

Supporting Information

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General Methods.

All reactions were carried out under a nitrogen atmosphere in glass vials fitted with rubber septa, unless otherwise stated. Analytical grade solvents and commercially available reagents were purchased from commercial sources and used directly without further purification unless otherwise stated. HPLC grade acetonitrile and methanol were obtained from Sigma-Aldrich. Light irradiation was performed with the Blue LEDs (910 mW, $\lambda_{\text{max}} = 447.5$ nm), which were purchased from Luxeon Star LEDs Quadica Developments Inc (Canada). UV LEDs were purchased from Lixada LED lamp (5 W, $\lambda_{\text{max}} = 365\text{nm}$). Thin-layer chromatography (TLC) was carried out on Merck 60 F₂₅₄ precoated, glass Silica flash plates which were visualized with ultraviolet light. Flash chromatography was performed using ZEOPrep 60 ECO 40-63 μm Silica flash. ¹H-NMR and ¹³C-NMR spectra were recorded at room temperature using a Varian I400 (¹H-NMR at 400MHz and ¹³C-NMR at 100MHz), Varian VXR400 (¹H-NMR at 400MHz and ¹³C-NMR at 100MHz), Varian I500 (¹H-NMR at 500MHz and ¹³C-NMR at 125MHz), Varian I600 (¹H-NMR at 600MHz). ¹⁹F-NMR spectra were recorded at room temperature using a VarianI400 or VXR400 (¹⁹F-NMR at 376 MHz). Chemical shifts are reported in ppm with reference to solvent signals [¹H-NMR: CDCl₃ (7.26 ppm); ¹³C-NMR: CDCl₃ (77.16 ppm)]. Signal patterns are indicated as s, singlet; d, doublet; t, triplet; q, quartet; and m, multiplet. High Resolution Mass (HRMS) analysis was obtained using Electron Impact Ionization (EI) and reported as m/z (relative intensity) for the molecular ion [M], or with Electrospray Ionization (ESI) and reporting the molecular ion [M+H]⁺ or a suitable fragment ion.

Synthesis and Characterization of New Substrates.

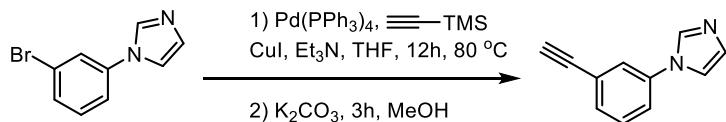
Copper complex bpyCu(CF₃)₃ was synthesized according to the reported procedure.¹⁻² The following compounds were synthesized according to literature procedures: *N*-(4-ethynylphenyl)acetamide (**1r**),³ 5-ethynylbenzofuran (**1u**),⁴ 2,6-dichloro-4-ethynylpyridine (**1w**),⁵ methyl (*S*)-2-((*tert*-butoxycarbonyl)amino)-3-(4-ethynylphenyl)propanoate (**S1**),⁶ (8*R*,9*S*,13*S*,14*S*)-3-ethynyl-13-methyl-6,7,8,9,11,12,13,14,15,16-decahydro-17*H*-cyclopenta-[a]phenanthren-17-one (**S2**).⁷

Synthesis of terminal alkynes:

General Procedure A: To an oven-dried screw cap reaction tube equipped with a Teflon®-coated stir bar was added aromatic bromide or trifluoromethanesulfonate (4.00 mmol, 1.0 equiv), Pd(PPh₃)₄ (231 mg, 0.20 mmol, 5 mol%), CuI (76 mg, 0.40 mmol, 10 mol%) and THF (2.0 mL). Under nitrogen atmosphere, triethylamine (26.0 mL) and trimethylsilylacetylene (5.20 mmol; 740 µL, 1.3 equiv) were added to the reaction mixture before sealing and stirring at 80 °C for 12 h. The reaction was monitored by TLC and, upon completion, quenched with saturated aqueous NH₄Cl solution and extracted with EtOAc (50 mL x 3). After drying the organic layer over anhydrous MgSO₄ and removing the solvent under reduced pressure, the residue was purified by silica flash chromatography (purification details for each substrate disclosed below). To remove the TMS group and reveal the terminal alkyne, the purified material was dissolved in 15.0 mL of MeOH before adding anhydrous K₂CO₃ (1.10 g, 8.00 mmol, 2.0 equiv) and stirred under N₂ atmosphere at room temperature for 3 h. Upon completion the reaction was filtered through Celite® and the filtrate was evaporated under reduced pressure and purified by silica chromatography (details for each substrate is disclosed individually).

General Procedure B: General procedure A was followed to make the TMS-acetylene. To remove the TMS group and reveal the terminal alkyne, the purified material was dissolved in 10.0 ml THF before treating with TBAF (4.20 mmol, 1.05 equiv, 1 M in THF) at room temperature for 18 h. Upon completion, the reaction was quenched with saturated aqueous NH₄Cl solution and extracted with EtOAc (3 × 100 mL). The organic phases were combined and dried over anhydrous Na₂SO₄, filtered and concentrated under reduced pressure. The residue was then purified by silica chromatography (purification details for each substrate disclosed below).

1-(3-Ethynylphenyl)-1*H*-imidazole (1v**)**



1-(3-Bromophenyl)-1*H*-imidazole (892 mg, 4.00 mmol) was subjected to General Procedure A. Silica flash chromatography (0-30% EtOAc in hexanes) provided **1v** (367 mg, 55% yield after two steps) as a colorless liquid.

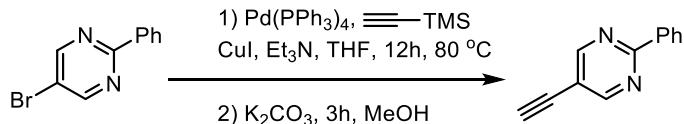
¹H NMR (400 MHz, CDCl₃) δ 7.93 (d, *J* = 2.4 Hz, 1H), 7.82 (s, 1H), 7.76 – 7.66 (m, 2H), 7.46 – 7.37 (m, 2H), 6.50 – 6.46 (m, 1H), 3.13 (s, 1H).

¹³C NMR (126 MHz, CDCl₃) δ 141.4, 140.2, 130.0, 129.5, 126.8, 123.5, 122.6, 119.6, 108.0, 82.8, 78.3.

HRMS (EI): Calcd. for C₁₁H₈N₂ [M], 168.0687. Found: 168.0681.

TLC: R_f = 0.15, 20% EtOAc in hexanes.

1-(3-Ethynylphenyl)-1H-imidazole (1x)



5-Bromo-2-phenylpyrimidine (940 mg, 4.00 mmol) was subjected to General Procedure A. Silica flash chromatography (0-8% EtOAc in hexanes) provided **1x** (503 mg, 70% yield after two steps) as a white solid.

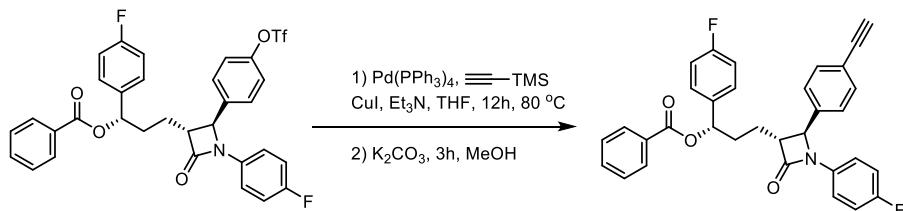
¹H NMR (400 MHz, CDCl₃) δ 8.87 (s, 2H), 8.47 – 8.42 (m, 2H), 7.52 – 7.48 (m, 3H), 3.41 (s, 1H).

¹³C NMR (126 MHz, CDCl₃) δ 163.2, 159.8, 136.9, 131.4, 128.8, 128.6, 116.1, 84.2, 77.9.

HRMS (EI): Calcd. for C₁₂H₈N₂ [M], 180.0687. Found: 180.0685.

TLC: R_f = 0.30, 10% EtOAc in hexanes.

(S)-3-((2*S*,3*R*)-2-(4-ethynylphenyl)-1-(4-fluorophenyl)-4-oxoazetidin-3-yl)-1-(4-fluoro-phenyl)propyl benzoate (S3)



(S)-1-(4-fluorophenyl)-3-((3*R*,4*S*)-1-(4-fluorophenyl)-2-oxo-4-(4-((trifluoromethyl)sulfonyl)-oxy)phenyl)azetidin-3-yl)propyl benzoate (2.58 g, 4.00 mmol) was subjected to General Procedure A. Silica flash chromatography (0-20% EtOAc in hexanes) provided **S3** (1.42 g, 68% yield after two steps) as a white solid.

¹H NMR (400 MHz, CDCl₃) δ 8.04 (d, *J* = 7.1 Hz, 2H), 7.61 – 7.53 (m, 1H), 7.52 – 7.40 (m, 4H), 7.37 (dd, *J* = 8.6, 5.4 Hz, 2H), 7.27 (d, *J* = 5.7 Hz, 2H), 7.19 (dd, *J* = 9.0, 4.7 Hz, 2H), 7.08 – 7.00 (m, 2H), 6.97 – 6.88 (m, 2H), 5.97 (t, *J* = 6.9 Hz, 1H), 4.59 (d, *J* = 2.2 Hz, 1H), 3.16 – 3.05 (m, 2H), 2.25 – 2.11 (m, 2H), 2.02 – 1.88 (m, 2H).

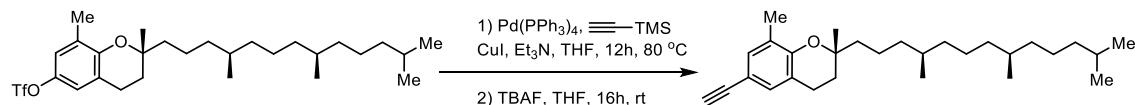
¹³C NMR (126 MHz, CDCl₃) δ 166.7, 165.8, 162.6 (d, *J* = 246.9 Hz), 159.2 (d, *J* = 243.8 Hz), 138.3, 135.8 (d, *J* = 3.1 Hz), 133.8 (d, *J* = 2.8 Hz), 133.4, 133.2, 130.1, 129.8, 128.6, 128.3 (d, *J* = 8.2 Hz), 126.0, 122.8, 118.4 (d, *J* = 7.9 Hz), 116.1 (d, *J* = 22.7 Hz), 115.8 (d, *J* = 21.6 Hz), 83.0, 78.3, 75.5, 61.1, 60.3, 33.9, 25.2.

¹⁹F NMR (376 MHz, CDCl₃) δ -113.63 – -113.79 (m, 1F), -117.70 – -117.80 (m, 1F).

HRMS (ESI): Calcd. for $C_{33}H_{25}O_3NF_2Na [M+Na]^+$, 544.1695. Found: 544.1696.

TLC: $R_f = 0.10$, 10% EtOAc in hexanes.

(R)-6-ethynyl-2,8-dimethyl-2-((4*R*,8*R*)-4,8,12-trimethyltridecyl)chroman (S4**)⁸**



(*R*)-2,8-Dimethyl-2-((4*R*,8*R*)-4,8,12-trimethyltridecyl)chroman-6-yl trifluoromethanesulfonate (2.14 g, 4.00 mmol) was subjected to General Procedure B. Silica flash chromatography (0-2% EtOAc in hexanes) provided **S4** (756 mg, 46% yield after two steps) as a colorless liquid.

¹H NMR (400 MHz, CDCl₃) δ 7.10 (s, 1H), 7.07 (s, 1H), 2.93 (s, 1H), 2.77 – 2.61 (m, 2H), 2.12 (s, 3H), 1.89 – 1.68 (m, 3H), 1.63 – 1.00 (m, 23H), 0.91 – 0.77 (m, 12H).

¹³C NMR (126 MHz, CDCl₃) δ 153.1, 132.2, 131.2, 126.7, 120.7, 112.1, 84.6, 76.8, 74.9, 40.2, 39.5, 37.6, 37.6, 37.4, 33.0, 32.8, 31.2, 28.1, 25.0, 24.6, 24.4, 22.9, 22.8, 22.2, 21.1, 19.9, 19.81, 16.01.

TLC: $R_f = 0.20$, 2% EtOAc in hexanes.

Experimental Procedures and Characterization.

Bis-Trifluoromethylation of Arylacetylenes. General Procedure C

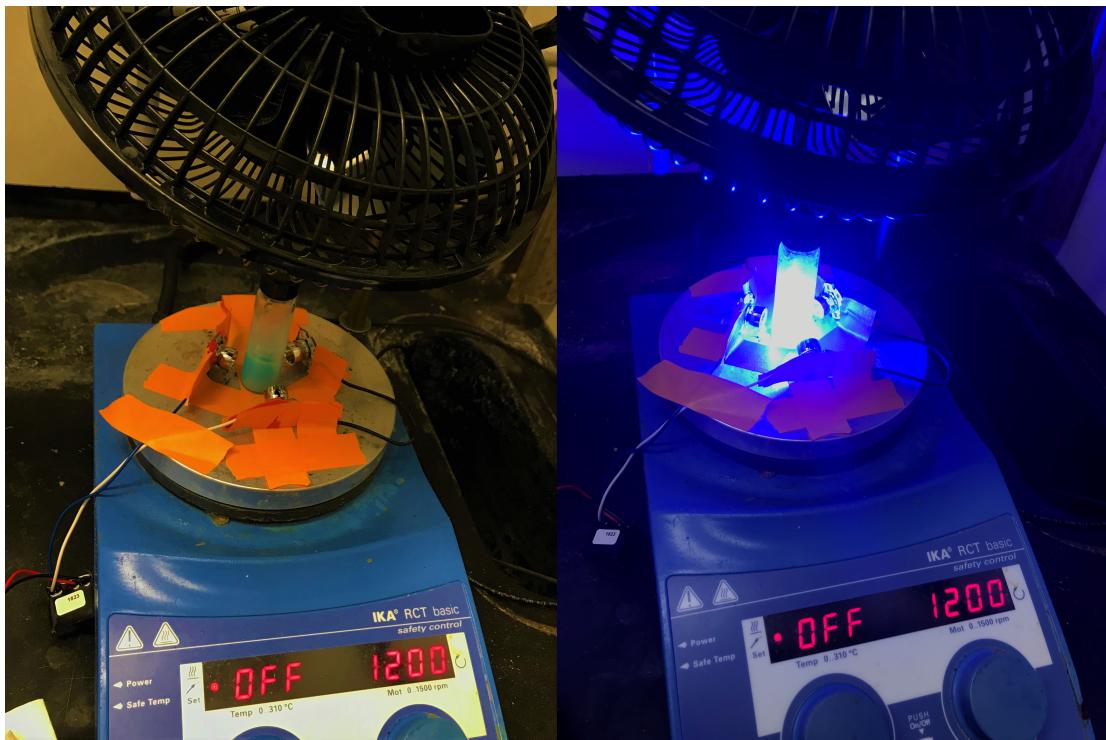
To an 11.0 mL screw-cap test tube equipped with a Teflon®-coated stir bar in an N₂ glovebox were added K₂S₂O₈ (65.0 mg, 0.240 mmol, 1.5 equiv), bpyCu(CF₃)₃ (68.5 mg, 0.160 mmol, 1.0 equiv) and the alkyne substrate (0.160 mmol, 1.0 equiv) (if solid). Degassed acetonitrile (1.2 mL), degassed methanol (1.6 mL) and the alkyne substrate (0.160 mmol, 1.0 equiv) (if liquid) were added via syringe. The tube was sealed with a screw cap, brought outside the glovebox, and irradiated with blue light (LED, 3 x 910 mW, $\lambda_{max} = 447.5$ nm) placed 1-2 cm away from the reaction vial with cooling fan to keep the reaction at room temperature for 1 h (**Figure S1**). The mixture was filtered by Celite® and washed by dichloromethane or diethyl ether (10.0 mL). Then saturated aqueous NH₄Cl (8 mL) was added. The organic layer was extracted with dichloromethane or diethyl ether (3 x 10 mL), combined, dried over anhydrous Na₂SO₄. The filtrate was concentrated under reduced pressure, and the residue was purified by silica flash chromatography to give the desired product (purification details for each substrate disclosed below).

Bis-Trifluoromethylation of Arylacetylenes. General Procedure D (for low boiling point products)

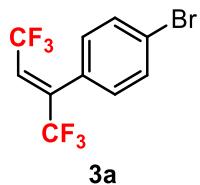
To an 11.0 mL screw-cap test tube equipped with a Teflon®-coated stir bar in an N₂ glovebox was added K₂S₂O₈ (65.0 mg, 0.24 mmol, 1.5 equiv), bpyCu(CF₃)₃ (68.5 mg, 0.16 mmol, 1.0 equiv) and alkyne substrate (0.16 mmol, 1.0 equiv) (if solid). Degassed acetonitrile (1.2 mL), degassed methanol (1.6 mL) and alkyne substrate (0.16 mmol, 1.0 equiv) (if liquid) were added via syringe. The tube was sealed with a screw cap, brought outside the glovebox, and irradiated with blue light (LED, 3 x 910 mW, $\lambda_{max} = 447.5$

nm) placed 1-2 cm away from the reaction vial with cooling fan to keep the reaction at room temperature for 1 h (**Figure S1**). The mixture was filtered by silica and washed with dichloromethane or diethyl ether (10 mL). The filtrate was concentrated at “low” temperature (bath below 25 °C) by rotary evaporation in an attempt to mitigate product evaporation. The residue was purified by silica flash chromatography to give the desired product (details for each substrate is disclosed individually).

Figure S1. Typical Reaction Set Up



(E)-1,1,1,4,4,4-Hexafluoro-2-(4-bromophenyl)but-2-ene (3a)



4-Bromophenylacetylene **1a** (29.0 mg, 0.160 mmol) was subjected to General Procedure D. Silica flash chromatography (*n*-pentane) provided **3a** (43.5 mg, 85% yield, *E/Z* = 15:1) as a colorless liquid.

¹H NMR (400 MHz, CDCl₃) δ 7.56 (d, *J* = 8.5 Hz, 2H), 7.15 (d, *J* = 8.4 Hz, 2H), 6.49 (q, *J* = 7.2 Hz, 1H).

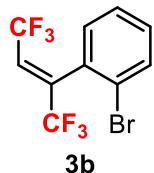
¹³C NMR (126 MHz, CDCl₃) δ 141.4 – 139.3 (m), 131.9, 130.5, 127.9, 124.7, 123.6 (qq, *J* = 35.8, 5.6 Hz), 121.8 (q, *J* = 275.1 Hz), 121.5 (q, *J* = 272.1 Hz).

¹⁹F NMR (376 MHz, CDCl₃) δ -58.11 (dq, *J* = 7.2, 1.3 Hz, 3F), -68.35 (s, 3F).

HRMS (EI): Calcd. for $C_{10}H_5BrF_6$ [M], 317.9479. Found: 317.9477.

TLC: $R_f = 0.5$, *n*-pentane.

(E)-1,1,1,4,4,4-Hexafluoro-2-(2-bromophenyl)but-2-ene (3b)



2-Bromophenylacetylene **1b** (29.0 mg, 0.160 mmol) was subjected to General Procedure D. Silica flash chromatography (*n*-pentane) provided **3b** (36.0 mg, 71% yield, *E/Z* > 20:1) as a colorless liquid.

¹H NMR (400 MHz, $CDCl_3$) δ 7.67 (dd, $J = 7.9, 1.0$ Hz, 1H), 7.41 – 7.35 (m, 1H), 7.34 – 7.28 (m, 1H), 7.22 (dd, $J = 7.5, 0.6$ Hz, 1H), 6.58 (q, $J = 7.1$ Hz, 1H).

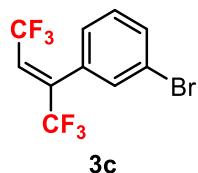
¹³C NMR (126 MHz, $CDCl_3$) δ 140.1 – 138.8 (m), 133.2, 131.4, 130.6, 130.3, 127.3, 124.6 (qq, $J = 35.8, 5.3$ Hz), 123.3, 121.66 (q, $J = 275.8$ Hz), 121.3 (q, $J = 272.2$ Hz).

¹⁹F NMR (376 MHz, $CDCl_3$) δ -60.71 (dq, $J = 7.0, 1.5$ Hz, 3F), -67.91 (s, 3F).

HRMS (EI): Calcd. for $C_{10}H_5BrF_6$ [M], 317.9479. Found: 317.9476.

TLC: $R_f = 0.50$, *n*-pentane.

(E)-1,1,1,4,4,4-Hexafluoro-2-(3-bromophenyl)but-2-ene (3c)



3-Bromophenylacetylene **1c** (29.0 mg, 0.160 mmol) was subjected to General Procedure D. Silica flash chromatography (*n*-pentane) provided **3c** (40.1 mg, 79% yield, *E/Z* = 15:1) as a colorless liquid.

¹H NMR (400 MHz, $CDCl_3$) δ 7.61 (d, $J = 8.0$ Hz, 1H), 7.45 (s, 1H), 7.36 – 7.28 (m, 1H), 7.23 (d, $J = 7.7$ Hz, 1H), 6.52 (qq, $J = 7.1, 1.3$ Hz, 1H).

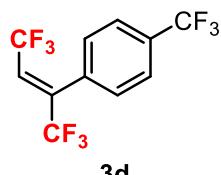
¹³C NMR (126 MHz, $CDCl_3$) δ 139.9 (qq, $J = 31.9, 4.9$ Hz), 133.3, 131.7, 130.8, 130.1, 127.6, 123.8 (qq, $J = 35.9, 5.6$ Hz), 122.6, 121.8 (q, $J = 275.2$ Hz), 121.4 (q, $J = 272.1$ Hz).

¹⁹F NMR (376 MHz, $CDCl_3$) δ -58.18 (dq, $J = 7.1, 1.1$ Hz, 3F), -68.26 (s, 3F).

HRMS (EI): Calcd. for $C_{10}H_5BrF_6$ [M], 317.9479. Found: 317.9478.

TLC: $R_f = 0.40$, *n*-pentane.

(E)-1,1,1,4,4,4-Hexafluoro-2-(4-trifluoromethylphenyl)but-2-ene (3d)



4-Trifluoromethylphenylacetylene **1d** (27.2 mg, 0.160 mmol) was subjected to General Procedure D. Silica flash chromatography (*n*-pentane) provided **3d** (27.3 mg, 55% yield, *E/Z* = 15:1) as a colorless liquid.

¹H NMR (400 MHz, CDCl₃) δ 7.71 (d, *J* = 8.2 Hz, 2H), 7.43 (d, *J* = 8.1 Hz, 2H), 6.57 (q, *J* = 7.1 Hz, 1H).

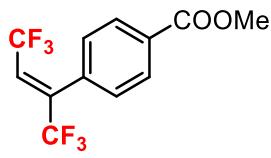
¹³C NMR (126 MHz, CDCl₃) δ 140.2 (qq, *J* = 32.2, 5.0 Hz), 132.8, 132.4 (q, *J* = 33.0 Hz), 129.5, 125.6 (q, *J* = 3.6 Hz), 124.1 (qq, *J* = 36.1, 5.7 Hz), 123.9 (d, *J* = 272.3 Hz), 121.8 (q, *J* = 275.0 Hz), 121.5 (q, *J* = 272.0 Hz).

¹⁹F NMR (376 MHz, CDCl₃) δ -58.19 (dq, *J* = 7.0, 1.4 Hz, 3F), -63.11 (s, 3F), -68.23 (s, 3F).

HRMS (EI): Calcd. for C₁₁H₅F₉ [M], 308.0248. Found: 308.0246.

TLC: R_f = 0.4, *n*-pentane.

(E)-methyl-4-(1,1,1,4,4-hexafluorobut-2-en-2-yl)benzoate (3e)



Methyl-4-ethynylbenzoate **1e** (25.6 mg, 0.160 mmol) was subjected to General Procedure C. Silica flash chromatography (0-10% EtOAc in hexanes) provided **3e** (29.5 mg, 62% yield, *E/Z* = 20:1) as a colorless liquid.

¹H NMR (400 MHz, CDCl₃) δ 8.10 (d, *J* = 8.3 Hz, 2H), 7.38 (d, *J* = 8.2 Hz, 2H), 6.54 (q, *J* = 7.2 Hz, 1H), 3.95 (s, 3H).

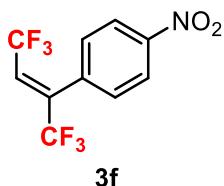
¹³C NMR (126 MHz, CDCl₃) δ 166.4, 140.6 (qq, *J* = 32.0, 5.1 Hz), 133.5, 131.8, 129.7, 129.0, 123.7 (qq, *J* = 35.9, 5.7 Hz), 121.8 (q, *J* = 275.2 Hz), 121.4 (q, *J* = 272.1 Hz), 52.5.

¹⁹F NMR (376 MHz, CDCl₃) δ -58.20 (dq, *J* = 7.2, 1.6 Hz, 3F), -68.12 (s, 3F).

HRMS (EI): Calcd. for C₁₂H₈F₆O₂ [M], 298.0428. Found: 298.0428.

TLC: R_f = 0.20, 10% EtOAc in hexanes.

(E)-1,1,1,4,4-Hexafluoro-2-(4-nitrophenyl)but-2-ene (3f)



4-Nitrophenylacetylene **1f** (23.5 mg, 0.160 mmol) was subjected to General Procedure C. Silica flash chromatography (0-15% EtOAc in hexanes) provided **3f** (34.2 mg, 75% yield, *E/Z* = 20:1) as a colorless liquid.

¹H NMR (400 MHz, CDCl₃) δ 8.31 (d, *J* = 8.8 Hz, 2H), 7.50 (d, *J* = 8.6 Hz, 2H), 6.62 (qq, *J* = 7.1, 1.3 Hz, 1H).

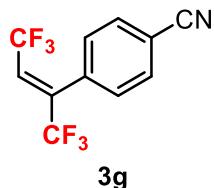
¹³C NMR (126 MHz, CDCl₃) δ 148.9, 139.3 (qq, *J* = 32.4, 5.0 Hz), 135.2, 130.1, 124.4 (qq, *J* = 36.1, 5.5 Hz), 123.6, 121.4 (q, *J* = 275.3 Hz), 121.1 (q, *J* = 272.3 Hz).

¹⁹F NMR (376 MHz, CDCl₃) δ -58.21 (dq, *J* = 6.9, 1.3 Hz, 3F), -68.01 (s, 3F).

HRMS (EI): Calcd. for C₁₀H₅F₆NO₂ [M], 285.0224. Found: 285.0222.

TLC: R_f = 0.35, 20% EtOAc in hexanes.

(E)-1,1,1,4,4,4-Hexafluoro-2-(4-cyanophenyl)but-2-ene (3g)



4-Cyanophenylacetylene **1g** (20.3 mg, 0.160 mmol) was subjected to General Procedure D. Silica flash chromatography (0-10% EtOAc in hexanes) provided **3g** (35.0 mg, 82% yield, *E/Z* = 15:1) as a colorless liquid.

¹H NMR (400 MHz, CDCl₃) δ 7.75 (d, *J* = 8.4 Hz, 2H), 7.43 (d, *J* = 8.1 Hz, 2H), 6.59 (qq, *J* = 7.1, 1.2 Hz, 1H).

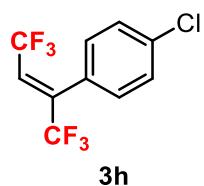
¹³C NMR (126 MHz, CDCl₃) δ 139.5 (qq, *J* = 32.2, 5.1 Hz), 133.4, 132.2, 129.6 (q, *J* = 1.4 Hz), 124.2 (qq, *J* = 36.0, 5.5 Hz), 121.4 (q, *J* = 275.2 Hz), 121.1 (q, *J* = 272.3 Hz), 117.8, 114.3.

¹⁹F NMR (376 MHz, CDCl₃) δ -58.20 (dq, *J* = 7.1, 1.3 Hz, 3F), -68.06 (s, 3F).

HRMS (EI): Calcd. for C₁₁H₅F₆N [M], 265.0326. Found: 265.0323.

TLC: R_f = 0.20, 10% EtOAc in hexanes.

(E)-1,1,1,4,4,4-Hexafluoro-2-(4-chlorophenyl)but-2-ene (3h)



4-Chlorophenylacetylene **1h** (21.8 mg, 0.160 mmol) was subjected to General Procedure D. Silica flash chromatography (*n*-pentane) provided **3h** (30.8 mg, 70% yield, *E/Z* = 15:1) as a colorless liquid.

¹H NMR (400 MHz, CDCl₃) δ 7.40 (d, *J* = 8.4 Hz, 2H), 7.21 (d, *J* = 8.3 Hz, 2H), 6.49 (q, *J* = 6.4 Hz, 1H).

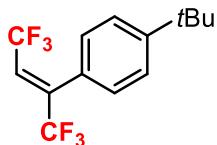
¹³C NMR (126 MHz, CDCl₃) δ 140.4 (qq, *J* = 31.8, 5.1 Hz), 136.5, 130.3, 129.0, 127.4, 123.6 (qq, *J* = 35.8, 5.6 Hz), 121.9 (q, *J* = 275.1 Hz), 121.5 (q, *J* = 272.0 Hz).

¹⁹F NMR (376 MHz, CDCl₃) δ -58.12 (dq, *J* = 7.2, 1.3 Hz, 3F), -68.36 (s, 3F).

HRMS (EI): Calcd. for C₁₀H₅ClF₆ [M], 273.9984. Found: 273.9984.

TLC: R_f = 0.50, *n*-pentane.

(E)-1,1,1,4,4,4-Hexafluoro-2-(4-tertbutylphenyl)but-2-ene (3i)



3i

4-Tertbutylphenylacetylene **1i** (25.3 mg, 0.160 mmol) was subjected to General Procedure C. Silica flash chromatography (*n*-pentane) provided **3i** (40.6 mg, 86% yield, *E/Z* = 19:1) as a colorless liquid.

¹H NMR (400 MHz, CDCl₃) δ 7.42 (d, *J* = 8.4 Hz, 2H), 7.22 (d, *J* = 8.2 Hz, 2H), 6.46 (qq, *J* = 7.3, 1.2 Hz, 1H), 1.34 (s, 9H).

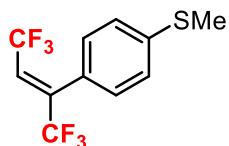
¹³C NMR (126 MHz, CDCl₃) δ 153.2, 141.6 (qq, *J* = 31.4, 5.2 Hz), 128.6, 126.1, 125.5, 122.7 (qq, *J* = 35.7, 5.8 Hz), 122.2 (q, *J* = 275.2 Hz), 121.8 (q, *J* = 271.8 Hz), 34.9, 31.3.

¹⁹F NMR (376 MHz, CDCl₃) δ -58.02 (d, *J* = 7.2 Hz, 3F), -68.23 (s, 3F).

HRMS (EI): Calcd. for C₁₄H₁₄F₆ [M], 296.1000. Found: 296.0996.

TLC: R_f = 0.4, *n*-pentane.

(E)-1,1,4,4,4-Hexafluoro-2-(4-methylthiophenyl)but-2-ene (3j)



3j

4-Methylthiophenylacetylene **1j** (23.7 mg, 0.160 mmol) was subjected to General Procedure C. Silica flash chromatography (0-2% EtOAc in hexanes) provided **3j** (34.5 mg, 75% yield, *E/Z* = 16:1) as a colorless liquid.

¹H NMR (400 MHz, CDCl₃) δ 7.27 (d, *J* = 8.4 Hz, 2H), 7.20 (d, *J* = 8.4 Hz, 2H), 6.47 (qq, *J* = 7.2, 1.3 Hz, 1H), 2.51 (s, 3H).

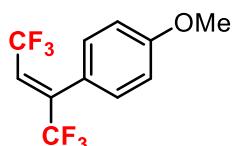
¹³C NMR (126 MHz, CDCl₃) δ 141.7, 141.0 (qq, *J* = 31.5, 5.3 Hz), 129.2, 125.7, 125.2, 123.0 (qq, *J* = 35.6, 5.6 Hz), 122.1 (q, *J* = 275.2 Hz), 121.7 (q, *J* = 271.8 Hz), 15.2.

¹⁹F NMR (376 MHz, CDCl₃) δ -58.02 (dq, *J* = 7.2, 1.6 Hz, 3F), -68.23 (s, 3F).

HRMS (EI): Calcd. for C₁₁H₈F₆S [M], 286.0251. Found: 286.0248.

TLC: R_f = 0.25, 4% EtOAc in hexanes.

(E)-1,1,4,4,4-Hexafluoro-2-(4-methoxyphenyl)but-2-ene (3k)



3k

4-Methoxyphenylacetylene **1k** (21.2 mg, 0.160 mmol) was subjected to General Procedure C. Silica flash chromatography (0-8% EtOAc in hexanes) provided **3k** (31.2 mg, 72% yield, *E/Z* = 15:1) as a colorless liquid.

¹H NMR (400 MHz, CDCl₃) δ 7.23 (d, *J* = 8.6 Hz, 2H), 6.94 (d, *J* = 8.8 Hz, 2H), 6.45 (qq, *J* = 7.3, 1.3 Hz, 1H), 3.84 (s, 3H).

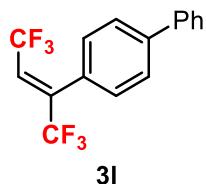
¹³C NMR (126 MHz, CDCl₃) δ 160.9, 141.3 (qq, *J* = 31.5, 5.1 Hz), 130.3, 122.6 (qq, *J* = 35.5, 5.6 Hz), 122.2 (q, *J* = 275.4 Hz), 121.8 (q, *J* = 271.8 Hz), 121.1, 114.0, 55.4.

¹⁹F NMR (376 MHz, CDCl₃) δ -58.02 (dq, *J* = 7.2, 1.6 Hz, 3F), -68.23 (s, 3F).

HRMS (EI): Calcd. for C₁₁H₈F₆O [M], 270.0479. Found: 270.0475.

TLC: R_f = 0.3, 10% EtOAc in hexanes.

(E)-1,1,4,4,4-Hexafluoro-2-(4-phenylphenyl)but-2-ene (**3l**)



4-Phenylphenylacetylene **1l** (28.5 mg, 0.160 mmol) was subjected to General Procedure D. Silica flash chromatography (0-4% EtOAc in hexanes.) provided **3l** (44.9 mg, 89% yield, *E/Z* = 14:1) as a white solid.

¹H NMR (400 MHz, CDCl₃) δ 7.63 (d, *J* = 8.3 Hz, 2H), 7.60 (d, *J* = 7.4 Hz, 2H), 7.47 – 7.41 (m, 2H), 7.40 – 7.31 (m, 3H), 6.50 (q, *J* = 5.9 Hz, 1H).

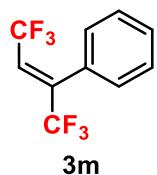
¹³C NMR (126 MHz, CDCl₃) δ 142.9, 141.2 (qq, *J* = 31.6, 5.1 Hz), 140.2, 129.3, 129.0, 128.1, 127.9, 127.3, 127.2, 123.1 (qq, *J* = 35.7, 5.7 Hz), 122.1 (q, *J* = 275.2 Hz), 121.7 (q, *J* = 271.9 Hz).

¹⁹F NMR (376 MHz, CDCl₃) δ -57.99 (dq, *J* = 7.2, 1.5 Hz, 3F), -68.13 (s, 3F).

HRMS (EI): Calcd. for C₁₆H₁₀F₆ [M], 316.0687. Found: 316.0681.

TLC: R_f = 0.20, 4% EtOAc in hexanes.

(E)-1,1,4,4,4-Hexafluoro-2-phenylbut-2-ene (**3m**)⁹



Phenylacetylene **1m** (16.4 mg, 0.160 mmol) was subjected to General Procedure D. Silica flash chromatography (*n*-pentane) provided **3m** (16.0 mg, 42% yield, *E/Z* = 15:1) as a colorless liquid.

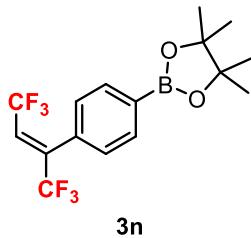
¹H NMR (400 MHz, CDCl₃) δ 7.53 – 7.37 (m, 3H), 7.33 – 7.27 (m, 2H), 6.49 (q, *J* = 7.2 Hz, 1H).

¹³C NMR (126 MHz, CDCl₃) δ 141.7 – 140.8 (m), 130.0, 129.1, 128.8 (q, *J* = 1.3 Hz), 128.5, 123.0 (qq, *J* = 35.7, 5.7 Hz), 122.1 (q, *J* = 275.1 Hz), 121.7 (q, *J* = 271.9 Hz).

¹⁹F NMR (376 MHz, CDCl₃) δ -58.13 (dd, *J* = 7.2, 1.7 Hz, 3F), -68.36 (s, 3F).

TLC: $R_f = 0.5$, *n*-pentane.

2-((E)-4-(1,1,1,4,4,4-hexafluorobut-2-en-2-yl)phenyl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane (3n)



2-(4-Ethynylphenyl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane **1n** (36.5 mg, 0.160 mmol) was subjected to General Procedure C. Silica flash chromatography (0-40% EtOAc in hexanes) provided **3n** (38.2 mg, 65% yield, *E/Z* = 15:1) as a colorless liquid.

¹H NMR (400 MHz, CDCl₃) δ 7.86 (d, *J* = 8.1 Hz, 2H), 7.29 (d, *J* = 7.8 Hz, 2H), 6.49 (qq, *J* = 7.2, 1.3 Hz, 1H), 1.35 (s, 12H).

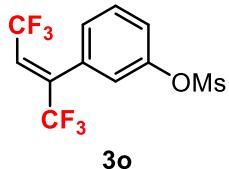
¹³C NMR (126 MHz, CDCl₃) δ 141.4 (qq, *J* = 31.7, 5.1 Hz), 134.8, 134.6, 131.7, 128.1, 123.0 (qq, *J* = 35.8, 5.7 Hz), 122.0 (q, *J* = 275.2 Hz), 121.6 (q, *J* = 272.0 Hz), 84.3, 25.0.

¹⁹F NMR (376 MHz, CDCl₃) δ -58.13 (dq, *J* = 7.1, 1.5 Hz, 3F), -68.21 (s, 3F).

HRMS (EI): Calcd. for C₁₆H₁₇BF₆O₂ [M], 366.1226. Found: 366.1226.

TLC: $R_f = 0.25$, 50% EtOAc in hexanes.

(E)-3-(1,1,1,4,4-Hexafluorobut-2-en-2-yl)phenyl-methanesulfonate (3o)



3-Ethynylphenyl methanesulfonate **1o** (31.4 mg, 0.160 mmol) was subjected to General Procedure C. Silica flash chromatography (0-40% EtOAc in hexanes) provided **3o** (49.0 mg, 92% yield, *E/Z* = 14:1) as a colorless liquid.

¹H NMR (400 MHz, CDCl₃) δ 7.54 – 7.48 (m, 1H), 7.47 – 7.41 (m, 1H), 7.31 – 7.22 (m, 2H), 6.55 (q, *J* = 7.1 Hz, 1H), 3.15 (s, 3H).

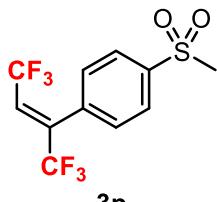
¹³C NMR (126 MHz, CDCl₃) δ 149.1, 139.7 (qq, *J* = 32.2, 5.1 Hz), 130.8, 130.4, 127.9, 124.06 (qq, *J* = 35.9, 5.6 Hz), 123.9, 122.7, 121.7 (q, *J* = 275.1 Hz), 121.4 (q, *J* = 272.2 Hz), 37.5.

¹⁹F NMR (376 MHz, CDCl₃) δ -58.12 (dq, *J* = 7.1, 1.3 Hz, 3F), -68.20 (s, 3F).

HRMS (EI): Calcd. for C₁₁H₈F₆O₃S [M], 334.0098. Found: 334.0092.

TLC: $R_f = 0.35$, 50% EtOAc in hexanes.

(E)-1-(1,1,1,4,4-hexafluorobut-2-en-2-yl)-4-(methylsulfonyl)benzene (3p)



3p

1-Ethynyl-4-(methylsulfonyl)benzene **1p** (28.9 mg, 0.160 mmol) was subjected to General Procedure C. Silica flash chromatography (0-50% EtOAc in hexanes) provided **3p** (41.0 mg, 81% yield, *E/Z* = 13:1) as a colorless liquid.

¹H NMR (400 MHz, CDCl₃) δ 8.05 (d, *J* = 8.3 Hz, 2H), 7.54 (d, *J* = 8.3 Hz, 2H), 6.63 (q, *J* = 7.1 Hz, 1H), 3.13 (s, 3H).

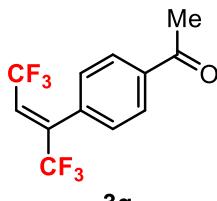
¹³C NMR (126 MHz, CDCl₃) δ 142.3, 139.6 (qq, *J* = 32.3, 5.0 Hz), 134.5, 130.1 (q, *J* = 1.2 Hz), 127.7, 124.4 (qq, *J* = 36.1, 5.5 Hz), 121.6 (q, *J* = 275.2 Hz), 121.2 (q, *J* = 272.2 Hz), 44.5.

¹⁹F NMR (376 MHz, CDCl₃) δ -58.16 (dq, *J* = 7.1, 1.4 Hz, 3F), -68.04 (s, 3F).

HRMS (EI): Calcd. for C₁₁H₈F₆O₂S [M], 318.0149. Found: 318.0155.

TLC: R_f = 0.2, 50% EtOAc in hexanes.

(E)-1,1,4,4,4-Hexafluoro-2-(4-acetylphenyl)but-2-ene (**3q**)



3q

4-Acetylphenylacetylene **1q** (23.1 mg, 0.160 mmol) was subjected to General Procedure C. Silica flash chromatography (15% EtOAc in hexanes) provided **3q** (37.6 mg, 83% yield, *E/Z* = 19:1) as a colorless liquid.

¹H NMR (400 MHz, CDCl₃) δ 8.02 (d, *J* = 8.2 Hz, 2H), 7.41 (d, *J* = 8.1 Hz, 2H), 6.55 (q, *J* = 6.7 Hz, 1H), 2.64 (s, 3H).

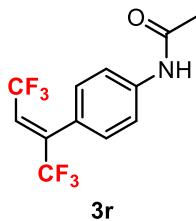
¹³C NMR (126 MHz, CDCl₃) δ 197.3, 140.5 (qq, *J* = 31.7, 5.0 Hz), 138.2, 133.5, 129.3, 128.4, 123.7 (qq, *J* = 35.8, 5.6 Hz), 121.8 (q, *J* = 275.1 Hz), 121.4 (q, *J* = 272.0 Hz), 26.7.

¹⁹F NMR (376 MHz, CDCl₃) δ -58.18 (dq, *J* = 7.1, 1.6 Hz, 3F), -68.09 (s, 3F).

HRMS (EI): Calcd. for C₁₂H₈F₆O [M], 282.0479. Found: 282.0476.

TLC: R_f = 0.25, 20% EtOAc in hexanes.

(E)-N-(4-(1,1,4,4,4-hexafluorobut-2-en-2-yl)phenyl)acetamide (**3r**)



N-(4-ethynylphenyl)acetamide **1r** (25.5 mg, 0.160 mmol) was subjected to General Procedure C. Silica flash chromatography (0-85% EtOAc in hexanes) provided **3r** (35.9 mg, 75% yield, *E/Z* = 13:1) as a white solid.

¹H NMR (400 MHz, CDCl₃) 7.59 (d, *J* = 8.4 Hz, 2H), 7.25 (d, *J* = 8.4 Hz, 2H), 7.20 (br, 1H), 6.47 (q, *J* = 7.1 Hz, 1H), 2.21 (s, 3H).

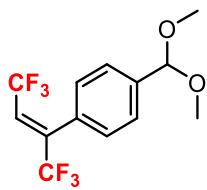
¹³C NMR (126 MHz, CDCl₃) δ 168.7, 140.8, 139.7 (qq, *J* = 31.3, 5.6 Hz), 129.2, 123.5 (qq, *J* = 34.7, 5.5 Hz), 122.0 (q, *J* = 275.3 Hz), 121.7 (d, *J* = 272.0 Hz), 122.7, 118.6, 24.0.

¹⁹F NMR (376 MHz, CDCl₃) δ -58.03 (dq, *J* = 7.2, 1.2 Hz, 3F), -68.26 (s, 3F).

HRMS (ESI): Calcd. for C₁₂H₁₀ONF₆ [M+H]⁺, 298.0661. Found: 298.0663.

TLC: R_f = 0.20, 80% EtOAc in hexanes.

(E)-1-(Dimethoxymethyl)-4-(1,1,1,4,4-hexafluorobut-2-en-2-yl)benzene (**3s**)



4-Ethynylbenzaldehyde **1s** (20.9 mg, 0.160 mmol) was subjected to General Procedure C. Silica flash chromatography (10% EtOAc in hexanes) provided **3s** (47.6 mg, 95% yield, *E/Z* = 19:1) as a white solid.

¹H NMR (400 MHz, CDCl₃) δ 7.52 (d, *J* = 7.9 Hz, 2H), 7.30 (d, *J* = 7.9 Hz, 2H), 6.50 (q, *J* = 7.2 Hz, 1H), 5.43 (s, 1H), 3.34 (s, 6H).

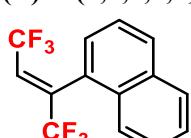
¹³C NMR (126 MHz, CDCl₃) δ 141.2 (qq, *J* = 31.6, 5.2 Hz), 140.1, 129.1, 128.8 (q, *J* = 1.3 Hz), 126.9, 123.1 (qq, *J* = 35.6, 5.6 Hz), 122.0 (q, *J* = 275.1 Hz), 121.6 (q, *J* = 272.0 Hz), 102.6, 52.9.

¹⁹F NMR (376 MHz, CDCl₃) δ -58.12 (d, *J* = 7.1 Hz, 3F), -68.29 (s, 3F).

HRMS (EI): Calcd. for C₁₃H₁₂F₆O₂ [M], 314.0741. Found: 314.0704.

TLC: R_f = 0.20, 10% EtOAc in hexanes.

(E)-1-(1,1,1,4,4-hexafluorobut-2-en-2-yl)naphthalene (**3t**)



1-Ethynylnaphthalene **1t** (24.3 mg, 0.160 mmol) was subjected to General Procedure D. Silica flash chromatography (0-5% EtOAc in hexanes.) provided **3t** (26.0 mg, 54% yield, *E/Z* > 20:1) as a colorless liquid.

¹H NMR (400 MHz, CDCl₃) δ 7.95 (d, *J* = 8.3 Hz, 1H), 7.92 – 7.86 (m, 1H), 7.75 – 7.68 (m, 1H), 7.59 – 7.48 (m, 3H), 7.37 (d, *J* = 7.1 Hz, 1H), 6.78 (q, *J* = 7.1 Hz, 1H).

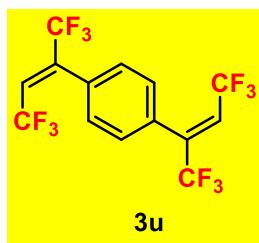
¹³C NMR (126 MHz, CDCl₃) δ 140.1 (qq, *J* = 32.3, 4.8 Hz), 133.5, 131.5, 130.4, 128.6, 127.5, 127.1, 126.5, 126.4, 125.7 – 124.4 (m), 125.0, 124.9, 122.2 (q, *J* = 275.8 Hz), 121.5 (q, *J* = 272.2 Hz).

¹⁹F NMR (376 MHz, CDCl₃) δ -59.98 (dq, *J* = 7.0, 1.4 Hz, 3F), -67.95 (s, 3F).

HRMS (EI): Calcd. for C₁₄H₈F₆ [M], 290.0530. Found: 290.0529.

TLC: R_f = 0.40, 10% EtOAc in hexanes.

1,4-Bis((E)-1,1,1,4,4,4-hexafluorobut-2-en-2-yl)benzene (**3u**)



1,4-Diethynylbenzene **1u** (20.2 mg, 0.160 mmol) was subjected to General Procedure D. Silica flash chromatography (*n*-pentane) provided **3u** (26.2 mg, 41% yield, *E/Z* = 20:1) as a colorless liquid (volatile).

¹H NMR (400 MHz, CDCl₃) δ 7.36 (s, 4H), 6.54 (q, *J* = 7.0 Hz, 2H).

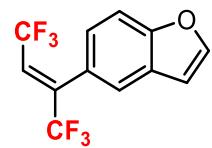
¹³C NMR (126 MHz, CDCl₃) δ 141.3 – 139.6 (m), 130.8, 129.0, 123.8 (qq, *J* = 35.8, 5.6 Hz), 121.9 (q, *J* = 275.1 Hz), 121.5 (q, *J* = 272.1 Hz).

¹⁹F NMR (376 MHz, CDCl₃) δ -58.32 (dq, *J* = 7.0, 1.4 Hz, 6F), -68.21 (s, 6F).

HRMS (EI): Calcd. for C₁₄H₆F₁₂ [M], 402.0278. Found: 402.0276.

TLC: R_f = 0.6, hexanes.

(E)-5-(1,1,1,4,4,4-hexafluorobut-2-en-2-yl)benzofuran (**3v**)



5-Ethynylbenzofuran **1v** (22.8 mg, 0.160 mmol) was subjected to General Procedure D. Silica flash chromatography (0-8% EtOAc in hexanes) provided **3v** (23.5 mg, 52% yield, *E/Z* = 13:1) as a colorless liquid.

¹H NMR (400 MHz, CDCl₃) δ 7.69 (d, *J* = 2.1 Hz, 1H), 7.58 – 7.54 (m, 1H), 7.54 (s, 1H), 7.21 (d, *J* = 9.1 Hz, 1H), 6.81 (d, *J* = 2.0 Hz, 1H), 6.53 (q, *J* = 7.2 Hz, 1H).

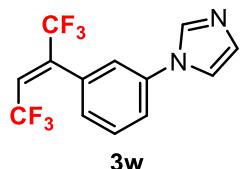
¹³C NMR (126 MHz, CDCl₃) δ 155.6, 146.2, 141.7 (qq, *J* = 31.6, 5.2 Hz), 127.7, 125.0, 123.5, 123.1 (qq, *J* = 35.0, 5.0 Hz), 122.2 (q, *J* = 275.3 Hz), 122.1, 121.7 (q, *J* = 271.9 Hz), 111.7, 106.8.

¹⁹F NMR (376 MHz, CDCl₃) δ -58.03 (dq, *J* = 7.2, 1.2 Hz, 3F), -68.37 (s, 3F).

HRMS (EI): Calcd. for C₁₂H₆F₆O [M], 280.0323. Found: 280.0324.

TLC: R_f = 0.20, 8% EtOAc in hexanes.

(E)-1-(3-(1,1,1,4,4,4-Hexafluorobut-2-en-2-yl)phenyl)-1H-imidazole (3w)



1-(3-Ethynylphenyl)-1H-imidazole **1w** (26.9 mg, 0.160 mmol) was subjected to General Procedure C. Silica flash chromatography (0-20% EtOAc in hexanes) provided **3w** (26.8 mg, 55% yield, *E/Z* = 14:1) as a white solid.

¹H NMR (400 MHz, CDCl₃) δ 7.95 (d, *J* = 2.5 Hz, 1H), 7.80 (dd, *J* = 7.8, 1.8 Hz, 1H), 7.75 (d, *J* = 1.5 Hz, 1H), 7.68 (s, 1H), 7.56 – 7.49 (m, 1H), 7.21 (d, *J* = 7.7 Hz, 1H), 6.55 (q, *J* = 7.2 Hz, 1H), 6.51 – 6.48 (m, 1H).

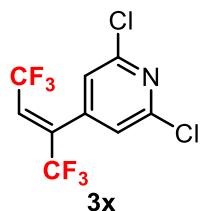
¹³C NMR (126 MHz, CDCl₃) δ 141.7, 141.2 – 139.7 (m), 140.4, 130.3, 129.8, 126.9, 126.8, 123.7 (qq, *J* = 35.8, 5.7 Hz), 121.9 (q, *J* = 275.2 Hz), 121.5 (q, *J* = 275.2 Hz), 120.4, 119.4, 108.3.

¹⁹F NMR (376 MHz, CDCl₃) δ -58.13 (dq, *J* = 7.1, 1.6 Hz, 3F), -68.13 (s, 3F).

HRMS (ESI): Calcd. for C₁₃H₉N₂F₆ [M+H]⁺, 307.0664. Found: 307.0667.

TLC: R_f = 0.20, 20% EtOAc in hexanes.

(E)-2,6-dichloro-4-(1,1,1,4,4,4-hexafluorobut-2-en-2-yl)pyridine (3x)



2,6-Dichloro-4-ethynylpyridine **1x** (27.5 mg, 0.160 mmol) was subjected to General Procedure C. Silica flash chromatography (0-5% EtOAc in hexanes) provided **3x** (29.5 mg, 59% yield, *E/Z* = 16:1) as a white solid.

¹H NMR (400 MHz, CDCl₃) δ 7.21 (s, 2H), 6.63 (q, *J* = 6.9 Hz, 1H).

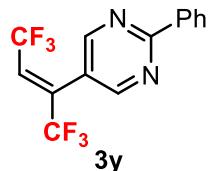
¹³C NMR (126 MHz, CDCl₃) δ 151.3, 142.1, 136.5 (qq, *J* = 33.0, 5.0 Hz), 125.6 (qq, *J* = 36.7, 5.5 Hz), 122.7 (q, *J* = 1.4 Hz), 121.1 (q, *J* = 275.5 Hz), 120.0 (q, *J* = 272.5 Hz).

¹⁹F NMR (376 MHz, CDCl₃) δ -58.31 (dq, *J* = 7.1, 1.2 Hz, 3F), -67.64 (s, 3F).

HRMS (EI): Calcd. for C₉H₃Cl₂F₆N [M], 308.9547. Found: 308.9545.

TLC: R_f = 0.20, 5% EtOAc in hexanes.

(E)-5-(1,1,1,4,4,4-hexafluorobut-2-en-2-yl)-2-phenylpyrimidine (3y)



5-Ethynyl-2-phenylpyrimidine **1y** (28.9 mg, 0.160 mmol) was subjected to General Procedure C. Silica flash chromatography (0-5% EtOAc in hexanes) provided **3y** (34.4 mg, 68% yield, *E/Z* = 13:1) as a colorless liquid.

¹H NMR (400 MHz, CDCl₃) δ 8.75 (s, 2H), 8.55 – 8.46 (m, 2H), 7.57 – 7.47 (m, 3H), 6.71 (qd, *J* = 7.0, 1.4 Hz, 1H).

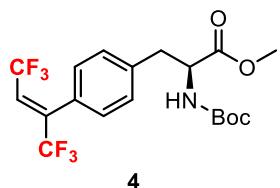
¹³C NMR (126 MHz, CDCl₃) δ 165.9, 156.6, 136.5, 135.9 (qq, *J* = 33.0, 4.9 Hz), 131.9, 128.9, 128.7, 125.9 (qq, *J* = 36.0, 5.4 Hz), 121.6 (q, *J* = 275.3 Hz) 121.3, 121.3 (q, *J* = 272.1 Hz).

¹⁹F NMR (376 MHz, CDCl₃) δ -57.82 (dq, *J* = 7.0, 1.5 Hz, 3F), -68.36 (s, 3F).

HRMS (EI): Calcd. for C₁₄H₈F₆N₂ [M], 318.0592. Found: 318.0591.

TLC: R_f = 0.3, 10% EtOAc in hexanes.

Methyl (*S, E*)-2-((tert-butoxycarbonyl)amino)-3-(4-(1,1,1,4,4,4-hexafluorobut-2-en-2-yl)phenyl)propanoate (4)



S1 (48.6 mg, 0.160 mmol) was subjected to General Procedure C. Silica flash chromatography (0-25% EtOAc in hexanes) provided **4** (60.3 mg, 85% yield, *E/Z* = 17:1) as a white solid.

¹H NMR (400 MHz, CDCl₃) δ 7.25 – 7.17 (m, 4H), 6.48 (q, *J* = 7.2 Hz, 1H), 5.02 (d, *J* = 8.4 Hz, 1H), 4.62 (q, *J* = 8.7 Hz, 1H), 3.67 (s, 3H), 3.21 – 2.97 (m, 2H), 1.41 (s, 9H).

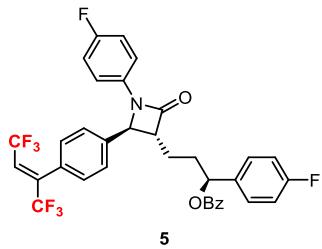
¹³C NMR (126 MHz, CDCl₃) δ 172.3, 155.1, 141.1 (qq, *J* = 31.6, 5.2 Hz), 138.5, 129.4, 128.9, 127.6, 123.5 – 122.4 (m), 120.0 (q, *J* = 275.1 Hz), 121.6 (q, *J* = 271.9 Hz), 80.1, 54.4, 52.2, 38.6, 28.3.

¹⁹F NMR (376 MHz, CDCl₃) δ -58.10 (d, *J* = 6.3 Hz, 3F), -68.27 (s, 3F).

HRMS (ESI): Calcd. for C₁₉H₂₁O₄NF₆Na [M+Na]⁺, 464.1267. Found: 464.1263.

TLC: R_f = 0.20, 25% EtOAc in hexanes.

(*S*)-1-(4-fluorophenyl)-3-((2*S*,3*R*)-1-(4-fluorophenyl)-2-((*E*)-1,1,1,4,4,4-hexafluorobut-2-en-2-yl)phenyl)-4-oxoazetidin-3-yl)propyl benzoate (5)



S3 (83.4 mg, 0.160 mmol) was subjected to General Procedure C. Silica flash chromatography (20% EtOAc in hexanes) provided **5** (90.7 mg, 86%, *E/Z*= 13:1) as a white solid.

¹H NMR (400 MHz, CDCl₃) δ 8.06 (d, *J* = 7.1 Hz, 2H), 7.62 – 7.53 (m, 1H), 7.49 – 7.42 (m, 2H), 7.41 – 7.34 (m, 4H), 7.30 (d, *J* = 8.1 Hz, 2H), 7.24 – 7.15 (m, 2H), 7.07 – 7.00 (m, 2H), 6.98 – 6.91 (m, 2H), 6.51 (q, *J* = 7.3 Hz, 1H), 5.97 (t, *J* = 6.7 Hz, 1H), 4.64 (d, *J* = 2.1 Hz, 1H), 3.14 (t, *J* = 6.6 Hz, 1H), 2.22 (dd, *J* = 15.1, 7.4 Hz, 2H), 2.11 – 1.82 (m, 2H).

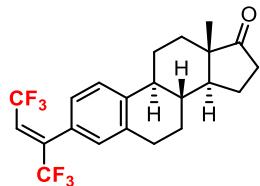
¹³C NMR (126 MHz, CDCl₃) δ 166.6, 165.8, 162.7 (d, *J* = 246.9 Hz), 159.3 (d, *J* = 243.9 Hz), 140.9 – 140.3 (m), 139.6, 135.8 (d, *J* = 3.2 Hz), 133.8, 133.4, 130.2, 129.9, 129.8, 129.4, 128.6, 128.4 (d, *J* = 8.2 Hz), 126.0, 123.5 (qq, *J* = 35.8, 5.6 Hz), 121.9 (q, *J* = 275.2 Hz), 121.5 (q, *J* = 272.0 Hz), 118.4 (d, *J* = 7.8 Hz), 116.1 (d, *J* = 22.8 Hz), 115.8 (d, *J* = 21.6 Hz), 75.5, 60.8, 60.2, 33.9, 25.2.

¹⁹F NMR (376 MHz, CDCl₃) δ -58.11 (d, *J* = 5.9 Hz, 3F), -68.19 (s, 3F), -113.64 – -113.75 (m, 1F), -117.65 – -117.76 (m, 1F).

HRMS (ESI): Calcd. for C₃₅H₂₅O₃NF₈Na [M+Na]⁺, 682.1599. Found: 682.1602.

TLC: R_f = 0.15, 10% EtOAc in hexanes.

(8R,9S,13S,14S)-3-((E)-1,1,1,4,4,4-hexafluorobut-2-en-2-yl)-13-methyl-6,7,8,9,11,12,13,14,15,16-decahydro-17H-cyclopenta[a]phenanthren-17-one (6)



S2 (44.6 mg, 0.160 mmol) was subjected to General Procedure C. Silica flash chromatography (0-40% EtOAc in hexanes) provided **6** (46.6 mg, 70% yield, *E/Z*= 14:1) as a white solid.

¹H NMR (400 MHz, CDCl₃) δ 7.30 (d, *J* = 8.1 Hz, 1H), 7.04 (d, *J* = 8.1 Hz, 1H), 6.99 (s, 1H), 6.43 (q, *J* = 7.1 Hz, 1H), 2.91 (dd, *J* = 8.7, 3.9 Hz, 2H), 2.50 (dd, *J* = 18.7, 8.7 Hz, 1H), 2.44 – 2.37 (m, 1H), 2.35 – 2.25 (m, 1H), 2.15 (dd, *J* = 18.5, 9.3 Hz, 1H), 2.10 – 1.90 (m, 3H), 1.70 – 1.40 (m, 6H), 0.91 (s, 3H).

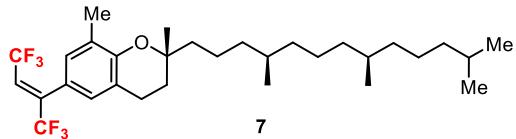
¹³C NMR (126 MHz, CDCl₃) δ 220.6, 141.7, 141.3 (qq, *J* = 31.3, 5.4 Hz), 136.7, 129.0, 126.3, 126.1, 125.3, 122.4 (qq, *J* = 35.5, 5.6 Hz), 122.0 (q, *J* = 275.3 Hz), 121.60 (q, *J* = 271.8 Hz), 50.6, 47.9, 44.4, 37.8, 35.8, 31.6, 29.2, 26.3, 25.5, 21.6, 13.9.

¹⁹F NMR (376 MHz, CDCl₃) δ -57.94 (dq, *J* = 7.3, 1.5 Hz, 3F), -68.16 (s, 3F).

HRMS (EI): Calcd. for C₂₂H₂₂F₆O [M], 416.1575. Found: 416.1578.

TLC: $R_f = 0.35$, 50% EtOAc in hexanes.

(R)-6-((E)-1,1,1,4,4,4-hexafluorobut-2-en-2-yl)-2,8-dimethyl-2-((4*R*,8*R*)-4,8,12-trimethyltridecyl)chromane (7)



S4 (65.7 mg, 0.160 mmol) was subjected to General Procedure C. Silica flash chromatography (0–15% EtOAc in hexanes) provided **7** (56.2 mg, 64% yield, *E/Z* = 12:1) as a colorless liquid.

¹H NMR (400 MHz, CDCl₃) δ 6.86 (s, 1H), 6.82 (s, 1H), 6.37 (q, *J* = 7.3 Hz, 1H), 2.79 – 2.69 (m, 2H), 2.16 (s, 3H), 1.92 – 1.69 (m, 2H), 1.62 – 1.55 (m, 2H), 1.52 – 1.31 (m, 7H), 1.28 (s, 3H), 1.25 – 1.01 (m, 12H), 0.87 (s, 3H), 0.87 (m, 3H), 0.86 (s, 3H), 0.85 (s, 3H).

¹³C NMR (126 MHz, CDCl₃) δ 153.8, 141.8 (qq, *J* = 30.9, 5.2 Hz), 128.7, 127.6, 126.5, 122.4 (q, *J* = 275.4 Hz), 122.0 (q, *J* = 271.7 Hz), 121.7 (qq, *J* = 35.3, 5.7 Hz), 120.5, 119.2, 40.6, 39.6, 37.6, 37.6, 37.6, 37.5, 33.0, 32.9, 31.2, 28.2, 25.0, 24.6, 24.4, 22.9, 22.8, 22.4, 21.1, 19.9, 19.8, 16.2.

¹⁹F NMR (376 MHz, CDCl₃) δ -57.82 (d, *J* = 7.3 Hz, 3F), -67.99 (s, 3F).

HRMS (EI): Calcd. for C₃₁H₄₆F₆O [M], 548.3453. Found: 548.3456.

TLC: $R_f = 0.15$, 10% EtOAc in hexanes.

Table S1. TEMPO control experiments

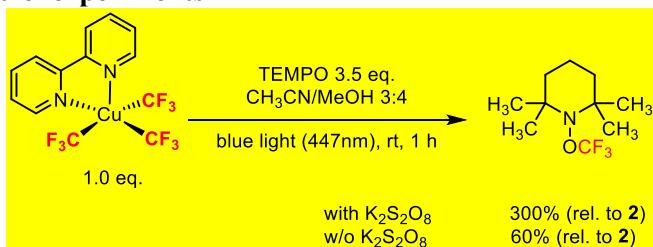


Table S2. Varying the 1a:2 ratio

1.0 eq.	1.0 eq.	w/o $\text{K}_2\text{S}_2\text{O}_8$	31% (rel. to 1a)
1.0 eq.	2.0 eq.	w/o $\text{K}_2\text{S}_2\text{O}_8$	66% (rel. to 1a)
1.0 eq.	3.0 eq.	w/o $\text{K}_2\text{S}_2\text{O}_8$	82% (rel. to 1a)
1.0 eq.	1.0 eq.	with $\text{K}_2\text{S}_2\text{O}_8$	94% (rel. to 1a)
3.0 eq.	1.0 eq.	w/o $\text{K}_2\text{S}_2\text{O}_8$	20% (rel. to 2)
3.0 eq.	1.0 eq.	with $\text{K}_2\text{S}_2\text{O}_8$	120% (rel. to 2)

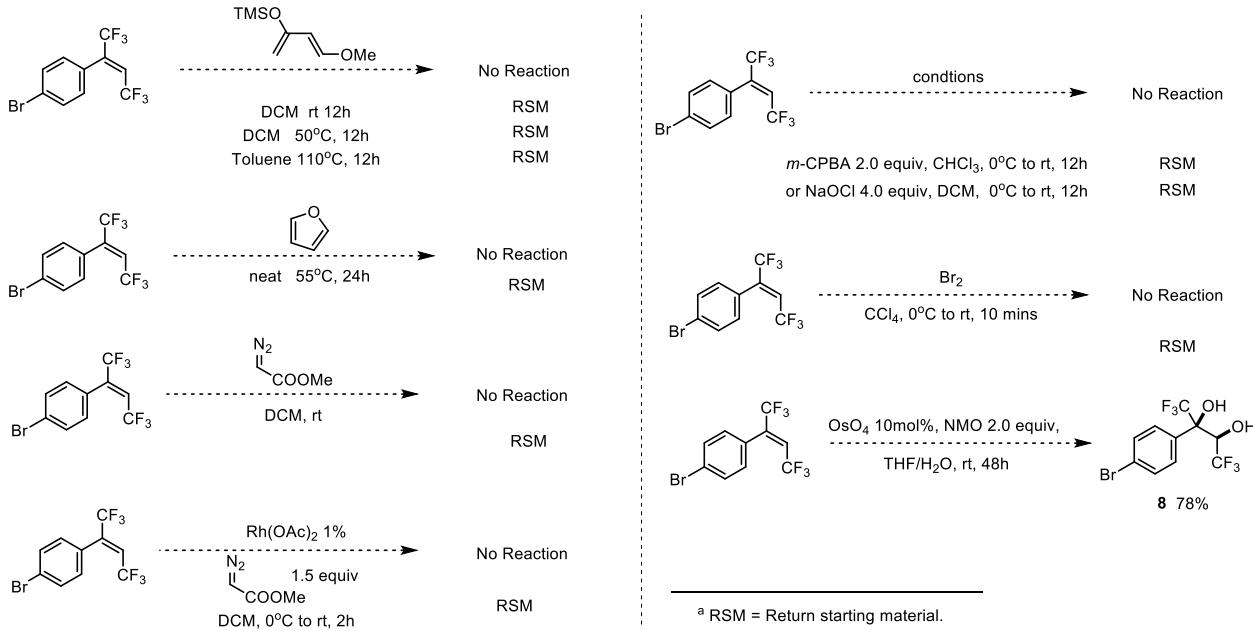
To an 2.0 mL screw-cap test tube equipped with a Teflon®-coated stir bar in an N_2 glovebox was added $\text{K}_2\text{S}_2\text{O}_8$ (16.3 mg, 0.06 mmol, 1.5 equiv), bpyCu(CF_3)₃ (x equiv) and 4-bromophenylacetylene **1a** (y equiv). Degassed acetonitrile (0.3 mL) and degassed methanol (0.4 mL) were added via syringe. The tube was sealed with a screw cap, brought outside the glovebox, and irradiated with blue light (LED, 3 x 910 mW, $\lambda_{\text{max}} = 447.5$ nm) placed 1-2 cm away from the reaction vial with cooling fan to keep the reaction at room temperature for 1 h. When the reaction was completed, 1-fluoro-4-methylbenzene (6.0 μL , 0.0545 mmol, internal standard) and acetone- d_6 (0.6 mL) were added. The NMR yield of (*E*)-1,1,1,4,4,4-hexafluoro-2-(4-bromophenyl)but-2-ene **3a** was determined by comparing the integration of the ¹⁹F NMR (*E*)-1,1,1,4,4,4-hexafluoro-2-(4-bromophenyl)but-2-ene **3a** with that of 1-fluoro-4-methylbenzene (-121.3 ppm).

Table S3. Isotope-labeling experiments



E-HFB Reactivity Studies.

Scheme S1. The study of reactivity of *E*-HFBs^a



2-(4-Bromophenyl)-1,1,4,4,4-hexafluorobutane-2,3-diol (**8**)



In a 50 mL one-neck round-bottom flask were added **3c** (95.7 mg, 0.30 mmol, 1.0 equiv), THF (0.3 mL), and deionized water (0.1 mL). The flask was cooled to 0 °C in an ice bath. After cooling for 10 min, 50% w/w NMO in H_2O (138 mg, 0.60 mmol, 2.0 equiv) was added to the flask followed by 4% w/w OsO_4 (this reagent is extremely toxic, please consults MSDS and handle in a well ventilated hood) in H_2O (191 mg, 0.03 mmol, 0.1 equiv). Five minutes after this addition, the ice bath was removed, and the solution was stirred for 48 h at room temperature. When the reaction was completed, the mixture was diluted with deionized water (5 mL) and Et_2O (5 mL). The phases were separated, and the aqueous layer was extracted with Et_2O (3 × 10 mL). The combined organic layers were washed with brine and dried with anhydrous Na_2SO_4 . The filtrate was concentrated under reduced pressure, and the crude product was purified by column chromatography on silica flash (0-20% EtOAc in hexanes) to give the compound **8** (83.0 mg, 78% yield).

¹H NMR (400 MHz, CDCl_3) δ 7.56 (d, J = 8.7 Hz, 2H), 7.46 (d, J = 8.6 Hz, 2H), 4.80 – 4.65 (m, 1H), 3.75 (s, 1H), 3.02 (d, J = 5.4 Hz, 1H).

¹³C NMR (126 MHz, CDCl_3) δ 131.8, 131.4, 127.7, 124.4 (q, J = 287.7 Hz), 123.9, 123.17 (q, J = 284.2 Hz), 71.2 (q, J = 29.3 Hz).

¹⁹F NMR (376 MHz, CDCl_3) δ -71.50 (d, J = 6.3 Hz, 3F), -75.23 (s, 3F).

HRMS (EI): Calcd. for $\text{C}_{10}\text{H}_6\text{O}_2\text{BrF}_6$ [M-H]⁻, 350.9461. Found: 350.9457.

TLC: R_f = 0.50, 33% EtOAc in hexanes.

Computational Methods.

Geometry Optimization, Single-Point Energy, and Frequency Calculations

All calculations were performed by using DFT, as implemented in the Jaguar 9.1 suite of ab initio quantum chemistry programs.¹⁰ Geometry optimizations were performed with the M06¹¹ functional using the 6-31G** basis set. Cu was represented by using the Los Alamos LACVP¹²⁻¹³ basis set that included relativistic core potentials. More accurate single-point energies were computed from the optimized geometries by using Dunning's correlation consistent triple- ζ basis set, cc-pVTZ(-f),¹⁴⁻¹⁵ which included a double set of polarization functions. Cu was represented by using a modified version of LACVP, designated as LACV3P, in which the exponents were decontracted to match the effective core potential with triple- ζ quality. Vibrational frequencies were computed at the M06/6-31G** level of theory to derive the zero-point energy (ZPE) and vibrational entropy corrections from unscaled frequencies. Entropy herein referred specifically to the vibrational/rotational/translational entropy of the solutes because the continuum model included the entropy of the solvent implicitly. All intermediates were confirmed as local minima on the potential energy surface with zero imaginary frequencies. Transition states were confirmed to possess only one imaginary frequency. Solvation energies were evaluated by using a self-consistent reaction field (SCRF)¹⁶⁻¹⁸ approach based on accurate numerical solutions of the linearized Poisson–Boltzmann equation. Solvation calculations were carried out on the optimized gas-phase geometries by using a dielectric constant of $\epsilon = 32.63$ for methanol. The change in solution-phase free energy, $\Delta G(\text{sol})$, was calculated from Equations (S1)–(S5).

$$G(\text{sol}) = G(\text{gas}) + \Delta G(\text{solv}) \quad (\text{S1})$$

$$G(\text{gas}) = H(\text{gas}) - TS(\text{gas}) \quad (\text{S2})$$

$$H(\text{gas}) = E(\text{SCF}) + ZPE \quad (\text{S3})$$

$$\Delta E(\text{SCF}) = \sum E(\text{SCF}) \text{ for products} - \sum E(\text{SCF}) \text{ for reactants} \quad (\text{S4})$$

$$\Delta G(\text{sol}) = \sum G(\text{sol}) \text{ for products} - \sum G(\text{sol}) \text{ for reactants} \quad (\text{S5})$$

TDDFT Calculations

All calculations were performed by using DFT and TDDFT, as implemented in the Gaussian 09 Suite of programs.¹⁹ Geometry optimization for bpyCu(CF₃)₃ was performed with the M06¹¹ functional using the 6-311++G(d,2p) basis set. A frequency calculation was performed at the same level of theory to confirm the nature of the convergence as a minimum. TDDFT calculations were performed on the optimized geometry using both M06 with the 6-311++G(d,2p) basis set, and using the M06 and ω b97xd functionals with the cc-PVTZ.¹⁴⁻¹⁵

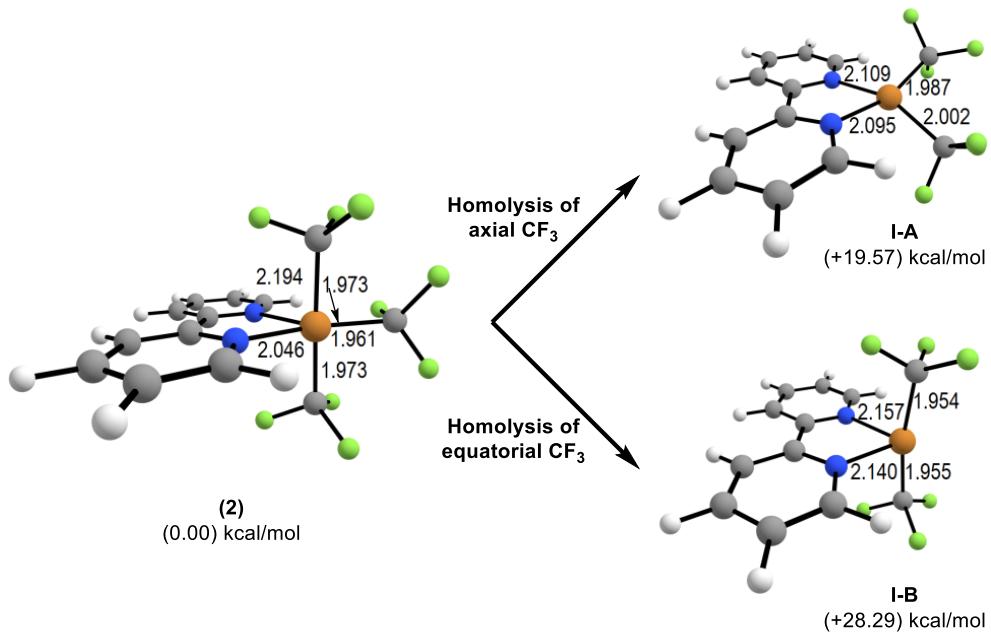


Figure S2: We calculated the B.D.E. for CF_3 from $\text{bpyCu}(\text{CF}_3)_3$ (2). We found two different pathways for bond homolysis: (i) the homolysis of the axial CF_3 results in a square planar species (**I-A**), and (ii) the homolysis of the equatorial CF_3 results in the formation of a T-shaped intermediate (**I-B**). **I-A** was calculated to be more stable than **I-B** by 8.7 kcal/mol.

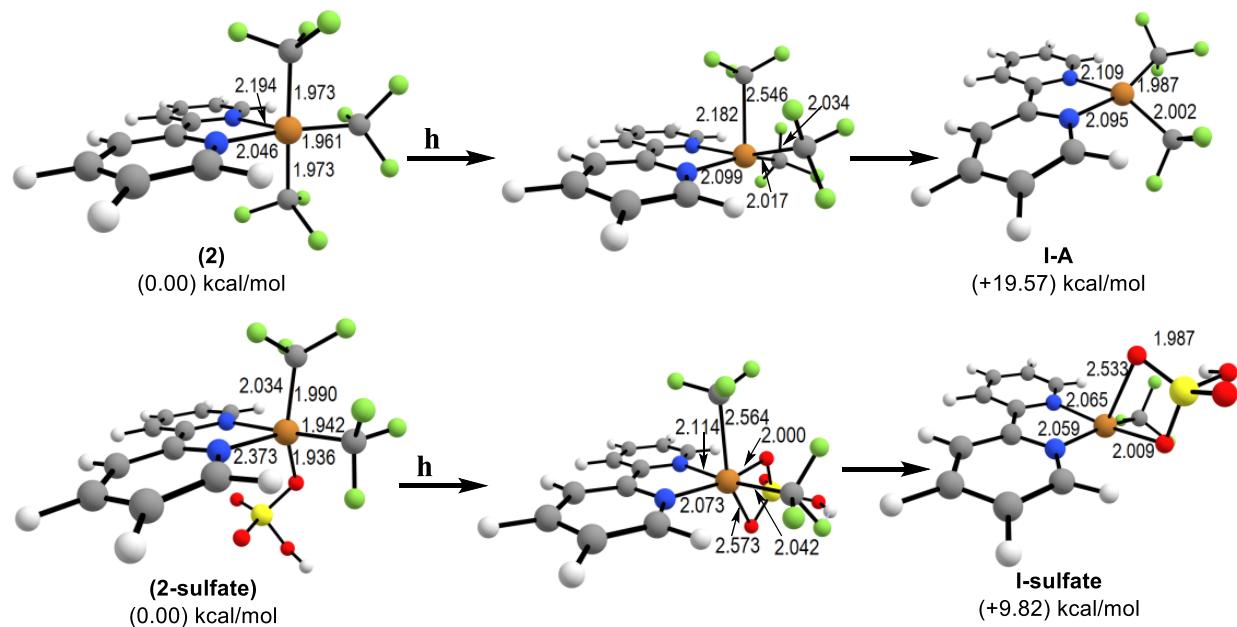


Figure S3: The presence of sulfate ligand results in a significant decrease in the bond-

dissociation energy (BDE). The BDE of Cu-CF₃ in (**2**) was 19.6 kcal/mol, while the Cu-CF₃ in **2-sulfate** was 9.8 kcal/mol.

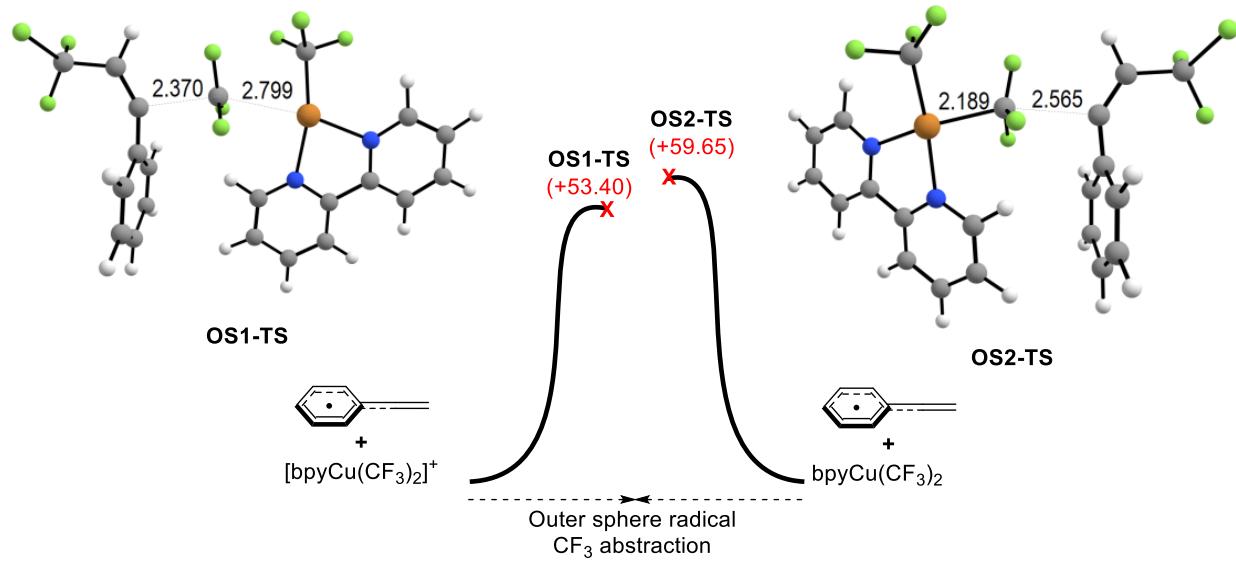


Figure S4: Similar to our previous study,{Guo, 2018 #970} the barriers to outer sphere radical abstraction are too high to achieve under these reaction conditions.

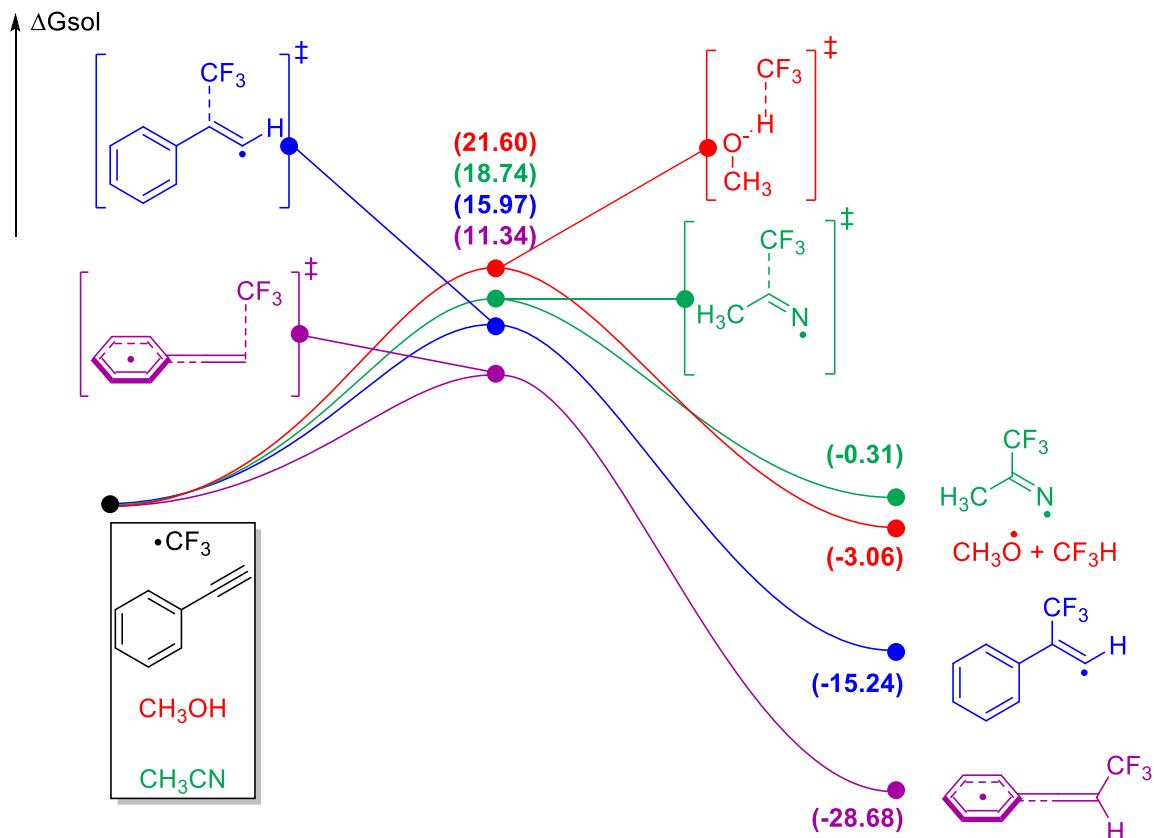
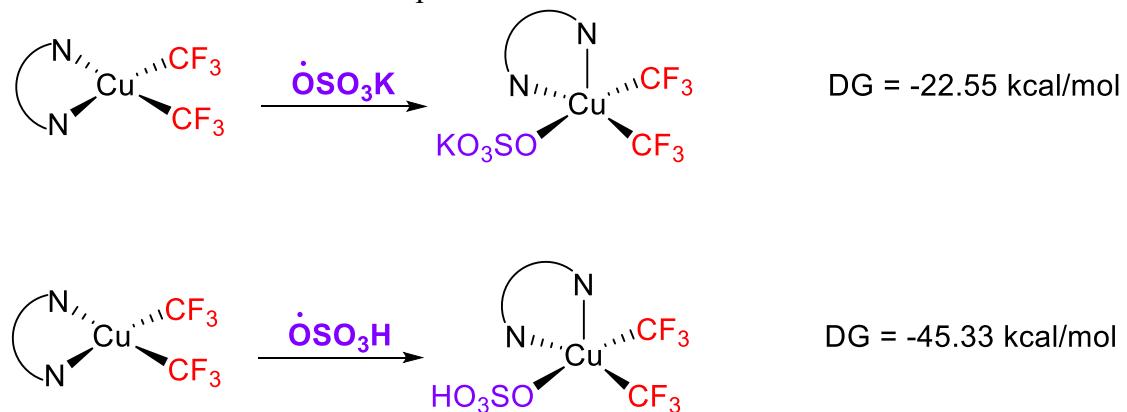


Figure S5: Evaluation of potential side reactions for trifluoromethyl radical . There exist several competing pathways; and while these pathways have a significantly higher barrier, they involve abundant solvent. The surfaces in **blue** and **purple** support the formation of a conjugated allenyl radical over a vinyl radical upon addition of CF_3 to the alkyne. The $\Delta\Delta G^\ddagger$ for this process favors the allenyl radical transition state by 4.6 kcal/mol, in addition to the allenyl radical being thermodynamically more stable than its vinylic isomer by 13.4 kcal/mol. The surfaces in **green** and **red** support the feasibility trifluoromethyl radical reacting with solvent—rendering the reaction inefficient in the absence of persulfate.



Scheme S2: Both sulfonic acid- and potassium sulfate-based oxy-radical addition into $\text{bpyCu}(\text{CF}_3)_2$ is highly exergonic.

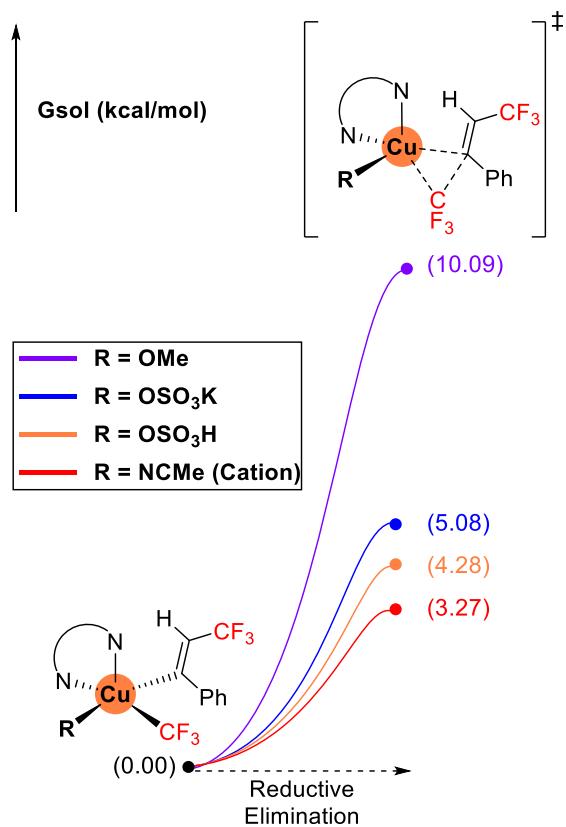


Figure S6: Evaluation of the reductive elimination with various ligands. All ligands proved viable in this reaction pathway.

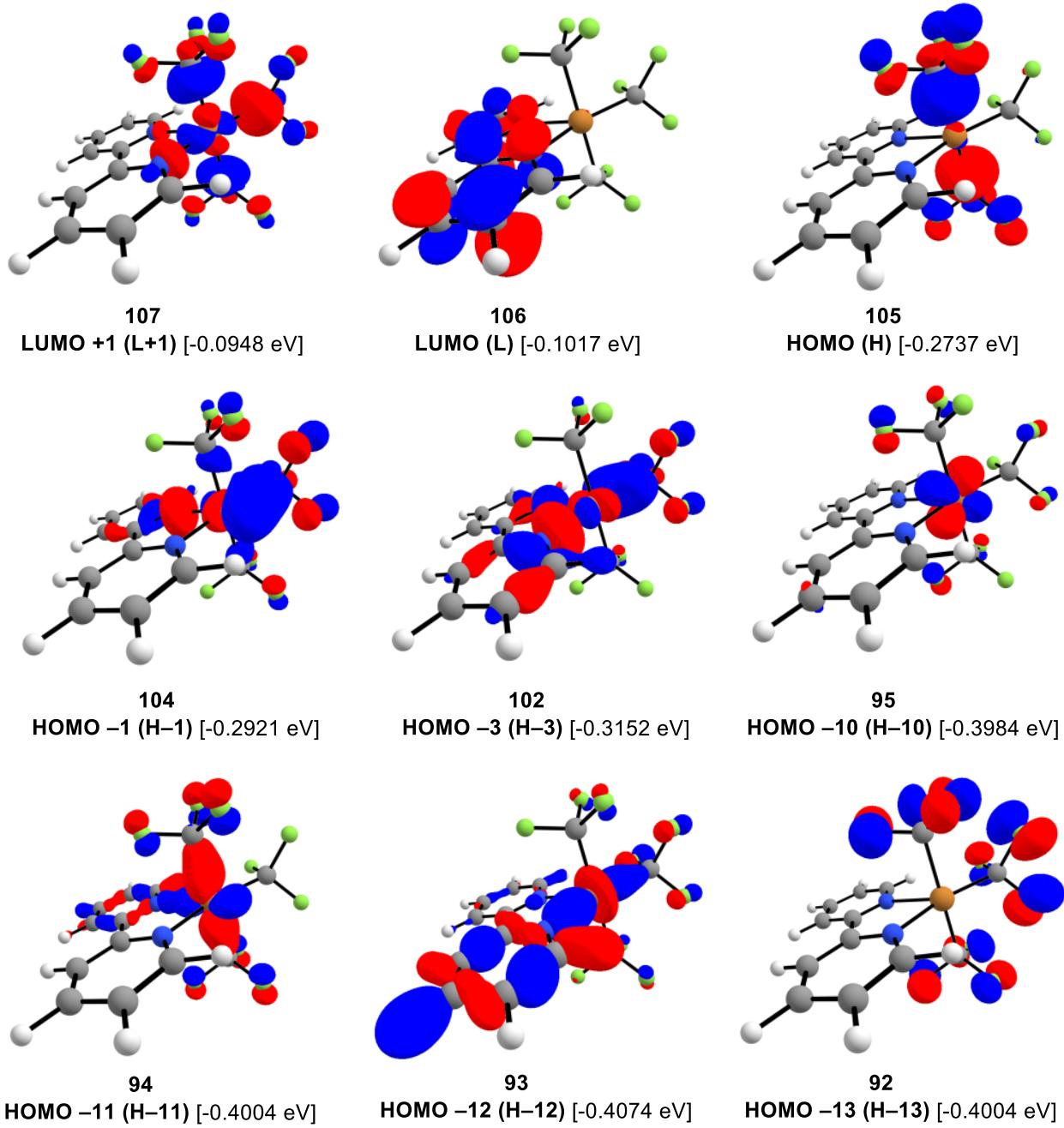
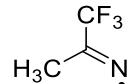
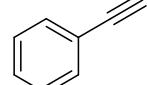
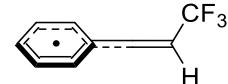
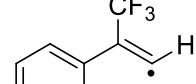


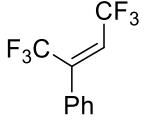
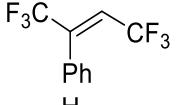
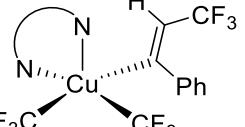
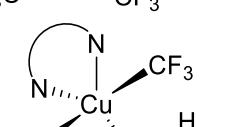
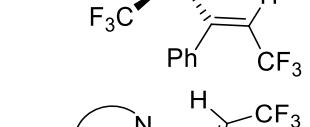
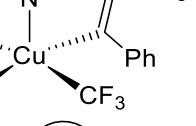
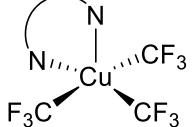
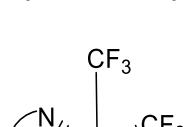
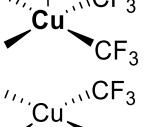
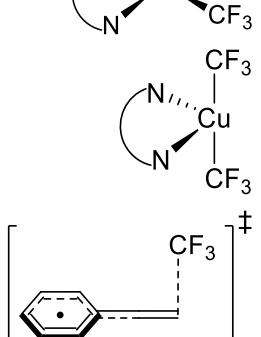
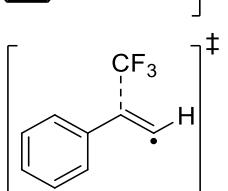
Figure S7: Relevant orbitals for $\text{bpyCu}(\text{CF}_3)_3$ calculated with M06/6-311++G(d,2p) and plotted at isovalue 0.05.

Table S4: TDDFT calculated first singlet and first triplet excitations.

Functional/ Basis Set	Relevant Triplet Excitation Wavelength (nm)	First Singlet Excitations Wavelength (nm)
M06/ 6-311++G(d,2p)	100% H → (L+1) 486.28	6.6% (H-11)→(L+1) 24.3% (H-3)→(L+1) 63.8% (H-1)→(L+1) 362.62
M06/ cc-PVTZ	100% H → (L+1) 488.50	2.7% (H-12)→(L+1) 5.9% (H-11)→(L+1) 27.7% (H-3)→(L+1) 56.5% (H-1)→(L+1) 4.7% (H)→(L) 353.79
ωb97xd/ cc-pVTZ	100% H → (L+1) 488.18	5.2% (H-13)→(L+1) 6.6% (H-10)→(L+1) 26.7% (H-3)→(L+1) 56.7% (H-1)→(L+1) 344.41

Table S5: Calculated Energy Components (M06)

Species	E	E	Z	S	S	G
<i>CF₃ Radical</i>	-9182.18	-9185.25	7.931	65.323	-0.3	-9185.76
<i>CF₃H</i>	-9200.61	-9203.67	16.182	64.108	-2.64	-9203.92
<i>MeO Radical</i>	-3128.74	-3129.78	22.726	56.662	-3.83	-3129.69
<i>Acetonitrile</i>	-3609.78	-3610.92	28.382	60.018	-8.43	-3610.83
<i>MeOH</i>	-3147.02	-3148.1	32.222	56.903	-6.34	-3147.71
	-12793	-12797	38.49	84.313	-4.5	-12796.6
	8385.106	-8387.56	68.549	79.631	-4.98	-8385.83
	-17569.4	-17574.7	78.345	106.231	-4.25	-17572.8
	-17569	-17574.2	78.801	102.275	-3.74	-17572.3

	-26755.8	-26763.9	90.744	118.473	-4.49	-26761.7
	-26756	-26764	90.488	120.062	-4.35	-26761.8
	-54748.5	-54764	198.505	195.292	-14.71	-54758.6
	-54748.6	-54764.1	198.115	205.311	-14.07	-54758.7
	-64599.1	-64615.5	208.236	200.626	-26.57	-64610.2
	-46361.3	-46374.7	126.817	160.405	-13.99	-46371.9
	-46360.2	-46373.3	125.34	183.026	-13.74	-46370.9
	-37177.5	-37187.7	116.989	153.538	-14.67	-37185.2
	-37176.9	-37187.3	116.755	154.476	-14.43	-37184.9
	-17567.4	-17572.8	76.376	108.276	-4.66	-17571.1
	-17567.2	-17572.6	76.357	108.715	-4.38	-17570.9

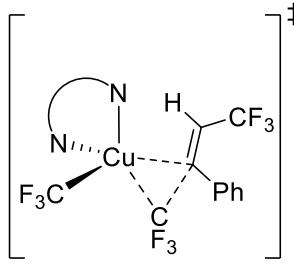
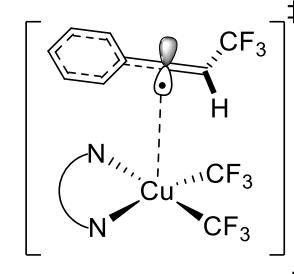
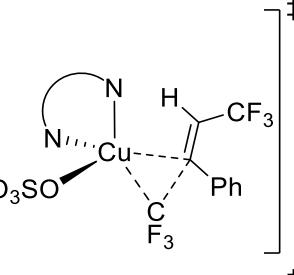
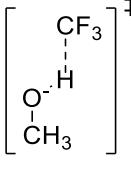
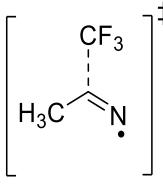
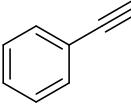
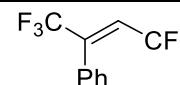
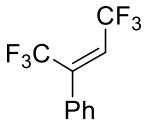
	-54748.1	-54763.4	198.036	199.572	-15.62	-54758
	-54747.3	-54762.7	195.406	201.67	-16.67	-54757.5
	-64599.1	-64615.4	208.032	195.398	-25.9	-64610
	-12328.9	-12333	37.169	82.197	-3.07	-12332.5
	-12791.8	-12795.9	36.636	89.984	-6.6	-12795.8

Table S6: Cartesian Coordinates of the Optimized Geometries.

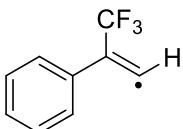
			
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C	0.083234532	0.135065950	-1.835660920
C	2.499632615	0.135068558	-1.836609080
C	0.086736492	0.135054082	-0.447824616
C	2.496300143	0.135056717	-0.448992373
C	1.291909851	0.135048111	0.249048081
H	-0.853358786	0.135078294	-2.38789484
H	3.436118620	0.135069741	-2.389113438
H	-0.856539339	0.135047725	0.092917878
H	3.440144652	0.135053358	0.091142896
H	1.292860551	0.135034830	1.336421534
C	1.291553602	0.135048250	-3.971748333
C	1.292809772	0.135045568	-5.180886518
H	1.294174406	0.135037908	-6.247125461
			
C	1.369519600	-0.267984383	-2.736765185
C	0.264652948	-0.041762967	-1.916683519
C	2.656285550	-0.080408026	-2.235328302
C	0.447157958	0.391263350	-0.609790462
C	2.834913120	0.352803099	-0.927066519
C	1.731624723	0.591168804	-0.114579794
H	-0.736206027	-0.199964907	-2.31380917
H	3.513442212	-0.269005605	-2.87859445
H	-0.416759074	0.575972541	0.023965646
H	3.839915831	0.506760057	-0.541830016

H	1.872661991	0.933601432	0.907723095
C	1.169939436	-0.732014489	-4.132280541
C	1.002583323	0.024428043	-5.213472476
H	0.862703656	-0.438257579	-6.18765419
C	1.006443257	1.515296883	-5.278377951
F	1.108825599	2.117393297	-4.098783105
F	2.026677007	1.930954591	-6.040164801
F	-0.119832619	1.944516577	-5.861160644
C	1.155044986	-2.231162789	-4.284930410
F	0.950985645	-2.629512342	-5.542263177
F	2.321674288	-2.745221187	-3.880730461
F	0.193816735	-2.767489695	-3.529772699

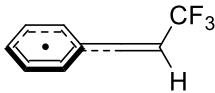


C	1.466652088	-0.390392481	-2.595472114
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C	2.687250771	-0.537984045	-1.926641264
C	0.577015209	0.754618617	-0.652357161
C	2.847377534	-0.037617500	-0.641490666
C	1.795292082	0.607232007	0.000461347
H	-0.544687689	0.355713308	-2.44366378
H	3.520436769	-1.027404998	-2.42045753
H	-0.254701690	1.248237058	-0.15564176
H	3.805083334	-0.149810433	-0.13919640
H	1.924652876	0.991911952	1.009209364
C	1.266656439	-0.833082771	-3.994840827
C	0.709681668	0.007887925	-4.874428915
H	0.508809139	1.027627314	-4.552174295
C	0.317941443	-0.235128497	-6.300639350

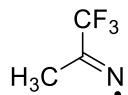
F	-0.598776232	0.676591550	-6.652481945
F	1.353447937	-0.095545472	-7.132668031
F	-0.219357746	-1.436792564	-6.507914550
C	1.597690124	-2.263282374	-4.370371029
F	2.053924577	-2.359530573	-5.619014806
F	2.531626370	-2.790395315	-3.572104177
F	0.511482061	-3.030719027	-4.262891811



C	1.718165924	-0.792872239	-2.842123477
C	0.725564776	-1.125657109	-1.914049445
C	2.884804044	-1.563448496	-2.885711313
C	0.897986954	-2.208365093	-1.060853699
C	3.051627784	-2.647062330	-2.035771092
C	2.056471743	-2.974793743	-1.119857340
H	-0.188449238	-0.541569663	-1.86442884
H	3.676736774	-1.291669191	-3.58156541
H	0.116394902	-2.456706556	-0.34670191
H	3.967550976	-3.231639608	-2.08086388
H	2.186771972	-3.821637527	-0.45030506
C	1.550622864	0.329962881	-3.793887570
C	2.071099777	0.354627032	-5.004994584
H	2.653656074	-0.315681488	-5.62288165
C	0.743976921	1.527236867	-3.358131043
F	0.860967684	2.542140176	-4.212817415
F	-0.564426129	1.231477846	-3.273337628
F	1.124995522	1.958677916	-2.152257360

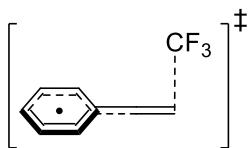


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C	0.630211379	-2.301185398	-1.348943361
C	3.026416787	-2.306107374	-1.676925099
C	1.908247340	-2.675622145	-0.923450012
H	-0.533187310	-1.274408957	-2.83935573
H	3.750556243	-1.282998526	-3.42558392
H	-0.240598453	-2.587759964	-0.76390280
H	4.021267678	-2.596256788	-1.34710828
H	2.032130479	-3.251473279	-0.00993411
C	1.433060005	-0.450510982	-4.433798627
C	1.276660702	0.199802818	-5.549025714
H	1.147265898	-0.292129773	-6.51806046
C	1.276870612	1.697087118	-5.628568987
F	1.403655799	2.271767428	-4.434476818
F	2.279756864	2.131401003	-6.402995362
F	0.141134523	2.141840092	-6.181291303

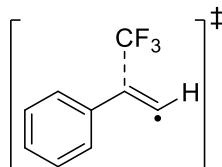


C	1.282951357	0.082110254	-3.951961400
N	1.417861620	0.103240430	-5.195722498
C	1.853378922	1.105806992	-3.012470632
H	1.049465752	1.542859574	-2.411116864
H	2.562486983	0.624214336	-2.330522710
H	2.362606054	1.891931916	-3.572074252

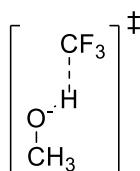
C	0.490712648	-1.042541187	-3.299067522
F	-0.545485499	-0.532410490	-2.626723234
F	0.034593420	-1.915860837	-4.180490030
F	1.264605367	-1.685077441	-2.419631752



C	1.389077772	-1.050626434	-3.031059832
C	0.304555562	-1.397502042	-2.211086510
C	2.642990471	-1.634666594	-2.795198145
C	0.474974877	-2.309672217	-1.180736457
C	2.803085568	-2.545766036	-1.762264384
C	1.722105281	-2.885517029	-0.953093325
H	-0.665909034	-0.944663902	-2.39889768
H	3.479985366	-1.365149988	-3.43466061
H	-0.370665099	-2.575499931	-0.55104039
H	3.777134980	-2.996187104	-1.58721520
H	1.851578398	-3.600963494	-0.14458997
C	1.218164562	-0.123224954	-4.092717084
C	1.049177447	0.582010934	-5.072411600
H	0.954965862	1.399645157	-5.753900032
C	0.517217490	-1.045016293	-6.847991913
F	-0.687143774	-0.824425854	-7.341668141
F	1.421110689	-0.986944682	-7.808425234
F	0.561236695	-2.212318873	-6.243098655

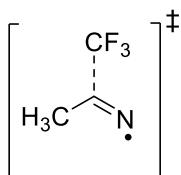


C	0.596493929	0.710966912	-2.426034272
C	-0.106493287	1.865631259	-2.792969958
C	1.368500837	0.722174103	-1.260061531
C	-0.036385810	3.007235570	-2.008287126
C	1.429803745	1.866574490	-0.476609607
C	0.730770889	3.010639803	-0.847189675
H	-0.704819171	1.848733539	-3.70060982
H	1.914741176	-0.170529745	-0.96876812
H	-0.584219977	3.89765783	-2.304552743
H	2.028562578	1.863945459	0.430870537
H	0.784206726	3.905550251	-0.231827617
C	0.468671696	-0.460400262	-3.259095332
C	-0.106572294	-1.251314252	-4.00475735
H	-0.377806808	-2.044081643	-4.66676349
C	2.632835322	-1.194789059	-3.351894792
F	3.462906869	-0.181856787	-3.511326088
F	2.947113144	-1.871635226	-2.256075017
F	2.681341655	-1.995522607	-4.396604080

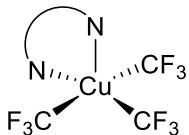


C	0.409178619	-1.047175464	-3.338291853
F	-0.663974928	-0.812826206	-2.600042444
F	0.066266209	-1.669048992	-4.449381110
F	1.266594208	-1.783245386	-2.651407345

C	1.509156645	1.483049547	-2.140906665
H	0.500034113	1.655379342	-1.736025552
H	2.031001866	0.742863388	-1.513551560
H	2.065910896	2.426996149	-2.060223505
O	1.509562598	1.147055149	-3.491832331
H	0.985445549	0.115991085	-3.600452316

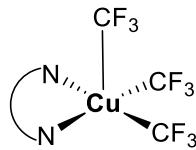


C	1.340338530	0.156624662	-4.142056855
N	1.237610949	-0.167679089	-5.27097460
C	1.748032359	0.960471037	-2.983335001
H	0.867818760	1.313240527	-2.437822092
H	2.355062832	0.359615302	-2.299678831
H	2.331113411	1.820982751	-3.321284796
C	0.250087507	-1.383651769	-3.036185859
F	-0.709624305	-0.775298535	-2.362602765
F	-0.242079628	-2.264947508	-3.864023797
F	1.107320012	-1.942068510	-2.200667584



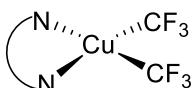
Cu	-0.717828211	-0.245194336	0.00256064
N	1.038629502	-1.294371079	0.014444416
C	1.064990821	-2.624792574	0.039578925
H	0.096680991	-3.123428301	0.045385533
C	2.253678739	-3.340464040	0.057540725
H	2.238537266	-4.425395877	0.077619859

C	3.446063841	-2.628858048	0.049668112
H	4.400254048	-3.149098056	0.063658830
C	3.412254551	-1.242090773	0.024697920
H	4.337884185	-0.674837579	0.020075347
C	2.181770010	-0.590181414	0.007555931
N	0.790723863	1.348245490	-0.019264091
C	2.045963219	0.886610532	-0.017176876
C	3.131854169	1.759219584	-0.038104510
H	4.152415121	1.388162285	-0.037883989
C	2.889413173	3.126523012	-0.060906822
H	3.721999790	3.825191518	-0.077529670
C	1.580606570	3.590585536	-0.063012596
H	1.355399819	4.652430218	-0.080968877
C	0.553580670	2.654553911	-0.042007358
H	-0.496138052	2.945789763	-0.04359768
C	-0.749053924	-0.247913193	-1.97027674
C	-2.628593598	0.194576579	0.001598651
C	-0.744434187	-0.218476497	1.975604161
F	-1.351876447	-1.332735980	-2.484628169
F	0.511232815	-0.257467591	-2.467494920
F	-1.333475341	0.842295589	-2.495087028
F	-2.666218019	1.541924455	0.001297957
F	-3.313966396	-0.225366299	-1.061529632
F	-3.311517663	-0.225703120	1.066350823
F	-1.339424138	0.869827520	2.491099232
F	-1.333581350	-1.304801327	2.503450436
F	0.517266662	-0.208237311	2.469500057



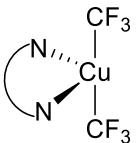
Cu	-0.506502692	0.133239812	-0.56297229
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H	0.542323519	-2.867131739	-0.77590127
C	2.633342511	-3.014559658	-0.225268012
H	2.682621238	-4.093789123	-0.33314252
C	3.741130552	-2.273895686	0.162689601
H	4.691105540	-2.762760011	0.364530064
C	3.627085174	-0.896409084	0.292293193
H	4.488720636	-0.306436367	0.588961962
C	2.397385230	-0.293984780	0.032955303
N	0.947993047	1.602636069	-0.202033997
C	2.169658153	1.166330628	0.151358964
C	3.146331380	2.052081002	0.599414682
H	4.125091318	1.694493785	0.903452564
C	2.850435630	3.406662115	0.664012502
H	3.600651066	4.110833997	1.014353498
C	1.591607901	3.847327806	0.280621439
H	1.322027385	4.898071959	0.314220189
C	0.663950087	2.904451368	-0.140712169
H	-0.343507639	3.184537433	-0.4378307
C	-1.537801949	-1.318745668	-1.51060528
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F	-1.824434100	-2.361057648	-0.686810883
F	-0.746327160	-1.850656790	-2.488555128

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F	-2.312919918	2.244097529	-1.048763974
F	-3.312166891	0.645157863	0.012783547
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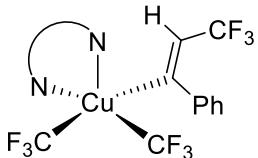
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C	2.469158965	-3.181704116	0.405075333
H	2.495224956	-4.250388131	0.593647136
C	3.621384729	-2.472012448	0.092147014
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H	4.433923827	-0.535784549	-0.36955684
C	2.295303884	-0.482658462	-0.061748455
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C	2.093963600	0.966699558	-0.293018207
C	3.089175881	1.811114118	-0.779945330
H	4.070218253	1.424110833	-1.039401043
C	2.804202183	3.160151527	-0.942227691
H	3.567631589	3.835644794	-1.319680857
C	1.538413905	3.633913316	-0.622537777
H	1.280721753	4.682547738	-0.732730407
C	0.592279316	2.728755800	-0.160761683
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C	-2.192962529	0.973487799	0.125448305
C	-1.416302795	-1.242810932	1.897959615
F	-2.322158486	2.014829927	0.998211571
F	-2.086342916	1.558628735	-1.103558387
F	-3.363510860	0.327170853	0.131099608
F	-2.468053817	-0.780705665	2.581836378
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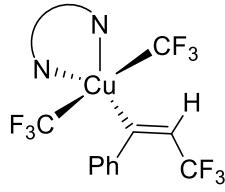
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C	3.583745614	-2.657154530	0.163680959
H	4.549474007	-3.153849893	0.210688174
C	3.518891783	-1.273450777	0.091915737
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N	0.869625711	1.307925882	-0.030962322
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C	3.211000310	1.692424925	-0.115753750
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C	2.987529144	3.060045594	-0.181442934
H	3.828871965	3.745906353	-0.239322655
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H	1.469559704	4.602570091	-0.234394101

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H	-0.392207231	2.928941892	-0.11759939
C	-0.851863884	-0.026212650	-1.93779845
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F	-1.716970256	-0.883332829	-2.527181222
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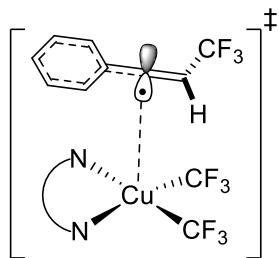
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C	1.846979003	-3.388300177	1.696934368
H	1.639696544	-4.355247893	2.145375999
C	3.137196752	-3.014464989	1.345406524
H	3.973031543	-3.690105672	1.509396860
C	3.356236733	-1.763249251	0.785426620
H	4.364152002	-1.459912333	0.520069753
C	2.266109623	-0.916842360	0.583126067
N	1.273186855	1.181537590	-0.063939334
C	2.399263346	0.454081959	0.030725951
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H	4.530419983	0.405728857	-0.307671225
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C	2.506808281	3.052770772	-0.877321382
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C	1.321133270	2.442529572	-0.494674962
H	0.368913488	2.967845692	-0.557512098
C	-2.352632609	-0.348319249	0.481644817
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F	-3.139975278	-0.246066834	-0.598418361
F	-2.226311126	-1.665493846	0.756248146
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C	-1.473372635	3.082352387	-3.102212876
C	-0.393048864	3.285628378	-3.956444339
H	1.271064973	0.373309267	-3.397001667
H	-2.406780798	1.761731062	-1.67682069
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H	-0.057884419	-2.778317082	1.43208620
C	2.052273381	-3.126831269	1.732160040
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C	2.336581867	3.131058132	-1.316427644
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C	1.170182091	2.443421679	-0.998477522
H	0.197613839	2.854475678	-1.259230144
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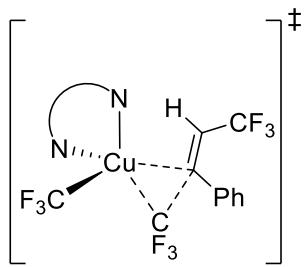
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C	-2.182244842	3.463657323	-2.497691391
C	-1.805814628	4.334390882	-0.284573171
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H	-2.548716168	1.340257237	-2.62002049
H	-1.854544184	2.896650034	1.316807571
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H	4.493162383	-0.813892120	0.438291726
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N	1.213032869	1.645294543	0.130884213
C	2.398539279	1.009960275	0.158988587
C	3.583285754	1.698178608	-0.096094478
H	4.538746254	1.182754023	-0.077275099
C	3.535816241	3.060325427	-0.358470395
H	4.453798682	3.609912247	-0.551699245
C	2.308883010	3.709085966	-0.364659163
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C	-0.475556933	-0.618036540	-2.15045200
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H	-0.828188365	-2.247594098	-0.89797690
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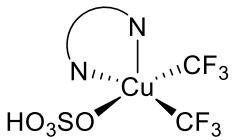
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H	1.899793197	0.151531368	-3.072743739
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H	4.397497259	-1.174823758	1.603038170
C	2.393753202	-0.922084630	0.827196052
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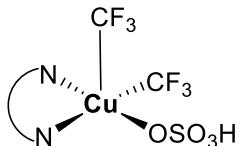
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F	-3.186036870	-0.586620962	-1.112759756
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F	-1.218698771	-1.224141900	-4.322604261
F	0.834663893	-1.731056214	-3.904764190
F	-0.715614232	-3.193059561	-3.601821830
C	-0.962293643	1.037582911	-2.309342654
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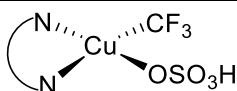
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H	-0.326431477	-3.097220018	0.10810259
C	1.781336563	-3.341183676	-0.295998845
H	1.747239939	-4.425228473	-0.30358917
C	2.959354027	-2.647816378	-0.530099087
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C	1.665589859	0.893286402	-0.292131133
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H	3.736114392	1.265671634	-0.816215233
C	2.606730465	3.074227453	-0.617094300
H	3.450936784	3.715821472	-0.858200411
C	1.359687323	3.614342680	-0.339368673
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C	0.317798535	2.741179555	-0.046835924
H	-0.678516331	3.117630786	0.176729570
C	-2.629515713	0.925976785	0.459487733
C	-1.104676259	-0.502980900	2.118104069
F	-2.352951872	1.862463348	1.370726868

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F	-3.765415634	0.330255770	0.772370123
F	-2.142517219	-0.191228610	2.879082558
F	-0.875124478	-1.812940889	2.293593850
F	-0.047974168	0.170224985	2.561648548
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S	-0.860440855	-0.685781444	-2.806160527
O	0.041112916	-1.806931647	-2.98821770
O	-0.303926241	0.663049864	-2.82893169
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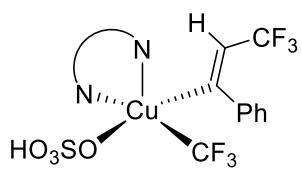
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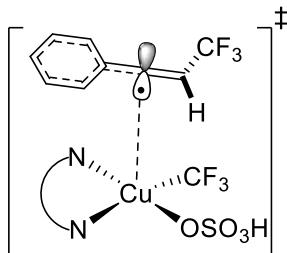
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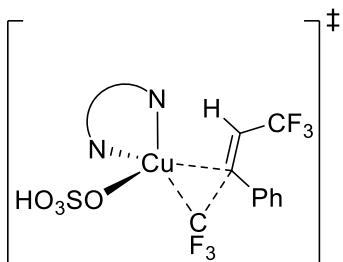
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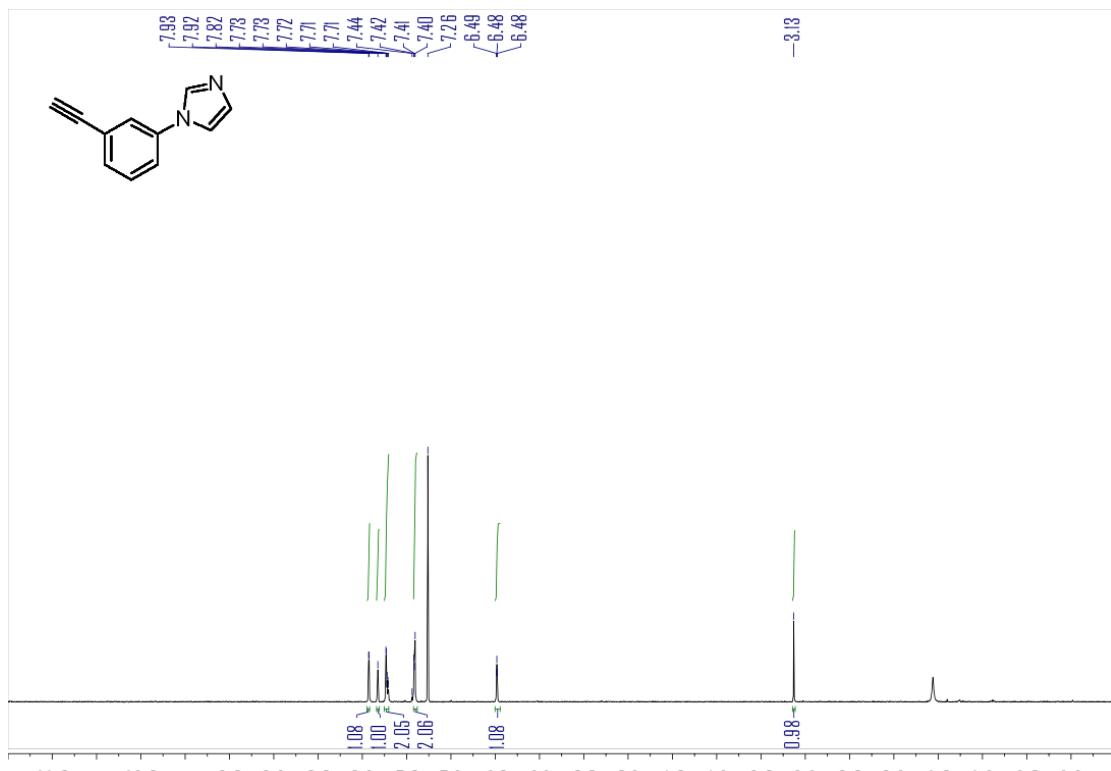
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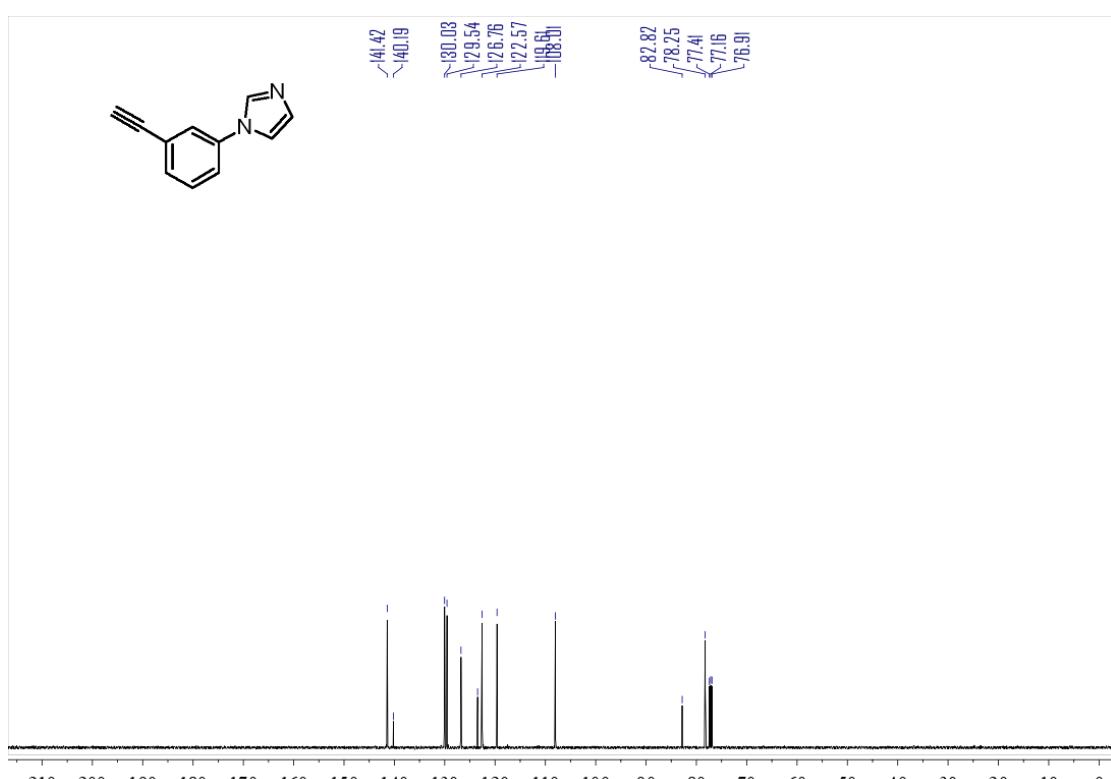
1. Romine, A. M.; Nebra, N.; Konovalov, A. I.; Martin, E.; Benet-Buchholz, J.; Grushin, V. V., Easy Access to the Copper(III) Anion $[\text{Cu}(\text{CF}_3)_4]^-$. *Angew. Chem., Int. Ed.* **2015**, *54*, 2745-2749.
2. Zhang, S. L.; Bie, W. F., Isolation and characterization of copper(III) trifluoromethyl complexes and reactivity studies of aerobic trifluoromethylation of arylboronic acids. *RSC Adv.* **2016**, *6*, 70902-70906.
3. Chan, W.-K.; Ho, C.-M.; Wong, M.-K.; Che, C.-M., Oxidative Amide Synthesis and N-Terminal α -Amino Group Ligation of Peptides in Aqueous Medium. *J. Am. Chem. Soc.* **2006**, *128*, 14796-14797.
4. Wender, P. A.; Lesser, A. B.; Sirois, L. E., Rhodium Dinaphthocyclooctatetraene Complexes: Synthesis, Characterization and Catalytic Activity in [5+2] Cycloadditions. *Angew. Chem., Int. Ed.* **2012**, *51*, 2736-2740.
5. Hübscher, J.; Seichter, W.; Gruber, T.; Kortus, J.; Weber, E., Synthesis and Structural Characterization of Ethynylene-Bridged Bisazines Featuring Various α -Substitution. *J. Heterocycl. Chem.* **2015**, *52*, 1062-1074.
6. Santandrea, J.; Minozzi, C.; Cruché, C.; Collins, S. K., Photochemical Dual-Catalytic Synthesis of Alkynyl Sulfides. *Angew. Chem., Int. Ed.* **2017**, *56*, 12255-12259.
7. Zhang, Z.; Jiang, X., Oxidative Coupling of Terminal Alkyne with α -Hydroxy Ketone: An Expedient Approach toward Ynediones. *Org. Lett.* **2014**, *16*, 4400-4403.
8. Shi, S.-L.; Buchwald, S. L., Copper-catalysed selective hydroamination reactions of alkynes. *Nat. Chem.* **2014**, *7*, 38-44.
9. Duan, J.; Dolbier, W. R.; Chen, Q.-Y., A New and Improved Synthesis of *trans*-1,2-Diodoalkenes and Their Stereospecific and Highly Regioselective Trifluoromethylation. *J. Org. Chem.* **1998**, *63*, 9486-9489.
10. Bochevarov, A. D.; Harder, E.; Hughes, T. F.; Greenwood, J. R.; Braden, D. A.; Philipp, D. M.; Rinaldo, D.; Halls, M. D.; Zhang, J.; Friesner, R. A., Jaguar: A high-performance quantum chemistry software program with strengths in life and materials sciences. *Int. J. Quantum Chem.* **2013**, *113*, 2110-2142.
11. Zhao, Y.; Truhlar, D. G., The M06 suite of density functionals for main group thermochemistry, thermochemical kinetics, noncovalent interactions, excited states, and transition elements: two new functionals and systematic testing of four M06-class functionals and 12 other functionals. *Theor. Chem. Acc.* **2008**, *120*, 215-241.
12. Hay, P. J.; Wadt, W. R., Ab initio effective core potentials for molecular calculations. Potentials for the transition metal atoms Sc to Hg. *J. Chem. Phys.* **1985**, *82*, 270-283.
13. Hay, P. J.; Wadt, W. R., Ab initio effective core potentials for molecular calculations. Potentials for K to Au including the outermost core orbitals. *J. Chem. Phys.* **1985**, *82*, 299-310.
14. Kendall, R. A.; Dunning, T. H.; Harrison, R. J., Electron affinities of the first-row atoms revisited. Systematic basis sets and wave functions. *J. Chem. Phys.* **1992**, *96*, 6796-6806.
15. Dunning, T. H., Gaussian basis sets for use in correlated molecular calculations. I. The atoms boron through neon and hydrogen. *J. Chem. Phys.* **1989**, *90*, 1007-1023.

16. Friedrichs, M.; Zhou, R.; Edinger, S. R.; Friesner, R. A., Poisson–Boltzmann Analytical Gradients for Molecular Modeling Calculations. *J. Phys. Chem. B* **1999**, *103*, 3057-3061.
17. Edinger, S. R.; Cortis, C.; Shenkin, P. S.; Friesner, R. A., Solvation Free Energies of Peptides: Comparison of Approximate Continuum Solvation Models with Accurate Solution of the Poisson–Boltzmann Equation. *J. Phys. Chem. B* **1997**, *101*, 1190-1197.
18. Marten, B.; Kim, K.; Cortis, C.; Friesner, R. A.; Murphy, R. B.; Ringnalda, M. N.; Sitkoff, D.; Honig, B., New Model for Calculation of Solvation Free Energies: Correction of Self-Consistent Reaction Field Continuum Dielectric Theory for Short-Range Hydrogen-Bonding Effects. *J. Chem. Phys.* **1996**, *100*, 11775-11788.
19. Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Mennucci, B.; Petersson, G. A.; Nakatsuji, H.; Caricato, M.; Li, X.; Hratchian, H. P.; Izmaylov, A. F.; Bloino, J.; Zheng, G.; Sonnenberg, J. L.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Montgomery, J. A.; Peralta, J. E.; Ogliaro, F.; Bearpark, M.; Heyd, J. J.; Brothers, E.; Kudin, K. N.; Staroverov, V. N.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Rega, N.; Millam, J. M.; Klene, M.; Knox, J. E.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Zakrzewski, V. G.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Dapprich, S.; Daniels, A. D.; Farkas; Foresman, J. B.; Ortiz, J. V.; Cioslowski, J.; Fox, D. J., Gaussian 09, Revision B.01. Wallingford CT, **2009**.

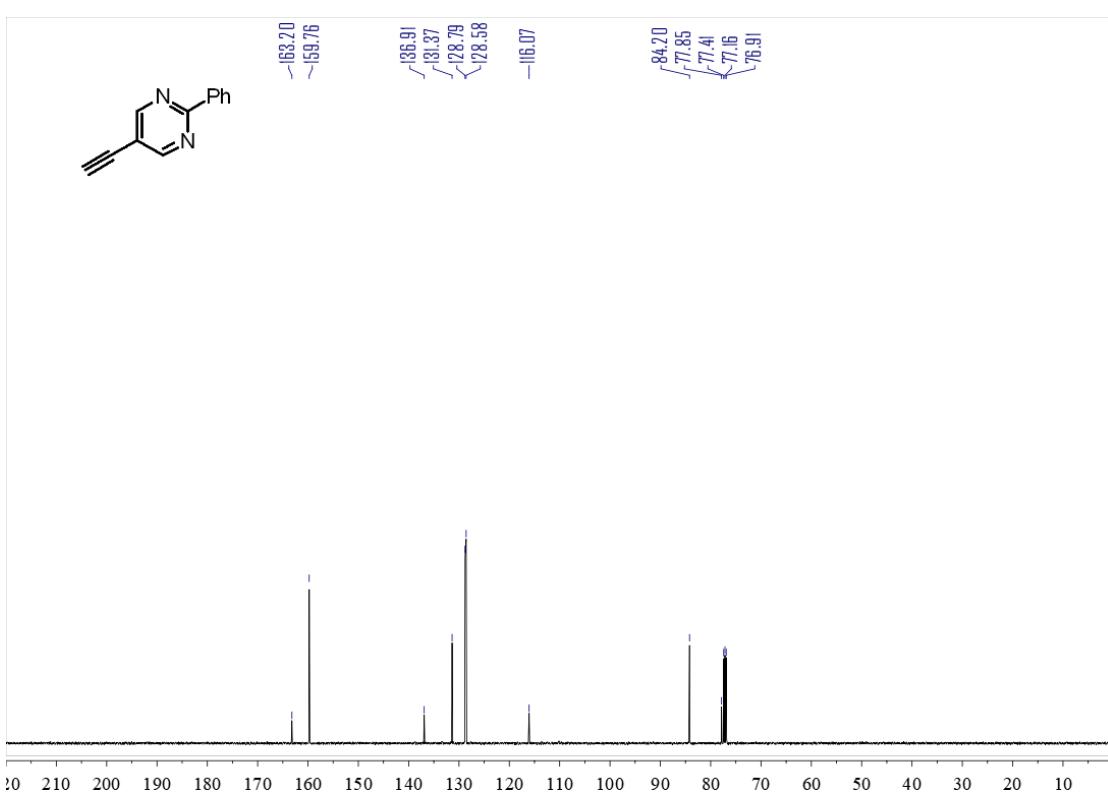
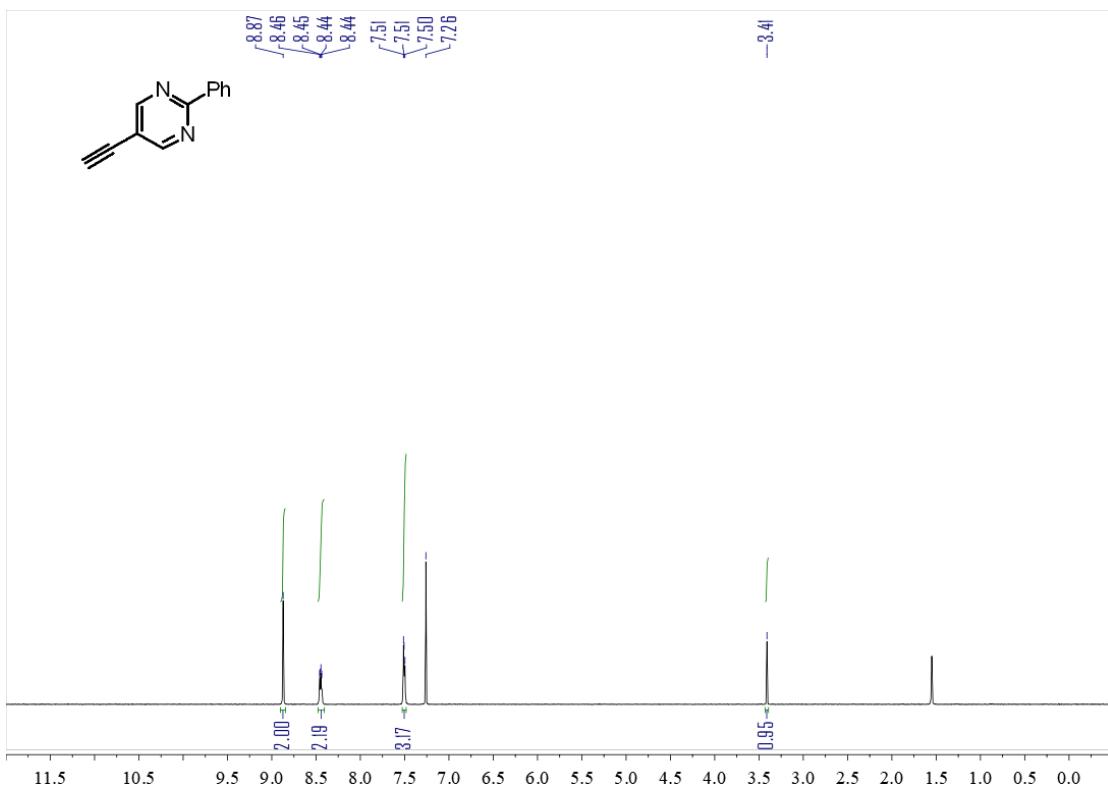
NMR Spectra.



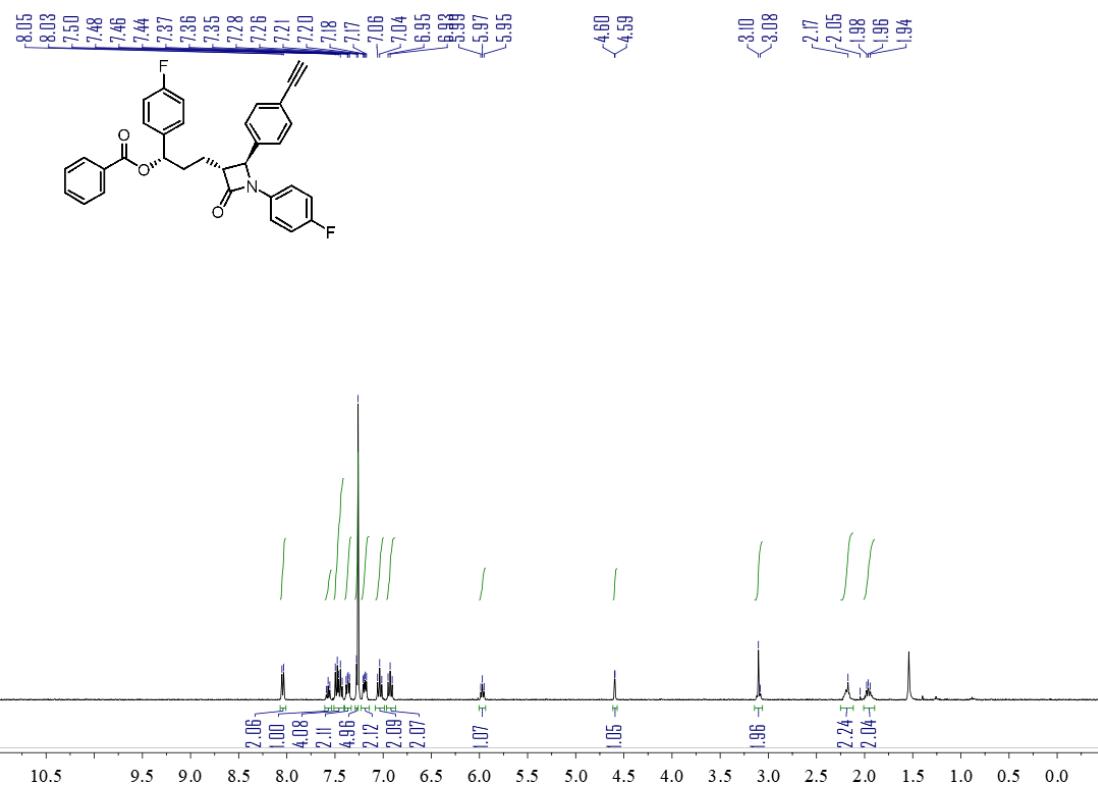
¹H NMR spectrum (400 MHz, CDCl₃, 23 °C) of **1v**



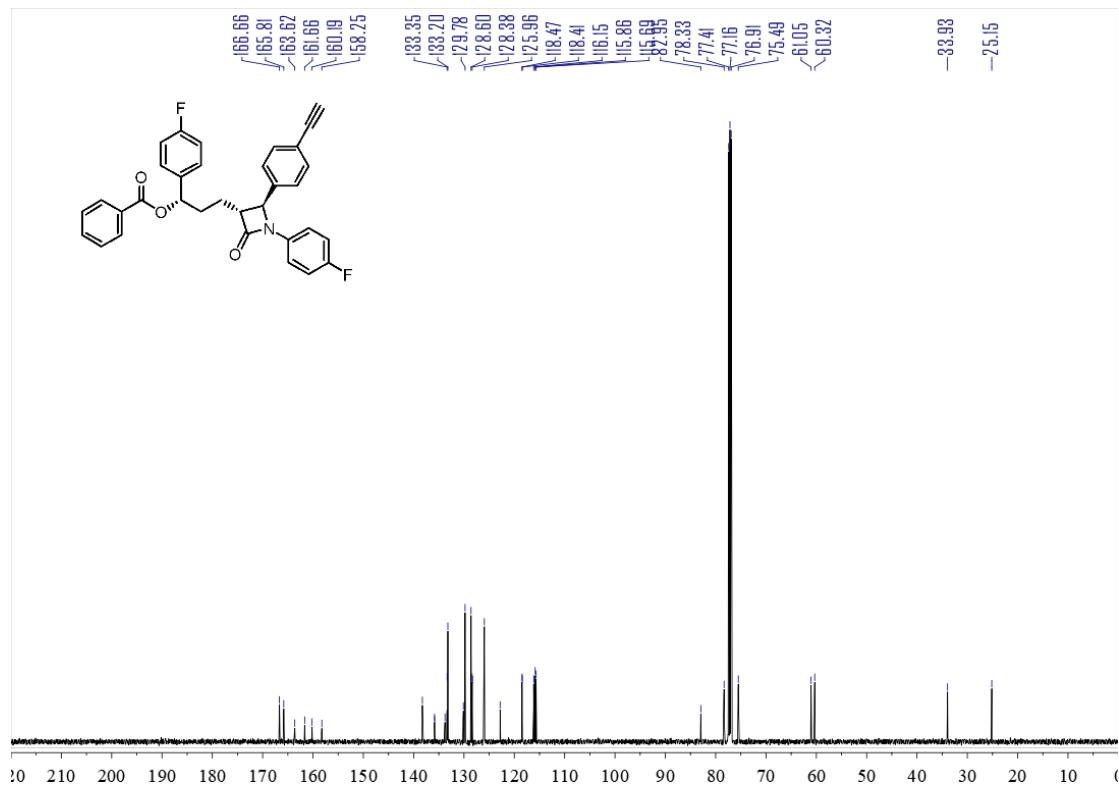
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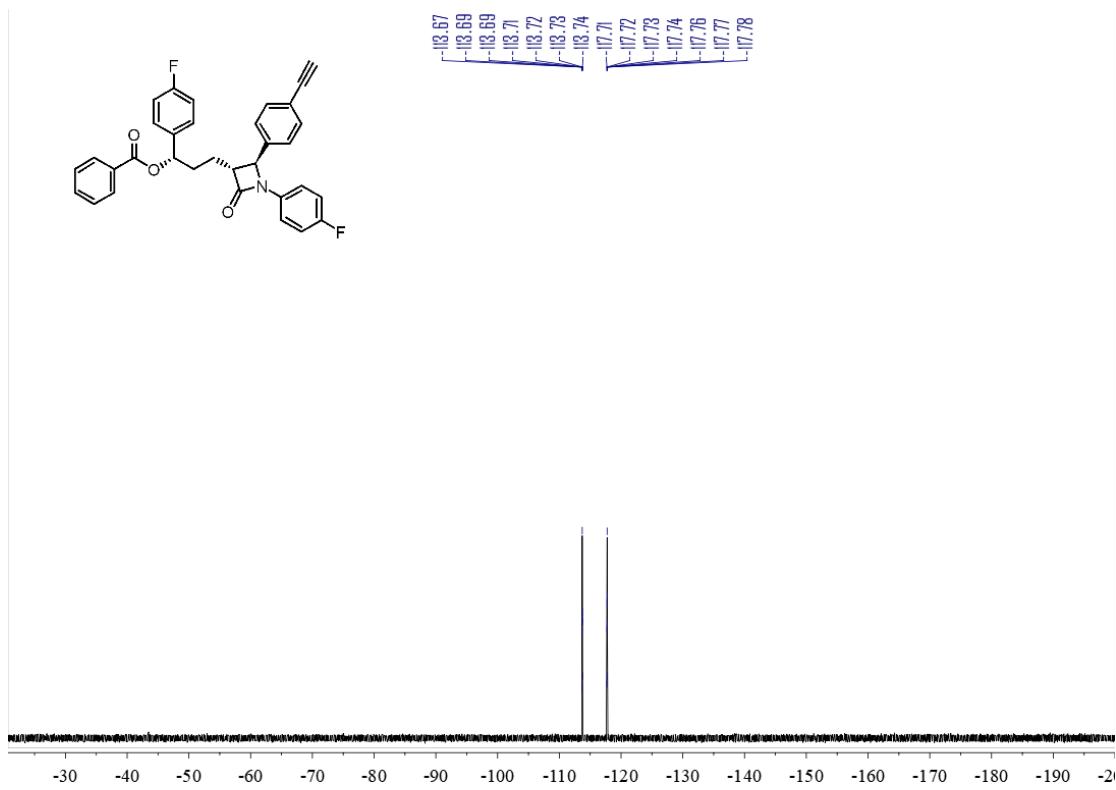
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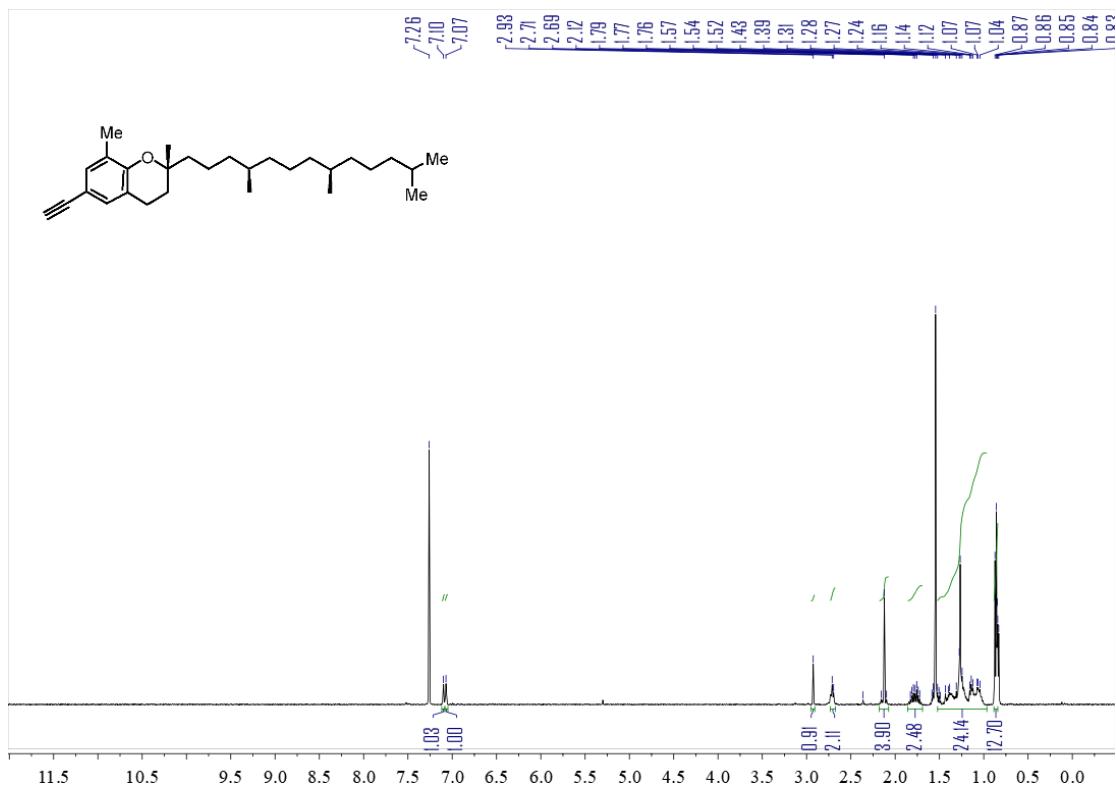
¹H NMR spectrum (400 MHz, CDCl₃, 23 °C) of S3



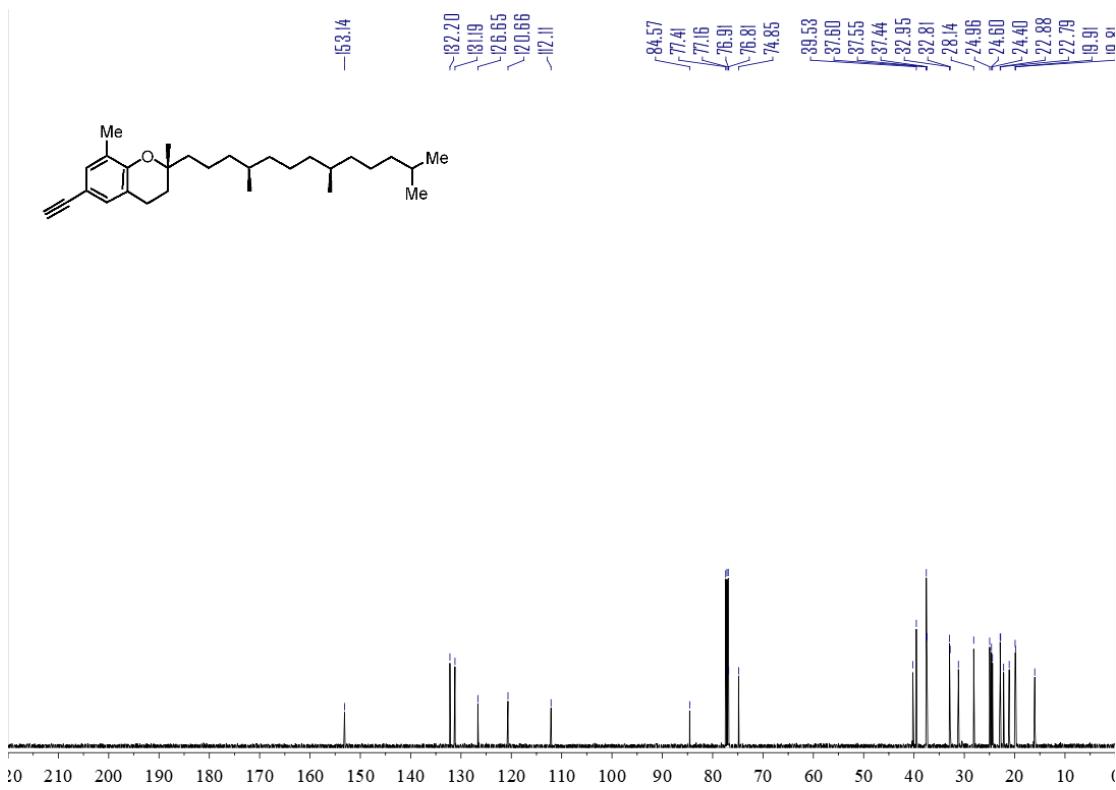
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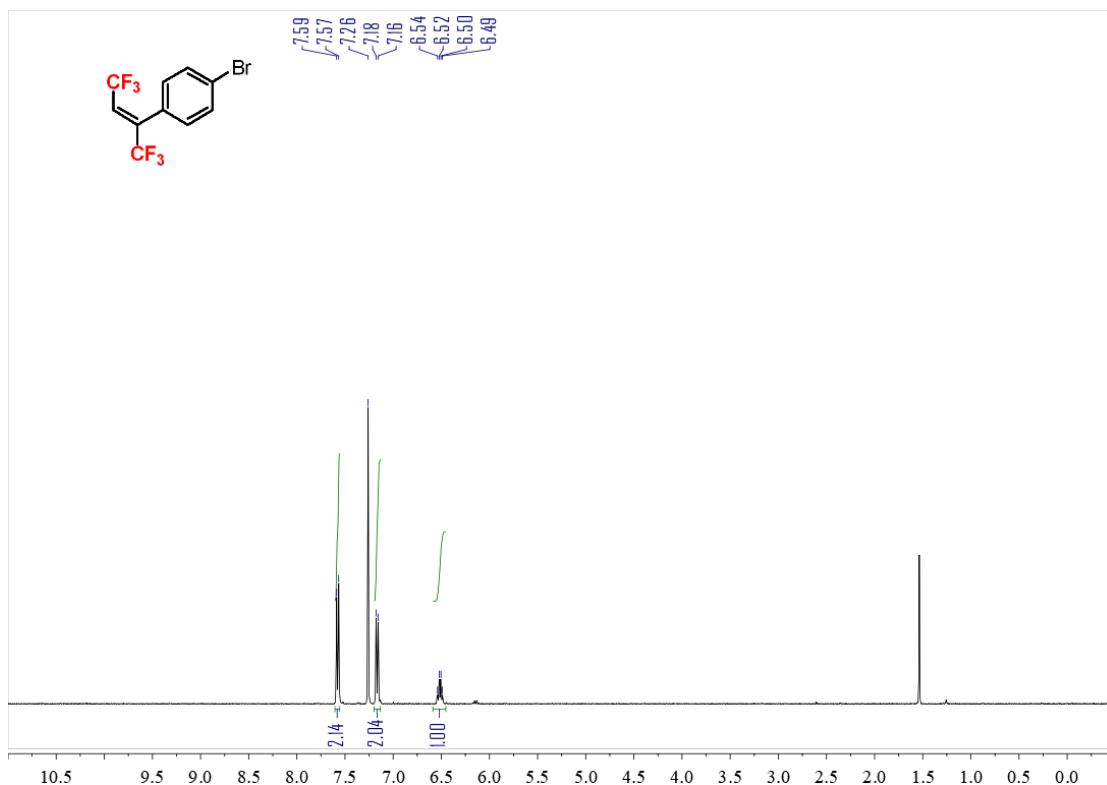
^{19}F NMR spectrum (375 MHz, CDCl_3 , 23 °C) of S3



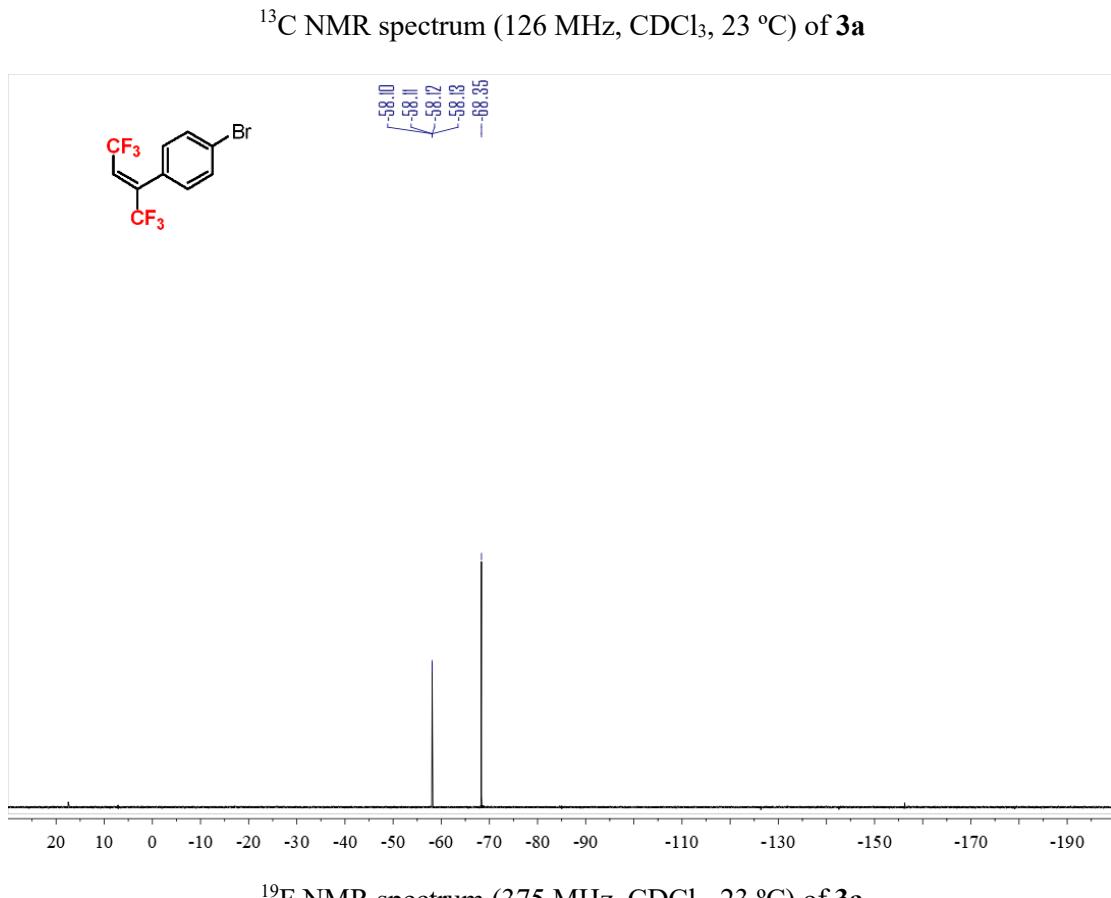
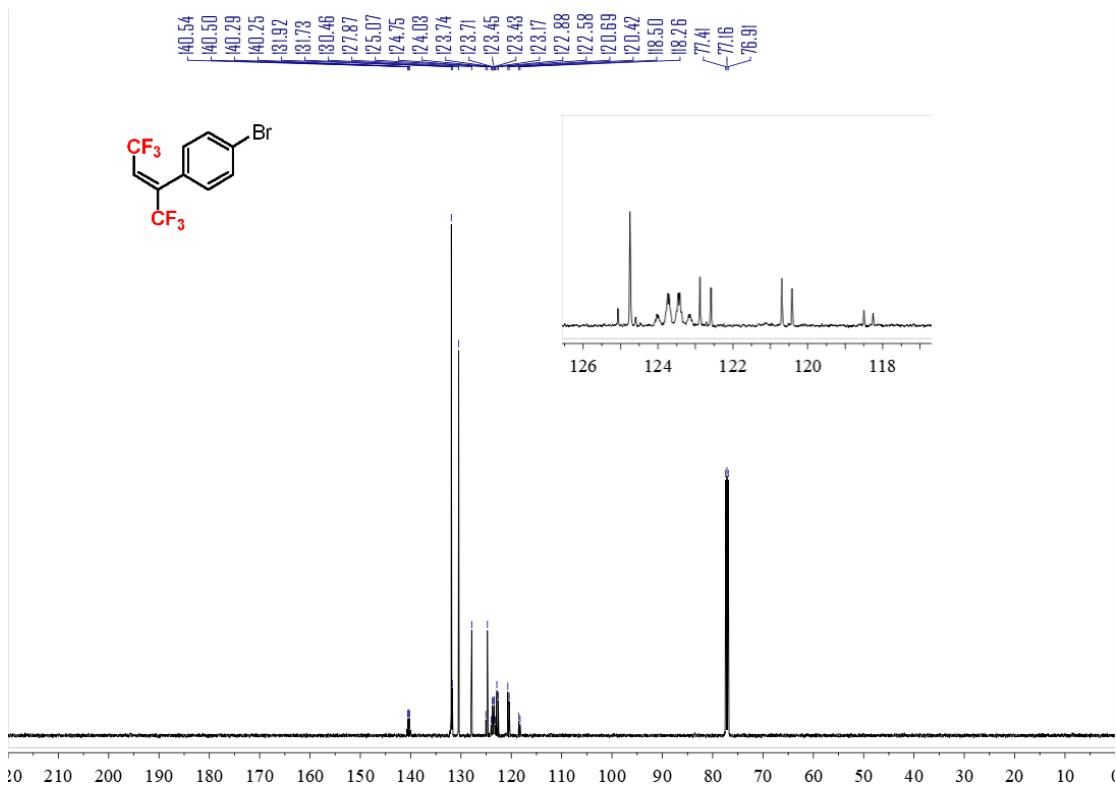
^1H NMR spectrum (400 MHz, CDCl_3 , 23 °C) of S4

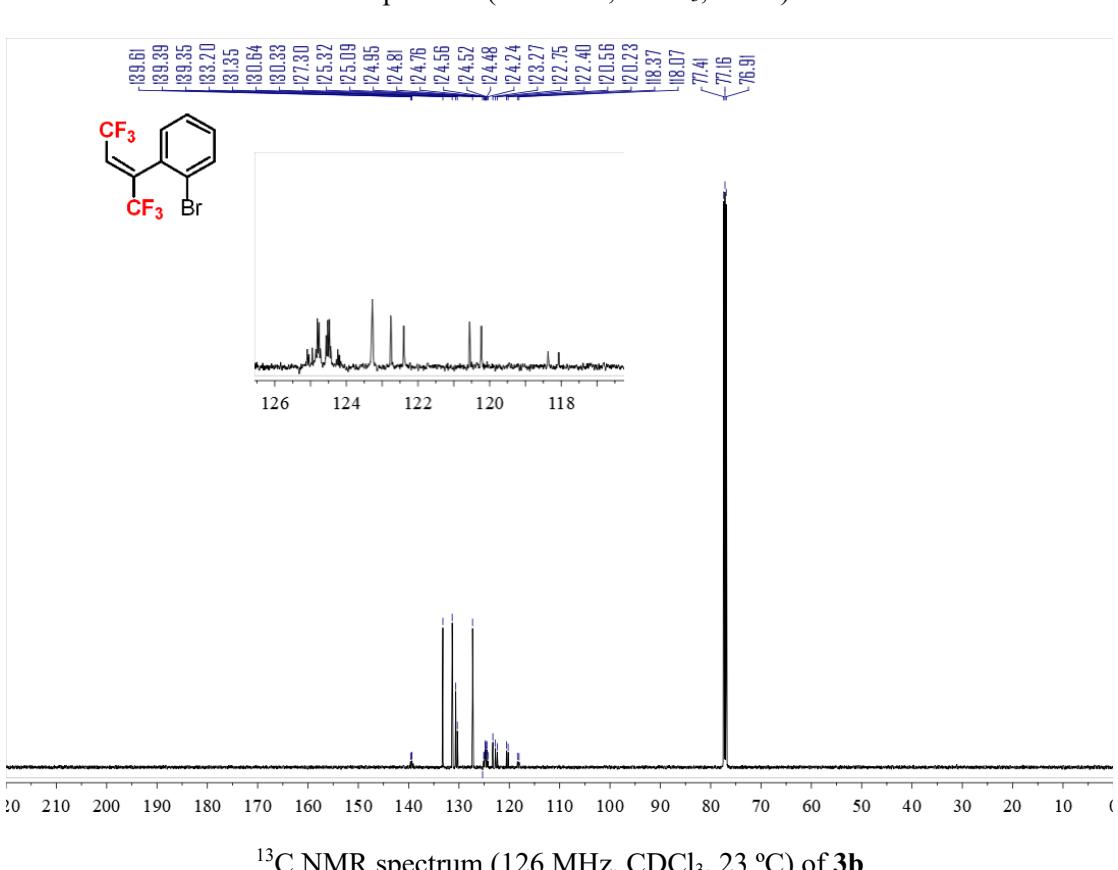
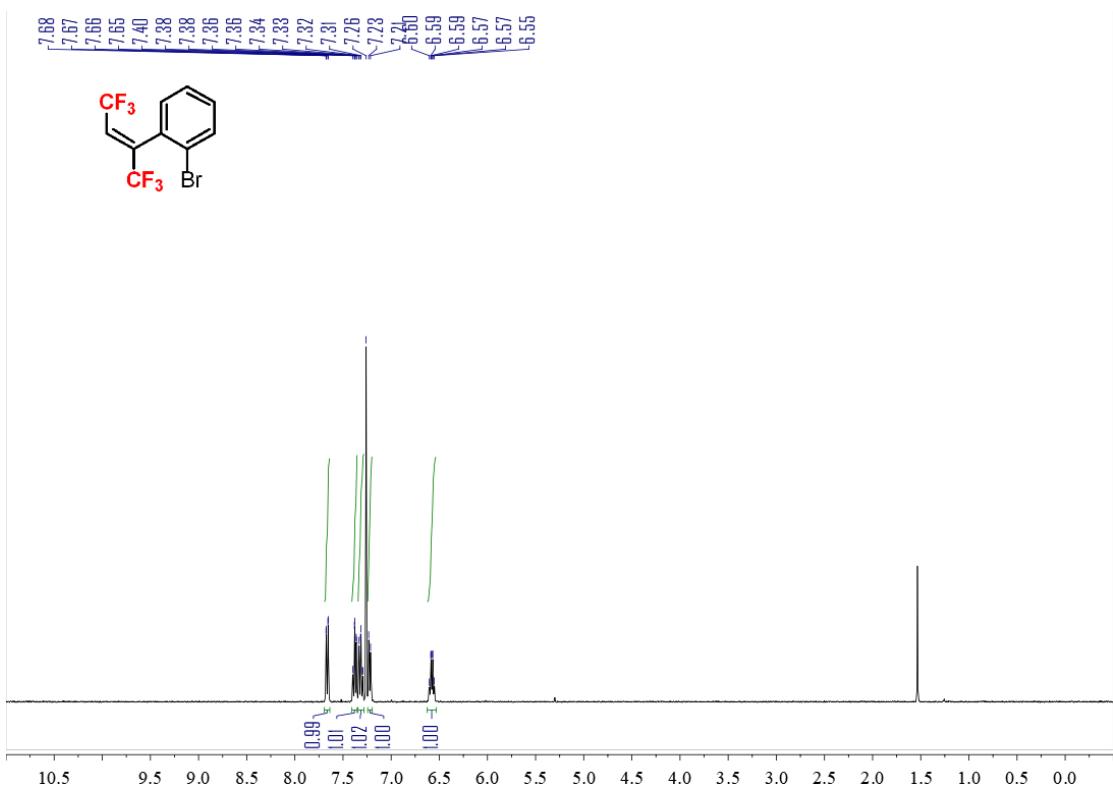


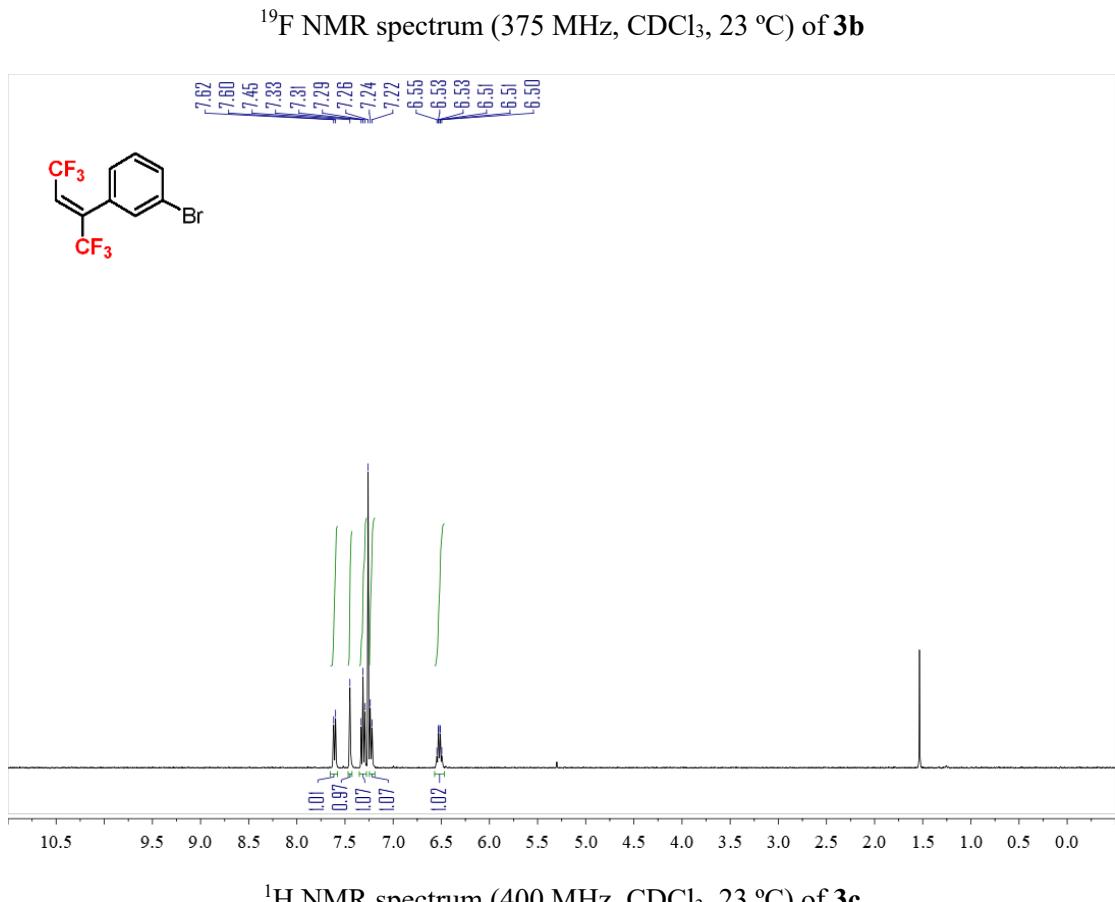
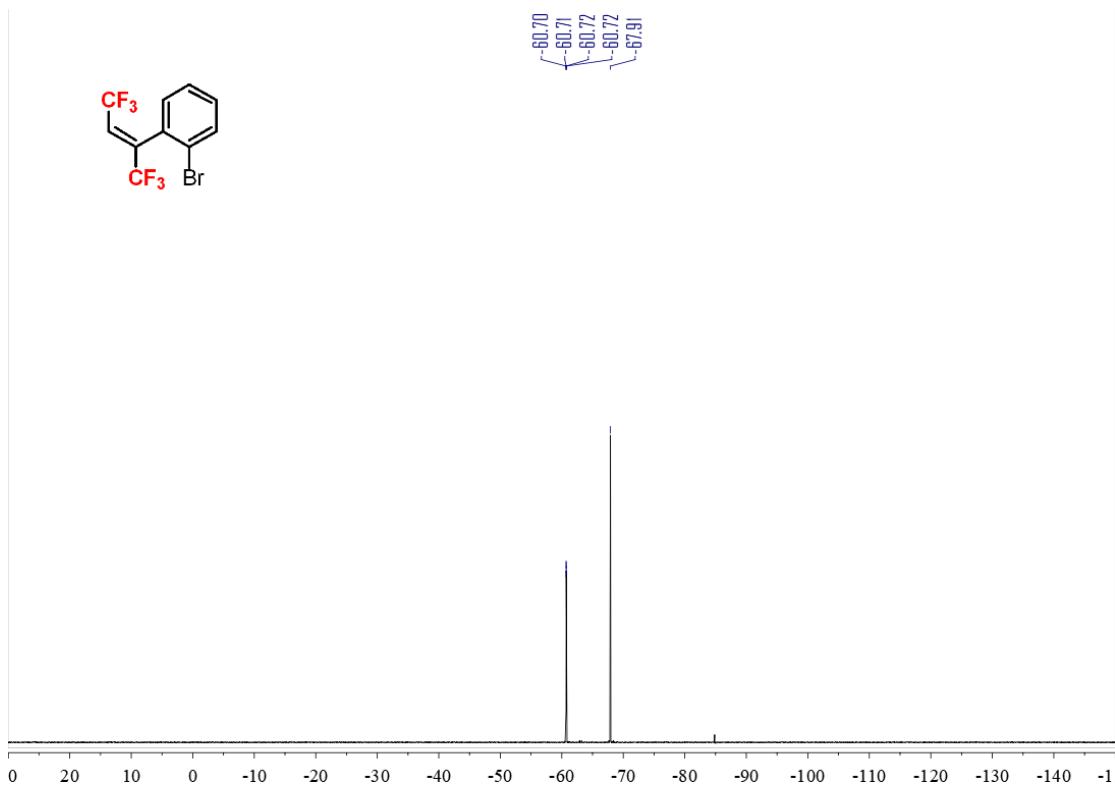
¹³C NMR spectrum (126 MHz, CDCl₃, 23 °C) of **S4**

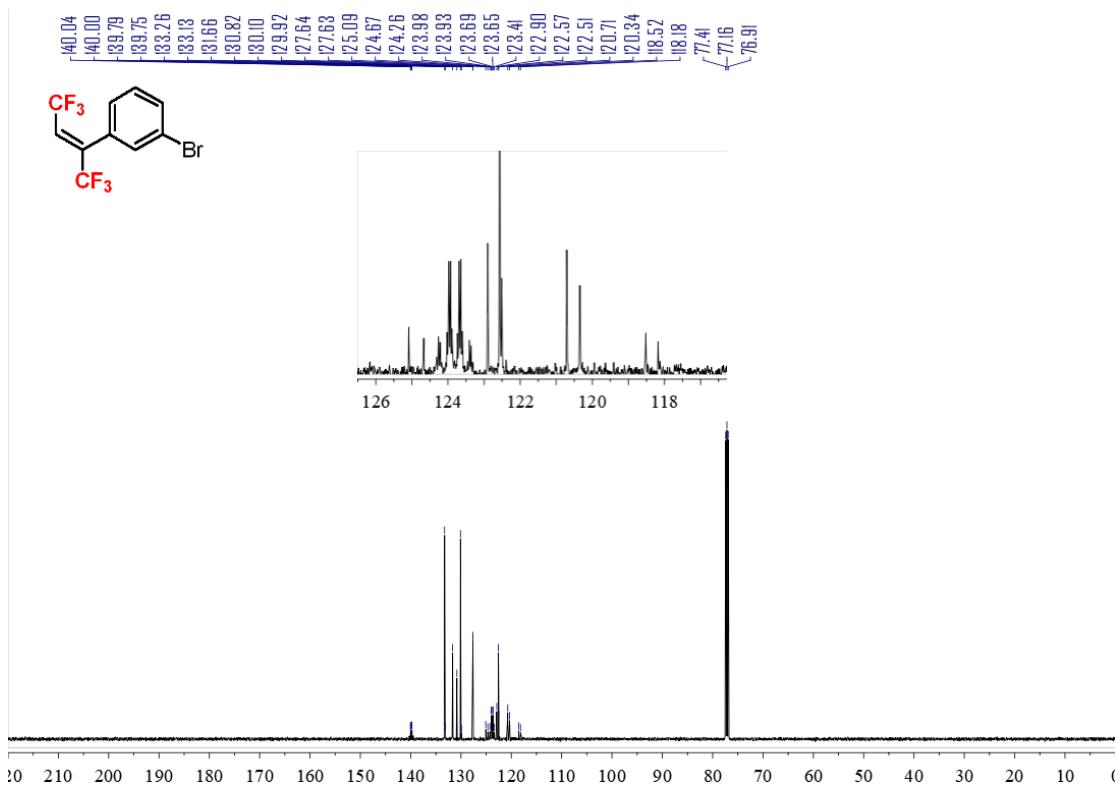


¹H NMR spectrum (400 MHz, CDCl₃, 23 °C) of **3a**

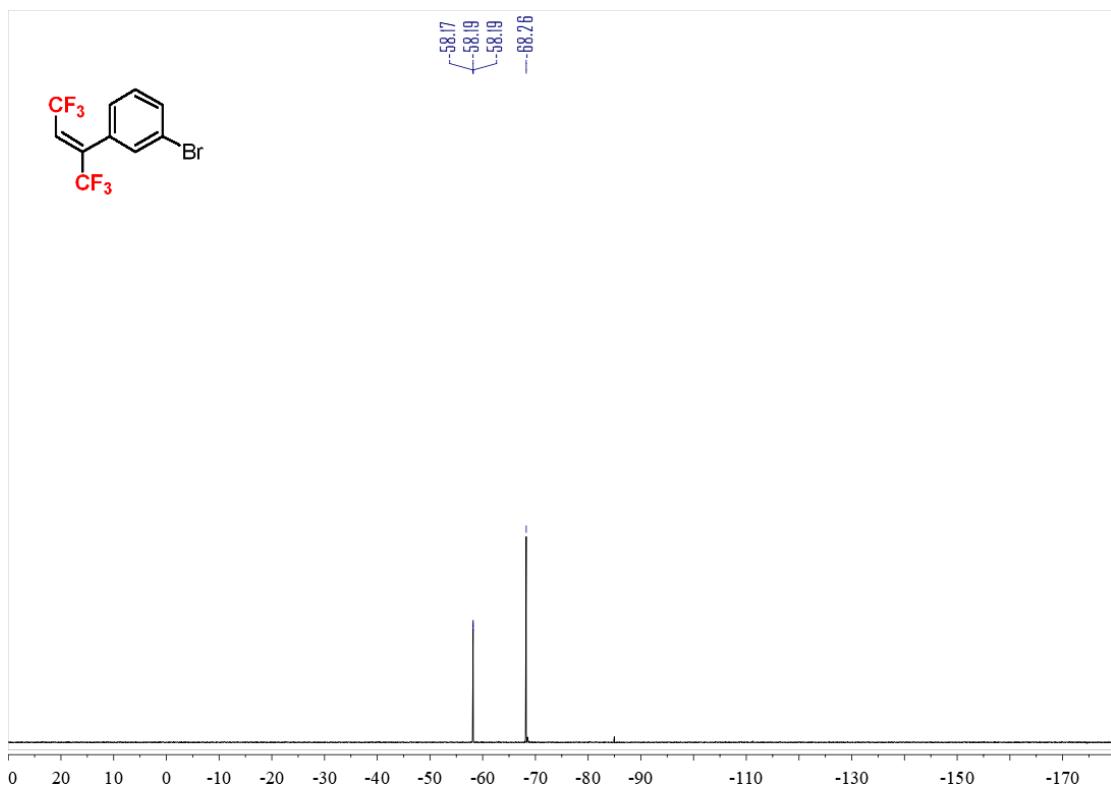




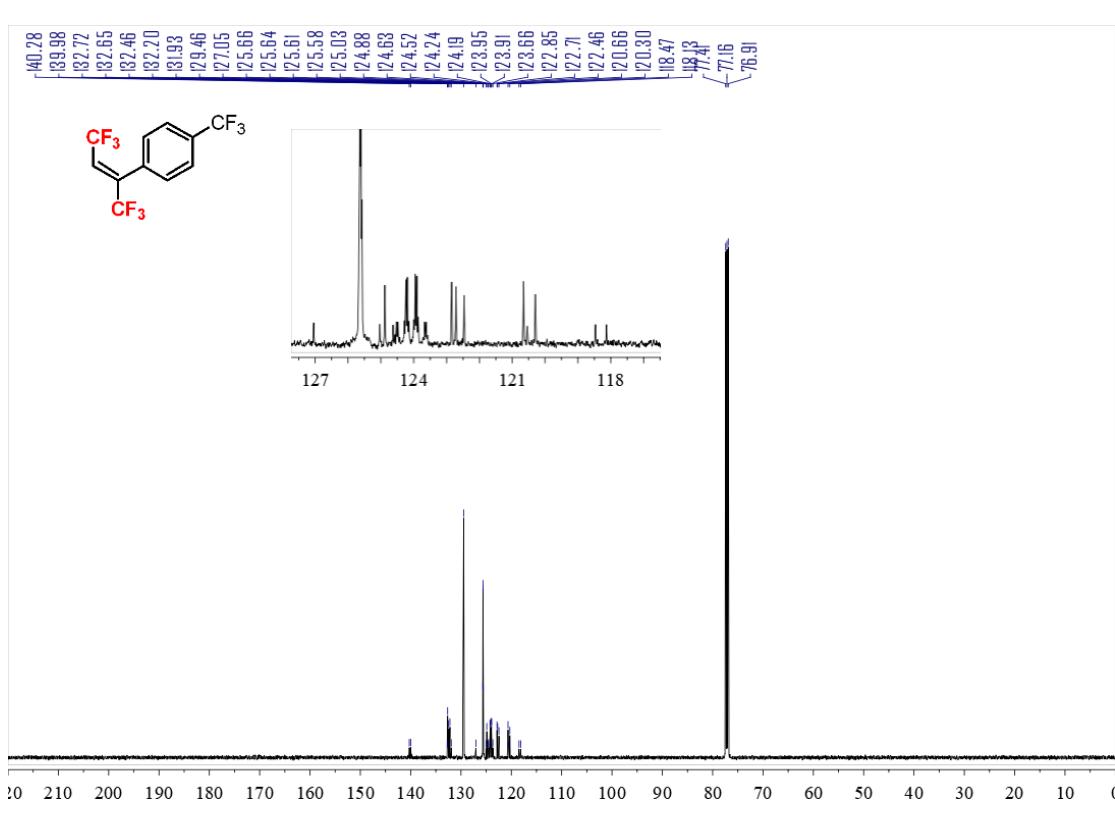
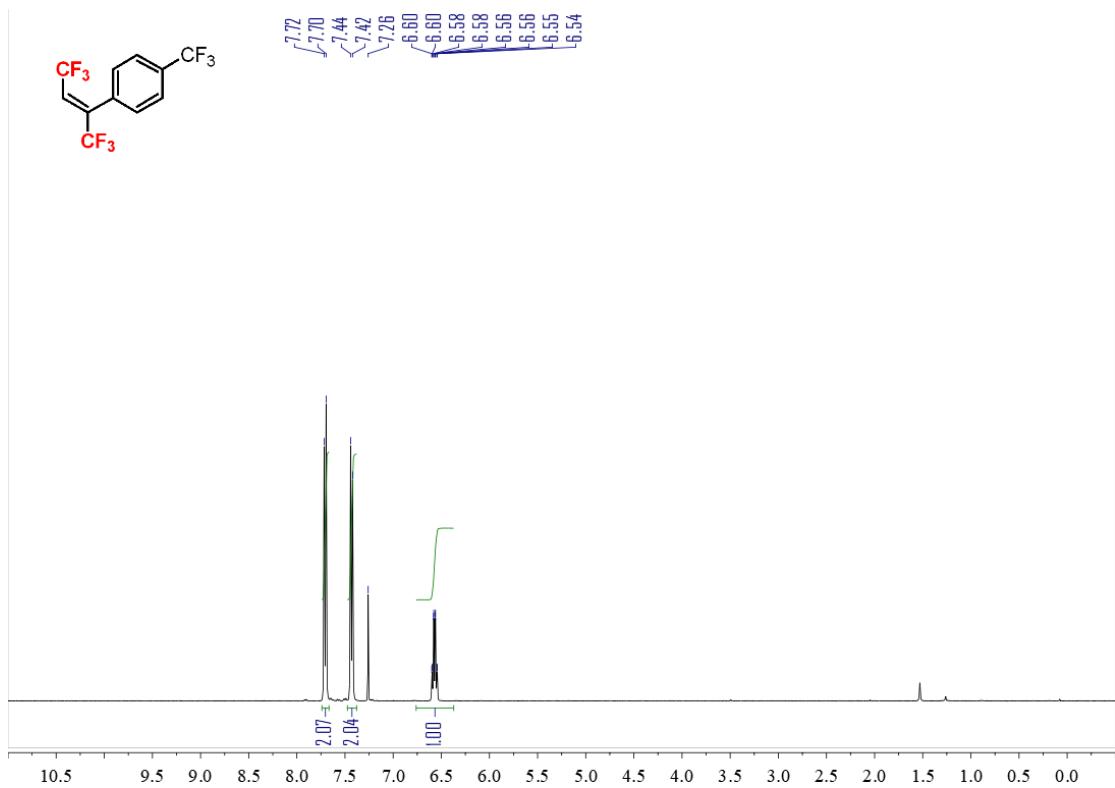


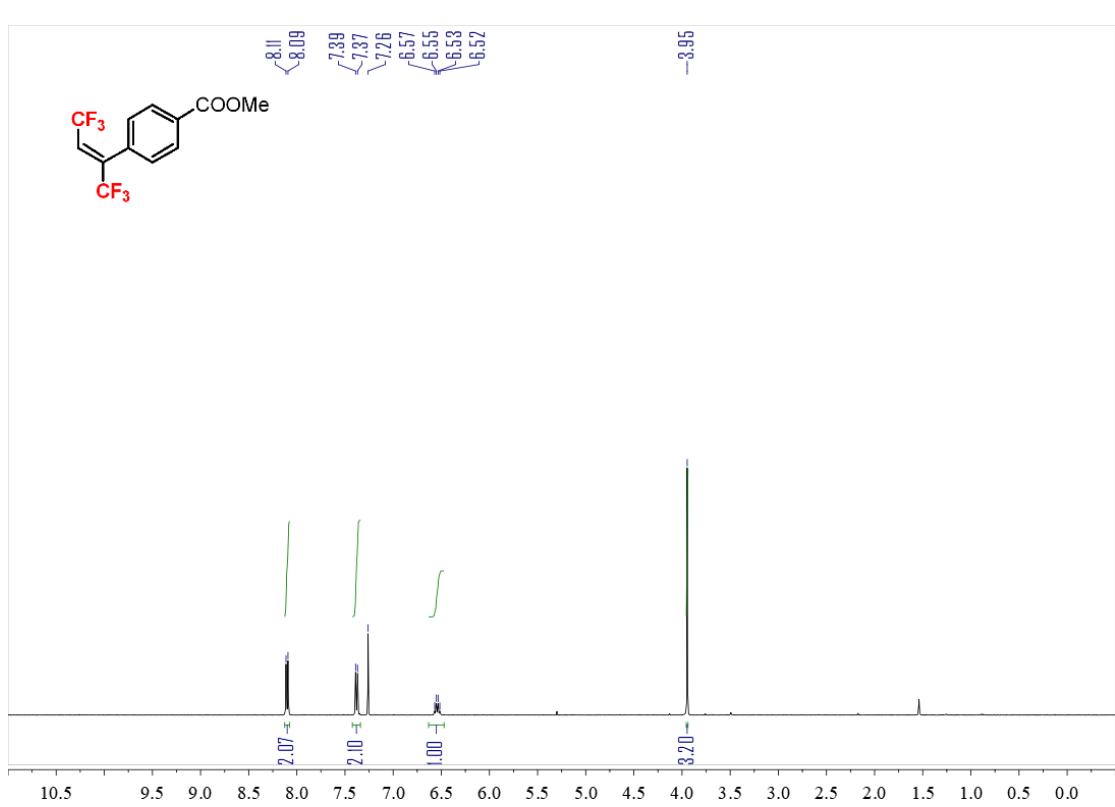
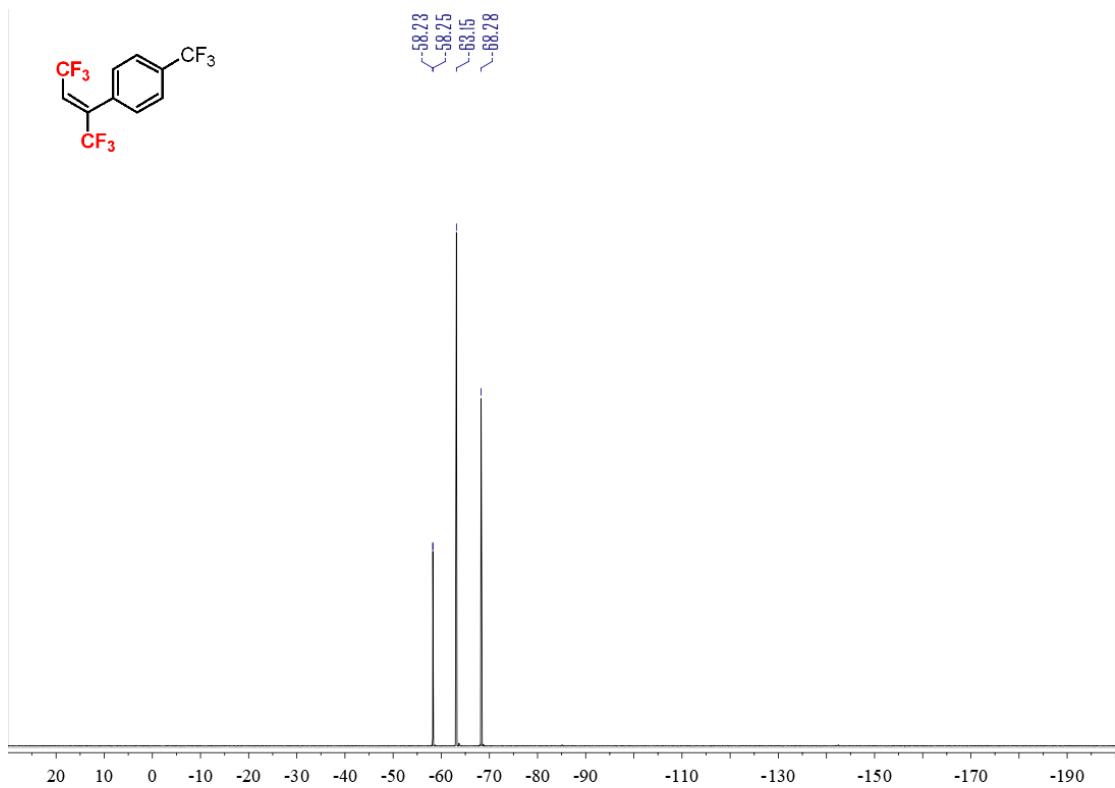


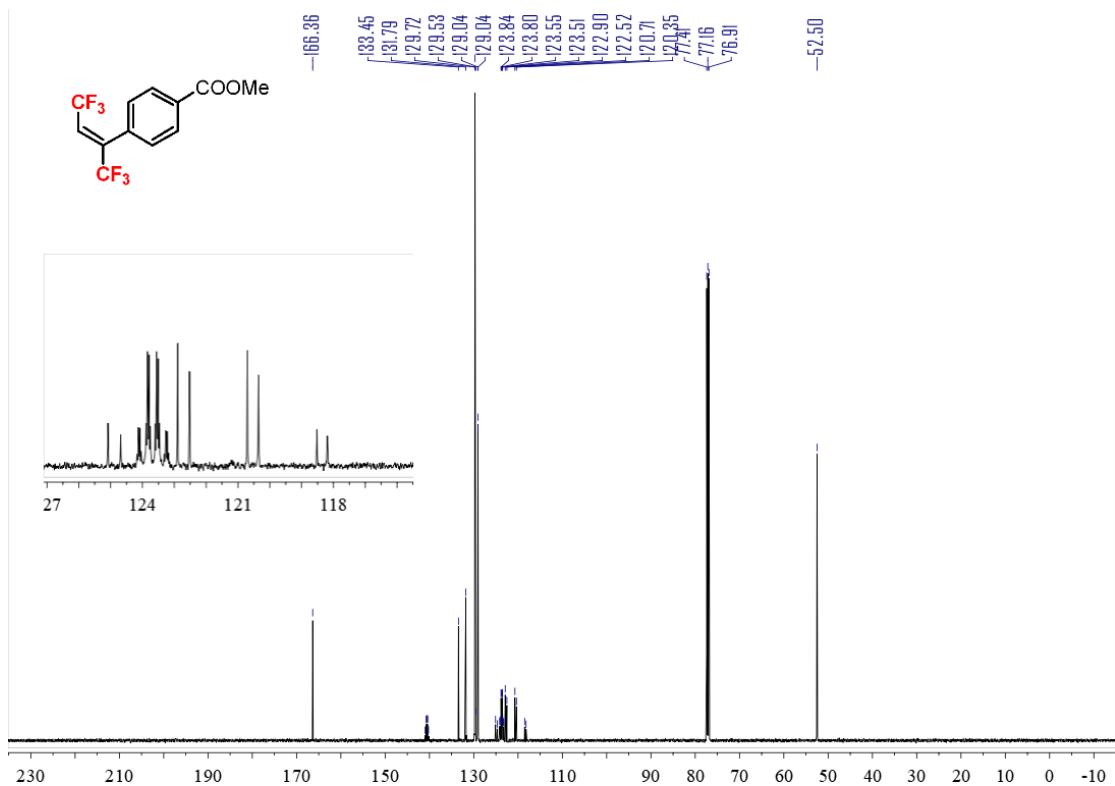
¹³C NMR spectrum (126 MHz, CDCl₃, 23 °C) of **3c**



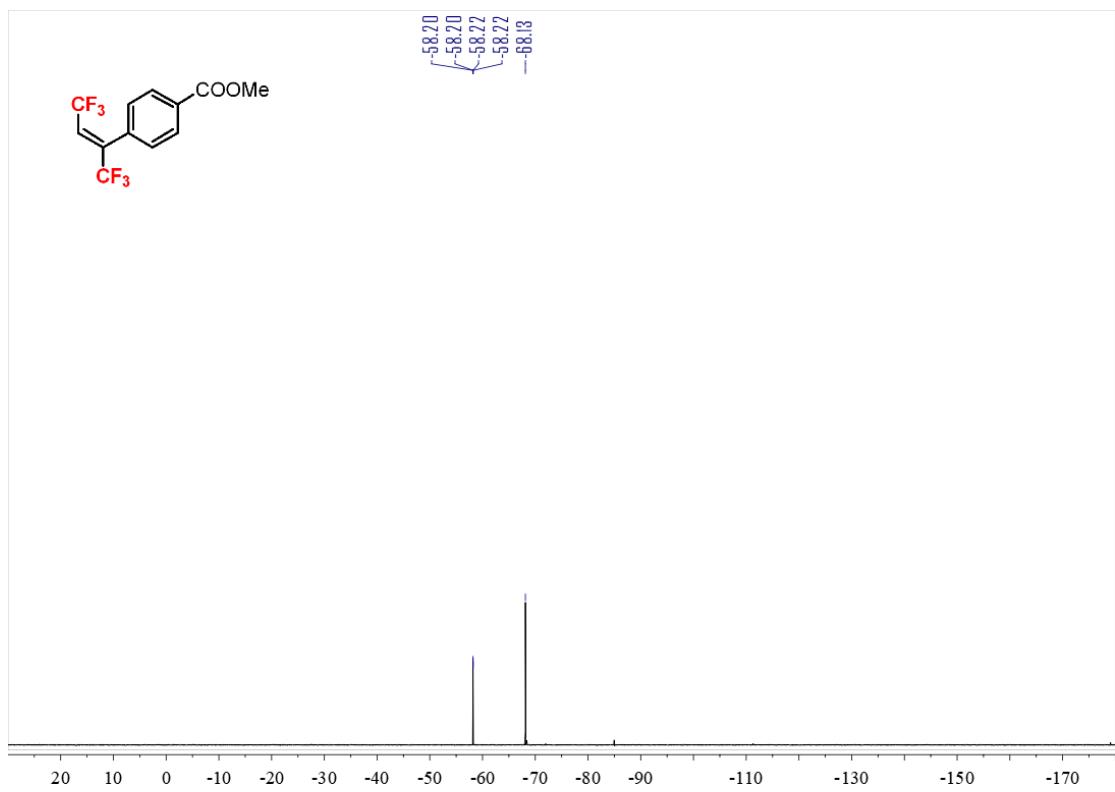
¹⁹F NMR spectrum (375 MHz, CDCl₃, 23 °C) of **3c**



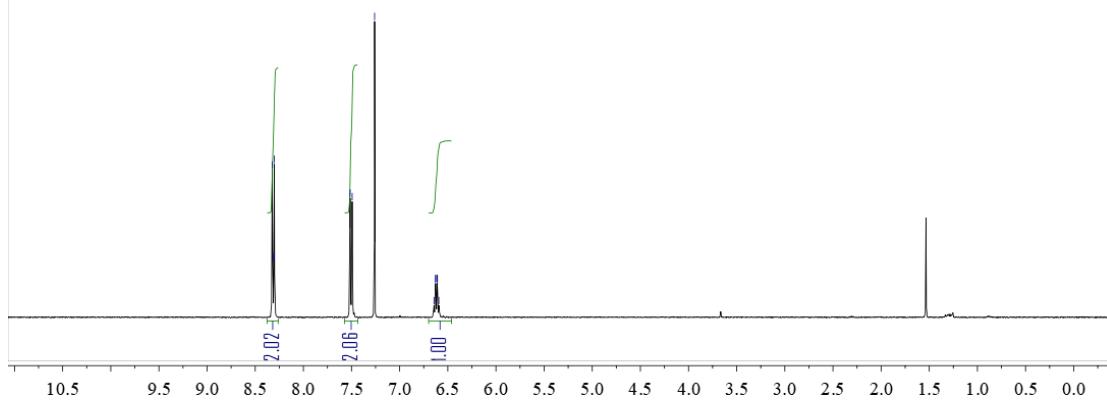
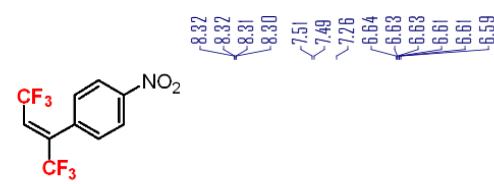




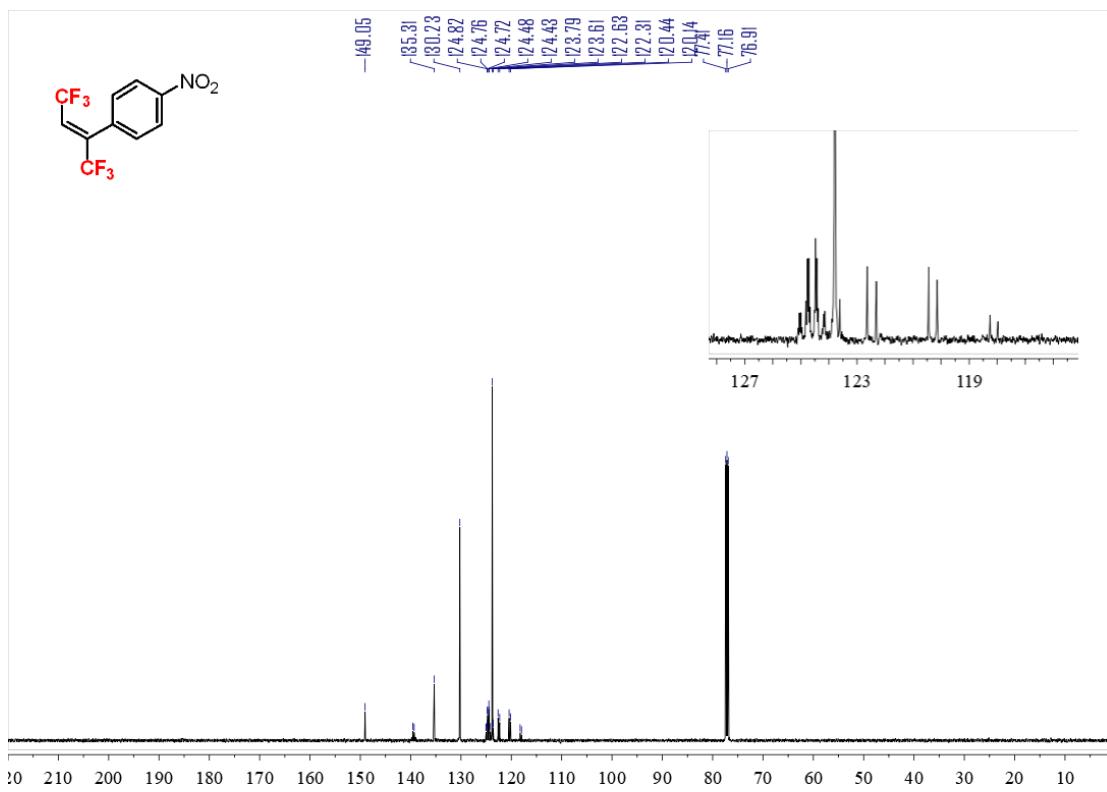
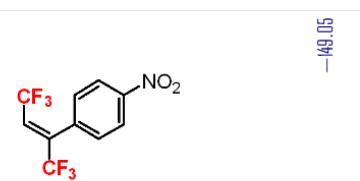
¹³C NMR spectrum (126 MHz, CDCl₃, 23 °C) of **3e**



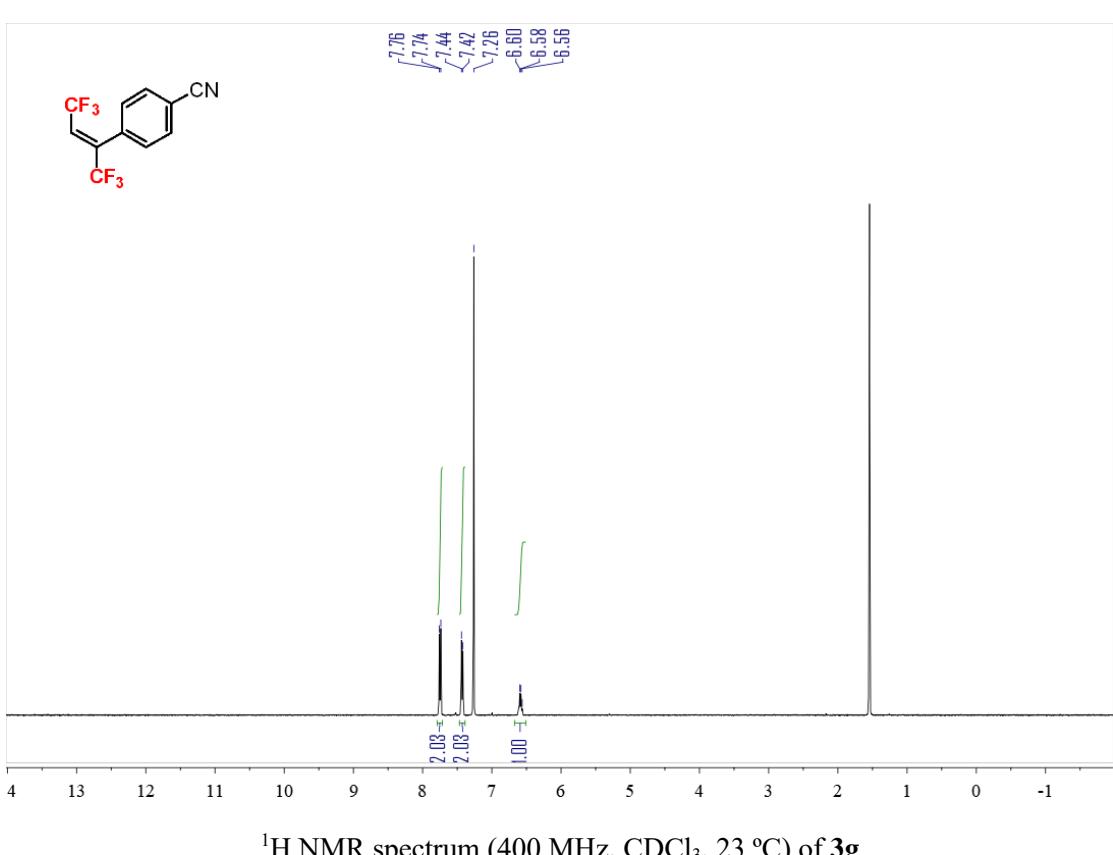
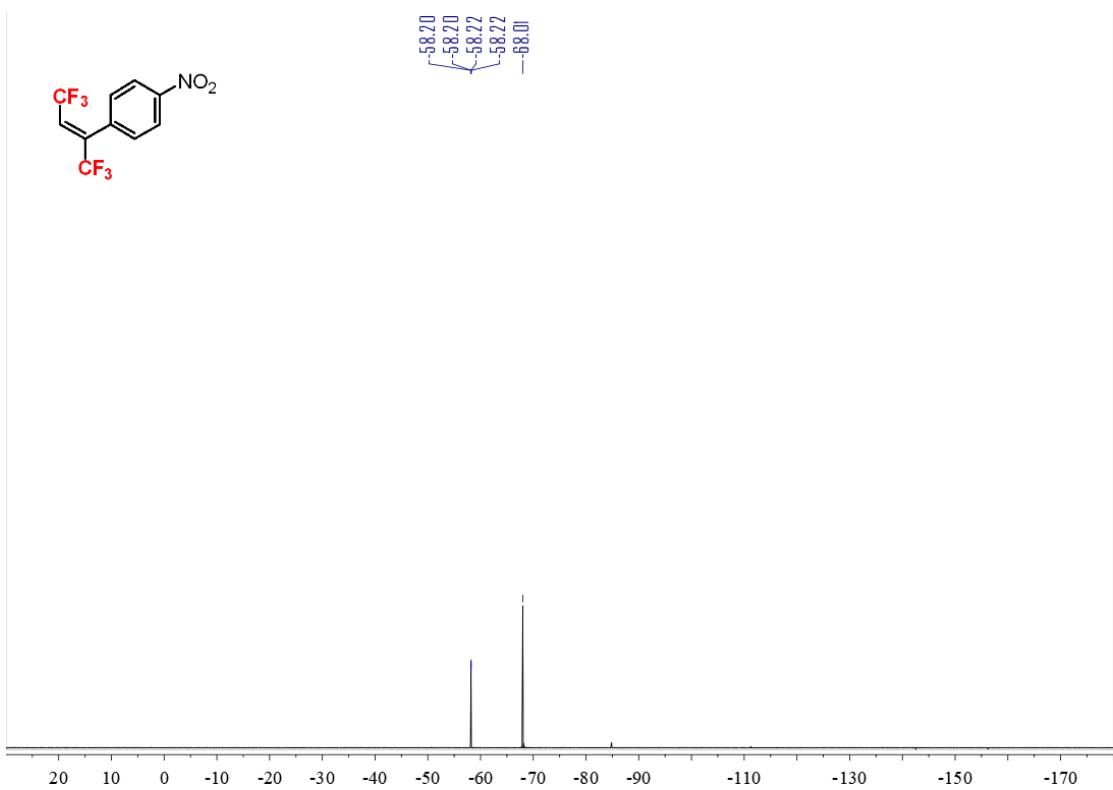
¹⁹F NMR spectrum (375 MHz, CDCl₃, 23 °C) of **3e**

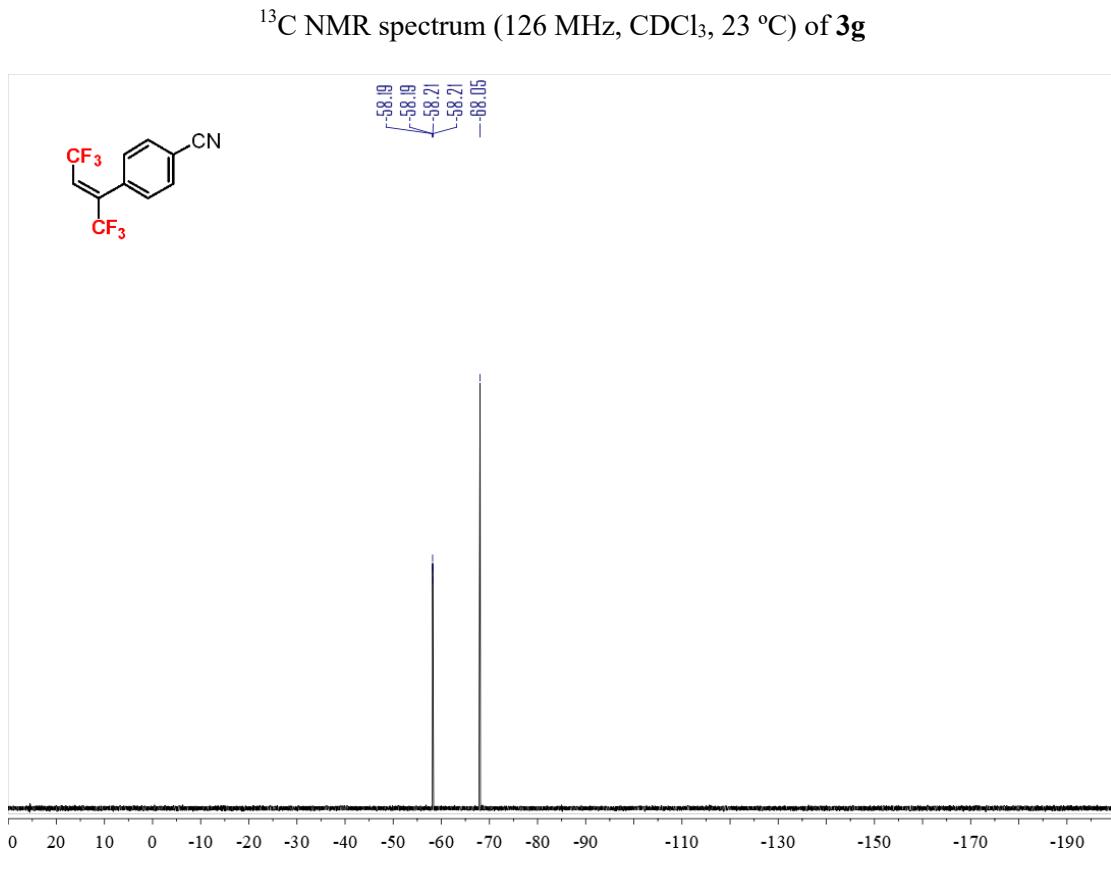
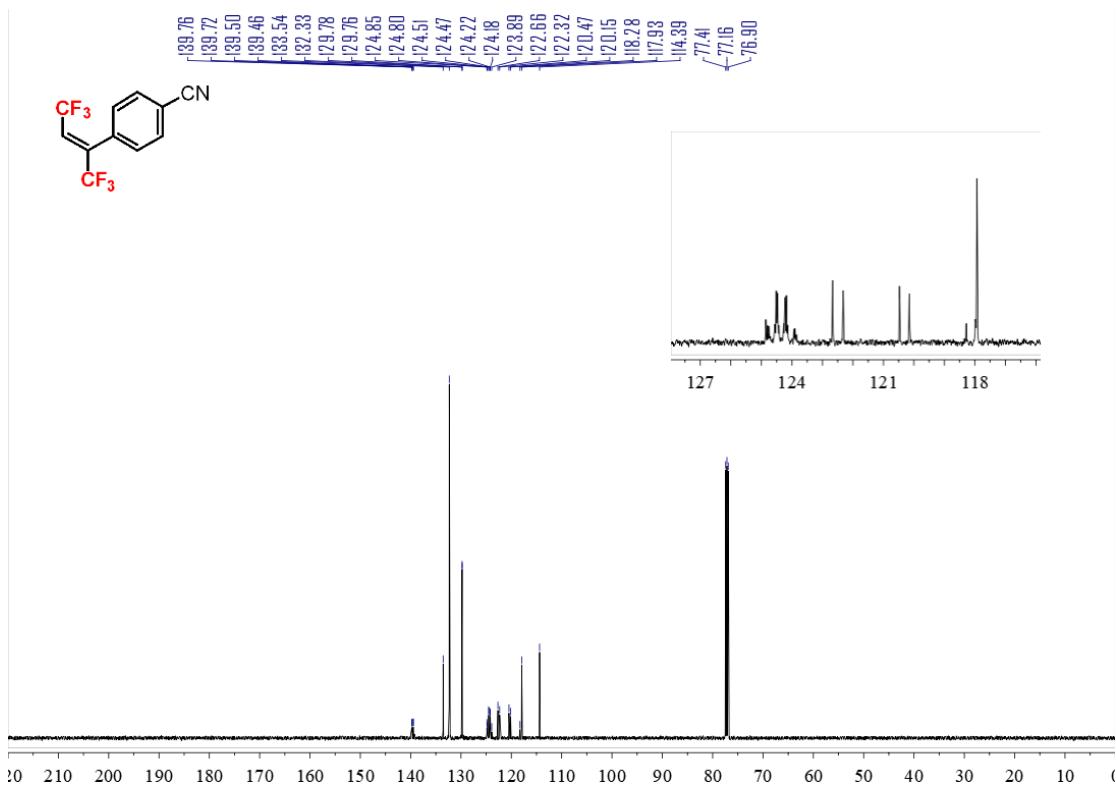


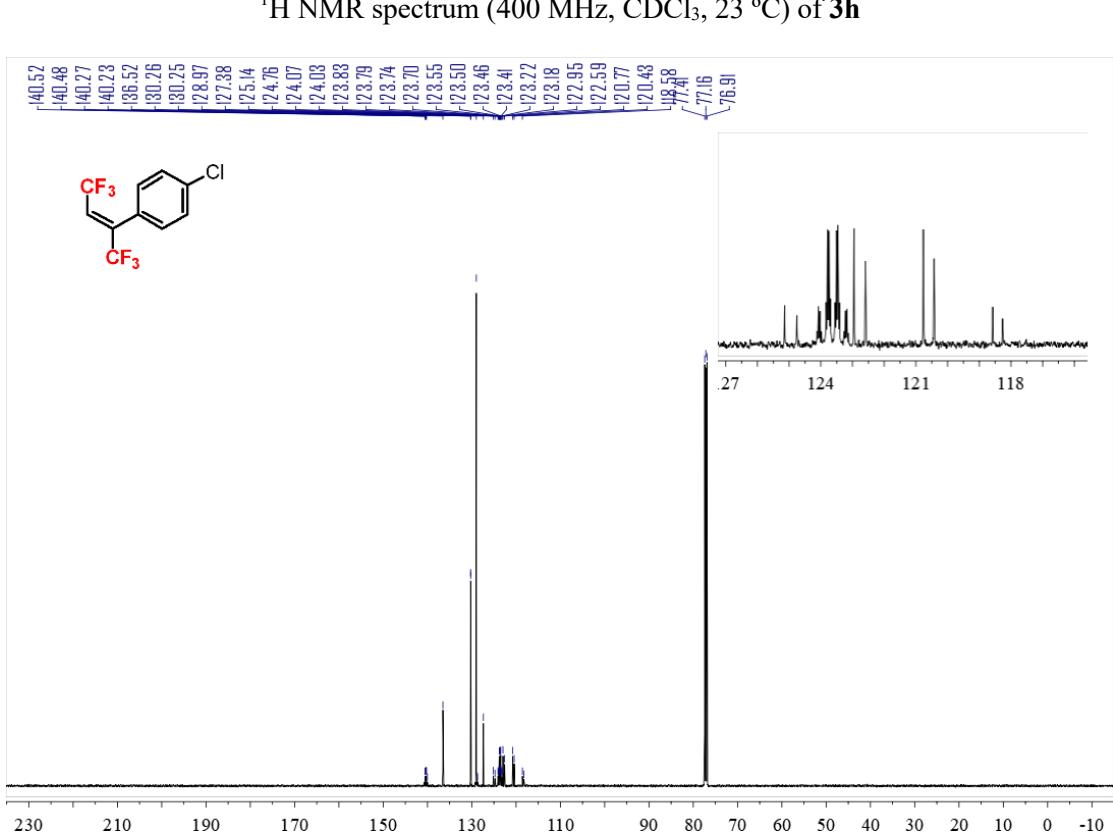
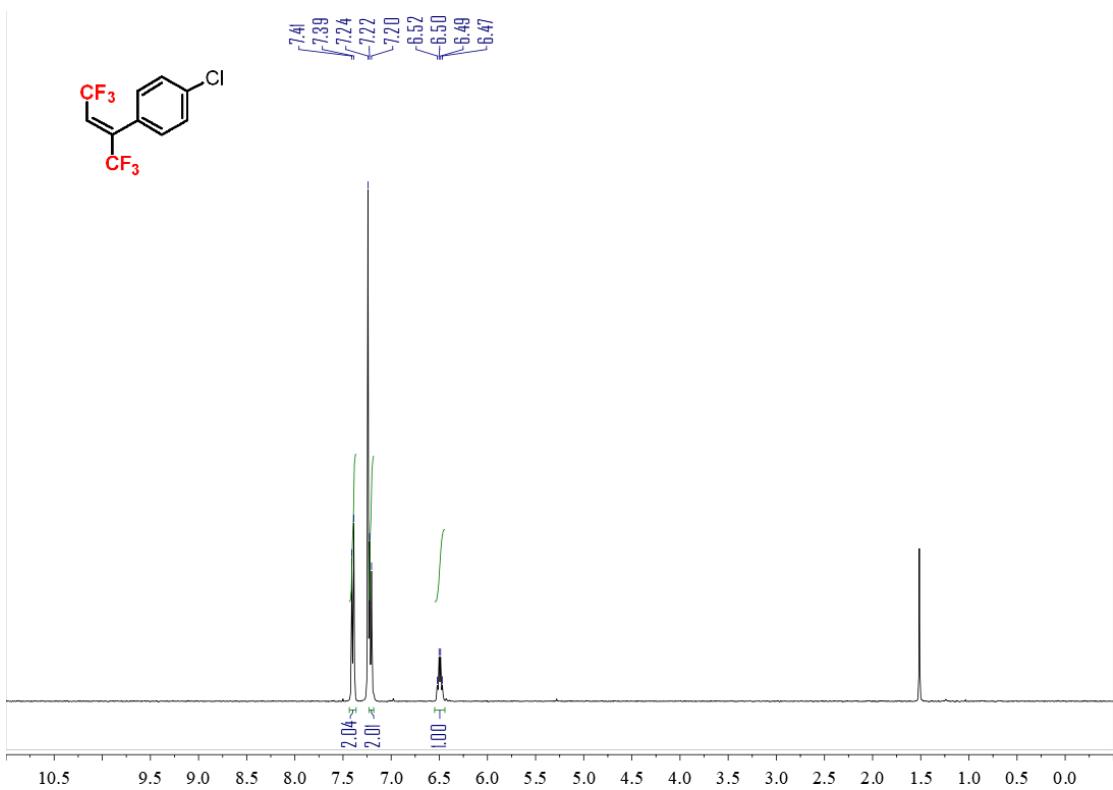
¹H NMR spectrum (400 MHz, CDCl₃, 23 °C) of **3f**



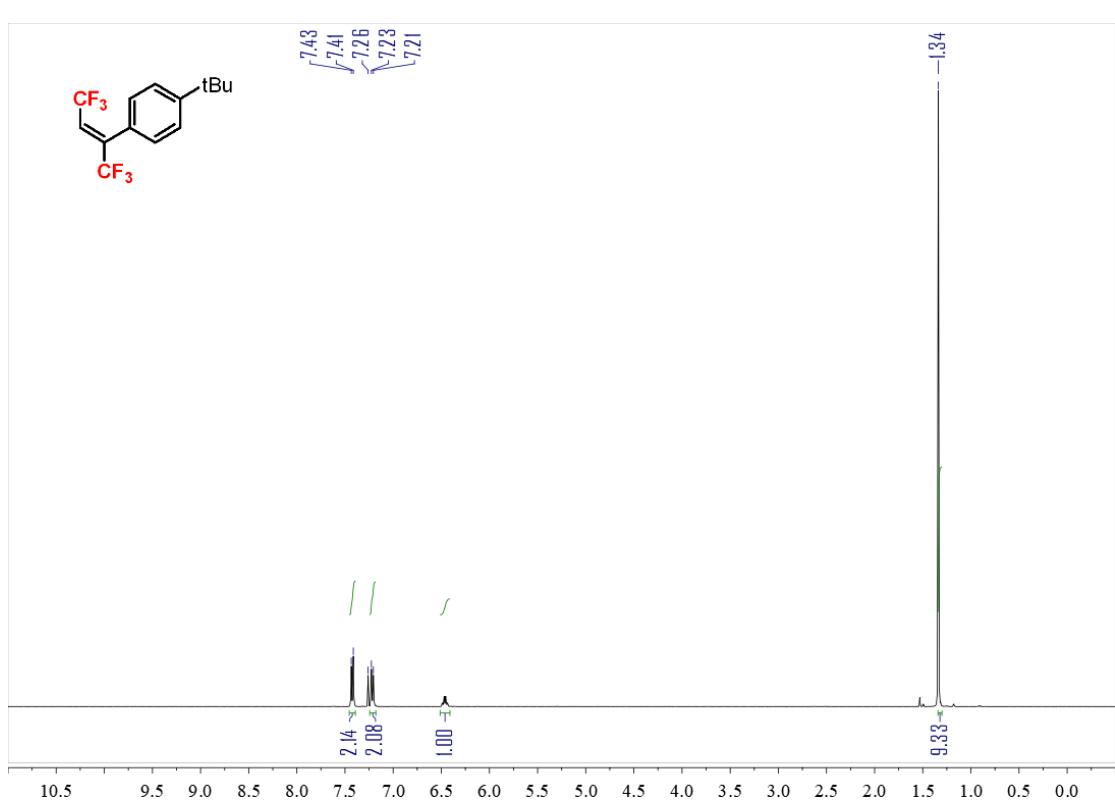
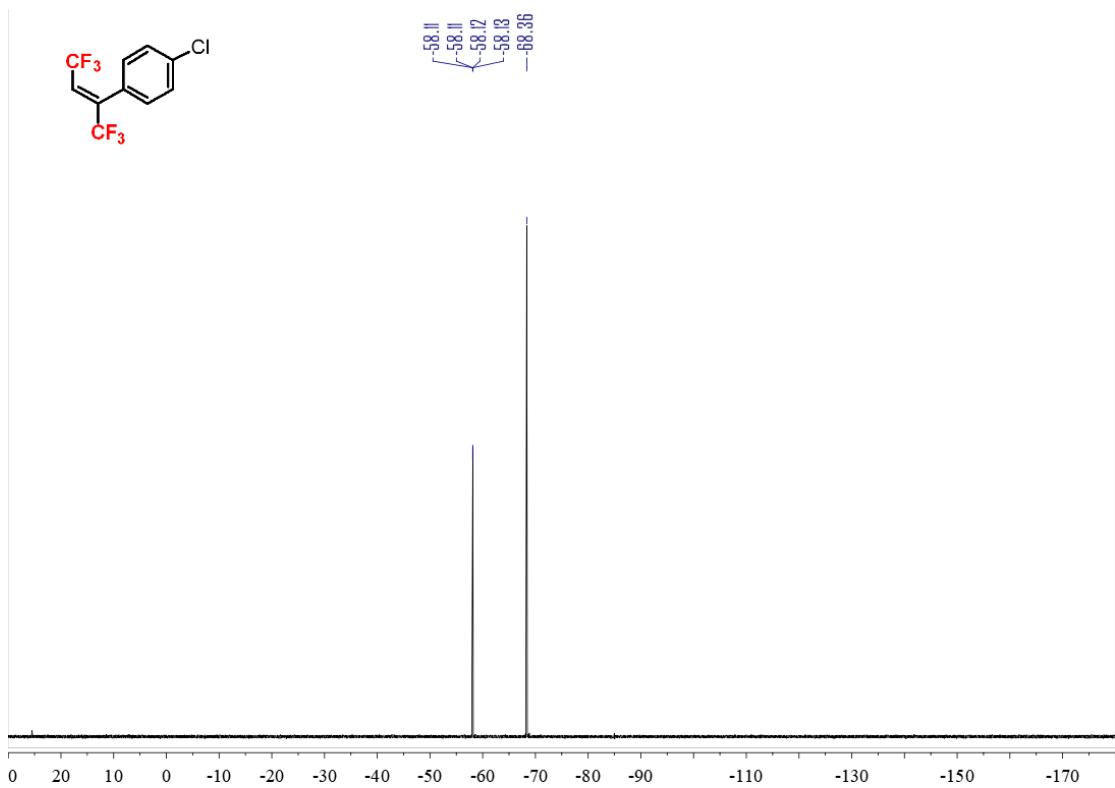
¹³C NMR spectrum (126 MHz, CDCl₃, 23 °C) of **3f**

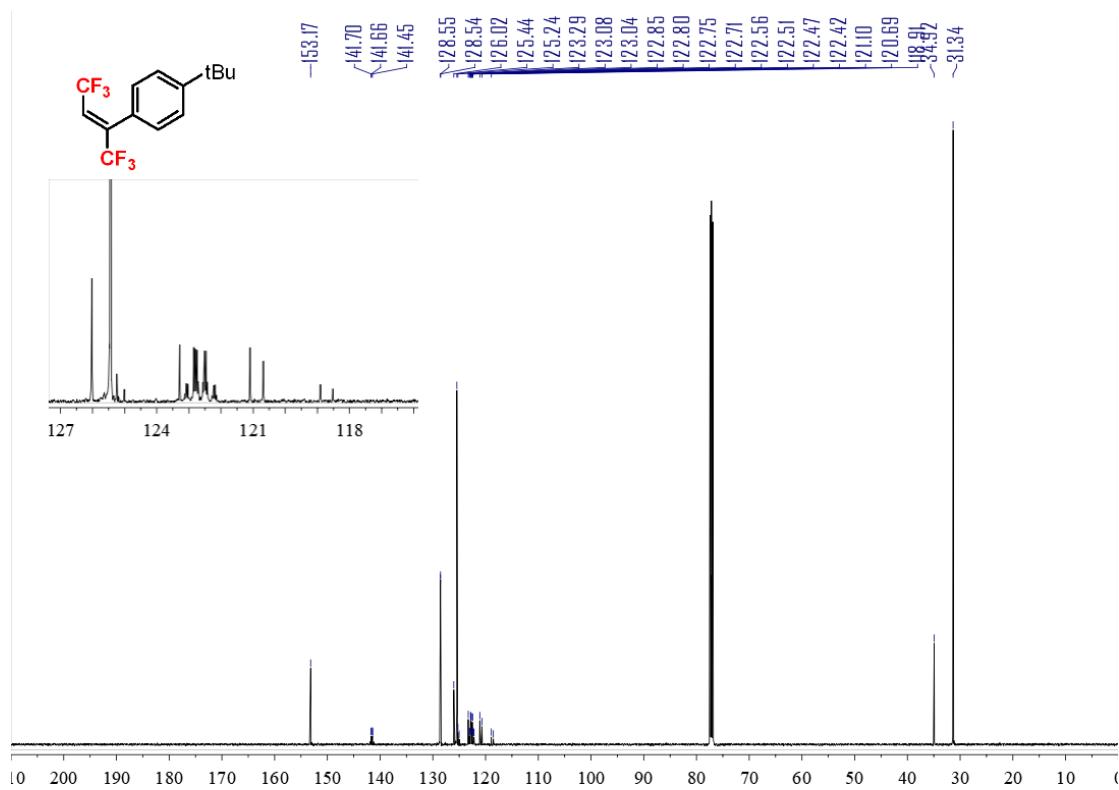




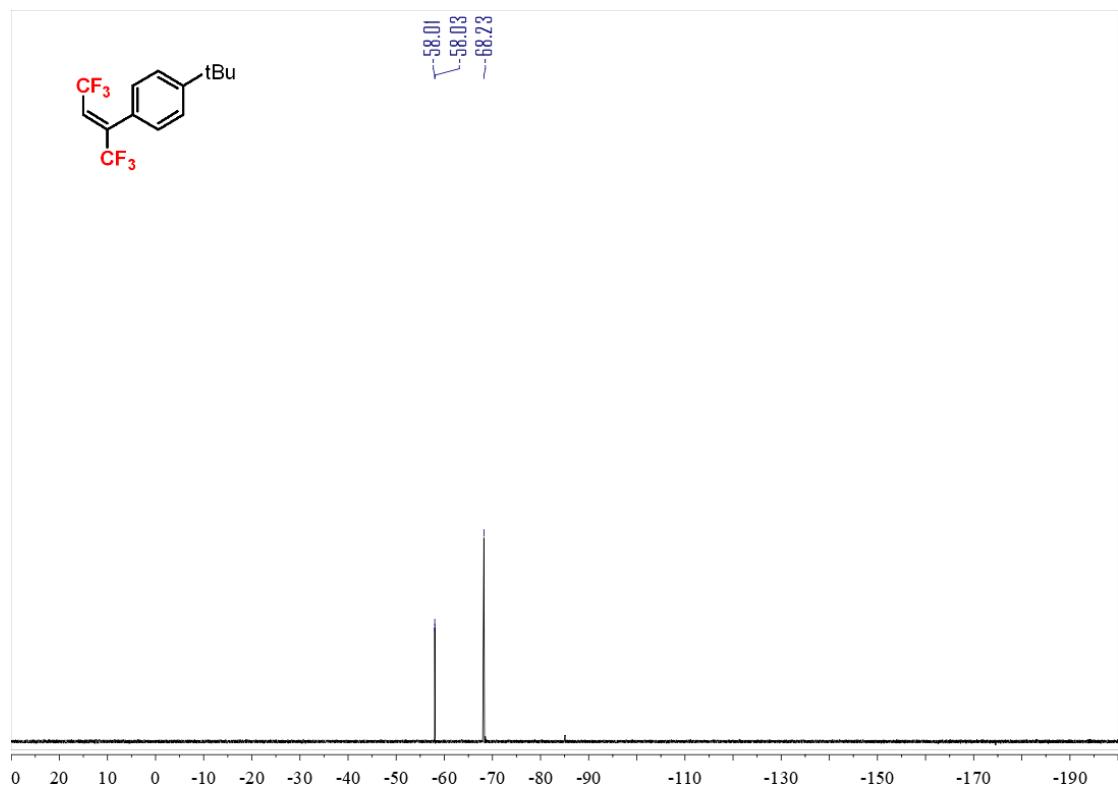


¹³C NMR spectrum (126 MHz, CDCl₃, 23 °C) of **3h**

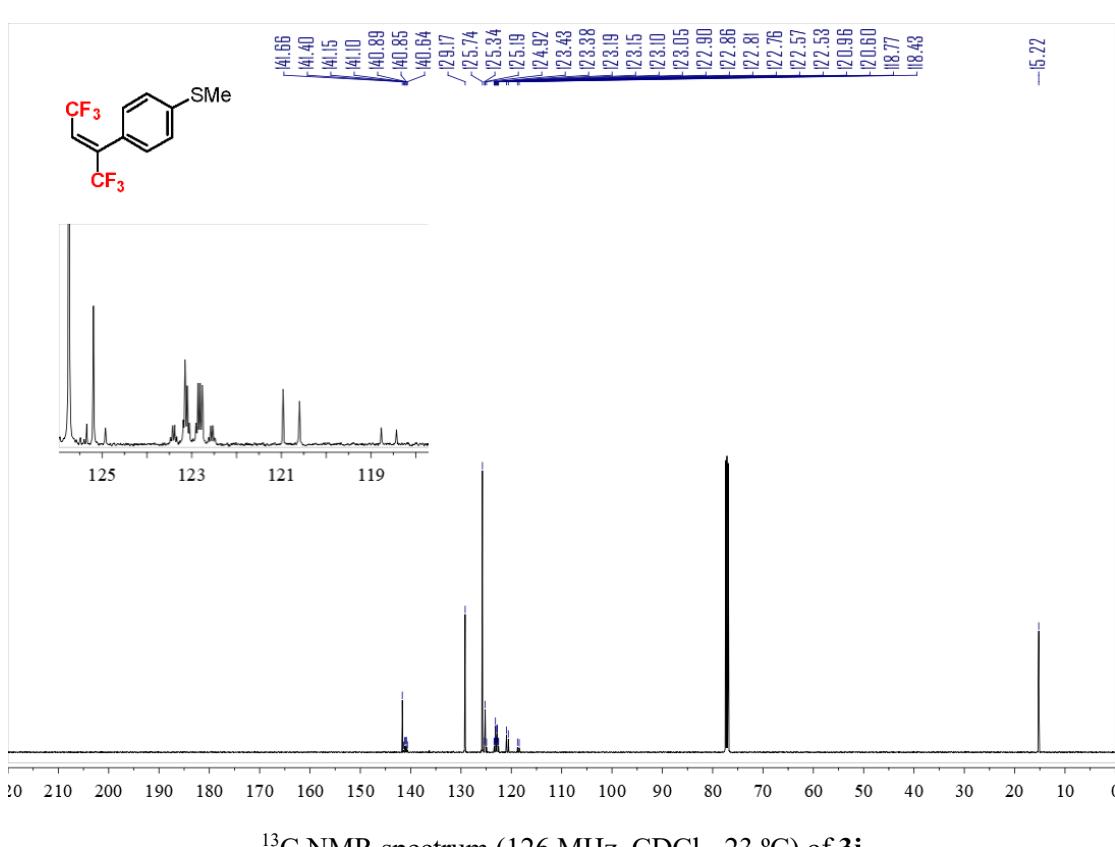
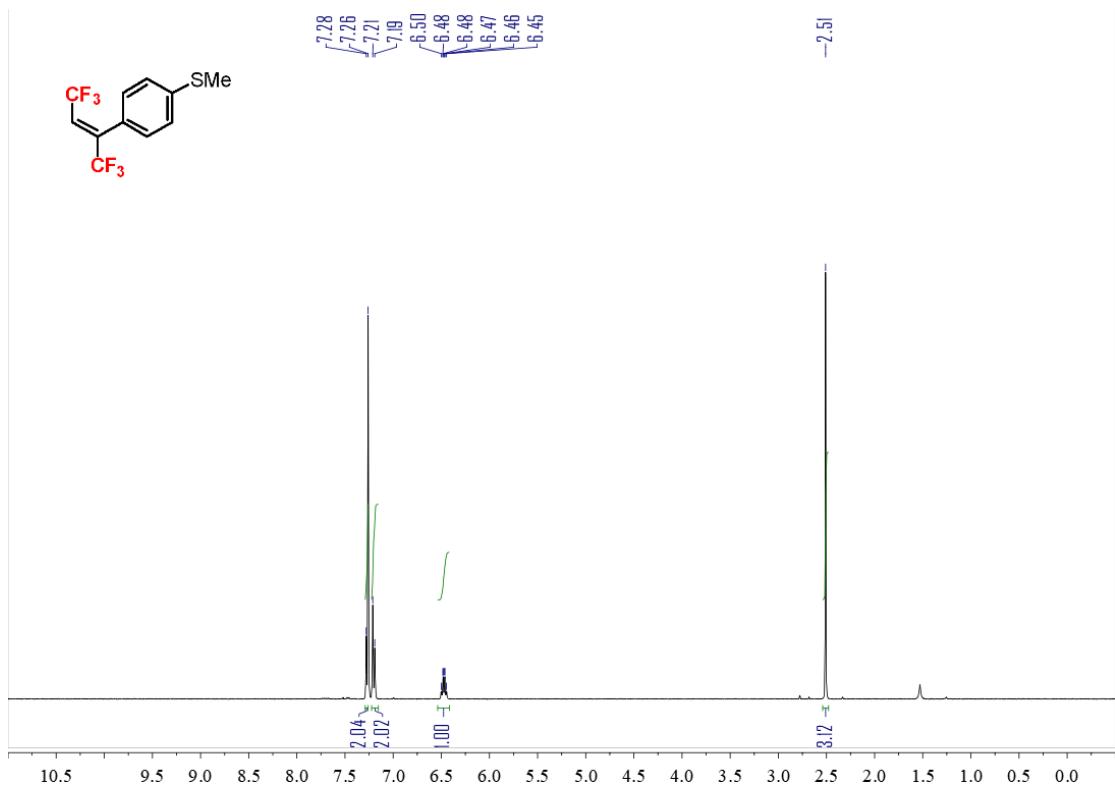


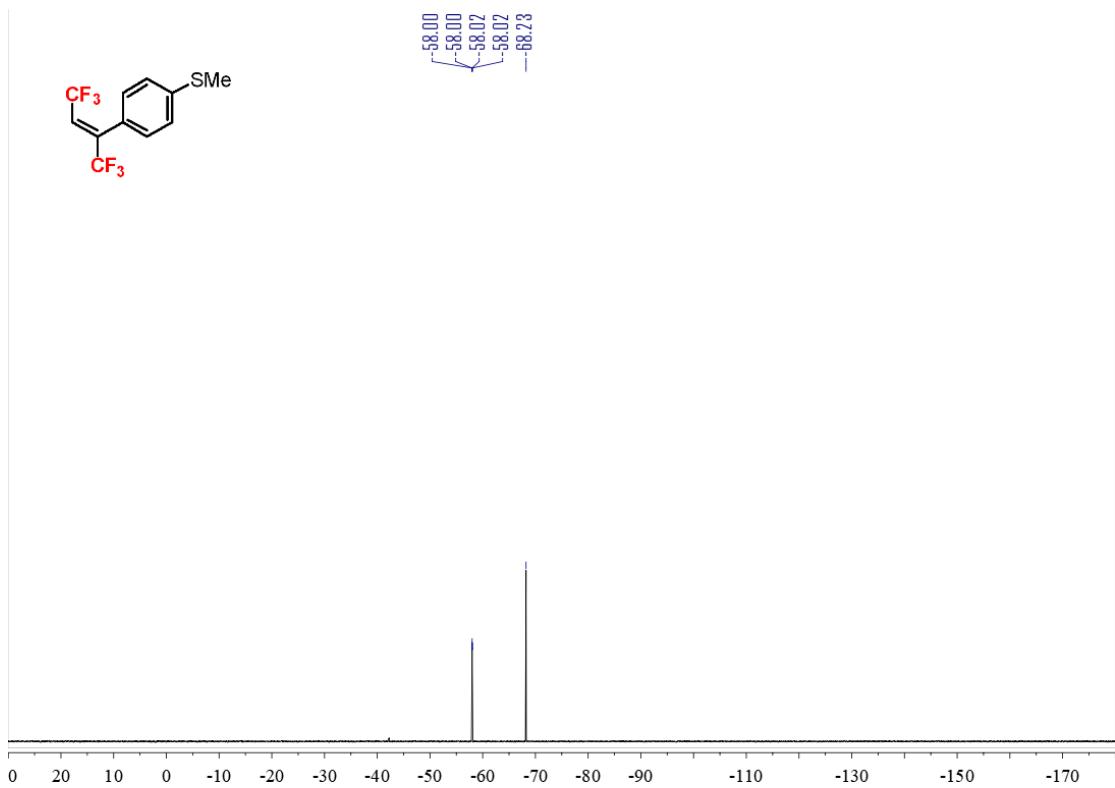


¹³C NMR spectrum (126 MHz, CDCl₃, 23 °C) of **3i**

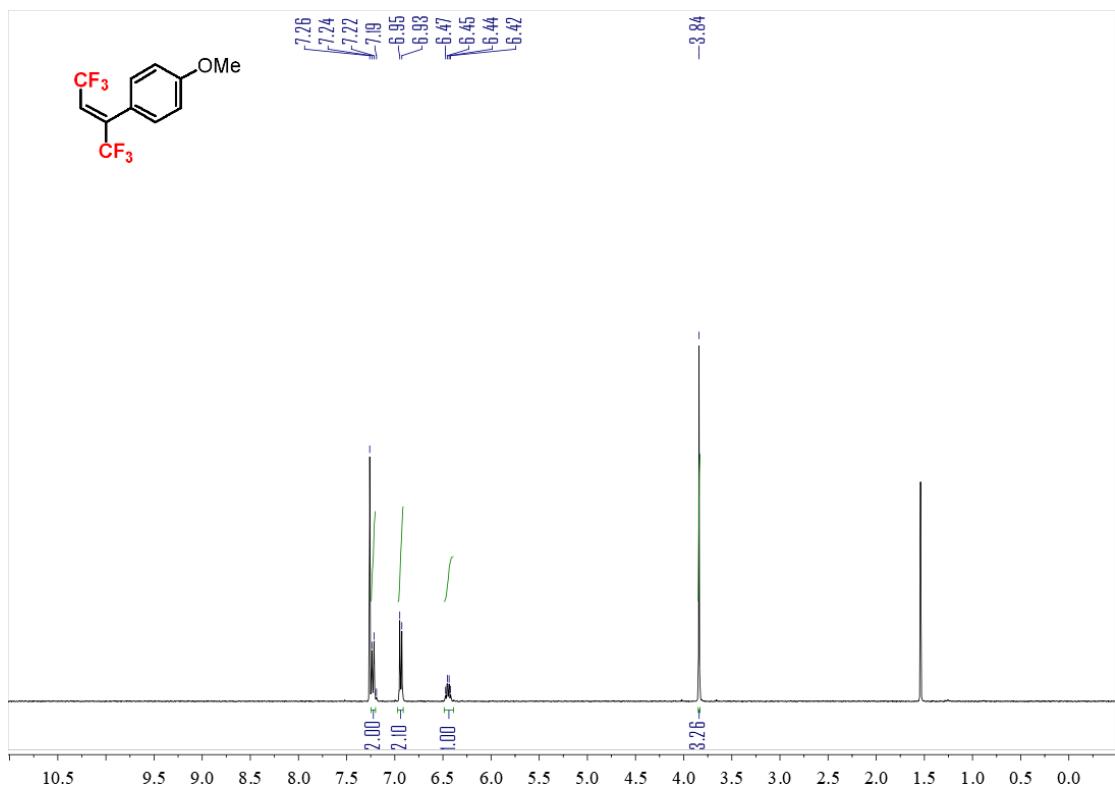


¹⁹F NMR spectrum (375 MHz, CDCl₃, 23 °C) of **3i**

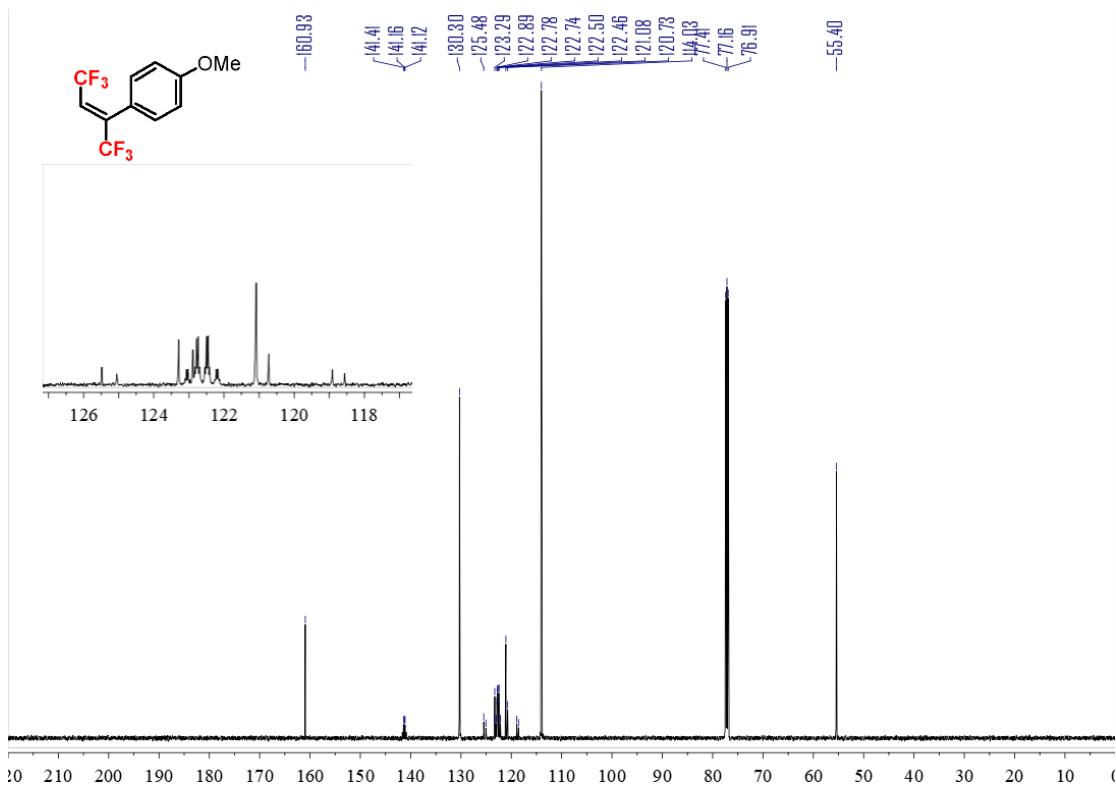




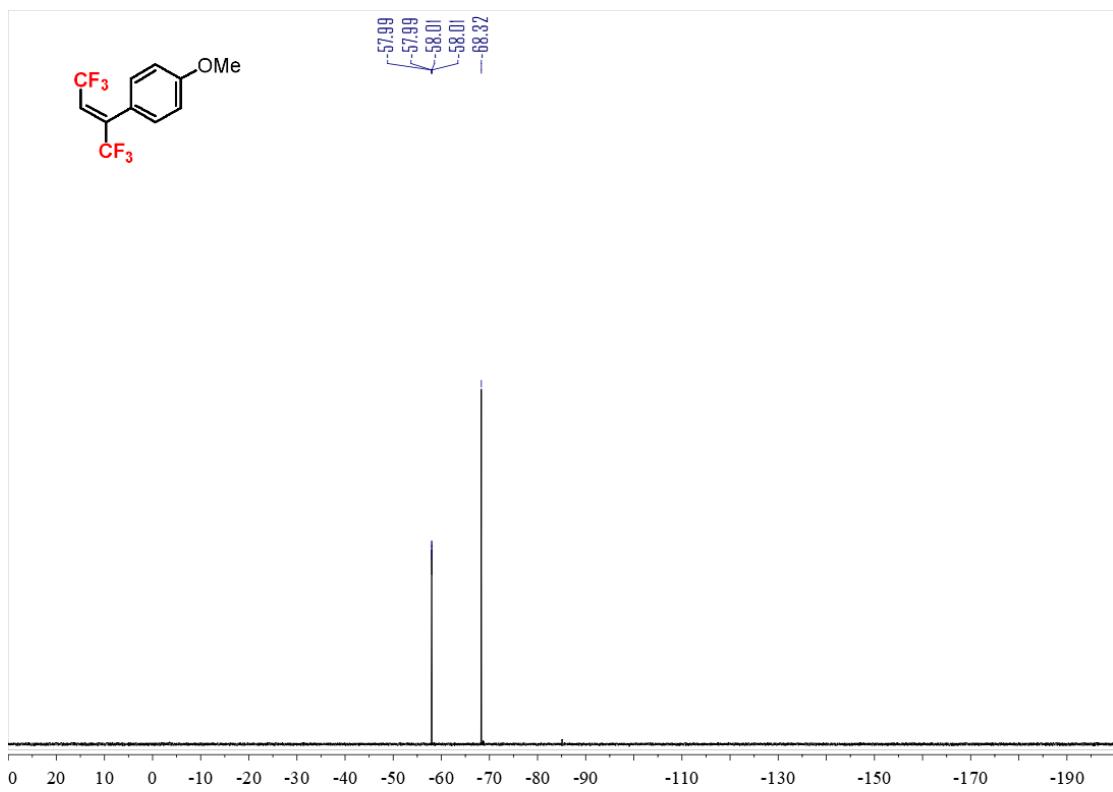
^{19}F NMR spectrum (375 MHz, CDCl_3 , 23 °C) of **3j**



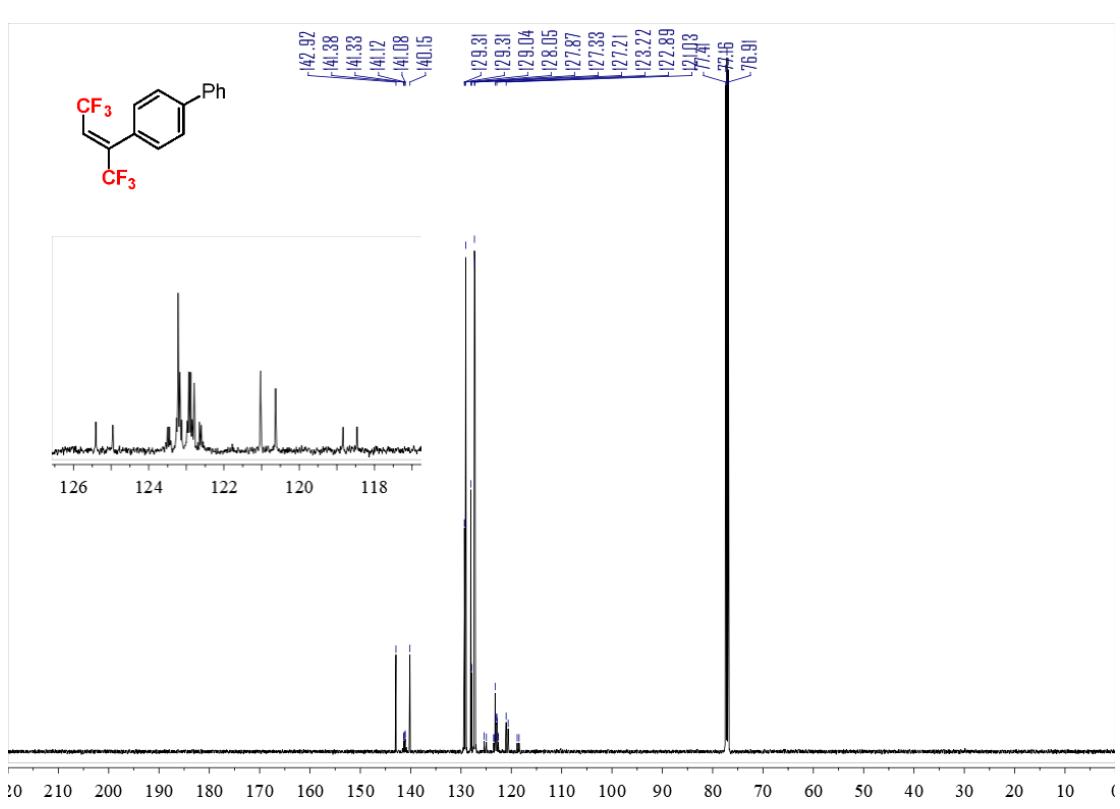
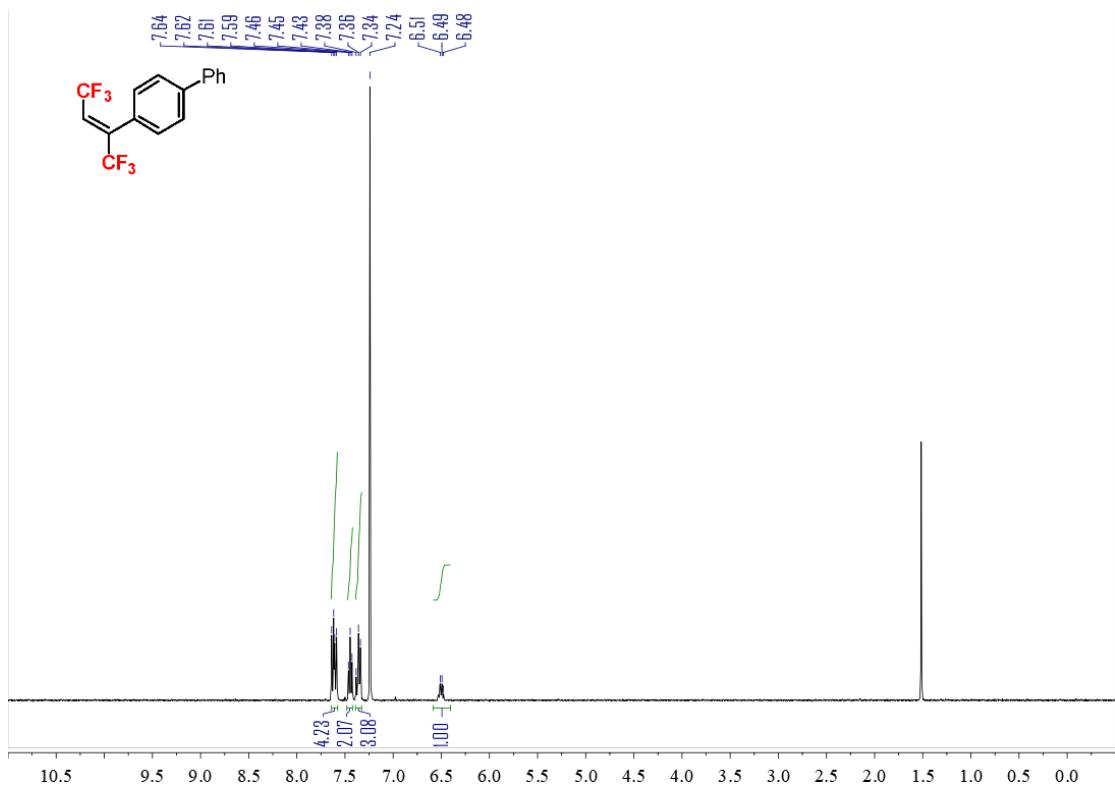
^1H NMR spectrum (400 MHz, CDCl_3 , 23 °C) of **3k**

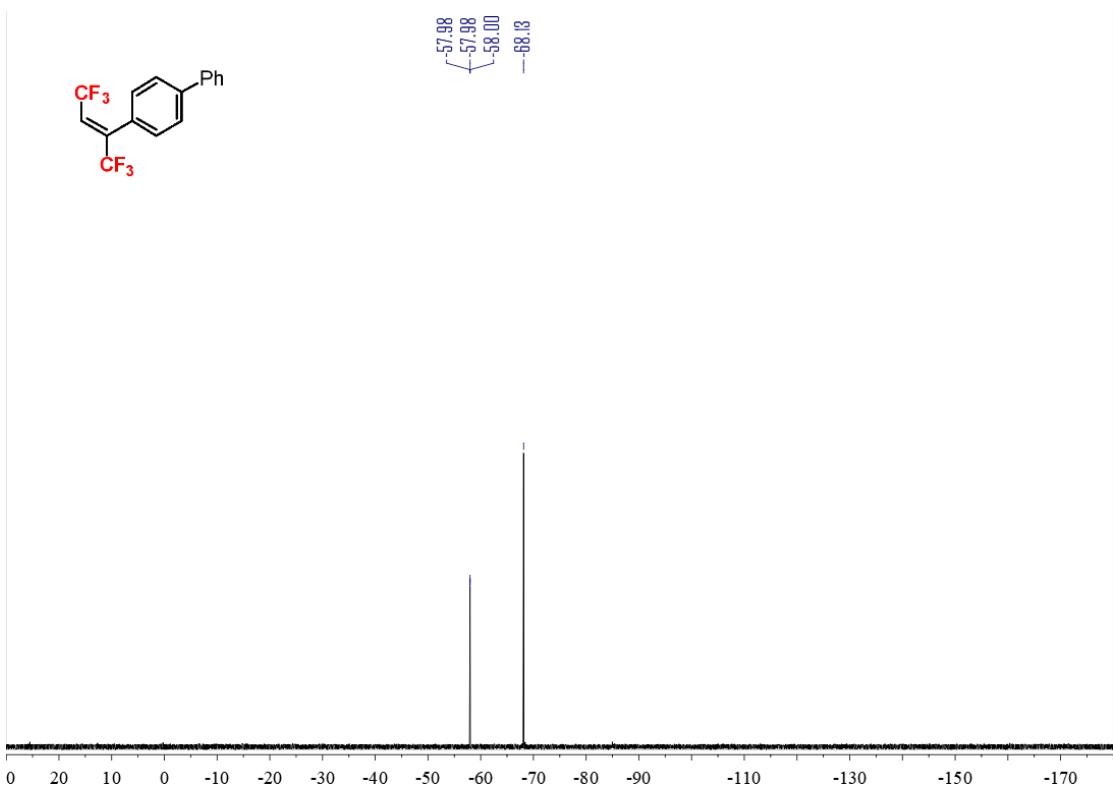


¹³C NMR spectrum (126 MHz, CDCl₃, 23 °C) of **3k**

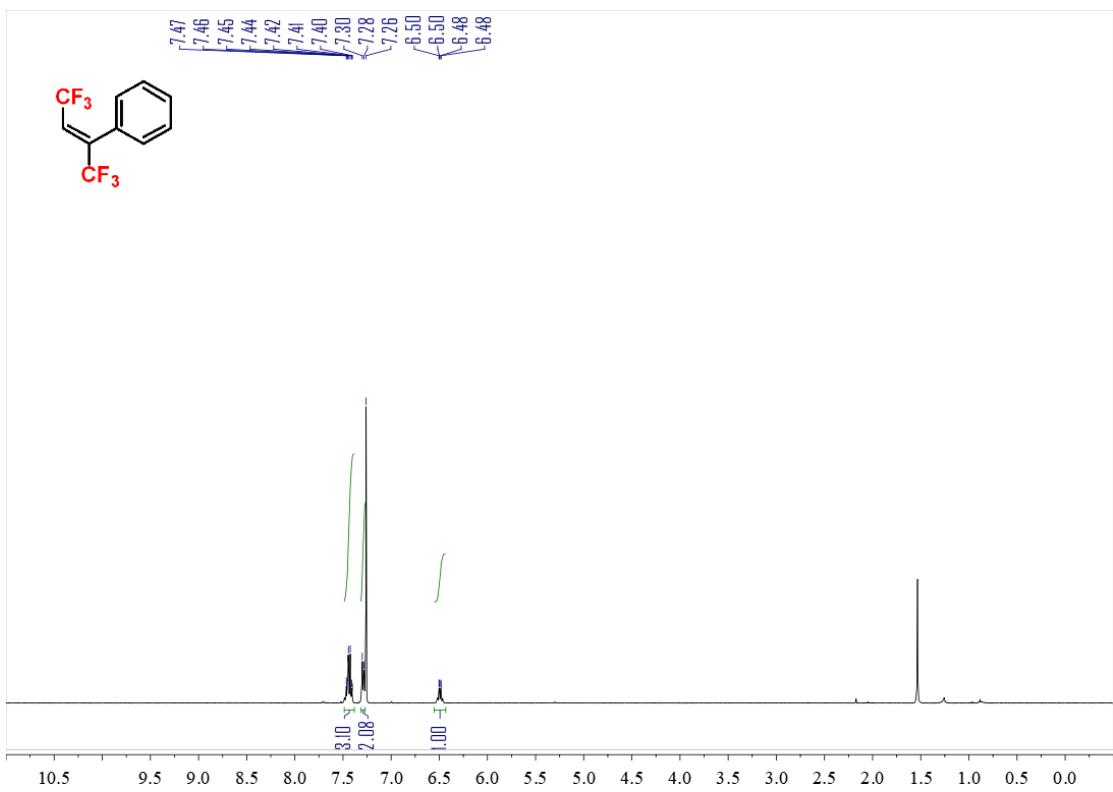


¹⁹F NMR spectrum (375 MHz, CDCl₃, 23 °C) of **3k**

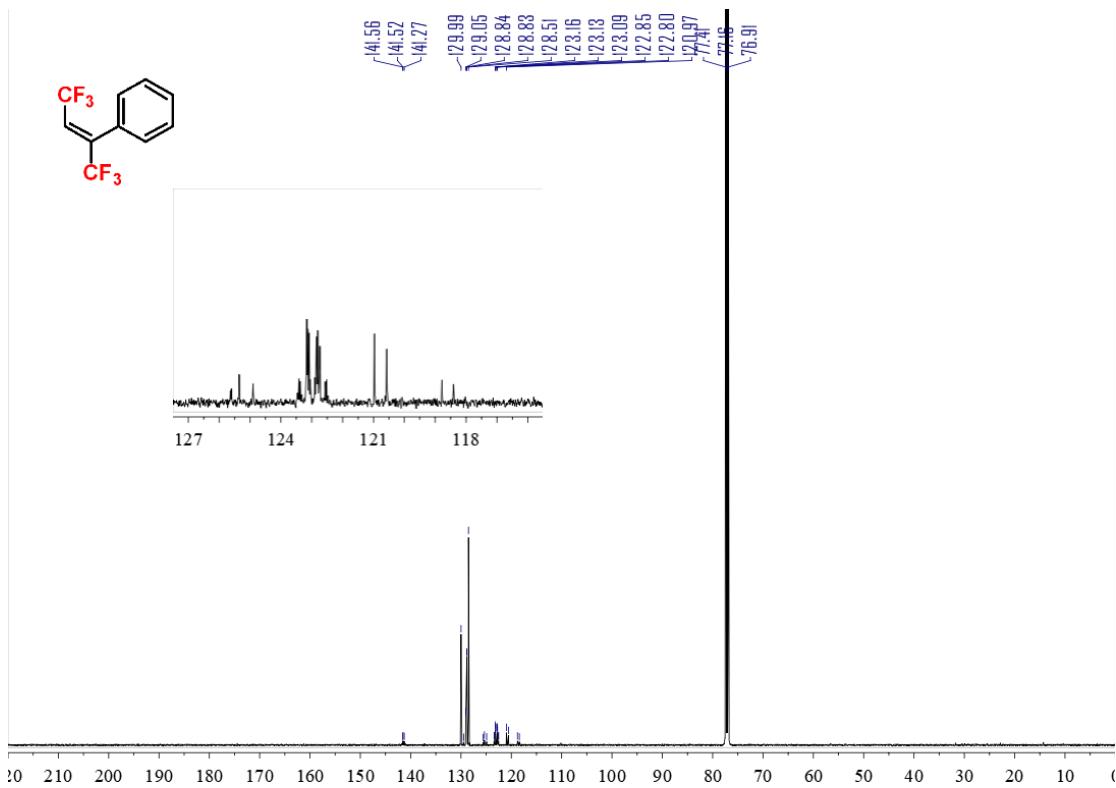




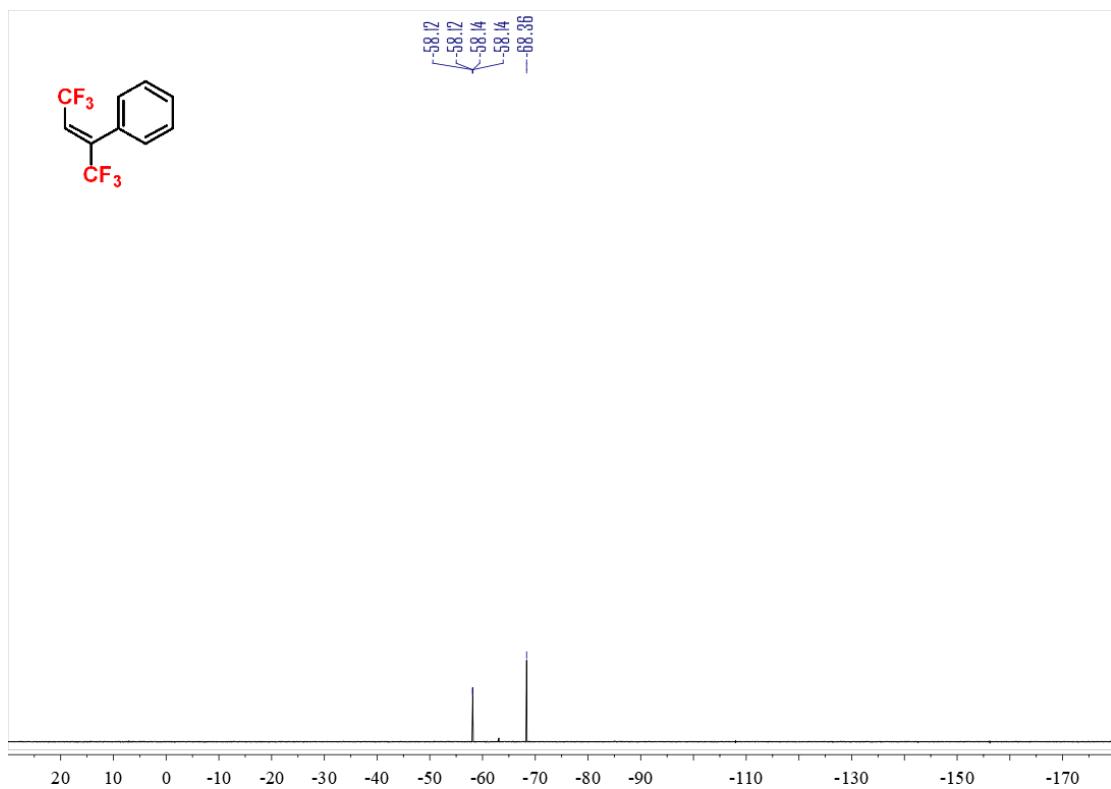
¹⁹F NMR spectrum (375 MHz, CDCl₃, 23 °C) of **3l**



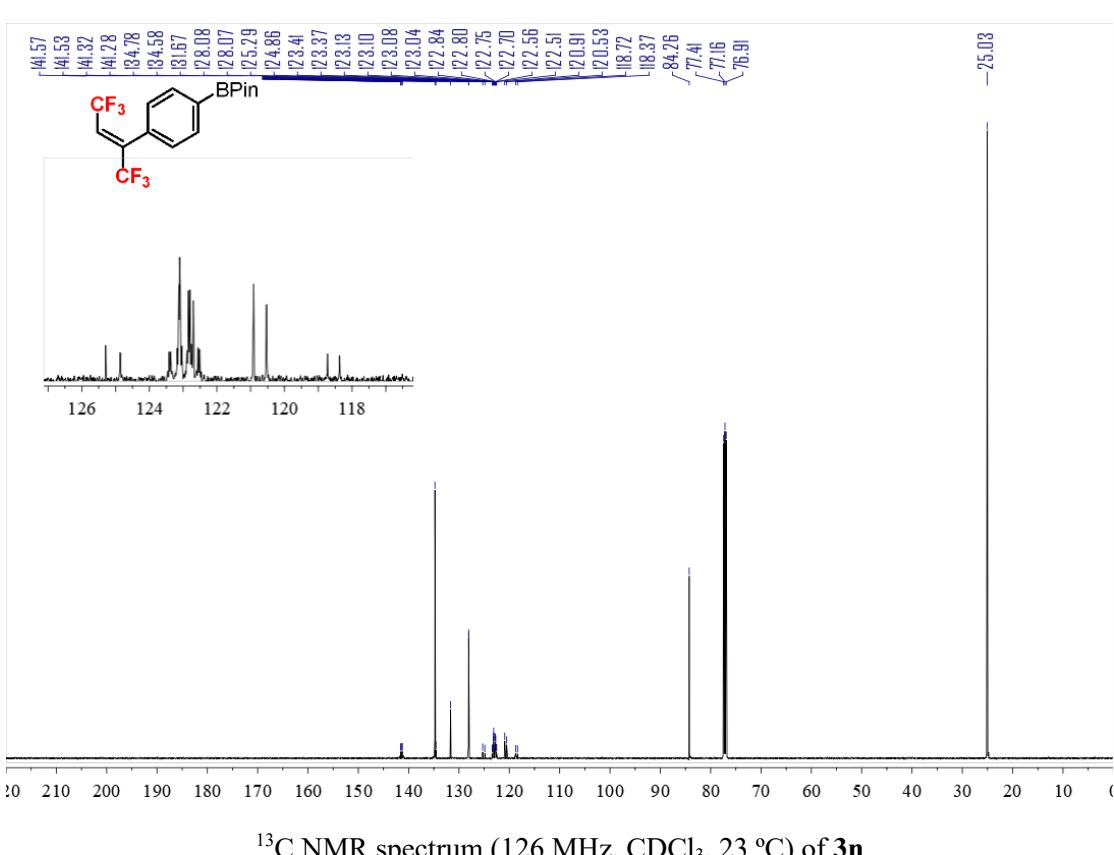
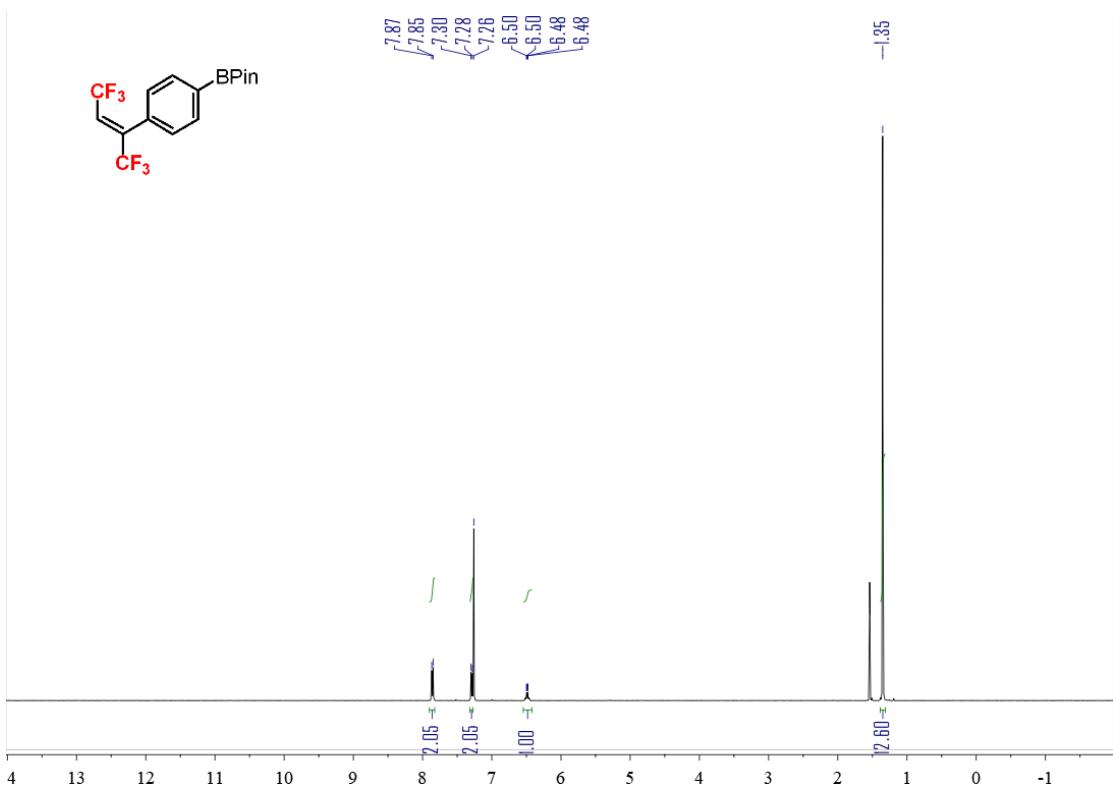
¹H NMR spectrum (400 MHz, CDCl₃, 23 °C) of **3m**

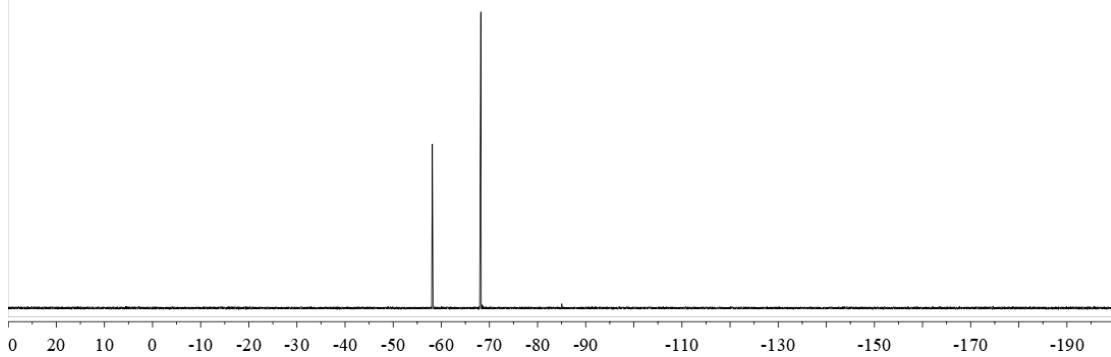


¹³C NMR spectrum (126 MHz, CDCl₃, 23 °C) of **3m**

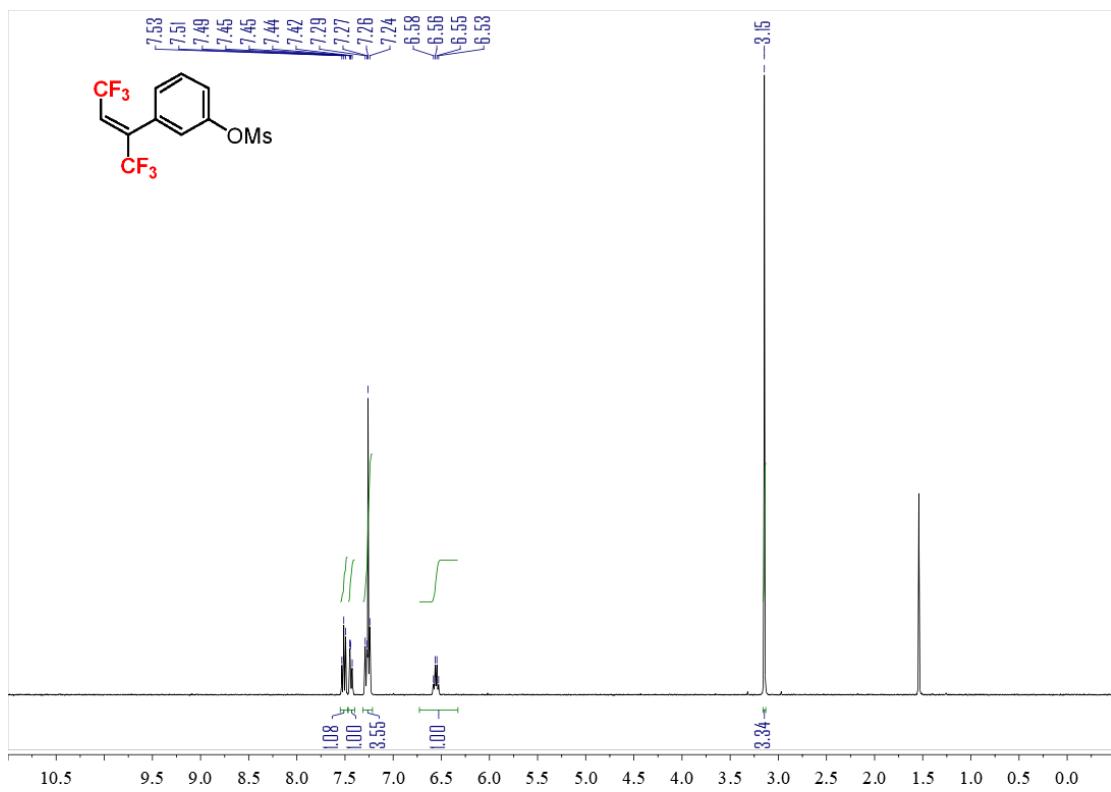
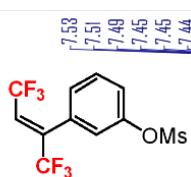


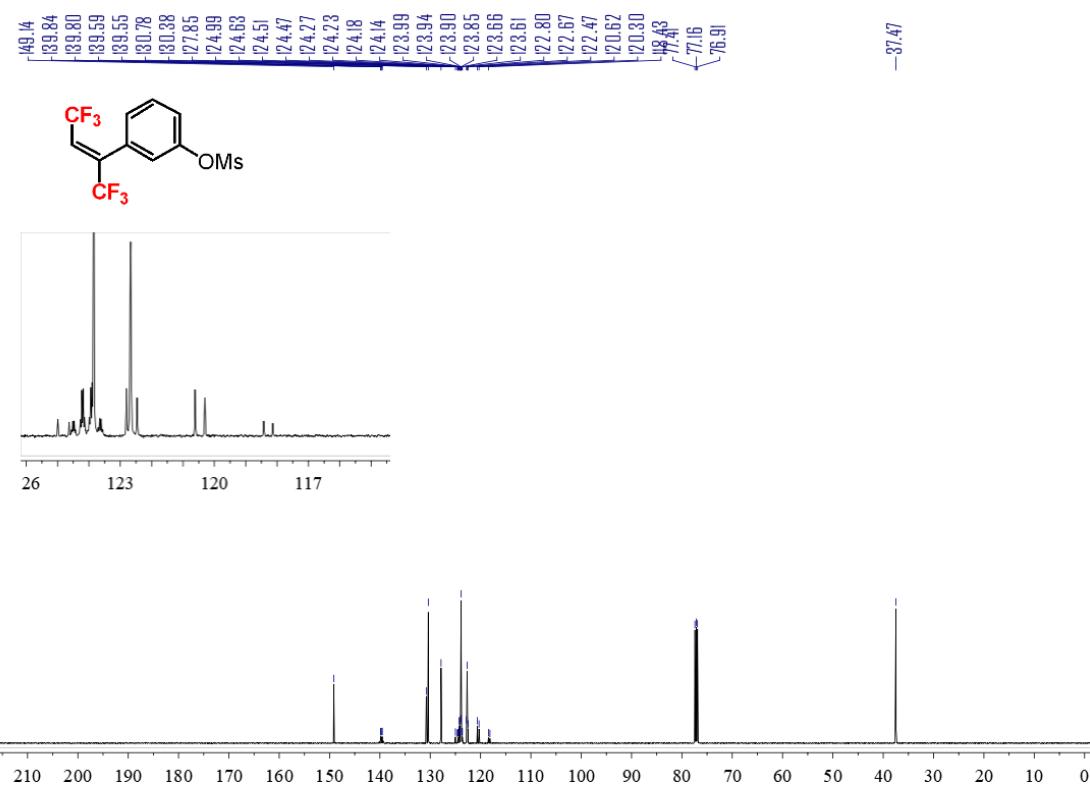
¹⁹F NMR spectrum (375 MHz, CDCl₃, 23 °C) of **3m**



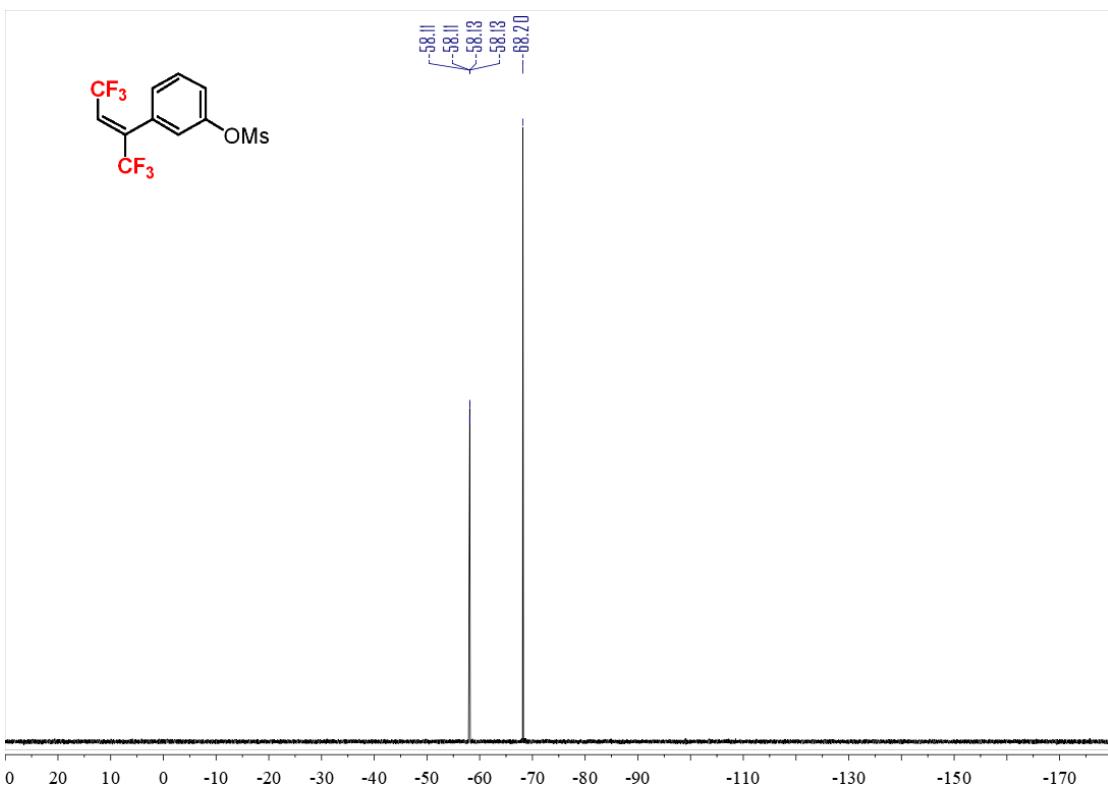


¹⁹F NMR spectrum (375 MHz, CDCl₃, 23 °C) of **3n**

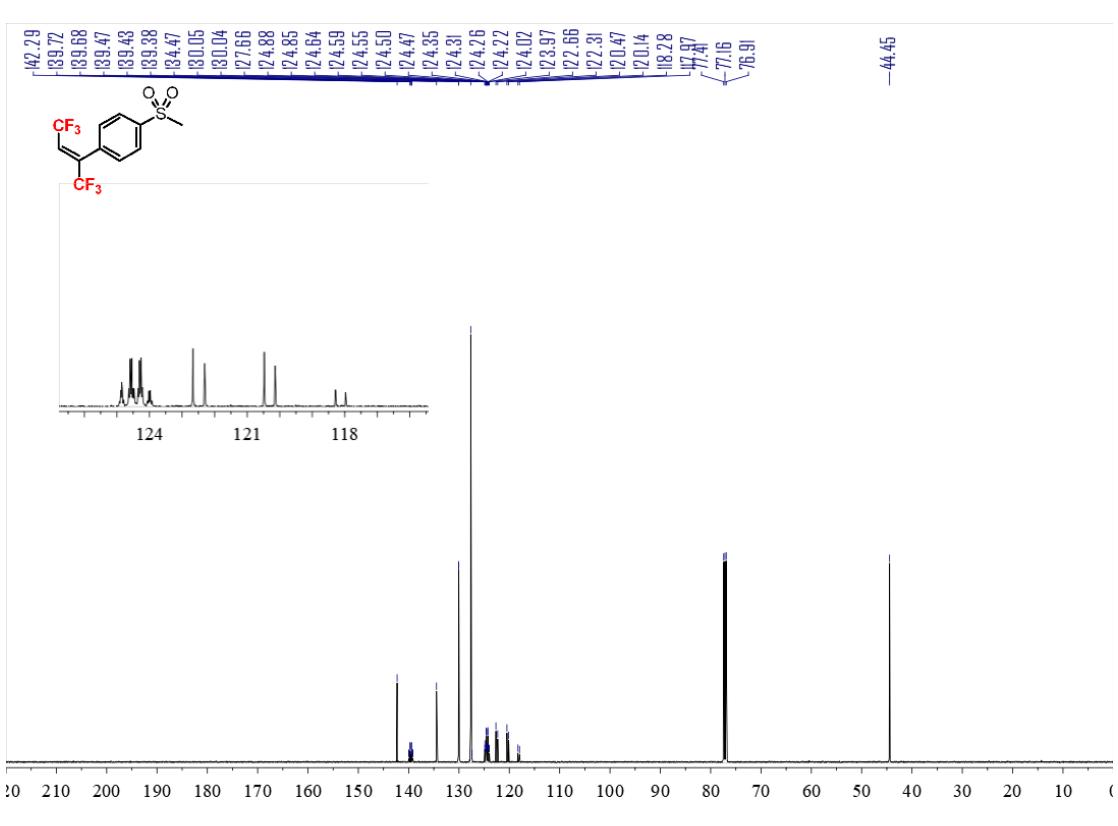
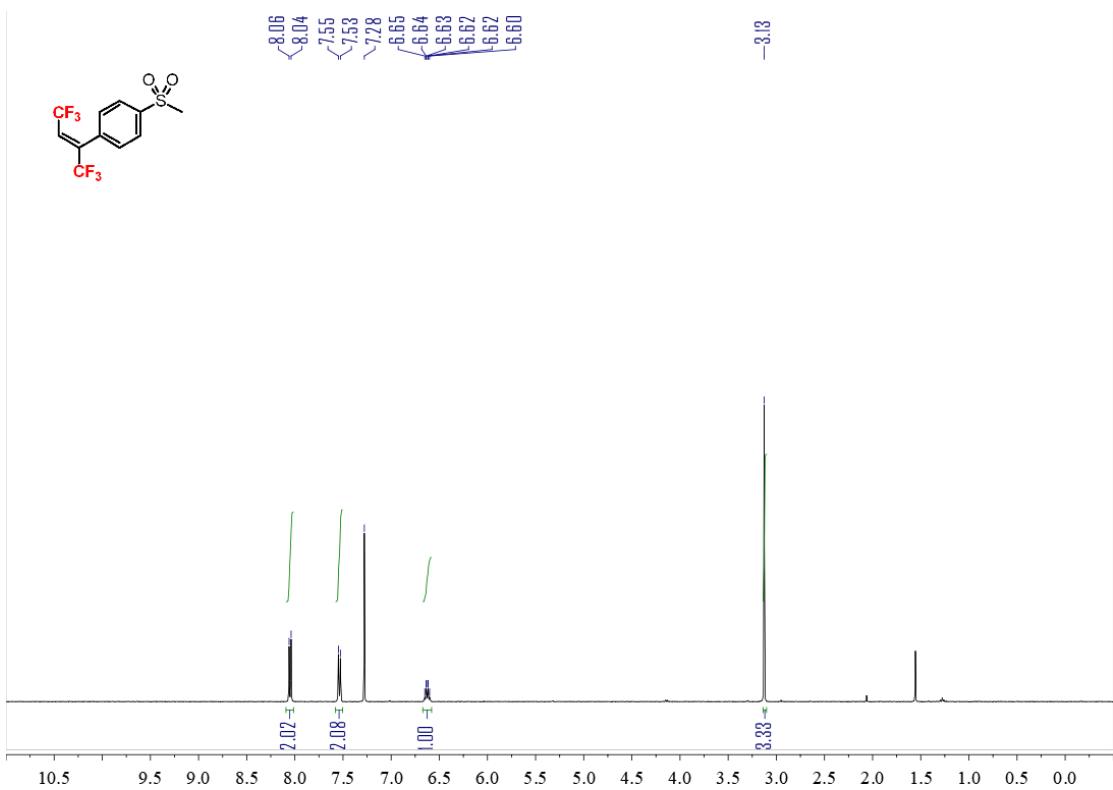


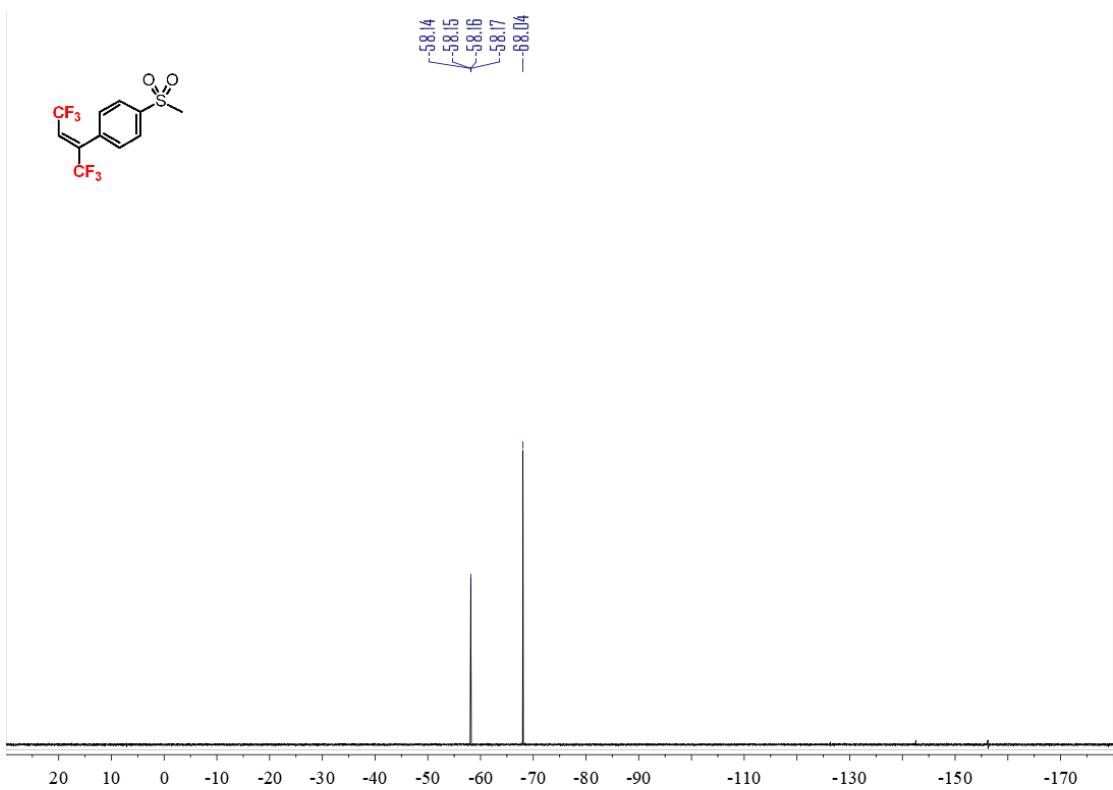


¹³C NMR spectrum (126 MHz, CDCl₃, 23 °C) of **3o**

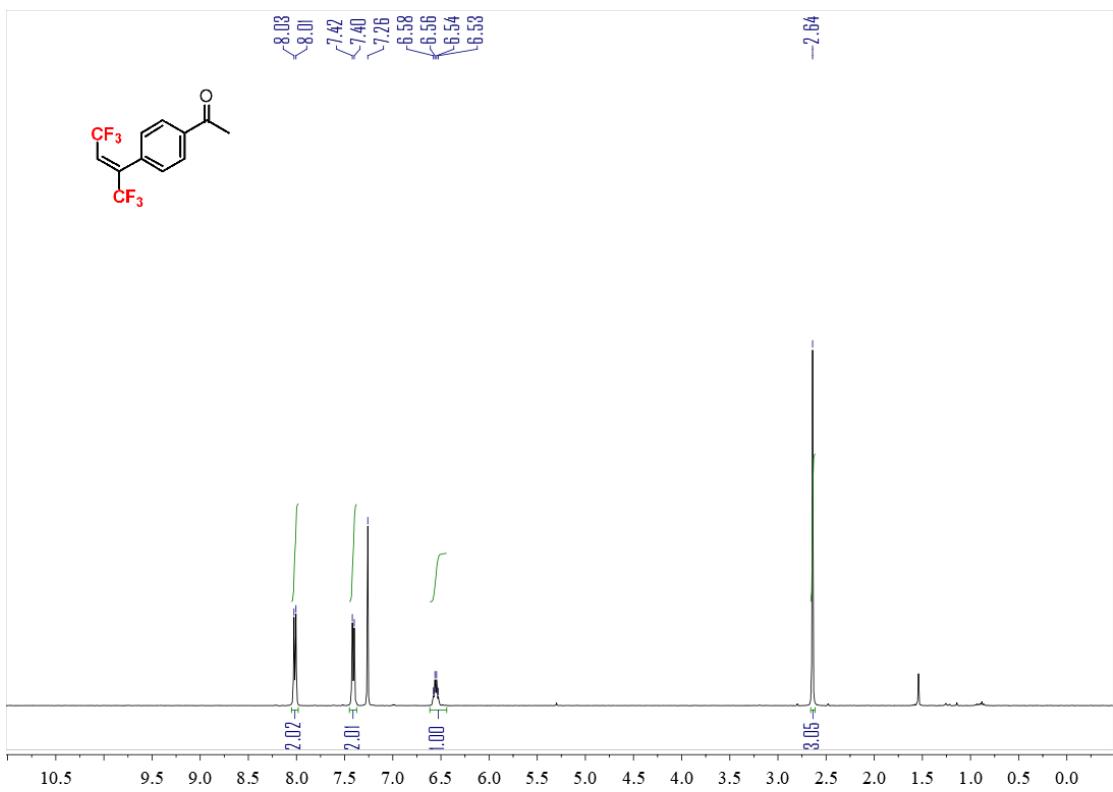


¹⁹F NMR spectrum (375 MHz, CDCl₃, 23 °C) of **3o**

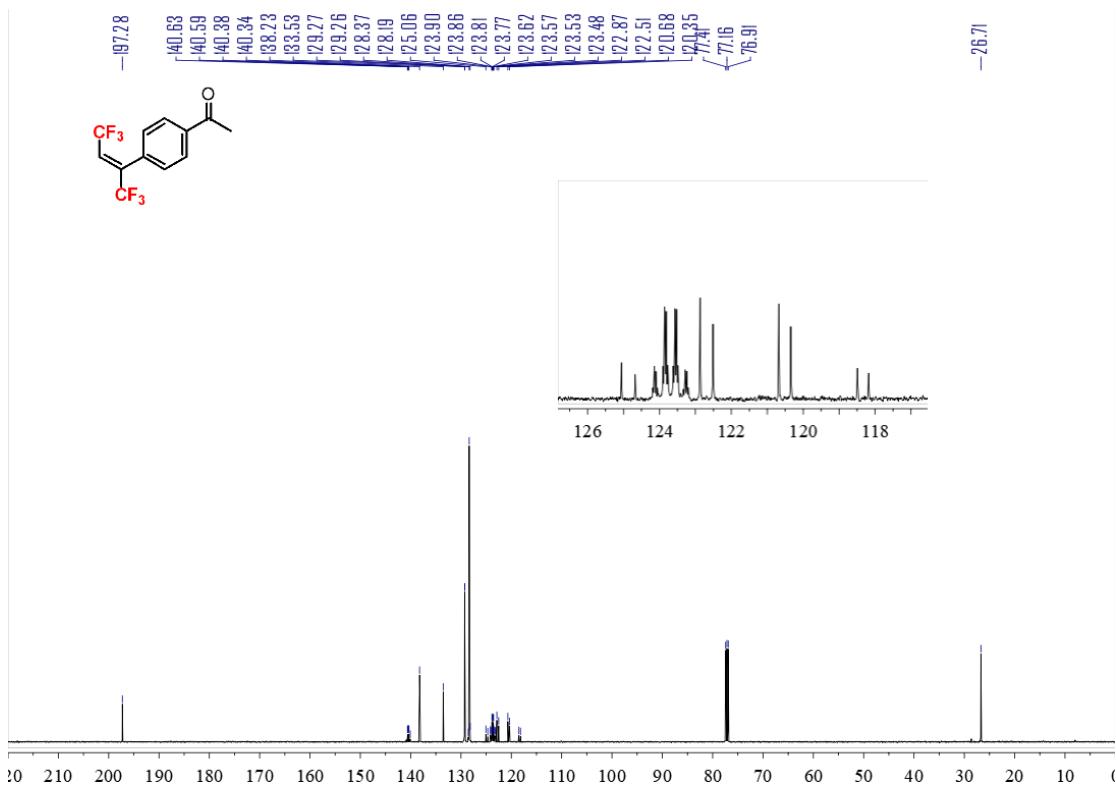




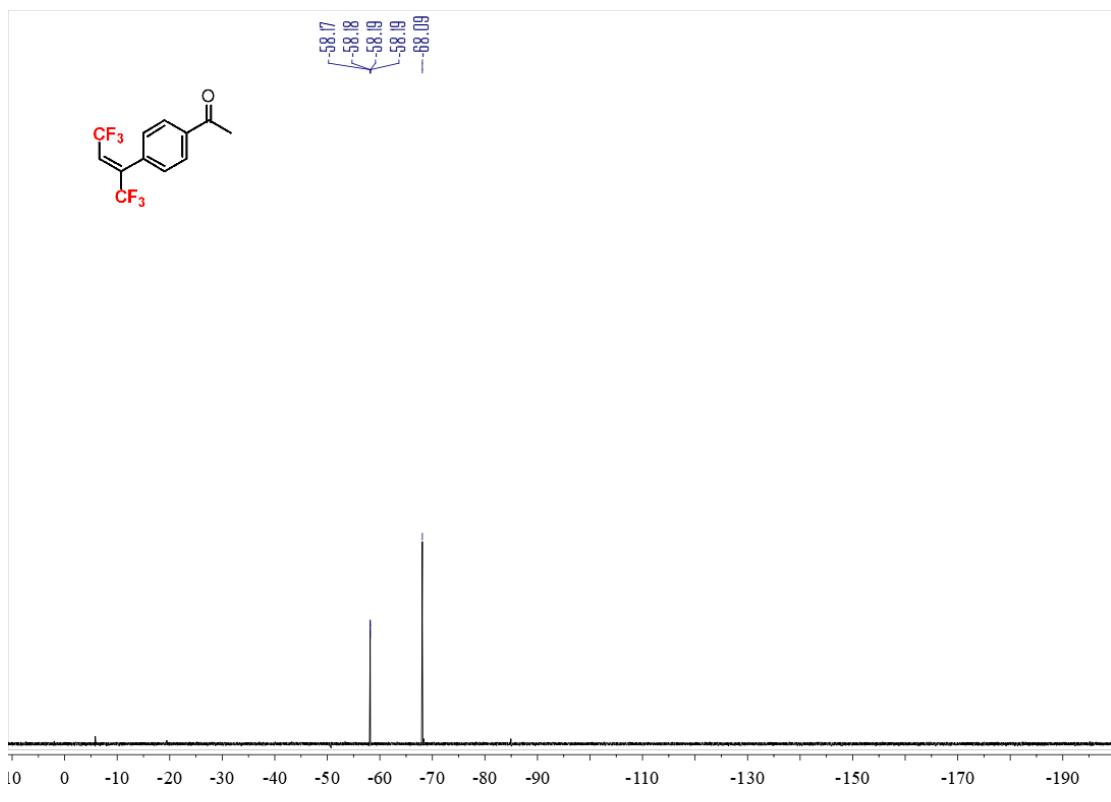
^{19}F NMR spectrum (375 MHz, CDCl_3 , 23 °C) of **3p**



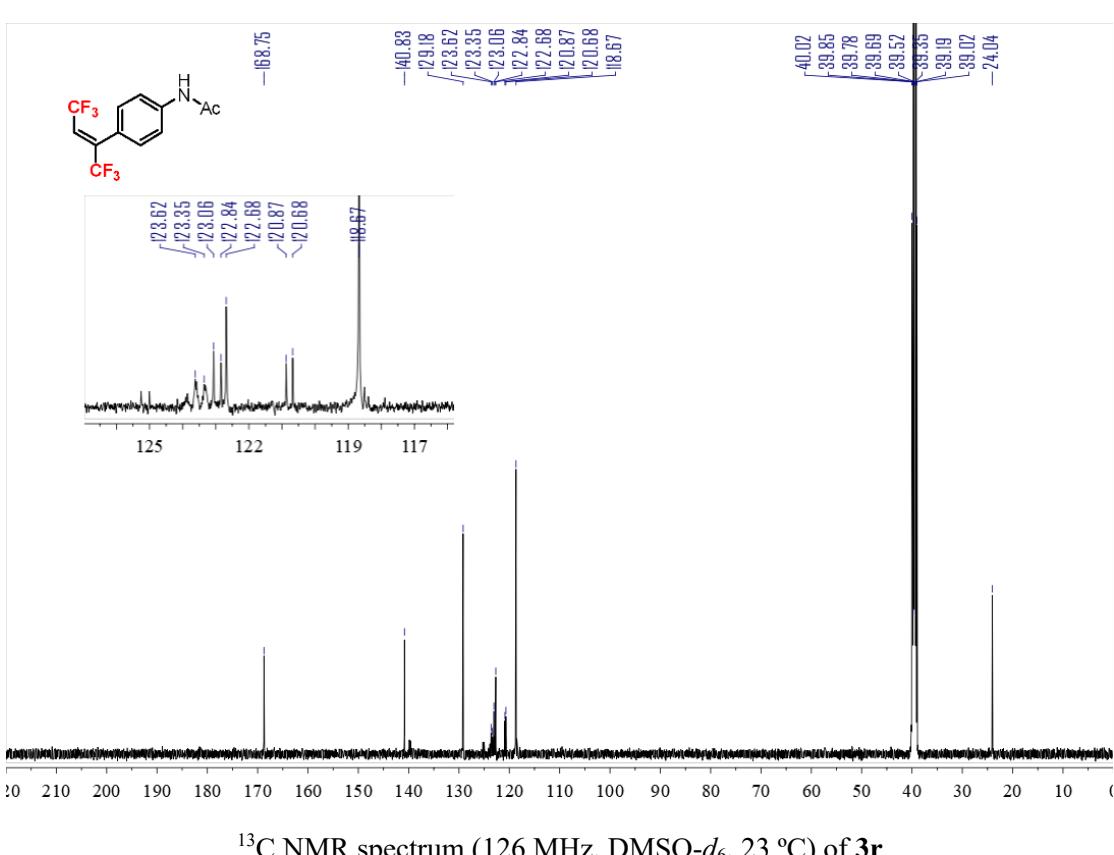
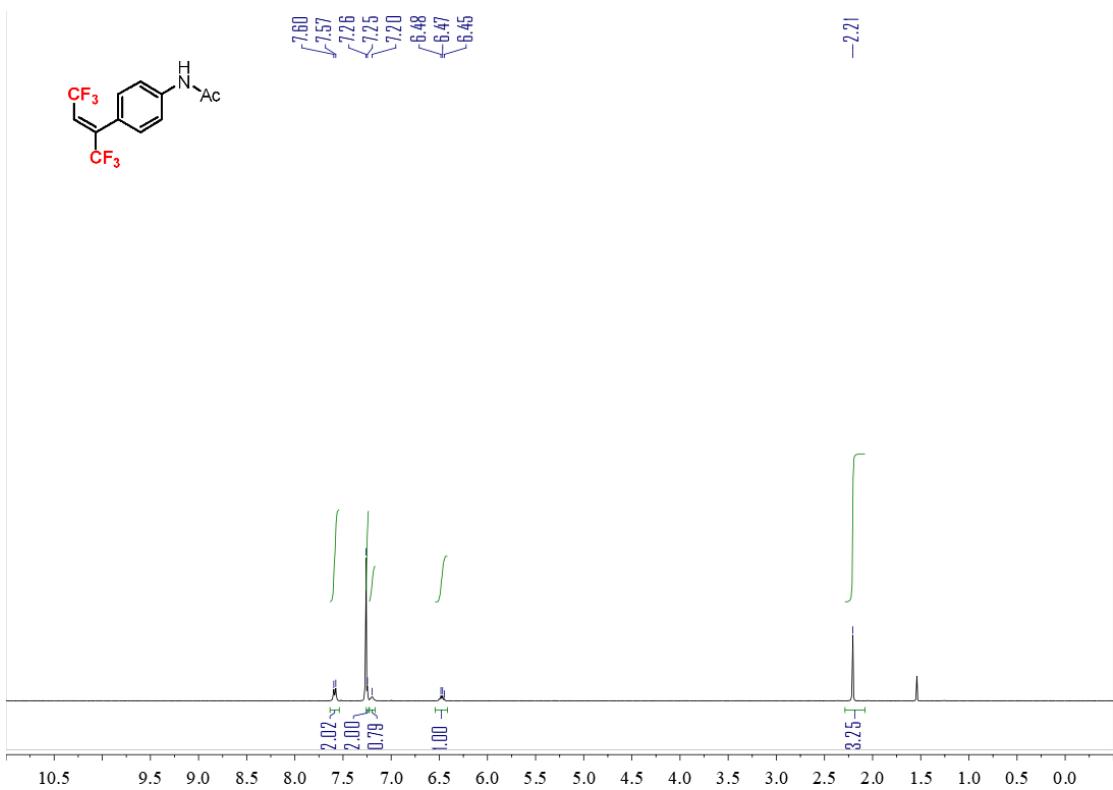
^1H NMR spectrum (400 MHz, CDCl_3 , 23 °C) of **3q**

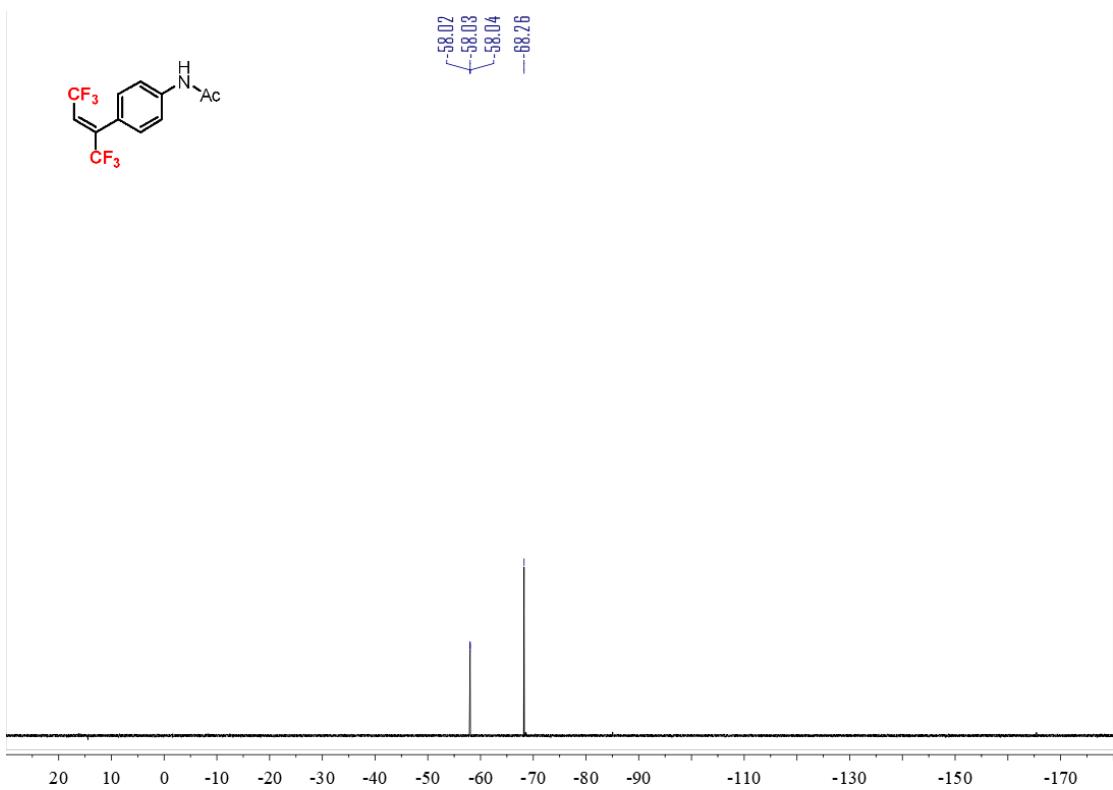


¹³C NMR spectrum (126 MHz, CDCl₃, 23 °C) of **3q**

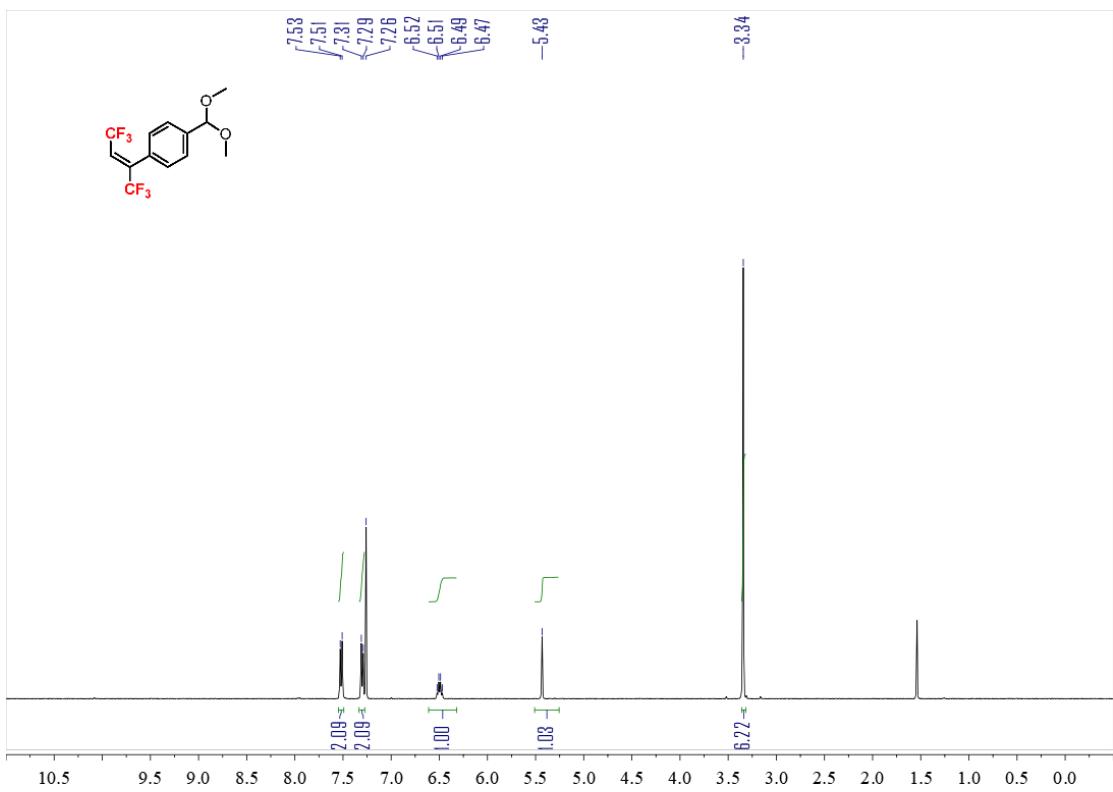


¹⁹F NMR spectrum (375 MHz, CDCl₃, 23 °C) of **3q**

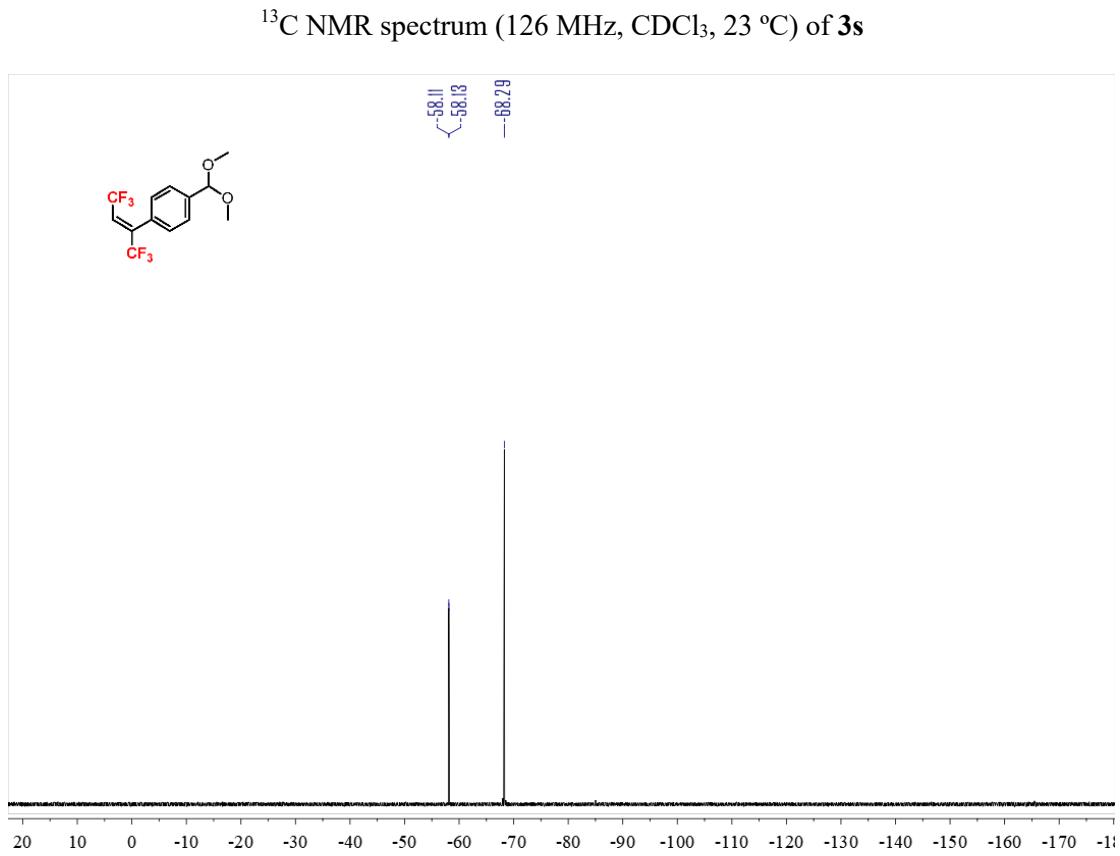
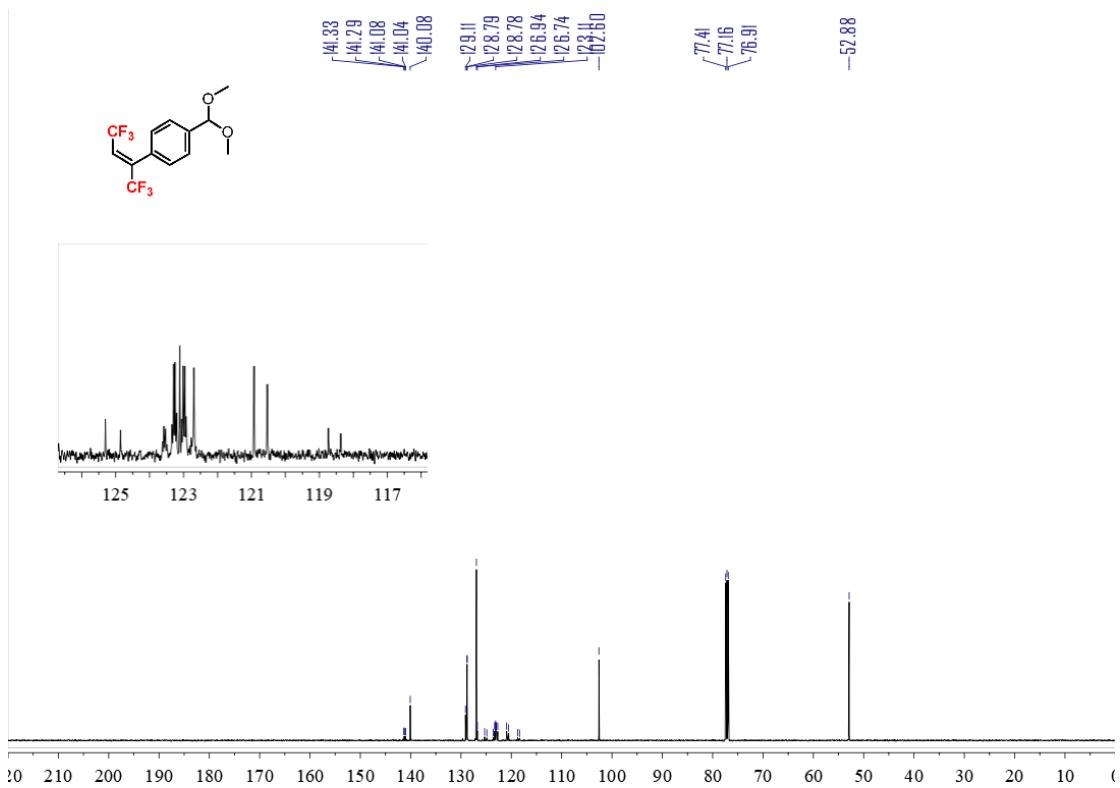




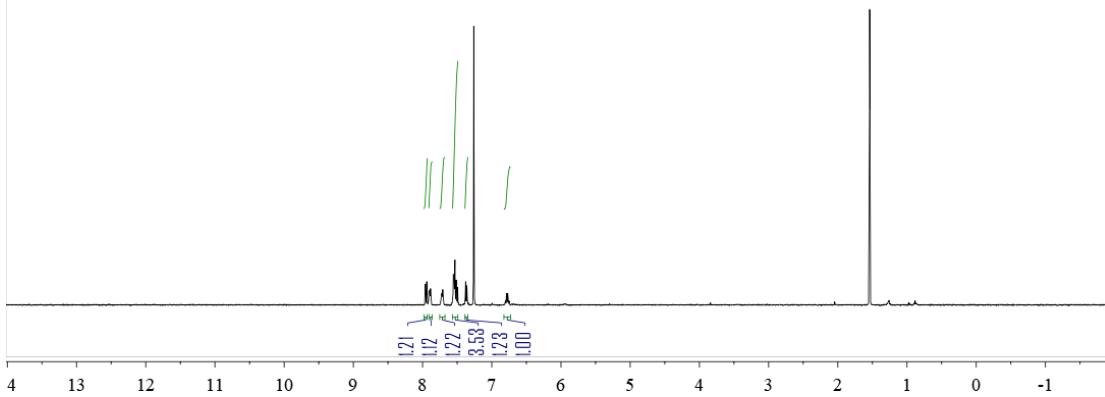
^{19}F NMR spectrum (375 MHz, CDCl_3 , 23 °C) of **3r**



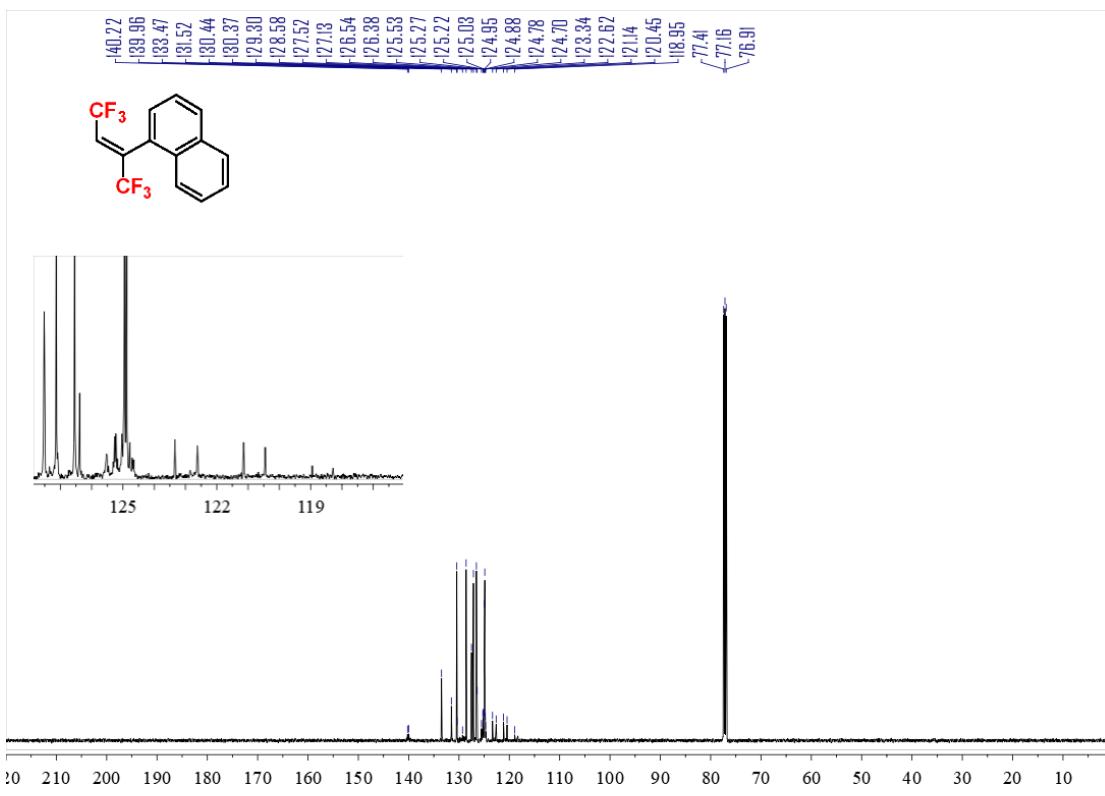
^1H NMR spectrum (400 MHz, CDCl_3 , 23 °C) of **3s**



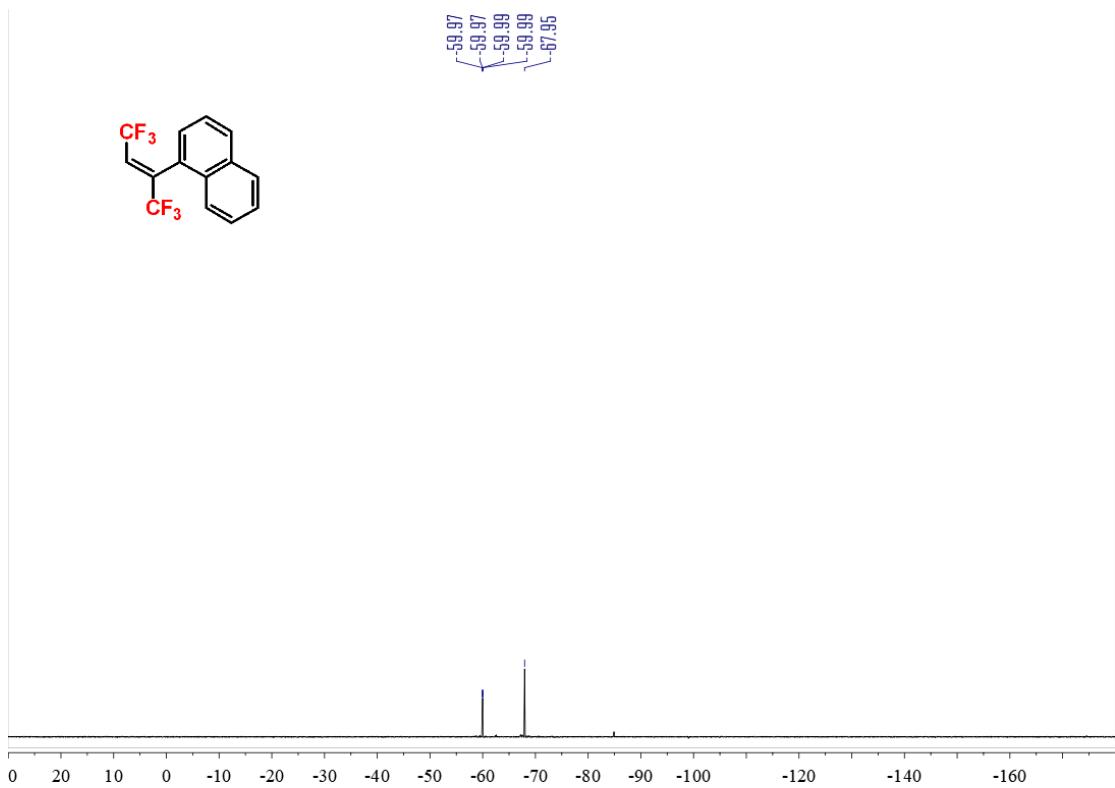
¹⁹F NMR spectrum (375 MHz, CDCl₃, 23 °C) of **3s**



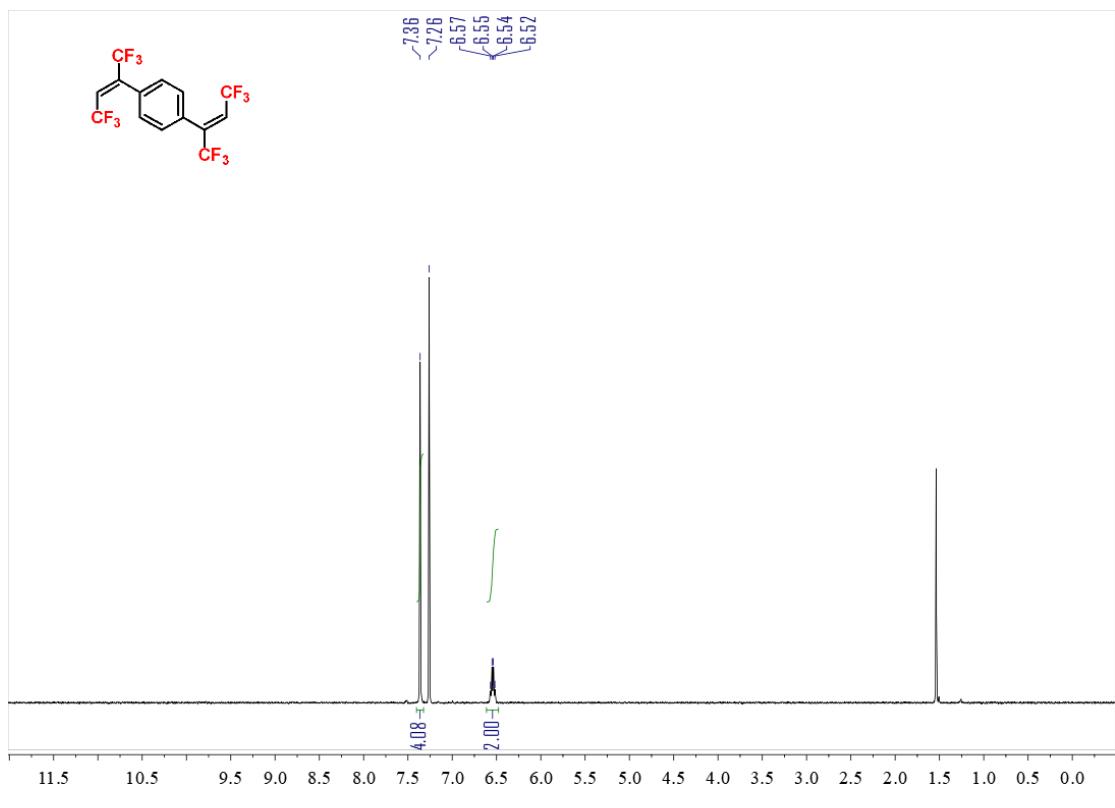
^1H NMR spectrum (400 MHz, CDCl_3 , 23 °C) of **3t**



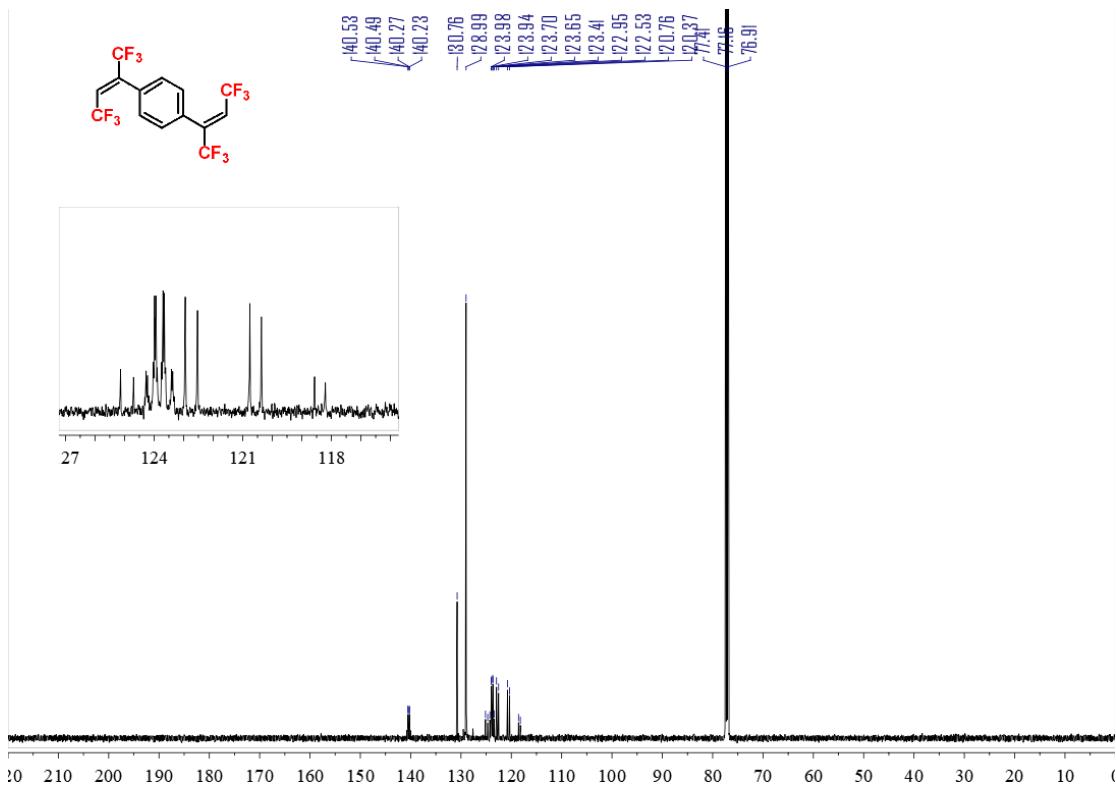
^{13}C NMR spectrum (101 MHz, CDCl_3 , 23 °C) of **3t**



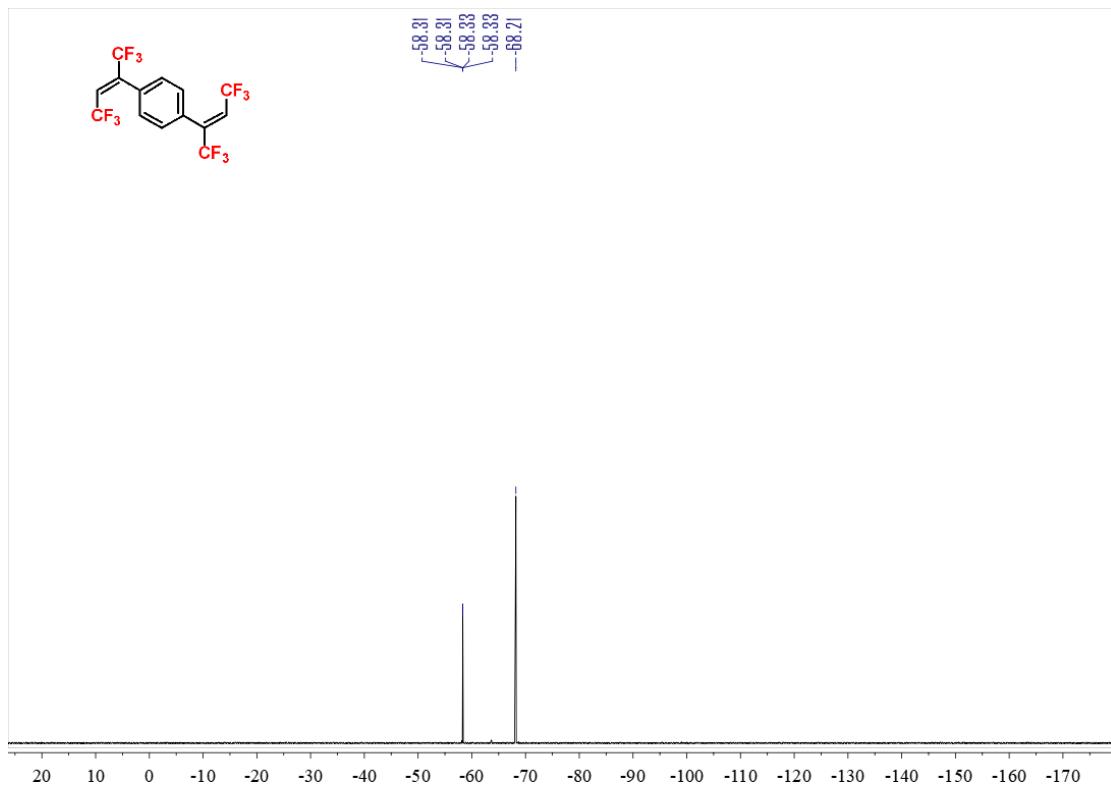
¹⁹F NMR spectrum (375 MHz, CDCl₃, 23 °C) of **3t**



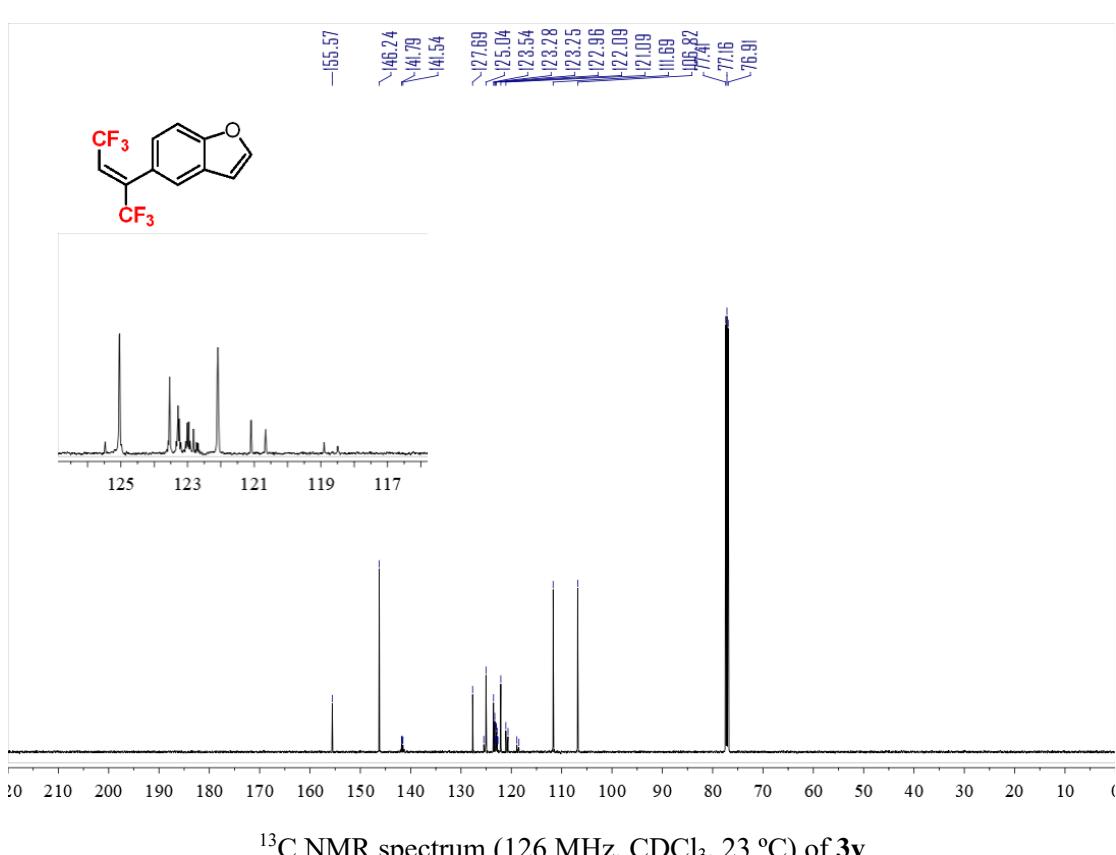
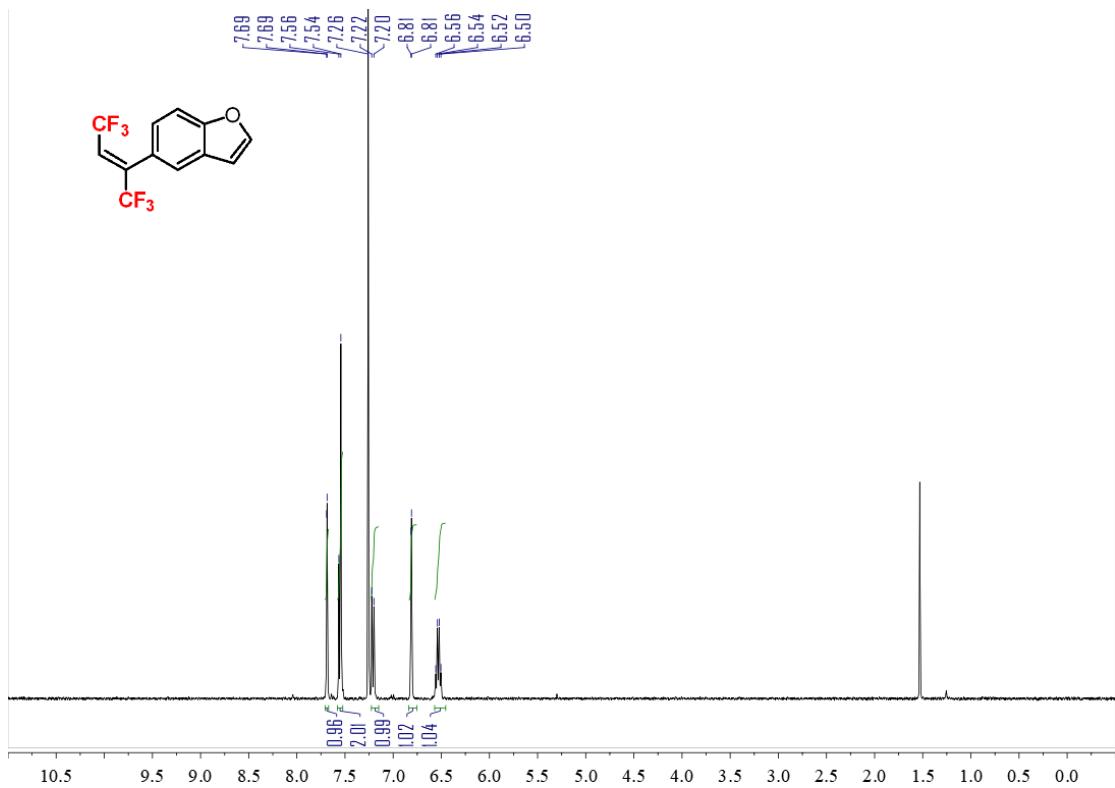
¹H NMR spectrum (400 MHz, CDCl₃, 23 °C) of **3u**

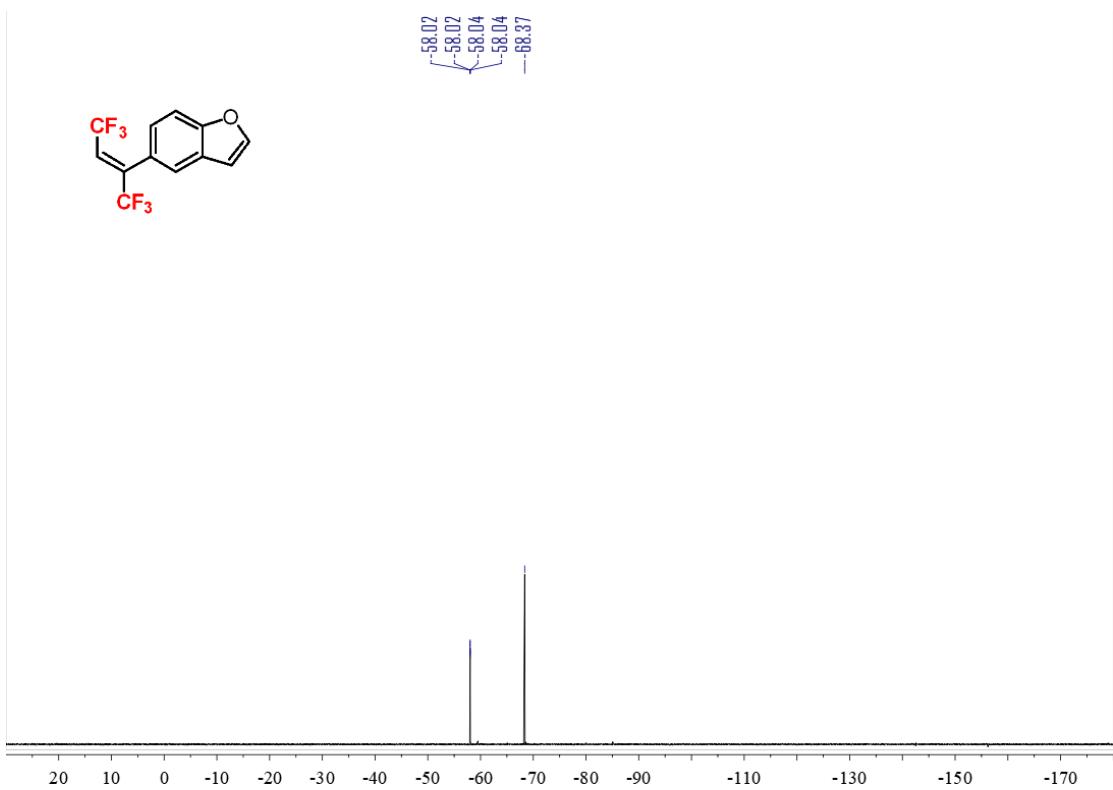


^{13}C NMR spectrum (126 MHz, CDCl_3 , 23 °C) of **3u**

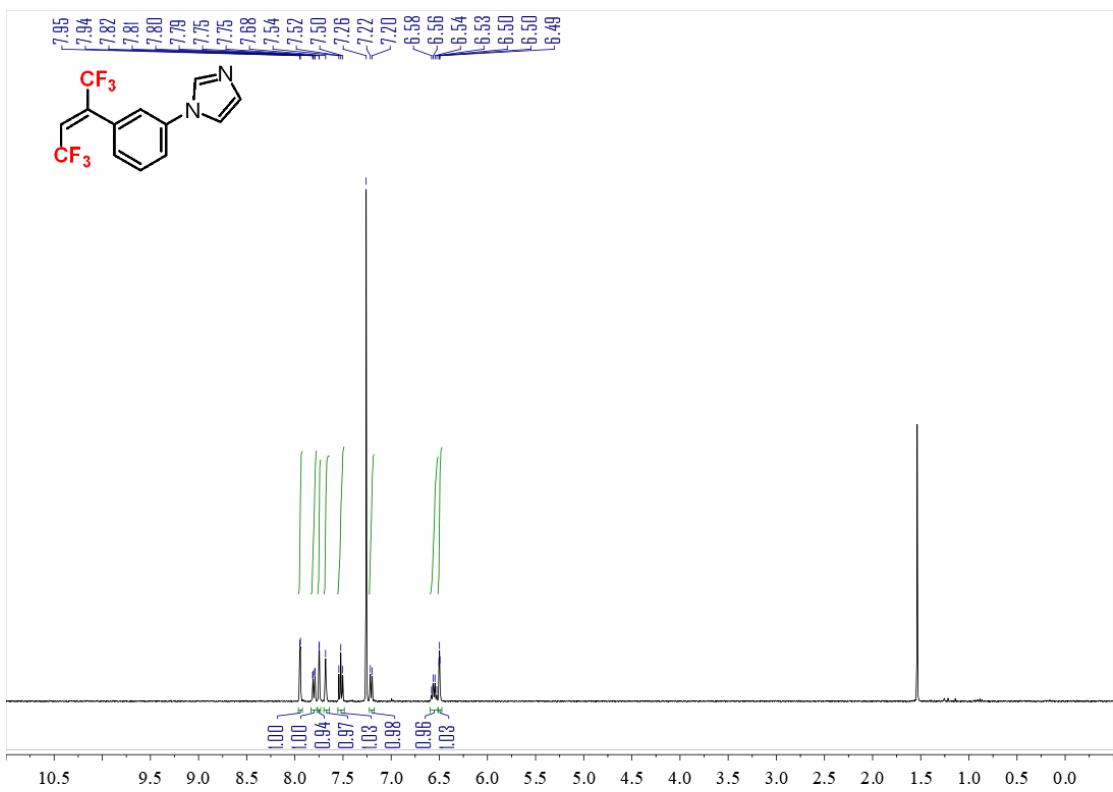


^{19}F NMR spectrum (375 MHz, CDCl_3 , 23 °C) of **3u**

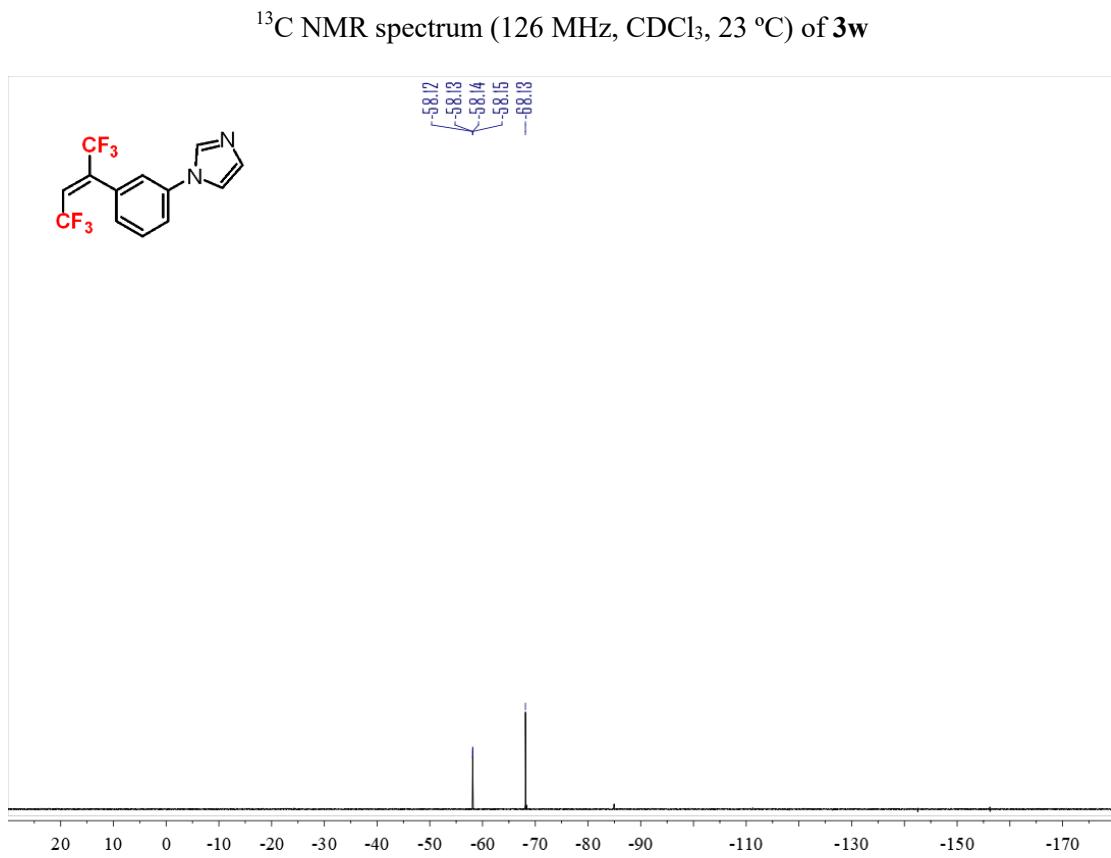
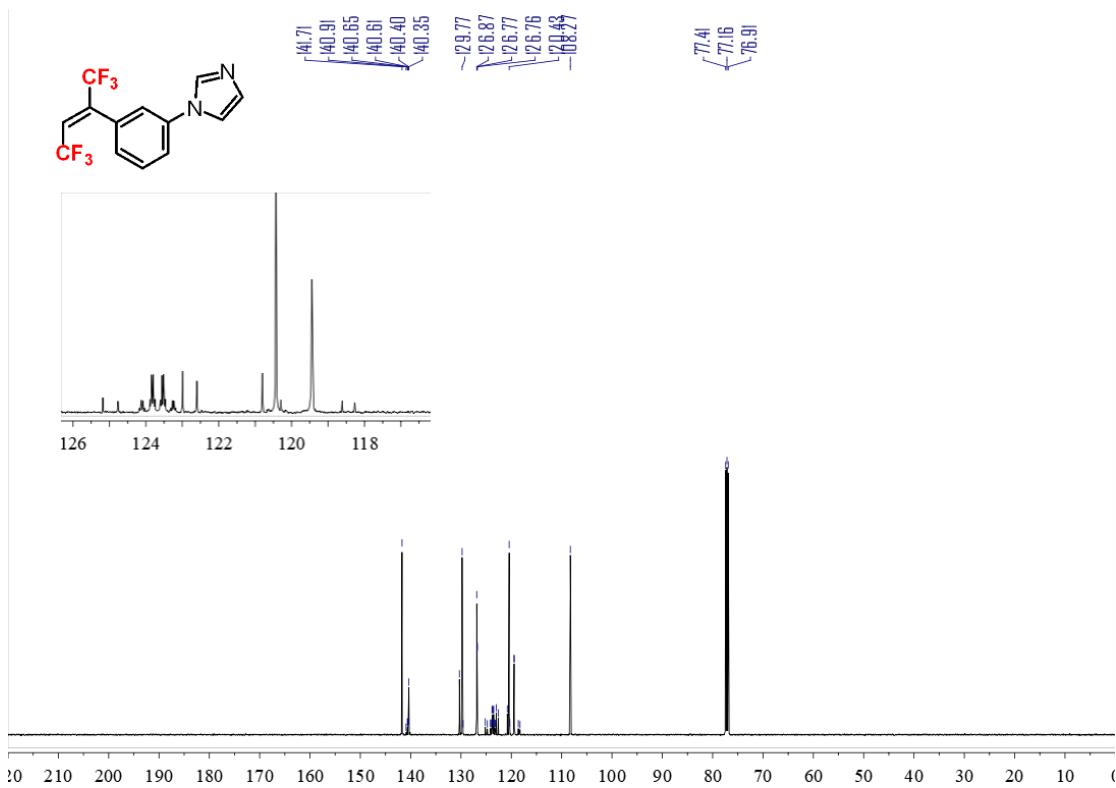


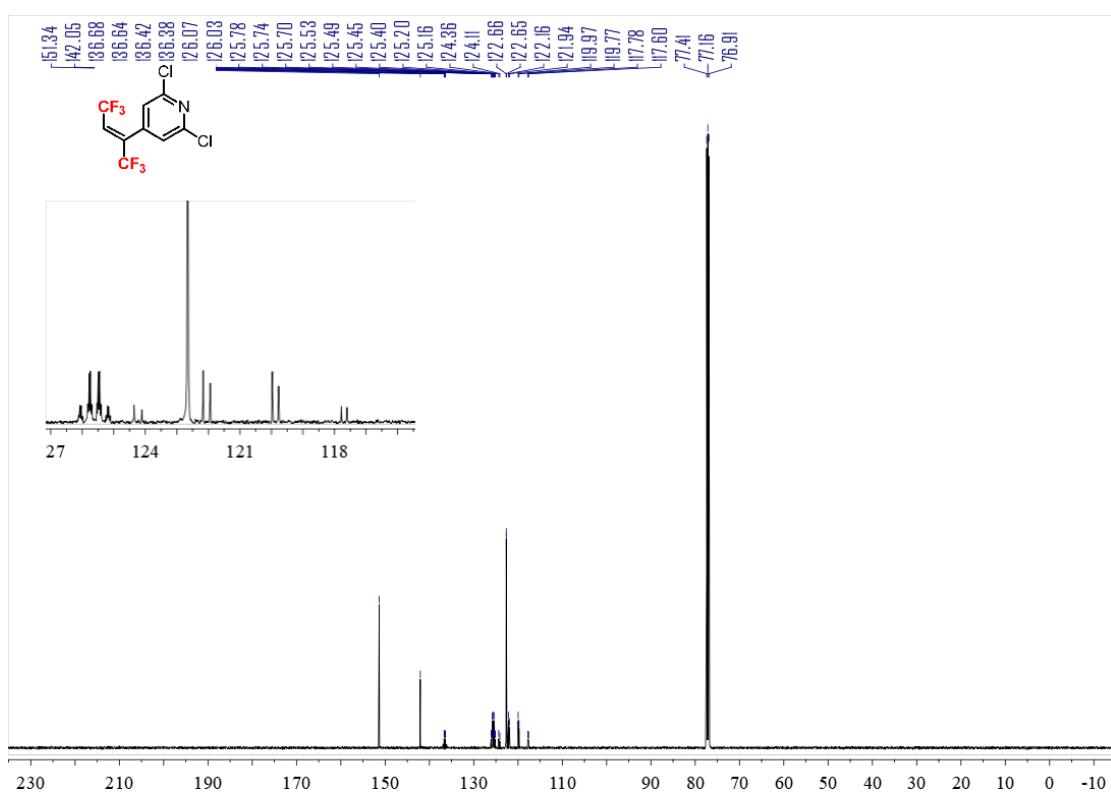
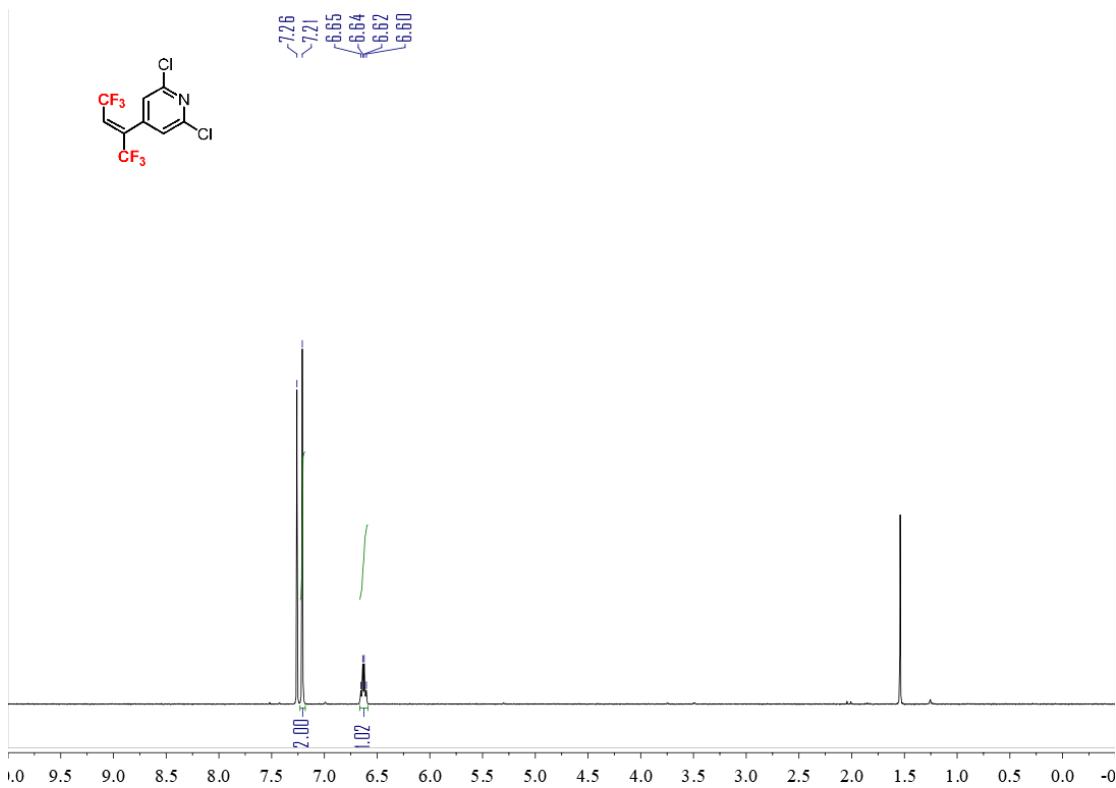


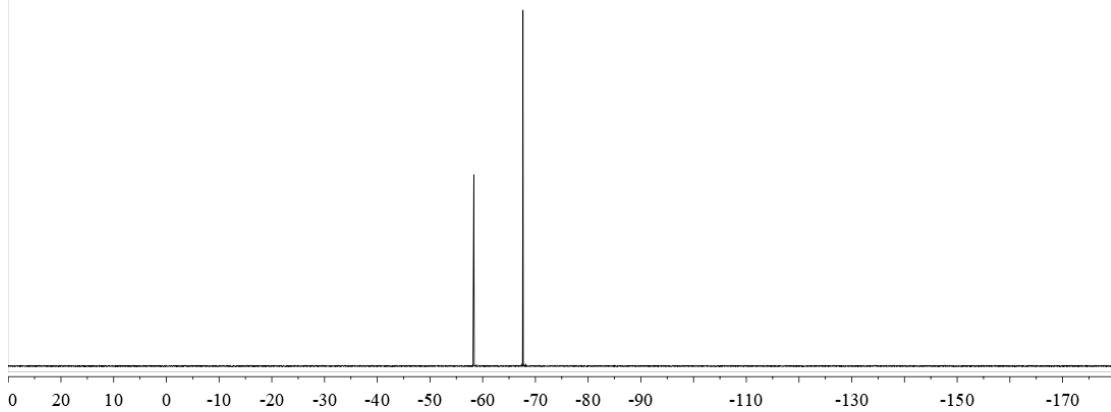
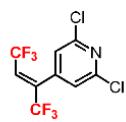
¹⁹F NMR spectrum (375 MHz, CDCl₃, 23 °C) of **3v**



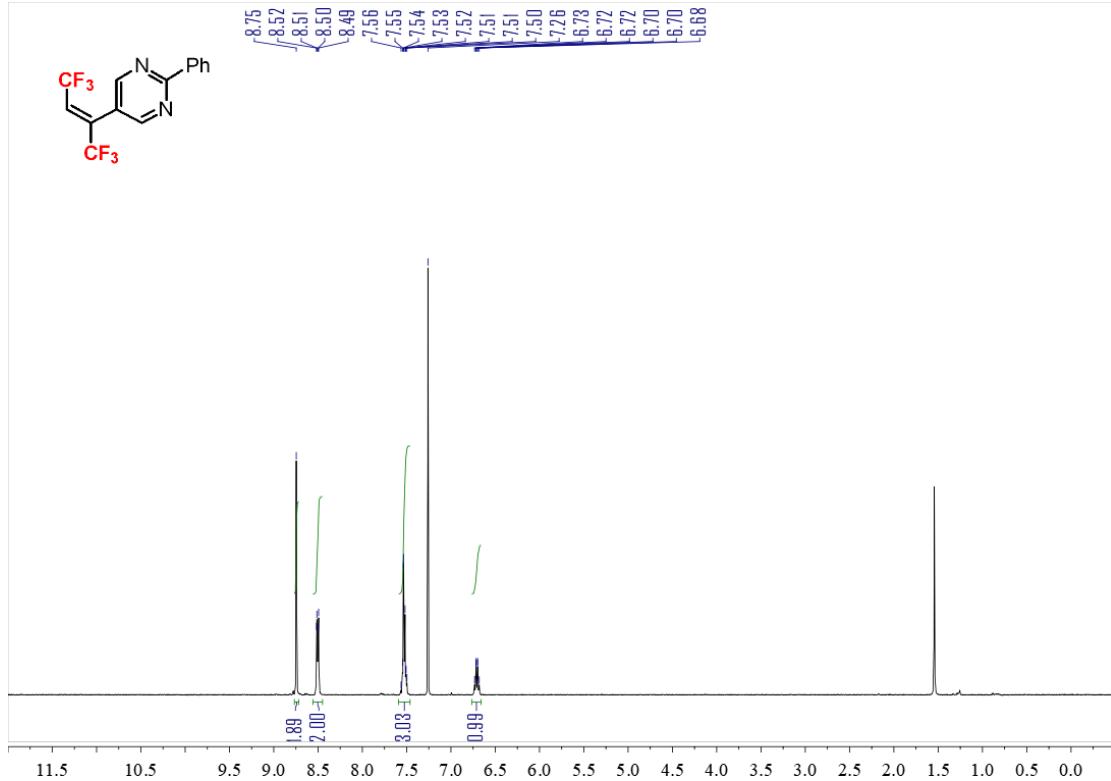
¹H NMR spectrum (400 MHz, CDCl₃, 23 °C) of **3w**



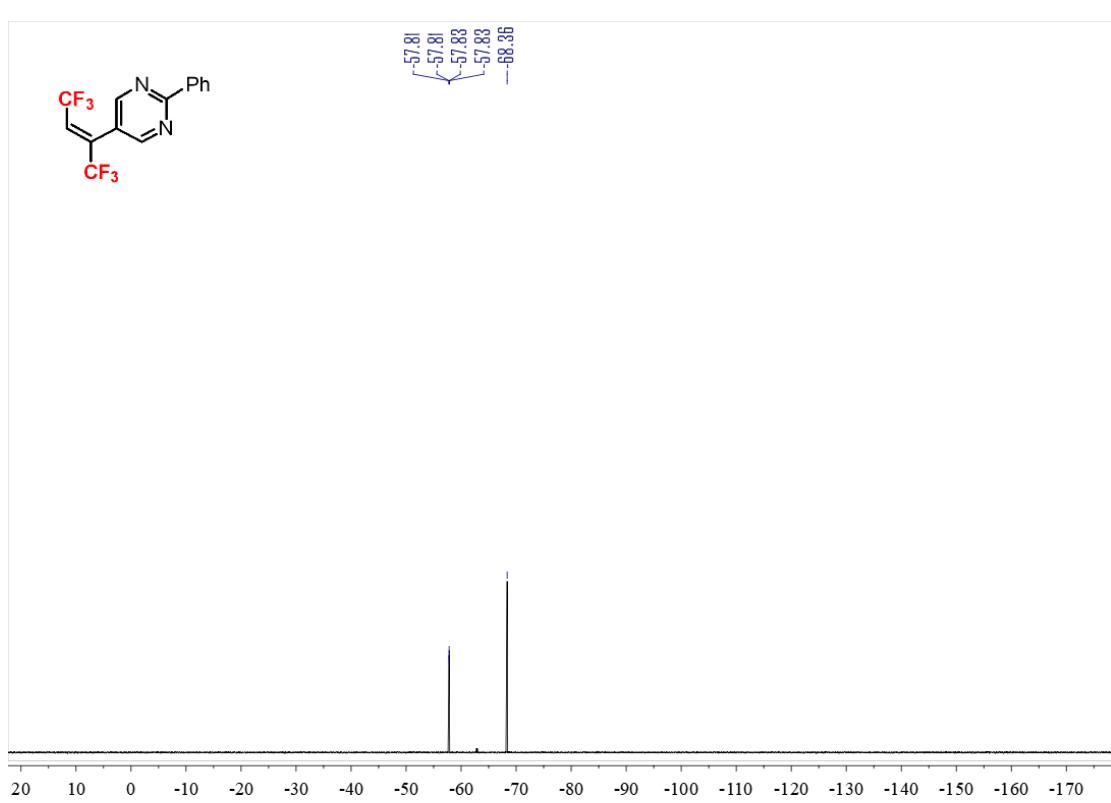
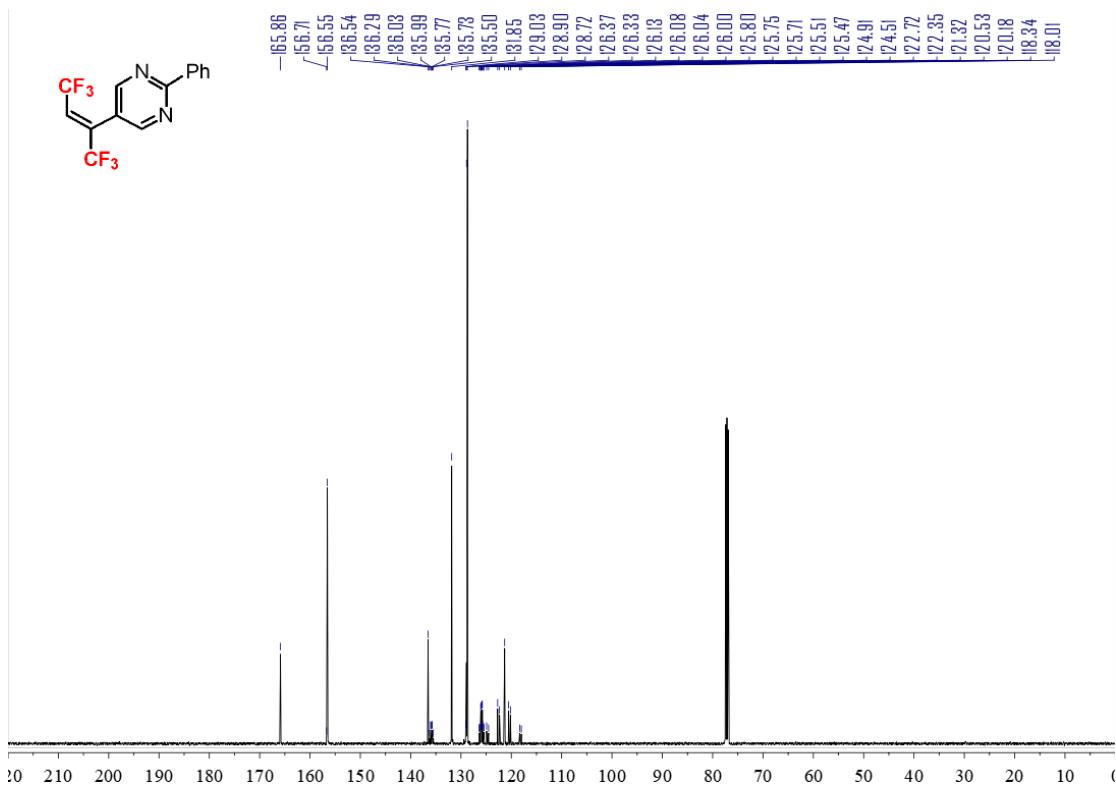


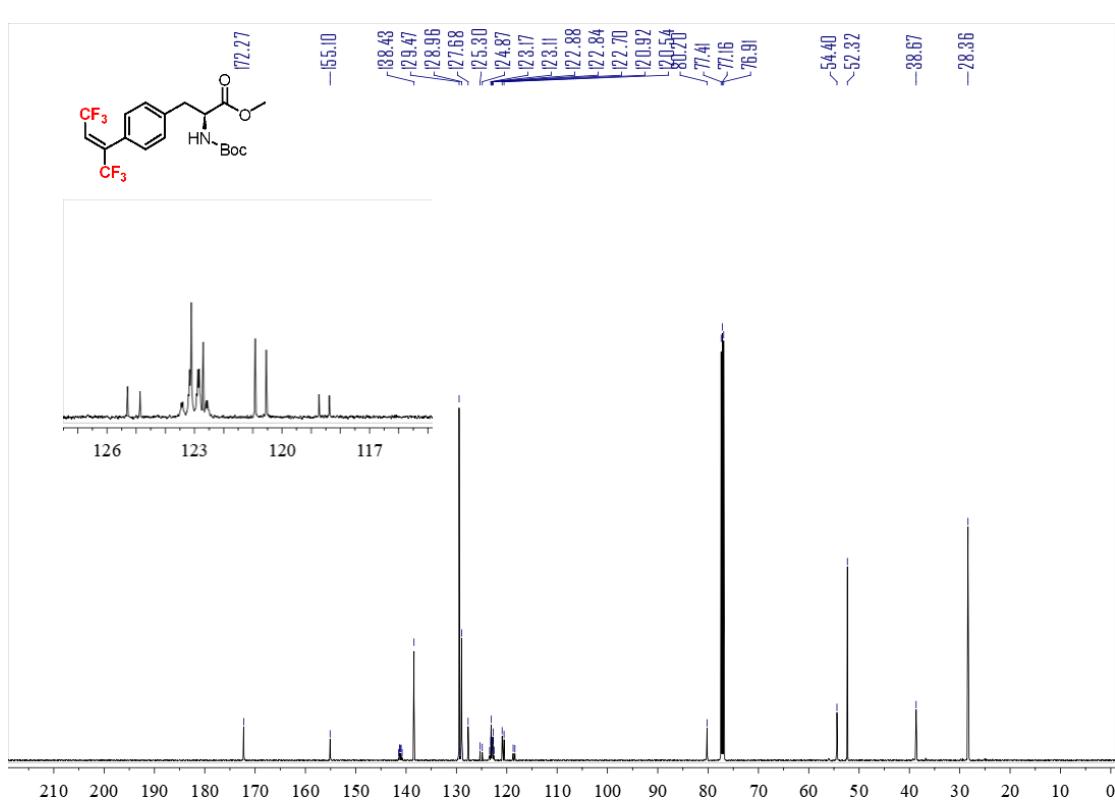
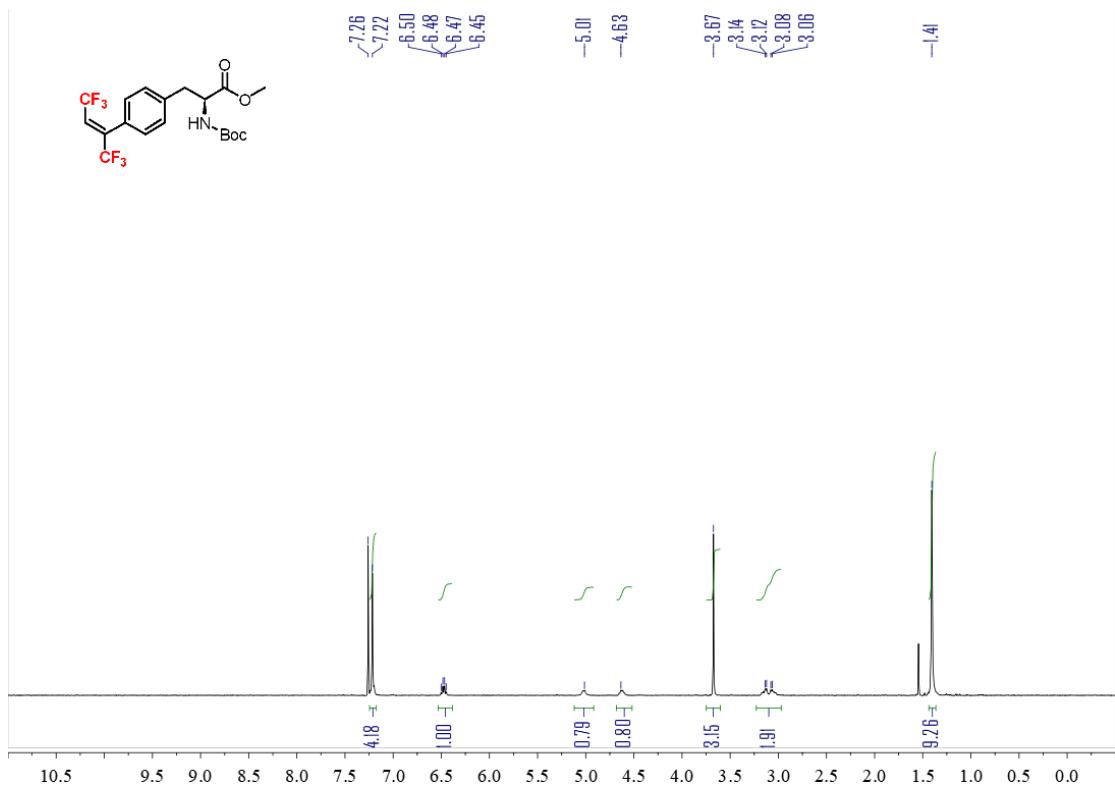


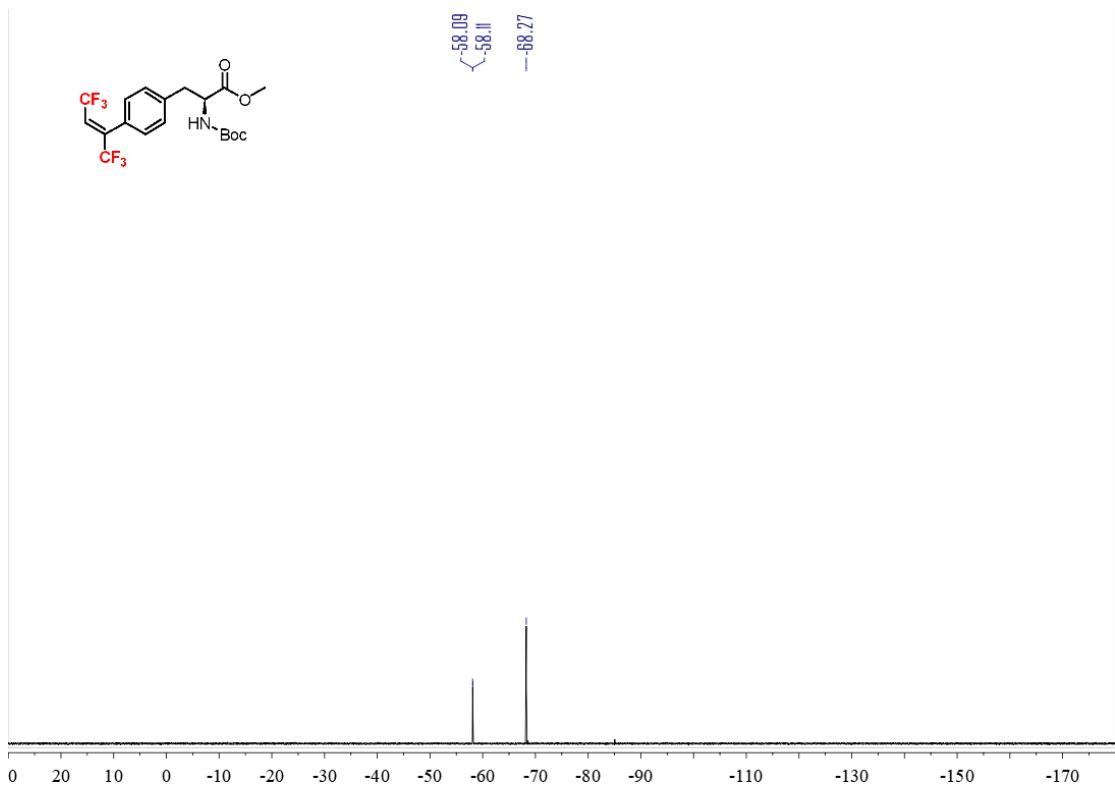
¹⁹F NMR spectrum (375 MHz, CDCl₃, 23 °C) of **3x**



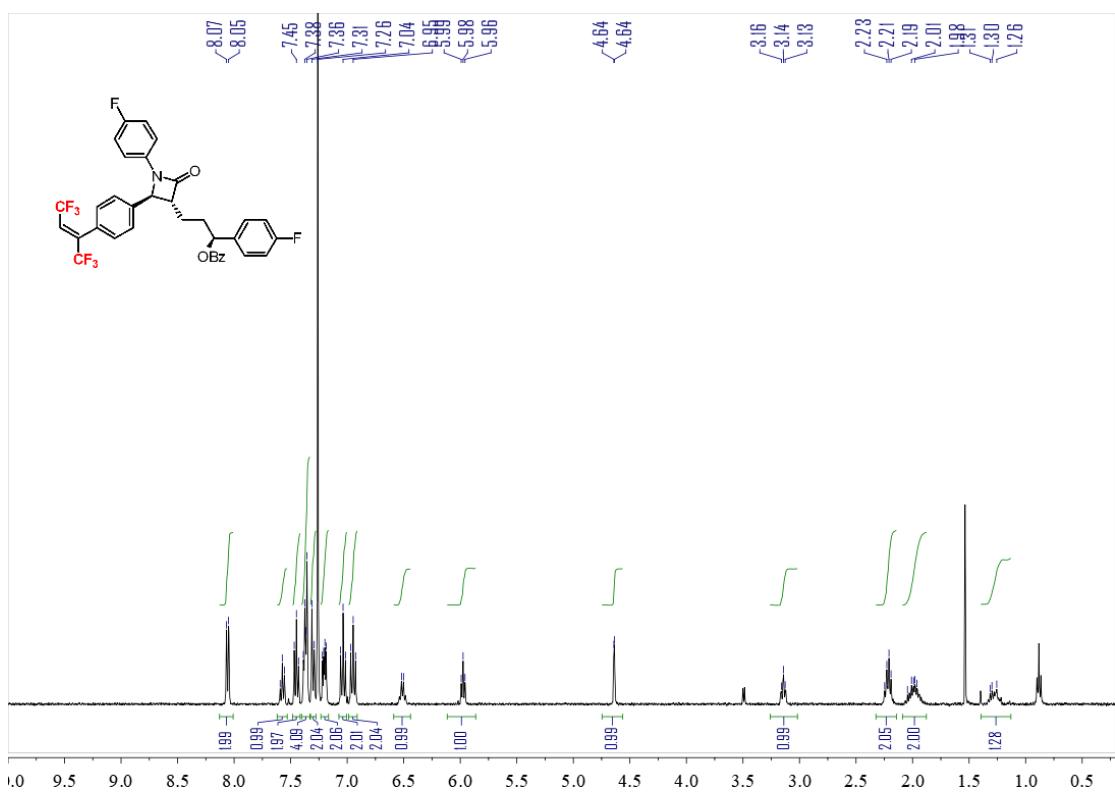
¹H NMR spectrum (400 MHz, CDCl₃, 23 °C) of **3y**



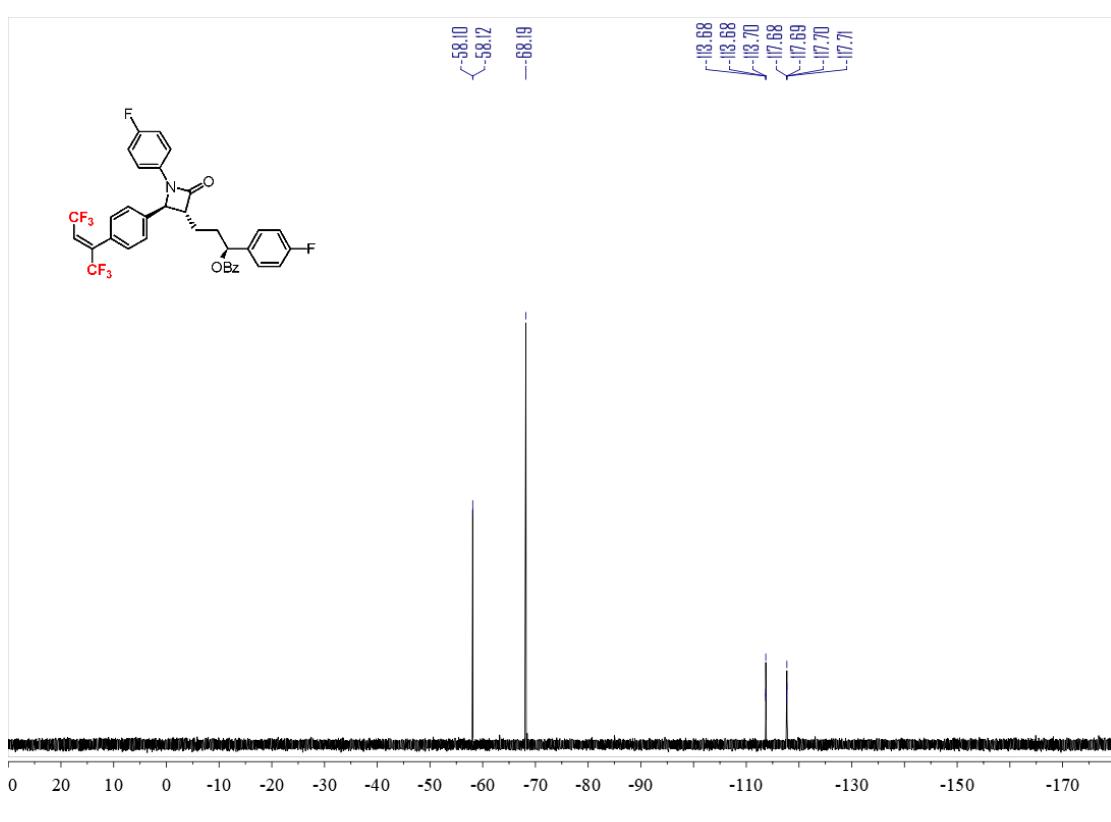
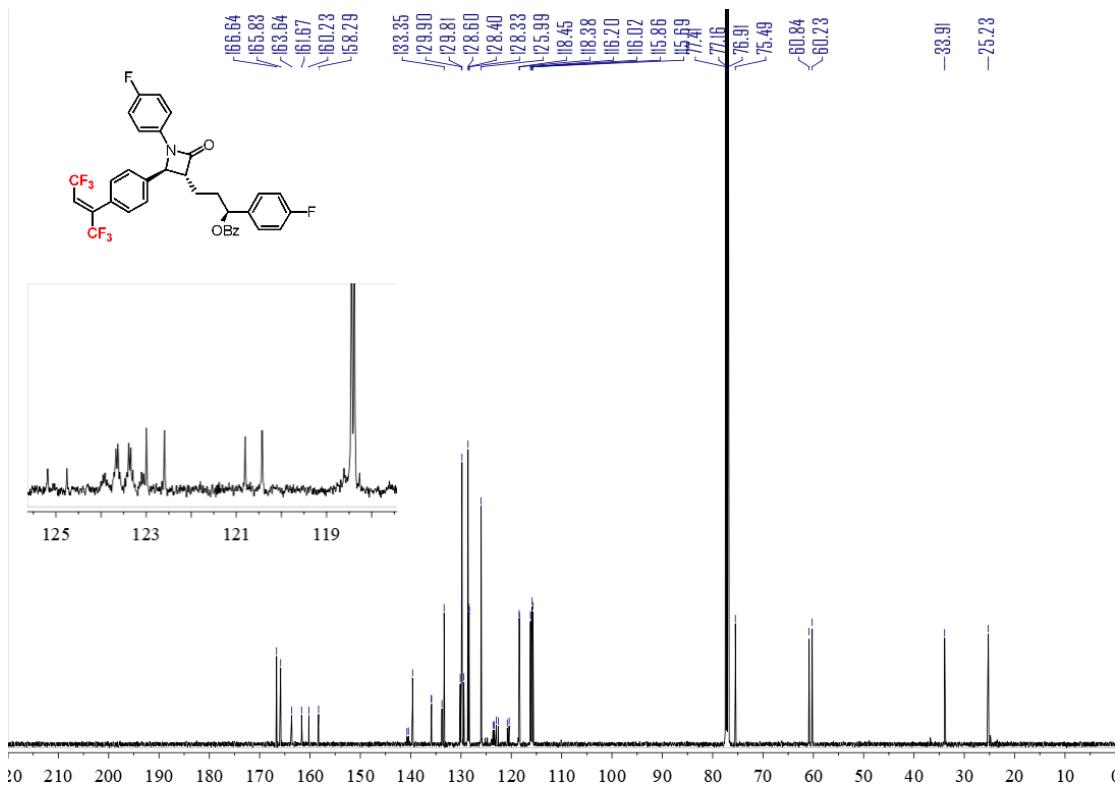


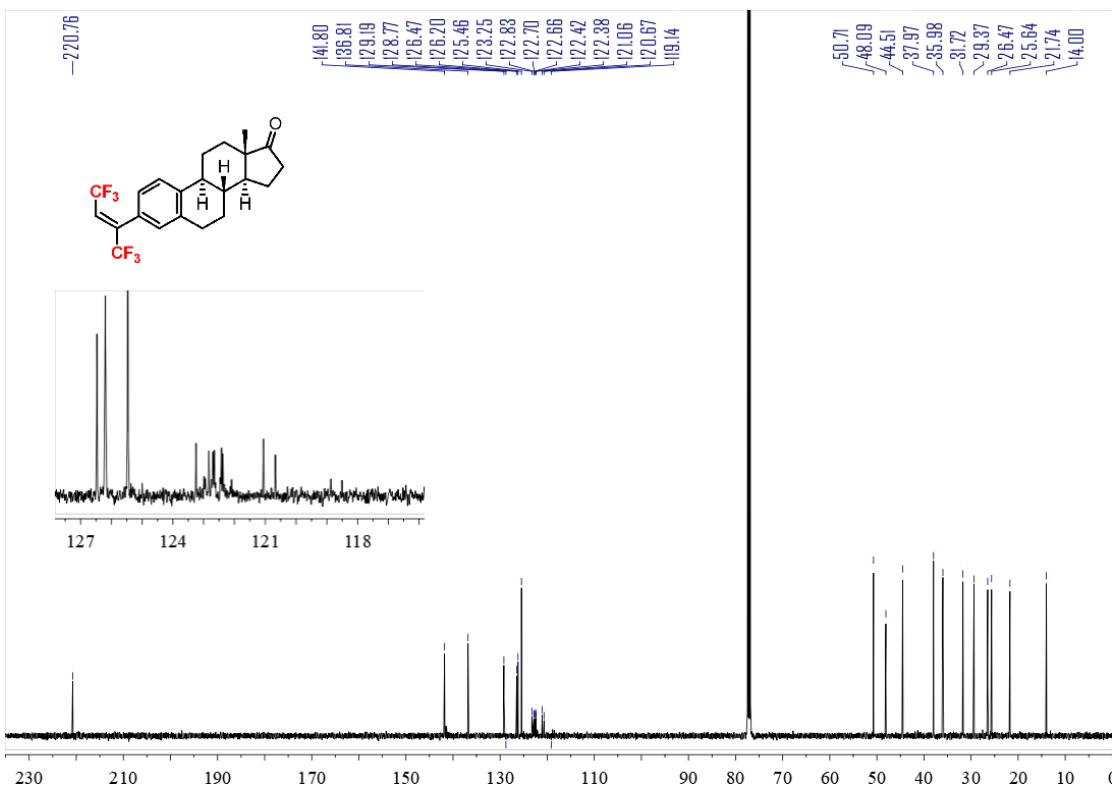
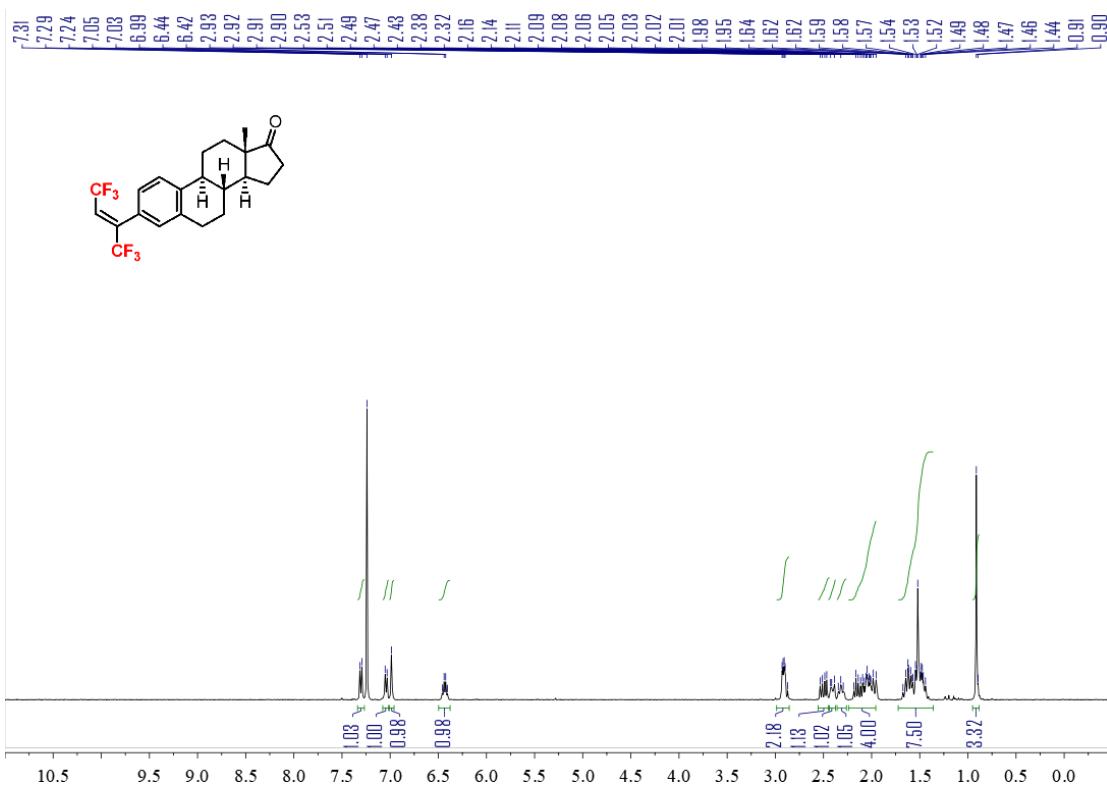


¹⁹F NMR spectrum (375 MHz, CDCl₃, 23 °C) of **4**

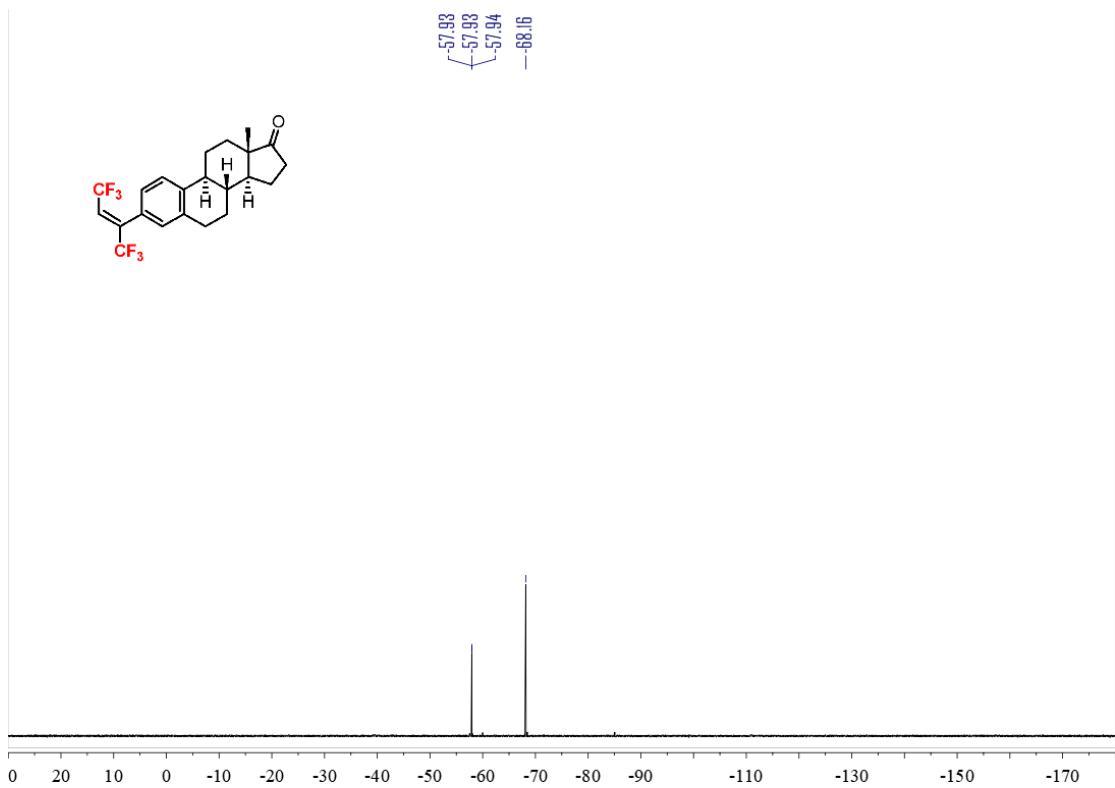


¹H NMR spectrum (400 MHz, CDCl₃, 23 °C) of **5**

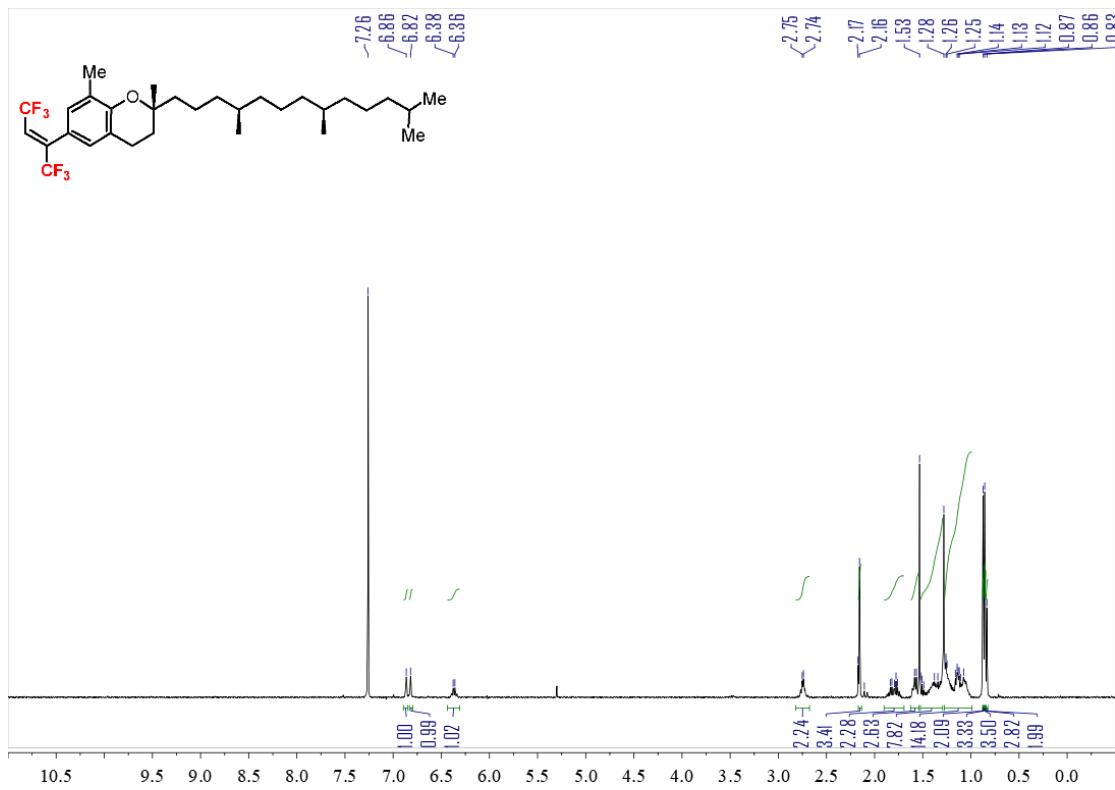




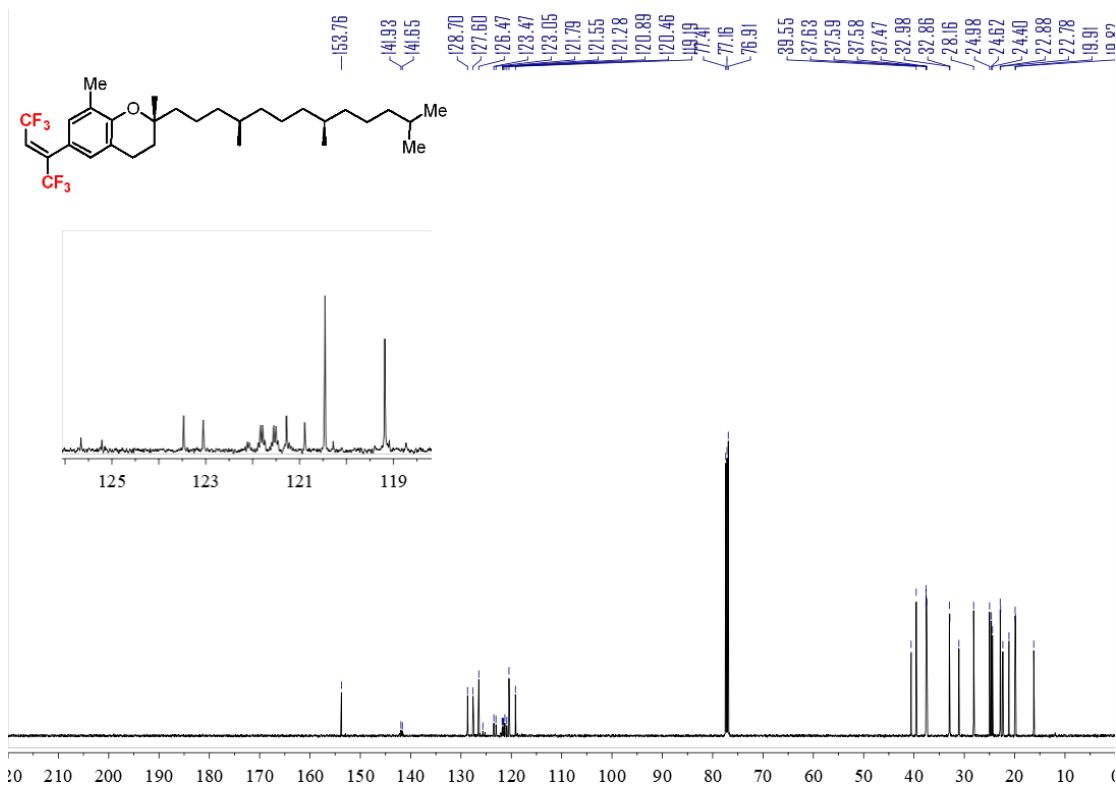
¹³C NMR spectrum (126 MHz, CDCl₃, 23 °C) of **6**



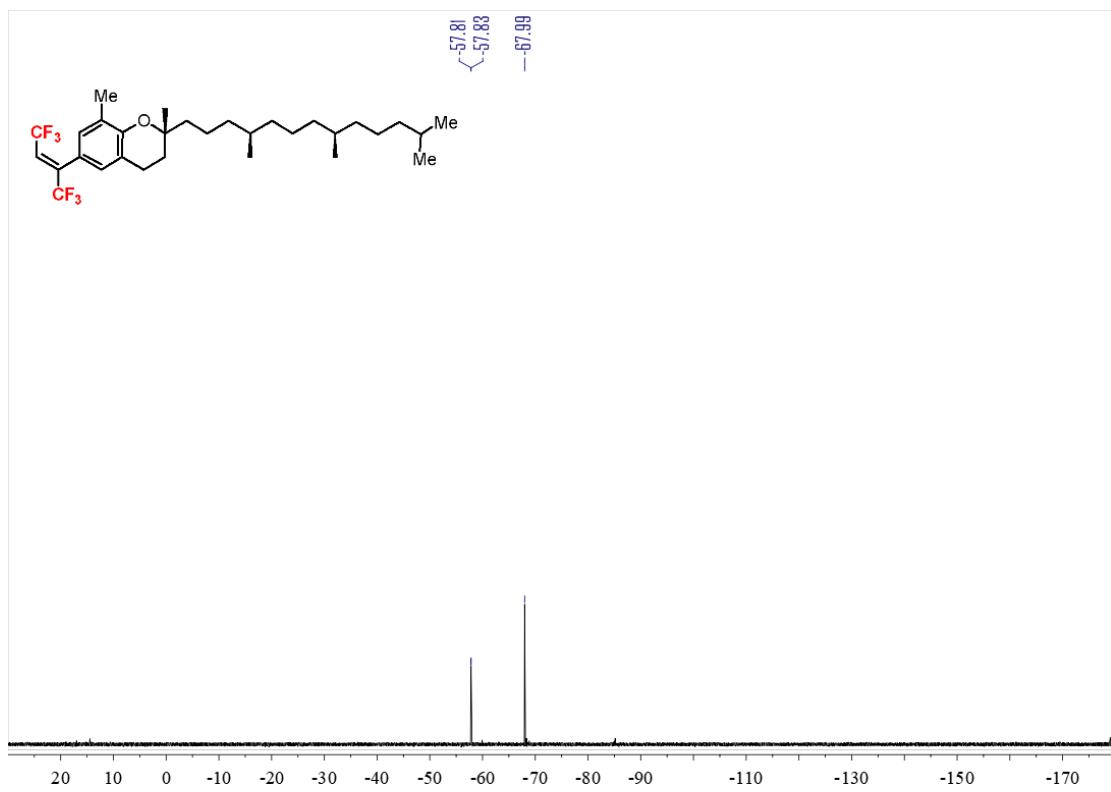
^{19}F NMR spectrum (375 MHz, CDCl_3 , 23 °C) of **6**



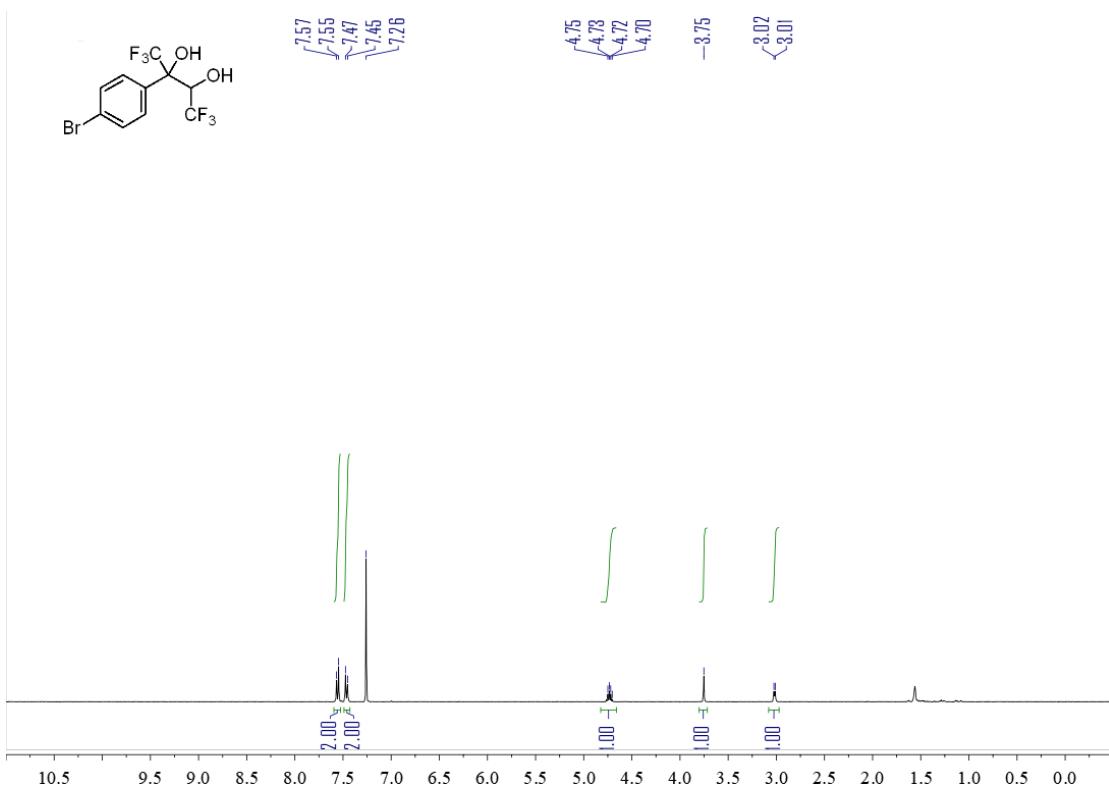
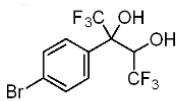
^1H NMR spectrum (400 MHz, CDCl_3 , 23 °C) of **7**



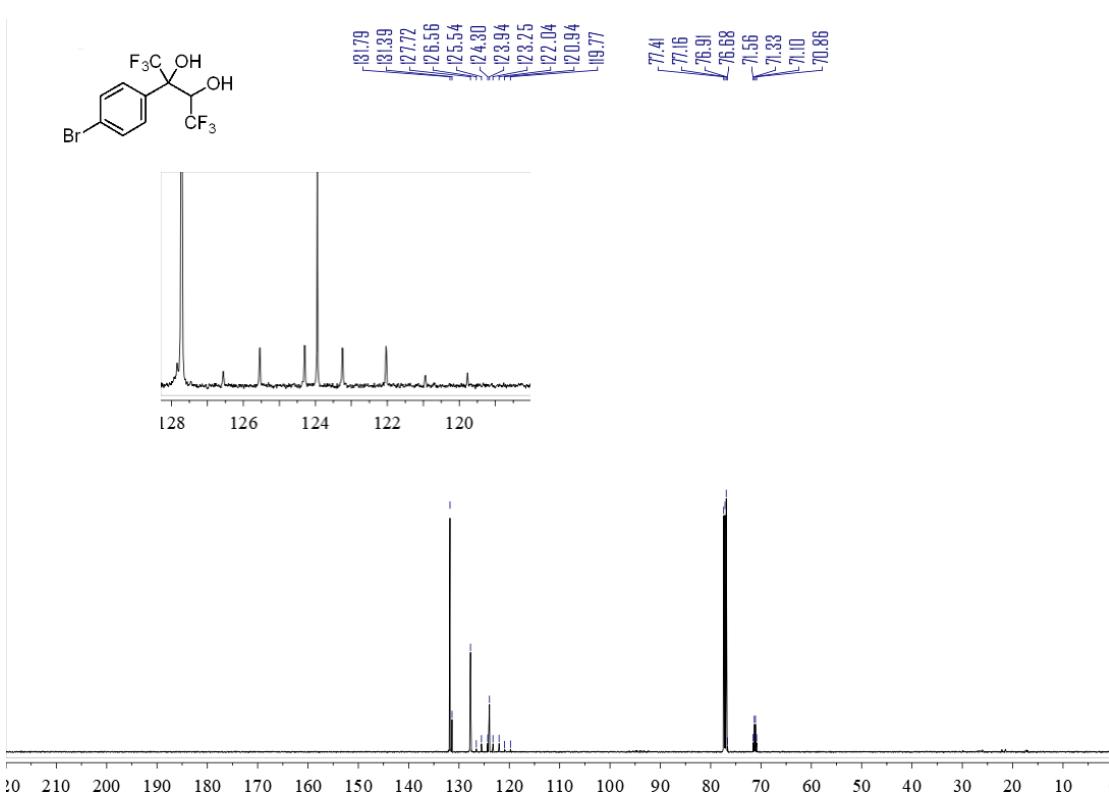
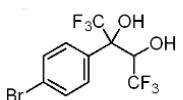
^{13}C NMR spectrum (126 MHz, CDCl_3 , 23 °C) of 7



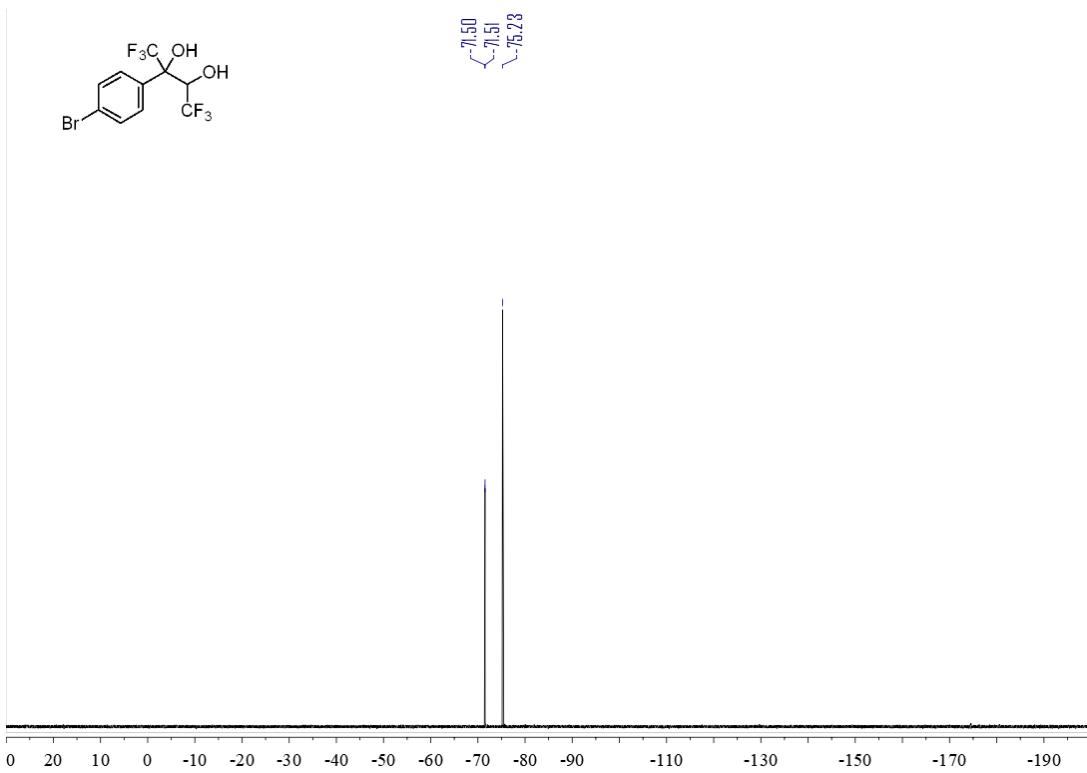
^{19}F NMR spectrum (375 MHz, CDCl_3 , 23 °C) of 7



¹H NMR spectrum (400 MHz, CDCl₃, 23 °C) of **8**



¹³C NMR spectrum (126 MHz, CDCl₃, 23 °C) of **8**



^{19}F NMR spectrum (375 MHz, CDCl_3 , 23 °C) of **8**