Electronic Supplementary Material (ESI) for Organic Chemistry Frontiers.

Supporting Information

Visible-Light-Mediated C−F Bond Cleavage for the Synthesis of Polyfluorinated Compounds

Bin Wang, Cui-Tian Wang, Xue-Song Li, Wen-Hui Sun, Xue-Yuan Liu*, and Yong-Min Liang*

State Key Laboratory of Applied Organic Chemistry and College of Chemistry and Chemical Engineering, Lanzhou University, Lanzhou 730000, P.R. China

E-mail: liuxuey@lzu.edu.cn; liangym@lzu.edu.cn

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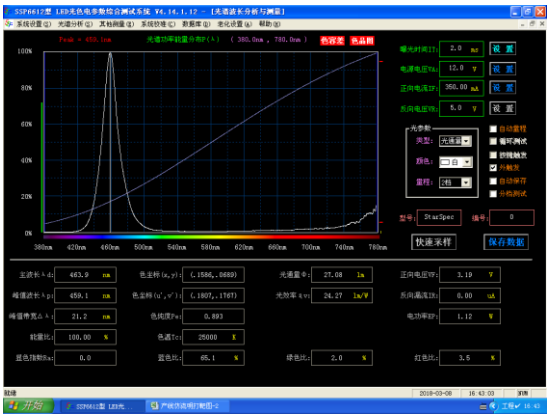
1. General information

Raw materials **1a-u**, **2d, and 2f** were prepared according to reported methods[1-3]. All solvents are commercially available and anhydrous. Unless otherwise noted, all of these reactions were carried out under an argon atmosphere. Analytical thin layer chromatography (TLC) was performed using silica gel plate, and plates were observed by UV radiation (254 nm). Silica gel (200-300 mesh) was employed for column chromatography.

^{1}H NMR and ^{13}C NMR spectra were recorded on BRUKER AVANCE III 400, BRUKER AVANCE III HD 400, or BRUKER AVANCE NEO 600 with 400 MHz or 600 MHz frequencies and 100 MHz or 150 MHz frequencies.^{19}F NMR spectra were recorded on BRUKER AVANCE III HD 400 with 376 MHz or BRUKER AVANCE NEO 600 with 565 MHz frequencies. Chemical shifts of ^{1}H NMR and ^{13}C NMR spectra were recorded with TMS (tetramethyl silane) as the internal reference standard (TMS δ=0.00 for ^{1}H NMR and $CDCl_3$ δ=77.0 for ^{13}C NMR). Data collection for HRMS was obtained from the Q-TOF instrument equipped with an ESI source. All of melting points were measured of micro melting point apparatus.

Light source in detail. We used the following light source, and the distance from the light source to the irradiation vessel is 4-6cm. The material of the irradiation vessel is ordinary glass. Detailed light source information：



2. Experimental procedures

General procedures for the synthesis of polyfluorinated compounds

α-trifluoromethyl alkenes 1 (if solid, 0.2 mmol), $[Ir(ppy)_2(dtbbpy)]PF_6$ (0.5 mol%), DABCO (15-20 mol%), HCO_2Na (0.22-0.25 mmol) were added in a 10 mL pre-dried reaction tube with stir bar. The tube was charged with argon (repeated six times). Then, the solvent (DMSO, 3mL), **2** (1.0 mmol) and **1** (if liquid, 0.2 mmol) were injected. The resulting light-yellow suspension were irradiated by 2*18 W blue LEDs, stirring at room temperature (cooled by fan) for 5 h. After the reaction was complete, water was added and the reaction mixture was extracted with ethyl acetate for 3 times, then dried with anhydrous Na_2SO_4, an appropriate amount of silica gel was added and concentrated in vacuo. The residue was purified with chromatography column on silica gel.

3. 1.0 mmol scale experiment

1a (1.0 mmol), $[Ir(ppy)_2(dtbbpy)]PF_6$ (0.5 mol%), DABCO (15 mol%), HCO_2Na (1.1 mmol) were added in a 50 mL pre-dried round bottom bottle with stir bar. The round bottom bottle was charged with argon (repeated six times), and then the solvent (DMSO, 15 mL) and **2a** (5.0 mmol) were injected. The resulting light-yellow suspension were irradiated by 2*18 W blue LEDs, stirring at room temperature (cooled by fan) for 5 h. After the reaction was complete, water was added and the reaction mixture was extracted with ethyl acetate for 3 times, then dried with anhydrous Na_2SO_4, an appropriate amount of silica gel was added and concentrated in vacuo. The residue was purified with chromatography column on silica gel (eluent: petroleum ether/ethyl acetate = 20:1), and 69% isolated yield of **3aa** (265.2 mg) has been obtained.

4. 10.0 mmol scale experiment

1bf (10.0 mmol), $[Ir(ppy)_2(dtbbpy)]PF_6$ (0.5 mol%), DABCO (15 mol%), HCO_2Na (11.0 mmol) were added in a 250 mL pre-dried round bottom bottle with stir bar. The round bottom bottle was charged with argon (repeated six times), and then the solvent (DMSO, 150 mL) and **2a** (50.0 mmol) were injected. The resulting light-yellow suspension were irradiated by 2*18 W blue LEDs, stirring at room temperature (cooled by fan) for 5 h. After the reaction was complete, water was added and the reaction mixture was extracted with ethyl acetate for 3 times, then dried with anhydrous Na_2SO_4, concentrated in vacuo. The residue was purified with chromatography column on silica gel (eluent: petroleum ether/ethyl acetate = 10:1-3:1), and 44% isolated yield of **3bf** (2.1g) has been obtained.

5. Determination of quantum yield.

(a) Determination of the light intensity at 400 nm:

The photon flux of the spectrophotometer was determined by standard ferrioxalate actinometry. A 0.15 M solution of ferrioxalate was prepared by dissolving 2.21 g of potassium ferrioxalate hydrate in 30 mL of 0.05 M H_2SO_4. A buffered solution of phenanthroline was prepared by dissolving 50 mg of phenanthroline and 11.25 g of sodium acetate in 50 mL of 0.5 M H_2SO_4. Both solutions were stored in the dark. To determine the photon flux of the spectrophotometer, 2.7 mL of the ferrioxalate solution was placed in a cuvette and irradiated for 90.0 seconds at λ = 400 nm with an emission slit width at 5.0 nm. After irradiation, 0.35 mL of the phenanthroline solution was added to the cuvette. The solution was then allowed to rest for 1 h to allow the ferrous ions to completely coordinate to the phenanthroline. The absorbance of the solution was measured at 510 nm. A non-irradiated sample was also prepared and the absorbance at 510 nm measured. Conversion was calculated using eq 1.

$$\text{mol } Fe^{2+} = \frac{V*\Delta A}{L*\mathcal{E}} \quad (1)$$

Where V is the total volume (0.00305 L) of the solution after addition of phenanthroline, ΔA is the difference in absorbance at 510 nm between the irradiated and non-irradiated solutions, L is the path length (1.000 cm), and ε is the molar absorptivity at 510 nm (11,100 L mol^{-1} cm^{-1}). The photon flux can be calculated using eq 2.

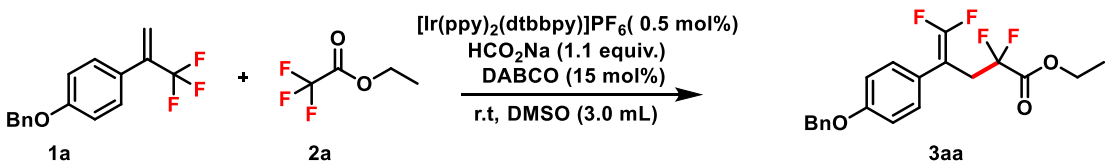
$$\text{photon flux} = \frac{\text{mol } Fe^{2+}}{\Phi*t*f} \quad (2)$$

Where Φ is the quantum yield for the ferrioxalate actinometer (1.13 for a 0.15 M solution at λ = 400 nm), t is the time (90.0 s), and f is the fraction of light absorbed at λ = 400 nm (1). The photon flux was calculated (average of two experiments) to be 5.4356 × 10^{-10} $einsteins^{-1}$.

Sample calculation:

$$\text{mol } Fe^{2+} = \frac{0.00305L*0.2012}{1.0000cm*11100\ L*mol^{-1}cm^{-1}} = 5.528*10^{-8}\ \text{mol}$$

$$\text{photon flux} = \frac{5.528*10^{-8}\ \text{mol}}{1.13*90s*1} = 5.4356*10^{-10}\ \text{einstein}^{-1}$$



1a (0.2 mmol), **2a** (1.0 mmol), [Ir(ppy)$_2$(dtbbpy)]PF_6 (0.5 mol%), DABCO (15 mol%) and HCO_2Na (0.22 mmol) were dissolved in DMSO (3.0 mL), the above system

solution was placed in a cuvette. Irradiated sample (λ = 400 nm, slit width= 5.0 nm) for 1800 s (30 min). After irradiation, the yield of the product formed was determined by ^{1}H NMR. f ($f = 1 - 10^{-Abs}$) is the fraction of light absorbed at λ = 400 nm (Abs = 1.797). The quantum yield was determined using eq 3.

Sample calculation:

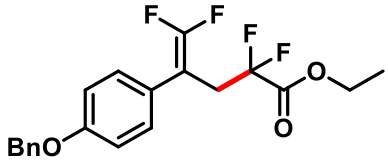
$$\Phi = \frac{\text{mol product}}{\text{flux} * t * f} \quad (3)$$

$$\Phi = \frac{3.14 * 10^{-6}\text{mol}}{5.4356 * 10^{-10}\ \text{einstein}^{-1} * 1800s * 0.98404} = 3.26$$

Thus, 3.26 equivalents of product are formed for every proton absorbed by the photocatalyst.

6. Characteristic data of compounds

ethyl 4-(4-(benzyloxy)phenyl)-2,2,5,5-tetrafluoropent-4-enoate (**3aa**).



56.3 mg, 74% yield, white solid, m.p: 63-65 ℃. eluent: petroleum ether/ethyl acetate 20:1 (v/v).

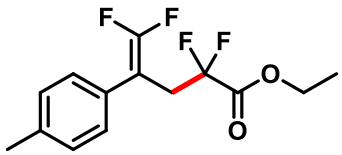
^{1}H NMR (600 MHz, $CDCl_3$) δ 7.41 (d, *J* = 7.1 Hz, 2H), 7.37 (td, *J* = 6.5, 1.9 Hz, 2H), 7.31 (tt, *J* = 7.2, 1.2 Hz, 1H), 7.20 (dd, *J* = 8.7, 2.7 Hz, 2H), 6.95 (dt, *J* = 8.8, 2.6 Hz, 2H), 5.04 (s, 2H), 3.97 (q, *J* = 7.2 Hz, 2H), 3.15 (tt, *J* = 15.0, 1.8 Hz, 2H), 1.16 (t, *J* = 7.1 Hz, 3H).

^{13}C NMR (150 MHz, $CDCl_3$) δ 163.4 (t, *J* = 32.0 Hz), 158.3, 155.2 (t, *J* = 289.8 Hz), 136.7, 129.7 (t, *J* = 2.5 Hz), 128.6, 128.0, 127.4, 124.3, 114.8, 114.5 (tt, *J* = 251.2, 3.4 Hz), 84.3 (tt, *J* = 20.1, 4.8 Hz), 69.9, 62.9, 34.1 (t, *J* = 25.4 Hz), 13.6.

^{19}F NMR (565 MHz, $CDCl_3$) δ -87.52 (s), -104.22 (t, *J* = 15.0 Hz).

HRMS (ESI) m/z: $[M + Na]^+$ Calcd for $C_{20}H_{18}F_4O_3Na^+$ 405.1084; found 405.1091.

ethyl 2,2,5,5-tetrafluoro-4-(p-tolyl)pent-4-enoate (**3ab**).



35.5 mg, 61% yield, yellow oil. eluent: petroleum ether/ethyl acetate 20:1 (v/v).

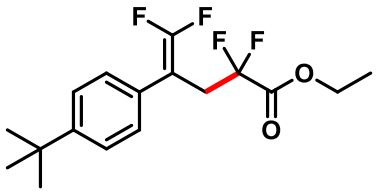
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.19 – 7.14 (m, 4H), 4.00 (q, *J* = 7.2 Hz, 2H), 3.18 (tt, *J* = 15.0, 1.8 Hz, 2H), 2.33 (s, 3H), 1.18 (t, *J* = 7.2 Hz, 3H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 163.4 (t, *J* = 32.1 Hz), 155.2 (t, *J* = 290.0 Hz), 137.7, 129.1, 129.0, 128.3 (t, *J* = 2.8 Hz), 114.5 (tt, *J* = 251.1, 3.9 Hz), 84.6 (tt, *J* = 20.2, 4.8 Hz), 62.9, 34.0 (td, *J* = 25.4, 1.3 Hz), 21.0, 13.6.

^{19}F NMR (376 MHz, $CDCl_3$) δ -87.21 – -87.24 (m), -104.28 – -104.30 (m).

All data matched that reported in the literature[3].

ethyl 4-(4-(tert-butyl)phenyl)-2,2,5,5-tetrafluoropent-4-enoate (**3ac**).



42.5 mg, 64% yield, yellow oil. eluent: petroleum ether/ethyl acetate 20:1 (v/v).

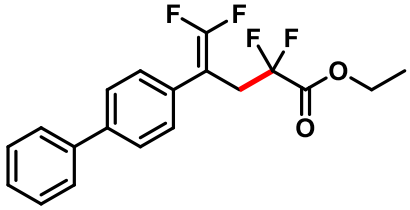
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.31 – 7.27 (m, 2H), 7.16 – 7.13 (m, 2H), 3.83 (q, *J* = 7.2 Hz, 2H), 3.11 (tt, *J* = 14.9, 2.0 Hz, 2H), 1.23 (s, 9H), 1.05 (t, *J* = 7.2 Hz, 3H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 163.4 (t, *J* = 32.1 Hz), 155.3 (t, *J* = 290.2 Hz), 150.9, 128.9, 128.1 (t, *J* = 2.8 Hz), 125.4, 114.5 (tt, *J* = 251.0, 3.7 Hz), 84.5 (tt, *J* = 20.1, 5.0 Hz), 62.8, 34.5, 34.0 (t, *J* = 25.5 Hz), 31.2, 13.6.

^{19}F NMR (376 MHz, $CDCl_3$) δ -86.98 – -87.01 (m), -104.37 (d, *J* = 3.6 Hz).

All data matched that reported in the literature[3].

ethyl 4-([1,1'-biphenyl]-4-yl)-2,2,5,5-tetrafluoropent-4-enoate (**3ad**).



42.3 mg, 60% yield, white solid, m.p: 32-34 ℃. eluent: petroleum ether/ethyl acetate 20:1 (v/v).

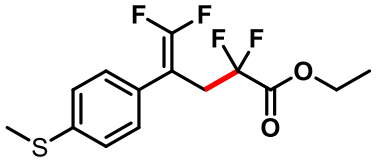
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.60 – 7.57 (m, 4H), 7.44 (t, *J* = 7.5 Hz, 2H), 7.38 – 7.36 (m, 3H), 4.03 (q, *J* = 7.2 Hz, 2H), 3.24 (tt, *J* = 15.0, 1.9 Hz, 2H), 1.19 (t, *J* = 7.2 Hz, 3H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 163.4 (t, *J* = 32.0 Hz), 155.4 (t, *J* = 290.9 Hz), 140.7, 140.3, 131.0 (t, *J* = 2.4 Hz), 128.8, 127.6, 127.1, 127.0, 114.5 (t, *J* = 251.8 Hz), 84.6 (t, *J* = 20.0 Hz), 63.0, 33.9 (td, *J* = 25.6, 1.9 Hz), 13.7.

^{19}F NMR (376 MHz, $CDCl_3$) δ -86.10 – -86.15 (m), -104.25 (d, *J* = 4.5 Hz).

All data matched that reported in the literature[3].

ethyl 2,2,5,5-tetrafluoro-4-(4-(methylthio)phenyl)pent-4-enoate (**3ae**).



34.8 mg, 54% yield, yellow oil. eluent: petroleum ether/ethyl acetate 20:1 (v/v).

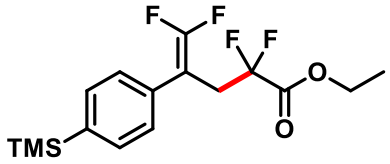
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.24 – 7.19 (m, 4H), 4.04 (q, *J* = 7.2 Hz, 2H), 3.17 (tt, *J* = 15.1, 2.0 Hz, 2H), 2.47 (s, 3H), 1.21 (t, *J* = 7.2 Hz, 3H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 163.3 (t, *J* = 32.1 Hz), 155.2 (t, *J* = 290.5 Hz), 138.6, 128.8 (t, *J* = 2.9 Hz), 128.5, 126.1, 114.4 (tt, *J* = 251.3, 3.7 Hz), 84.4 (tt, *J* = 20.2, 4.6 Hz), 62.9, 33.8 (t, *J* = 25.6 Hz), 15.4, 13.6.

^{19}F NMR (376 MHz, $CDCl_3$) δ -86.54 (d, *J* = 2.9 Hz), -104.28 – -104.29 (m).

All data matched that reported in the literature[3].

ethyl 2,2,5,5-tetrafluoro-4-(4-(trimethylsilyl)phenyl)pent-4-enoate (**3af**).



43.1 mg, 62% yield, yellow oil. eluent: petroleum ether/ethyl acetate 20:1 (v/v).

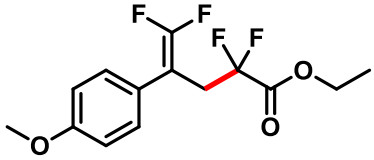
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.51 (d, *J* = 8.0 Hz, 2H), 7.27 (d, *J* = 7.4 Hz, 2H), 3.94 (q, *J* = 7.2 Hz, 2H), 3.21 (tt, *J* = 15.0, 1.8 Hz, 2H), 1.13 (t, *J* = 7.2 Hz, 3H), 0.26 (s, 9H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 163.4 (t, *J* = 32.1 Hz), 155.3 (t, *J* = 290.5 Hz), 140.4, 133.4, 132.4 (t, *J* = 2.5 Hz), 127.7 (t, *J* = 2.8 Hz), 114.4 (tt, *J* =251.3, 3.7 Hz), 84.8 (tt, *J* = 19.8, 5.0 Hz), 62.9, 33.9 (td, *J* = 25.9, 1.9 Hz), 13.5, -1.3.

^{19}F NMR (376 MHz, $CDCl_3$) δ -86.42 – -86.47 (m), -104.30 (d, *J* = 4.0 Hz).

HRMS (ESI) m/z: $[M + Na]^+$ Calcd for $C_{16}H_{20}F_4O_2SiNa^+$ 371.1061; found 371.1050.

ethyl 2,2,5,5-tetrafluoro-4-(4-methoxyphenyl)pent-4-enoate (**3ag**).



46.0 mg, 75% yield, colorless oil. eluent: petroleum ether/ethyl acetate 20:1 (v/v).

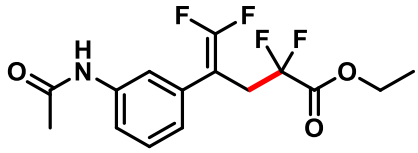
^{1}H NMR (600 MHz, $CDCl_3$) δ 7.21 (d, *J* = 8.6 Hz, 2H), 6.88 (d, *J* = 8.7 Hz, 2H), 4.01 (q, *J* = 7.1 Hz, 2H), 3.79 (s, 3H), 3.16 (t, *J* = 14.9 Hz, 2H), 1.19 (t, *J* = 7.1 Hz, 3H).

^{13}C NMR (150 MHz, $CDCl_3$) δ 163.4 (t, *J* = 32.2 Hz), 159.1, 155.1 (t, *J* = 289.4 Hz), 129.6 (t, *J* = 2.8 Hz), 124.0, 114.5 (tt, *J* = 251.3, 3.6 Hz), 113.8, 84.3 (tt, *J* = 20.1, 4.7 Hz), 62.9, 55.1, 34.0 (t, *J* = 25.4, Hz), 13.6.

^{19}F NMR (565 MHz, $CDCl_3$) δ -78.77, -104.32 (td, *J* = 16.3, 2.9 Hz).

All data matched that reported in the literature[3].

ethyl 4-(4-acetamidophenyl)-2,2,5,5-tetrafluoropent-4-enoate (**3ah**).



42.9 mg, 64% yield, colorless oil. eluent: petroleum ether/ethyl acetate 1:1 (v/v).

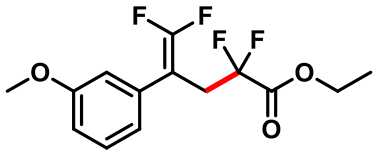
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.07 (s, 1H), 7.43 (d, *J* = 8.1 Hz, 1H), 7.40 (s, 1H), 7.19 (t, *J* = 7.9 Hz, 1H), 6.94 (d, *J* = 7.6 Hz, 1H), 3.97 (q, *J* = 7.2 Hz, 2H), 3.07 (t, *J* = 15.2 Hz, 2H), 2.06 (s, 3H), 1.12 (t, *J* = 7.2 Hz, 3H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 169.0, 163.4 (t, *J* = 32.1 Hz), 155.2 (t, *J* = 290.7 Hz), 138.3, 132.8 (t, *J* = 3.2 Hz), 128.9, 124.2, 119.7, 119.4, 114.4 (tt, *J* =250.9, 3.9 Hz), 84.6 (tt, *J* = 20.1, 4.4 Hz), 63.0, 33.8 (td, *J* = 25.4, 1.8 Hz), 24.3, 13.5.

^{19}F NMR (376 MHz, $CDCl_3$) δ -86.14 (d, *J* = 29.2 Hz), -86.38 (dt, *J* = 29.5, 4.4 Hz), -104.26 (d, *J* = 4.6 Hz).

HRMS (ESI) m/z: $[M + Na]^+$ Calcd for $C_{15}H_{15}F_4NO_3Na^+$ 356.0880; found 356.0863.

ethyl 2,2,5,5-tetrafluoro-4-(3-methoxyphenyl)pent-4-enoate (**3ai**).



31.5 mg, 51% yield, colorless oil. eluent: petroleum ether/ethyl acetate 10:1 (v/v).

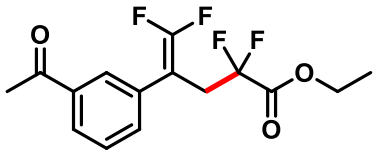
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.29 – 7.25 (m, 1H), 6.87 (dd, *J* = 7.7, 1.0 Hz, 1H), 6.85 – 6.83 (m, 2H), 4.02 (q, *J* = 7.2 Hz, 2H), 3.80 (s, 3H), 3.19 (tt, *J* = 15.1, 2.0 Hz, 2H), 1.19 (t, *J* = 7.2 Hz, 3H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 163.4 (t, *J* = 32.1 Hz), 159.5, 155.3 (t, *J* = 290.4 Hz), 133.4 (t, *J* = 3.4 Hz), 129.4, 120.8 (t, *J* = 2.8 Hz), 114.5 (tt, *J* =247.2, 4.3 Hz), 114.4 (t, *J* = 3.0 Hz), 113.3, 84.8 (tt, *J* = 20.0, 4.9 Hz), 62.9, 55.2, 34.0 (td, *J* = 25.6, 2.2 Hz), 13.6.

^{19}F NMR (376 MHz, $CDCl_3$) δ -86.04 (d, *J* = 29.6 Hz), -86.53 (dt, *J* = 29.7, 4.4 Hz), -104.34 (d, *J* = 4.8 Hz).

All data matched that reported in the literature[3].

ethyl 4-(3-acetylphenyl)-2,2,5,5-tetrafluoropent-4-enoate (**3aj**).



19.0 mg, 30% yield, colorless oil. eluent: petroleum ether/ethyl acetate 5:1 (v/v).

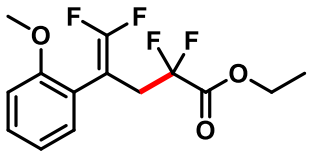
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.83 – 7.80 (m, 2H), 7.45 – 7.38 (m, 2H), 4.01 (q, *J* = 7.1 Hz, 2H), 3.16 (tt, *J* = 15.2, 2.0 Hz, 2H), 2.54 (s, 3H), 1.15 (t, *J* = 7.1 Hz, 3H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 197.5, 163.3 (t, *J* = 32.0 Hz), 155.5 (t, *J* = 291.2 Hz), 137.3, 133.1 (t, *J* = 2.8 Hz), 132.9, 128.8, 128.2 (t, *J* = 2.8 Hz), 127.9, 114.4 (tt, *J* =251.3, 3.6 Hz), 84.4 (tt, *J* = 20.3, 4.4 Hz), 63.0, 33.8 (td, *J* = 25.5, 1.5 Hz), 26.6, 13.7.

^{19}F NMR (376 MHz, $CDCl_3$) δ -85.70 – -85.73 (m), -104.24 (d, *J* = 3.8 Hz).

All data matched that reported in the literature[3].

ethyl 2,2,5,5-tetrafluoro-4-(2-methoxyphenyl)pent-4-enoate (**3ak**).



46.7 mg, 76% yield, colorless oil. eluent: petroleum ether/ethyl acetate 5:1 (v/v).

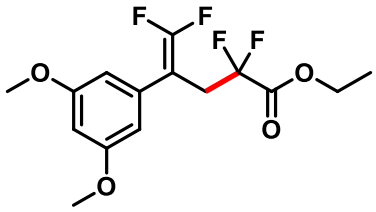
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.29 (td, *J* = 7.9, 1.7 Hz, 1H), 7.14 (d, *J* = 7.5 Hz, 1H), 6.92 (t, *J* = 7.5 Hz, 1H), 6.88 (d, *J* = 8.3 Hz, 1H), 3.98 (q, *J* = 7.2 Hz, 2H), 3.81 (s, 3H), 3.21 (tt, *J* = 15.3, 1.8 Hz, 2H), 1.17 (t, *J* = 7.2 Hz, 3H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 163.4 (t, *J* = 32.2 Hz), 157.2 (d, *J* = 2.9 Hz), 155.1 (td, *J* = 288.8, 3.1 Hz), 131.5, 129.8, 120.4, 120.4, 117.3 – 112.3 (m), 110.7, 82.4 (tt, *J* = 21.9, 5.5 Hz), 62.7, 55.3, 33.1 (td, *J* = 25.3, 2.2 Hz), 13.6.

^{19}F NMR (376 MHz, $CDCl_3$) δ -86.17 (d, *J* = 31.2 Hz), -89.27 (dt, *J* = 31.2, 3.9 Hz), -103.99 (d, *J* = 3.8 Hz).

All data matched that reported in the literature[3].

ethyl 4-(3,5-dimethoxyphenyl)-2,2,5,5-tetrafluoropent-4-enoate (**3al**).



38.9 mg, 58% yield, colorless oil. eluent: petroleum ether/ethyl acetate 10:1 (v/v).

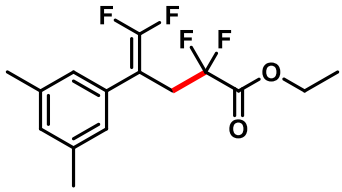
^{1}H NMR (400 MHz, $CDCl_3$) δ 6.43 (s, 2H), 6.40 (d, *J* = 2.0 Hz, 1H), 4.06 (q, *J* = 7.2 Hz, 2H), 3.78 (s, 6H), 3.17 (t, *J* = 15.1, 2H), 1.21 (t, *J* = 7.2 Hz, 3H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 163.4 (t, *J* = 32.1 Hz), 160.7, 155.3 (t, *J* = 290.5 Hz), 134.0 (t, *J* = 3.7 Hz), 114.4 (tt, *J* =251.4, 3.9 Hz), 106.8 (t, *J* = 2.9 Hz), 99.8, 84.9 (tt, *J* = 20.5, 4.7 Hz), 62.9, 55.3, 34.0 (td, *J* = 25.7, 2.4 Hz), 13.6.

^{19}F NMR (376 MHz, $CDCl_3$) δ -85.38 (d, *J* = 29.0 Hz), -86.33 – -86.43 (m), -104.30 (d, *J* = 5.1 Hz).

All data matched that reported in the literature[3].

ethyl 4-(3,5-dimethylphenyl)-2,2,5,5-tetrafluoropent-4-enoate (**3am**).



41.2 mg, 68% yield, colorless oil. eluent: petroleum ether/ethyl acetate 20:1 (v/v).

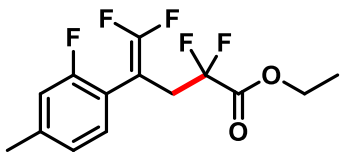
^{1}H NMR (400 MHz, $CDCl_3$) δ 6.92 (s, 1H), 6.89 (s, 2H), 3.98 (q, *J* = 7.2 Hz, 2H), 3.17 (tt, *J* = 15.0, 1.8 Hz, 2H), 2.30 (s, 6H), 1.17 (t, *J* = 7.2 Hz, 3H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 163.4 (t, *J* = 32.1 Hz), 155.2 (t, *J* = 289.8 Hz), 137.9, 131.8 (t, *J* = 3.2 Hz), 129.5, 126.2 (t, *J* = 2.6 Hz), 114.5 (tt, *J* = 251.1, 3.5 Hz), 84.8 (tt, *J* = 20.1, 4.9 Hz), 62.8, 34.0 (td, *J* = 25.6, 2.4 Hz), 21.1, 13.5.

^{19}F NMR (376 MHz, $CDCl_3$) δ -86.92 (d, *J* = 31.2 Hz), -87.28 (dt, *J* = 31.2, 5.1 Hz), -104.37 (d, *J* = 4.7 Hz).

HRMS (ESI) m/z: $[M + Na]^+$ Calcd for $C_{15}H_{16}F_4O_2Na^+$ 327.0979; found 327.0989.

ethyl 2,2,5,5-tetrafluoro-4-(2-fluoro-4-methylphenyl)pent-4-enoate (**3an**).



40.1 mg, 65% yield, yellow oil. eluent: petroleum ether/ethyl acetate 20:1 (v/v).

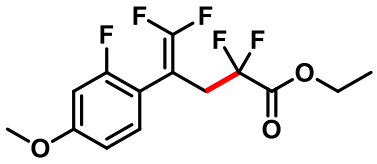
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.11 (t, *J* = 7.8 Hz, 1H), 6.94 (d, *J* = 7.9 Hz, 1H), 6.90 (d, *J* = 11.3 Hz, 1H), 4.07 (q, *J* = 7.2 Hz, 2H), 3.18 (tt, *J* = 15.1, 1.8 Hz, 2H), 2.33 (s, 3H), 1.22 (t, *J* = 7.2 Hz, 3H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 163.3 (t, *J* = 32.1 Hz), 160.0 (d, *J* = 244.0 Hz), 155.2 (t, *J* = 289.8 Hz), 141.0 (d, *J* = 8.1 Hz), 130.9, 124.9 (d, *J* = 3.1 Hz), 116.4, 116.2, 114.5 (tt, *J* = 254.2, 4.1 Hz), 79.8 (tt, *J* = 23.0, 5.0 Hz), 63.0, 33.6 (tt, *J* = 25.0, 2.3 Hz) 21.1 (d, *J* = 1.2 Hz), 13.6.

^{19}F NMR (376 MHz, $CDCl_3$) δ -84.24 (dd, *J* = 26.8, 8.5 Hz), -87.16 (dt, *J* = 26.8, 3.7 Hz), -104.42 (d, *J* = 3.6 Hz), -114.97 (d, *J* = 8.5 Hz).

HRMS (ESI) m/z: $[M+Na]^+$ Calcd for $C_{14}H_{13}F_5O_2Na^+$ 331.0728; found 331.0728.

ethyl 2,2,5,5-tetrafluoro-4-(2-fluoro-4-methoxyphenyl)pent-4-enoate (**3ao**).



42.0 mg, 65% yield, colorless oil. eluent: petroleum ether/ethyl acetate 20:1 (v/v).

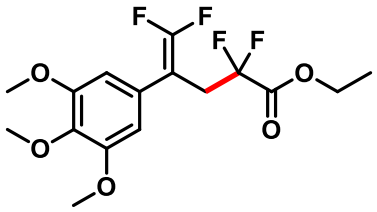
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.13 (t, *J* = 8.6 Hz, 1H), 6.69 (dd, *J* = 8.5, 2.5 Hz, 1H), 6.64 (dd, *J* = 12, 2.5 Hz, 1H), 4.10 (q, *J* = 7.2 Hz, 2H), 3.79 (s, 3H), 3.16 (tt, *J* = 15.1, 1.8 Hz, 2H), 1.24 (t, *J* = 7.2 Hz, 3H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 163.3 (t, *J* = 32.1 Hz), 161.1 (d, *J* =11.0 Hz), 160.8 (dd, *J* = 246.5, 2.3 Hz), 155.2 (td, *J* = 290.1, 2.1 Hz), 131.6 (t, *J* = 2.5 Hz), 114.5 (tt, *J* = 250.9, 3.6 Hz), 111.4 (dq, *J* = 14.9, 2.2Hz), 110.0 (d, *J* = 2.9 Hz), 101.7 (d, *J* = 25.5 Hz), 79.5 (tt, *J* = 23.2, 5.1 Hz), 62.9, 55.5, 33.6 (tt, *J* = 25.1, 2.1 Hz), 13.6.

^{19}F NMR (376 MHz, $CDCl_3$) δ -84.63 (dd, *J* = 27.4, 8.5 Hz), -87.44 (dt, *J* = 27.6, 3.6 Hz), -104.45 (d, *J* = 3.6 Hz), -111.78 (d, *J* = 8.3 Hz).

HRMS (ESI) m/z: $[M+Na]^+$ Calcd for $C_{14}H_{13}F_5O_3Na^+$ 347.0677; found 347.0674.

ethyl 2,2,5,5-tetrafluoro-4-(3,4,5-trimethoxyphenyl)pent-4-enoate (**3ap**).



43.2 mg, 59% yield, colorless oil. eluent: petroleum ether/ethyl acetate 5:1 (v/v).

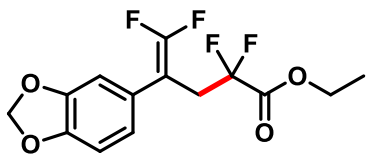
^{1}H NMR (400 MHz, $CDCl_3$) δ 6.50 (s, 2H), 4.05 (q, *J* = 7.2 Hz, 2H), 3.86 (s, 6H), 3.85 (s, 3H), 3.18 (t, *J* = 15.0 Hz, 2H), 1.20 (t, *J* = 7.2 Hz, 3H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 163.3 (t, *J* = 32.1 Hz), 155.2 (t, *J* = 290.2 Hz), 153.0, 137.6, 127.4 (t, *J* = 3.3 Hz), 114.4 (tt, *J* =250.2, 3.0 Hz), 105.9 (t, *J* = 2.4 Hz), 84.9 (tt, *J* = 20.4, 4.6 Hz), 62.9, 60.7, 56.1, 34.2 (td, *J* = 25.6, 2.0 Hz), 13.6.

^{19}F NMR (376 MHz, $CDCl_3$) δ -85.90 (d, *J* = 30.5 Hz), -86.93 (dt, *J* = 30.1, 5.2 Hz), -104.28 (d, *J* = 4.9 Hz).

HRMS (ESI) m/z: $[M+Na]^+$ Calcd for $C_{16}H_{18}F_4O_5Na^+$ 389.0983; found 389.0981.

ethyl 4-(benzo[*d*][1,3]dioxol-5-yl)-2,2,5,5-tetrafluoropent-4-enoate (**3aq**).



45.3 mg, 71% yield, colorless oil. eluent: petroleum ether/ethyl acetate 5:1 (v/v).

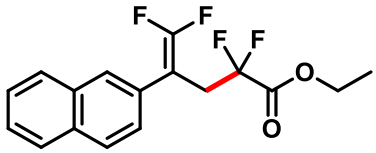
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.80 – 7.74 (m, 3H), 5.95 (s, 2H), 4.11 (q, *J* = 7.2 Hz, 2H), 3.13 (tt, *J* = 15.1, 1.9 Hz, 2H), 1.24 (t, *J* = 7.2 Hz, 3H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 163.4 (t, *J* = 32.1 Hz), 155.2 (t, *J* = 290.0 Hz), 147.7, 147.2, 125.6 (t, *J* = 3.3 Hz), 122.2 (t, *J* = 2.8 Hz), 114.5 (tt, *J* =249.7, 3.93 Hz), 109.0 (t, *J* = 2.9 Hz), 108.2, 101.2, 84.6 (tt, *J* = 20.6, 5.0 Hz), 62.9, 34.2 (td, *J* = 25.3, 2.1 Hz), 13.6.

^{19}F NMR (376 MHz, $CDCl_3$) δ -86.89 (d, *J* = 31.5 Hz), -87.34 (dt, *J* = 32.1, 4.7 Hz), -104.26 (d, *J* = 4.7 Hz).

All data matched that reported in the literature[3].

ethyl 2,2,5,5-tetrafluoro-4-(naphthalen-2-yl)pent-4-enoate (**3ar**).



32.1 mg, 49% yield, yellow oil. eluent: petroleum ether/ethyl acetate 20:1 (v/v).

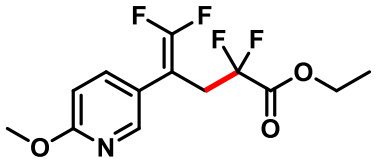
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.84 – 7.81 (m, 3H), 7.76 (s, 1H), 7.50 – 7.48 (m, 2H), 7.40 (d, *J* = 8.6 Hz, 1H), 3.89 (q, *J* = 7.1 Hz, 2H), 3.31 (t, *J* = 15.0 Hz, 2H), 1.09 (t, *J* = 7.2 Hz, 3H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 163.4 (t, *J* = 32.0 Hz), 155.5 (t, *J* = 290.8 Hz), 133.0, 132.6, 129.4 (t, *J* = 3.0 Hz), 128.2, 127.9, 127.6 (t, *J* = 2.8 Hz), 127.6, 126.5 (d, *J* = 2.8 Hz), 126.0 (t, *J* = 2.7 Hz), 114.5 (tt, *J* = 252.0, 3.8 Hz), 84.9 (t, *J* = 20.0 Hz), 62.9, 34.1 (td, *J* = 25.6, 2.1 Hz), 13.5.

^{19}F NMR (376 MHz, $CDCl_3$) δ -86.13 (dt, *J* = 28.7, 5.1 Hz), -86.34 (d, *J* = 29.4 Hz), -104.26 (d, *J* = 4.7 Hz).

All data matched that reported in the literature[3].

ethyl 2,2,5,5-tetrafluoro-4-(6-methoxypyridin-3-yl)pent-4-enoate (**3as**).



30.6 mg, 50% yield, colorless oil. eluent: petroleum ether/ethyl acetate 5:1 (v/v).

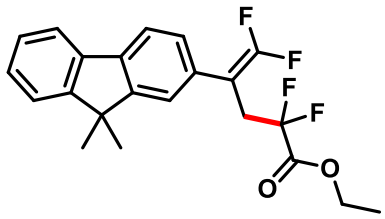
^{1}H NMR (600 MHz, $CDCl_3$) δ 8.12 – 8.10 (m, 1H), 7.52 – 7.50 (m, 1H), 6.75 (d, *J* = 8.6 Hz, 1H), 4.14 (q, *J* = 7.2 Hz, 2H), 3.94 (s, 3H), 3.16 (tt, *J* = 15.1,1.9 Hz, 3H), 1.26 (t, *J* = 7.1 Hz, 3H).

^{13}C NMR (150 MHz, $CDCl_3$) δ 163.5, 163.3 (t, *J* = 32.3 Hz), 155.3 (t, *J* = 290.5 Hz), 146.6 (t, *J* = 2.9 Hz), 138.6, 121.1 (t, *J* =3.2 Hz), 114.4 (tt, *J* = 251.5, 3.6 Hz), 110.7, 81.9 (tt, *J* = 21.2, 4.4 Hz), 63.1, 53.5, 33.8 (td, *J* = 25.1, 1.8 Hz), 13.7.

^{19}F NMR (565 MHz, $CDCl_3$) δ -86.02 (d, *J* = 30.3 Hz), -86.30 (d, *J* = 29.7 Hz), -104.26 – -104.28 (m).

HRMS (ESI) m/z: $[M + H]^+$ Calcd for $C_{13}H_{14}F_4NO_3^+$ 308.0904; found 308.0891.

ethyl 4-(9,9-dimethyl-9H-fluoren-2-yl)-2,2,5,5-tetrafluoropent-4-enoate (**3at**).



47.9 mg, 61% yield, yellow oil. eluent: petroleum ether/ethyl acetate 20:1 (v/v).

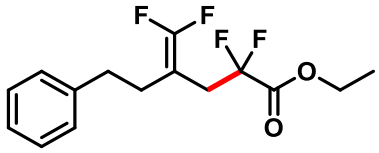
^{1}H NMR (600 MHz, $CDCl_3$) δ 7.71 – 7.68 (m, 2H), 7.43 – 7.42 (m, 1H), 7.35 – 7.32 (m, 3H), 7.26 (d, *J* = 7.9 Hz, 1H), 3.93 (q, *J* = 7.1 Hz, 2H), 3.26 (t, *J* = 14.9 Hz, 2H), 1.48 (s, 6H), 1.11 (t, *J* = 7.1 Hz, 3H).

^{13}C NMR (150 MHz, $CDCl_3$) δ 163.4 (t, *J* = 31.9 Hz), 155.4 (t, *J* = 290.5 Hz), 153.8 (d, *J* = 4.4 Hz), 139.0, 138.4, 130.8 (t, *J* = 3.1 Hz), 127.6, 127.4 (t, *J* = 2.6 Hz), 127.0, 122.8 (t, *J* = 2.7 Hz), 122.6, 120.1, 119.9, 114.5 (tt, *J* = 250.9, 3.1 Hz), 85.2 (tt, *J* = 20.1, 5.0 Hz), 62.8, 46.9, 34.2 (td, *J* = 25.9, 1.6 Hz), 27.0, 13.6.

^{19}F NMR (565 MHz, $CDCl_3$) δ -86.36 (d, *J* = 30.1 Hz), -86.55 (d, *J* = 30.2 Hz), -104.22 – -104.24 (m).

HRMS (ESI) m/z: $[M + Na]^+$ Calcd for $C_{22}H_{20}F_4O_2Na^+$ 415.1292; found 415.1289.

ethyl 4-(difluoromethylene)-2,2-difluoro-6-phenylhexanoate **(3au)**.



42.1 mg, 69% yield, colorless oil. eluent: petroleum ether/ethyl acetate 20:1 (v/v).

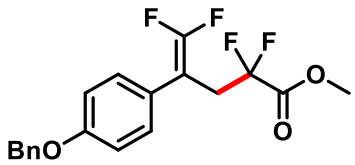
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.27 (t, *J* = 7.2 Hz, 2H), 7.19 (d, *J* = 7.3 Hz, 1H), 7.16 (d, *J* = 7.2 Hz, 2H), 4.29 (q, *J* = 7.2 Hz, 2H), 2.78 – 2.69 (m, 4H), 2.37 (t, *J* = 8.2 Hz, 2H), 1.31 (t, *J* = 7.2Hz, 3H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 163.5 (t, *J* = 32.1 Hz), 155.3 (td, *J* = 286.2, 1.9 Hz), 140.6, 128.4, 128.3, 126.2, 115.1 (tt, *J* = 251.1, 3.7 Hz), 81.6 – 81.1 (m), 63.0, 33.4, 31.7 (td, *J* = 24.6, 3.4 Hz), 28.4, 13.7.

^{19}F NMR (376 MHz, $CDCl_3$) -89.52 (d, *J* = 41.5 Hz), -90.17 (dt, *J* = 41.1, 3.7 Hz), -103.95 (d, *J* = 3.1 Hz).

HRMS (ESI) m/z: $[M + Na]^+$ Calcd for $C_{15}H_{16}F_4O_2Na^+$ 327.0979; found 327.0972.

methyl 4-(4-(benzyloxy)phenyl)-2,2,5,5-tetrafluoropent-4-enoate (**3av**).



33.5 mg, 46% yield, white solid, m.p: 62-64 ℃. eluent: petroleum ether/ethyl acetate 20:1 (v/v).

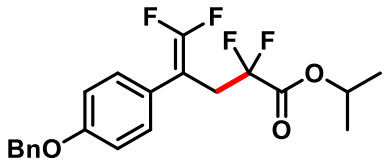
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.43 – 7.36 (m, 4H), 7.34 – 7.30 (m, 1H), 7.20 (d, *J* = 8.7 Hz, 2H), 6.96 (d, *J* = 8.8 Hz, 2H), 5.06 (s, 2H), 3.50 (s, 3H), 3.16 (t, *J* = 14.2 Hz, 2H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 163.8 (t, *J* = 32.2 Hz), 158.2, 155.2 (t, *J* = 289.8 Hz), 136.7, 129.7 (t, *J* = 2.8 Hz), 128.6, 128.0, 127.4, 124.2 (t, *J* = 3.1 Hz), 114.8, 114.5 (tt, *J* = 250.9, 3.7 Hz), 84.2 (tt, *J* = 20.3, 4.7 Hz), 69.9, 53.1, 34.1 (td, *J* = 25.5, 2.1 Hz).

^{19}F NMR (376 MHz, $CDCl_3$) -87.39 – -87.71 (m), -104.43 (d, *J* = 3.4 Hz).

HRMS (ESI) m/z: $[M + Na]^+$ Calcd for $C_{19}H_{16}F_4O_3Na^+$ 391.0928; found 391.0934.

isopropyl 4-(4-(benzyloxy)phenyl)-2,2,5,5-tetrafluoropent-4-enoate (**3aw**).



42.1 mg, 53% yield, white solid, m.p: 66-68 ℃. eluent: petroleum ether/ethyl acetate 20:1 (v/v).

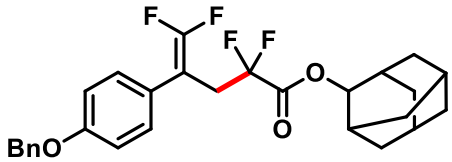
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.43 – 7.30 (m, 5H), 7.23 – 7.20 (m, 2H), 6.97 – 6.93 (m, 2H), 5.05 (s, 2H), 4.92 – 4.83 (m, 1H), 3.14 (tt, *J* = 14.9, 1.7 Hz, 2H), 1.17 (d, *J* = 6.3 Hz, 6H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 162.9 (t, *J* = 32.0 Hz), 158.3, 155.1 (t, *J* = 289.6 Hz), 136.7, 129.7 (t, *J* = 2.7 Hz), 128.6, 128.0, 127.4, 124.5 (t, *J* = 3.2 Hz), 114.8, 114.5 (tt, *J* = 251.2, 4.3 Hz), 84.4 (tt, *J* = 20.2, 4.8 Hz), 71.4, 69.9, 34.0 (td, *J* = 25.5, 2.1 Hz), 21.2.

^{19}F NMR (376 MHz, $CDCl_3$) δ -87.28 (dt, *J* = 32.3, 5.0 Hz), -87.52 (d, *J* = 32.4 Hz), -103.93 (d, *J* = 4.8 Hz).

HRMS (ESI) m/z: $[M + Na]^+$ Calcd for $C_{21}H_{20}F_4O_3Na^+$ 419.1241; found 419.1245.

adamantan-2-yl 4-(4-(benzyloxy)phenyl)-2,2,5,5-tetrafluoropent-4-enoate (**3ax**).



50.3 mg, 53% yield, colorless oil. eluent: petroleum ether/ethyl acetate 20:1 (v/v).

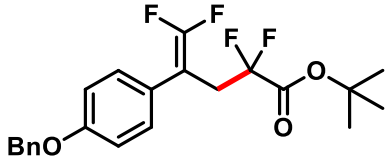
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.43 – 7.31 (m, 5H), 7.22 (dd, *J* = 8.6, 3.0 Hz, 2H), 6.95 (d, *J* = 8.8 Hz, 2H), 5.04 (s, 2H), 4.84 (s, 1H), 3.18 (t, *J* = 15.2 Hz, 2H), 1.95 – 1.82 (m, 8H), 1.72 – 1.68 (m, 4H), 1.53 (dd, *J* = 12.2, 8.2 Hz, 2H).

^{13}C NMR (150 MHz, $CDCl_3$) δ 162.8 (t, *J* = 32.1 Hz), 158.3, 155.1 (t, *J* = 289.9 Hz), 136.7, 129.7 (t, *J* = 2.7 Hz), 128.6, 128.0, 127.4, 124.6, 114.7, 114.6 (tt, *J* = 251.3, 3.5 Hz), 84.4 (tt, *J* = 20.2, 4.4 Hz), 80.4, 70.0, 37.1, 36.1, 34.1 (t, *J* = 25.1 Hz), 31.4 (d, *J* = 4.8 Hz), 26.9, 26.7.

^{19}F NMR (565 MHz, $CDCl_3$) δ -87.29 – -87.37 (m), -103.86 – -103.92 (m).

HRMS (ESI) m/z: $[M + Na]^+$ Calcd for $C_{28}H_{28}F_4O_3Na^+$ 511.1867; found 511.1875.

tert-butyl 4-(4-(benzyloxy)phenyl)-2,2,5,5-tetrafluoropent-4-enoate (**3ay**).



20.1 mg, 25% yield, white solid, m.p: 72-74 ℃. eluent: petroleum ether/ethyl acetate 20:1 (v/v).

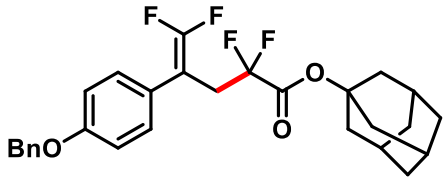
^{1}H NMR (600 MHz, $CDCl_3$) δ 7.42 (d, *J* = 7.3 Hz, 2H), 7.39 (t, *J* = 7.3Hz, 2H), 7.33 (t, *J* = 7.2 Hz, 1H), 7.22 (d, *J* = 8.4 Hz, 2H), 6.96 (d, *J* = 8.8 Hz, 2H), 5.06 (s, 2H), 3.12 (t, *J* = 14.9 Hz, 2H), 1.38 (s, 9H).

^{13}C NMR (150 MHz, $CDCl_3$) δ 162.3 (t, *J* = 31.5 Hz), 158.3, 155.1 (t, *J* = 289.5 Hz), 136.7, 129.7 (t, *J* = 2.7 Hz), 128.6, 128.0, 127.4, 124.7 (t, *J* = 3.2 Hz), 114.8, 114.4 (t, *J* = 252.3 Hz), 84.7, 84.5 (dt, *J* = 20.1, 4.5 Hz), 70.0, 33.8 (td, *J* = 25.0, 1.7 Hz), 27.5.

^{19}F NMR (565 MHz, $CDCl_3$) δ -87.19 (d, *J* = 32.1 Hz), -87.72 (d, *J* = 32.3 Hz), -103.40 (td, *J* = 14.5, 4.4 Hz).

HRMS (ESI) m/z: $[M +Na]^+$ Calcd for $C_{22}H_{22}F_4O_3^+$ 433.1397; found 433.1390.

adamantan-1-yl 4-(4-(benzyloxy)phenyl)-2,2,5,5-tetrafluoropent-4-enoate (**3az**).



22.1 mg, 23% yield, colorless oil. eluent: petroleum ether/ethyl acetate 20:1 (v/v).

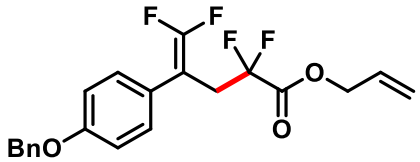
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.43 – 7.31 (m, 5H), 7.23 (dd, *J* = 8.4, 3.4 Hz, 2H), 6.96 (d, *J* = 8.7 Hz, 2H), 5.04 (s, 2H), 3.13 (t, *J* = 15.0 Hz, 2H), 2.16 (s, 3H), 2.00 (s, 6H), 1.63 (s, 6H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 161.8 (t, *J* = 31.3 Hz), 158.4, 155.1 (t, *J* = 289.6 Hz), 136.7, 129.7, 128.6, 128.0, 127.5, 124.7 (t, *J* = 3.3 Hz), 114.8, 84.7, 70.0, 40.6, 35.8, 33.9 (t, *J* = 25.6 Hz), 30.8.

^{19}F NMR (565 MHz, $CDCl_3$) δ -87.10 (d, *J* = 32.5 Hz), -87.70 (d, *J* = 32.3 Hz), -103.31 – -103.37 (m).

HRMS (ESI) m/z: $[M + Na]^+$ Calcd for $C_{28}H_{28}F_4O_3Na^+$511.1867; found 511.1863.

allyl 4-(4-(benzyloxy)phenyl)-2,2,5,5-tetrafluoropent-4-enoate (**3ba**).



10.4 mg, 13% yield, yellow solid, m.p: 46-48 ℃. eluent: petroleum ether/ethyl acetate 50:1 (v/v).

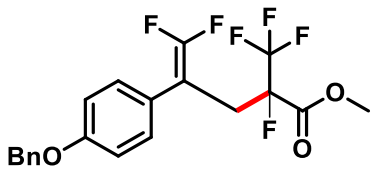
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.26 – 7.13 (m, 5H), 7.03 (d, *J* = 8.6 Hz, 2H), 6.78 (d, *J* = 8.6 Hz, 2H), 5.64 – 5.54 (m, 1H), 5.13 – 5.07 (m, 2H), 4.89 (s, 2H), 4.21 (d, *J* = 5.9 Hz, 2H), 3.00 (t, *J* = 14.9 Hz, 2H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 163.1 (t, *J* = 32.2 Hz), 158.3, 155.2 (t, *J* = 289.9 Hz), 136.7, 130.3, 129.8, 128.7, 128.1, 127.5, 124.3, 120.1, 114.9, 84.2 (t, *J* = 20.3 Hz), 70.0, 67.2, 34.2 (t, *J* = 25.4 Hz).

^{19}F NMR (376 MHz, $CDCl_3$) δ -87.39 (d, *J* = 2.9 Hz), -104.20 (t, *J* = 2.7 Hz).

HRMS (ESI) m/z: $[M + Na]^+$ Calcd for $C_{21}H_{18}F_4O_3Na^+$ 417.1084; found 417.1093..

methyl 4-(4-(benzyloxy)phenyl)-2,5,5-trifluoro-2-(trifluoromethyl)pent-4-enoate (**3bb**).



17.5 mg, 21% yield, white solid, m.p: 62-64 ℃. eluent: petroleum ether/ethyl acetate 20:1 (v/v).

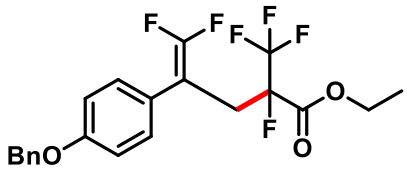
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.43 – 7.30 (m, 5H), 7.18 (d, *J* = 8.3 Hz, 2H), 6.96 (d, *J* = 8.7 Hz, 2H), 5.07 (s, 2H), 3.27 (s, 3H), 3.27 – 3.10 (m, 2H).

^{13}C NMR (150 MHz, $CDCl_3$) δ 163.6 (d, *J* = 25.6 Hz), 158.3, 155.2 (t, *J* = 289.8 Hz), 136.6, 130.1, 128.6, 128.1, 127.5, 123.6 (t, *J* = 2.9 Hz), 121.3 (qd, *J* = 283.9, 27.7 Hz), 114.9, 91.60 (dq, *J* = 202.7, 31.2 Hz), 84.3 (t, *J* = 20.1 Hz), 69.9, 53.1, 30.4 (d, *J* = 21.5 Hz).

^{19}F NMR (565 MHz, $CDCl_3$) δ -78.22 (d, *J* = 7.7 Hz), -87.20 (d, *J* = 31.6 Hz), -87.94 (dd, *J* = 32.0, 7.7 Hz).

HRMS (ESI) m/z: $[M + Na]^+$ Calcd for $C_{20}H_{16}F_6O_3Na^+$ 441.0896; found 441.0904.

ethyl 4-(4-(benzyloxy)phenyl)-2,5,5-trifluoro-2-(trifluoromethyl)pent-4-enoate (**3bc**).



52.1 mg, 60% yield, white solid, m.p: 62-64 ℃.. eluent: petroleum ether/ethyl acetate 10:1 (v/v).

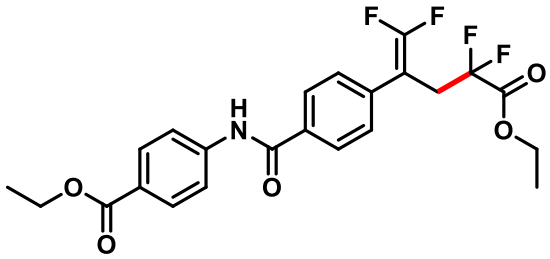
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.43 – 7.31 (m, 5H), 7.18 (d, *J* = 8.4 Hz, 2H), 6.95 (d, *J* = 8.4 Hz, 2H), 5.06 (s, 2H), 3.86 – 3.78 (m, 1H), 3.67– 3.59 (m, 1H), 3.25 – 3.12 (m, 2H), 1.06 (t, *J* = 7.1 Hz, 3H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 163.2 (d, *J* = 25.4 Hz), 158.3, 155.1 (t, *J* = 289.8 Hz), 136.6, 130.0 (t, *J* = 2.3 Hz), 128.6, 128.1, 127.4, 123.7 (t, *J* = 3.0 Hz), 121.4 (qd, *J* = 284.3, 28.5 Hz), 114.7, 91.7 (dq, *J* = 202.7, 30.7 Hz), 84.4 (t, *J* = 20.4 Hz), 69.9, 62.9, 30.4 (d, *J* = 21.5 Hz), 13.4.

^{19}F NMR (376 MHz, $CDCl_3$) -78.22 (d, *J* = 6.9 Hz), -87.31 (d, *J* = 31.6 Hz), -87.80 (dd, *J* = 32.1, 7.6 Hz).

HRMS (ESI) m/z: $[M + Na]^+$ Calcd for $C_{21}H_{18}F_6O_3Na^+$ 455.1052; found 455.1042.

ethyl 4-(4-(5-ethoxy-1,1,4,4-tetrafluoro-5-oxopent-1-en-2-yl)benzamido)benzoate **(3be)**.



24.1 mg, 25% yield, white solid, m.p: 81-83 ℃.eluent: petroleum ether/ethyl acetate 5:1 (v/v).

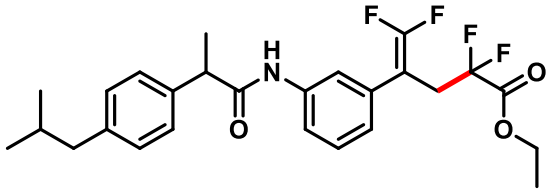
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.30 (s, 1H), 8.04 (dd, *J* = 6.9, 1.8 Hz, 2H), 7.87 (d, *J* = 8.4 Hz, 2H), 7.76 (dd, *J* = 7.0, 1.8 Hz, 2H), 7.40 (d, *J* = 7.6 Hz, 2H), 4.36 (q, *J* = 7.1 Hz, 2H), 4.12 (q, *J* = 7.2 Hz, 2H), 3.22 (t, *J* = 15.2 Hz, 2H), 1.39 (t, *J* = 7.1 Hz, 3H), 1.25 (t, *J* = 7.2 Hz, 3H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 166.1, 165.2, 163.3 (t, *J* = 32.0 Hz), 155.5 (t, *J* = 292.1 Hz), 142.0, 136.3 (t, *J* = 3.7 Hz), 133.8, 130.8, 128.8, 127.3, 126.2, 119.3, 114.3 (t, *J* = 248.7 Hz), 84.4 (t, *J* = 18.8 Hz), 63.2, 60.9, 33.6 (t, *J* =23.6 Hz), 14.3, 13.7.

^{19}F NMR (376 MHz, $CDCl_3$) -84.31 (dt, *J* = 25.6, 4.5 Hz), -84.60 (d, *J* = 25.6 Hz), -104.21 (d, *J* = 4.9 Hz).

HRMS (ESI) m/z: $[M + Na]^+$ Calcd for $C_{22}H_{21}F_4NO_5Na^+$ 490.1248; found 490.1273.

ethyl 2,2,5,5-tetrafluoro-4-(3-(2-(4-isobutylphenyl)propanamido)phenyl)pent-4-enoate **(3bf)**.



48.0 mg, 50% yield, colorless oil, eluent: petroleum ether/ethyl acetate 5:1 (v/v).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.44 (s, 1H), 7.34 (d, *J* = 8.2 Hz, 1H), 7.27 – 7.24 (m, 3H), 7.18 – 7.14 (m, 3H), 6.99 (d, *J* = 7.4 Hz, 1H), 4.02 (q, *J* = 7.2 Hz, 2H), 3.68 (q, *J* = 7.1 Hz, 1H), 3.15 (tt, *J* = 15.1,

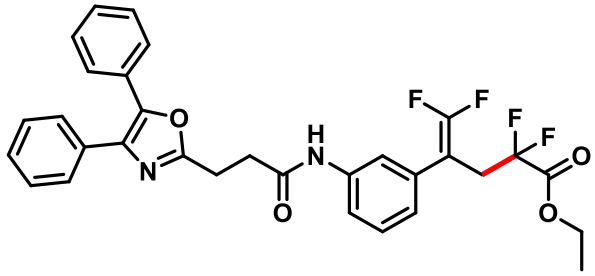
1.8 Hz, 2H), 2.47 (d, *J* = 7.2 Hz, 2H), 1.86 (sep, *J* = 6.8 Hz, 1H), 1.58 (d, *J* = 7.2 Hz, 3H), 1.18 (t, *J* = 7.2 Hz, 3H), 0.91 (d, *J* = 6.6Hz, 6H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 172.7, 163.3 (t, *J* = 32.1 Hz), 155.3 (t, *J* = 290.8 Hz), 141.1, 138.2, 137.9, 132.9 (t, *J* = 3.3 Hz), 129.9, 129.0, 127.3, 124.3, 119.4, 119.0, 114.4 (td, *J* = 251.0, 4.0 Hz), 84.6 (t, *J* = 20.0 Hz), 63.0, 47.7, 45.0, 33.9 (td, *J* = 25.5, 2.0 Hz), 30.1, 22.3, 18.4, 13.6, 14.3, 13.7.

^{19}F NMR (376 MHz, $CDCl_3$) -86.00 (d, *J* = 29.0 Hz), -86.39 (dt, *J* = 28.9, 4.4 Hz), -104.35 (d, *J* = 4.9 Hz).

HRMS (ESI) m/z: $[M + Na]^+$ Calcd for $C_{26}H_{29}F_4NO_3Na^+$ 502.1976; found 502.1963.

ethyl 4-(3-(3-(4,5-diphenyloxazol-2-yl)propanamido)phenyl)-2,2,5,5-tetrafluoropent-4-enoate **(3bg)**.



50.6 mg, 45% yield, colorless oil, eluent: petroleum ether/ethyl acetate 3:1 (v/v).

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.95 (s, 1H), 7.65 – 7.63 (m, 2H), 7.57 – 7.53 (m, 3H), 7.41 – 7.33 (m, 7H), 7.26 (s, 1H), 6.98 (d, *J* = 7.7 Hz, 1H), 4.01 (q, *J* = 7.2 Hz, 2H), 3.27 (t, *J* = 6.4 Hz, 2H), 3.08 (t, *J* = 15.1 Hz, 2H), 2.95 (t, *J* = 7.0 Hz, 2H), 1.17 (t, *J* = 7.2 Hz, 3H).

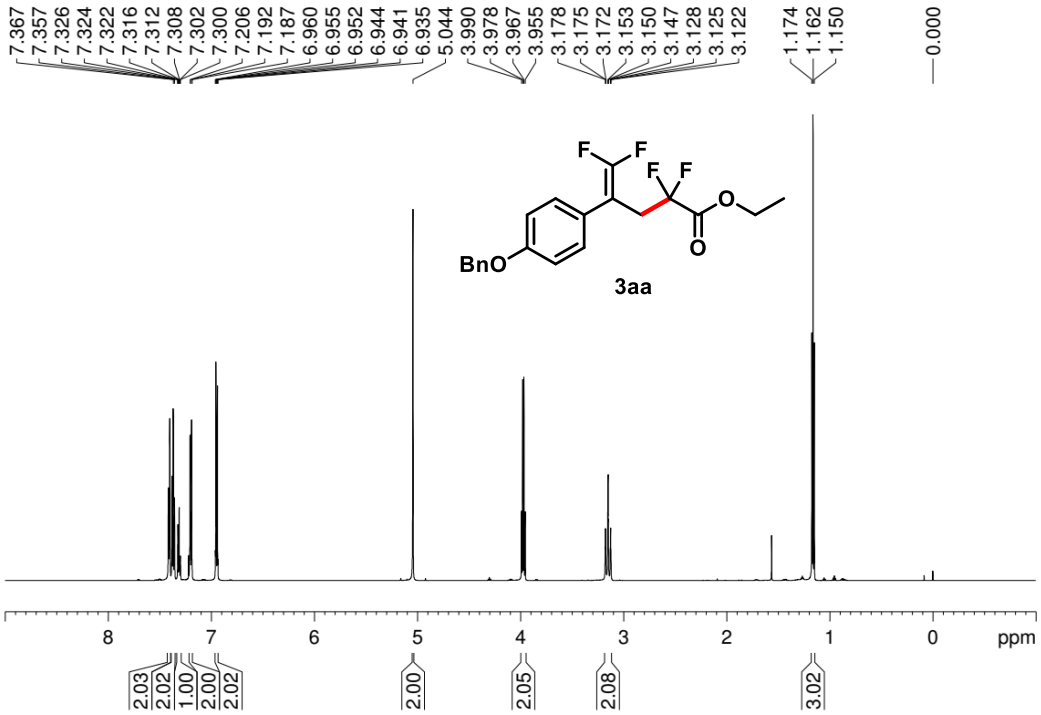
^{13}C NMR (100 MHz, $CDCl_3$) δ 169.9, 163.3 (t, *J* = 32.1 Hz), 162.5, 155.2 (t, *J* = 290.7 Hz), 145.7, 138.4, 134.7, 132.8, 132.1, 129.1, 128.7, 128.6, 128.3, 127.8, 126.4, 124.1, 119.4, 119.1, 114.4 (t, *J* = 252.0 Hz), 84.6 (t, *J* = 19.8 Hz), 62.9, 34.1, 33.9 (t, *J* = 25.5 Hz), 24.0, 13.6.

^{19}F NMR (376 MHz, $CDCl_3$) -86.11 (d, *J* = 29.0 Hz), -86.49 (dt, *J* = 28.8, 4.3 Hz), -104.30 (d, *J* = 4.8 Hz).

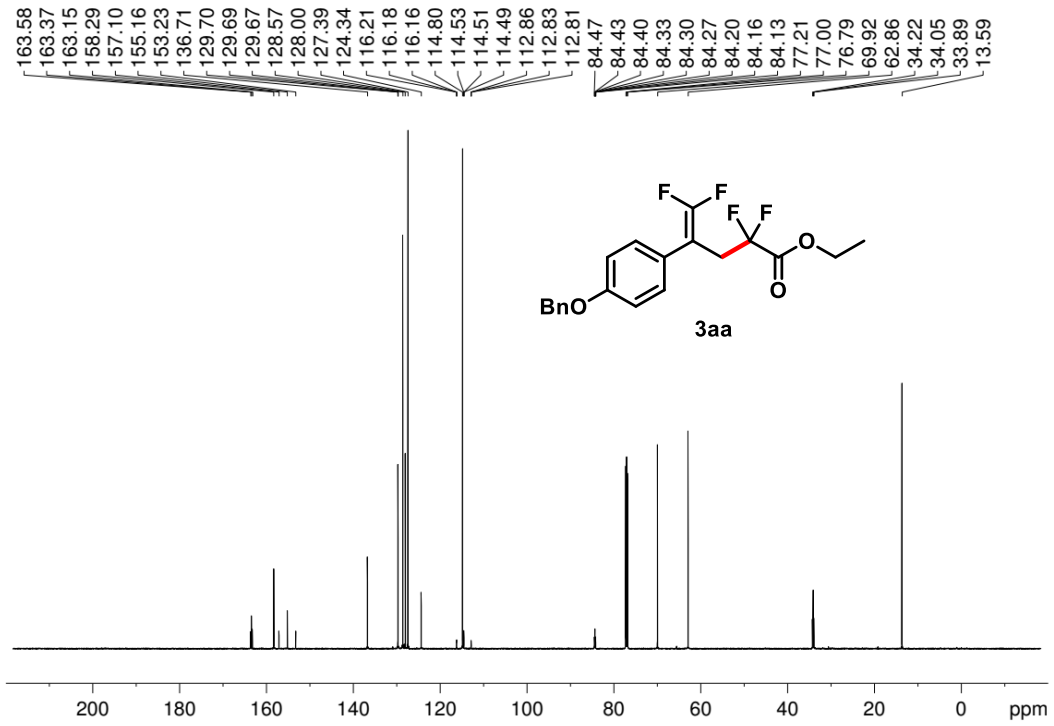
HRMS (ESI) m/z: $[M + H]^+$ Calcd for $C_{31}H_{27}F_4N_2O_4^+$ 567.1901; found 567.1906.

7. ^{1}H, ^{13}C and ^{19}F NMR spectra of the products

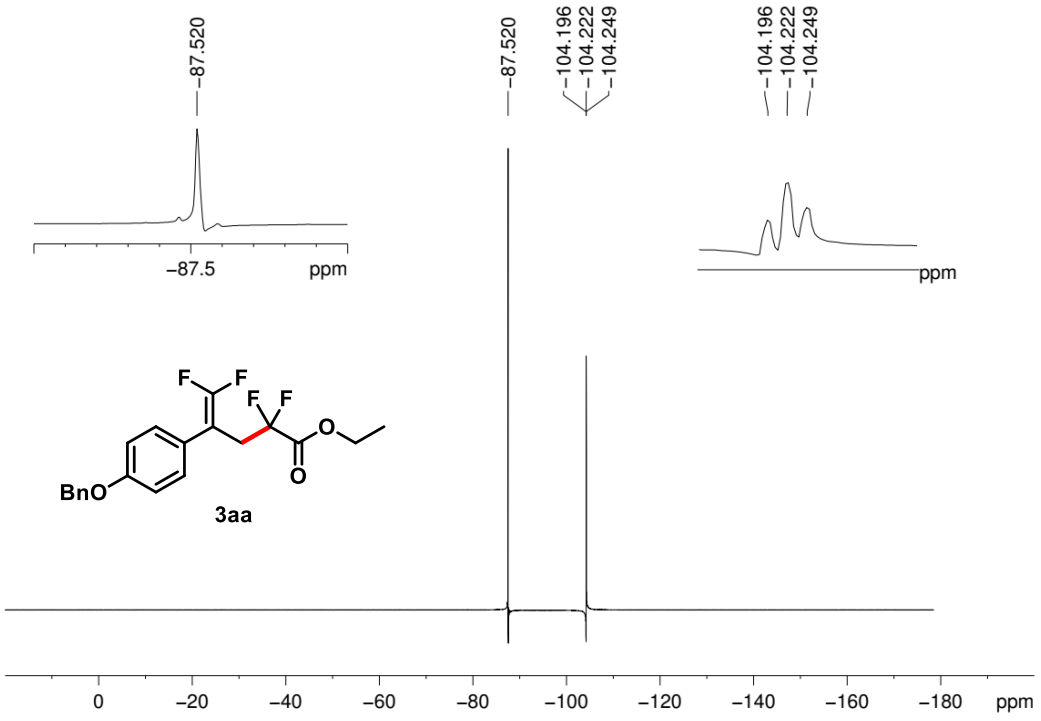
^{1}H NMR (600 MHz, $CDCl_3$)



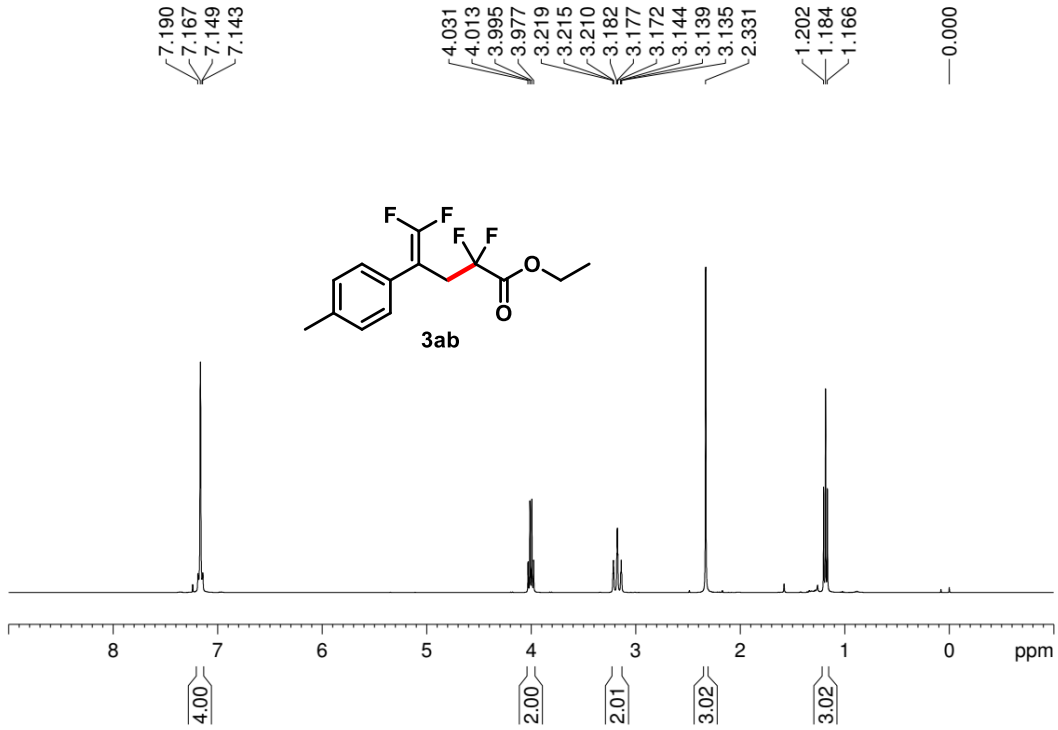
^{13}C NMR (150 MHz, $CDCl_3$)



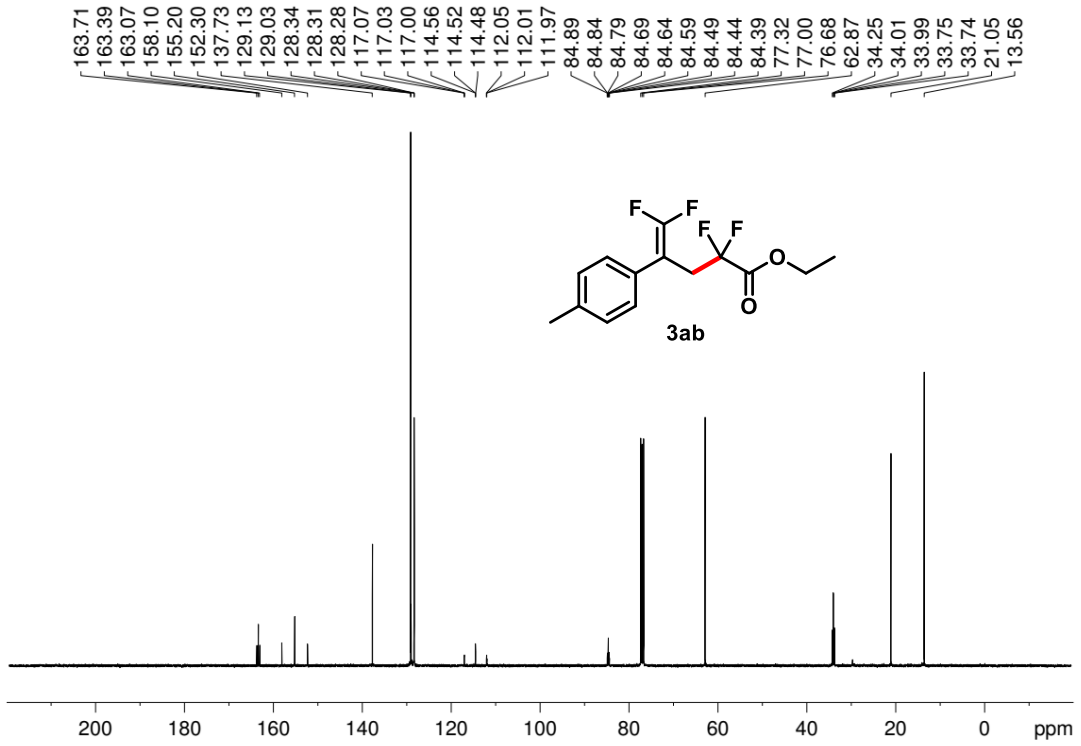
^{19}F NMR (565 MHz, CDCl$_3$)



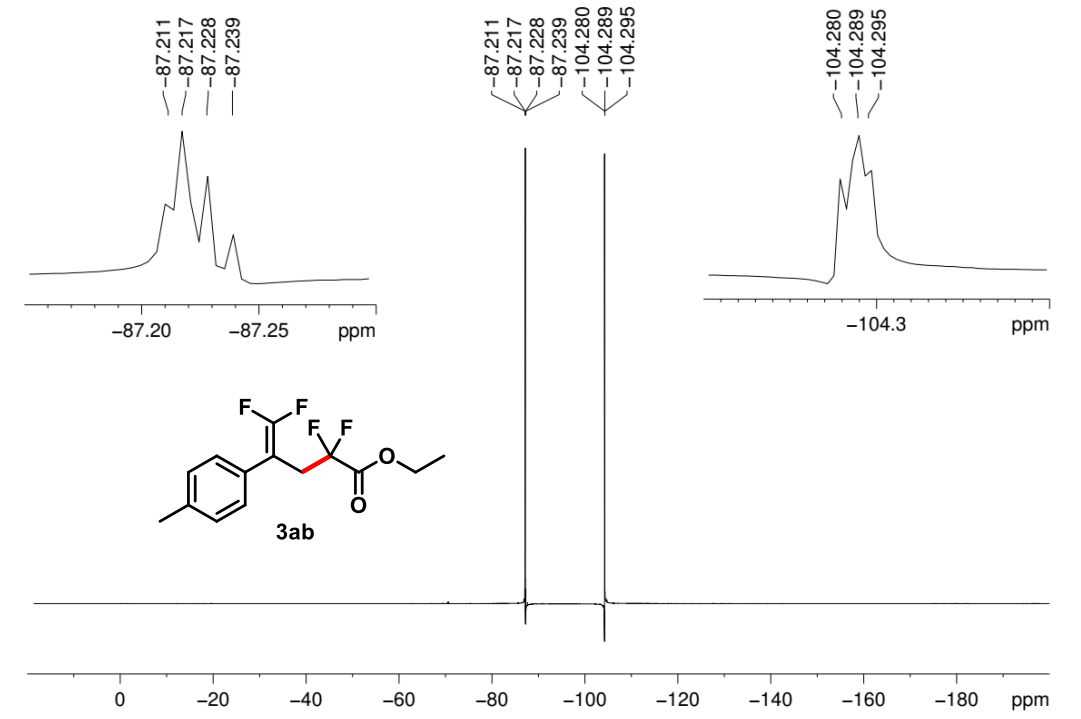
^{1}H NMR (400 MHz, CDCl$_3$)



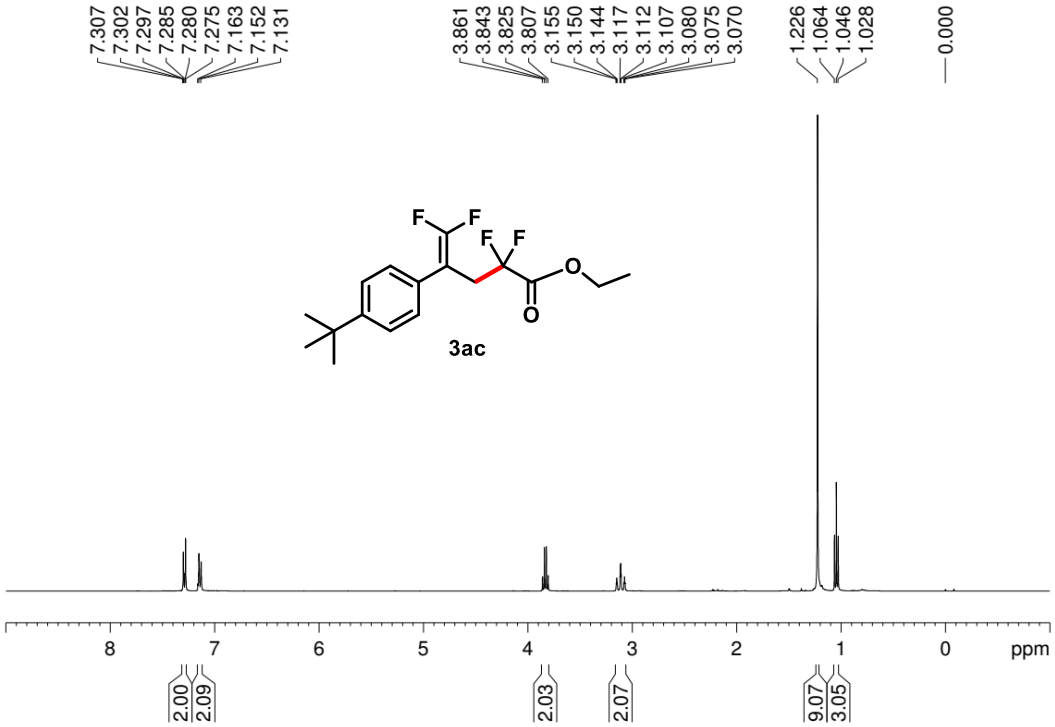
^{13}C NMR (100 MHz, $CDCl_3$)



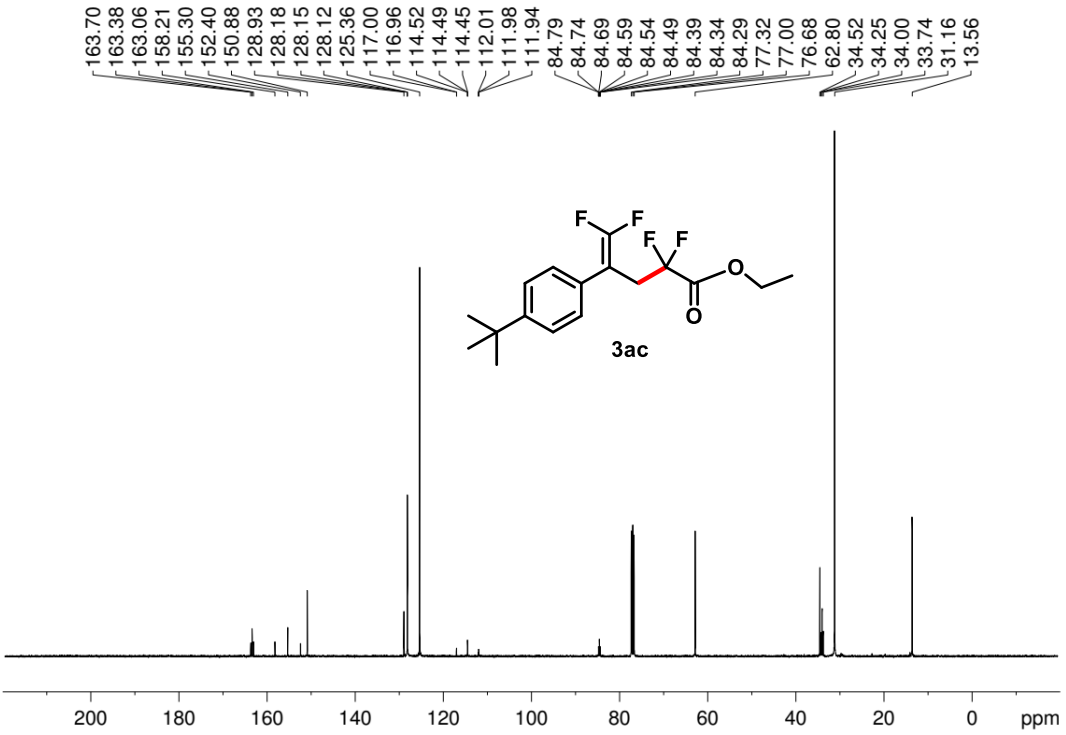
^{19}F NMR (376 MHz, $CDCl_3$)



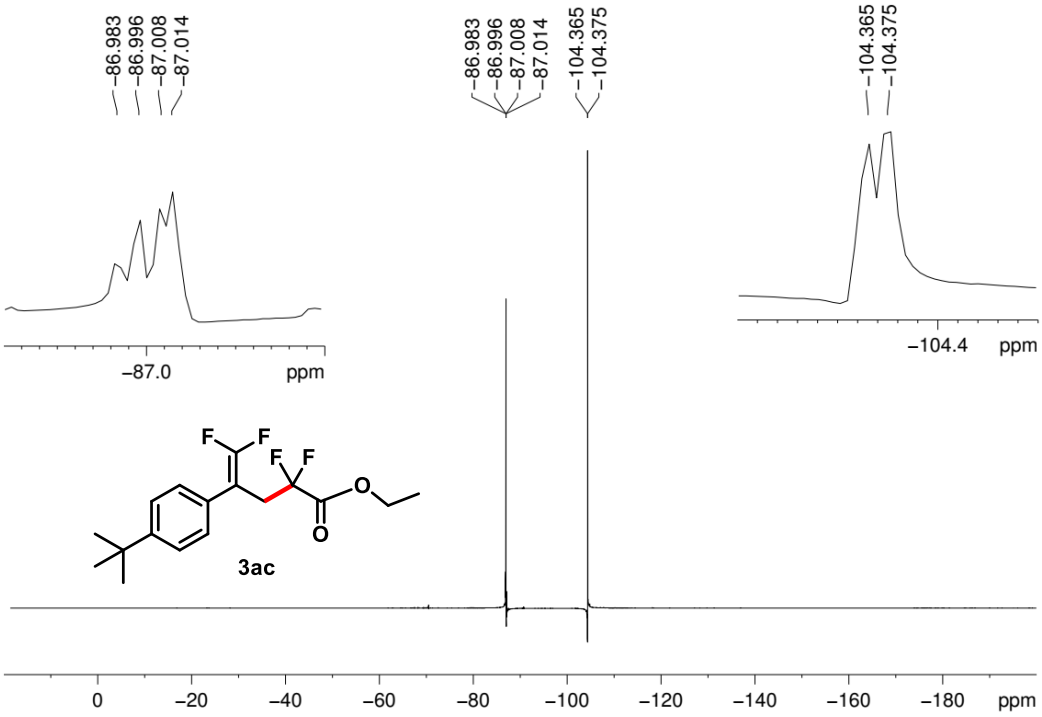
^{1}H NMR (400 MHz, $CDCl_3$)



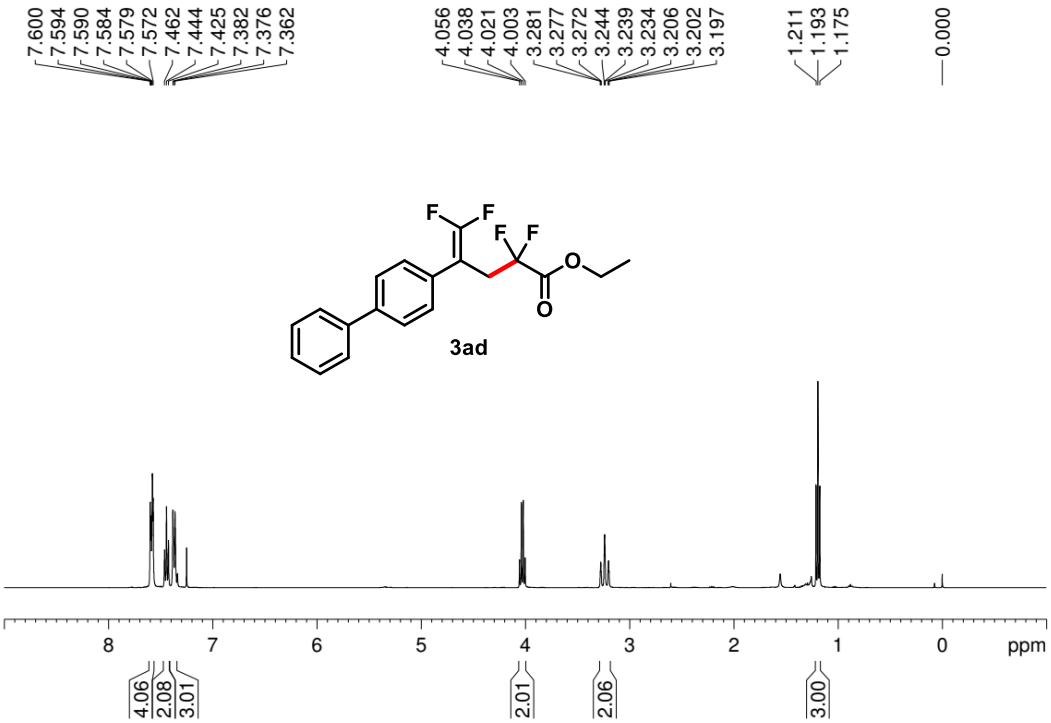
^{13}C NMR (100 MHz, $CDCl_3$)



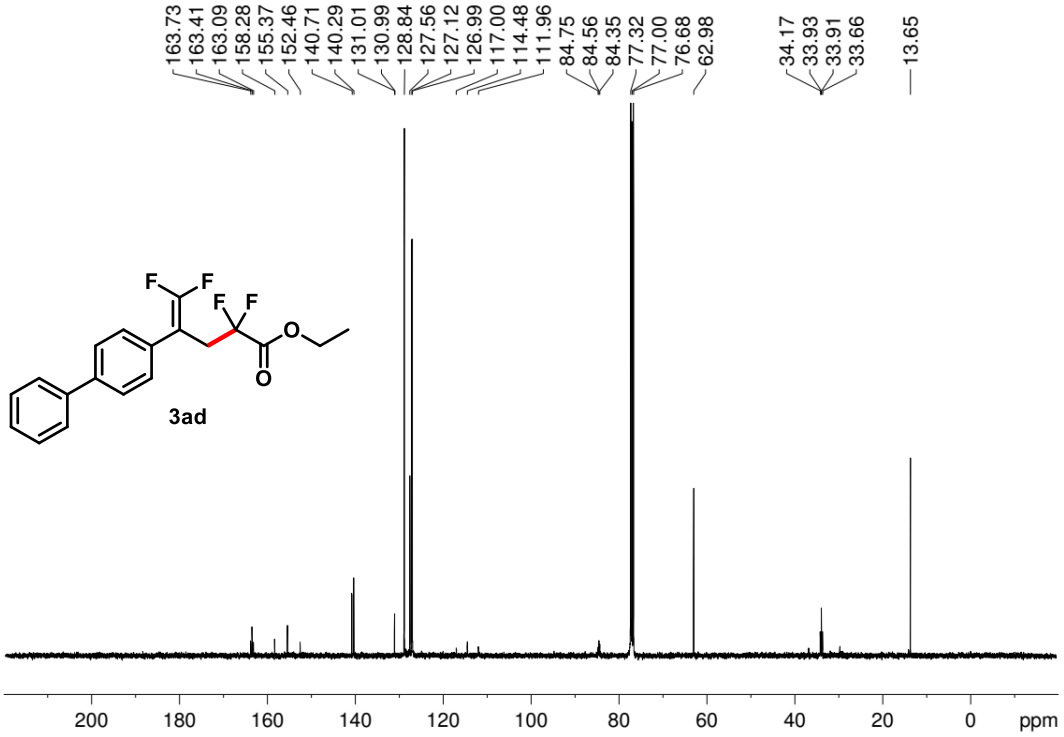
^{19}F NMR (376 MHz, CDCl$_3$)



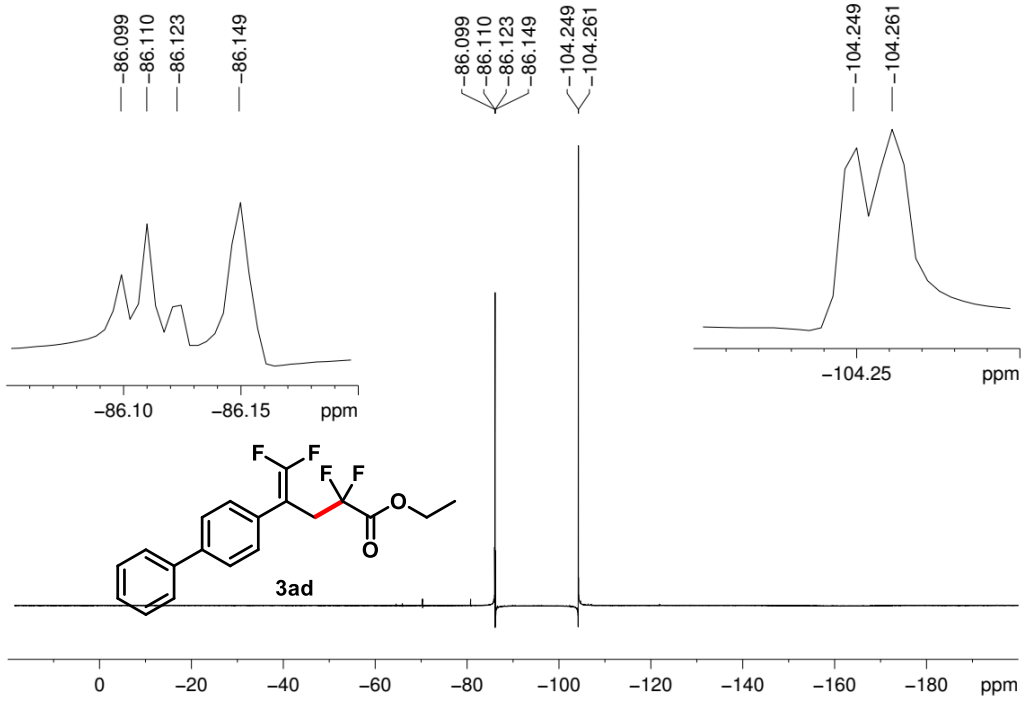
^{1}H NMR (400 MHz, CDCl$_3$)



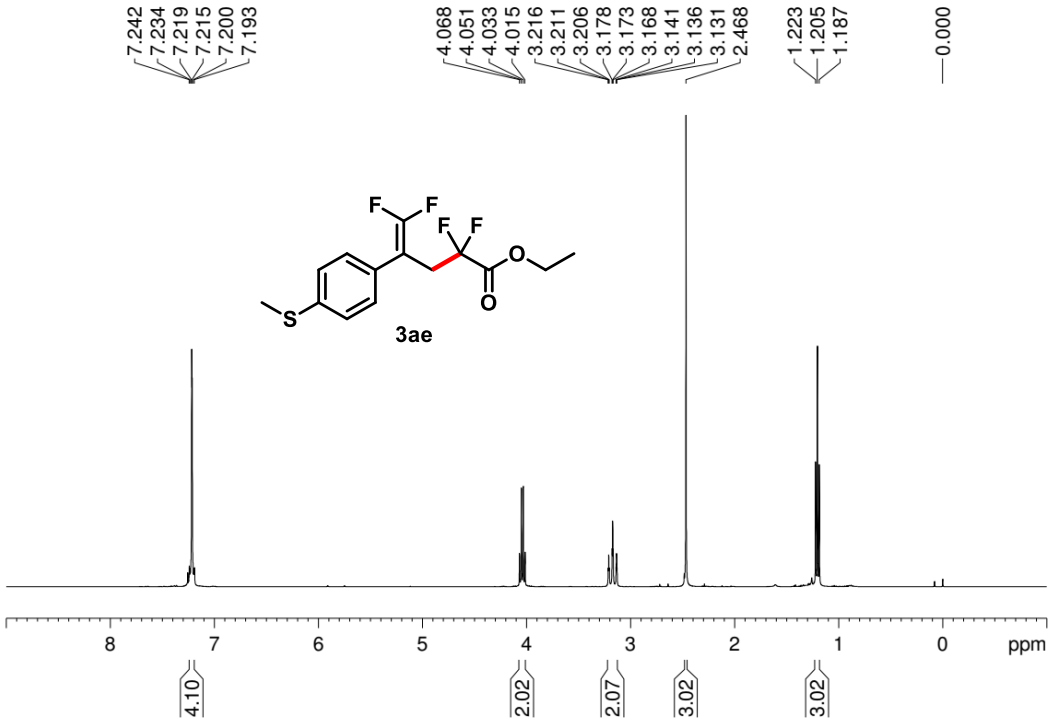
^{13}C NMR (100 MHz, $CDCl_3$)



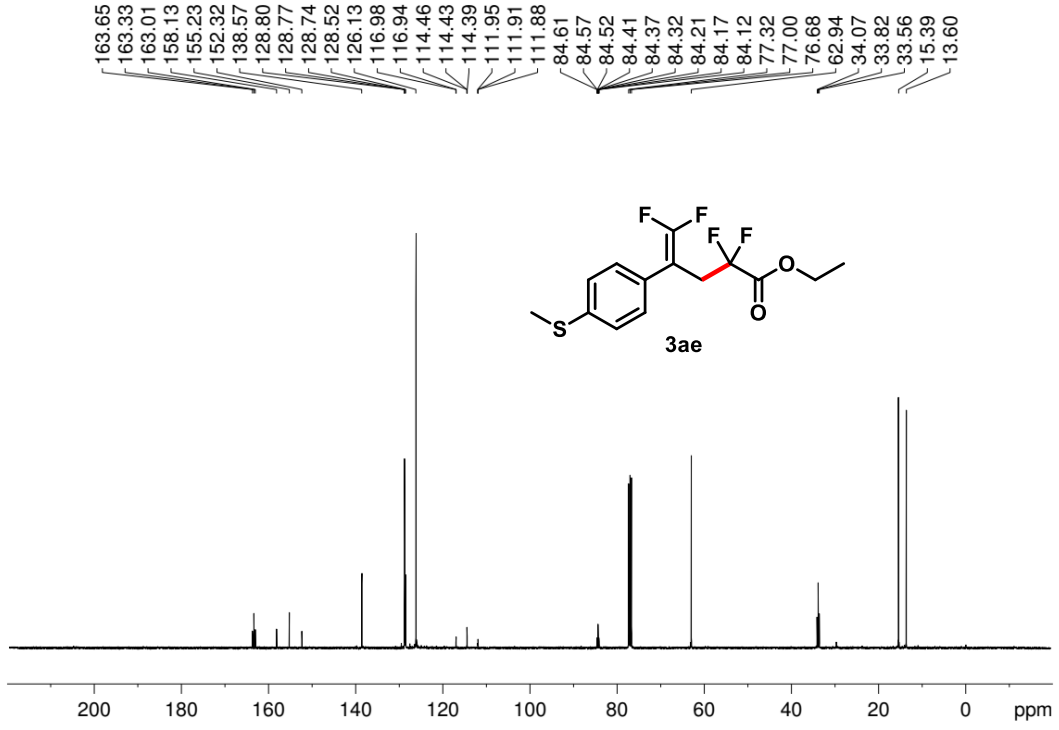
^{19}F NMR (376 MHz, $CDCl_3$)



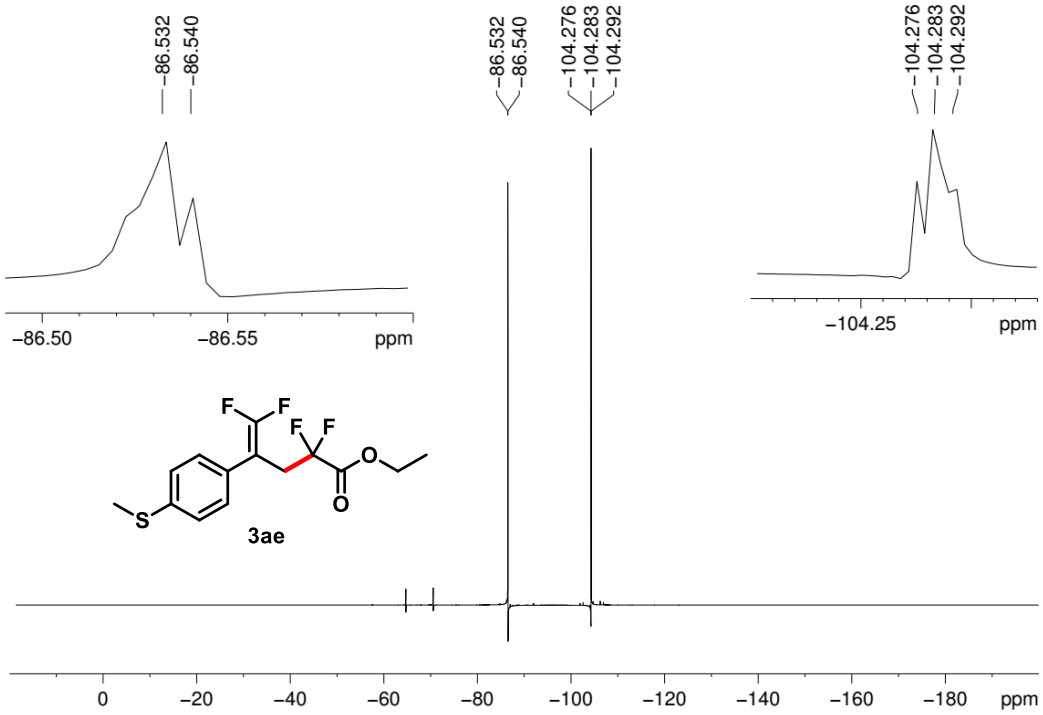
^{1}H NMR (400 MHz, $CDCl_3$)



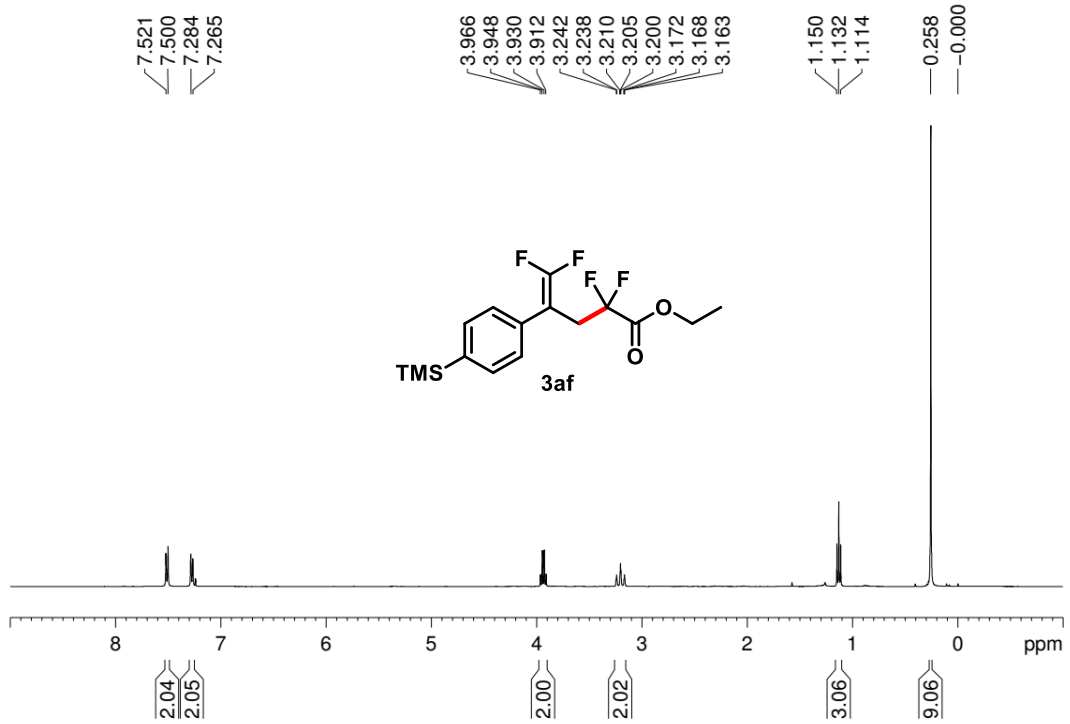
^{13}C NMR (100 MHz, $CDCl_3$)



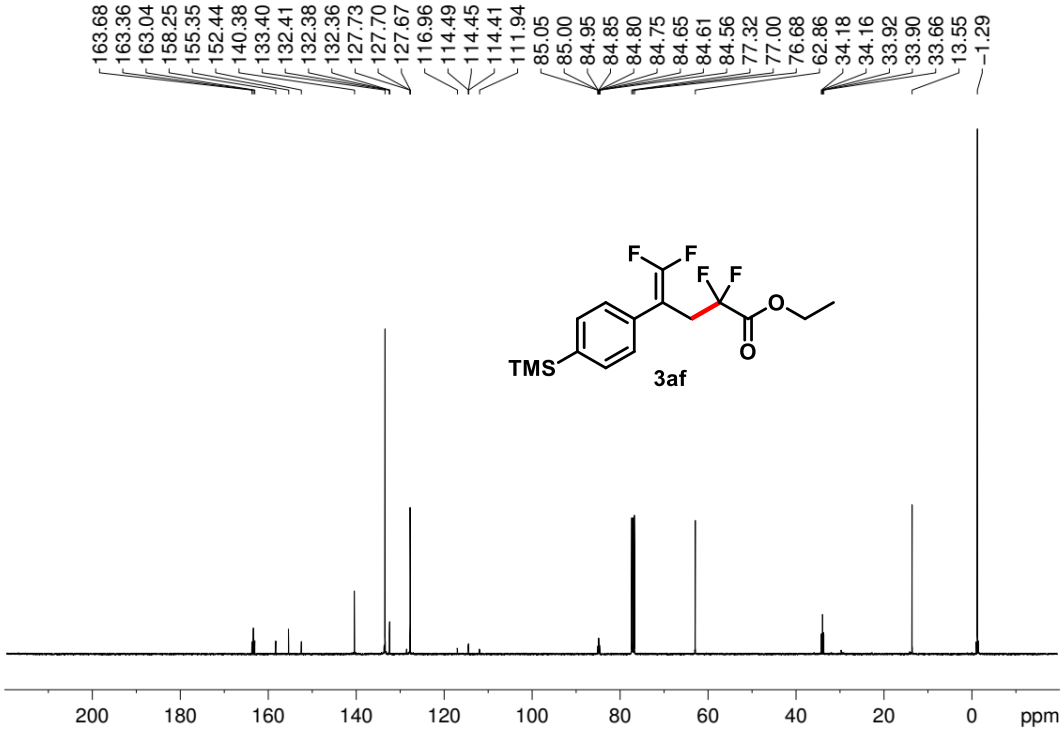
^{19}F NMR (376 MHz, $CDCl_3$)



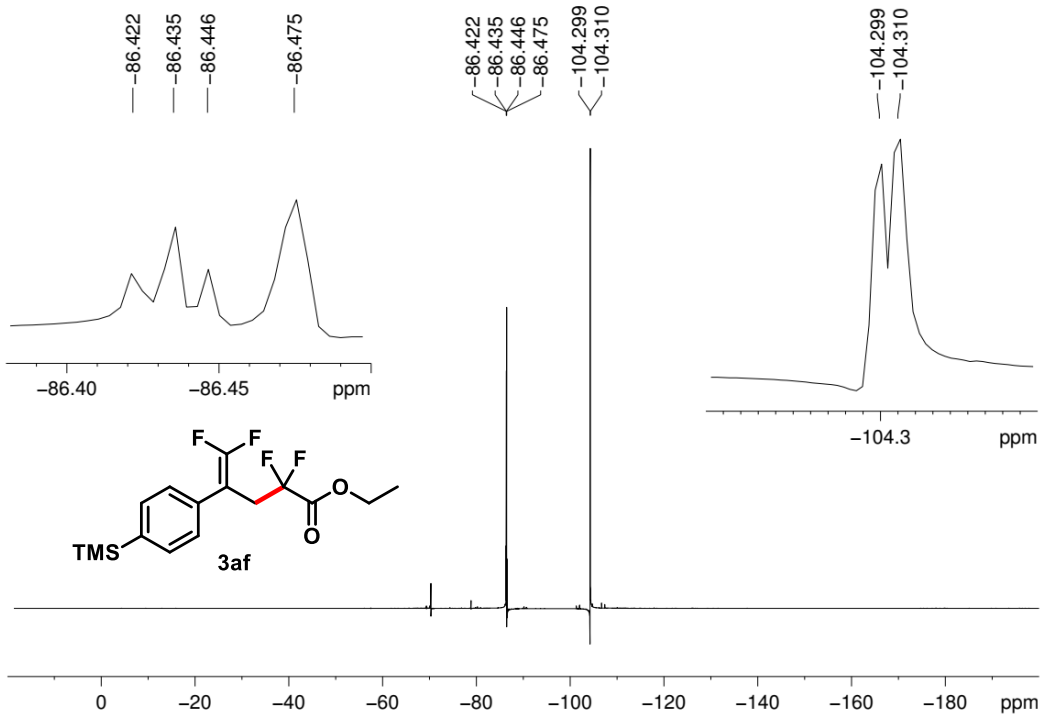
^{1}H NMR (400 MHz, $CDCl_3$)



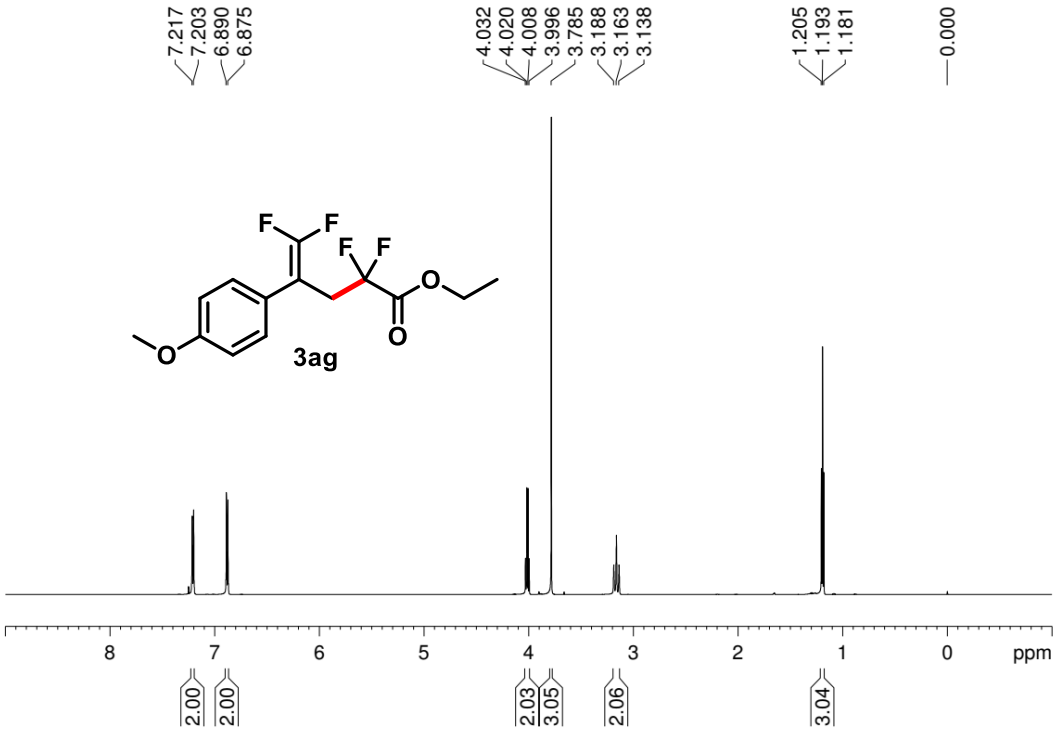
^{13}C NMR (100 MHz, $CDCl_3$)



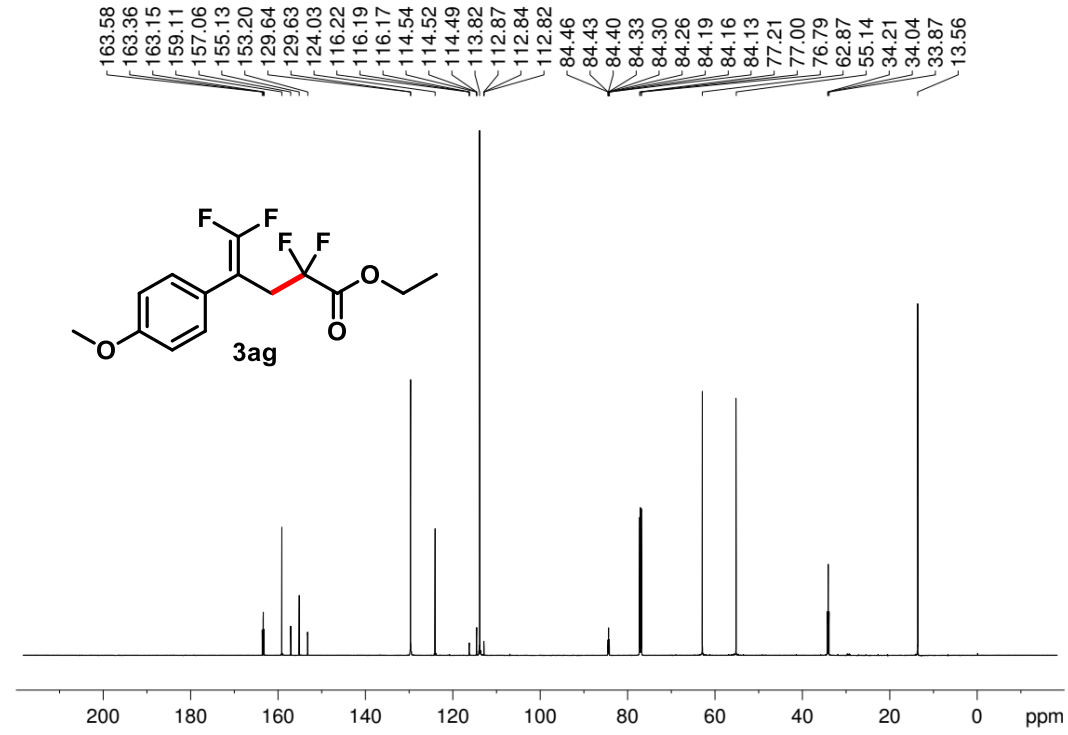
^{19}F NMR (376 MHz, $CDCl_3$)



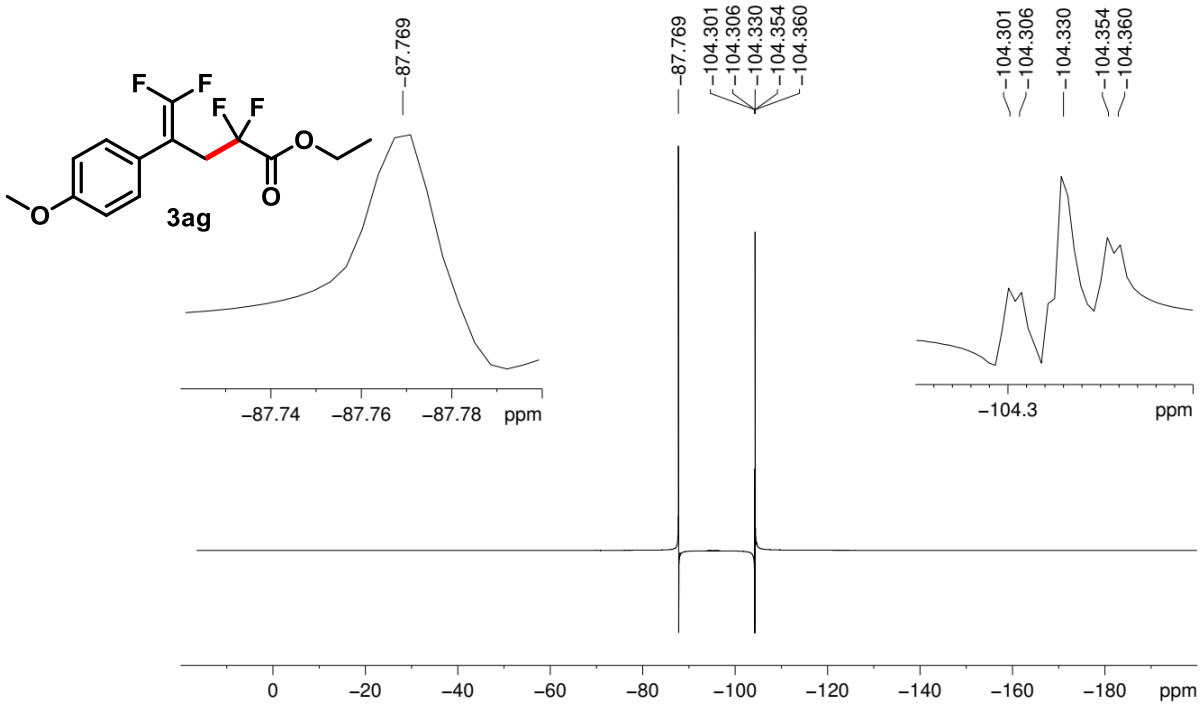
^{1}H NMR (600 MHz, $CDCl_3$)



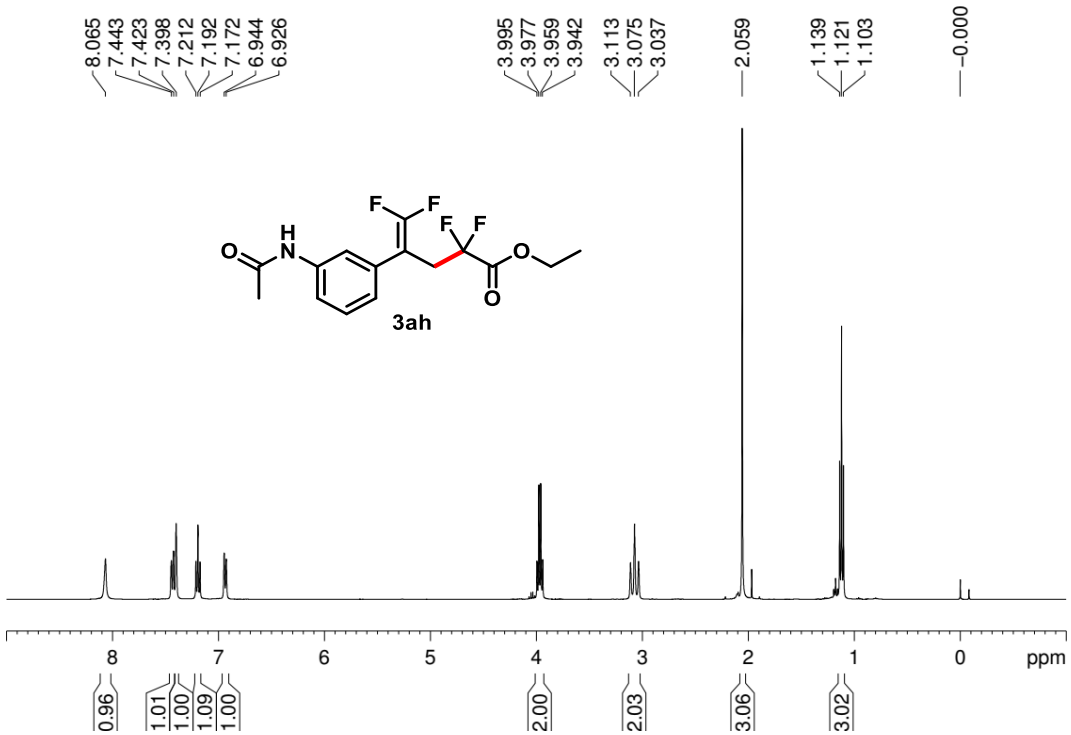
^{13}C NMR (150 MHz, $CDCl_3$)



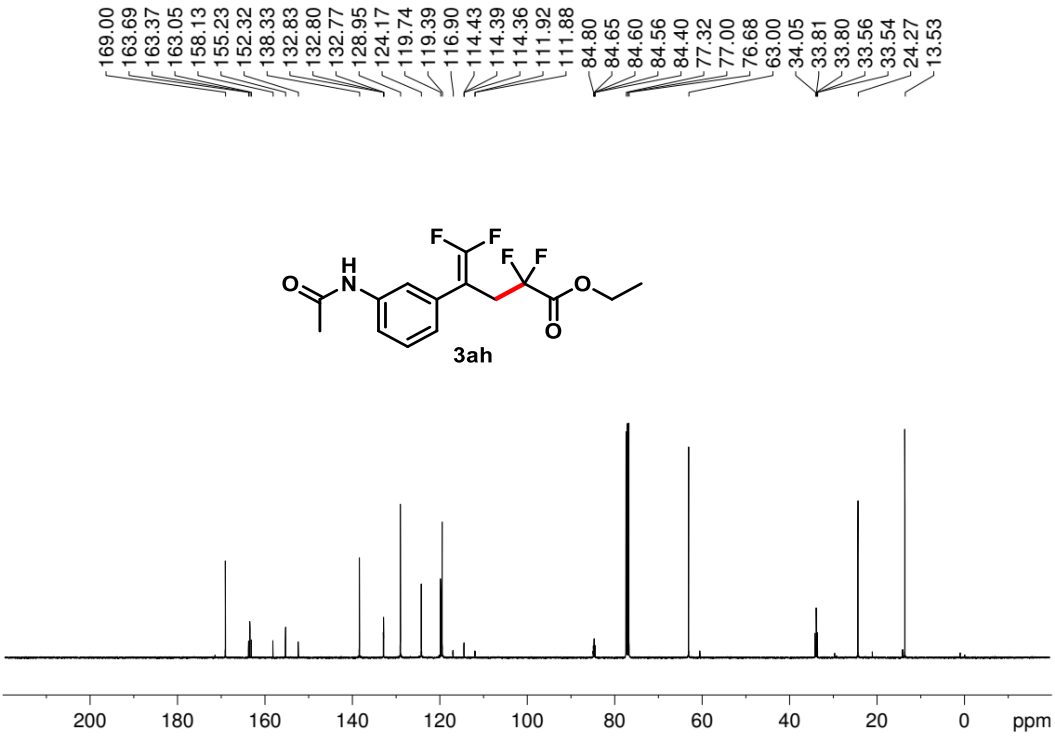
^{19}F NMR (565 MHz, $CDCl_3$)



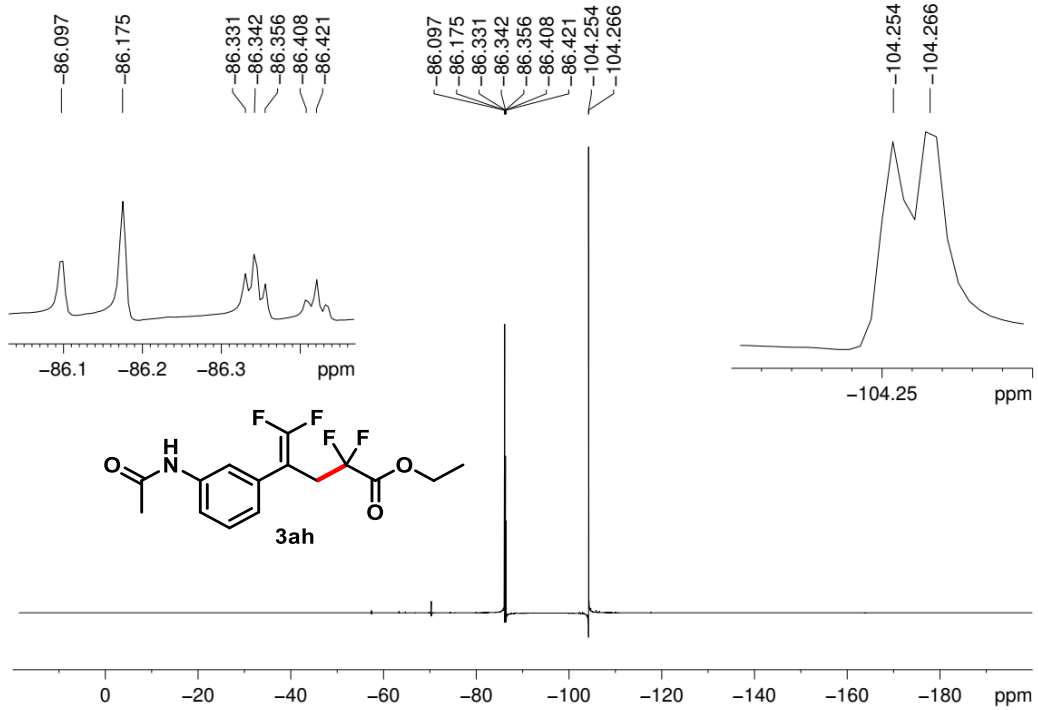
^{1}H NMR (400 MHz, $CDCl_3$)



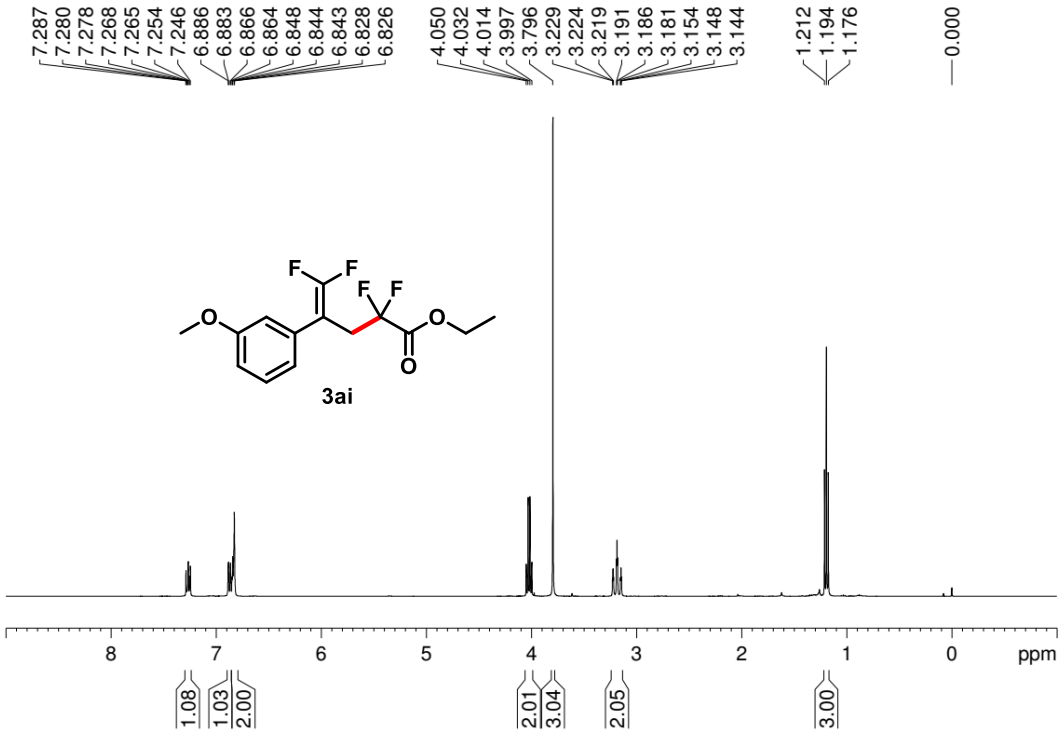
^{13}C NMR (100 MHz, $CDCl_3$)



^{19}F NMR (376 MHz, $CDCl_3$)



^{1}H NMR (400 MHz, $CDCl_3$)



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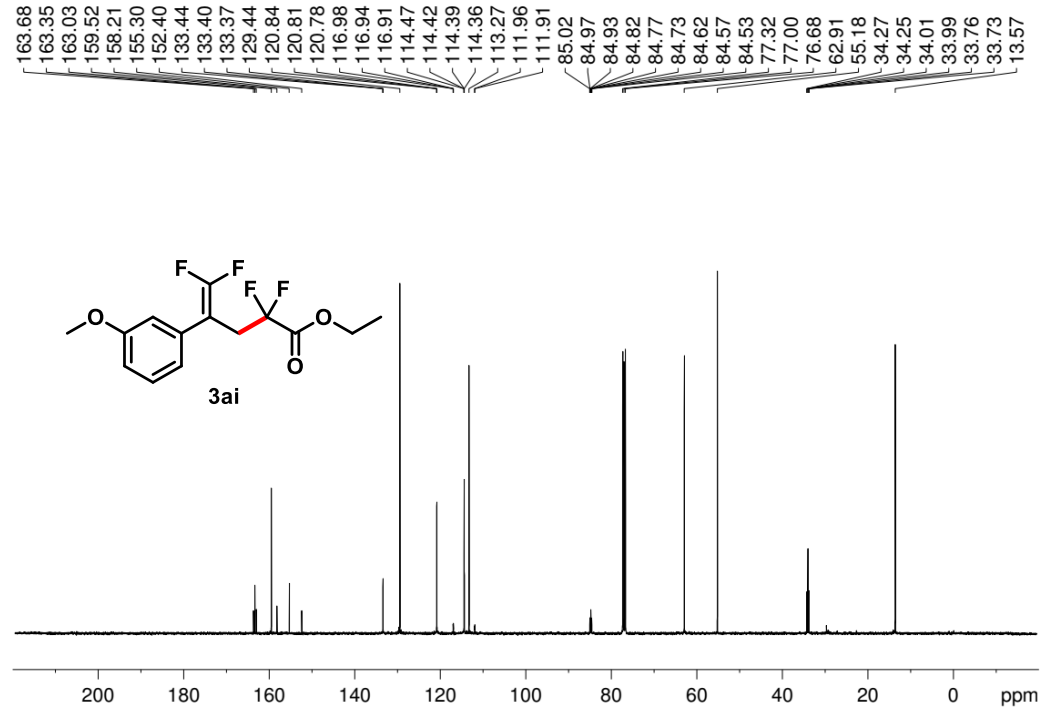

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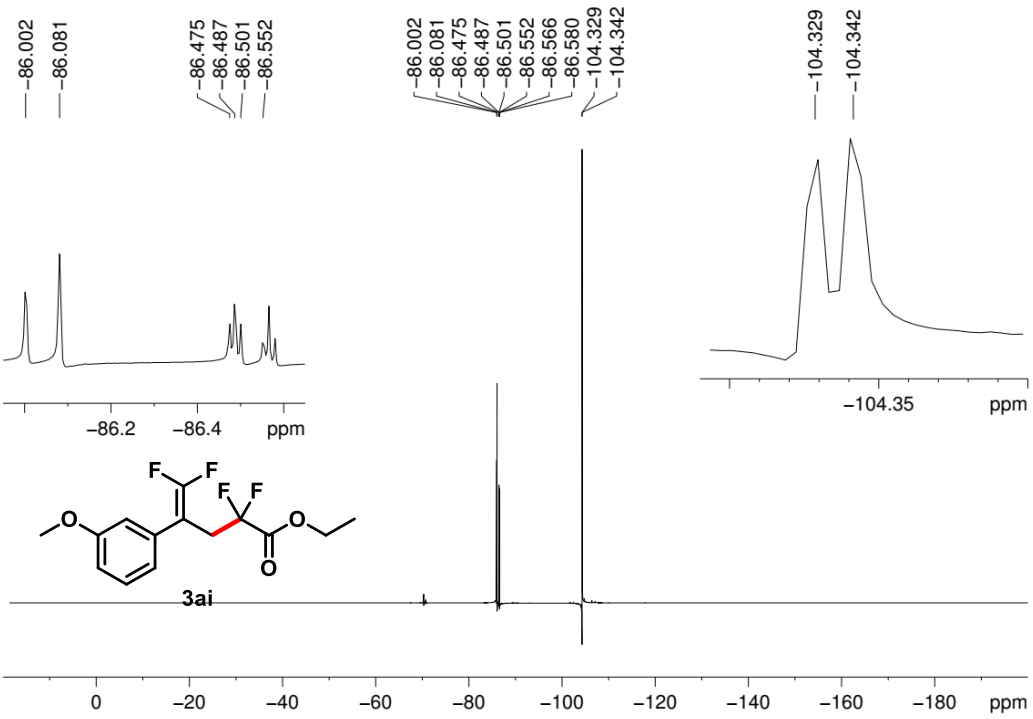

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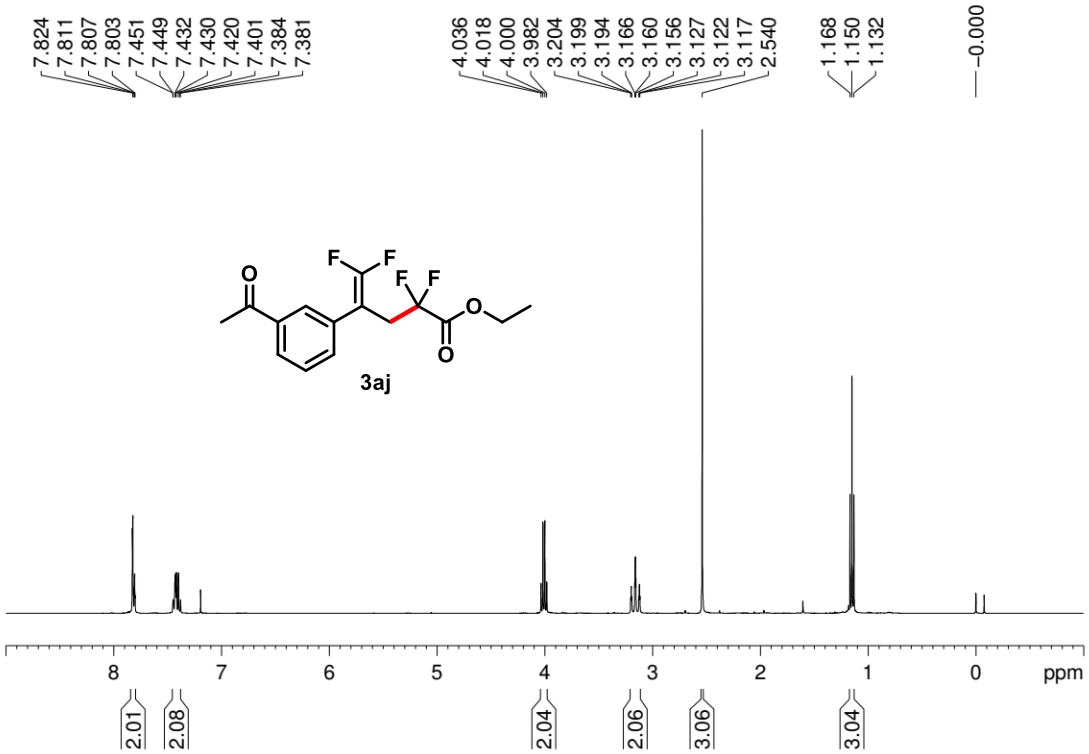

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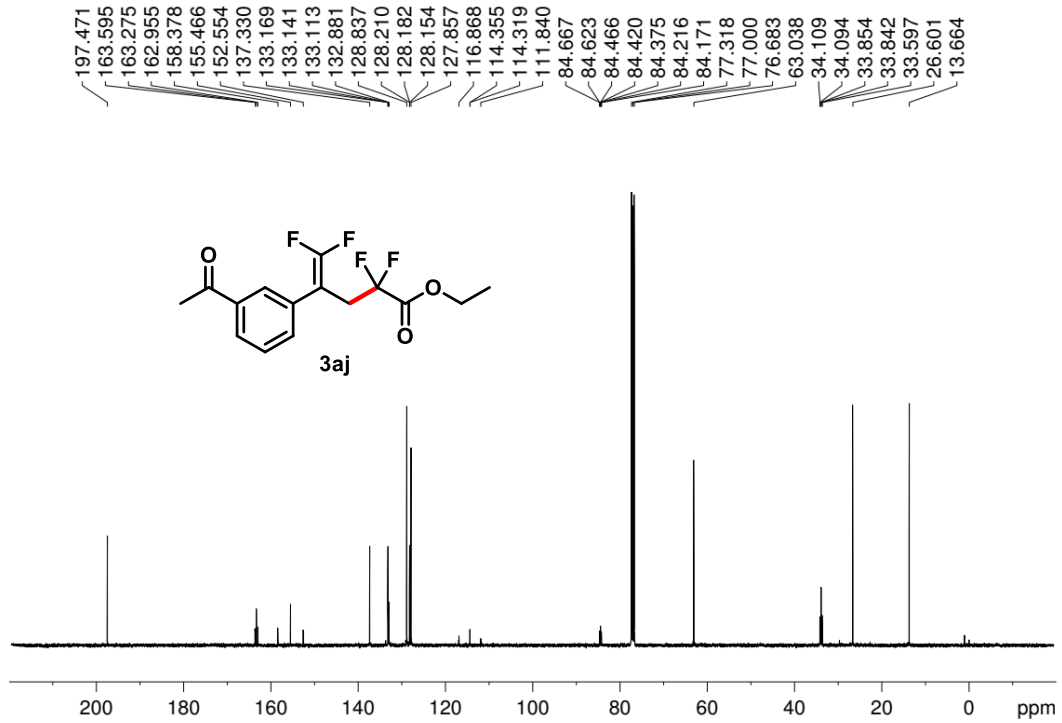

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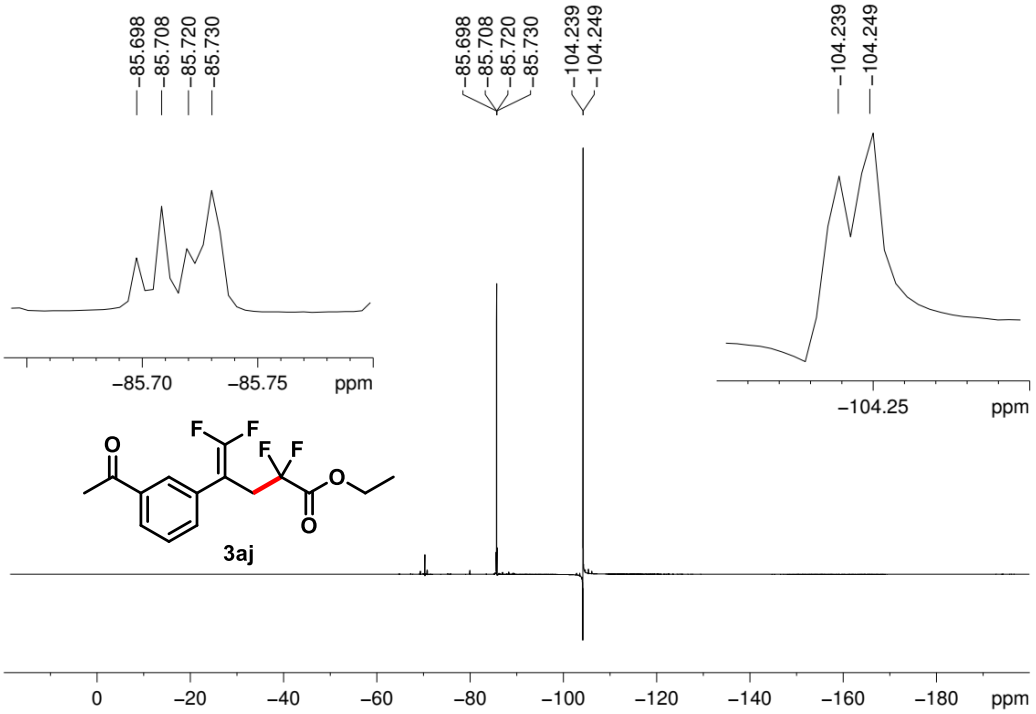

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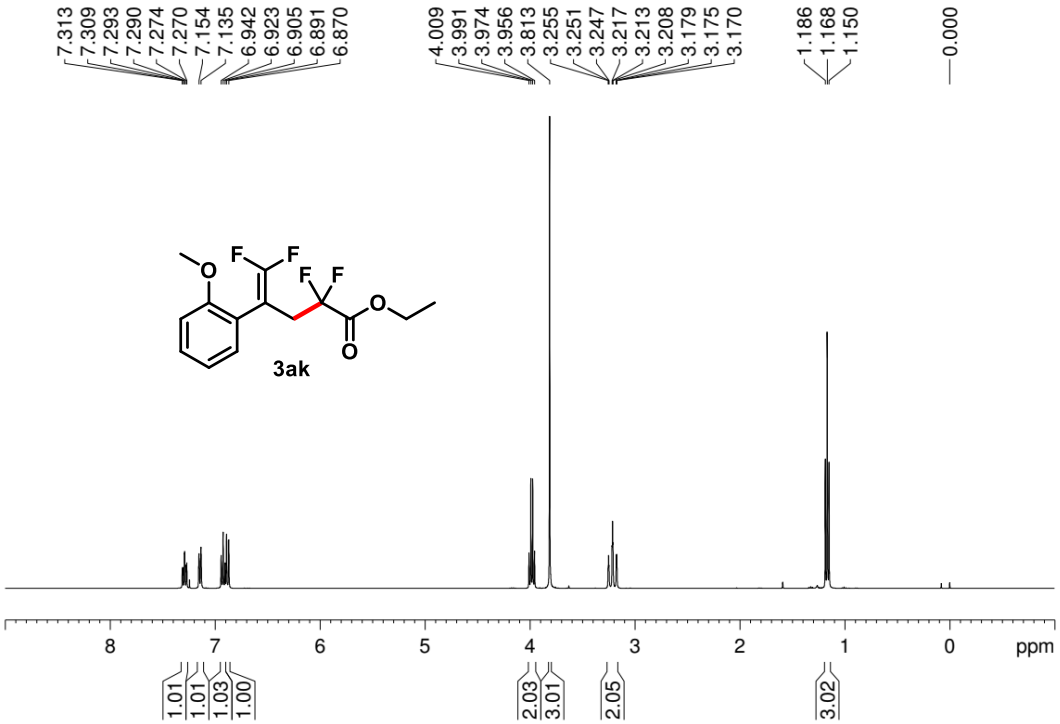

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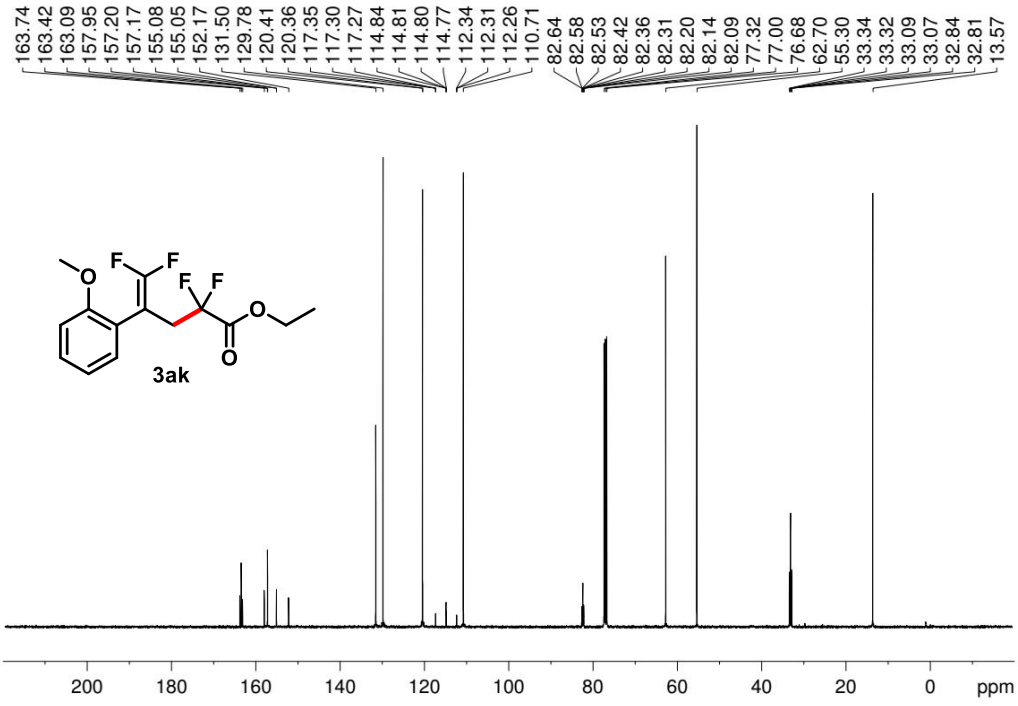

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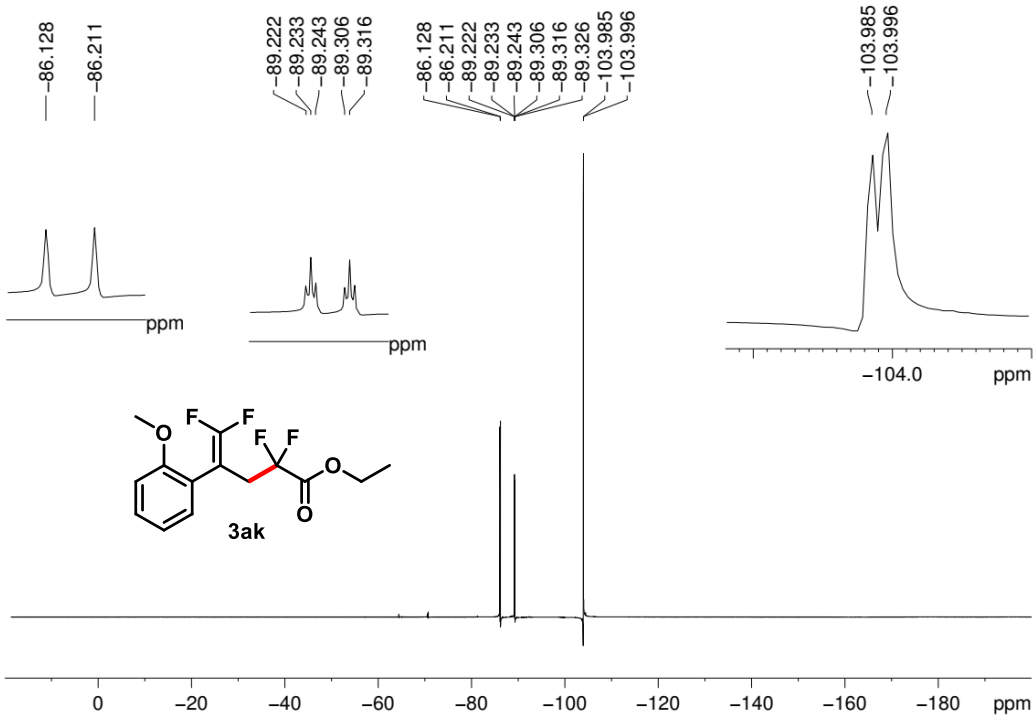

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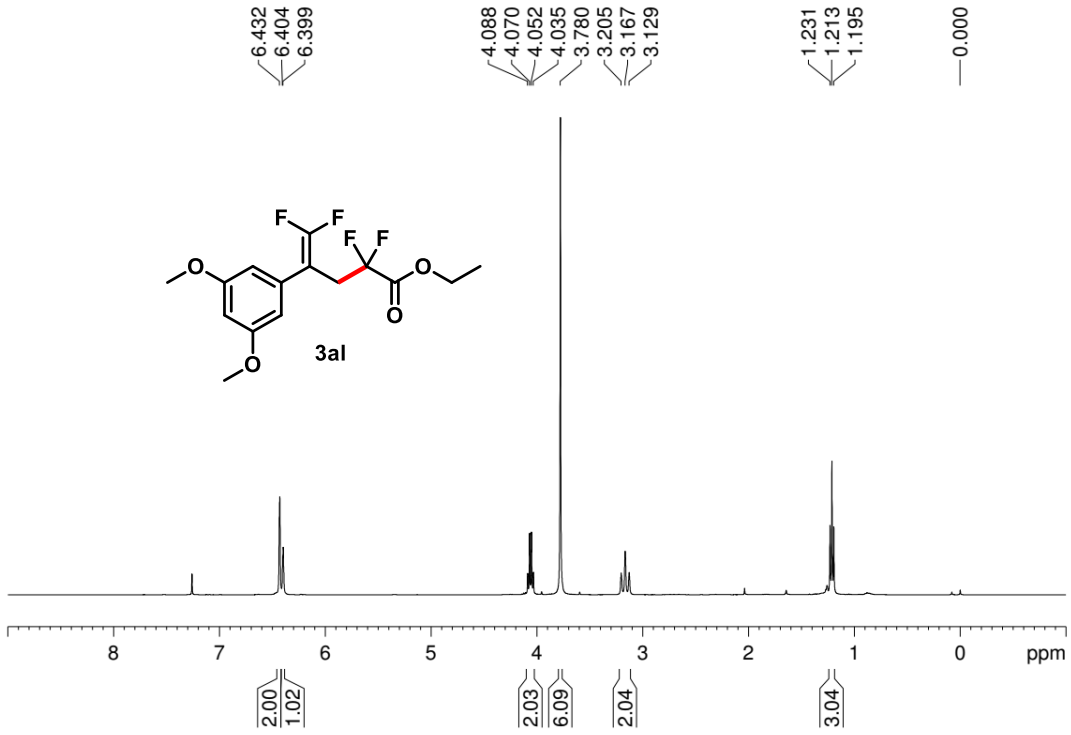

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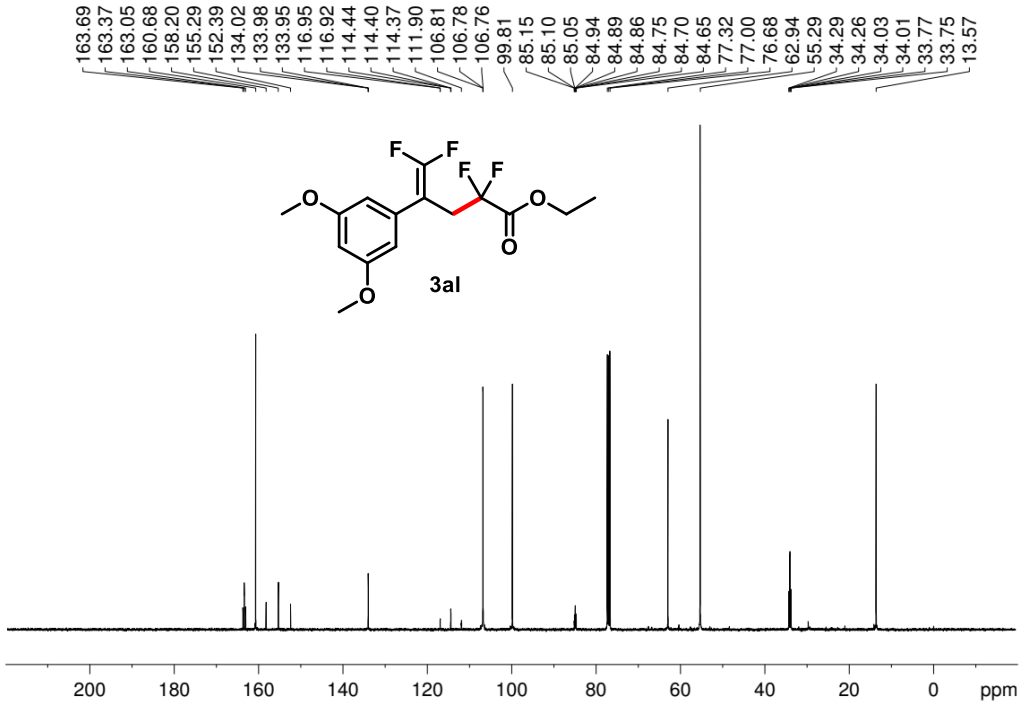

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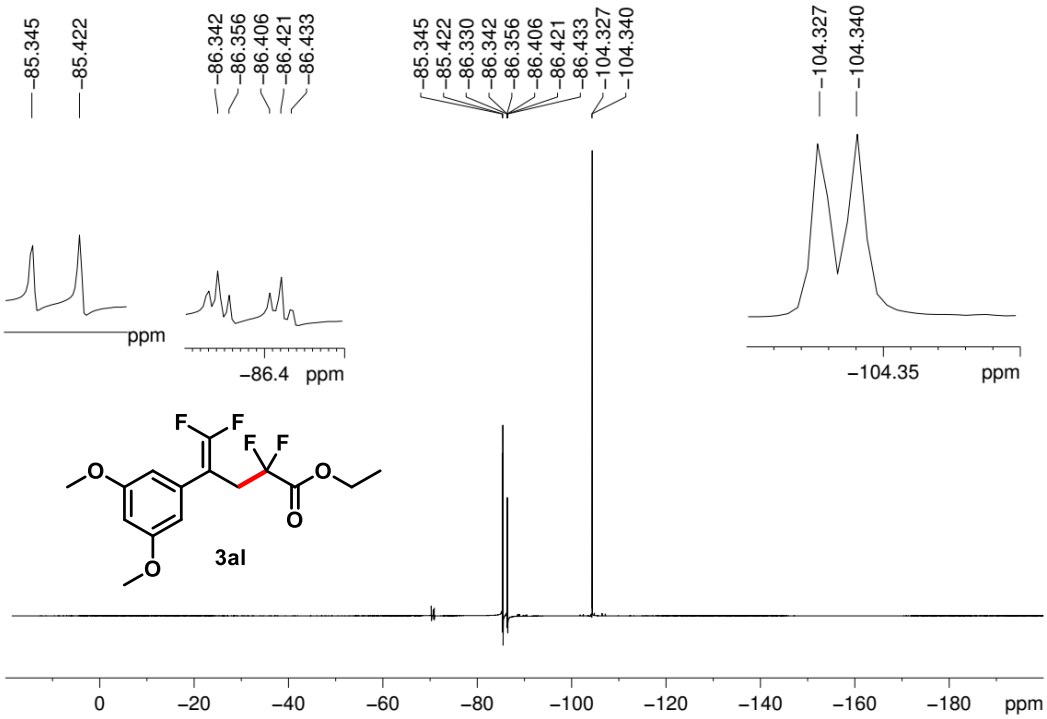

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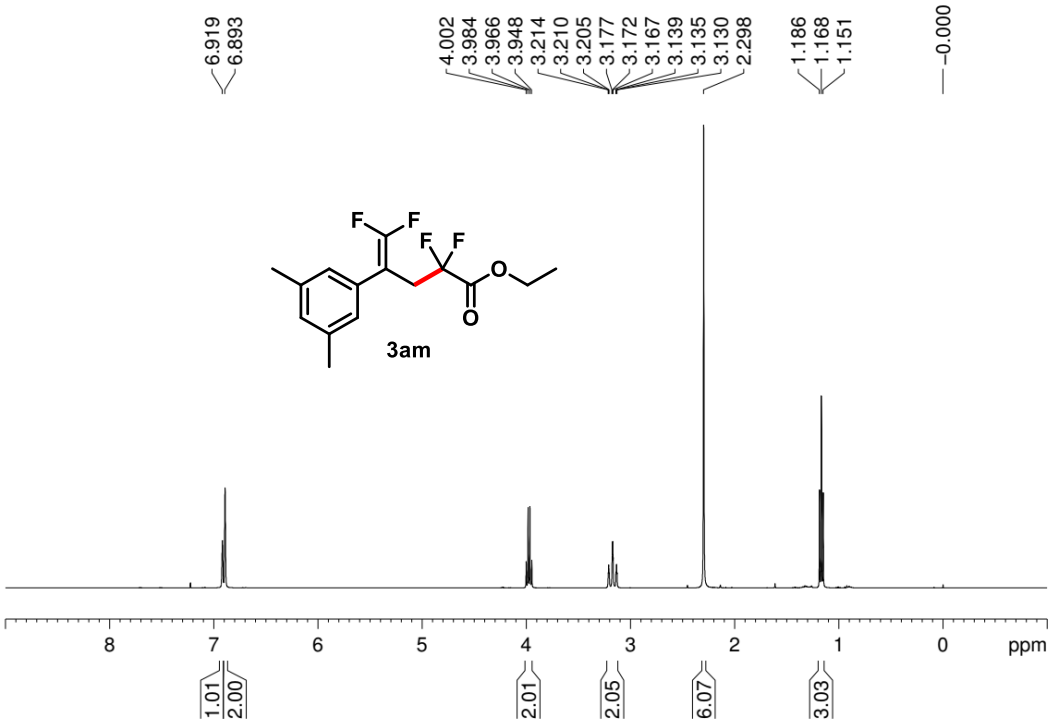

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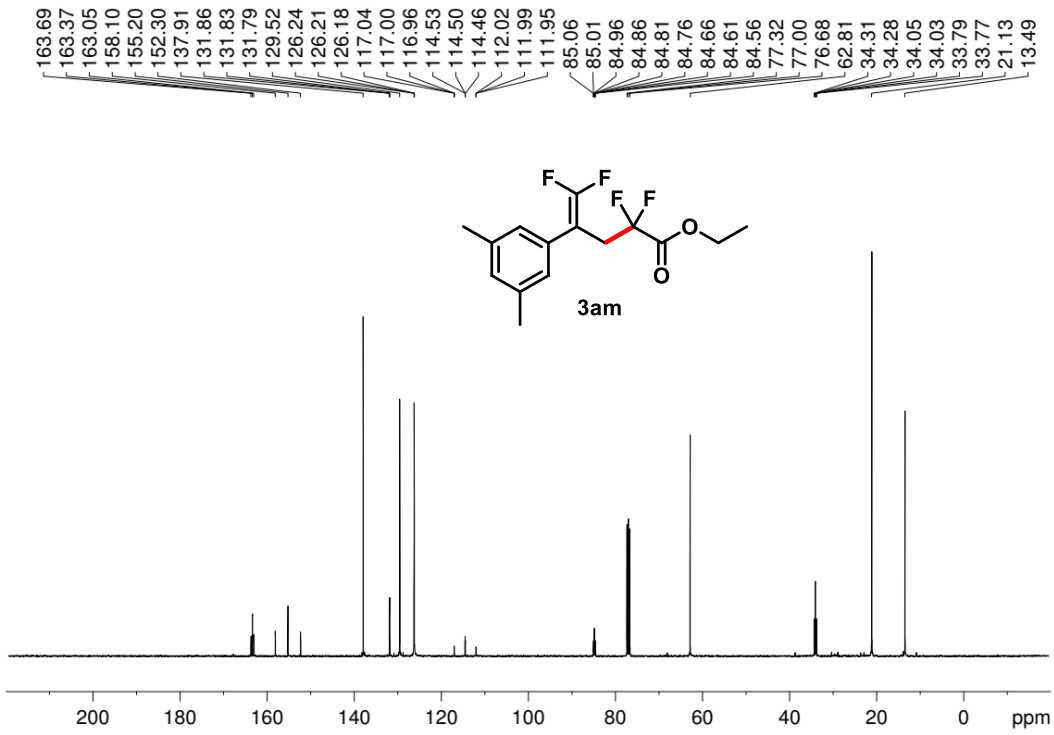

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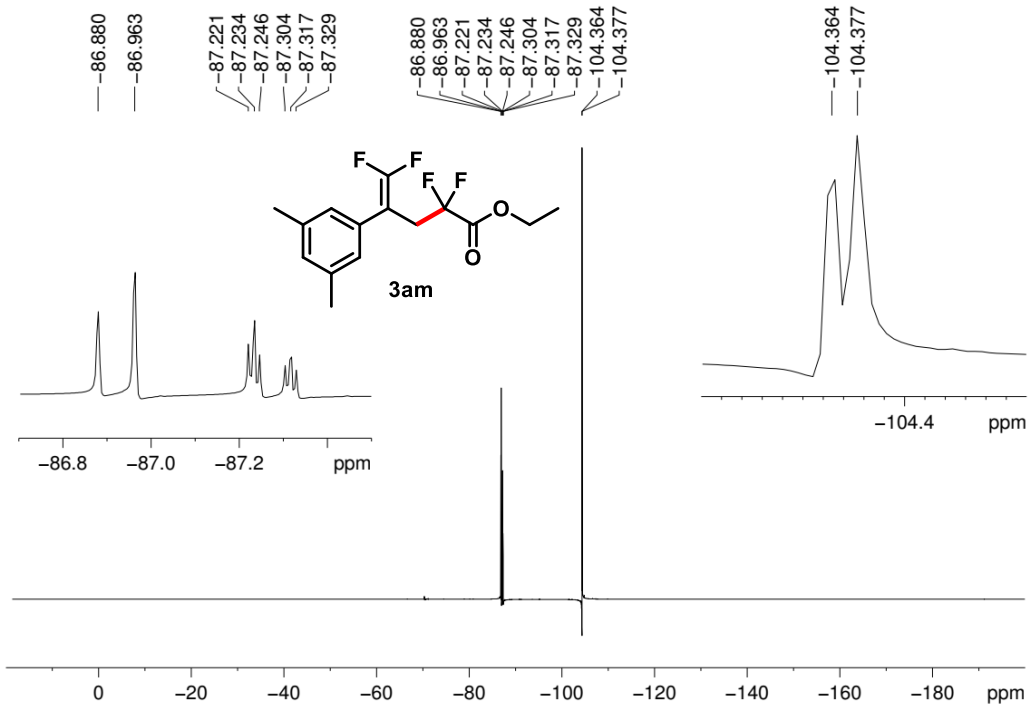

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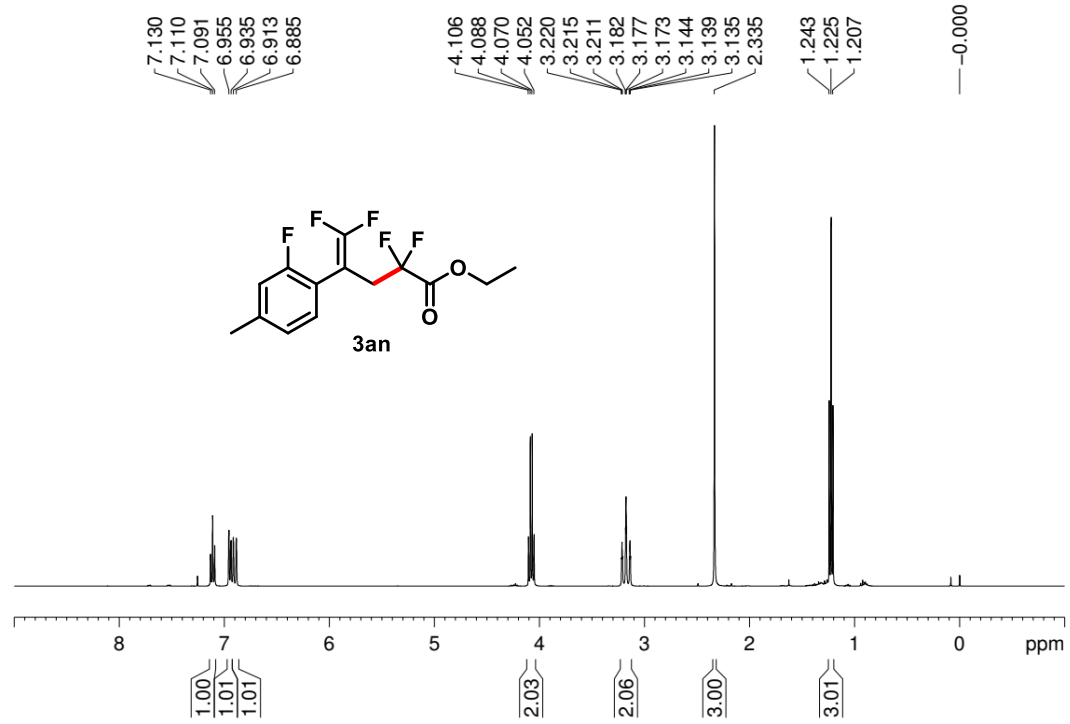

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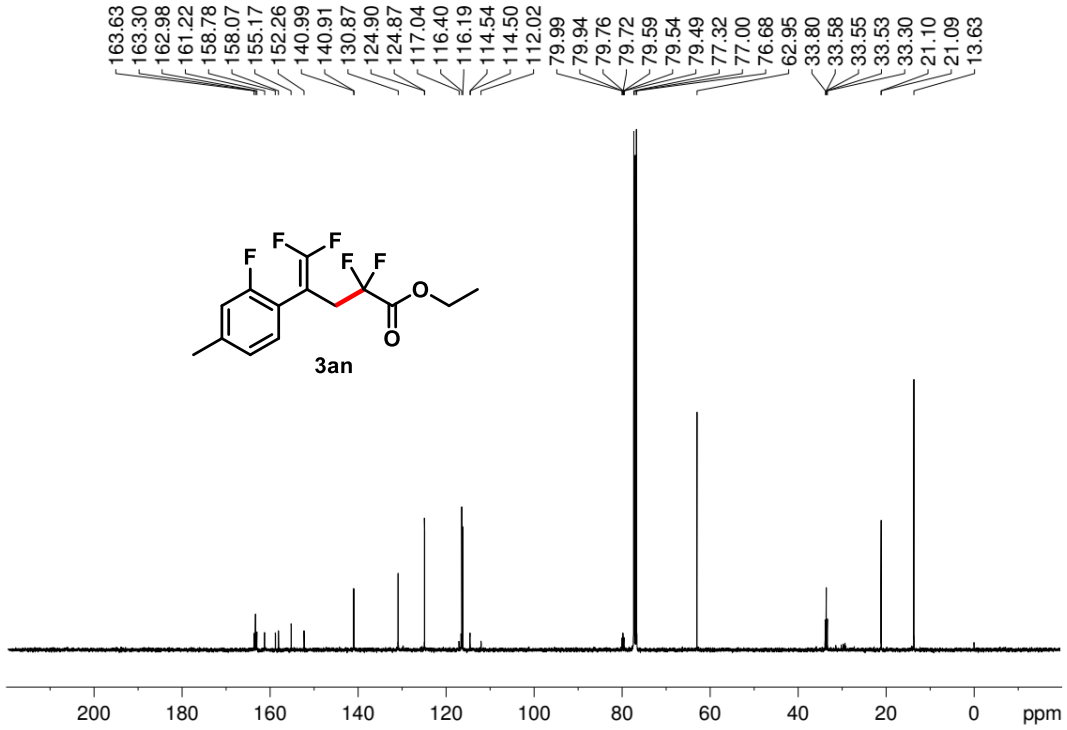

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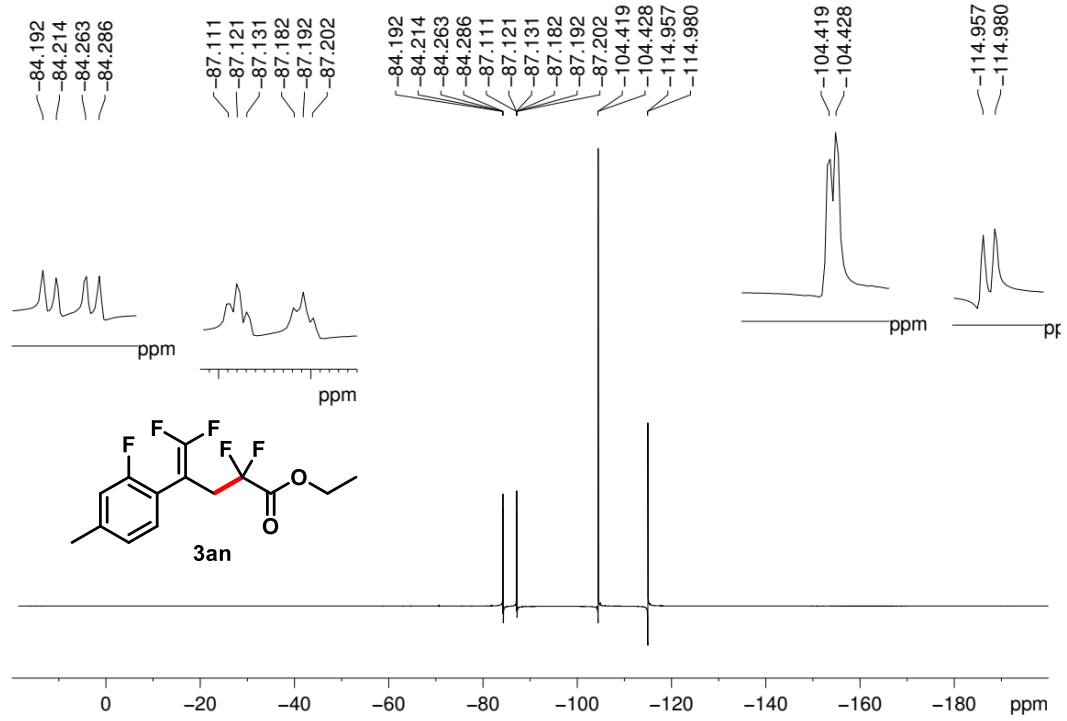

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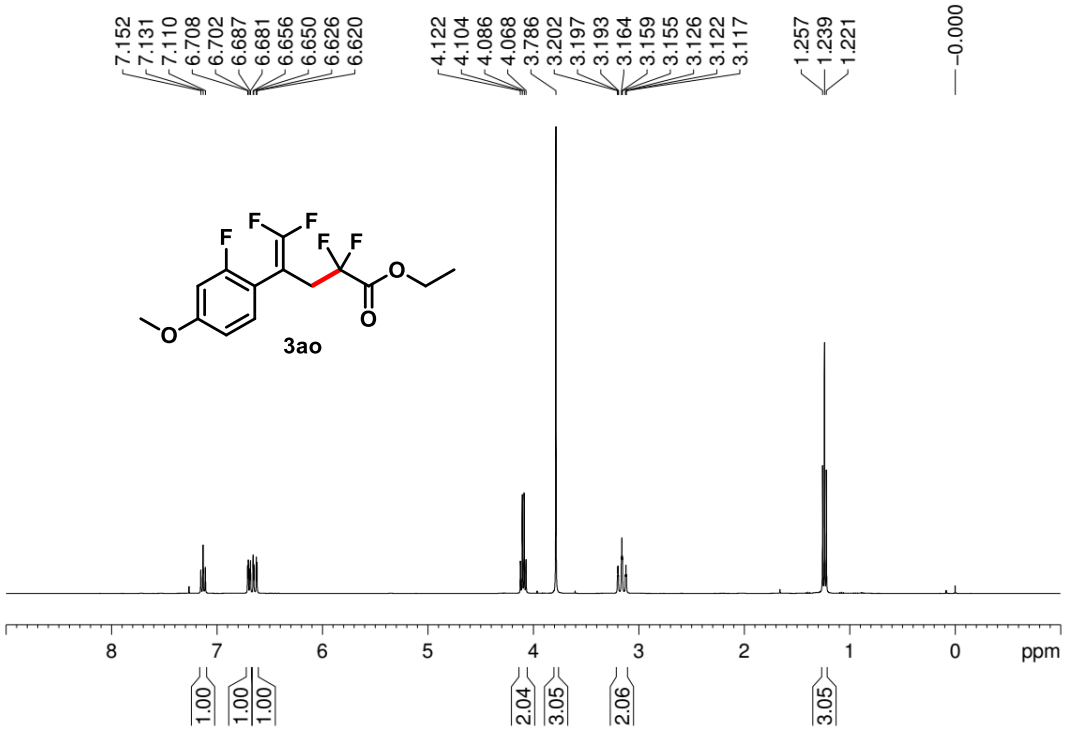

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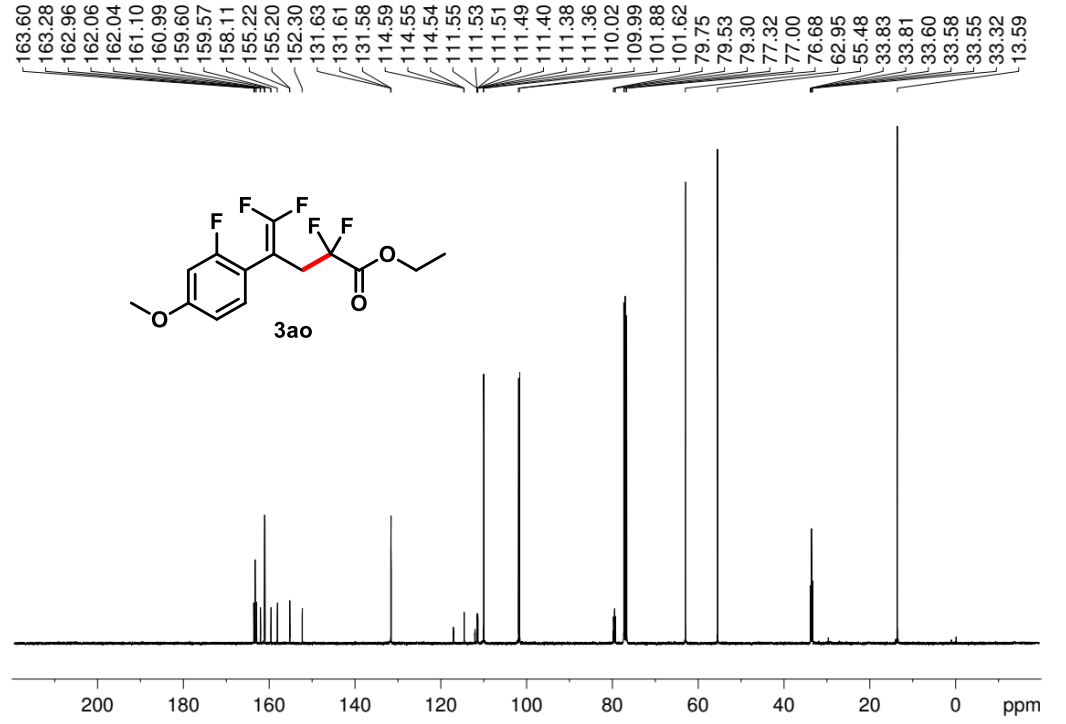

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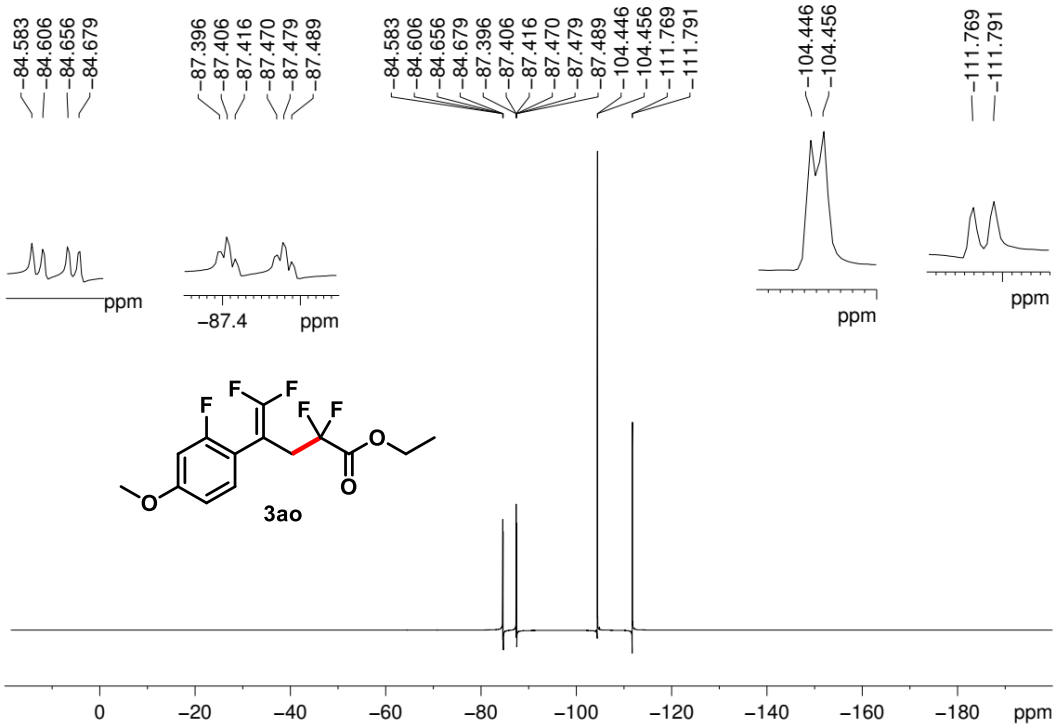

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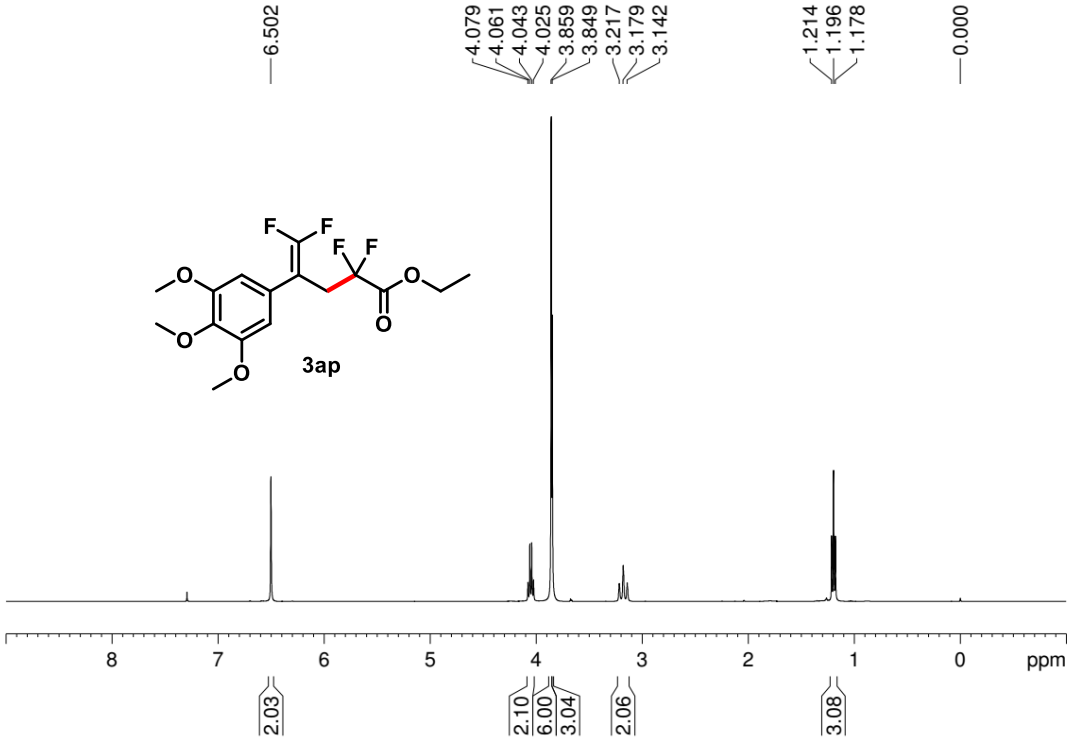

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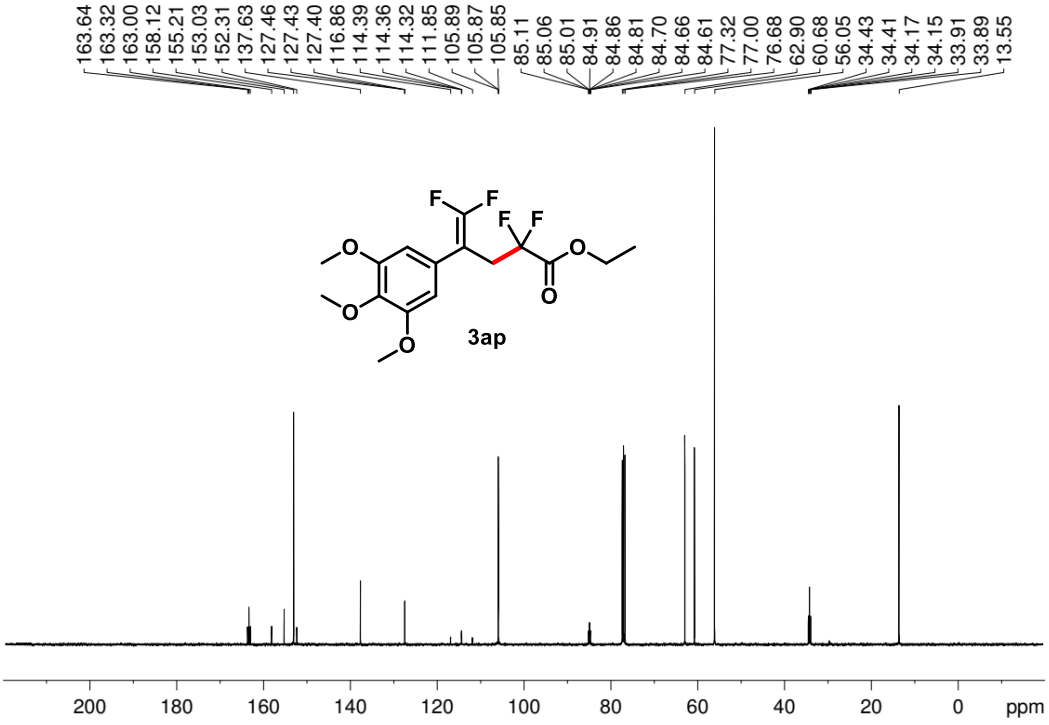

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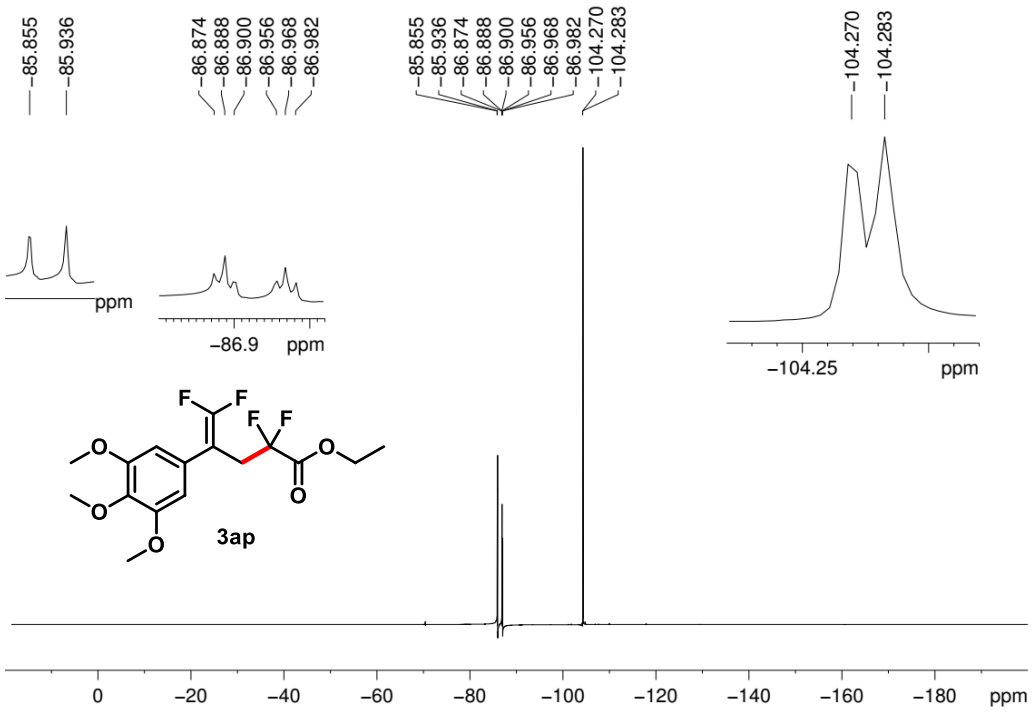

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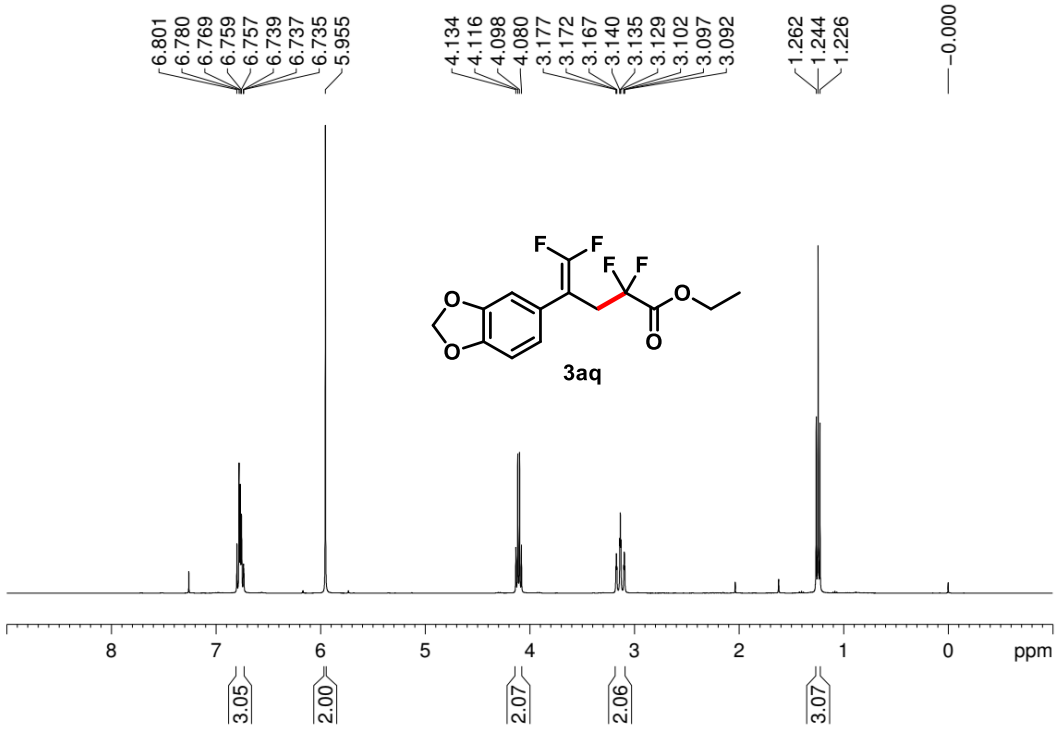

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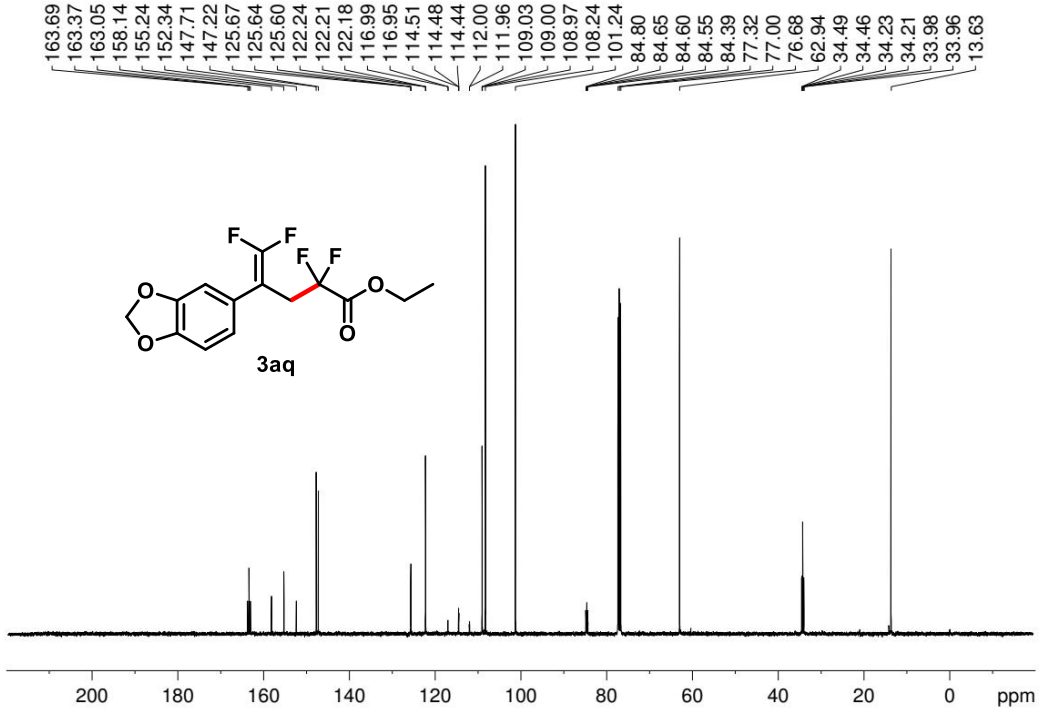
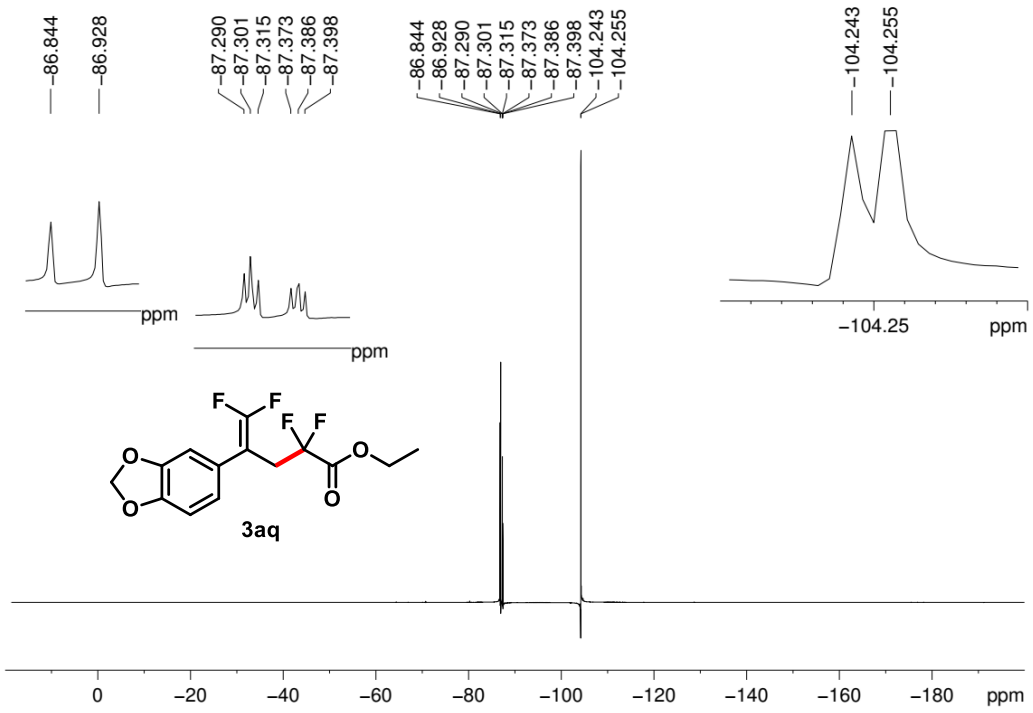
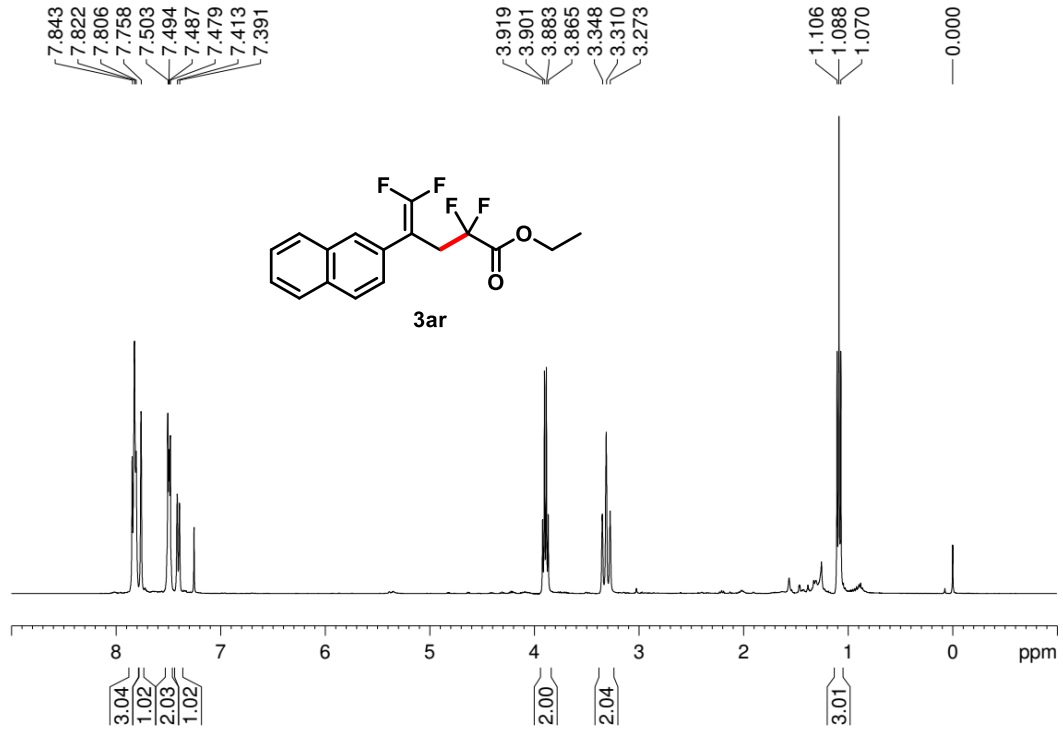


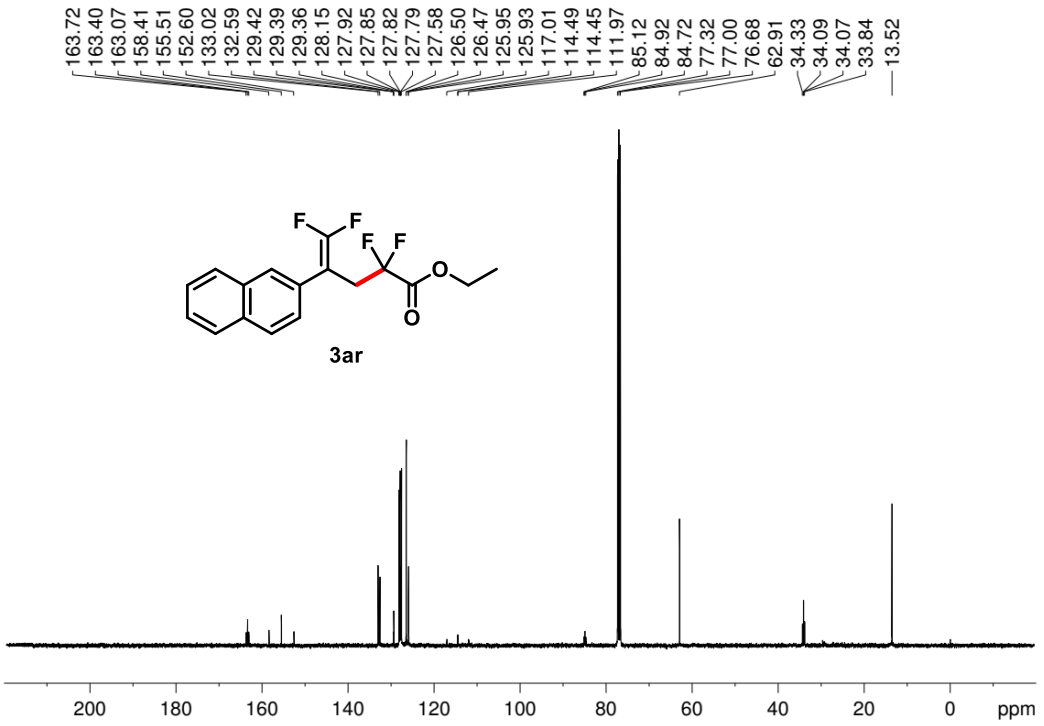
^{19}F NMR (376 MHz, $CDCl_3$)



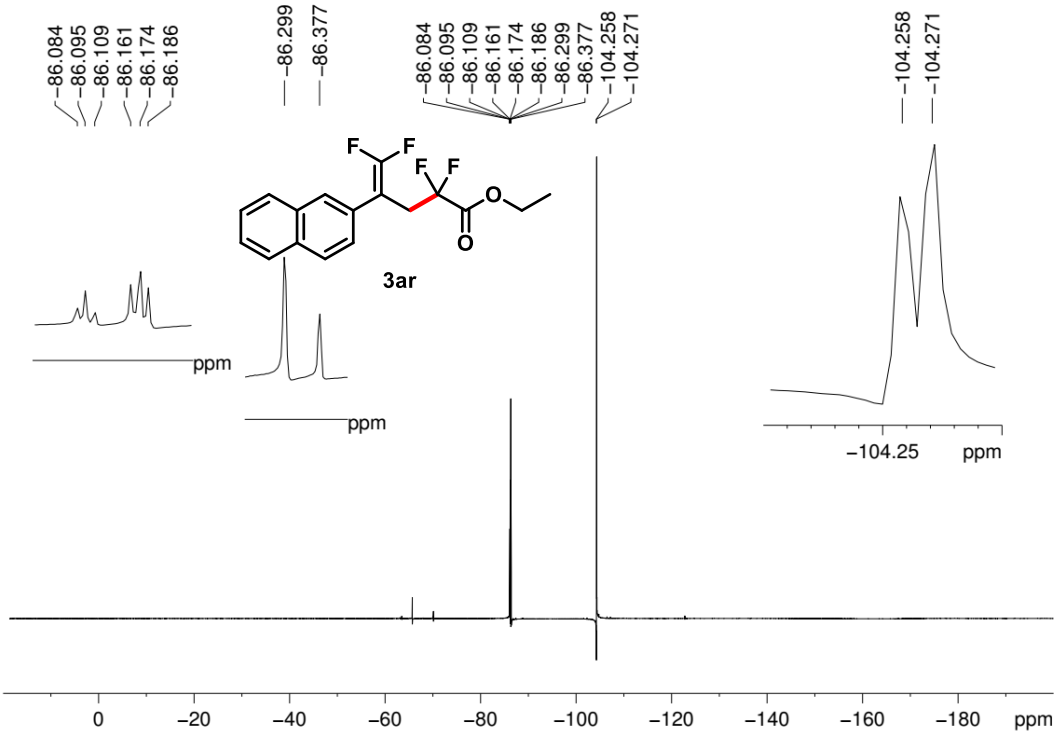
^{1}H NMR (400 MHz, $CDCl_3$)



^{13}C NMR (100 MHz, $CDCl_3$)



^{19}F NMR (376 MHz, $CDCl_3$)



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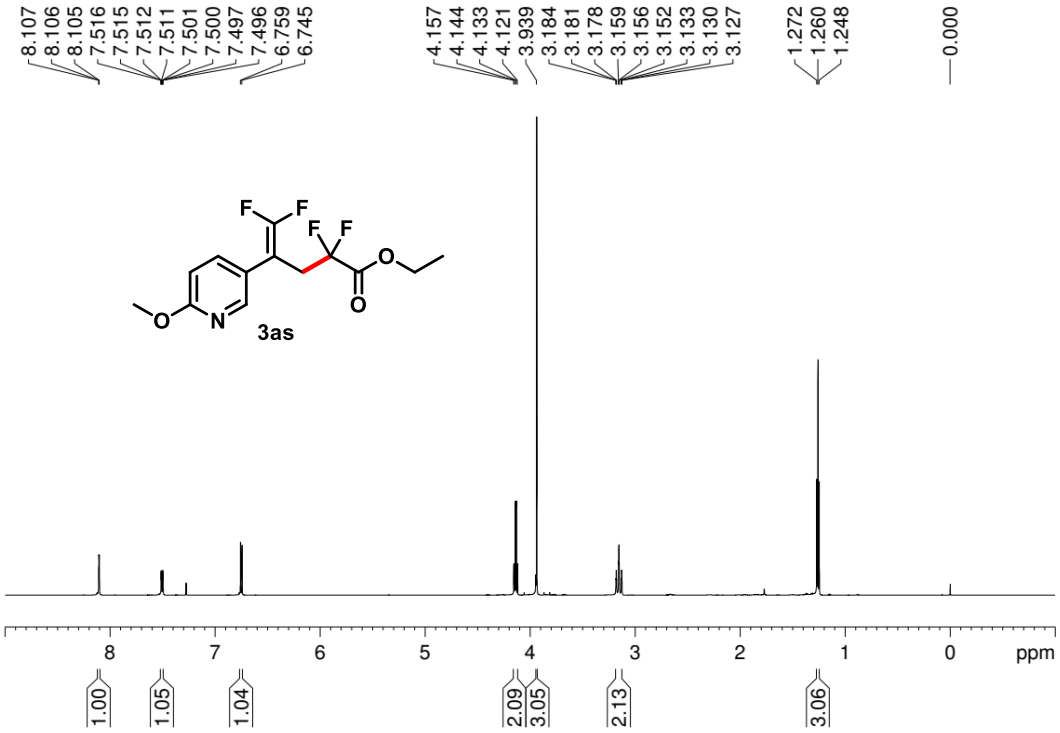

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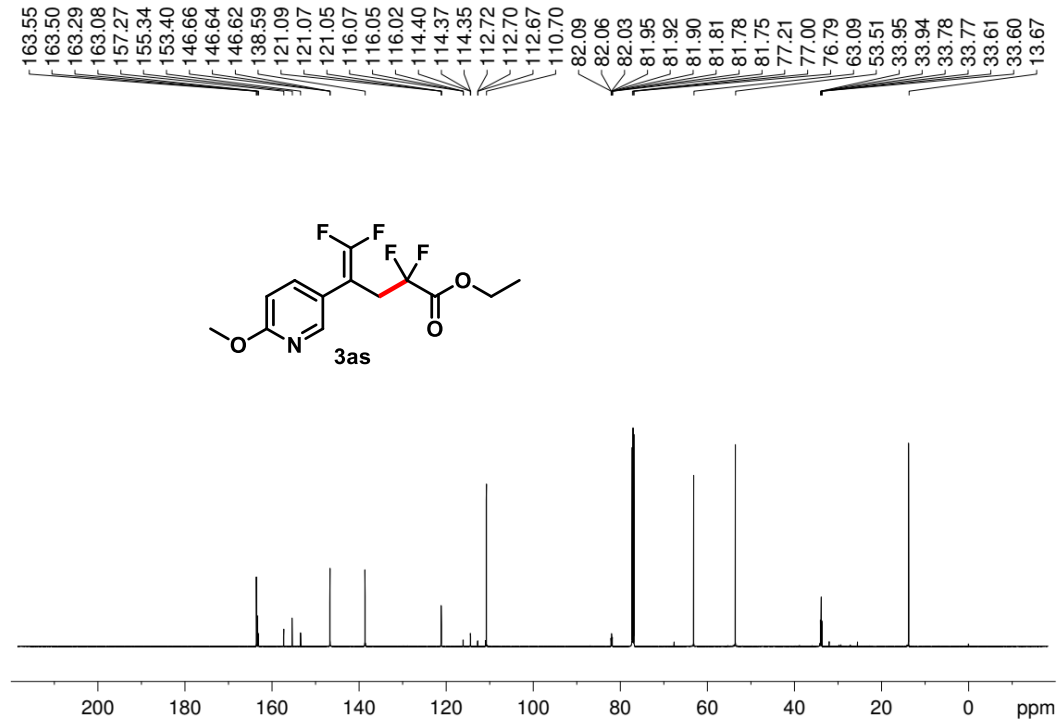
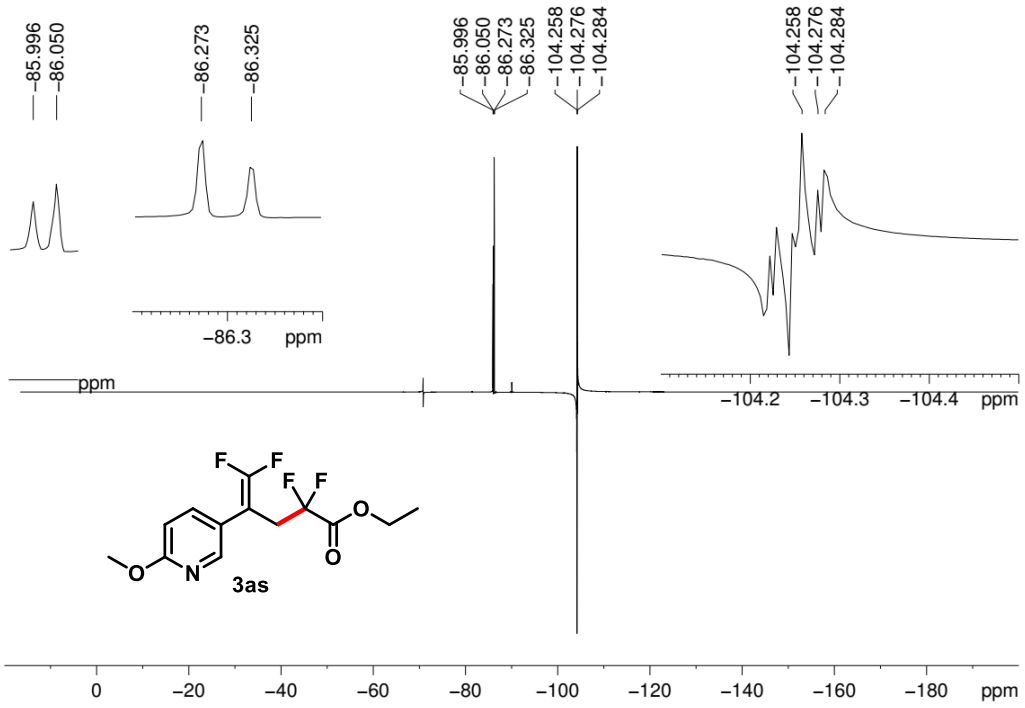
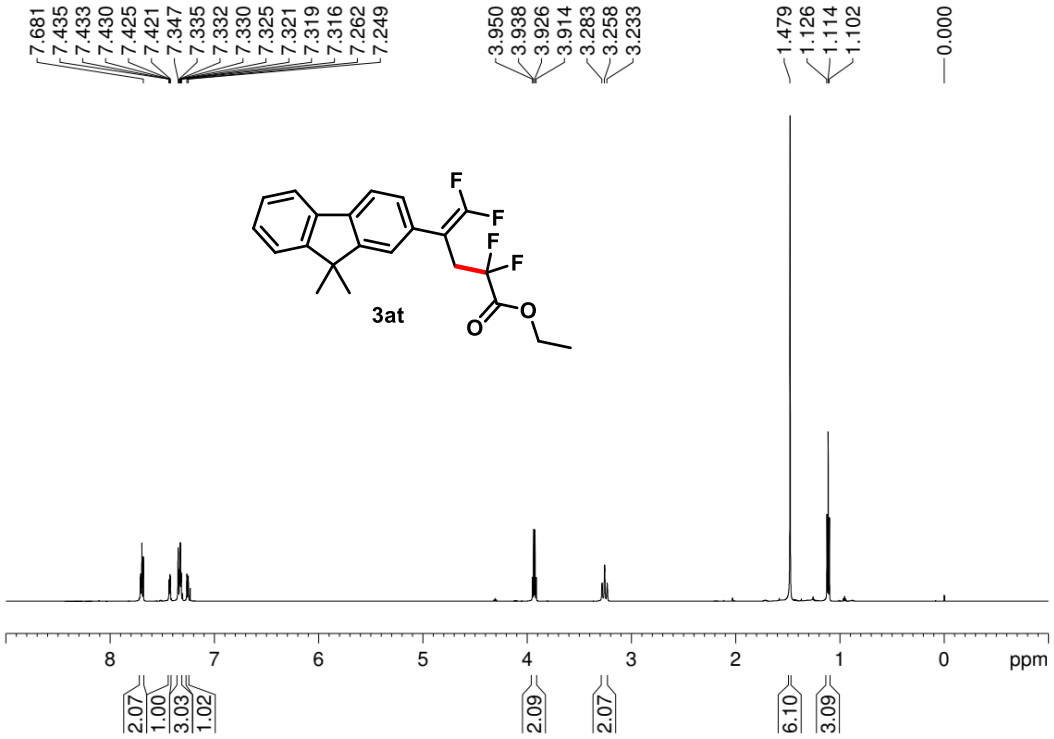


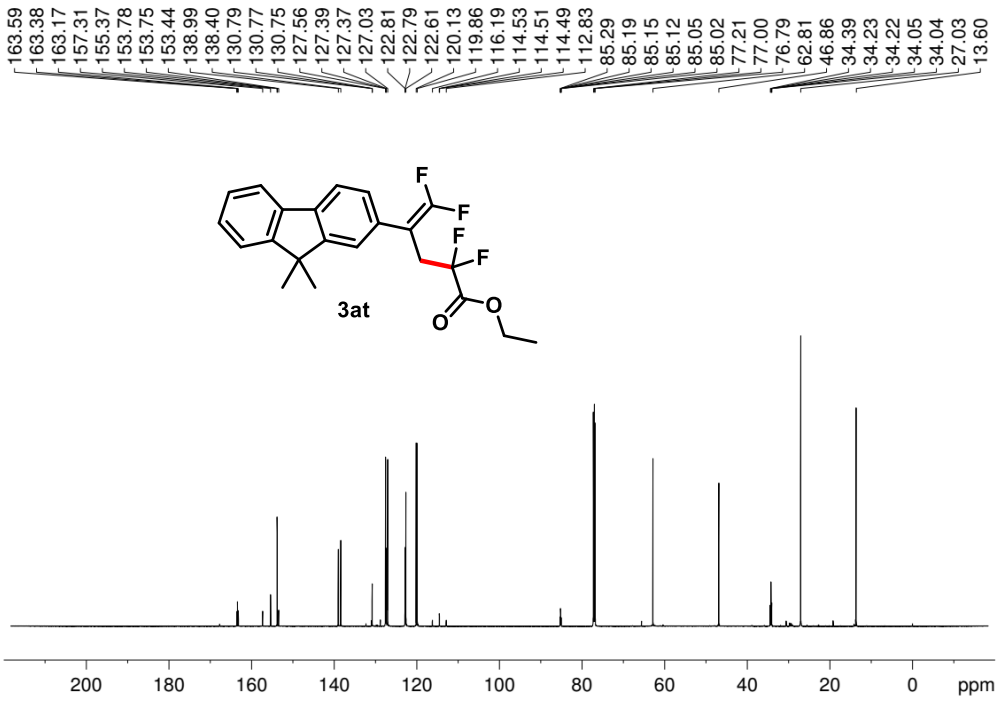
^{19}F NMR (565 MHz, $CDCl_3$)



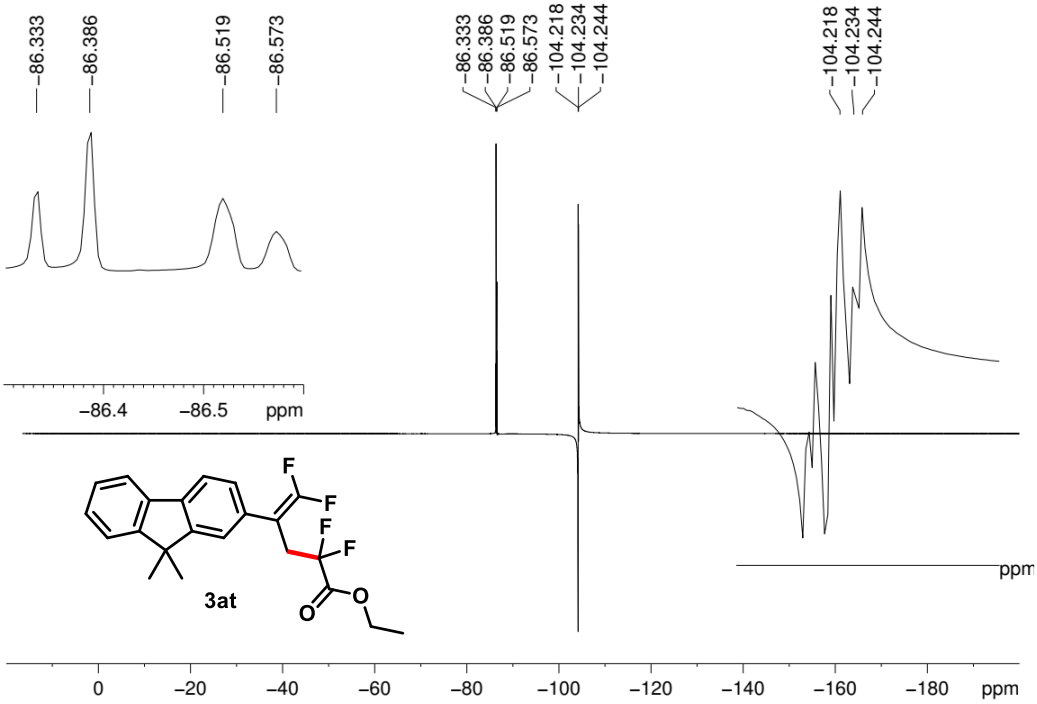
^{1}H NMR (600 MHz, $CDCl_3$)



^{13}C NMR (150 MHz, $CDCl_3$)



^{19}F NMR (565 MHz, $CDCl_3$)



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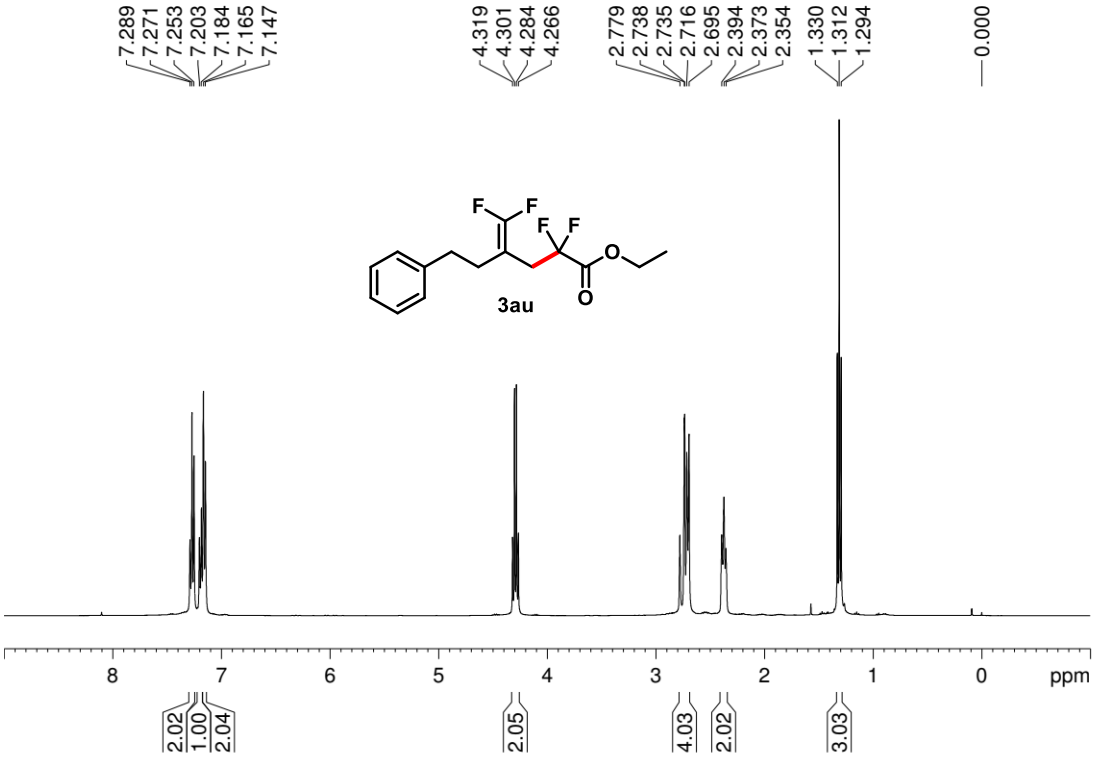
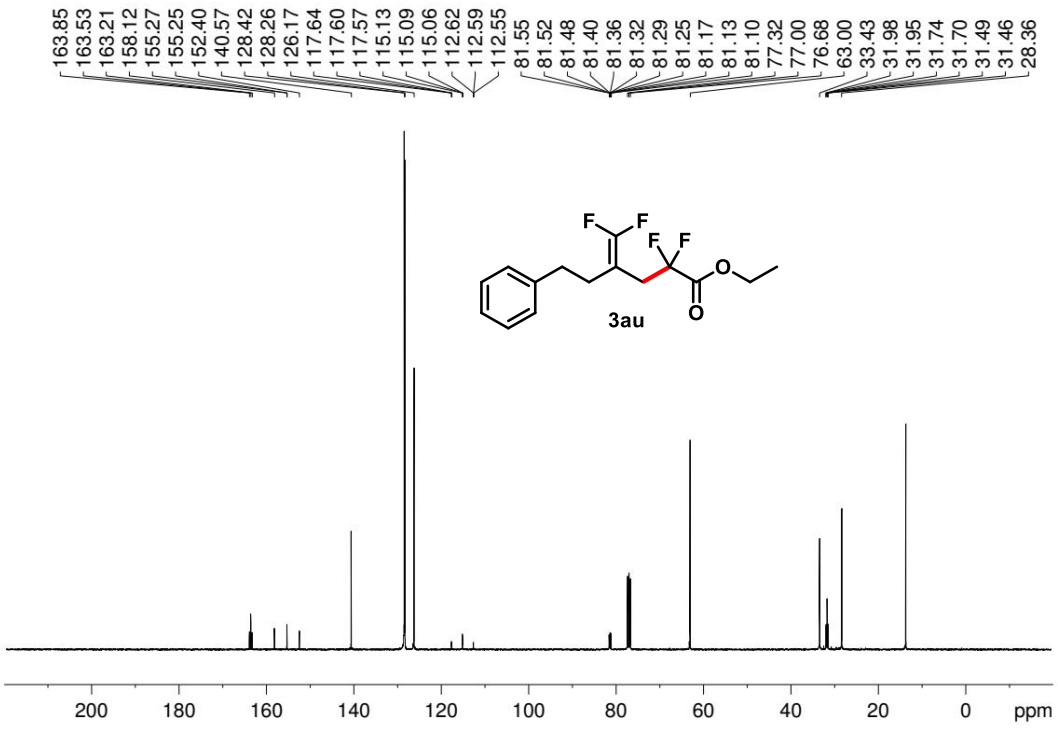
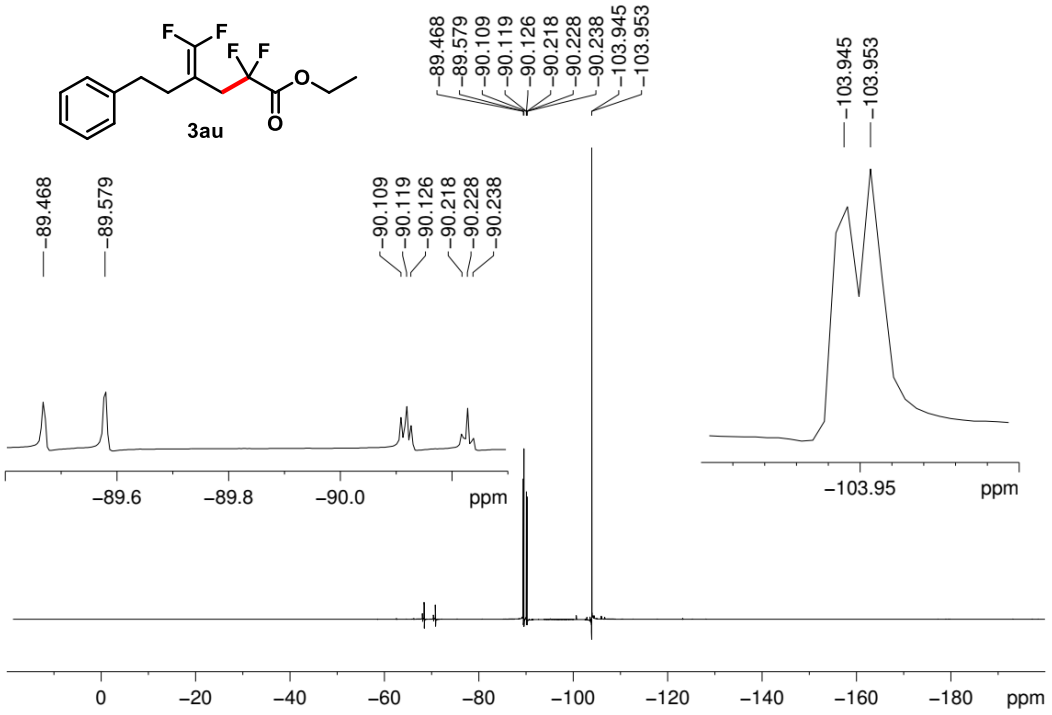


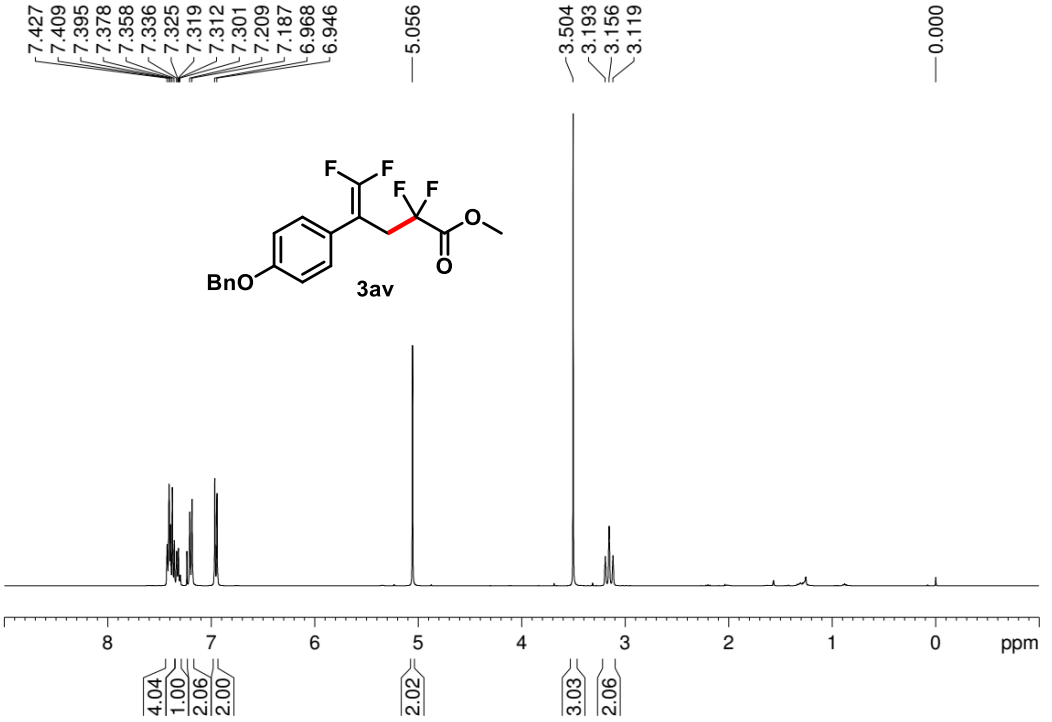
^{13}C NMR (100 MHz, $CDCl_3$)



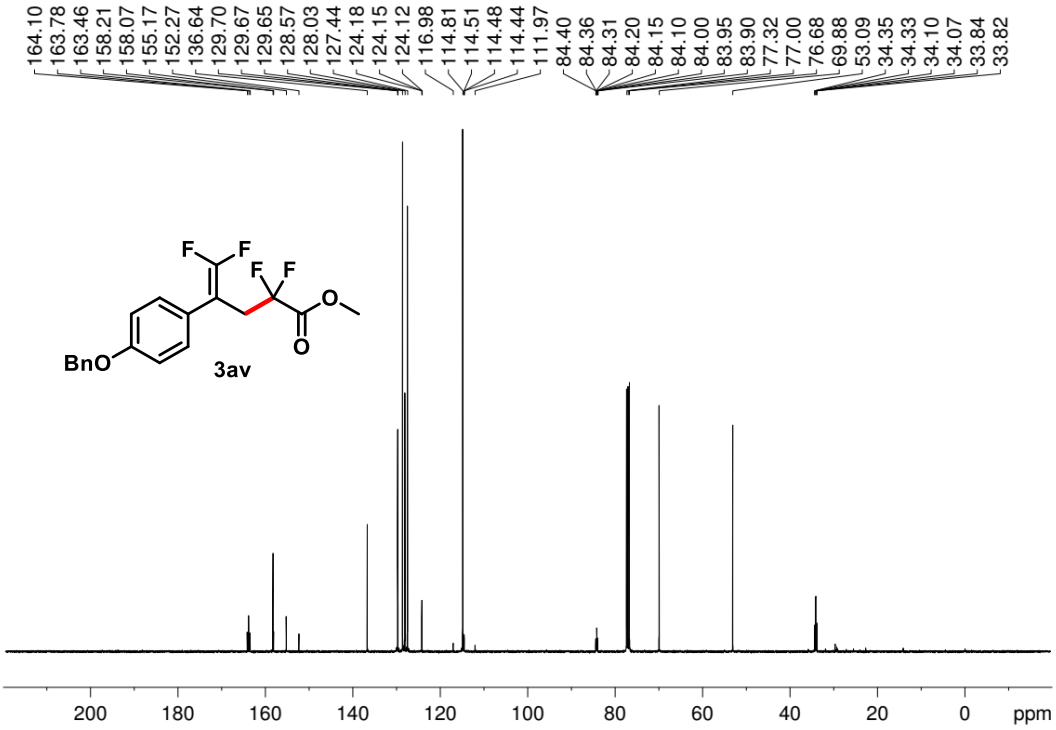
^{19}F NMR (376 MHz, CDCl$_3$)



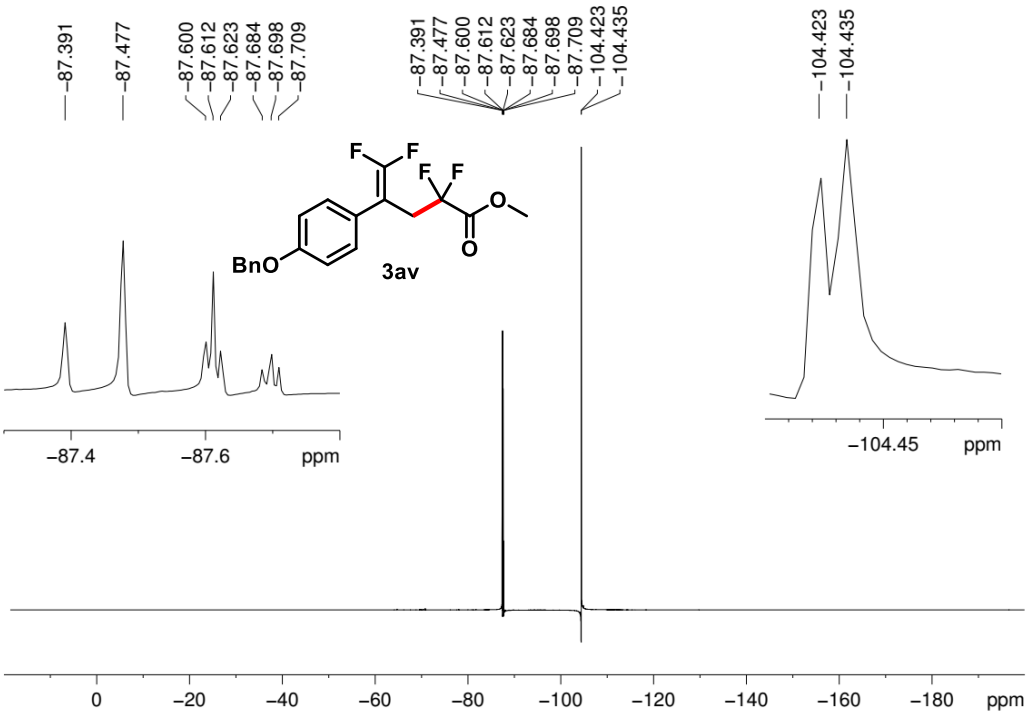
^{1}H NMR (400 MHz, CDCl$_3$)



^{13}C NMR (100 MHz, $CDCl_3$)



^{19}F NMR (376 MHz, $CDCl_3$)



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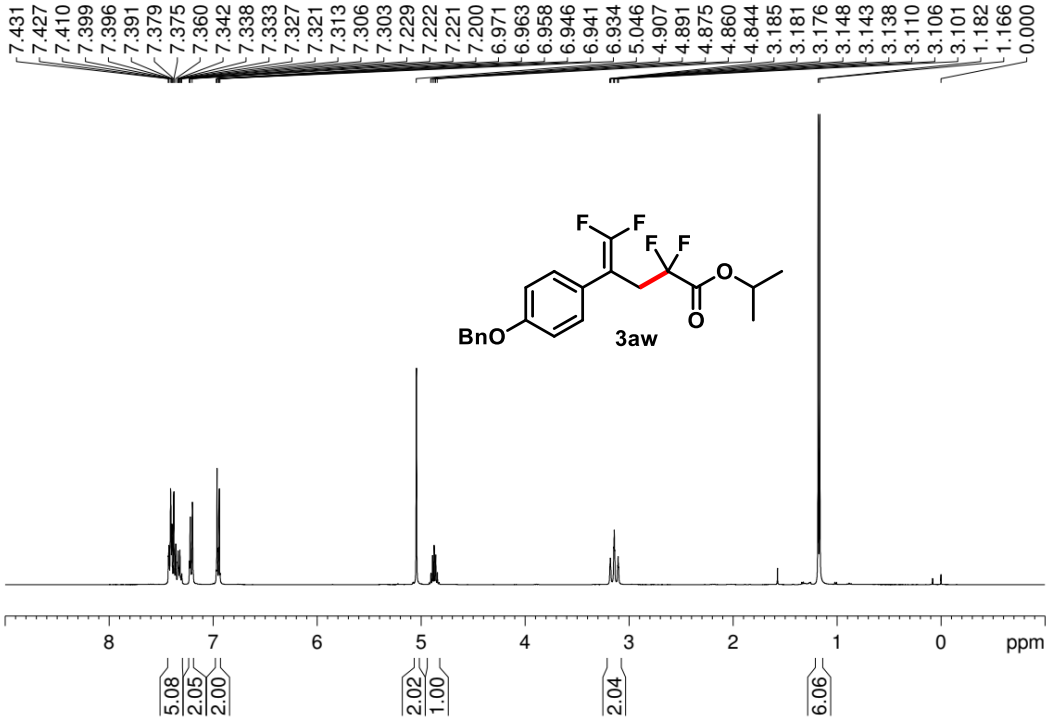
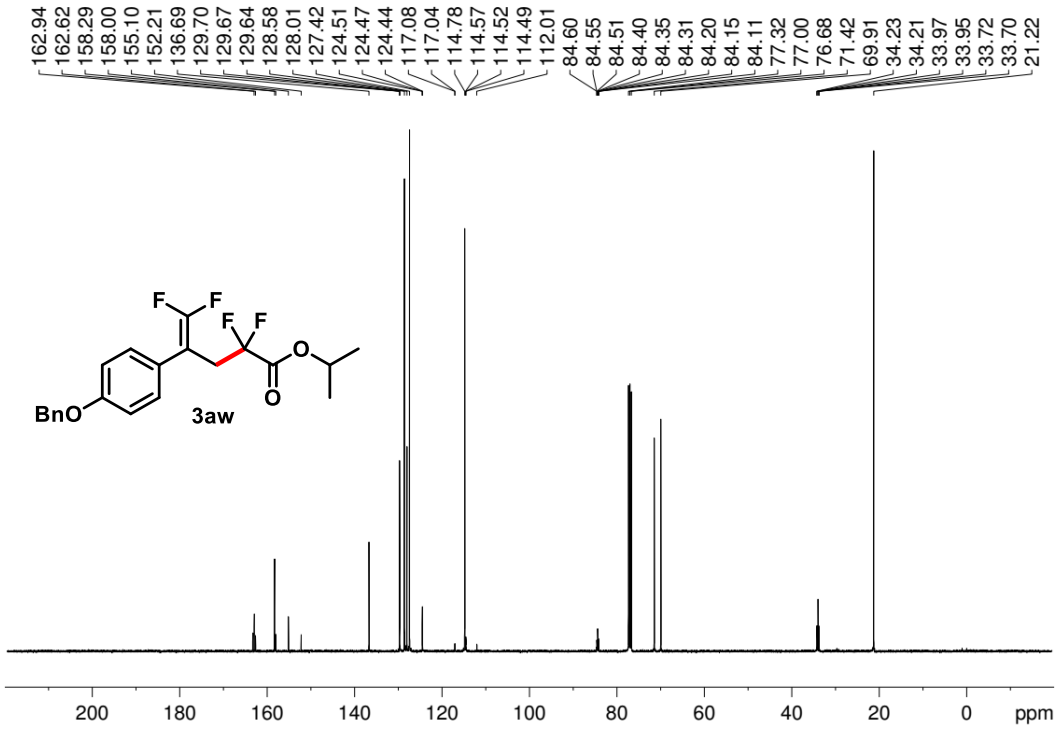
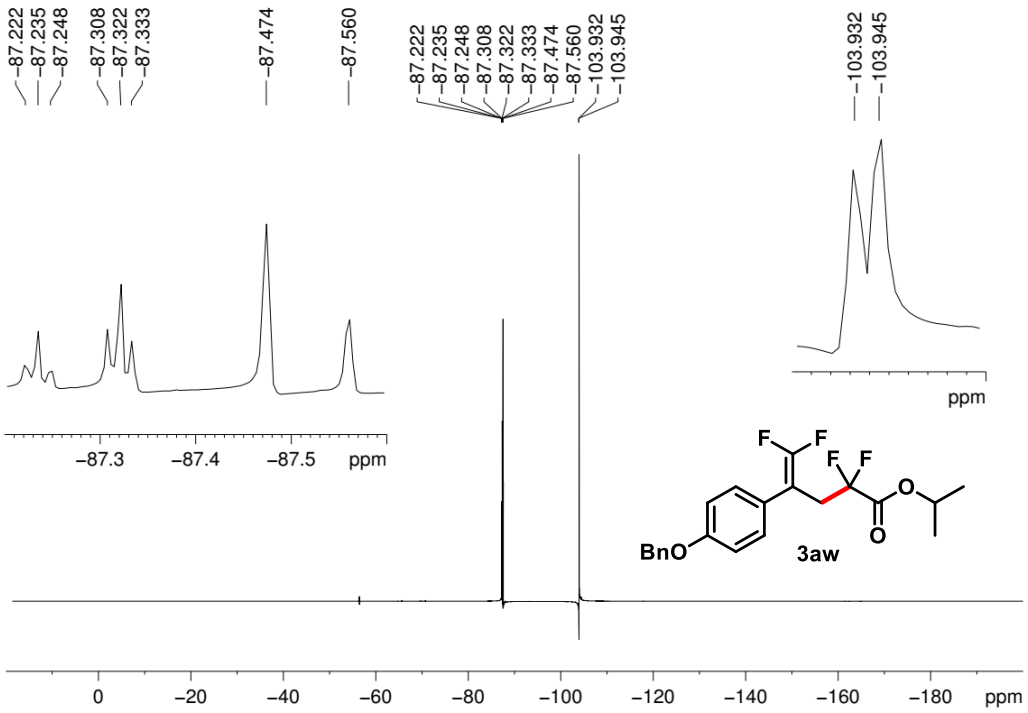


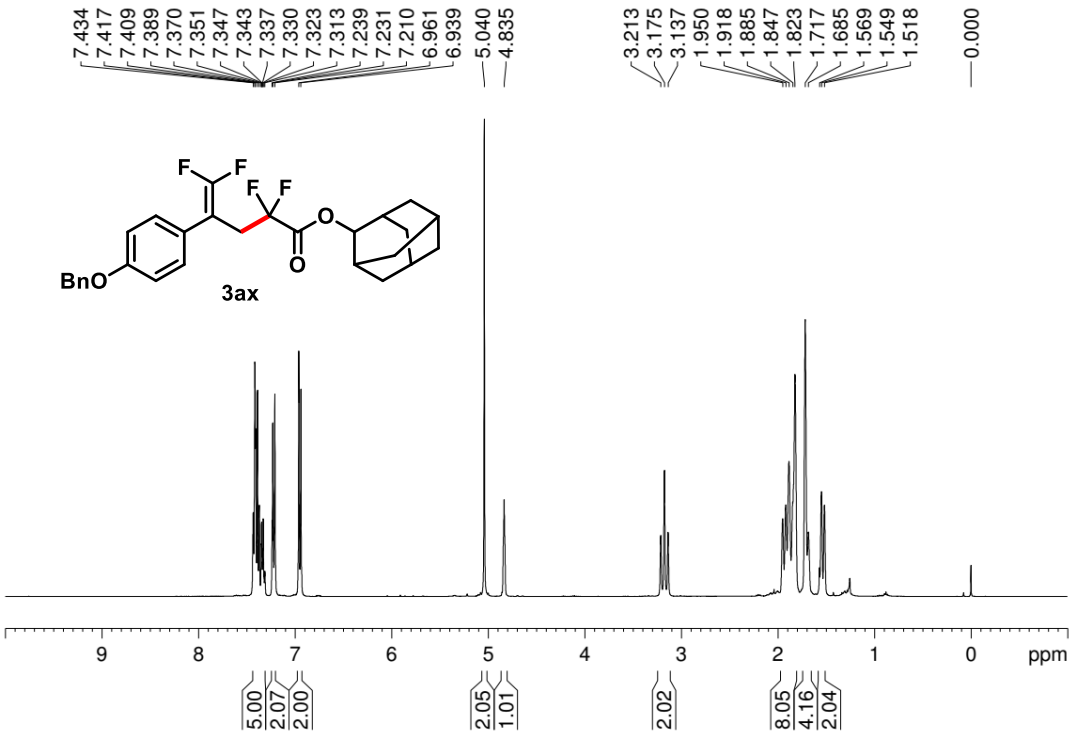
^{13}C NMR (100 MHz, $CDCl_3$)



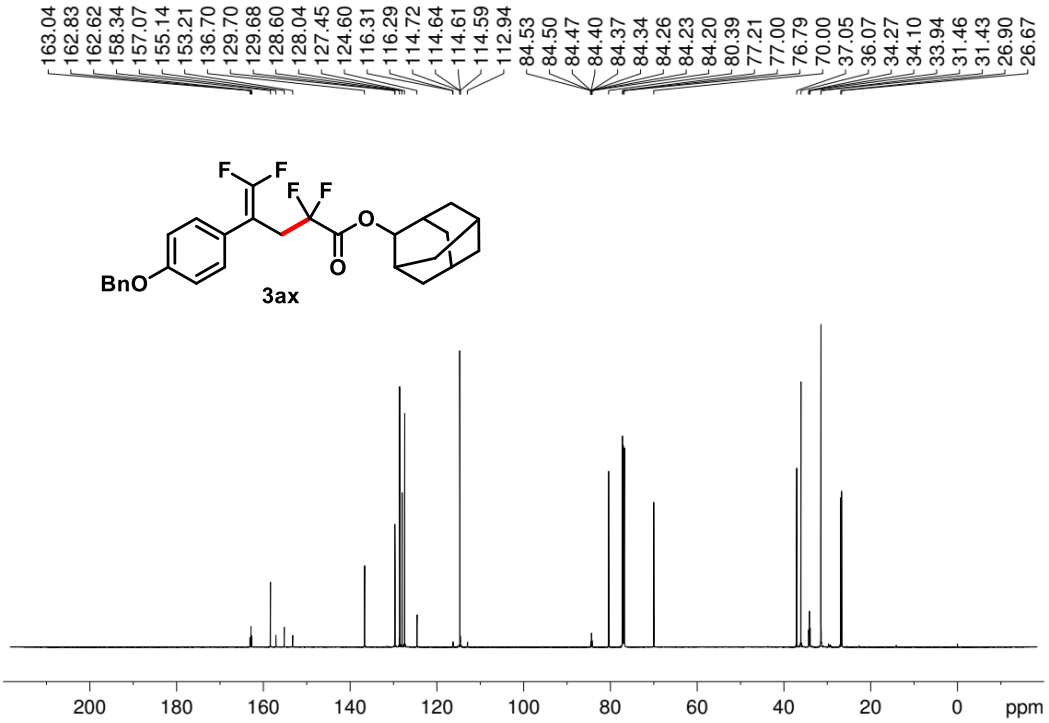
^{19}F NMR (376 MHz, $CDCl_3$)



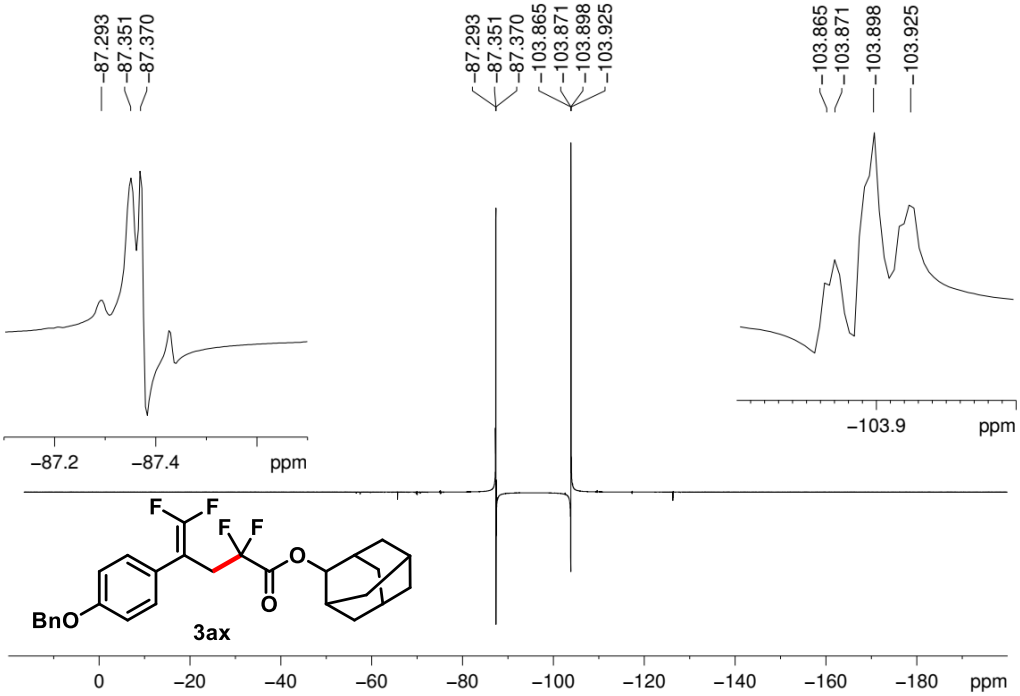
^{1}H NMR (400 MHz, $CDCl_3$)



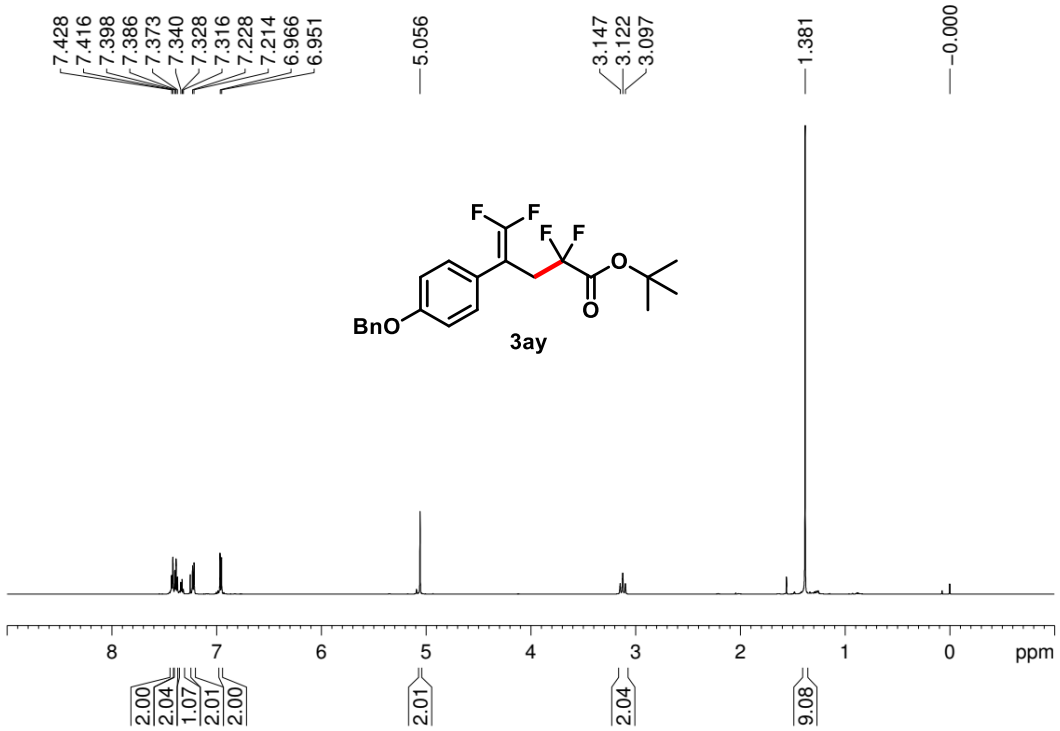
^{13}C NMR (150 MHz, $CDCl_3$)



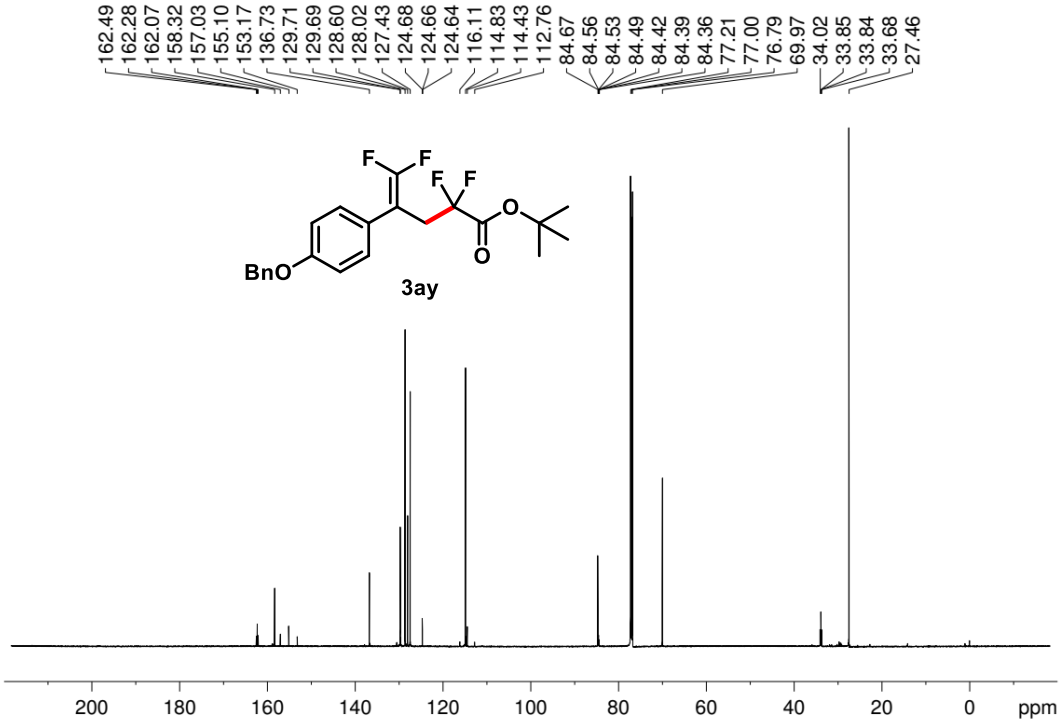
^{19}F NMR (565 MHz, $CDCl_3$)



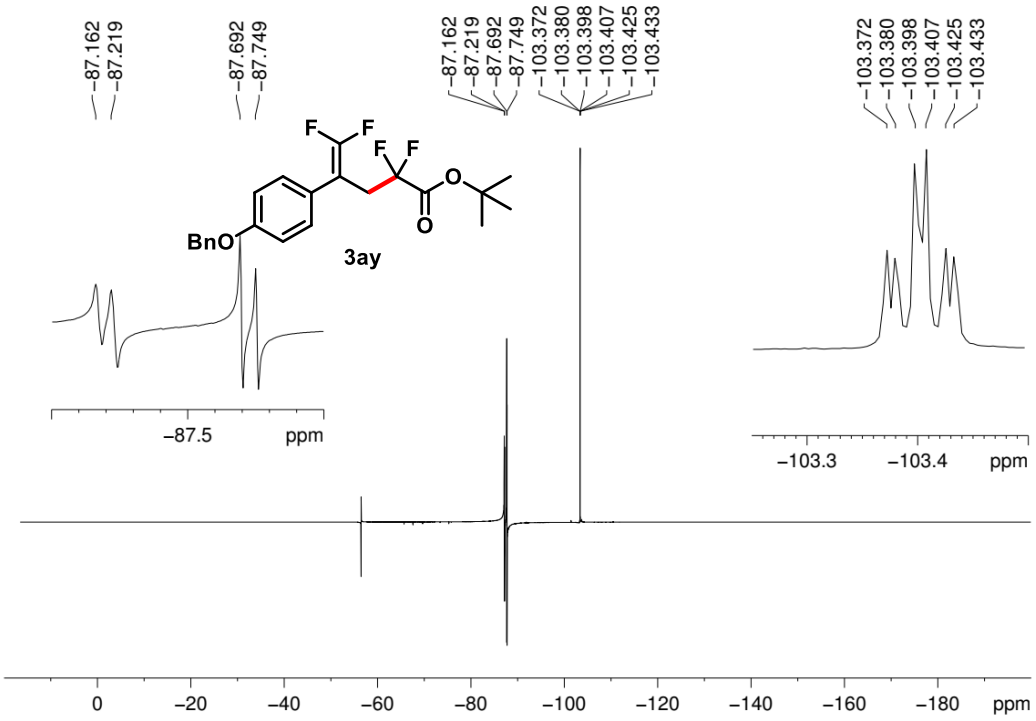
^{1}H NMR (600 MHz, $CDCl_3$)



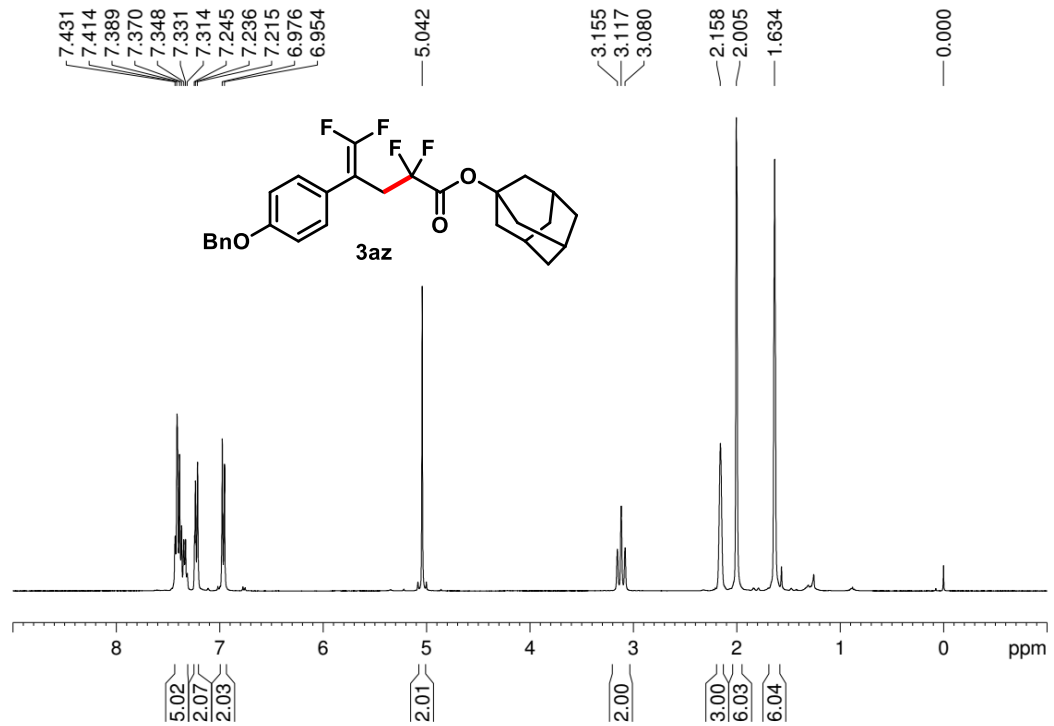
^{13}C NMR (150 MHz, $CDCl_3$)



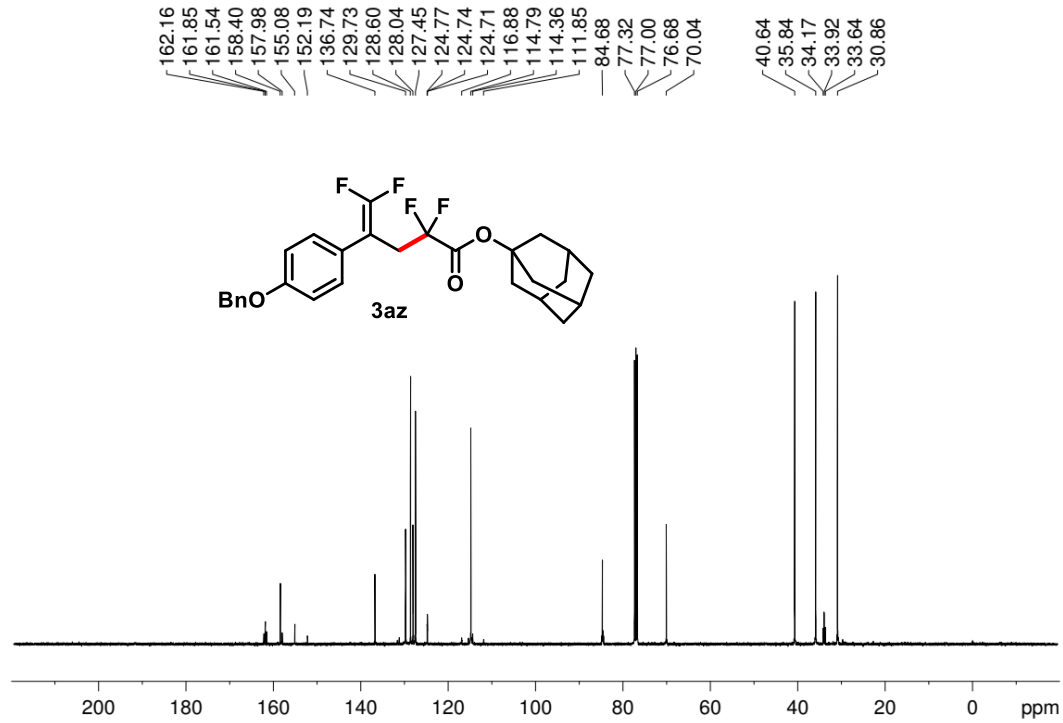
^{19}F NMR (565 MHz, $CDCl_3$)



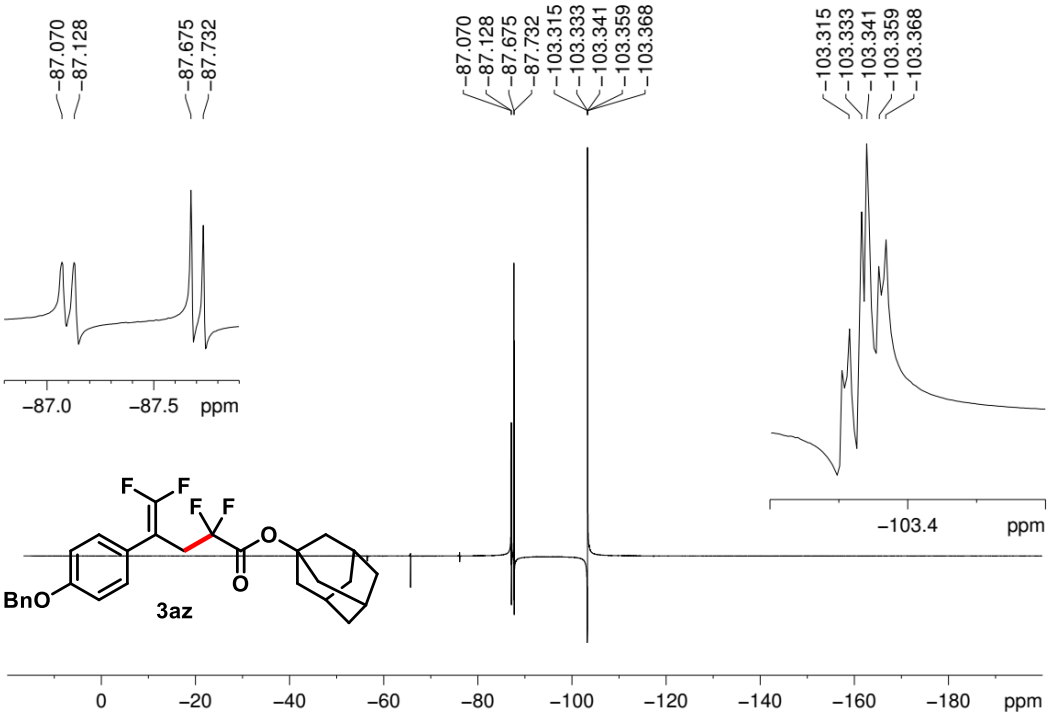
^{1}H NMR (400 MHz, $CDCl_3$)



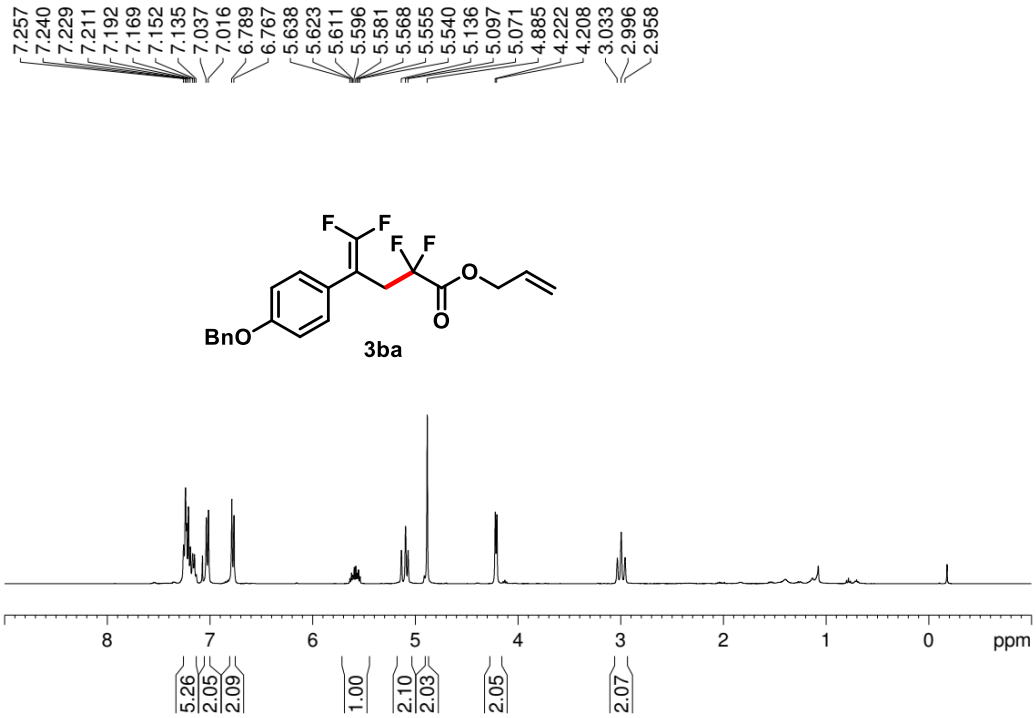
^{13}C NMR (100 MHz, $CDCl_3$)



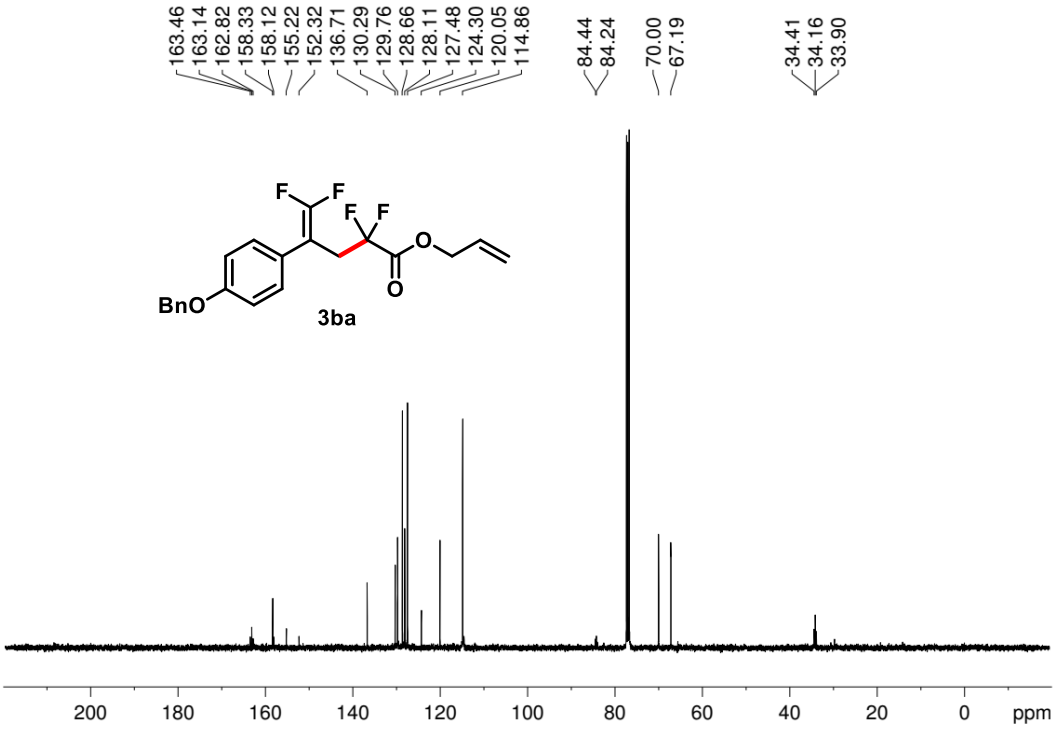
^{19}F NMR (565 MHz, $CDCl_3$)



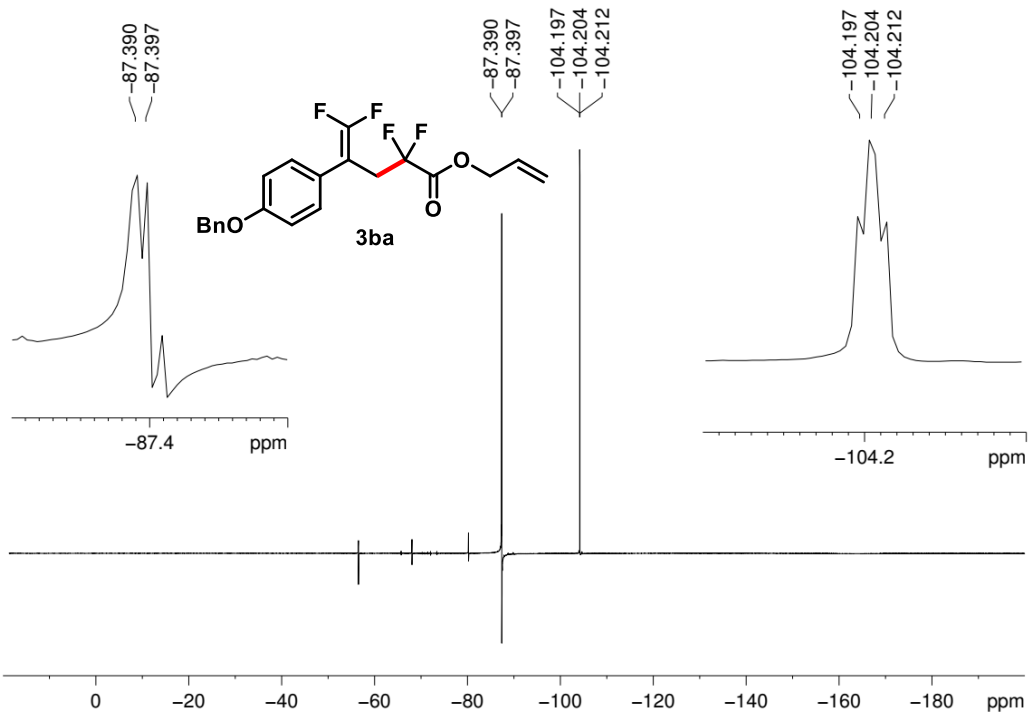
^{1}H NMR (400 MHz, $CDCl_3$)



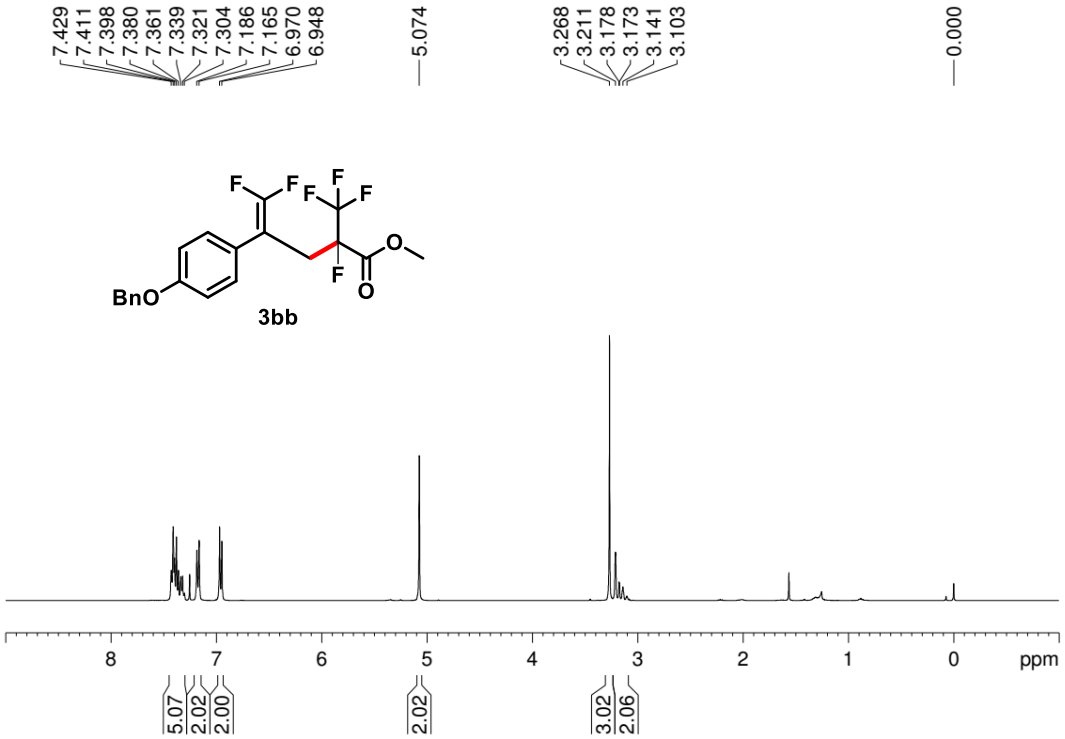
^{13}C NMR (100 MHz, $CDCl_3$)



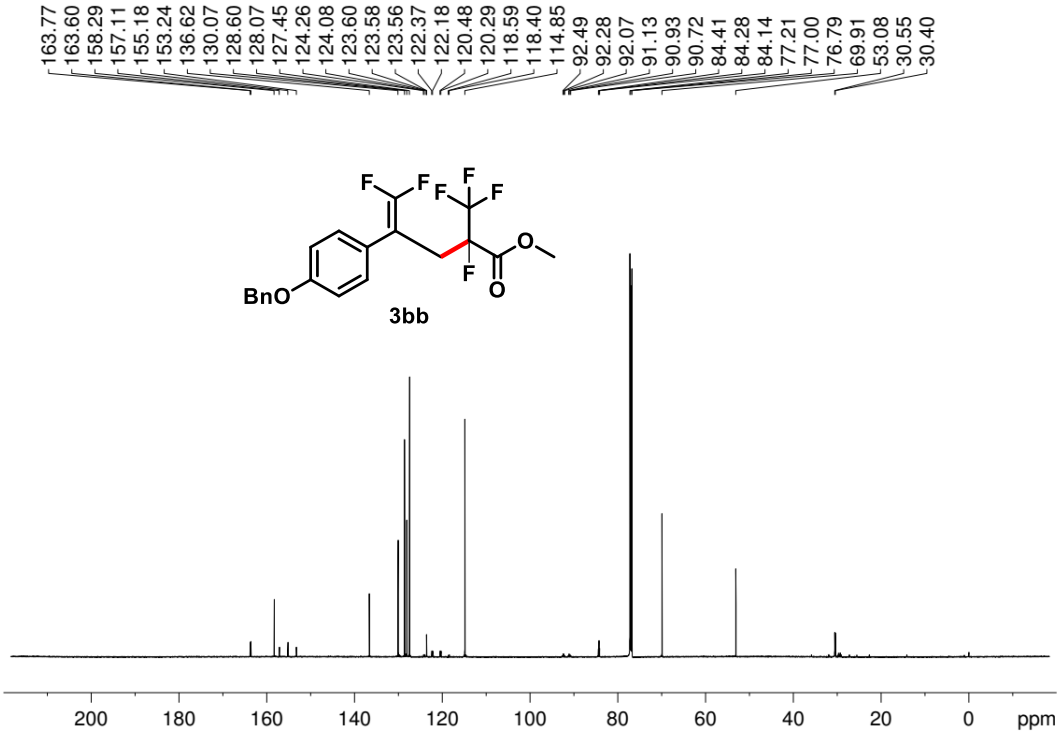
^{19}F NMR (376 MHz, $CDCl_3$)



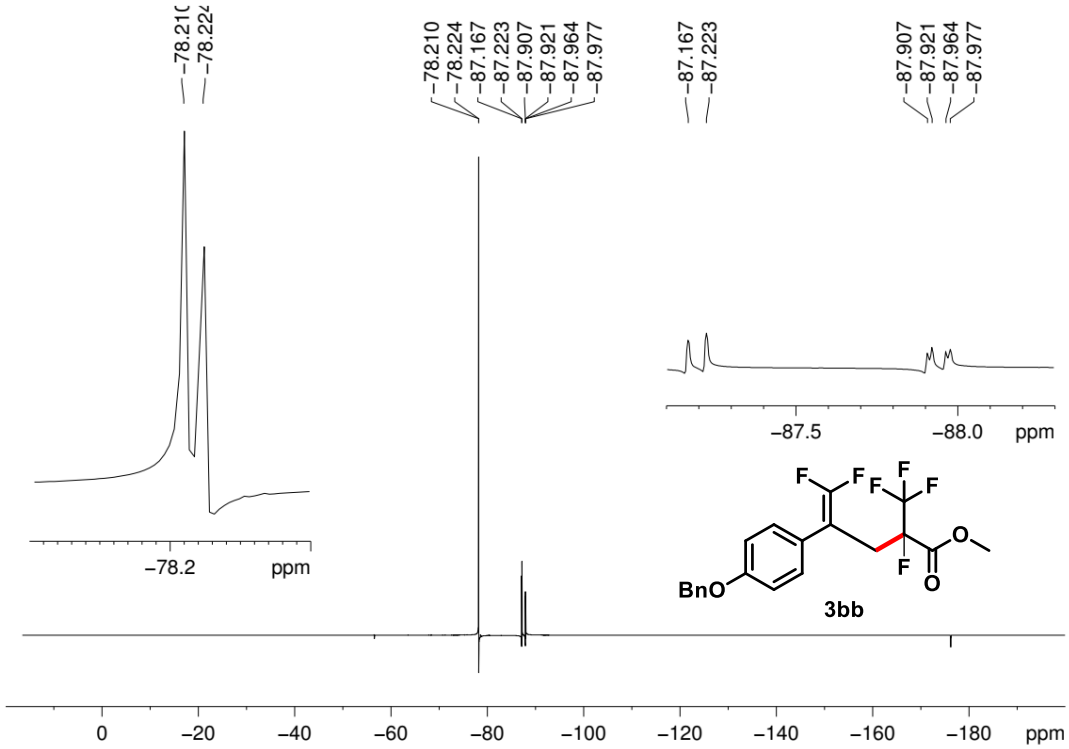
^{1}H NMR (400 MHz, $CDCl_3$)



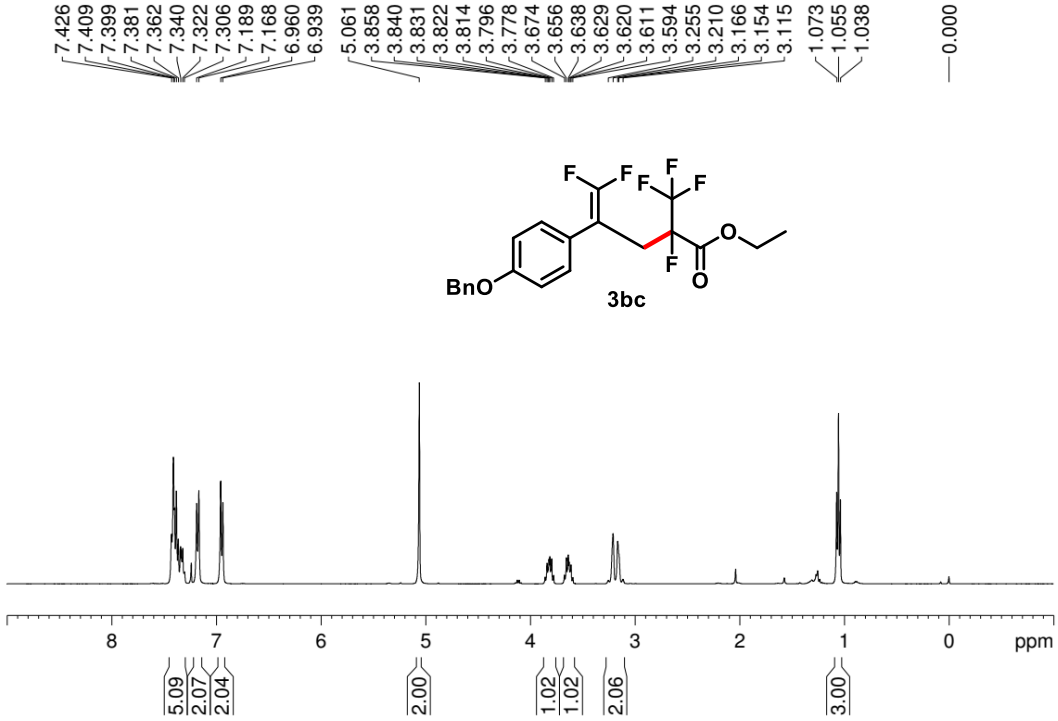
^{13}C NMR (150 MHz, $CDCl_3$)



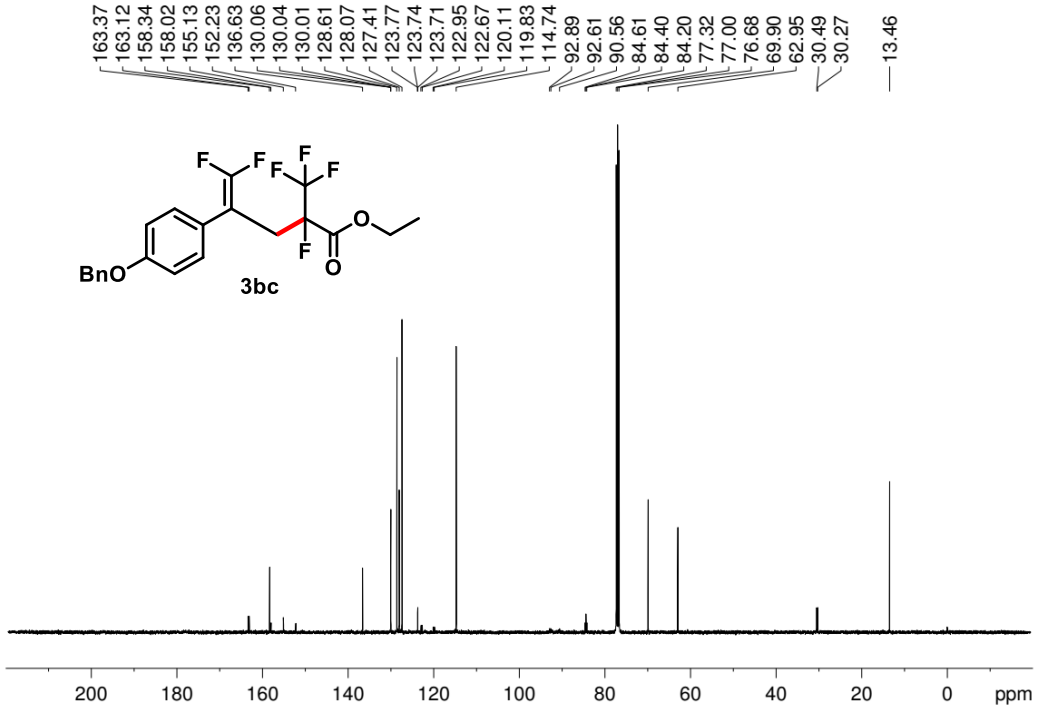
^{19}F NMR (565 MHz, $CDCl_3$)



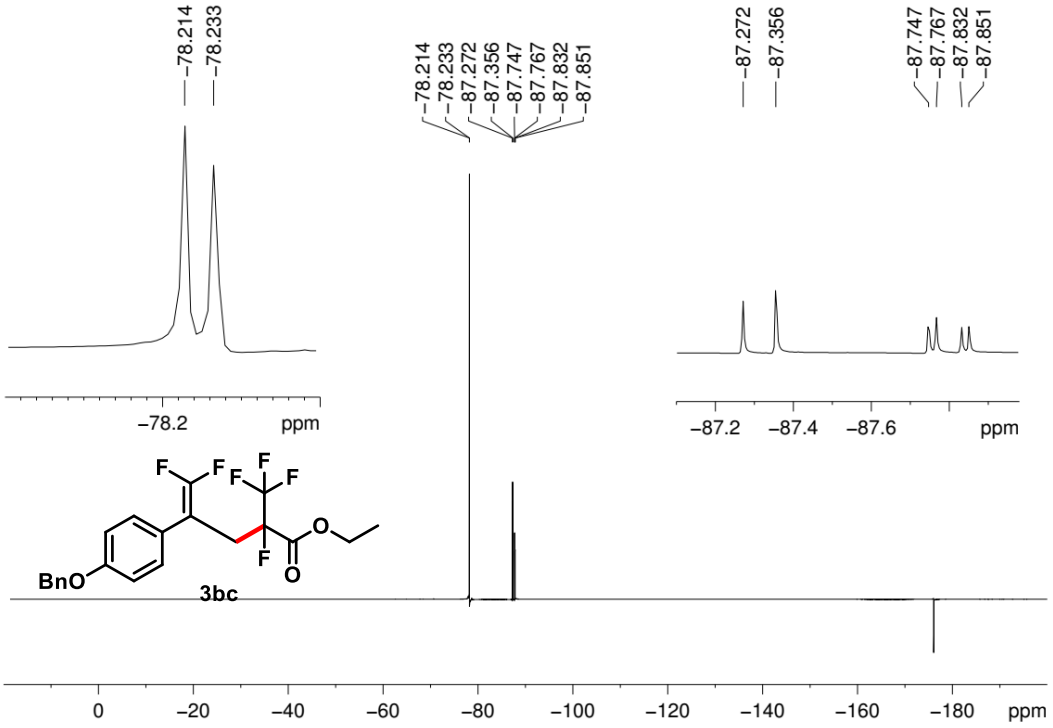
^{1}H NMR (400 MHz, $CDCl_3$)



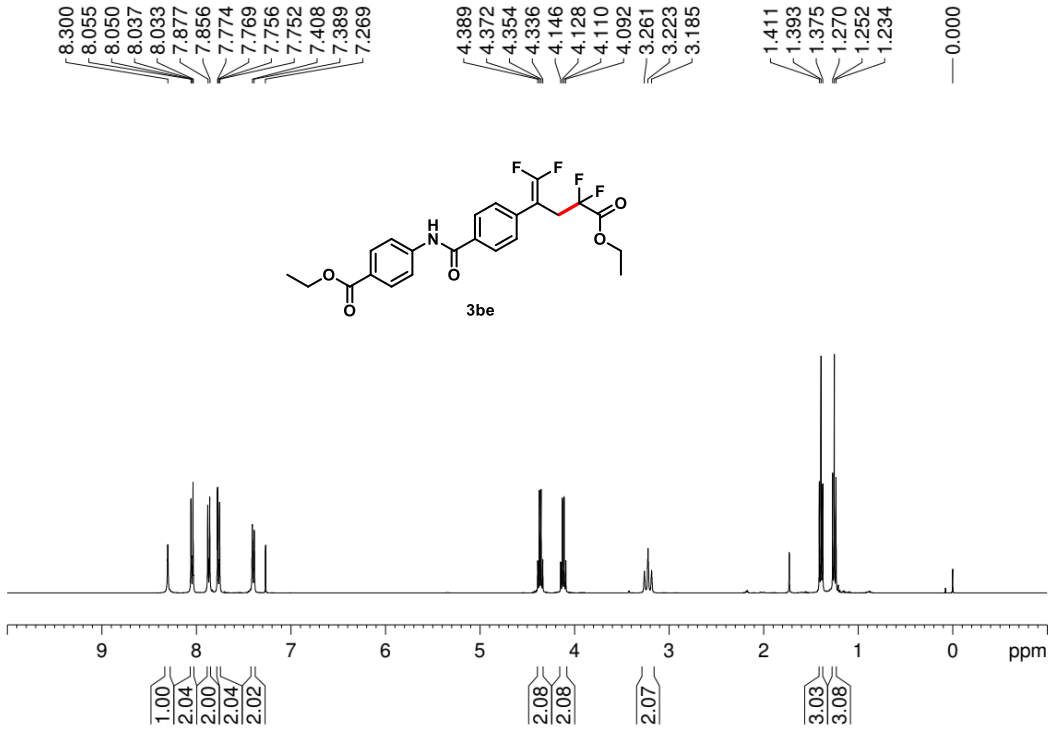
^{13}C NMR (100 MHz, $CDCl_3$)



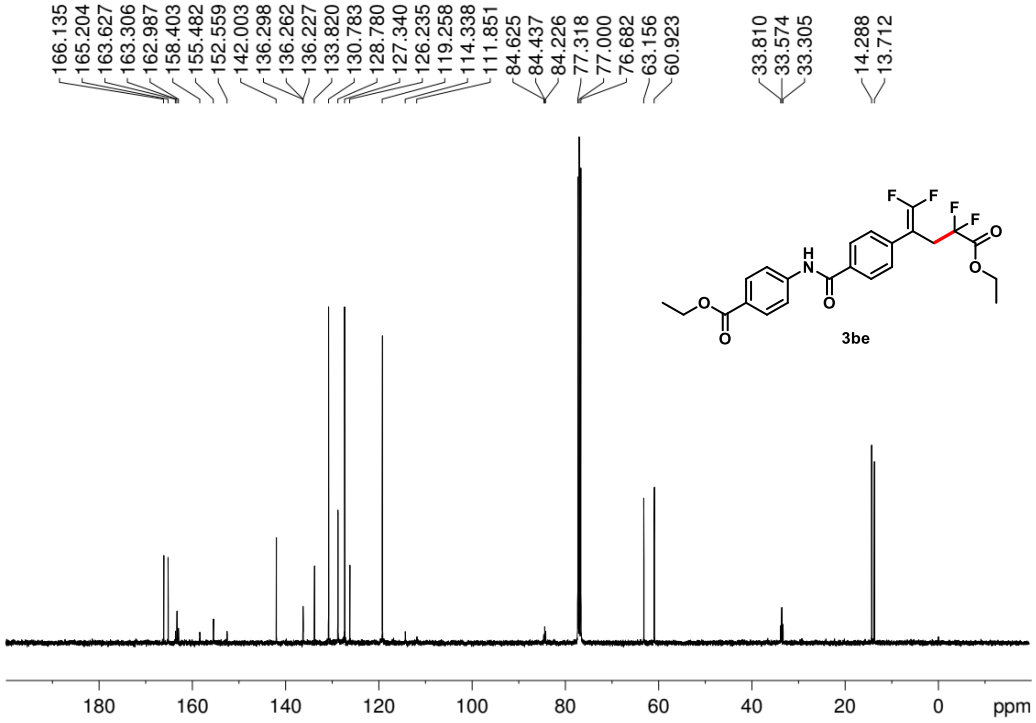
^{19}F NMR (376 MHz, $CDCl_3$)



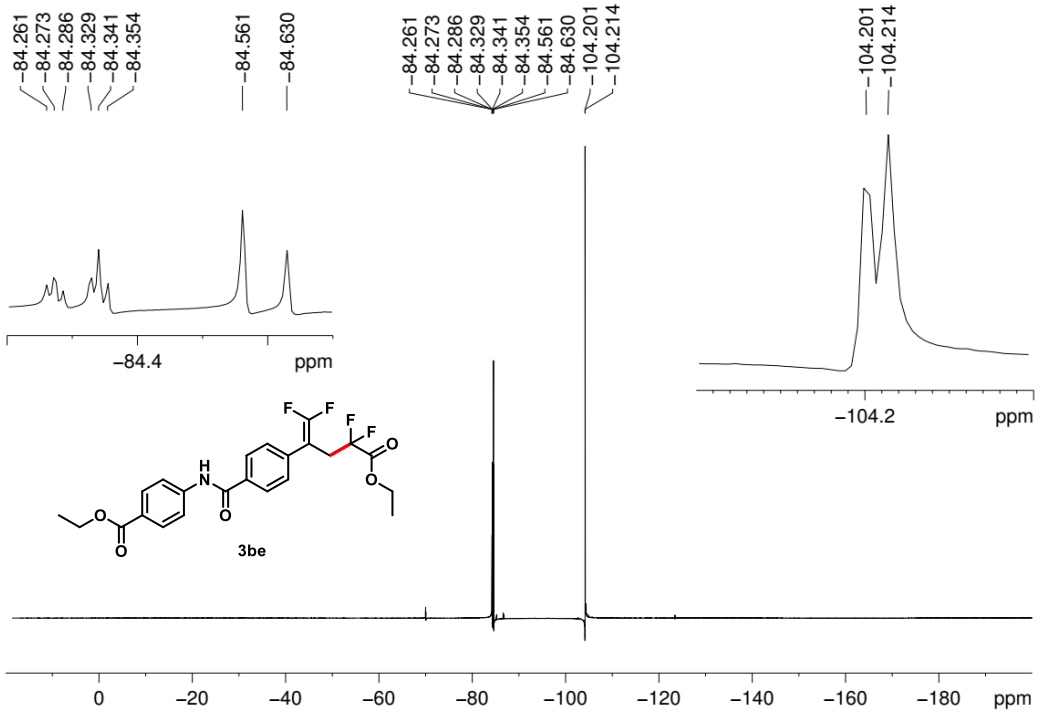
^{1}H NMR (400 MHz, $CDCl_3$)



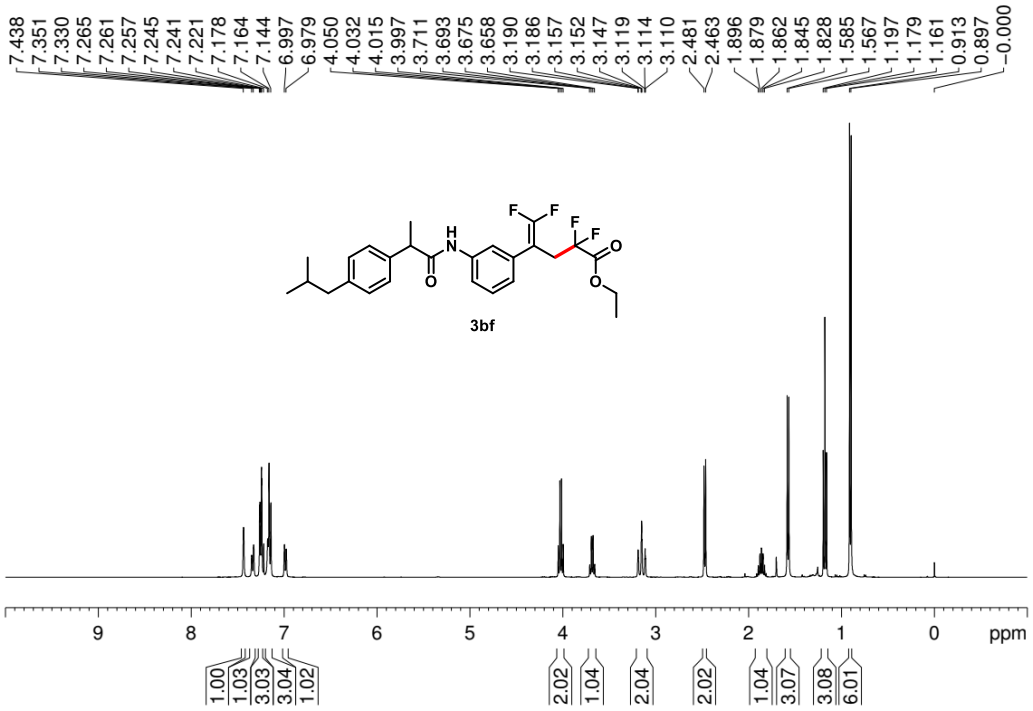
^{13}C NMR (100 MHz, $CDCl_3$)



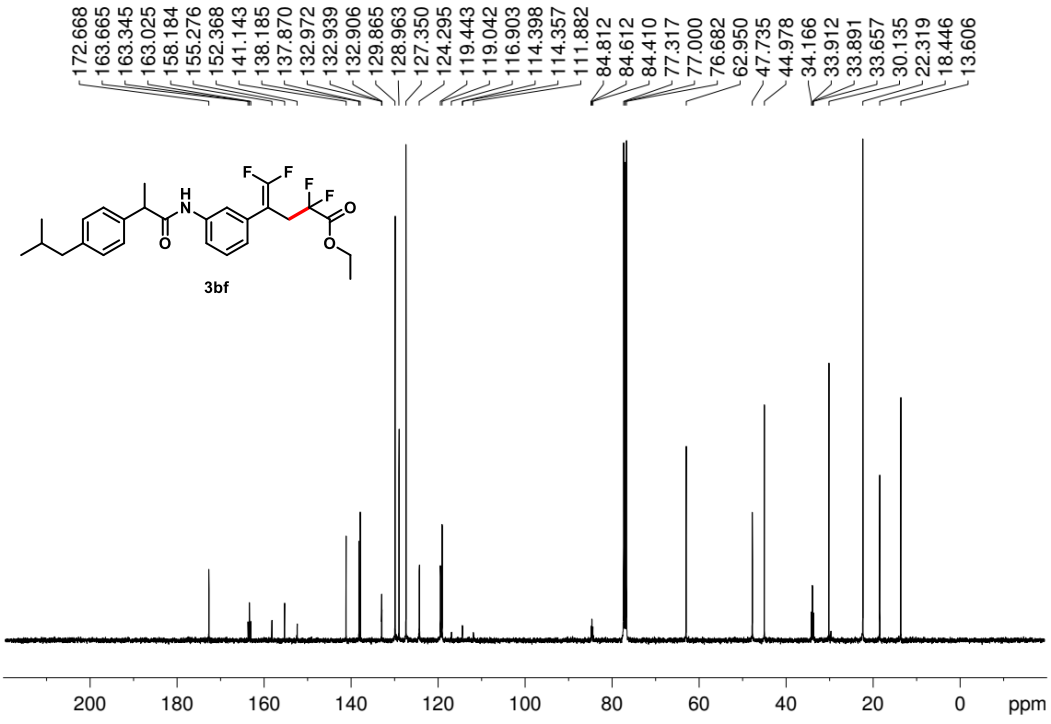
^{19}F NMR (376 MHz, $CDCl_3$)



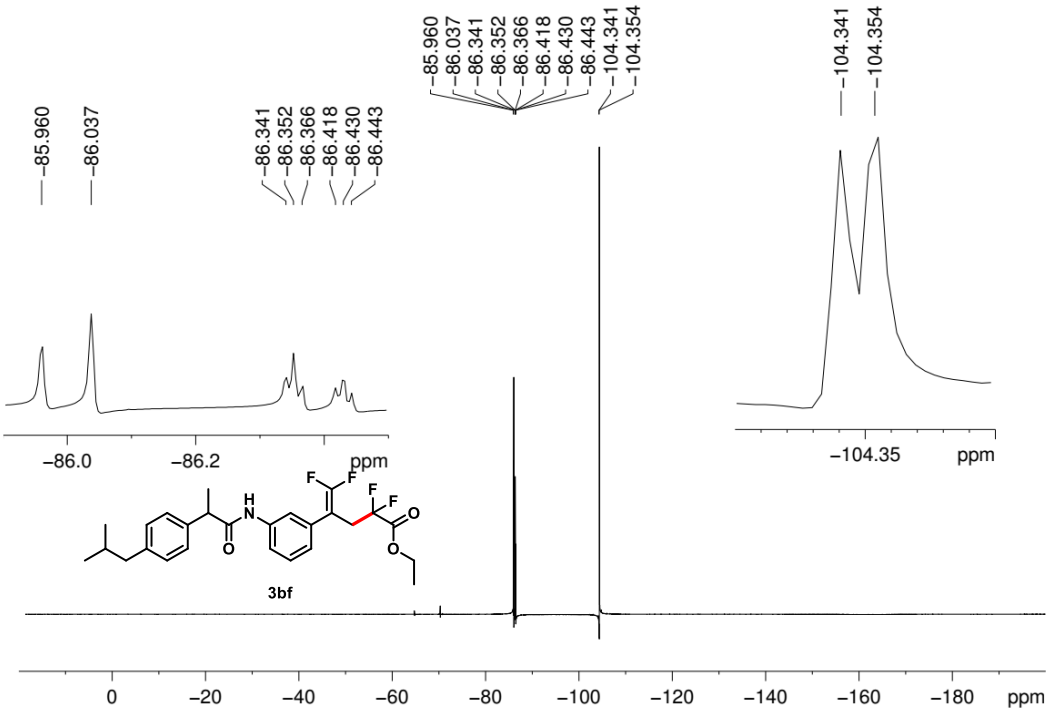
^{1}H NMR (400 MHz, $CDCl_3$)



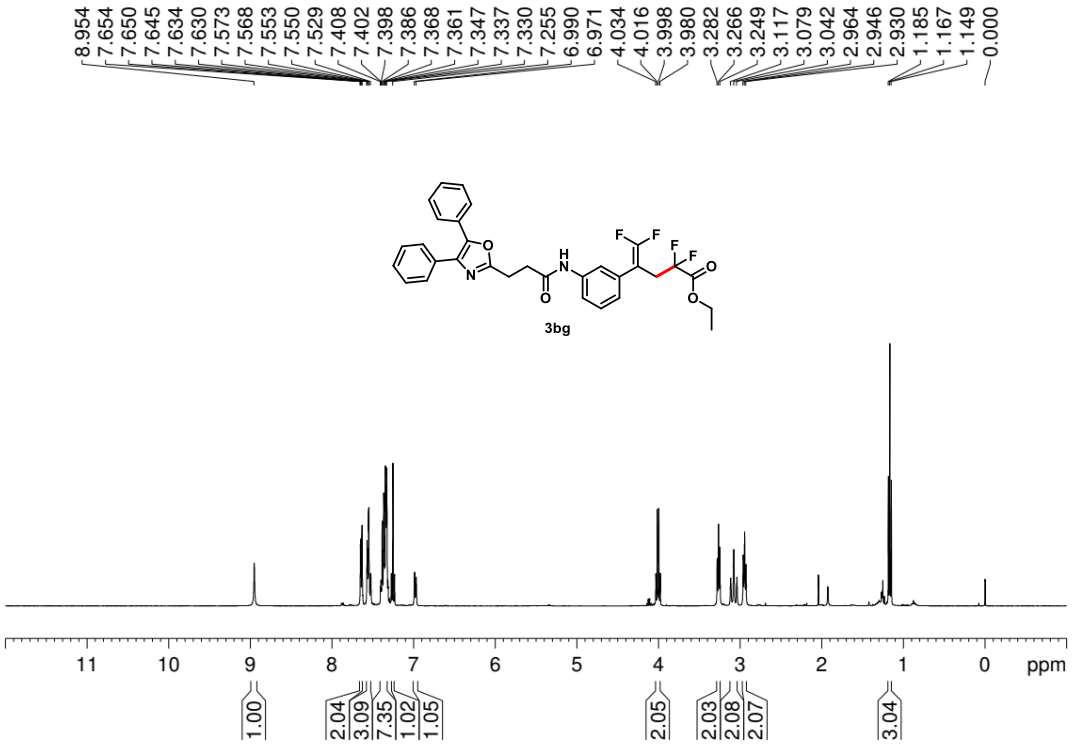
^{13}C NMR (100 MHz, $CDCl_3$)



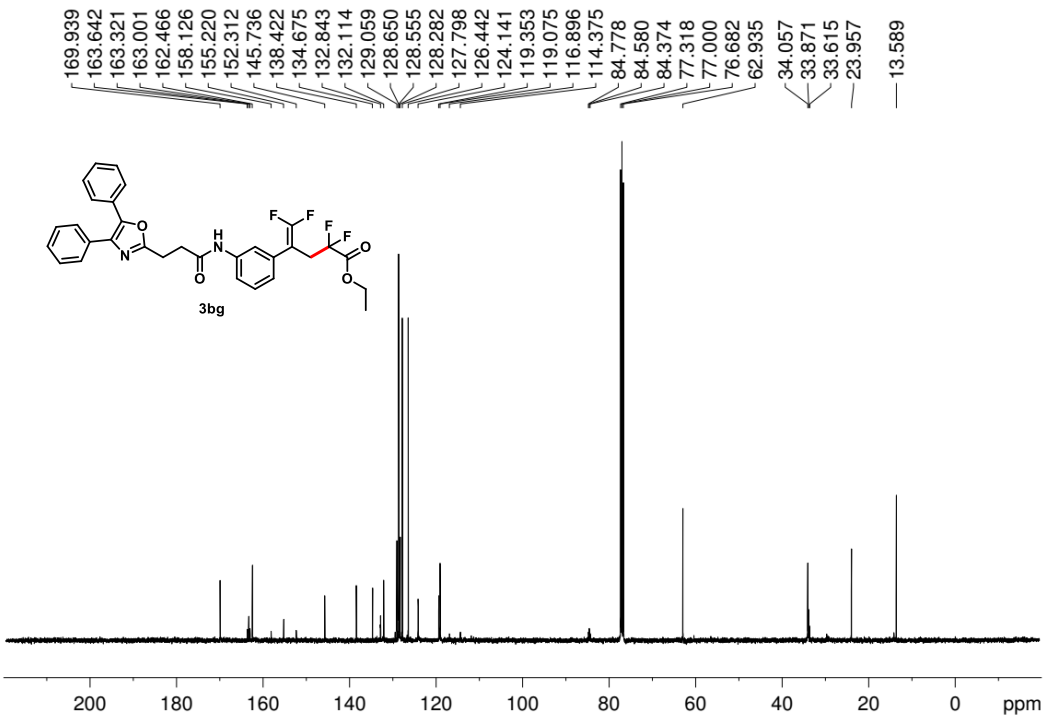
^{19}F NMR (376 MHz, $CDCl_3$)



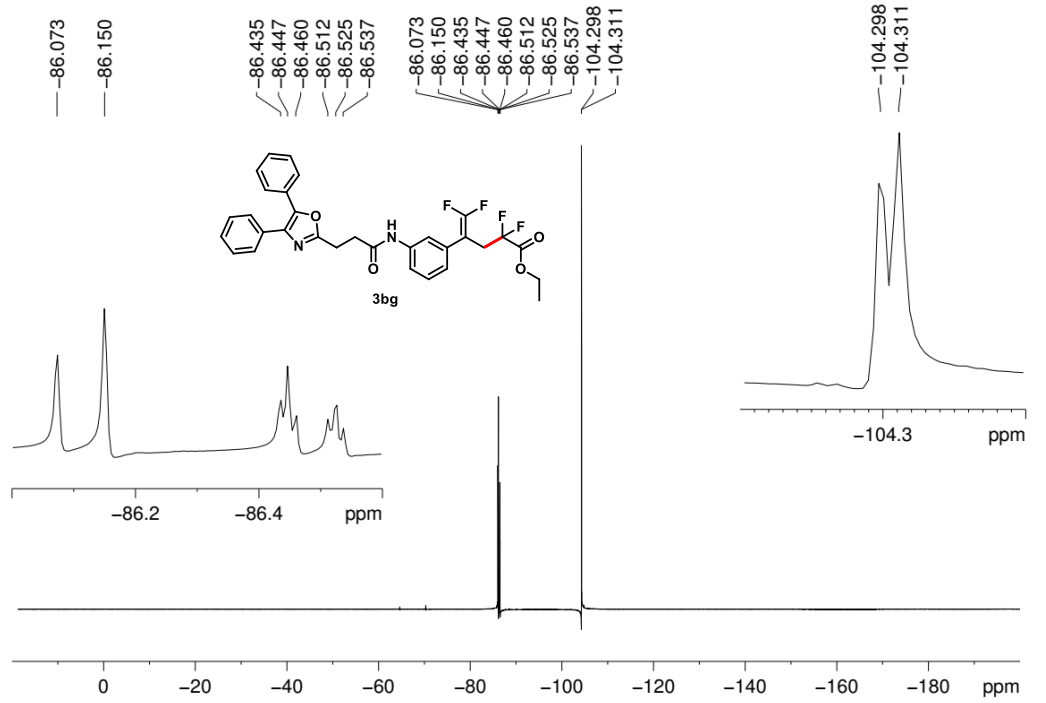
^{1}H NMR (400 MHz, $CDCl_3$)



^{13}C NMR (100 MHz, $CDCl_3$)



^{19}F NMR (376 MHz, $CDCl_3$)



8. Computational details

All the calculations were performed using the Gaussian 09 programs[4]. All of the structures were

fully optimized with the B3LYP[5,6] method and Ahlrichs' split-valence def2-SVP basis set[7]. Grimmes's DFT-D3 dispersion correction was used to describe the van der waals interaction[8]. Single-point corrections were calculated using B3LYP functional with def2tzvp basis set and Grimmes's DFT-D3 dispersion correction in Polarizable Continuum Model (PCM)[9]. The DMSO is used as a model solvent. The Vibrational frequency calculations were performed to ensure that a transition state has only one imaginary frequency and a local minimum has no imaginary frequency. Transition states connecting relevant minima were further examined by running intrinsic reaction coordinate (IRC) calculations.

Cartesian Coordinates

1a

C	1.71299	-2.02511	3.06299
C	0.35614	-1.92114	2.71160
C	-0.11216	-0.72816	2.13907
C	0.77206	0.33349	1.93464
C	2.12700	0.25243	2.29372
C	2.58044	-0.96073	2.85578
C	3.02568	1.41504	2.08485
C	2.64255	2.69583	2.20211
F	5.12883	2.21107	1.29532
C	4.46195	1.11793	1.69761
F	4.52605	0.21793	0.70149
F	5.15761	0.60076	2.73786
O	-0.40838	-3.01315	2.95192
C	-2.42719	-4.31066	3.00155
C	-1.70330	-5.35483	3.58833
C	-2.34110	-6.55680	3.91560
C	-3.70390	-6.72677	3.66086
C	-4.43176	-5.68511	3.07404
C	-3.79629	-4.48616	2.74715
C	-1.78386	-2.99355	2.63174
H	2.06386	-2.95990	3.50425
H	-1.15236	-0.61749	1.83412
H	0.39595	1.24173	1.45843
H	3.62465	-1.06887	3.14867
H	1.62991	2.95114	2.52106
H	3.32968	3.51626	1.99114
H	-0.63960	-5.22027	3.78616
H	-1.76530	-7.36549	4.37336
H	-4.19944	-7.66650	3.91742
H	-5.49861	-5.80802	2.87023
H	-4.37105	-3.67539	2.28801
H	-1.92184	-2.80338	1.54905

H	-2.28990	-2.16834	3.17076

Na^+

Na	0.14950	-0.77450	0.00000

NaF

F	1.06904	-0.38040	0.00000
Na	-0.82084	-0.38040	0.00000

A

C	0.17539	0.81816	-0.10983
O	-0.11818	1.44192	0.95413
O	-0.87645	0.46598	-1.05903
C	1.13212	-0.32511	-0.06937
C	-2.16921	0.48178	-0.51154
H	-2.87324	0.41714	-1.36454
H	-2.35741	1.43663	0.01779
C	-2.41190	-0.66944	0.46734
H	-3.45132	-0.66386	0.84658
H	-2.20983	-1.64006	-0.01479
H	-1.72001	-0.55560	1.31433
F	2.26253	-0.01176	0.61086
F	0.67418	-1.49413	0.55808
F	1.52394	-0.76195	-1.29863

TS1

C	0.19653	0.77636	-0.12680
O	0.15251	1.80406	0.52877
O	-0.84124	0.34360	-0.93143
C	1.35869	-0.02739	-0.33546
C	-2.13853	0.44696	-0.35706
H	-2.83146	0.70930	-1.17931
H	-2.14769	1.27858	0.36793
C	-2.51233	-0.86857	0.31743
H	-3.46321	-0.77092	0.87380
H	-2.62867	-1.66795	-0.43530
H	-1.66515	-1.13406	0.98208
F	2.47919	0.19042	0.33725
F	0.21977	-0.99101	1.32550
F	1.39213	-1.15056	-1.03792

B

C	0.21737	0.35845	0.18339
O	0.07175	1.33680	0.92706

O	-0.78418	0.08249	-0.82907
C	1.54634	0.21646	-0.56878
C	-2.09320	0.37269	-0.41799
H	-2.69186	0.52202	-1.33818
H	-2.10348	1.31792	0.15737
C	-2.70279	-0.74662	0.43018
H	-3.74728	-0.51329	0.71035
H	-2.68716	-1.69983	-0.12488
H	-2.09234	-0.88185	1.33346
F	2.63811	0.46185	0.17189
F	0.22907	-0.99227	0.97378
F	1.76026	-0.89701	-1.29116

10

C	2.42223	2.87006	-0.21619
C	1.76774	4.12671	-0.55275
O	2.43295	4.76952	-1.52847
C	1.91527	6.05975	-1.90216
F	3.36257	2.33087	-0.95480
F	1.84607	2.02366	0.59809
O	0.78103	4.53544	0.02217
C	2.80348	6.61224	-2.99609
H	0.87007	5.94346	-2.23403
H	1.89838	6.70928	-1.01092
H	2.43954	7.60222	-3.31170
H	3.84018	6.71852	-2.64170
H	2.80479	5.94576	-3.87214

TS2

C	-1.77591	1.93212	-0.35823
C	-2.20913	0.60225	-0.20954
C	-1.25439	-0.42680	-0.15728
C	0.10225	-0.12266	-0.26454
C	0.55314	1.20253	-0.42889
C	-0.42435	2.22552	-0.46100
C	1.98962	1.49070	-0.55452
C	2.91104	0.59515	-1.01111
C	3.55045	-0.52977	0.99562
C	3.53791	-1.89728	0.45921
O	4.72679	-2.22098	-0.06711
C	4.79782	-3.48336	-0.75848
F	4.69243	0.05851	1.29190
F	2.58441	-0.18944	1.82013
O	2.53414	-2.57785	0.39993

C	6.20059	-3.62814	-1.30716
F	3.82678	2.88225	0.02646
C	2.48679	2.83169	-0.05570
F	2.00162	3.11867	1.16449
F	2.10819	3.84139	-0.87447
O	-3.54639	0.41842	-0.11392
C	-5.57986	-0.83767	0.04374
C	-6.28380	0.21789	-0.55094
C	-7.68181	0.21963	-0.55444
C	-8.39107	-0.83376	0.03028
C	-7.69347	-1.88955	0.62583
C	-6.29638	-1.88786	0.63565
C	-4.07066	-0.89055	0.01700
H	-2.52915	2.72152	-0.39122
H	-1.54896	-1.46579	-0.01255
H	0.81796	-0.94125	-0.17185
H	-0.12248	3.26513	-0.58675
H	2.57986	-0.31956	-1.50409
H	3.95794	0.87599	-1.12273
H	4.54067	-4.29053	-0.05308
H	4.03383	-3.49570	-1.55375
H	6.29714	-4.58432	-1.84418
H	6.43332	-2.81042	-2.00631
H	6.94194	-3.60844	-0.49389
H	-5.72802	1.04183	-1.00105
H	-8.22019	1.05107	-1.01697
H	-9.48403	-0.83026	0.02671
H	-8.23893	-2.71395	1.09231
H	-5.75687	-2.71182	1.11286
H	-3.69062	-1.36775	0.93988
H	-3.73335	-1.51543	-0.83420

4

C	-1.87115	1.80591	0.02421
C	-2.45237	0.53269	-0.15647
C	-1.63411	-0.53976	-0.55624
C	-0.27727	-0.33544	-0.77491
C	0.33823	0.93979	-0.60974
C	-0.52335	2.00682	-0.19351
C	1.73052	1.13021	-0.85491
C	2.63270	0.03424	-1.33990
C	3.23744	-0.80573	-0.21413
C	4.06613	-1.98672	-0.76741
O	5.19933	-2.16879	-0.10447

C	6.02551	-3.27867	-0.52303
F	3.97793	-0.03155	0.61249
F	2.24405	-1.36478	0.54569
O	3.67444	-2.65404	-1.69223
C	7.25544	-3.29273	0.35744
F	3.68496	2.46586	-0.82475
C	2.36583	2.46217	-0.56283
F	2.21869	2.83201	0.72799
F	1.82465	3.46240	-1.30299
O	-3.77877	0.44530	0.08225
C	-5.92422	-0.61462	0.18551
C	-6.55831	0.61959	-0.01128
C	-7.93326	0.74807	0.20479
C	-8.68996	-0.35443	0.61351
C	-8.06225	-1.58815	0.81187
C	-6.68638	-1.71484	0.60329
C	-4.45053	-0.79131	-0.09186
H	-2.51806	2.62634	0.34088
H	-2.04354	-1.54062	-0.69096
H	0.32792	-1.19763	-1.05151
H	-0.11883	3.00649	-0.04557
H	2.10910	-0.66088	-2.00889
H	3.47662	0.45048	-1.90797
H	5.43550	-4.20566	-0.43736
H	6.27236	-3.14829	-1.58928
H	7.91291	-4.12732	0.06892
H	7.81920	-2.35297	0.25621
H	6.97732	-3.41676	1.41500
H	-5.96477	1.48019	-0.32399
H	-8.41627	1.71693	0.05321
H	-9.76495	-0.25178	0.78202
H	-8.64396	-2.45378	1.13893
H	-6.19962	-2.68045	0.77135
H	-4.02445	-1.55792	0.58183
H	-4.30389	-1.15058	-1.12999

9. References

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