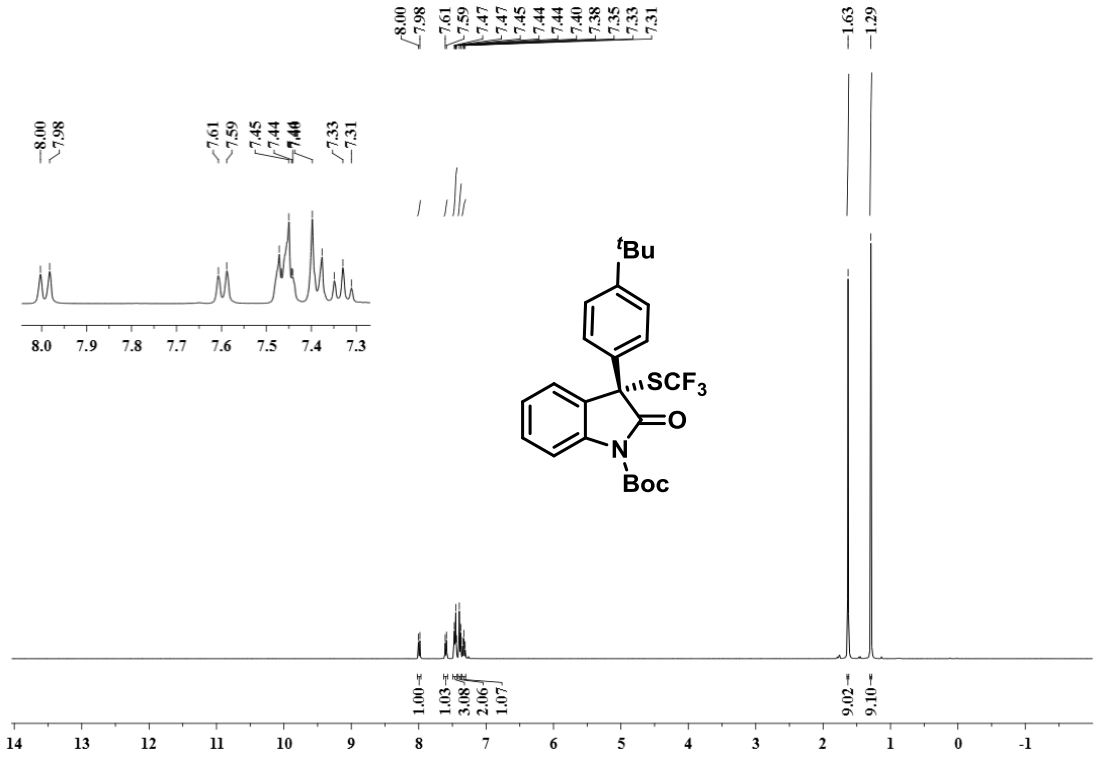
^{19}F NMR Spectrum for

(S)-*tert*-Butyl-3-(4-chlorophenyl)-2-oxo-3-((trifluoromethyl)thio)indoline-1-carboxylate 4m



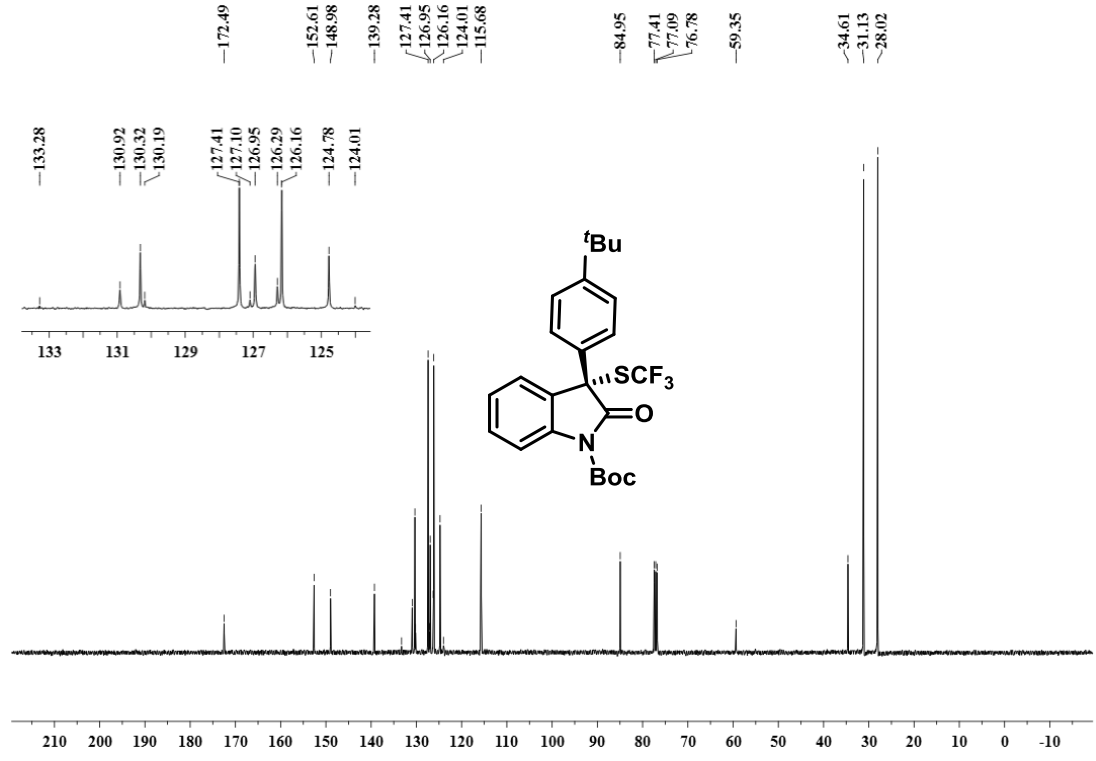
^{1}H NMR Spectrum for

(S)-*tert*-Butyl-3-(4-(*tert*-butyl)phenyl)-2-oxo-3-((trifluoromethyl)thio)indoline-1-carboxylate 4n



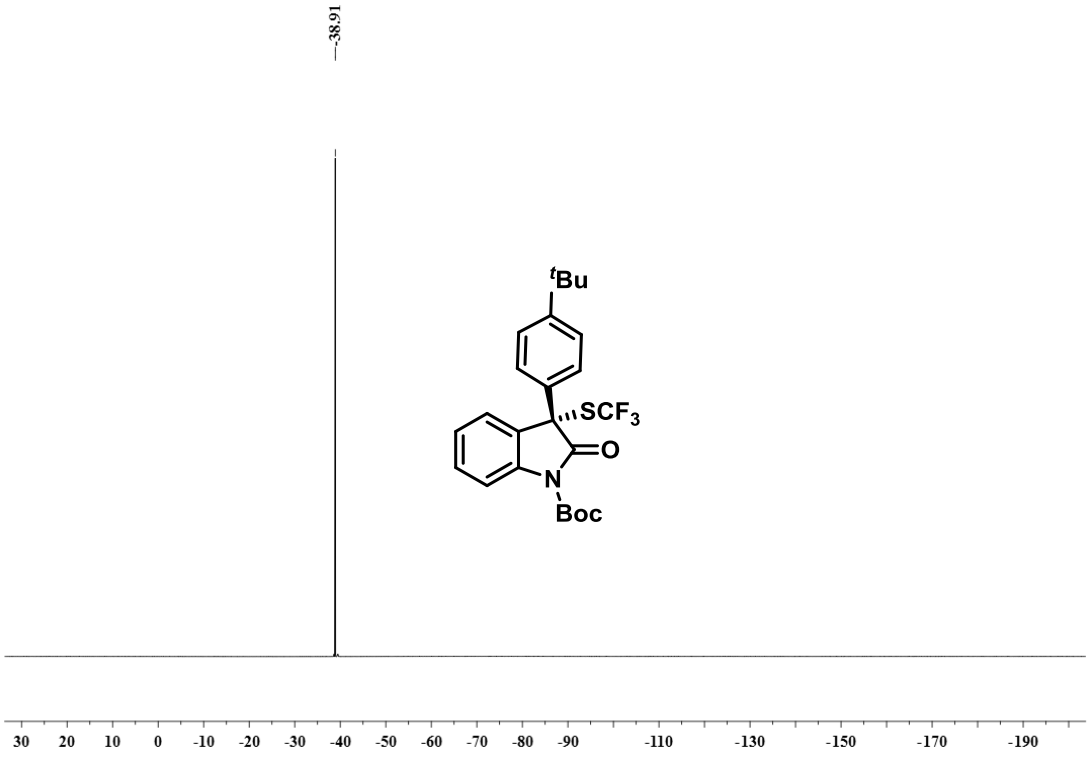
^{13}C NMR Spectrum for

(S)-*tert*-Butyl-3-(4-(*tert*-butyl)phenyl)-2-oxo-3-((trifluoromethyl)thio)indoline-1-carboxylate 4n



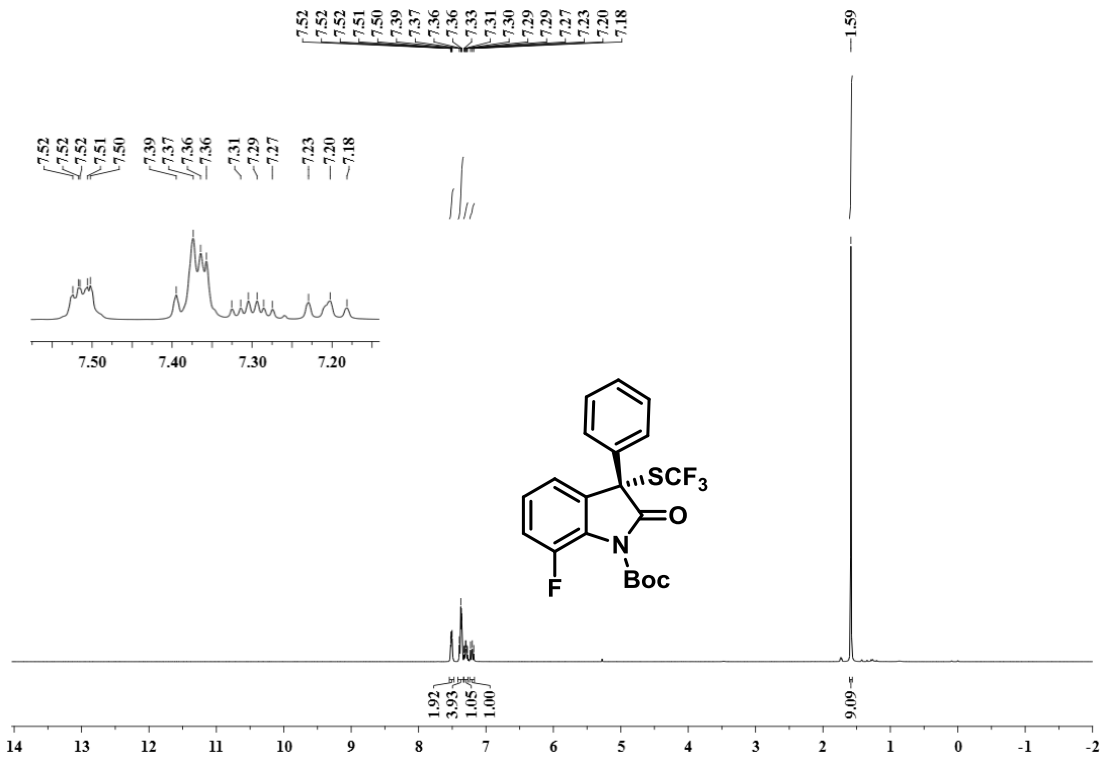
^{19}F NMR Spectrum for

(S)-*tert*-Butyl-3-(4-(*tert*-butyl)phenyl)-2-oxo-3-((trifluoromethyl)thio)indoline-1-carboxylate 4n



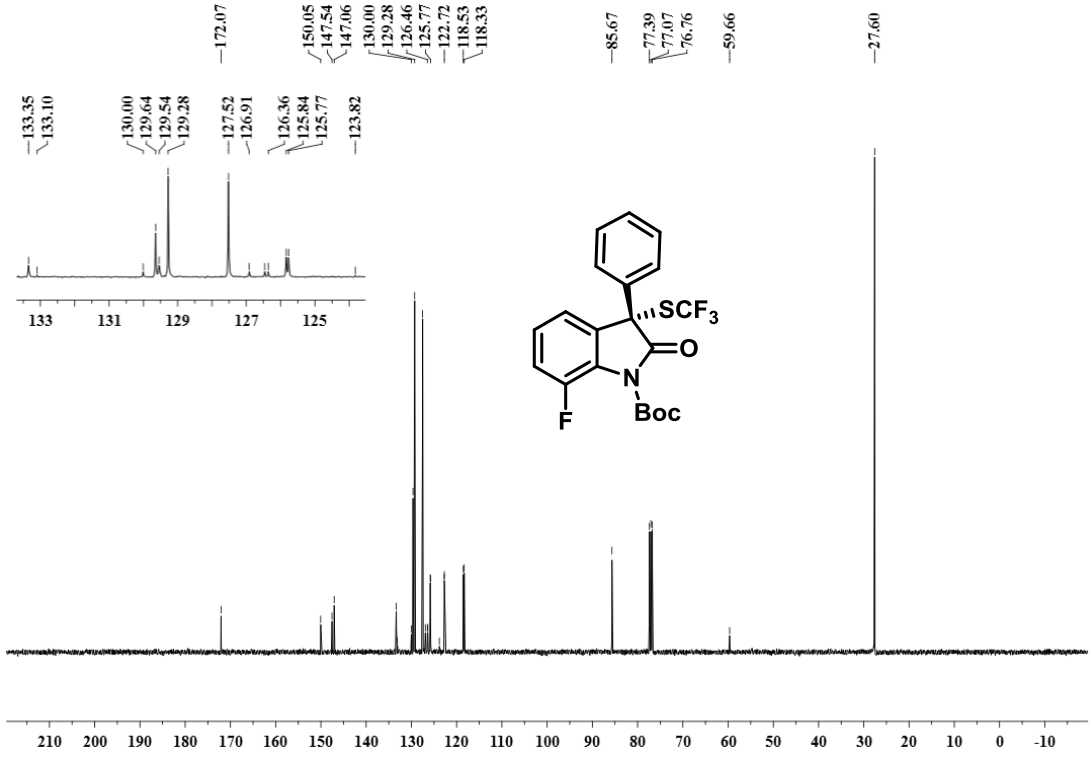
^{1}H NMR Spectrum for

(S)-*tert*-Butyl-7-fluoro-2-oxo-3-phenyl-3-((trifluoromethyl)thio)indoline-1-carboxylate 4o



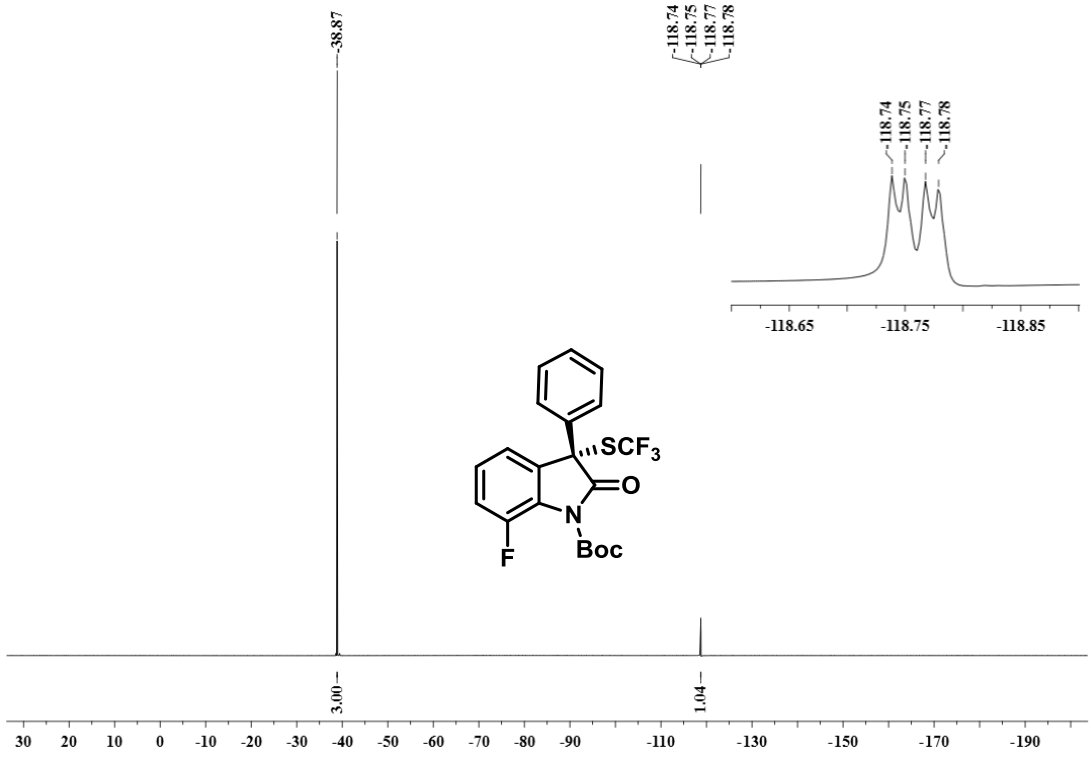
^{13}C NMR Spectrum for

(S)-*tert*-Butyl-7-fluoro-2-oxo-3-phenyl-3-((trifluoromethyl)thio)indoline-1-carboxylate 4o



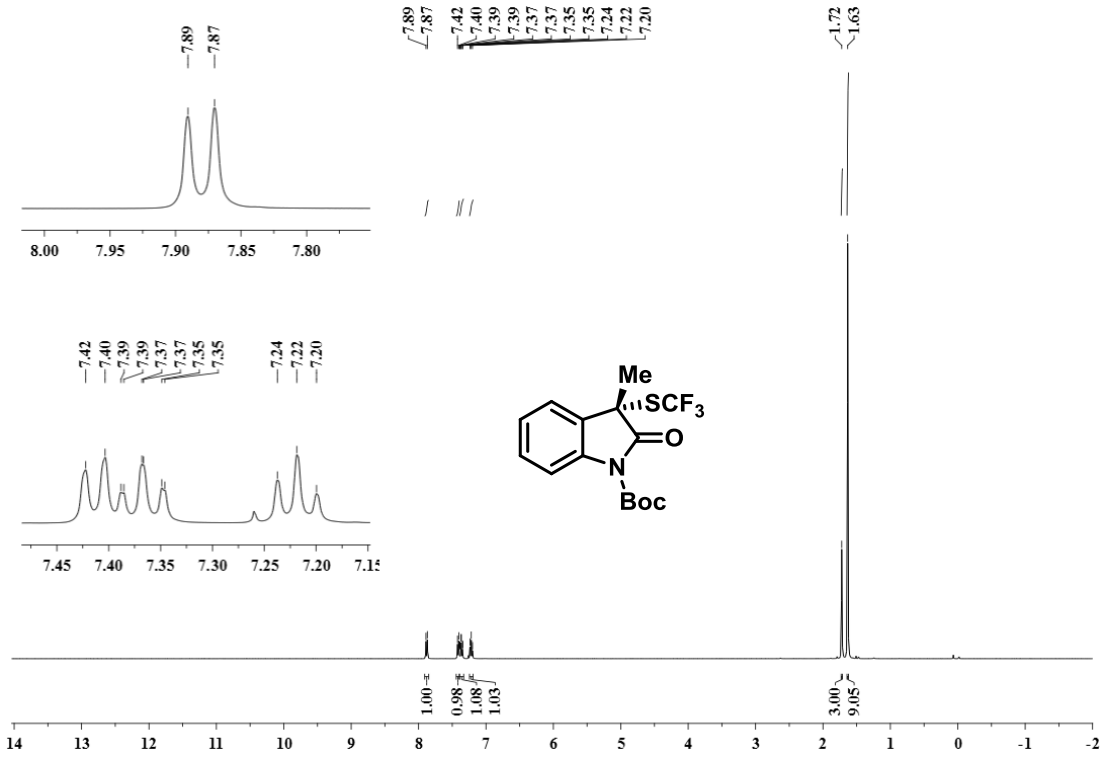
^{19}F NMR Spectrum for

(S)-*tert*-Butyl-7-fluoro-2-oxo-3-phenyl-3-((trifluoromethyl)thio)indoline-1-carboxylate 4o



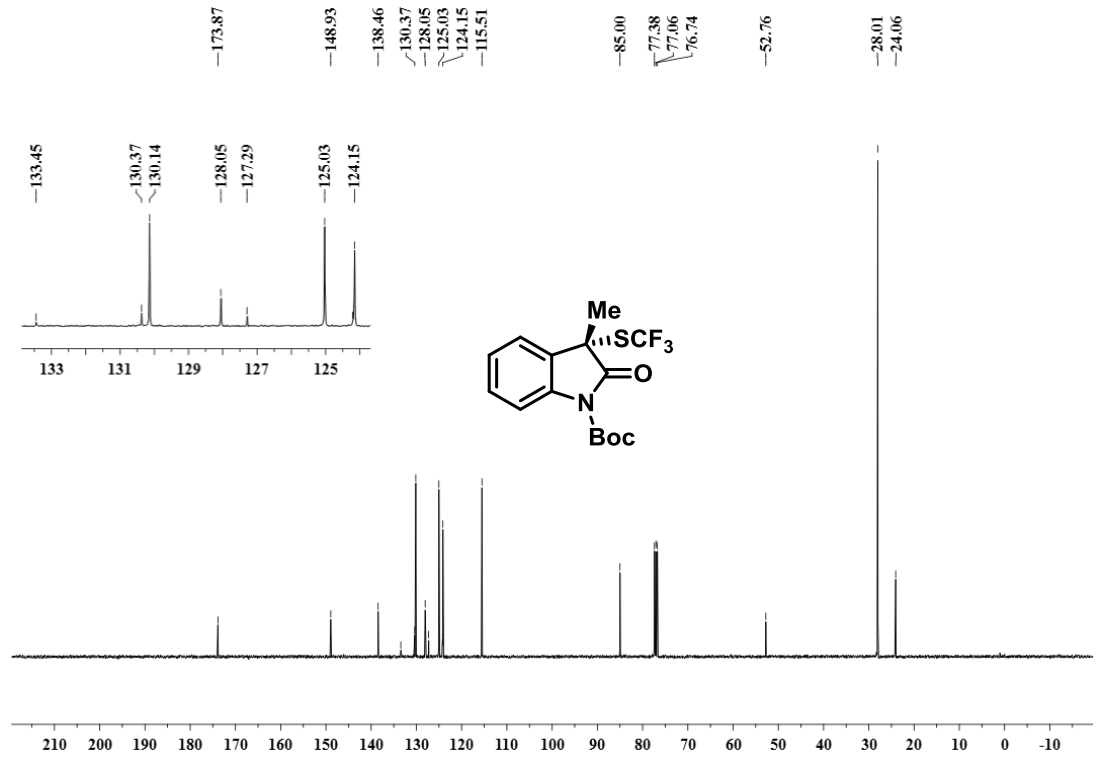
^{1}H NMR Spectrum for

(S)-*tert*-Butyl-3-methyl-2-oxo-3-((trifluoromethyl)thio)indoline-1-carboxylate 4p



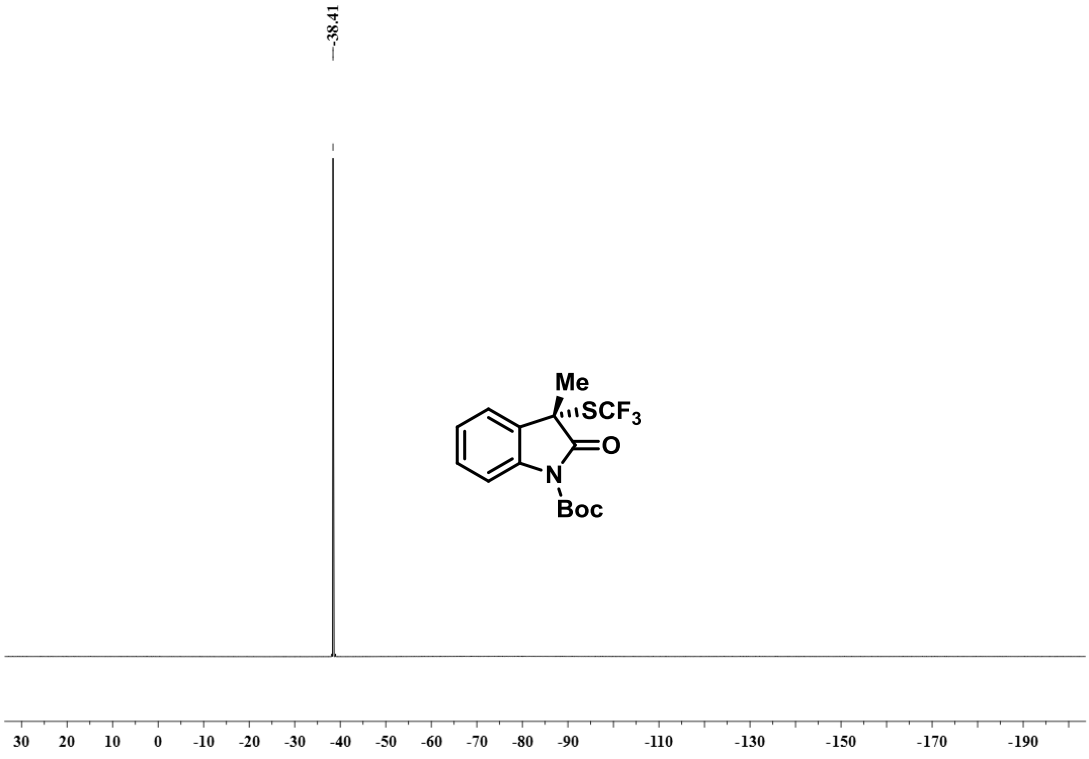
^{13}C NMR Spectrum for

(S)-*tert*-Butyl-3-methyl-2-oxo-3-((trifluoromethyl)thio)indoline-1-carboxylate 4p

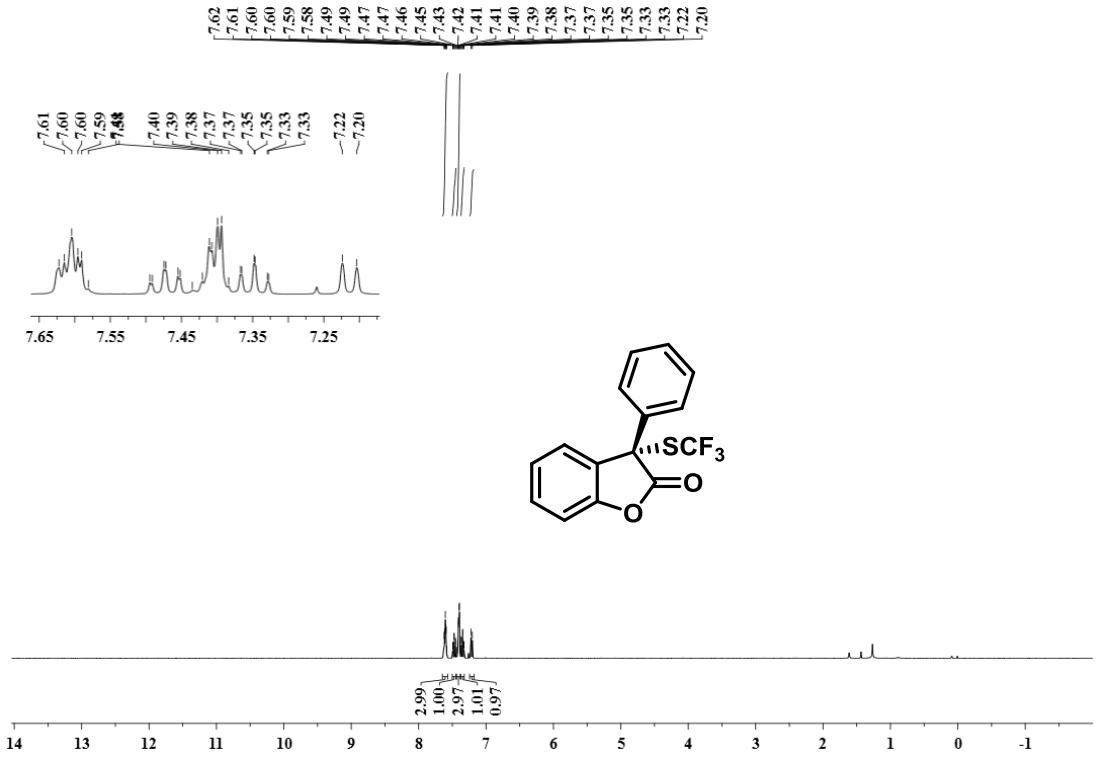


^{19}F NMR Spectrum for

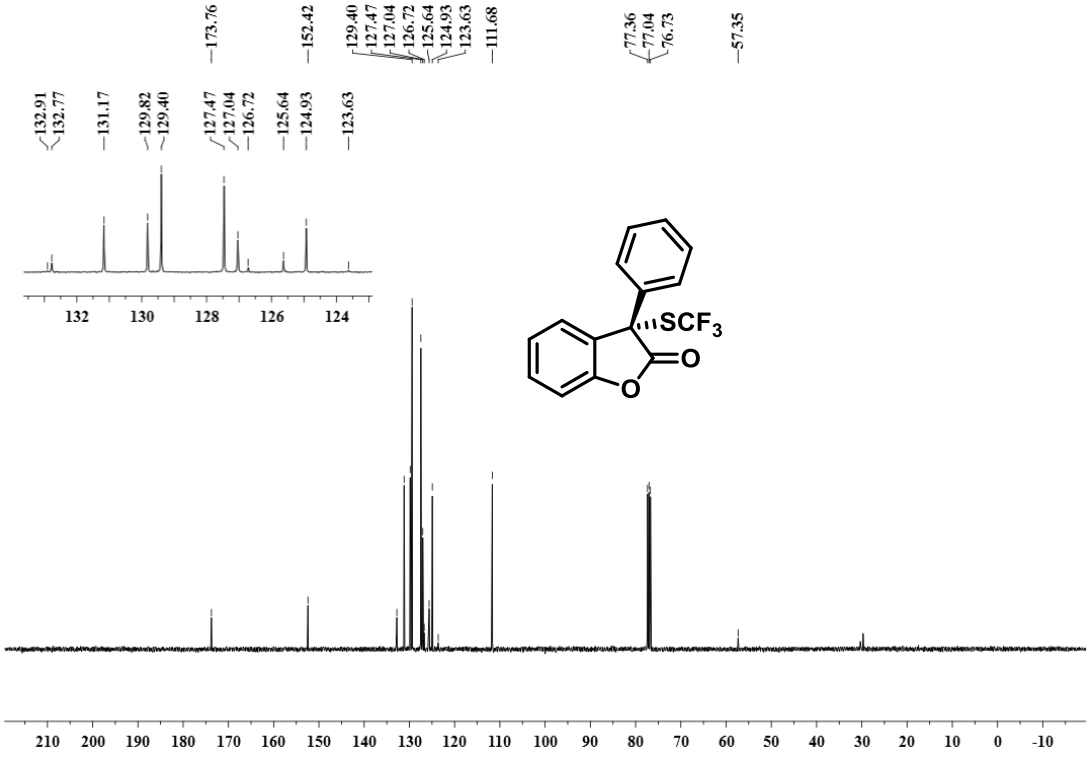
(S)-*tert*-Butyl-3-methyl-2-oxo-3-((trifluoromethyl)thio)indoline-1-carboxylate 4p



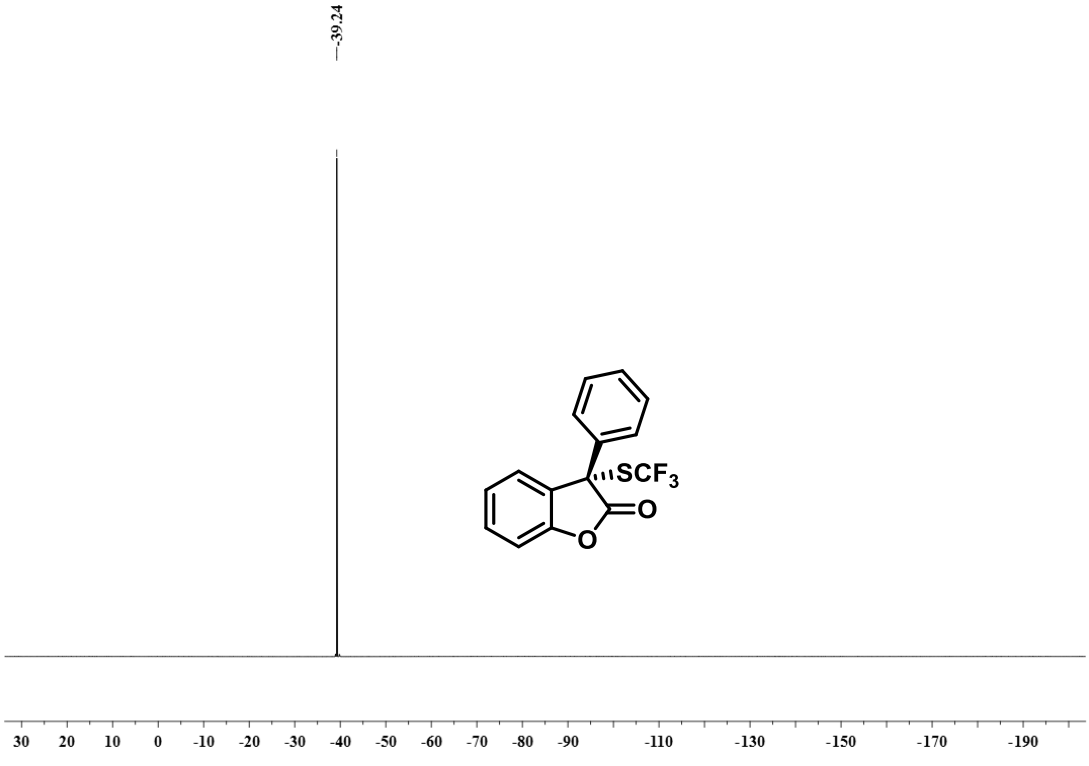
^{1}H NMR Spectrum for 3-Phenyl-3-((trifluoromethyl)thio)benzofuran-2(3*H*)-one 5a



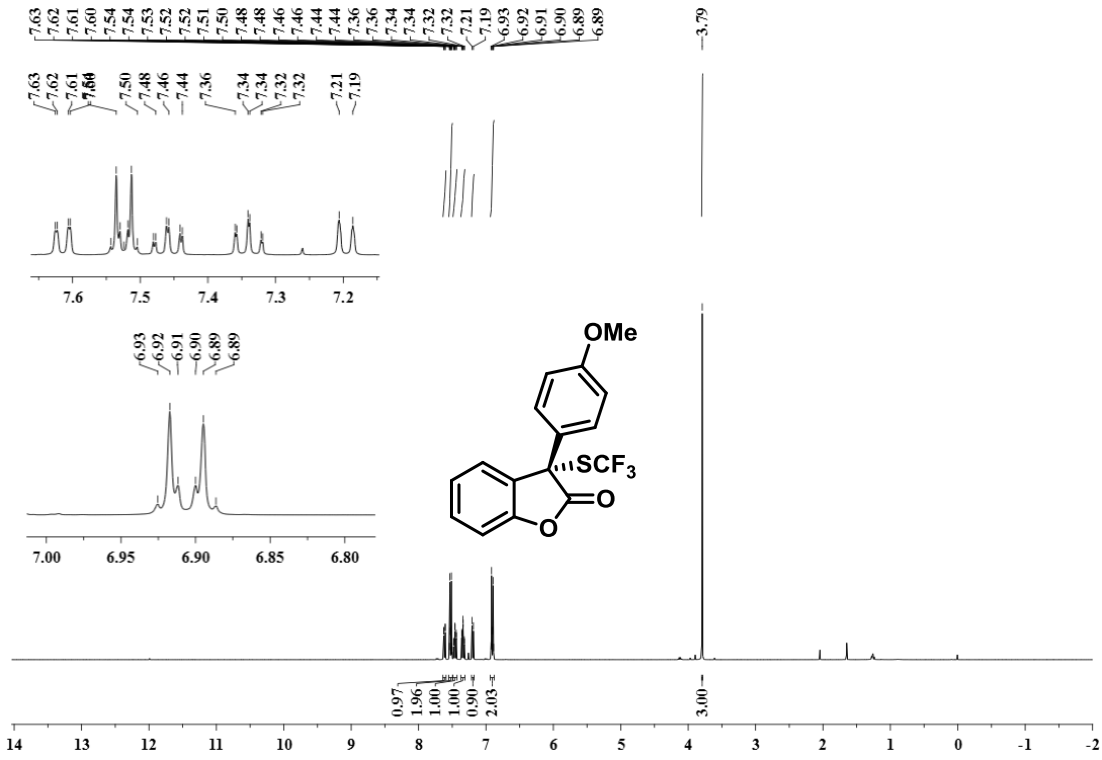
^{13}C NMR Spectrum for 3-Phenyl-3-((trifluoromethyl)thio)benzofuran-2(3H)-one 5a



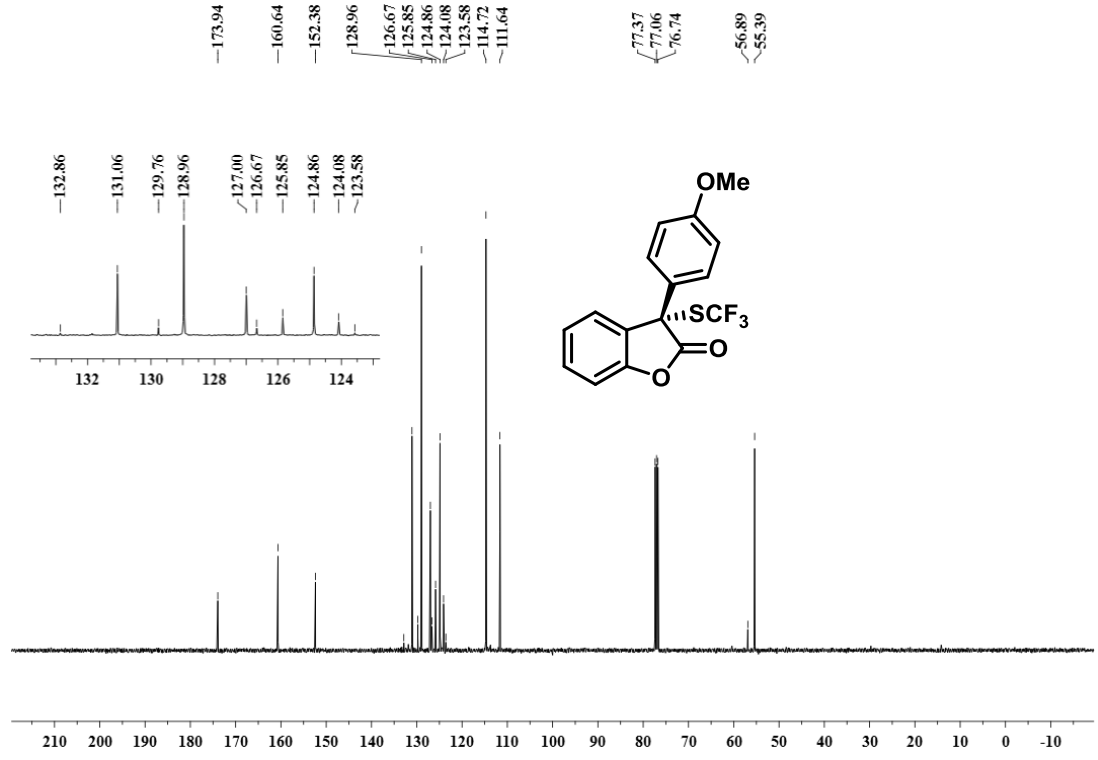
^{19}F NMR Spectrum for 3-Phenyl-3-((trifluoromethyl)thio)benzofuran-2(3H)-one 5a



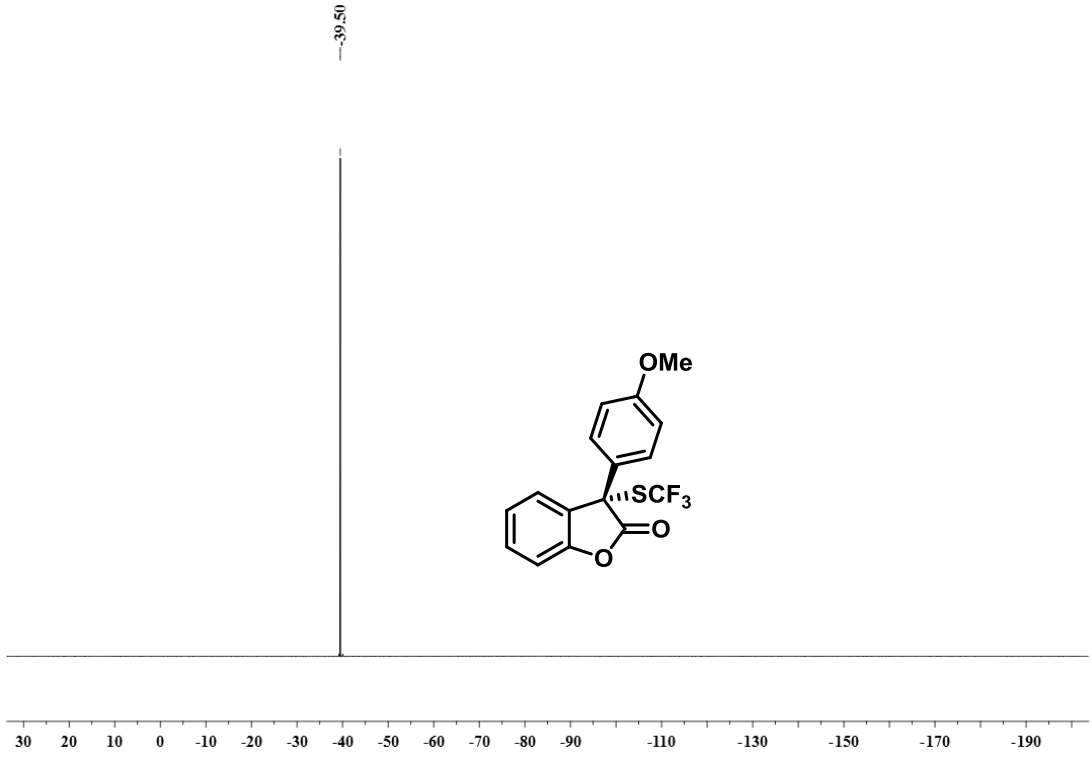
^{1}H NMR Spectrum for 3-(4-Methoxyphenyl)-3-((trifluoromethyl)thio)benzofuran-2(3*H*)-one 5b



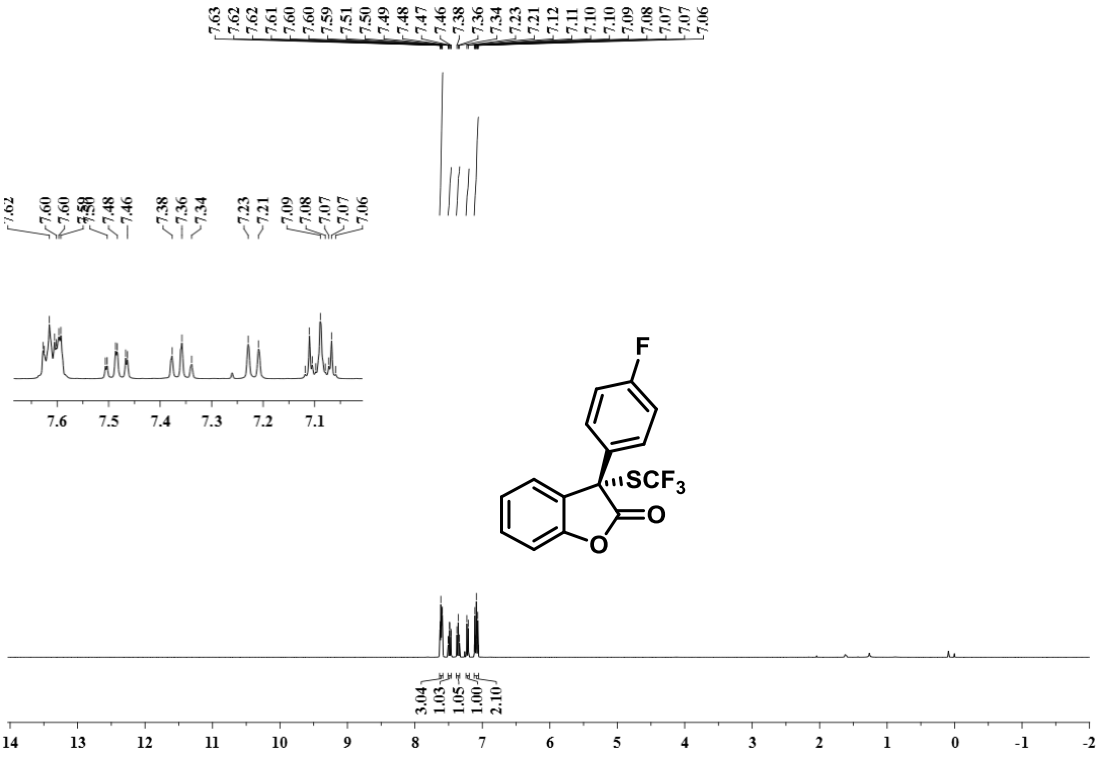
^{13}C NMR Spectrum for 3-(4-Methoxyphenyl)-3-((trifluoromethyl)thio)benzofuran-2(3*H*)-one 5b



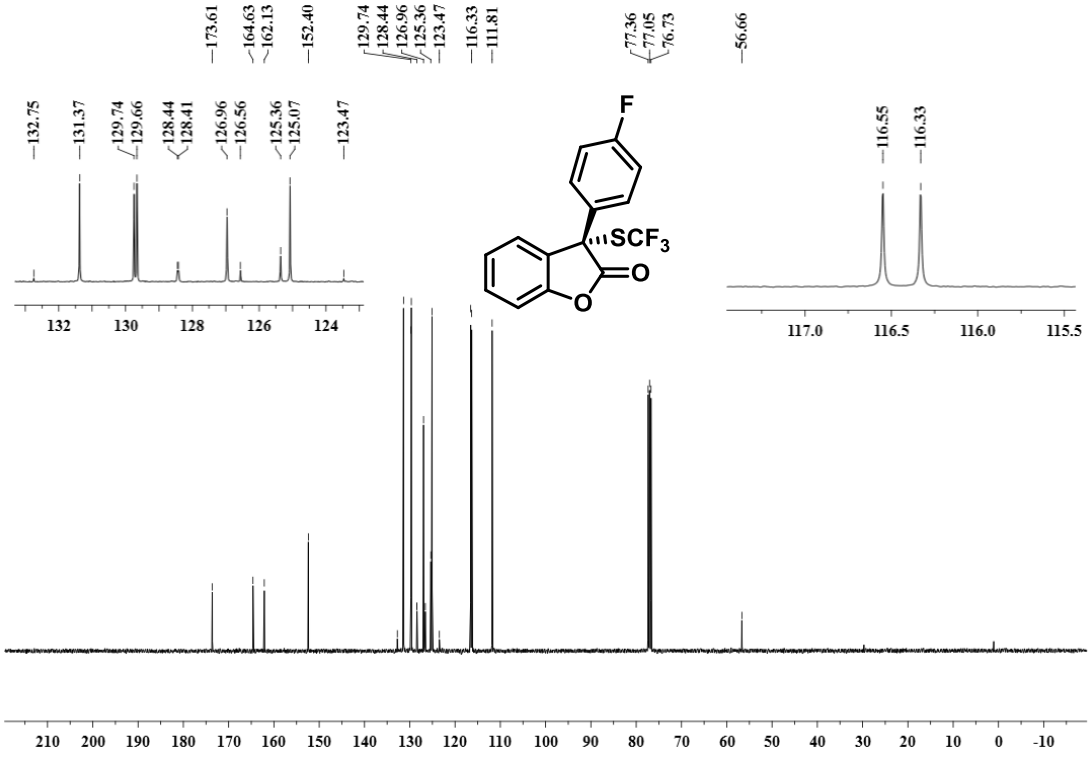
^{19}F NMR Spectrum for 3-(4-Methoxyphenyl)-3-((trifluoromethyl)thio)benzofuran-2(3*H*)-one 5b



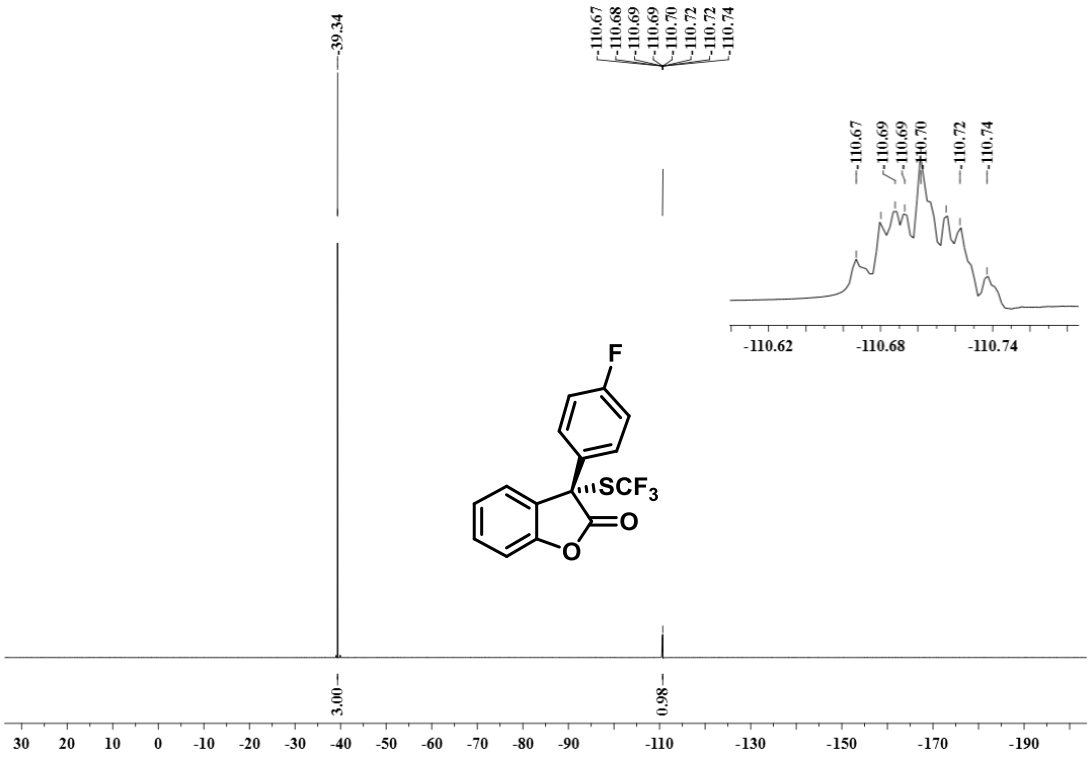
^{1}H NMR Spectrum for 3-(4-Fluorophenyl)-3-((trifluoromethyl)thio)benzofuran-2(3*H*)-one 5c



^{13}C NMR Spectrum for 3-(4-Fluorophenyl)-3-((trifluoromethyl)thio)benzofuran-2(3*H*)-one 5c

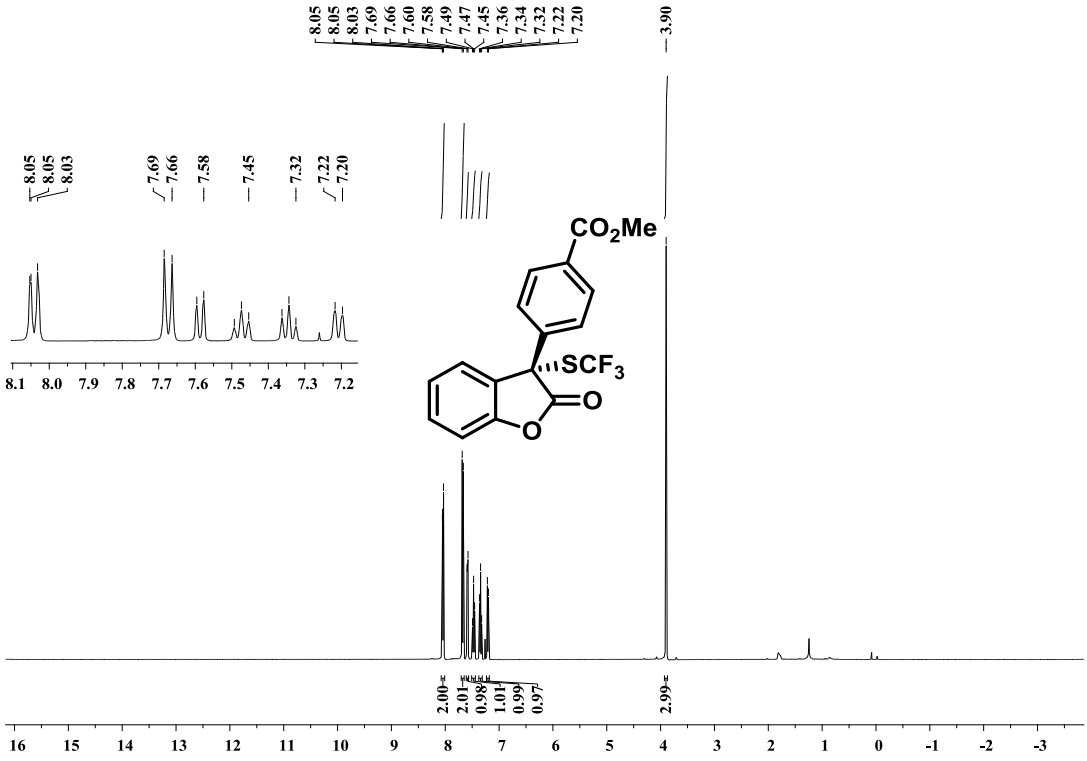


^{19}F NMR Spectrum for 3-(4-Fluorophenyl)-3-((trifluoromethyl)thio)benzofuran-2(3*H*)-one 5c



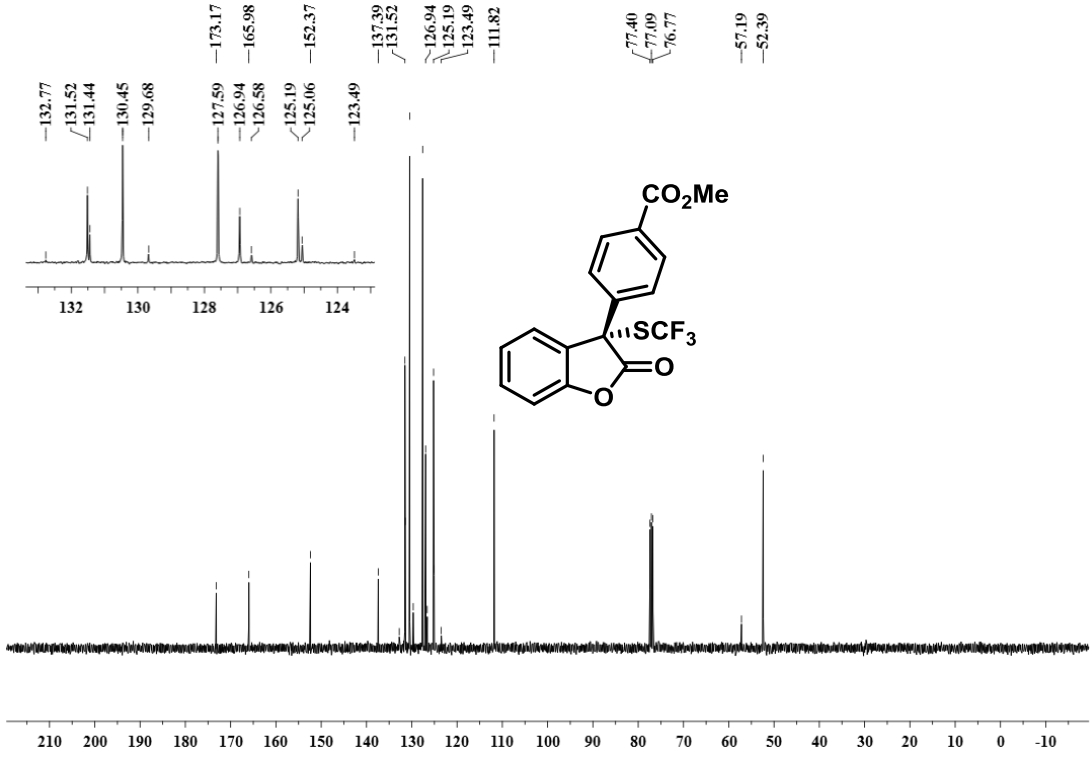
^{1}H NMR Spectrum for

Methyl-4-(2-oxo-3-((trifluoromethyl)thio)-2,3-dihydrobenzofuran-3-yl)benzoate 5d



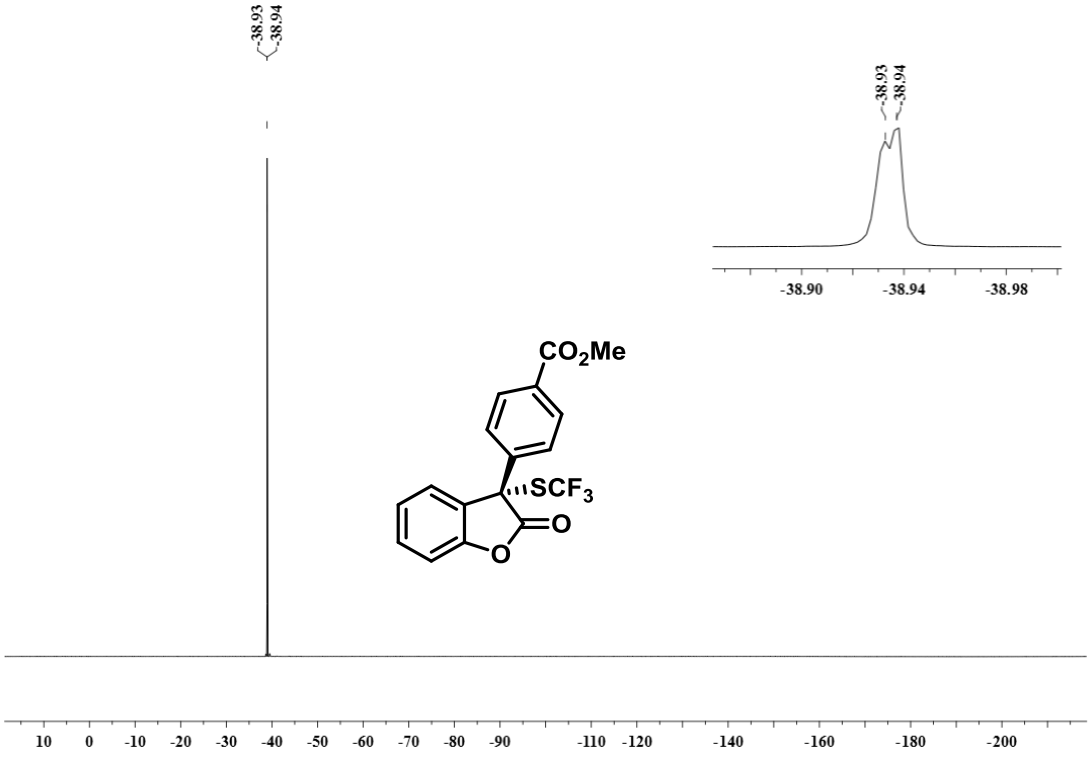
^{13}C NMR Spectrum for

Methyl-4-(2-oxo-3-((trifluoromethyl)thio)-2,3-dihydrobenzofuran-3-yl)benzoate 5d

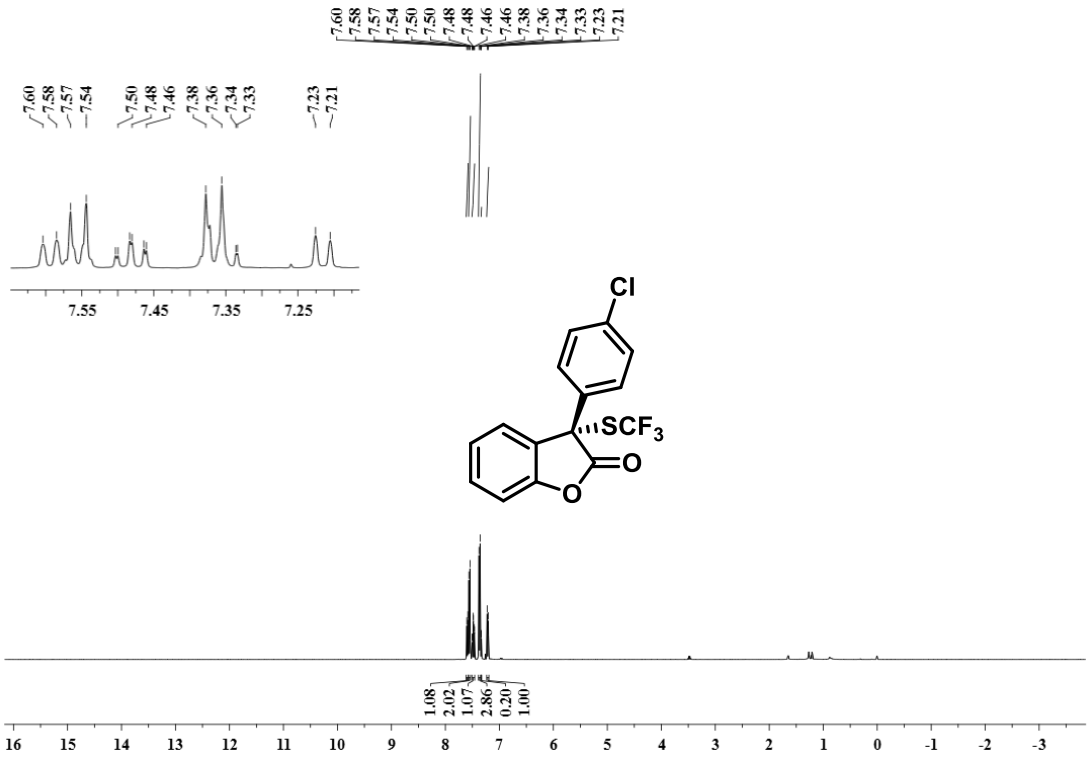


^{19}F NMR Spectrum for

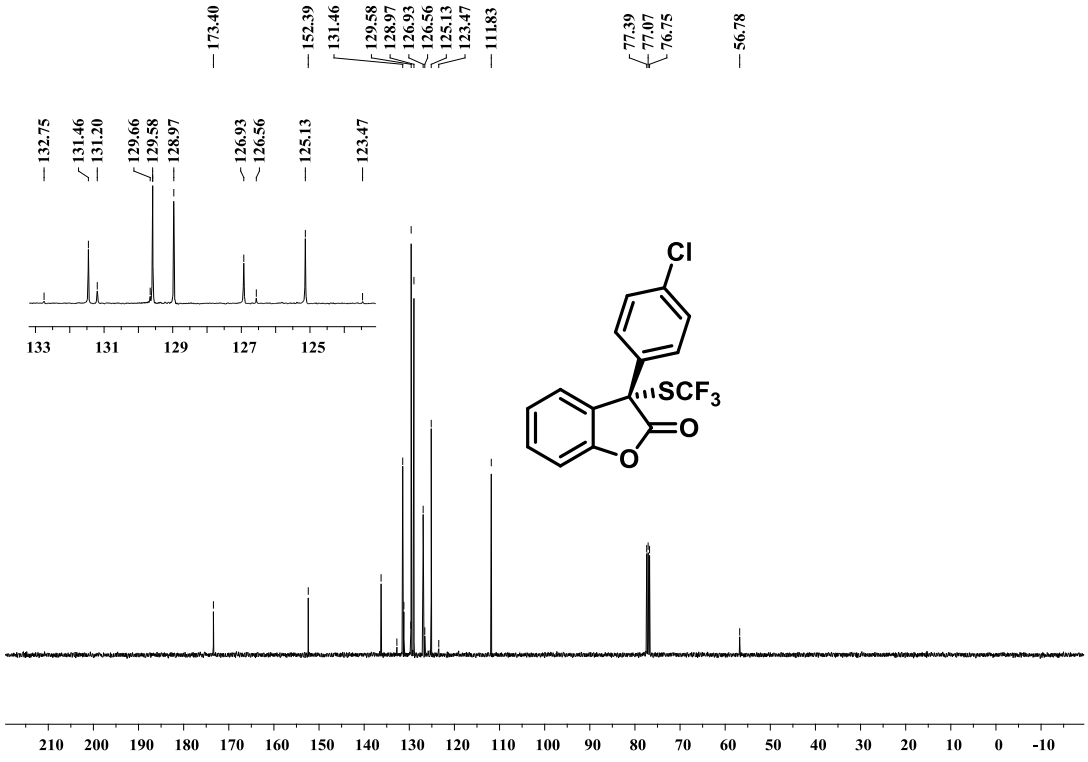
Methyl-4-(2-oxo-3-((trifluoromethyl)thio)-2,3-dihydrobenzofuran-3-yl)benzoate 5d



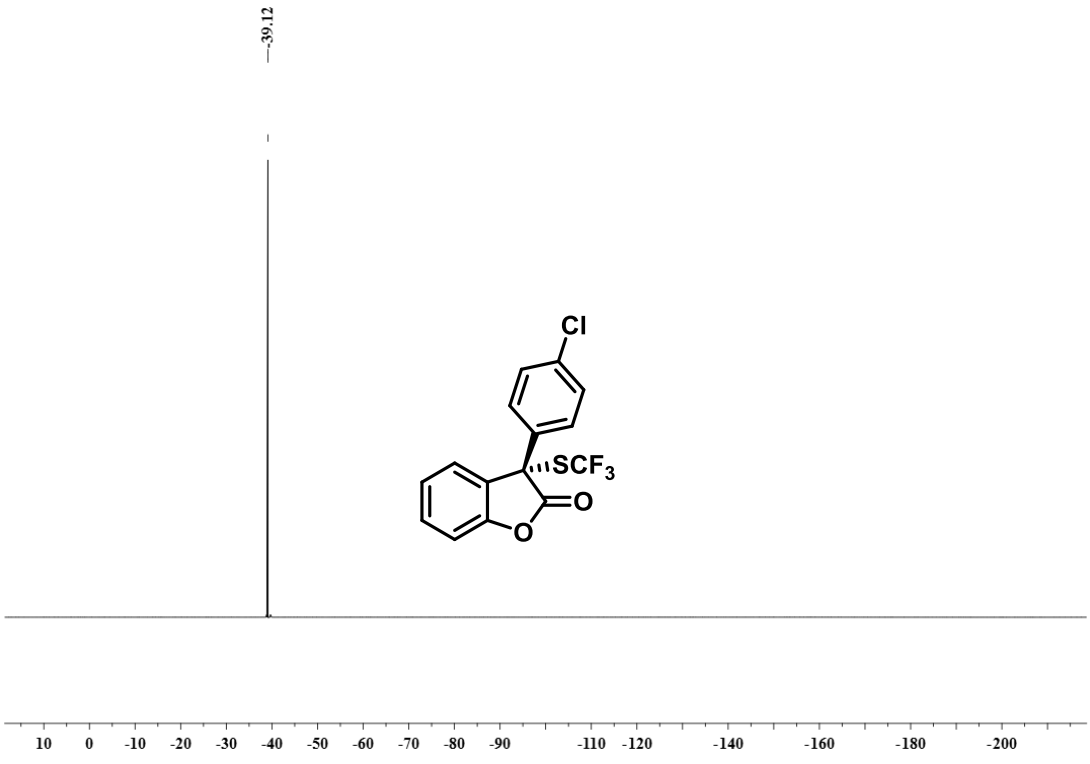
^{1}H NMR Spectrum for 3-(4-Chlorophenyl)-3-((trifluoromethyl)thio)benzofuran-2(3*H*)-one 5e



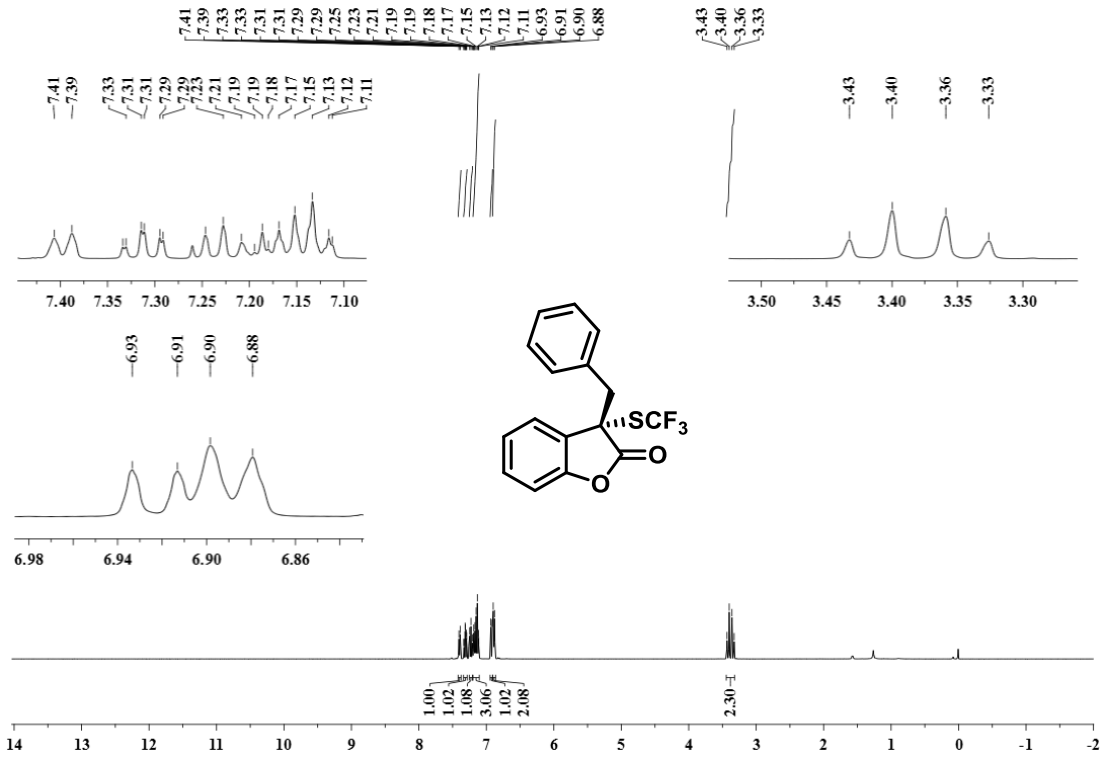
^{13}C NMR Spectrum for 3-(4-Chlorophenyl)-3-((trifluoromethyl)thio)benzofuran-2(3*H*)-one 5e



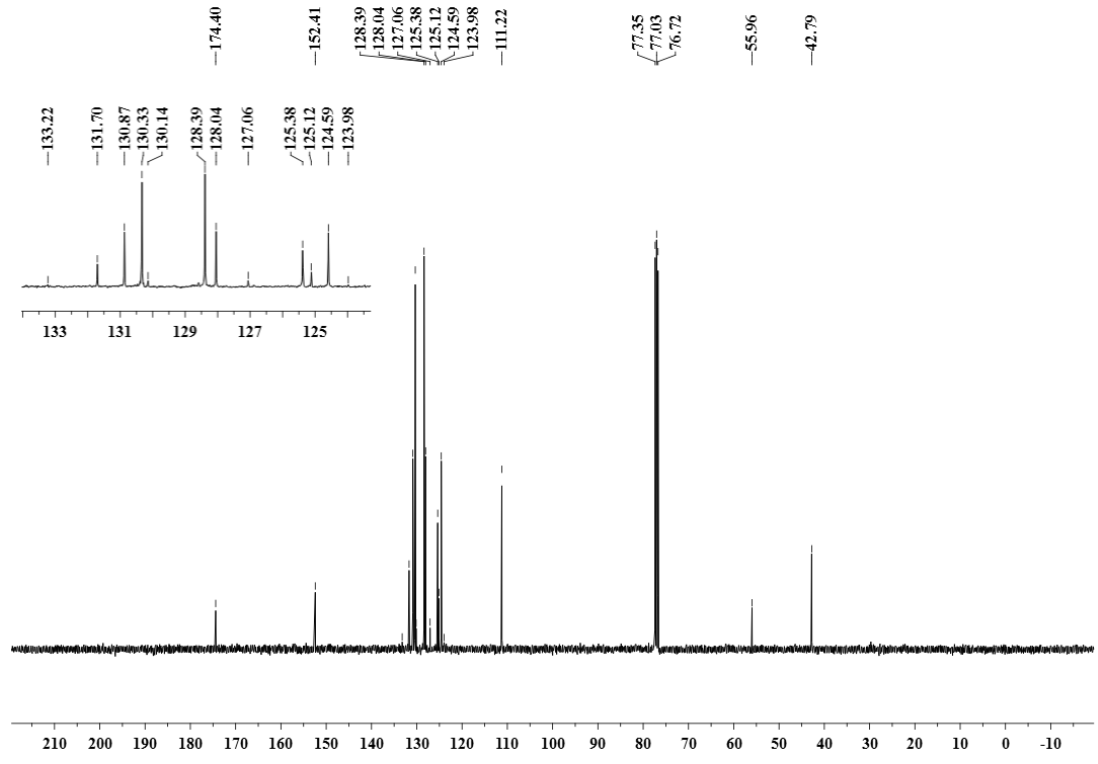
^{19}F NMR Spectrum for 3-(4-Chlorophenyl)-3-((trifluoromethyl)thio)benzofuran-2(3*H*)-one 5e



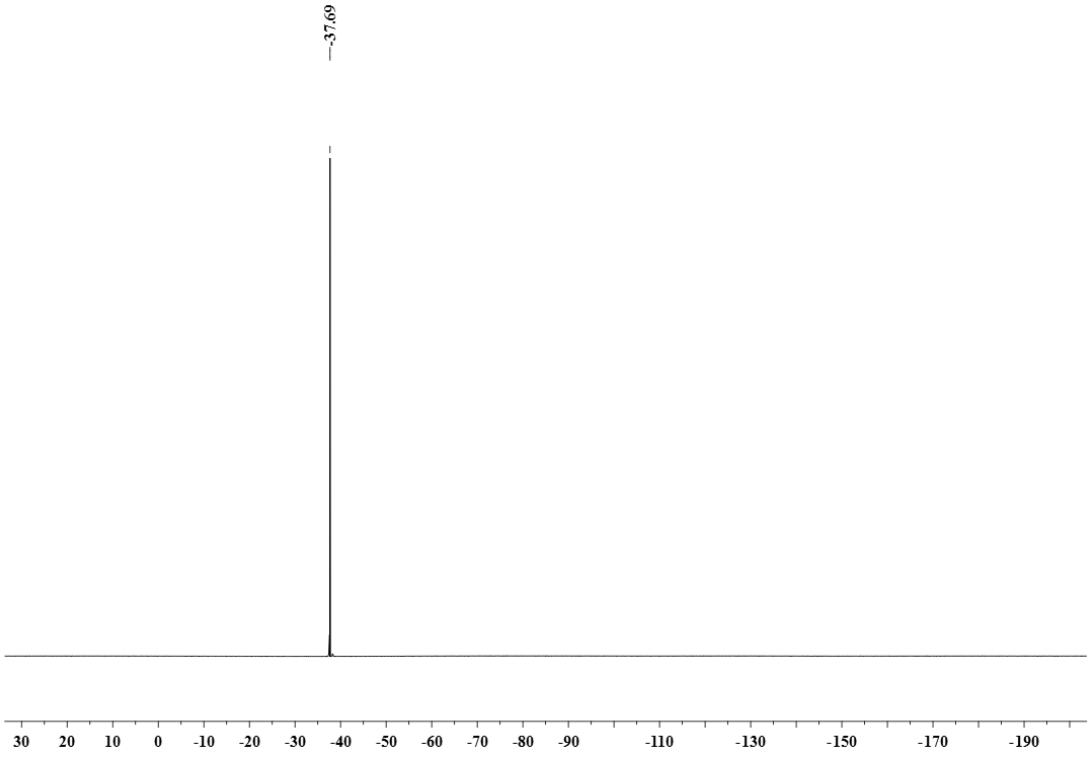
^{1}H NMR Spectrum for 3-Benzyl-3-((trifluoromethyl)thio)benzofuran-2(3*H*)-one 5f



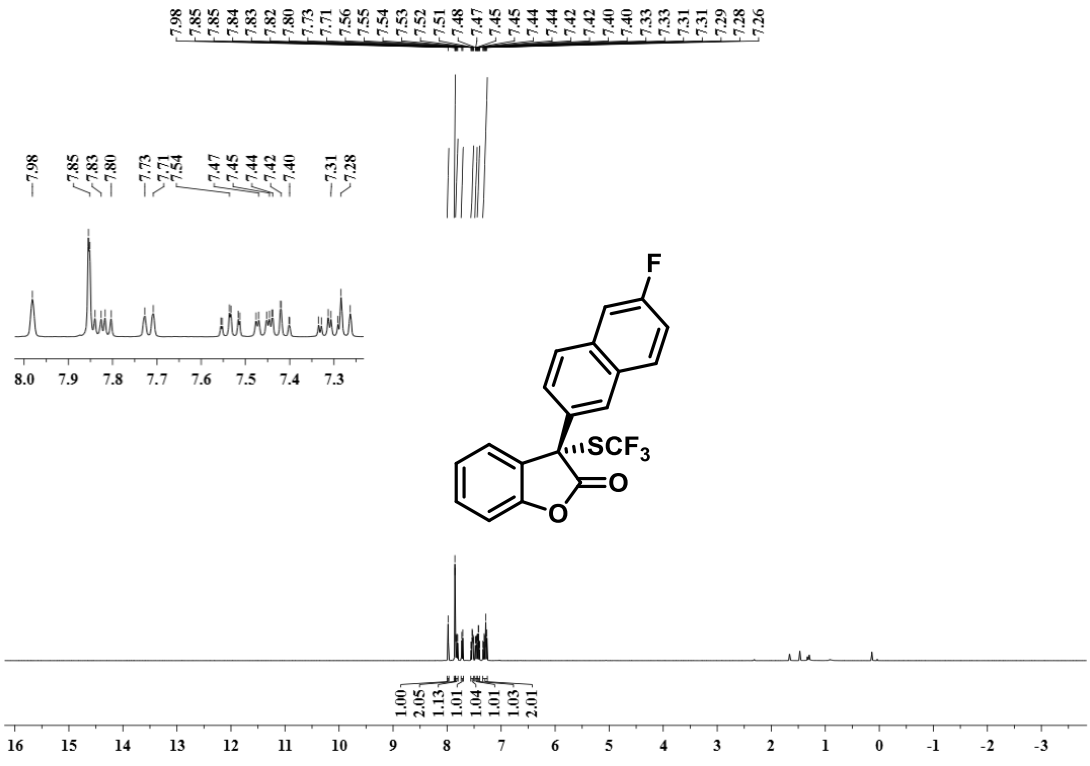
^{13}C NMR Spectrum for 3-Benzyl-3-((trifluoromethyl)thio)benzofuran-2(3*H*)-one 5f



^{19}F NMR Spectrum for 3-Benzyl-3-((trifluoromethyl)thio)benzofuran-2(3*H*)-one 5f

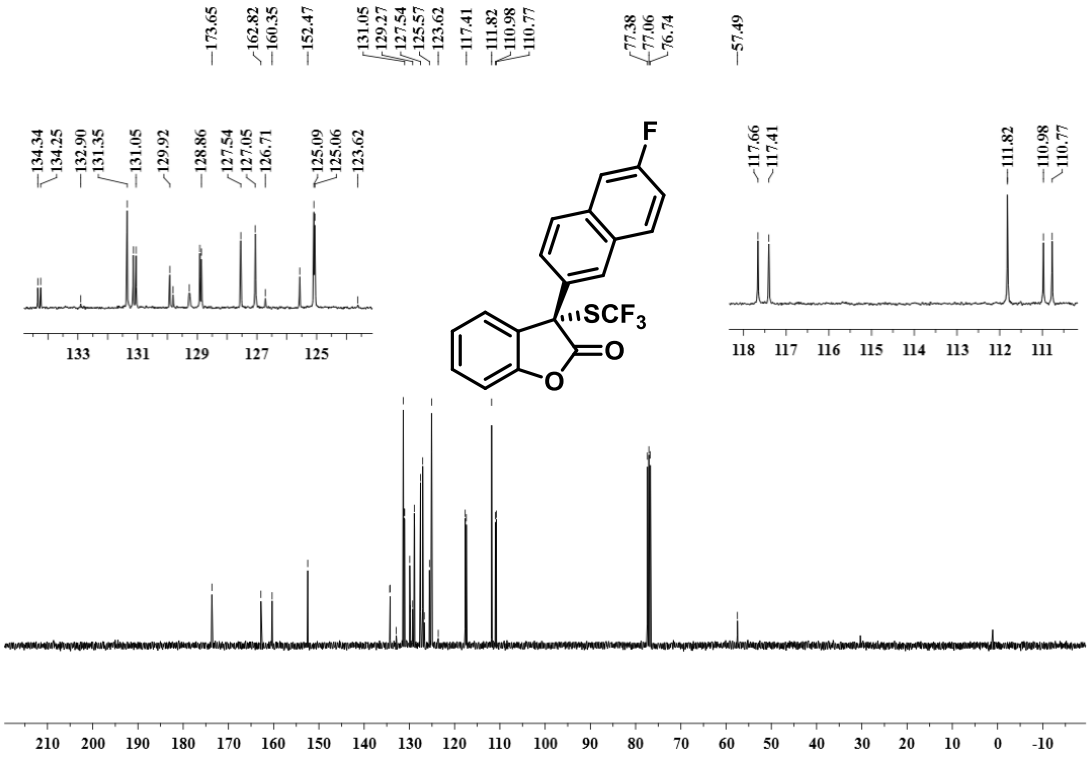


^{1}H NMR Spectrum for
3-(6-Fluoronaphthalen-2-yl)-3-((trifluoromethyl)thio)benzofuran-2(3*H*)-one 5g



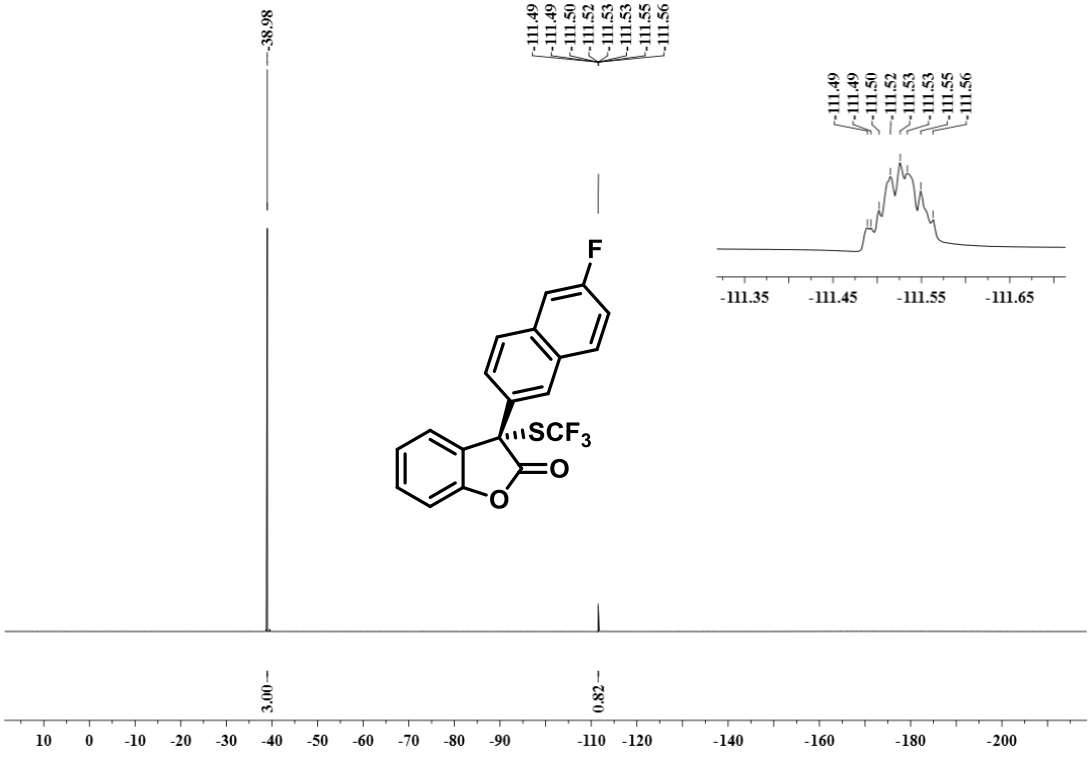
^{13}C NMR Spectrum for

3-(6-Fluoronaphthalen-2-yl)-3-((trifluoromethyl)thio)benzofuran-2(3*H*)-one 5g



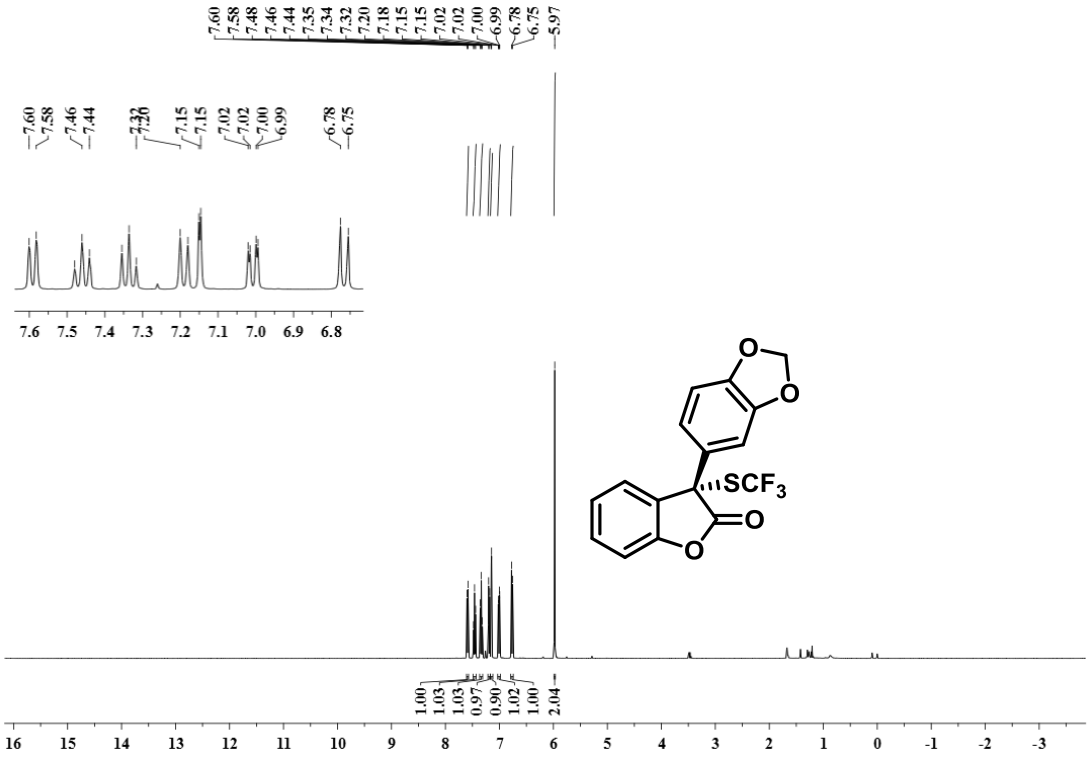
^{19}F NMR Spectrum for

3-(6-Fluoronaphthalen-2-yl)-3-((trifluoromethyl)thio)benzofuran-2(3*H*)-one 5g



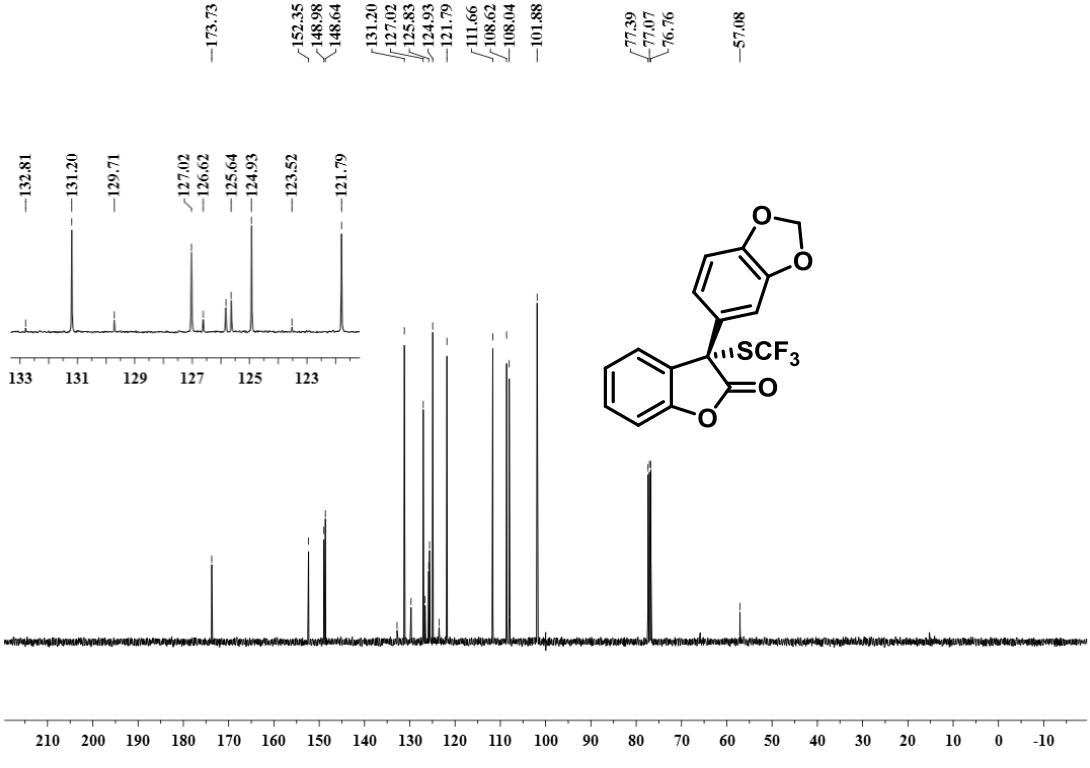
^{1}H NMR Spectrum for

3-(Benzo[d][1,3]dioxol-5-yl)-3-((trifluoromethyl)thio)benzofuran-2(3*H*)-one 5h



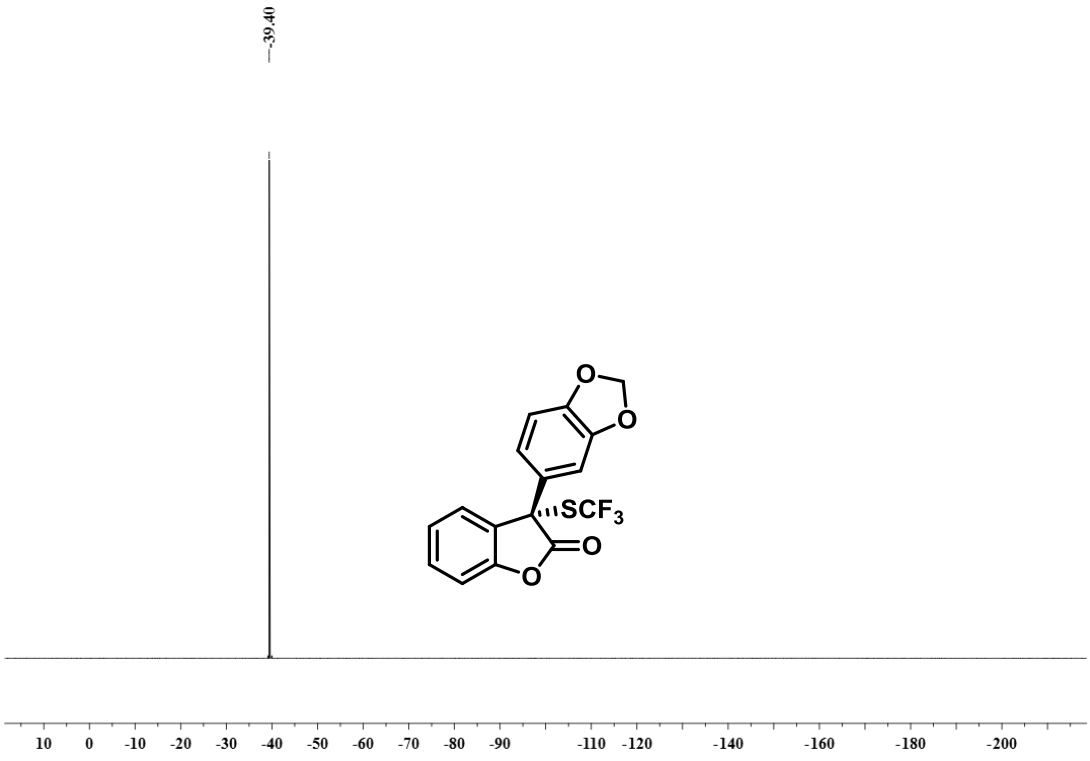
^{13}C NMR Spectrum for

3-(Benzo[d][1,3]dioxol-5-yl)-3-((trifluoromethyl)thio)benzofuran-2(3*H*)-one 5h



^{19}F NMR Spectrum for

3-(Benzo[d][1,3]dioxol-5-yl)-3-((trifluoromethyl)thio)benzofuran-2(3*H*)-one 5h



X-ray structures of compound 1a-c, 3n, 4i, 5g

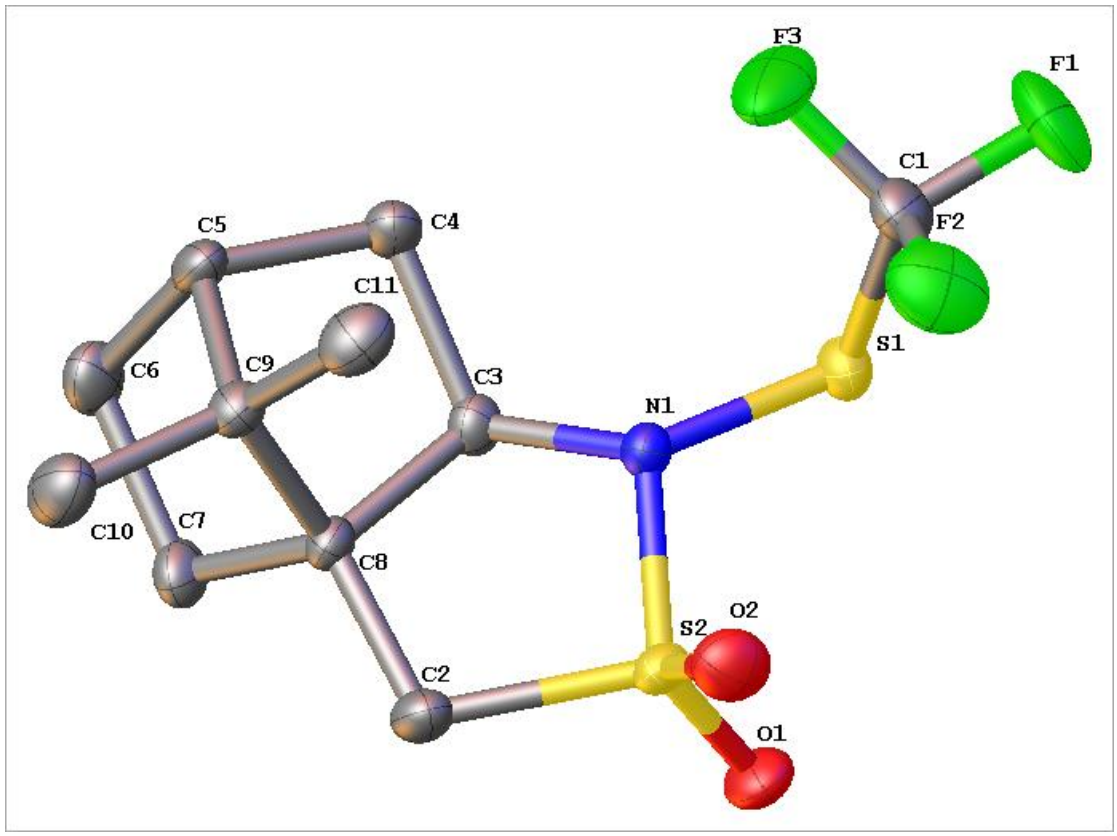


Figure S1. X-ray structure of (1S)-(-)-*N*-trifluoromethylthio-2,10-camphorsultam 1a.

Table S1. Crystal data and structure refinement for compound **1a** (dm16677).

Identification code	dm16677	
Empirical formula	C11 H16 F3 N O2 S2	
Formula weight	315.37	
Temperature	130 K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	C 1 2 1	
Unit cell dimensions	a = 11.500(4) Å	α= 90 °.
	b = 10.460(4) Å	β= 95.060(8) °.
	c = 11.413(5) Å	γ = 90 °.
Volume	1367.6(9) $Å^3$	
Z	4	
Density (calculated)	1.532 Mg/m^3	
Absorption coefficient	0.421 mm^{-1}	
F(000)	656	
Crystal size	0.33 x 0.25 x 0.2 mm^3	
Theta range for data collection	1.791 to 27.200 °.	
Index ranges	-14<=h<=14, -13<=k<=10, -14<=l<=14	
Reflections collected	5043	
Independent reflections	2368 [R(int) = 0.0352]	
Completeness to theta = 25.242 °	99.7 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7455 and 0.6267	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	2368 / 1 / 174	
Goodness-of-fit on F^2	1.108	
Final R indices [I>2sigma(I)]	R1 = 0.0404, wR2 = 0.0934	
R indices (all data)	R1 = 0.0455, wR2 = 0.0982	
Absolute structure parameter	-0.03(7)	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.405 and -0.468 e.$Å^{-3}$	

Table S2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for dm16677. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
S(1)	-784(1)	-5097(1)	-6519(1)	24(1)
S(2)	-2228(1)	-6968(1)	-5580(1)	21(1)
F(1)	-1196(3)	-2970(3)	-7524(3)	53(1)
F(2)	-2780(3)	-3976(4)	-7225(3)	50(1)
F(3)	-1787(4)	-4546(4)	-8619(2)	57(1)
O(1)	-1511(3)	-6782(4)	-4499(2)	32(1)
O(2)	-3346(3)	-6355(4)	-5684(3)	34(1)
N(1)	-1488(3)	-6509(4)	-6734(3)	21(1)
C(1)	-1703(4)	-4126(5)	-7519(4)	30(1)
C(2)	-2293(4)	-8629(5)	-5955(3)	27(1)
C(3)	-843(3)	-7616(4)	-7188(3)	21(1)
C(4)	-675(4)	-7576(5)	-8521(4)	26(1)
C(5)	-1260(4)	-8839(5)	-8957(3)	25(1)
C(6)	-544(4)	-9953(5)	-8412(4)	31(1)
C(7)	-833(4)	-9948(5)	-7093(4)	28(1)
C(8)	-1640(3)	-8785(4)	-7065(3)	19(1)
C(9)	-2372(4)	-8872(4)	-8284(3)	22(1)
C(10)	-3065(4)	-10136(6)	-8436(4)	35(1)
C(11)	-3227(4)	-7776(6)	-8579(4)	32(1)

Table S3. Bond lengths [Å] and angles [°] for dm16677.

S(1)-N(1)	1.692(4)
S(1)-C(1)	1.799(5)
S(2)-O(1)	1.436(3)
S(2)-O(2)	1.432(3)
S(2)-N(1)	1.700(3)
S(2)-C(2)	1.790(5)
F(1)-C(1)	1.342(6)
F(2)-C(1)	1.321(6)
F(3)-C(1)	1.325(6)
N(1)-C(3)	1.492(5)
C(2)-H(2A)	0.9900
C(2)-H(2B)	0.9900
C(2)-C(8)	1.537(5)
C(3)-H(3)	1.0000
C(3)-C(4)	1.552(5)
C(3)-C(8)	1.542(6)
C(4)-H(4A)	0.9900
C(4)-H(4B)	0.9900
C(4)-C(5)	1.545(6)
C(5)-H(5)	1.0000
C(5)-C(6)	1.527(7)
C(5)-C(9)	1.550(6)
C(6)-H(6A)	0.9900
C(6)-H(6B)	0.9900
C(6)-C(7)	1.570(6)
C(7)-H(7A)	0.9900
C(7)-H(7B)	0.9900
C(7)-C(8)	1.533(6)
C(8)-C(9)	1.564(5)
C(9)-C(10)	1.545(7)
C(9)-C(11)	1.528(7)
C(10)-H(10A)	0.9800
C(10)-H(10B)	0.9800
C(10)-H(10C)	0.9800
C(11)-H(11A)	0.9800
C(11)-H(11B)	0.9800

C(11)-H(11C)	0.9800

N(1)-S(1)-C(1)	98.9(2)
O(1)-S(2)-N(1)	109.78(18)
O(1)-S(2)-C(2)	110.3(2)
O(2)-S(2)-O(1)	117.0(2)
O(2)-S(2)-N(1)	108.46(19)
O(2)-S(2)-C(2)	113.4(2)
N(1)-S(2)-C(2)	95.86(18)
S(1)-N(1)-S(2)	113.62(19)
C(3)-N(1)-S(1)	118.8(3)
C(3)-N(1)-S(2)	110.4(3)
F(1)-C(1)-S(1)	106.3(4)
F(2)-C(1)-S(1)	114.7(3)
F(2)-C(1)-F(1)	108.2(4)
F(2)-C(1)-F(3)	106.7(4)
F(3)-C(1)-S(1)	113.8(3)
F(3)-C(1)-F(1)	106.9(4)
S(2)-C(2)-H(2A)	110.4
S(2)-C(2)-H(2B)	110.4
H(2A)-C(2)-H(2B)	108.6
C(8)-C(2)-S(2)	106.7(3)
C(8)-C(2)-H(2A)	110.4
C(8)-C(2)-H(2B)	110.4
N(1)-C(3)-H(3)	110.7
N(1)-C(3)-C(4)	115.4(4)
N(1)-C(3)-C(8)	105.4(3)
C(4)-C(3)-H(3)	110.7
C(8)-C(3)-H(3)	110.7
C(8)-C(3)-C(4)	103.7(3)
C(3)-C(4)-H(4A)	111.4
C(3)-C(4)-H(4B)	111.4
H(4A)-C(4)-H(4B)	109.3
C(5)-C(4)-C(3)	101.8(3)
C(5)-C(4)-H(4A)	111.4
C(5)-C(4)-H(4B)	111.4
C(4)-C(5)-H(5)	114.0
C(4)-C(5)-C(9)	102.4(3)

C(6)-C(5)-C(4)	108.5(4)
C(6)-C(5)-H(5)	114.0
C(6)-C(5)-C(9)	102.7(3)
C(9)-C(5)-H(5)	114.0
C(5)-C(6)-H(6A)	111.0
C(5)-C(6)-H(6B)	111.0
C(5)-C(6)-C(7)	103.7(3)
H(6A)-C(6)-H(6B)	109.0
C(7)-C(6)-H(6A)	111.0
C(7)-C(6)-H(6B)	111.0
C(6)-C(7)-H(7A)	111.4
C(6)-C(7)-H(7B)	111.4
H(7A)-C(7)-H(7B)	109.3
C(8)-C(7)-C(6)	101.7(4)
C(8)-C(7)-H(7A)	111.4
C(8)-C(7)-H(7B)	111.4
C(2)-C(8)-C(3)	109.2(3)
C(2)-C(8)-C(9)	118.4(3)
C(3)-C(8)-C(9)	104.1(3)
C(7)-C(8)-C(2)	116.2(4)
C(7)-C(8)-C(3)	105.2(3)
C(7)-C(8)-C(9)	102.4(3)
C(5)-C(9)-C(8)	92.1(3)
C(10)-C(9)-C(5)	113.8(4)
C(10)-C(9)-C(8)	112.4(4)
C(11)-C(9)-C(5)	114.7(4)
C(11)-C(9)-C(8)	115.9(4)
C(11)-C(9)-C(10)	107.6(4)
C(9)-C(10)-H(10A)	109.5
C(9)-C(10)-H(10B)	109.5
C(9)-C(10)-H(10C)	109.5
H(10A)-C(10)-H(10B)	109.5
H(10A)-C(10)-H(10C)	109.5
H(10B)-C(10)-H(10C)	109.5
C(9)-C(11)-H(11A)	109.5
C(9)-C(11)-H(11B)	109.5
C(9)-C(11)-H(11C)	109.5
H(11A)-C(11)-H(11B)	109.5

H(11A)-C(11)-H(11C)	109.5
H(11B)-C(11)-H(11C)	109.5

Symmetry transformations used to generate equivalent atoms:

Table S4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for dm16677. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ...\ \ + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
S(1)	30(1)	18(1)	24(1)	-1(1)	2(1)	-2(1)
S(2)	28(1)	20(1)	15(1)	-1(1)	5(1)	2(1)
F(1)	65(2)	19(2)	75(2)	10(2)	2(2)	-5(2)
F(2)	41(2)	50(2)	57(2)	13(2)	2(1)	12(2)
F(3)	103(3)	43(2)	22(1)	3(1)	-4(2)	24(2)
O(1)	47(2)	33(2)	16(1)	-1(1)	-1(1)	-2(2)
O(2)	33(2)	35(2)	35(2)	2(2)	12(1)	5(2)
N(1)	28(2)	16(2)	18(2)	-2(1)	4(1)	0(1)
C(1)	42(3)	19(2)	30(2)	3(2)	5(2)	3(2)
C(2)	39(2)	25(2)	19(2)	-1(2)	9(2)	-6(2)
C(3)	22(2)	18(2)	22(2)	-3(2)	4(1)	2(2)
C(4)	34(2)	22(2)	23(2)	-2(2)	11(2)	-5(2)
C(5)	37(2)	24(2)	17(2)	-4(2)	9(2)	-7(2)
C(6)	36(2)	24(3)	34(2)	-5(2)	12(2)	4(2)
C(7)	39(2)	17(2)	26(2)	-2(2)	3(2)	5(2)
C(8)	26(2)	17(2)	15(2)	-2(2)	3(1)	1(2)
C(9)	28(2)	22(2)	17(2)	-1(2)	2(2)	-1(2)
C(10)	40(2)	35(3)	29(2)	-8(2)	7(2)	-11(2)
C(11)	30(2)	39(3)	25(2)	-3(2)	1(2)	0(2)

Table S5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^{3}) for dm16677.

	x	y	z	U(eq)
H(2A)	-1917	-9150	-5304	33
H(2B)	-3115	-8909	-6111	33
H(3)	-77	-7738	-6715	25
H(4A)	-1069	-6826	-8907	31
H(4B)	163	-7560	-8661	31
H(5)	-1419	-8894	-9832	30
H(6A)	301	-9817	-8473	37
H(6B)	-781	-10770	-8801	37
H(7A)	-1236	-10744	-6890	33
H(7B)	-120	-9839	-6551	33
H(10A)	-3496	-10154	-9216	52
H(10B)	-3615	-10196	-7830	52
H(10C)	-2522	-10860	-8360	52
H(11A)	-3835	-7785	-8029	48
H(11B)	-3587	-7880	-9384	48
H(11C)	-2807	-6960	-8512	48

Table S6. Torsion angles [°] for dm16677.

S(1)-N(1)-C(3)-C(4)	-76.3(4)
S(1)-N(1)-C(3)-C(8)	169.9(2)
S(2)-N(1)-C(3)-C(4)	149.9(3)
S(2)-N(1)-C(3)-C(8)	36.2(4)
S(2)-C(2)-C(8)-C(3)	19.1(4)
S(2)-C(2)-C(8)-C(7)	137.8(3)
S(2)-C(2)-C(8)-C(9)	-99.6(4)
O(1)-S(2)-N(1)-S(1)	-45.0(3)
O(1)-S(2)-N(1)-C(3)	91.3(3)
O(1)-S(2)-C(2)-C(8)	-112.1(3)
O(2)-S(2)-N(1)-S(1)	84.0(3)
O(2)-S(2)-N(1)-C(3)	-139.7(3)
O(2)-S(2)-C(2)-C(8)	114.5(3)
N(1)-S(1)-C(1)-F(1)	-175.0(3)
N(1)-S(1)-C(1)-F(2)	65.6(4)
N(1)-S(1)-C(1)-F(3)	-57.7(4)
N(1)-S(2)-C(2)-C(8)	1.5(3)
N(1)-C(3)-C(4)-C(5)	-122.2(4)
N(1)-C(3)-C(8)-C(2)	-34.6(4)
N(1)-C(3)-C(8)-C(7)	-160.0(3)
N(1)-C(3)-C(8)-C(9)	92.7(4)
C(1)-S(1)-N(1)-S(2)	-108.2(2)
C(1)-S(1)-N(1)-C(3)	119.4(3)
C(2)-S(2)-N(1)-S(1)	-159.0(2)
C(2)-S(2)-N(1)-C(3)	-22.7(3)
C(2)-C(8)-C(9)-C(5)	173.5(4)
C(2)-C(8)-C(9)-C(10)	-69.7(5)
C(2)-C(8)-C(9)-C(11)	54.7(5)
C(3)-C(4)-C(5)-C(6)	-66.1(4)
C(3)-C(4)-C(5)-C(9)	42.0(4)
C(3)-C(8)-C(9)-C(5)	52.1(4)
C(3)-C(8)-C(9)-C(10)	169.0(3)
C(3)-C(8)-C(9)-C(11)	-66.7(4)
C(4)-C(3)-C(8)-C(2)	-156.3(4)
C(4)-C(3)-C(8)-C(7)	78.4(4)
C(4)-C(3)-C(8)-C(9)	-28.9(4)

C(4)-C(5)-C(6)-C(7)	73.4(4)
C(4)-C(5)-C(9)-C(8)	-57.2(4)
C(4)-C(5)-C(9)-C(10)	-172.8(4)
C(4)-C(5)-C(9)-C(11)	62.7(4)
C(5)-C(6)-C(7)-C(8)	-2.3(4)
C(6)-C(5)-C(9)-C(8)	55.3(4)
C(6)-C(5)-C(9)-C(10)	-60.3(4)
C(6)-C(5)-C(9)-C(11)	175.2(4)
C(6)-C(7)-C(8)-C(2)	168.6(4)
C(6)-C(7)-C(8)-C(3)	-70.5(4)
C(6)-C(7)-C(8)-C(9)	38.0(4)
C(7)-C(8)-C(9)-C(5)	-57.2(4)
C(7)-C(8)-C(9)-C(10)	59.6(4)
C(7)-C(8)-C(9)-C(11)	-176.0(4)
C(8)-C(3)-C(4)-C(5)	-7.5(4)
C(9)-C(5)-C(6)-C(7)	-34.5(4)

Symmetry transformations used to generate equivalent atoms:

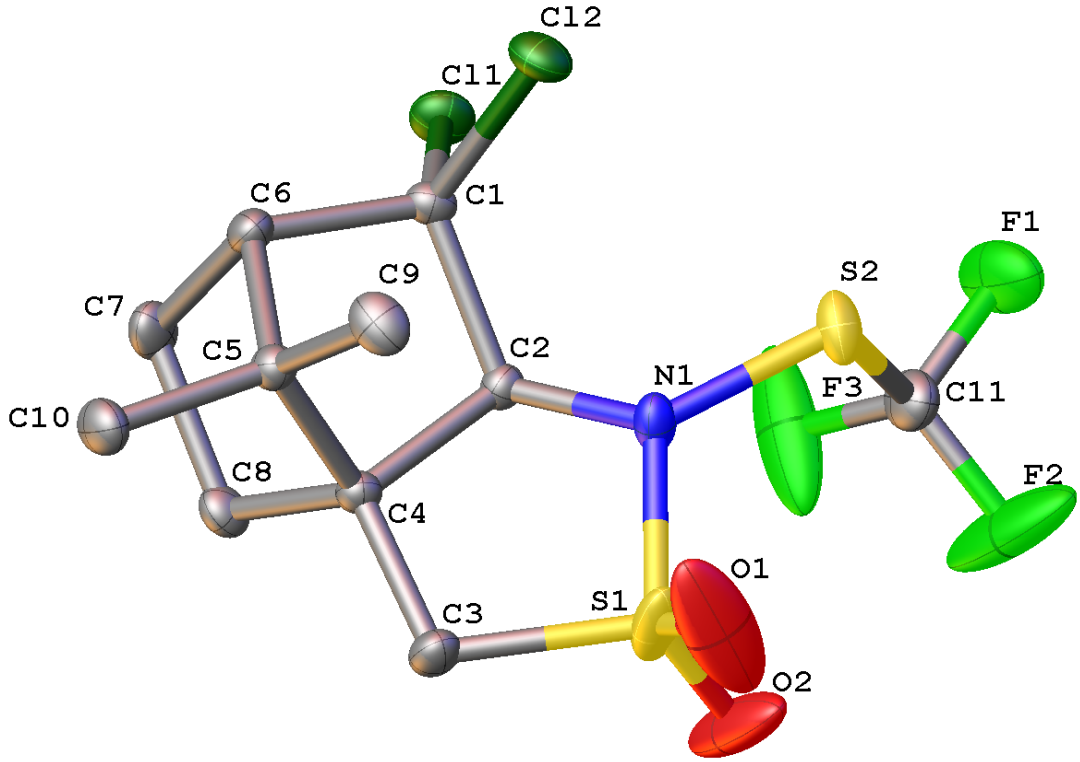


Figure S2. X-ray structure of (3aS,6S,7aS)-7,7-Dichloro-8,8-dimethyl-1-((trifluoromethyl)thio)hexahydro-1H-3a,6-methanobenzo[c]isothiazole-2,2-dioxide 1b.

Table S7. Crystal data and structure refinement for compound **1b** (dm16474_0m).

Identification code	mo_dm16474_0m	
Empirical formula	C11 H14 Cl2 F3 N O2 S2	
Formula weight	384.25	
Temperature	130 K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P 1 21 1	
Unit cell dimensions	a = 7.7869(6) Å	α= 90 °.
	b = 10.8732(8) Å	β= 95.0620(10) °.
	c = 8.8809(7) Å	γ = 90 °.
Volume	749.00(10) $Å^3$	
Z	2	
Density (calculated)	1.704 Mg/m^3	
Absorption coefficient	0.746 mm^{-1}	
F(000)	392	
Crystal size	0.3 x 0.25 x 0.22 mm^3	
Theta range for data collection	2.302 to 30.672 °.	
Index ranges	-11<=h<=11, -15<=k<=15, -12<=l<=10	
Reflections collected	7661	
Independent reflections	4461 [R(int) = 0.0147]	
Completeness to theta = 25.242 °	100.0 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7461 and 0.6619	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	4461 / 1 / 192	
Goodness-of-fit on F^2	1.035	
Final R indices [I>2sigma(I)]	R1 = 0.0285, wR2 = 0.0720	
R indices (all data)	R1 = 0.0292, wR2 = 0.0725	
Absolute structure parameter	0.056(19)	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.428 and -0.616 e.$Å^{-3}$	

Table S8. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for mo_dm16474_0m. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Cl(1)	3879(1)	7466(1)	8116(1)	24(1)
Cl(2)	4481(1)	10053(1)	8109(1)	23(1)
S(1)	8309(1)	9279(1)	4522(1)	41(1)
S(2)	4653(1)	9760(1)	4467(1)	25(1)
F(1)	2163(2)	8526(2)	3153(2)	47(1)
F(2)	4329(4)	8432(4)	1940(3)	91(1)
F(3)	4275(5)	7403(2)	3960(4)	94(1)
O(1)	8782(4)	10518(4)	4268(5)	96(2)
O(2)	8084(3)	8469(5)	3265(3)	93(2)
N(1)	6480(3)	9292(2)	5429(2)	19(1)
C(1)	5556(3)	8603(2)	8051(2)	16(1)
C(2)	6557(3)	8351(2)	6620(2)	14(1)
C(3)	9633(3)	8578(2)	6023(3)	21(1)
C(4)	8481(3)	8281(2)	7282(2)	14(1)
C(5)	8555(3)	9149(2)	8687(2)	16(1)
C(6)	7004(3)	8494(2)	9346(2)	18(1)
C(7)	7629(3)	7139(2)	9418(3)	23(1)
C(8)	8688(3)	7002(2)	8022(3)	19(1)
C(9)	8401(3)	10533(2)	8309(3)	23(1)
C(10)	10212(3)	9029(2)	9761(3)	23(1)
C(11)	3875(3)	8455(3)	3310(3)	27(1)

Table S9. Bond lengths [Å] and angles [º] for mo_dm16474_0m.

Cl(1)-C(1)	1.802(2)
Cl(2)-C(1)	1.788(2)
S(1)-O(1)	1.420(4)
S(1)-O(2)	1.420(4)
S(1)-N(1)	1.697(2)
S(1)-C(3)	1.782(3)
S(2)-N(1)	1.673(2)
S(2)-C(11)	1.824(3)
F(1)-C(11)	1.331(3)
F(2)-C(11)	1.297(3)
F(3)-C(11)	1.306(4)
N(1)-C(2)	1.469(3)
C(1)-C(2)	1.573(3)
C(1)-C(6)	1.543(3)
C(2)-H(2)	1.0000
C(2)-C(4)	1.562(3)
C(3)-H(3A)	0.9900
C(3)-H(3B)	0.9900
C(3)-C(4)	1.529(3)
C(4)-C(5)	1.561(3)
C(4)-C(8)	1.540(3)
C(5)-C(6)	1.560(3)
C(5)-C(9)	1.544(3)
C(5)-C(10)	1.540(3)
C(6)-H(6)	1.0000
C(6)-C(7)	1.550(3)
C(7)-H(7A)	0.9900
C(7)-H(7B)	0.9900
C(7)-C(8)	1.555(3)
C(8)-H(8A)	0.9900
C(8)-H(8B)	0.9900
C(9)-H(9A)	0.9800
C(9)-H(9B)	0.9800
C(9)-H(9C)	0.9800
C(10)-H(10A)	0.9800
C(10)-H(10B)	0.9800

C(10)-H(10C)	0.9800

O(1)-S(1)-N(1)	107.9(2)
O(1)-S(1)-C(3)	112.53(18)
O(2)-S(1)-O(1)	118.6(3)
O(2)-S(1)-N(1)	109.17(15)
O(2)-S(1)-C(3)	110.2(2)
N(1)-S(1)-C(3)	95.93(10)
N(1)-S(2)-C(11)	106.06(12)
S(2)-N(1)-S(1)	118.13(11)
C(2)-N(1)-S(1)	110.65(15)
C(2)-N(1)-S(2)	123.96(16)
Cl(2)-C(1)-Cl(1)	105.15(11)
C(2)-C(1)-Cl(1)	108.57(15)
C(2)-C(1)-Cl(2)	116.32(15)
C(6)-C(1)-Cl(1)	114.05(15)
C(6)-C(1)-Cl(2)	111.10(15)
C(6)-C(1)-C(2)	101.95(17)
N(1)-C(2)-C(1)	117.94(18)
N(1)-C(2)-H(2)	109.6
N(1)-C(2)-C(4)	106.39(17)
C(1)-C(2)-H(2)	109.6
C(4)-C(2)-C(1)	103.37(16)
C(4)-C(2)-H(2)	109.6
S(1)-C(3)-H(3A)	110.2
S(1)-C(3)-H(3B)	110.2
H(3A)-C(3)-H(3B)	108.5
C(4)-C(3)-S(1)	107.40(16)
C(4)-C(3)-H(3A)	110.2
C(4)-C(3)-H(3B)	110.2
C(3)-C(4)-C(2)	108.62(17)
C(3)-C(4)-C(5)	118.27(19)
C(3)-C(4)-C(8)	117.20(19)
C(5)-C(4)-C(2)	103.78(16)
C(8)-C(4)-C(2)	105.41(17)
C(8)-C(4)-C(5)	102.09(17)
C(6)-C(5)-C(4)	92.77(17)
C(9)-C(5)-C(4)	114.75(18)

C(9)-C(5)-C(6)	118.60(19)
C(10)-C(5)-C(4)	114.42(18)
C(10)-C(5)-C(6)	111.27(18)
C(10)-C(5)-C(9)	105.18(19)
C(1)-C(6)-C(5)	102.97(17)
C(1)-C(6)-H(6)	114.3
C(1)-C(6)-C(7)	108.07(19)
C(5)-C(6)-H(6)	114.3
C(7)-C(6)-C(5)	101.46(18)
C(7)-C(6)-H(6)	114.3
C(6)-C(7)-H(7A)	110.9
C(6)-C(7)-H(7B)	110.9
C(6)-C(7)-C(8)	104.17(18)
H(7A)-C(7)-H(7B)	108.9
C(8)-C(7)-H(7A)	110.9
C(8)-C(7)-H(7B)	110.9
C(4)-C(8)-C(7)	102.15(17)
C(4)-C(8)-H(8A)	111.3
C(4)-C(8)-H(8B)	111.3
C(7)-C(8)-H(8A)	111.3
C(7)-C(8)-H(8B)	111.3
H(8A)-C(8)-H(8B)	109.2
C(5)-C(9)-H(9A)	109.5
C(5)-C(9)-H(9B)	109.5
C(5)-C(9)-H(9C)	109.5
H(9A)-C(9)-H(9B)	109.5
H(9A)-C(9)-H(9C)	109.5
H(9B)-C(9)-H(9C)	109.5
C(5)-C(10)-H(10A)	109.5
C(5)-C(10)-H(10B)	109.5
C(5)-C(10)-H(10C)	109.5
H(10A)-C(10)-H(10B)	109.5
H(10A)-C(10)-H(10C)	109.5
H(10B)-C(10)-H(10C)	109.5
F(1)-C(11)-S(2)	107.09(19)
F(2)-C(11)-S(2)	116.0(2)
F(2)-C(11)-F(1)	104.9(2)
F(2)-C(11)-F(3)	108.9(3)

F(3)-C(11)-S(2)	112.22(18)
F(3)-C(11)-F(1)	107.1(3)

Symmetry transformations used to generate equivalent atoms:

Table S10. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for mo_dm16474_0m. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Cl(1)	18(1)	25(1)	29(1)	1(1)	7(1)	-5(1)
Cl(2)	19(1)	21(1)	30(1)	-5(1)	3(1)	5(1)
S(1)	21(1)	79(1)	22(1)	24(1)	2(1)	-7(1)
S(2)	27(1)	20(1)	25(1)	4(1)	-10(1)	0(1)
F(1)	23(1)	74(2)	43(1)	-18(1)	-4(1)	-5(1)
F(2)	60(2)	183(4)	34(1)	-49(2)	23(1)	-54(2)
F(3)	138(3)	30(1)	95(2)	-18(1)	-90(2)	14(2)
O(1)	32(1)	110(3)	146(4)	104(3)	5(2)	-11(2)
O(2)	31(1)	227(5)	22(1)	-33(2)	3(1)	8(2)
N(1)	18(1)	21(1)	17(1)	6(1)	-2(1)	-2(1)
C(1)	14(1)	15(1)	19(1)	-1(1)	3(1)	0(1)
C(2)	15(1)	15(1)	13(1)	1(1)	1(1)	-1(1)
C(3)	17(1)	30(1)	16(1)	2(1)	5(1)	0(1)
C(4)	13(1)	16(1)	14(1)	0(1)	2(1)	0(1)
C(5)	15(1)	18(1)	15(1)	-1(1)	1(1)	0(1)
C(6)	17(1)	25(1)	13(1)	1(1)	2(1)	1(1)
C(7)	22(1)	25(1)	22(1)	10(1)	3(1)	2(1)
C(8)	18(1)	15(1)	23(1)	2(1)	1(1)	4(1)
C(9)	21(1)	17(1)	30(1)	-4(1)	-3(1)	-3(1)
C(10)	17(1)	30(1)	20(1)	-3(1)	-3(1)	0(1)
C(11)	24(1)	37(2)	20(1)	-5(1)	-4(1)	1(1)

Table S11. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for mo_dm16474_0m.

	x	y	z	U(eq)
H(2)	6195	7539	6169	17
H(3A)	10161	7816	5664	25
H(3B)	10567	9146	6400	25
H(6)	6700	8833	10335	22
H(7A)	6639	6565	9352	28
H(7B)	8359	6979	10368	28
H(8A)	9913	6817	8332	23
H(8B)	8207	6349	7332	23
H(9A)	8154	10990	9216	35
H(9B)	7464	10660	7513	35
H(9C)	9487	10826	7959	35
H(10A)	11186	9374	9275	34
H(10B)	10433	8158	9991	34
H(10C)	10070	9476	10699	34

Table S12. Torsion angles [°] for mo_dm16474_0m.

Cl(1)-C(1)-C(2)-N(1)	116.04(18)
Cl(1)-C(1)-C(2)-C(4)	-126.94(15)
Cl(1)-C(1)-C(6)-C(5)	157.24(15)
Cl(1)-C(1)-C(6)-C(7)	50.4(2)
Cl(2)-C(1)-C(2)-N(1)	-2.2(3)
Cl(2)-C(1)-C(2)-C(4)	114.78(17)
Cl(2)-C(1)-C(6)-C(5)	-84.13(18)
Cl(2)-C(1)-C(6)-C(7)	169.03(15)
S(1)-N(1)-C(2)-C(1)	150.09(16)
S(1)-N(1)-C(2)-C(4)	34.7(2)
S(1)-C(3)-C(4)-C(2)	15.7(2)
S(1)-C(3)-C(4)-C(5)	-102.1(2)
S(1)-C(3)-C(4)-C(8)	134.98(18)
S(2)-N(1)-C(2)-C(1)	-60.5(3)
S(2)-N(1)-C(2)-C(4)	-175.85(16)
O(1)-S(1)-N(1)-S(2)	69.5(2)
O(1)-S(1)-N(1)-C(2)	-139.0(2)
O(1)-S(1)-C(3)-C(4)	115.5(3)
O(2)-S(1)-N(1)-S(2)	-60.6(3)
O(2)-S(1)-N(1)-C(2)	90.8(3)
O(2)-S(1)-C(3)-C(4)	-109.6(2)
N(1)-S(1)-C(3)-C(4)	3.33(19)
N(1)-S(2)-C(11)-F(1)	149.20(19)
N(1)-S(2)-C(11)-F(2)	-94.1(3)
N(1)-S(2)-C(11)-F(3)	31.9(3)
N(1)-C(2)-C(4)-C(3)	-31.6(2)
N(1)-C(2)-C(4)-C(5)	95.10(19)
N(1)-C(2)-C(4)-C(8)	-157.96(17)
C(1)-C(2)-C(4)-C(3)	-156.46(18)
C(1)-C(2)-C(4)-C(5)	-29.8(2)
C(1)-C(2)-C(4)-C(8)	77.16(19)
C(1)-C(6)-C(7)-C(8)	73.7(2)
C(2)-C(1)-C(6)-C(5)	40.4(2)
C(2)-C(1)-C(6)-C(7)	-66.4(2)
C(2)-C(4)-C(5)-C(6)	52.07(18)
C(2)-C(4)-C(5)-C(9)	-71.3(2)

C(2)-C(4)-C(5)-C(10)	166.96(18)
C(2)-C(4)-C(8)-C(7)	-70.2(2)
C(3)-S(1)-N(1)-S(2)	-174.49(15)
C(3)-S(1)-N(1)-C(2)	-23.05(18)
C(3)-C(4)-C(5)-C(6)	172.42(19)
C(3)-C(4)-C(5)-C(9)	49.1(3)
C(3)-C(4)-C(5)-C(10)	-72.7(3)
C(3)-C(4)-C(8)-C(7)	168.83(19)
C(4)-C(5)-C(6)-C(1)	-56.80(19)
C(4)-C(5)-C(6)-C(7)	55.01(19)
C(5)-C(4)-C(8)-C(7)	37.9(2)
C(5)-C(6)-C(7)-C(8)	-34.2(2)
C(6)-C(1)-C(2)-N(1)	-123.3(2)
C(6)-C(1)-C(2)-C(4)	-6.2(2)
C(6)-C(7)-C(8)-C(4)	-2.2(2)
C(8)-C(4)-C(5)-C(6)	-57.34(18)
C(8)-C(4)-C(5)-C(9)	179.29(18)
C(8)-C(4)-C(5)-C(10)	57.5(2)
C(9)-C(5)-C(6)-C(1)	63.5(2)
C(9)-C(5)-C(6)-C(7)	175.26(19)
C(10)-C(5)-C(6)-C(1)	-174.38(18)
C(10)-C(5)-C(6)-C(7)	-62.6(2)
C(11)-S(2)-N(1)-S(1)	79.55(17)
C(11)-S(2)-N(1)-C(2)	-67.8(2)

Symmetry transformations used to generate equivalent atoms:

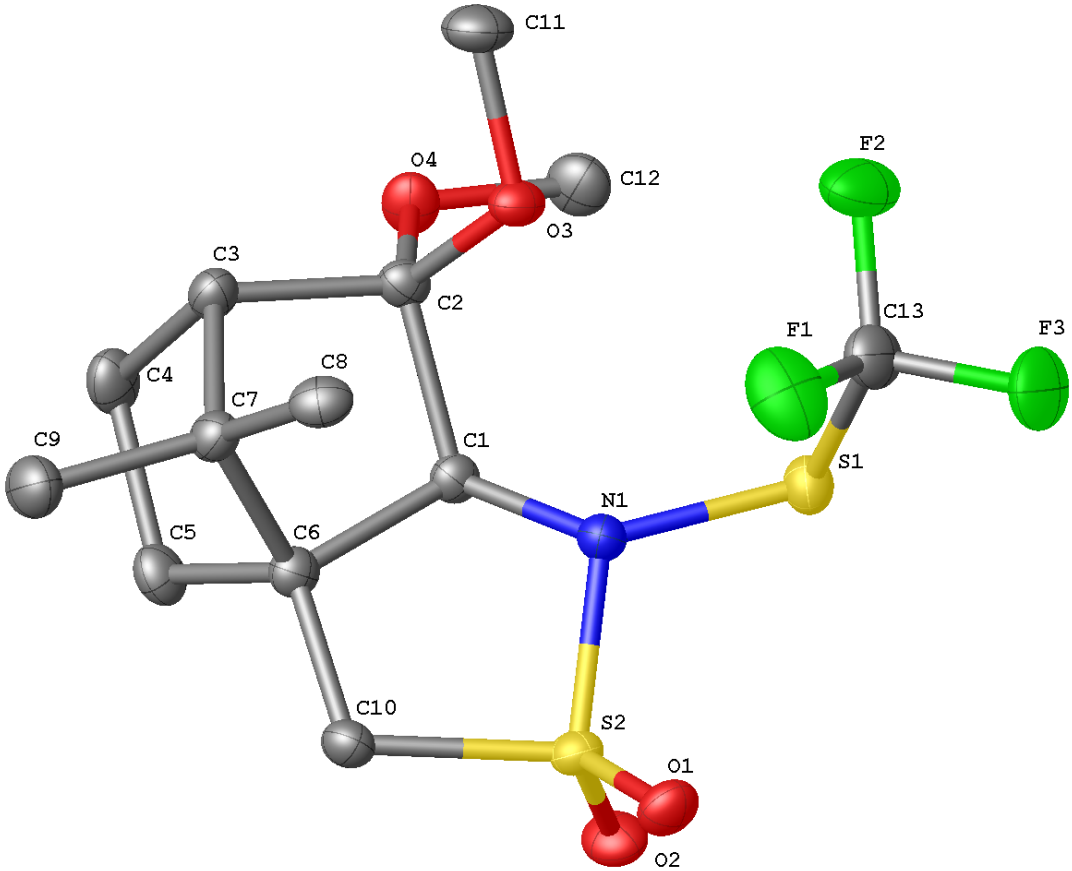


Figure S3. X-ray structure of (3aS,6S,7aS)-7,7-Dimethoxy-8,8-dimethyl-1-((trifluoromethyl)thio)hexahydro-1*H*-3a,6-methanobenzo[c]isothiazole 2,2-dioxide 1c.

Table S13. Crystal data and structure refinement for compound **1c**_(dm16194_0m).

Identification code	mo_dm16194_0m	
Empirical formula	C13 H20 F3 N O4 S2	
Formula weight	375.42	
Temperature	130 K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P 1 21 1	
Unit cell dimensions	a = 12.4266(17) Å	α= 90 °.
	b = 8.8229(12) Å	β= 105.700(3) °.
	c = 15.107(2) Å	γ = 90 °.
Volume	1594.5(4) $Å^3$	
Z	4	
Density (calculated)	1.564 Mg/m^3	
Absorption coefficient	0.384 mm^{-1}	
F(000)	784	
Crystal size	0.2 x 0.12 x 0.08 mm^3	
Theta range for data collection	1.400 to 30.554 °.	
Index ranges	-17<=h<=17, -12<=k<=12, -21<=l<=21	
Reflections collected	16180	
Independent reflections	9395 [R(int) = 0.0251]	
Completeness to theta = 26.000 °	100.0 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7461 and 0.7012	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	9395 / 1 / 423	
Goodness-of-fit on F^2	1.033	
Final R indices [I>2sigma(I)]	R1 = 0.0379, wR2 = 0.0862	
R indices (all data)	R1 = 0.0445, wR2 = 0.0904	
Absolute structure parameter	0.02(3)	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.642 and -0.480 e.$Å^{-3}$	

Table S14. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for mo_dm16194_0m. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
S(1)	6862(1)	2362(1)	2573(1)	21(1)
S(2)	5760(1)	2739(1)	3963(1)	17(1)
F(1)	8481(2)	995(3)	3820(2)	42(1)
F(2)	9015(2)	1970(2)	2707(2)	42(1)
F(3)	7988(2)	-4(2)	2466(2)	42(1)
O(1)	5917(2)	1195(2)	4270(2)	23(1)
O(2)	4725(2)	3120(3)	3296(1)	24(1)
O(3)	8814(2)	4619(2)	3616(1)	19(1)
O(4)	7932(2)	6795(2)	2925(1)	22(1)
N(1)	6857(2)	3276(3)	3568(2)	18(1)
C(1)	6904(2)	4953(3)	3630(2)	16(1)
C(2)	8035(2)	5758(3)	3649(2)	17(1)
C(3)	8266(2)	6670(3)	4556(2)	19(1)
C(4)	7332(3)	7883(3)	4429(2)	25(1)
C(5)	6295(3)	6974(3)	4517(2)	22(1)
C(6)	6731(2)	5332(3)	4595(2)	17(1)
C(7)	7950(2)	5529(3)	5231(2)	18(1)
C(8)	8632(2)	4063(3)	5440(2)	20(1)
C(9)	7976(3)	6226(4)	6170(2)	26(1)
C(10)	6013(2)	4109(3)	4867(2)	18(1)
C(11)	9933(3)	5125(4)	3733(2)	27(1)
C(12)	7696(3)	6157(4)	2019(2)	26(1)
C(13)	8163(3)	1292(4)	2929(2)	27(1)
S(3)	2624(1)	3426(1)	1602(1)	19(1)
S(4)	3994(1)	4636(1)	568(1)	19(1)
F(4)	958(2)	4090(4)	168(2)	71(1)
F(5)	478(2)	3941(3)	1405(2)	59(1)
F(6)	874(2)	1929(3)	803(2)	56(1)
O(5)	4936(2)	3842(3)	1144(2)	30(1)
O(6)	3420(2)	3953(3)	-286(2)	34(1)
O(7)	2898(2)	7302(2)	3109(1)	19(1)
O(8)	1583(2)	6758(2)	1739(1)	19(1)
N(2)	3059(2)	5030(3)	1174(2)	16(1)

C(14)	3513(2)	6312(3)	1790(2)	15(1)
C(15)	3999(2)	7442(3)	1198(2)	15(1)
C(16)	4870(2)	8385(3)	1897(2)	19(1)
C(17)	4115(2)	9356(3)	2355(2)	20(1)
C(18)	2913(2)	8910(3)	1819(2)	16(1)
C(19)	2664(2)	7310(3)	2136(2)	15(1)
C(20)	3034(2)	8599(3)	833(2)	17(1)
C(21)	2004(2)	7993(3)	110(2)	22(1)
C(22)	3408(3)	10007(3)	394(2)	22(1)
C(23)	4379(3)	6560(3)	468(2)	20(1)
C(24)	2727(3)	5865(3)	3495(2)	22(1)
C(25)	688(2)	7688(4)	1858(2)	26(1)
C(26)	1163(3)	3368(4)	945(2)	31(1)

Table S15. Bond lengths [Å] and angles [°] for mo_dm16194_0m.

S(1)-N(1)	1.707(2)
S(1)-C(13)	1.823(3)
S(2)-O(1)	1.436(2)
S(2)-O(2)	1.443(2)
S(2)-N(1)	1.696(2)
S(2)-C(10)	1.787(3)
F(1)-C(13)	1.322(4)
F(2)-C(13)	1.336(4)
F(3)-C(13)	1.327(4)
O(3)-C(2)	1.406(3)
O(3)-C(11)	1.425(3)
O(4)-C(2)	1.406(3)
O(4)-C(12)	1.435(4)
N(1)-C(1)	1.483(3)
C(1)-H(1)	1.0000
C(1)-C(2)	1.567(4)
C(1)-C(6)	1.567(4)
C(2)-C(3)	1.548(4)
C(3)-H(3)	1.0000
C(3)-C(4)	1.552(4)
C(3)-C(7)	1.556(4)
C(4)-H(4A)	0.9900
C(4)-H(4B)	0.9900
C(4)-C(5)	1.553(4)
C(5)-H(5A)	0.9900
C(5)-H(5B)	0.9900
C(5)-C(6)	1.541(4)
C(6)-C(7)	1.568(4)
C(6)-C(10)	1.526(4)
C(7)-C(8)	1.532(4)
C(7)-C(9)	1.538(4)
C(8)-H(8A)	0.9800
C(8)-H(8B)	0.9800
C(8)-H(8C)	0.9800
C(9)-H(9A)	0.9800
C(9)-H(9B)	0.9800

C(9)-H(9C)	0.9800
C(10)-H(10A)	0.9900
C(10)-H(10B)	0.9900
C(11)-H(11A)	0.9800
C(11)-H(11B)	0.9800
C(11)-H(11C)	0.9800
C(12)-H(12A)	0.9800
C(12)-H(12B)	0.9800
C(12)-H(12C)	0.9800
S(3)-N(2)	1.704(2)
S(3)-C(26)	1.819(3)
S(4)-O(5)	1.438(2)
S(4)-O(6)	1.427(2)
S(4)-N(2)	1.698(2)
S(4)-C(23)	1.781(3)
F(4)-C(26)	1.299(4)
F(5)-C(26)	1.335(4)
F(6)-C(26)	1.321(4)
O(7)-C(19)	1.419(3)
O(7)-C(24)	1.436(3)
O(8)-C(19)	1.401(3)
O(8)-C(25)	1.432(3)
N(2)-C(14)	1.477(3)
C(14)-H(14)	1.0000
C(14)-C(15)	1.565(4)
C(14)-C(19)	1.569(4)
C(15)-C(16)	1.536(4)
C(15)-C(20)	1.558(4)
C(15)-C(23)	1.525(4)
C(16)-H(16A)	0.9900
C(16)-H(16B)	0.9900
C(16)-C(17)	1.564(4)
C(17)-H(17A)	0.9900
C(17)-H(17B)	0.9900
C(17)-C(18)	1.544(4)
C(18)-H(18)	1.0000
C(18)-C(19)	1.549(4)
C(18)-C(20)	1.561(4)

C(20)-C(21)	1.537(4)
C(20)-C(22)	1.538(4)
C(21)-H(21A)	0.9800
C(21)-H(21B)	0.9800
C(21)-H(21C)	0.9800
C(22)-H(22A)	0.9800
C(22)-H(22B)	0.9800
C(22)-H(22C)	0.9800
C(23)-H(23A)	0.9900
C(23)-H(23B)	0.9900
C(24)-H(24A)	0.9800
C(24)-H(24B)	0.9800
C(24)-H(24C)	0.9800
C(25)-H(25A)	0.9800
C(25)-H(25B)	0.9800
C(25)-H(25C)	0.9800

N(1)-S(1)-C(13)	101.50(14)
O(1)-S(2)-O(2)	117.63(13)
O(1)-S(2)-N(1)	109.06(12)
O(1)-S(2)-C(10)	114.53(13)
O(2)-S(2)-N(1)	109.80(13)
O(2)-S(2)-C(10)	108.39(13)
N(1)-S(2)-C(10)	95.08(12)
C(2)-O(3)-C(11)	115.5(2)
C(2)-O(4)-C(12)	116.1(2)
S(2)-N(1)-S(1)	111.89(13)
C(1)-N(1)-S(1)	121.14(18)
C(1)-N(1)-S(2)	106.12(17)
N(1)-C(1)-H(1)	109.9
N(1)-C(1)-C(2)	118.2(2)
N(1)-C(1)-C(6)	105.0(2)
C(2)-C(1)-H(1)	109.9
C(6)-C(1)-H(1)	109.9
C(6)-C(1)-C(2)	103.5(2)
O(3)-C(2)-O(4)	110.8(2)
O(3)-C(2)-C(1)	107.4(2)
O(3)-C(2)-C(3)	116.0(2)

O(4)-C(2)-C(1)	112.8(2)
O(4)-C(2)-C(3)	107.9(2)
C(3)-C(2)-C(1)	101.7(2)
C(2)-C(3)-H(3)	114.3
C(2)-C(3)-C(4)	107.2(2)
C(2)-C(3)-C(7)	103.0(2)
C(4)-C(3)-H(3)	114.3
C(4)-C(3)-C(7)	102.4(2)
C(7)-C(3)-H(3)	114.3
C(3)-C(4)-H(4A)	110.9
C(3)-C(4)-H(4B)	110.9
C(3)-C(4)-C(5)	104.1(2)
H(4A)-C(4)-H(4B)	109.0
C(5)-C(4)-H(4A)	110.9
C(5)-C(4)-H(4B)	110.9
C(4)-C(5)-H(5A)	111.4
C(4)-C(5)-H(5B)	111.4
H(5A)-C(5)-H(5B)	109.2
C(6)-C(5)-C(4)	102.1(2)
C(6)-C(5)-H(5A)	111.4
C(6)-C(5)-H(5B)	111.4
C(1)-C(6)-C(7)	104.0(2)
C(5)-C(6)-C(1)	105.2(2)
C(5)-C(6)-C(7)	101.8(2)
C(10)-C(6)-C(1)	109.7(2)
C(10)-C(6)-C(5)	117.8(2)
C(10)-C(6)-C(7)	116.9(2)
C(3)-C(7)-C(6)	92.5(2)
C(8)-C(7)-C(3)	117.2(2)
C(8)-C(7)-C(6)	114.9(2)
C(8)-C(7)-C(9)	106.0(2)
C(9)-C(7)-C(3)	113.6(2)
C(9)-C(7)-C(6)	112.7(2)
C(7)-C(8)-H(8A)	109.5
C(7)-C(8)-H(8B)	109.5
C(7)-C(8)-H(8C)	109.5
H(8A)-C(8)-H(8B)	109.5
H(8A)-C(8)-H(8C)	109.5

H(8B)-C(8)-H(8C)	109.5
C(7)-C(9)-H(9A)	109.5
C(7)-C(9)-H(9B)	109.5
C(7)-C(9)-H(9C)	109.5
H(9A)-C(9)-H(9B)	109.5
H(9A)-C(9)-H(9C)	109.5
H(9B)-C(9)-H(9C)	109.5
S(2)-C(10)-H(10A)	110.6
S(2)-C(10)-H(10B)	110.6
C(6)-C(10)-S(2)	105.48(18)
C(6)-C(10)-H(10A)	110.6
C(6)-C(10)-H(10B)	110.6
H(10A)-C(10)-H(10B)	108.8
O(3)-C(11)-H(11A)	109.5
O(3)-C(11)-H(11B)	109.5
O(3)-C(11)-H(11C)	109.5
H(11A)-C(11)-H(11B)	109.5
H(11A)-C(11)-H(11C)	109.5
H(11B)-C(11)-H(11C)	109.5
O(4)-C(12)-H(12A)	109.5
O(4)-C(12)-H(12B)	109.5
O(4)-C(12)-H(12C)	109.5
H(12A)-C(12)-H(12B)	109.5
H(12A)-C(12)-H(12C)	109.5
H(12B)-C(12)-H(12C)	109.5
F(1)-C(13)-S(1)	113.5(2)
F(1)-C(13)-F(2)	107.8(3)
F(1)-C(13)-F(3)	109.1(3)
F(2)-C(13)-S(1)	113.2(2)
F(3)-C(13)-S(1)	106.5(2)
F(3)-C(13)-F(2)	106.4(3)
N(2)-S(3)-C(26)	100.85(14)
O(5)-S(4)-N(2)	109.73(13)
O(5)-S(4)-C(23)	108.77(15)
O(6)-S(4)-O(5)	117.86(15)
O(6)-S(4)-N(2)	109.03(13)
O(6)-S(4)-C(23)	113.94(15)
N(2)-S(4)-C(23)	95.11(12)

C(19)-O(7)-C(24)	114.5(2)
C(19)-O(8)-C(25)	115.7(2)
S(4)-N(2)-S(3)	111.61(13)
C(14)-N(2)-S(3)	120.22(18)
C(14)-N(2)-S(4)	107.23(16)
N(2)-C(14)-H(14)	110.0
N(2)-C(14)-C(15)	105.6(2)
N(2)-C(14)-C(19)	117.6(2)
C(15)-C(14)-H(14)	110.0
C(15)-C(14)-C(19)	103.4(2)
C(19)-C(14)-H(14)	110.0
C(16)-C(15)-C(14)	105.1(2)
C(16)-C(15)-C(20)	102.7(2)
C(20)-C(15)-C(14)	103.9(2)
C(23)-C(15)-C(14)	109.3(2)
C(23)-C(15)-C(16)	118.4(2)
C(23)-C(15)-C(20)	116.0(2)
C(15)-C(16)-H(16A)	111.4
C(15)-C(16)-H(16B)	111.4
C(15)-C(16)-C(17)	101.8(2)
H(16A)-C(16)-H(16B)	109.3
C(17)-C(16)-H(16A)	111.4
C(17)-C(16)-H(16B)	111.4
C(16)-C(17)-H(17A)	111.0
C(16)-C(17)-H(17B)	111.0
H(17A)-C(17)-H(17B)	109.0
C(18)-C(17)-C(16)	103.9(2)
C(18)-C(17)-H(17A)	111.0
C(18)-C(17)-H(17B)	111.0
C(17)-C(18)-H(18)	114.1
C(17)-C(18)-C(19)	108.5(2)
C(17)-C(18)-C(20)	102.5(2)
C(19)-C(18)-H(18)	114.1
C(19)-C(18)-C(20)	102.3(2)
C(20)-C(18)-H(18)	114.1
O(7)-C(19)-C(14)	112.0(2)
O(7)-C(19)-C(18)	108.8(2)
O(8)-C(19)-O(7)	110.3(2)

O(8)-C(19)-C(14)	108.4(2)
O(8)-C(19)-C(18)	115.7(2)
C(18)-C(19)-C(14)	101.5(2)
C(15)-C(20)-C(18)	92.4(2)
C(21)-C(20)-C(15)	115.9(2)
C(21)-C(20)-C(18)	117.5(2)
C(21)-C(20)-C(22)	105.4(2)
C(22)-C(20)-C(15)	112.8(2)
C(22)-C(20)-C(18)	112.8(2)
C(20)-C(21)-H(21A)	109.5
C(20)-C(21)-H(21B)	109.5
C(20)-C(21)-H(21C)	109.5
H(21A)-C(21)-H(21B)	109.5
H(21A)-C(21)-H(21C)	109.5
H(21B)-C(21)-H(21C)	109.5
C(20)-C(22)-H(22A)	109.5
C(20)-C(22)-H(22B)	109.5
C(20)-C(22)-H(22C)	109.5
H(22A)-C(22)-H(22B)	109.5
H(22A)-C(22)-H(22C)	109.5
H(22B)-C(22)-H(22C)	109.5
S(4)-C(23)-H(23A)	110.4
S(4)-C(23)-H(23B)	110.4
C(15)-C(23)-S(4)	106.43(18)
C(15)-C(23)-H(23A)	110.4
C(15)-C(23)-H(23B)	110.4
H(23A)-C(23)-H(23B)	108.6
O(7)-C(24)-H(24A)	109.5
O(7)-C(24)-H(24B)	109.5
O(7)-C(24)-H(24C)	109.5
H(24A)-C(24)-H(24B)	109.5
H(24A)-C(24)-H(24C)	109.5
H(24B)-C(24)-H(24C)	109.5
O(8)-C(25)-H(25A)	109.5
O(8)-C(25)-H(25B)	109.5
O(8)-C(25)-H(25C)	109.5
H(25A)-C(25)-H(25B)	109.5
H(25A)-C(25)-H(25C)	109.5

H(25B)-C(25)-H(25C)	109.5
F(4)-C(26)-S(3)	113.7(2)
F(4)-C(26)-F(5)	106.7(3)
F(4)-C(26)-F(6)	110.3(3)
F(5)-C(26)-S(3)	112.9(2)
F(6)-C(26)-S(3)	107.6(2)
F(6)-C(26)-F(5)	105.3(3)

Symmetry transformations used to generate equivalent atoms:

Table S16. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for mo_dm16194_0m. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ...\ \ + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
S(1)	23(1)	20(1)	20(1)	-3(1)	6(1)	1(1)
S(2)	15(1)	18(1)	20(1)	0(1)	5(1)	-2(1)
F(1)	42(1)	43(1)	36(1)	6(1)	5(1)	20(1)
F(2)	31(1)	31(1)	72(2)	-6(1)	29(1)	-1(1)
F(3)	49(1)	20(1)	61(1)	-13(1)	22(1)	3(1)
O(1)	25(1)	18(1)	27(1)	1(1)	8(1)	-5(1)
O(2)	15(1)	32(1)	24(1)	-1(1)	2(1)	0(1)
O(3)	16(1)	17(1)	26(1)	1(1)	8(1)	0(1)
O(4)	32(1)	18(1)	18(1)	4(1)	9(1)	-2(1)
N(1)	17(1)	18(1)	19(1)	-2(1)	7(1)	-2(1)
C(1)	18(1)	13(1)	18(1)	1(1)	6(1)	0(1)
C(2)	18(1)	14(1)	19(1)	2(1)	7(1)	0(1)
C(3)	22(1)	17(1)	20(1)	-2(1)	8(1)	-4(1)
C(4)	34(2)	14(1)	28(2)	-1(1)	13(1)	0(1)
C(5)	25(1)	18(1)	24(1)	-1(1)	9(1)	5(1)
C(6)	18(1)	14(1)	19(1)	1(1)	6(1)	1(1)
C(7)	19(1)	19(1)	17(1)	-2(1)	5(1)	-3(1)
C(8)	16(1)	23(1)	21(1)	4(1)	2(1)	0(1)
C(9)	28(2)	30(2)	21(1)	-5(1)	8(1)	-4(1)
C(10)	18(1)	21(1)	18(1)	0(1)	8(1)	-1(1)
C(11)	19(1)	32(2)	35(2)	1(1)	12(1)	-3(1)
C(12)	32(2)	28(2)	19(1)	4(1)	9(1)	-2(1)
C(13)	29(2)	18(1)	37(2)	-4(1)	14(1)	2(1)
S(3)	19(1)	15(1)	23(1)	-1(1)	4(1)	-4(1)
S(4)	24(1)	15(1)	20(1)	-3(1)	10(1)	1(1)
F(4)	44(1)	100(2)	50(2)	27(2)	-21(1)	-30(2)
F(5)	24(1)	64(2)	89(2)	-30(2)	14(1)	-8(1)
F(6)	34(1)	31(1)	95(2)	-15(1)	3(1)	-16(1)
O(5)	28(1)	28(1)	39(1)	10(1)	18(1)	10(1)
O(6)	47(2)	34(1)	24(1)	-14(1)	16(1)	-10(1)
O(7)	26(1)	18(1)	14(1)	-1(1)	7(1)	-1(1)
O(8)	16(1)	21(1)	22(1)	-1(1)	6(1)	-1(1)
N(2)	18(1)	14(1)	17(1)	-2(1)	6(1)	-2(1)

C(14)	16(1)	14(1)	17(1)	-2(1)	6(1)	-1(1)
C(15)	17(1)	15(1)	16(1)	1(1)	8(1)	0(1)
C(16)	18(1)	17(1)	21(1)	0(1)	6(1)	-4(1)
C(17)	24(1)	18(1)	18(1)	-4(1)	5(1)	-4(1)
C(18)	19(1)	13(1)	16(1)	0(1)	7(1)	1(1)
C(19)	15(1)	18(1)	13(1)	-1(1)	4(1)	0(1)
C(20)	19(1)	16(1)	16(1)	2(1)	7(1)	2(1)
C(21)	21(1)	26(2)	17(1)	0(1)	3(1)	1(1)
C(22)	28(2)	19(1)	21(1)	4(1)	11(1)	2(1)
C(23)	25(1)	17(1)	23(1)	0(1)	13(1)	1(1)
C(24)	28(1)	21(1)	18(1)	3(1)	9(1)	1(1)
C(25)	18(1)	32(2)	29(2)	1(1)	9(1)	5(1)
C(26)	24(2)	27(2)	37(2)	-1(2)	1(1)	-9(1)

Table S17. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for mo_dm16194_0m.

	x	y	z	U(eq)
H(1)	6283	5403	3134	19
H(3)	9042	7083	4774	23
H(4A)	7186	8371	3818	30
H(4B)	7539	8672	4911	30
H(5A)	6068	7278	5071	26
H(5B)	5654	7109	3967	26
H(8A)	8549	3491	4870	31
H(8B)	8361	3449	5876	31
H(8C)	9422	4310	5708	31
H(9A)	8752	6313	6544	39
H(9B)	7559	5575	6487	39
H(9C)	7633	7235	6079	39
H(10A)	5301	4543	4925	22
H(10B)	6412	3642	5461	22
H(11A)	10339	4383	3464	41
H(11B)	10304	5236	4391	41
H(11C)	9925	6105	3426	41
H(12A)	7630	6972	1567	38
H(12B)	6993	5588	1888	38
H(12C)	8305	5474	1983	38
H(14)	4124	5949	2326	18
H(16A)	5309	9034	1588	22
H(16B)	5386	7731	2353	22
H(17A)	4260	9108	3016	24
H(17B)	4245	10452	2290	24
H(18)	2335	9687	1842	19
H(21A)	1788	7009	311	33
H(21B)	2182	7873	-479	33
H(21C)	1383	8709	38	33
H(22A)	2780	10715	203	33
H(22B)	3654	9701	-143	33
H(22C)	4027	10501	843	33

H(23A)	5198	6648	574	24
H(23B)	4009	6955	-153	24
H(24A)	1977	5487	3187	33
H(24B)	2798	5987	4154	33
H(24C)	3287	5140	3410	33
H(25A)	624	8594	1472	38
H(25B)	840	7989	2504	38
H(25C)	-14	7116	1678	38

Table S18. Torsion angles [°] for mo_dm16194_0m.

S(1)-N(1)-C(1)-C(2)	-72.2(3)
S(1)-N(1)-C(1)-C(6)	173.14(17)
S(2)-N(1)-C(1)-C(2)	158.91(19)
S(2)-N(1)-C(1)-C(6)	44.2(2)
O(1)-S(2)-N(1)-S(1)	68.69(17)
O(1)-S(2)-N(1)-C(1)	-157.17(17)
O(1)-S(2)-C(10)-C(6)	134.00(19)
O(2)-S(2)-N(1)-S(1)	-61.54(17)
O(2)-S(2)-N(1)-C(1)	72.6(2)
O(2)-S(2)-C(10)-C(6)	-92.5(2)
O(3)-C(2)-C(3)-C(4)	178.3(2)
O(3)-C(2)-C(3)-C(7)	-74.2(3)
O(4)-C(2)-C(3)-C(4)	53.3(3)
O(4)-C(2)-C(3)-C(7)	160.8(2)
N(1)-S(1)-C(13)-F(1)	25.5(3)
N(1)-S(1)-C(13)-F(2)	-97.8(2)
N(1)-S(1)-C(13)-F(3)	145.6(2)
N(1)-S(2)-C(10)-C(6)	20.4(2)
N(1)-C(1)-C(2)-O(3)	-0.9(3)
N(1)-C(1)-C(2)-O(4)	121.4(3)
N(1)-C(1)-C(2)-C(3)	-123.3(2)
N(1)-C(1)-C(6)-C(5)	-157.2(2)
N(1)-C(1)-C(6)-C(7)	96.2(2)
N(1)-C(1)-C(6)-C(10)	-29.5(3)
C(1)-C(2)-C(3)-C(4)	-65.6(3)
C(1)-C(2)-C(3)-C(7)	42.0(3)
C(1)-C(6)-C(7)-C(3)	51.4(2)
C(1)-C(6)-C(7)-C(8)	-70.3(3)
C(1)-C(6)-C(7)-C(9)	168.2(2)
C(1)-C(6)-C(10)-S(2)	3.0(3)
C(2)-C(1)-C(6)-C(5)	78.3(2)
C(2)-C(1)-C(6)-C(7)	-28.3(3)
C(2)-C(1)-C(6)-C(10)	-154.1(2)
C(2)-C(3)-C(4)-C(5)	76.0(3)
C(2)-C(3)-C(7)-C(6)	-57.2(2)
C(2)-C(3)-C(7)-C(8)	62.5(3)

C(2)-C(3)-C(7)-C(9)	-173.3(2)
C(3)-C(4)-C(5)-C(6)	-4.9(3)
C(4)-C(3)-C(7)-C(6)	54.0(2)
C(4)-C(3)-C(7)-C(8)	173.7(2)
C(4)-C(3)-C(7)-C(9)	-62.1(3)
C(4)-C(5)-C(6)-C(1)	-68.3(3)
C(4)-C(5)-C(6)-C(7)	40.0(3)
C(4)-C(5)-C(6)-C(10)	169.1(2)
C(5)-C(6)-C(7)-C(3)	-57.8(2)
C(5)-C(6)-C(7)-C(8)	-179.4(2)
C(5)-C(6)-C(7)-C(9)	59.1(3)
C(5)-C(6)-C(10)-S(2)	123.2(2)
C(6)-C(1)-C(2)-O(3)	114.5(2)
C(6)-C(1)-C(2)-O(4)	-123.1(2)
C(6)-C(1)-C(2)-C(3)	-7.8(3)
C(7)-C(3)-C(4)-C(5)	-32.0(3)
C(7)-C(6)-C(10)-S(2)	-115.0(2)
C(10)-S(2)-N(1)-S(1)	-173.17(15)
C(10)-S(2)-N(1)-C(1)	-39.03(19)
C(10)-C(6)-C(7)-C(3)	172.5(2)
C(10)-C(6)-C(7)-C(8)	50.8(3)
C(10)-C(6)-C(7)-C(9)	-70.7(3)
C(11)-O(3)-C(2)-O(4)	63.3(3)
C(11)-O(3)-C(2)-C(1)	-173.1(2)
C(11)-O(3)-C(2)-C(3)	-60.2(3)
C(12)-O(4)-C(2)-O(3)	52.9(3)
C(12)-O(4)-C(2)-C(1)	-67.5(3)
C(12)-O(4)-C(2)-C(3)	-179.0(2)
C(13)-S(1)-N(1)-S(2)	-116.82(16)
C(13)-S(1)-N(1)-C(1)	116.8(2)
S(3)-N(2)-C(14)-C(15)	170.91(17)
S(3)-N(2)-C(14)-C(19)	-74.5(3)
S(4)-N(2)-C(14)-C(15)	42.1(2)
S(4)-N(2)-C(14)-C(19)	156.72(19)
O(5)-S(4)-N(2)-S(3)	-57.64(18)
O(5)-S(4)-N(2)-C(14)	76.0(2)
O(5)-S(4)-C(23)-C(15)	-95.1(2)
O(6)-S(4)-N(2)-S(3)	72.82(17)

O(6)-S(4)-N(2)-C(14)	-153.57(19)
O(6)-S(4)-C(23)-C(15)	131.2(2)
N(2)-S(3)-C(26)-F(4)	24.0(3)
N(2)-S(3)-C(26)-F(5)	-97.8(3)
N(2)-S(3)-C(26)-F(6)	146.4(3)
N(2)-S(4)-C(23)-C(15)	17.7(2)
N(2)-C(14)-C(15)-C(16)	-157.0(2)
N(2)-C(14)-C(15)-C(20)	95.4(2)
N(2)-C(14)-C(15)-C(23)	-29.0(3)
N(2)-C(14)-C(19)-O(7)	120.1(2)
N(2)-C(14)-C(19)-O(8)	-1.8(3)
N(2)-C(14)-C(19)-C(18)	-124.0(2)
C(14)-C(15)-C(16)-C(17)	-69.7(2)
C(14)-C(15)-C(20)-C(18)	52.2(2)
C(14)-C(15)-C(20)-C(21)	-70.1(3)
C(14)-C(15)-C(20)-C(22)	168.2(2)
C(14)-C(15)-C(23)-S(4)	4.4(3)
C(15)-C(14)-C(19)-O(7)	-124.1(2)
C(15)-C(14)-C(19)-O(8)	114.1(2)
C(15)-C(14)-C(19)-C(18)	-8.2(2)
C(15)-C(16)-C(17)-C(18)	-3.2(3)
C(16)-C(15)-C(20)-C(18)	-57.2(2)
C(16)-C(15)-C(20)-C(21)	-179.5(2)
C(16)-C(15)-C(20)-C(22)	58.8(3)
C(16)-C(15)-C(23)-S(4)	124.6(2)
C(16)-C(17)-C(18)-C(19)	74.7(2)
C(16)-C(17)-C(18)-C(20)	-33.1(3)
C(17)-C(18)-C(19)-O(7)	52.9(3)
C(17)-C(18)-C(19)-O(8)	177.6(2)
C(17)-C(18)-C(19)-C(14)	-65.3(2)
C(17)-C(18)-C(20)-C(15)	54.3(2)
C(17)-C(18)-C(20)-C(21)	175.3(2)
C(17)-C(18)-C(20)-C(22)	-61.8(3)
C(19)-C(14)-C(15)-C(16)	78.9(2)
C(19)-C(14)-C(15)-C(20)	-28.7(2)
C(19)-C(14)-C(15)-C(23)	-153.1(2)
C(19)-C(18)-C(20)-C(15)	-58.1(2)
C(19)-C(18)-C(20)-C(21)	62.9(3)

C(19)-C(18)-C(20)-C(22)	-174.1(2)
C(20)-C(15)-C(16)-C(17)	38.8(2)
C(20)-C(15)-C(23)-S(4)	-112.6(2)
C(20)-C(18)-C(19)-O(7)	160.7(2)
C(20)-C(18)-C(19)-O(8)	-74.6(3)
C(20)-C(18)-C(19)-C(14)	42.5(2)
C(23)-S(4)-N(2)-S(3)	-169.68(15)
C(23)-S(4)-N(2)-C(14)	-36.1(2)
C(23)-C(15)-C(16)-C(17)	168.0(2)
C(23)-C(15)-C(20)-C(18)	172.1(2)
C(23)-C(15)-C(20)-C(21)	49.8(3)
C(23)-C(15)-C(20)-C(22)	-71.9(3)
C(24)-O(7)-C(19)-O(8)	53.6(3)
C(24)-O(7)-C(19)-C(14)	-67.2(3)
C(24)-O(7)-C(19)-C(18)	-178.5(2)
C(25)-O(8)-C(19)-O(7)	67.1(3)
C(25)-O(8)-C(19)-C(14)	-170.0(2)
C(25)-O(8)-C(19)-C(18)	-56.9(3)
C(26)-S(3)-N(2)-S(4)	-113.09(17)
C(26)-S(3)-N(2)-C(14)	120.1(2)

Symmetry transformations used to generate equivalent atoms:

Table S19. Hydrogen bonds for mo_dm16194_0m [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
C(8)-H(8A)...O(3)	0.98	2.24	2.868(3)	120.7
C(21)-H(21A)...O(8)	0.98	2.25	2.865(4)	119.6

Symmetry transformations used to generate equivalent atoms:

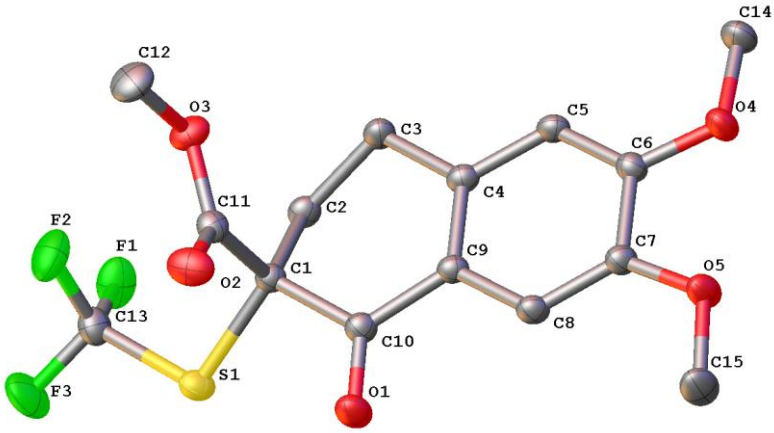


Figure S4. X-ray structure of (R)-Adamantan-1-yl-8-methoxy-1-oxo-2-((trifluoromethyl)thio) -1,2,3,4-tetrahydronaphthalene-2-carboxylate 3n.

Table S20. Crystal data and structure refinement for compound **3m** (mo_dm16808_0m).

Identification code	mo_dm16808_0m	
Empirical formula	C15 H15 F3 O5 S	
Formula weight	364.33	
Temperature	130(2) K	
Wavelength	0.71073 Å	
Crystal system	Orthorhombic	
Space group	P 21 21 21	
Unit cell dimensions	a = 7.5426(6) Å	α= 90 °.
	b = 13.2312(10) Å	β= 90 °.
	c = 15.9887(13) Å	γ = 90 °.
Volume	1595.6(2) $Å^3$	
Z	4	
Density (calculated)	1.517 Mg/m^3	
Absorption coefficient	0.258 mm^{-1}	
F(000)	752	
Crystal size	0.200 x 0.120 x 0.100 mm^3	
Theta range for data collection	1.998 to 30.677 °.	
Index ranges	-10<=h<=10, -18<=k<=15, -22<=l<=22	
Reflections collected	16260	
Independent reflections	4902 [R(int) = 0.0238]	
Completeness to theta = 26.000 °	99.6 %	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	4902 / 0 / 220	
Goodness-of-fit on F^2	1.033	
Final R indices [I>2sigma(I)]	R1 = 0.0273, wR2 = 0.0700	
R indices (all data)	R1 = 0.0307, wR2 = 0.0719	
Absolute structure parameter	-0.017(19)	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.273 and -0.221 e.$Å^{-3}$	

Table S21. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for mo_dm16808_0m. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
S(1)	384(1)	7175(1)	8460(1)	23(1)
F(1)	-466(2)	8983(1)	9055(1)	36(1)
F(2)	2134(2)	8510(1)	9374(1)	40(1)
F(3)	-119(2)	7787(1)	9944(1)	47(1)
O(1)	1255(2)	6027(1)	7109(1)	29(1)
O(2)	4435(2)	7037(1)	8034(1)	32(1)
O(3)	4227(2)	8717(1)	7862(1)	26(1)
O(4)	2120(2)	7939(1)	3515(1)	27(1)
O(5)	1975(2)	6068(1)	3922(1)	28(1)
C(1)	1634(2)	7735(1)	7586(1)	18(1)
C(2)	828(2)	8729(1)	7265(1)	20(1)
C(3)	1705(2)	9082(1)	6452(1)	22(1)
C(4)	1784(2)	8250(1)	5807(1)	19(1)
C(5)	1925(2)	8504(1)	4960(1)	20(1)
C(6)	1994(2)	7766(1)	4349(1)	20(1)
C(7)	1915(2)	6726(1)	4579(1)	21(1)
C(8)	1766(2)	6470(1)	5408(1)	20(1)
C(9)	1706(2)	7231(1)	6029(1)	18(1)
C(10)	1504(2)	6904(1)	6905(1)	20(1)
C(11)	3600(2)	7774(1)	7852(1)	21(1)
C(12)	6059(2)	8798(2)	8136(1)	32(1)
C(13)	501(2)	8159(1)	9229(1)	25(1)
C(14)	2012(3)	8974(1)	3250(1)	30(1)
C(15)	1769(3)	5018(1)	4115(1)	35(1)

Table S22. Bond lengths [Å] and angles [°] for mo_dm16808_0m.

S(1)-C(1)	1.8417(14)
S(1)-C(13)	1.7933(17)
F(1)-C(13)	1.341(2)
F(2)-C(13)	1.337(2)
F(3)-C(13)	1.3307(19)
O(1)-C(10)	1.2197(18)
O(2)-C(11)	1.1972(19)
O(3)-C(11)	1.3337(19)
O(3)-C(12)	1.453(2)
O(4)-C(6)	1.3562(18)
O(4)-C(14)	1.4346(18)
O(5)-C(7)	1.3644(18)
O(5)-C(15)	1.4314(19)
C(1)-C(2)	1.536(2)
C(1)-C(10)	1.551(2)
C(1)-C(11)	1.544(2)
C(2)-H(2A)	0.9900
C(2)-H(2B)	0.9900
C(2)-C(3)	1.532(2)
C(3)-H(3A)	0.9900
C(3)-H(3B)	0.9900
C(3)-C(4)	1.509(2)
C(4)-C(5)	1.399(2)
C(4)-C(9)	1.3957(19)
C(5)-H(5)	0.9500
C(5)-C(6)	1.383(2)
C(6)-C(7)	1.426(2)
C(7)-C(8)	1.373(2)
C(8)-H(8)	0.9500
C(8)-C(9)	1.4150(19)
C(9)-C(10)	1.474(2)
C(12)-H(12A)	0.9800
C(12)-H(12B)	0.9800
C(12)-H(12C)	0.9800
C(14)-H(14A)	0.9800
C(14)-H(14B)	0.9800

C(14)-H(14C)	0.9800
C(15)-H(15A)	0.9800
C(15)-H(15B)	0.9800
C(15)-H(15C)	0.9800

C(13)-S(1)-C(1)	101.69(7)
C(11)-O(3)-C(12)	114.16(13)
C(6)-O(4)-C(14)	116.55(12)
C(7)-O(5)-C(15)	116.77(12)
C(2)-C(1)-S(1)	113.28(10)
C(2)-C(1)-C(10)	110.37(12)
C(2)-C(1)-C(11)	116.34(12)
C(10)-C(1)-S(1)	102.35(9)
C(11)-C(1)-S(1)	107.20(10)
C(11)-C(1)-C(10)	106.16(11)
C(1)-C(2)-H(2A)	109.2
C(1)-C(2)-H(2B)	109.2
H(2A)-C(2)-H(2B)	107.9
C(3)-C(2)-C(1)	111.91(12)
C(3)-C(2)-H(2A)	109.2
C(3)-C(2)-H(2B)	109.2
C(2)-C(3)-H(3A)	109.2
C(2)-C(3)-H(3B)	109.2
H(3A)-C(3)-H(3B)	107.9
C(4)-C(3)-C(2)	112.05(12)
C(4)-C(3)-H(3A)	109.2
C(4)-C(3)-H(3B)	109.2
C(5)-C(4)-C(3)	119.29(13)
C(9)-C(4)-C(3)	121.87(13)
C(9)-C(4)-C(5)	118.83(13)
C(4)-C(5)-H(5)	119.4
C(6)-C(5)-C(4)	121.11(13)
C(6)-C(5)-H(5)	119.4
O(4)-C(6)-C(5)	125.28(13)
O(4)-C(6)-C(7)	114.84(13)
C(5)-C(6)-C(7)	119.88(13)
O(5)-C(7)-C(6)	114.59(13)
O(5)-C(7)-C(8)	126.04(14)

C(8)-C(7)-C(6)	119.37(13)
C(7)-C(8)-H(8)	119.8
C(7)-C(8)-C(9)	120.35(13)
C(9)-C(8)-H(8)	119.8
C(4)-C(9)-C(8)	120.46(13)
C(4)-C(9)-C(10)	122.08(13)
C(8)-C(9)-C(10)	117.44(12)
O(1)-C(10)-C(1)	119.80(13)
O(1)-C(10)-C(9)	123.38(13)
C(9)-C(10)-C(1)	116.82(12)
O(2)-C(11)-O(3)	124.95(14)
O(2)-C(11)-C(1)	123.04(14)
O(3)-C(11)-C(1)	112.01(12)
O(3)-C(12)-H(12A)	109.5
O(3)-C(12)-H(12B)	109.5
O(3)-C(12)-H(12C)	109.5
H(12A)-C(12)-H(12B)	109.5
H(12A)-C(12)-H(12C)	109.5
H(12B)-C(12)-H(12C)	109.5
F(1)-C(13)-S(1)	114.94(12)
F(2)-C(13)-S(1)	114.65(11)
F(2)-C(13)-F(1)	104.68(14)
F(3)-C(13)-S(1)	107.70(12)
F(3)-C(13)-F(1)	106.76(14)
F(3)-C(13)-F(2)	107.65(14)
O(4)-C(14)-H(14A)	109.5
O(4)-C(14)-H(14B)	109.5
O(4)-C(14)-H(14C)	109.5
H(14A)-C(14)-H(14B)	109.5
H(14A)-C(14)-H(14C)	109.5
H(14B)-C(14)-H(14C)	109.5
O(5)-C(15)-H(15A)	109.5
O(5)-C(15)-H(15B)	109.5
O(5)-C(15)-H(15C)	109.5
H(15A)-C(15)-H(15B)	109.5
H(15A)-C(15)-H(15C)	109.5
H(15B)-C(15)-H(15C)	109.5

Table S23. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for mo_dm16808_0m. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ... \quad + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
S(1)	26(1)	20(1)	23(1)	0(1)	7(1)	-1(1)
F(1)	42(1)	34(1)	34(1)	-10(1)	-2(1)	15(1)
F(2)	28(1)	56(1)	36(1)	-15(1)	-5(1)	-2(1)
F(3)	73(1)	41(1)	26(1)	0(1)	22(1)	-2(1)
O(1)	46(1)	17(1)	25(1)	1(1)	3(1)	-2(1)
O(2)	23(1)	28(1)	44(1)	8(1)	0(1)	6(1)
O(3)	19(1)	23(1)	35(1)	-3(1)	-3(1)	-1(1)
O(4)	42(1)	19(1)	19(1)	3(1)	2(1)	-2(1)
O(5)	47(1)	17(1)	21(1)	-3(1)	7(1)	-2(1)
C(1)	19(1)	16(1)	19(1)	0(1)	1(1)	1(1)
C(2)	22(1)	15(1)	23(1)	-1(1)	-1(1)	3(1)
C(3)	30(1)	15(1)	21(1)	0(1)	-2(1)	0(1)
C(4)	20(1)	15(1)	22(1)	0(1)	0(1)	0(1)
C(5)	24(1)	14(1)	23(1)	1(1)	-1(1)	-1(1)
C(6)	23(1)	18(1)	20(1)	1(1)	1(1)	0(1)
C(7)	25(1)	16(1)	20(1)	-1(1)	3(1)	-1(1)
C(8)	25(1)	14(1)	22(1)	0(1)	2(1)	0(1)
C(9)	19(1)	14(1)	21(1)	0(1)	1(1)	0(1)
C(10)	22(1)	16(1)	21(1)	-1(1)	1(1)	2(1)
C(11)	19(1)	23(1)	20(1)	0(1)	2(1)	1(1)
C(12)	18(1)	37(1)	42(1)	-3(1)	-4(1)	-3(1)
C(13)	26(1)	29(1)	21(1)	-1(1)	2(1)	3(1)
C(14)	45(1)	19(1)	25(1)	6(1)	-1(1)	-3(1)
C(15)	61(1)	16(1)	28(1)	-3(1)	4(1)	-1(1)

Table S24. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for mo_dm16808_0m.

	x	y	z	U(eq)
H(2A)	-457	8632	7169	24
H(2B)	973	9258	7697	24
H(3A)	1028	9659	6221	26
H(3B)	2922	9318	6574	26
H(5)	1974	9196	4802	24
H(8)	1702	5779	5566	24
H(12A)	6796	8333	7809	49
H(12B)	6139	8623	8730	49
H(12C)	6476	9492	8053	49
H(14A)	2103	9008	2640	44
H(14B)	2984	9359	3502	44
H(14C)	876	9260	3429	44
H(15A)	1848	4620	3599	53
H(15B)	609	4907	4376	53
H(15C)	2707	4807	4501	53

Table S25. Torsion angles [°] for mo_dm16808_0m.

S(1)-C(1)-C(2)-C(3)	-170.43(10)
S(1)-C(1)-C(10)-O(1)	-24.47(17)
S(1)-C(1)-C(10)-C(9)	155.91(11)
S(1)-C(1)-C(11)-O(2)	59.63(17)
S(1)-C(1)-C(11)-O(3)	-119.64(11)
O(4)-C(6)-C(7)-O(5)	-0.1(2)
O(4)-C(6)-C(7)-C(8)	-179.26(14)
O(5)-C(7)-C(8)-C(9)	-179.57(15)
C(1)-S(1)-C(13)-F(1)	70.77(14)
C(1)-S(1)-C(13)-F(2)	-50.63(14)
C(1)-S(1)-C(13)-F(3)	-170.41(12)
C(1)-C(2)-C(3)-C(4)	50.11(17)
C(2)-C(1)-C(10)-O(1)	-145.33(15)
C(2)-C(1)-C(10)-C(9)	35.06(17)
C(2)-C(1)-C(11)-O(2)	-172.42(14)
C(2)-C(1)-C(11)-O(3)	8.31(18)
C(2)-C(3)-C(4)-C(5)	157.00(14)
C(2)-C(3)-C(4)-C(9)	-22.5(2)
C(3)-C(4)-C(5)-C(6)	-179.73(14)
C(3)-C(4)-C(9)-C(8)	179.35(14)
C(3)-C(4)-C(9)-C(10)	1.3(2)
C(4)-C(5)-C(6)-O(4)	179.60(15)
C(4)-C(5)-C(6)-C(7)	0.2(2)
C(4)-C(9)-C(10)-O(1)	172.40(16)
C(4)-C(9)-C(10)-C(1)	-8.0(2)
C(5)-C(4)-C(9)-C(8)	-0.1(2)
C(5)-C(4)-C(9)-C(10)	-178.16(14)
C(5)-C(6)-C(7)-O(5)	179.30(14)
C(5)-C(6)-C(7)-C(8)	0.2(2)
C(6)-C(7)-C(8)-C(9)	-0.5(2)
C(7)-C(8)-C(9)-C(4)	0.5(2)
C(7)-C(8)-C(9)-C(10)	178.65(15)
C(8)-C(9)-C(10)-O(1)	-5.7(2)
C(8)-C(9)-C(10)-C(1)	173.91(13)
C(9)-C(4)-C(5)-C(6)	-0.2(2)
C(10)-C(1)-C(2)-C(3)	-56.34(16)

C(10)-C(1)-C(11)-O(2)	-49.20(19)
C(10)-C(1)-C(11)-O(3)	131.53(12)
C(11)-C(1)-C(2)-C(3)	64.66(16)
C(11)-C(1)-C(10)-O(1)	87.78(17)
C(11)-C(1)-C(10)-C(9)	-91.84(15)
C(12)-O(3)-C(11)-O(2)	-1.2(2)
C(12)-O(3)-C(11)-C(1)	178.09(13)
C(13)-S(1)-C(1)-C(2)	-59.74(12)
C(13)-S(1)-C(1)-C(10)	-178.57(10)
C(13)-S(1)-C(1)-C(11)	69.97(11)
C(14)-O(4)-C(6)-C(5)	-5.9(2)
C(14)-O(4)-C(6)-C(7)	173.54(14)
C(15)-O(5)-C(7)-C(6)	-175.55(16)
C(15)-O(5)-C(7)-C(8)	3.5(3)

Symmetry transformations used to generate equivalent atoms:

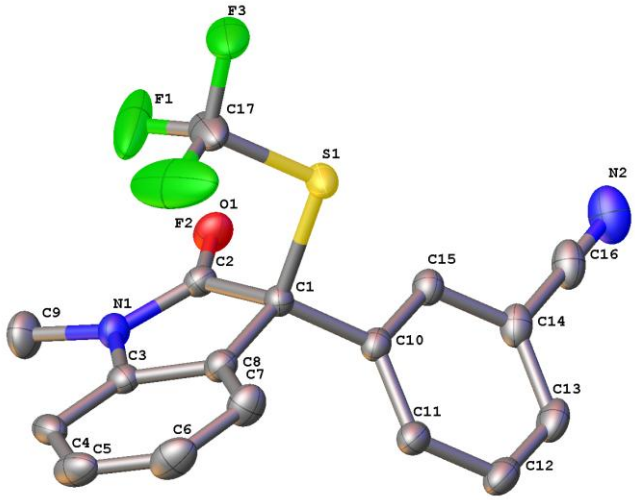


Figure S5. X-ray structure of compound (S)-3-(1-Methyl-2-oxo-3-((trifluoromethyl) -thio)indolin-3-yl)benzonitrile 4i

Table S26. Crystal data and structure refinement for compound **4i** (mo_dm16829_0m).

Identification code	mo_dm16829_0m	
Empirical formula	C17 H11 F3 N2 O S	
Formula weight	348.34	
Temperature	130 K	
Wavelength	0.71073 Å	
Crystal system	Orthorhombic	
Space group	P 21 21 21	
Unit cell dimensions	a = 8.5502(8) Å	α= 90 °.
	b = 11.0835(11) Å	β= 90 °.
	c = 16.8212(16) Å	γ = 90 °.
Volume	1594.1(3) $Å^3$	
Z	4	
Density (calculated)	1.451 Mg/m^3	
Absorption coefficient	0.241 mm^{-1}	
F(000)	712	
Crystal size	0.18 x 0.15 x 0.12 mm^3	
Theta range for data collection	2.201 to 30.801 °.	
Index ranges	-12<=h<=12, -15<=k<=15, -19<=l<=24	
Reflections collected	16232	
Independent reflections	4949 [R(int) = 0.0416]	
Completeness to theta = 25.242 °	100.0 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7461 and 0.6370	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	4949 / 0 / 218	
Goodness-of-fit on F^2	1.036	
Final R indices [I>2sigma(I)]	R1 = 0.0397, wR2 = 0.0975	
R indices (all data)	R1 = 0.0471, wR2 = 0.1022	
Absolute structure parameter	0.01(3)	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.364 and -0.392 e.$Å^{-3}$	

Table S27. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for mo_dm16829_0m. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
S(1)	3385(1)	3388(1)	5503(1)	27(1)
F(1)	3443(5)	2883(2)	7021(1)	98(1)
F(2)	1451(3)	2208(2)	6437(2)	113(1)
F(3)	3681(2)	1391(1)	6236(1)	48(1)
O(1)	4767(2)	5614(2)	6603(1)	30(1)
N(1)	2276(2)	5522(2)	7119(1)	22(1)
N(2)	7676(3)	6778(2)	3766(1)	43(1)
C(1)	2538(3)	4856(2)	5796(1)	20(1)
C(2)	3388(3)	5377(2)	6546(1)	22(1)
C(3)	796(3)	5137(2)	6863(1)	21(1)
C(4)	-574(3)	5071(2)	7300(1)	26(1)
C(5)	-1904(3)	4631(2)	6921(2)	34(1)
C(6)	-1857(3)	4265(3)	6131(2)	35(1)
C(7)	-460(3)	4314(2)	5702(1)	29(1)
C(8)	867(3)	4757(2)	6072(1)	22(1)
C(9)	2606(3)	6052(2)	7895(1)	33(1)
C(10)	2866(3)	5654(2)	5072(1)	21(1)
C(11)	1683(3)	6226(2)	4650(1)	25(1)
C(12)	2034(3)	6969(2)	4001(1)	31(1)
C(13)	3565(3)	7125(2)	3765(1)	31(1)
C(14)	4767(3)	6546(2)	4181(1)	27(1)
C(15)	4427(3)	5812(2)	4833(1)	23(1)
C(16)	6386(3)	6682(2)	3946(1)	32(1)
C(17)	2962(4)	2445(2)	6341(2)	46(1)

Table S28. Bond lengths [Å] and angles [°] for mo_dm16829_0m.

S(1)-C(1)	1.848(2)
S(1)-C(17)	1.793(3)
F(1)-C(17)	1.309(4)
F(2)-C(17)	1.327(4)
F(3)-C(17)	1.331(3)
O(1)-C(2)	1.212(3)
N(1)-C(2)	1.364(3)
N(1)-C(3)	1.403(3)
N(1)-C(9)	1.459(3)
N(2)-C(16)	1.149(4)
C(1)-C(2)	1.566(3)
C(1)-C(8)	1.506(3)
C(1)-C(10)	1.531(3)
C(3)-C(4)	1.385(3)
C(3)-C(8)	1.397(3)
C(4)-H(4)	0.9500
C(4)-C(5)	1.392(4)
C(5)-H(5)	0.9500
C(5)-C(6)	1.390(4)
C(6)-H(6)	0.9500
C(6)-C(7)	1.396(3)
C(7)-H(7)	0.9500
C(7)-C(8)	1.385(3)
C(9)-H(9A)	0.9800
C(9)-H(9B)	0.9800
C(9)-H(9C)	0.9800
C(10)-C(11)	1.388(3)
C(10)-C(15)	1.405(3)
C(11)-H(11)	0.9500
C(11)-C(12)	1.400(3)
C(12)-H(12)	0.9500
C(12)-C(13)	1.378(4)
C(13)-H(13)	0.9500
C(13)-C(14)	1.399(3)
C(14)-C(15)	1.396(3)
C(14)-C(16)	1.448(4)

C(15)-H(15)	0.9500

C(17)-S(1)-C(1)	102.99(11)
C(2)-N(1)-C(3)	112.06(17)
C(2)-N(1)-C(9)	123.1(2)
C(3)-N(1)-C(9)	124.85(19)
C(2)-C(1)-S(1)	110.95(14)
C(8)-C(1)-S(1)	112.95(15)
C(8)-C(1)-C(2)	102.59(16)
C(8)-C(1)-C(10)	117.48(18)
C(10)-C(1)-S(1)	102.99(13)
C(10)-C(1)-C(2)	110.04(17)
O(1)-C(2)-N(1)	126.6(2)
O(1)-C(2)-C(1)	126.5(2)
N(1)-C(2)-C(1)	106.85(18)
C(4)-C(3)-N(1)	128.0(2)
C(4)-C(3)-C(8)	121.8(2)
C(8)-C(3)-N(1)	110.15(18)
C(3)-C(4)-H(4)	121.1
C(3)-C(4)-C(5)	117.8(2)
C(5)-C(4)-H(4)	121.1
C(4)-C(5)-H(5)	119.4
C(6)-C(5)-C(4)	121.1(2)
C(6)-C(5)-H(5)	119.4
C(5)-C(6)-H(6)	119.8
C(5)-C(6)-C(7)	120.5(2)
C(7)-C(6)-H(6)	119.8
C(6)-C(7)-H(7)	120.6
C(8)-C(7)-C(6)	118.9(2)
C(8)-C(7)-H(7)	120.6
C(3)-C(8)-C(1)	108.28(18)
C(7)-C(8)-C(1)	131.7(2)
C(7)-C(8)-C(3)	119.9(2)
N(1)-C(9)-H(9A)	109.5
N(1)-C(9)-H(9B)	109.5
N(1)-C(9)-H(9C)	109.5
H(9A)-C(9)-H(9B)	109.5
H(9A)-C(9)-H(9C)	109.5

H(9B)-C(9)-H(9C)	109.5
C(11)-C(10)-C(1)	122.5(2)
C(11)-C(10)-C(15)	119.3(2)
C(15)-C(10)-C(1)	118.24(18)
C(10)-C(11)-H(11)	119.6
C(10)-C(11)-C(12)	120.7(2)
C(12)-C(11)-H(11)	119.6
C(11)-C(12)-H(12)	119.9
C(13)-C(12)-C(11)	120.1(2)
C(13)-C(12)-H(12)	119.9
C(12)-C(13)-H(13)	120.2
C(12)-C(13)-C(14)	119.7(2)
C(14)-C(13)-H(13)	120.2
C(13)-C(14)-C(16)	121.2(2)
C(15)-C(14)-C(13)	120.5(2)
C(15)-C(14)-C(16)	118.3(2)
C(10)-C(15)-H(15)	120.2
C(14)-C(15)-C(10)	119.6(2)
C(14)-C(15)-H(15)	120.2
N(2)-C(16)-C(14)	179.1(3)
F(1)-C(17)-S(1)	114.0(2)
F(1)-C(17)-F(2)	105.8(3)
F(1)-C(17)-F(3)	107.2(3)
F(2)-C(17)-S(1)	114.0(2)
F(2)-C(17)-F(3)	107.0(3)
F(3)-C(17)-S(1)	108.32(18)

Symmetry transformations used to generate equivalent atoms:

Table S29. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for mo_dm16829_0m. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
S(1)	38(1)	21(1)	24(1)	3(1)	8(1)	6(1)
F(1)	226(4)	41(1)	26(1)	8(1)	17(1)	40(2)
F(2)	72(2)	81(2)	185(3)	95(2)	63(2)	25(1)
F(3)	80(1)	25(1)	40(1)	8(1)	13(1)	19(1)
O(1)	21(1)	39(1)	29(1)	5(1)	-4(1)	-2(1)
N(1)	25(1)	23(1)	19(1)	-1(1)	-1(1)	0(1)
N(2)	47(1)	42(1)	39(1)	-5(1)	9(1)	-17(1)
C(1)	22(1)	20(1)	17(1)	1(1)	1(1)	2(1)
C(2)	22(1)	22(1)	20(1)	2(1)	-2(1)	2(1)
C(3)	23(1)	18(1)	22(1)	3(1)	1(1)	2(1)
C(4)	26(1)	24(1)	27(1)	5(1)	7(1)	8(1)
C(5)	21(1)	36(1)	44(1)	14(1)	5(1)	4(1)
C(6)	22(1)	40(1)	42(1)	12(1)	-6(1)	-6(1)
C(7)	28(1)	33(1)	28(1)	2(1)	-5(1)	-5(1)
C(8)	22(1)	22(1)	22(1)	3(1)	-1(1)	1(1)
C(9)	42(1)	35(1)	22(1)	-7(1)	-2(1)	-4(1)
C(10)	27(1)	18(1)	17(1)	0(1)	0(1)	0(1)
C(11)	31(1)	23(1)	21(1)	0(1)	-1(1)	4(1)
C(12)	44(1)	25(1)	24(1)	3(1)	-4(1)	5(1)
C(13)	48(2)	23(1)	21(1)	4(1)	2(1)	-3(1)
C(14)	37(1)	22(1)	21(1)	-1(1)	3(1)	-7(1)
C(15)	28(1)	21(1)	20(1)	1(1)	2(1)	-1(1)
C(16)	44(1)	28(1)	24(1)	-1(1)	6(1)	-11(1)
C(17)	67(2)	29(1)	41(2)	16(1)	23(1)	19(1)

Table S30. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for mo_dm16829_0m.

	x	y	z	U(eq)
H(4)	-604	5317	7841	31
H(5)	-2860	4580	7207	40
H(6)	-2782	3980	5881	42
H(7)	-422	4047	5166	35
H(9A)	2015	6804	7955	49
H(9B)	3728	6222	7939	49
H(9C)	2298	5485	8314	49
H(11)	624	6113	4804	30
H(12)	1216	7366	3723	37
H(13)	3803	7623	3322	37
H(15)	5247	5422	5115	28

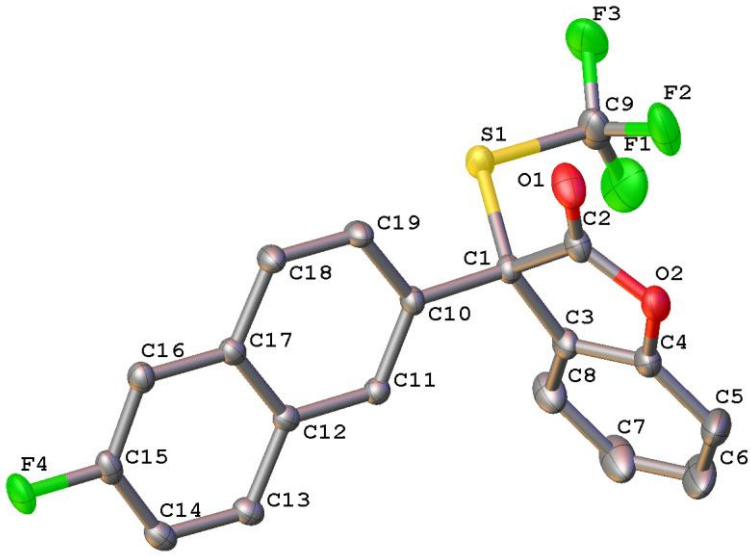


Figure S6. X-ray structure of (S)-3-(6-Fluoronaphthalen-2-yl)-3-((trifluoro methyl)thio)benzofuran-2(3*H*)-one 5g

Table S31. Crystal data and structure refinement for compound **7i** (mo_dm16671_0m).

Identification code	mo_dm16671_0m	
Empirical formula	C19 H10 F4 O2 S	
Formula weight	378.33	
Temperature	130 K	
Wavelength	0.71073 Å	
Crystal system	Orthorhombic	
Space group	P 21 21 21	
Unit cell dimensions	a = 6.6977(5) Å	α= 90 °.
	b = 8.1914(6) Å	β= 90 °.
	c = 30.513(2) Å	γ = 90 °.
Volume	1674.0(2) $Å^3$	
Z	4	
Density (calculated)	1.501 Mg/m^3	
Absorption coefficient	0.246 mm^{-1}	
F(000)	768	
Crystal size	0.25 x 0.22 x 0.2 mm^3	
Theta range for data collection	2.575 to 30.677 °.	
Index ranges	-9<=h<=9, -11<=k<=7, -43<=l<=41	
Reflections collected	17063	
Independent reflections	5168 [R(int) = 0.0202]	
Completeness to theta = 26.000 °	99.7 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7461 and 0.6139	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	5168 / 0 / 235	
Goodness-of-fit on F^2	1.067	
Final R indices [I>2sigma(I)]	R1 = 0.0334, wR2 = 0.0865	
R indices (all data)	R1 = 0.0353, wR2 = 0.0875	
Absolute structure parameter	0.004(19)	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.327 and -0.250 e.$Å^{-3}$	

Table S32. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for mo_dm16671_0m. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
S(1)	858(1)	2490(1)	6149(1)	24(1)
F(1)	320(3)	2658(2)	7008(1)	53(1)
F(2)	2669(2)	1052(2)	6810(1)	48(1)
F(3)	-411(2)	384(2)	6698(1)	51(1)
F(4)	2887(2)	8983(2)	3981(1)	29(1)
O(1)	5596(3)	1626(2)	5998(1)	33(1)
O(2)	6126(2)	3358(2)	6554(1)	25(1)
C(1)	3097(2)	3789(2)	6154(1)	16(1)
C(2)	5037(3)	2758(2)	6210(1)	21(1)
C(3)	3252(3)	4927(2)	6538(1)	20(1)
C(4)	5050(3)	4630(2)	6746(1)	25(1)
C(5)	5706(5)	5475(3)	7109(1)	43(1)
C(6)	4435(6)	6660(3)	7269(1)	55(1)
C(7)	2582(5)	6969(3)	7072(1)	47(1)
C(8)	1974(4)	6113(2)	6703(1)	31(1)
C(9)	875(4)	1620(3)	6693(1)	34(1)
C(10)	3102(3)	4580(2)	5698(1)	17(1)
C(11)	3113(2)	6250(2)	5646(1)	16(1)
C(12)	3094(2)	6960(2)	5219(1)	15(1)
C(13)	3097(3)	8679(2)	5160(1)	20(1)
C(14)	3042(3)	9339(2)	4746(1)	22(1)
C(15)	2985(3)	8283(2)	4386(1)	21(1)
C(16)	2997(3)	6621(2)	4417(1)	19(1)
C(17)	3052(3)	5926(2)	4845(1)	17(1)
C(18)	3064(3)	4204(2)	4908(1)	20(1)
C(19)	3091(3)	3549(2)	5321(1)	20(1)

Table S33. Bond lengths [Å] and angles [°] for mo_dm16671_0m.

S(1)-C(1)	1.8386(17)
S(1)-C(9)	1.805(2)
F(1)-C(9)	1.336(3)
F(2)-C(9)	1.337(3)
F(3)-C(9)	1.330(3)
F(4)-C(15)	1.3626(19)
O(1)-C(2)	1.192(2)
O(2)-C(2)	1.369(2)
O(2)-C(4)	1.396(2)
C(1)-C(2)	1.559(2)
C(1)-C(3)	1.501(2)
C(1)-C(10)	1.535(2)
C(3)-C(4)	1.383(3)
C(3)-C(8)	1.389(3)
C(4)-C(5)	1.379(3)
C(5)-H(5)	0.9500
C(5)-C(6)	1.380(4)
C(6)-H(6)	0.9500
C(6)-C(7)	1.402(5)
C(7)-H(7)	0.9500
C(7)-C(8)	1.388(3)
C(8)-H(8)	0.9500
C(10)-C(11)	1.378(2)
C(10)-C(19)	1.427(2)
C(11)-H(11)	0.9500
C(11)-C(12)	1.425(2)
C(12)-C(13)	1.419(2)
C(12)-C(17)	1.421(2)
C(13)-H(13)	0.9500
C(13)-C(14)	1.373(2)
C(14)-H(14)	0.9500
C(14)-C(15)	1.400(3)
C(15)-C(16)	1.364(2)
C(16)-H(16)	0.9500
C(16)-C(17)	1.426(2)
C(17)-C(18)	1.423(2)

C(18)-H(18)	0.9500
C(18)-C(19)	1.369(2)
C(19)-H(19)	0.9500

C(9)-S(1)-C(1)	102.48(9)
C(2)-O(2)-C(4)	108.30(14)
C(2)-C(1)-S(1)	111.55(11)
C(3)-C(1)-S(1)	114.92(12)
C(3)-C(1)-C(2)	101.07(14)
C(3)-C(1)-C(10)	116.47(13)
C(10)-C(1)-S(1)	103.84(11)
C(10)-C(1)-C(2)	109.10(13)
O(1)-C(2)-O(2)	121.90(17)
O(1)-C(2)-C(1)	128.54(17)
O(2)-C(2)-C(1)	109.56(14)
C(4)-C(3)-C(1)	108.02(15)
C(4)-C(3)-C(8)	119.50(17)
C(8)-C(3)-C(1)	132.47(18)
C(3)-C(4)-O(2)	112.87(16)
C(5)-C(4)-O(2)	123.2(2)
C(5)-C(4)-C(3)	123.9(2)
C(4)-C(5)-H(5)	121.9
C(4)-C(5)-C(6)	116.2(2)
C(6)-C(5)-H(5)	121.9
C(5)-C(6)-H(6)	119.3
C(5)-C(6)-C(7)	121.5(2)
C(7)-C(6)-H(6)	119.3
C(6)-C(7)-H(7)	119.5
C(8)-C(7)-C(6)	121.0(2)
C(8)-C(7)-H(7)	119.5
C(3)-C(8)-H(8)	121.1
C(7)-C(8)-C(3)	117.9(2)
C(7)-C(8)-H(8)	121.1
F(1)-C(9)-S(1)	114.07(16)
F(1)-C(9)-F(2)	106.2(2)
F(2)-C(9)-S(1)	112.91(16)
F(3)-C(9)-S(1)	107.99(15)
F(3)-C(9)-F(1)	107.14(19)

F(3)-C(9)-F(2)	108.24(19)
C(11)-C(10)-C(1)	121.60(14)
C(11)-C(10)-C(19)	119.65(15)
C(19)-C(10)-C(1)	118.75(14)
C(10)-C(11)-H(11)	119.6
C(10)-C(11)-C(12)	120.71(14)
C(12)-C(11)-H(11)	119.6
C(13)-C(12)-C(11)	121.40(15)
C(13)-C(12)-C(17)	119.28(15)
C(17)-C(12)-C(11)	119.31(14)
C(12)-C(13)-H(13)	119.8
C(14)-C(13)-C(12)	120.49(16)
C(14)-C(13)-H(13)	119.8
C(13)-C(14)-H(14)	120.7
C(13)-C(14)-C(15)	118.67(16)
C(15)-C(14)-H(14)	120.7
F(4)-C(15)-C(14)	116.96(15)
F(4)-C(15)-C(16)	118.87(17)
C(16)-C(15)-C(14)	124.16(17)
C(15)-C(16)-H(16)	121.2
C(15)-C(16)-C(17)	117.52(17)
C(17)-C(16)-H(16)	121.2
C(12)-C(17)-C(16)	119.87(15)
C(12)-C(17)-C(18)	118.89(15)
C(18)-C(17)-C(16)	121.23(15)
C(17)-C(18)-H(18)	119.6
C(19)-C(18)-C(17)	120.77(15)
C(19)-C(18)-H(18)	119.6
C(10)-C(19)-H(19)	119.7
C(18)-C(19)-C(10)	120.66(15)
C(18)-C(19)-H(19)	119.7

Symmetry transformations used to generate equivalent atoms:

Table S34. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for mo_dm16671_0m. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ...\ \ + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
S(1)	25(1)	27(1)	21(1)	6(1)	-3(1)	-6(1)
F(1)	65(1)	69(1)	26(1)	6(1)	12(1)	-12(1)
F(2)	40(1)	59(1)	45(1)	31(1)	-11(1)	-5(1)
F(3)	48(1)	54(1)	50(1)	27(1)	-7(1)	-26(1)
F(4)	34(1)	32(1)	22(1)	14(1)	0(1)	0(1)
O(1)	41(1)	34(1)	23(1)	1(1)	3(1)	18(1)
O(2)	24(1)	27(1)	25(1)	5(1)	-5(1)	1(1)
C(1)	19(1)	17(1)	14(1)	1(1)	0(1)	2(1)
C(2)	22(1)	24(1)	18(1)	6(1)	1(1)	4(1)
C(3)	29(1)	19(1)	13(1)	0(1)	0(1)	1(1)
C(4)	34(1)	21(1)	20(1)	4(1)	-6(1)	-2(1)
C(5)	64(2)	31(1)	34(1)	-1(1)	-27(1)	0(1)
C(6)	105(3)	33(1)	27(1)	-11(1)	-28(1)	11(1)
C(7)	87(2)	33(1)	21(1)	-6(1)	-4(1)	19(1)
C(8)	45(1)	28(1)	19(1)	0(1)	3(1)	12(1)
C(9)	33(1)	42(1)	28(1)	15(1)	-3(1)	-11(1)
C(10)	19(1)	17(1)	14(1)	2(1)	-1(1)	2(1)
C(11)	17(1)	16(1)	15(1)	-1(1)	0(1)	0(1)
C(12)	14(1)	16(1)	17(1)	0(1)	0(1)	0(1)
C(13)	20(1)	16(1)	23(1)	1(1)	1(1)	1(1)
C(14)	21(1)	18(1)	26(1)	5(1)	1(1)	0(1)
C(15)	17(1)	24(1)	20(1)	8(1)	0(1)	-1(1)
C(16)	20(1)	21(1)	17(1)	3(1)	-1(1)	-1(1)
C(17)	16(1)	17(1)	18(1)	2(1)	0(1)	0(1)
C(18)	28(1)	16(1)	16(1)	-1(1)	-1(1)	0(1)
C(19)	29(1)	14(1)	17(1)	-1(1)	0(1)	0(1)

Table S35. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^{3}) for mo_dm16671_0m.

	x	y	z	U(eq)
H(5)	6960	5254	7242	51
H(6)	4825	7280	7518	66
H(7)	1728	7778	7194	56
H(8)	725	6330	6568	37
H(11)	3133	6936	5896	19
H(13)	3137	9378	5408	24
H(14)	3042	10488	4706	26
H(16)	2969	5952	4163	23
H(18)	3054	3501	4660	24
H(19)	3102	2397	5356	24

Table S36. Torsion angles [°] for mo_dm16671_0m.

S(1)-C(1)-C(2)-O(1)	54.1(2)
S(1)-C(1)-C(2)-O(2)	-126.82(13)
S(1)-C(1)-C(3)-C(4)	123.97(14)
S(1)-C(1)-C(3)-C(8)	-55.4(2)
S(1)-C(1)-C(10)-C(11)	123.19(15)
S(1)-C(1)-C(10)-C(19)	-56.68(18)
F(4)-C(15)-C(16)-C(17)	-178.51(14)
O(2)-C(4)-C(5)-C(6)	-177.7(2)
C(1)-S(1)-C(9)-F(1)	74.73(18)
C(1)-S(1)-C(9)-F(2)	-46.66(19)
C(1)-S(1)-C(9)-F(3)	-166.30(16)
C(1)-C(3)-C(4)-O(2)	-2.3(2)
C(1)-C(3)-C(4)-C(5)	178.9(2)
C(1)-C(3)-C(8)-C(7)	-180.0(2)
C(1)-C(10)-C(11)-C(12)	-179.27(14)
C(1)-C(10)-C(19)-C(18)	179.00(16)
C(2)-O(2)-C(4)-C(3)	-0.6(2)
C(2)-O(2)-C(4)-C(5)	178.3(2)
C(2)-C(1)-C(3)-C(4)	3.73(17)
C(2)-C(1)-C(3)-C(8)	-175.7(2)
C(2)-C(1)-C(10)-C(11)	-117.76(17)
C(2)-C(1)-C(10)-C(19)	62.4(2)
C(3)-C(1)-C(2)-O(1)	176.71(19)
C(3)-C(1)-C(2)-O(2)	-4.21(17)
C(3)-C(1)-C(10)-C(11)	-4.2(2)
C(3)-C(1)-C(10)-C(19)	175.92(16)
C(3)-C(4)-C(5)-C(6)	1.0(4)
C(4)-O(2)-C(2)-O(1)	-177.73(18)
C(4)-O(2)-C(2)-C(1)	3.12(18)
C(4)-C(3)-C(8)-C(7)	0.7(3)
C(4)-C(5)-C(6)-C(7)	0.4(4)
C(5)-C(6)-C(7)-C(8)	-1.3(5)
C(6)-C(7)-C(8)-C(3)	0.7(4)
C(8)-C(3)-C(4)-O(2)	177.24(17)
C(8)-C(3)-C(4)-C(5)	-1.6(3)
C(9)-S(1)-C(1)-C(2)	63.83(14)

C(9)-S(1)-C(1)-C(3)	-50.44(15)
C(9)-S(1)-C(1)-C(10)	-178.80(12)
C(10)-C(1)-C(2)-O(1)	-60.0(2)
C(10)-C(1)-C(2)-O(2)	119.05(14)
C(10)-C(1)-C(3)-C(4)	-114.30(16)
C(10)-C(1)-C(3)-C(8)	66.3(3)
C(10)-C(11)-C(12)-C(13)	179.74(16)
C(10)-C(11)-C(12)-C(17)	0.4(2)
C(11)-C(10)-C(19)-C(18)	-0.9(3)
C(11)-C(12)-C(13)-C(14)	-178.81(16)
C(11)-C(12)-C(17)-C(16)	178.89(15)
C(11)-C(12)-C(17)-C(18)	-1.1(2)
C(12)-C(13)-C(14)-C(15)	-0.1(3)
C(12)-C(17)-C(18)-C(19)	0.8(3)
C(13)-C(12)-C(17)-C(16)	-0.5(2)
C(13)-C(12)-C(17)-C(18)	179.55(17)
C(13)-C(14)-C(15)-F(4)	178.58(16)
C(13)-C(14)-C(15)-C(16)	-0.5(3)
C(14)-C(15)-C(16)-C(17)	0.6(3)
C(15)-C(16)-C(17)-C(12)	-0.1(3)
C(15)-C(16)-C(17)-C(18)	179.90(19)
C(16)-C(17)-C(18)-C(19)	-179.15(18)
C(17)-C(12)-C(13)-C(14)	0.6(3)
C(17)-C(18)-C(19)-C(10)	0.2(3)
C(19)-C(10)-C(11)-C(12)	0.6(3)

Symmetry transformations used to generate equivalent atoms: