Supporting Information

Effect of Trifluoromethyl Group on Torquoselectivity in 4π Ring-Opening Reaction of Oxetenes: Stereoselective Synthesis of Tetrasubstituted Olefins

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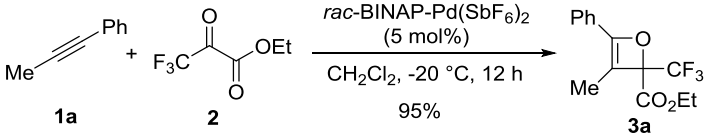
General Information:

^{1}H, ^{13}C, and ^{19}F NMR spectra were measured on Bruker AV300M (300 MHz) spectrometers. Chemical shifts of ^{1}H NMR were expressed in parts per million relative to the singlet (δ = 7.26) for $CDCl_3$. Chemical shifts of ^{13}C NMR were expressed in parts per million relative to the central line of the triplet (δ = 77.0) for $CDCl_3$. Chemical shifts of ^{19}F NMR were expressed in parts per million relative to the singlet (δ = -63.24) for BTF as an external standard. IR spectra were measured on a JASCO FT/IR-4200 spectrometer. Mass spectra were measured on a JEOL JMS-T100CS (Accu-TOF) spectrometer. X-ray crystal analyses were measured on Rigaku XtaLAB mini diffractometer (graphite monochromated MoKα radiation, λ = 0.71075 Å). All experiments were carried out under argon atmosphere unless otherwise noted.

Experimental Procedures:

Oxetenes **3b**, **3d-e**, and **3g-o** were synthesized employing procedure published from our laboratory.[1]

General Procedure for Catalytic Asymmetric [2+2]Cycloaddition (Scheme 2)

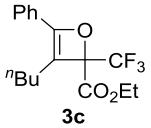


To a solution of *rac*-BINAP-$PdCl_2$ (60.0 mg, 0.075 mmol) in CH_2Cl_2 (10.0 mL) was added $AgSbF_6$ (51.5 mg, 0.15 mmol) at room temperature under argon atmosphere. After stirring for 30 min, ethyl trifluoropyruvate **2** (399 μL, 3.0 mmol) and alkyne **1a** (174 mg, 1.5 mmol) were added to the mixture at –20 °C. The reaction mixture was stirred at -20 °C for 12 h, and then directly loaded onto a short silica-gel column (hexane/AcOEt = 3/1) to remove the catalyst. Purification by silica-gel chromatography (hexane/AcOEt = 10/1) gave oxetene **3a** (409 mg, 95% yield).

Ethyl 3-methyl-4-phenyl-2-(trifluoromethyl)-2H-oxete-2-carboxylate (3a)[1]

^{1}H NMR (300 MHz, $CDCl_3$) δ 1.36 (t, J = 7.2 Hz, 3H), 2.10 (s, 3H), 4.34-4.42 (m, 2H), 7.38-7.45 (m, 3H), 7.51-7.54 (m, 2H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 9.2, 14.0, 62.7, 86.2 (q, J_{C-F} = 33.2 Hz), 111.1, 122.0 (q, J_{C-F} = 280.6 Hz), 124.8, 128.4, 128.6, 129.9, 162.2, 163.5; ^{19}F NMR (282 MHz, $CDCl_3$) δ -76.1; FT-IR (neat, cm^{-1}) 3071, 2975, 2940, 1758, 1452, 1281, 1192, 1089, 1022, 761; HRMS (APCI-TOF) calcd for $C_{14}H_{14}F_3O_3$ $[M+H]^+$: 287.0895, found: 287.0893.

Ethyl 3-butyl-4-phenyl-2-(trifluoromethyl)-2H-oxete-2-carboxylate (3c)

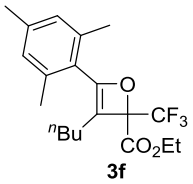


3c

^{1}H NMR (300 MHz, $CDCl_3$) δ 0.94 (t, J = 7.2 Hz, 3H), 1.36 (t, J = 7.2 Hz, 3H), 1.27-1.46 (m, 2H), 1.51-1.65 (m, 2H), 2.47 (t, J = 7.7 Hz, 2H), 4.37 (q, J = 7.1 Hz, 2H), 7.40-7.43 (m, 3H), 7.52-7.55 (m,

2H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 13.8, 14.0, 22.5, 24.3, 30.1, 62.8, 86.2 (q, J_{C-F} = 33.5 Hz), 116.2, 122.1 (q, J_{C-F} = 282.1 Hz), 124.9, 128.5, 128.6, 129.9, 162.7, 163.8; ^{19}F NMR (282 MHz, $CDCl_3$) δ -75.77; FT-IR (neat, cm^{-1}) 2960, 2935, 2874, 1745, 1452, 1369, 1269, 1176, 1088, 1026; HRMS (APCI-TOF) calcd for $C_{17}H_{20}F_3O_3$ $[M+H]^+$: 329.1365, found: 329.1348.

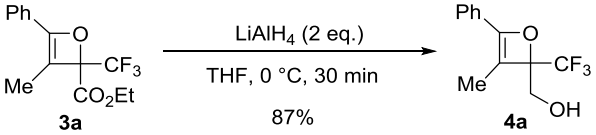
Ethyl 3-butyl-4-mesityl-2-(trifluoromethyl)-2H-oxete-2-carboxylate (3f)



3f

^{1}H NMR (300 MHz, $CDCl_3$) δ 0.85 (t, J = 7.2 Hz, 3H), 1.40 (t, J = 7.2 Hz, 3H), 1.24-1.48 (m, 4H), 2.24 (t, J = 7.2 Hz, 2H), 2.31 (s, 3H), 2.43 (s, 6H), 4.33-4.50 (m, 2H), 6.91 (s, 2H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 13.4, 13.9, 19.6, 21.1, 22.3, 24.1, 28.8, 62.5, 85.8 (q, J_{C-F} = 33.0 Hz), 121.2, 122.3 (q, J_{C-F} = 281.4 Hz), 125.5, 128.3, 138.5, 140.4, 164.3, 164.8; ^{19}F NMR (282 MHz, $CDCl_3$) δ -75.45; FT-IR (neat, cm^{-1}) 2959, 2932, 2872, 1746, 1315, 1286, 1268, 1174, 1075, 1031; HRMS (APCI-TOF) calcd for $C_{20}H_{26}F_3O_3$ $[M+H]^+$: 371.1834, found: 371.1819.

General Procedure for Reduction of Ester (Scheme 2)

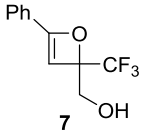


To a solution of $LiAlH_4$ (75.9 mg, 2.0 mmol) in THF (10 mL) was added oxetene **3a** (286.2 mg, 1.0 mmol) in THF (1 mL) at -78 °C, and the reaction mixture was warmed up to 0 °C. After stirring for 30 min, the reaction mixture was quenched by $Na_2SO_4 \cdot 10H_2O$, filtered through celite, and then concentrated under reduced pressure. Purification by silica-gel chromatography (hexane/AcOEt = 5/1) gave the product **4a** (212.4 mg, 87% yield).

(3-Methyl-4-phenyl-2-(trifluoromethyl)-2H-oxet-2-yl)methanol (4a)

^{1}H NMR (300 MHz, $CDCl_3$) δ 2.07 (s, 3H), 3.84 (s, 1H), 4.12 (d, J = 13.2 Hz, 1H), 4.24 (d, J = 13.2 Hz, 1H), 7.35-7.44 (m, 3H), 7.53-7.56 (m, 2H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 8.9, 60.0, 89.4 (q, J_{C-F} = 30.5 Hz), 111.1, 124.0 (q, J_{C-F} = 282.4 Hz), 124.6, 128.6, 129.0, 129.4, 158.6; ^{19}F NMR (282 MHz, $CDCl_3$) δ -76.76; FT-IR (neat, cm^{-1}) 3412, 3065, 2933, 1450, 1340, 1312, 1239, 1151, 1067, 1032, 989; HRMS (APCI-TOF) calcd for $C_{12}H_{12}F_3O_2$ $[M+H]^+$: 245.0789, found: 245.0786.

(4-Phenyl-2-(trifluoromethyl)-2H-oxet-2-yl)methanol (7)

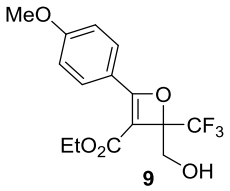


7

^{1}H NMR (300 MHz, $CDCl_3$) δ 2.77 (dd, J = 6.9, 6.9 Hz, 1H), 4.10 (dd, J = 12.9, 6.9 Hz, 1H), 4.19 (dd,

J = 12.9, 6.9 Hz, 1H), 5.98 (s, 1H), 7.39-7.44 (m, 3H), 7.52-7.55 (m, 2H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 61.1, 88.7 (q, J_{C-F} = 31.7 Hz), 98.6, 123.6 (q, J_{C-F} = 281.6 Hz), 124.4, 127.8, 128.6, 130.6, 165.8; ^{19}F NMR (282 MHz, $CDCl_3$) δ -77.29; FT-IR (KBr pellet, cm^{-1}) 3503, 3110, 2949, 2850, 1745, 1685, 1601, 1459, 1312, 1261, 1185, 1135, 1027; HRMS (APCI-TOF) calcd for $C_{11}H_9F_3NaO_2$ $[M+Na]^+$: 253.0452, found: 253.0461.

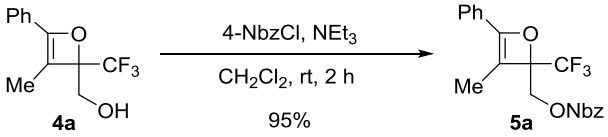
Ethyl 2-(hydroxymethyl)-4-(4-methoxyphenyl)-2-(trifluoromethyl)-2H-oxete-3-carboxylate (9)



9

To a solution of $NaBH_4$ (113.5 mg, 3.0 mmol) in THF (15 mL) was added the oxetene with ester group (561.5 mg, 1.5 mmol) in THF (1 mL) at 0 °C, and the reaction mixture was warmed up to room temperature. After stirring for 1 h, the reaction mixture was quenched by water and extracted with diethyl ether. The organic layer was washed with brine, dried over Na_2SO_4, and concentrated under reduced pressure. Purification by silica-gel chromatography gave **9** (295.5 mg, 59% yield).
^{1}H NMR (300 MHz, $CDCl_3$) δ 1.29 (t, *J* = 7.2 Hz, 3H), 3.83 (s, 3H), 4.13-4.31 (m, 2H), 4.22 (s, 2H), 6.92 (d, *J* = 9.0 Hz, 2H), 8.10 (d, *J* = 9.0 Hz, 2H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 14.14, 55.45, 60.19, 60.44, 91.24 (q, J_{C-F} = 32.0Hz), 101.8, 114.1, 119.1, 123.0 (q, J_{C-F} = 282.4 Hz), 130.1, 160.2, 163.5, 172.6; ^{19}F NMR (282 MHz, $CDCl_3$) δ -76.34; FT-IR (neat, cm^{-1}) 3452, 2936, 2841, 1658, 1603, 1513, 1316, 1263, 1216, 1174, 1122, 1101, 1071, 987; HRMS (APCI-TOF) calcd for $C_{15}H_{15}F_3NaO_5$ $[M+Na]^+$: 355.0769, found: 355.0755.

General Procedure for Protection of Alcohol with 4-Nitrobenzoyl Group (Scheme 2)

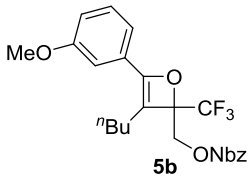


To a solution of **4a** (212.4 mg, 0.9 mmol) in CH_2Cl_2 (9 mL) were added NEt_3 (250.9 μL, 1.8 mmol) and 4-nitrobenzoyl chloride (185.6 mg, 1.0 mmol) at 0 °C, and the reaction mixture was warmed up to room temperature. After stirring for 2 h, the reaction mixture was quenched by water and extracted with diethyl ether. The organic layer was washed with brine, dried over Na_2SO_4, and concentrated under reduced pressure. Purification by silica-gel chromatography gave **5a** (336.0 mg, 95% yield). The structure of **5a** was clarified by X-ray analysis of the single crystal (*vide infra*).

(3-Methyl-4-phenyl-2-(trifluoromethyl)-2H-oxet-2-yl)methyl 4-nitrobenzoate (5a)
^{1}H NMR (300 MHz, $CDCl_3$) δ 2.09 (s, 3H), 4.90 (d, *J* = 12.6 Hz, 1H), 4.99 (d, *J* = 12.6 Hz, 1H), 7.36-7.42 (m, 3H), 7.46-7.50 (m, 2H), 8.17 (d, *J* = 9.0 Hz, 2H), 8.22 (d, *J* = 9.0 Hz, 2H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 9.2, 62.4, 86.6 (q, J_{C-F} = 32.2 Hz), 110.8, 123.4 (q, J_{C-F} = 282.4 Hz), 123.6, 124.6,

128.6 (2C), 129.8, 130.9, 134.6, 150.7, 160.0, 163.9; ^{19}F NMR (282 MHz, $CDCl_3$) δ -76.77; FT-IR (KBr pellet, cm^{-1}) 2958, 2923, 2852, 1728, 1523, 1344, 1279, 1186, 1161, 1116, 1106, 874; HRMS (APCI-TOF) calcd for $C_{19}H_{15}F_3NO_5$ $[M+H]^+$: 394.0902, found: 394.0905.

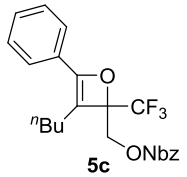
(3-Butyl-4-(3-methoxyphenyl)-2-(trifluoromethyl)-2H-oxet-2-yl)methyl 4-nitrobenzoate (5b)



5b

^{1}H NMR (300 MHz, $CDCl_3$) δ 0.91 (t, *J* = 7.2 Hz, 3H), 1.32-1.44 (m, 2H), 1.47-1.59 (m, 2H), 2.44 (t, *J* = 7.8 Hz, 2H), 3.82 (s, 3H), 4.92 (s, 2H), 6.93 (ddd, *J* = 7.8, 2.7, 1.2 Hz, 1H), 7.00 (dd, *J* = 2.7, 1.2 Hz, 1H), 7.08 (ddd, *J* = 7.8, 1.2, 1.2 Hz, 1H), 7.32 (dd, *J* = 7.8, 7.8 Hz, 1H), 8.18 (d, *J* = 9.0 Hz, 2H), 8.26 (d, *J* = 9.0 Hz, 2H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 13.8, 22.7, 24.3, 30.3, 55.3, 62.7, 86.7 (q, J_{C-F} = 32.5 Hz), 109.8, 115.8, 116.0, 117.4, 123.5 (q, J_{C-F} = 282.4 Hz), 123.7, 129.8, 129.9, 130.9, 134.6, 150.8, 159.7, 159.9, 163.9; ^{19}F NMR (282 MHz, $CDCl_3$) δ -76.24; FT-IR (KBr pellet, cm^{-1}) 2954, 2863, 2835, 1726, 1601, 1579, 1523, 1433, 1344, 1289, 1239, 1172, 1148; HRMS (APCI-TOF) calcd for $C_{23}H_{23}F_3NO_6$ $[M+H]^+$: 466.1478, found: 466.1498.

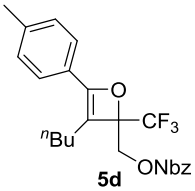
(3-Butyl-4-phenyl-2-(trifluoromethyl)-2H-oxet-2-yl)methyl 4-nitrobenzoate (5c)



5c

^{1}H NMR (300 MHz, $CDCl_3$) δ 0.92 (t, *J* = 7.2 Hz, 3H), 1.38-1.48 (m, 2H), 1.50-1.60 (m, 2H), 2.46 (t, *J* = 7.5 Hz, 2H), 4.94 (s, 2H), 7.39-7.41 (m, 3H), 7.49-7.52 (m, 2H), 8.18 (d, *J* = 9.0 Hz, 2H), 8.25 (d, *J* = 9.0 Hz, 2H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 13.7, 22.7, 24.4, 30.4, 62.7, 86.7 (q, J_{C-F} = 32.5 Hz), 115.8, 123.5 (q, J_{C-F} = 282.4 Hz), 123.6, 124.8, 128.65, 128.70, 129.8, 130.9, 134.6, 150.8, 160.1, 163.9; ^{19}F NMR (282 MHz, $CDCl_3$) δ -76.27; FT-IR (KBr pellet, cm^{-1}) 2958, 2934, 2860, 1726, 1527, 1347, 1281, 1174, 1153, 1123, 1077; HRMS (APCI-TOF) calcd for $C_{22}H_{21}F_3NO_5$ $[M+H]^+$: 436.1372, found: 436.1357.

(3-Butyl-4-(*p*-tolyl)-2-(trifluoromethyl)-2H-oxet-2-yl)methyl 4-nitrobenzoate (5d)

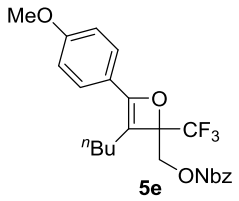


5d

^{1}H NMR (300 MHz, $CDCl_3$) δ 0.91 (t, *J* = 7.2 Hz, 3H), 1.34-1.44 (m, 2H), 1.46-1.61 (m, 2H), 2.38 (s,

3H), 2.42 (t, *J* = 7.8 Hz, 2H), 4.91 (s, 2H), 7.22 (d, *J* = 8.1 Hz, 2H), 7.38 (d, *J* = 8.1 Hz, 2H), 8.19 (d, *J* = 9.0 Hz, 2H), 8.26 (d, *J* = 9.0 Hz, 2H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 13.8, 21.5, 22.6, 24.3, 30.4, 62.8, 86.7 (q, J_{C-F} = 32.5 Hz), 114.5, 123.5 (q, J_{C-F} = 282.4 Hz), 123.7, 124.7, 126.0, 129.3, 130.9, 134.7, 140.1, 150.8, 160.3, 163.9; ^{19}F NMR (282 MHz, $CDCl_3$) δ -76.30; FT-IR (KBr pellet, cm^{-1}) 2962, 2930, 2861, 1726, 1530, 1339, 1282, 1176, 1155, 1125, 1069, 994; HRMS (APCI-TOF) calc for $C_{23}H_{23}F_3NO_5$ $[M+H]^+$: 450.1528, found: 450.1543.

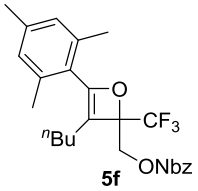
(3-Butyl-4-(4-methoxyphenyl)-2-(trifluoromethyl)-2H-oxet-2-yl)methyl 4-nitrobenzoate (5e)



5e

^{1}H NMR (300 MHz, $CDCl_3$) δ 0.90 (t, *J* = 7.2 Hz, 3H), 1.33-1.43 (m, 2H), 1.46-1.55 (m, 2H), 2.41 (t, *J* = 7.7 Hz, 3H), 3.82 (s, 3H), 4.91 (s, 2H), 6.91 (d, *J* = 9.0 Hz, 2H), 7.42 (d, *J* = 9.0 Hz, 2H), 8.18 (d, *J* = 9.0 Hz, 2H), 8.24 (d, *J* = 9.0 Hz, 2H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 13.7, 22.6, 24.3, 30.5, 55.3, 62.8, 86.7 (q, J_{C-F} = 32.5 Hz), 113.1, 114.1, 121.5, 123.59 (q, J_{C-F} = 282.4 Hz), 123.61, 126.4, 130.9, 134.7, 150.7, 160.0, 160.7, 163.9; ^{19}F NMR (282 MHz, $CDCl_3$) δ -76.36; FT-IR (KBr pellet, cm^{-1}) 2954, 2860, 2838, 1729, 1528, 1509, 1351, 1283, 1256, 1173, 1155, 1123, 1095, 833; HRMS (APCI-TOF) calcd for $C_{23}H_{23}F_3NO_6$ $[M+H]^+$: 466.1478, found: 466.1489.

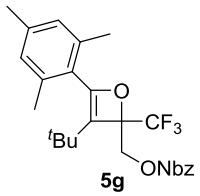
(3-Butyl-4-mesityl-2-(trifluoromethyl)-2H-oxet-2-yl)methyl 4-nitrobenzoate (5f)



5f

^{1}H NMR (300 MHz, $CDCl_3$) δ 0.82 (t, *J* = 7.2 Hz, 3H), 1.22-1.32 (m, 2H), 1.34-1.44 (m, 2H), 2.19 (t, *J* = 7.8 Hz, 2H), 2.28 (s, 3H), 2.33 (s, 6H), 4.95 (d, *J* = 12.6 Hz, 1H), 5.03 (d, *J* = 12.6 Hz, 1H), 6.87 (s, 2H), 8.25 (d, *J* = 9.0 Hz, 2H), 8.30 (d, *J* = 9.0 Hz, 2H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 13.7, 19.9, 21.3, 22.6, 24.5, 29.1, 63.5, 86.2 (q, J_{C-F} = 32.2 Hz), 120.7, 123.7, 123.8 (q, J_{C-F} = 282.1 Hz), 125.7, 128.5, 131.1, 134.8, 138.4, 140.4, 151.0, 161.8, 164.1; ^{19}F NMR (282 MHz, $CDCl_3$) δ -75.96; FT-IR (neat, cm^{-1}) 2959, 2929, 2863, 1738, 1611, 1530, 1347, 1316, 1270, 1159, 1101, 1079; HRMS (APCI-TOF) calcd for $C_{25}H_{26}F_3NNaO_5$ $[M+Na]^+$: 500.1661, found: 500.1681.

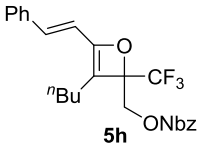
(3-(*tert*-Butyl)-4-mesityl-2-(trifluoromethyl)-2H-oxet-2-yl)methyl 4-nitrobenzoate (5g)



5g

^{1}H NMR (300 MHz, $CDCl_3$) δ 1.10 (s, 9H), 2.27 (s, 3H), 2.32 (s, 3H), 2.40 (s, 3H), 4.97 (d, *J* = 12.6 Hz, 1H), 5.06 (d, *J* = 12.6 Hz, 1H), 6.84 (s, 1H), 6.88 (s, 1H), 8.25 (d, *J* = 9.0 Hz, 1H), 8.30 (d, *J* = 9.0 Hz, 1H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 19.7, 20.0, 21.3, 28.8, 31.2, 64.2, 86.2 (q, $J_{C\text{-}F}$ = 32.5 Hz), 123.6, 123.8 (q, $J_{C\text{-}F}$ = 282.4 Hz), 126.9, 128.0, 128.2, 129.3, 131.0, 134.8, 137.7, 138.4, 140.2, 150.8, 160.0, 164.0; ^{19}F NMR (282 MHz, $CDCl_3$) δ -74.03; FT-IR (KBr pellet, cm^{-1}) 2966, 2926, 2867, 1735, 1608, 1540, 1270, 1184, 1157, 1082, 984, 960, 860; HRMS (APCI-TOF) calcd for $C_{25}H_{26}F_3NNaO_5$ $[M+Na]^+$: 500.1661, found: 500.1651.

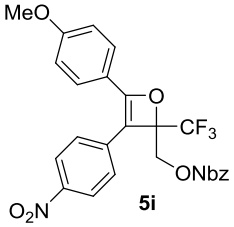
(*E*)-(3-Butyl-4-styryl-2-(trifluoromethyl)-2H-oxet-2-yl)methyl 4-nitrobenzoate (5h)



5h

Oxetene **3h** of *E*/*Z* = 10/1 was used for the reduction followed by the protection of alcohol group.
E-isomer: ^{1}H NMR (300 MHz, $CDCl_3$) δ 0.93 (t, *J* = 7.2 Hz, 3H), 1.34-1.46 (m, 2H), 1.49-1.60 (m, 2H), 2.28 (t, *J* = 7.7 Hz, 2H), 4.89 (s, 2H), 6.53 (d, *J* = 16.2 Hz, 1H), 6.92 (d, *J* = 16.2 Hz, 1H), 7.26-7.38 (m, 3H), 7.43-7.48 (m, 2H), 8.22 (d, *J* = 9.0 Hz, 2H), 8.29 (d, *J* = 9.0 Hz, 2H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 13.7, 22.5, 24.1, 29.9, 62.6, 87.1 (q, $J_{C\text{-}F}$ = 32.5 Hz), 112.6, 117.7, 123.4 (q, $J_{C\text{-}F}$ = 283.1 Hz), 123.7, 127.0, 128.8, 129.0, 130.9, 132.6, 134.6, 135.4, 150.8, 159.9, 163.9; ^{19}F NMR (282 MHz, $CDCl_3$) δ *E*-isomer: -76.51, *Z*-isomer: -76.30; FT-IR (neat, cm^{-1}) 2958, 2931, 2861, 1735, 1606, 1527, 1345, 1319, 1270, 1163, 1101; HRMS (APCI-TOF) calcd for $C_{24}H_{23}F_3NO_5$ $[M+H]^+$: 462.1528, found: 462.1544.

(4-(4-Methoxyphenyl)-3-(4-nitrophenyl)-2-(trifluoromethyl)-2H-oxet-2-yl)methyl 4-nitrobenzoate (5i)

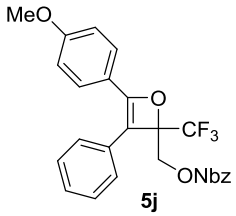


5i

^{1}H NMR (300 MHz, $CDCl_3$) δ 3.89 (s, 3H), 5.11 (s, 2H), 6.99 (d, *J* = 9.0 Hz, 2H), 7.50 (d, *J* = 9.0 Hz, 2H), 7.69 (d, *J* = 9.0 Hz, 2H), 8.10 (d, *J* = 9.0 Hz, 2H), 8.18 (d, *J* = 9.0 Hz, 2H), 8.23 (d, *J* = 9.0 Hz,

2H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 55.6, 61.9, 87.9 (q, J_{C-F} = 33.2 Hz), 110.8, 114.6, 120.1, 123.1 (q, J_{C-F} = 282.9 Hz), 123.7, 124.5, 124.8, 127.9, 130.9, 134.2, 136.1, 145.9, 150.8, 162.6, 163.7, 163.8; ^{19}F NMR (282 MHz, $CDCl_3$) δ -75.69; FT-IR (KBr pellet, cm^{-1}) 3080, 2960, 2924, 2847, 1740, 1595, 1518, 1343, 1264, 1172, 1098, 1022, 851; HRMS (APCI-TOF) calcd for $C_{25}H_{18}F_3N_2O_8$ $[M+H]^+$: 531.1015, found: 531.1011.

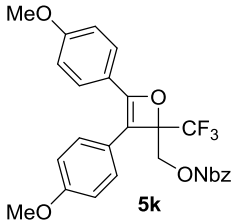
(4-(4-Methoxyphenyl)-3-phenyl-2-(trifluoromethyl)-2H-oxet-2-yl)methyl 4-nitrobenzoate (5j)



5j

^{1}H NMR (300 MHz, $CDCl_3$) δ 3.87 (s, 3H), 5.08 (d, J = 12.9 Hz, 1H), 5.15 (d, J = 12.9 Hz, 1H), 6.97 (d, J = 9.0 Hz, 2H), 7.25-7.31 (m, 1H), 7.35-7.40 (m, 2H), 7.44-7.47 (m, 2H), 7.71 (d, J = 9.0 Hz, 2H), 8.12 (d, J = 9.0 Hz, 2H), 8.23 (d, J = 9.0 Hz, 2H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 55.4, 62.8, 87.3 (q, J_{C-F} = 32.5 Hz), 113.1, 114.3, 121.1, 123.5 (q, J_{C-F} = 282.3 Hz), 123.6, 125.3, 127.2, 127.5, 129.0, 129.7, 130.9, 134.6, 150.7, 160.0, 161.6, 163.8; ^{19}F NMR (282 MHz, $CDCl_3$) δ -75.70; FT-IR (neat, cm^{-1}) 2959, 2933, 2842, 1733, 1668, 1603, 1520, 1458, 1359, 1313, 1264, 1119, 1031; HRMS (APCI-TOF) calcd for $C_{25}H_{19}F_3NO_6$ $[M+H]^+$: 486.1165, found: 486.1172.

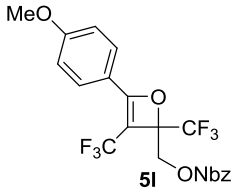
(3,4-Bis(4-methoxyphenyl)-2-(trifluoromethyl)-2H-oxet-2-yl)methyl 4-nitrobenzoate (5k)



5k

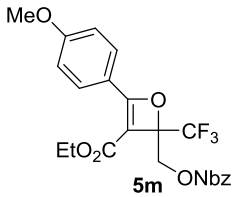
^{1}H NMR (300 MHz, $CDCl_3$) δ 3.81 (s, 3H), 3.84 (s, 3H), 5.03 (d, J = 12.6 Hz, 1H), 5.08 (d, J = 12.6 Hz, 1H), 6.89 (d, J = 8.7 Hz, 2H), 6.93 (d, J = 8.7 Hz, 2H), 7.34 (d, J = 9.0 Hz, 2H), 7.64 (d, J = 9.0 Hz, 2H), 8.10 (d, J = 9.0 Hz, 2H), 8.21 (d, J = 9.0 Hz, 2H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 55.3, 55.4, 62.8, 87.1 (q, J_{C-F} = 32.8 Hz), 112.9, 114.2, 114.5, 121.2, 122.2, 123.5 (q, J_{C-F} = 283.2 Hz), 123.6, 126.9, 127.0, 130.9, 134.6, 150.7, 158.6, 159.0, 161.3, 163.8; ^{19}F NMR (282 MHz, $CDCl_3$) δ -75.79; FT-IR (KBr pellet, cm^{-1}) 2956, 2939, 2841, 1732, 1523, 1279, 1249, 1186, 1131, 1089, 1026, 833; HRMS (APCI-TOF) calcd for $C_{26}H_{21}F_3NO_7$ $[M+H]^+$: 516.1270, found: 516.1258.

(4-(4-Methoxyphenyl)-2,3-bis(trifluoromethyl)-2H-oxet-2-yl)methyl 4-nitrobenzoate (5l)



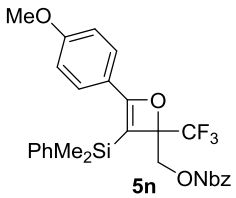
^{1}H NMR (300 MHz, $CDCl_3$) δ 3.88 (s, 3H), 4.95 (d, J = 12.9 Hz, 1H), 5.05 (d, J = 12.9 Hz, 1H), 6.98 (d, J = 9.0 Hz, 2H), 7.66 (d, J = 9.0 Hz, 2H), 8.17 (d, J = 9.0 Hz, 2H), 8.26 (d, J = 9.0 Hz, 2H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 55.6, 61.5, 87.2 (q, $J_{C\text{-}F}$ = 34.2 Hz), 98.4 (q, $J_{C\text{-}F}$ = 43.8 Hz), 114.5, 117.7, 119.8 (q, $J_{C\text{-}F}$ = 264.3 Hz), 122.2 (q, $J_{C\text{-}F}$ = 282.4 Hz), 123.7, 128.8 (q, $J_{C\text{-}F}$ = 2.3 Hz), 130.9, 134.2, 150.9, 163.3, 163.6, 167.1 (q, $J_{C\text{-}F}$ = 6.3 Hz); ^{19}F NMR (282 MHz, $CDCl_3$) δ -77.10, -57.12; FT-IR (KBr pellet, cm^{-1}) 3083, 3061, 2968, 2933, 2844, 1728, 1683, 1530, 1343, 1267, 1171, 1094, 1038; HRMS (APCI-TOF) calcd for $C_{20}H_{14}F_6NO_6$ $[M+H]^+$: 478.0725, found: 478.0741. The structure of **5l** was clarified by X-ray analysis of the single crystal (*vide infra*).

Ethyl 4-(4-methoxyphenyl)-2-(((4-nitrobenzoyl)oxy)methyl)-2-(trifluoromethyl)-2H-oxete-3-carboxylate (5m)



^{1}H NMR (300 MHz, $CDCl_3$) δ 1.30 (t, J = 7.2 Hz, 3H), 3.88 (s, 3H), 4.15-4.34 (m, 2H), 4.99 (d, J = 12.9 Hz, 1H), 5.11 (d, J = 12.9 Hz, 1H), 6.97 (d, J = 9.0 Hz, 2H), 8.13-8.17 (m, 4H), 8.23-8.26 (m, 2H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 14.3, 55.6, 60.4, 61.9, 88.7 (q, $J_{C\text{-}F}$ = 33.5 Hz), 101.9, 114.2, 118.8, 122.6 (q, $J_{C\text{-}F}$ = 282.4 Hz), 123.7, 130.2, 130.9, 134.5, 150.8, 159.6, 163.7, 163.8, 173.4; ^{19}F NMR (282 MHz, $CDCl_3$) δ -75.99; FT-IR (neat, cm^{-1}) 2964, 2936, 2848, 2360, 1739, 1700, 1654, 1605, 1530, 1512, 1348, 1266, 1175, 1101; HRMS (APCI-TOF) calcd for $C_{22}H_{18}F_3NNaO_8$ $[M+Na]^+$: 504.0882, found: 504.0886.

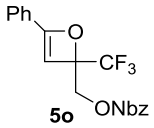
(3-(Dimethyl(phenyl)silyl)-4-(4-methoxyphenyl)-2-(trifluoromethyl)-2H-oxet-2-yl)methyl 4-nitrobenzoate (5n)



^{1}H NMR (300 MHz, $CDCl_3$) δ 0.48 (s, 3H), 0.52 (s, 3H), 3.82 (s, 3H), 4.85 (d, J = 12.9 Hz, 1H), 4.90

(d, J = 12.9 Hz, 1H), 6.80 (d, J = 9.0 Hz, 2H), 7.28-7.42 (m, 5H), 7.59 (d, J = 9.0 Hz, 2H), 8.18 (d, J = 9.0 Hz, 2H), 8.27 (d, J = 9.0 Hz, 2H); ^{13}C NMR (75 MHz, $CDCl_3$) δ -2.0, 29.7, 55.4, 63.0, 88.3 (q, J_{C-F} = 32.5 Hz), 106.7, 113.9, 121.6, 123.59 (q, J_{C-F} = 282.4 Hz), 123.60, 127.3, 128.2, 129.7, 130.9, 133.9, 134.7, 136.6, 150.7, 161.7, 163.9, 173.7; ^{19}F NMR (282 MHz, $CDCl_3$) δ -76.15; FT-IR (neat, cm^{-1}) 2956, 2925, 2852, 1735, 1619, 1530, 1504, 1460, 1342, 1264, 1166, 1122; HRMS (APCI-TOF) calcd for $C_{27}H_{25}F_3NO_6Si$ $[M+H]^+$: 544.1403, found: 544.1422.

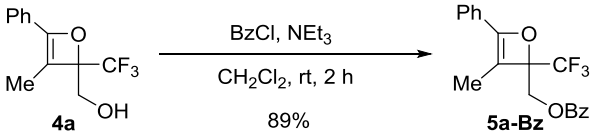
(4-Phenyl-2-(trifluoromethyl)-2H-oxet-2-yl)methyl 4-nitrobenzoate (5o)



5o

^{1}H NMR (300 MHz, $CDCl_3$) δ 4.90 (d, J = 12.6 Hz, 1H), 5.00 (d, J = 12.6 Hz, 1H), 6.07 (s, 1H), 7.39-7.41 (m, 3H), 7.50-7.53 (m, 2H), 8.17 (d, J = 8.7 Hz, 2H), 8.22 (d, J = 8.7 Hz, 2H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 62.8, 86.6 (q, J_{C-F} = 33.2 Hz), 98.7, 123.2 (q, J_{C-F} = 281.6 Hz), 123.6, 124.4, 124.7, 127.6, 128.6, 130.9, 134.6, 150.7, 163.9, 166.8; ^{19}F NMR (282 MHz, $CDCl_3$) δ -77.32; FT-IR (KBr pellet, cm^{-1}) 3150, 3107, 2949, 2855, 1740, 1525, 1348, 1271, 1193, 1158, 1086, 1015, 872; HRMS (APCI-TOF) calcd for $C_{18}H_{13}F_3NO_5$ $[M+H]^+$: 380.0746, found: 380.0751.

Procedure for Protection of Alcohol with Benzoyl Group (Scheme 2)



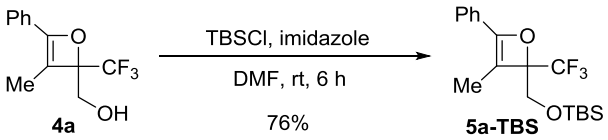
4a **5a-Bz**

To a solution of **4a** (122.1 mg, 0.5 mmol) in CH_2Cl_2 (5 mL) were added NEt_3 (139.4 μL, 1.0 mmol) and benzoyl chloride (69.6 μL, 0.6 mmol) at 0 °C, and the reaction mixture was warmed up to room temperature. After stirring for 2 h, the reaction mixture was quenched by water and extracted with diethyl ether. The organic layer was washed with brine, dried over Na_2SO_4, and concentrated under reduced pressure. Purification by silica-gel chromatography gave **5a-Bz** (154.4 mg, 89% yield).

(3-Methyl-4-phenyl-2-(trifluoromethyl)-2H-oxet-2-yl)methyl benzoate (5a-Bz)

^{1}H NMR (300 MHz, $CDCl_3$) δ 2.09 (s, 3H), 4.85 (d, J = 12.6 Hz, 1H), 4.97 (d, J = 12.6 Hz, 1H), 7.37-7.60 (m, 8H), 8.03-8.07 (m, 2H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 9.3, 61.9, 86.8 (q, J_{C-F} = 32.0 Hz), 111.2, 123.6 (q, J_{C-F} = 282.1 Hz), 124.7, 128.5, 128.6, 128.9, 129.3, 129.6, 129.8, 133.4, 159.8, 165.8.
^{19}F NMR (282 MHz, $CDCl_3$) δ -76.89; FT-IR (KBr pellet, cm^{-1}) 3069, 2999, 2950, 2925, 1732, 1450, 1341, 1270, 1191, 1118, 1071, 1028, 989, 971; HRMS (APCI-TOF) calcd for $C_{19}H_{16}F_3O_3$ $[M+H]^+$: 349.1052, found: 349.1035.

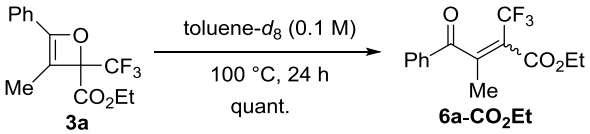
Procedure for Protection of Alcohol with tert-Butyldimethylsilyl Group (Scheme 2)



To a solution of **4a** (122.1 mg, 0.5 mmol) in DMF (5 mL) were added imidazole (102.1 mg, 1.5 mmol) and *tert*-butyldimethylsilyl chloride (113.0 mg, 0.75 mmol) at 0 °C, and the reaction mixture was warmed up to room temperature. After stirring for 6 h, the reaction mixture was quenched by water and extracted with diethyl ether. The organic layer was washed with brine, dried over Na_2SO_4, and concentrated under reduced pressure. Purification by silica-gel chromatography gave **5a-TBS** (136.8 mg, 76% yield).

***tert*-Butyldimethyl((3-methyl-4-phenyl-2-(trifluoromethyl)-2H-oxet-2-yl)methoxy)silane (5a-TBS)**
^{1}H NMR (300 MHz, $CDCl_3$) δ 0.08 (s, 3H), 0.11 (s, 3H), 0.89 (s, 9H), 2.08 (s, 3H), 4.12 (d, J = 11.4 Hz, 1H), 4.24 (d, J = 11.4 Hz, 1H), 7.32-7.43 (m, 3H), 7.48-7.51 (m, 2H); ^{13}C NMR (75 MHz, $CDCl_3$) δ -5.7, -5.6, 9.6, 18.1, 25.6, 62.4, 88.2 (q, $J_{C\text{-}F}$ = 30.2 Hz), 112.5, 123.9 (q, $J_{C\text{-}F}$ = 282.6 Hz), 124.5, 128.5, 129.0, 129.4, 158.6; ^{19}F NMR (282 MHz, $CDCl_3$) δ -76.68; FT-IR (neat, cm^{-1}) 2953, 2930, 2886, 2857, 1258, 1186, 1163, 1150, 1111, 839; HRMS (APCI-TOF) calcd for $C_{18}H_{26}F_3O_2Si$ $[M+H]^+$: 359.1654, found: 359.1663.

General Procedure for 4π Ring-Opening Reaction of Oxetenes (Table 1, 3-4, and Scheme 3)



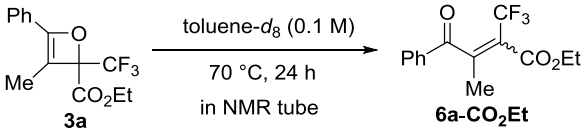
A solution of oxetene **3a** (409 mg, 1.4 mmol) in toluene (14 mL, 0.1 M) was heated at 100 °C. After stirring for 8 h at 100 °C, the solvent were removed under reduced pressure (*Z*/*E* = 77/23). Purification by silica-gel chromatography (hexane/AcOEt = 10/1) gave olefin **6a-CO_2Et** quantitatively, to separate *Z*- and *E*-isomers. This method was applied to 4π ring-opening reactions for all of oxetenes.

The *Z*- and *E*-configuration of **6a-CO_2Et** was determined on the base of NMR spectra according to previous literature.[2] In ^{1}H NMR, the coupling constant between Me and CF_3 groups in *Z*-isomer is smaller than that in *E*-isomer. The *Z*- and *E*-configurations of **6a** and **6l** were determined by X-ray analysis of the single crystal. The *Z*- and *E*-configurations of other olefins were determined by NOE analysis.

Ethyl 3-methyl-4-oxo-4-phenyl-2-(trifluoromethyl)but-2-enoate (6a-CO_2Et)
Z-isomer : *E*-isomer (at 70 °C) = 81 : 19; *Z*-isomer : *E*-isomer (at 100 °C) = 77 : 23
Z-isomer: ^{1}H NMR (300 MHz, $CDCl_3$) δ 1.37 (t, J = 7.2 Hz, 3H), 2.27 (q, J = 1.8 Hz, 3H), 4.37 (q, J = 7.2 Hz, 2H), 7.51 (t, J = 7.5 Hz, 2H), 7.63 (t, J = 7.5 Hz, 1H), 7.87 (t, J = 7.5 Hz, 2H); ^{1}H NMR (300 MHz, toluene-d_8) δ 1.25 (t, J = 7.2 Hz, 3H), 2.26 (q, J = 1.8 Hz, 3H), 4.27 (q, J = 7.2 Hz, 2H),

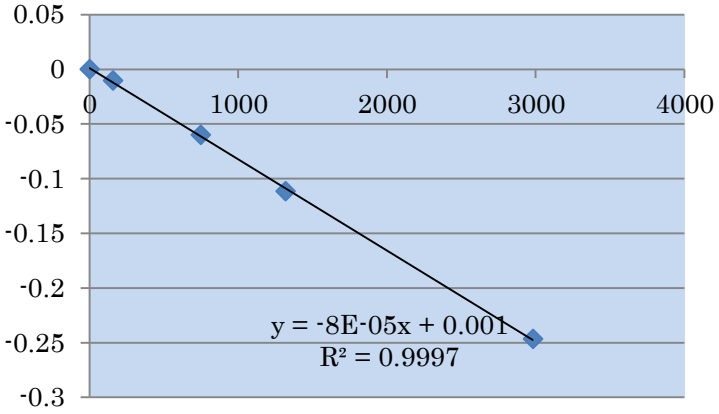
7.24-7.38 (m, 3H), 7.97-8.03 (m, 2H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 14.0, 19.5, 62.1, 121.4 (q, J_{C-F} = 274.8 Hz), 122.1 (q, J_{C-F} = 32.5 Hz), 129.0, 129.2, 133.3, 134.5, 152.9 (q, J_{C-F} = 3.0 Hz), 162.5 (q, J_{C-F} = 1.5 Hz), 194.6; ^{19}F NMR (282 MHz, $CDCl_3$) δ -58.26; ^{19}F NMR (282 MHz, toluene-d_8) δ -58.02; FT-IR (neat, cm^{-1}) 2920, 2882, 2851, 1759, 1689, 1587, 1328, 1209, 1101, 1032, 942; HRMS (APCI-TOF) calcd for $C_{14}H_{13}F_3NaO_3$ $[M+Na]^+$: 309.0715, found: 309.0712.
E-isomer: ^{1}H NMR (300 MHz, toluene-d_8) δ 0.89 (t, *J* = 7.2 Hz, 3H), 2.13 (q, *J* = 2.7 Hz, 3H), 3.87 (q, *J* = 7.2 Hz, 2H), 7.24-7.38 (m, 3H), 7.97-8.03 (m, 2H); ^{19}F NMR (282 MHz, toluene-d_8) δ -57.81.

General Procedure for Determination of Half-Life of Oxetenes (Table 1, 3-4, and Scheme 3)



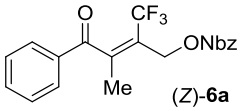
A solution of oxetene **3a** (21.5 mg, 0.075 mmol) in toluene-d_8 (0.75 mL, 0.1 M) in sealed NMR tube was heated at 70 °C. The progress of 4π ring-opening reaction was monitored by ^{19}F NMR analysis at four different times.

Run	t (min)	Maj (%)	[a]/[a$_0$]	ln([a]/[a$_0$])
0	0	100	1	0
1	157	98.97	0.9897	-0.0104
2	747	94.17	0.9417	-0.0601
3	1317	89.44	0.8944	-0.1116
4	2981	78.14	0.7814	-0.2467



$k = 5.0 \times 10^{-3}$ h^{-1}
$t_{1/2}$ at 70 °C = 138 h
E-isomer : *Z*-isomer (at 70 °C) = 81 : 19

3-Methyl-4-oxo-4-phenyl-2-(trifluoromethyl)but-2-en-1-yl 4-nitrobenzoate (6a)

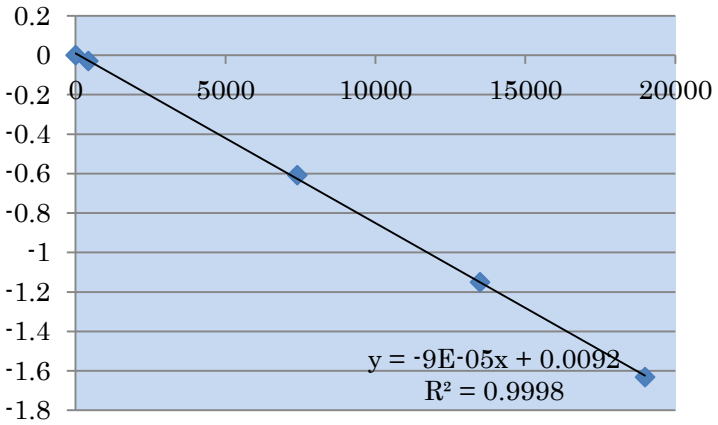


Z-isomer : *E*-isomer (at 70 °C) = 97 : 3; *Z*-isomer : *E*-isomer (at 100 °C) = 96 : 4
^{1}H NMR (300 MHz, $CDCl_3$) δ 2.24 (s, 3H), 5.20 (s, 2H), 7.52 (t, *J* = 7.5 Hz, 2H), 7.64 (t, *J* = 7.5 Hz, 1H), 7.85-7.88 (m, 2H), 8.26 (d, *J* = 9.0 Hz, 2H), 8.34 (d, *J* = 9.0 Hz, 2H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 18.0, 59.1 (q, J_{C-F} = 1.5 Hz), 121.5 (q, J_{C-F} = 30.5 Hz), 122.9 (q, J_{C-F} = 275.3 Hz), 123.7, 129.0, 129.2, 131.0, 133.6, 134.4, 134.7, 148.9 (q, J_{C-F} = 3.3 Hz), 150.8, 164.3, 195.7; ^{19}F NMR (282 MHz, $CDCl_3$) δ *Z*-isomer: -60.49, *E*-isomer: -59.33; FT-IR (KBr pellet, cm^{-1}) 2925, 2860, 1718, 1667, 1532, 1263, 1198, 1122, 1099, 722; HRMS (APCI-TOF) calcd for $C_{19}H_{15}F_3NO_5$ $[M+H]^+$: 394.0902, found: 394.0894. The structure of (*Z*)-**6a** was clarified by X-ray analysis of the single crystal (*vide infra*).

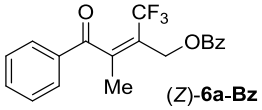
Run	t (min)	Maj (%)	[a]/[a$_0$]	ln([a]/[a$_0$])
0	0	100	1	0
1	424	97.09	0.9709	-0.0295
2	7391	54.43	0.5443	-0.6083
3	13485	31.64	0.3164	-1.1507
4	18989	19.56	0.1956	-1.6317

$k = 5.16 \times 10^{-3}$ h^{-1}

$t_{1/2}$ at 70 °C = 134 h



(*Z*)-3-Methyl-4-oxo-4-phenyl-2-(trifluoromethyl)but-2-en-1-yl benzoate (6a-Bz)



(*Z*)-**6a-Bz**

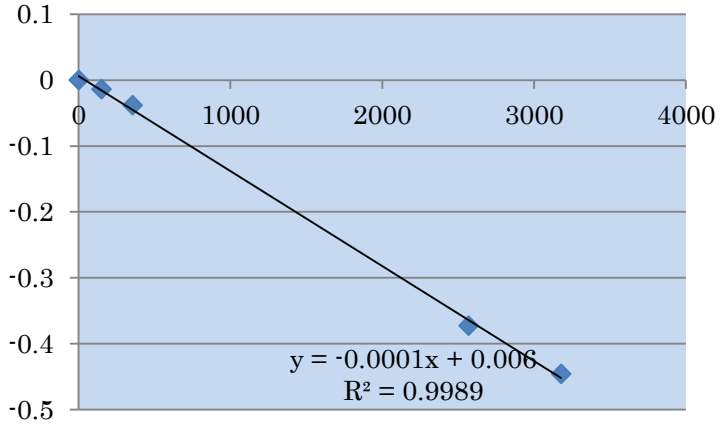
Z-isomer : *E*-isomer (at 70 °C) = 97 : 3; *Z*-isomer : *E*-isomer (at 100 °C) = 97 : 3

^{1}H NMR (300 MHz, $CDCl_3$) δ 2.22 (q, *J* = 1.8 Hz, 3H), 5.14 (s, 2H), 7.46-7.53 (m, 4H), 7.59-7.65 (m, 2H), 7.88 (d, *J* = 7.5 Hz, 2H), 8.09 (d, *J* = 7.5 Hz, 2H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 18.0, 58.3 (q, $J_{C\text{-}F}$ = 1.5 Hz), 122.1 (q, $J_{C\text{-}F}$ = 30.5 Hz), 123.0 (q, $J_{C\text{-}F}$ = 275.3 Hz), 128.6, 129.0, 129.2, 129.4, 129.8, 133.5, 133.7 (q, $J_{C\text{-}F}$ = 1.3 Hz), 134.3, 148.2 (q, $J_{C\text{-}F}$ = 3.8 Hz), 166.2, 196.0; ^{19}F NMR (282 MHz, $CDCl_3$) δ *Z*-isomer: -60.64, *E*-isomer: -59.25; FT-IR (neat, cm^{-1}) 3064, 2959, 2928, 2854, 1726, 1684, 1450, 1333, 1261, 1193, 1125, 1048; HRMS (APCI-TOF) calcd for $C_{19}H_{16}F_3O_3$ $[M+H]^+$: 349.1052, found: 349.1040.

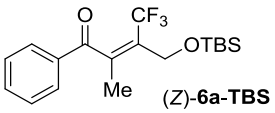
Run	t (min)	Maj (%)	[a]/[a$_0$]	ln([a]/[a$_0$])
0	0	100	1	0
1	150	98.62	0.9862	-0.0139
2	355	96.24	0.9624	-0.0383
3	2568	68.88	0.6888	-0.3728
4	3178	64.02	0.6402	-0.4460

$k = 8.65 \times 10^{-3}$ h^{-1}

$t_{1/2}$ at 70 °C = 80 h



3-(((*tert*-Butyldimethylsilyl)oxy)methyl)-4,4,4-trifluoro-2-methyl-1-phenylbut-2-en-1-one (6a-TBS)



(*Z*)-**6a-TBS**

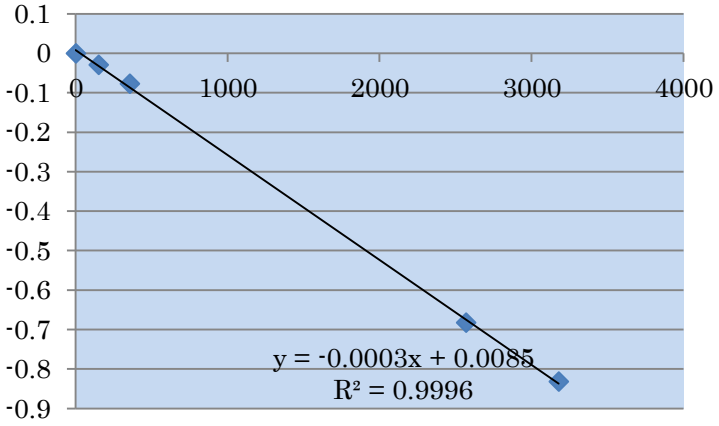
Z-isomer : *E*-isomer (at 70 °C) = 98 : 2; *Z*-isomer : *E*-isomer (at 100 °C) = 98 : 2

^{1}H NMR (300 MHz, $CDCl_3$) δ 0.14 (s, 6H), 0.94 (s, 9H), 2.11 (q, *J* = 2.1 Hz, 3H), 4.39 (s, 2H), 7.49 (t, *J* = 7.5 Hz, 2H), 7.61 (t, *J* = 7.5 Hz, 1H), 7.89 (d, *J* = 7.5 Hz, 2H); ^{13}C NMR (75 MHz, $CDCl_3$) δ -5.5, 17.5, 18.2, 25.7, 57.2 (q, J_{C-F} = 1.8 Hz), 123.4 (q, J_{C-F} = 274.8 Hz), 126.2 (q, J_{C-F} = 28.7 Hz), 128.9, 129.2, 134.0, 134.2, 144.9 (q, J_{C-F} = 3.8 Hz), 196.8; ^{19}F NMR (282 MHz, $CDCl_3$) δ *Z*-isomer: -61.09, *E*-isomer: -58.97; FT-IR (KBr pellet, cm^{-1}) 2957, 2928, 2857, 1681, 1335, 1266, 1182, 1119, 1073, 1040; HRMS (APCI-TOF) calcd for $C_{18}H_{26}F_3O_2Si$ $[M+H]^+$: 359.1654, found: 359.1658.

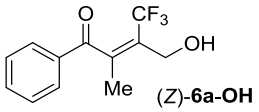
Run	t (min)	Maj (%)	[a]/[a$_0$]	ln([a]/[a$_0$])
0	0	100	1	0
1	150	97.13	0.9713	-0.0291
2	355	92.59	0.9259	-0.0770
3	2568	50.54	0.5054	-0.6824
4	3178	43.53	0.4353	-0.8317

$k = 1.60 \times 10^{-2}$ h^{-1}

$t_{1/2}$ at 70 °C = 43 h



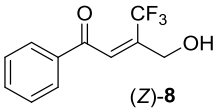
4,4,4-Trifluoro-3-(hydroxymethyl)-2-methyl-1-phenylbut-2-en-1-one (6a-OH)



(*Z*)-**6a-OH**

Purification by silica-gel column chromatography gave the product in 36% yield.
Z-isomer : *E*-isomer (at 70 °C) = 100 : 0
^{1}H NMR (300 MHz, $CDCl_3$) δ 2.16 (q, *J* = 2.1 Hz, 3H), 4.45 (s, 2H), 7.50 (t, *J* = 7.2 Hz, 2H), 7.63 (t, *J* = 7.2 Hz, 1H), 7.89 (d, *J* = 7.2 Hz, 2H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 17.5, 56.9 (q, J_{C-F} = 1.5 Hz), 123.5 (q, J_{C-F} = 274.8 Hz), 125.9 (q, J_{C-F} = 36.5 Hz), 128.9, 129.2, 133.9, 134.2, 146.2 (q, J_{C-F} = 3.8 Hz), 196.5; ^{19}F NMR (282 MHz, $CDCl_3$) δ -61.07; FT-IR (neat, cm^{-1}) 3432, 3012, 2934, 2893, 2850, 1739, 1656, 1503, 1364, 1259, 1192, 1123; HRMS (APCI-TOF) calcd for $C_{12}H_{11}F_3NaO_2$ $[M+Na]^+$: 267.0609, found: 267.0618.

4,4,4-Trifluoro-3-(hydroxymethyl)-1-phenylbut-2-en-1-one (8)

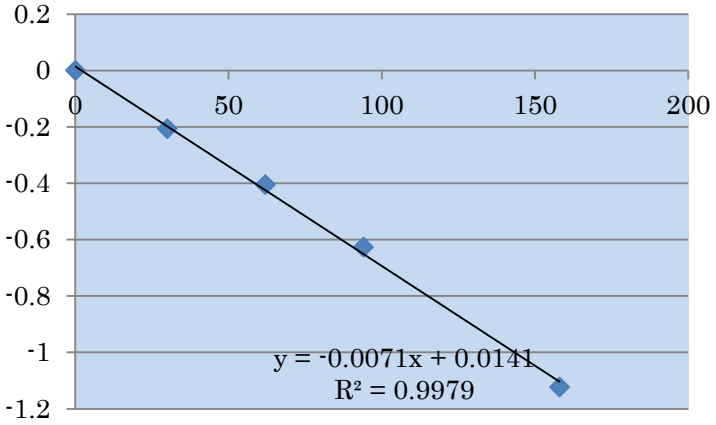


(*Z*)-**8**

Z-isomer : *E*-isomer (at 70 °C) = 100 : 0
^{1}H NMR (300 MHz, $CDCl_3$) δ 3.78 (br s, 1H), 4.46 (s, 2H), 7.03-7.05 (m, 1H), 7.43-7.48 (m, 2H), 7.57-7.63 (m, 1H), 7.90-7.93 (m, 2H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 59.4 (q, J_{C-F} = 3.0 Hz), 122.4 (q, J_{C-F} = 276.1 Hz), 128.8, 129.2, 130.8 (q, J_{C-F} = 3.8 Hz), 134.5, 135.4, 136.2 (q, J_{C-F} = 29.4 Hz), 194.4.
^{19}F NMR (282 MHz, $CDCl_3$) δ -62.34; FT-IR (KBr pellet, cm^{-1}) 3427, 2937, 2938, 2877, 1656, 1599,

1452, 1348, 1264, 1178, 1125, 1022; HRMS (APCI-TOF) calcd for $C_{11}H_9F_3NaO_2$ $[M+Na]^+$: 253.0452, found: 253.0467.

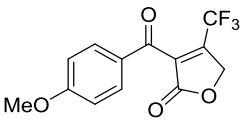
Run	t (min)	Maj (%)	$[a]/[a_0]$	$\ln([a]/[a_0])$
0	0	100	1	0
1	30	81.31	0.8131	-0.2069
2	62	66.67	0.6667	-0.4054
3	94	53.41	0.5341	-0.6272
4	158	32.51	0.3251	-1.1236



$k = 4.25 \times 10^{-1}$ h^{-1}

$t_{1/2}$ at 70 °C = 1.6 h

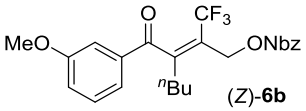
3-(4-Methoxybenzoyl)-4-(trifluoromethyl)furan-2(5H)-one (10)



10

^{1}H NMR (300 MHz, $CDCl_3$) δ 3.83 (s, 3H), 5.09 (s, 2H), 6.93 (d, J = 9.0 Hz, 2H), 7.81 (d, J = 9.0 Hz, 2H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 55.6, 67.9 (q, $J_{C\text{-}F}$ = 1.5 Hz), 114.4, 119.7 (q, $J_{C\text{-}F}$ = 272.63 Hz), 127.7, 132.0, 134.7 (q, $J_{C\text{-}F}$ = 3.0 Hz), 148.0 (q, $J_{C\text{-}F}$ = 37.8 Hz), 165.4, 167.8, 184.9; ^{19}F NMR (282 MHz, $CDCl_3$) δ -62.81; FT-IR (neat, cm^{-1}) 2938, 2846, 1779, 1664, 1600, 1574, 1514, 1375, 1344, 1262, 1152, 1041, 1026; HRMS (APCI-TOF) calcd for $C_{13}H_{10}F_3O_4$ $[M+H]^+$: 287.0531, found: 287.0535.

3-(3-Methoxybenzoyl)-2-(trifluoromethyl)hept-2-en-1-yl 4-nitrobenzoate (6b)



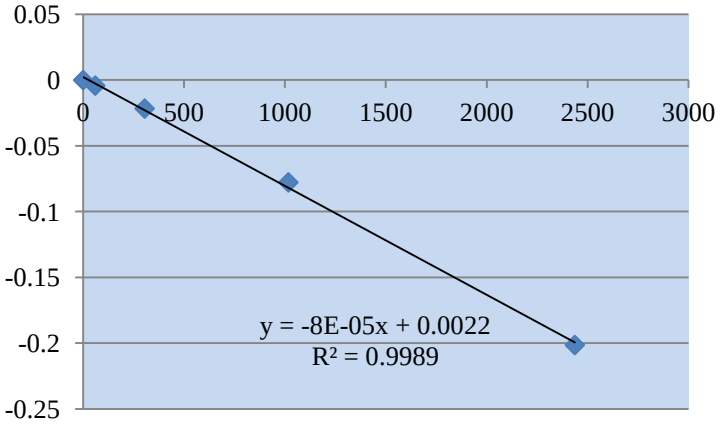
(*Z*)-**6b**

Z-isomer : *E*-isomer (at 70 °C) = 98 : 2; *Z*-isomer : *E*-isomer (at 100 °C) = 96 : 4

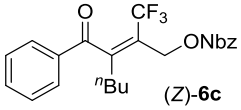
^{1}H NMR (300 MHz, $CDCl_3$) δ 0.84 (t, J = 7.2 Hz, 3H), 1.27-1.39 (m, 2H), 1.42-1.52 (m, 2H), 2.54 (br s, 2 H), 3.84 (s, 3H), 5.18 (s, 2H), 7.13-7.19 (m, 1H), 7.39-7.40 (m, 2H), 7.43-7.44 (m, 1H), 8.25 (d, J = 9.0 Hz, 2H), 8.33 (d, J = 9.0 Hz, 2H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 13.6, 22.7, 30.2, 31.6, 55.5, 59.0, 112.7, 121.0, 121.3 (q, $J_{C\text{-}F}$ = 30.2 Hz), 122.1, 123.0 (q, $J_{C\text{-}F}$ = 275.6 Hz), 123.7, 129.9, 130.9, 134.7, 135.6, 150.8, 152.9 (q, $J_{C\text{-}F}$ = 3.5 Hz), 160.0, 164.3, 195.0; ^{19}F NMR (282 MHz, $CDCl_3$) δ *Z*-isomer: -60.23, *E*-isomer: -58.34; FT-IR (KBr pellet, cm^{-1}) 3013, 2963, 2875, 2844, 1727, 1674, 1523, 1337, 1297, 1265, 1236, 1175, 1146, 1101; HRMS (APCI-TOF) calcd for $C_{23}H_{23}F_3NO_6$ $[M+H]^+$: 466.1478, found: 466.1466.

Run	t (min)	Maj (%)	[a]/[a$_0$]	ln([a]/[a$_0$])
0	0	100	1	0
1	60	99.58	0.9958	-0.0042
2	305	97.86	0.9786	-0.0246
3	1017	92.52	0.9252	-0.0778
4	2436	81.76	0.8176	-0.2014

$k = 4.97 \times 10^{-3}$ h^{-1}
$t_{1/2}$ at 70 °C = 140 h



3-Benzoyl-2-(trifluoromethyl)hept-2-en-1-yl 4-nitrobenzoate (6c)

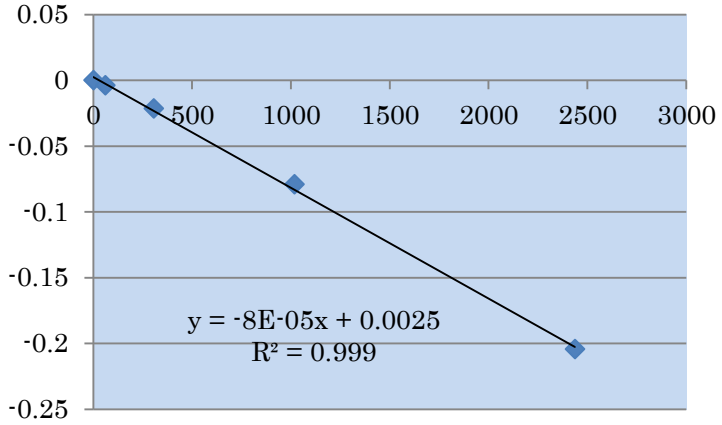


(*Z*)-**6c**

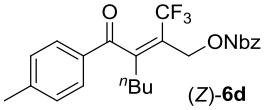
Z-isomer : *E*-isomer (at 70 °C) = 98 : 2; *Z*-isomer : *E*-isomer (at 100 °C) = 96 : 4
^{1}H NMR (300 MHz, $CDCl_3$) δ 0.84 (t, *J* = 7.2 Hz, 3H), 1.27-1.42 (m, 2H), 1.44-1.56 (m, 2H), 2.54 (br s, 2H), 5.19 (s, 2H), 7.51 (t, *J* = 7.5 Hz, 2H), 7.63 (t, *J* = 7.5 Hz, 1H), 7.87 (d, *J* = 7.5 Hz, 2H), 8.25 (d, *J* = 9.0 Hz, 2H), 8.33 (d, *J* = 9.0 Hz, 2H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 13.6, 22.7, 30.2, 31.6, 59.0, 121.4 (q, J_{C-F} = 30.2 Hz), 123.0 (q, J_{C-F} = 275.6 Hz), 123.7, 128.9, 129.2, 130.9, 134.26, 134.31, 134.7, 150.8, 153.0 (q, J_{C-F} = 3.5 Hz), 164.3, 195.2; ^{19}F NMR (282 MHz, $CDCl_3$) δ *Z*-isomer: -60.24, *E*-isomer: -58.40; FT-IR (KBr pellet, cm^{-1}) 3113, 2963, 2944, 2874, 1719, 1676, 1527, 1343, 1279, 1261, 1188, 1125, 1102; HRMS (APCI-TOF) calcd for $C_{22}H_{20}F_3NNaO_5$ $[M+Na]^+$: 458.1191, found: 456.1173.

Run	t (min)	Maj (%)	[a]/[a$_0$]	ln([a]/[a$_0$])
0	0	100	1	0
1	60	99.61	0.9961	-0.0039
2	305	97.87	0.9787	-0.0215
3	1017	92.39	0.9239	-0.0792
4	2436	81.51	0.8151	-0.2044

$k = 5.05 \times 10^{-3}$ h^{-1}
$t_{1/2}$ at 70 °C = 137 h



3-(4-Methylbenzoyl)-2-(trifluoromethyl)hept-2-en-1-yl 4-nitrobenzoate (6d)



(*Z*)-**6d**

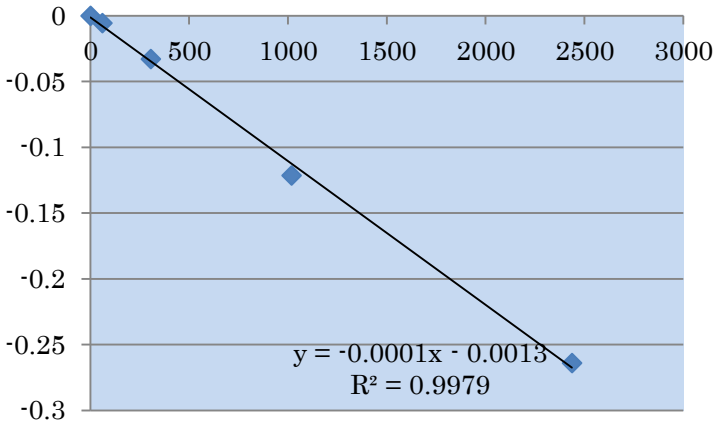
Z-isomer : *E*-isomer (at 70 °C) = 98 : 2; *Z*-isomer : *E*-isomer (at 100 °C) = 96 : 4

^{1}H NMR (300 MHz, $CDCl_3$) δ 0.84 (t, *J* = 7.2 Hz, 3H), 1.29-1.38 (m, 2H), 1.41-1.49 (m, 2H), 2.43 (s, 3H), 2.83 (br s, 2H), 5.18 (s, 2H), 7.30 (d, *J* = 7.8 Hz, 2H), 7.77 (d, *J* = 7.8 Hz, 2H), 8.25 (d, *J* = 9.0 Hz, 2H), 8.34 (d, *J* = 9.0 Hz, 2H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 13.6, 21.8, 22.7, 30.2, 31.7, 59.0 (q, J_{C-F} = 1.5 Hz), 121.1 (q, J_{C-F} = 30.2 Hz), 123.0 (q, J_{C-F} = 275.6 Hz), 123.7, 129.3, 129.7, 130.9, 131.9, 134.8, 145.4, 150.8, 153.2 (q, J_{C-F} = 3.3 Hz), 164.3, 194.9; ^{19}F NMR (282 MHz, $CDCl_3$) δ *Z*-isomer: -60.27, *E*-isomer: -58.34; FT-IR (KBr pellet, cm^{-1}) 3112, 2962, 1940, 2876, 1718, 1673, 1606, 1527, 1340, 1278, 1259, 1180, 1118, 1101; HRMS (APCI-TOF) calcd for $C_{23}H_{22}F_3NNaO_5$ $[M+Na]^+$: 472.1348, found: 472.1329.

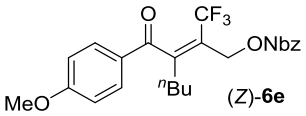
Run	t (min)	Maj (%)	[a]/[a_0]	ln([a]/[a_0])
0	0	100	1	0
1	60	99.45	0.9945	-0.0055
2	305	96.77	0.9677	-0.0328
3	1017	88.57	0.8857	-0.1214
4	2436	76.8	0.768	-0.2640

$k = 6.55 \times 10^{-3}$ h^{-1}

$t_{1/2}$ at 70 °C = 106 h



3-(4-Methoxybenzoyl)-2-(trifluoromethyl)hept-2-en-1-yl 4-nitrobenzoate (6e)



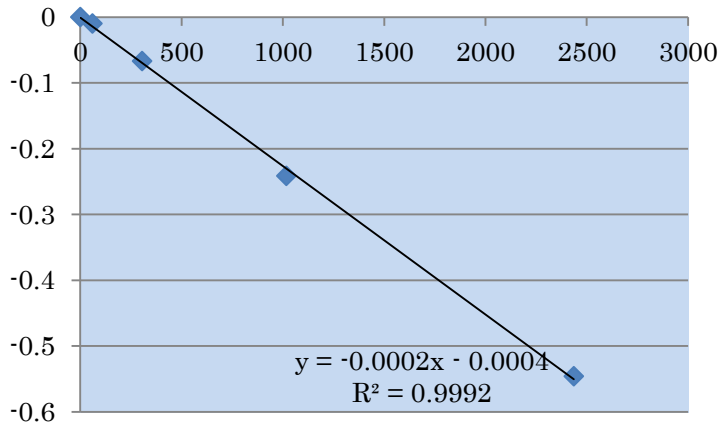
Z-isomer : *E*-isomer (at 70 °C) = 98 : 2; *Z*-isomer : *E*-isomer (at 100 °C) = 96 : 4

^{1}H NMR (300 MHz, $CDCl_3$) δ 0.83 (t, *J* = 7.2 Hz, 3H), 1.27-1.38 (m, 2H), 1.46 (br s, 2H), 2.52 (br s, 2H), 3.88 (s, 3H), 5.18 (s, 2H), 6.97 (d, *J* = 9.0 Hz, 2H), 7.84 (d, *J* = 9.0 Hz, 2H), 8.25 (d, *J* = 9.0 Hz, 2H), 8.33 (d, *J* = 9.0 Hz, 2H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 13.6, 22.7, 30.2, 31.8, 55.6, 59.1, 114.2, 120.9 (q, J_{C-F} = 30.2 Hz), 123.0 (q, J_{C-F} = 275.6 Hz), 123.7, 127.5, 130.9, 131.6, 134.8, 150.8, 153.3 (q, J_{C-F} = 3.5 Hz), 164.3, 164.4, 193.9; ^{19}F NMR (282 MHz, $CDCl_3$) δ *Z*-isomer: -60.30, *E*-isomer: -58.27; FT-IR (KBr pellet, cm^{-1}) 2958, 2934, 2876, 2859, 1716, 1604, 1530, 1344, 1264, 1182, 1172, 1126, 1101; HRMS (APCI-TOF) calcd for $C_{23}H_{23}F_3NO_6$ $[M+H]^+$: 466.1478, found: 466.1483.

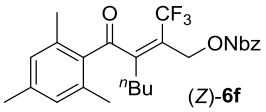
Run	t (min)	Maj (%)	[a]/[a_0]	ln([a]/[a_0])
0	0	100	1	0
1	60	99.03	0.9903	-0.0097
2	305	93.53	0.9353	-0.0669
3	1017	78.55	0.7855	-0.2414
4	2436	57.92	0.5792	-0.5461

$k = 1.36 \times 10^{-2}$ h^{-1}

$t_{1/2}$ at 70 °C = 51 h



4,4-Dimethyl-2-(trifluoromethyl)-3-(2,4,6-trimethylbenzoyl)pent-2-en-1-yl 4-nitrobenzoate (6f)

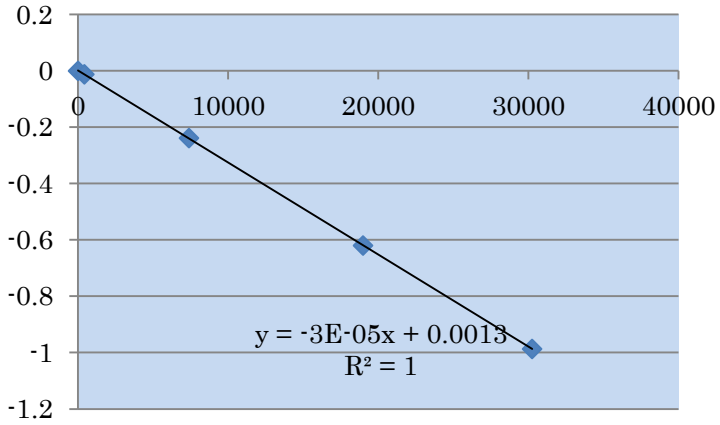


(*Z*)-**6f**

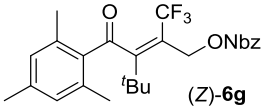
Z-isomer : *E*-isomer (at 70 °C) = 96 : 4; *Z*-isomer : *E*-isomer (at 100 °C) = 96 : 4
^{1}H NMR (300 MHz, $CDCl_3$) δ 0.80 (t, *J* = 7.2 Hz, 3H), 1.21-1.33 (m, 2H), 1.35-1.45 (m, 2H), 2.29 (s, 3H), 2.36 (s, 6H), 2.42 (t, *J* = 7.8 Hz, 2H), 5.13 (s, 2H), 6.89 (s, 2H), 8.20 (d, *J* = 9.0 Hz, 2H), 8.31 (d, *J* = 9.0 Hz, 2H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 13.6, 21.2, 21.3, 22.6, 31.2, 31.3, 59.8 (q, J_{C-F} = 2.3 Hz), 123.0 (q, J_{C-F} = 276.1 Hz), 123.3 (q, J_{C-F} = 30.7 Hz), 123.7, 130.4, 130.9, 133.2, 134.7, 138.1, 141.7, 150.8, 156.6 (q, J_{C-F} = 3.0 Hz), 164.1, 198.2; ^{19}F NMR (282 MHz, $CDCl_3$) δ *Z*-isomer: -59.13, *E*-isomer: -58.93; FT-IR (neat, cm^{-1}) 2961, 2933, 2871, 1729, 1608, 1530, 1349, 1273, 1242, 1170, 1098, 1052; HRMS (APCI-TOF) calcd for $C_{25}H_{27}F_3NO_5$ $[M+H]^+$: 478.1841, found: 478.1846.

Run	t (min)	Maj (%)	$[a]/[a_0]$	$\ln([a]/[a_0])$
0	0	100	1	0
1	424	98.79	0.9879	-0.0122
2	7391	78.79	0.7879	-0.2384
3	18989	53.82	0.5382	-0.6195
4	30253	37.29	0.3729	-0.9864

$k = 1.96 \times 10^{-3}$ h^{-1}
$t_{1/2}$ at 70 °C = 354 h



2-(Trifluoromethyl)-3-(2,4,5-trimethylbenzoyl)hept-2-en-1-yl 4-nitrobenzoate (6g)

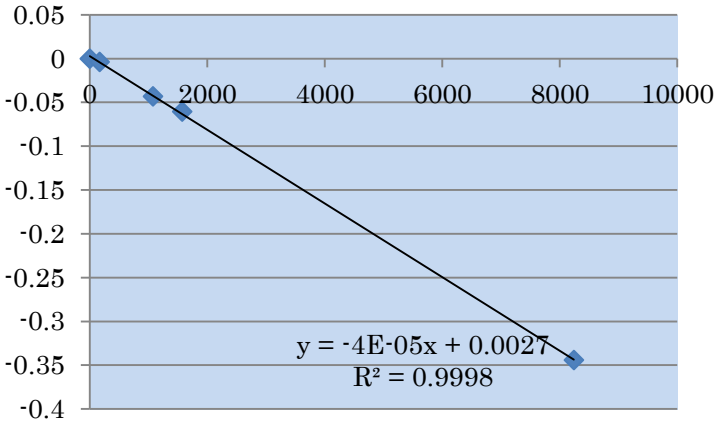


(*Z*)-**6g**

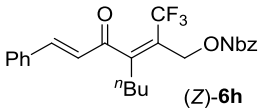
Z-isomer : *E*-isomer (at 100 °C) = 98 : 2
^{1}H NMR (300 MHz, $CDCl_3$) δ 1.31 (s, 9H), 2.32 (s, 3H), 2.56 (s, 6H), 5.27 (s, 2H), 6.95 (s, 2H), 8.21 (d, *J* = 9.0 Hz, 2H), 8.32 (d, *J* = 9.0 Hz, 2H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 22.2, 23.7, 31.7, 36.8, 60.1 (q, J_{C-F} = 1.8 Hz), 120.5 (q, J_{C-F} = 28.9 Hz), 123.7 (q, J_{C-F} = 277.1 Hz), 123.8, 130.8, 131.8, 133.23, 133.25, 134.9, 142.5, 150.8, 164.1, 165.3 (q, J_{C-F} = 3.0 Hz), 196.9; ^{19}F NMR (282 MHz, $CDCl_3$) δ *Z*-isomer: -58.81, *E*-isomer: -54.83; FT-IR (KBr pellet, cm^{-1}) 2978, 2963, 2927, 1726, 1608, 1531, 1350, 1322, 1279, 1249, 1178, 1110; HRMS (APCI-TOF) calcd for $C_{25}H_{26}F_3NNaO_5$ $[M+Na]^+$: 500.1661, found: 500.1658.

Run	t (min)	Maj (%)	[a]/[a$_0$]	ln([a]/[a$_0$])
0	0	100	1	0
1	168	99.63	0.9963	-0.0037
2	1076	95.79	0.9579	-0.0430
3	1573	94.14	0.9414	-0.0603
4	8241	70.89	0.7089	-0.3440

$k = 2.52 \times 10^{-3}$ h^{-1}
$t_{1/2}$ at 100 °C = 275 h



3-Cinnamoyl-2-(trifluoromethyl)hept-2-en-1-yl 4-nitrobenzoate (6h)

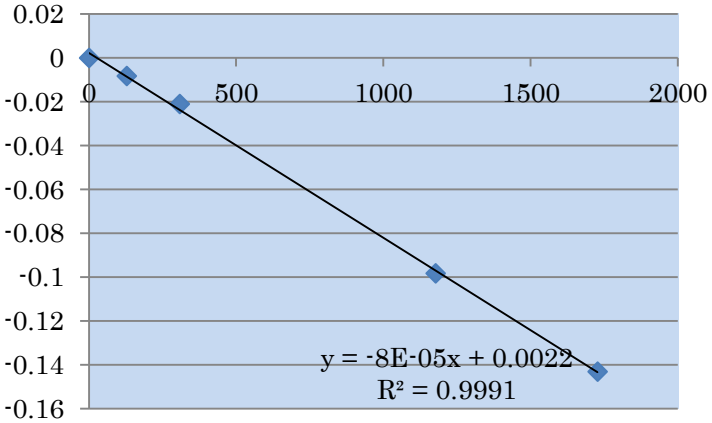


(*Z*)-**6h**

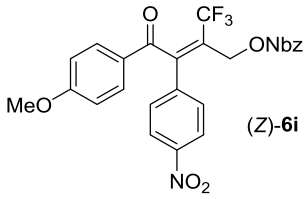
Z-isomer : *E*-isomer (at 70 °C) = 97 : 3; *Z*-isomer : *E*-isomer (at 100 °C) = 96 : 4
^{1}H NMR (300 MHz, $CDCl_3$) δ 0.88 (t, *J* = 7.2 Hz, 3H), 1.31-1.43 (m, 2H), 1.45-1.60 (m, 2H), 2.54 (t, *J* = 7.8 Hz, 2H), 5.15 (s, 2H), 6.79 (d, *J* = 16.2 Hz, 1H), 7.45 (d, *J* = 16.2 Hz, 1H), 7.36-7.47 (m, 3H), 7.53-7.55 (m, 2H), 8.25 (d, *J* = 8.7 Hz, 2H), 8.33 (d, *J* = 8.7 Hz, 2H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 13.7, 22.7, 30.2, 31.7, 59.1, 121.0 (q, $J_{C\text{-}F}$ = 30.2 Hz), 123.8, 125.2, 126.7 (q, $J_{C\text{-}F}$ = 280.1 Hz), 128.6, 129.1, 130.9, 131.4, 133.8, 134.8, 147.1, 150.8, 153.3 (q, $J_{C\text{-}F}$ = 3.0 Hz), 164.3, 195.6; ^{19}F NMR (282 MHz, $CDCl_3$) δ *Z*-isomer: -59.98 (*E*: Ph-CH=CH-), -59.70 (*Z*: Ph-CH=CH-), *E*-isomer: -58.34; FT-IR (KBr pellet, cm^{-1}) 3111, 2963, 2938, 2874, 1719, 1653, 1526, 1339, 1260, 1186, 1118, 1100; HRMS (APCI-TOF) calcd for $C_{24}H_{23}F_3NO_5$ $[M+H]^+$: 462.1528, found: 462.1516.

Run	t (min)	Maj (%)	[a]/[a$_0$]	ln([a]/[a$_0$])
0	0	100	1	0
1	128	99.18	0.9918	-0.0082
2	308	97.92	0.9792	-0.0210
3	1177	90.64	0.9064	-0.0983
4	1727	86.67	0.8667	-0.1431

$k = 5.06 \times 10^{-3}$ h^{-1}
$t_{1/2}$ at 70 °C = 137 h



4-(4-Methoxyphenyl)-3-(4-nitrophenyl)-4-oxo-2-(trifluoromethyl)but-2-en-1-yl 4-nitrobenzoate (6i)

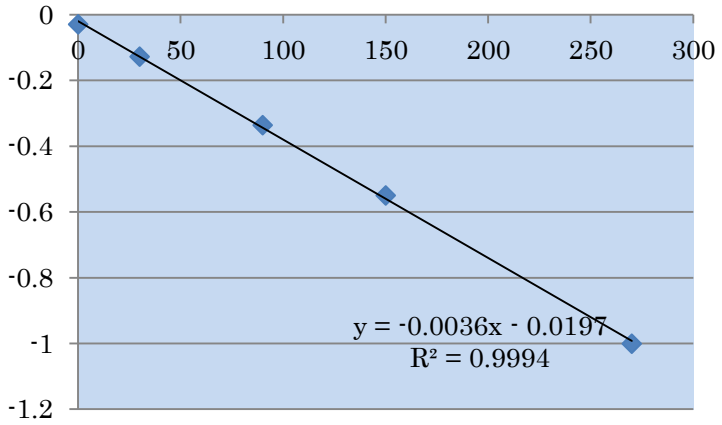


(*Z*)-**6i**

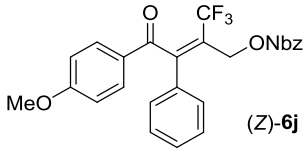
Z-isomer : *E*-isomer (at 70 °C) = 99 : 1; *Z*-isomer : *E*-isomer (at 100 °C) = 98 : 2
^{1}H NMR (300 MHz, $CDCl_3$) δ 3.87 (s, 3H), 5.02 (s, 2H), 6.98 (d, *J* = 9.0 Hz, 2H), 7.66 (d, *J* = 9.0 Hz, 2H), 7.92 (d, *J* = 9.0 Hz, 2H), 8.22 (d, *J* = 9.0 Hz, 2H), 8.25 (d, *J* = 9.0 Hz, 2H), 8.33 (d, *J* = 9.0 Hz, 2H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 55.7, 60.4, 114.5, 122.7 (q, J_{C-F} = 276.3 Hz), 123.8, 124.29, 124.34 (q, J_{C-F} = 30.5 Hz), 126.8, 129.3, 130.9, 132.1, 134.4, 139.2, 148.4, 150.1 (q, J_{C-F} = 3.3 Hz), 150.9, 163.9, 164.9, 190.4; ^{19}F NMR (282 MHz, $CDCl_3$) δ *Z*-isomer: -60.27, *E*-isomer: -57.46; FT-IR (KBr pellet, cm^{-1}) 3110, 3019, 2935, 2846, 1736, 1599, 1518, 1350, 1331, 1262, 1172, 1118; HRMS (APCI-TOF) calcd for $C_{25}H_{18}F_3N_2O_8$ $[M+H]^+$: 531.1015, found: 531.1000.

Run	t (min)	Maj (%)	$[a]/[a_0]$	$\ln([a]/[a_0])$
0	0	97.09	0.9709	-0.0295
1	30	88.01	0.8801	-0.1277
2	90	71.45	0.7145	-0.3362
3	150	57.70	0.5770	-0.5499
4	270	36.76	0.3676	-1.0008

$k = 2.16 \times 10^{-1}$ h^{-1}
$t_{1/2}$ at 70 °C = 3.2 h



4-(4-Methoxyphenyl)-4-oxo-3-phenyl-2-(trifluoromethyl)but-2-en-1-yl 4-nitrobenzoate (6j)

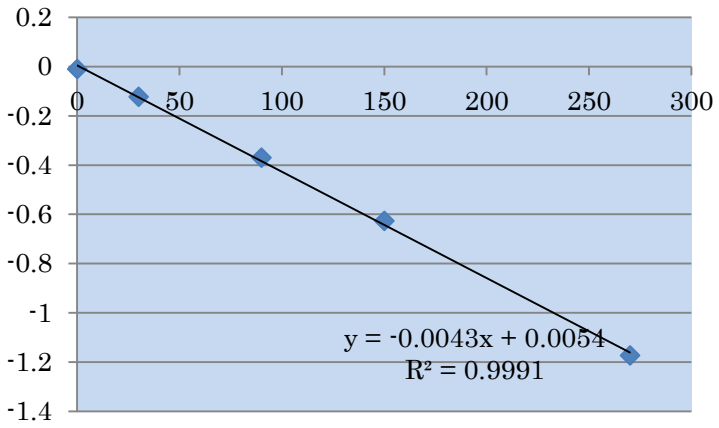


(*Z*)-**6j**

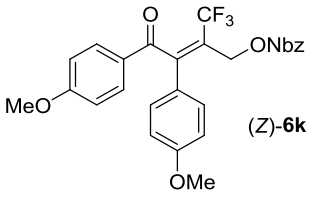
Z-isomer : *E*-isomer (at 70 °C) = 99 : 1; *Z*-isomer : *E*-isomer (at 100 °C) = 98 : 2
^{1}H NMR (300 MHz, $CDCl_3$) δ 3.84 (s, 3H), 5.07 (s, 2H), 6.94 (d, *J* = 9.0 Hz, 2H), 7.35-7.40 (m, 3H), 7.41-7.44 (m, 2H), 7.93 (d, *J* = 9.0 Hz, 2H), 8.22 (d, *J* = 8.7 Hz, 2H), 8.27 (d, *J* = 8.7 Hz, 2H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 55.6, 60.8, 114.2, 122.6 (q, J_{C-F} = 30.2 Hz), 123.2 (q, J_{C-F} = 276.3 Hz), 123.7, 127.4, 128.1, 129.2, 129.8, 130.9, 132.0, 132.8, 134.8, 150.8, 152.6 (q, J_{C-F} = 3.3 Hz), 163.9, 164.4, 191.6; ^{19}F NMR (282 MHz, $CDCl_3$) δ *Z*-isomer: -60.02, *E*-isomer: -57.22; FT-IR (KBr pellet, cm^{-1}) 3064, 2924, 2850, 1726, 1662, 1599, 1574, 1525, 1339, 1265, 1177, 1124; HRMS (APCI-TOF) calcd for $C_{25}H_{18}F_3NNaO_6$ $[M+Na]^+$: 508.0984, found: 508.0996.

Run	t (min)	Maj (%)	[a]/[a$_0$]	ln([a]/[a$_0$])
0	0	98.95	0.9895	-0.0106
1	30	88.40	0.8840	-0.1233
2	90	69.05	0.6905	-0.3703
3	150	53.42	0.5342	-0.6270
4	270	30.94	0.3094	-1.1731

$k = 2.59 \times 10^{-1}$ h^{-1}
$t_{1/2}$ at 70 °C = 2.7 h



3,4-Bis(4-methoxyphenyl)-4-oxo-2-(trifluoromethyl)but-2-en-1-yl 4-nitrobenzoate (6k)

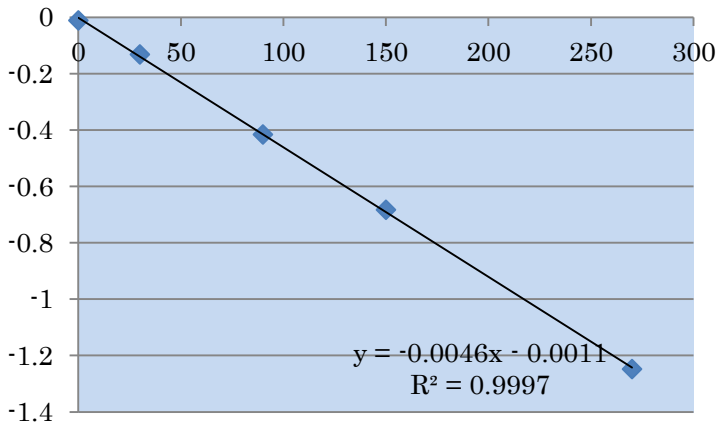


(*Z*)-**6k**

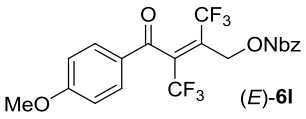
Z-isomer : *E*-isomer (at 70 °C) = 99 : 1; *Z*-isomer : *E*-isomer (at 100 °C) = 98 : 2
^{1}H NMR (300 MHz, $CDCl_3$) δ 3.76 (s, 3H), 3.84 (s, 3H), 5.10 (s, 2H), 6.88 (d, *J* = 8.7 Hz, 2H), 6.93 (d, *J* = 8.7 Hz, 2H), 7.34 (d, *J* = 8.7 Hz, 2H), 7.90 (d, *J* = 8.7 Hz, 2H), 8.24 (d, *J* = 9.0 Hz, 2H), 8.32 (d, *J* = 9.0 Hz, 2H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 55.3, 55.6, 61.1, 114.2, 114.6, 121.6 (q, $J_{C\text{-}F}$ = 30.2 Hz), 123.3 (q, $J_{C\text{-}F}$ = 276.3 Hz), 123.7, 124.8, 127.6, 129.7, 130.9, 132.0, 134.9, 150.8, 152.5 (q, $J_{C\text{-}F}$ = 3.8 Hz), 160.8, 164.0, 164.3, 191.9; ^{19}F NMR (282 MHz, $CDCl_3$) δ *Z*-isomer: -59.79, *E*-isomer: -57.14; FT-IR (KBr pellet, cm^{-1}) 3078, 3006, 2939, 2845, 1726, 1604, 1526, 1510, 1259, 1171, 1115, 1030; HRMS (APCI-TOF) calcd for $C_{26}H_{20}F_3NNaO_7$ [M+Na]$^+$: 538.1090, found: 538.1063.

Run	t (min)	Maj (%)	[a]/[a$_0$]	ln([a]/[a$_0$])
0	0	98.91	0.9891	-0.0110
1	30	87.67	0.8767	-0.1316
2	90	65.99	0.6599	-0.4157
3	150	50.52	0.5052	-0.6828
4	270	28.71	0.2871	-1.2479

$k = 2.76 \times 10^{-1}$ h^{-1}
$t_{1/2}$ at 70 °C = 2.5 h



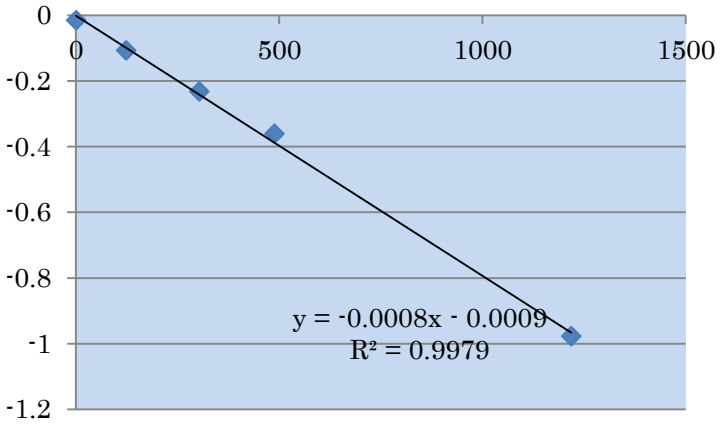
4,4,4-Trifluoro-3-(4-methoxybenzoyl)-2-(trifluoromethyl)but-2-en-1-yl 4-nitrobenzoate (6l)



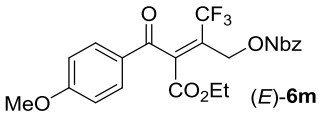
E-isomer : *Z*-isomer (at 70 °C) = 100 : 0; *E*-isomer : *Z*-isomer (at 100 °C) = 100 : 0
^{1}H NMR (300 MHz, $CDCl_3$) δ 3.91 (s, 3H), 5.27 (d, *J* = 12.9 Hz, 1H), 5.35 (d, *J* = 12.9 Hz, 1H), 7.03 (d, *J* = 9.0 Hz, 2H), 7.88 (d, *J* = 9.0 Hz, 2H), 8.25 (d, *J* = 8.7 Hz, 2H), 8.34 (d, *J* = 8.7 Hz, 2H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 55.7, 58.4, 114.6, 120.7 (q, J_{C-F} = 277.8 Hz), 121.7 (q, J_{C-F} = 277.8 Hz), 123.8, 127.5, 131.0, 131.8, 131.9 (q, J_{C-F} = 32.5 Hz), 134.1, 140.3 (q, J_{C-F} = 32.5 Hz), 151.0, 163.7, 165.3, 185.4; ^{19}F NMR (282 MHz, $CDCl_3$) δ -61.18, -56.77; FT-IR (KBr pellet, cm^{-1}) 2977, 2933, 2837, 1735, 1602, 1526, 1353, 1267, 1215, 1142, 1096; HRMS (APCI-TOF) calcd for $C_{20}H_{14}F_6NO_6$ $[M+H]^+$: 478.0725, found: 478.0703. The structure of (*E*)-**6l** was clarified by X-ray analysis of the single crystal (*vide infra*).

Run	t (min)	Maj (%)	$[a]/[a_0]$	$\ln([a]/[a_0])$
0	0	98.48	0.9848	-0.0153
1	123	89.84	0.8984	-0.1071
2	303	79.27	0.7927	-0.2323
3	488	69.70	0.6970	-0.3610
4	1218	37.63	0.3763	-0.9774

$k = 4.75 \times 10^{-2}$ h^{-1}
$t_{1/2}$ at 70 °C = 15 h



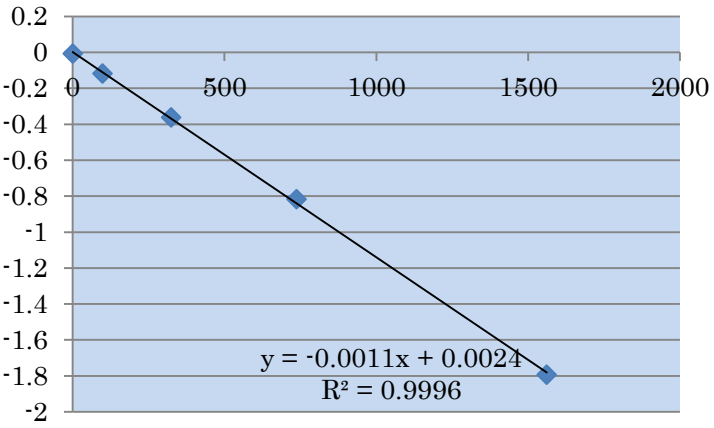
4-Ethoxy-3-(4-methoxybenzoyl)-4-oxo-2-(trifluoromethyl)but-2-en-1-yl 4-nitrobenzoate (6m)



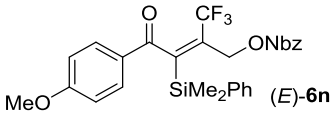
E-isomer : *Z*-isomer (at 70 °C) = 100 : 0; *E*-isomer : *Z*-isomer (at 100 °C) = 100 : 0
^{1}H NMR (300 MHz, $CDCl_3$) δ 1.15 (t, *J* = 7.2 Hz, 3H), 3.88 (s, 3H), 4.21 (q, *J* = 7.2 Hz, 2H), 5.42 (s, 2H), 6.97 (d, *J* = 8.7 Hz, 2H), 7.88 (d, *J* = 8.7 Hz, 2H), 8.23 (d, *J* = 8.7 Hz, 2H), 8.31 (d, *J* = 8.7 Hz, 2H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 13.8, 55.6, 59.5, 63.1, 114.3, 122.2 (q, J_{C-F} = 277.8 Hz), 123.7, 127.9, 131.0, 131.6 (q, J_{C-F} = 31.7 Hz), 131.8, 134.5, 142.7 (q, J_{C-F} = 3.8 Hz), 150.8, 162.6, 163.9, 164.7, 187.6; ^{19}F NMR (282 MHz, $CDCl_3$) δ -60.98; FT-IR (neat, cm^{-1}) 2936, 2848, 1732, 1675, 1599, 1577, 1530, 1513, 1348, 1319, 1264, 1173, 1141, 1101, 1030; HRMS (APCI-TOF) calcd for $C_{22}H_{19}F_3NO_8$ $[M+H]^+$: 482.1063, found: 482.1065.

Run	t (min)	Maj (%)	[a]/[a$_0$]	ln([a]/[a$_0$])
0	0	99.31	0.9931	-0.0069
1	98	88.89	0.8889	-0.1178
2	324	69.64	0.6964	-0.3618
3	737	44.18	0.4418	-0.8169
4	1561	16.64	0.1664	-1.7934

$k = 6.86 \times 10^{-2}$ h^{-1}
$t_{1/2}$ at 70 °C = 10 h



3-(Dimethyl(phenyl)silyl)-4-(4-methoxyphenyl)-4-oxo-2-(trifluoromethyl)but-2-en-1-yl 4-nitrobenzoate (6n)

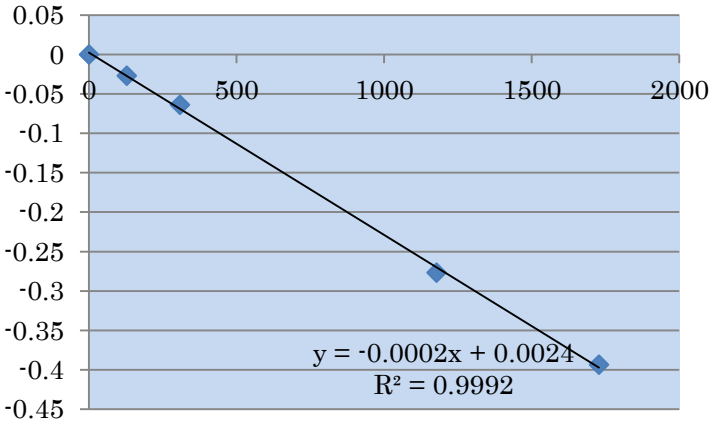


(*E*)-**6n**

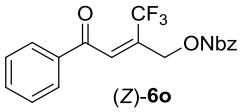
E-isomer : *Z*-isomer (at 70 °C) = 99 : 1
^{1}H NMR (300 MHz, $CDCl_3$) δ 0.38 (s, 3H), 0.52 (s, 3H), 3.92 (s, 3H), 4.91 (d, *J* = 12.6 Hz, 1H), 4.99 (d, *J* = 12.6 Hz, 1H), 7.02 (d, *J* = 8.7 Hz, 2H), 7.22-7.31 (m, 3H), 7.58-7.60 (m, 2H), 7.89 (d, *J* = 8.7 Hz, 2H), 8.06 (d, *J* = 8.7 Hz, 2H), 8.29 (d, *J* = 8.7 Hz, 2H); ^{13}C NMR (75 MHz, $CDCl_3$) δ -2.5, -1.7, 55.6, 61.9, 114.2, 122.4 (q, J_{C-F} = 279.4 Hz), 123.5, 128.3, 129.0, 130.1, 130.8, 131.2, 131.7 (q, J_{C-F} = 29.7 Hz), 133.9, 134.6, 134.9, 150.7, 157.9 (q, J_{C-F} = 2.3 Hz), 163.6, 164.2, 195.4; ^{19}F NMR (282 MHz, $CDCl_3$) δ *E*-isomer: -60.88, *Z*-isomer: -58.97; FT-IR (KBr pellet, cm^{-1}) 3016, 2965, 2937, 2845, 1726, 1604, 1526, 1354, 1314, 1270, 1170, 1124; HRMS (APCI-TOF) calcd for $C_{27}H_{24}F_3NO_6Si$ $[M+H]^+$: 544.1403, found: 544.1399.

Run	t (min)	Maj (%)	[a]/[a$_0$]	ln([a]/[a$_0$])
0	0	100	1	0
1	128	97.35	0.9735	-0.0269
2	308	93.82	0.9382	-0.0638
3	1177	75.83	0.7583	-0.2767
4	1727	67.47	0.6747	-0.3934

$k = 1.39 \times 10^{-2}$ h^{-1}
$t_{1/2}$ at 70 °C = 50 h



4-Oxo-4-phenyl-2-(trifluoromethyl)but-2-en-1-yl 4-nitrobenzoate (6o)

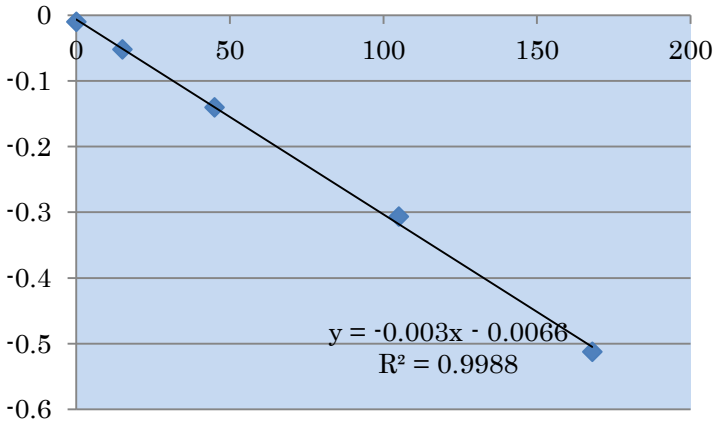


(*Z*)-**6o**

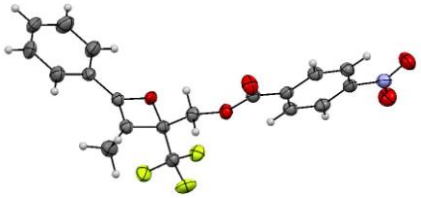
Z-isomer : *E*-isomer (at 70 °C) = 99 : 1; *Z*-isomer : *E*-isomer (at 100 °C) = 99 : 1
^{1}H NMR (300 MHz, $CDCl_3$) δ 5.15 (s, 2H), 7.06 (s, 1H), 7.46 (t, *J* = 7.2 Hz, 2H), 7.59 (t, *J* = 7.2 Hz, 1H), 7.88 (d, *J* = 7.2 Hz, 2H), 8.22 (d, *J* = 9.0 Hz, 2H), 8.26 (d, *J* = 9.0 Hz, 2H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 62.6 (q, J_{C-F} = 2.3 Hz), 122.0 (q, J_{C-F} = 275.8 Hz), 123.7, 128.9, 129.1, 129.7 (q, J_{C-F} = 31.5 Hz), 130.9, 134.5, 135.1 (2C), 136.3 (q, J_{C-F} = 3.8 Hz), 150.8, 163.9, 191.5; ^{19}F NMR (282 MHz, $CDCl_3$) δ *Z*-isomer: -61.95, *E*-isomer: -60.85; FT-IR (KBr pellet, cm^{-1}) 3118, 2955, 2923, 1728, 1667, 1536, 1348, 1266, 1189, 1134, 1121, 1097, 719; HRMS (APCI-TOF) calcd for $C_{18}H_{13}F_3NO_5$ $[M+H]^+$: 380.0746, found: 380.0737.

Run	t (min)	Maj (%)	$[a]/[a_0]$	$\ln([a]/[a_0])$
0	0	99	0.99	-0.0100
1	15	94.93	0.9493	-0.0520
2	45	86.91	0.8691	-0.1403
3	105	73.60	0.7360	-0.3065
4	168	59.91	0.5991	-0.5123

$k = 1.78 \times 10^{-1}$ h^{-1}
$t_{1/2}$ at 70 °C = 3.9 h



X-ray analysis of oxetene 5a



CCDC 948159 (**5a**) contains the supplementary crystallographic data for this paper. The data can be obtained free of charge from The Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/data_request/cif

Crystal Data

Empirical Formula	$C_{19}H_{14}F_3NO_5$
Formula Weight	393.32
Crystal Color, Habit	colorless, block
Crystal Dimensions	0.200 x 0.150 x 0.100 mm
Crystal System	triclinic
Lattice Type	Primitive
Lattice Parameters	a = 5.512(3) Å
	b = 10.789(7) Å
	c = 14.890(9) Å
	α = 88.566(12) °
	β = 81.672(12) °
	γ = 83.072(9) °
	V = 869.7(9) $Å^3$
Space Group	P-1 (#2)
Z value	2
Dcalc	1.502 g/cm^3
F000 404.00	
μ(MoKα)	1.295 cm^{-1}

Intensity Measurements

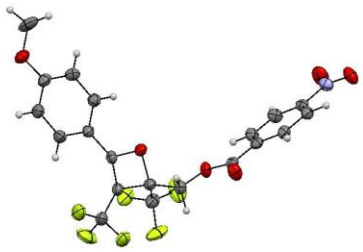
Diffractometer	XtaLAB mini
Radiation	MoKα (λ = 0.71075 Å)
	graphite monochromated
Voltage, Current	50kV, 12mA
Temperature	-180.0 °C
Detector Aperture	75 mm (diameter)
Data Images	1080 exposures
ω oscillation Range	-60.0 - 120.0°

Exposure Rate	32.0 sec%
Detector Swing Angle	29.95°
ω oscillation Range	-60.0 - 120.0°
Exposure Rate	32.0 sec%
Detector Swing Angle	29.95o
ω oscillation Range	-60.0 - 120.0°
Exposure Rate	32.0 sec%
Detector Swing Angle	29.95°
Detector Position	49.90 mm
Pixel Size	0.146 mm
2θmax	55.1°
No. of Reflections Measured	Total: 9198
	Unique: 3982 (Rint = 0.0297)
Corrections	Lorentz-polarization
	Absorption
	(trans. factors: 0.881 - 0.987)

Structure Solution and Refinement

Structure Solution	Direct Methods
Refinement	Full-matrix least-squares on F^2
Function Minimized	Σ w $(Fo^2 - Fc^2)^2$
Least Squares Weights	$w = 1/ [\sigma^2(Fo^2) + (0.0666 . P)^2 + 0.1265 . P]$
	where $P = (Max(Fo^2,0) + 2Fc^2)/3$
2θmax cutoff	55.1°
Anomalous Dispersion	All non-hydrogen atoms
No. Observations (All reflections)	3982
No. Variables	254
Reflection/Parameter Ratio	15.68
Residuals: R1 (I>2.00σ(I))	0.0454
Residuals: R (All reflections)	0.0621
Residuals: wR2 (All reflections)	0.1266
Goodness of Fit Indicator	1.054
Max Shift/Error in Final Cycle	0.000
Maximum peak in Final Diff. Map	0.27 e-/$Å^3$
Minimum peak in Final Diff. Map	-0.32 e-/$Å^3$

X-ray analysis of oxetene 5l



CCDC 948160 (**5l**) contains the supplementary crystallographic data for this paper. The data can be obtained free of charge from The Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/data_request/cif

Crystal Data

Empirical Formula	$C_{20}H_{13}F_6NO_6$
Formula Weight	477.32
Crystal Color, Habit	colorless, plate
Crystal Dimensions	0.260 x 0.090 x 0.060 mm
Crystal System	monoclinic
Lattice Type	C-centered
Lattice Parameters	a = 22.067(11) Å b = 6.117(3) Å c = 29.455(15) Å β = 92.449(6) ° V = 3972(3) $Å^3$
Space Group	C2/c (#15)
Z value	8
Dcalc	1.596 g/cm^3
F000	1936.00
μ(MoKα)	1.532 cm^{-1}

Intensity Measurements

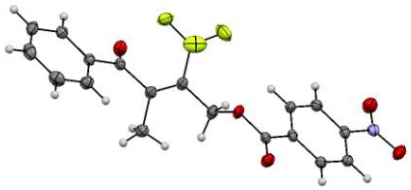
Diffractometer	XtaLAB mini
Radiation	MoKα (λ = 0.71075 Å) graphite monochromated
Voltage, Current	50kV, 12mA
Temperature	-180.0°C
Detector Aperture	75 mm (diameter)
Data Images	1440 exposures
ω oscillation Range	-60.0 - 120.0°
Exposure Rate	256.0 sec%

Detector Swing Angle	29.99°
ω oscillation Range	-60.0 - 120.0°
Exposure Rate	256.0 sec%
Detector Swing Angle	29.99°
Detector Position	49.91 mm
Pixel Size	0.146 mm
2θmax	55.0°
No. of Reflections Measured	Total: 13294
	Unique: 4538 (Rint = 0.0249)
Corrections	Lorentz-polarization
	Absorption
	(trans. factors: 0.903 - 0.991)

Structure Solution and Refinement

Structure Solution	Direct Methods
Refinement	Full-matrix least-squares on F^2
Function Minimized	$\Sigma\ w\ (Fo^2 - Fc^2)^2$
Least Squares Weights	$w = 1/\ [\ \sigma^2(Fo^2) + (0.0514\ .\ P)^2 + 4.4287\ .\ P\ ]$
	where $P = (Max(Fo^2,0) + 2Fc^2)/3$
2θmax cutoff	55.0°
Anomalous Dispersion	All non-hydrogen atoms
No. Observations (All reflections)	4538
No. Variables	299
Reflection/Parameter Ratio	15.18
Residuals: R1 (I>2.00σ(I))	0.0417
Residuals: R (All reflections)	0.0602
Residuals: wR2 (All reflections)	0.1140
Goodness of Fit Indicator	1.048
Max Shift/Error in Final Cycle	0.001
Maximum peak in Final Diff. Map	0.34 e-/$Å^3$
Minimum peak in Final Diff. Map	-0.29 e-/$Å^3$

X-ray analysis of olefin (Z)-6a



CCDC 948161 (**6a**) contains the supplementary crystallographic data for this paper. The data can be obtained free of charge from The Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/data_request/cif

Crystal Data

Empirical Formula	$C_{19}H_{14}F_3NO_5$
Formula Weight	393.32
Crystal Color, Habit	colorless, block
Crystal Dimensions	0.240 x 0.140 x 0.140 mm
Crystal System	triclinic
Lattice Type	Primitive
Lattice Parameters	a = 5.877(4) Å b = 11.649(8) Å c = 12.864(8) Å α = 87.422(12) ° β = 81.769(12) ° γ = 83.004(14) ° V = 864.8(10) $Å^3$
Space Group	P-1 (#2)
Z value	2
Dcalc	1.510 g/cm^3
F000	404.00
μ(MoKα)	1.302 cm^{-1}

Intensity Measurements

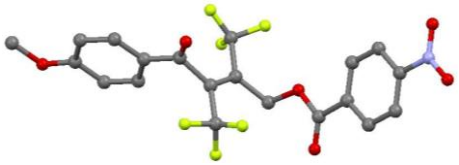
Diffractometer	XtaLAB mini
Radiation	MoKα (λ = 0.71075 Å) graphite monochromated
Voltage, Current	50kV, 12mA
Temperature	-180.0°C
Detector Aperture	75 mm (diameter)
Data Images	1080 exposures
ω oscillation Range	-72.0 - 108.0°
Exposure Rate	64.0 sec%
Detector Swing Angle	29.91°

ω oscillation Range	-72.0 - 108.0°
Exposure Rate	64.0 sec%
Detector Swing Angle	29.91°
ω oscillation Range	-72.0 - 108.0°
Exposure Rate	64.0 sec%
Detector Swing Angle	29.91°
Detector Position	49.97 mm
Pixel Size	0.146 mm
2θmax	54.9°
No. of Reflections Measured	Total: 9140
	Unique: 3934 (Rint = 0.0312)
Corrections	Lorentz-polarization
	Absorption
	(trans. factors: 0.877 - 0.982)

Structure Solution and Refinement

Structure Solution	Direct Methods
Refinement	Full-matrix least-squares on F^2
Function Minimized	$\Sigma\ w\ (Fo^2 - Fc^2)^2$
Least Squares Weights	$w = 1/ [\ \sigma^2(Fo^2) + (0.0543\ .\ P)^2 + 0.2995\ .\ P\ ]$
	where $P = (Max(Fo^2,0) + 2Fc^2)/3$
2θmax cutoff	54.9°
Anomalous Dispersion	All non-hydrogen atoms
No. Observations (All reflections)	3934
No. Variables	254
Reflection/Parameter Ratio	15.49
Residuals: R1 (I>2.00σ(I))	0.0401
Residuals: R (All reflections)	0.0466
Residuals: wR2 (All reflections)	0.1097
Goodness of Fit Indicator	1.047
Max Shift/Error in Final Cycle	0.001
Maximum peak in Final Diff. Map	0.40 e-/$Å^3$
Minimum peak in Final Diff. Map	-0.25 e-/$Å^3$

X-ray analysis of olefin (E)-6l



CCDC 948162 (**6l**) contains the supplementary crystallographic data for this paper. The data can be obtained free of charge from The Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/data_request/cif

Crystal Data

Empirical Formula	$C_{20}H_{13}F_6NO_6$
Formula Weight	477.32
Crystal Color, Habit	colorless, needle
Crystal Dimensions	0.260 x 0.090 x 0.090 mm
Crystal System	monoclinic
Lattice Type	Primitive
Lattice Parameters	a = 10.5731(7) Å b = 28.9962(19) Å c = 13.1962(9) Å β = 94.339(4) ° V = 4034.1(5) $Å^3$
Space Group	P21/c (#14)
Z value	8
Dcalc	1.572 g/cm^3
F000	1936.00
μ(MoKα)	1.508 cm^{-1}

Intensity Measurements

Diffractometer	XtaLAB mini
Radiation	MoKα (λ = 0.71075 Å) graphite monochromated
Voltage, Current	50kV, 12mA
Temperature	-180.0°C
Detector Aperture	75 mm (diameter)
Data Images	1440 exposures
ω oscillation Range	-72.0 - 108.0°
Exposure Rate	64.0 sec%
Detector Swing Angle	29.96°
ω oscillation Range	-72.0 - 108.0°
Exposure Rate	64.0 sec%

Detector Swing Angle	29.96°
Detector Position	49.88 mm
Pixel Size	0.146 mm
2θmax	55.0°
No. of Reflections Measured	Total: 28233
	Unique: 9229 (Rint = 0.0547)
Corrections	Lorentz-polarization
	Absorption
	(trans. factors: 0.875 - 0.987)

Structure Solution and Refinement

Structure Solution	Direct Methods
Refinement	Full-matrix least-squares on F^2
Function Minimized	Σ w $(Fo^2 - Fc^2)^2$
Least Squares Weights	$w = 1/ [\sigma^2(Fo^2) + (0.0437 . P)^2 + 2.9187 . P]$
	where $P = (Max(Fo^2,0) + 2Fc^2)/3$
2θmax cutoff	55.0°
Anomalous Dispersion	All non-hydrogen atoms
No. Observations (All reflections)	9229
No. Variables	635
Reflection/Parameter Ratio	14.53
Residuals: R1 (I>2.00σ(I))	0.0590
Residuals: R (All reflections)	0.0965
Residuals: wR2 (All reflections)	0.1363
Goodness of Fit Indicator	1.061
Max Shift/Error in Final Cycle	0.000
Maximum peak in Final Diff. Map	0.56 e-/$Å^3$
Minimum peak in Final Diff. Map	-0.56 e-/$Å^3$

Full citation of the Gaussian 09 program

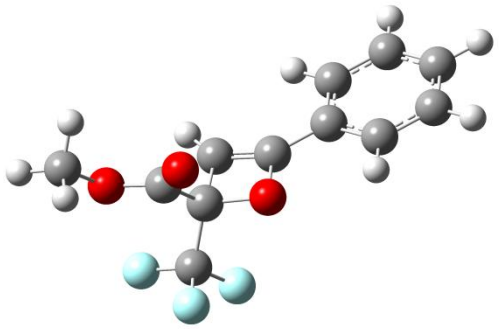
Gaussian 09, Revision A.02, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, O. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2009.

Computational Method

All the calculations were performed with Gaussian 09, Revision A.02 program package. All the structures were optimized with B3LYP/6-31G(d) level. Gibbs free energies contain zero-point, thermal entropy effects at 273.15 K and 1 atm pressure. Natural bond orbital (NBO) analysis was performed with Gaussian NBO Version 3.1.

Molecular Geometries and Energies

Cartesian coordinates of Oxetene A

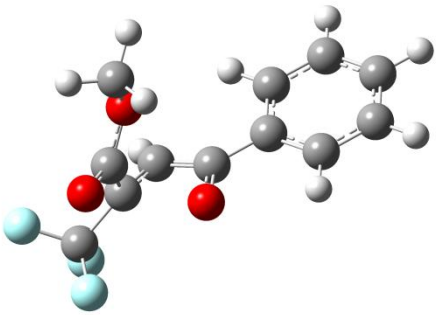


E(RB3LYP) = -987.836701969 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.999563	-1.053552	-0.364908
2	8	0	-1.836271	-1.772583	-1.317865
3	6	0	-1.809821	1.465277	0.036774
4	8	0	-2.985321	-1.176671	0.541651
5	6	0	-3.909465	-2.255422	0.301280
6	1	0	-4.637347	-2.198242	1.110248
7	1	0	-4.397226	-2.128795	-0.668269
8	1	0	-3.385507	-3.214396	0.317767
9	6	0	-1.084380	0.113209	0.022507
10	8	0	0.062256	0.192805	-0.876607
11	6	0	-0.123850	-0.152112	1.159543
12	6	0	0.864332	-0.060474	0.246129
13	1	0	-0.233868	-0.335915	2.215653
14	6	0	2.308635	-0.144286	0.135547
15	6	0	3.096946	-0.387268	1.272868
16	6	0	2.924263	0.018434	-1.115313
17	6	0	4.480911	-0.466245	1.157403
18	1	0	2.621051	-0.512100	2.241792
19	6	0	4.311226	-0.061200	-1.223035
20	1	0	2.309645	0.203670	-1.990196
21	6	0	5.091220	-0.303149	-0.090422
22	1	0	5.086306	-0.654264	2.039670
23	1	0	4.783805	0.065219	-2.193016
24	1	0	6.172486	-0.364901	-0.177618
25	9	0	-0.943826	2.483862	0.135417
26	9	0	-2.656996	1.539586	1.080596
27	9	0	-2.526664	1.633445	-1.094202

Rotational constants (GHZ): 0.8220669 0.2323528 0.2120007

Cartesian coordinates of TSEa

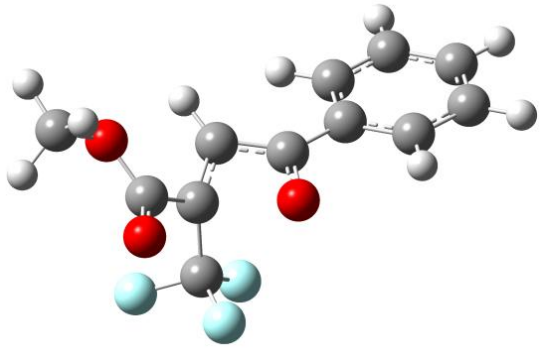


E(RB3LYP) = -987.791871356 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.665230	1.194009	0.065614
2	8	0	-2.579392	1.590353	0.752292
3	6	0	-2.630863	-1.147398	-0.031210
4	8	0	-0.833214	1.982159	-0.635616
5	6	0	-1.012306	3.392178	-0.414043
6	1	0	-0.291953	3.881290	-1.069747
7	1	0	-2.032766	3.691227	-0.665866
8	1	0	-0.812999	3.640601	0.631773
9	6	0	-1.373951	-0.282257	-0.160429
10	8	0	0.043783	-0.112601	1.171640
11	6	0	-0.230010	-0.788720	-0.860547
12	6	0	0.719535	-0.444952	0.083123
13	1	0	-0.207120	-1.393875	-1.754968
14	6	0	2.176842	-0.355743	0.042777
15	6	0	2.870368	-0.448103	-1.175862
16	6	0	2.894429	-0.173507	1.236364
17	6	0	4.259179	-0.363649	-1.198032
18	1	0	2.314722	-0.571535	-2.101184
19	6	0	4.283129	-0.074517	1.207758
20	1	0	2.349254	-0.114767	2.172966
21	6	0	4.966770	-0.173574	-0.006926
22	1	0	4.791398	-0.436169	-2.142295
23	1	0	4.834536	0.069897	2.132544
24	1	0	6.051103	-0.105048	-0.026474
25	9	0	-2.388815	-2.401167	-0.459541
26	9	0	-3.624349	-0.648626	-0.798624
27	9	0	-3.052718	-1.210597	1.234297

Rotational constants (GHZ): 0.7568282 0.2423495 0.2124470

Cartesian coordinates of TSZa

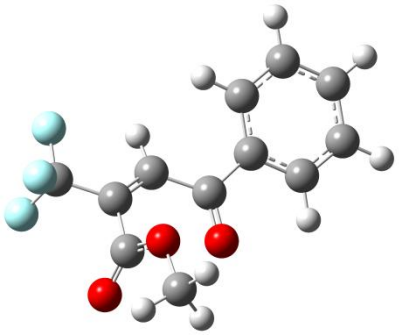


E(RB3LYP) = -987.793518014 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.559596	-0.640158	0.353230
2	8	0	3.311152	-0.173640	1.178024
3	6	0	1.456531	1.508452	-0.384842
4	8	0	2.727847	-1.822684	-0.264569
5	6	0	3.929492	-2.532718	0.092206
6	1	0	3.920967	-3.438312	-0.513800
7	1	0	4.810841	-1.925502	-0.129064
8	1	0	3.920261	-2.778005	1.157079
9	6	0	1.268568	0.015843	-0.079942
10	8	0	-0.213620	0.436543	1.133469
11	6	0	0.191889	-0.751240	-0.627898
12	6	0	-0.815352	-0.241100	0.179525
13	1	0	0.254703	-1.600633	-1.291259
14	6	0	-2.273796	-0.306912	0.100568
15	6	0	-2.911076	-0.820227	-1.041490
16	6	0	-3.047293	0.150271	1.180051
17	6	0	-4.300270	-0.879776	-1.099498
18	1	0	-2.313285	-1.156856	-1.883874
19	6	0	-4.437080	0.101894	1.112056
20	1	0	-2.542931	0.537353	2.059532
21	6	0	-5.064469	-0.416306	-0.024124
22	1	0	-4.789298	-1.277091	-1.984424
23	1	0	-5.032666	0.460183	1.946944
24	1	0	-6.149204	-0.460268	-0.072237
25	9	0	0.370684	2.079617	-0.923656
26	9	0	2.444947	1.575511	-1.321702
27	9	0	1.848495	2.232565	0.664987

Rotational constants (GHZ): 0.7964857 0.2322939 0.2076239

Cartesian coordinates of (E)-Enone via TSEa

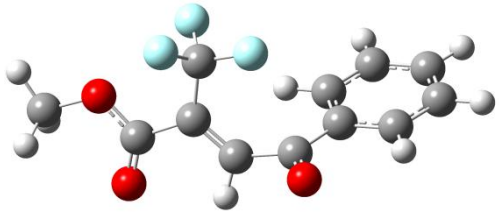


E(RB3LYP) = -987.875858298 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.004822	1.031813	-0.120344
2	8	0	2.747973	1.421455	-0.990537
3	6	0	2.446267	-1.462300	-0.032673
4	8	0	1.660363	1.716158	0.977950
5	6	0	2.115492	3.082252	1.011996
6	1	0	1.793691	3.470042	1.978346
7	1	0	3.203100	3.126486	0.917741
8	1	0	1.654139	3.644733	0.196519
9	6	0	1.417274	-0.358092	-0.110762
10	8	0	-0.617678	1.531672	-0.799865
11	6	0	0.114550	-0.641925	-0.232382
12	6	0	-0.933389	0.410064	-0.418235
13	1	0	-0.188473	-1.682930	-0.242497
14	6	0	-2.360708	0.054383	-0.162960
15	6	0	-3.346037	0.968262	-0.573756
16	6	0	-2.752339	-1.128755	0.483999
17	6	0	-4.692366	0.698367	-0.355588
18	1	0	-3.027608	1.882005	-1.064415
19	6	0	-4.102532	-1.393198	0.710593
20	1	0	-2.010659	-1.839808	0.833827
21	6	0	-5.073364	-0.484220	0.286912
22	1	0	-5.447506	1.407086	-0.683852
23	1	0	-4.395574	-2.307955	1.217821
24	1	0	-6.125521	-0.695018	0.458322
25	9	0	1.882737	-2.667806	0.196041
26	9	0	3.317892	-1.224183	0.971488
27	9	0	3.154164	-1.554550	-1.171194

Rotational constants (GHZ): 0.6988266 0.2346319 0.1924870

Cartesian coordinates of (Z)-Enone via TSZa

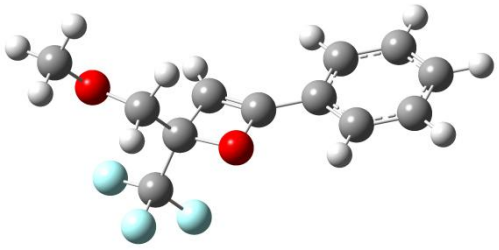


E(RB3LYP) = -987.876605118 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.560702	0.545716	-0.710604
2	8	0	2.767450	1.416920	-1.530146
3	6	0	1.124340	-0.716155	1.049129
4	8	0	3.459230	-0.389662	-0.363838
5	6	0	4.732508	-0.300981	-1.028231
6	1	0	5.323752	-1.124665	-0.629081
7	1	0	4.605247	-0.401999	-2.108952
8	1	0	5.207647	0.658852	-0.811136
9	6	0	1.258048	0.380731	0.019575
10	8	0	-1.264373	2.313020	1.073710
11	6	0	0.266709	1.222554	-0.302769
12	6	0	-1.106558	1.376964	0.305518
13	1	0	0.509892	1.973835	-1.053944
14	6	0	-2.219351	0.491610	-0.129400
15	6	0	-2.019888	-0.594570	-0.994221
16	6	0	-3.512363	0.778981	0.337127
17	6	0	-3.100267	-1.383628	-1.385630
18	1	0	-1.022439	-0.830245	-1.352246
19	6	0	-4.588152	-0.009633	-0.055591
20	1	0	-3.645564	1.624223	1.004523
21	6	0	-4.383283	-1.091512	-0.918634
22	1	0	-2.941176	-2.225828	-2.052934
23	1	0	-5.587155	0.215332	0.307221
24	1	0	-5.224713	-1.706687	-1.226141
25	9	0	-0.075168	-0.671326	1.670747
26	9	0	2.068458	-0.626356	2.003386
27	9	0	1.229087	-1.936263	0.477785

Rotational constants (GHZ): 0.8197549 0.2355801 0.2304155

Cartesian coordinates of Oxetene B

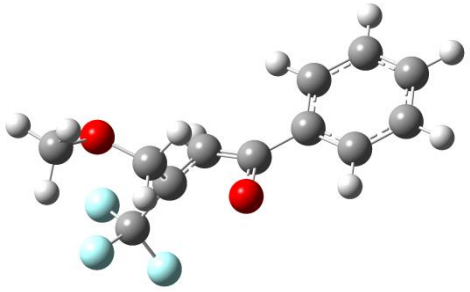


E(RB3LYP) = -913.801715206 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.049260	1.067168	-0.712219
2	6	0	1.930321	-1.326604	0.184204
3	8	0	3.024828	1.486901	0.214571
4	6	0	1.187708	-0.009015	-0.059345
5	8	0	0.019838	-0.271536	-0.920464
6	6	0	0.233056	0.411881	1.028547
7	6	0	-0.767584	0.145637	0.166367
8	1	0	0.345314	0.766368	2.040144
9	6	0	-2.216564	0.186096	0.070883
10	6	0	-2.990452	0.631517	1.155577
11	6	0	-2.852654	-0.223774	-1.111222
12	6	0	-4.377754	0.665474	1.056221
13	1	0	-2.500035	0.948842	2.071910
14	6	0	-4.242702	-0.186947	-1.204084
15	1	0	-2.250772	-0.569565	-1.945416
16	6	0	-5.007694	0.256693	-0.123614
17	1	0	-4.970566	1.010641	1.898768
18	1	0	-4.729538	-0.506408	-2.121379
19	1	0	-6.091336	0.283919	-0.198307
20	9	0	1.089455	-2.314859	0.532400
21	9	0	2.832835	-1.183708	1.172856
22	9	0	2.591986	-1.727221	-0.924780
23	6	0	3.882215	2.479254	-0.313457
24	1	0	3.325570	3.386247	-0.598345
25	1	0	4.599216	2.731528	0.471362
26	1	0	4.429125	2.114062	-1.196761
27	1	0	2.512612	0.665443	-1.627140
28	1	0	1.381656	1.893813	-0.999121

Rotational constants (GHZ): 0.9289476 0.2419384 0.2205638

Cartesian coordinates of TSEb

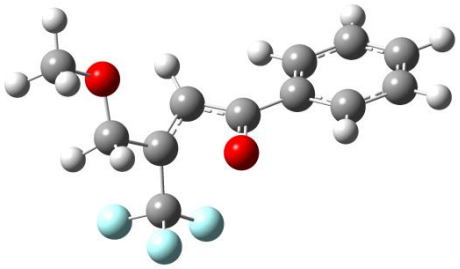


E(RB3LYP) = -913.755566548 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.646381	1.264296	-0.493962
2	6	0	2.371257	-1.126927	0.065099
3	8	0	2.561917	1.734695	0.488958
4	6	0	1.233619	-0.106626	0.006942
5	8	0	-0.280878	-0.152198	-1.285245
6	6	0	0.095511	-0.351231	0.845539
7	6	0	-0.886254	-0.194564	-0.116593
8	1	0	0.087724	-0.760703	1.845614
9	6	0	-2.339610	-0.036064	-0.013987
10	6	0	-2.958292	0.166532	1.230727
11	6	0	-3.125728	-0.086231	-1.176205
12	6	0	-4.340447	0.311217	1.310842
13	1	0	-2.349462	0.222844	2.128797
14	6	0	-4.506881	0.073499	-1.093991
15	1	0	-2.637001	-0.253094	-2.130736
16	6	0	-5.116193	0.267845	0.148362
17	1	0	-4.813831	0.467205	2.276236
18	1	0	-5.110785	0.037315	-1.996493
19	1	0	-6.194841	0.384030	0.212039
20	9	0	1.956163	-2.308074	-0.425581
21	9	0	2.746887	-1.319629	1.346500
22	9	0	3.462645	-0.762127	-0.639049
23	6	0	3.670895	2.442361	-0.040668
24	1	0	3.354108	3.347943	-0.579121
25	1	0	4.290915	2.734622	0.810425
26	1	0	4.263593	1.811741	-0.717891
27	1	0	0.780064	1.926496	-0.570650
28	1	0	2.124411	1.185448	-1.477390

Rotational constants (GHZ): 0.9823574 0.2246796 0.2108526

Cartesian coordinates of TSZb

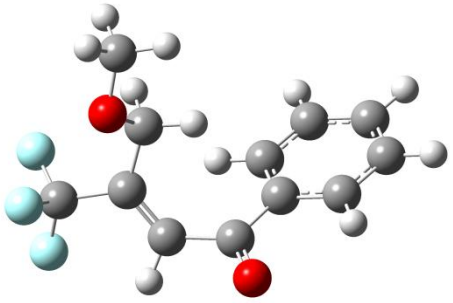


E(RB3LYP) = -913.759812494 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.747016	0.699625	-0.190983
2	6	0	1.690051	-1.547964	0.171957
3	8	0	2.591824	2.071724	0.058274
4	6	0	1.474293	-0.032707	0.130566
5	8	0	-0.010771	-0.293436	-1.172986
6	6	0	0.363964	0.583645	0.784245
7	6	0	-0.617731	0.206765	-0.120612
8	1	0	0.404192	1.365802	1.527909
9	6	0	-2.080571	0.264261	-0.047122
10	6	0	-2.730255	0.587058	1.155287
11	6	0	-2.843819	-0.009833	-1.192947
12	6	0	-4.120282	0.640915	1.208444
13	1	0	-2.140287	0.780095	2.046956
14	6	0	-4.234655	0.030646	-1.132852
15	1	0	-2.329326	-0.251824	-2.117332
16	6	0	-4.874327	0.359989	0.065073
17	1	0	-4.617787	0.891160	2.141376
18	1	0	-4.821533	-0.186804	-2.021050
19	1	0	-5.959582	0.398338	0.108567
20	9	0	0.606317	-2.277747	0.437023
21	9	0	2.579332	-1.791130	1.180479
22	9	0	2.259425	-2.004904	-0.961098
23	6	0	3.746017	2.815732	-0.282696
24	1	0	3.986286	2.721655	-1.353134
25	1	0	3.526126	3.861479	-0.056565
26	1	0	4.623683	2.497466	0.301833
27	1	0	2.973930	0.495739	-1.252922
28	1	0	3.582006	0.275831	0.394264

Rotational constants (GHZ): 0.7770374 0.2606836 0.2244596

Cartesian coordinates of (E)-Enone via TSEb

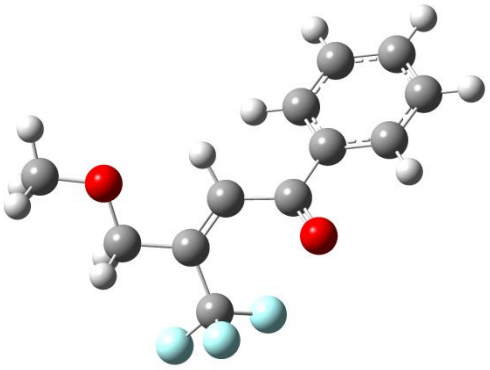


E(RB3LYP) = -913.832302909

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.937185	1.153805	-0.013236
2	6	0	2.624944	-0.704317	0.466771
3	8	0	1.911023	1.816076	-0.796309
4	6	0	1.238040	-0.326558	-0.010466
5	8	0	-1.133759	-1.585589	-2.134467
6	6	0	0.399212	-1.296128	-0.395558
7	6	0	-0.964763	-1.132611	-1.010926
8	1	0	0.745468	-2.326368	-0.379220
9	6	0	-2.080551	-0.496051	-0.249404
10	6	0	-1.994778	-0.220322	1.124241
11	6	0	-3.273172	-0.213303	-0.936227
12	6	0	-3.081450	0.337220	1.797408
13	1	0	-1.083979	-0.454758	1.666547
14	6	0	-4.351627	0.352505	-0.264897
15	1	0	-3.327094	-0.447090	-1.994535
16	6	0	-4.257521	0.628194	1.103594
17	1	0	-3.011184	0.541653	2.862056
18	1	0	-5.268490	0.576875	-0.802872
19	1	0	-5.102403	1.066285	1.628228
20	9	0	2.727986	-2.023468	0.748921
21	9	0	2.930430	-0.031334	1.602883
22	9	0	3.577533	-0.420160	-0.438143
23	6	0	1.748582	3.220339	-0.780883
24	1	0	2.543403	3.638074	-1.403064
25	1	0	0.772649	3.521388	-1.193964
26	1	0	1.836712	3.628188	0.238718
27	1	0	-0.072720	1.337642	-0.404578
28	1	0	0.961371	1.532231	1.023435

Rotational constants (GHZ): 0.7295835 0.2611358 0.2429374

Cartesian coordinates of (Z)-Enone via TSZb

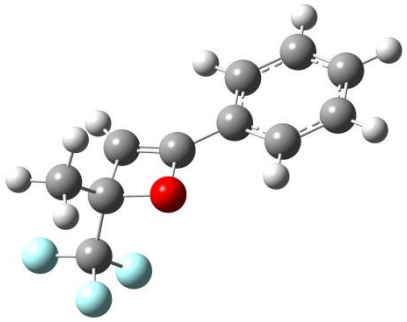


E(RB3LYP) = -913.834241586 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.739323	0.962037	0.062305
2	6	0	1.956657	-1.429061	0.381286
3	8	0	2.347753	2.214623	-0.443495
4	6	0	1.587960	-0.014173	-0.015447
5	8	0	-0.689158	-1.617882	-1.193789
6	6	0	0.369163	0.360011	-0.422053
7	6	0	-0.815091	-0.530302	-0.648131
8	1	0	0.240306	1.413153	-0.655741
9	6	0	-2.159483	-0.017308	-0.238819
10	6	0	-2.321257	1.142070	0.534608
11	6	0	-3.294055	-0.747273	-0.627881
12	6	0	-3.596179	1.565940	0.908796
13	1	0	-1.452516	1.706890	0.859537
14	6	0	-4.565379	-0.320157	-0.259399
15	1	0	-3.149418	-1.646398	-1.217954
16	6	0	-4.718627	0.838240	0.509497
17	1	0	-3.713092	2.461804	1.512295
18	1	0	-5.439163	-0.887693	-0.567702
19	1	0	-5.712006	1.170974	0.798769
20	9	0	0.962798	-2.090757	0.994031
21	9	0	3.004208	-1.404145	1.252234
22	9	0	2.358208	-2.153319	-0.680895
23	6	0	3.384200	3.175339	-0.383577
24	1	0	4.255785	2.867717	-0.981583
25	1	0	2.980620	4.104313	-0.792862
26	1	0	3.714842	3.351035	0.651961
27	1	0	3.083047	1.050601	1.106540
28	1	0	3.592521	0.555489	-0.510426

Rotational constants (GHZ): 0.6938318 0.2649977 0.2120400

Cartesian coordinates of Oxetene C

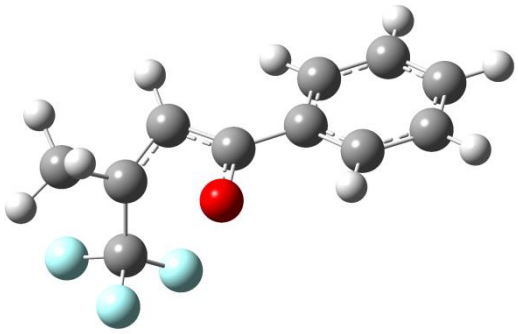


E(RB3LYP) = -799.292934232

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.324899	0.243226	1.944736
2	6	0	-2.575780	-0.134280	-0.541917
3	6	0	-1.620202	0.216705	0.600632
4	8	0	-0.508035	-0.759957	0.591698
5	6	0	-0.605021	1.289241	0.278553
6	6	0	0.331188	0.320506	0.290360
7	1	0	-0.649885	2.352617	0.104097
8	6	0	1.761348	0.135888	0.111002
9	6	0	2.592127	1.232594	-0.173201
10	6	0	2.321262	-1.146516	0.219336
11	6	0	3.960064	1.046549	-0.345597
12	1	0	2.160855	2.226407	-0.258503
13	6	0	3.692310	-1.326114	0.045141
14	1	0	1.674937	-1.990549	0.437426
15	6	0	4.513966	-0.233043	-0.236889
16	1	0	4.596993	1.898838	-0.565661
17	1	0	4.119793	-2.321437	0.129284
18	1	0	5.582578	-0.375581	-0.372432
19	9	0	-1.950741	-0.265025	-1.720790
20	9	0	-3.502394	0.846798	-0.668478
21	9	0	-3.236549	-1.286136	-0.298336
22	1	0	-2.812039	-0.716204	2.141448
23	1	0	-1.594698	0.445831	2.731467
24	1	0	-3.085282	1.030464	1.954782

Rotational constants (GHZ): 1.5831740 0.2951849 0.2906651

Cartesian coordinates of TSZc

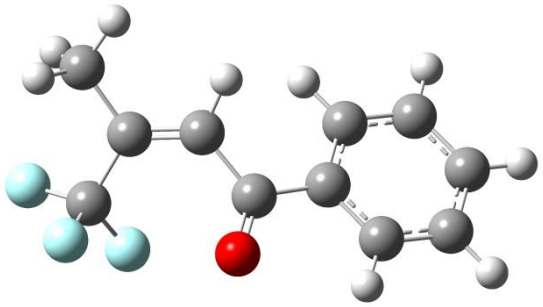


E(RB3LYP) = -799.251194826

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.860734	1.120185	1.445212
2	6	0	-2.397228	-0.379042	-0.537545
3	6	0	-1.835654	0.617393	0.476883
4	8	0	-0.420951	-0.713834	0.977147
5	6	0	-0.612235	1.319052	0.232115
6	6	0	0.270113	0.272799	0.458083
7	1	0	-0.476728	2.391411	0.187368
8	6	0	1.707553	0.139136	0.199403
9	6	0	2.398145	1.098927	-0.558106
10	6	0	2.403345	-0.965490	0.715113
11	6	0	3.763727	0.958884	-0.790013
12	1	0	1.856140	1.943100	-0.975361
13	6	0	3.766839	-1.109574	0.470508
14	1	0	1.858420	-1.697548	1.302398
15	6	0	4.449248	-0.146694	-0.277751
16	1	0	4.293087	1.703871	-1.377595
17	1	0	4.300632	-1.968307	0.868227
18	1	0	5.514557	-0.256946	-0.462343
19	9	0	-1.525230	-0.844367	-1.434783
20	9	0	-3.356837	0.296884	-1.235719
21	9	0	-3.009329	-1.419394	0.056347
22	1	0	-2.597228	0.714053	2.430714
23	1	0	-3.883953	0.818575	1.210371
24	1	0	-2.793471	2.210893	1.523017

Rotational constants (GHZ): 1.5056801 0.3052613 0.3001949

Cartesian coordinates of (Z)-Enone via TSZc

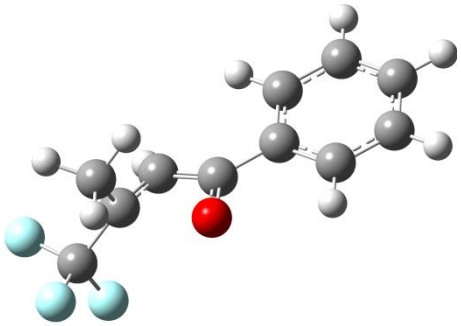


E(RB3LYP) = -799.322244163

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.777177	1.945027	-0.731622
2	6	0	2.566580	-0.328155	0.392869
3	6	0	1.883537	0.782884	-0.385503
4	8	0	0.001991	-1.562813	-0.815473
5	6	0	0.595111	0.733184	-0.754011
6	6	0	-0.358237	-0.414841	-0.596402
7	1	0	0.195940	1.600455	-1.277829
8	6	0	-1.775478	-0.100874	-0.234751
9	6	0	-2.177233	1.166787	0.212088
10	6	0	-2.726803	-1.129424	-0.326921
11	6	0	-3.508138	1.403517	0.555058
12	1	0	-1.448805	1.966158	0.311893
13	6	0	-4.055302	-0.890666	0.008880
14	1	0	-2.396639	-2.106536	-0.664238
15	6	0	-4.448611	0.377231	0.449575
16	1	0	-3.810072	2.386361	0.906144
17	1	0	-4.786905	-1.690136	-0.069729
18	1	0	-5.486380	0.563151	0.713325
19	9	0	1.750174	-0.973421	1.242164
20	9	0	3.576752	0.186053	1.141981
21	9	0	3.120724	-1.235314	-0.435742
22	1	0	3.134713	2.457800	0.167911
23	1	0	3.666618	1.596495	-1.271319
24	1	0	2.251137	2.664881	-1.363564

Rotational constants (GHZ): 1.4216234 0.3005958 0.2765938

Cartesian coordinates of TSEc

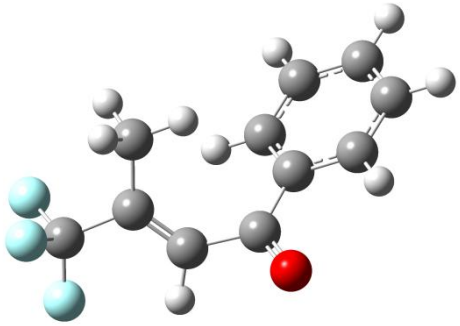


E(RB3LYP) = -799.244574049

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.911883	-0.729806	1.786472
2	6	0	-2.926935	0.170115	-0.353555
3	6	0	-1.657697	-0.039547	0.472672
4	8	0	-0.153889	-1.297412	-0.020146
5	6	0	-0.550102	0.835704	0.207097
6	6	0	0.434184	-0.126920	0.047510
7	1	0	-0.598800	1.869523	-0.108359
8	6	0	1.895842	-0.012361	-0.011053
9	6	0	2.540828	1.192930	0.311280
10	6	0	2.662297	-1.124693	-0.393337
11	6	0	3.928372	1.285177	0.246120
12	1	0	1.949429	2.048608	0.625327
13	6	0	4.051235	-1.033583	-0.443339
14	1	0	2.151196	-2.047416	-0.648693
15	6	0	4.685561	0.170999	-0.128315
16	1	0	4.421877	2.220387	0.495829
17	1	0	4.640464	-1.898201	-0.736319
18	1	0	5.768936	0.242943	-0.175401
19	9	0	-2.661439	0.389466	-1.647488
20	9	0	-3.567107	1.266002	0.130532
21	9	0	-3.774808	-0.871005	-0.272773
22	1	0	-2.365433	-1.714694	1.650796
23	1	0	-2.624650	-0.110601	2.352682
24	1	0	-0.991945	-0.819502	2.363554

Rotational constants (GHZ): 1.7001502 0.2663722 0.2579789

Cartesian coordinates of (E)-enone via TSEc

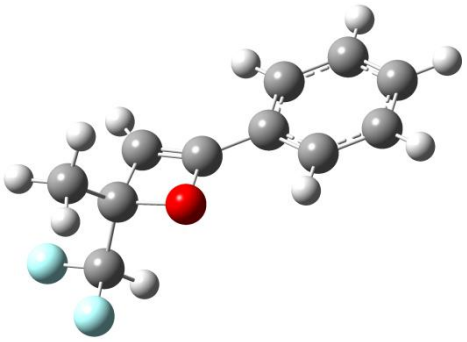


E(RB3LYP) = -799.325642594

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.004262	-0.707587	1.509245
2	6	0	2.900582	-0.241238	-0.095003
3	6	0	1.461034	0.027954	0.276571
4	8	0	-0.806513	2.589571	-0.058920
5	6	0	0.753508	0.895594	-0.459044
6	6	0	-0.642157	1.383544	-0.189364
7	1	0	1.245930	1.420203	-1.273229
8	6	0	-1.793461	0.432929	-0.136961
9	6	0	-1.696664	-0.892177	-0.588894
10	6	0	-3.027216	0.912172	0.333913
11	6	0	-2.814140	-1.725926	-0.562986
12	1	0	-0.751417	-1.263446	-0.972290
13	6	0	-4.137369	0.075106	0.370268
14	1	0	-3.088227	1.944169	0.663926
15	6	0	-4.032584	-1.245509	-0.079227
16	1	0	-2.734588	-2.748323	-0.921689
17	1	0	-5.086757	0.448667	0.743894
18	1	0	-4.901654	-1.897585	-0.055135
19	9	0	3.306689	0.415222	-1.198403
20	9	0	3.090184	-1.564809	-0.321971
21	9	0	3.737284	0.104599	0.911626
22	1	0	-0.025415	-0.463971	1.771550
23	1	0	1.081508	-1.791528	1.365823
24	1	0	1.650542	-0.449027	2.356131

Rotational constants (GHZ): 1.2703543 0.3029972 0.2716450

Cartesian coordinates of Oxetene D

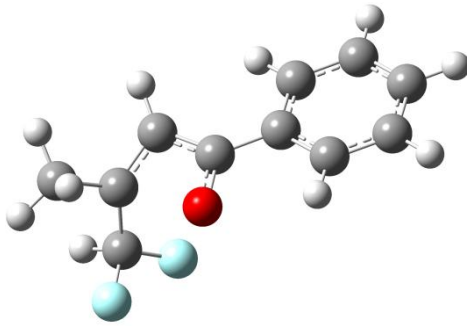


E(RB3LYP) = -700.044056036

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.573255	-0.033409	1.719957
2	6	0	-2.664820	-0.076206	-0.814709
3	6	0	-1.801425	0.118509	0.424753
4	8	0	-0.672637	-0.846716	0.339414
5	6	0	-0.780618	1.225129	0.288017
6	6	0	0.164806	0.266215	0.215572
7	1	0	-0.824405	2.302652	0.259147
8	6	0	1.603213	0.114680	0.062975
9	6	0	2.431826	1.242828	-0.057162
10	6	0	2.173163	-1.167650	0.033191
11	6	0	3.806675	1.088060	-0.204872
12	1	0	1.993241	2.236897	-0.034327
13	6	0	3.550939	-1.315999	-0.115874
14	1	0	1.528965	-2.035990	0.127042
15	6	0	4.370160	-0.191594	-0.234991
16	1	0	4.441540	1.965006	-0.296994
17	1	0	3.985902	-2.311436	-0.138549
18	1	0	5.444094	-0.309786	-0.350513
19	9	0	-3.554043	0.964823	-0.893567
20	9	0	-3.390489	-1.230407	-0.724406
21	1	0	-3.055482	-1.014097	1.761519
22	1	0	-1.897687	0.076335	2.571584
23	1	0	-3.348375	0.737702	1.778305
24	1	0	-2.069901	-0.106676	-1.731899

Rotational constants (GHZ): 1.9110646 0.3194416 0.3037720

Cartesian coordinates of TSZd1

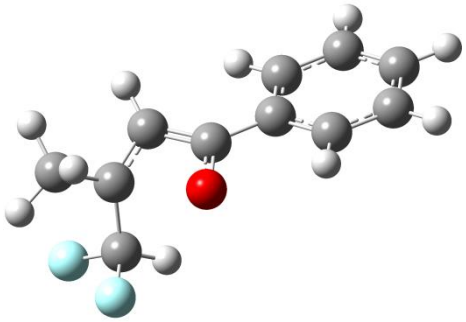


E(RB3LYP) = -699.998835147

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.161502	1.309661	-1.033222
2	6	0	2.650044	-0.376512	0.763951
3	6	0	2.102665	0.692350	-0.171670
4	8	0	0.738869	-0.587280	-0.899633
5	6	0	0.854216	1.352778	0.078943
6	6	0	0.006418	0.328756	-0.314522
7	1	0	0.694784	2.414074	0.217923
8	6	0	-1.443528	0.156315	-0.161534
9	6	0	-2.195958	1.029632	0.639929
10	6	0	-2.088786	-0.897531	-0.826913
11	6	0	-3.571561	0.856088	0.767421
12	1	0	-1.694349	1.833009	1.172444
13	6	0	-3.462910	-1.077274	-0.686676
14	1	0	-1.495945	-1.562932	-1.446233
15	6	0	-4.206715	-0.199140	0.105857
16	1	0	-4.148400	1.535310	1.389236
17	1	0	-3.956914	-1.897609	-1.200266
18	1	0	-5.279959	-0.336174	0.208869
19	9	0	1.718199	-0.991798	1.526330
20	9	0	3.343134	-1.322324	0.063337
21	1	0	2.995708	0.933709	-2.051696
22	1	0	4.184259	1.044002	-0.746742
23	1	0	3.042004	2.397643	-1.069640
24	1	0	3.363561	0.113562	1.446780

Rotational constants (GHZ): 1.6893068 0.3554556 0.3409730

Cartesian coordinates of TSZd2

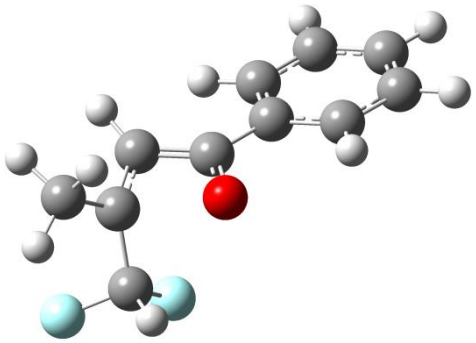


E(RB3LYP) = -700.005422426

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.047108	-0.497211	1.522278
2	6	0	2.455360	0.225989	-0.833494
3	6	0	1.983174	-0.368757	0.479472
4	8	0	0.557348	1.038994	0.527265
5	6	0	0.760682	-1.125283	0.519626
6	6	0	-0.131859	-0.075248	0.404814
7	1	0	0.641731	-2.157811	0.820011
8	6	0	-1.578815	-0.047095	0.158783
9	6	0	-2.276172	-1.211098	-0.203252
10	6	0	-2.277293	1.163811	0.285458
11	6	0	-3.649303	-1.165024	-0.428434
12	1	0	-1.734400	-2.145735	-0.320081
13	6	0	-3.648843	1.209594	0.046285
14	1	0	-1.728239	2.054982	0.572218
15	6	0	-4.337273	0.046065	-0.306480
16	1	0	-4.183168	-2.069069	-0.708230
17	1	0	-4.183966	2.150393	0.142203
18	1	0	-5.408573	0.081552	-0.485772
19	9	0	3.327400	-0.701932	-1.368109
20	9	0	3.174338	1.363858	-0.630570
21	1	0	2.870281	0.296417	2.260582
22	1	0	4.057180	-0.370858	1.124454
23	1	0	2.954319	-1.452386	2.048870
24	1	0	1.659816	0.408763	-1.554604

Rotational constants (GHZ): 1.7654505 0.3233206 0.3105707

Cartesian coordinates of TSZd3

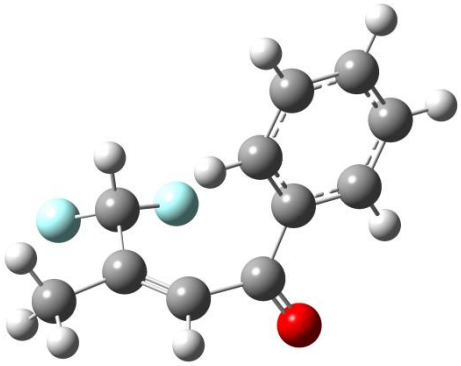


E(RB3LYP) = -700.001551522

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.122365	-1.683235	0.070243
2	6	0	-2.599811	0.762804	-0.356398
3	6	0	-2.092943	-0.596135	0.121171
4	8	0	-0.600638	-0.462520	-1.220670
5	6	0	-0.908512	-0.723207	0.918996
6	6	0	0.029187	-0.468829	-0.068316
7	1	0	-0.828459	-1.174672	1.898997
8	6	0	1.473570	-0.220209	0.006244
9	6	0	2.109614	-0.010021	1.240299
10	6	0	2.232571	-0.192308	-1.173983
11	6	0	3.482235	0.217182	1.292696
12	1	0	1.520116	-0.010064	2.152969
13	6	0	3.603419	0.048645	-1.119951
14	1	0	1.729546	-0.361402	-2.120634
15	6	0	4.230872	0.248975	0.112340
16	1	0	3.968441	0.379892	2.250708
17	1	0	4.185511	0.073364	-2.037197
18	1	0	5.301683	0.430135	0.153982
19	9	0	-1.712840	1.764561	-0.168254
20	9	0	-3.697726	1.042138	0.438067
21	1	0	-2.768068	-2.444770	-0.636158
22	1	0	-4.114722	-1.345470	-0.238551
23	1	0	-3.188722	-2.169819	1.050673
24	1	0	-2.932149	0.760702	-1.397780

Rotational constants (GHZ): 1.7447978 0.3403729 0.3362044

Cartesian coordinates of (Z)-enone via TSZd

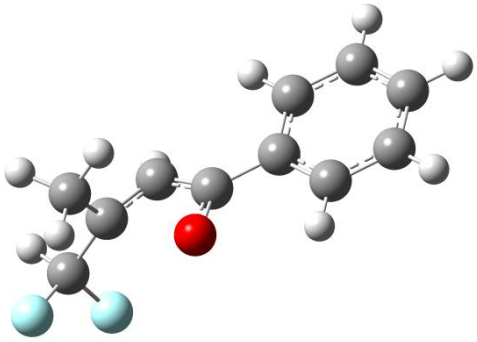


E(RB3LYP) = -700.070792170

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.386390	-0.094034	1.268111
2	6	0	1.841321	-0.902358	-0.580080
3	6	0	2.085095	0.094814	0.530003
4	8	0	-0.174761	2.555706	-0.315384
5	6	0	1.213150	1.063342	0.843106
6	6	0	-0.080862	1.436030	0.166289
7	1	0	1.495437	1.767623	1.624854
8	6	0	-1.244339	0.496040	0.182025
9	6	0	-1.270319	-0.654973	0.982233
10	6	0	-2.365371	0.815169	-0.599521
11	6	0	-2.395017	-1.479962	0.992648
12	1	0	-0.416933	-0.894128	1.610131
13	6	0	-3.482836	-0.013370	-0.596220
14	1	0	-2.333947	1.717031	-1.202175
15	6	0	-3.499765	-1.163120	0.200224
16	1	0	-2.410921	-2.366421	1.620945
17	1	0	-4.343762	0.234655	-1.211030
18	1	0	-4.374564	-1.808002	0.205421
19	9	0	0.979158	-0.413279	-1.519623
20	9	0	3.025453	-1.183754	-1.214398
21	1	0	3.480264	-1.118897	1.651311
22	1	0	4.240181	0.070323	0.601994
23	1	0	3.461930	0.595234	2.113042
24	1	0	1.434217	-1.855231	-0.218137

Rotational constants (GHZ): 1.1995505 0.4343734 0.3988123

Cartesian coordinates of TSEd1

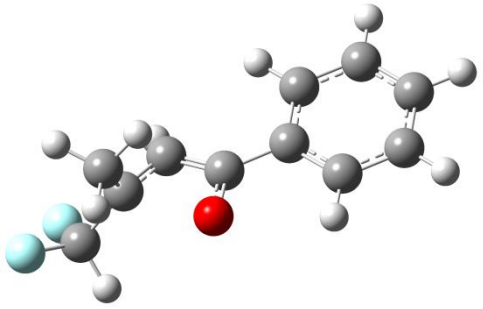


E(RB3LYP) = -699.994101432

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.240207	-0.590161	1.774246
2	6	0	-3.173071	0.487038	-0.324807
3	6	0	-1.941668	0.157854	0.501693
4	8	0	-0.505375	-1.164111	-0.050486
5	6	0	-0.775740	0.975923	0.297062
6	6	0	0.146225	-0.035036	0.074069
7	1	0	-0.756717	2.021592	0.016917
8	6	0	1.612892	0.000997	0.002462
9	6	0	2.330365	1.146526	0.383282
10	6	0	2.309869	-1.129191	-0.452842
11	6	0	3.720273	1.163203	0.303600
12	1	0	1.792712	2.014703	0.754579
13	6	0	3.701178	-1.114875	-0.518019
14	1	0	1.742899	-2.004893	-0.752066
15	6	0	4.407879	0.031268	-0.144527
16	1	0	4.269718	2.052860	0.599127
17	1	0	4.235971	-1.993630	-0.868059
18	1	0	5.493053	0.043841	-0.203076
19	9	0	-2.851286	0.659883	-1.633577
20	9	0	-4.115409	-0.496706	-0.241058
21	1	0	-2.753877	-1.533868	1.576160
22	1	0	-2.917315	0.029685	2.383701
23	1	0	-1.329907	-0.770276	2.345582
24	1	0	-3.621253	1.423000	0.045433

Rotational constants (GHZ): 1.9404852 0.3041846 0.3000929

Cartesian coordinates of TSEd2

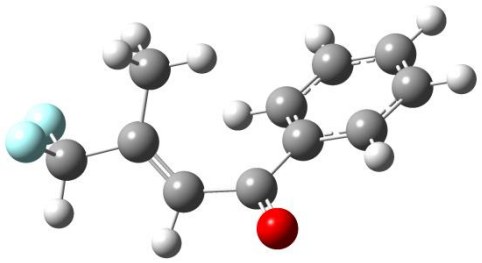


E(RB3LYP) = -699.996288239

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.209376	-1.006451	1.492002
2	6	0	-3.087607	0.156558	-0.607330
3	6	0	-1.913343	-0.110515	0.322575
4	8	0	-0.379647	-1.282298	-0.315013
5	6	0	-0.790089	0.787856	0.246878
6	6	0	0.199711	-0.138693	-0.034982
7	1	0	-0.829444	1.859145	0.108226
8	6	0	1.663392	-0.014412	-0.036714
9	6	0	2.295990	1.123845	0.488823
10	6	0	2.444010	-1.052324	-0.569237
11	6	0	3.684637	1.224529	0.475080
12	1	0	1.693827	1.919168	0.919534
13	6	0	3.833566	-0.955437	-0.568782
14	1	0	1.942504	-1.923629	-0.978121
15	6	0	4.455655	0.183724	-0.051319
16	1	0	4.168040	2.108102	0.882870
17	1	0	4.432994	-1.763682	-0.978937
18	1	0	5.539654	0.261625	-0.058143
19	9	0	-3.238894	1.503448	-0.787165
20	9	0	-4.266353	-0.331090	-0.115546
21	1	0	-2.667034	-1.951355	1.185375
22	1	0	-2.943146	-0.483748	2.124447
23	1	0	-1.310578	-1.197647	2.077737
24	1	0	-2.901687	-0.312897	-1.580454

Rotational constants (GHZ): 2.0227911 0.2981476 0.2819609

Cartesian coordinates of (E)-enone via TSEd

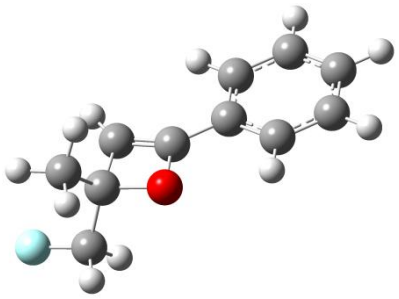


E(RB3LYP) = -700.074458904

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.328575	-0.685016	1.326101
2	6	0	3.152968	-0.104538	-0.334105
3	6	0	1.724722	0.094042	0.101157
4	8	0	-0.634495	2.618823	-0.263632
5	6	0	0.972615	0.956013	-0.600841
6	6	0	-0.428691	1.412357	-0.318240
7	1	0	1.438410	1.520646	-1.407958
8	6	0	-1.547244	0.432611	-0.163466
9	6	0	-1.441656	-0.903251	-0.580060
10	6	0	-2.764787	0.895663	0.362007
11	6	0	-2.533127	-1.763422	-0.464038
12	1	0	-0.510517	-1.262219	-1.007157
13	6	0	-3.848175	0.032549	0.489361
14	1	0	-2.835151	1.936256	0.661751
15	6	0	-3.734165	-1.298771	0.075455
16	1	0	-2.446936	-2.794289	-0.796098
17	1	0	-4.784123	0.394256	0.906177
18	1	0	-4.582515	-1.971390	0.170320
19	9	0	3.359850	-1.428686	-0.634623
20	9	0	4.010284	0.206412	0.689759
21	1	0	0.307744	-0.474864	1.644926
22	1	0	1.426713	-1.761237	1.142259
23	1	0	2.012378	-0.439267	2.146633
24	1	0	3.432547	0.492570	-1.208004

Rotational constants (GHZ): 1.3847496 0.3524175 0.3055156

Cartesian coordinates of Oxetene E

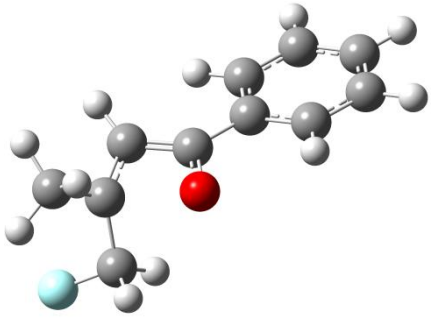


E(RB3LYP) = -600.799796801

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.877948	-0.595909	1.471650
2	6	0	-2.920597	-0.164142	-1.027279
3	6	0	-2.093200	-0.151065	0.252126
4	8	0	-0.907996	-1.024622	0.017217
5	6	0	-1.127481	1.004267	0.401827
6	6	0	-0.129652	0.128695	0.172544
7	1	0	-1.226733	2.060203	0.600055
8	6	0	1.319670	0.081218	0.056674
9	6	0	2.087808	1.247839	0.208696
10	6	0	1.963114	-1.137487	-0.209185
11	6	0	3.473616	1.193593	0.096091
12	1	0	1.593063	2.193355	0.414461
13	6	0	3.351592	-1.185359	-0.321866
14	1	0	1.366467	-2.036641	-0.324804
15	6	0	4.110020	-0.023008	-0.169821
16	1	0	4.060271	2.100463	0.215223
17	1	0	3.842593	-2.132545	-0.528236
18	1	0	5.192353	-0.062718	-0.257532
19	9	0	-3.956246	0.759398	-0.898133
20	1	0	-3.293048	-1.598722	1.317553
21	1	0	-2.237738	-0.608474	2.357461
22	1	0	-3.708387	0.097057	1.641585
23	1	0	-2.300559	0.114057	-1.884704
24	1	0	-3.359754	-1.155485	-1.194339

Rotational constants (GHZ): 2.3459093 0.3691468 0.3526140

Cartesian coordinates of TSZe1

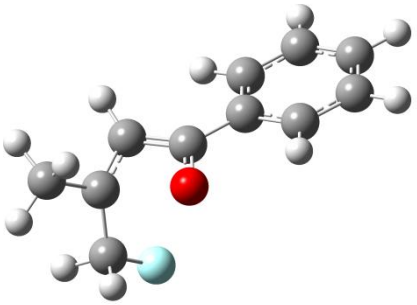


E(RB3LYP) = -600.762616916

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.323757	-0.101476	1.413240
2	6	0	-2.705880	-0.301169	-1.037766
3	6	0	-2.261043	0.054967	0.368465
4	8	0	-0.764333	-1.248826	0.139027
5	6	0	-1.081485	0.848590	0.615634
6	6	0	-0.132424	-0.102393	0.305732
7	1	0	-1.025884	1.788598	1.148718
8	6	0	1.321844	-0.010191	0.126121
9	6	0	1.969150	1.235119	0.074283
10	6	0	2.079590	-1.185005	0.001548
11	6	0	3.349672	1.302747	-0.092712
12	1	0	1.382781	2.146695	0.151142
13	6	0	3.459124	-1.114202	-0.179844
14	1	0	1.568965	-2.141417	0.050469
15	6	0	4.096899	0.128083	-0.222797
16	1	0	3.843885	2.269708	-0.131779
17	1	0	4.039559	-2.027428	-0.279768
18	1	0	5.174049	0.182292	-0.356907
19	9	0	-3.752272	0.581080	-1.349961
20	1	0	-3.147498	-1.066226	1.909518
21	1	0	-4.332560	-0.111022	0.990725
22	1	0	-3.240039	0.674122	2.180570
23	1	0	-3.100994	-1.320439	-1.089946
24	1	0	-1.907300	-0.164420	-1.766728

Rotational constants (GHZ): 2.1725472 0.3651951 0.3542887

Cartesian coordinates of TSZe2

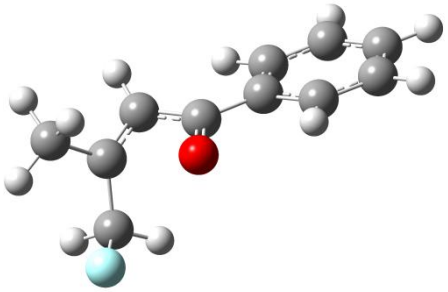


E(RB3LYP) = -600.758463378

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.487709	0.923437	-1.094981
2	6	0	2.936826	-0.680831	0.761005
3	6	0	2.426807	0.385579	-0.179258
4	8	0	0.956701	-0.829053	-0.860549
5	6	0	1.217786	1.130926	0.059074
6	6	0	0.301791	0.161371	-0.306045
7	1	0	1.130351	2.205526	0.157714
8	6	0	-1.159915	0.112452	-0.156702
9	6	0	-1.843315	1.066440	0.613791
10	6	0	-1.886307	-0.904512	-0.794556
11	6	0	-3.229120	1.008742	0.737255
12	1	0	-1.280155	1.841160	1.126882
13	6	0	-3.271351	-0.968541	-0.658806
14	1	0	-1.345833	-1.633450	-1.389829
15	6	0	-3.945463	-0.010403	0.102631
16	1	0	-3.751455	1.750378	1.335697
17	1	0	-3.827832	-1.761373	-1.151599
18	1	0	-5.026758	-0.057304	0.202661
19	9	0	1.990446	-1.172549	1.623178
20	1	0	3.195019	0.670640	-2.121737
21	1	0	4.489062	0.515966	-0.912985
22	1	0	3.516480	2.017514	-1.033323
23	1	0	3.731548	-0.204085	1.361882
24	1	0	3.389266	-1.507561	0.199979

Rotational constants (GHZ): 1.9061462 0.4146802 0.4074125

Cartesian coordinates of TSZe3

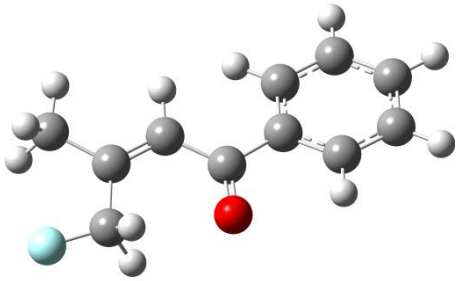


E(RB3LYP) = -600.760876575

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.339045	0.838063	-1.135012
2	6	0	2.727077	-0.201595	1.102648
3	6	0	2.272369	0.525834	-0.134499
4	8	0	0.872213	-0.907967	-0.527988
5	6	0	1.017109	1.233664	-0.107937
6	6	0	0.159429	0.152796	-0.244968
7	1	0	0.868792	2.291049	-0.287816
8	6	0	-1.302823	0.066803	-0.103452
9	6	0	-2.048608	1.138442	0.412735
10	6	0	-1.964359	-1.109203	-0.488844
11	6	0	-3.432224	1.037948	0.534368
12	1	0	-1.536190	2.042458	0.730623
13	6	0	-3.347077	-1.212753	-0.353545
14	1	0	-1.376164	-1.927912	-0.890897
15	6	0	-4.083526	-0.139101	0.153591
16	1	0	-4.003217	1.871428	0.934595
17	1	0	-3.853151	-2.127585	-0.650043
18	1	0	-5.162992	-0.218284	0.252362
19	9	0	3.568649	-1.260180	0.798924
20	1	0	3.115547	0.251332	-2.035580
21	1	0	4.344432	0.568503	-0.799961
22	1	0	3.291905	1.893876	-1.426684
23	1	0	3.311822	0.524791	1.693243
24	1	0	1.885197	-0.549687	1.703242

Rotational constants (GHZ): 2.1586388 0.3783491 0.3550527

Cartesian coordinates of (Z)-enone via TSZe

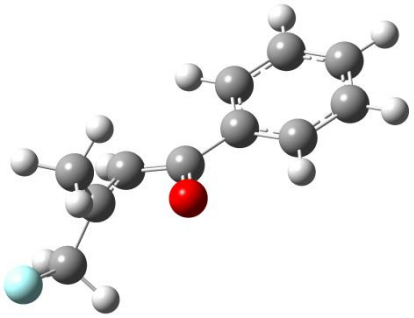


E(RB3LYP) = -600.839757271

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.289315	1.683460	0.244563
2	6	0	-3.012279	-0.828482	-0.112815
3	6	0	-2.354125	0.515658	0.095362
4	8	0	-0.424721	-1.597019	-0.025389
5	6	0	-1.013244	0.681028	0.156669
6	6	0	-0.045809	-0.423462	0.037720
7	1	0	-0.633448	1.683415	0.325675
8	6	0	1.424077	-0.116324	0.009701
9	6	0	1.946633	1.171732	-0.186477
10	6	0	2.313873	-1.191512	0.168102
11	6	0	3.325770	1.378505	-0.217768
12	1	0	1.285794	2.018869	-0.338381
13	6	0	3.689209	-0.983797	0.146352
14	1	0	1.897188	-2.183547	0.306923
15	6	0	4.199236	0.303587	-0.046356
16	1	0	3.717335	2.379392	-0.377705
17	1	0	4.366298	-1.823588	0.277369
18	1	0	5.273481	0.467259	-0.065688
19	9	0	-4.391501	-0.667924	-0.252687
20	1	0	-3.918252	1.791129	-0.646695
21	1	0	-3.979229	1.522874	1.081822
22	1	0	-2.741393	2.614729	0.409213
23	1	0	-2.625947	-1.333057	-1.003834
24	1	0	-2.824700	-1.492374	0.738283

Rotational constants (GHZ): 2.3315122 0.3467480 0.3047619

Cartesian coordinates of TSEe1

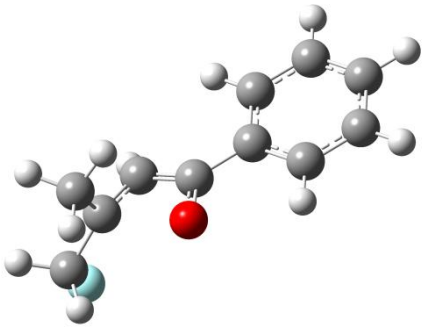


E(RB3LYP) = -600.760998082

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.621788	-0.292029	1.506283
2	6	0	-3.276837	0.306797	-0.881009
3	6	0	-2.204221	0.223461	0.159332
4	8	0	-0.719886	-1.170842	-0.036133
5	6	0	-1.004636	0.994610	-0.085101
6	6	0	-0.076753	-0.031452	-0.065498
7	1	0	-0.956108	1.999382	-0.486422
8	6	0	1.394379	0.008211	-0.052999
9	6	0	2.089138	1.213997	0.132384
10	6	0	2.117148	-1.181765	-0.227643
11	6	0	3.481615	1.229932	0.135074
12	1	0	1.532004	2.133755	0.288788
13	6	0	3.510142	-1.165764	-0.211346
14	1	0	1.567604	-2.106116	-0.374198
15	6	0	4.194633	0.039373	-0.034561
16	1	0	4.012660	2.167051	0.279055
17	1	0	4.063920	-2.091449	-0.343416
18	1	0	5.281405	0.052021	-0.028478
19	9	0	-4.532347	-0.071836	-0.428231
20	1	0	-3.142049	-1.250797	1.429890
21	1	0	-3.341089	0.429048	1.923828
22	1	0	-1.769896	-0.374721	2.180815
23	1	0	-2.987078	-0.352692	-1.709958
24	1	0	-3.328083	1.335567	-1.266263

Rotational constants (GHZ): 2.6671848 0.3407110 0.3245652

Cartesian coordinates of TSEe2

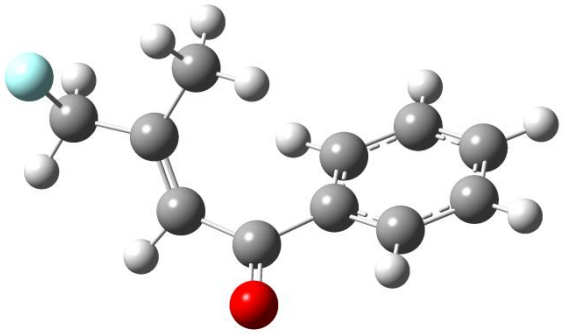


E(RB3LYP) = -600.757839631

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.578979	-1.216293	1.412609
2	6	0	-3.511597	0.221737	-0.425117
3	6	0	-2.299500	-0.151265	0.379276
4	8	0	-0.783134	-1.227339	-0.426937
5	6	0	-1.169060	0.741062	0.446658
6	6	0	-0.195160	-0.136340	0.005568
7	1	0	-1.203114	1.822049	0.438950
8	6	0	1.269918	-0.013218	-0.010444
9	6	0	1.917792	1.038369	0.657377
10	6	0	2.036073	-0.963983	-0.702104
11	6	0	3.306112	1.140853	0.627380
12	1	0	1.326929	1.763991	1.209709
13	6	0	3.425852	-0.867900	-0.718567
14	1	0	1.522498	-1.767572	-1.220135
15	6	0	4.062882	0.185922	-0.058339
16	1	0	3.800674	1.958033	1.145629
17	1	0	4.013718	-1.609492	-1.252907
18	1	0	5.146764	0.264301	-0.077972
19	9	0	-3.311034	1.350412	-1.192432
20	1	0	-3.077667	-2.090170	0.978191
21	1	0	-3.255237	-0.789736	2.169697
22	1	0	-1.663549	-1.535463	1.909823
23	1	0	-4.369817	0.399312	0.240874
24	1	0	-3.762819	-0.623907	-1.080264

Rotational constants (GHZ): 1.9766378 0.3806392 0.3643503

Cartesian coordinates of (E)-enone via TSEe

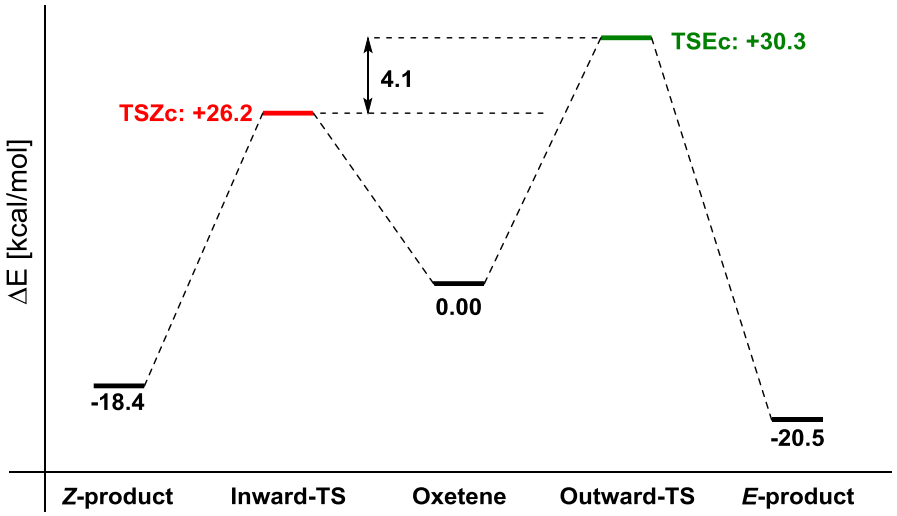


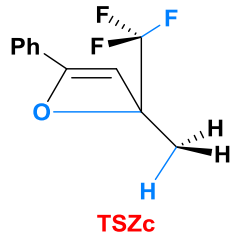
E(RB3LYP) = -600.830463791

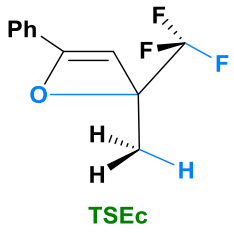
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.561544	-1.036356	1.083106
2	6	0	3.396410	-0.421494	-0.555340
3	6	0	2.005069	-0.141082	-0.043220
4	8	0	-0.205720	2.571154	-0.062806
5	6	0	1.302536	0.865076	-0.593569
6	6	0	-0.061152	1.365258	-0.230095
7	1	0	1.799543	1.514512	-1.312931
8	6	0	-1.233971	0.439498	-0.129639
9	6	0	-1.241647	-0.833018	-0.719996
10	6	0	-2.390063	0.901750	0.519755
11	6	0	-2.382149	-1.632935	-0.654162
12	1	0	-0.359351	-1.186442	-1.244444
13	6	0	-3.521961	0.096452	0.598828
14	1	0	-2.375587	1.896770	0.952652
15	6	0	-3.520385	-1.172473	0.010480
16	1	0	-2.383612	-2.613231	-1.122889
17	1	0	-4.408956	0.456227	1.113133
18	1	0	-4.406916	-1.798635	0.066838
19	9	0	4.303035	-0.506315	0.502647
20	1	0	0.592139	-0.754530	1.494516
21	1	0	1.506979	-2.083368	0.754389
22	1	0	2.310171	-0.997705	1.881905
23	1	0	3.738333	0.358870	-1.243480
24	1	0	3.420319	-1.388933	-1.077956

Rotational constants (GHZ): 1.6088581 0.4176665 0.3611451

Energy Diagram of CF_3-Oxetene (C) Ring Opening

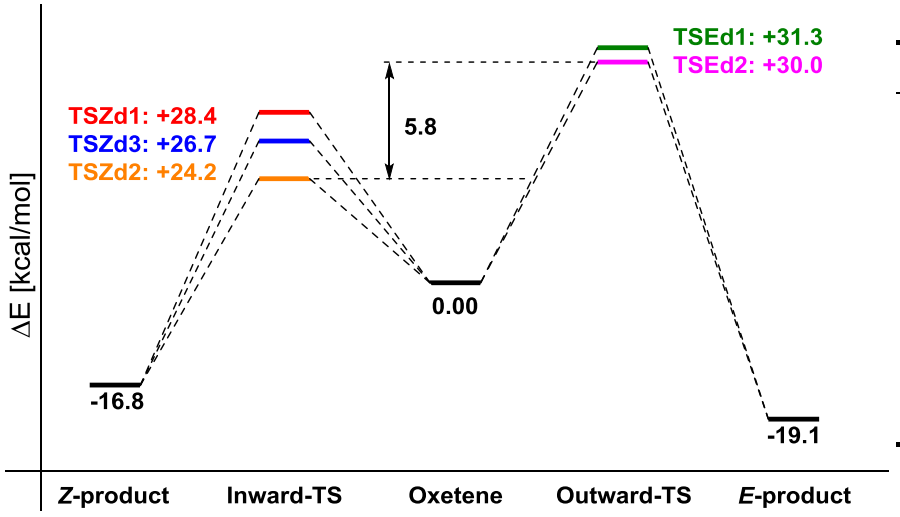


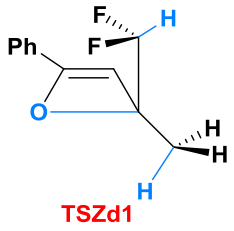


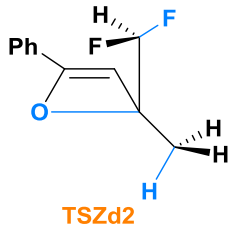


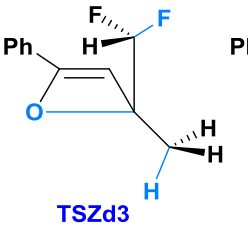
State	ΔE [kcal/mol]
Oxetene	0.00
TSZc	**+26.2**
Z-product	-18.4
TSEc	**+30.3**
E-product	-20.5

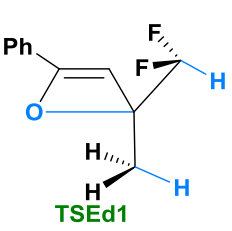
Energy Diagram of CF_2H-Oxetene (D) Ring Opening

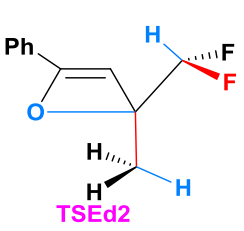






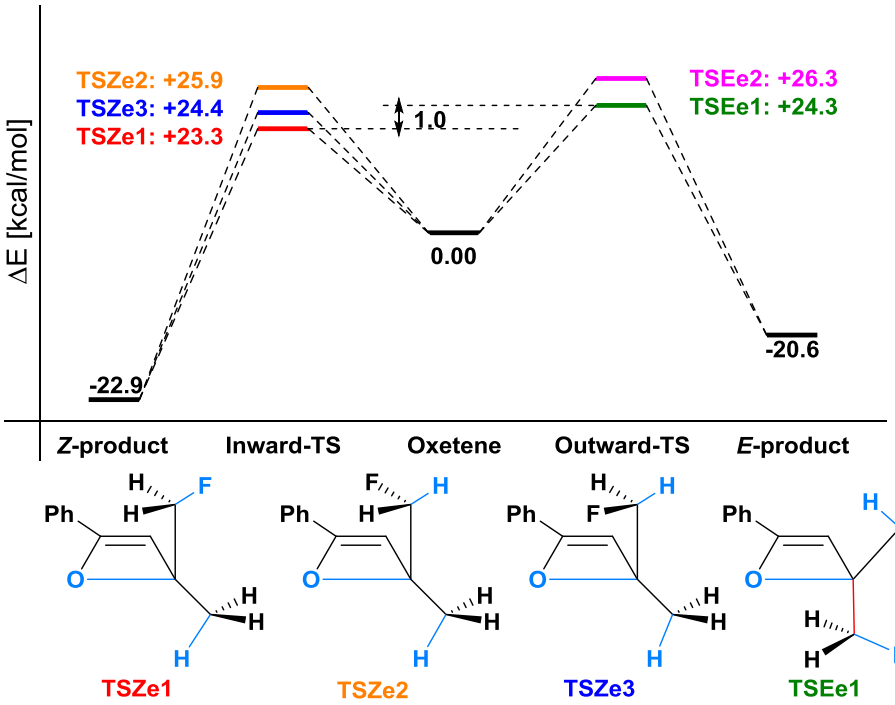






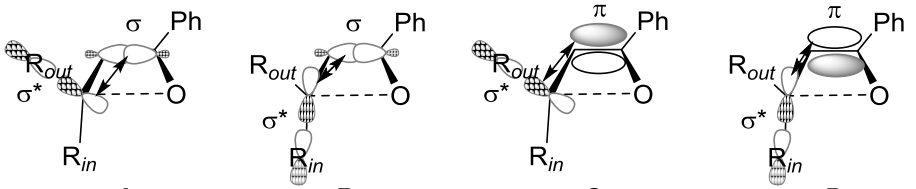
State	ΔE [kcal/mol]
Oxetene	0.00
TSZd1	+28.4
TSZd2	**+24.2**
TSZd3	+26.7
Z-product	-16.8
TSEd1	+31.3
TSEd2	**+30.0**
E-product	-19.1

Energy Diagram of CFH_2-Oxetene (E) Ring Opening

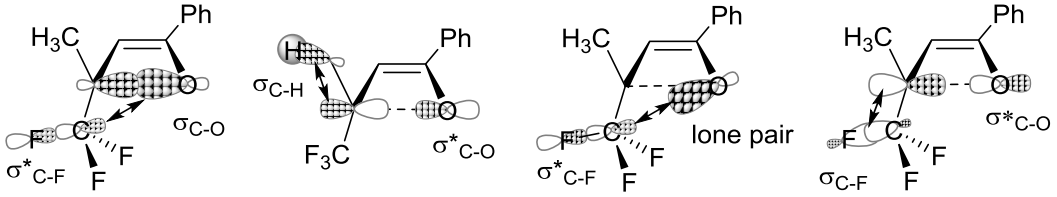


State	ΔE [kcal/mol]
Oxetene	0.00
TSZe1	**+23.3**
TSZe2	+25.9
TSZe3	+24.4
Z-product	-25.1
TSEe1	**+24.3**
TSEe2	+26.3
E-product	-19.2

Secondary interactions (**A**-**D** and **I**-**IV**) between NBOs of **TSZc** and **TSEc**, and these interaction energies in kcal/mol



	R_{in}	R_{out}	**A**	**B**	**C**	**D**
TSZc	CF_3	Me	-4.56	-0.18	-3.24	-7.24
TSEc	Me	CF_3	-3.80	-0.44	-4.22	-5.37

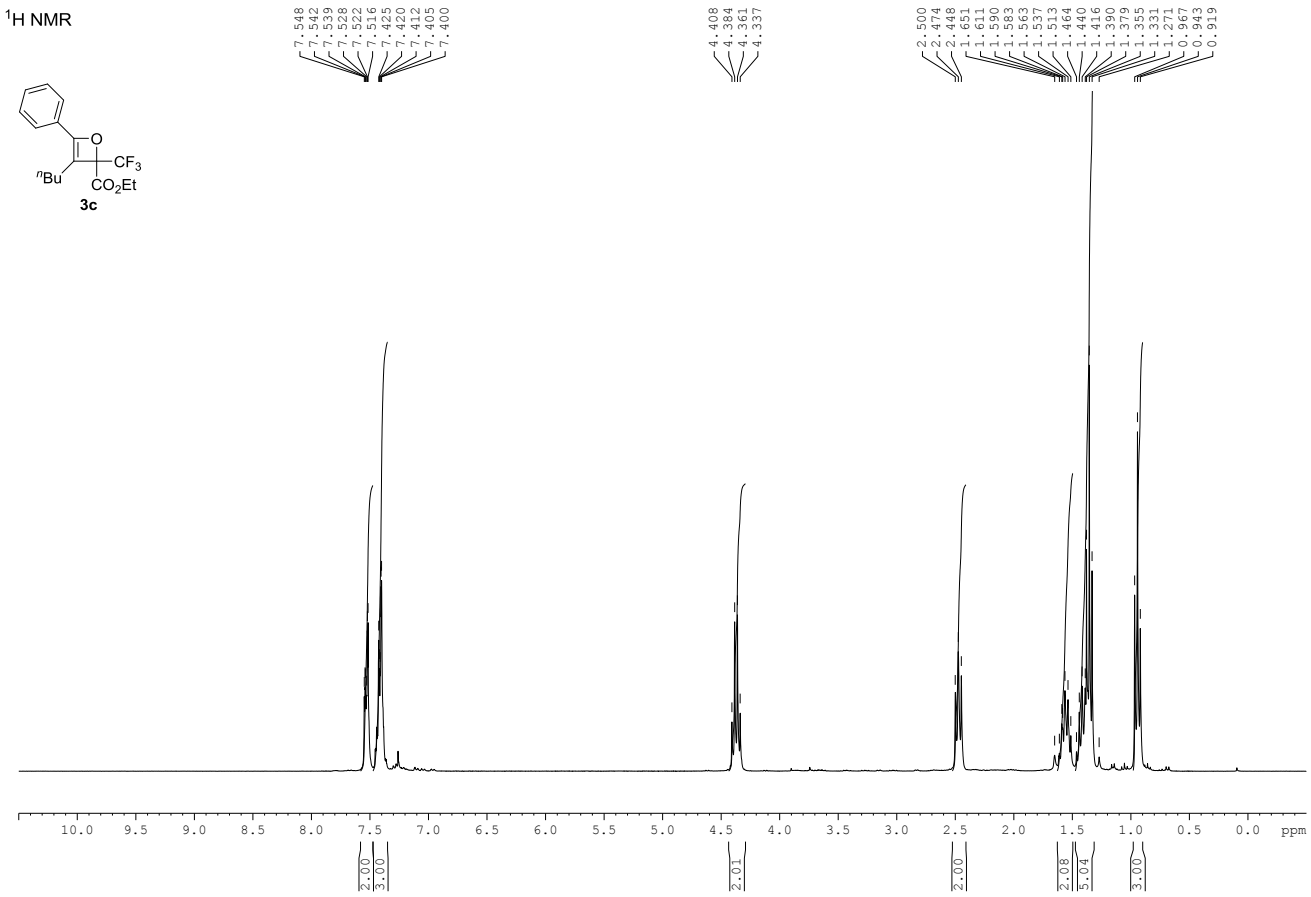


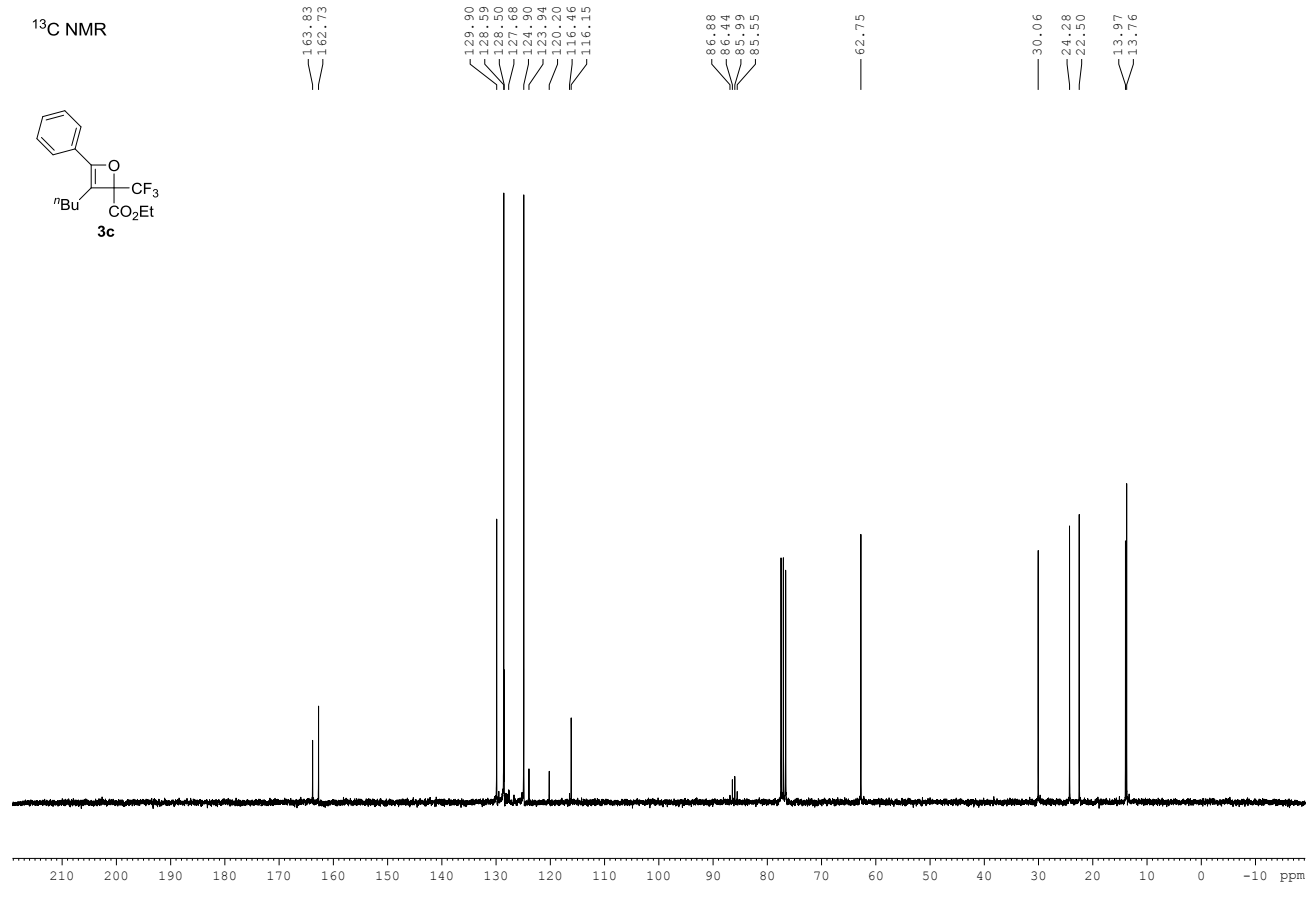
	I	**II**	**III**	**IV**
TSZc	-8.18	-6.10	-0.49	-1.94
TSEc	-2.56	-6.39	<-0.1	-2.66

References

[1] Aikawa, K.; Hioki, Y.; Shimizu, N.; Mikami, K. *J. Am. Chem. Soc.* **2011**, *133*, 20092.

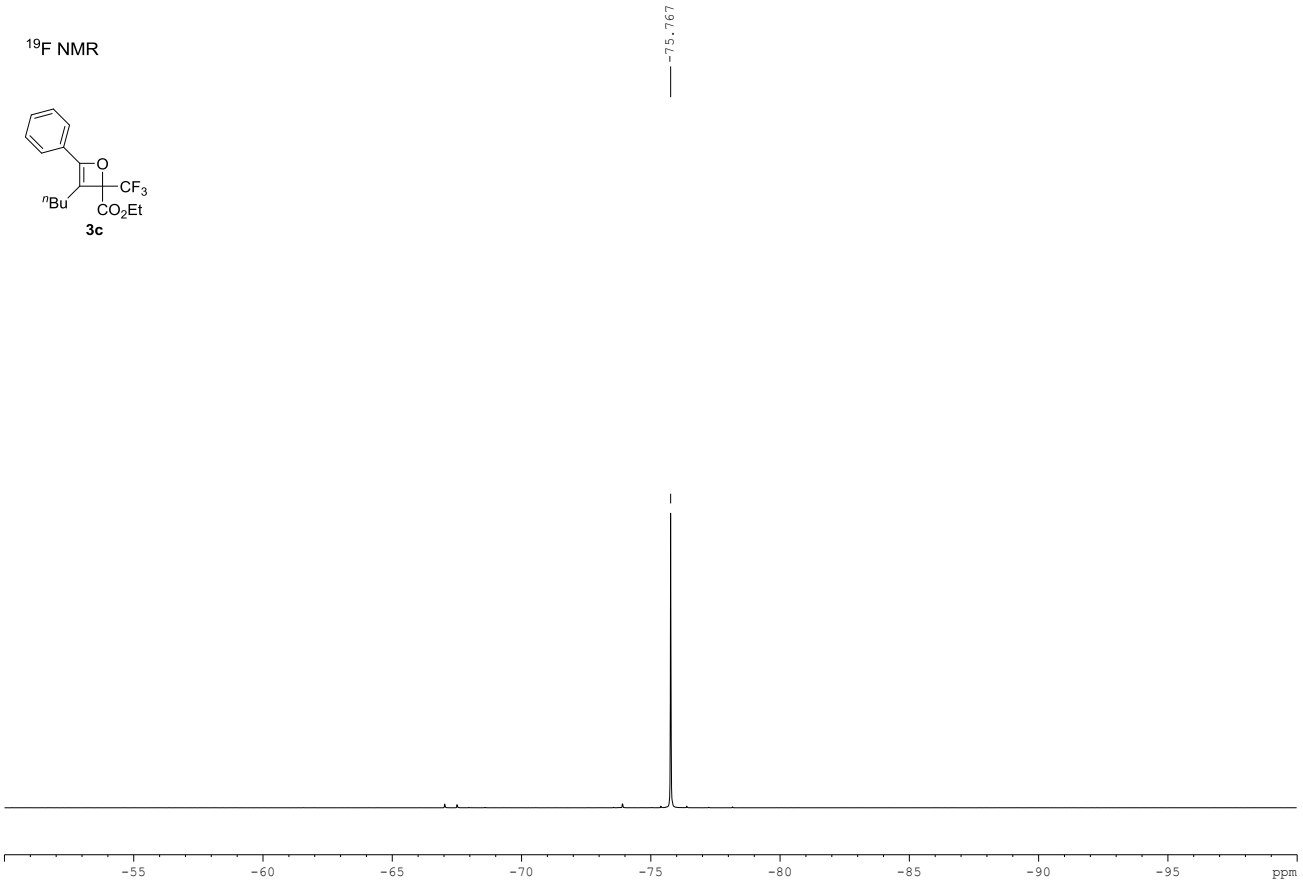
[2] Paleček, J.; Kvíčala, J.; Paleta, O. *J. Fluorine Chem.* **2002**, *113*, 177, and references therein.


1H NMR
7.548
7.542
7.539
7.528
7.522
7.516
7.425
7.420
7.412
7.405
7.400
4.408
4.384
4.361
4.337
2.500
2.474
2.448
1.651
1.611
1.590
1.583
1.563
1.537
1.513
1.464
1.440
1.416
1.390
1.379
1.355
1.331
1.271
0.967
0.943
0.919
O
CF3
nBu
CO2Et
3c
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 ppm
2.00
3.00
2.01
2.00
2.08
5.04
3.00


13C NMR
163.83
162.73
129.90
128.59
128.50
127.68
124.90
123.94
120.20
116.46
116.15
86.88
86.44
85.99
85.55
62.75
30.06
24.28
22.50
13.97
13.76
O
CF3
nBu
CO2Et
3c
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 ppm

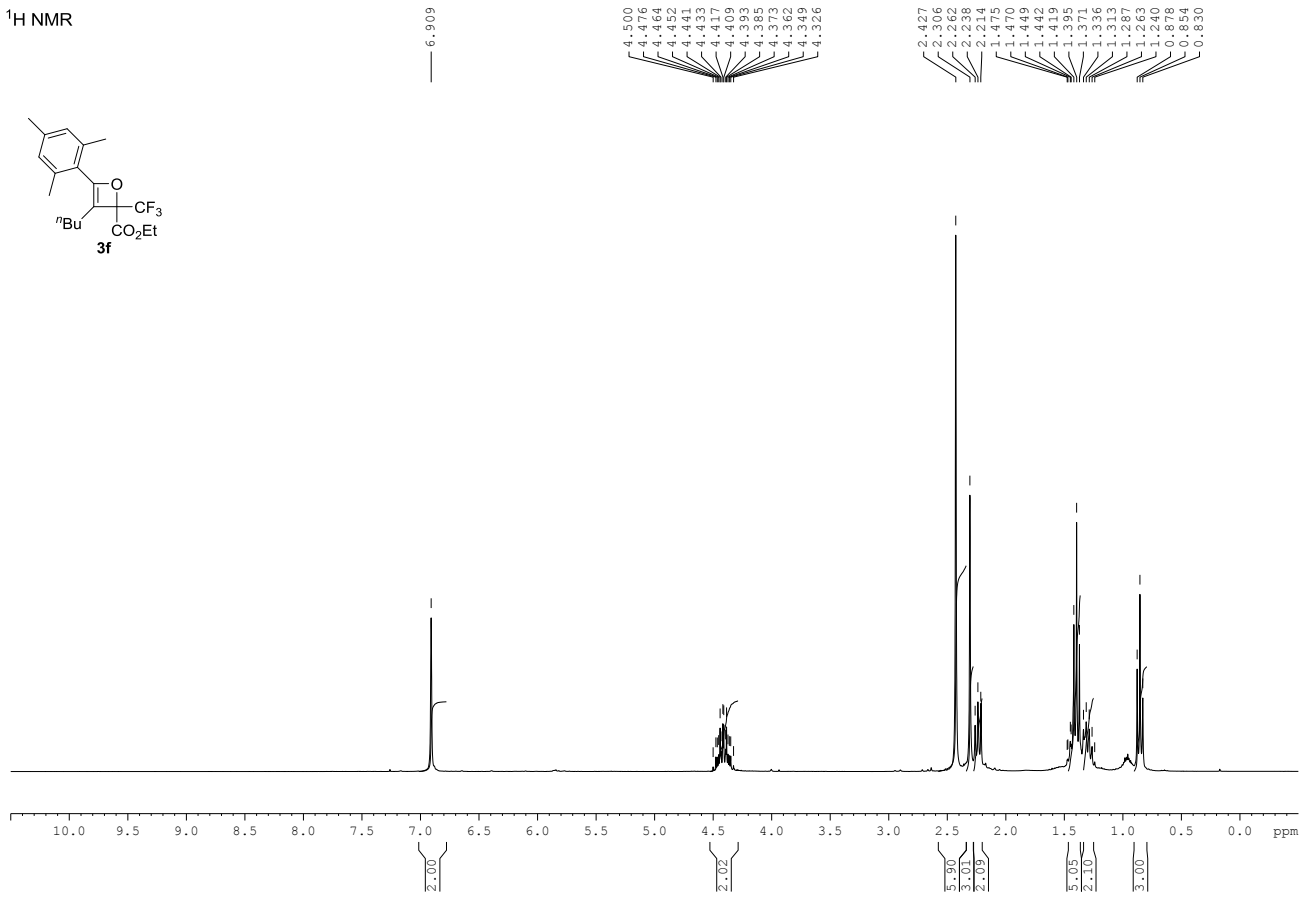
^{19}F NMR

3c



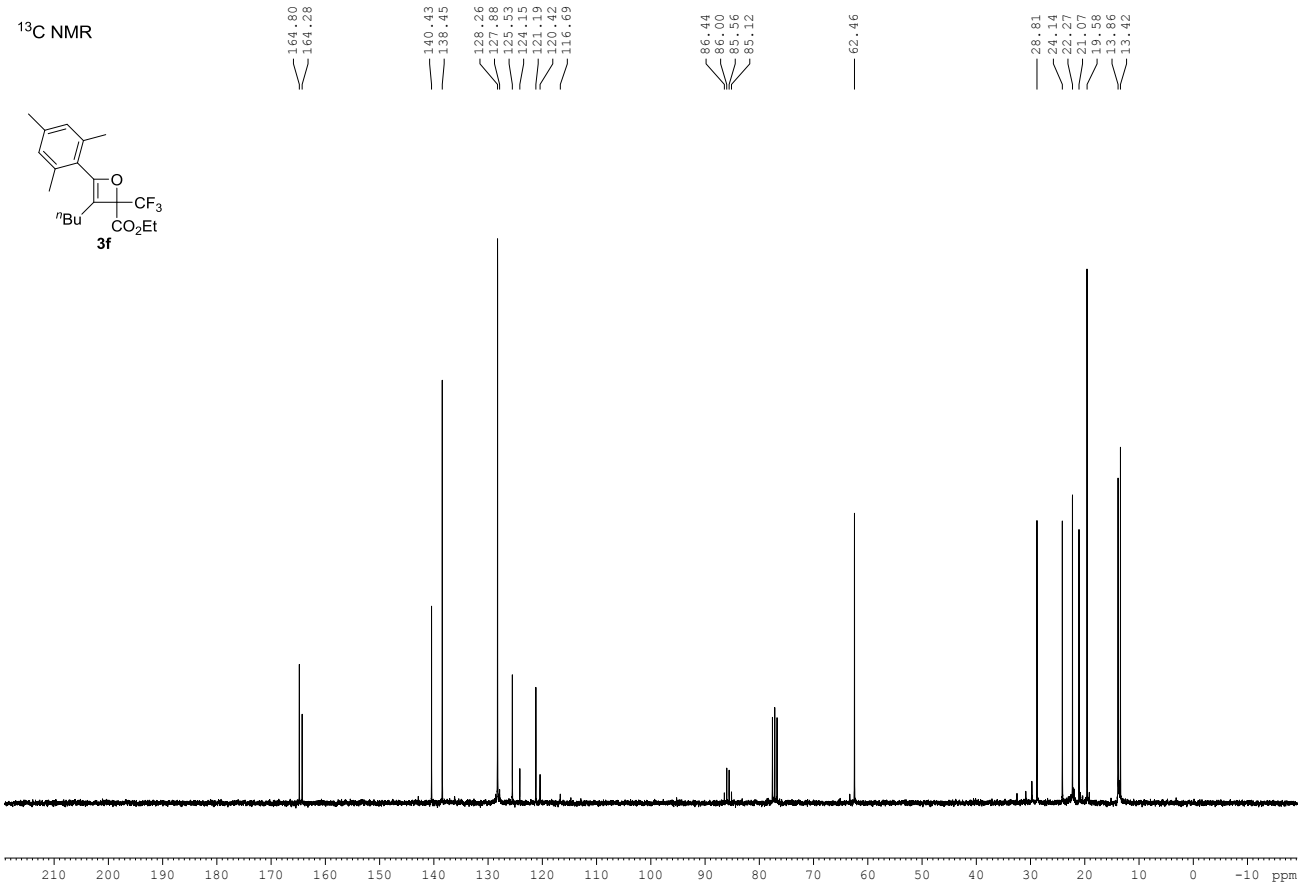
^{1}H NMR

3f



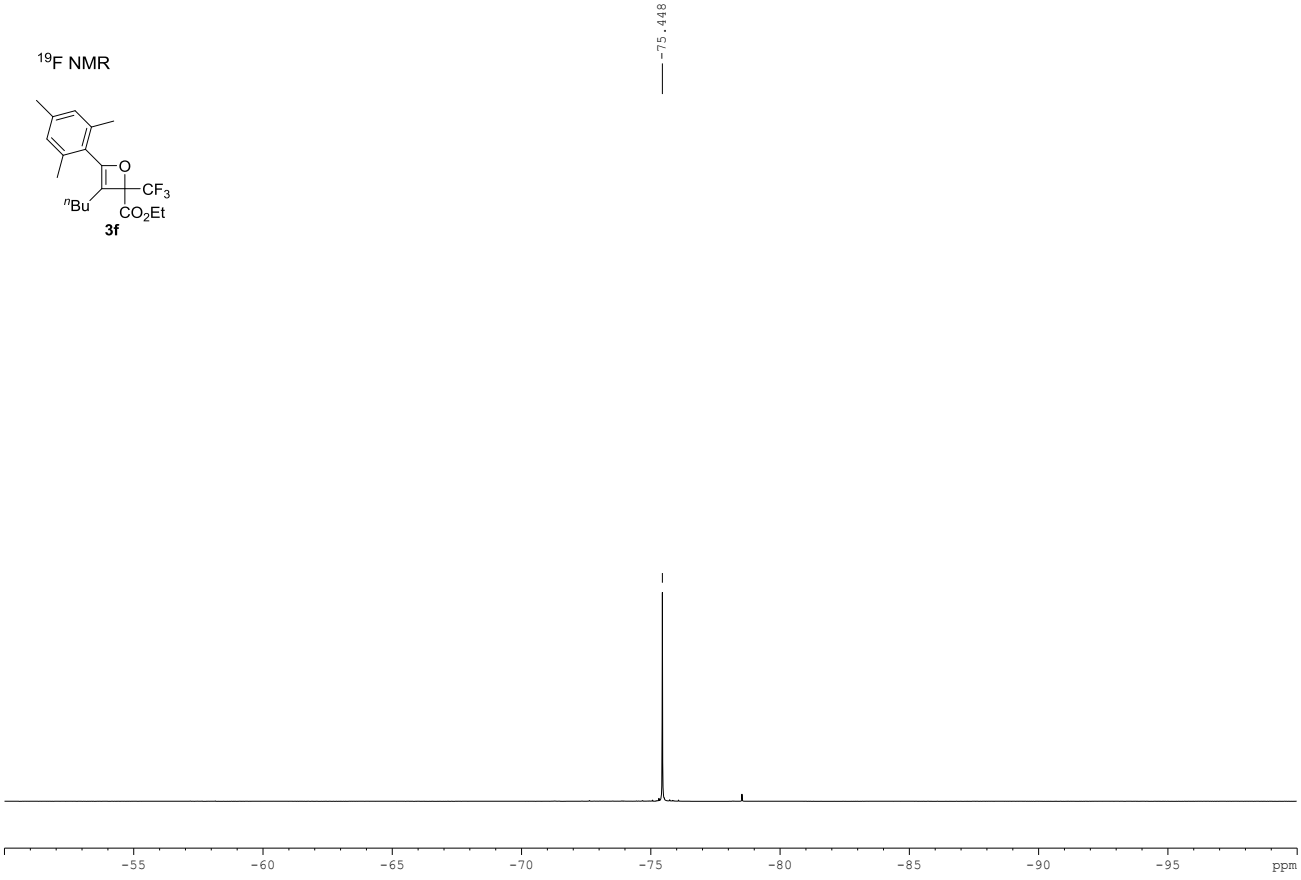
^{13}C NMR

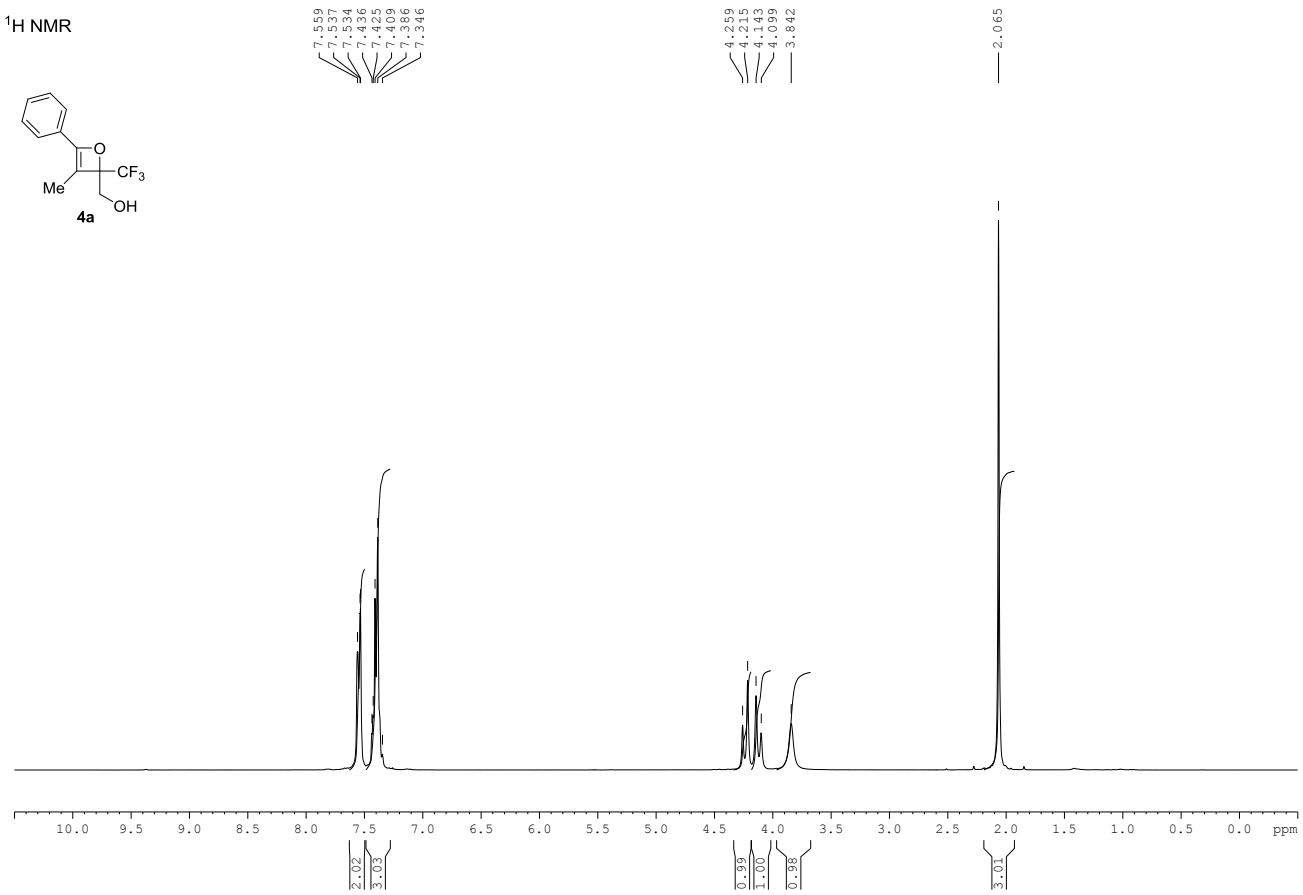
3f

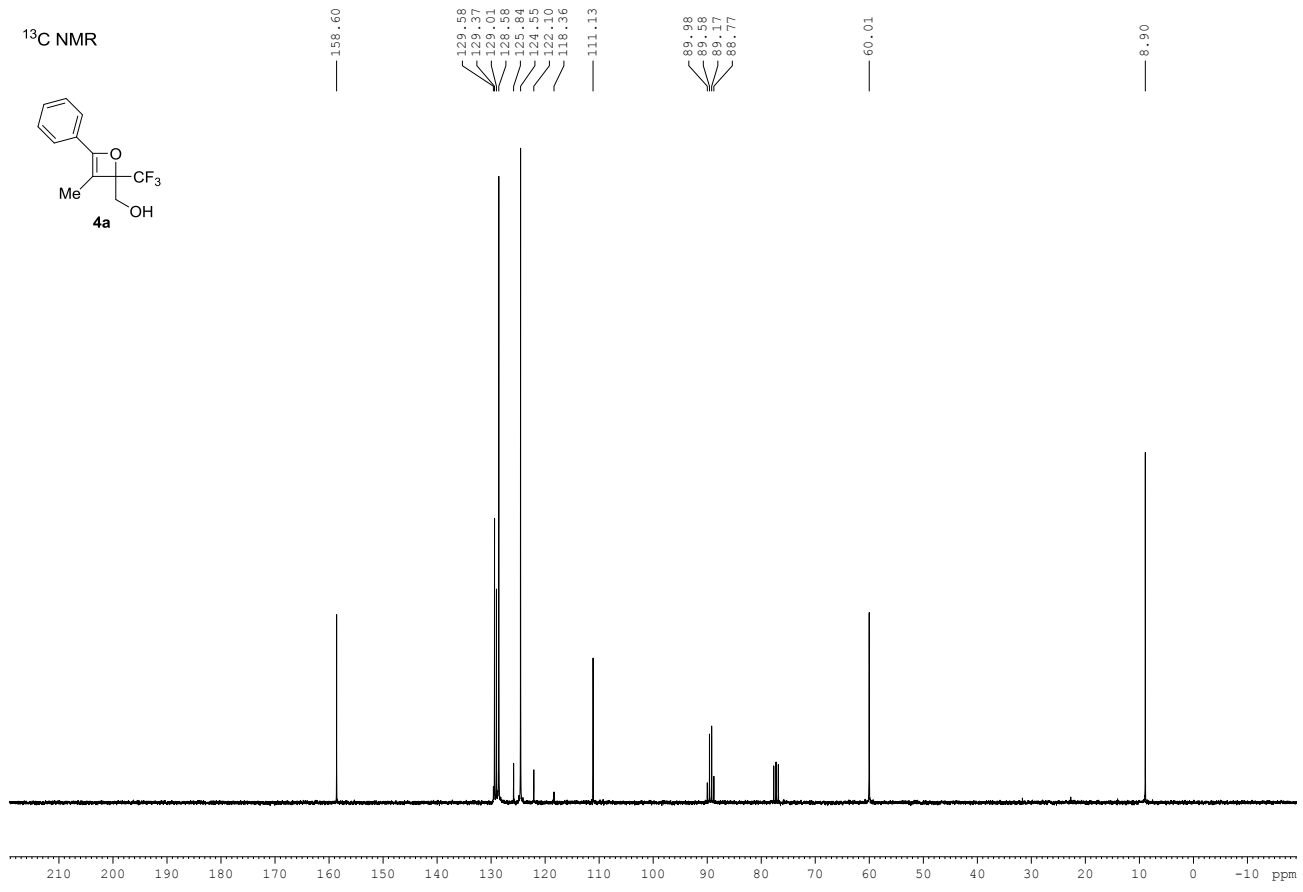


^{19}F NMR

3f

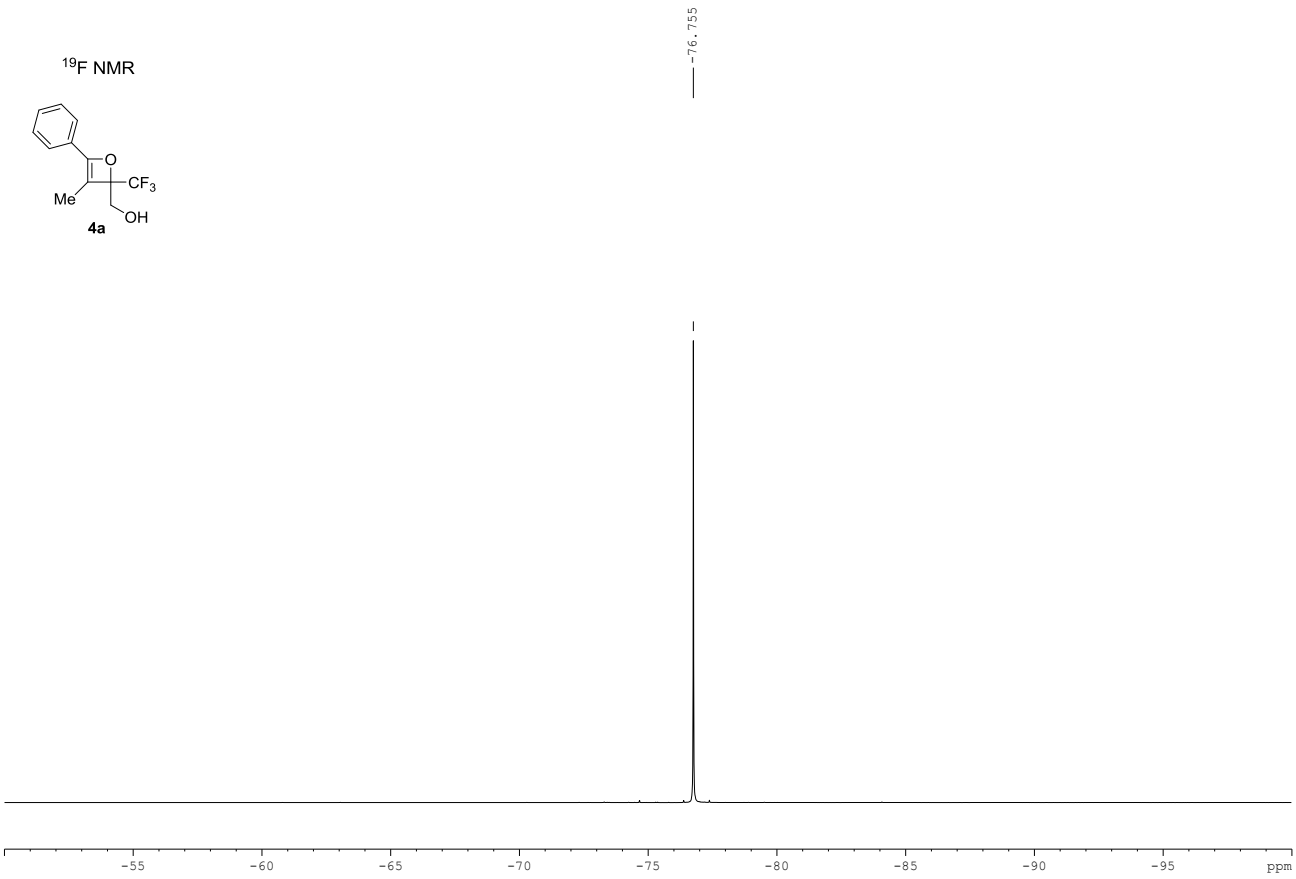



1H NMR
7.559
7.537
7.534
7.436
7.425
7.409
7.386
7.346
4.259
4.215
4.143
4.099
3.842
2.065
O
CF3
Me
OH
4a
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 ppm
2.02
3.03
0.99
1.00
0.98
3.01


13C NMR
158.60
129.58
129.37
129.01
128.58
125.84
124.55
122.10
118.36
111.13
89.98
89.58
89.17
88.77
60.01
8.90
O
CF3
Me
OH
4a
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 ppm

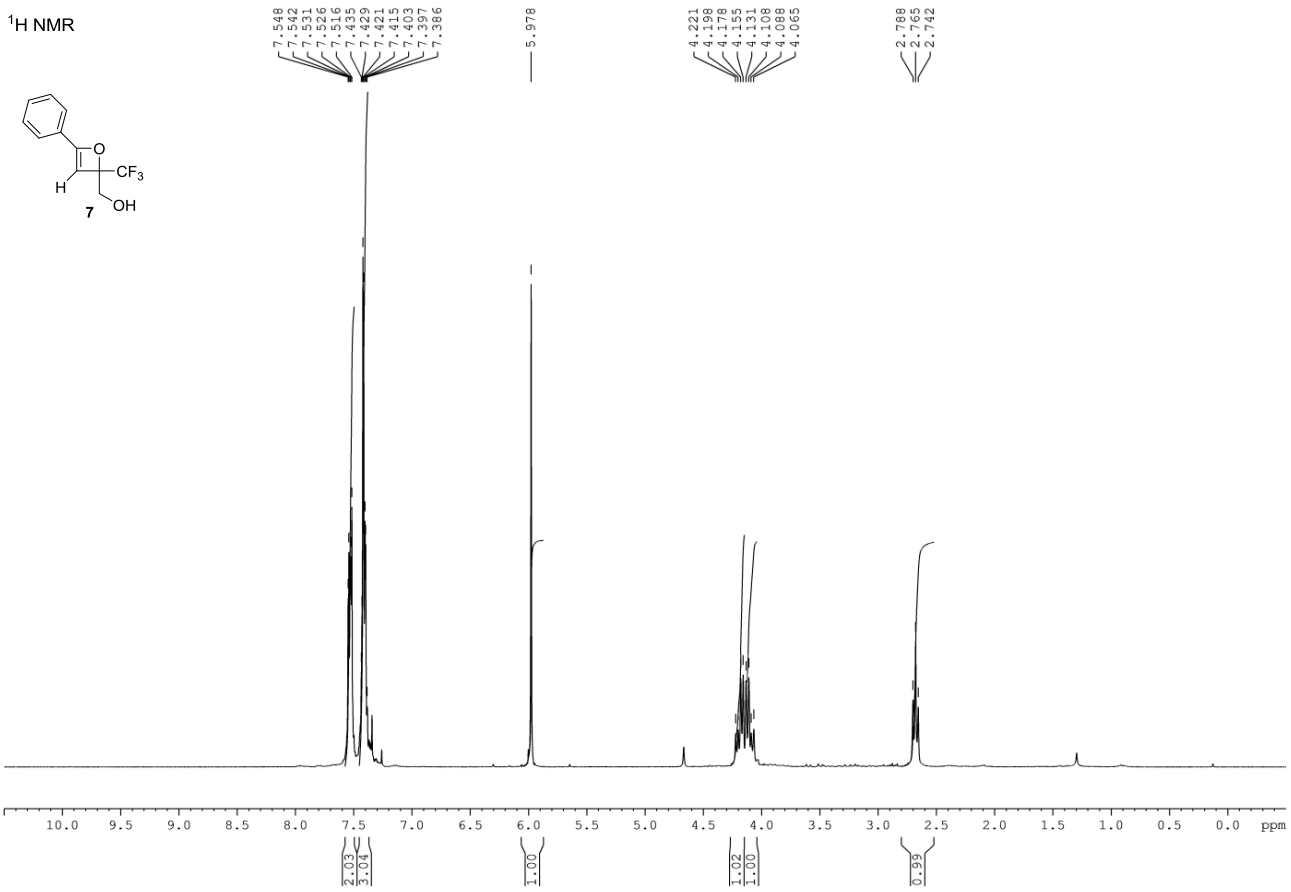
^{19}F NMR

4a

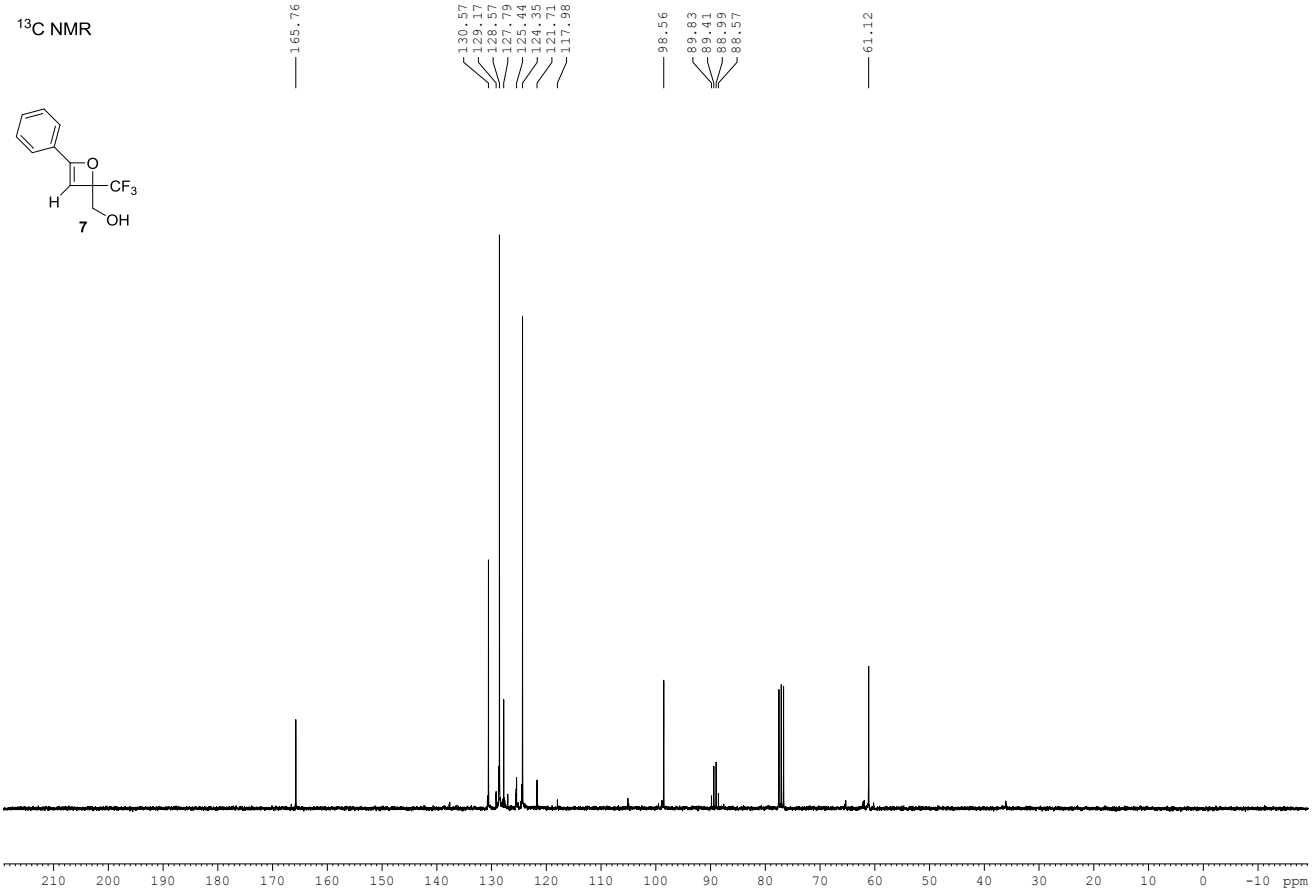


^{1}H NMR

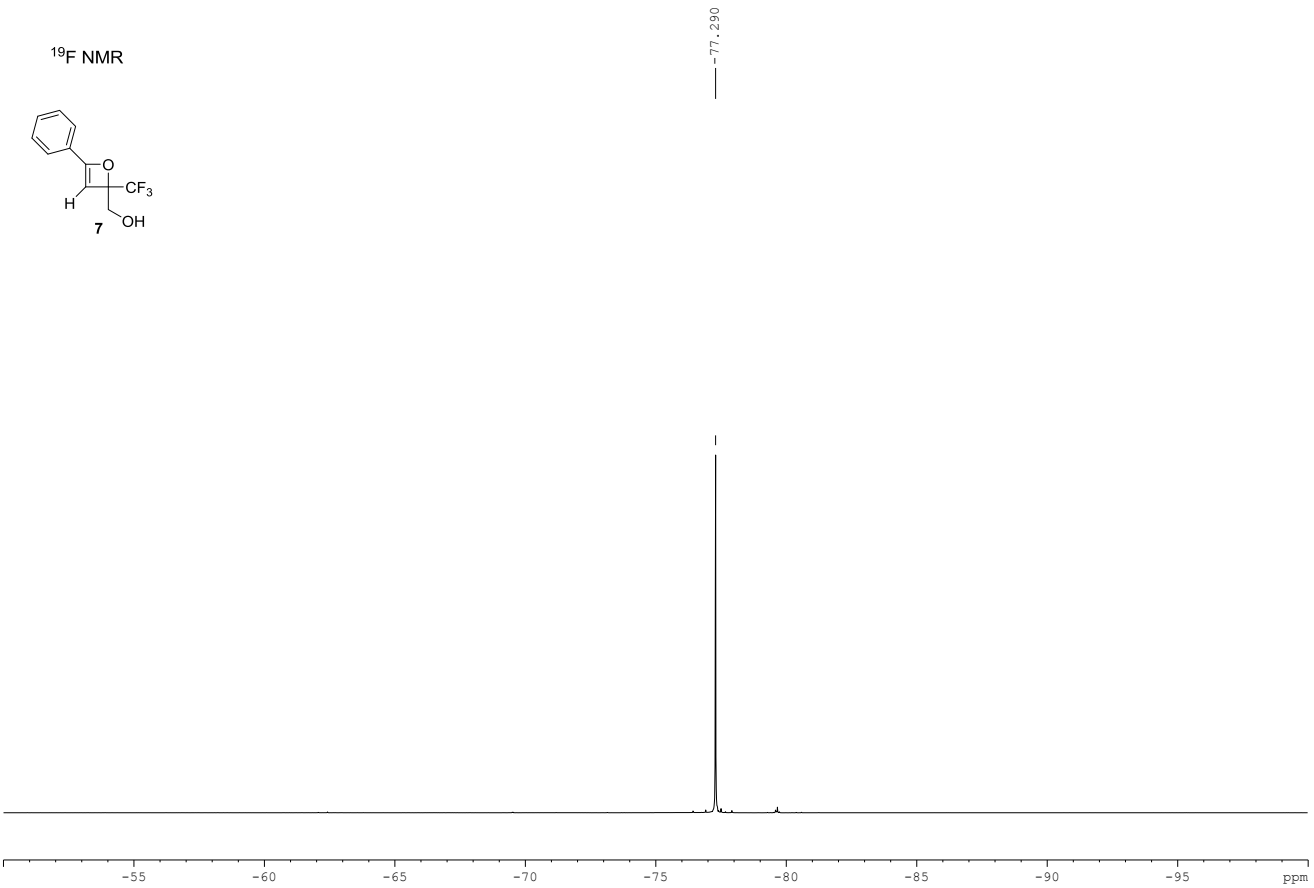
7



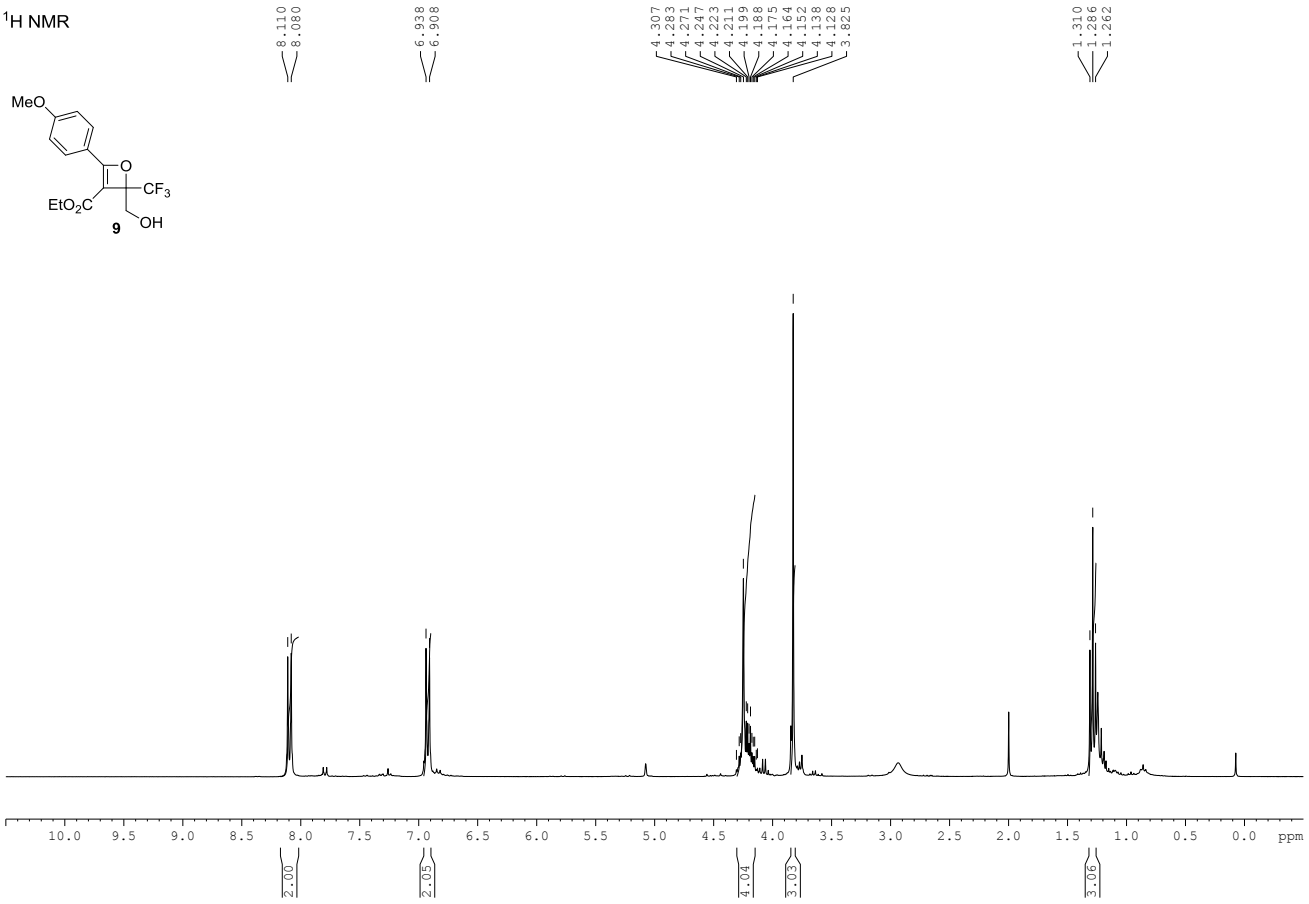
^{13}C NMR



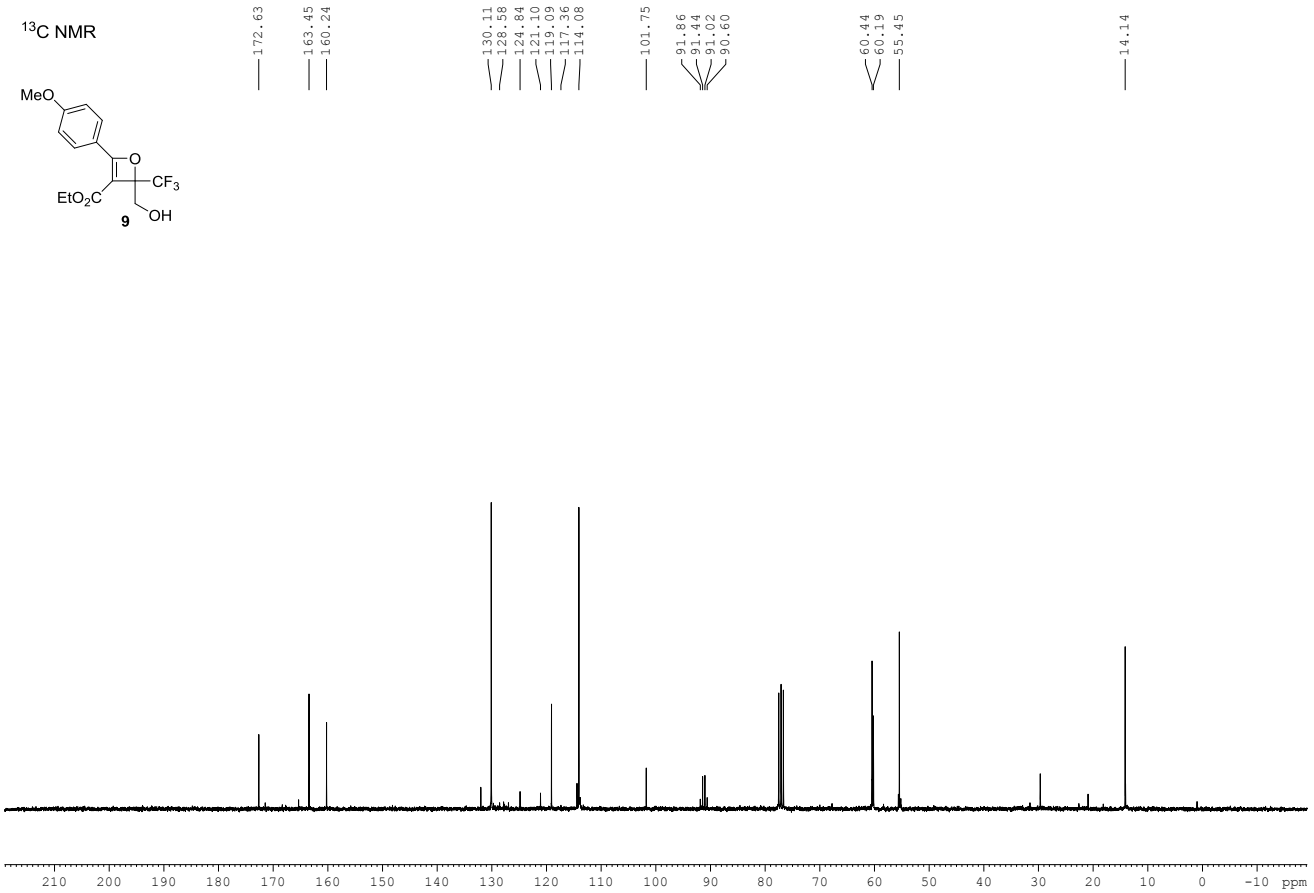
^{19}F NMR



^{1}H NMR

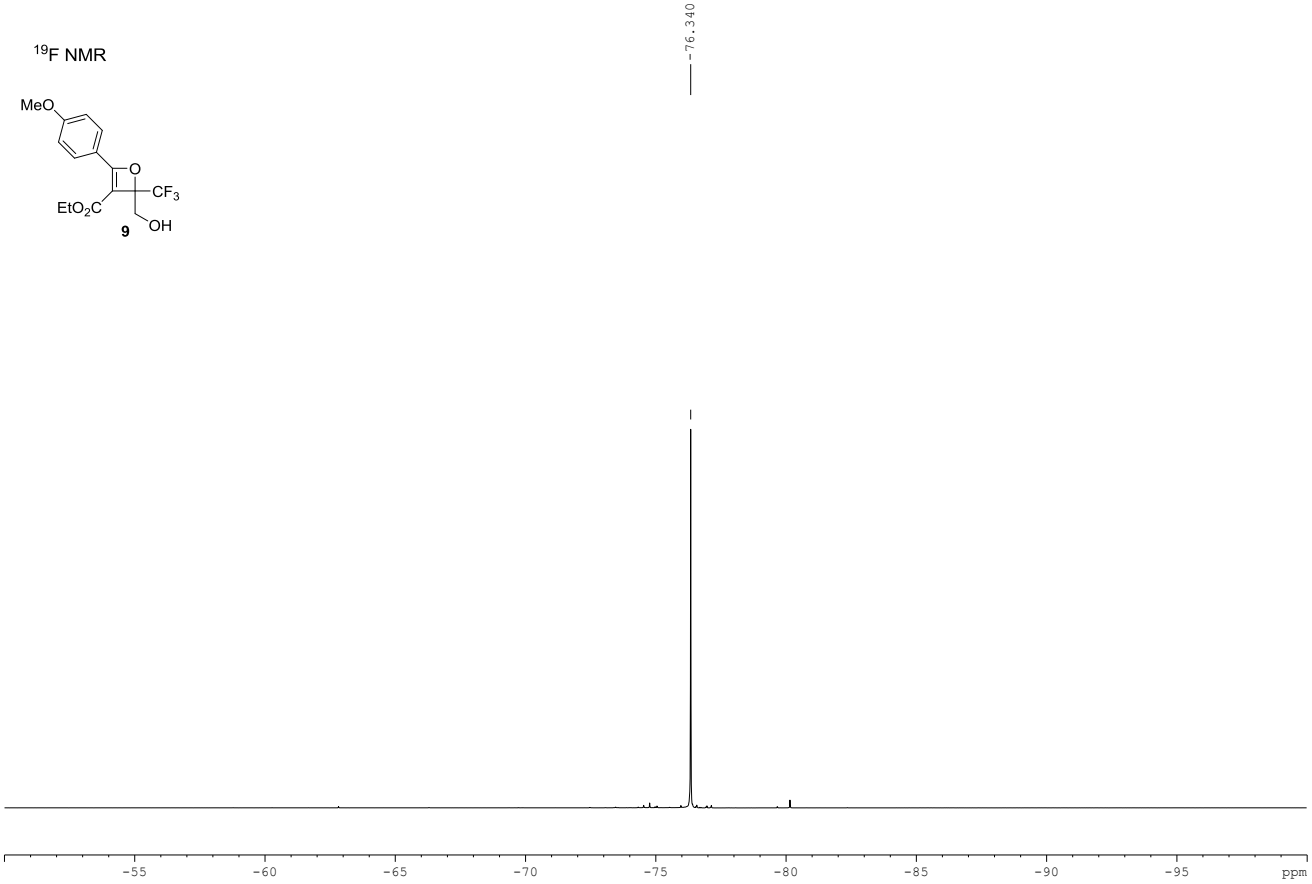


^{13}C NMR



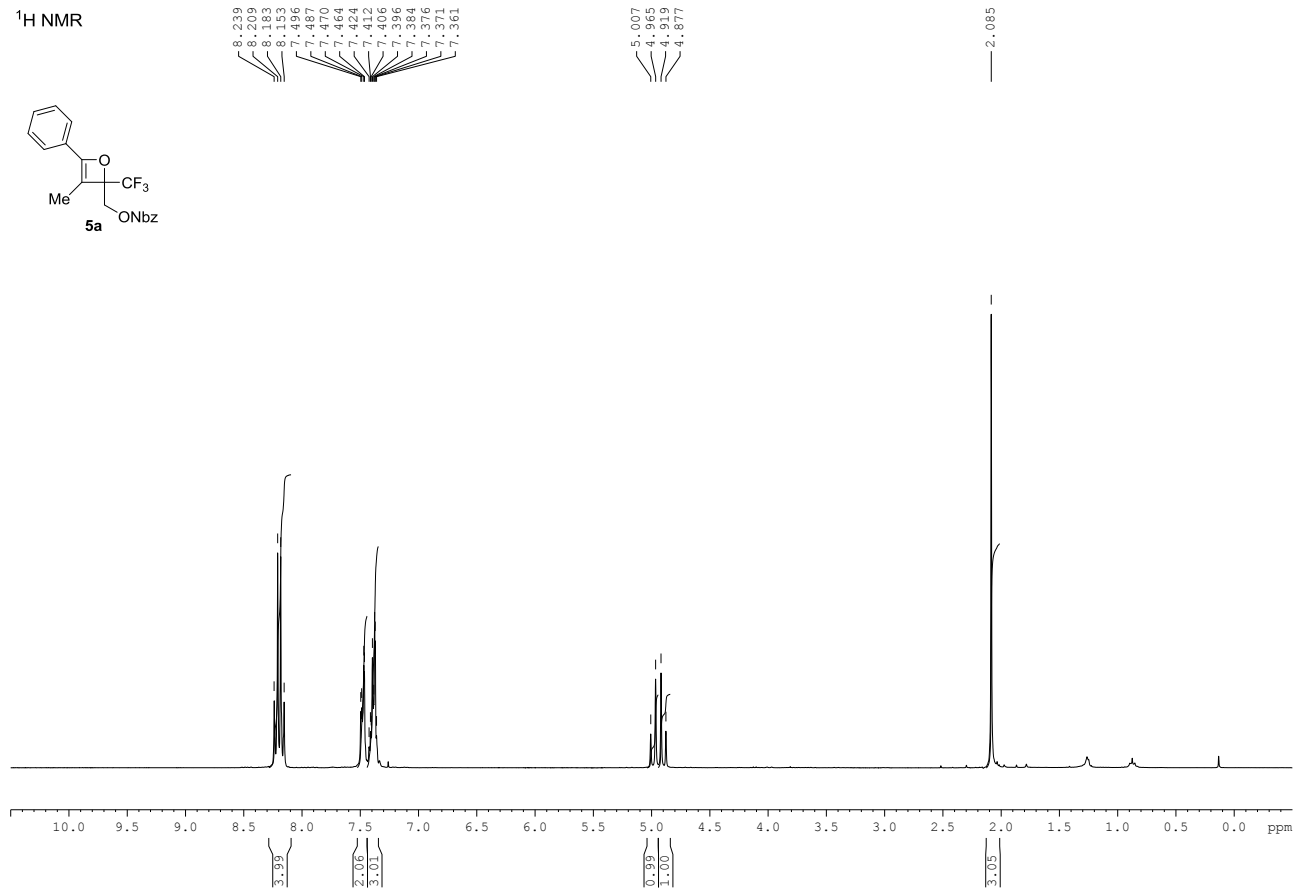
^{19}F NMR

9



^{1}H NMR

5a



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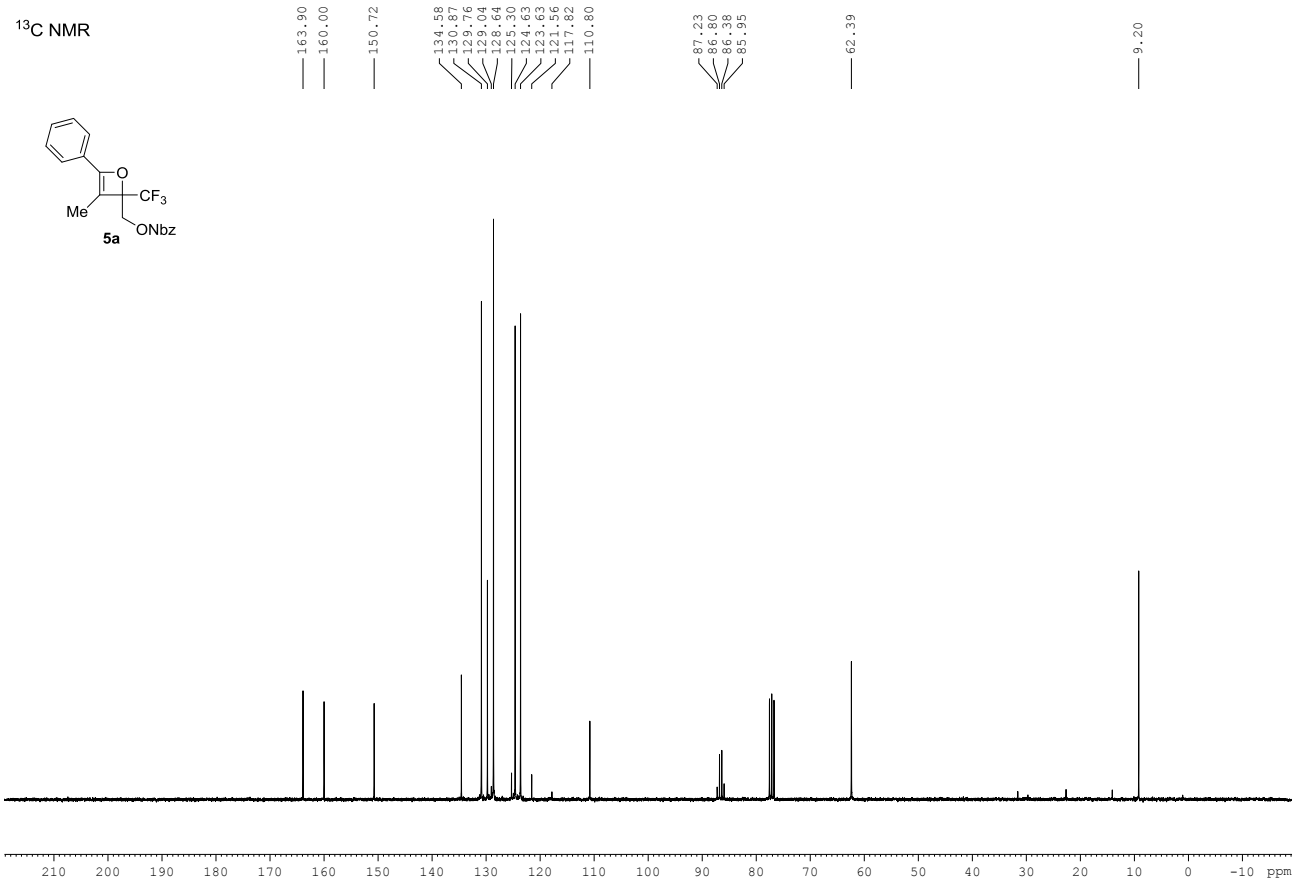

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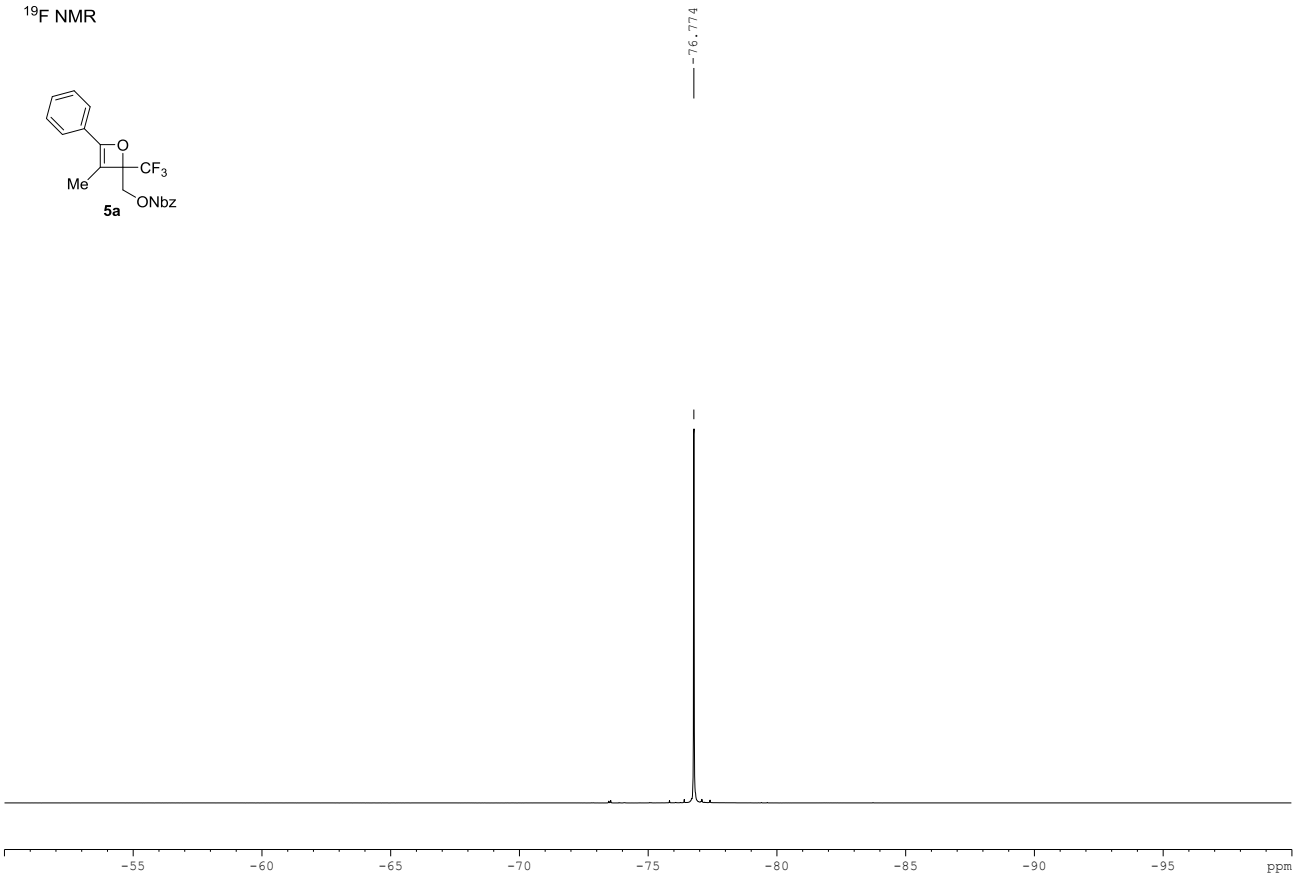
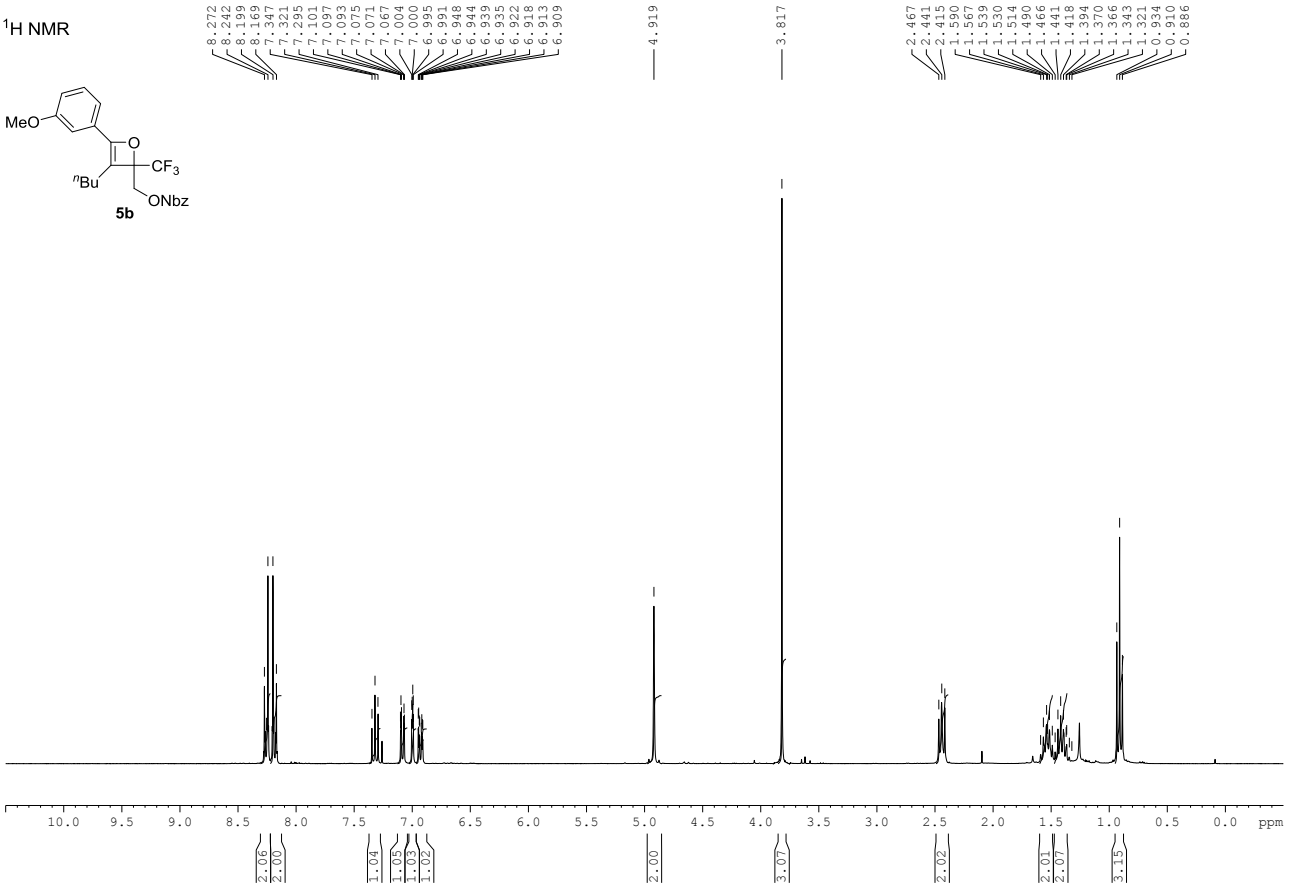


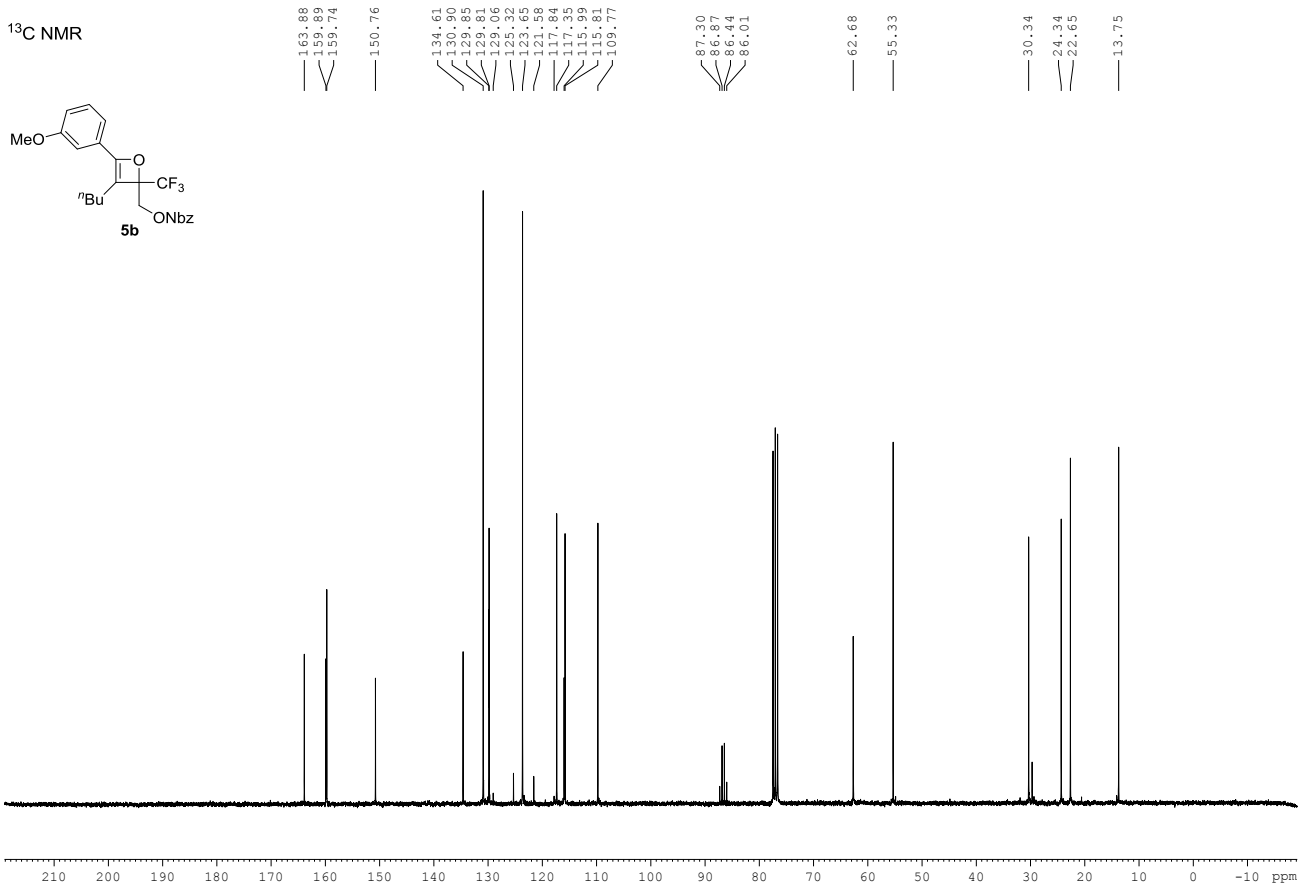
^{1}H NMR

5b



^{13}C NMR

5b



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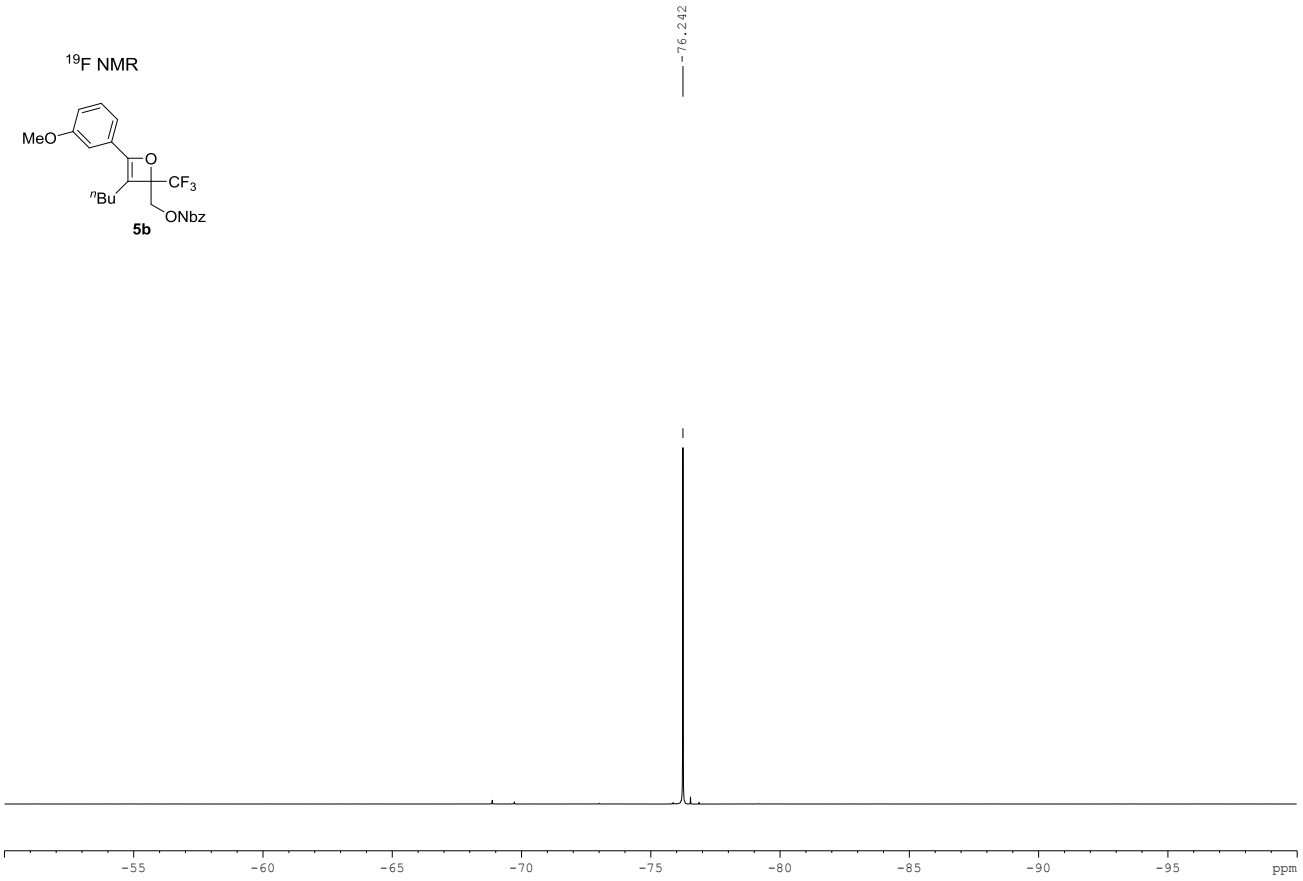
5b



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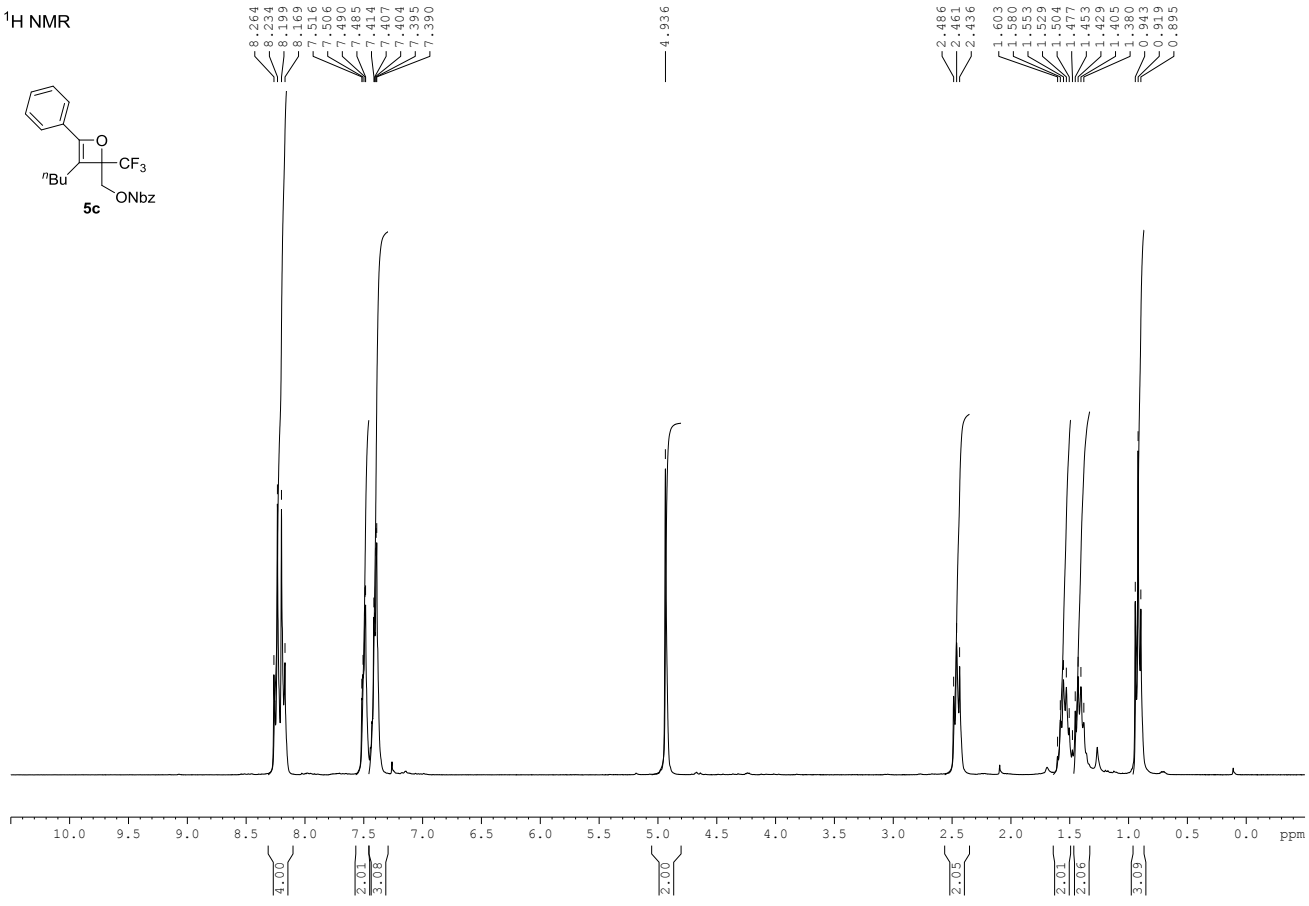

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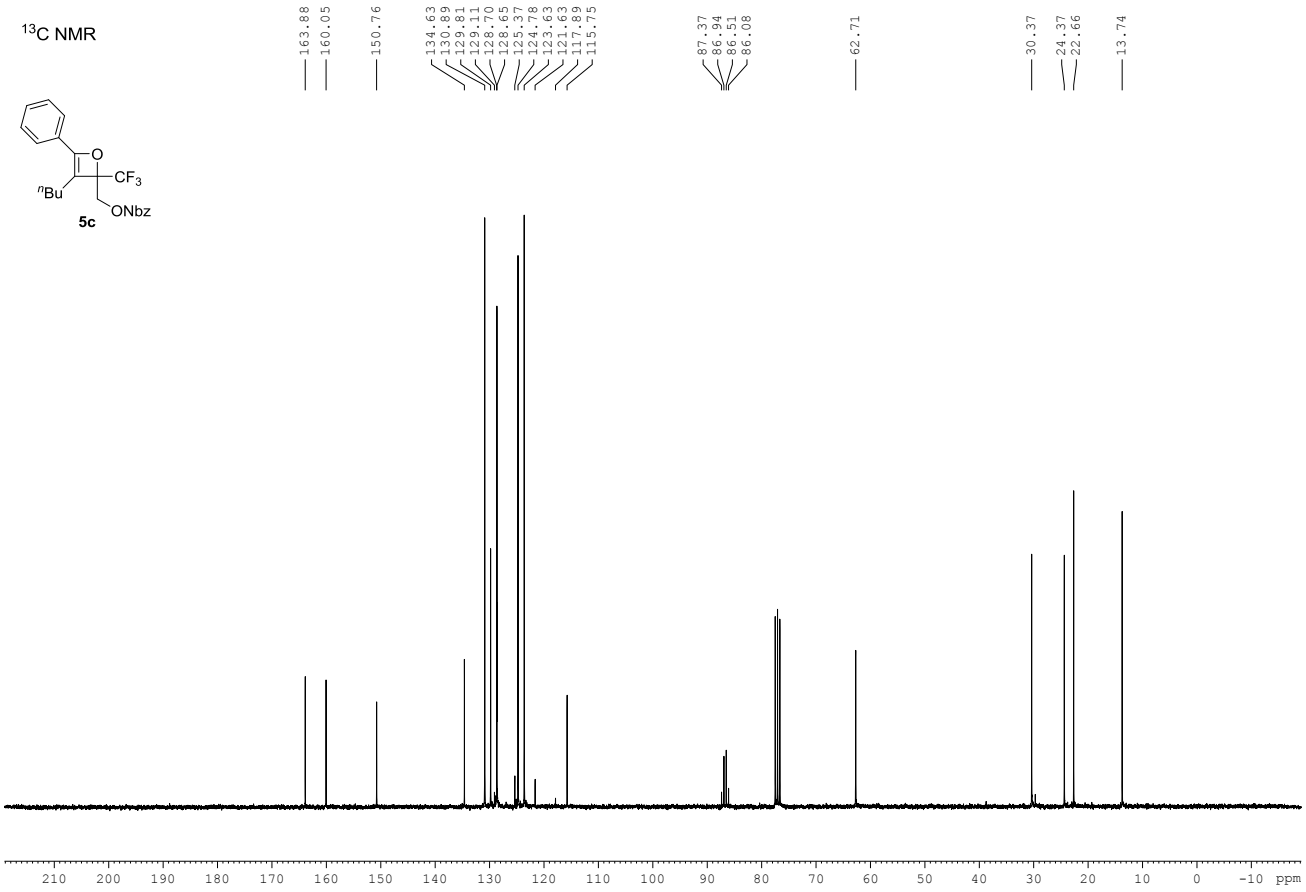
5c



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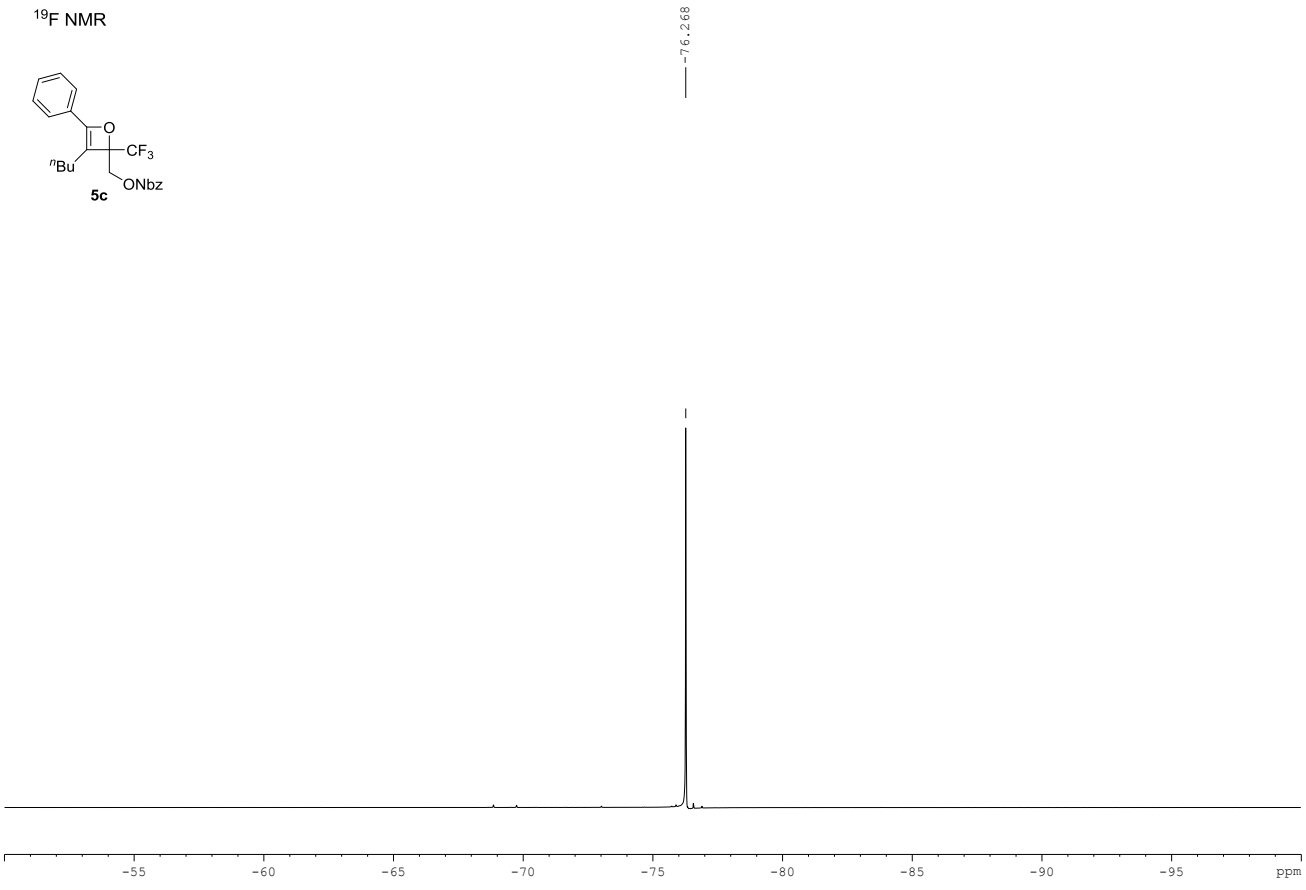
5c



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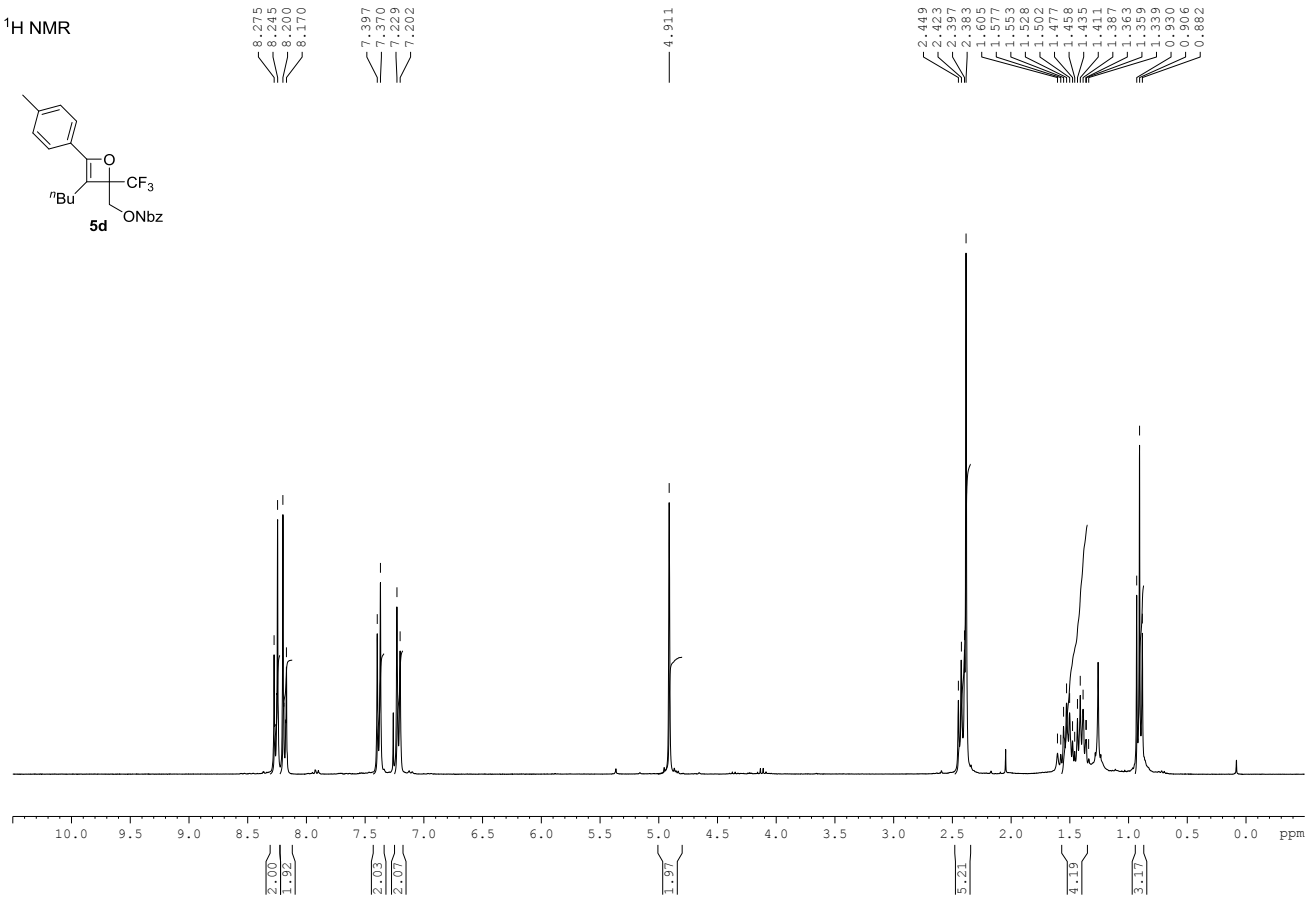

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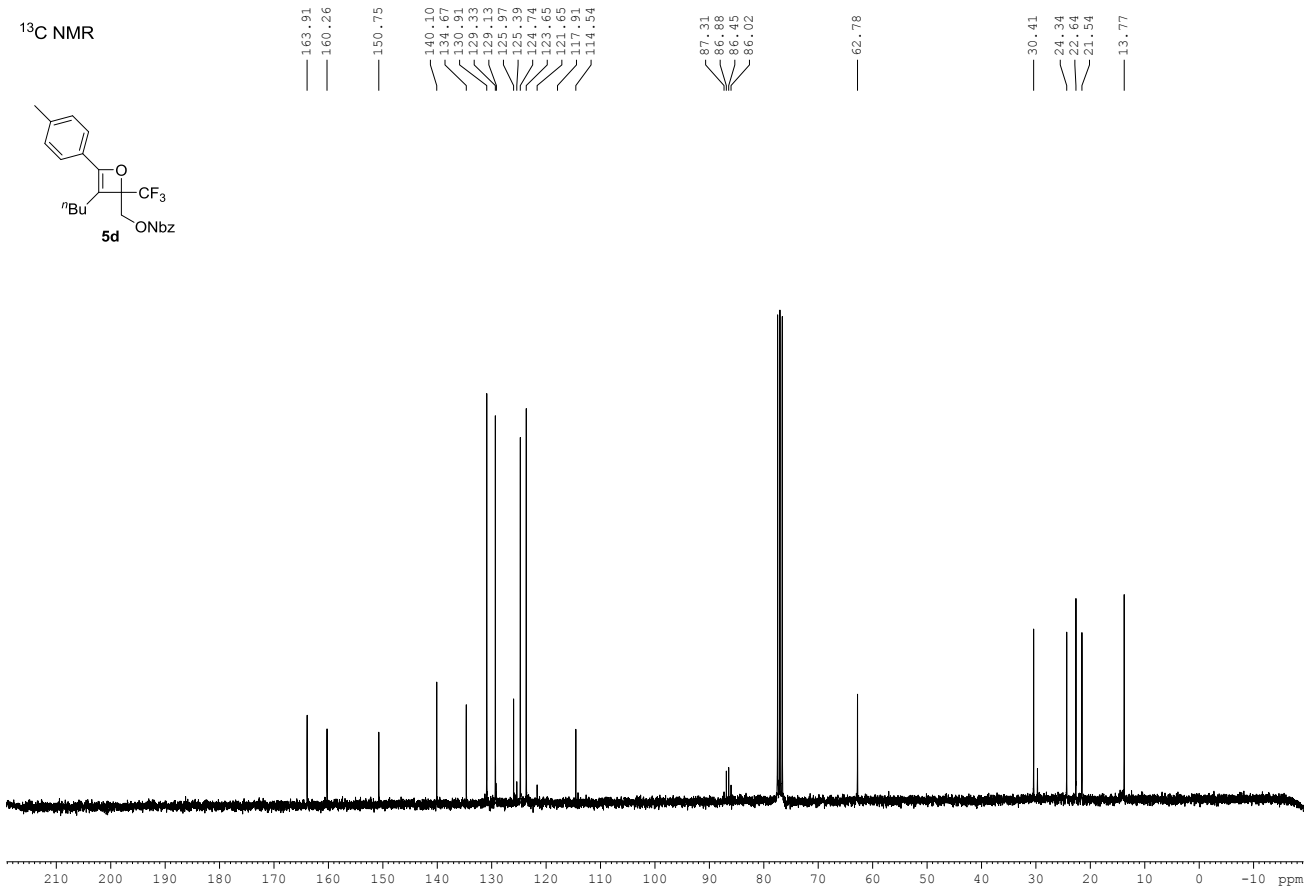

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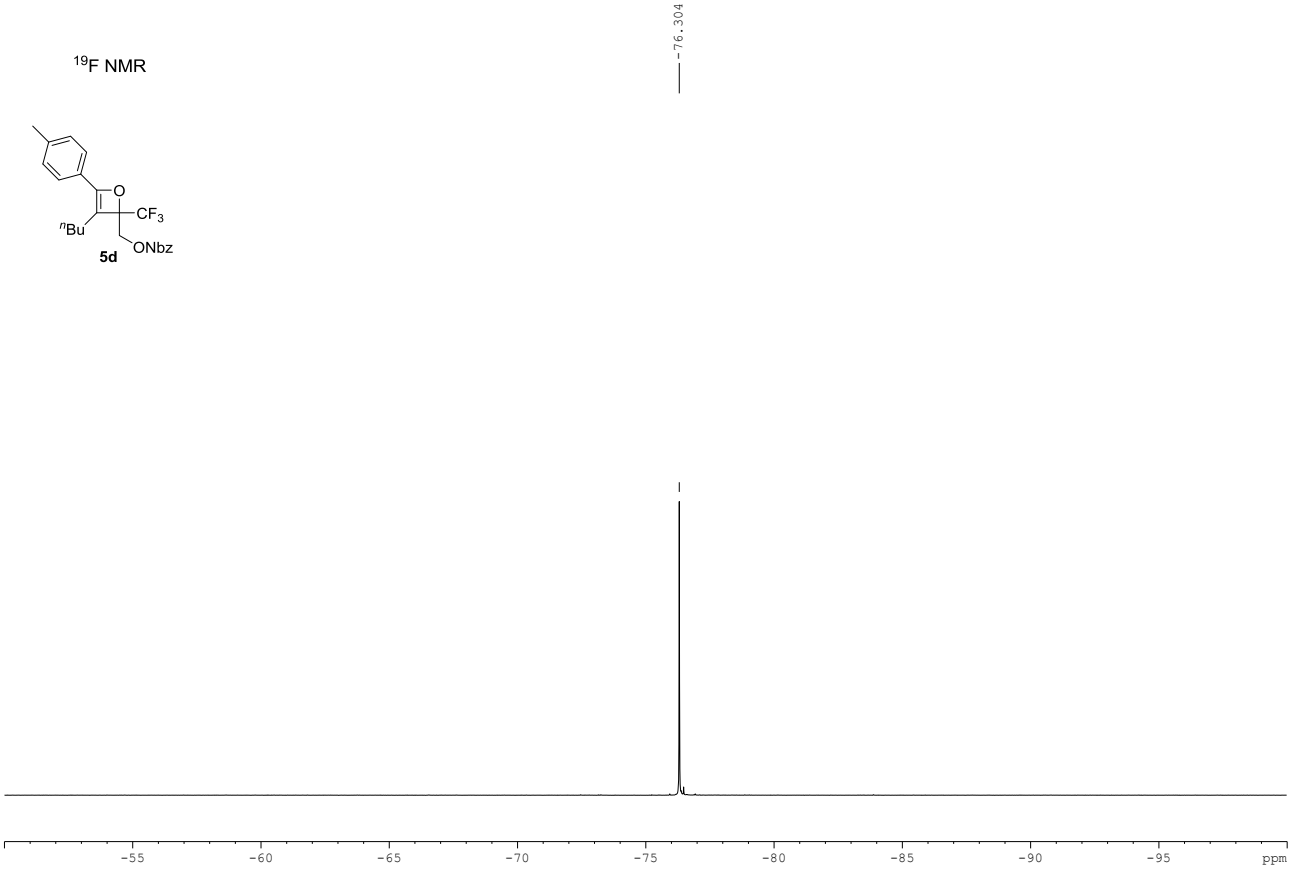
5d



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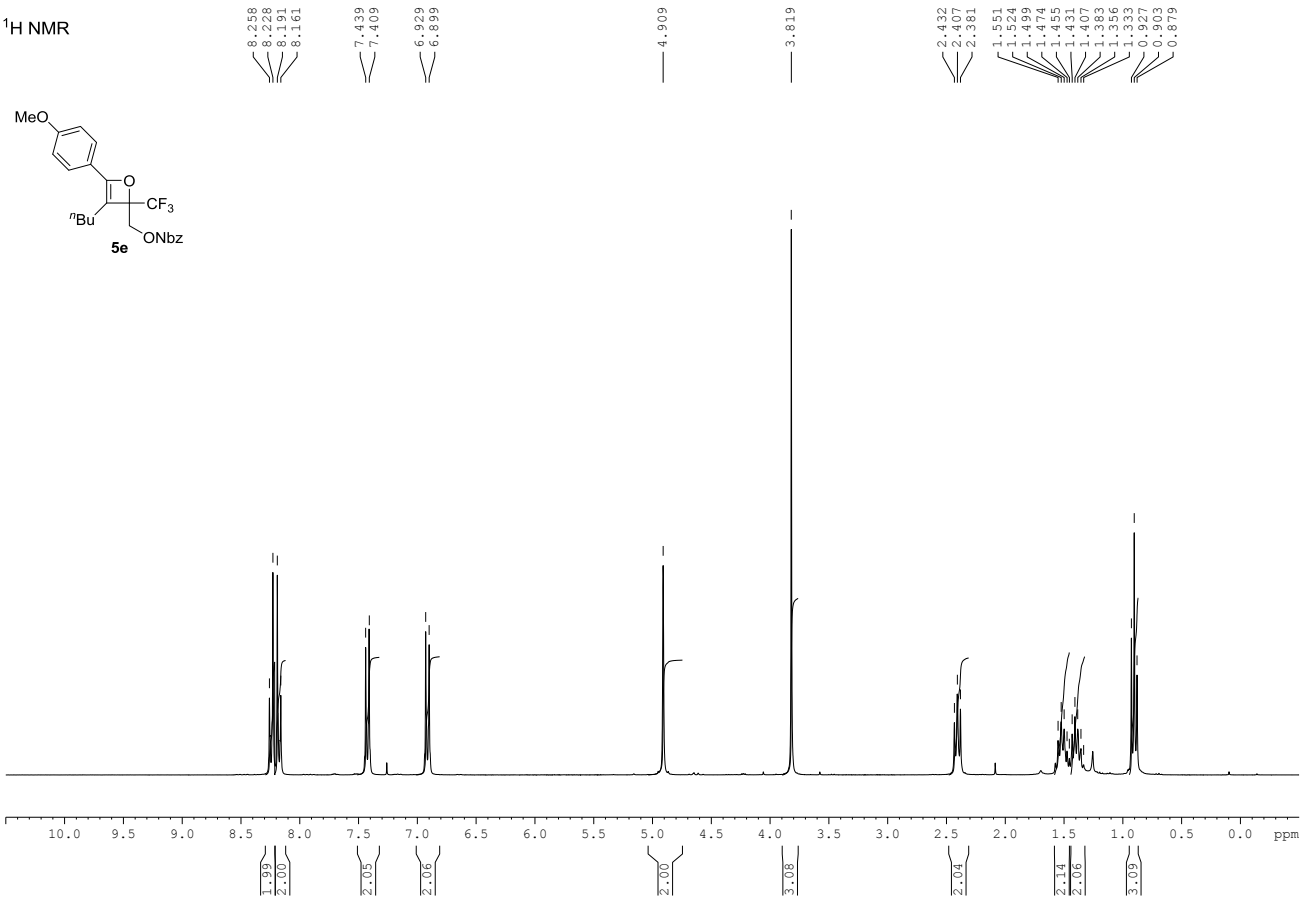
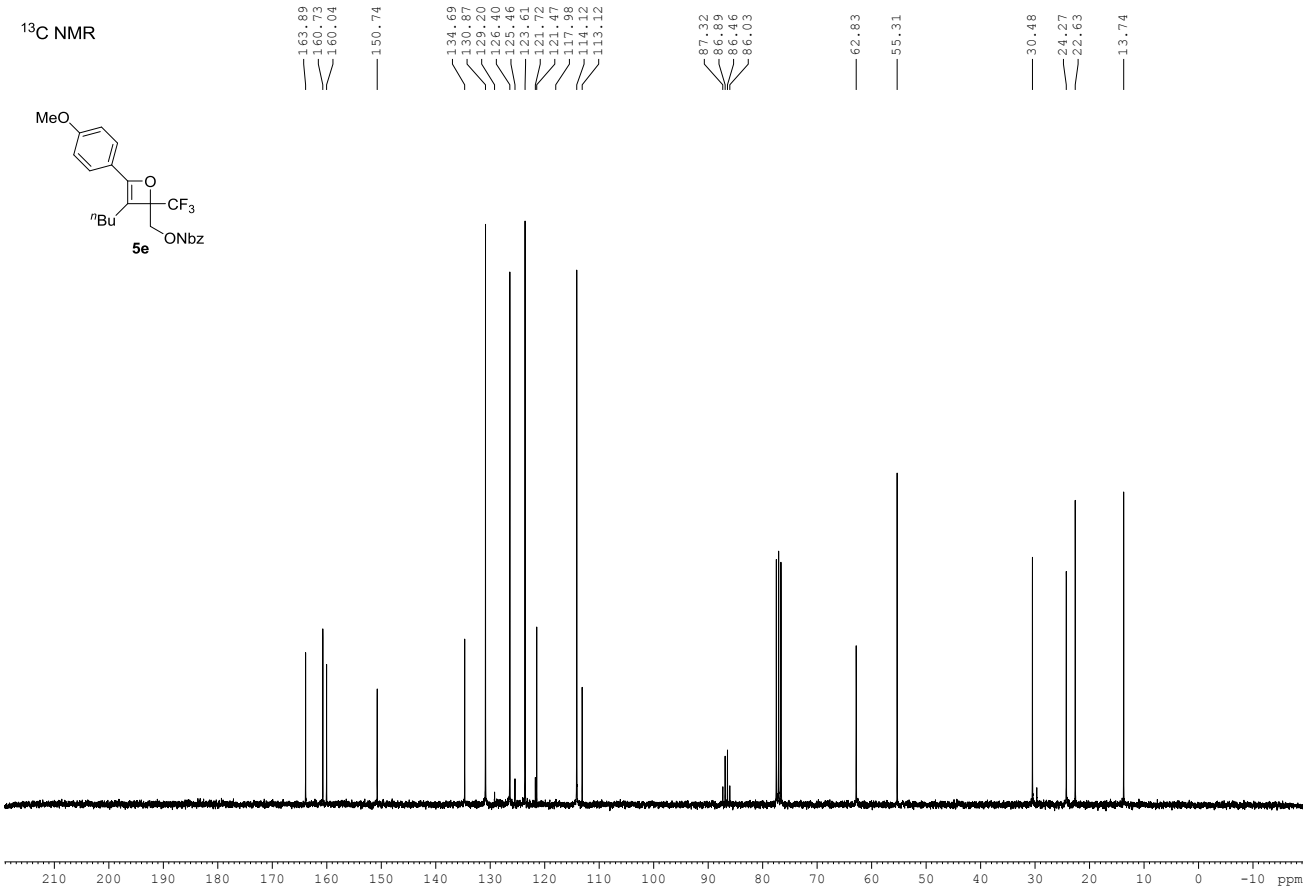
5e



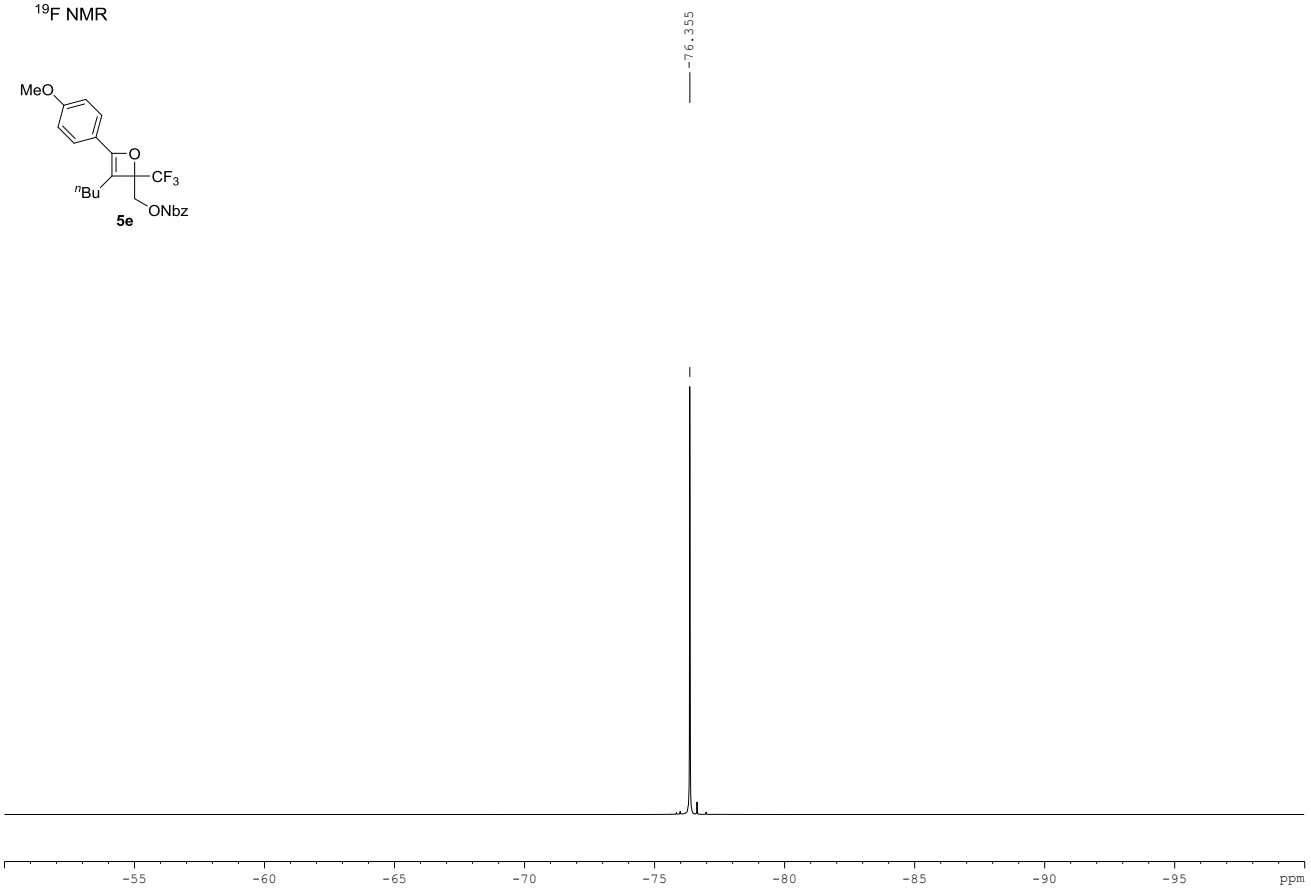
^{13}C NMR

5e

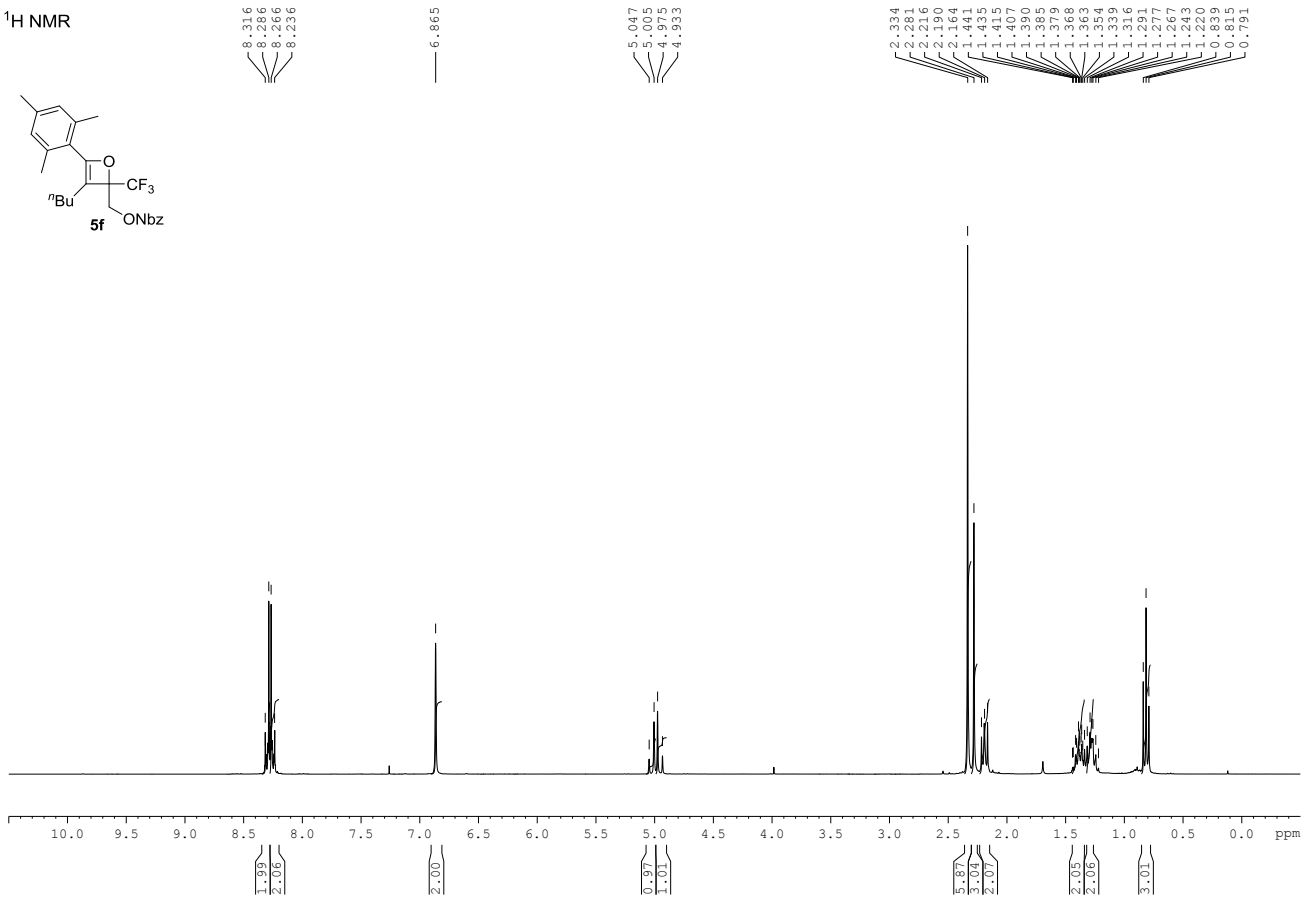


^{19}F NMR

5e



^{1}H NMR



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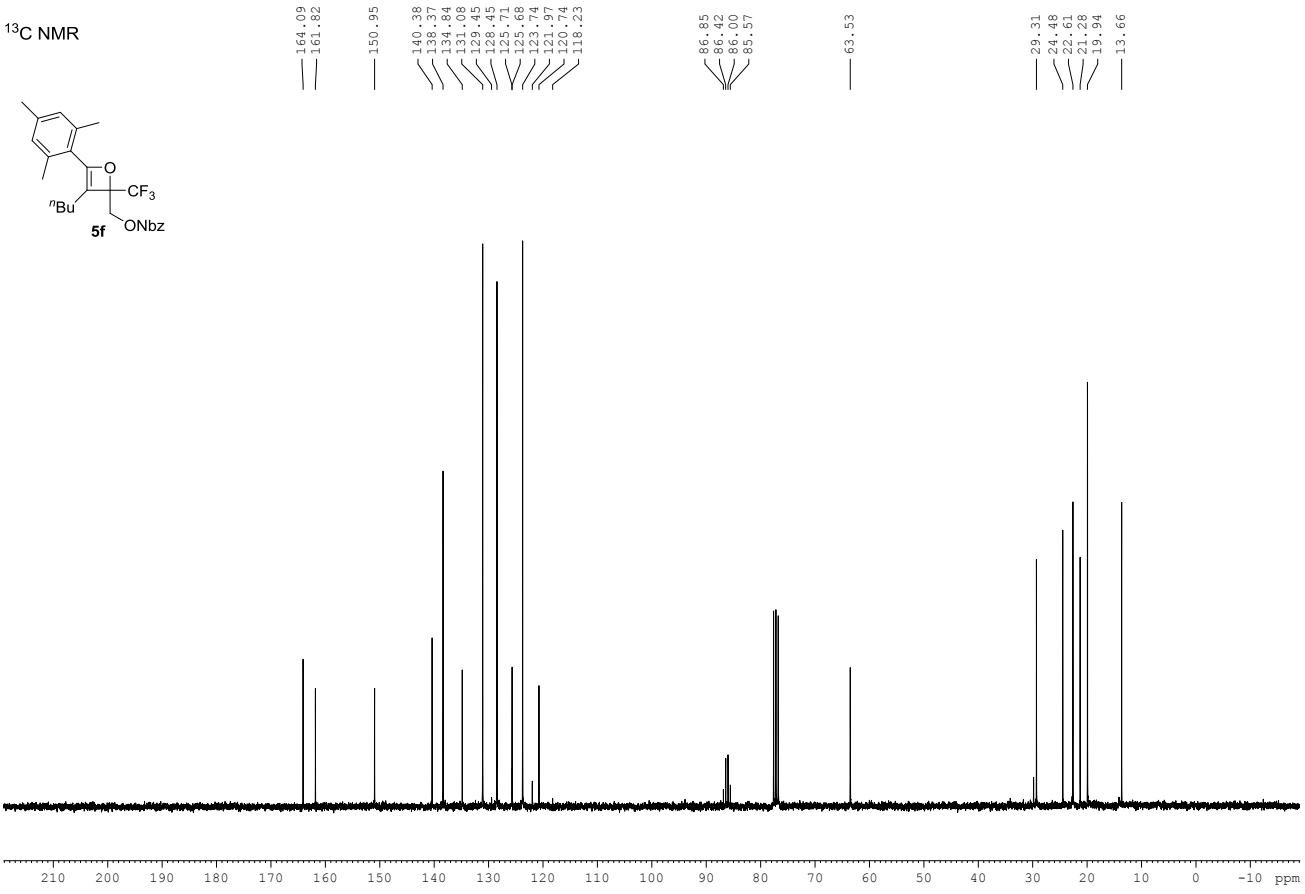
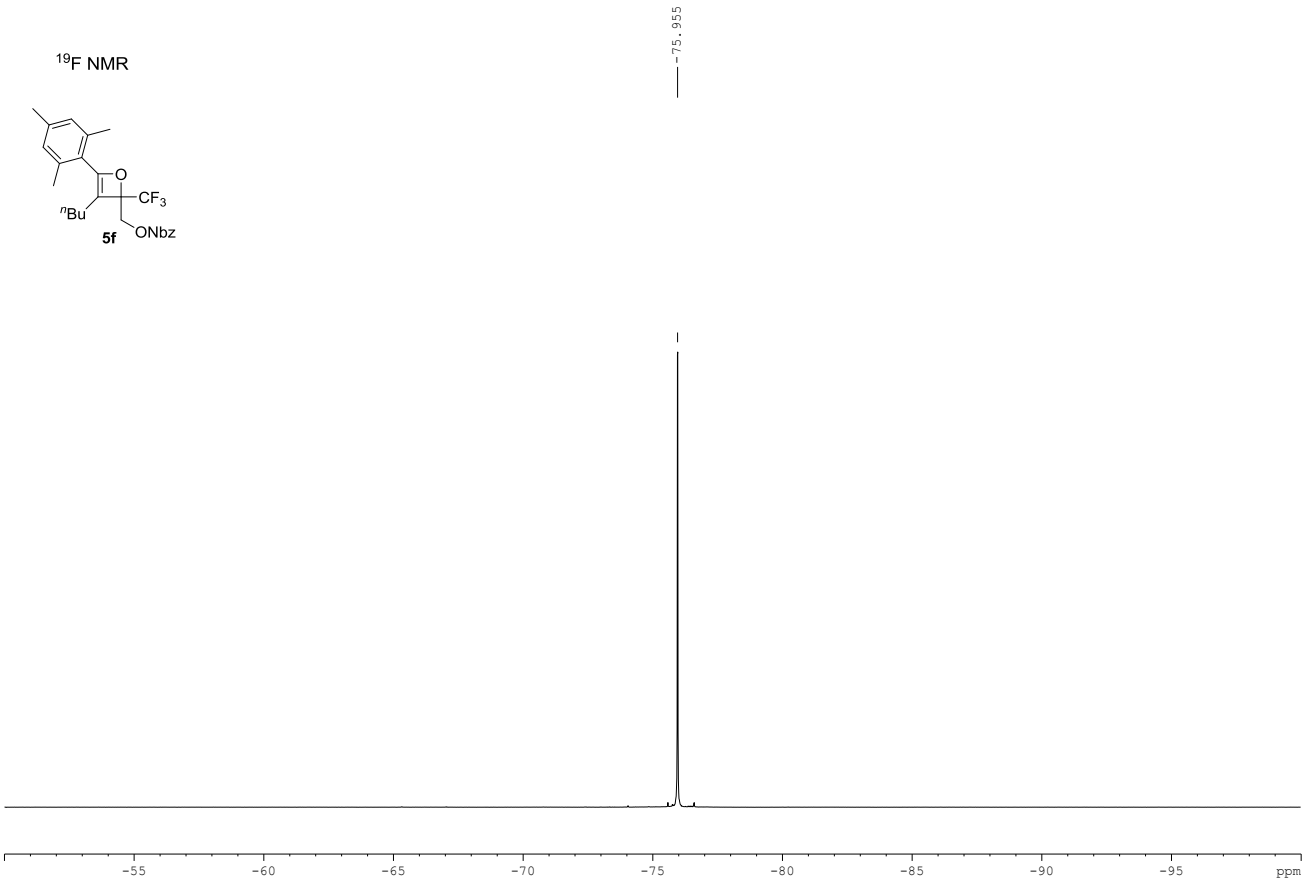


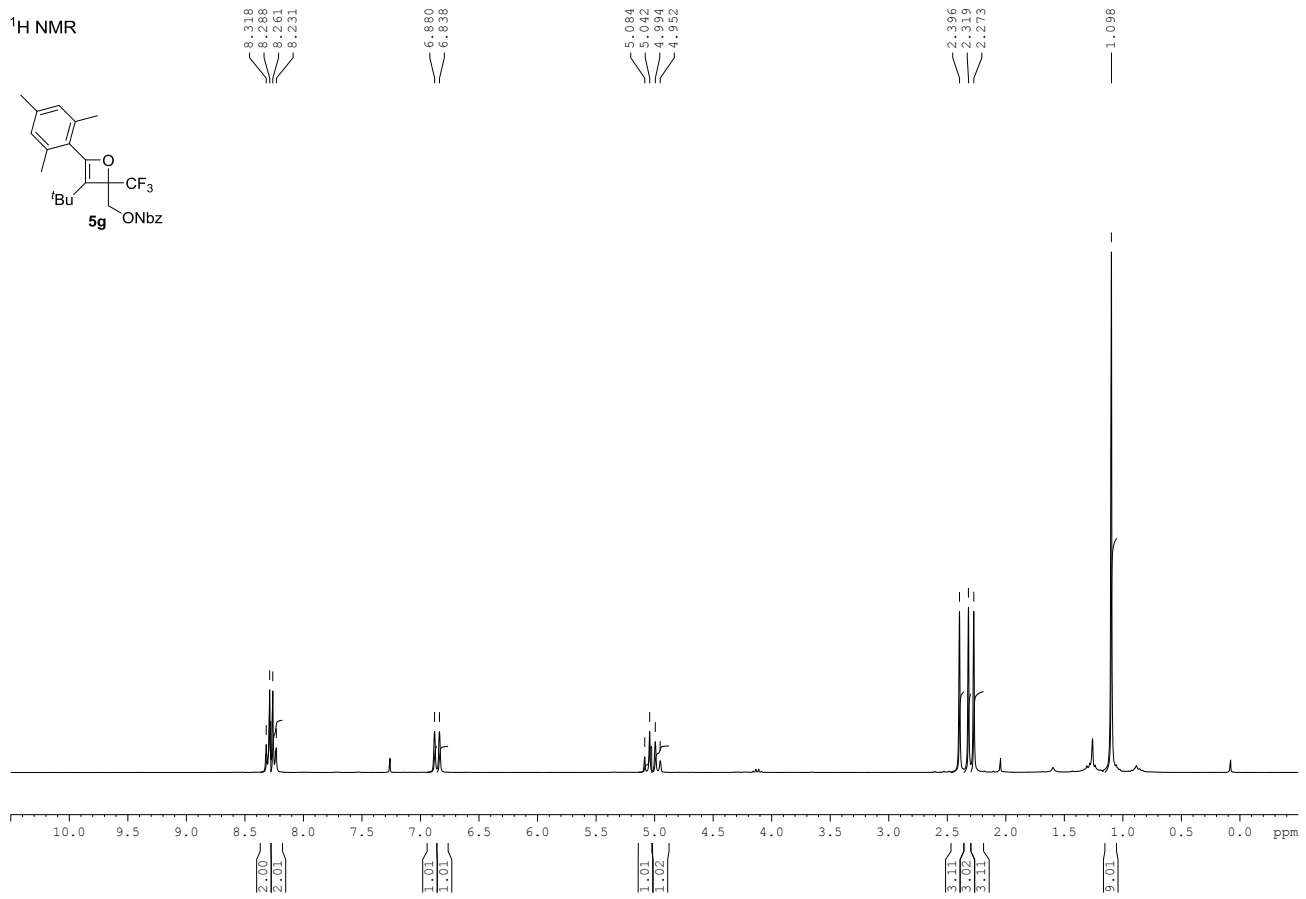
^{19}F NMR

5f

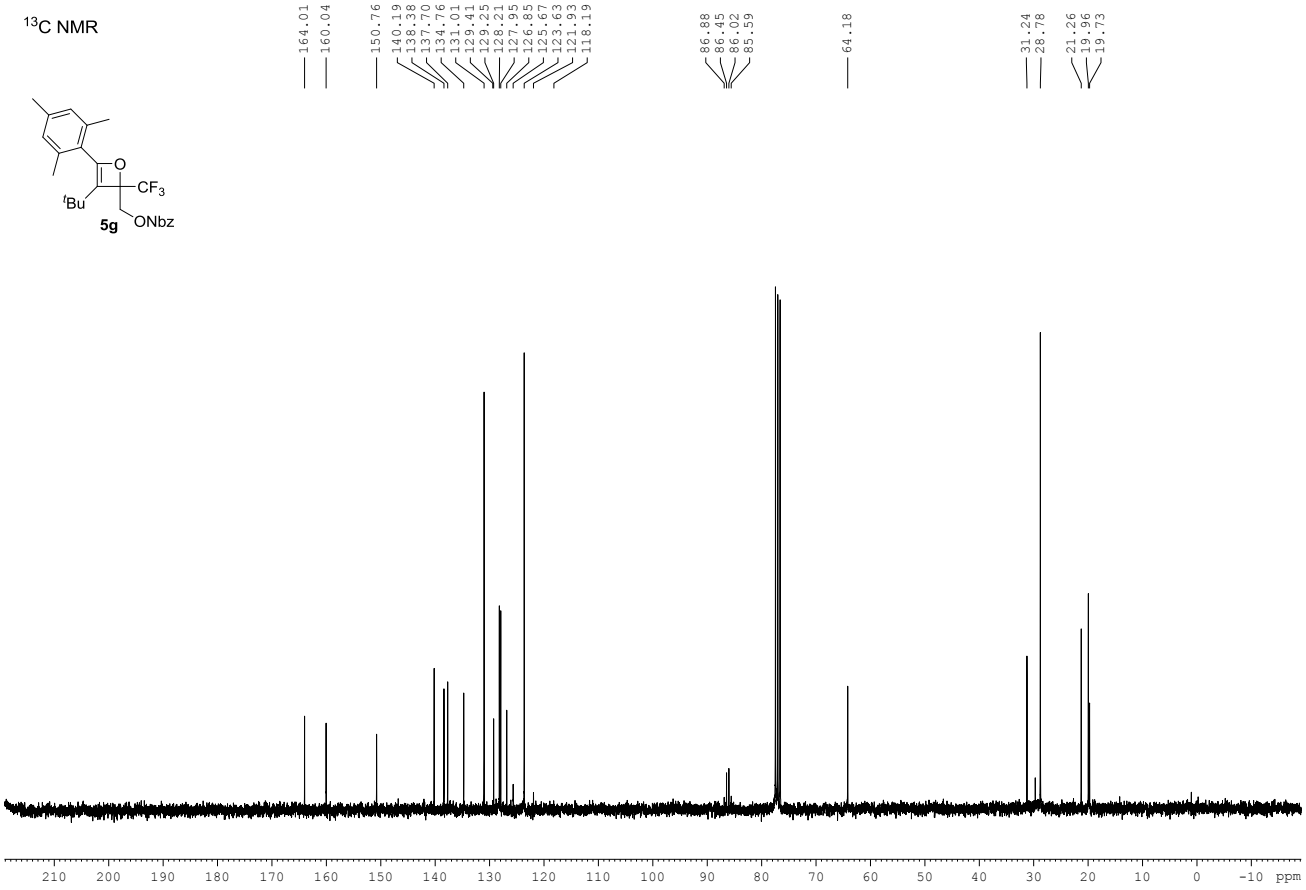


^{1}H NMR

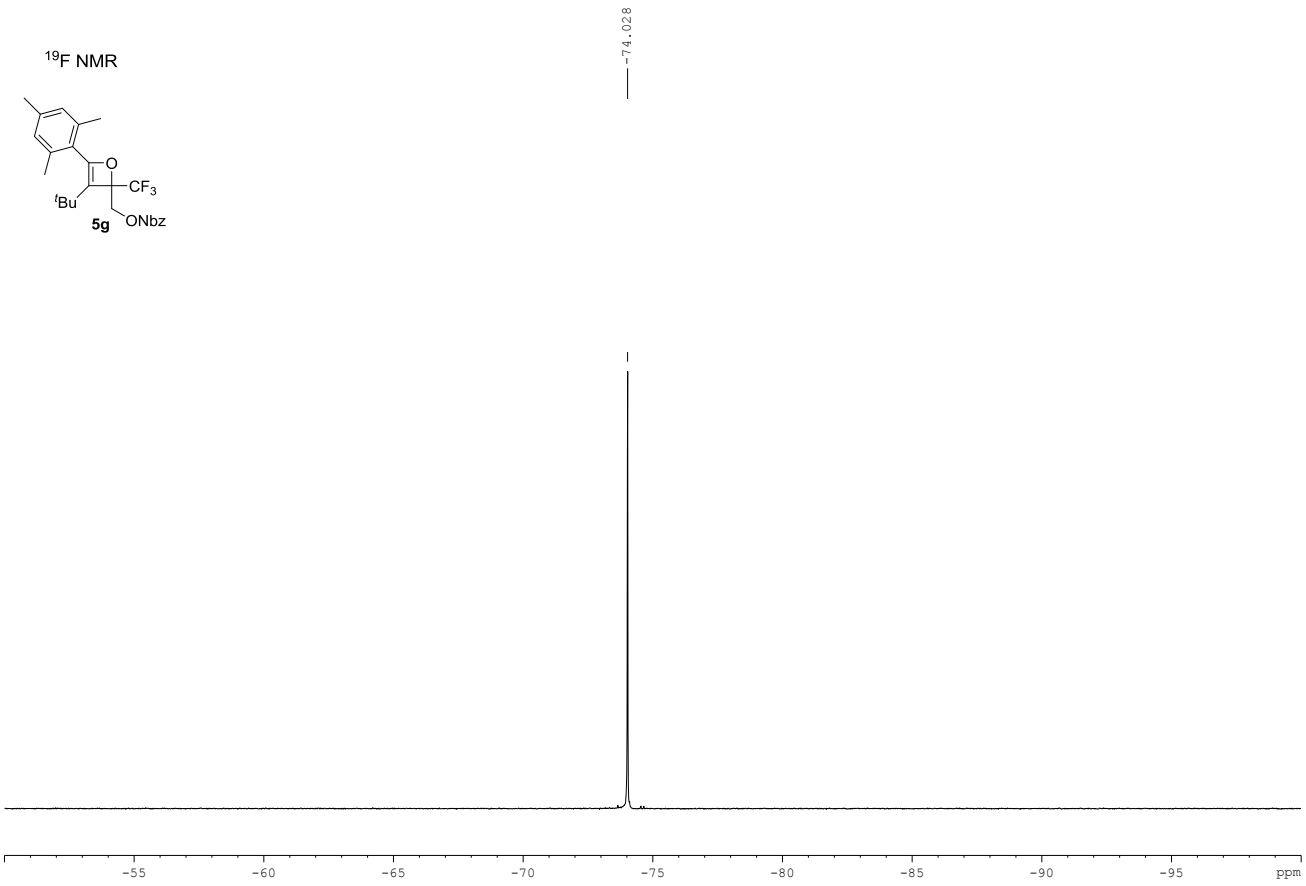
5g

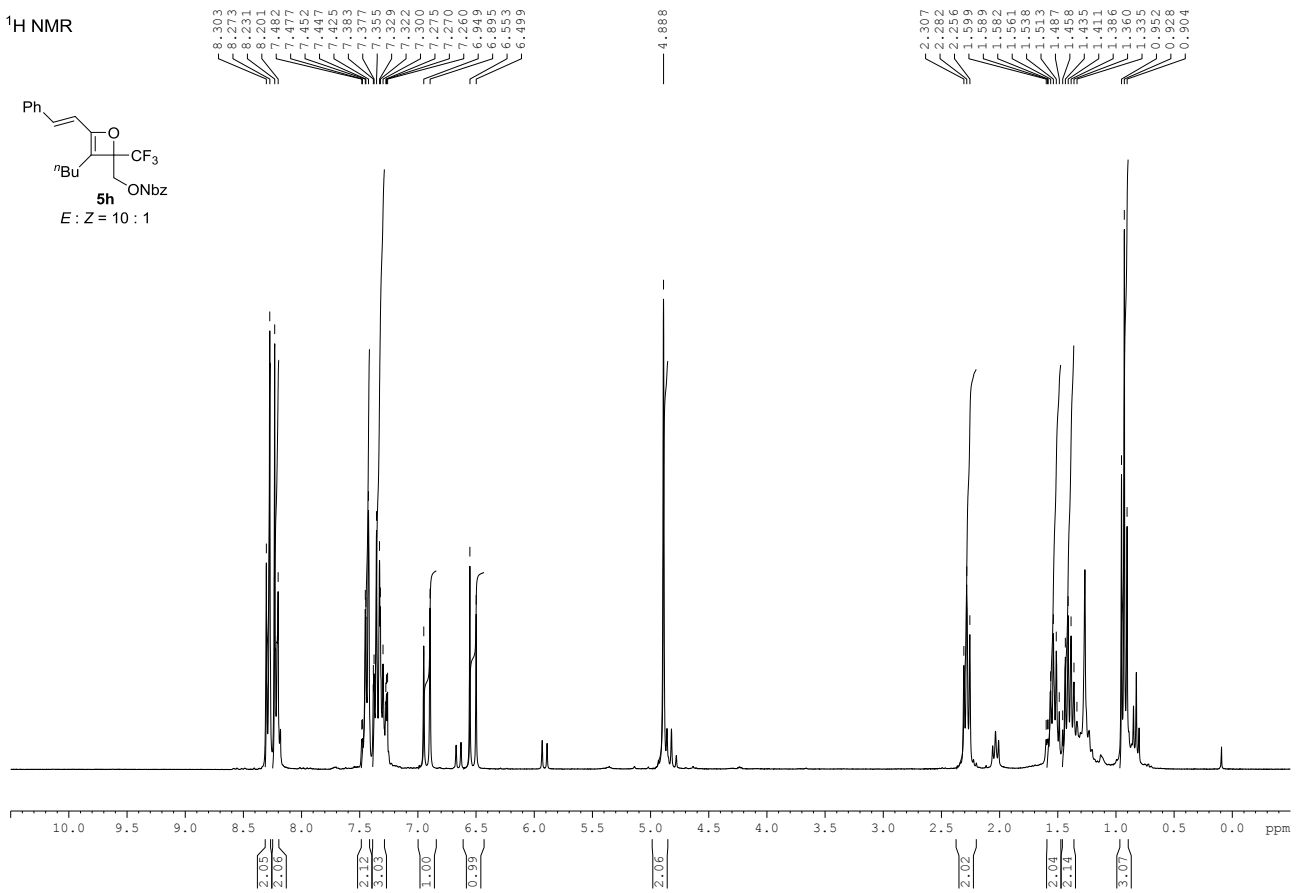


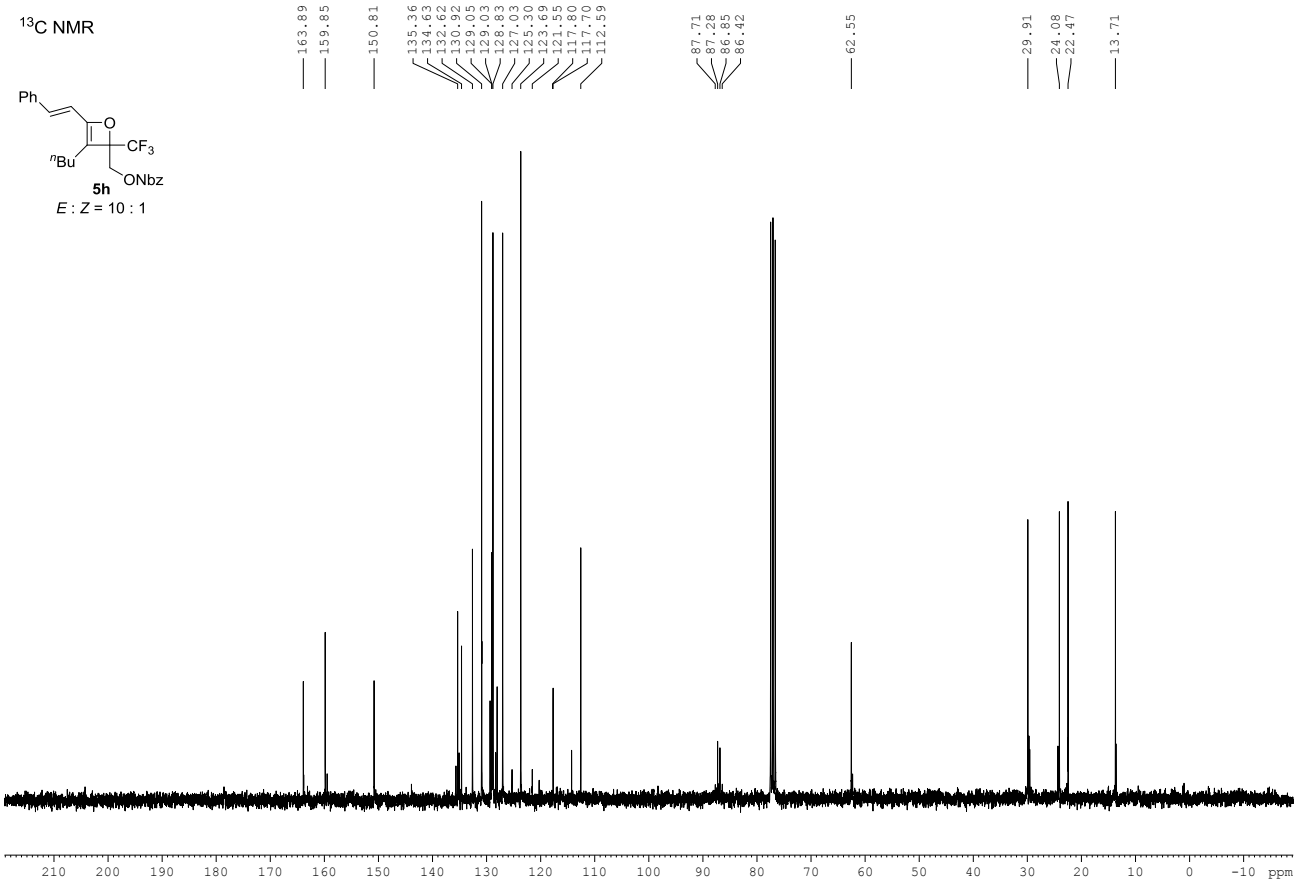
^{13}C NMR



^{19}F NMR



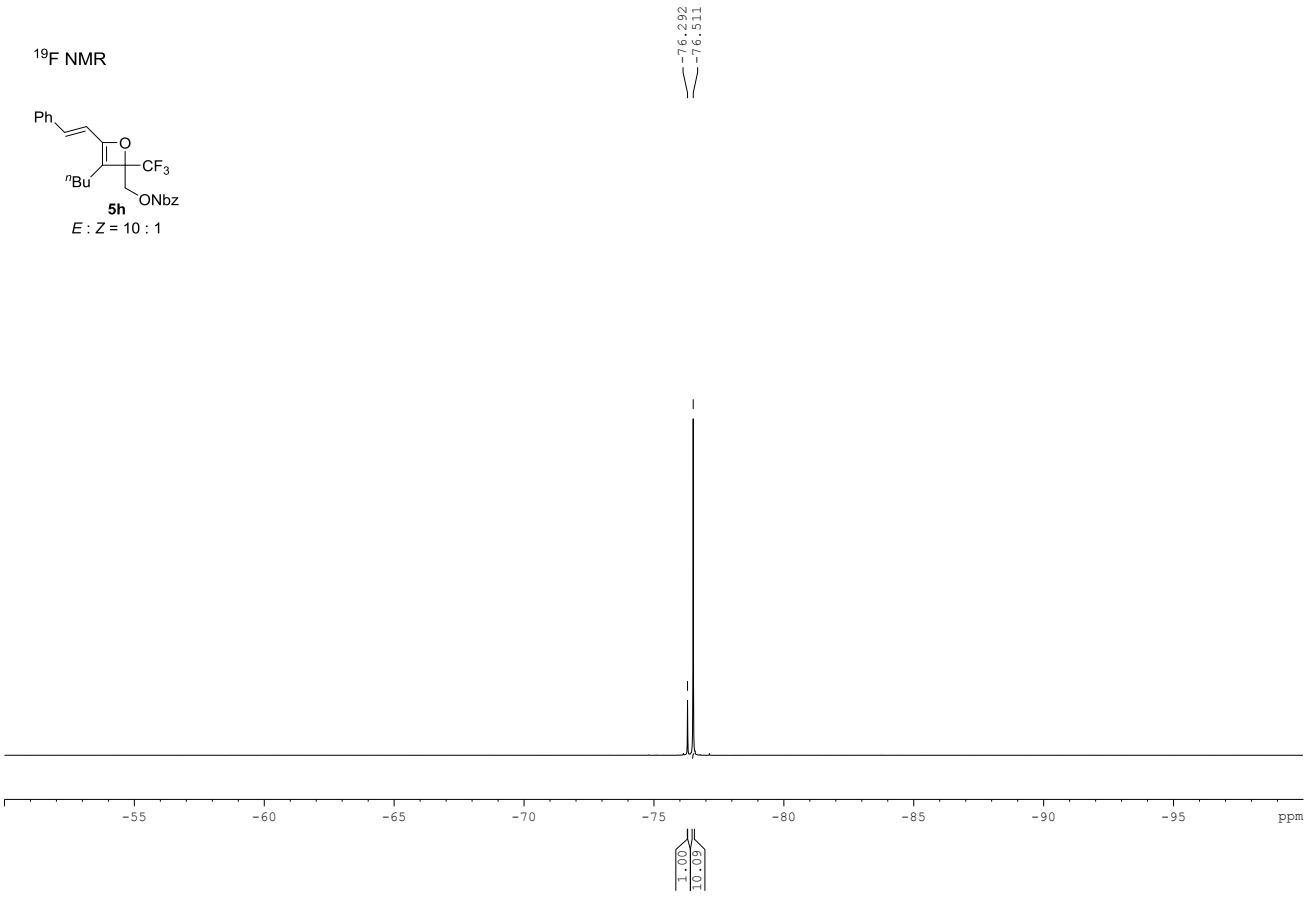

1H NMR
8.303
8.273
8.231
8.201
7.492
7.477
7.452
7.447
7.425
7.383
7.377
7.355
7.329
7.322
7.300
7.275
7.270
7.260
6.949
6.895
6.553
6.499
4.888
2.307
2.282
2.256
1.599
1.589
1.582
1.561
1.538
1.513
1.487
1.458
1.435
1.411
1.386
1.360
1.335
0.952
0.928
0.904
Ph
O
CF3
nBu
ONbz
5h
E : Z = 10 : 1
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
ppm
2.05
2.06
2.12
3.03
1.00
0.99
2.06
2.02
2.04
2.14
3.07


13C NMR
163.89
159.85
150.81
135.36
134.63
132.62
130.92
129.05
129.03
128.83
127.03
125.30
123.69
121.55
117.80
117.70
112.59
87.71
87.28
86.85
86.42
62.55
29.91
24.08
22.47
13.71
Ph
O
CF3
nBu
ONbz
5h
E : Z = 10 : 1
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
ppm

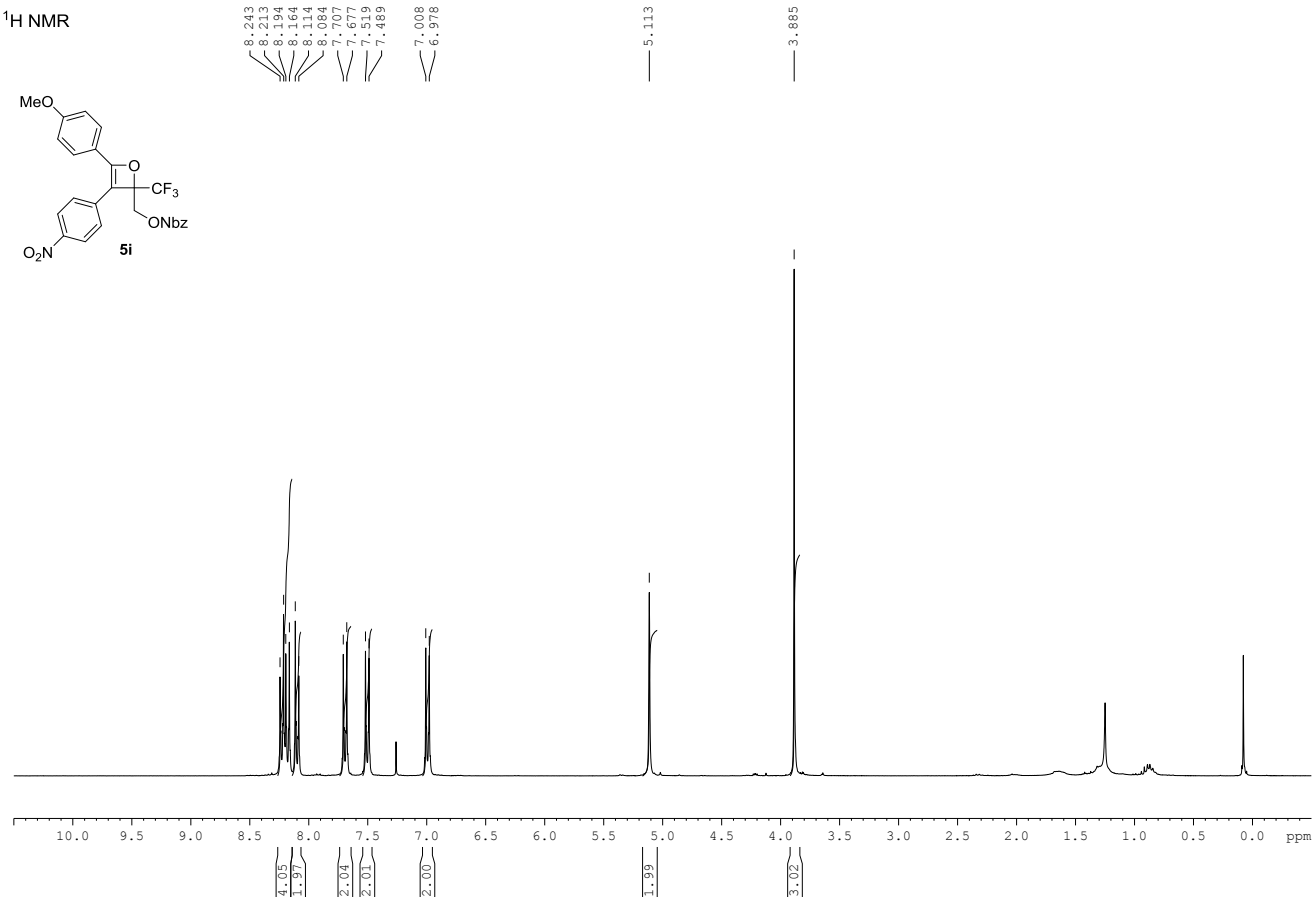
^{19}F NMR

5h

E : *Z* = 10 : 1



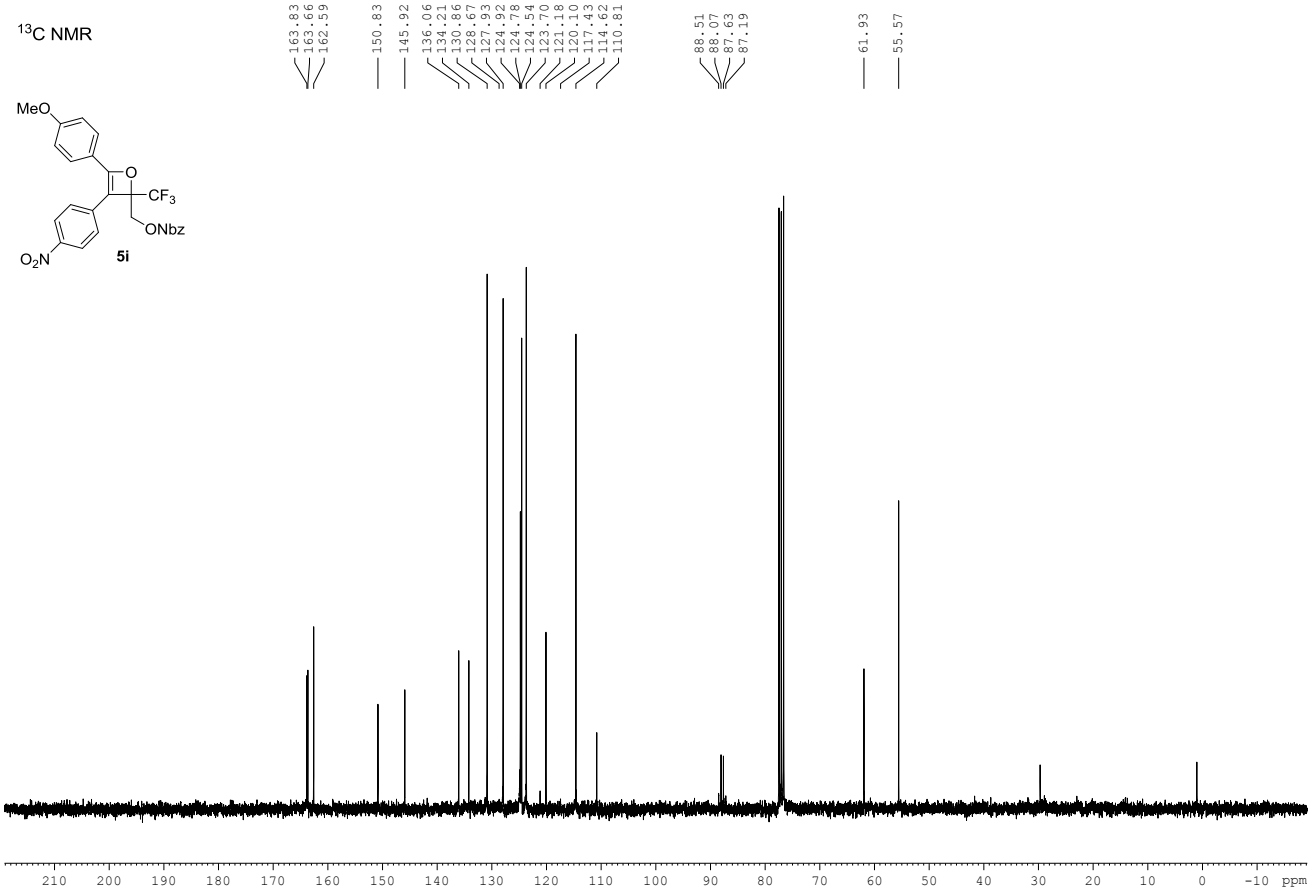
^{1}H NMR



5i

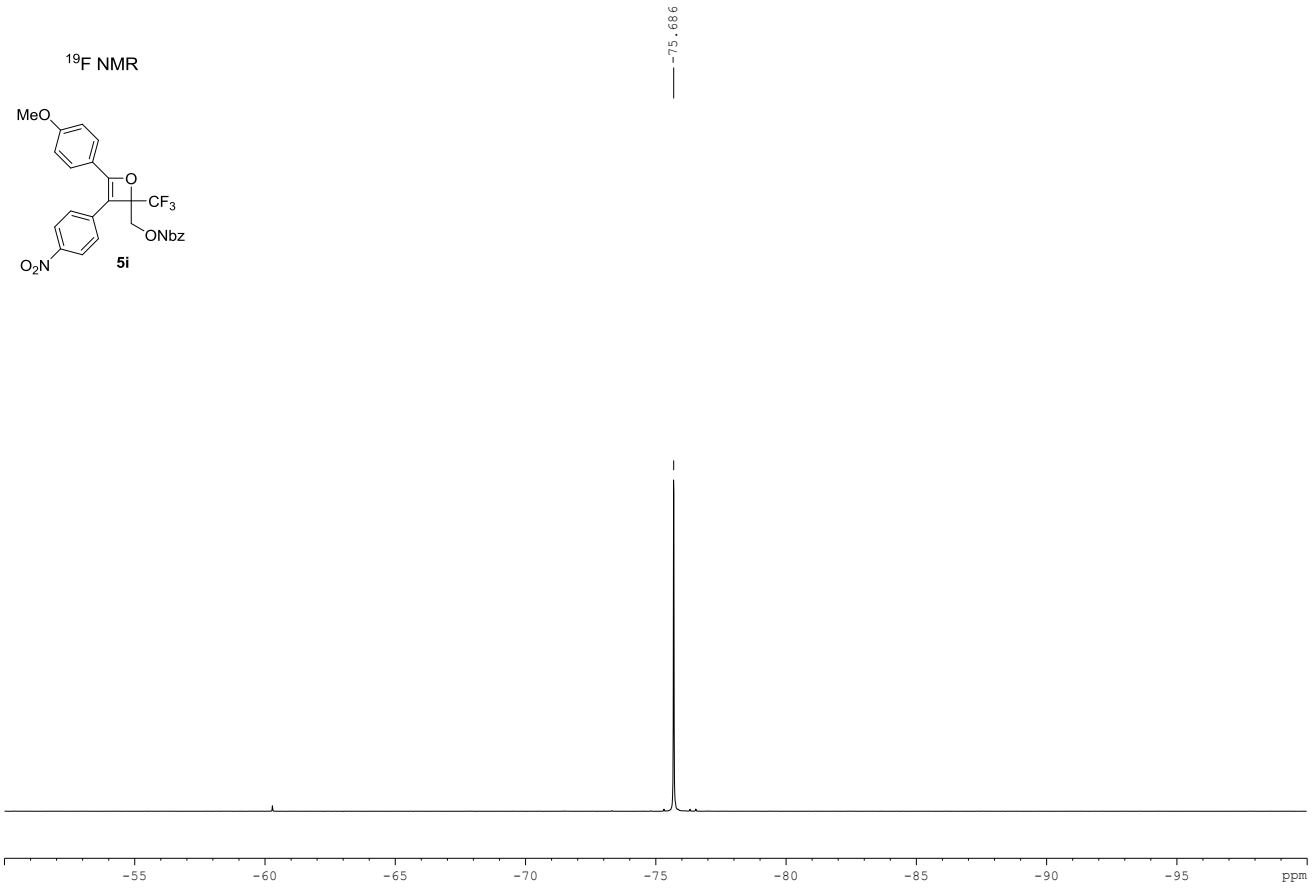
^{13}C NMR

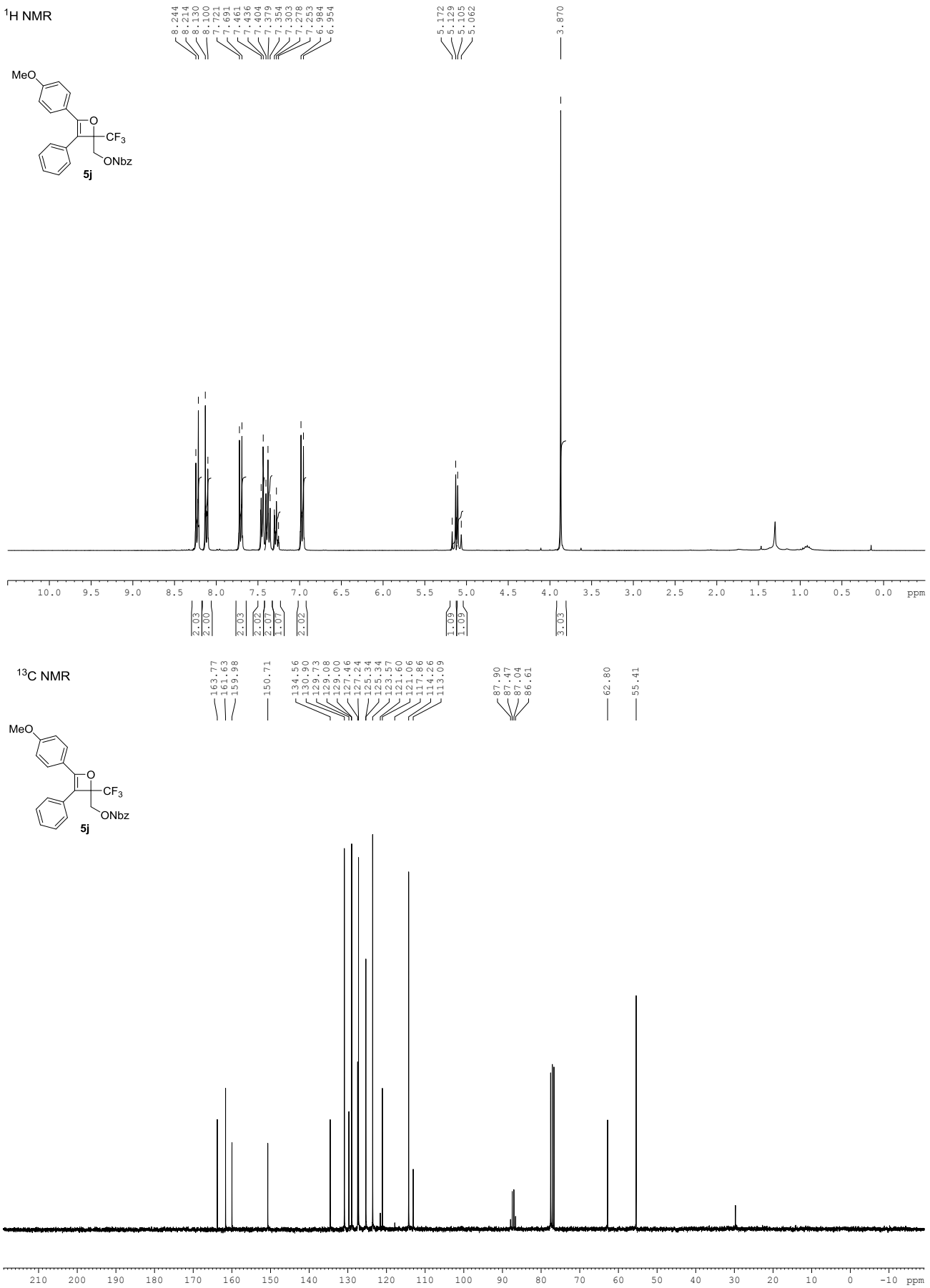
5i



^{19}F NMR

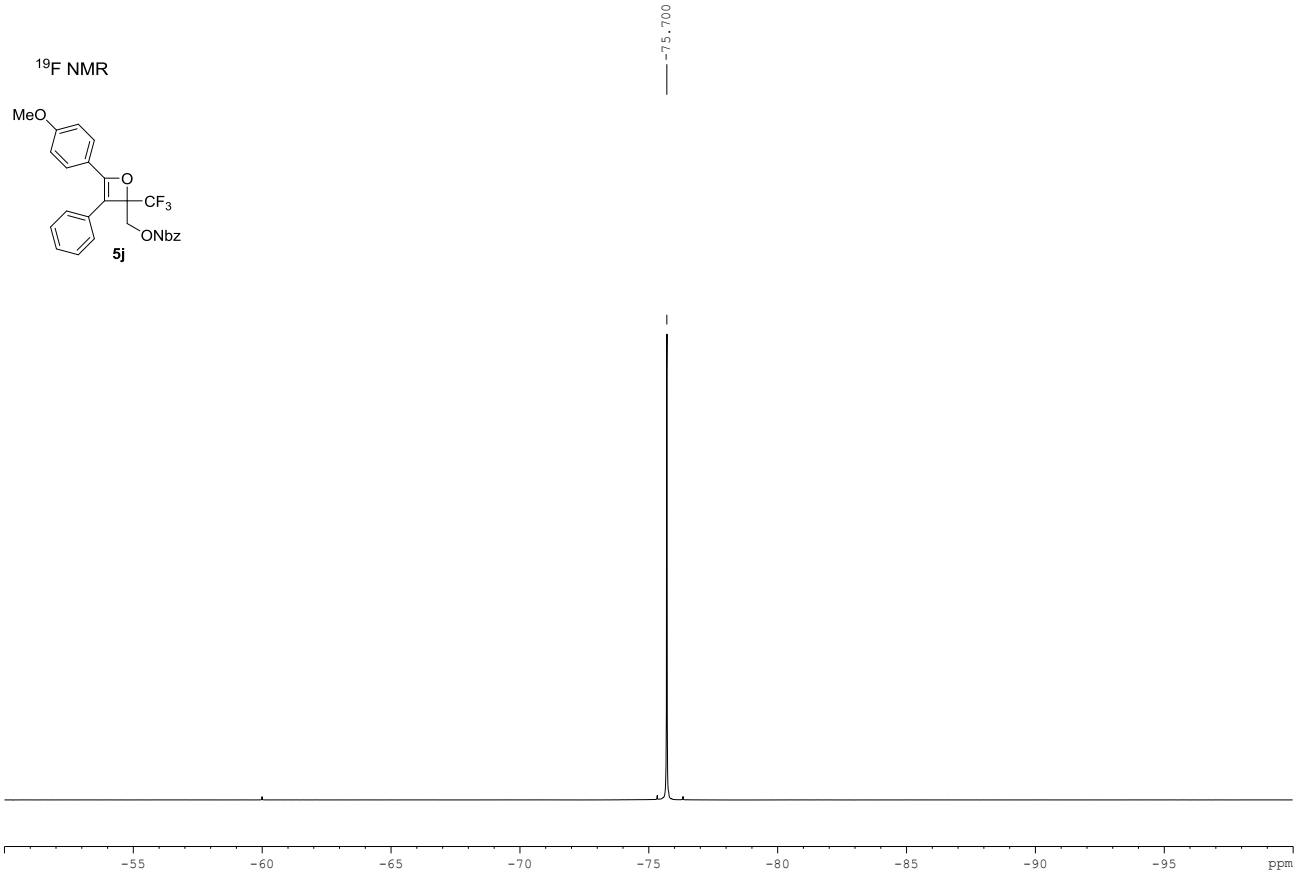
5i




1H NMR
8.244
8.214
8.130
8.100
7.721
7.691
7.461
7.436
7.404
7.379
7.354
7.303
7.278
7.253
6.984
6.954
5.172
5.129
5.105
5.062
3.870
MeO
O
CF3
ONbz
5j
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 ppm
2.03
2.00
2.03
2.02
2.07
1.07
2.02
1.09
1.09
3.03
13C NMR
163.77
161.63
159.98
150.71
134.56
130.90
129.73
129.08
129.00
127.46
127.24
125.34
125.34
123.57
121.60
121.06
117.86
114.26
113.09
87.90
87.47
87.04
86.61
62.80
55.41
MeO
O
CF3
ONbz
5j
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 ppm

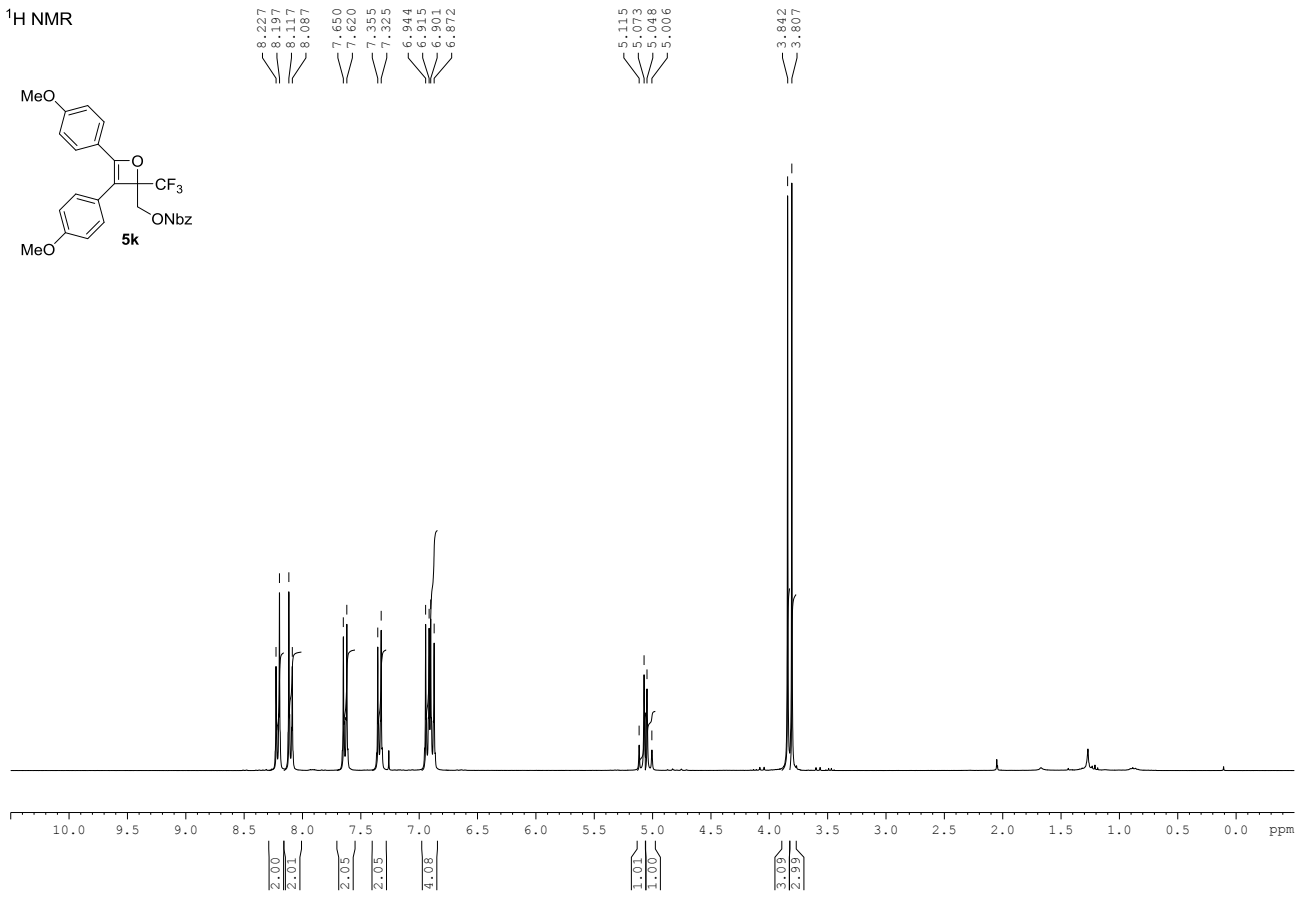
^{19}F NMR

5j

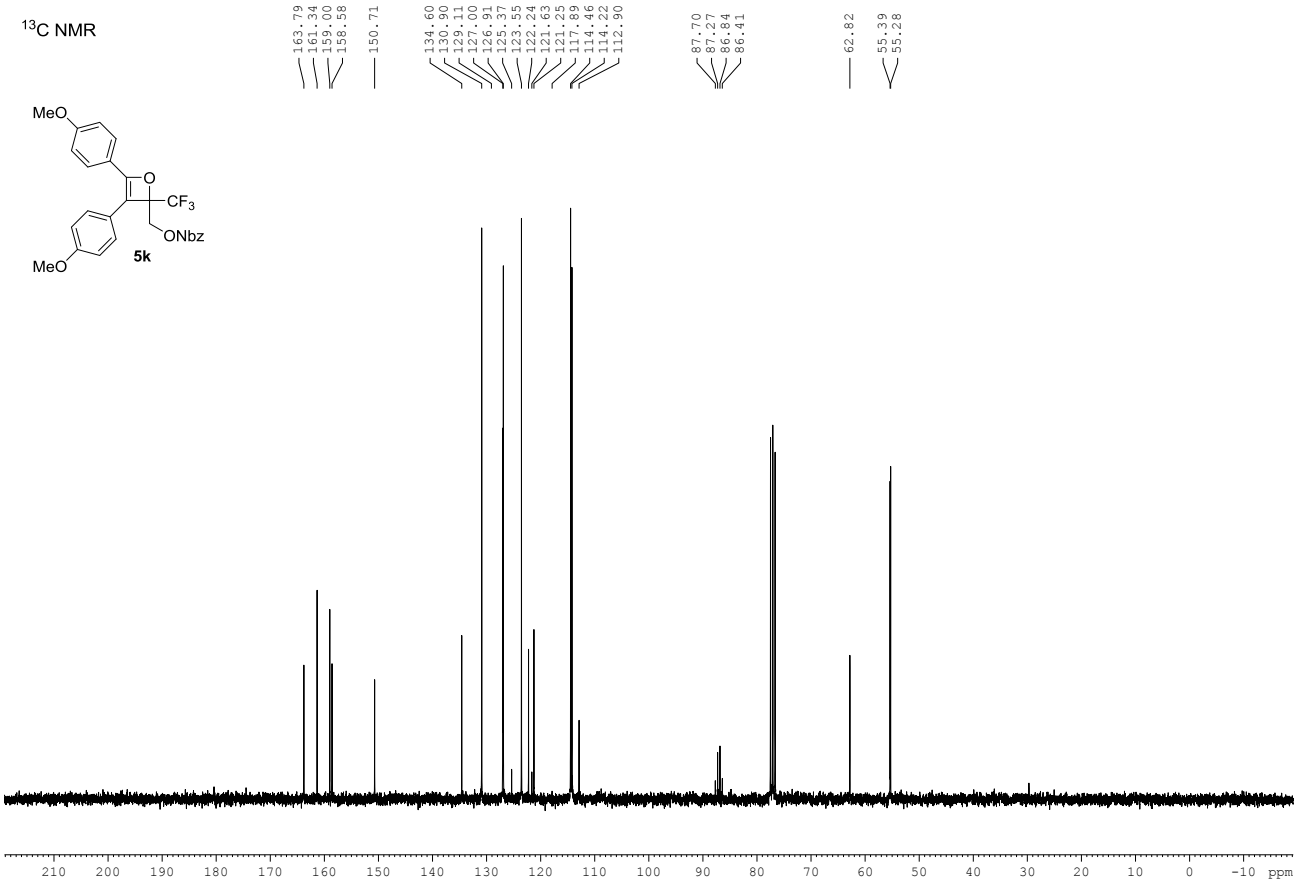


^{1}H NMR

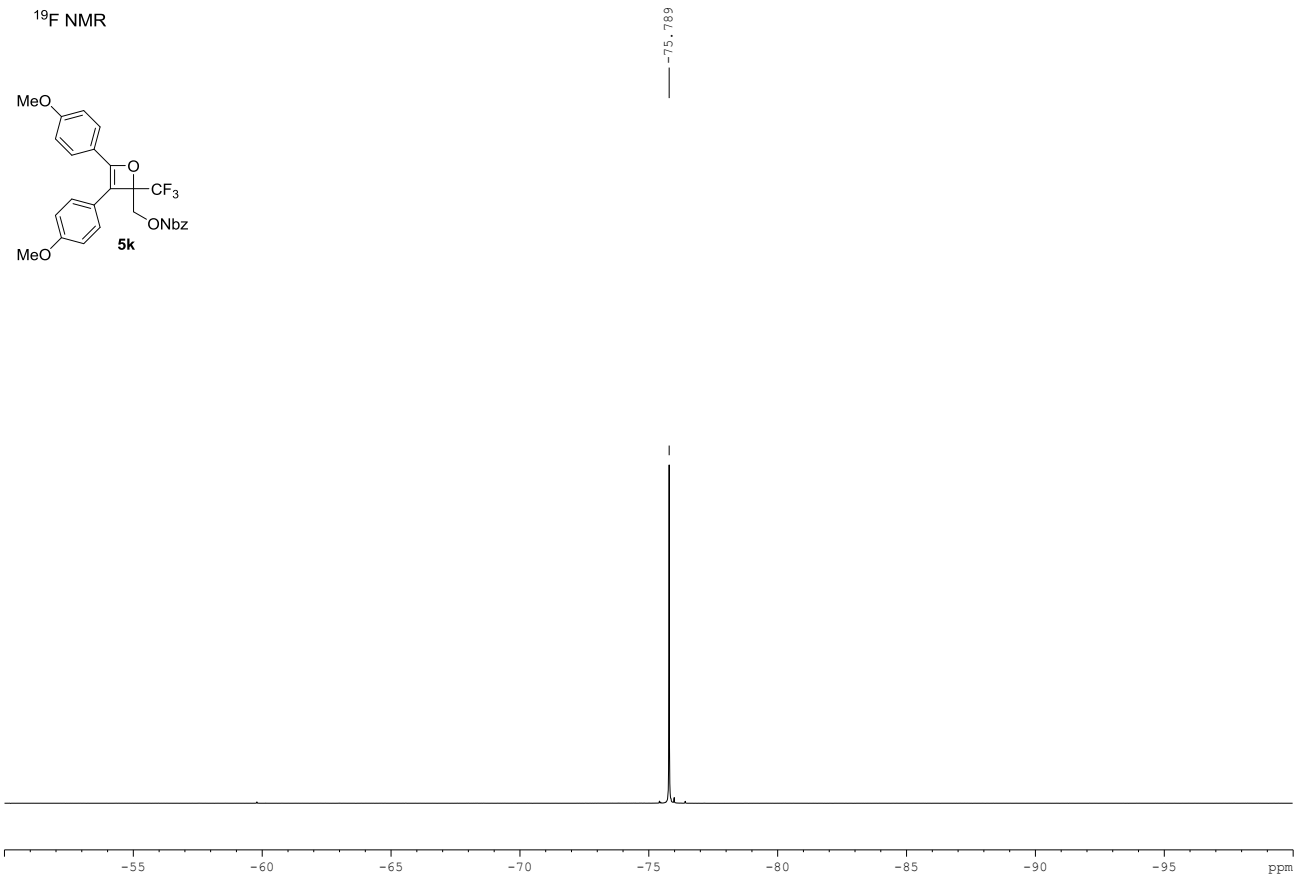
5k

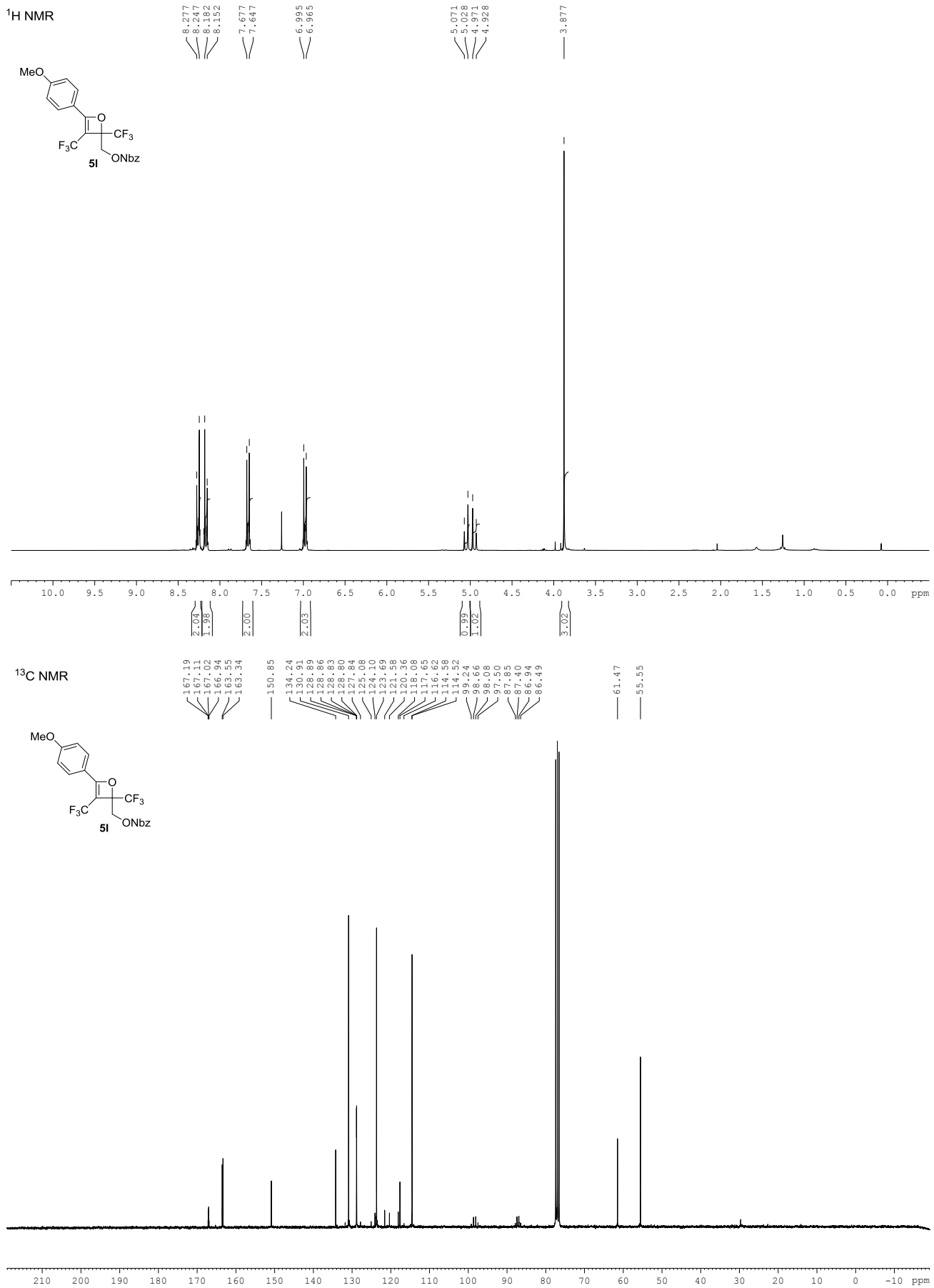


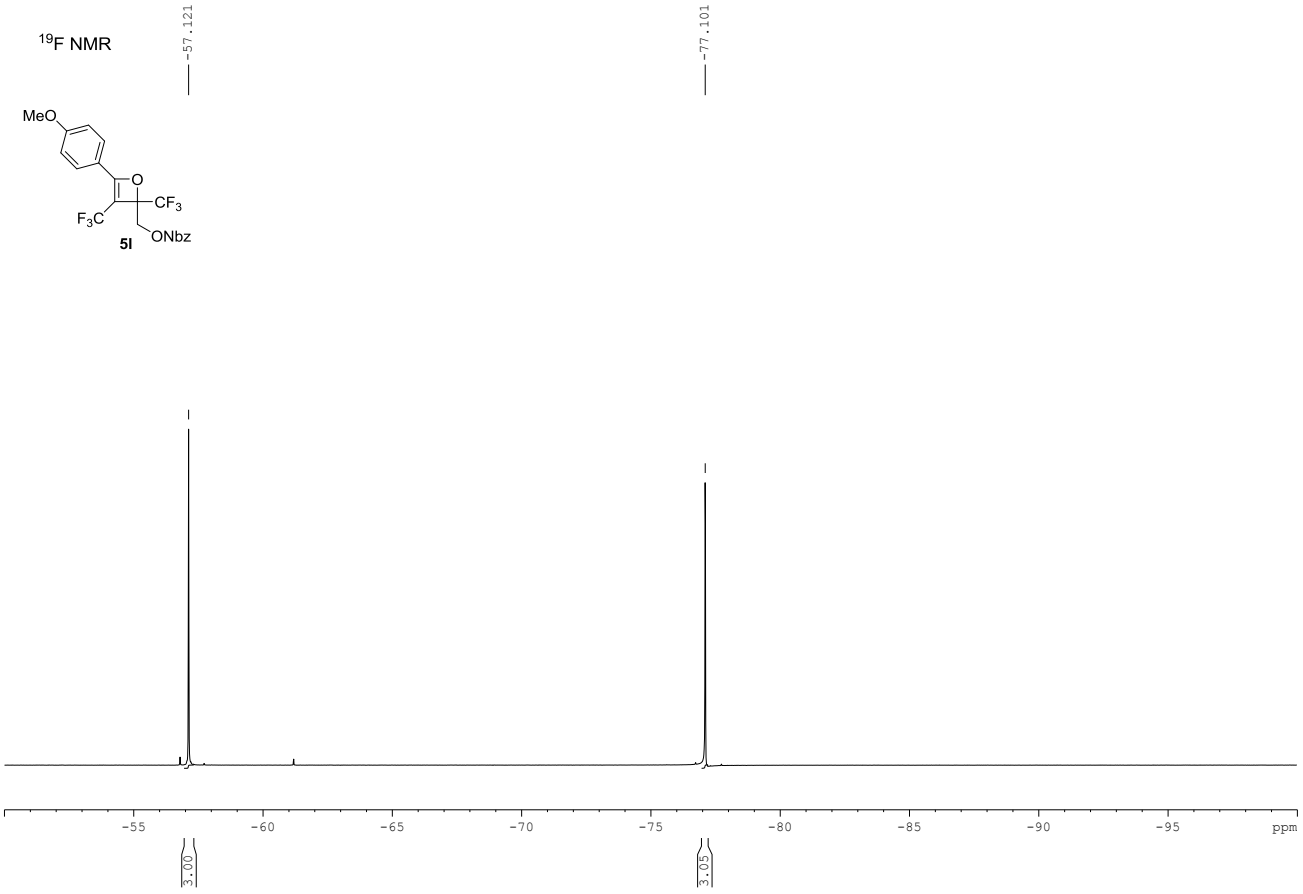
^{13}C NMR

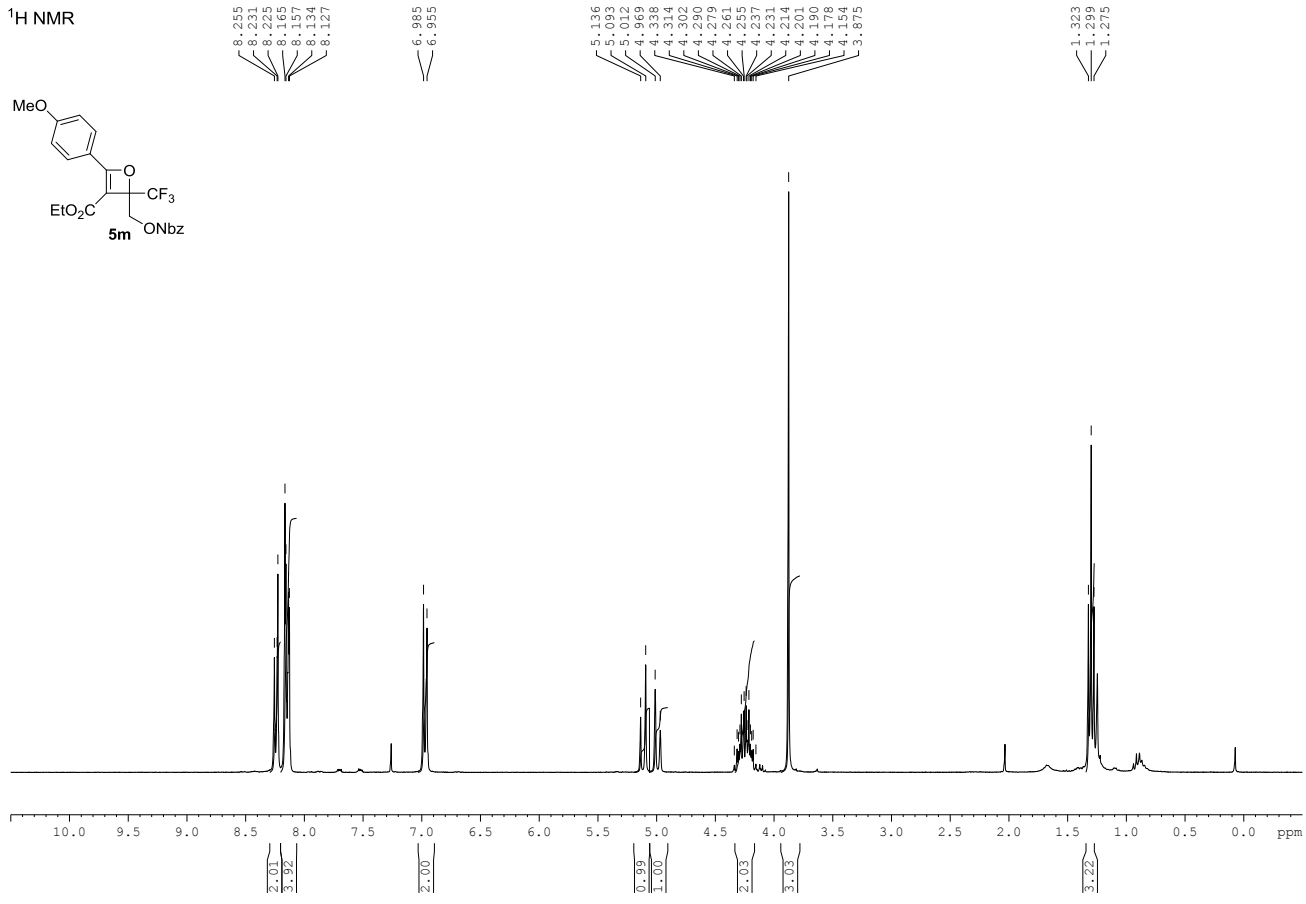


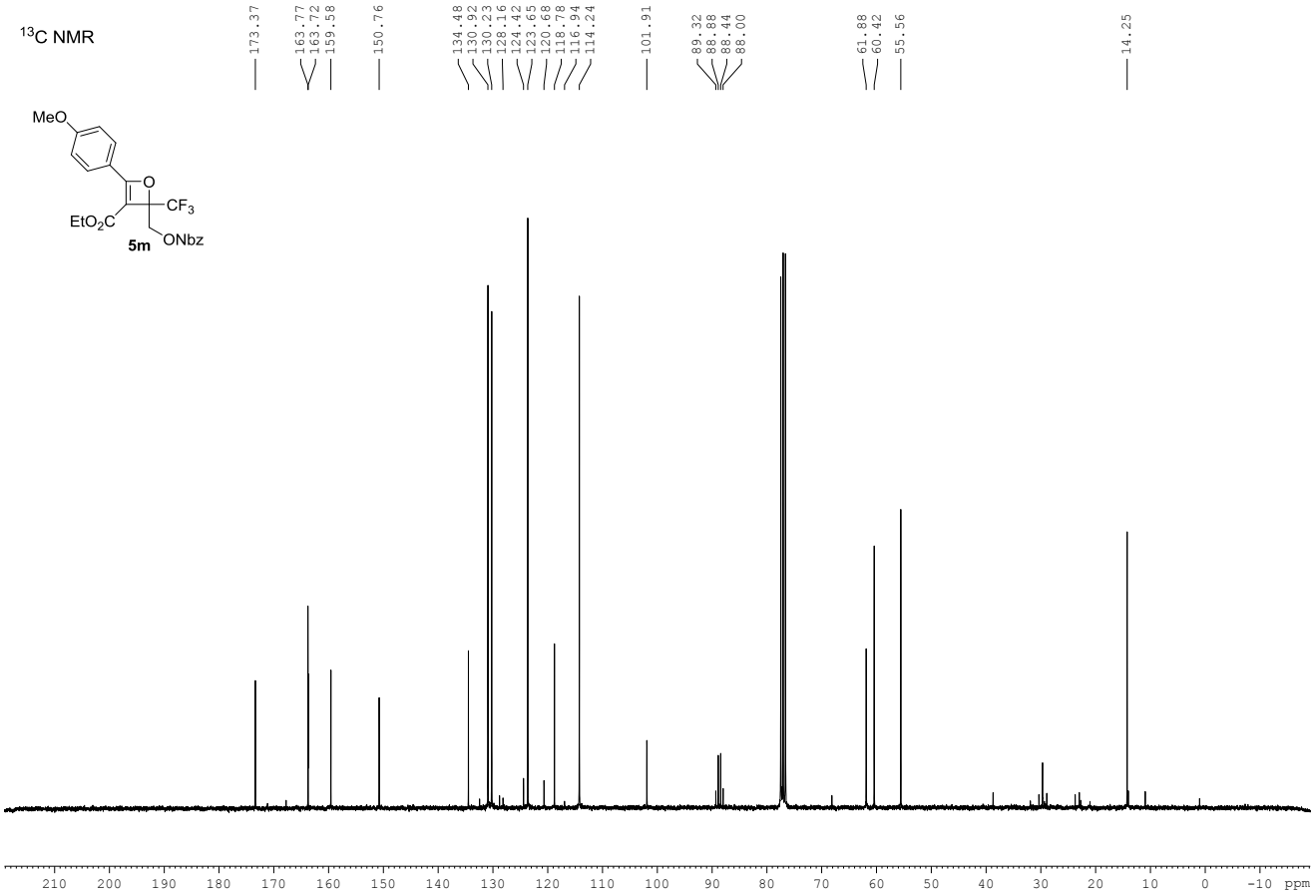
^{19}F NMR

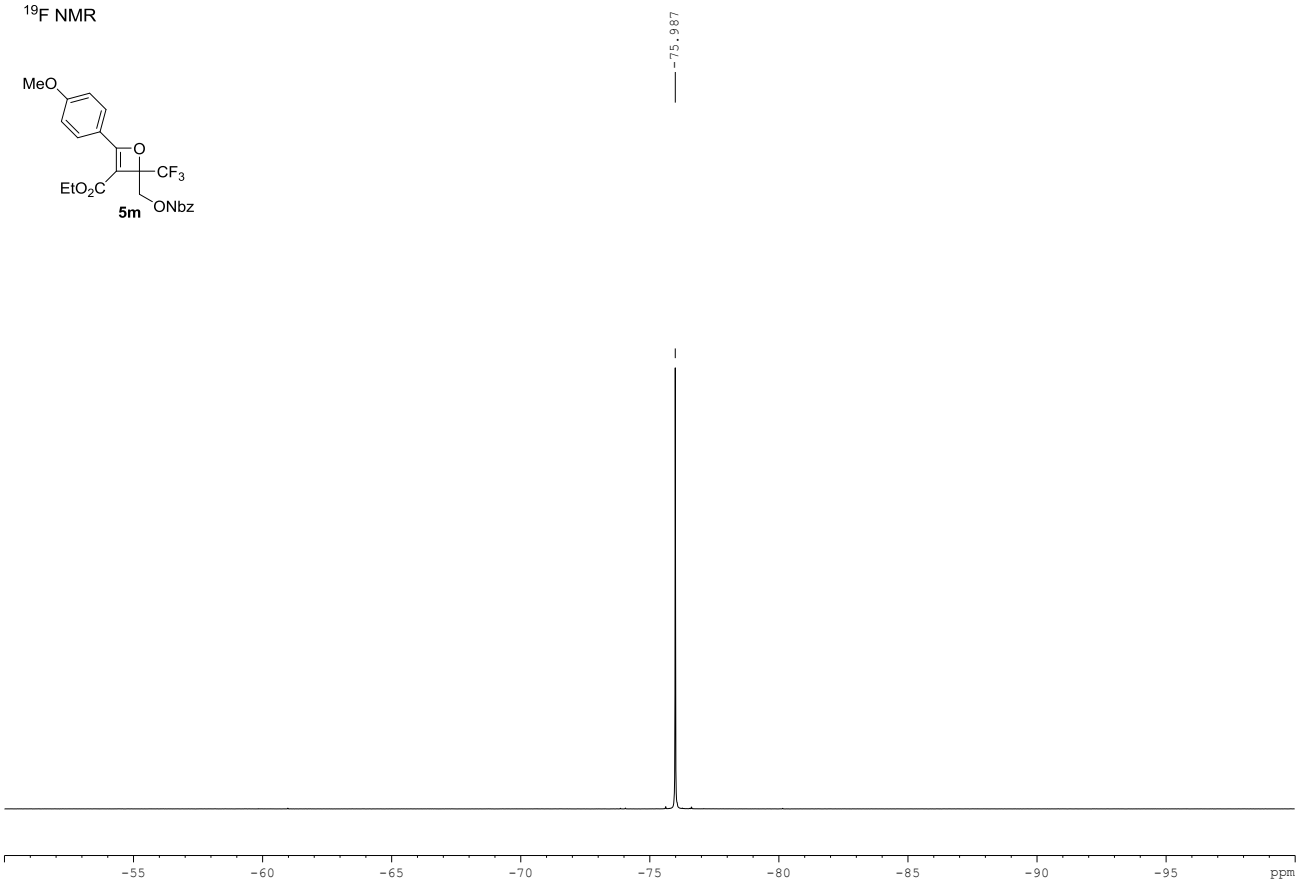



1H NMR
8.277
8.247
8.182
8.152
7.677
7.647
6.995
6.965
5.071
5.028
4.971
4.928
3.877
MeO
O
CF3
F3C
ONbz
5l
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 ppm
2.04
1.98
2.00
2.03
0.99
1.02
3.02
13C NMR
167.19
167.11
167.02
166.94
163.55
163.34
150.85
134.24
130.91
128.89
128.86
128.83
128.80
127.84
125.08
124.10
123.69
121.58
120.36
118.08
117.65
116.62
114.58
114.52
99.24
98.66
98.08
97.50
87.85
87.40
86.94
86.49
61.47
55.55
MeO
O
CF3
F3C
ONbz
5l
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 ppm

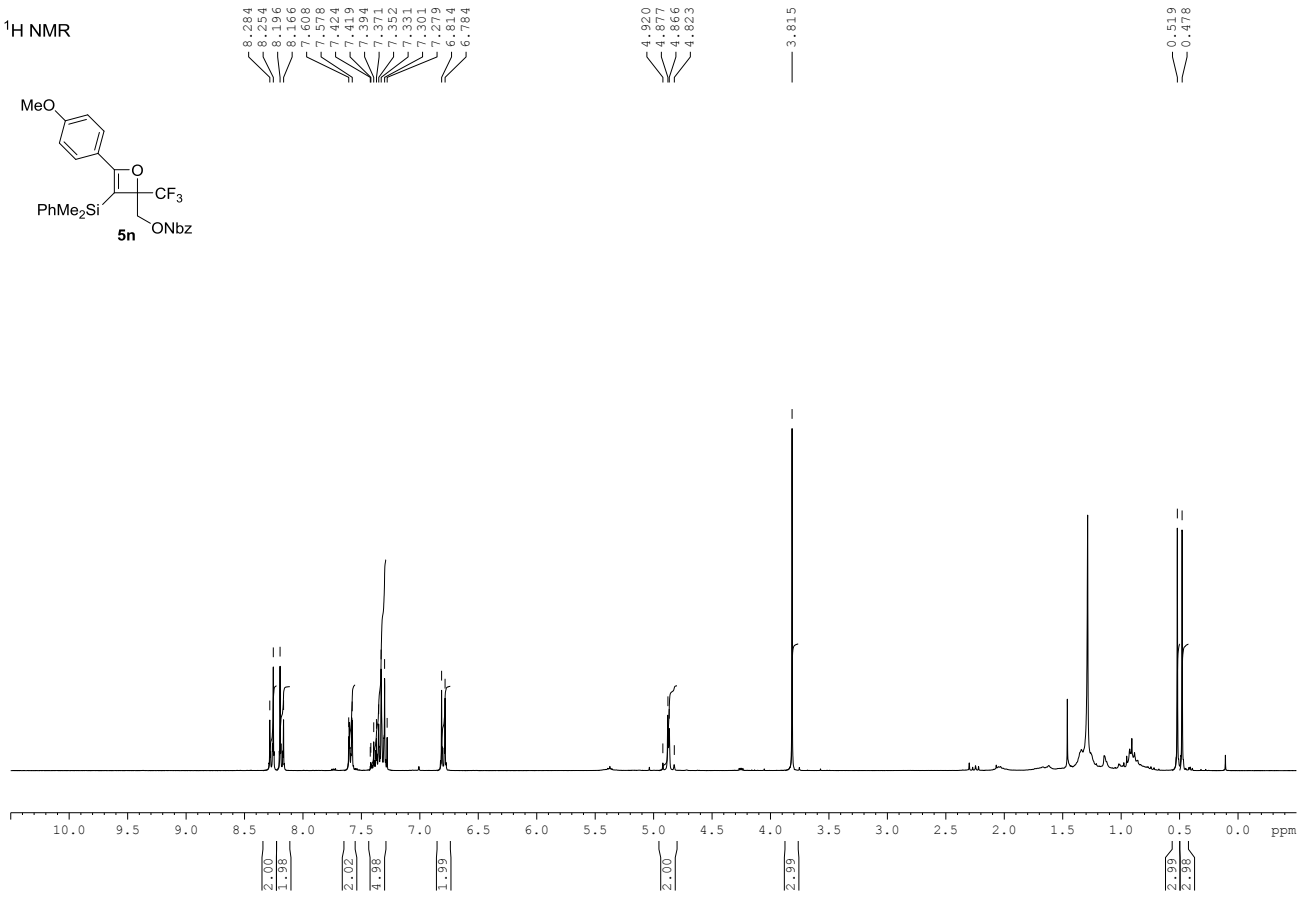

19F NMR
-57.121
-77.101
MeO
O
CF3
F3C
ONbz
5l
-55
-60
-65
-70
-75
-80
-85
-90
-95
ppm
3.00
3.05


1H NMR
8.255
8.231
8.225
8.165
8.157
8.134
8.127
6.985
6.955
5.136
5.093
5.012
4.969
4.338
4.314
4.302
4.290
4.279
4.261
4.255
4.237
4.231
4.214
4.201
4.190
4.178
4.154
3.875
1.323
1.299
1.275
MeO
O
CF3
EtO2C
ONbz
5m
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
ppm
2.01
3.92
2.00
0.99
1.00
2.03
3.03
3.22

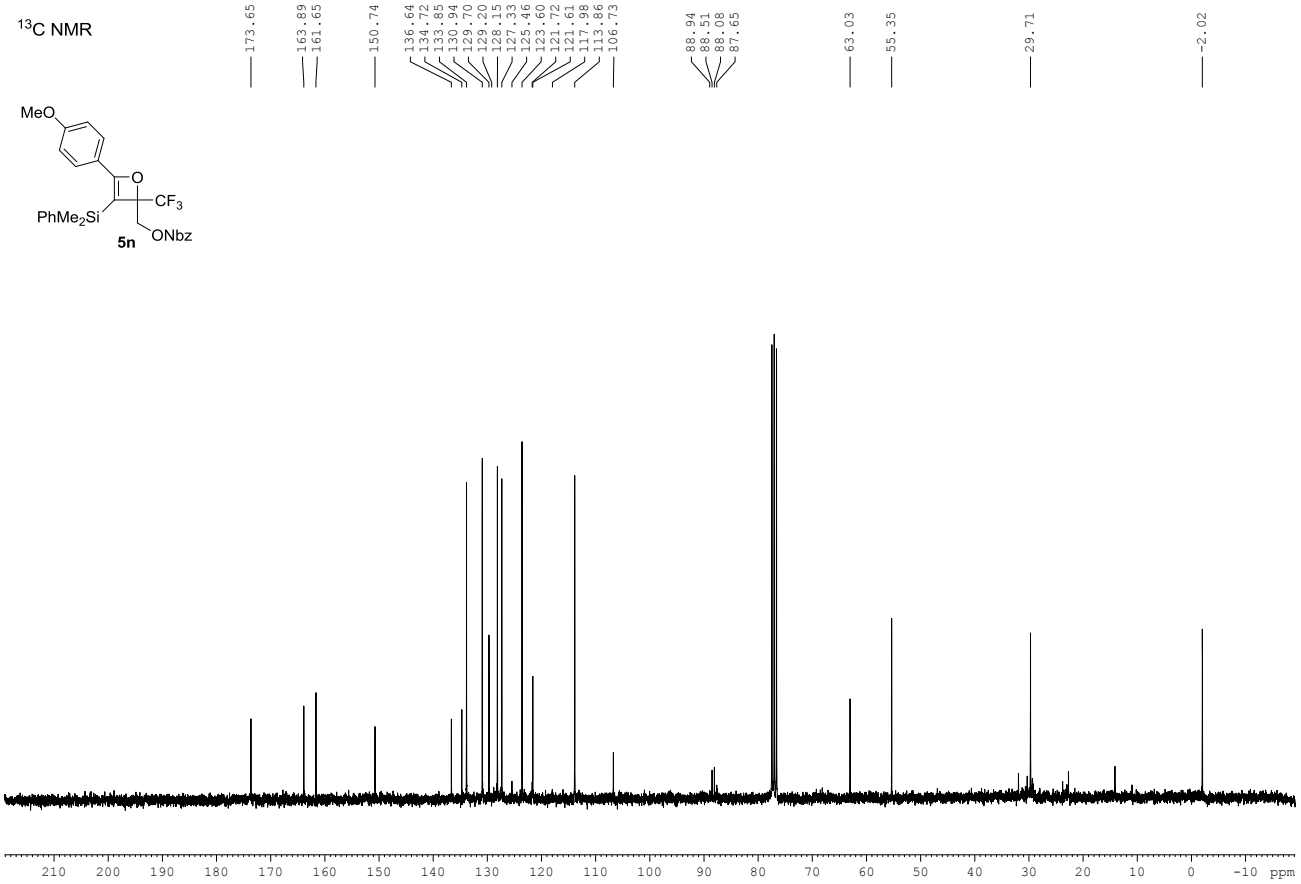

13C NMR
173.37
163.77
163.72
159.58
150.76
134.48
130.92
130.23
128.16
124.42
123.65
120.68
118.78
116.94
114.24
101.91
89.32
88.88
88.44
88.00
61.88
60.42
55.56
14.25
MeO
O
CF3
EtO2C
ONbz
5m
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 ppm


19F NMR
-75.987
MeO
O
CF3
EtO2C
ONbz
5m
-55 -60 -65 -70 -75 -80 -85 -90 -95 ppm

^{1}H NMR

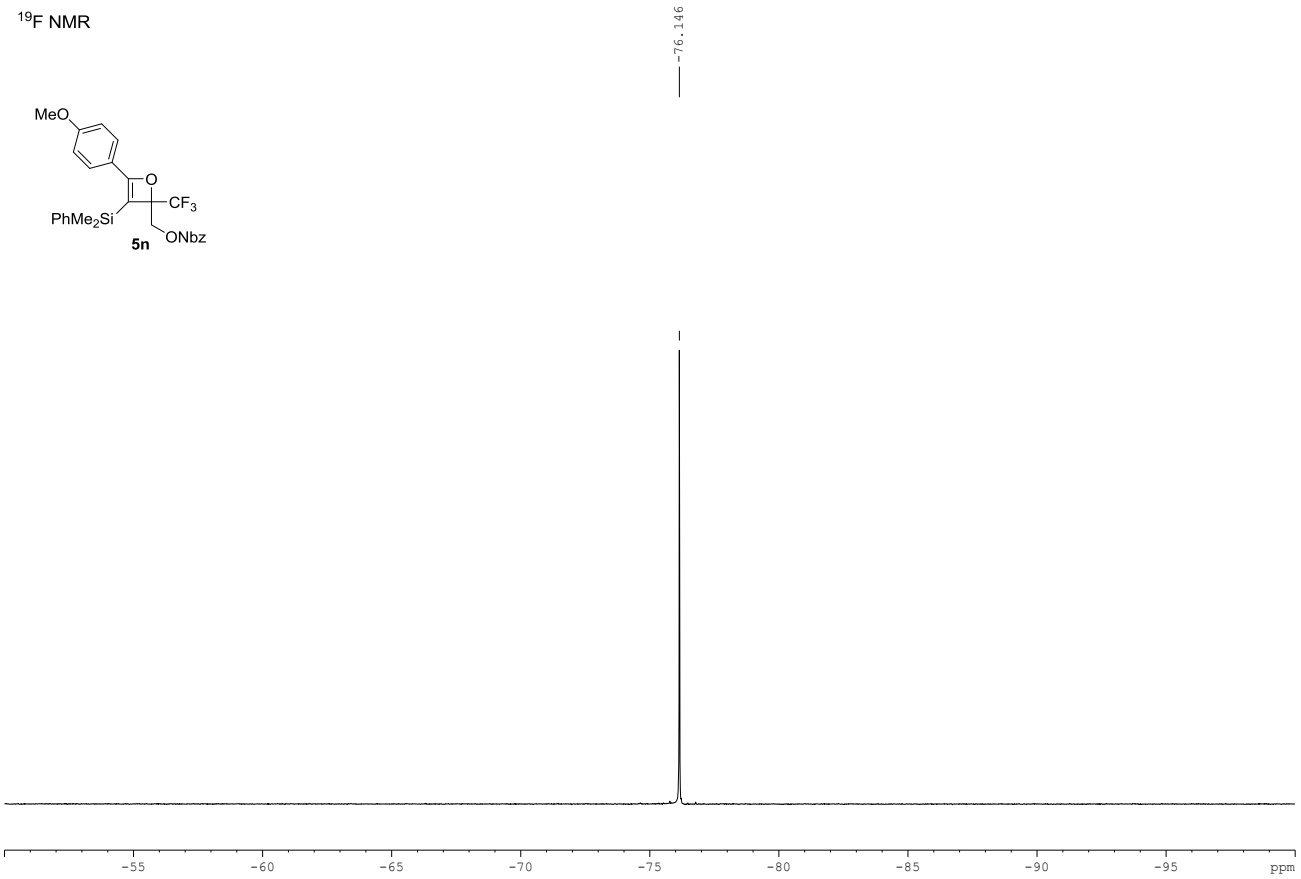


^{13}C NMR



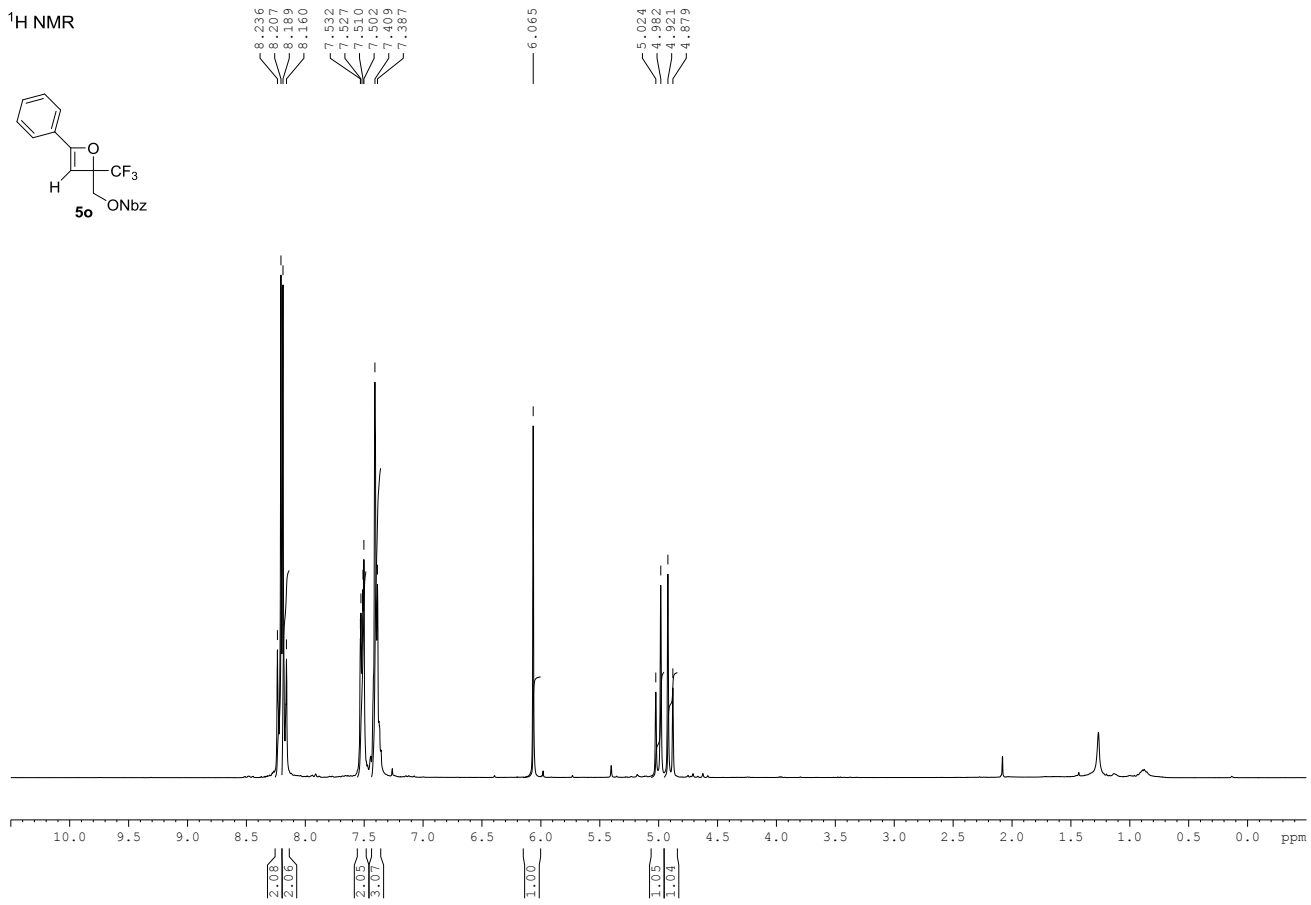
^{19}F NMR

5n



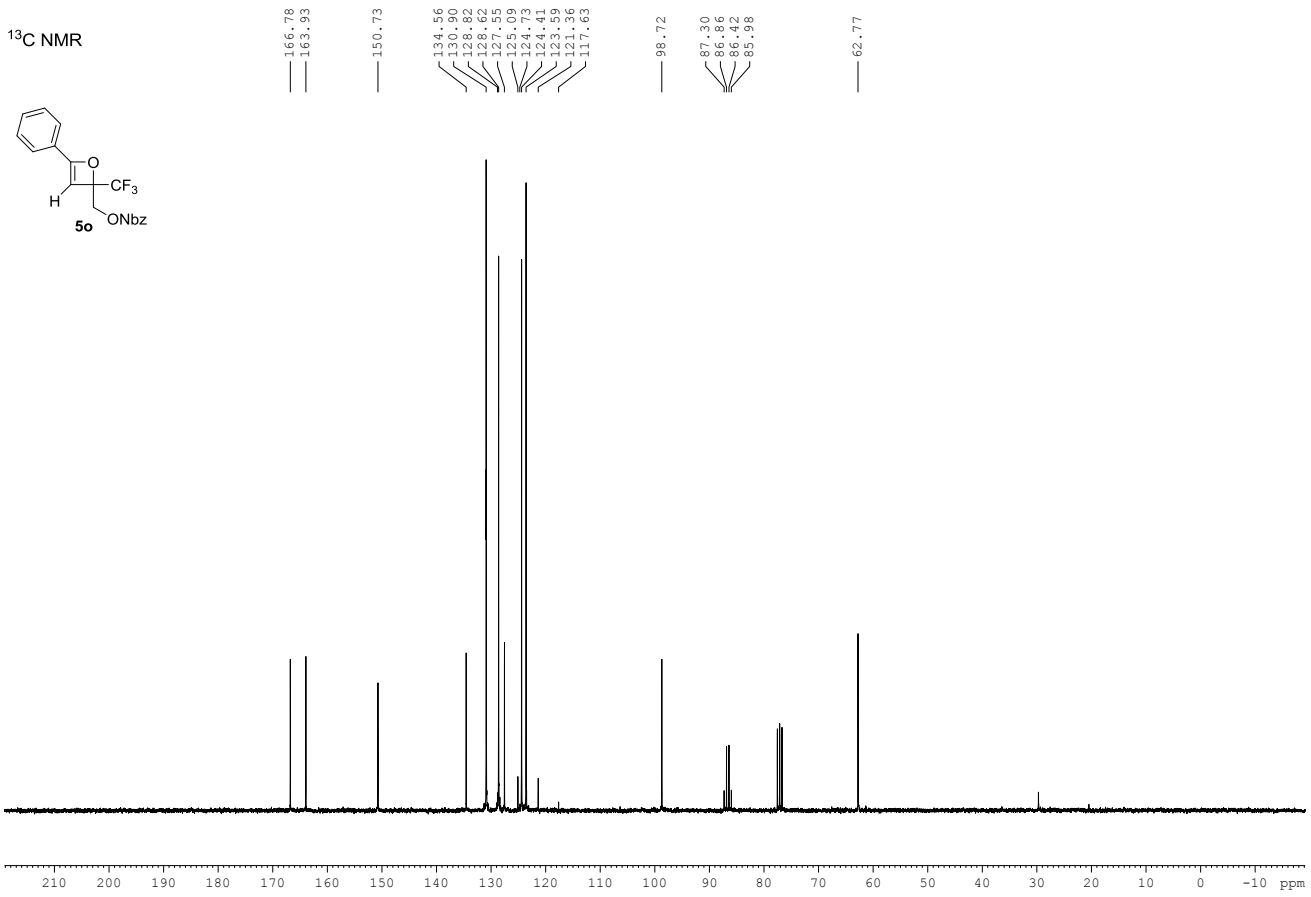
^{1}H NMR

5o



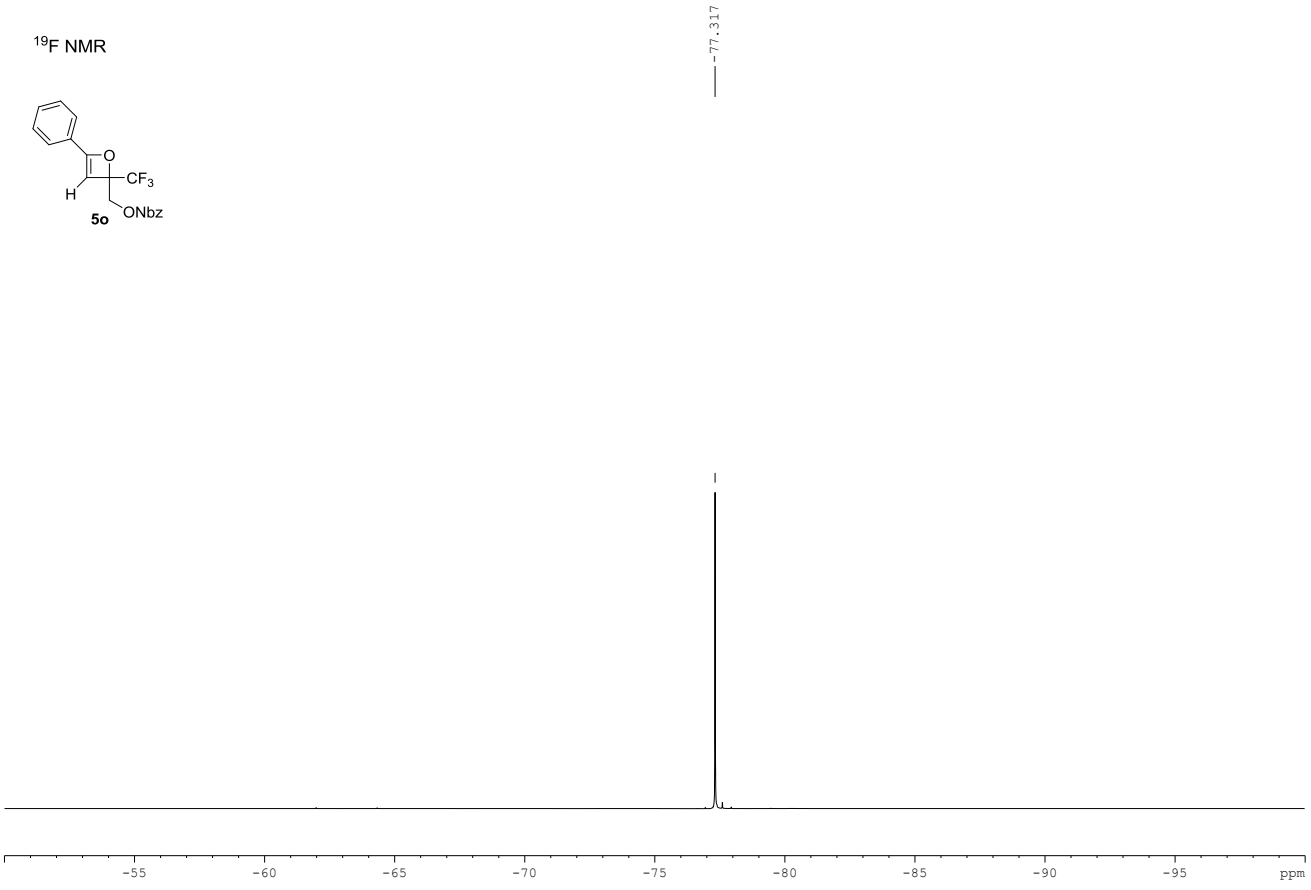
^{13}C NMR

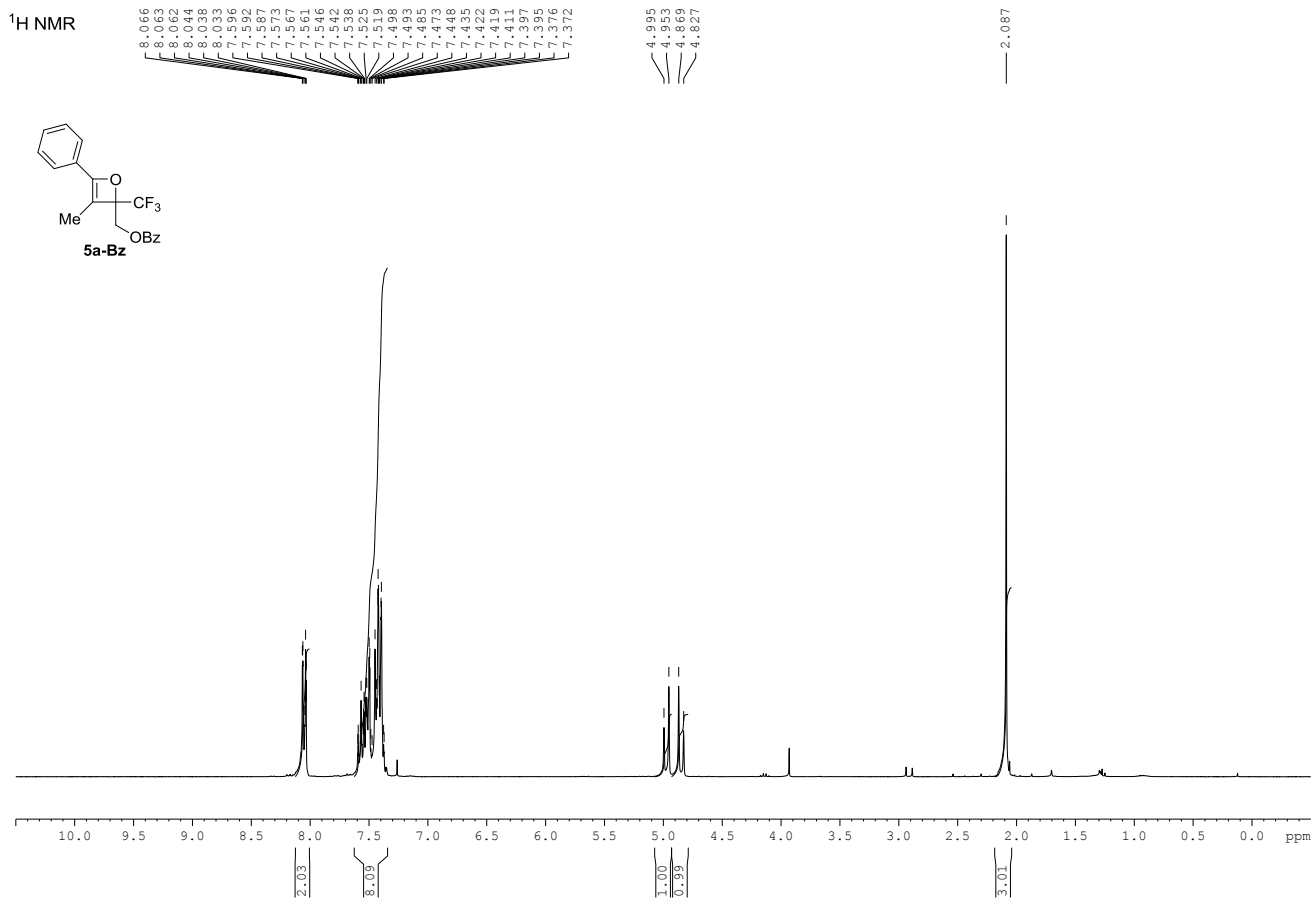
5o

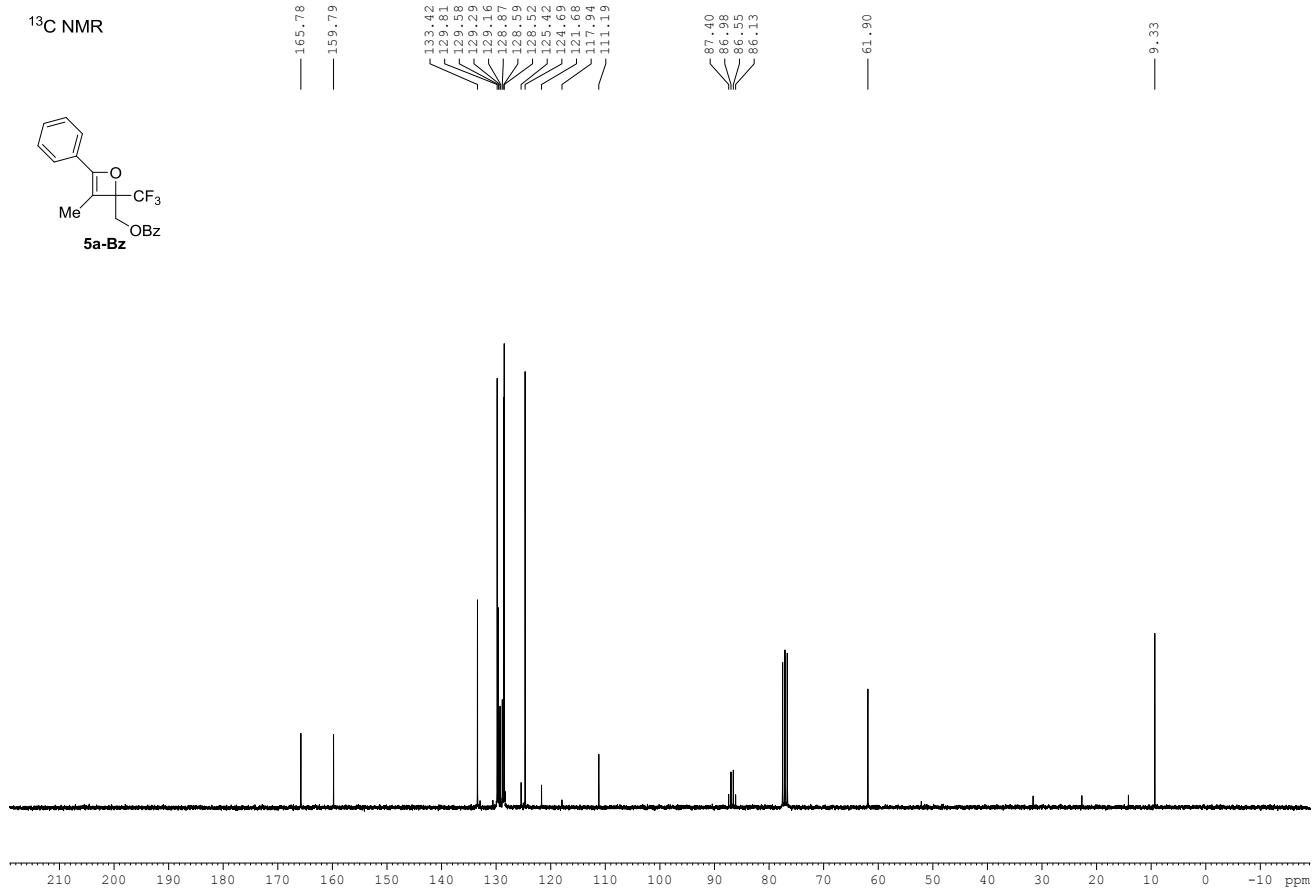


^{19}F NMR

5o

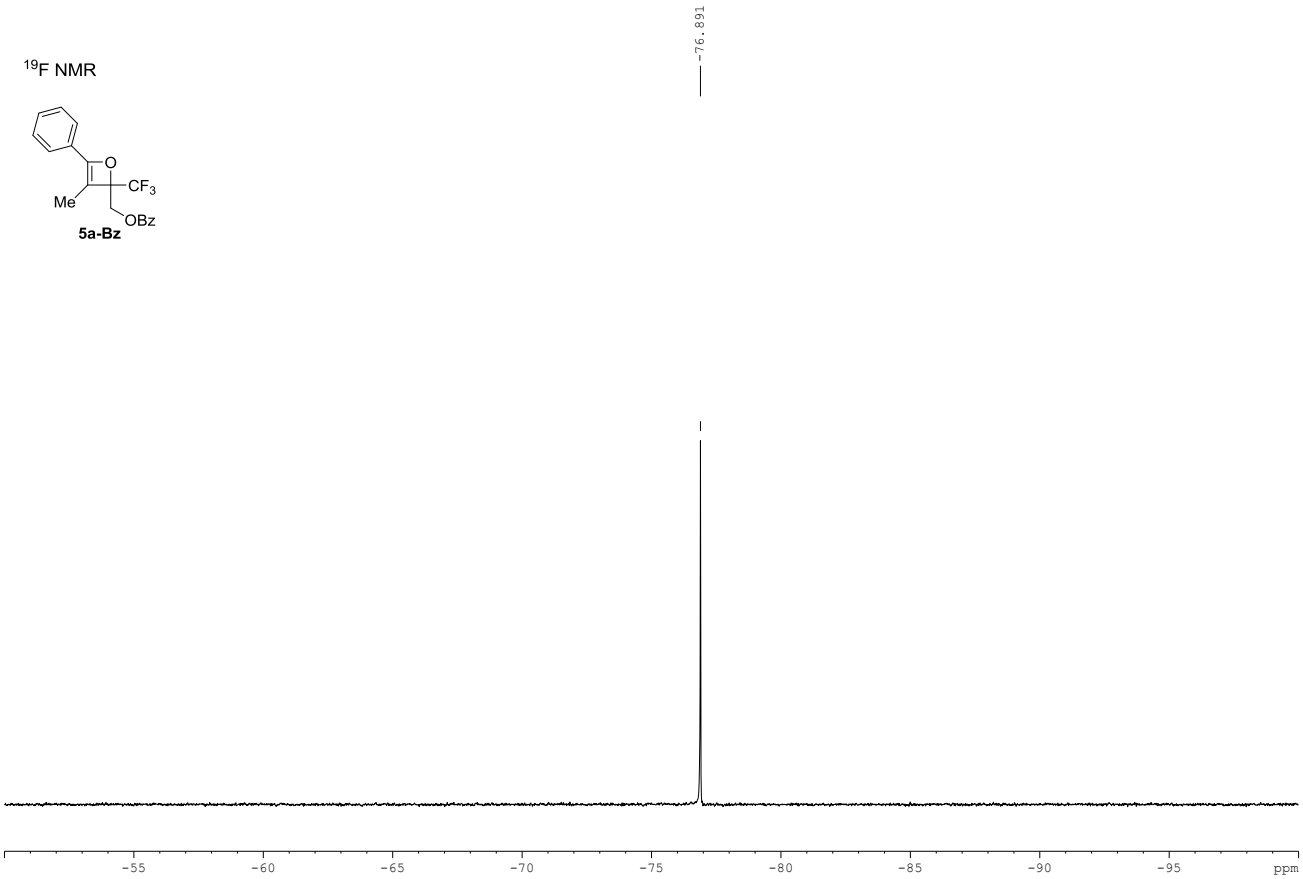



1H NMR
8.066
8.063
8.062
8.044
8.038
8.033
7.596
7.592
7.587
7.573
7.567
7.561
7.546
7.542
7.538
7.525
7.519
7.498
7.493
7.485
7.473
7.448
7.435
7.422
7.419
7.411
7.397
7.395
7.376
7.372
4.995
4.953
4.869
4.827
2.087
O
CF3
Me
OBz
5a-Bz
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
ppm
2.03
8.09
1.00
0.99
3.01


13C NMR
165.78
159.79
133.42
129.81
129.58
129.29
129.16
128.87
128.59
128.52
125.42
124.69
121.68
117.94
111.19
87.40
86.98
86.55
86.13
61.90
9.33
O
CF3
Me
OBz
5a-Bz
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
ppm

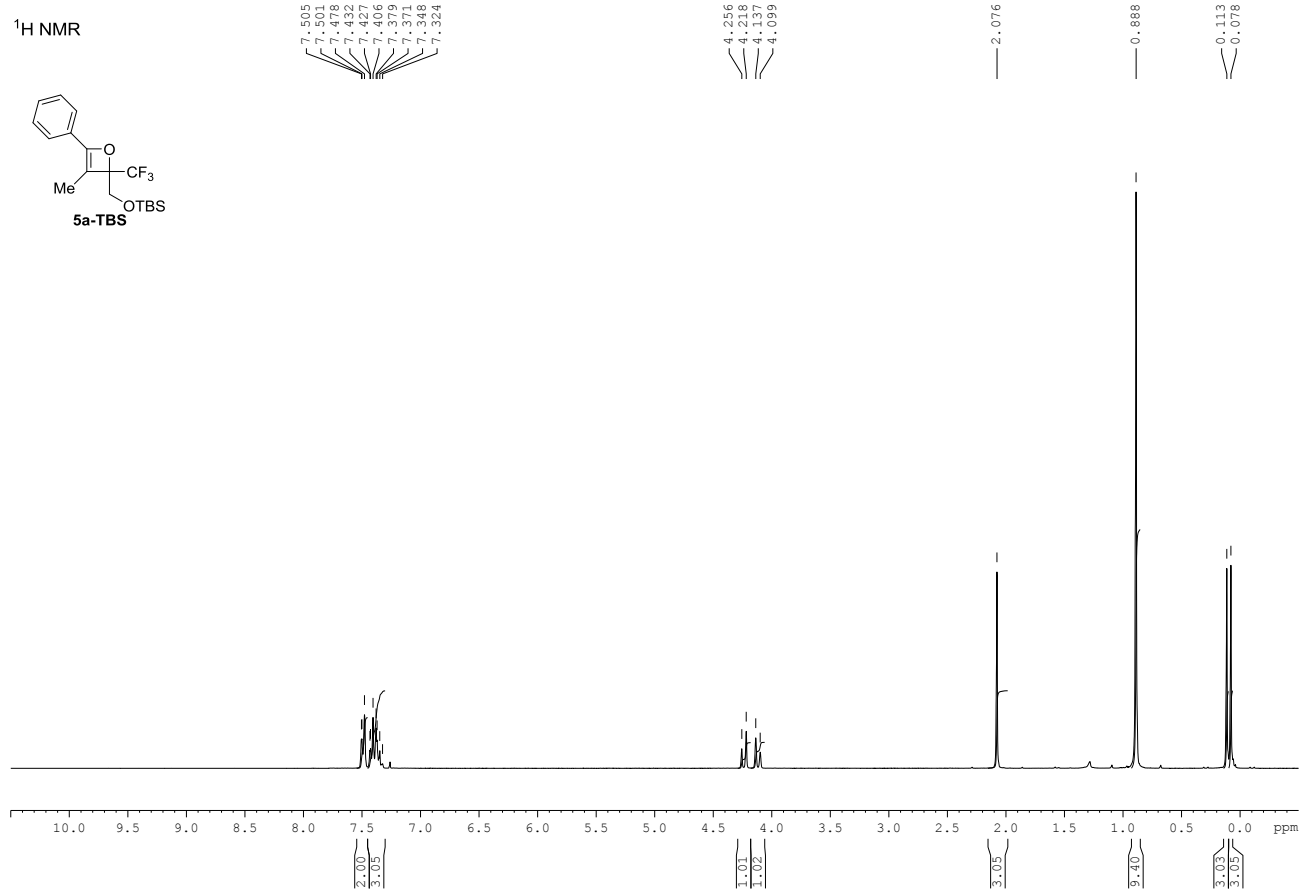
^{19}F NMR

5a-Bz

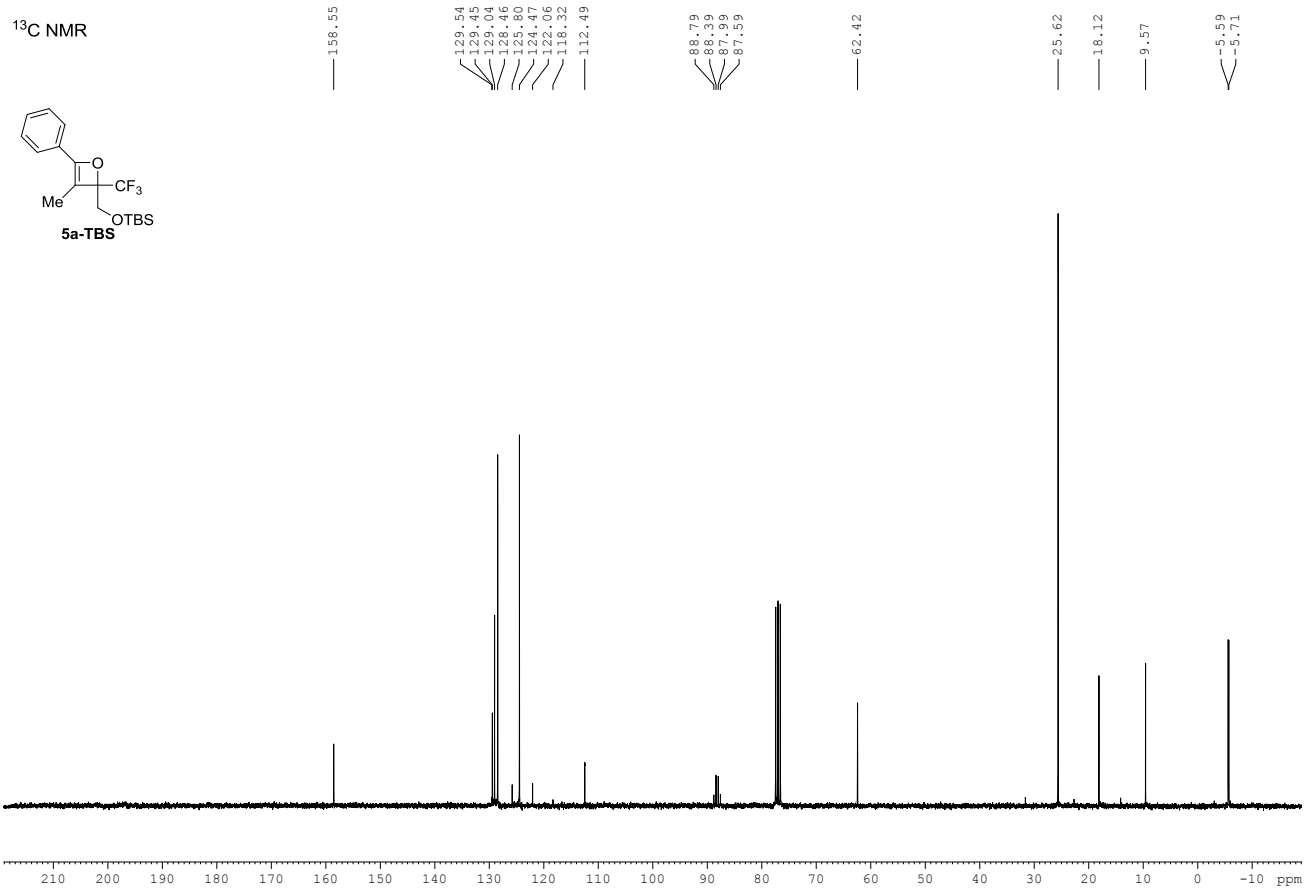


^{1}H NMR

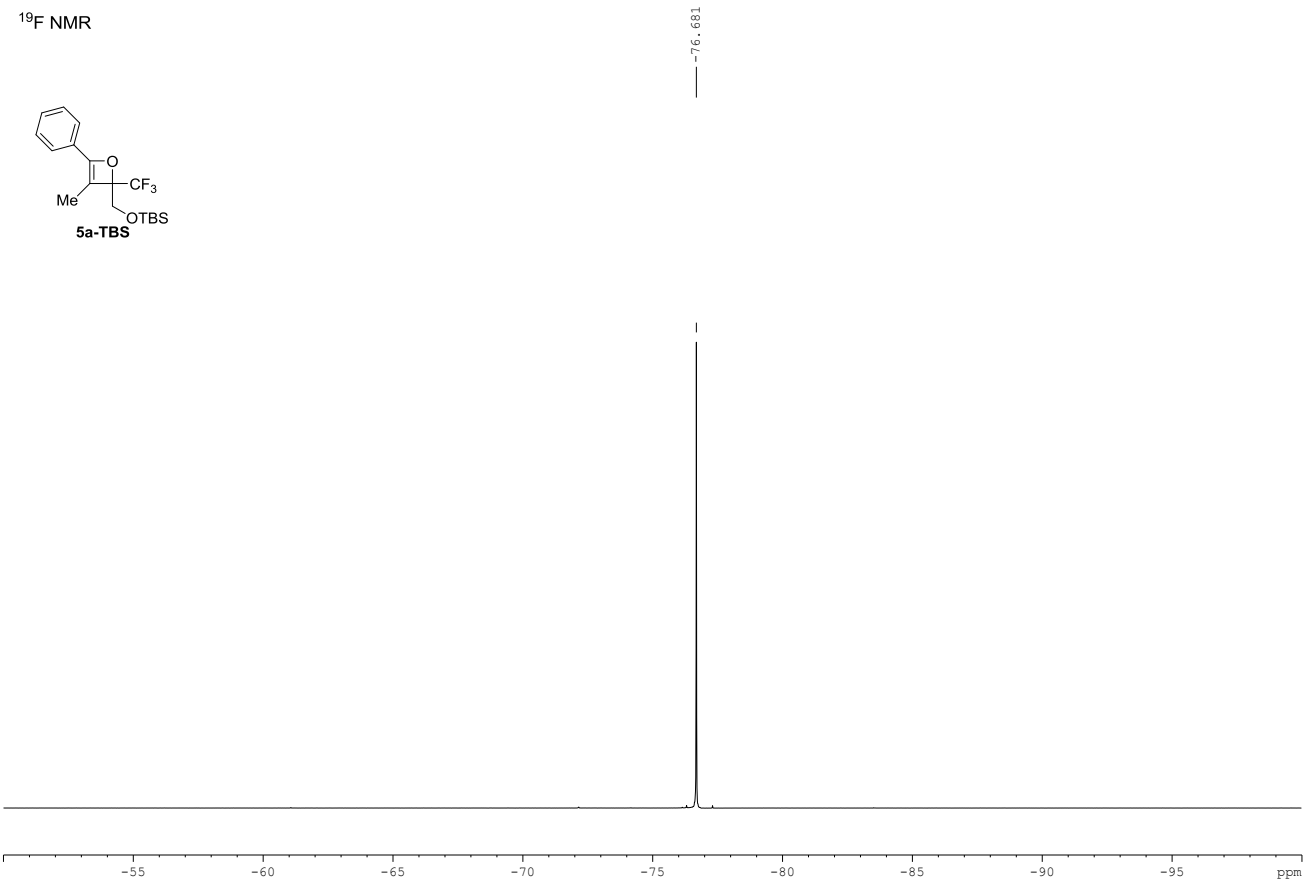
5a-TBS



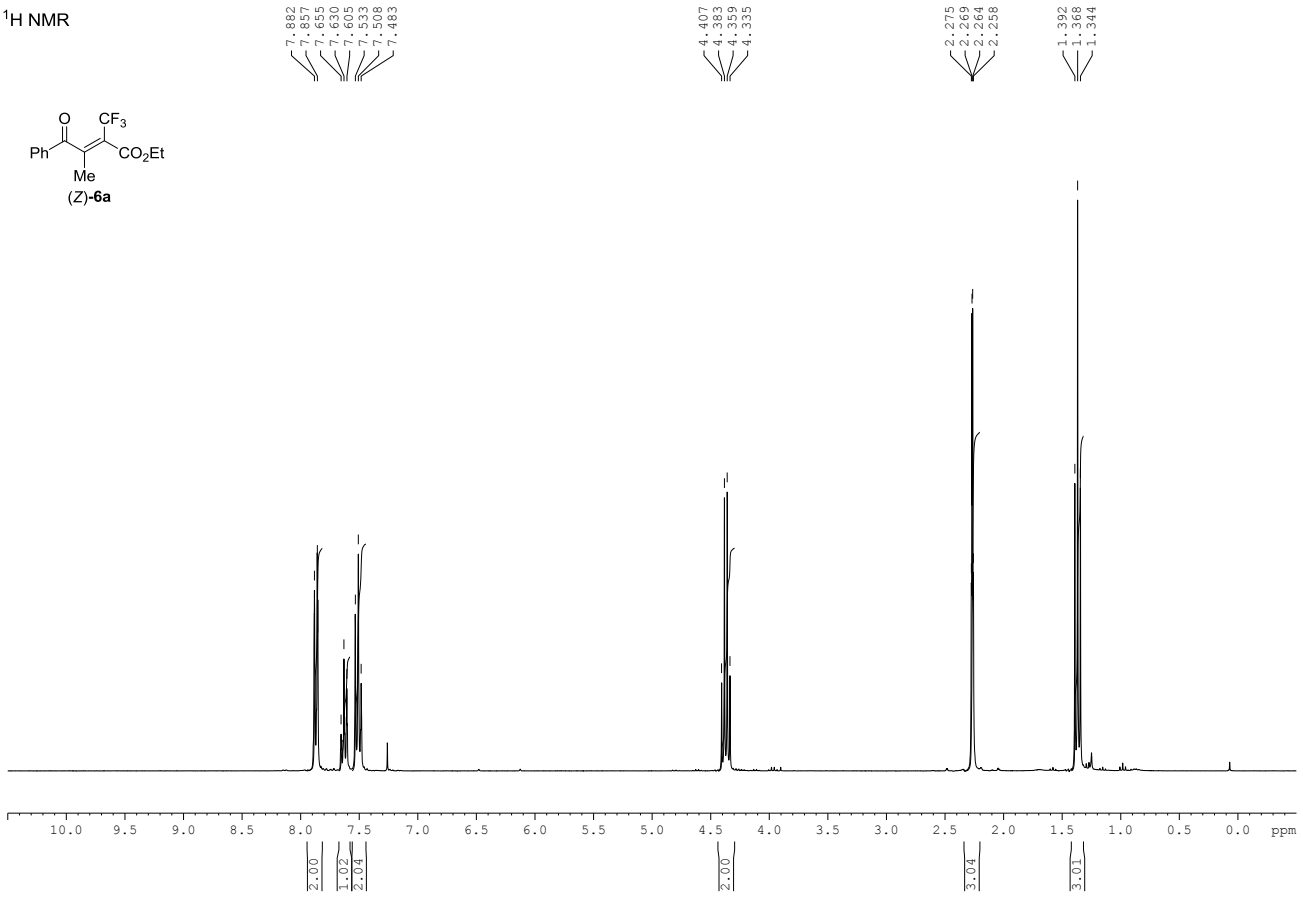
^{13}C NMR



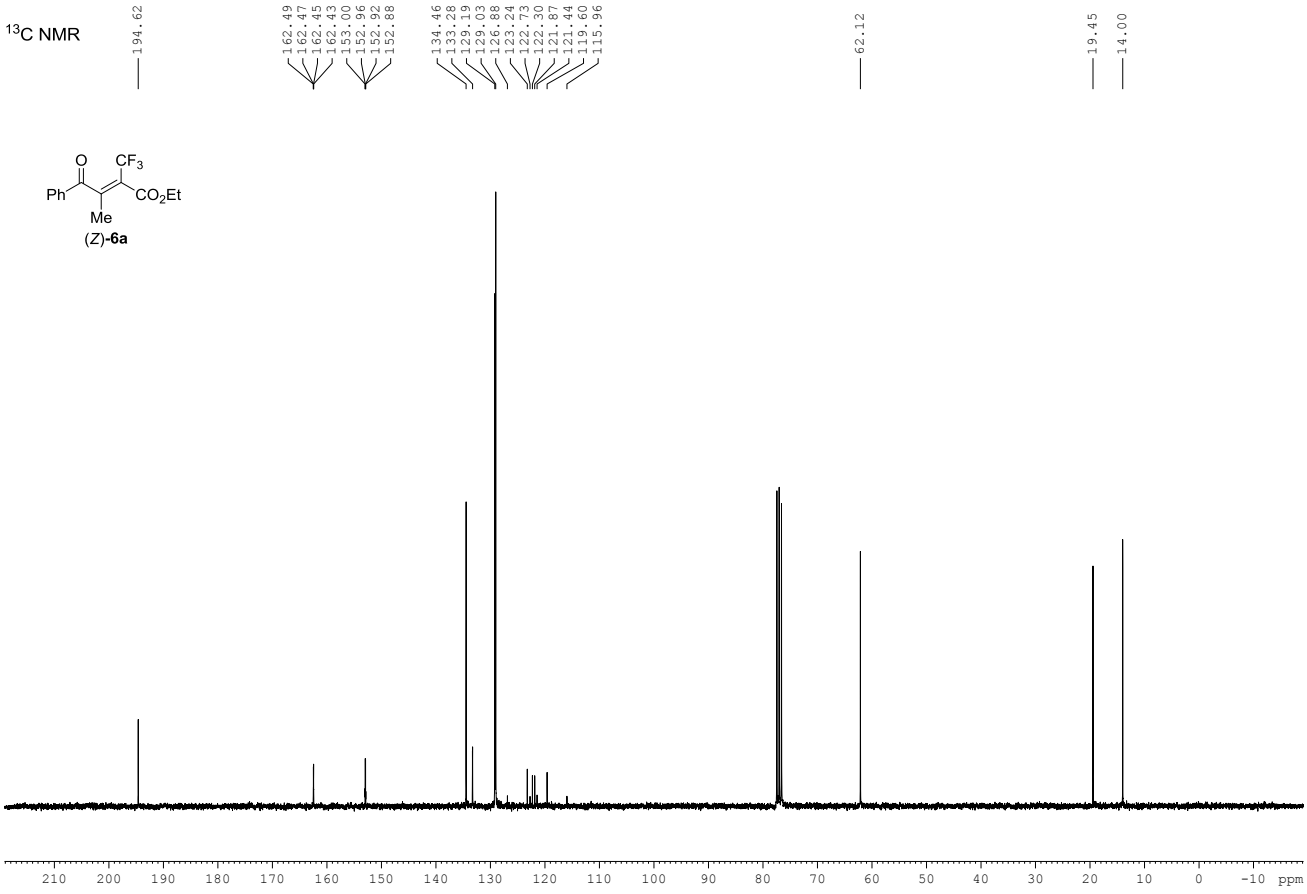
^{19}F NMR

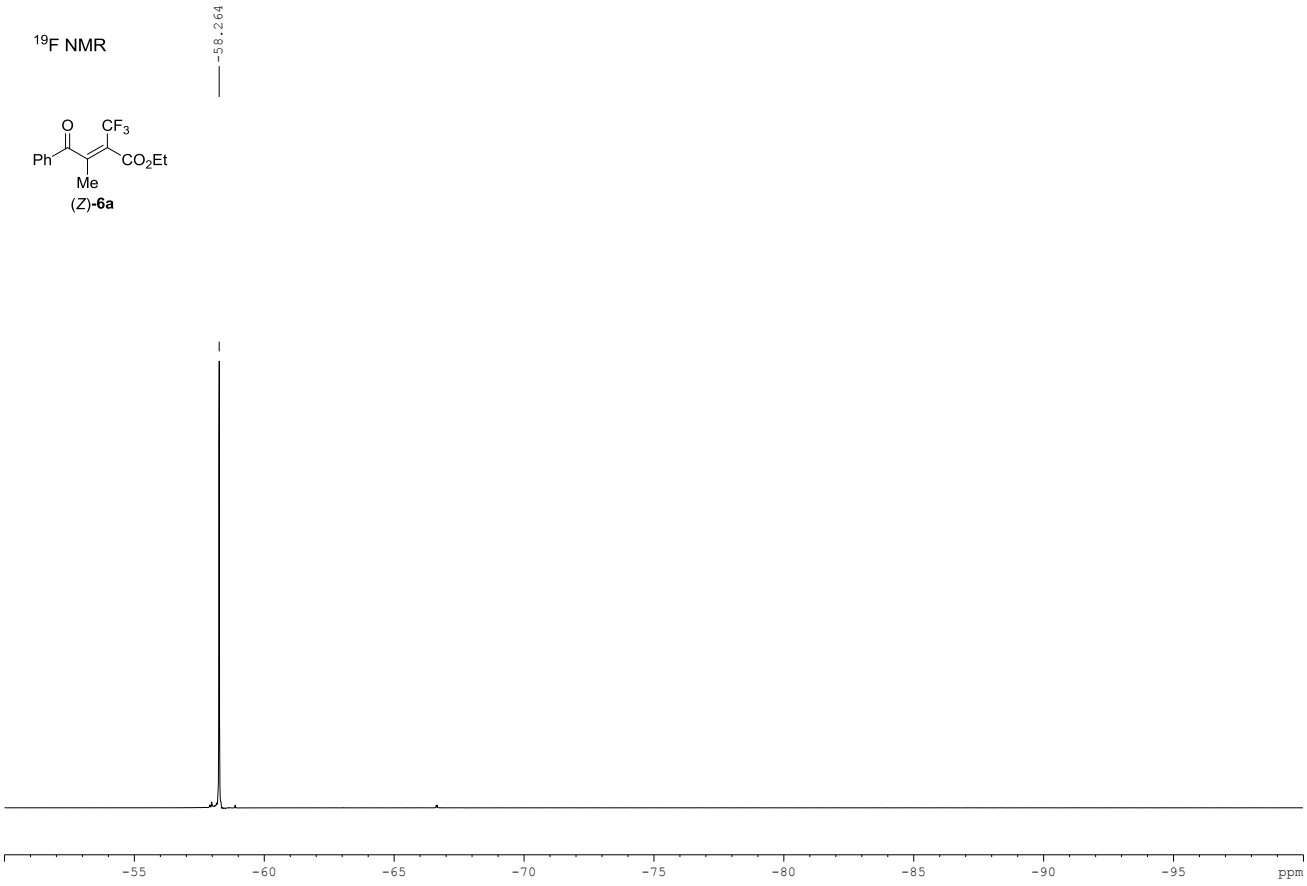


^{1}H NMR

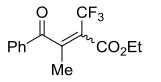


^{13}C NMR

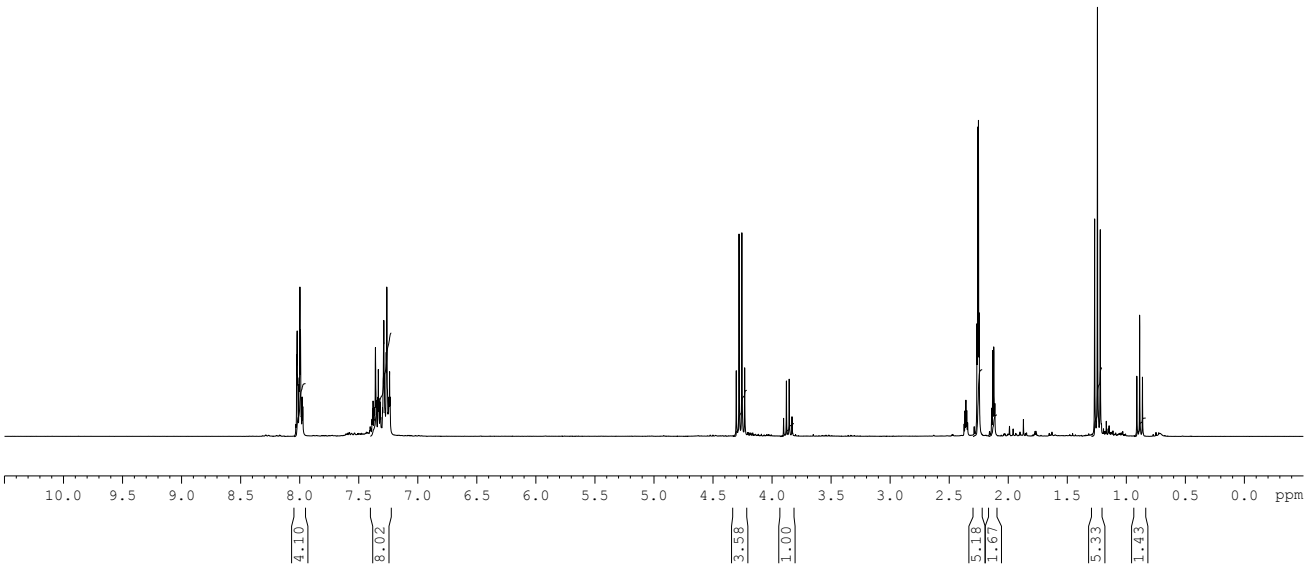



19F NMR
-58.264
O
CF3
Ph
CO2Et
Me
(Z)-6a
-55
-60
-65
-70
-75
-80
-85
-90
-95
ppm

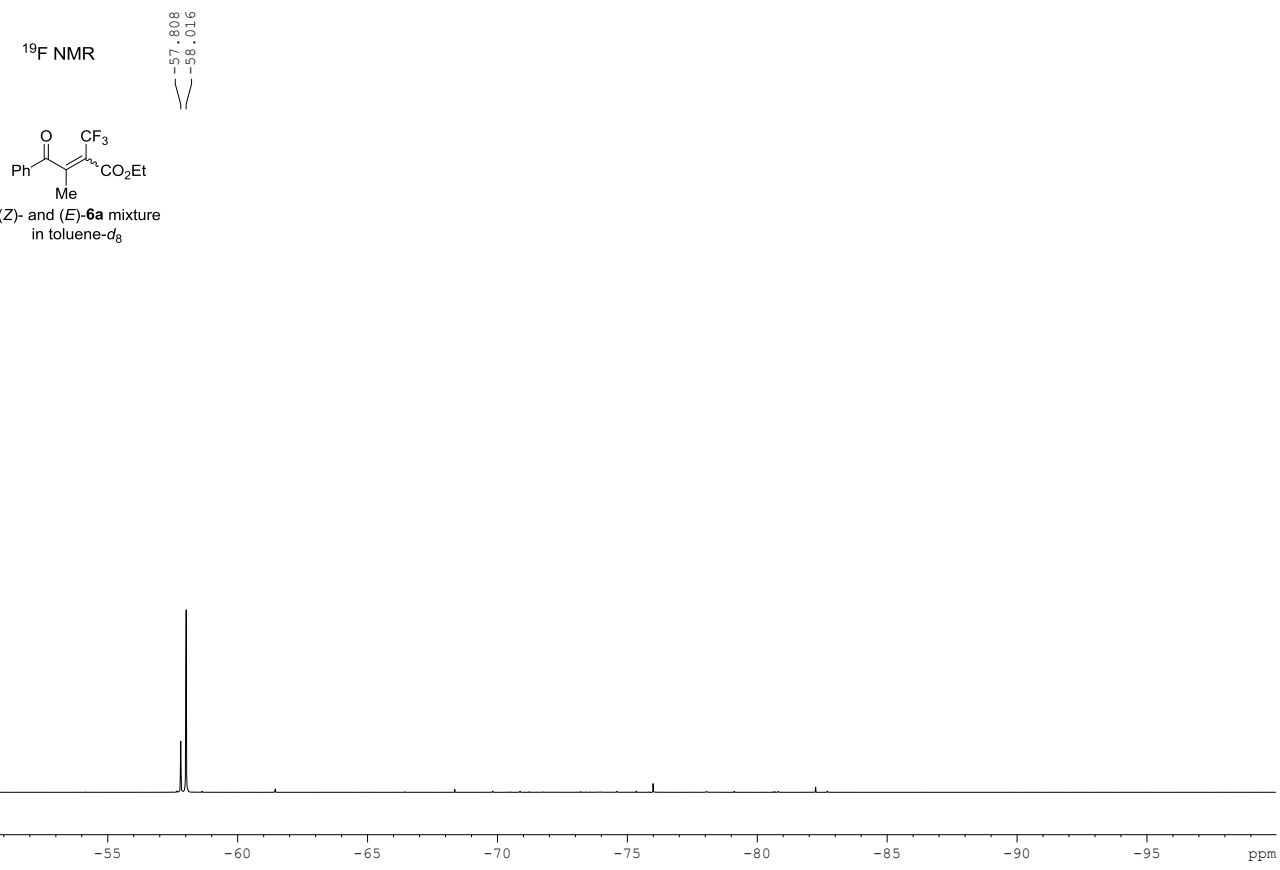
^{1}H NMR



(*Z*)- and (*E*)-**6a** mixture
in toluene-d_8



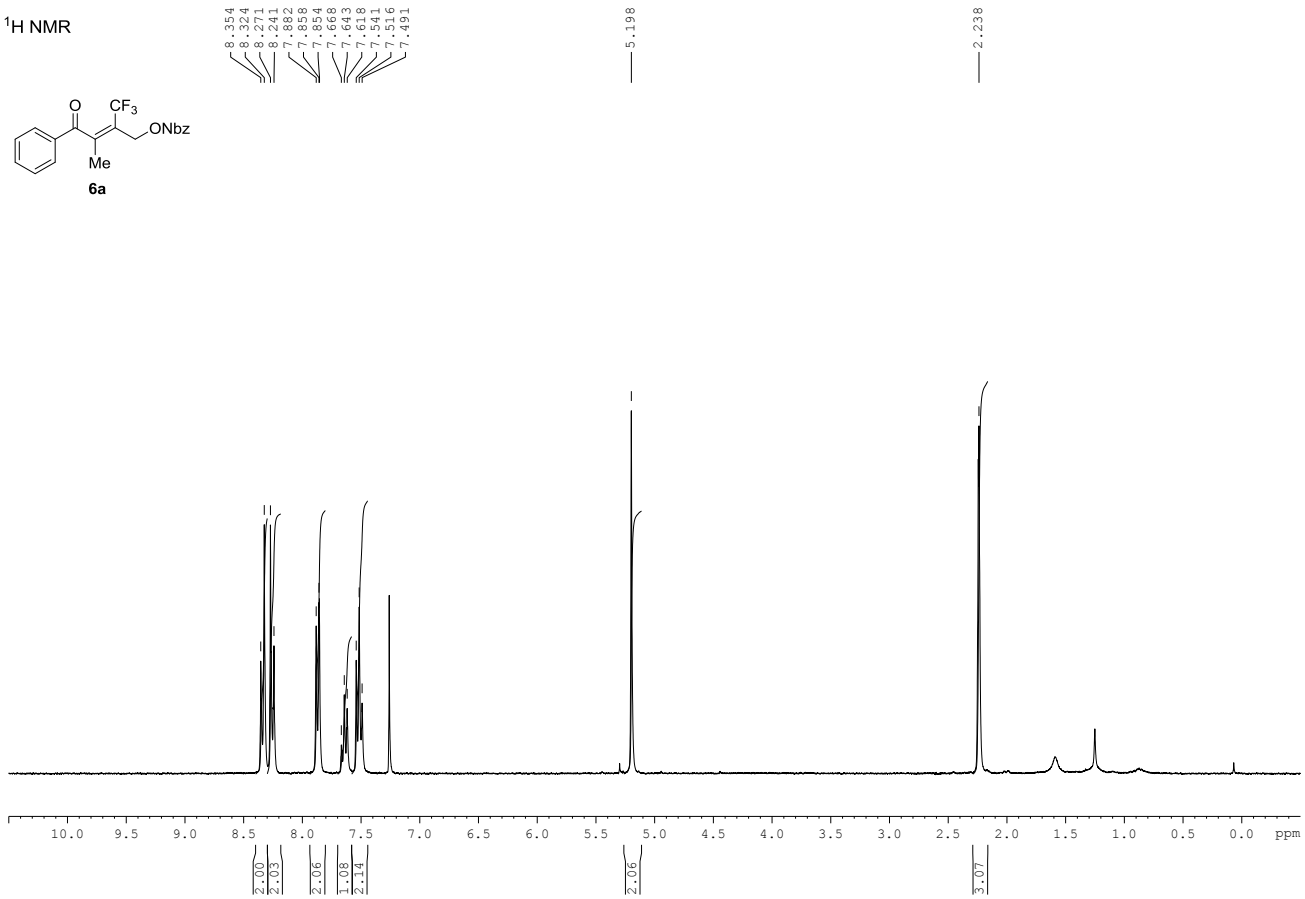
^{19}F NMR



(*Z*)- and (*E*)-**6a** mixture
in toluene-d_8

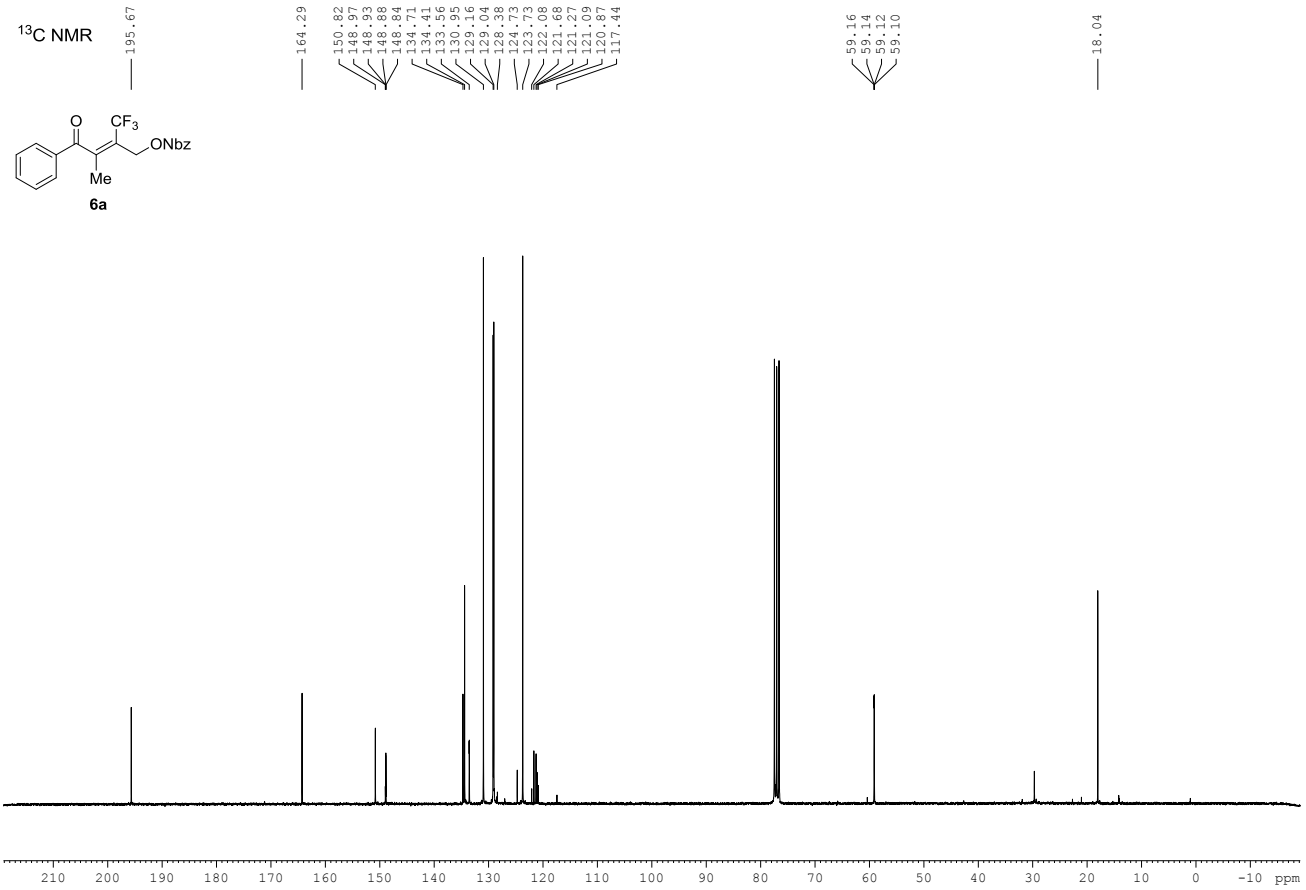
^{1}H NMR

6a



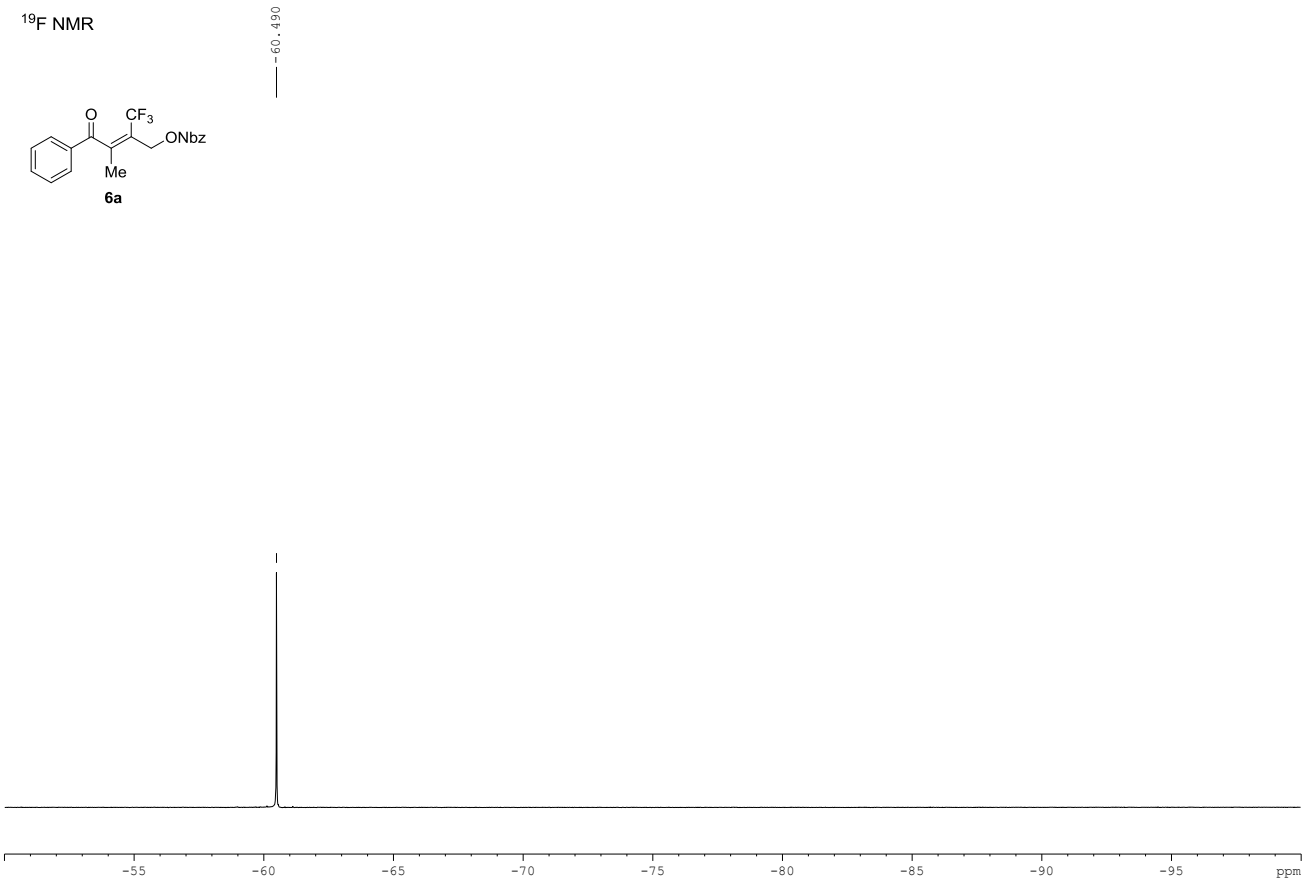
^{13}C NMR

6a



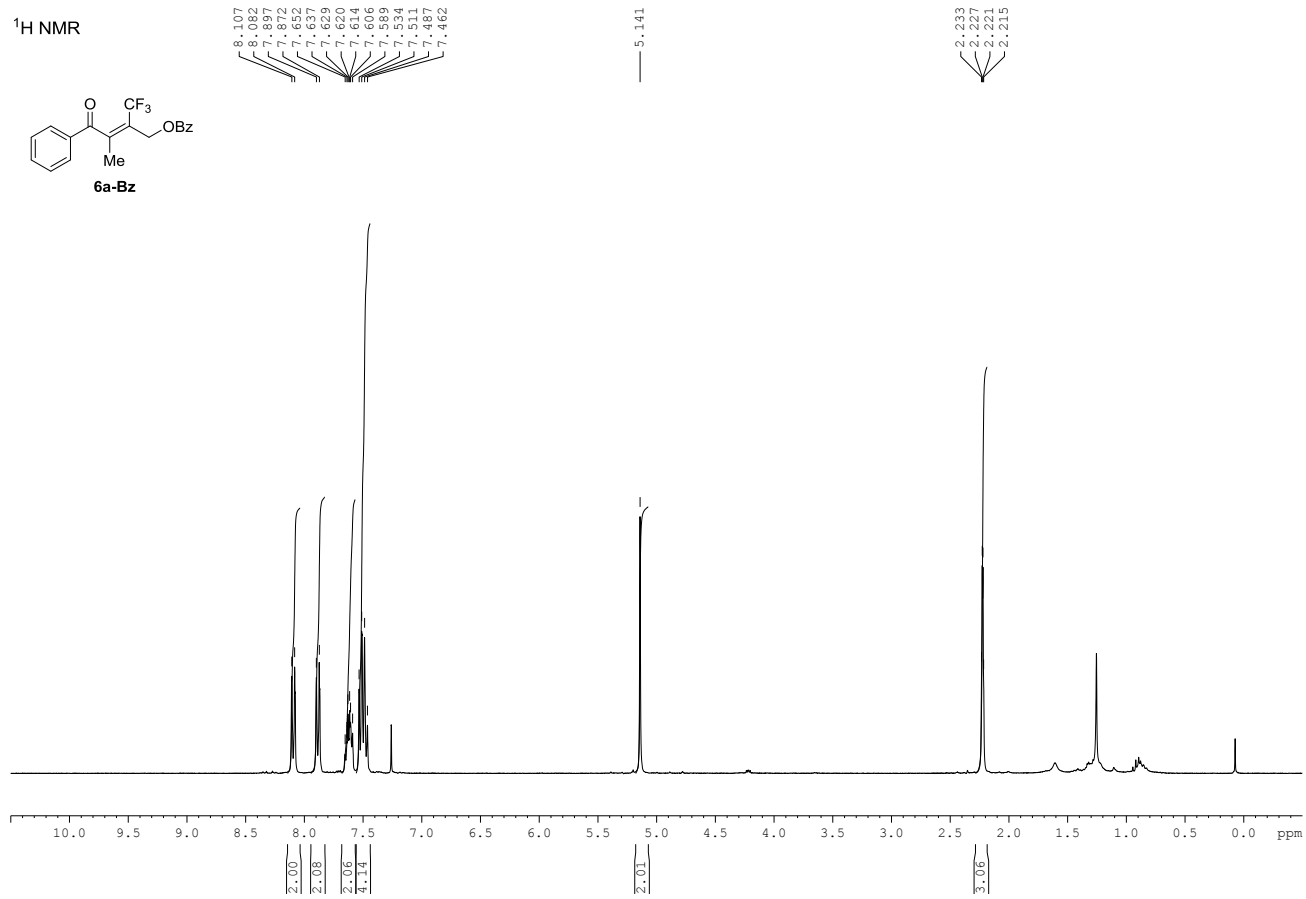
^{19}F NMR

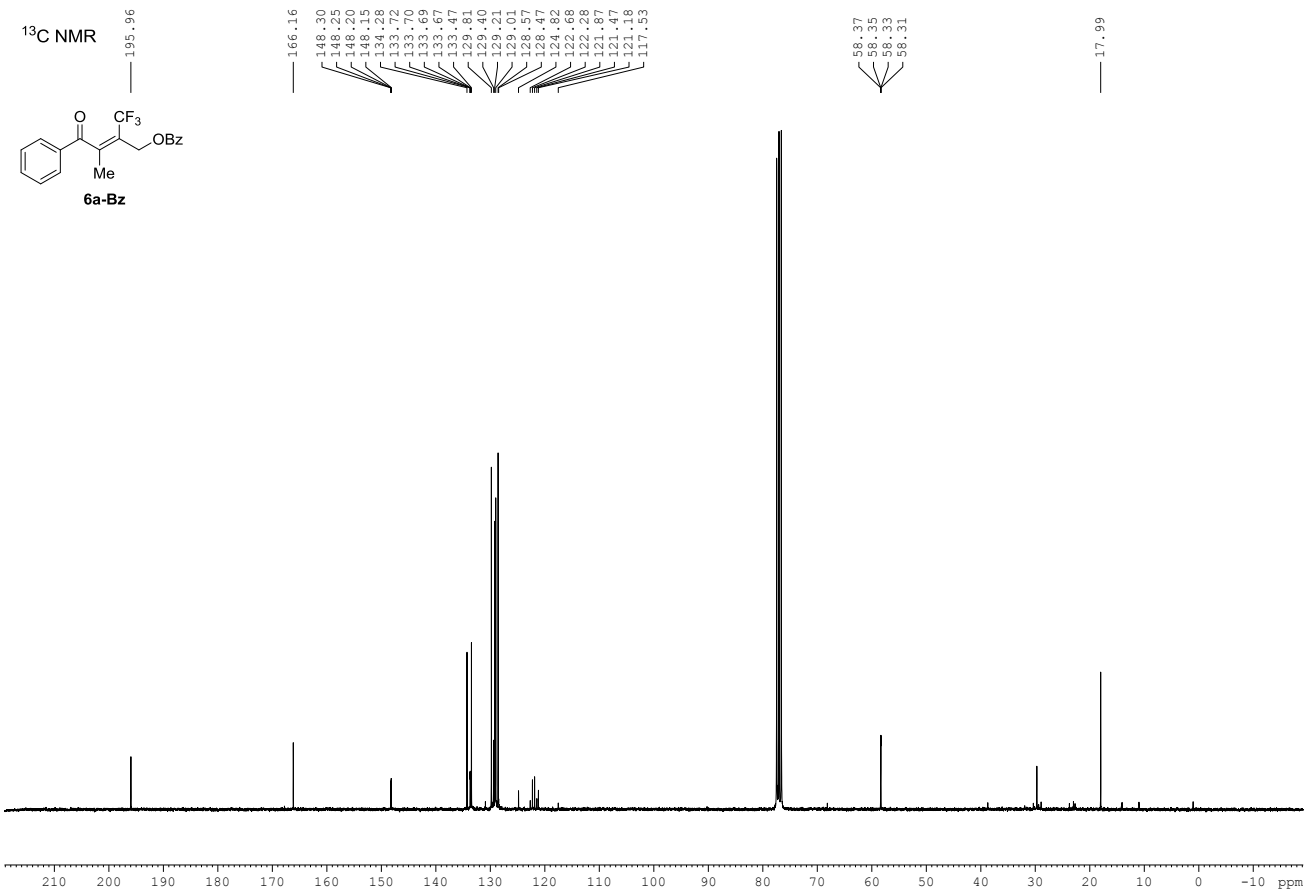
6a

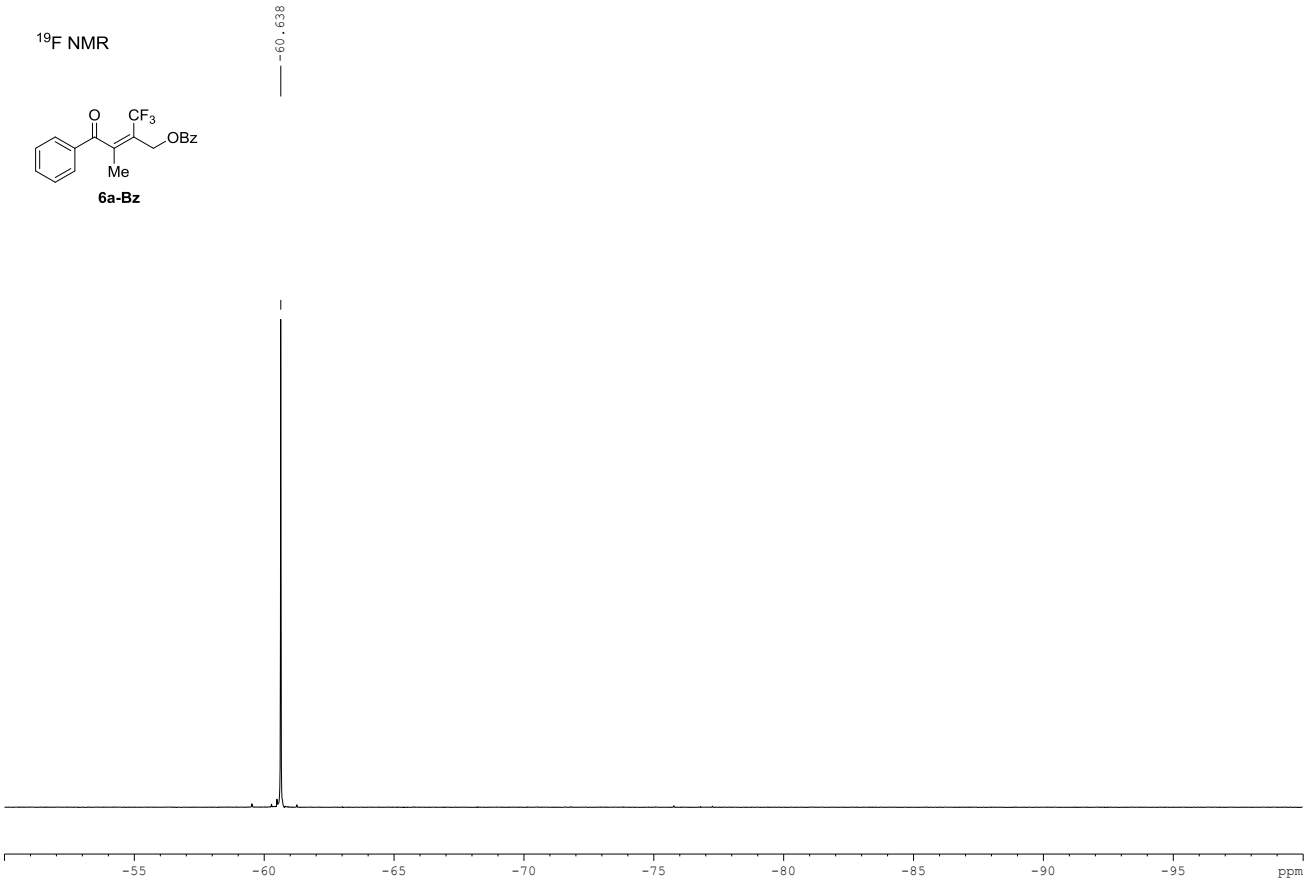


^{1}H NMR

6a-Bz

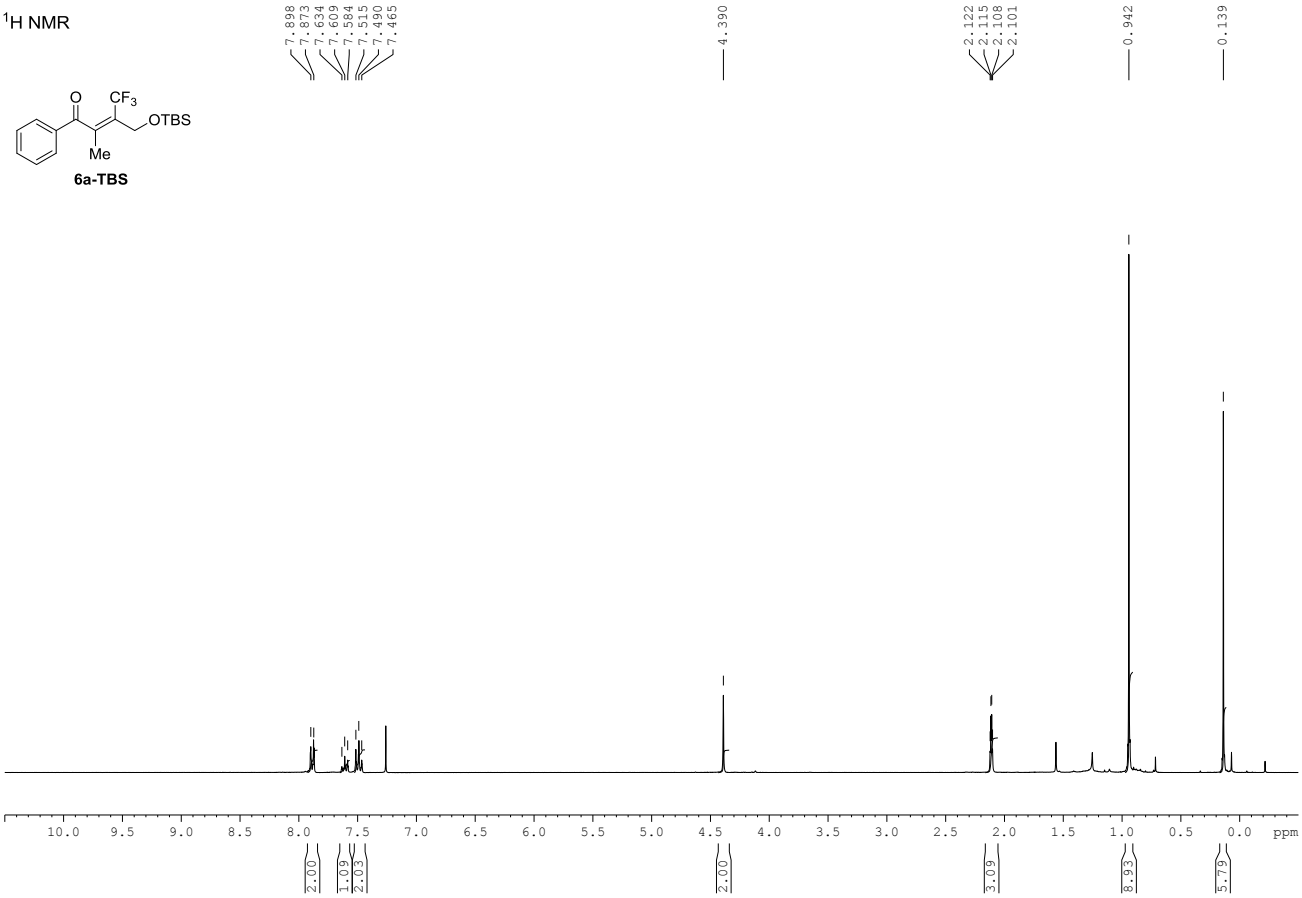



13C NMR
195.96
166.16
148.30
148.25
148.20
148.15
134.28
133.72
133.70
133.69
133.67
133.47
129.81
129.40
129.21
129.01
128.57
128.47
124.82
122.68
122.28
121.87
121.47
121.18
117.53
58.37
58.35
58.33
58.31
17.99
O
CF3
OBz
Me
6a-Bz
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 ppm

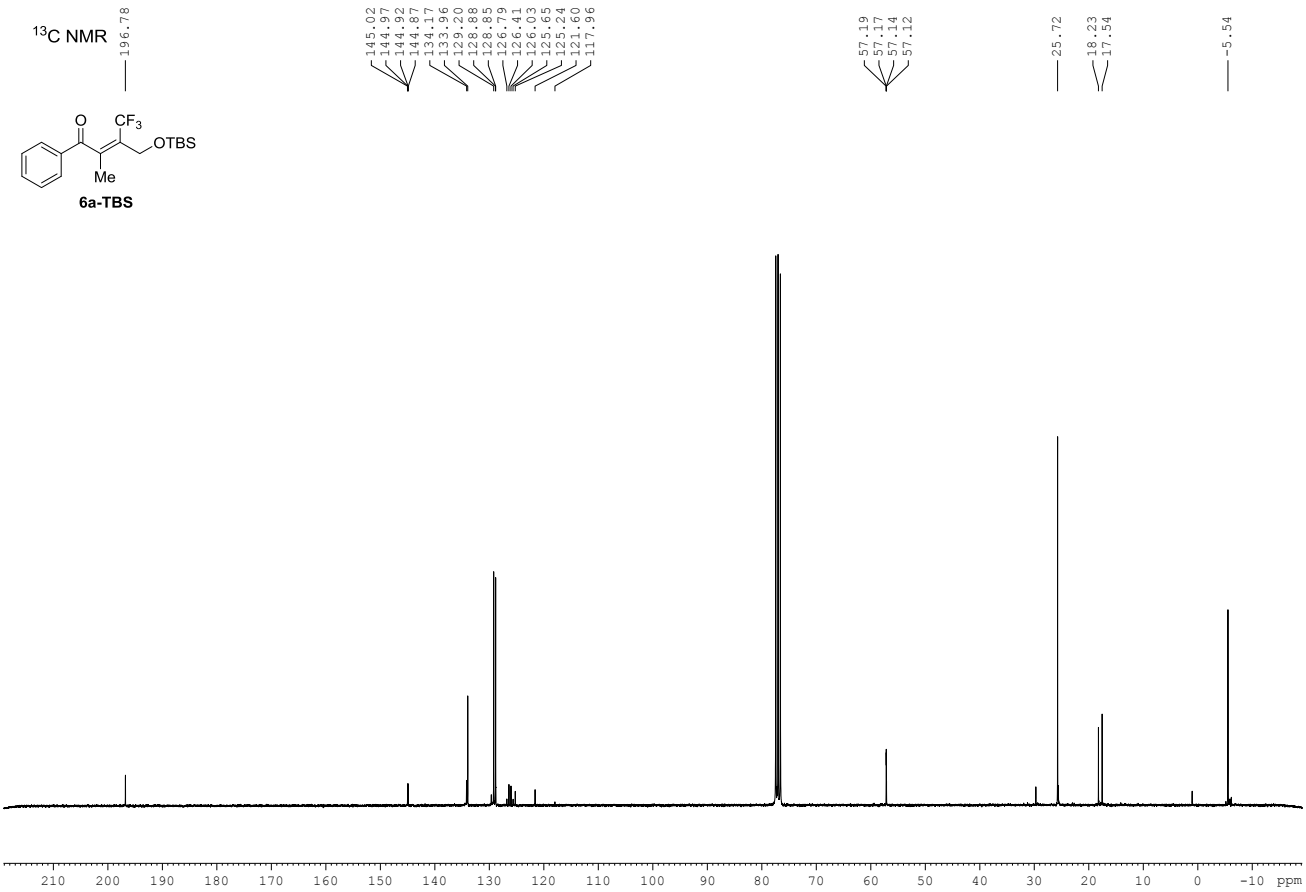

19F NMR
-60.638
O
CF3
OBz
Me
6a-Bz
-55 -60 -65 -70 -75 -80 -85 -90 -95 ppm

^{1}H NMR

6a-TBS



^{13}C NMR

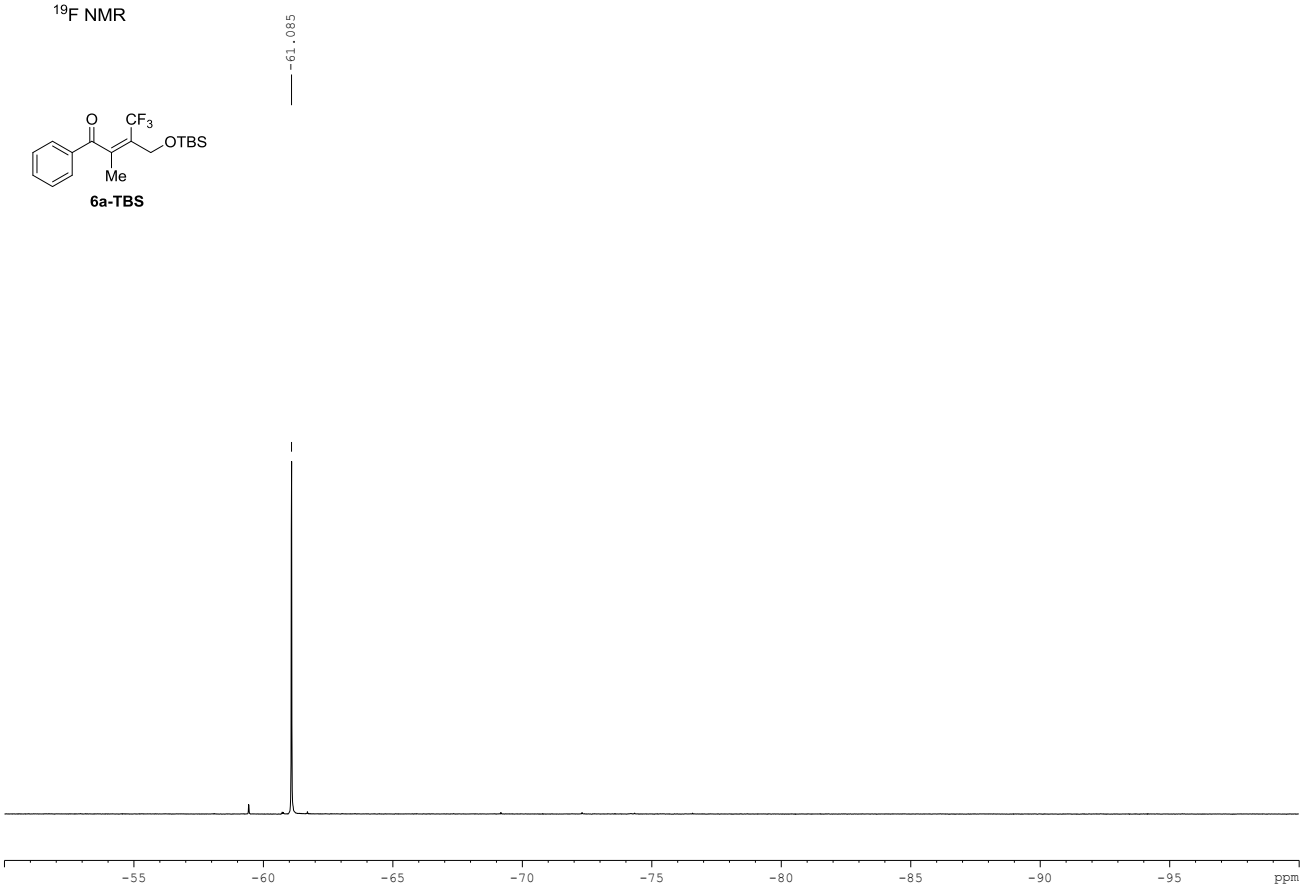


O
CF3
OTBS
Me

6a-TBS

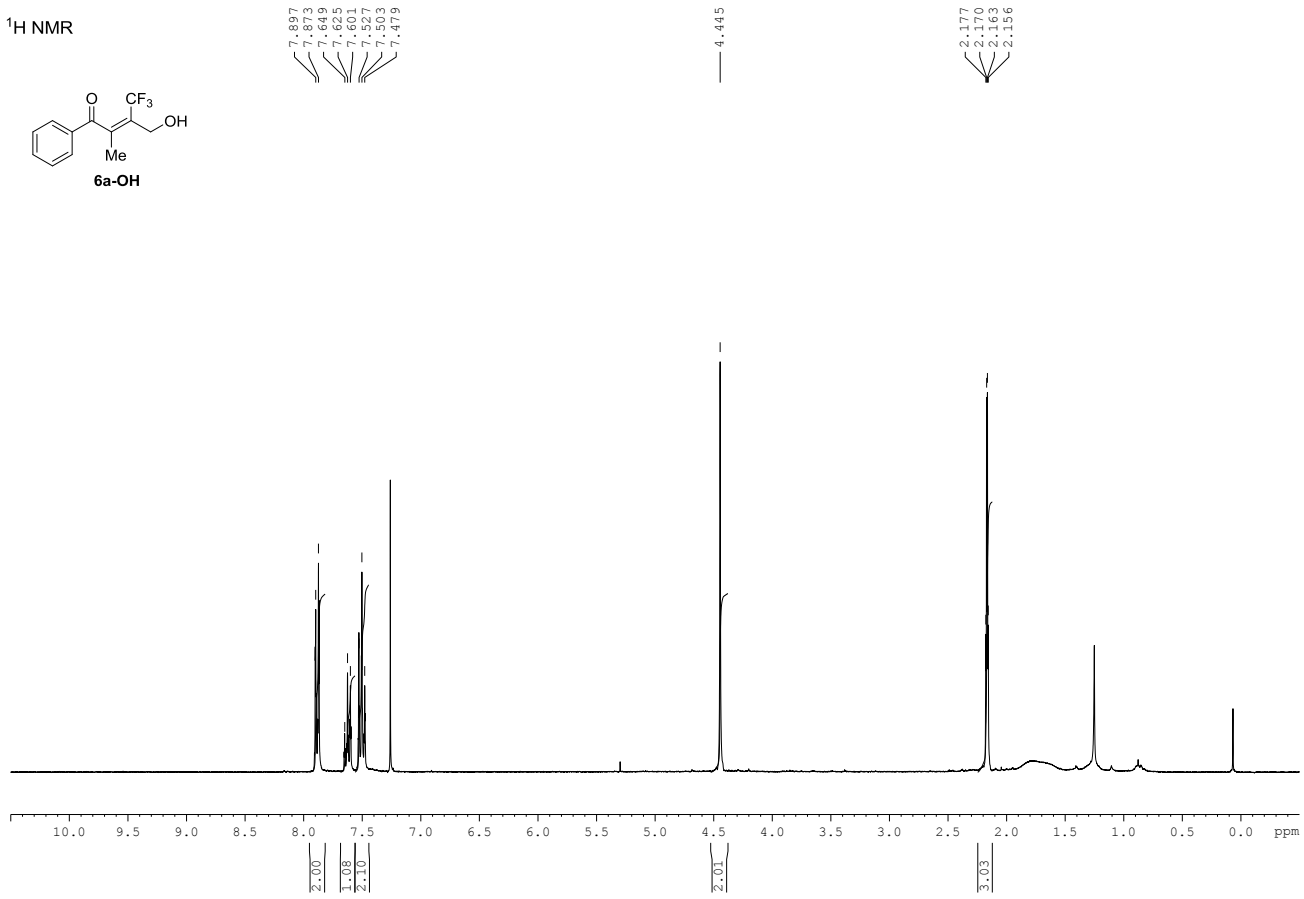
^{19}F NMR

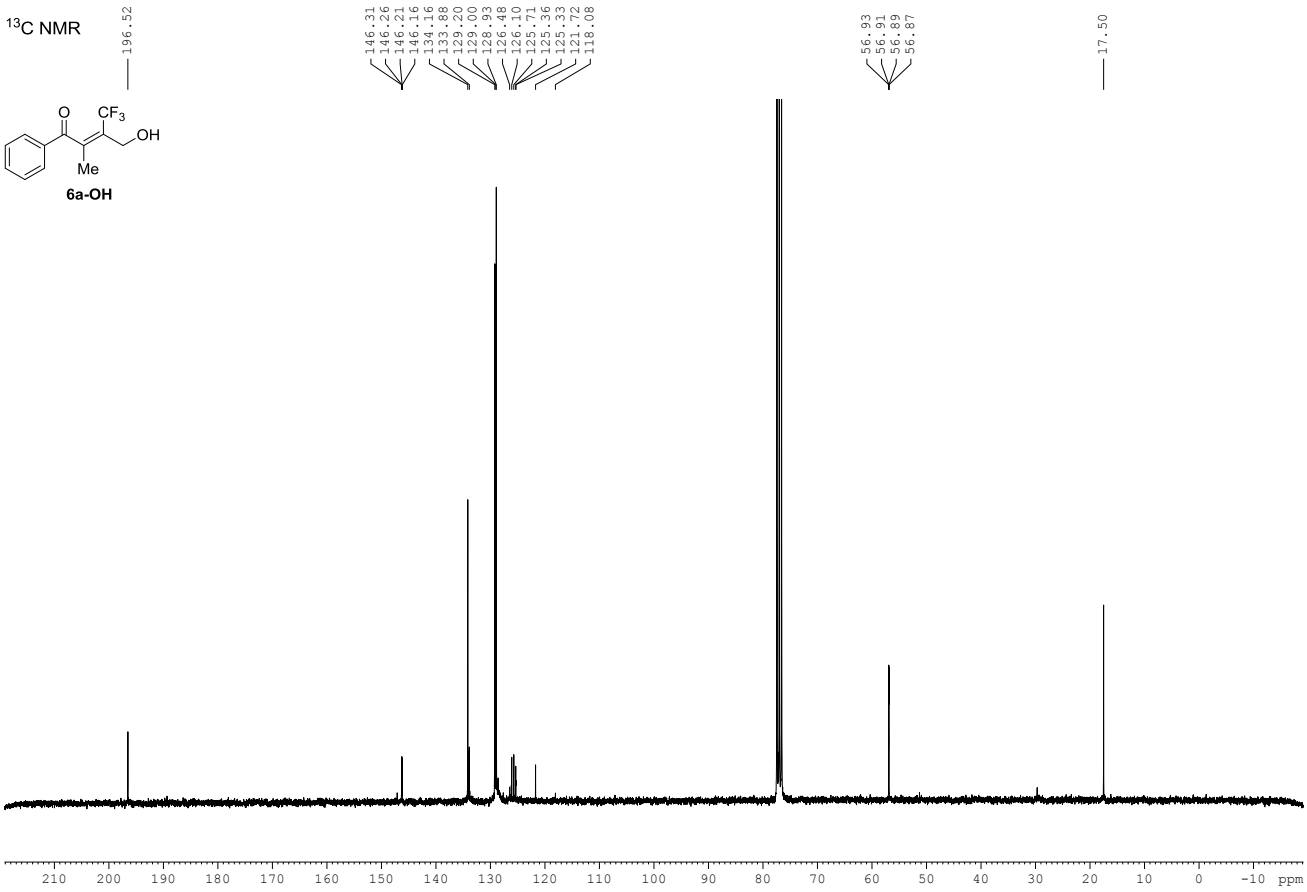
6a-TBS

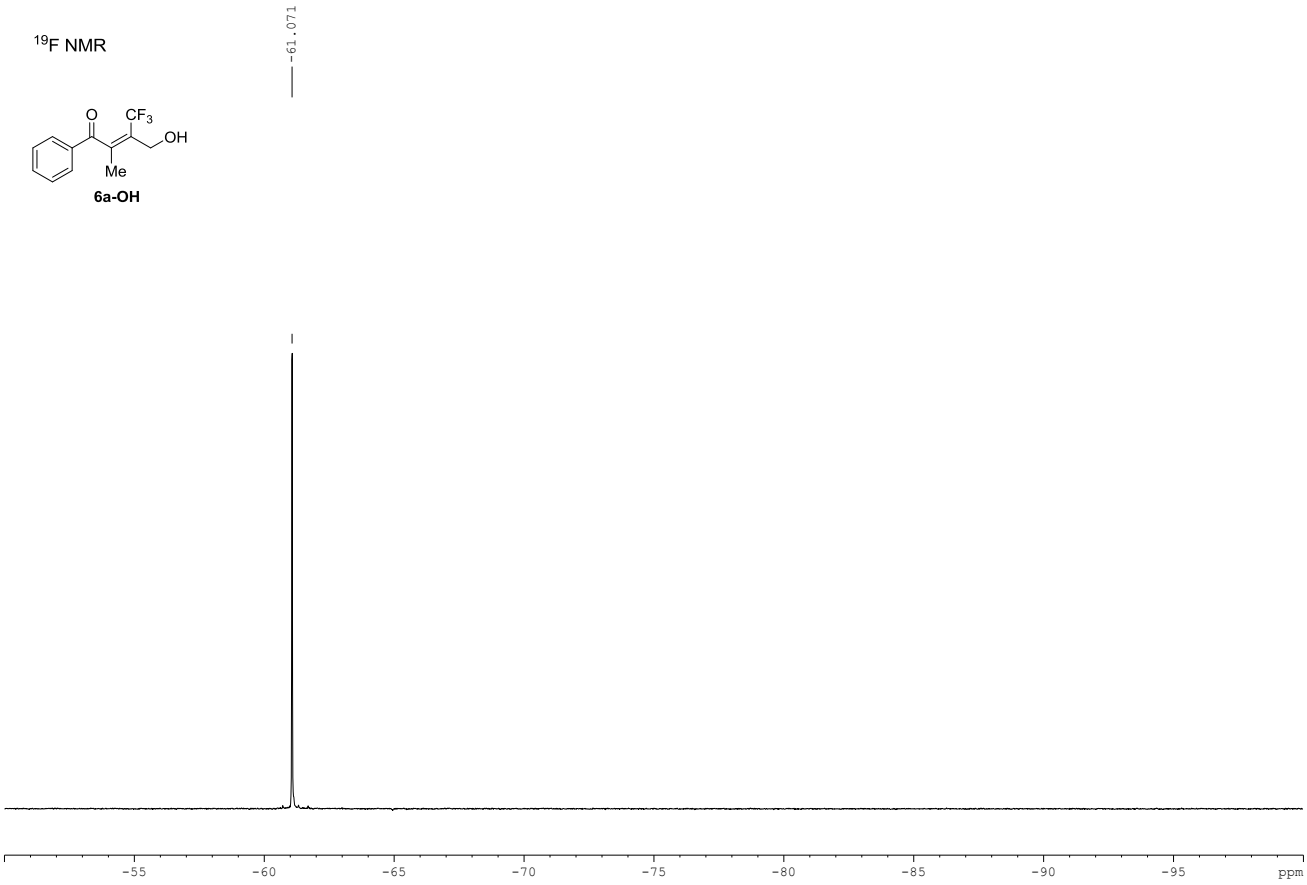


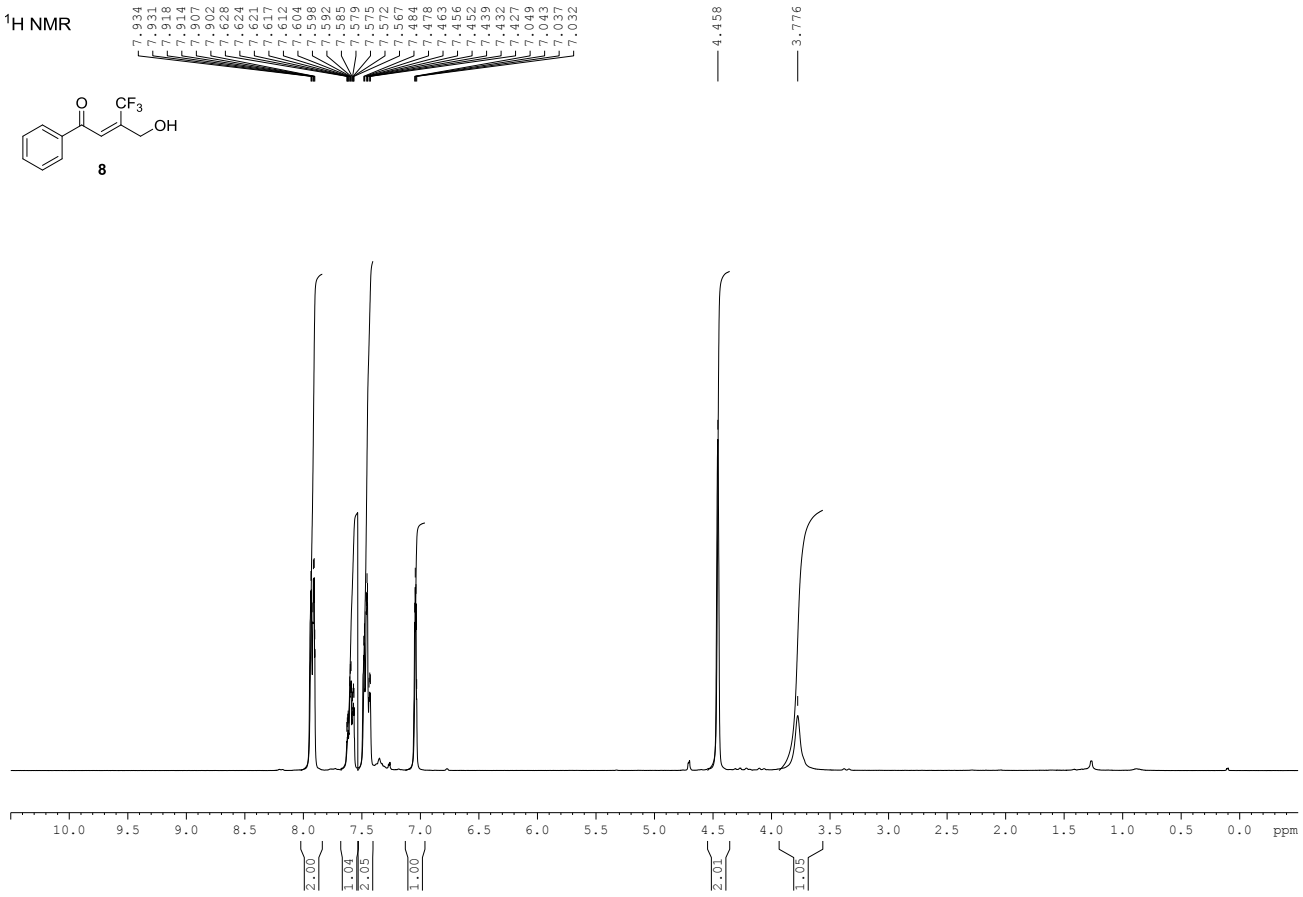
^{1}H NMR

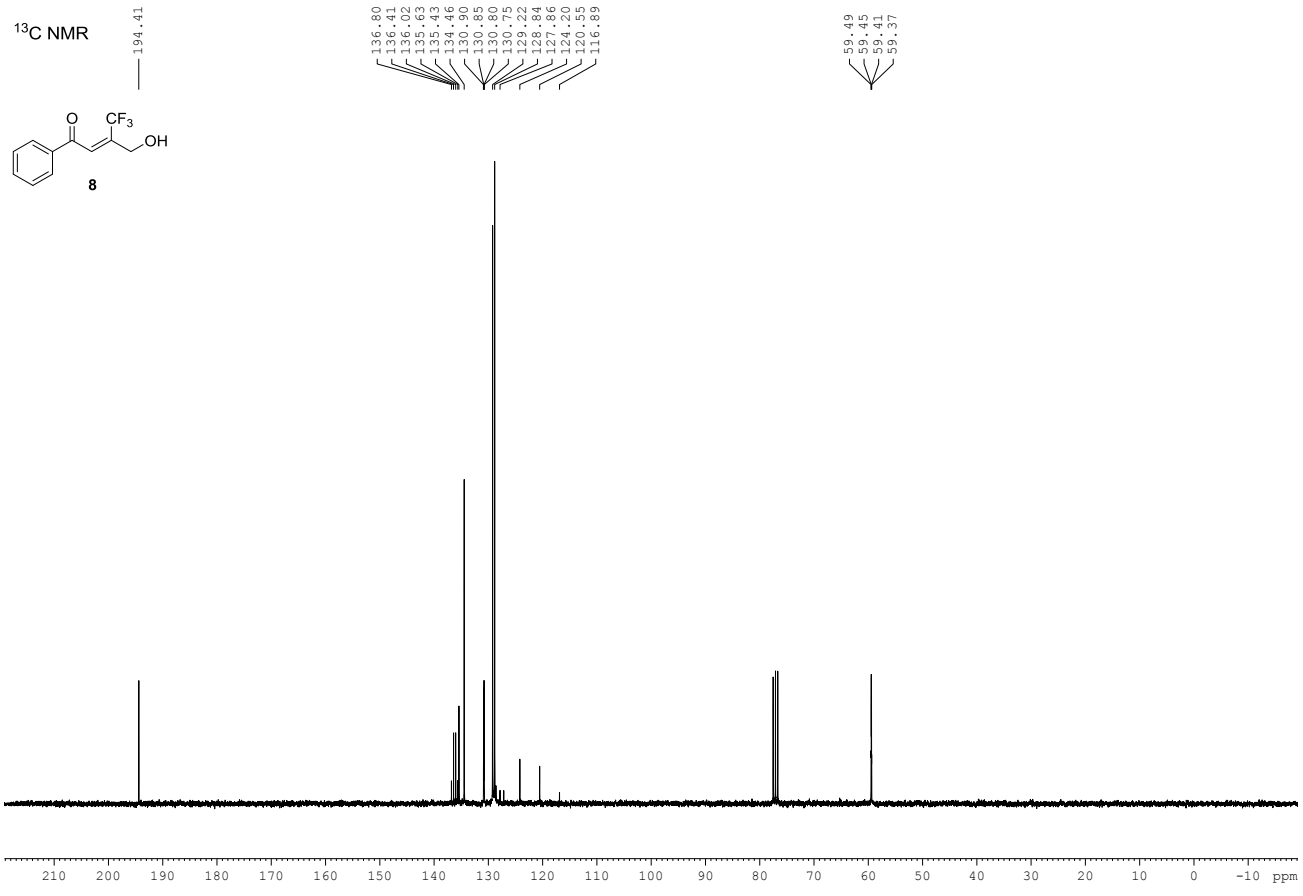
6a-OH




13C NMR
196.52
146.31
146.26
146.21
146.16
134.16
133.88
129.20
129.00
128.93
126.48
126.10
125.71
125.36
125.33
121.72
118.08
56.93
56.91
56.89
56.87
17.50
O
CF3
OH
Me
6a-OH
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 ppm

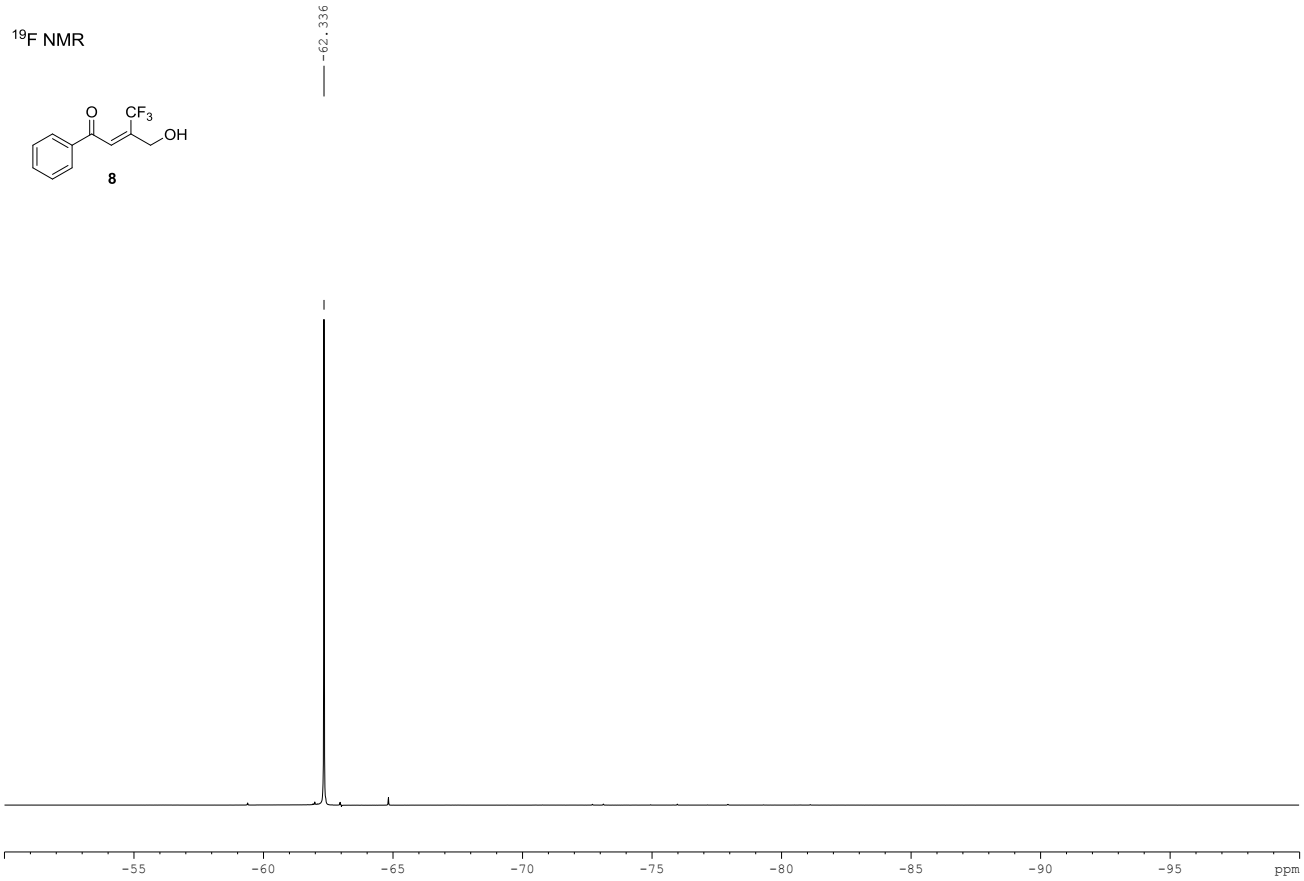

19F NMR
-61.071
O
CF3
OH
Me
6a-OH
-55 -60 -65 -70 -75 -80 -85 -90 -95 ppm


1H NMR
7.934
7.931
7.918
7.914
7.907
7.902
7.628
7.624
7.621
7.617
7.612
7.604
7.598
7.592
7.585
7.579
7.575
7.572
7.567
7.484
7.478
7.463
7.456
7.452
7.439
7.432
7.427
7.049
7.043
7.037
7.032
4.458
3.776
O
CF3
OH
8
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 ppm
2.00
1.04
2.05
1.00
2.01
1.05


13C NMR
194.41
136.80
136.41
136.02
135.63
135.43
134.46
130.90
130.85
130.80
130.75
129.22
128.84
127.86
124.20
120.55
116.89
59.49
59.45
59.41
59.37
O
CF3
OH
8
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 ppm

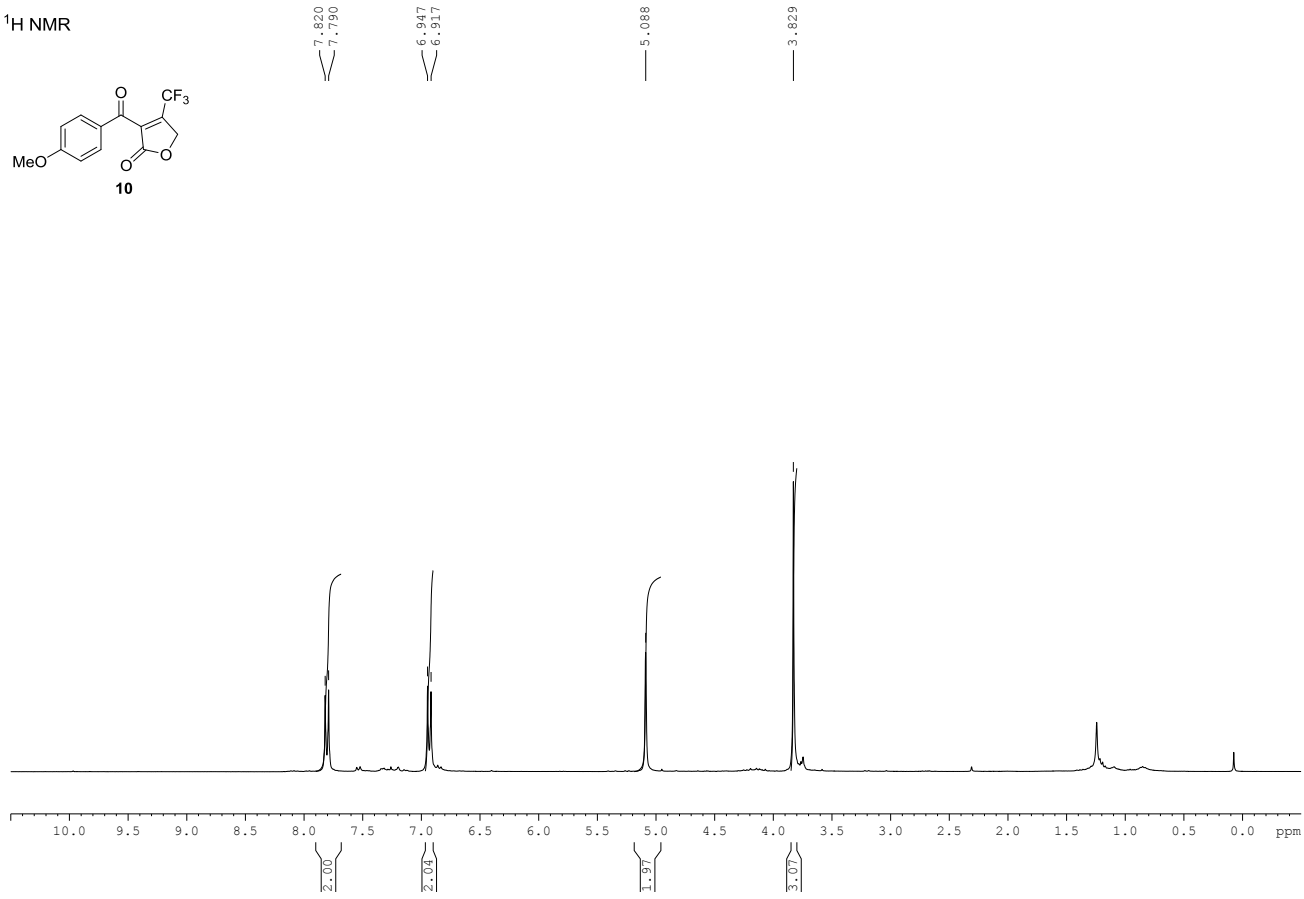
^{19}F NMR

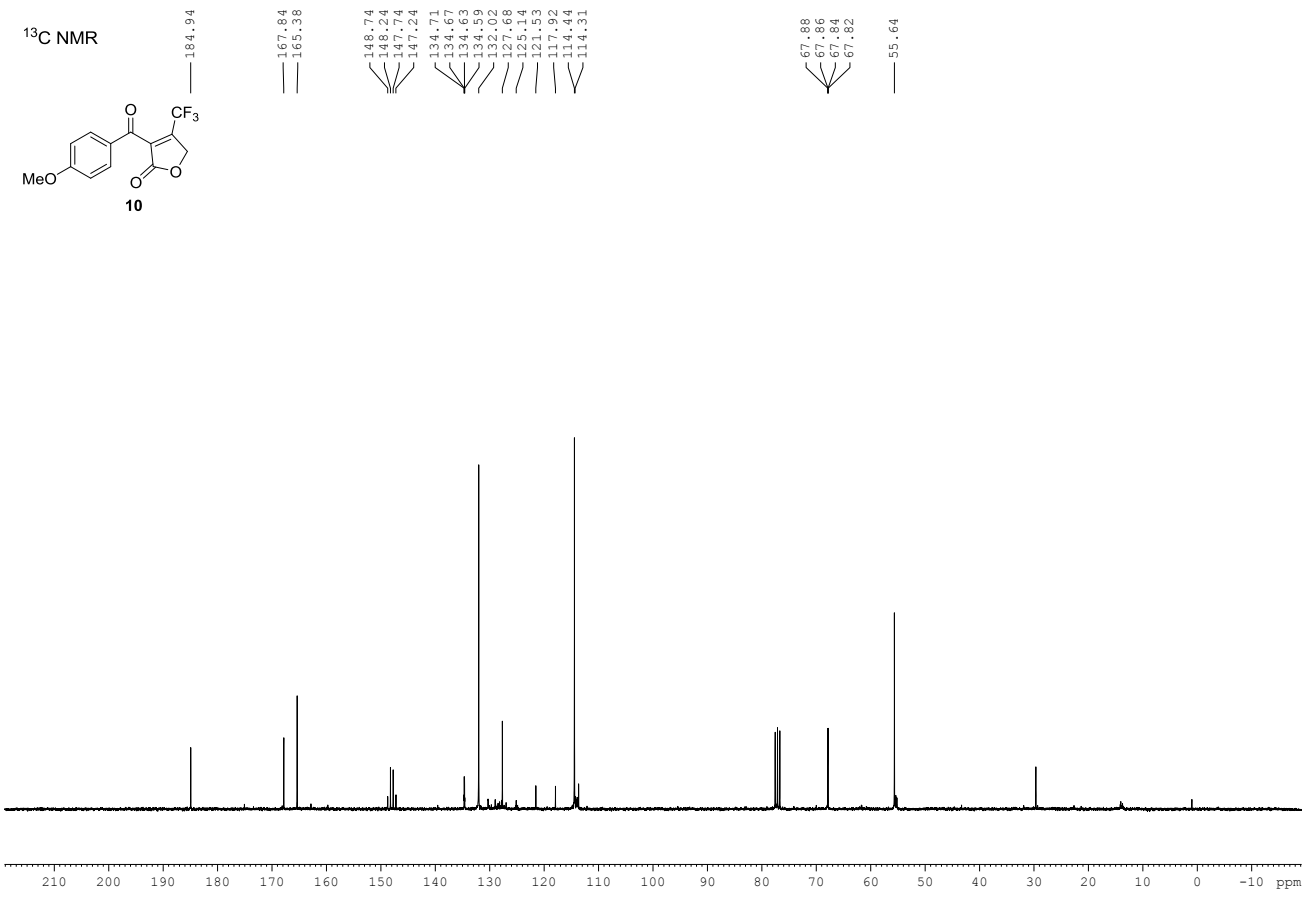
8

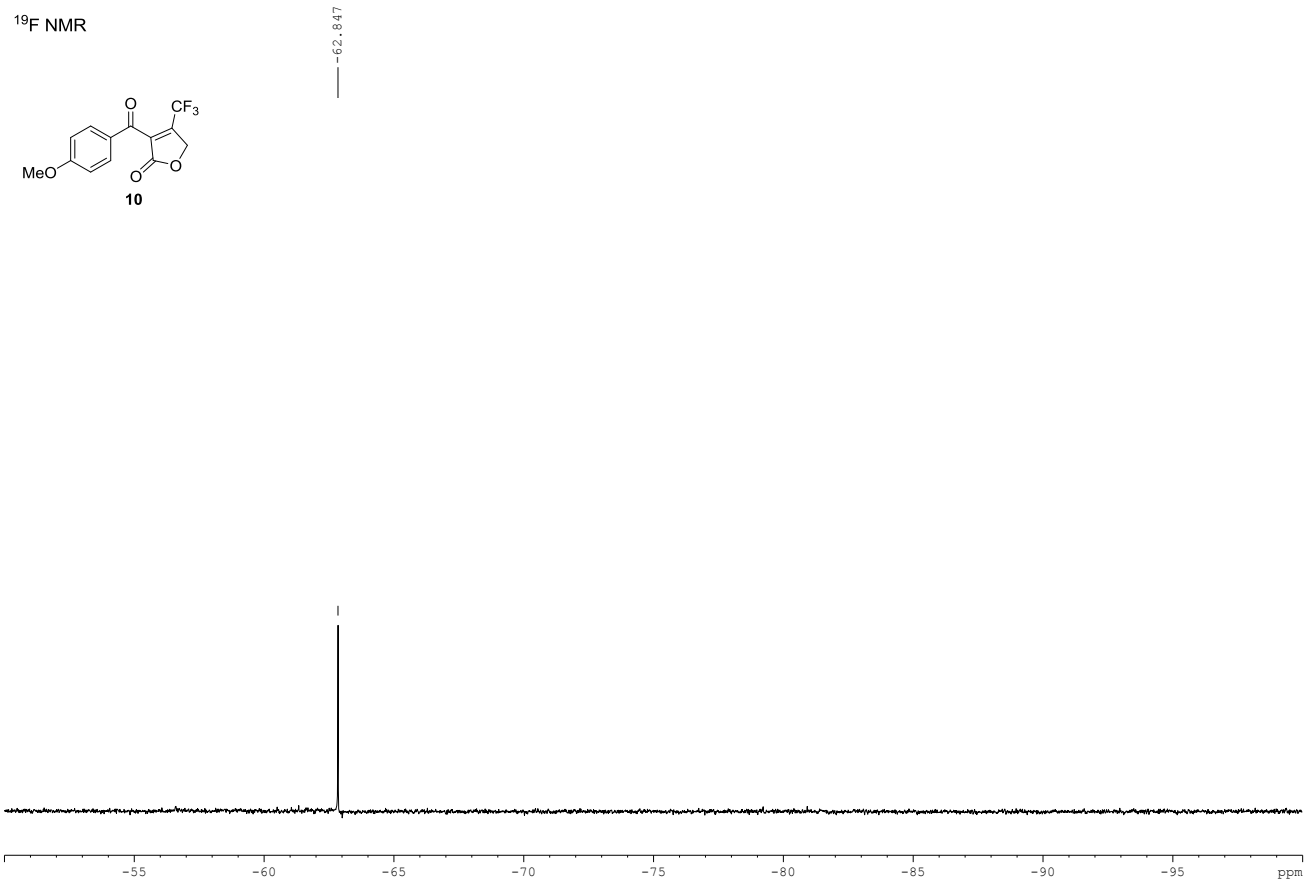


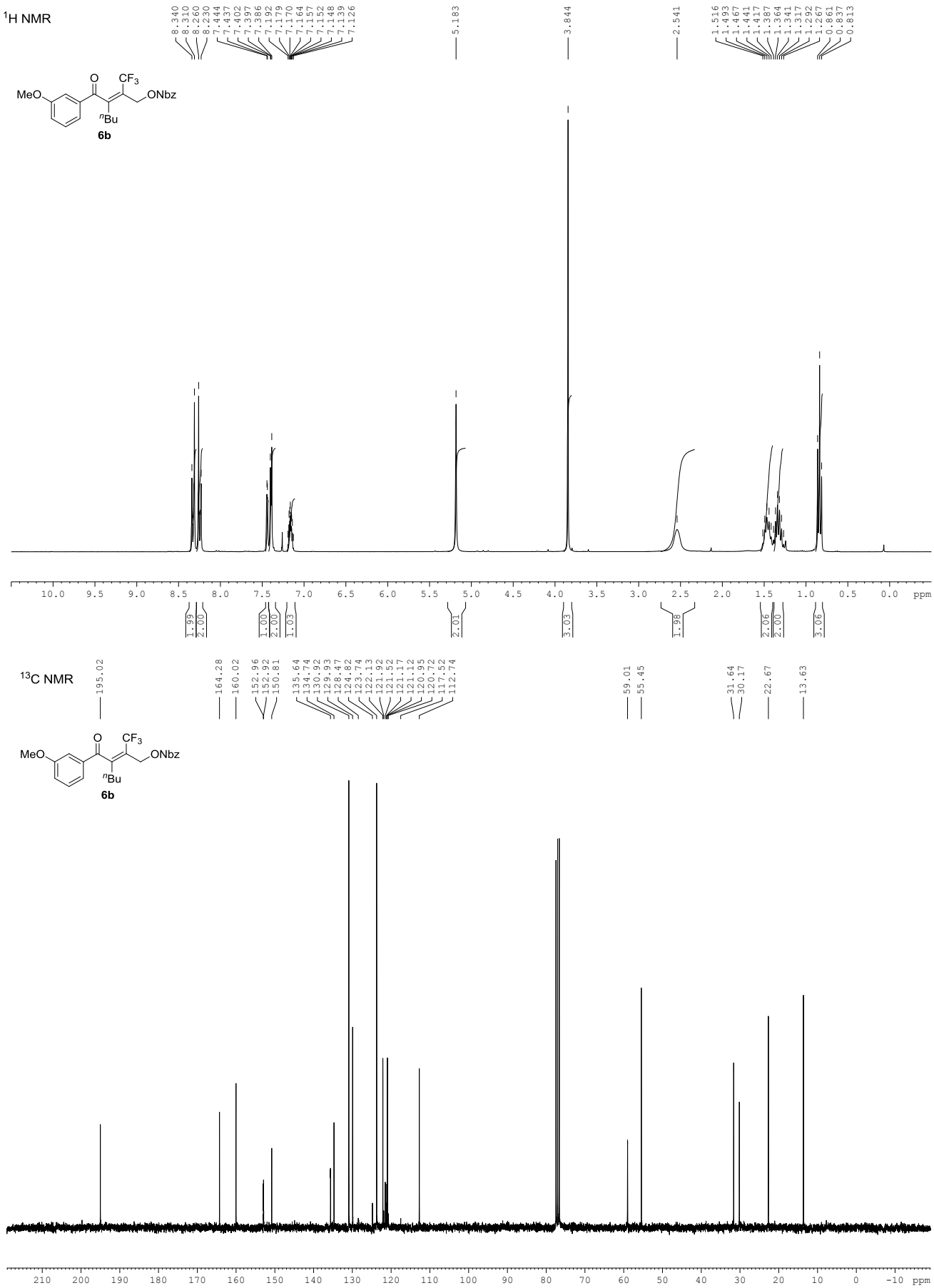
^{1}H NMR

10

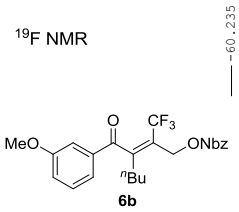



13C NMR
184.94
167.84
165.38
148.74
148.24
147.74
147.24
134.71
134.67
134.63
134.59
132.02
127.68
125.14
121.53
117.92
114.44
114.31
67.88
67.86
67.84
67.82
55.64
CF3
O
MeO
10
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 ppm

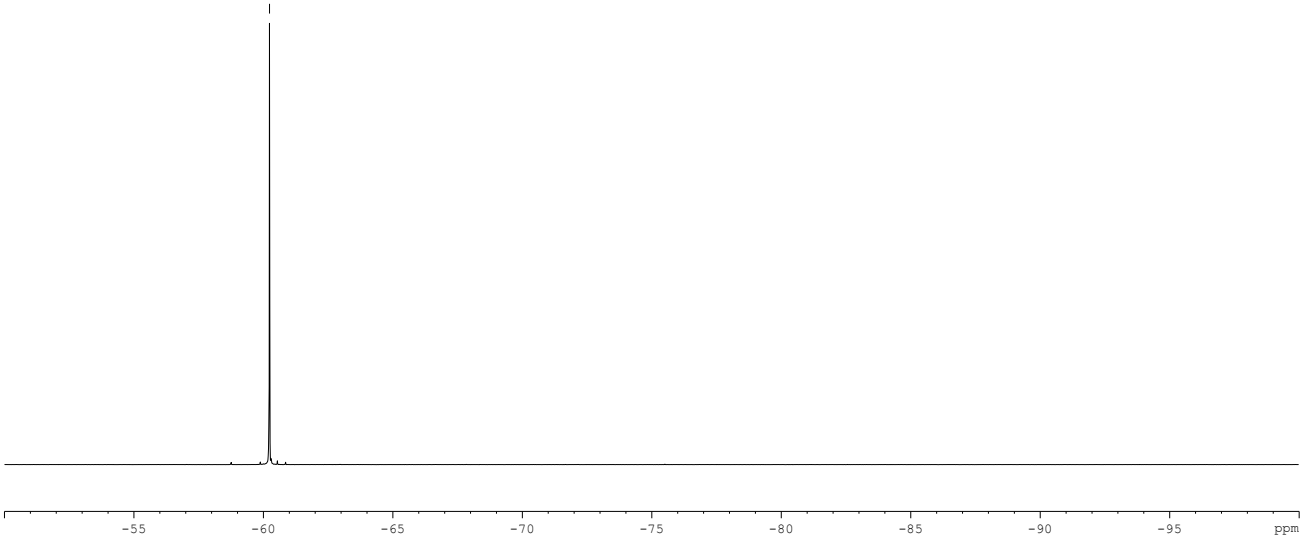

19F NMR
-62.847
CF3
O
MeO
10
-55 -60 -65 -70 -75 -80 -85 -90 -95 ppm


1H NMR
8.340
8.310
8.260
8.230
7.444
7.437
7.402
7.397
7.386
7.192
7.179
7.170
7.164
7.157
7.152
7.148
7.139
7.126
5.183
3.844
2.541
1.516
1.493
1.467
1.441
1.417
1.387
1.364
1.341
1.317
1.292
1.267
0.861
0.837
0.813
MeO
O
CF3
ONbz
nBu
6b
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 ppm
1.99
2.00
1.00
2.00
1.03
2.01
3.03
1.98
2.06
2.00
3.06
13C NMR
195.02
164.28
160.02
152.96
152.92
150.81
135.64
134.74
130.92
129.93
128.47
124.82
123.74
122.13
121.92
121.52
121.17
121.12
120.95
120.72
117.52
112.74
59.01
55.45
31.64
30.17
22.67
13.63
MeO
O
CF3
ONbz
nBu
6b
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 ppm

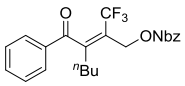
^{19}F NMR



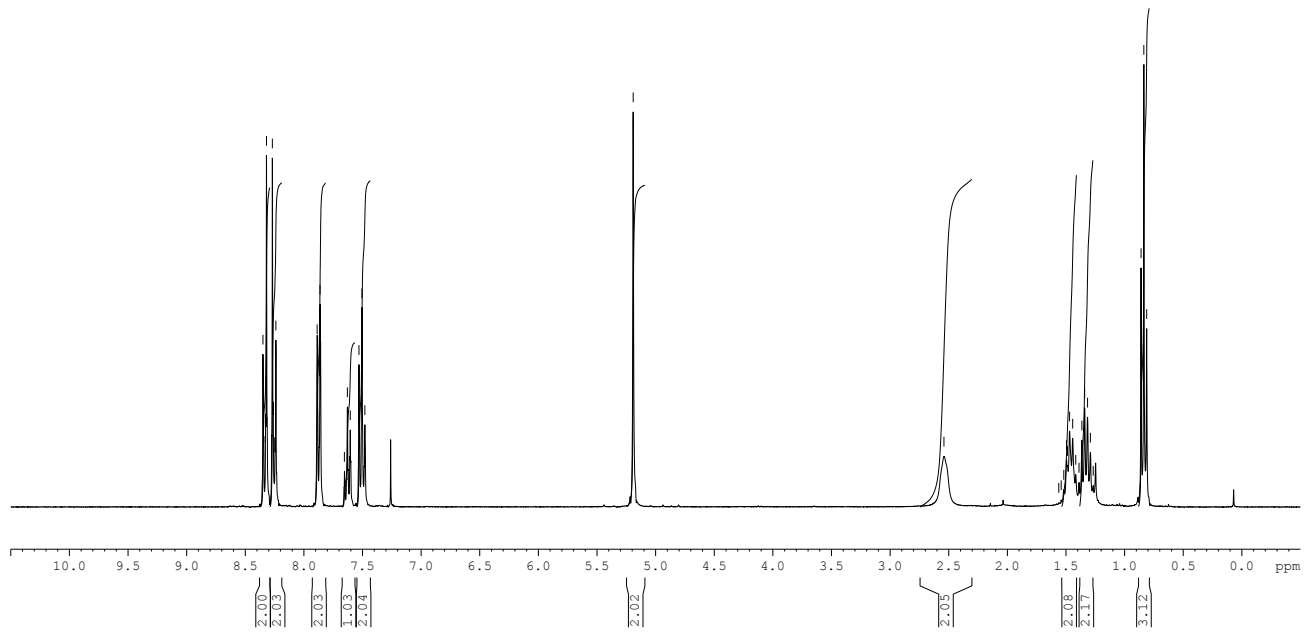
6b



^{1}H NMR

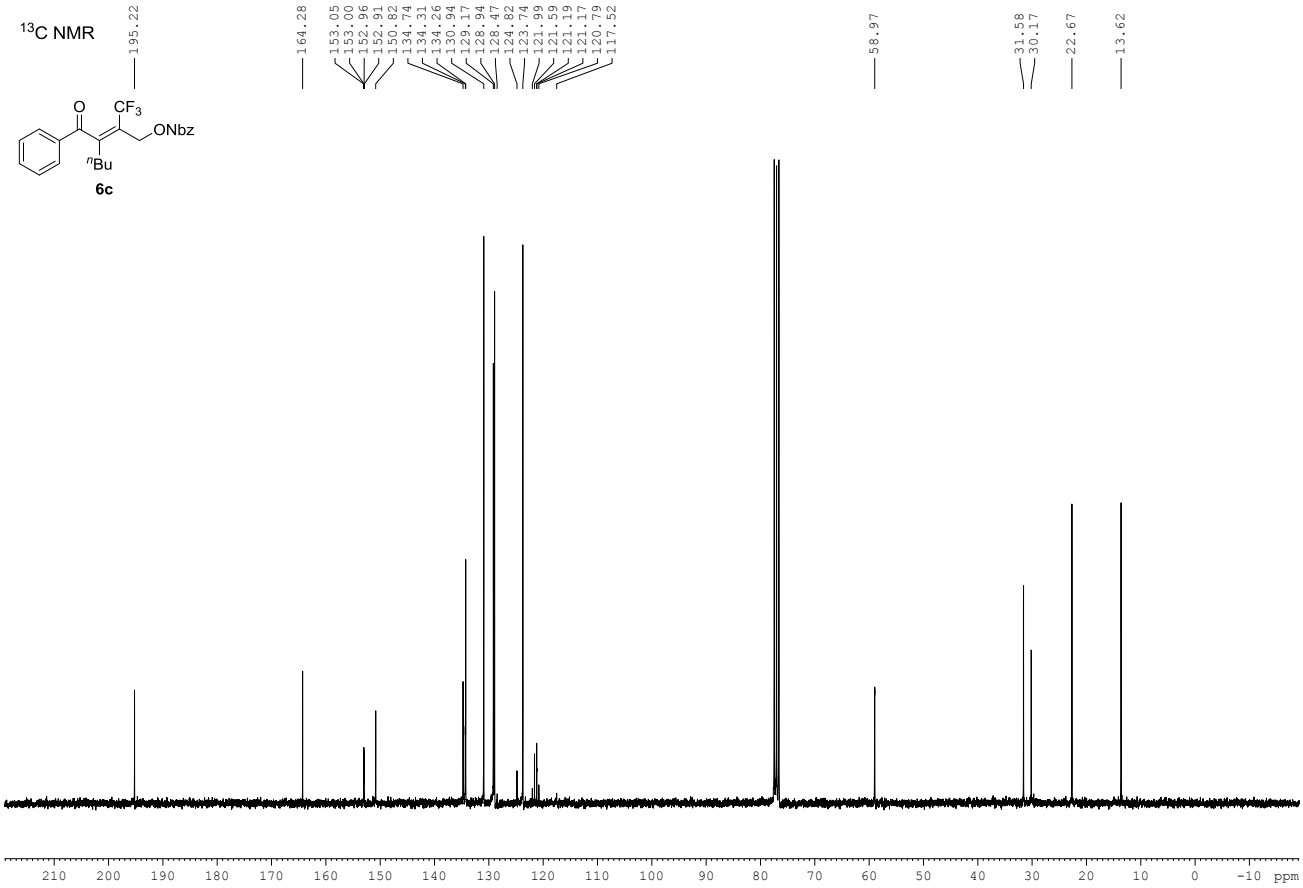


6c



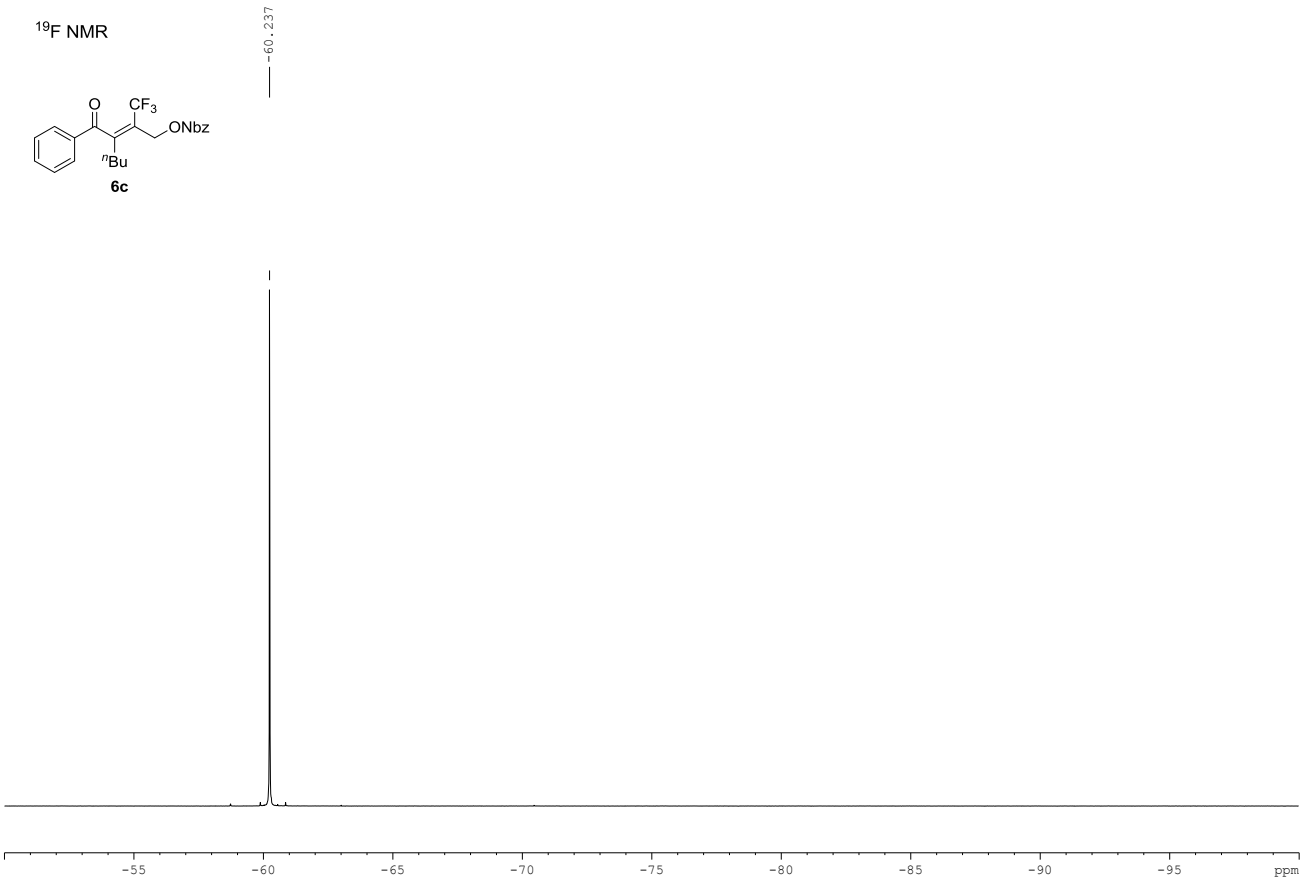
^{13}C NMR

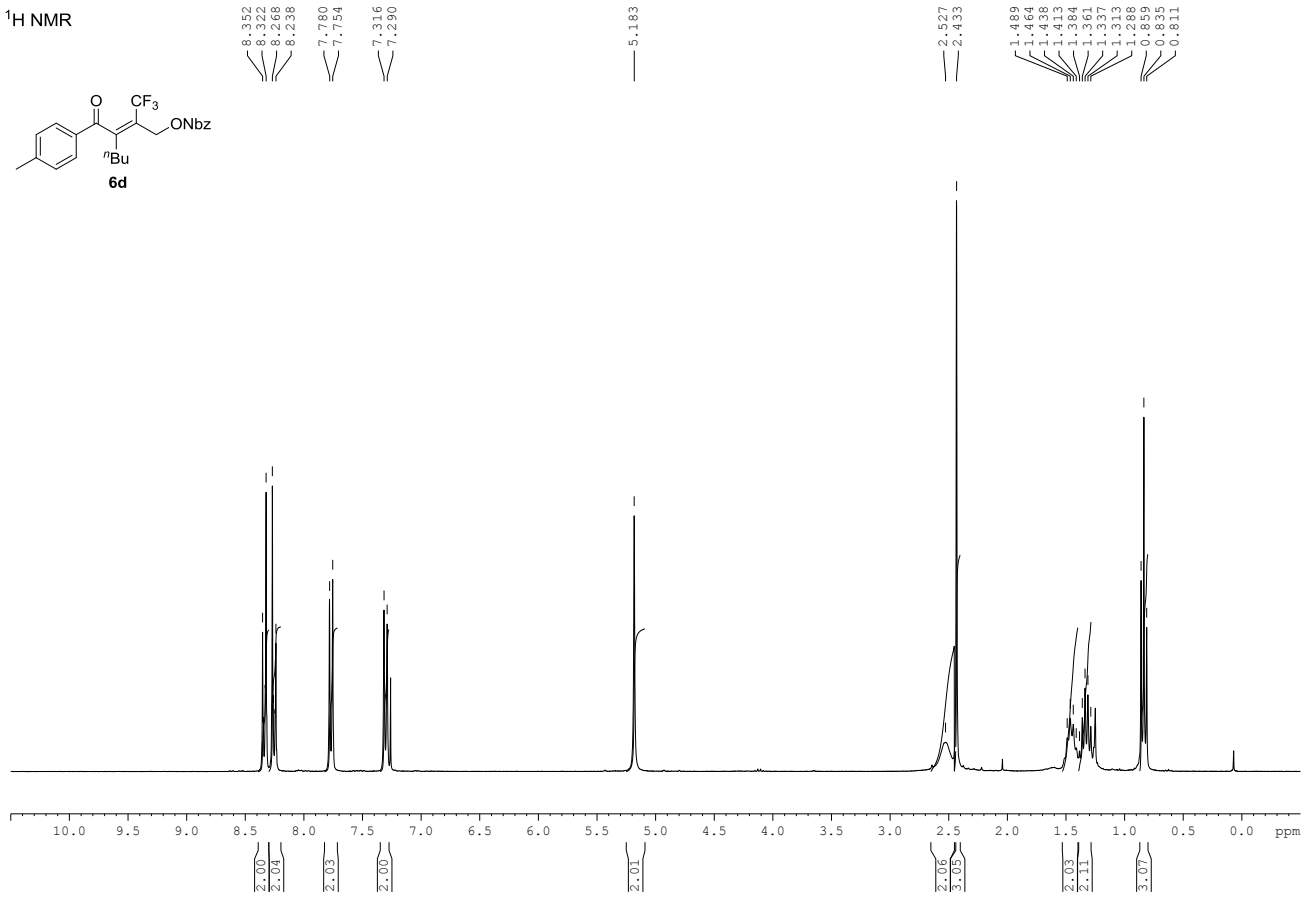
6c

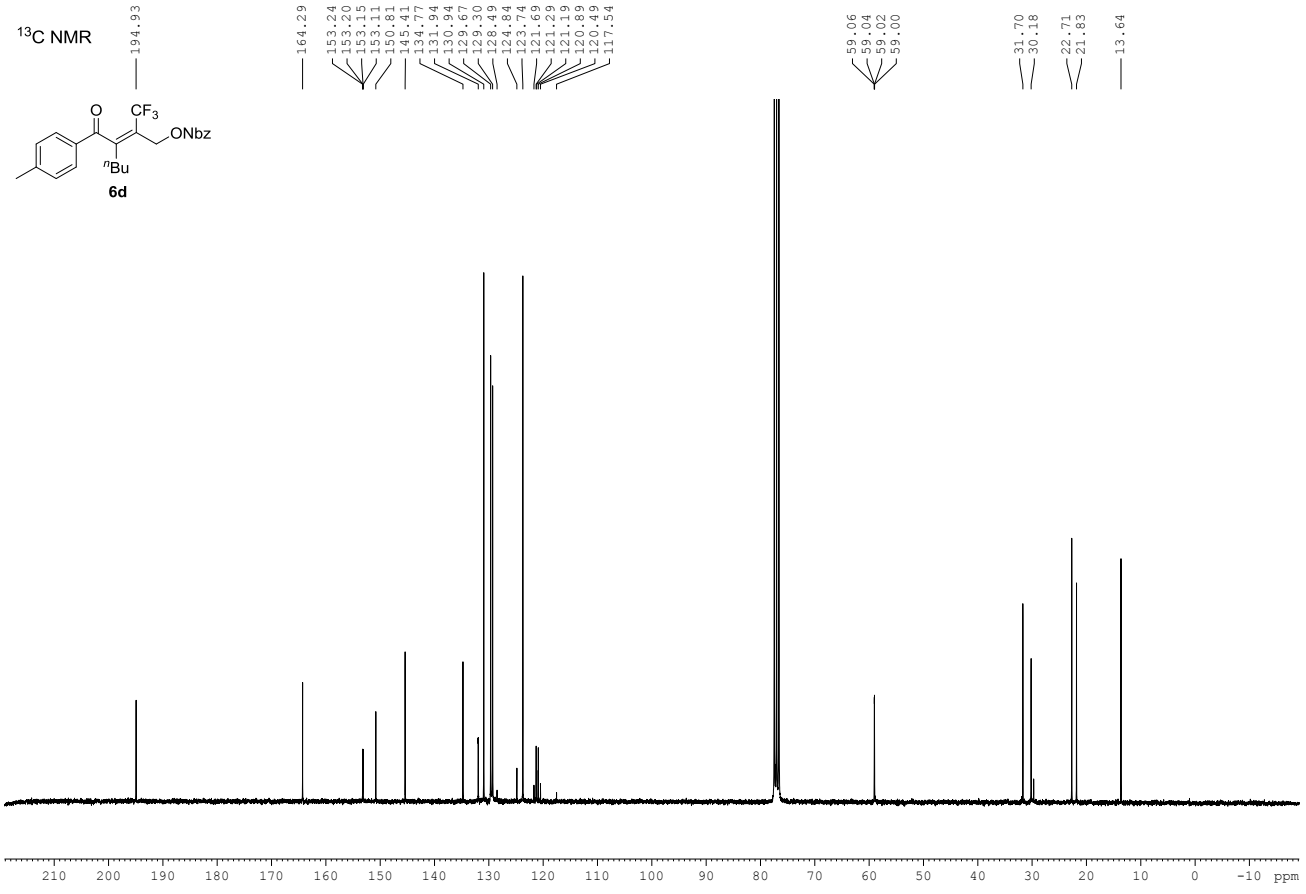


^{19}F NMR

6c

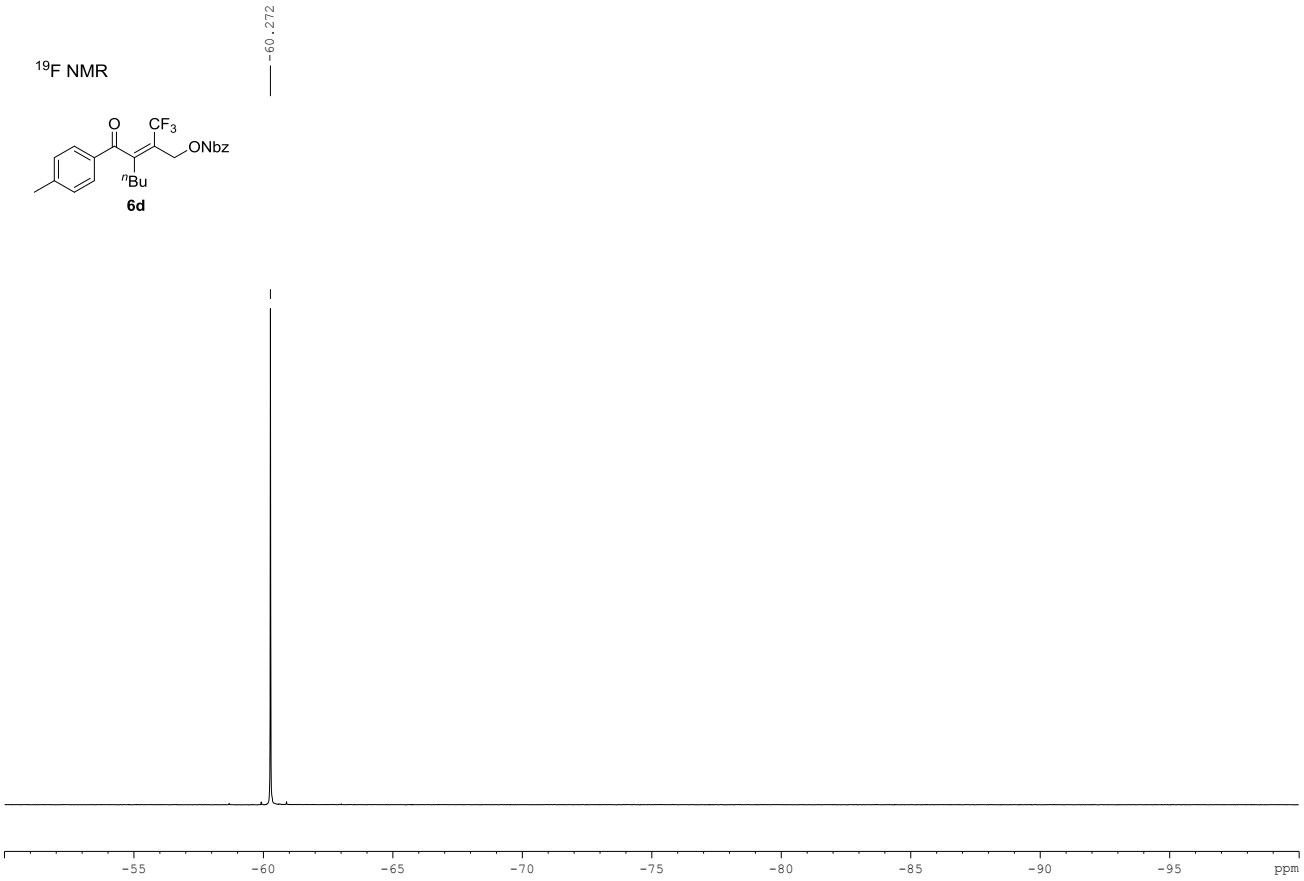



1H NMR
8.352
8.322
8.268
8.238
7.780
7.754
7.316
7.290
5.183
2.527
2.433
1.489
1.464
1.438
1.413
1.384
1.361
1.337
1.313
1.288
0.859
0.835
0.811
O
CF3
ONbz
nBu
6d
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 ppm
2.00
2.04
2.03
2.00
2.01
2.06
3.05
2.03
2.11
3.07


13C NMR
194.93
164.29
153.24
153.20
153.15
153.11
150.81
145.41
134.77
131.94
130.94
129.67
129.30
128.49
124.84
123.74
121.69
121.29
121.19
120.89
120.49
117.54
59.06
59.04
59.02
59.00
31.70
30.18
22.71
21.83
13.64
O
CF3
ONbz
nBu
6d
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 ppm

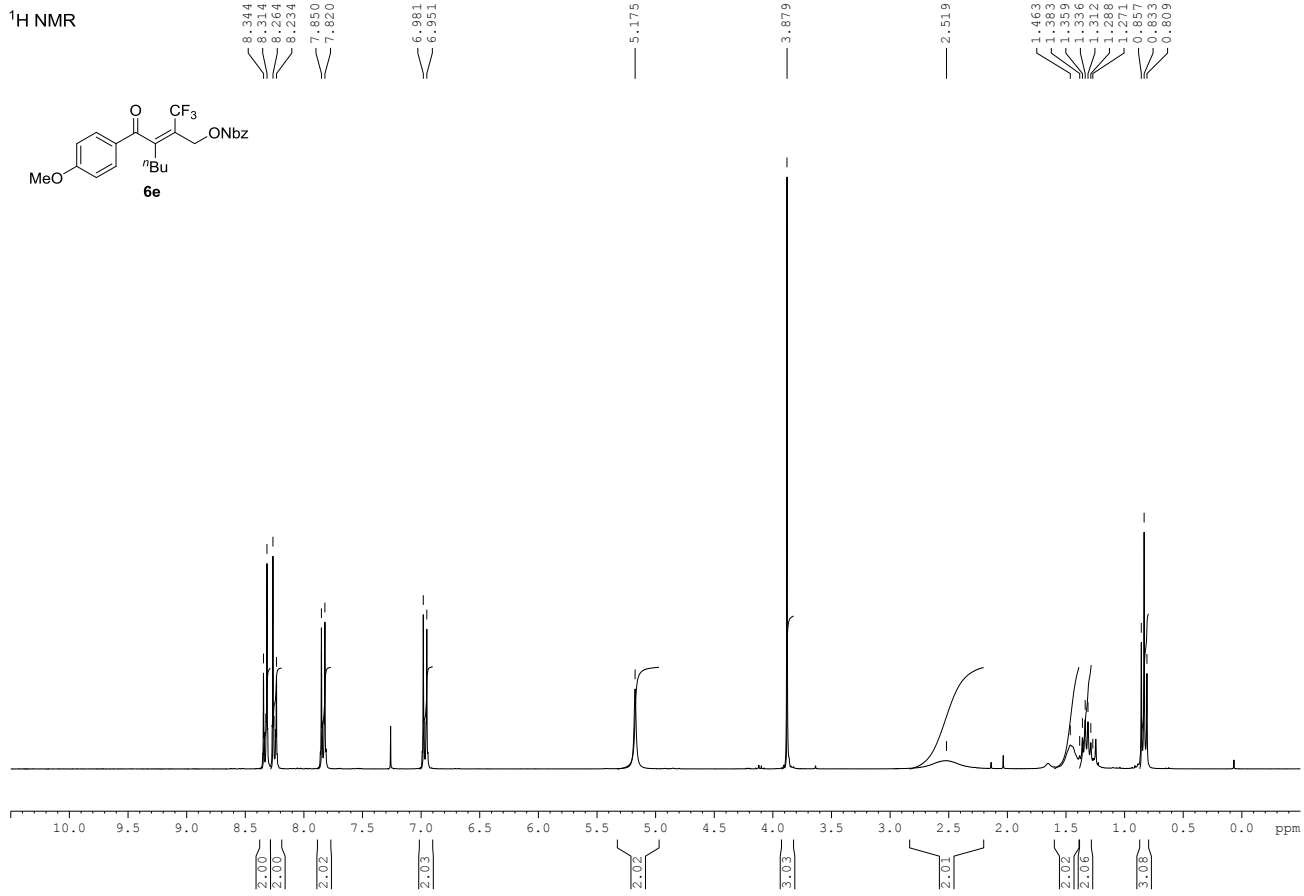
^{19}F NMR

6d



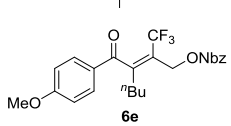
^{1}H NMR

6e

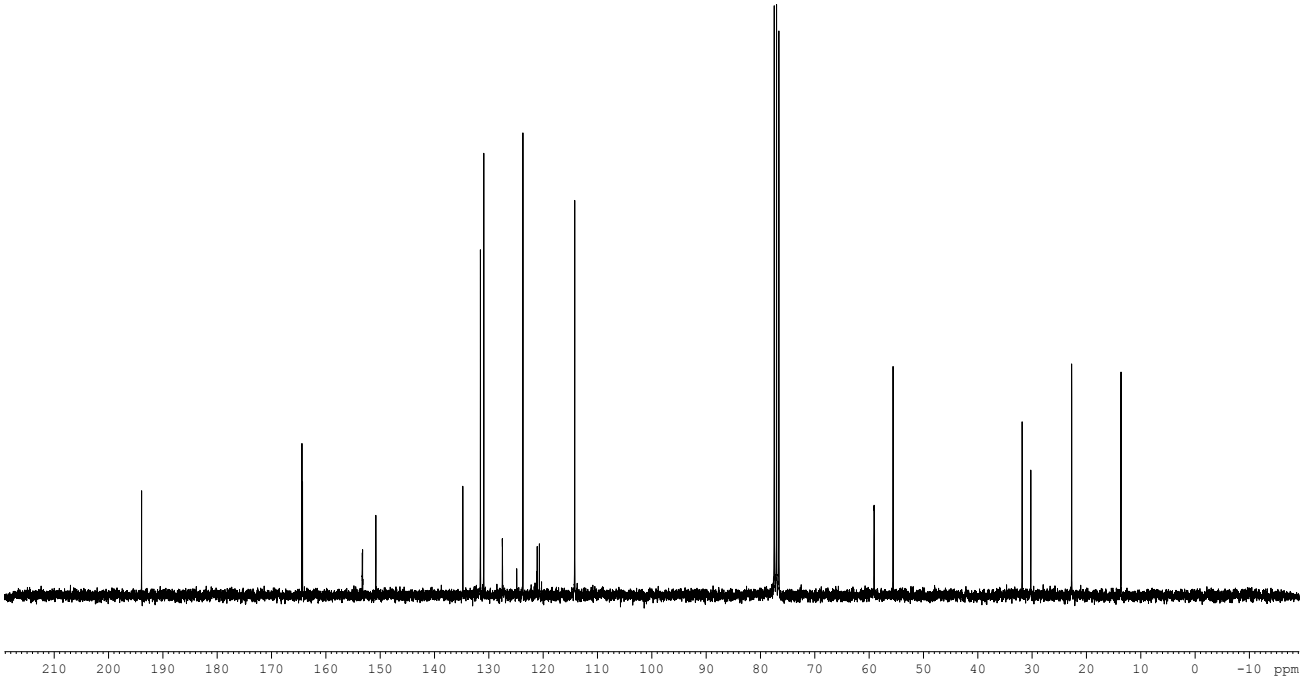


^{13}C NMR

193.92
164.41
164.30
153.34
153.29
153.25
153.20
150.80
134.79
131.55
130.93
128.52
127.51
124.87
123.73
123.50
121.22
121.10
120.70
120.30
117.57
114.19
59.09
55.59
31.83
30.24
22.72
13.64

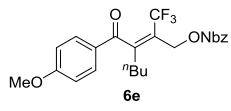


6e

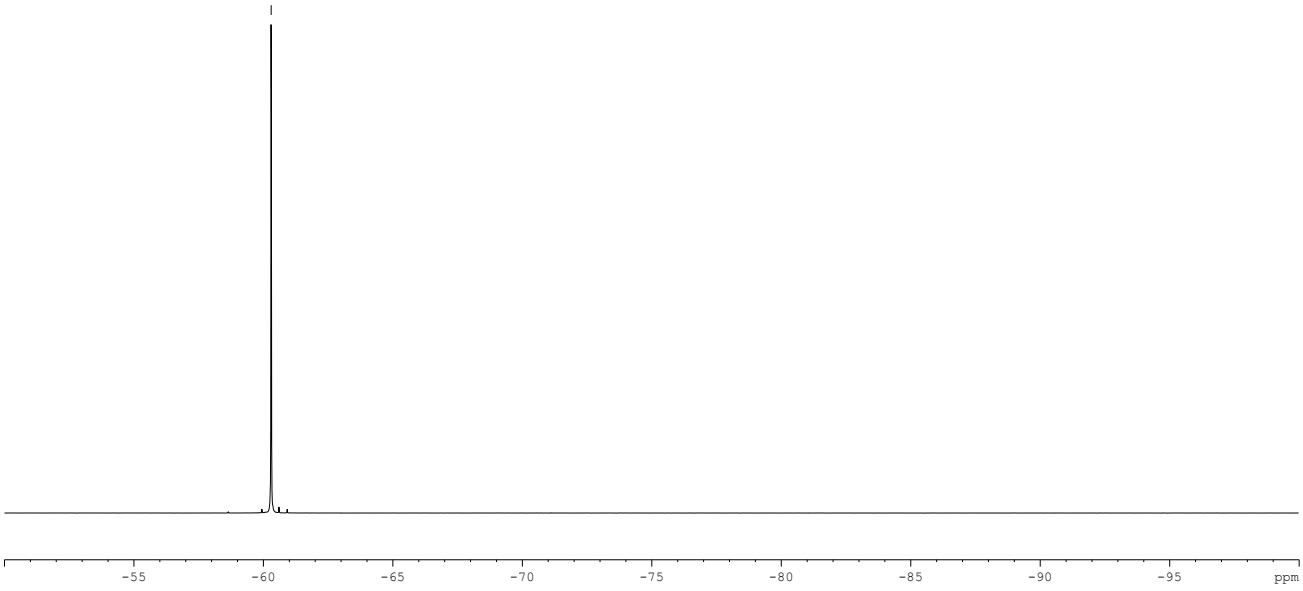


^{19}F NMR

-60.299

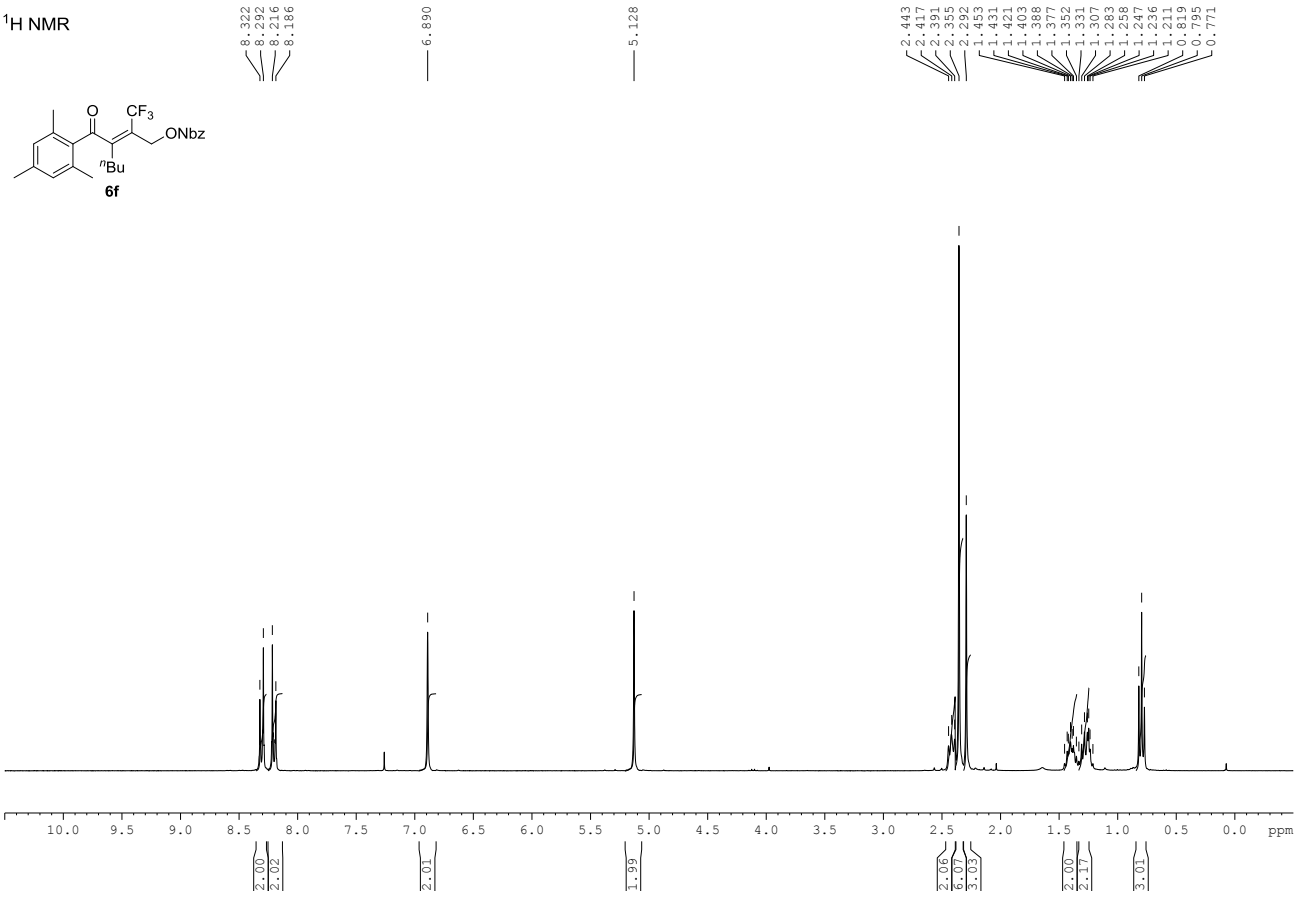


6e

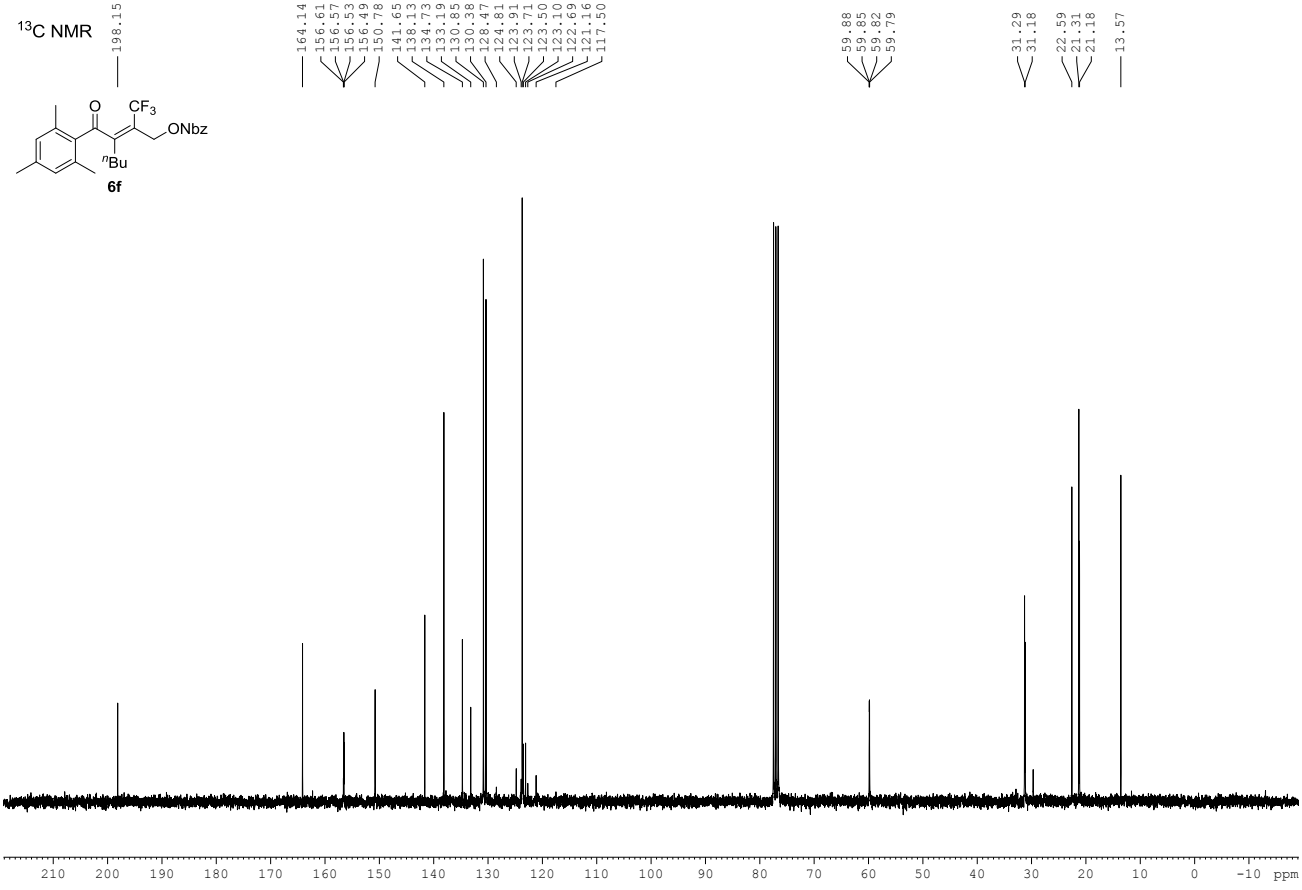


^{1}H NMR

6f



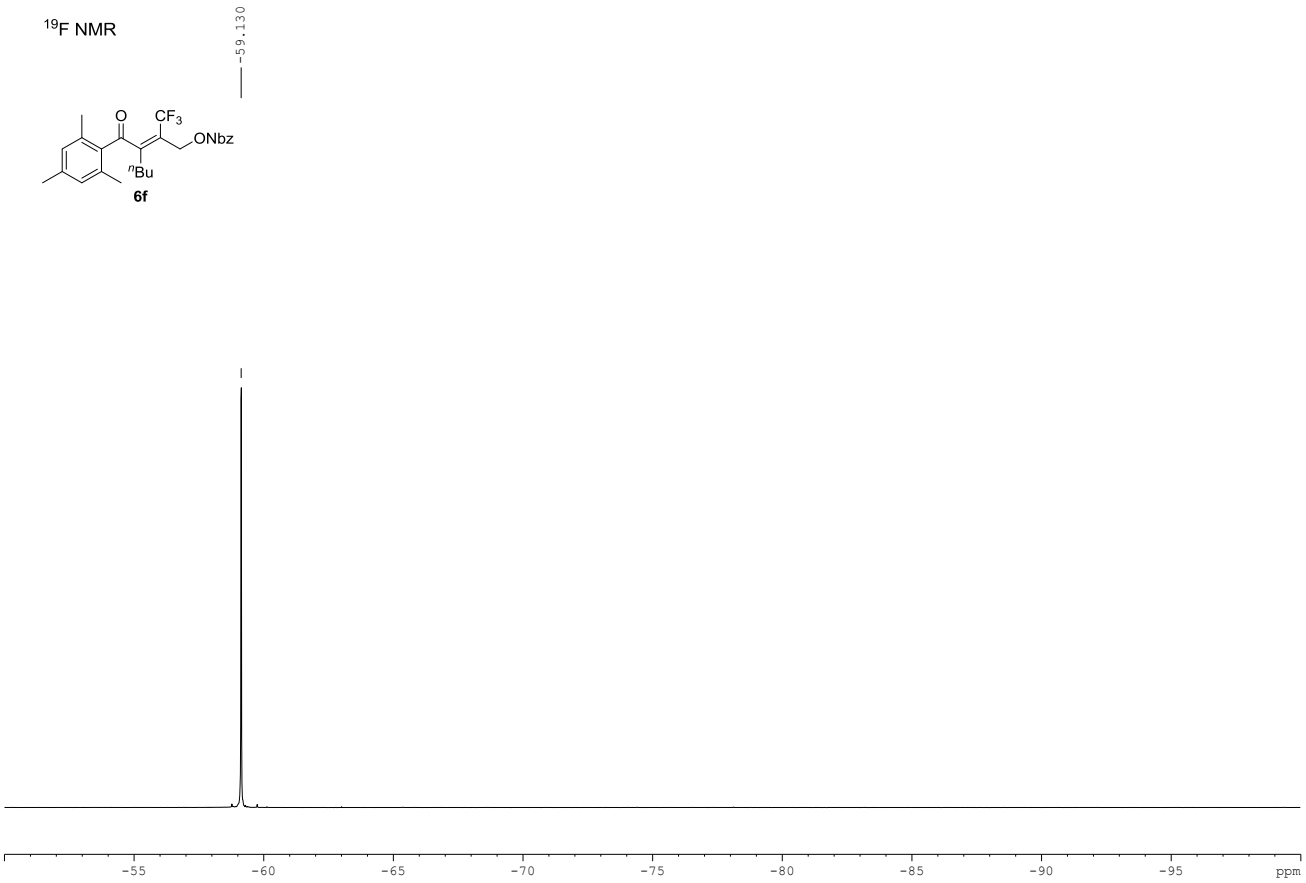
^{13}C NMR



6f

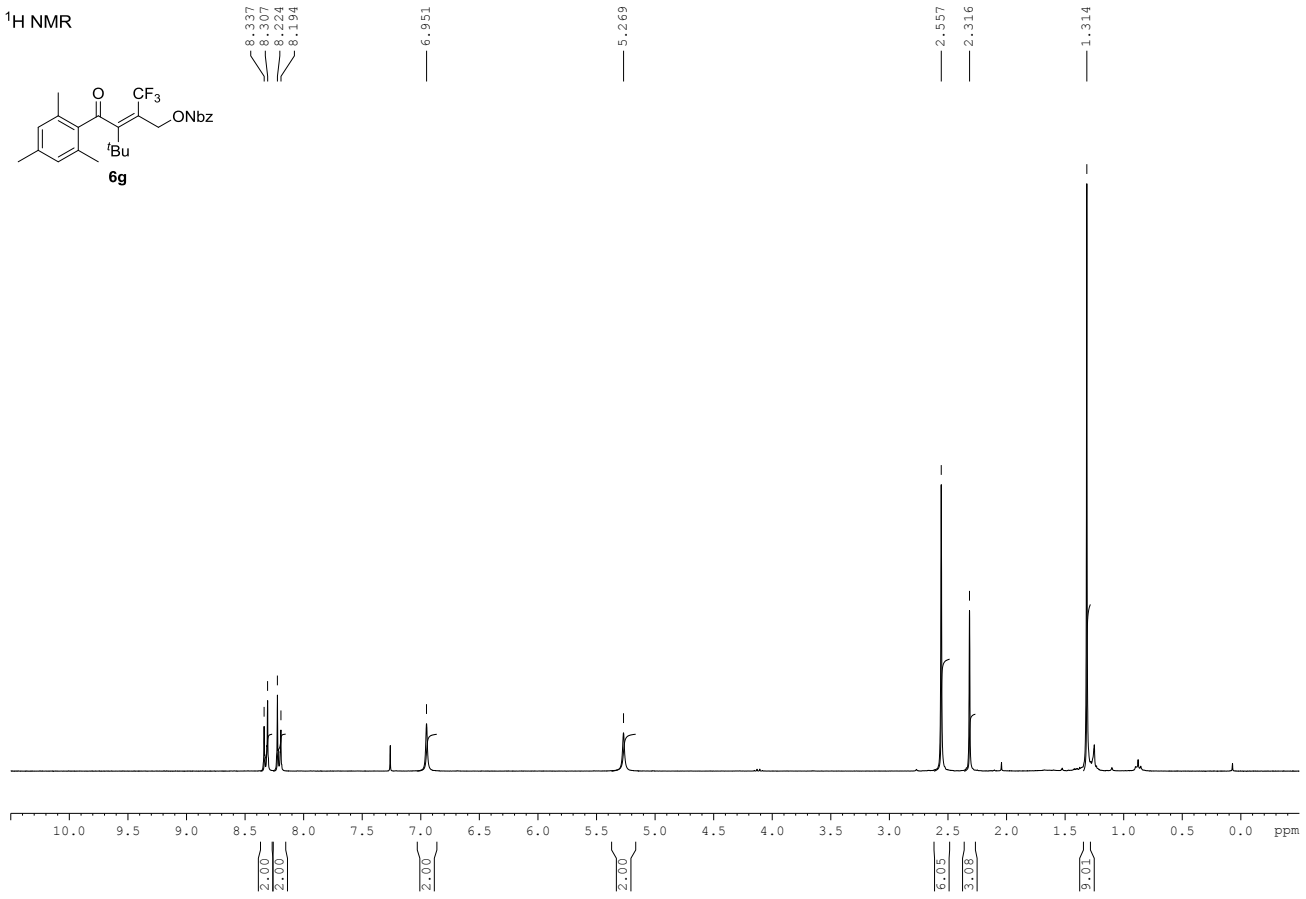
^{19}F NMR

6f

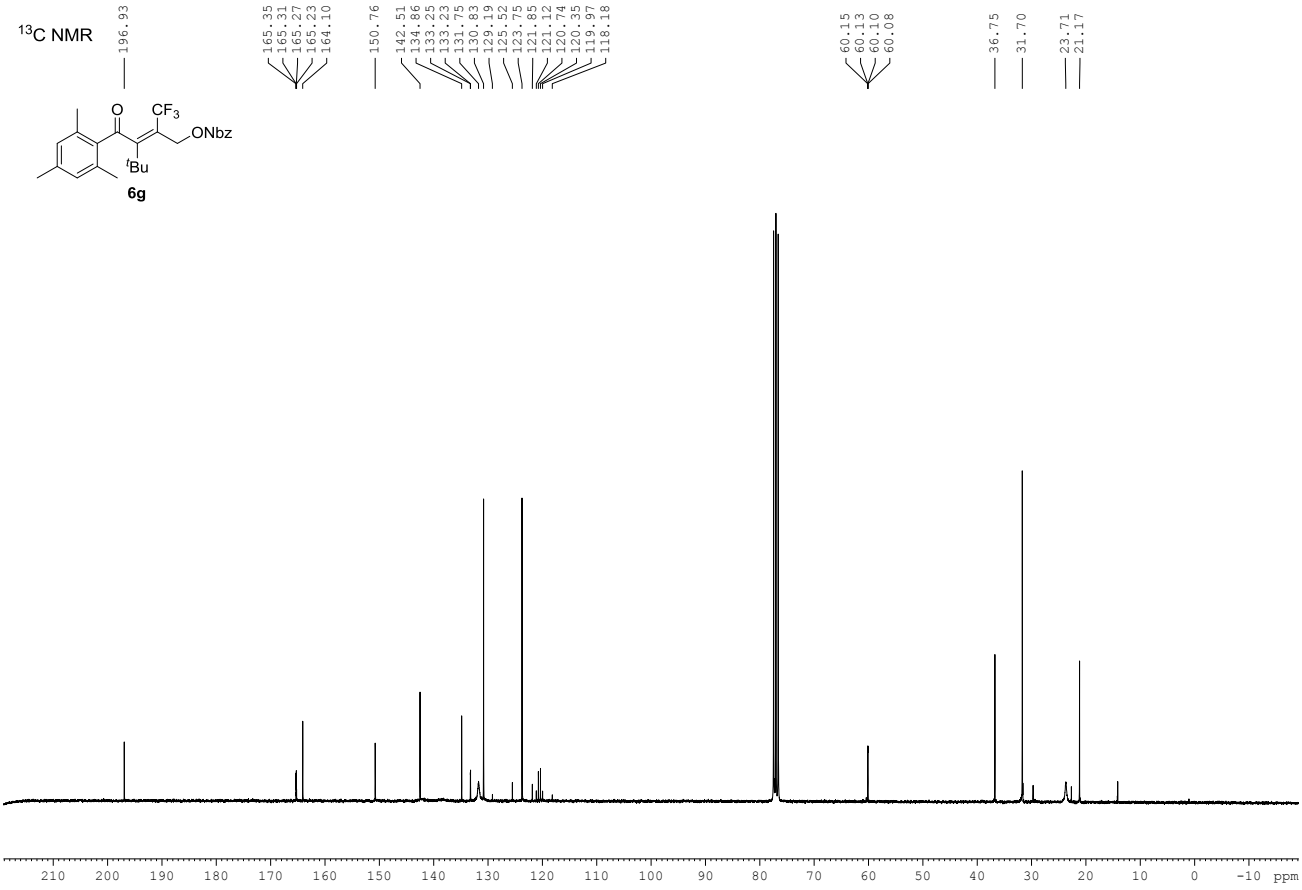


^{1}H NMR

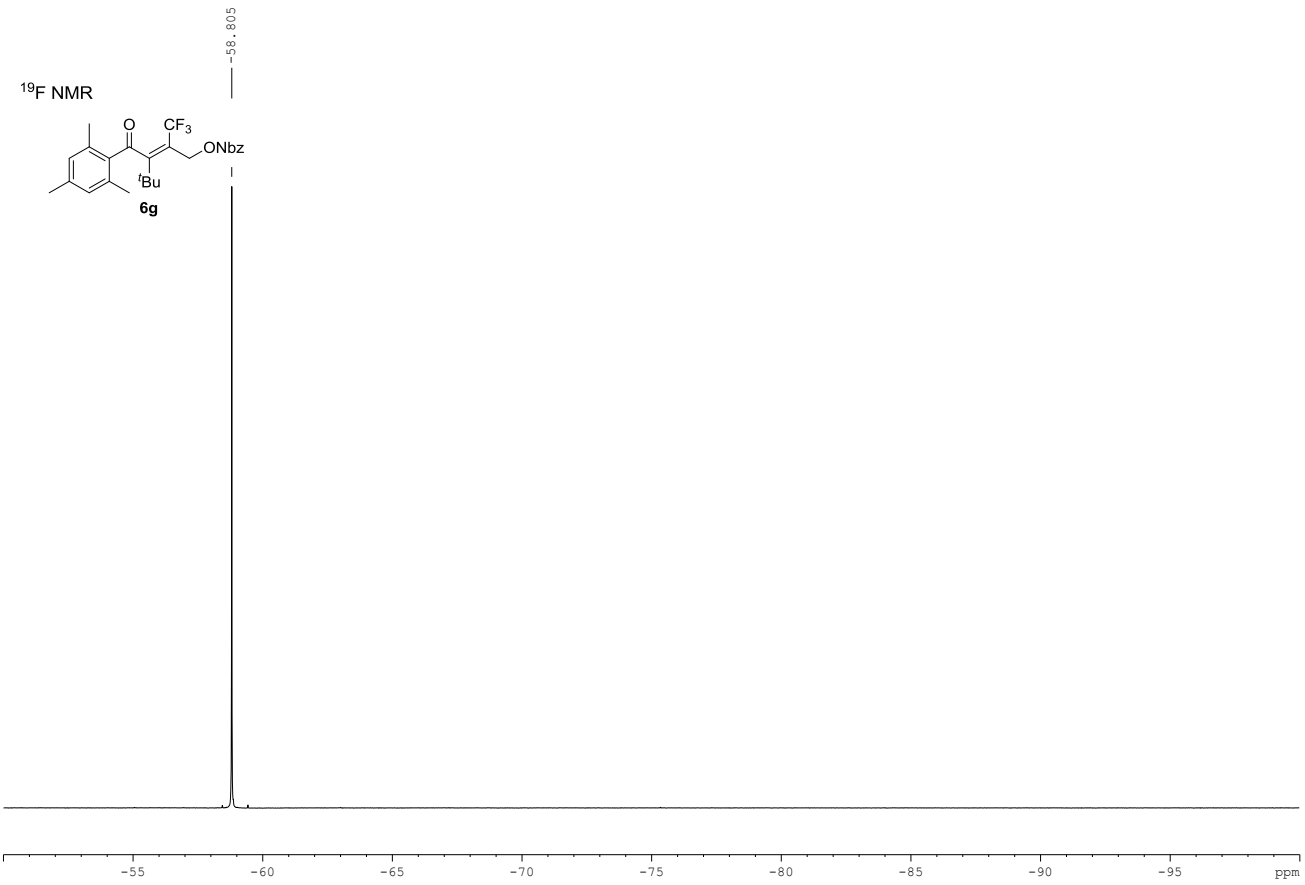
6g

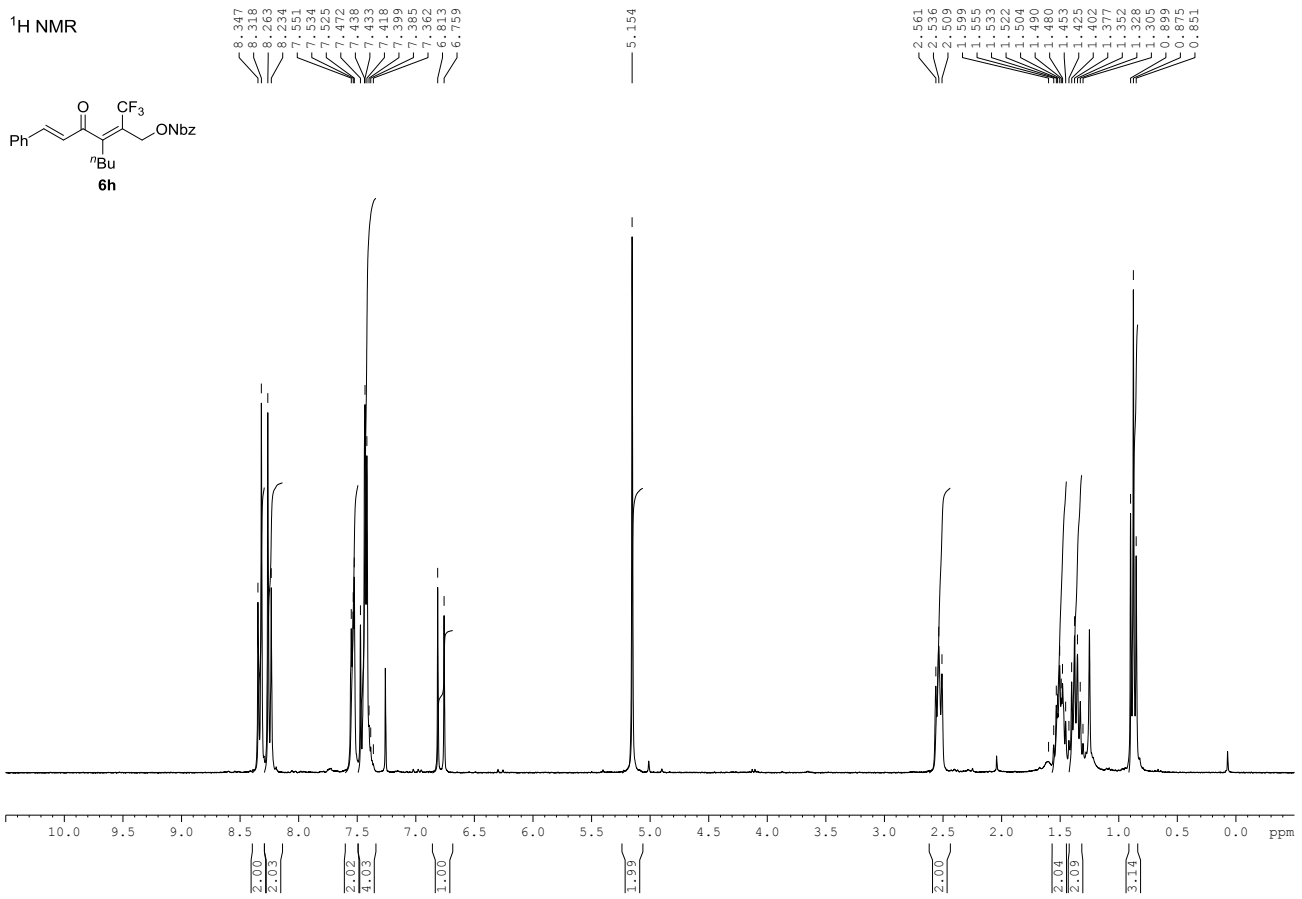


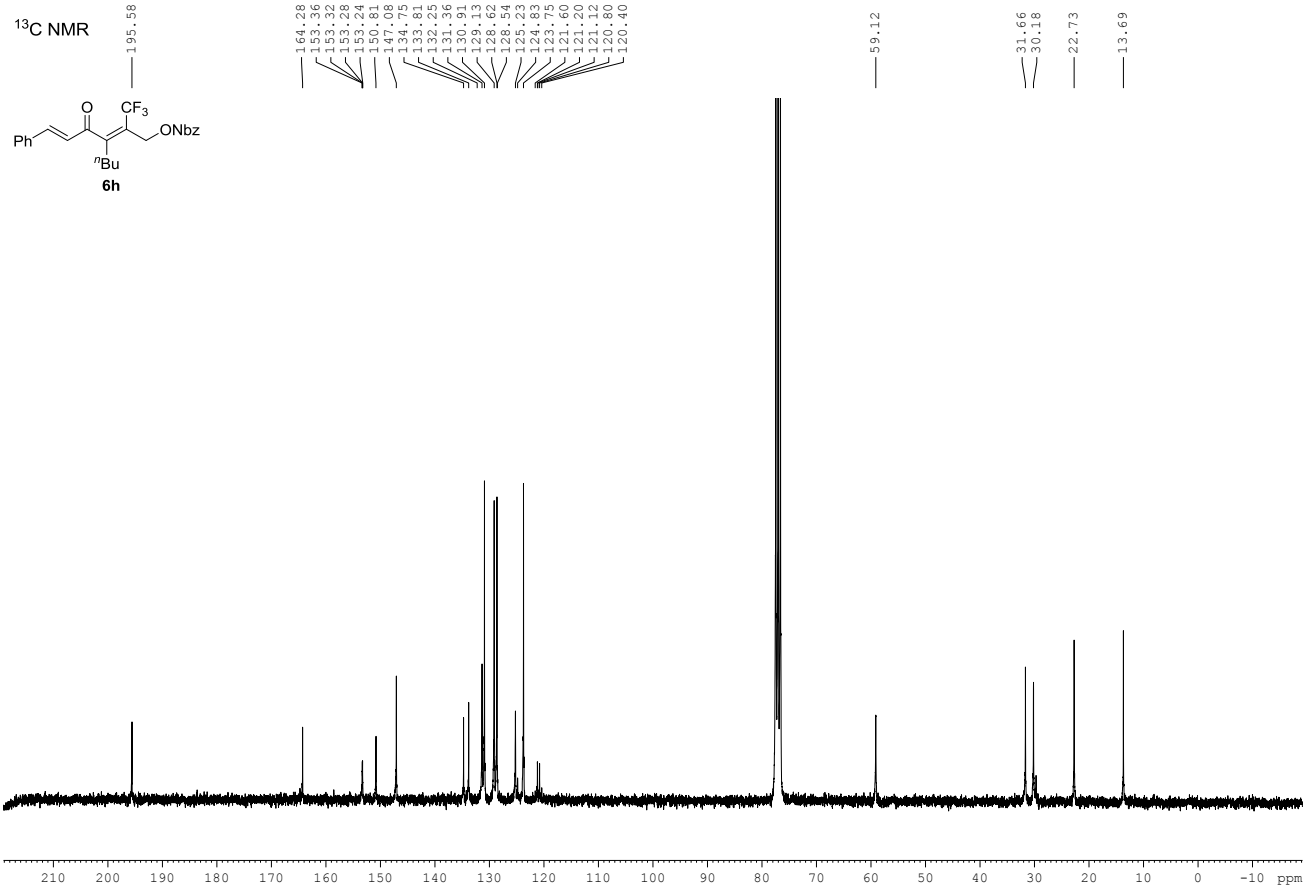
^{13}C NMR



^{19}F NMR

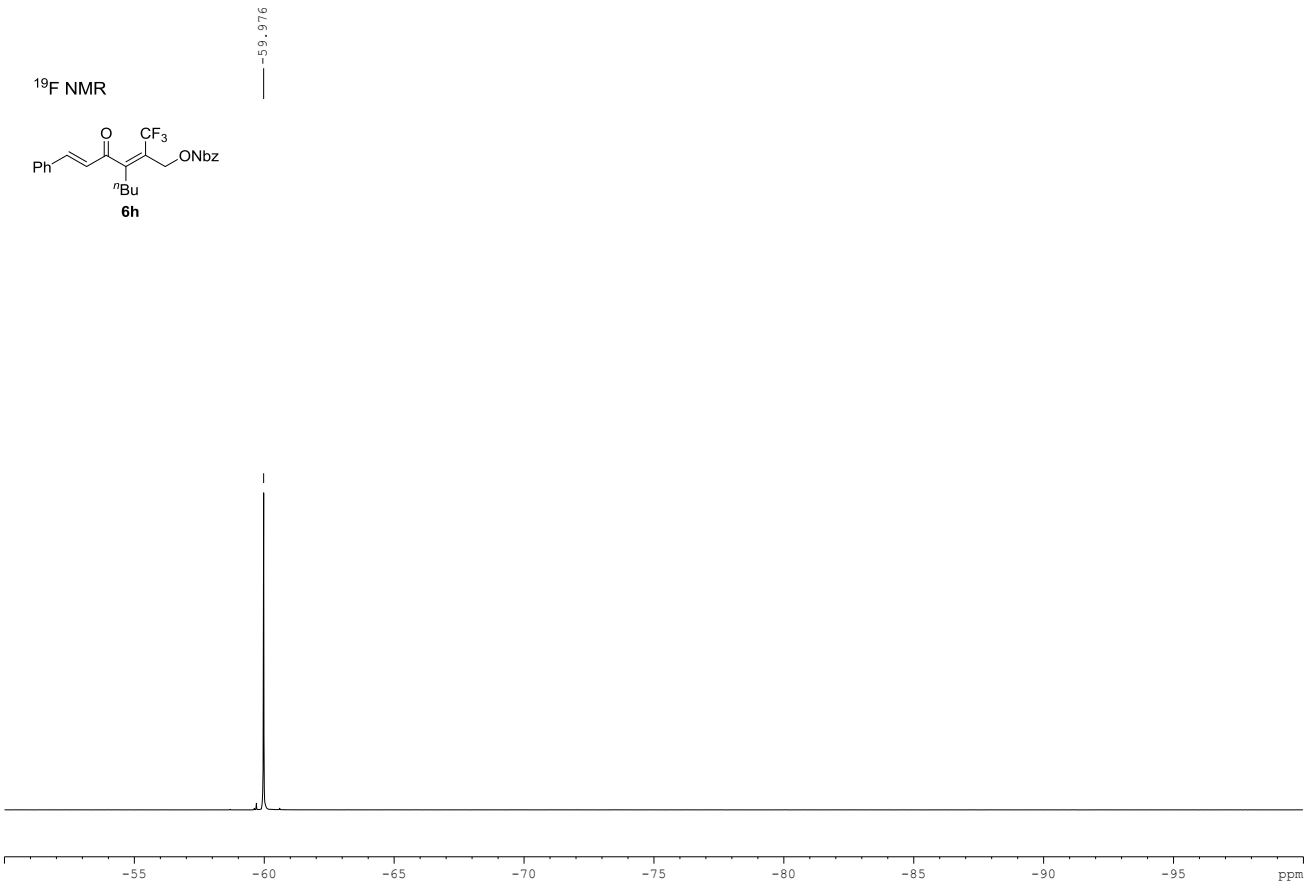



1H NMR
8.347
8.318
8.263
8.234
7.551
7.534
7.525
7.472
7.438
7.433
7.418
7.399
7.385
7.362
6.813
6.759
5.154
2.561
2.536
2.509
1.599
1.555
1.533
1.522
1.504
1.490
1.480
1.453
1.425
1.402
1.377
1.352
1.328
1.305
0.899
0.875
0.851
O
CF3
Ph
ONbz
nBu
6h
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
ppm
2.00
2.03
2.02
4.03
1.00
1.99
2.00
2.04
2.09
3.14


13C NMR
195.58
164.28
153.36
153.32
153.28
153.24
150.81
147.08
134.75
133.81
132.25
131.36
130.91
129.13
128.62
128.54
125.23
124.83
123.75
121.60
121.20
121.12
120.80
120.40
59.12
31.66
30.18
22.73
13.69
O
CF3
Ph
ONbz
nBu
6h
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
ppm

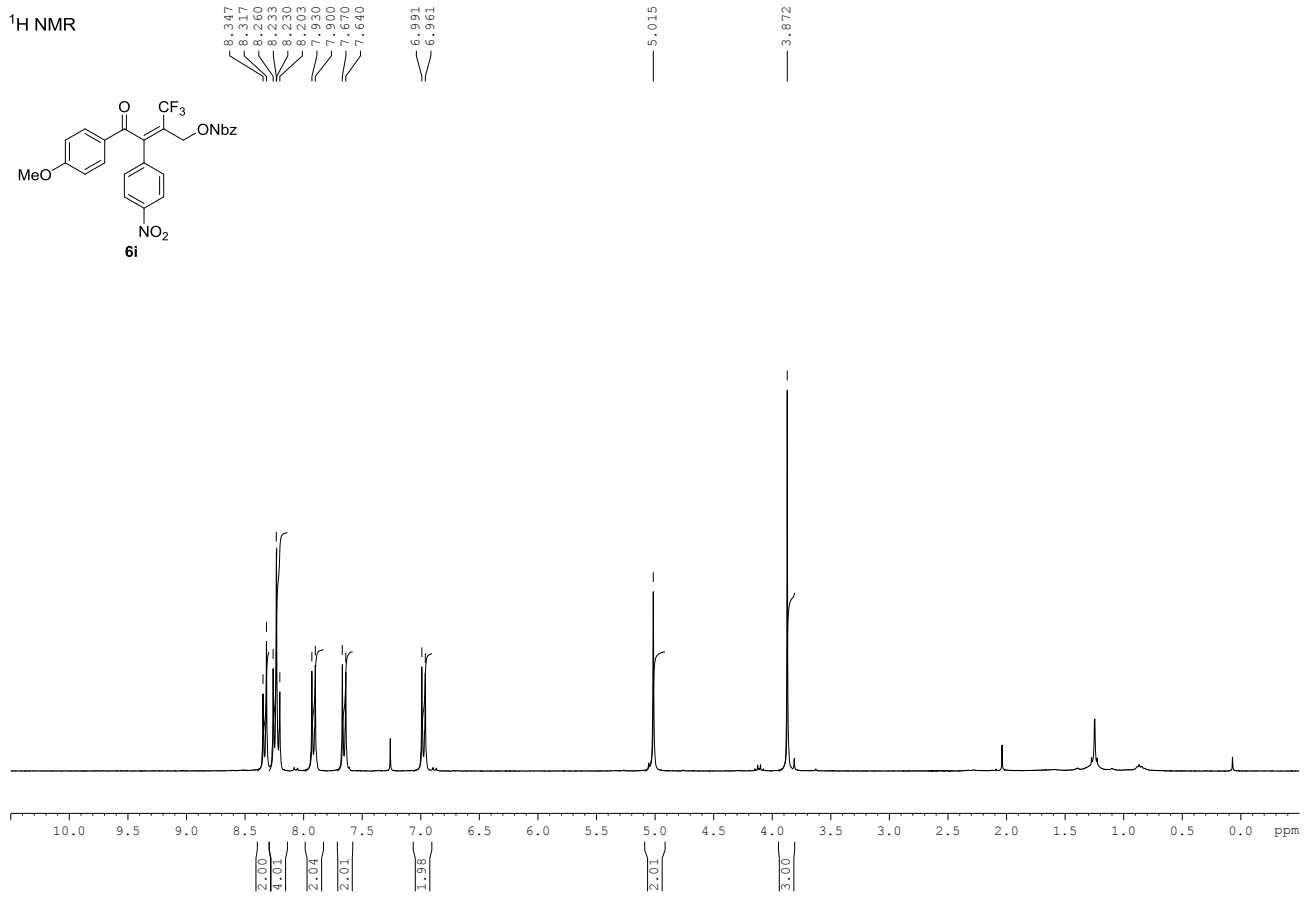
^{19}F NMR

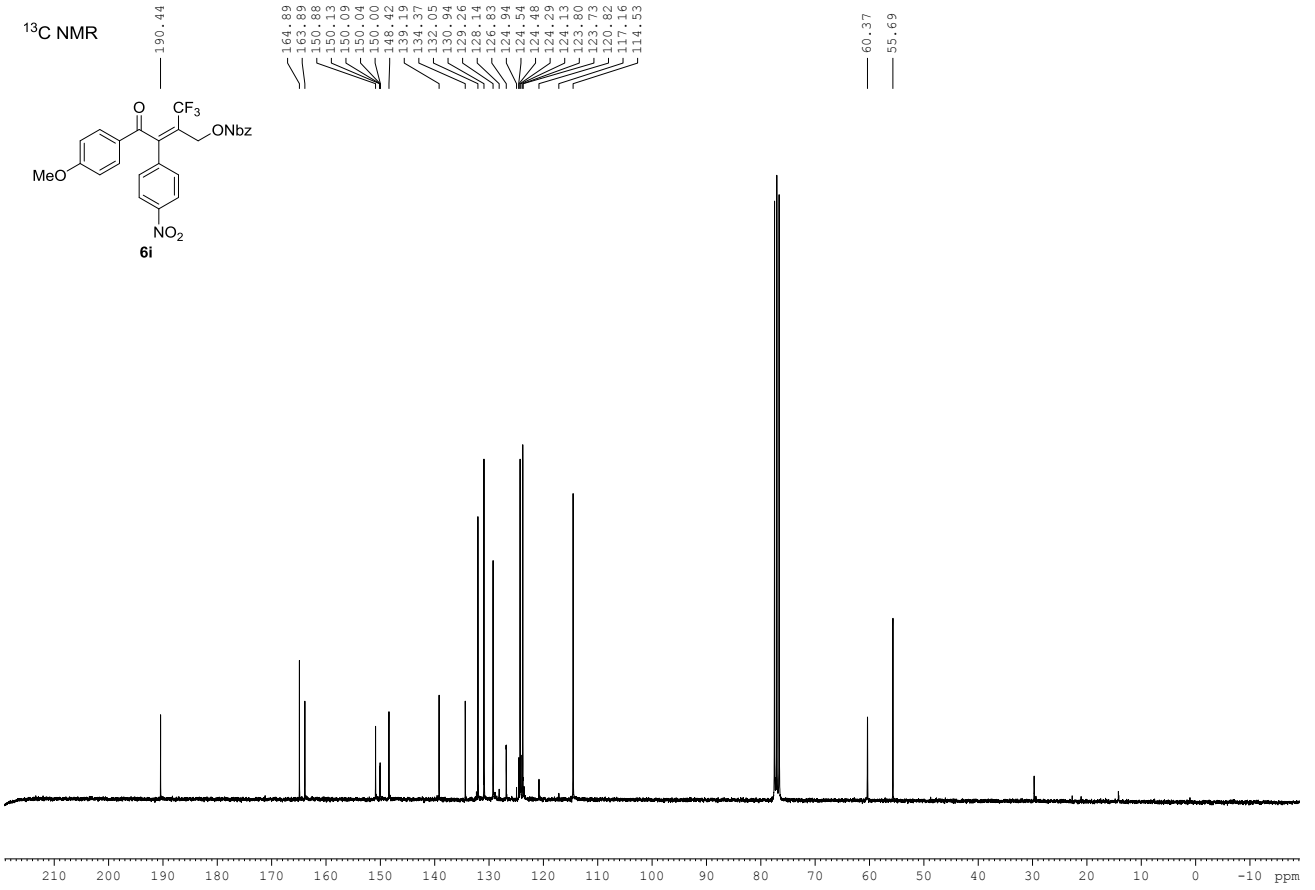
6h

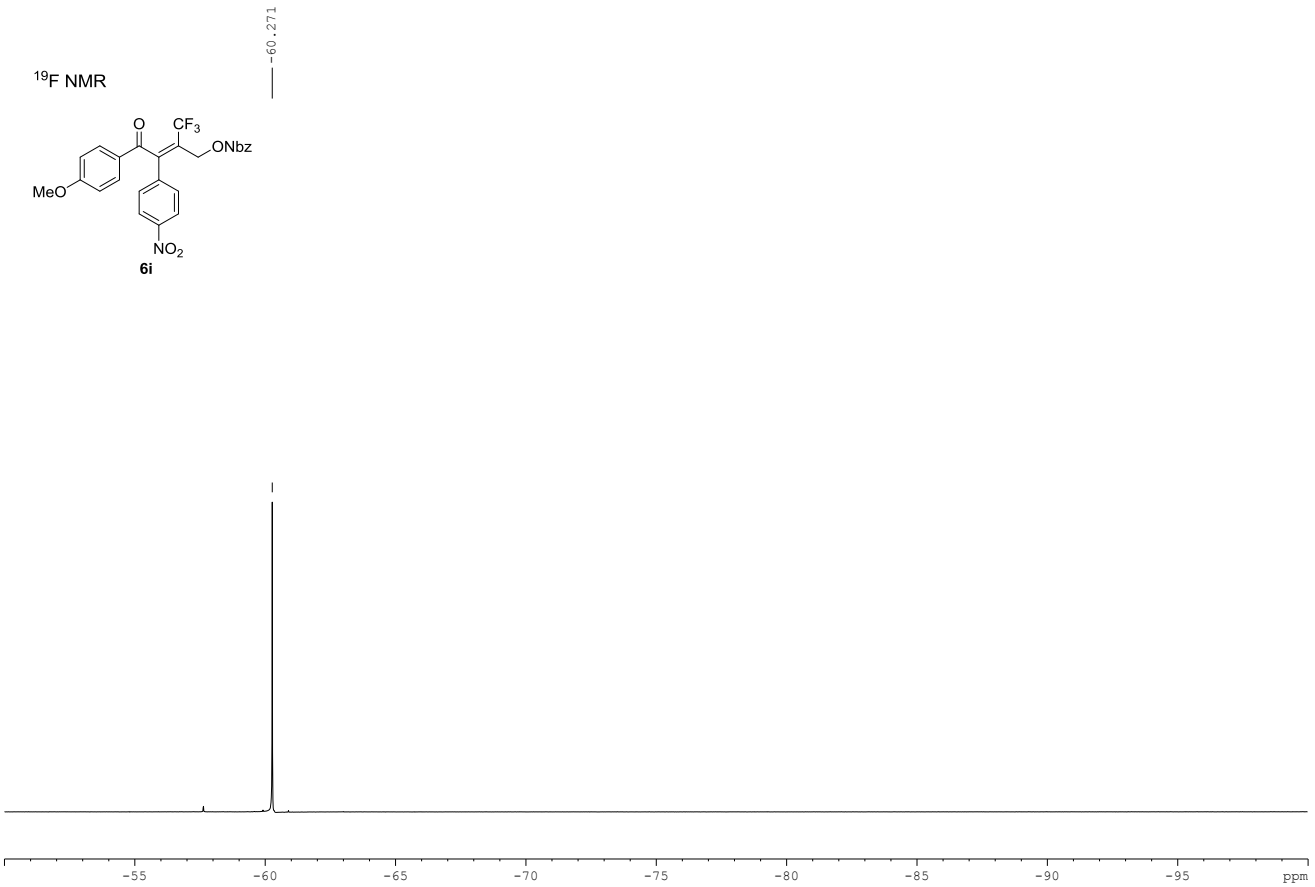


^{1}H NMR

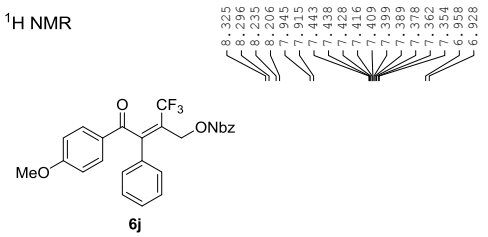
6i



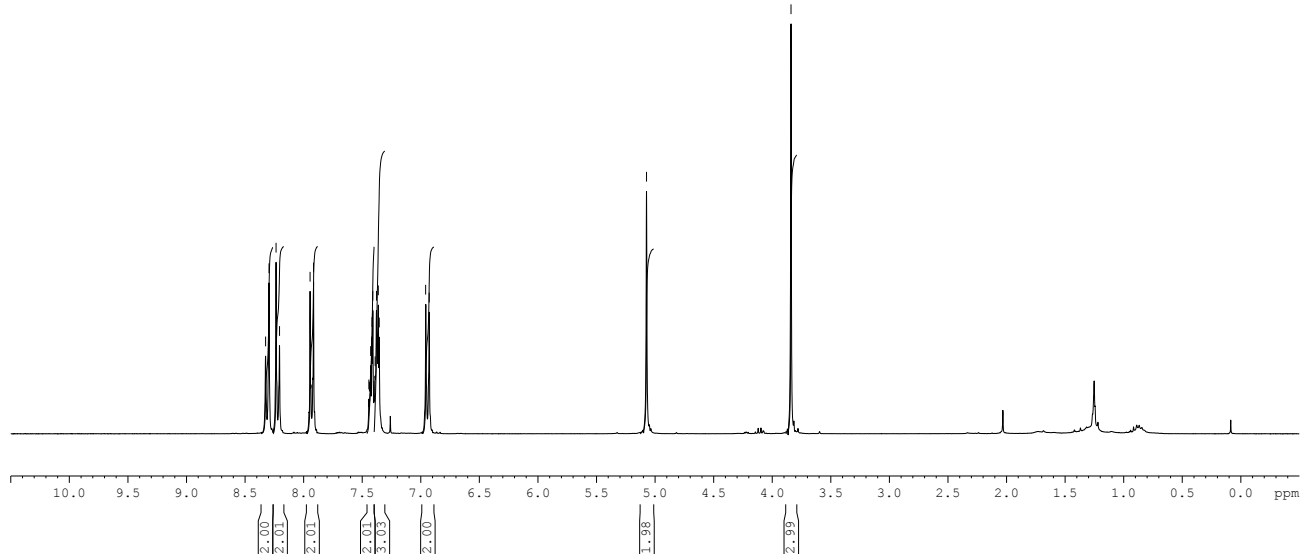

13C NMR
190.44
164.89
163.89
150.88
150.13
150.09
150.04
150.00
148.42
139.19
134.37
132.05
130.94
129.26
128.14
126.83
124.94
124.54
124.48
124.29
124.13
123.80
123.73
120.82
117.16
114.53
60.37
55.69
O
CF3
ONbz
MeO
NO2
6i
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
ppm


19F NMR
-60.271
O
CF3
ONbz
MeO
NO2
6i
-55
-60
-65
-70
-75
-80
-85
-90
-95
ppm

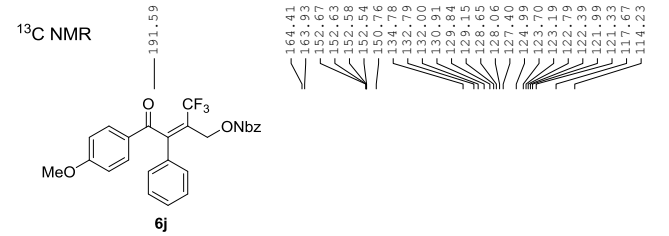
^{1}H NMR



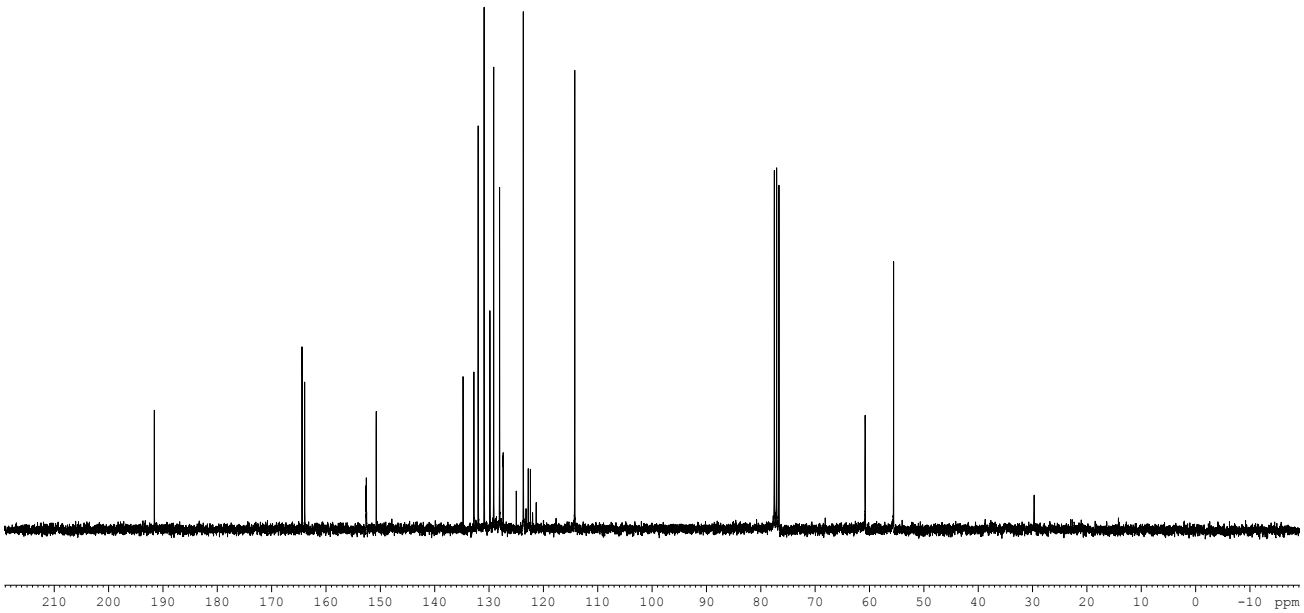
6j



^{13}C NMR

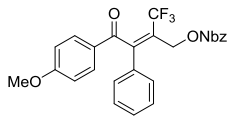


6j

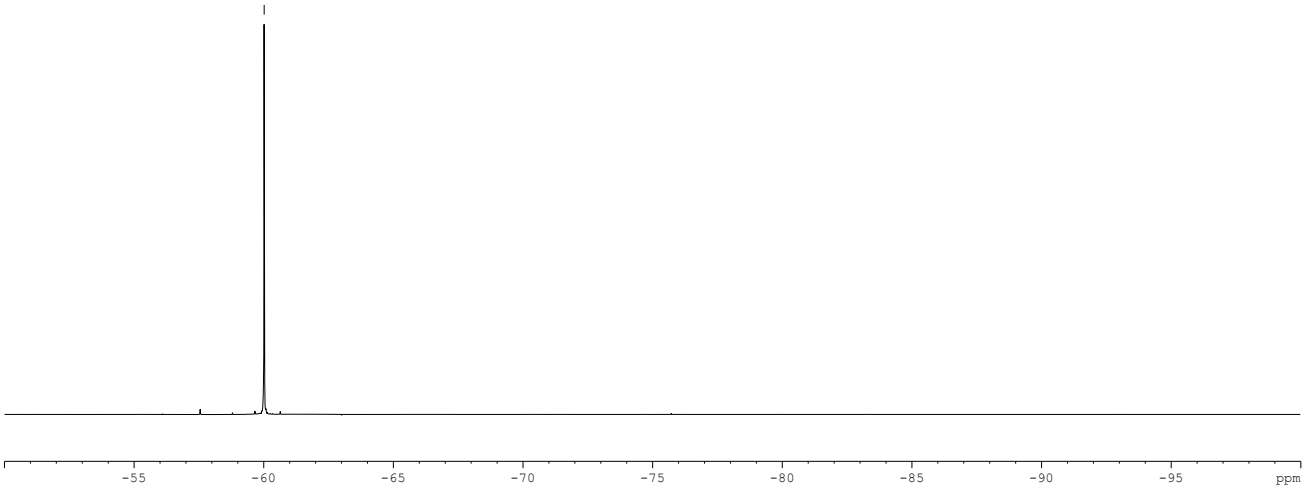


^{19}F NMR

-60.016

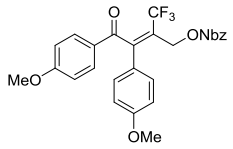


6j

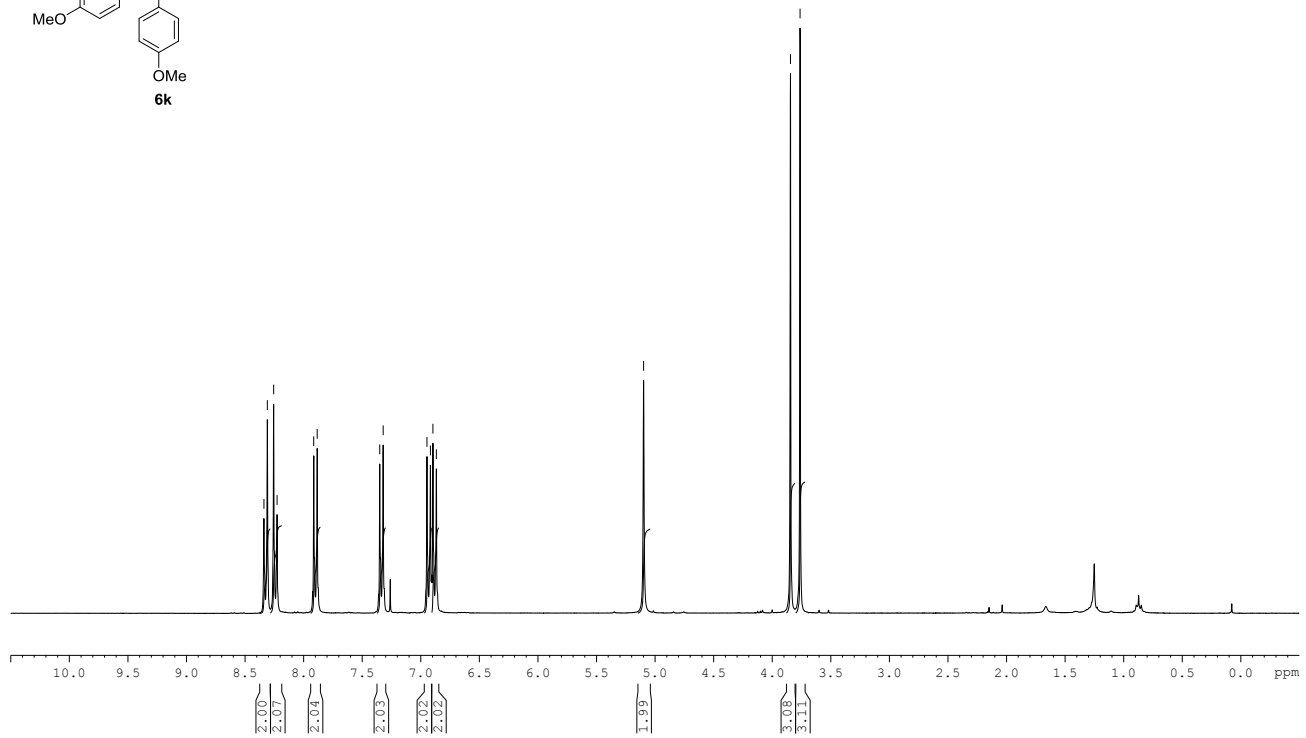


^{1}H NMR

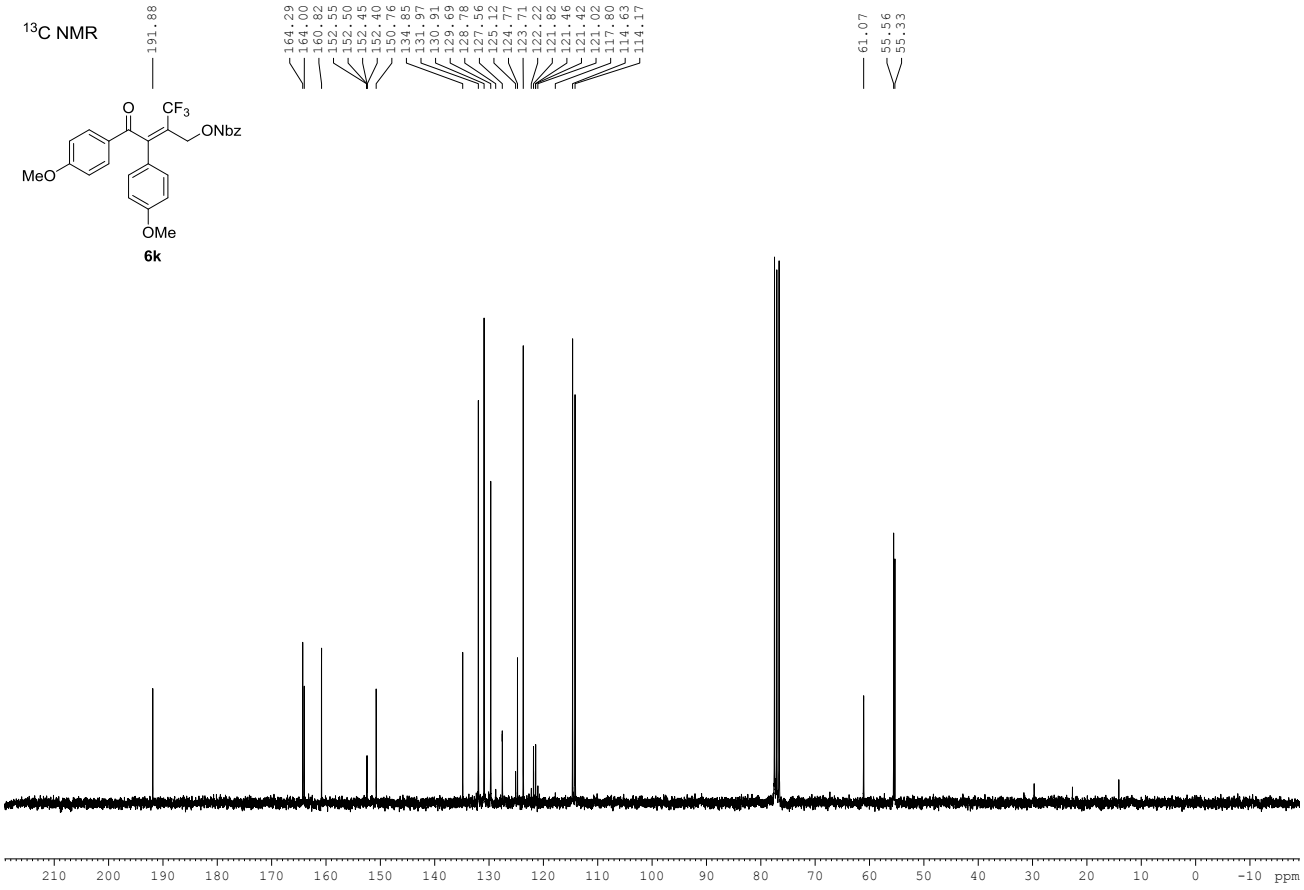
8.339
8.309
8.256
8.226
7.913
7.884
7.350
7.321
6.947
6.918
6.896
6.867
5.098
3.844
3.762

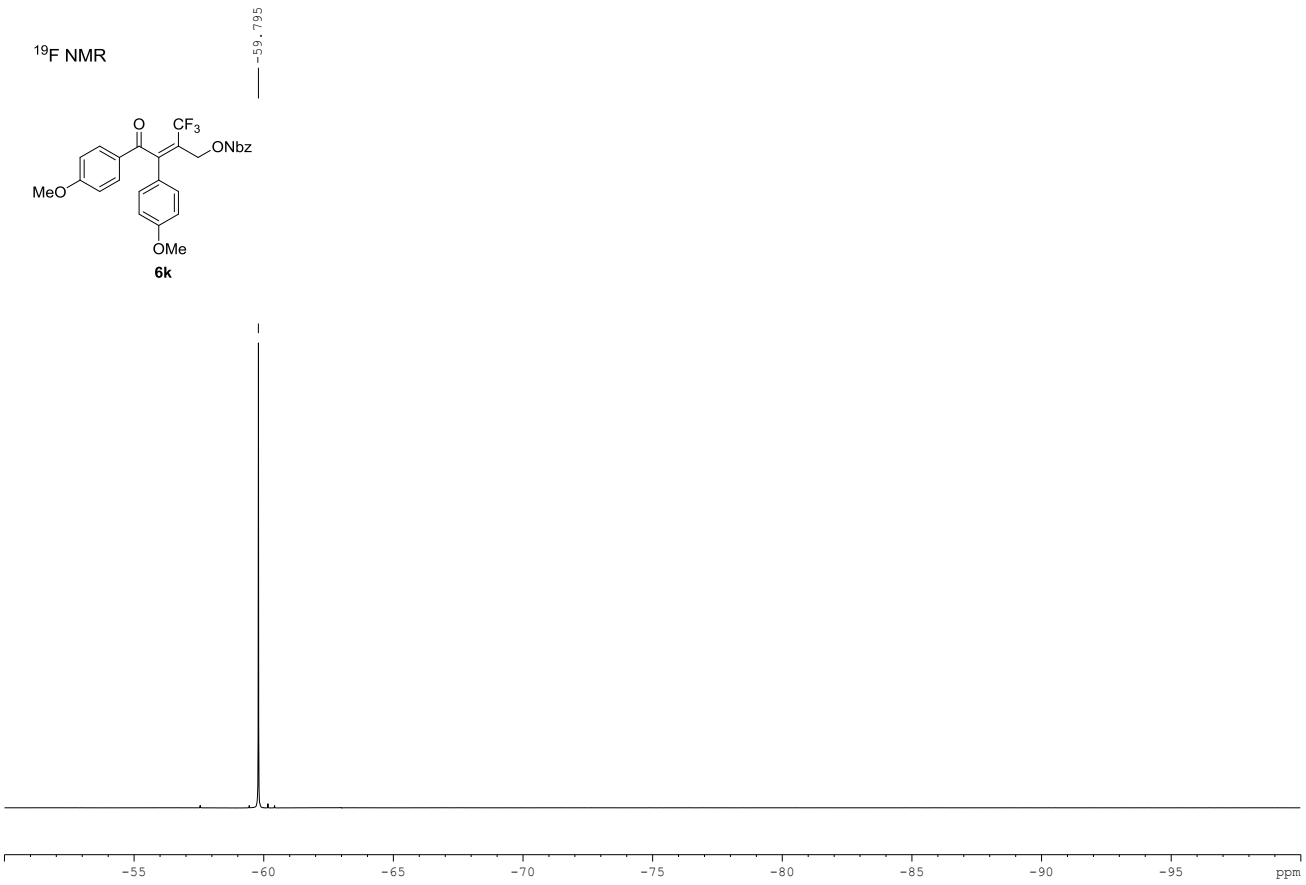


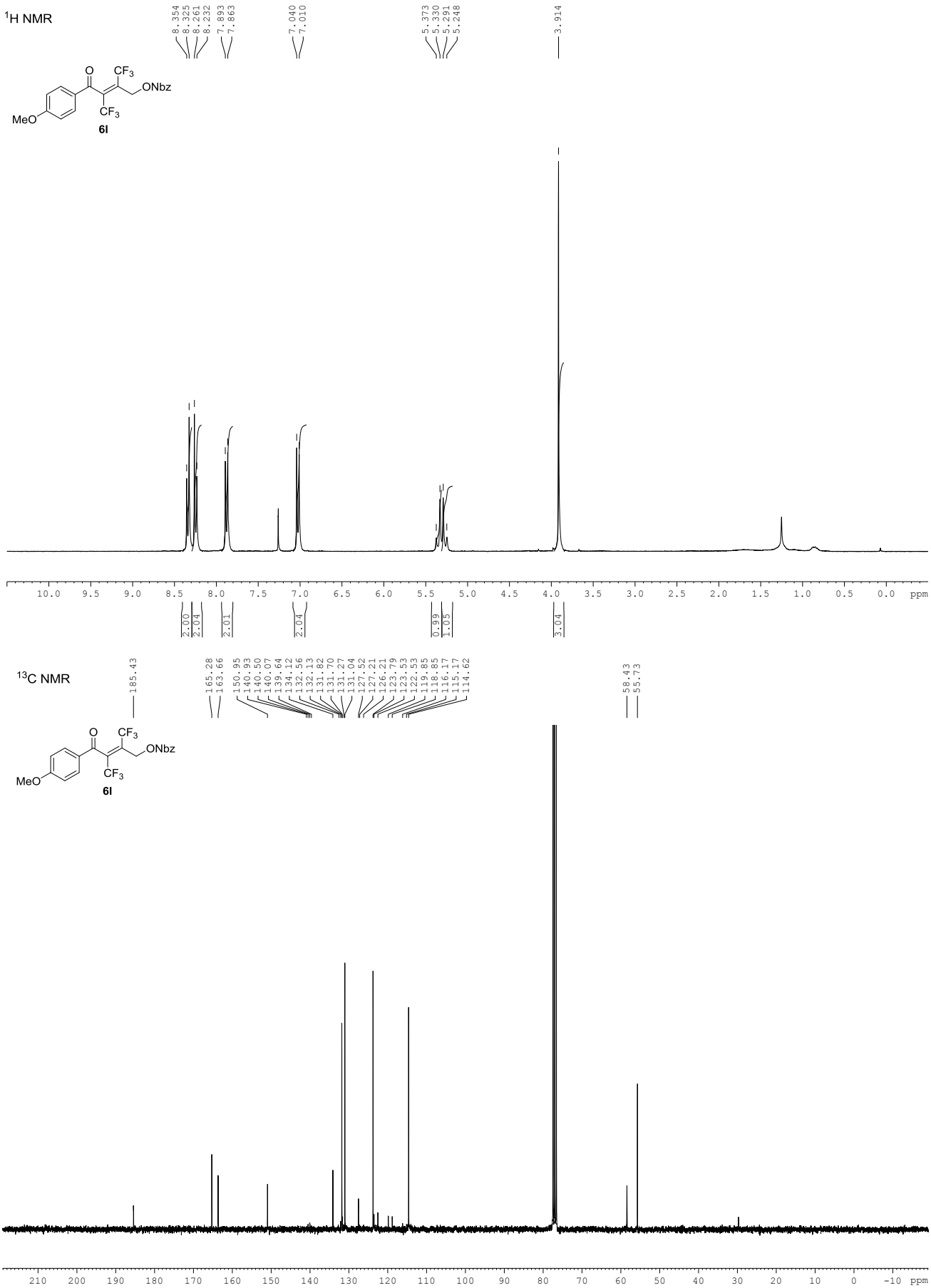
6k

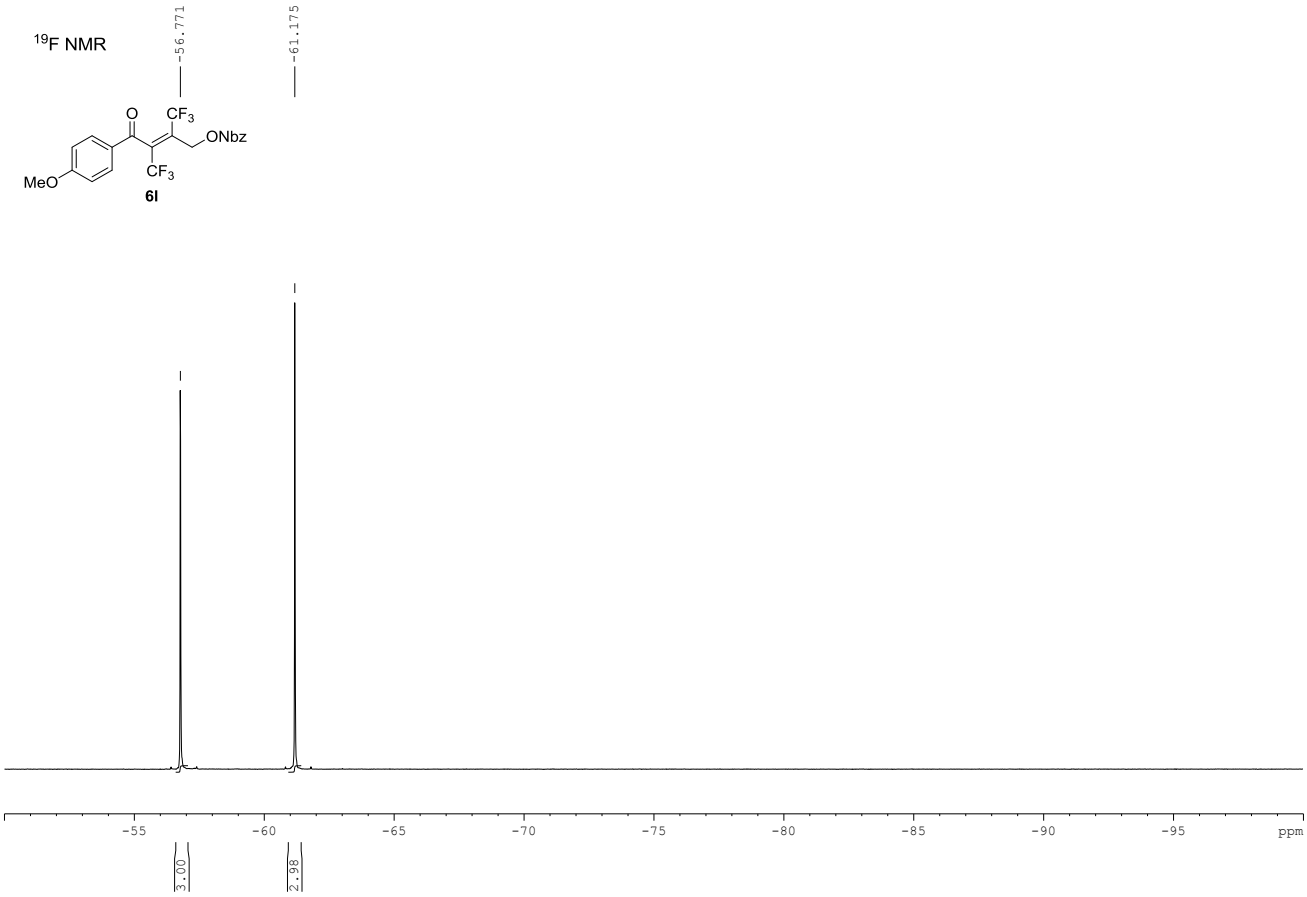


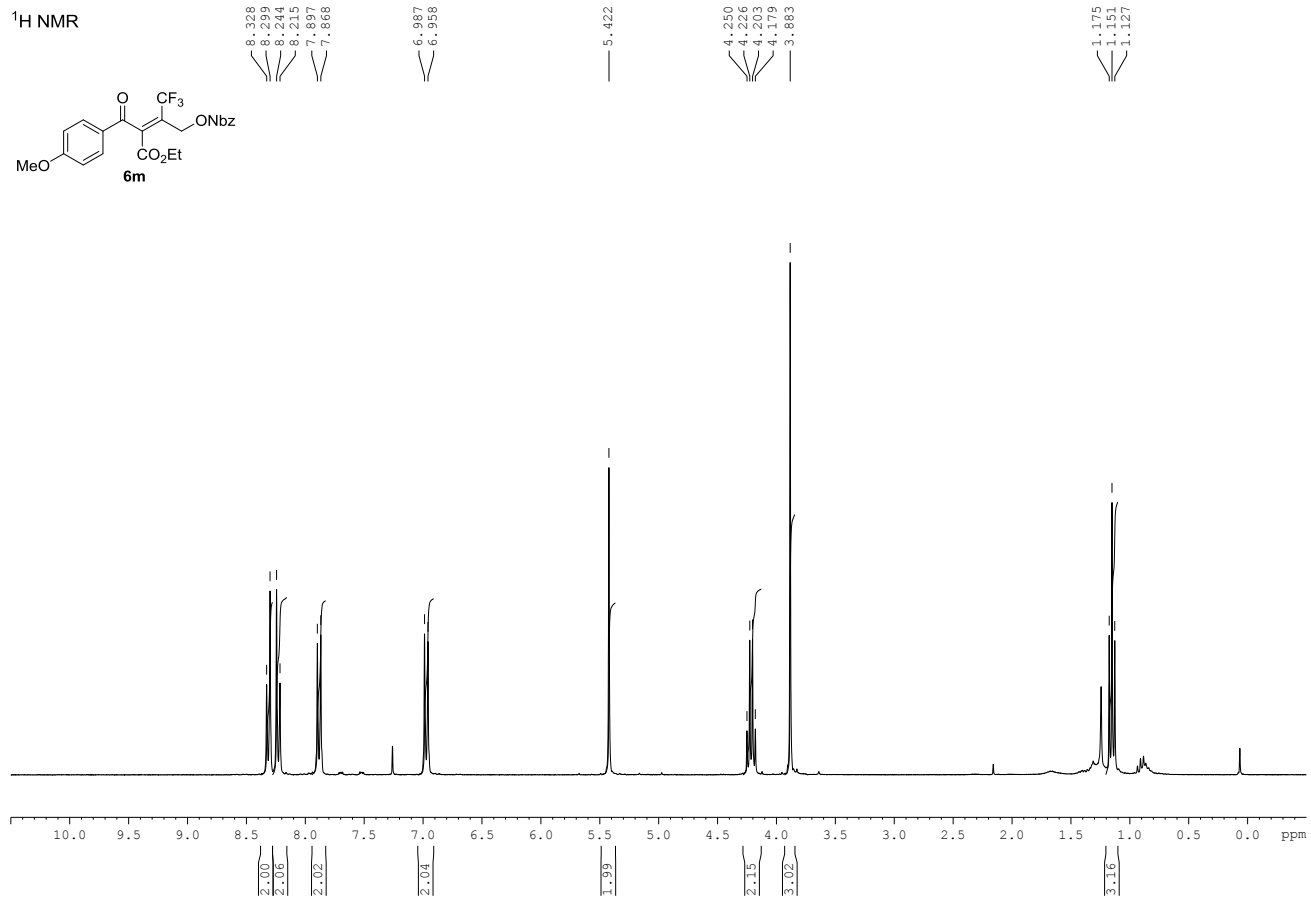
2.00
2.07
2.04
2.03
2.02
2.02
1.99
3.08
3.11


13C NMR
191.88
164.29
164.00
160.82
152.55
152.50
152.45
152.40
150.76
134.85
131.97
130.91
129.69
128.78
127.56
125.12
124.77
123.71
122.22
121.82
121.46
121.42
121.02
117.80
114.63
114.17
61.07
55.56
55.33
O
CF3
ONbz
MeO
OMe
6k
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 ppm

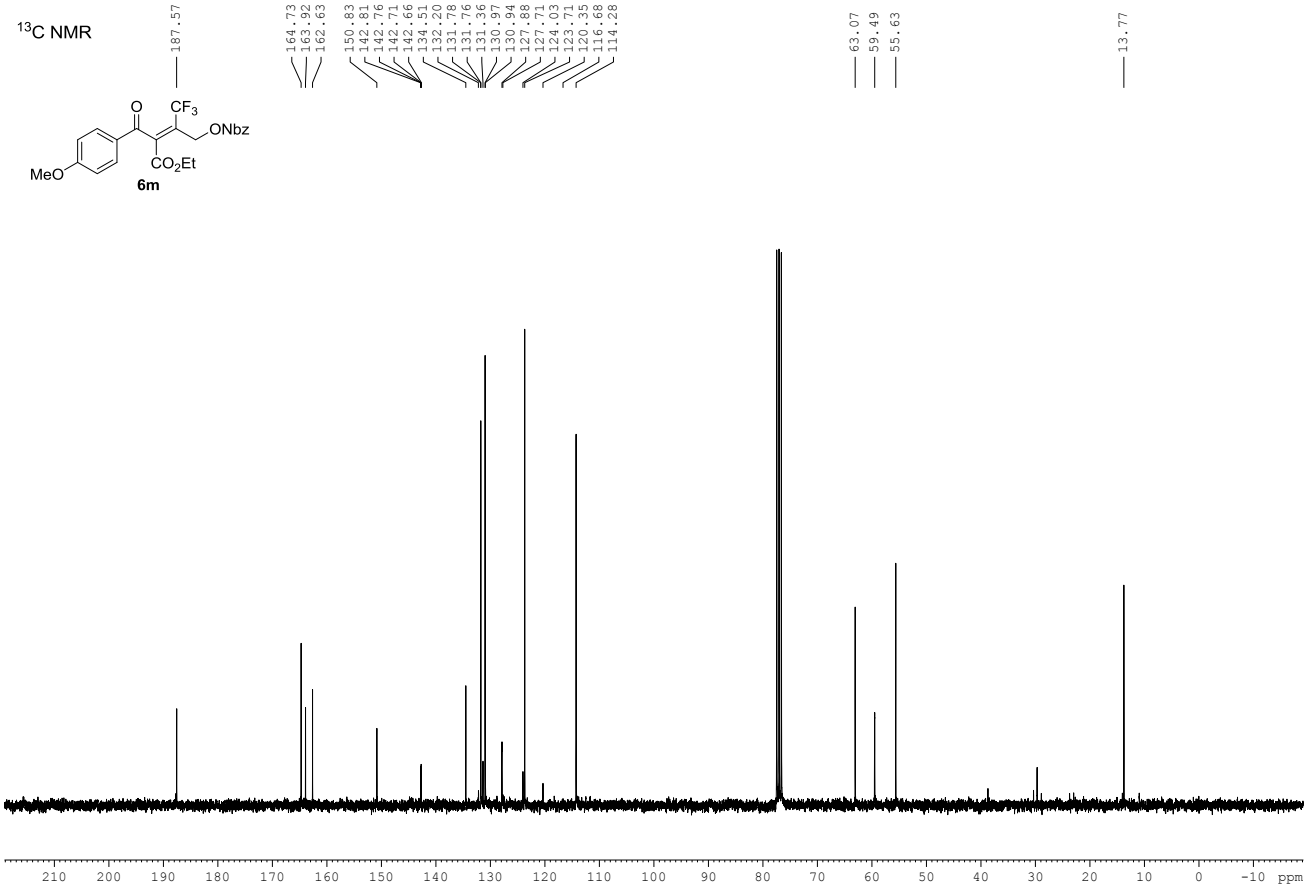

19F NMR
-59.795
O
CF3
ONbz
MeO
OMe
6k
-55 -60 -65 -70 -75 -80 -85 -90 -95 ppm


^{1}H NMR
8.354
8.325
8.261
8.232
7.893
7.863
7.040
7.010
5.373
5.330
5.291
5.248
3.914
O
CF3
ONbz
CF3
MeO
6l
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 ppm
2.00
2.04
2.01
2.04
0.99
1.05
3.04
^{13}C NMR
185.43
165.28
163.66
150.95
140.93
140.50
140.07
139.64
134.12
132.56
132.13
131.82
131.70
131.27
131.04
127.52
127.21
126.21
123.79
123.53
122.53
119.85
118.85
116.17
115.17
114.62
58.43
55.73
O
CF3
ONbz
CF3
MeO
6l
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 ppm

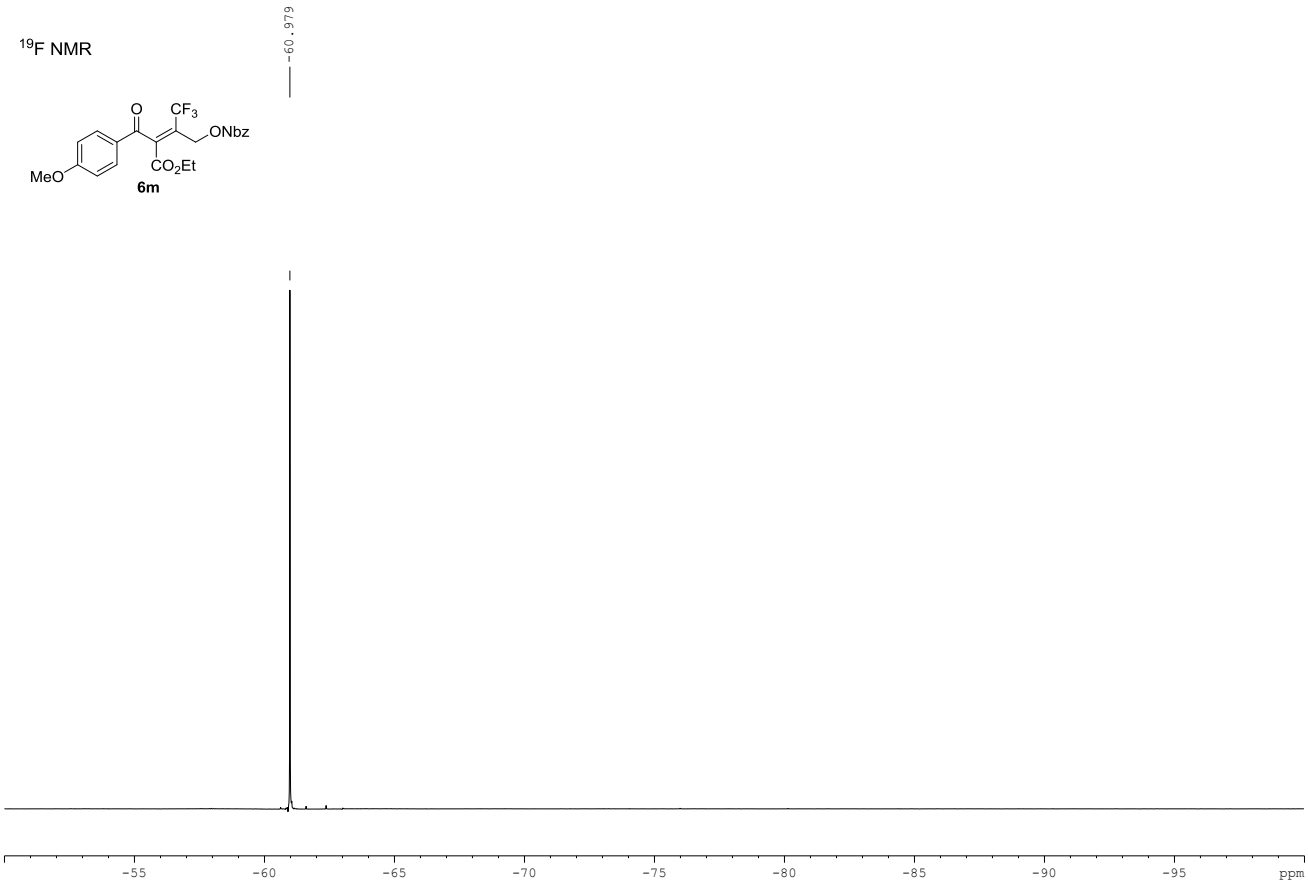

19F NMR
-56.771
-61.175
O
CF3
ONbz
CF3
MeO
6l
-55
-60
-65
-70
-75
-80
-85
-90
-95
ppm
3.00
2.98

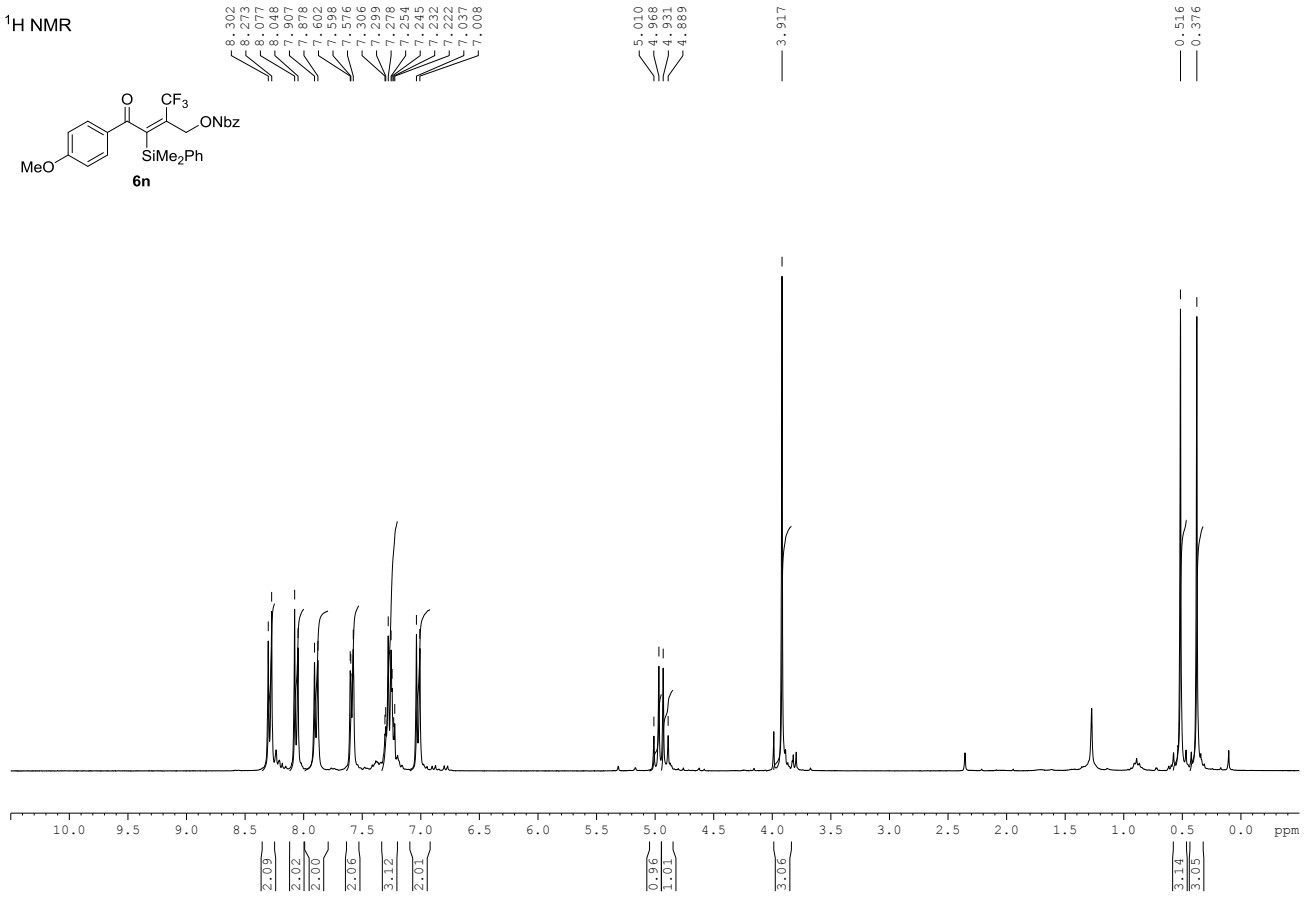

1H NMR
8.328
8.299
8.244
8.215
7.897
7.868
6.987
6.958
5.422
4.250
4.226
4.203
4.179
3.883
1.175
1.151
1.127
O
CF3
ONbz
CO2Et
MeO
6m
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
ppm
2.00
2.06
2.02
2.04
1.99
2.15
3.02
3.16

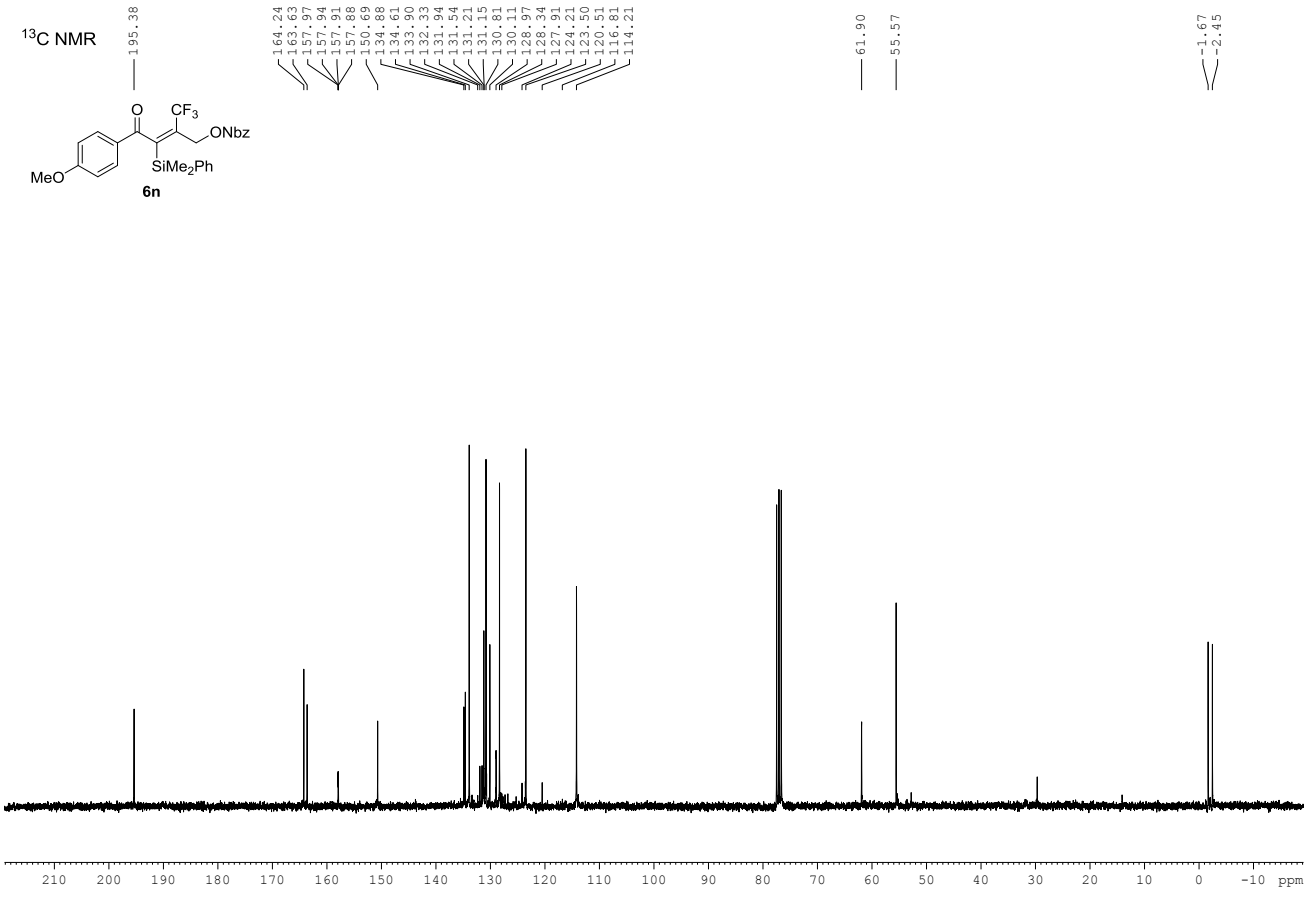
^{13}C NMR



^{19}F NMR

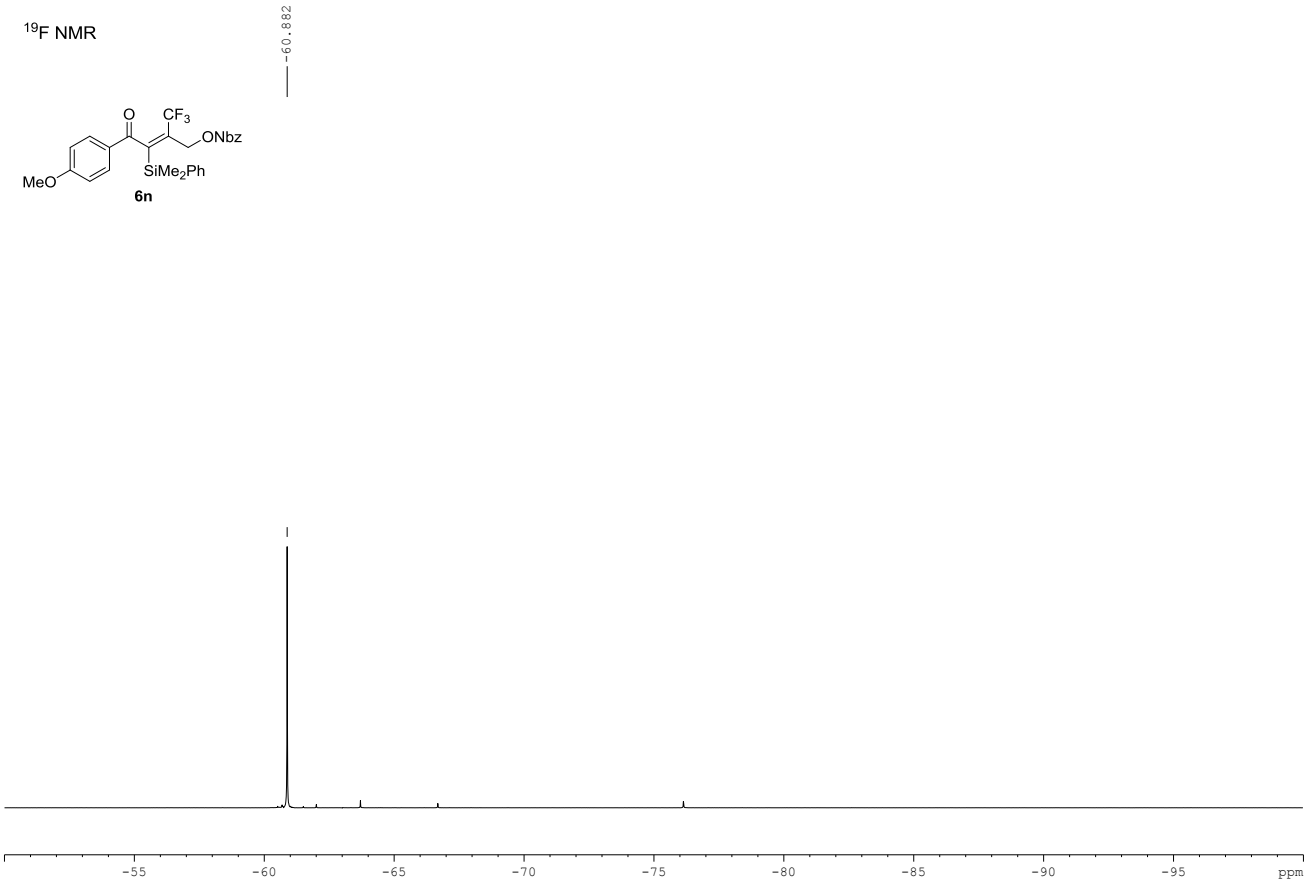



^{1}H NMR
8.302
8.273
8.077
8.048
7.907
7.878
7.602
7.598
7.576
7.306
7.299
7.278
7.254
7.245
7.232
7.222
7.037
7.008
5.010
4.968
4.931
4.889
3.917
0.516
0.376
O
CF3
ONbz
SiMe2Ph
MeO
6n
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 ppm
2.09
2.02
2.00
2.06
3.12
2.01
0.96
1.01
3.06
3.14
3.05


^{13}C NMR
195.38
164.24
163.63
157.97
157.94
157.91
157.88
150.69
134.88
134.61
133.90
132.33
131.94
131.54
131.21
131.15
130.81
130.11
128.97
128.34
127.91
124.21
123.50
120.51
116.81
114.21
61.90
55.57
-1.67
-2.45
O
CF3
ONbz
SiMe2Ph
MeO
6n
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 ppm

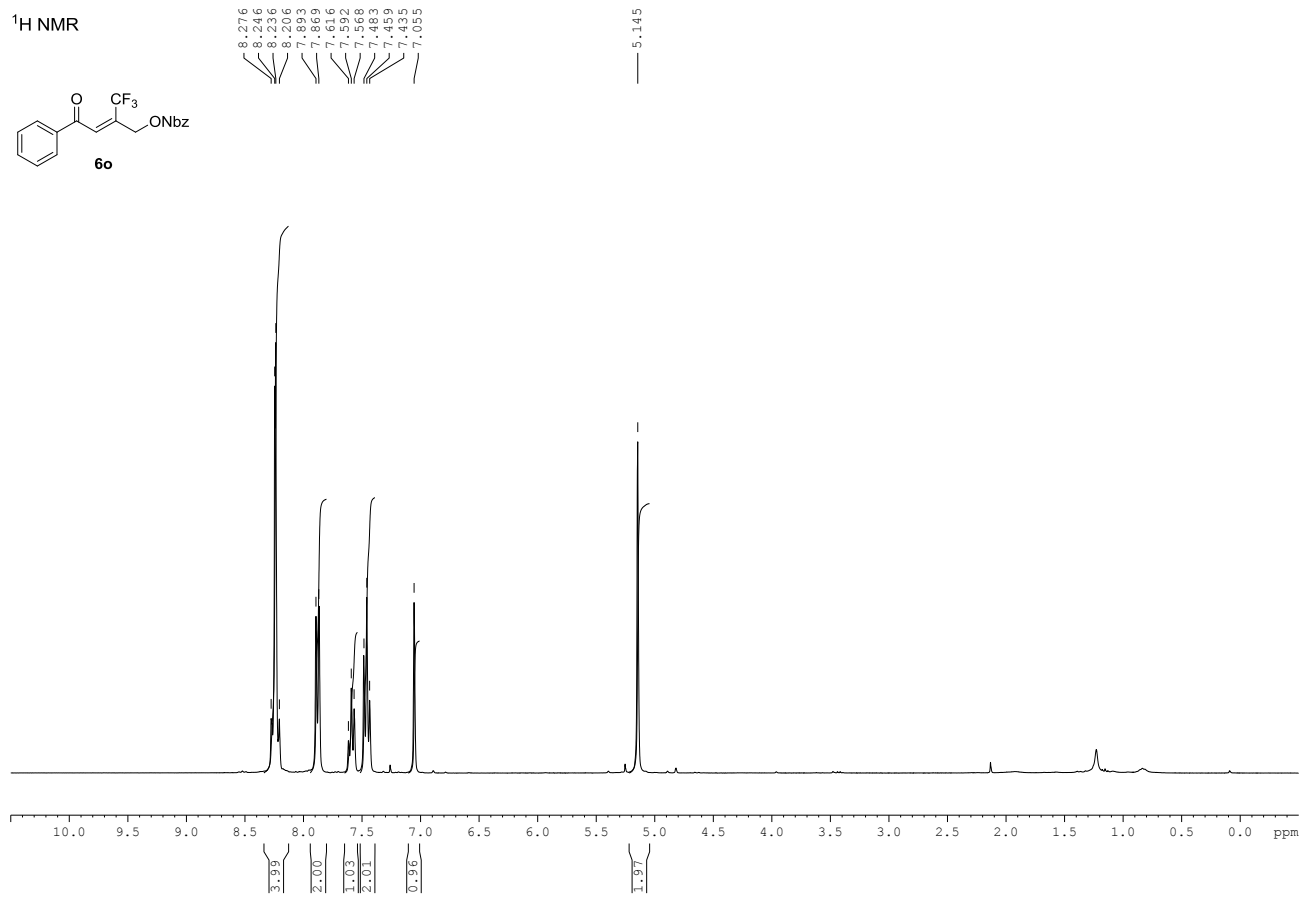
^{19}F NMR

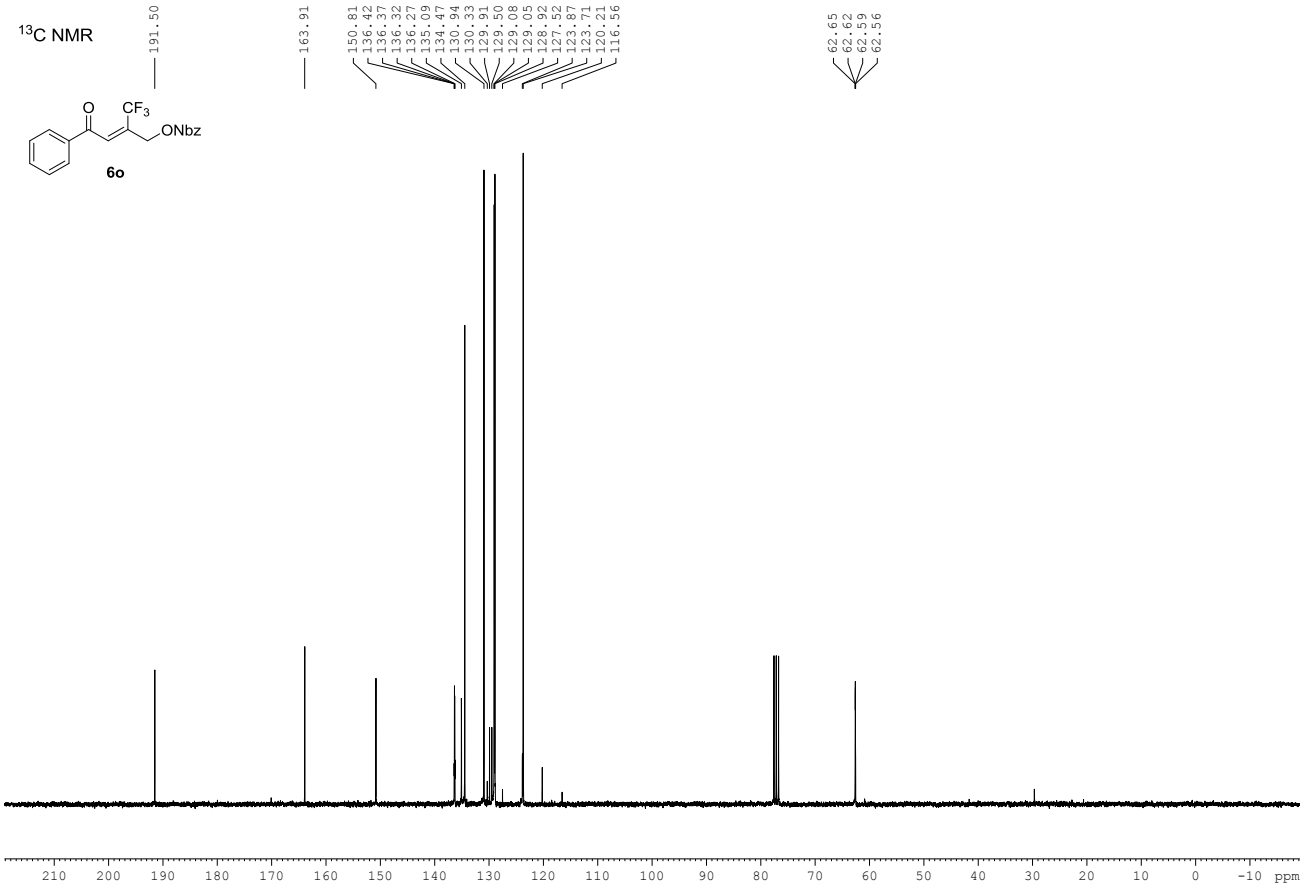
6n

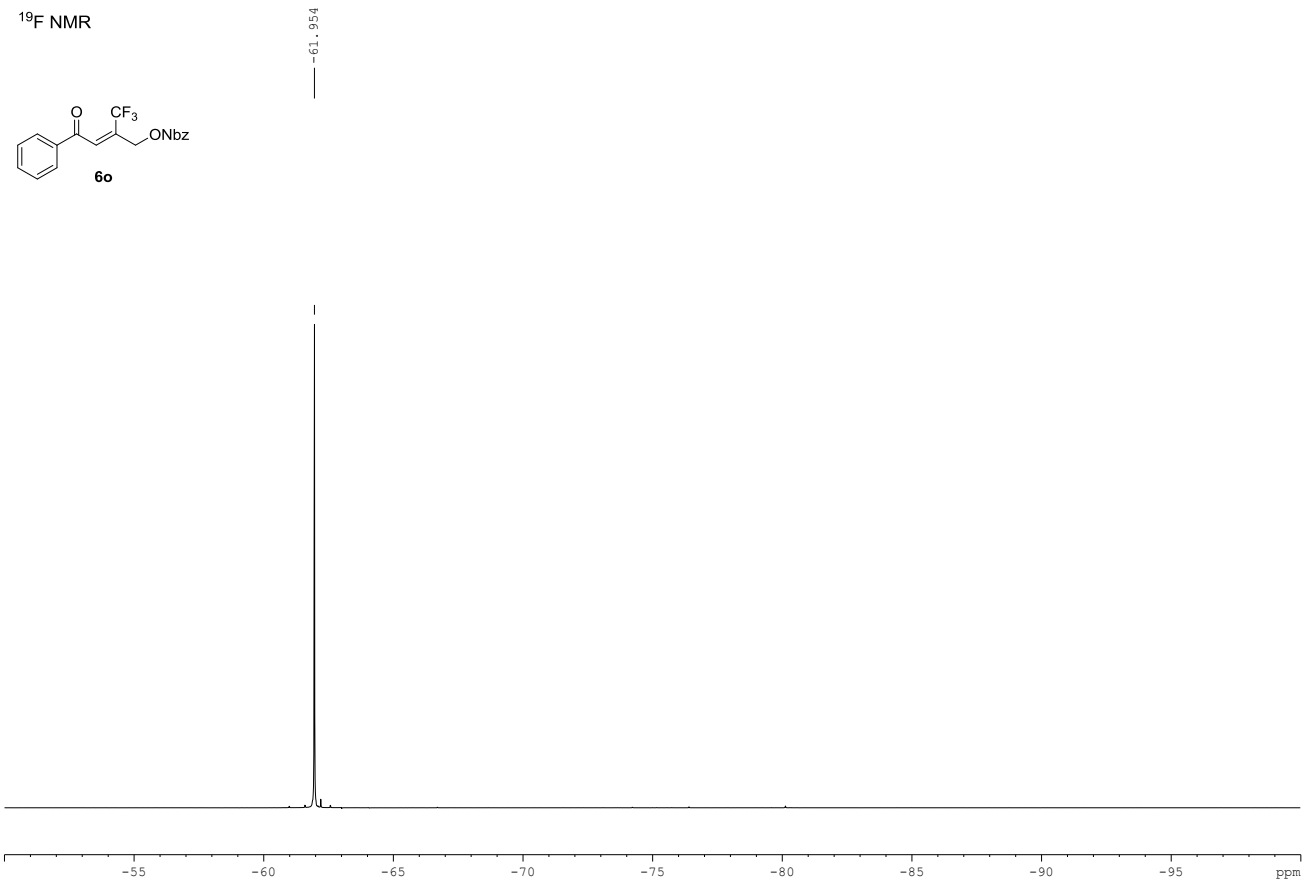


^{1}H NMR

6o




^{13}C NMR
191.50
163.91
150.81
136.42
136.37
136.32
136.27
135.09
134.47
130.94
130.33
129.91
129.50
129.08
129.05
128.92
127.52
123.87
123.71
120.21
116.56
62.65
62.62
62.59
62.56
O
CF3
ONbz
6o
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 ppm


^{19}F NMR
-61.954
O
CF3
ONbz
6o
-55 -60 -65 -70 -75 -80 -85 -90 -95 ppm