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Supplementary Information

Phosphine-Catalyzed Remote α-C-H Bond Activation of Alcohols or Amines Triggered by Radical Trifluoromethylation of Alkenes: Reaction Development and Mechanistic Insights

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General information.

All reactions were carried out under argon using Schlenk techniques. Reagents were purchased at the commercial quality and used without further purification. Analytical thin layer chromatography (TLC) was performed on precoated silica gel 60 GF254 plates. Flash column chromatography was performed using Tsingdao silica gel (60, particle size 0.040-0.063 mm). Visualization on TLC was achieved by use of UV light (254 nm) or iodine. NMR spectra were recorded on a Bruker DPX 400 spectrometer at 400 MHz for ^{1}H NMR, 100 MHz for ^{13}C NMR and 376 MHz for ^{19}F NMR in $CDCl_3$ with tetramethylsilane (TMS) as internal standard. Microwave irradiation experiments were carried out in a dedicated Biotage Initator Robot 8 auto microwave apparatus. The chemical shifts are expressed in ppm and coupling constants are given in Hz. Data for ^{1}H NMR are recorded as follows: chemical shift (ppm), multiplicity (s, singlet; d, doublet; t, triplet; q, quartet; m, multiplet), coupling constant (Hz), integration. Data for ^{13}C NMR are reported in terms of chemical shift (δ, ppm). ^{19}F NMR spectra were recorded on a Bruker DPX 400 MHz spectrometer ($CFCl_3$ as an external reference (0 ppm)). Mass spectrometric data were obtained using Bruker Apex IV RTMS.

Figure 1. The relative bond dissociation energy based on DFT calculations

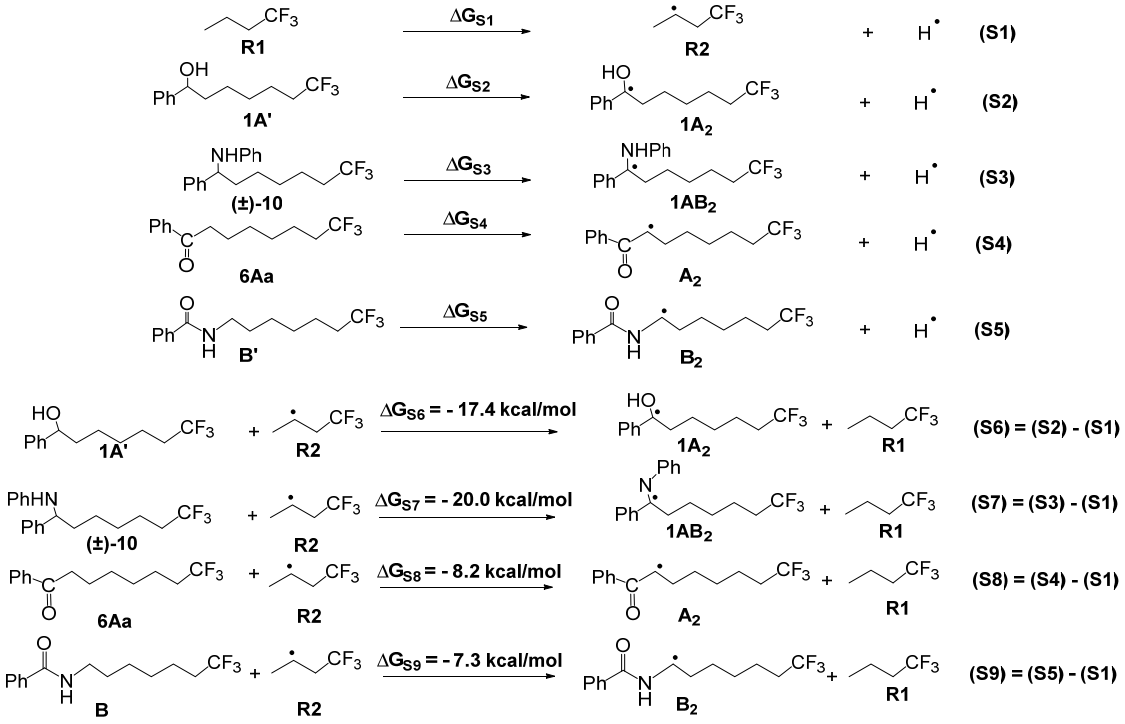
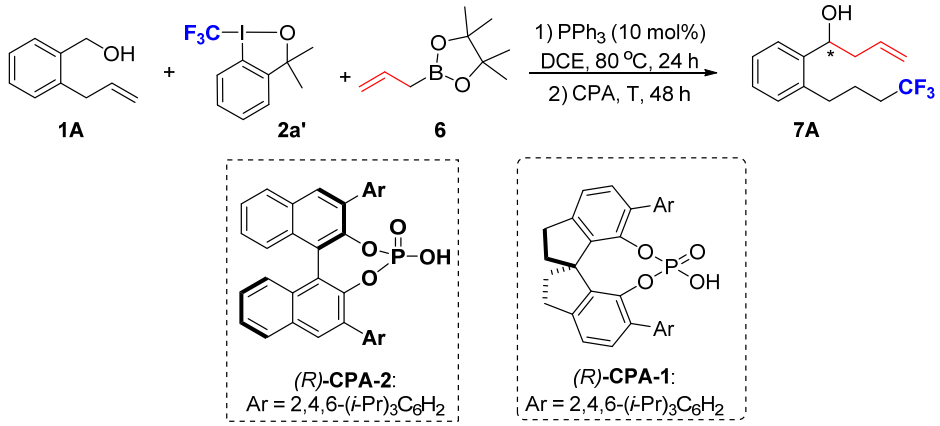


Table S1 Screening Results of Reaction Conditions for Further Transformation

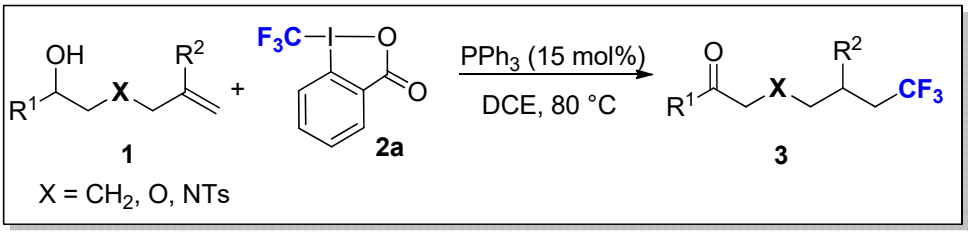


Entry	Catalyst	Solvent	T/(°C)	yield (%)	ee (%)
1	CPA-2	DCE	-20	70	70
2	CPA-1	DCE	-20	71	80
3	CPA-1	EtOAc	-35	67	45
4	CPA-1	DCE	-35	62	89
5	CPA-1	MeCN	-35	64	42

Reaction conditions: 1) **1A** (0.1 mmol, 1 equiv), Togni's reagent **2a'** (0.13 mmol, 1.3 equiv), PPh_3 (0.1 mmol, 0.1 equiv), DCE (2.0 mL) at 80 °C for 24 h under argon; 2) 2-allyl-4,4,5,5-tetramethyl-1,3,2-dioxaborolane (0.12 mmol, 1.2 equiv), CPA (0.2 mmol, 0.2 equiv) was added for 48 h under argon.

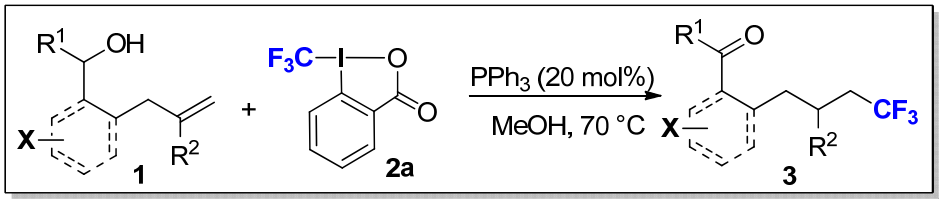
General procedure

General procedure 1 for catalytic trifluoromethylation reaction system



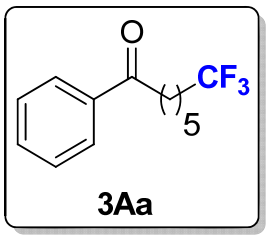
Under argon, a 25 mL Schlenk tube equipped with a magnetic stir bar were charged with **1** (0.2 mmol, 1.0 equiv), Togni's reagent **2a** (0.3 mmol, 1.5 equiv), triphenylphosphine (0.03 mmol, 0.15 equiv) and 1,2-dichloroethane (DCE, super dry, 2.0 mL). The sealed tube was then stirred at 80 °C for 16 hours. After completion (monitored by TLC), the reaction solution was concentrated *in vacuo*, and the residue was purified by silica gel column chromatography (petroleum ether/EtOAc) to give the desired products **3**.

General procedure 2 for catalytic trifluoromethylation reaction system



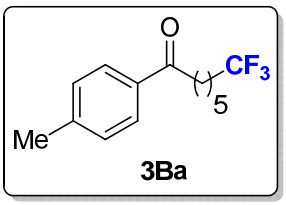
Under argon, a 25 mL Schlenk tube equipped with a magnetic stir bar were charged with **1** (0.2 mmol, 1.0 equiv), Togni's reagent **2a** (0.3 mmol, 1.5 equiv), triphenylphosphine (0.03 mmol, 0.15 equiv) and methanol (super dry, 2.0 mL). The sealed tube was then stirred at 70 °C for 16 hours. After completion (monitored by TLC), the reaction solution was concentrated *in vacuo*, and the residue was purified by silica gel column chromatography (petroleum ether/EtOAc) to give the desired products **3**.

7,7,7-trifluoro-1-phenylheptan-1-one (3Aa)



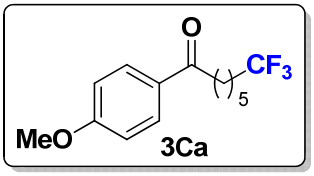
^{1}H NMR (400 MHz, CDCl3) δ 7.98 - 7.93 (m, 2H), 7.56 (t, *J* = 7.2 Hz, 1H), 7.46 (t, *J* = 7.6 Hz, 2H), 2.99 (t, *J* = 7.2 Hz, 2H), 2.16 - 2.01 (m, 2H), 1.82 - 1.72 (m, 2H), 1.66 - 1.56 (m, 2H), 1.50 - 1.41 (m, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 199.88, 136.88, 132.99, 128.56, 127.95, 127.15 (q, *J* = 274.6 Hz), 38.05, 33.51 (q, *J* = 28.2 Hz), 28.29, 23.64, 21.77 (q, *J* = 2.8 Hz). ^{19}F NMR (376 MHz, $CDCl_3$) δ -66.38. HRMS (ESI) m/z calcd. for $C_{13}H_{16}F_3O$ $[M+H]^+$ 245.1153, found 245.1142.

7,7,7-trifluoro-1-(p-tolyl)heptan-1-one (3Ba)



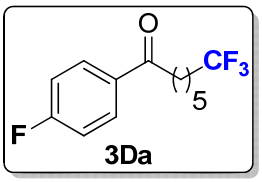
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.85 (d, *J* = 8.4 Hz, 2H), 7.25 (d, *J* = 8.0 Hz, 2H), 2.95 (t, *J* = 7.2 Hz, 2H), 2.40 (s, 3H), 2.14 - 2.03 (m, 2H), 1.71 - 1.80 (m, 2H), 1.65 - 1.55 (m, 2H), 1.40 - 1.49 (m, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 199.52, 143.73, 134.39, 129.20, 128.05, 127.14 (q, *J* = 274.7 Hz), 37.91, 33.48 (q, *J* = 28.2 Hz), 28.29, 23.72, 21.74 (q, *J* = 2.9 Hz), 21.49. ^{19}F NMR (376 MHz, $CDCl_3$) δ -66.39. HRMS (APCI) m/z calcd. for $C_{14}H_{18}OF_3$ $[M+H]^+$ 259.1310, found 259.1304.

7,7,7-trifluoro-1-(4-methoxyphenyl)heptan-1-one (3Ca)



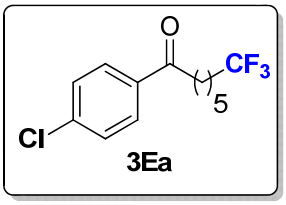
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.97 - 7.87 (m, 2H), 6.97 - 6.85 (m, 2H), 3.86 (s, 3H), 2.92 (t, *J* = 7.2 Hz, 2H), 2.13 - 2.01 (m, 2H), 1.79 - 1.71 (m, 2H), 1.55 - 1.66 (m, 2H), 1.51 - 1.40 (m, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 198.49, 163.38, 130.22, 129.99, 127.17 (q, *J* = 274.6 Hz), 113.67, 55.39, 37.71, 33.52 (q, *J* = 28.2 Hz), 28.35, 23.87, 21.77 (q, *J* = 2.8 Hz). ^{19}F NMR (376 MHz, $CDCl_3$) δ -66.38 (s). HRMS (APCI) m/z calcd. for $C_{14}H_{18}O_2F_3$ $[M+H]^+$ 275.1259, found 275.1255.

7,7,7-trifluoro-1-(4-fluorophenyl)heptan-1-one (3Da)



^{1}H NMR (400 MHz, $CDCl_3$) δ 8.03 - 7.92 (m, 2H), 7.18 - 7.06 (m, 2H), 2.96 (t, *J* = 7.2 Hz, 2H), 2.18 - 2.02 (m, 2H), 1.71 - 1.80 (m, 2H), 1.66 - 1.57 (m, 2H), 1.51 - 1.38 (m, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 198.24, 166.69 (d, *J* = 253.0 Hz), 133.34 (d, *J* = 3.0 Hz), 130.59 (d, *J* = 9.2 Hz), 127.15 (q, *J* = 274.6 Hz), 115.66 (d, *J* = 21.8 Hz), 38.00, 33.54 (q, *J* = 28.3 Hz), 28.29, 23.63, 21.79 (q, *J* = 2.9 Hz). ^{19}F NMR (376 MHz, $CDCl_3$) δ -66.38 (s, 3F), -105.44 (s, 1F). HRMS (APCI) m/z calcd. for $C_{13}H_{15}OF_4$ $[M+H]^+$ 263.1059, found 263.1053.

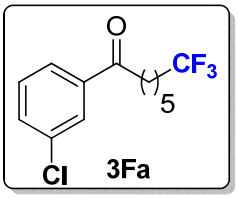
1-(4-chlorophenyl)-7,7,7-trifluoroheptan-1-one (3Ea)



^{1}H NMR (400 MHz, $CDCl_3$) δ 7.95 - 7.83 (m, 2H), 7.48 - 7.35 (m, 2H), 2.94 (t, *J* = 7.2 Hz, 2H),

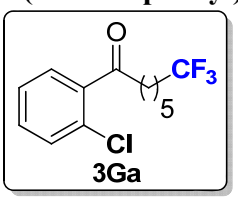
2.16 - 1.99 (m, 2H), 1.82 - 1.70 (m, 2H), 1.64 - 1.55 (m, 2H), 1.49 - 1.37 (m, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 198.57, 139.40, 135.17, 129.37, 128.86, 127.13 (q, *J* = 274.5 Hz), 38.04, 33.49 (q, *J* = 28.2 Hz), 28.24, 23.54, 21.76 (q, *J* = 2.9 Hz). ^{19}F NMR (376 MHz, $CDCl_3$) δ -66.37. HRMS (APCI) m/z calcd. for $C_{13}H_{15}ClF_3O$ $[M+H]^+$ 279.0764, found 279.0761.

1-(3-chlorophenyl)-7,7,7-trifluoroheptan-1-one (3Fa)



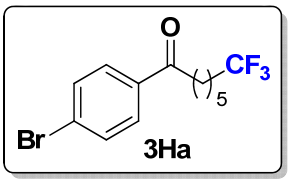
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.47 - 7.26 (m, 4H), 2.94 (t, *J* = 7.2 Hz, 2H), 2.14 - 1.99 (m, 2H), 1.79 - 1.68 (m, 2H), 1.64 - 1.54 (m, 2H), 1.50 - 1.37 (m, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 203.22, 139.55, 131.55, 130.67, 130.45, 128.63, 127.13 (q, *J* = 274.7 Hz), 126.90, 42.49, 33.49 (q, *J* = 28.3 Hz), 28.11, 23.55, 21.70 (q, *J* = 2.8 Hz). ^{19}F NMR (376 MHz, $CDCl_3$) δ -66.39. HRMS (APCI) m/z calcd. for $C_{13}H_{15}OF_3Cl$ $[M+H]^+$ 279.0764, found 279.0759.

1-(2-chlorophenyl)-7,7,7-trifluoroheptan-1-one (3Ga)



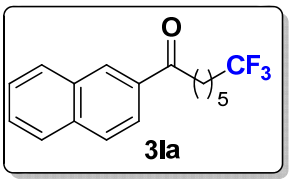
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.91 (t, *J* = 2.0 Hz, 1H), 7.81 (dt, *J* = 7.6, 1.2 Hz, 1H), 7.52 (dq, *J* = 8.0, 1.2 Hz, 1H), 7.40 (t, *J* = 8.0 Hz, 1H), 2.96 (t, *J* = 7.2 Hz, 2H), 2.18 - 1.99 (m, 2H), 1.81 - 1.69 (m, 2H), 1.65 - 1.56 (m, 2H), 1.50 - 1.39 (m, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 198.48, 138.43, 134.92, 132.90, 129.92, 128.09, 127.14 (q, *J* = 274.7 Hz), 126.03, 38.18, 33.51 (q, *J* = 28.3 Hz), 28.23, 23.48, 21.76 (q, *J* = 2.9 Hz). ^{19}F NMR (376 MHz, $CDCl_3$) δ -66.37. HRMS (APCI) m/z calcd. for $C_{13}H_{15}OF_3Cl$ $[M+H]^+$ 279.0764, found 279.0757.

1-(4-bromophenyl)-7,7,7-trifluoroheptan-1-one (3Ha)



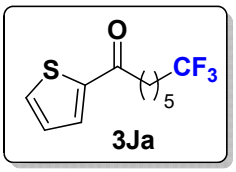
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.80 (d, *J* = 8.0 Hz, 2H), 7.58 (d, *J* = 8.0 Hz, 2H), 2.93 (t, *J* = 7.2 Hz, 2H), 2.15 - 2.01 (m, 2H), 1.79 - 1.70 (m, 2H), 1.64 - 1.55 (m, 2H), 1.48 - 1.39 (m, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 198.73, 135.55, 131.84, 129.47, 128.09, 127.11 (q, *J* = 274.6 Hz), 38.00, 33.47 (q, *J* = 28.2 Hz), 28.22, 23.50, 21.75 (q, *J* = 2.9 Hz). ^{19}F NMR (376 MHz, $CDCl_3$) δ -66.36. HRMS (ESI) m/z calcd. for $C_{13}H_{15}BrF_3O$ $[M+H]^+$ 323.0258, found 323.0246.

7,7,7-trifluoro-1-(naphthalen-2-yl)heptan-1-one (3Ia)



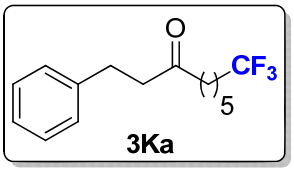
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.46 (s, 1H), 8.03 (dd, *J* = 8.4, 1.6 Hz, 1H), 7.97 (d, *J* = 8.0 Hz, 1H), 7.92 - 7.85 (m, 2H), 7.58 - 7.63 (m, 1H), 7.53 - 7.58 (m, 1H), 3.12 (t, *J* = 7.2 Hz, 2H), 2.18 - 2.03 (m, 2H), 1.78 - 1.86 (m, 2H), 1.69 - 1.61 (m, 2H), 1.55 - 1.46 (m, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 199.80, 135.53, 134.22, 132.50, 129.56, 129.45, 128.43, 128.39, 127.74, 127.17 (q, *J* = 274.6 Hz), 126.75, 123.80, 38.14, 33.55 (q, *J* = 28.2 Hz), 28.35, 23.81, 21.81 (q, *J* = 2.8 Hz). ^{19}F NMR (376 MHz, $CDCl_3$) δ -66.32. HRMS (APCI) m/z calcd. for $C_{17}H_{18}OF_3$ $[M+H]^+$ 295.1310, found 295.1305.

7,7,7-trifluoro-1-(thiophen-2-yl)heptan-1-one (3Ja)



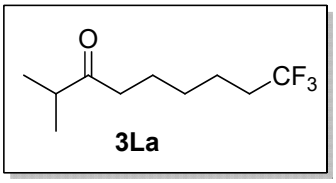
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.70 (dd, *J* = 3.6, 1.2 Hz, 1H), 7.62 (dd, *J* = 5.2, 1.2 Hz, 1H), 7.12 (dd, *J* = 4.8, 4.0 Hz, 1H), 2.92 (t, *J* = 7.2 Hz, 2H), 2.15 - 2.02 (m, 2H), 1.73 - 1.82 (m, 2H), 1.65 - 1.56 (m, 2H), 1.40 - 1.49 (m, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 192.84, 144.27, 133.47, 131.69, 128.06, 127.14 (q, *J* = 274.6 Hz), 38.84, 33.51 (q, *J* = 28.2 Hz), 28.26, 24.02, 21.73 (q, *J* = 2.9 Hz). ^{19}F NMR (376 MHz, $CDCl_3$) δ -66.38.
HRMS (APCI) m/z calcd. for $C_{11}H_{14}OF_3S$ $[M+H]^+$ 251.0717, found 251.0714.

9,9,9-trifluoro-1-phenylnonan-3-one (3Ka)



^{1}H NMR (400 MHz, $CDCl_3$) δ 7.31 - 7.24 (m, 2H), 7.22 - 7.12 (m, 3H), 2.89 (t, *J* = 7.6 Hz, 2H), 2.72 (t, *J* = 7.6 Hz, 2H), 2.38 (t, *J* = 7.2 Hz, 2H), 2.11 - 1.97 (m, 2H), 1.62 - 1.47 (m, 4H), 1.255 - 1.35 (m, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 209.69, 140.99, 128.49, 128.43, 127.11 (q, *J* = 274.8 Hz), 126.07, 44.21, 42.46, 33.44 (q, *J* = 28.2 Hz), 29.72, 28.09, 23.07, 21.65 (q, *J* = 2.9 Hz). ^{19}F NMR (376 MHz, $CDCl_3$) δ -66.40. HRMS (APCI) m/z calcd. for $C_{15}H_{20}OF_3$ $[M+H]^+$ 273.1466, found 273.1461.

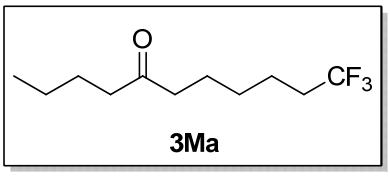
9,9,9-trifluoro-2-methylnonan-3-one (3La)



^{1}H NMR (400 MHz, $CDCl_3$) δ 2.63 - 2.53 (m, 1H), 2.45 (t, *J* = 7.2 Hz, 2H), 2.12 - 1.98 (m, 2H), 1.62 - 1.51 (m, 4H), 1.40 - 1.30 (m, 2H), 1.07 (d, *J* = 6.8 Hz, 6H). ^{13}C NMR (100 MHz, $CDCl_3$)

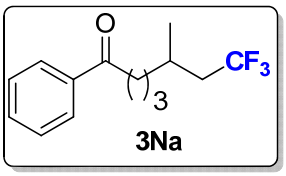
δ 214.49, 127.14 (q, *J* = 274.6 Hz), 40.82, 39.76, 33.50 (q, *J* = 28.2 Hz), 28.24, 23.13, 21.72 (q, *J* = 2.9 Hz), 18.18. ^{19}F NMR (376 MHz, $CDCl_3$) δ -66.44. HRMS (APCI) m/z calcd. for $C_{10}H_{18}F_3O$ $[M+H]^+$ 211.1304, found 211.1298.

11,11,11-trifluoroundecan-5-one (3Ma)



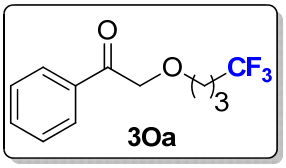
1H NMR (400 MHz, CDCl3) δ 2.47 - 2.29 (m, 4H), 2.13 - 1.97 (m, 2H), 1.62 - 1.49 (m, 6H), 1.37 - 1.25 (m, 4H), 0.88 (t, *J* = 7.2 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 210.99, 127.13 (q, *J* = 274.6 Hz), 42.55, 42.18, 33.48 (q, *J* = 28.2 Hz), 28.19, 25.91, 23.17, 22.30, 21.69 (q, *J* = 2.9 Hz), 13.78. ^{19}F NMR (376 MHz, $CDCl_3$) δ -66.47. HRMS (APCI) m/z calcd. for $C_{11}H_{20}F_3O$ $[M+H]^+$ 225.1461, found 225.1455.

7,7,7-trifluoro-5-methyl-1-phenylheptan-1-one (3Na)



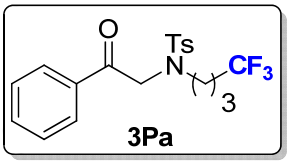
1H NMR (400 MHz, CDCl3) δ 8.01 - 7.90 (m, 2H), 7.59 - 7.50 (m, 1H), 7.50 - 7.38 (m, 2H), 2.96 (t, *J* = 7.2 Hz, 2H), 2.20 - 2.05 (m, 1H), 1.98 - 1.84 (m, 2H), 1.80 - 1.66 (m, 2H), 1.53 - 1.42 (m, 1H), 1.38 - 1.28 (m, 1H), 1.06 - 1.01 (m, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 199.86, 136.88, 132.95, 128.53, 127.91, 127.16 (q, *J* = 275.6 Hz), 39.98 (q, *J* = 26.7 Hz), 38.27, 36.25, 27.60 (q, *J* = 2.3 Hz), 21.07, 19.56. ^{19}F NMR (376 MHz, $CDCl_3$) δ -63.33. HRMS (APCI) m/z calcd. for $C_{14}H_{18}OF_3$ $[M+H]^+$ 259.1310, found 259.1302.

1-phenyl-2-(4,4,4-trifluorobutoxy)ethanone (3Oa)



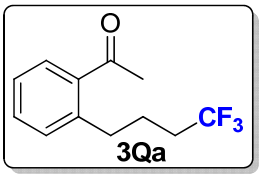
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.90 - 7.94 (m, 2H), 7.63 - 7.55 (m, 1H), 7.45 - 7.50 (m, 2H), 4.75 (s, 2H), 3.63 (t, *J* = 6.0 Hz, 2H), 2.33 - 2.21 (m, 2H), 1.94 - 1.87 (m, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 196.25, 134.82, 133.61, 128.73, 127.82, 127.21 (q, *J* = 272.3 Hz), 73.62, 69.86, 30.66 (q, *J* = 28.8 Hz), 22.47 (q, *J* = 3.0 Hz). ^{19}F NMR (376 MHz, $CDCl_3$) δ -66.38. HRMS (APCI) m/z calcd. for $C_{12}H_{14}O_2F_3$ $[M+H]^+$ 247.0946, found 247.0941.

4-methyl-N-(2-oxo-2-phenylethyl)-N-(4,4,4-trifluorobutyl)benzenesulfonamide (3Pa)



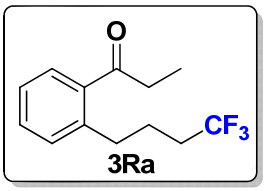
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.88 - 7.95 (m, 2H), 7.74 - 7.68 (m, 2H), 7.64 - 7.58 (m, 1H), 7.52 - 7.45 (m, 2H), 7.31 (d, *J* = 8.0 Hz, 2H), 4.73 (s, 2H), 3.32 (t, *J* = 7.2 Hz, 2H), 2.43 (s, 3H), 2.18 - 2.05 (m, 2H), 1.72 - 1.81 (m, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 193.66, 143.69, 136.22, 134.63, 133.94, 129.63, 128.87, 127.98, 127.51 (q, *J* = 274.8 Hz), 127.40, 53.22, 47.49, 30.96 (q, *J* = 28.9 Hz), 21.52, 20.82 (q, *J* = 2.6 Hz). ^{19}F NMR (376 MHz, $CDCl_3$) δ -66.21. HRMS (APCI) m/z calcd. for $C_{19}H_{21}NO_3F_3S$ $[M+H]^+$ 400.1194, found 400.1189.

1-(2-(4,4,4-trifluorobutyl)phenyl)ethanone (3Qa)



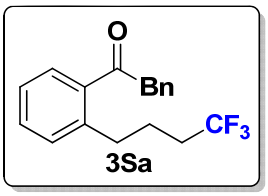
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.72 (dd, *J* = 7.6, 1.2 Hz, 1H), 7.43 (td, *J* = 7.6, 1.4 Hz, 1H), 7.31 (td, *J* = 7.6, 1.3 Hz, 1H), 7.27 - 7.23 (m, 1H), 3.02 - 2.86 (m, 2H), 2.59 (s, 3H), 2.22 - 2.07 (m, 2H), 1.92 - 1.80 (m, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 201.56, 141.38, 137.28, 131.77, 131.28, 129.77, 127.17 (q, *J* = 274.5 Hz), 126.30, 33.44 (q, *J* = 28.3 Hz), 32.94, 29.60, 23.80 (q, *J* = 2.8 Hz). ^{19}F NMR (376 MHz, $CDCl_3$) δ -66.20. HRMS (APCI) m/z calcd. for $C_{12}H_{14}OF_3$ $[M+H]^+$ 231.0997, found 231.0990.

1-(2-(4,4,4-trifluorobutyl)phenyl)propan-1-one (3Ra)



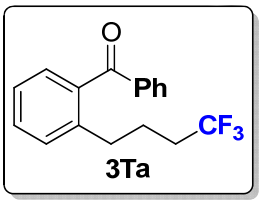
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.66 (dd, *J* = 7.6, 1.2 Hz, 1H), 7.42 (td, *J* = 7.6, 1.2 Hz, 1H), 7.29 (td, *J* = 7.2, 1.2 Hz, 2H), 7.24 - 7.27 (m, 1H), 2.94 (q, *J* = 7.2 Hz, 2H), 2.90 - 2.83 (m, 2H), 2.20 - 2.08 (m, 2H), 1.81 - 1.91 (m, 2H), 1.20 (t, *J* = 7.2 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 204.97, 140.84, 137.84, 131.31, 131.11, 128.64, 127.16 (q, *J* = 274.5 Hz), 126.26, 34.83, 33.41 (q, *J* = 28.2 Hz), 32.77, 23.91 (q, *J* = 2.8 Hz), 8.37. ^{19}F NMR (376 MHz, $CDCl_3$) δ -66.21 (s). HRMS (APCI) m/z calcd. for $C_{13}H_{16}F_3O$ $[M+H]^+$ 245.1153, found 245.1157.

2-phenyl-1-(2-(4,4,4-trifluorobutyl)phenyl)ethanone (3Sa)



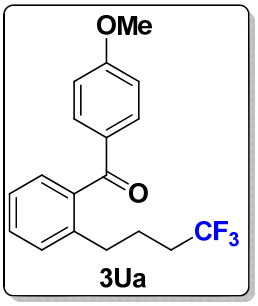
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.76 (dd, *J* = 7.6, 1.2 Hz, 1H), 7.42 (td, *J* = 7.6, 1.2 Hz, 1H), 7.35 - 7.28 (m, 3H), 7.28 - 7.20 (m, 4H), 4.21 (s, 2H), 2.84 (t, *J* = 7.6 Hz, 2H), 2.08 - 1.96 (m, 2H), 1.79 - 1.69 (m, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 201.43, 141.40, 137.44, 134.14, 131.57, 131.16, 129.51, 128.90, 128.68, 127.10 (q, *J* = 274.7 Hz), 127.01, 126.21, 48.64, 33.29 (q, *J* = 28.2 Hz), 32.53, 23.70 (q, *J* = 2.9 Hz). ^{19}F NMR (376 MHz, $CDCl_3$) δ -66.16. HRMS (APCI) m/z calcd. for $C_{18}H_{17}O_2F_3Na$ $[M+Na]^+$ 345.1078, found 345.1073.

phenyl(2-(4,4,4-trifluorobutyl)phenyl)methanone (3Ta)



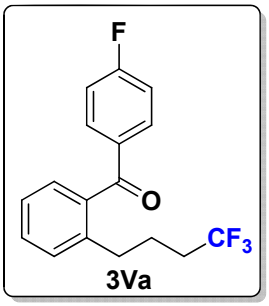
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.83 - 7.75 (m, 2H), 7.64 - 7.56 (m, 1H), 7.50 - 7.43 (m, 3H), 7.26 - 7.35 (m, 3H), 2.78 - 2.70 (m, 2H), 2.12 - 1.99 (m, 2H), 1.90 - 1.80 (m, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 198.35, 140.01, 138.34, 137.67, 133.30, 130.50, 130.14, 130.12, 128.97, 128.46, 127.02 (q, *J* = 274.5 Hz), 125.70, 33.21 (q, *J* = 28.4 Hz), 32.00, 23.76 (q, *J* = 2.8 Hz). ^{19}F NMR (376 MHz, $CDCl_3$) δ -66.22. HRMS (APCI) m/z calcd. for $C_{17}H_{16}OF_3$ $[M+H]^+$ 293.1153, found 293.1148.

(4-methoxyphenyl)(2-(4,4,4-trifluorobutyl)phenyl)methanone (3Ua)



^{1}H NMR (400 MHz, $CDCl_3$) δ 7.87 - 7.72 (m, 2H), 7.40 - 7.46 (m, 1H), 7.33 - 7.23 (m, 3H), 7.03 - 6.87 (m, 2H), 3.88 (s, 3H), 2.71 (t, *J* = 8.0 Hz, 2H), 2.09 - 1.95 (m, 2H), 1.89 - 1.71 (m, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 197.02, 163.80, 139.43, 138.93, 132.53, 130.46, 130.05, 129.92, 128.40, 126.75 (q, *J* = 275.6 Hz), 125.67, 113.70, 55.50, 33.18 (q, *J* = 28.3 Hz), 31.91, 23.65 (q, *J* = 2.9 Hz). ^{19}F NMR (376 MHz, $CDCl_3$) δ -66.21. HRMS (APCI) m/z calcd. for $C_{18}H_{18}O_2F_3$ $[M+H]^+$ 323.1259, found 323.1253.

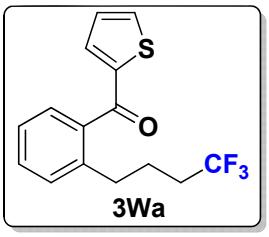
(4-fluorophenyl)(2-(4,4,4-trifluorobutyl)phenyl)methanone (3Va)



^{1}H NMR (400 MHz, $CDCl_3$) δ 7.87 - 7.77 (m, 2H), 7.50 - 7.42 (m, 1H), 7.35 - 7.27 (m, 3H), 7.17 - 7.10 (m, 2H), 2.73 (t, J = 7.6 Hz, 2H), 2.13 - 1.96 (m, 2H), 1.89 - 1.78 (m, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 196.71, 165.88 (d, *J* = 254.1 Hz), 139.94, 138.06, 134.02 (d, *J* = 2.9 Hz), 132.80 (d, *J* = 9.3 Hz), 130.60, 130.20, 128.73, 127.00 (q, *J* = 274.6 Hz), 125.77, 115.66 (q, *J* = 21.8 Hz), 33.19 (q, *J* = 28.3 Hz), 31.97, 23.77 (q, *J* = 2.9 Hz). ^{19}F NMR (376 MHz, $CDCl_3$) δ -66.22 (s, 3F), -104.48 (s, 1F).

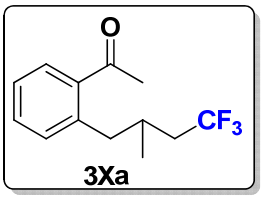
HRMS (APCI) m/z calcd. for $C_{17}H_{15}OF_4$ $[M+H]^+$ 311.1059, found 311.1054.

thiophen-2-yl(2-(4,4,4-trifluorobutyl)phenyl)methanone (3Wa)



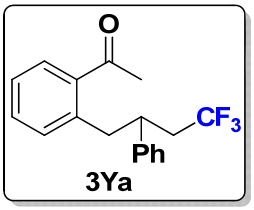
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.74 (d, *J* = 4.8 Hz, 1H), 7.50 - 7.40 (m, 3H), 7.35 - 7.28 (m, 2H), 7.12 (t, *J* = 3.6 Hz, 1H), 2.78 (t, *J* = 7.6 Hz, 2H), 2.13 - 2.00 (m, 2H), 1.92 - 1.83 (m, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 190.06, 144.91, 139.68, 138.22, 135.54, 135.09, 130.59, 130.14, 128.49, 128.14, 127.04 (q, *J* = 274.6 Hz), 125.68, 33.17 (q, *J* = 28.3 Hz), 31.83, 23.75 (q, *J* = 2.8 Hz). ^{19}F NMR (376 MHz, $CDCl_3$) δ -66.21. HRMS (APCI) m/z calcd. for $C_{15}H_{14}F_3OS$ $[M+H]^+$ 299.0717, found 299.0698

1-(2-(4,4,4-trifluoro-2-methylbutyl)phenyl)ethanone (3Xa)



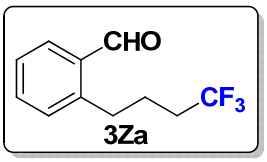
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.71 (d, *J* = 9.0 Hz, 1H), 7.42 (t, *J* = 7.6 Hz, 1H), 7.31 (t, *J* = 7.6 Hz, 1H), 7.21 (d, *J* = 7.6 Hz, 1H), 2.93 (dd, *J* = 13.2, 6.8 Hz, 1H), 2.81 (dd, *J* = 13.2, 7.6 Hz, 1H), 2.58 (s, 3H), 2.21 - 2.09 (m, 2H), 2.03 - 1.90 (m, 1H), 1.01 (d, *J* = 6.4 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 201.82, 139.97, 137.85, 132.09, 131.41, 129.07, 127.18 (q, *J* = 275.7 Hz), 126.38, 40.85, 39.56 (q, *J* = 26.9 Hz), 29.75, 29.72 (q, *J* = 2.3 Hz), 19.49. ^{19}F NMR (376 MHz, $CDCl_3$) δ -63.03. HRMS (APCI) m/z calcd. for $C_{13}H_{16}OF_3$ $[M+H]^+$ 245.1153, found 245.1147.

1-(2-(4,4,4-trifluoro-2-phenylbutyl)phenyl)ethanone (3Ya)

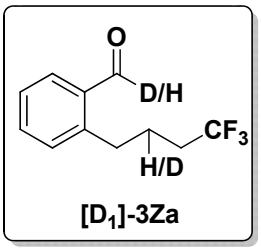


^{1}H NMR (400 MHz, $CDCl_3$) δ 7.63 (dd, *J* = 7.6, 1.6 Hz, 1H), 7.30 (td, *J* = 7.6, 1.6 Hz, 1H), 7.27 - 7.22 (m, 3H), 7.21 - 7.17 (m, 1H), 7.09 - 7.05 (m, 2H), 6.99 (dd, *J* = 7.6, 1.2 Hz, 1H), 3.32 - 3.15 (m, 3H), 2.62 - 2.47 (m, 2H), 2.43 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 201.87, 142.47, 139.19, 137.89, 132.11, 131.31, 129.44, 128.36, 127.61, 126.67, 126.35, 126.61 (q, *J* = 276.0 Hz), 41.90 (q, *J* = 2.4 Hz), 40.78, 39.04 (q, *J* = 27.1 Hz), 29.49. ^{19}F NMR (376 MHz, $CDCl_3$) δ -63.49. HRMS (APCI) m/z calcd. for $C_{18}H_{18}OF_3$ $[M+H]^+$ 307.1310, found 307.1303.

2-(4,4,4-trifluorobutyl)benzaldehyde (3Za)

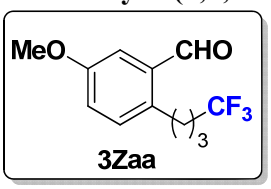


^{1}H NMR (400 MHz, $CDCl_3$) δ 10.18 (s, 1H), 7.82 (dd, *J* = 7.6, 1.2 Hz, 1H), 7.54 (td, *J* = 7.6, 1.2 Hz, 1H), 7.44 (t, *J* = 7.6 Hz, 1H), 7.31 - 7.27 (m, 1H), 3.12 (t, *J* = 7.6 Hz, 2H), 2.16 (m, 2H), 1.92 – 1.84 (m, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 192.81, 143.27, 134.04, 133.82, 133.70, 131.06, 127.06 (q, *J* = 271.7 Hz), 127.01, 33.34 (q, *J* = 28.4 Hz), 31.67, 23.78 (q, *J* = 2.9 Hz). ^{19}F NMR (376 MHz, $CDCl_3$) δ -66.16. HRMS (APCI) m/z calcd. for $C_{11}H_{12}OF_3$ $[M+H]^+$ 217.0840, found 217.0831.



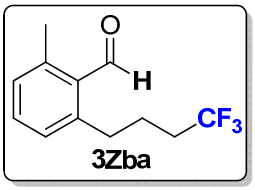
^{1}H NMR (400 MHz, $CDCl_3$) δ 10.18 (s, 0.1H), 7.82 (dd, *J* = 7.6, 1.6 Hz, 1H), 7.53 (td, *J* = 7.6, 1.6 Hz, 1H), 7.43 (td, *J* = 7.6, 1.2 Hz, 1H), 7.28 (d, *J* = 7.6 Hz, 1H), 3.14 – 3.11 (t, *J* = 7.6 Hz, 2H), 2.21 - 2.11 (m, 2H), 1.92 - 1.82 (m, 2H).
^{13}C NMR (101 MHz, $CDCl_3$) δ192.44 (t, *J* = 26.1 Hz), 143.29, 133.93, 133.81, 131.03, 127.05 (q, *J* = 274.6 Hz), 126.99, 33.33 (q, *J* = 28.5 Hz), 31.64, 23.78 (q, *J* = 2.9 Hz).
^{19}F NMR (376 MHz, $CDCl_3$) δ -66.17.
HRMS (APCI) m/z calcd. for $C_{11}H_{11}DF_3O$ $[M+H]^+$ 218.0903, found 218.0897.

5-methoxy-2-(4,4,4-trifluorobutyl)benzaldehyde (3Zaa)



^{1}H NMR (400 MHz, $CDCl_3$) δ 10.18 (s, 1H), 7.33 (d, *J* = 2.8 Hz, 1H), 7.18 (d, *J* = 8.4 Hz, 1H), 7.07 (dd, *J* = 8.4, 2.8 Hz, 1H), 3.85 (s, 3H), 3.03 (t, *J* = 7.6 Hz, 2H), 2.19 - 2.09 (m, 2H), 1.79 - 1.89 (m, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 191.93, 158.51, 135.56, 134.43, 132.19, 127.05 (q, *J* = 275.2 Hz), 120.40, 116.47, 55.48, 33.21 (q, *J* = 28.5 Hz), 30.51, 24.28. ^{19}F NMR (376 MHz, $CDCl_3$) δ -66.13. HRMS (APCI) m/z calcd. for $C_{12}H_{14}O_2F_3$ $[M+H]^+$ 247.0946, found 247.0941.

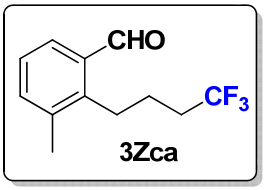
2-methyl-6-(4,4,4-trifluorobutyl)benzaldehyde (3Zba)



^{1}H NMR (400 MHz, $CDCl_3$) δ 10.61 (s, 1H), 7.39 (t, *J* = 7.6 Hz, 1H), 7.16 (d, *J* = 7.6 Hz, 1H),

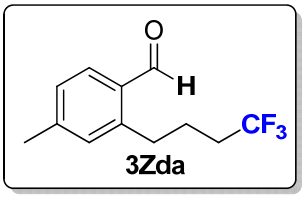
7.12 (d, J = 7.6 Hz, 1H), 3.05 - 3.00 (m, 2H), 2.65 (s, 3H), 2.14 - 2.22 (m, 2H), 1.91 - 1.85 (m, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 193.13, 143.60, 141.88, 133.19, 132.04, 130.25, 129.11, 127.08 (q, J = 274.7 Hz), 33.36 (q, J = 28.4 Hz), 32.40, 24.13 (q, J = 2.8 Hz), 20.23. 19F NMR (376 MHz, $CDCl_3$) δ -66.17. HRMS (APCI) m/z calcd. for $C_{12}H_{14}OF_3$ $[M+H]^+$ 231.0997, found 231.0991.

3-methyl-2-(4,4,4-trifluorobutyl)benzaldehyde (3Zca)



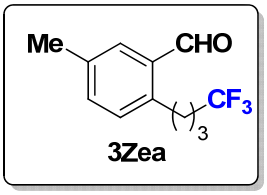
^{1}H NMR (400 MHz, $CDCl_3$) δ 10.16 (s, 1H), 7.65 (d, J = 7.6 Hz, 1H), 7.41 (d, J = 7.6 Hz, 1H), 7.32 (t, J = 7.6 Hz, 1H), 3.12 (d, J = 7.6 Hz, 2H), 2.39 (s, 3H), 2.32 - 2.18 (m, 2H), 1.81 - 1.72 (m, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 193.24, 141.67, 137.72, 135.95, 133.94, 132.33, 127.07 (q, J = 274.8 Hz), 126.55, 33.70 (q, J = 28.4 Hz), 27.17, 22.65 (q, J = 2.8 Hz), 19.04. ^{19}F NMR (376 MHz, $CDCl_3$) δ -66.10. HRMS (APCI) m/z calcd. for $C_{12}H_{14}OF_3$ $[M+H]^+$ 231.0997, found 231.0991.

4-methyl-2-(4,4,4-trifluorobutyl)benzaldehyde (3Zda)



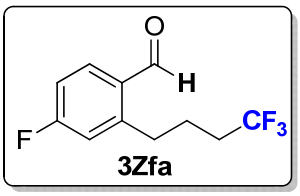
^{1}H NMR (400 MHz, $CDCl_3$) δ 10.10 (s, 1H), 7.69 (d, J = 8.0 Hz, 1H), 7.21 (d, J = 7.6 Hz, 1H), 7.07 (s, 1H), 3.06 (t, J = 8.0 Hz, 2H), 2.40 (s, 3H), 2.07 - 2.20 (m, 2H), 1.89 - 1.80 (m, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 192.31, 144.82, 143.24, 134.33, 131.81, 131.41, 127.66, 127.07 (q, J = 274.6 Hz), 33.32 (q, J = 28.4 Hz), 31.62, 23.74 (q, J = 2.8 Hz), 21.59. ^{19}F NMR (376 MHz, $CDCl_3$) δ -66.18. HRMS (APCI) m/z calcd. for $C_{12}H_{14}OF_3$ $[M+H]^+$ 231.0997, found 231.0993.

5-methyl-2-(4,4,4-trifluorobutyl)benzaldehyde (3Zea)



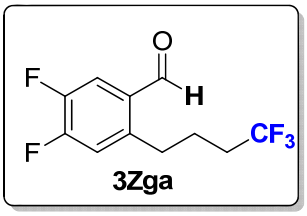
^{1}H NMR (400 MHz, $CDCl_3$) δ 10.15 (s, 1H), 7.62 (d, J = 1.2 Hz, 1H), 7.34 (dd, J = 7.6, 1.6 Hz, 1H), 7.16 (d, J = 7.6 Hz, 1H), 3.07 (t, J = 7.6 Hz, 2H), 2.41 (s, 3H), 2.06 - 2.20 (m, 2H), 1.80 - 1.89 (m, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 192.87, 140.29, 136.77, 134.58, 134.33, 133.56, 131.02, 127.08 (q, J = 274.5 Hz), 33.30 (q, J = 28.3 Hz), 32.87, 31.18, 23.87 (q, J = 2.9 Hz), 20.69. ^{19}F NMR (376 MHz, $CDCl_3$) δ -66.17.
HRMS (APCI) m/z calcd. for $C_{12}H_{14}OF_3$ $[M+H]^+$ 231.0997, found 231.0993.

4-fluoro-2-(4,4,4-trifluorobutyl)benzaldehyde (3Zfa)



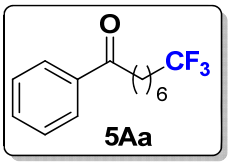
^{1}H NMR (400 MHz, $CDCl_3$) δ 10.08 (s, 1H), 7.81 (dd, *J* = 8.8, 6.0 Hz, 1H), 7.06 (td, *J* = 8.0, 2.4 Hz, 1H), 6.95 (dd, *J* = 9.6, 2.4 Hz, 1H), 3.16 - 3.04 (m, 2H), 2.21 - 2.10 (m, 2H), 1.79 - 1.89 (m, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 190.96, 165.57 (d, *J* = 255.5 Hz), 146.79 (d, *J* = 8.8 Hz), 136.62 (d, *J* = 10.1 Hz), 130.33 (d, *J* = 2.6 Hz), 126.93 (q, *J* = 274.6 Hz), 117.85 (d, *J* = 21.6 Hz), 114.04 (d, *J* = 21.6 Hz), 33.17 (q, *J* = 28.6 Hz), 31.42, 23.43 (q, *J* = 2.9 Hz). ^{19}F NMR (376 MHz, $CDCl_3$) δ -66.27 (s, 3F), -103.50 (s, 1F). HRMS (APCI) m/z calcd. for $C_{11}H_{11}OF_4$ $[M+H]^+$ 235.0746, found 235.0741.

4,5-difluoro-2-(4,4,4-trifluorobutyl)benzaldehyde (3Zga)



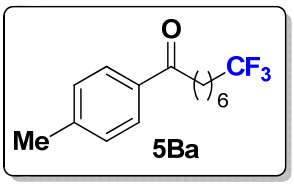
^{1}H NMR (400 MHz, $CDCl_3$) δ 10.09 (s, 1H), 7.64 (dd, *J* = 10.0, 8.0 Hz, 1H), 7.09 (dd, *J* = 10.8, 7.6 Hz, 1H), 3.10 - 3.02 (m, 2H), 2.24 - 2.10 (m, 2H), 1.81 - 1.90 (m, 2H).
^{13}C NMR (101 MHz, $CDCl_3$) δ 189.38, 153.48 (dd, *J* = 257.5, 12.8 Hz), 149.09 (dd, *J* = 249.1, 12.9 Hz), 141.36 (dd, *J* = 6.7, 3.9 Hz), 130.48 (t, *J* = 3.4 Hz), 126.85 (q, *J* = 274.6 Hz), 121.25 (d, *J* = 17.2 Hz), 119.78 (d, *J* = 17.6 Hz), 33.13 (q, *J* = 28.7 Hz), 30.57, 23.86 (q, *J* = 2.1 Hz). ^{19}F NMR (376 MHz, $CDCl_3$) δ -66.24 (s, 3F), -128.17 (d, *J* = 21.8 Hz, 1F), -139.00 (d, *J* = 21.8 Hz, 1F). HRMS (APCI) m/z calcd. for $C_{11}H_{10}OF_5$ $[M+H]^+$ 253.0652, found 253.0648.

8,8,8-trifluoro-1-phenyloctan-1-one (5Aa)



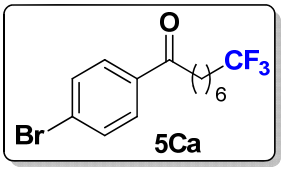
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.93 - 7.97 (m, 2H), 7.58 - 7.52 (m, 1H), 7.42 - 7.48 (m, 2H), 2.97 (t, *J* = 7.2 Hz, 2H), 2.11 - 2.01 (m, 2H), 1.78 - 1.71 (m, 2H), 1.53 - 1.60 (m, 2H), 1.38 - 1.44 (m, 4H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 200.16, 136.95, 132.91, 128.53, 127.96, 127.20 (q, *J* = 274.4 Hz), 38.30, 33.59 (q, *J* = 28.1 Hz), 28.83, 28.52, 23.89, 21.68 (q, *J* = 2.8 Hz). ^{19}F NMR (376 MHz, $CDCl_3$) δ -66.39. HRMS (APCI) m/z calcd. for $C_{14}H_{18}OF_3$ $[M+H]^+$ 259.1310, found 259.1306.

8,8,8-trifluoro-1-(p-tolyl)octan-1-one (5Ba)



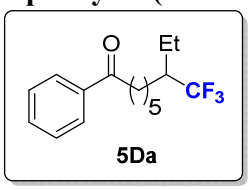
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.86 (d, *J* = 8.4 Hz, 2H), 7.25 (d, *J* = 7.6 Hz, 2H), 2.94 (t, *J* = 7.2 Hz, 2H), 2.41 (s, 3H), 2.00 - 2.13 (m, 2H), 1.69 - 1.77 (m, 2H), 1.62 - 1.53 (m, 2H), 1.37 - 1.45 (m, 4H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 199.87, 143.68, 134.47, 129.21, 128.10, 127.20 (q, *J* = 274.6 Hz), 38.20, 33.60 (q, *J* = 28.1 Hz), 28.86, 28.54, 24.02, 21.69 (q, *J* = 2.9 Hz), 21.56. ^{19}F NMR (376 MHz, $CDCl_3$) δ -66.39. HRMS (APCI) m/z calcd. for $C_{15}H_{20}OF_3$ $[M+H]^+$ 273.1466, found 273.1462.

1-(4-bromophenyl)-8,8,8-trifluorooctan-1-one (5Ca)



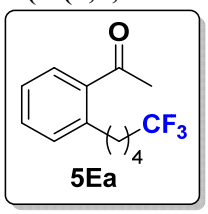
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.87 - 7.73 (m, 2H), 7.68 - 7.53 (m, 2H), 2.93 (t, *J* = 7.3 Hz, 2H), 1.99 - 2.13 (m, 2H), 1.78 - 1.68 (m, 2H), 1.61 - 1.50 (m, 2H), 1.39 - 1.46 (m, 4H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 199.04, 135.63, 131.84, 129.51, 128.05, 127.17 (q, *J* = 274.6 Hz), 38.27, 33.59 (q, *J* = 28.2 Hz), 28.79, 28.51, 23.77, 21.68 (q, *J* = 2.9 Hz). ^{19}F NMR (376 MHz, $CDCl_3$) δ -66.37. HRMS (APCI) m/z calcd. for $C_{14}H_{17}BrF_3O$ $[M]^+$ 337.0415, found 337.0409.

1-phenyl-7-(trifluoromethyl)nonan-1-one (5Da)



^{1}H NMR (400 MHz, $CDCl_3$) δ 8.01 - 7.95 (m, 2H), 7.61 - 7.55 (m, 1H), 7.52 - 7.36 (m, 2H), 3.00 (t, *J* = 7.2 Hz, 2H), 2.04 – 1.92 (m, 1H), 1.82 – 1.74 (m, 2H), 1.68 – 1.60 (m, 2H), 1.55 – 1.39 (m, 6H), 1.02 - 0.97 (m, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 200.34, 137.02, 132.98, 128.72 (q, *J* = 278.8 Hz), 128.60, 128.05, 43.86 (q, *J* = 24.4 Hz), 38.43, 29.43, 27.12 (q, *J* = 2.3 Hz), 26.77, 24.07, 20.70 (q, *J* = 2.7 Hz), 11.25. ^{19}F NMR (376 MHz, $CDCl_3$) δ -69.9. HRMS (APCI) m/z calcd. for $C_{16}H_{22}OF_3$ $[M+H]^+$ 287.1617, found 287.1610.

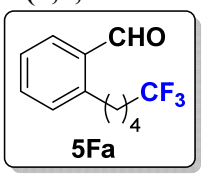
1-(2-(5,5,5-trifluoropentyl)phenyl)ethanone (5Ea)



1H NMR (400 MHz, CDCl3) δ 7.69 (dd, *J* = 7.6, 1.2 Hz, 1H), 7.41 (td, *J* = 7.6, 1.2 Hz, 1H), 7.28 (td, *J* = 7.6, 1.2 Hz, 1H), 7.24 (d, *J* = 7.6 Hz, 1H), 2.87 (t, *J* = 7.2 Hz, 2H), 2.58 (s, 3H), 2.17 -

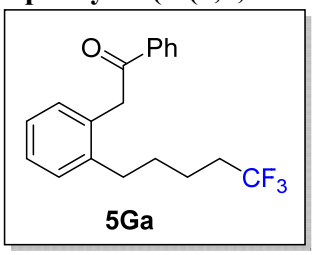
2.05 (m, 2H), 1.68 - 1.59 (m, 4H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 201.78, 142.15, 137.40, 131.58, 131.27, 129.50, 127.22 (q, *J* = 274.6 Hz), 125.97, 33.68, 33.48 (q, *J* = 28.2 Hz), 30.72, 29.66, 21.83 (q, *J* = 2.9 Hz). ^{19}F NMR (376 MHz, $CDCl_3$) δ -66.35. HRMS (APCI) m/z calcd. for $C_{13}H_{16}OF_3$ $[M+H]^+$ 245.1153, found 245.1149.

2-(5,5,5-trifluoropentyl)benzaldehyde (5Fa)



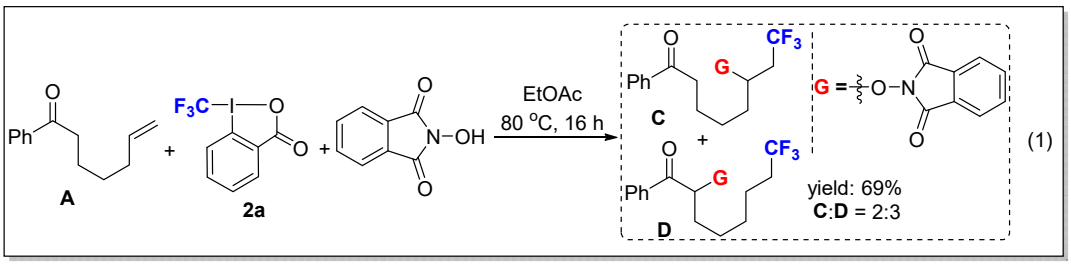
^{1}H NMR (400 MHz, $CDCl_3$) δ 10.21 (s, 1H), 7.82 (dd, *J* = 8.0, 1.6 Hz, 1H), 7.52 (td, *J* = 7.6, 1.6 Hz, 1H), 7.40 (td, *J* = 7.6, 1.2 Hz, 1H), 7.27 (d, *J* = 7.2 Hz, 1H), 3.06 (t, *J* = 7.2 Hz, 2H), 2.05 - 2.17 (m, 2H), 1.62 - 1.73 (m, 4H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 192.6, 144.35, 133.76, 133.61, 133.20, 131.02, 127.11 (q, *J* = 28.2 Hz), 126.69, 33.46 (q, *J* = 3.0 Hz), 32.37, 30.82, 21.74 (q, *J* = 2.9 Hz). ^{19}F NMR (376 MHz, $CDCl_3$) δ -66.33. HRMS (APCI) m/z calcd. for $C_{12}H_{14}OF_3$ $[M+H]^+$ 231.0997, found 231.0992.

1-phenyl-2-(2-(5,5,5-trifluoropentyl)phenyl)ethanone (5Ga)



^{1}H NMR (400 MHz, $CDCl_3$) δ 8.06 - 7.99 (m, 2H), 7.59 (t, *J* = 7.6 Hz, 1H), 7.49 (t, *J* = 7.6 Hz, 2H), 7.26 - 7.11 (m, 4H), 4.32 (s, 2H), 2.63 - 2.53 (m, 2H), 2.12 - 1.97 (m, 2H), 1.65 - 1.54 (m, 4H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 197.66, 140.26, 136.75, 133.26, 132.77, 130.86, 129.21, 128.70, 128.28, 127.35, 127.07 (q, *J* = 274.7 Hz), 126.33, 42.84, 33.93 (q, *J* = 33.51 Hz), 32.64, 29.61, 21.83 (q, *J* = 2.8 Hz). ^{19}F NMR (376 MHz, $CDCl_3$) δ -66.25. HRMS (APCI) m/z calcd. for $C_{19}H_{20}F_3O$ $[M+H]^+$ 321.1461, found 321.1455.

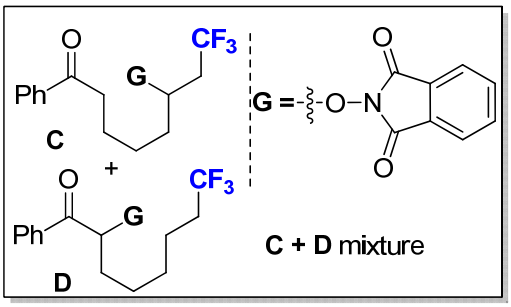
The Procedure with linear alkenyl ketone **A**、alkenyl amide **E**、alkenyl amine **1AB** and alkenyl alcohol **1A** as substrate



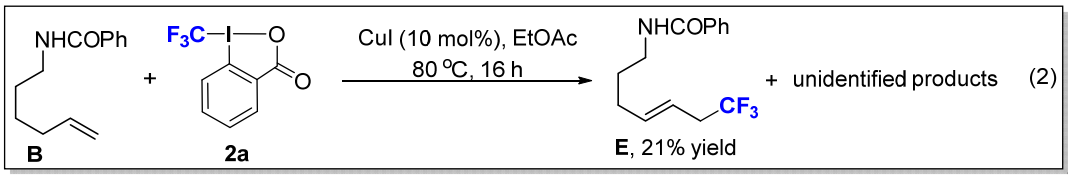
Procedure: Under argon, a 25 mL Schlenk tube equipped with a magnetic stir bar were charged with **A** (0.2 mmol, 1.0 equiv), Togni's reagent **2a** (0.4 mmol, 2.0 equiv), 2-hydroxyisoindoline-1,3-dione (0.4 mmol, 2.0 equiv) and EtOAc (super dry, 2.0 mL). The sealed tube was then stirred at 80 °C for 16 hours, after reaction completion (monitored by TLC),

concentrated *in vacuo*, and the residue was purified by silica gel column chromatography (petroleum ether/EtOAc) to give the mixture **C** and **D**.

2-((1,1,1-trifluoro-8-oxo-8-phenyloctan-3-yl)oxy)isoindoline-1,3-dione (C) and 2-((8,8,8-trifluoro-1-oxo-1-phenyloctan-2-yl)oxy)isoindoline-1,3-dione(D)

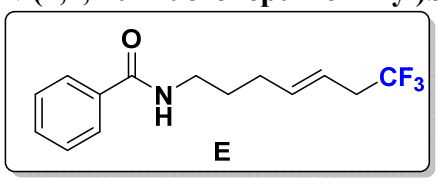


^{1}H NMR (400 MHz, $CDCl_3$) δ 8.10 - 8.05 (m, 2H), 7.99 - 7.94 (m, 1H), 7.85 - 7.71 (m, 6H), 7.63 - 7.53 (m, 2H), 7.52 - 7.43 (m, 3H), 5.62 - 5.56 (m, 1H), 4.56 - 4.48 (m, 0.48 H), 3.05 (t, *J* = 6.6 Hz, 1H), 2.83 - 2.71 (m, 0.49 H), 2.59 - 2.44 (m, 0.47 H), 2.12 - 1.99 (m, 4H), 1.90 - 1.72 (m, 3H), 1.68 - 1.53 (m, 4H), 1.52 - 1.42 (m, 2H). ^{13}C NMR (100 MHz, CDCl3) δ 199.87, 195.63, 163.99, 163.35, 136.85, 134.81, 134.64, 134.55, 133.70, 132.86, 128.84, 128.65, 128.47, 127.93, 127.09 (q, *J* = 275.3 Hz), 125.47 (q, *J* = 275.1 Hz), 123.58, 123.53, 87.88, 81.75 (q, *J* = 2.7 Hz), 38.20, 37.75 (q, *J* = 28.1 Hz), 33.40 (q, *J* = 28.2 Hz), 33.14, 31.04, 28.25, 24.56, 24.16, 23.76, 21.52 (q, *J* = 2.8 Hz). ^{19}F NMR (376 MHz, $CDCl_3$) δ -63.37 (s), -66.33 (s). HRMS (APCI) m/z calcd. for $C_{22}H_{21}NO_4F_3$ $[M+H]^+$ 420.1423, found 420.1415.

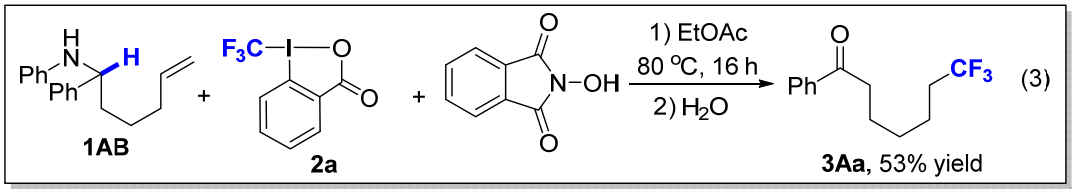


Procedure: Under argon, a 25 mL Schlenk tube equipped with a magnetic stir bar were charged with **B** (0.2 mmol, 1.0 equiv), Togni's reagent (0.4 mmol, 2.0 equiv), CuI (0.1 mmol, 0.1 equiv) and EtOAc (super dry, 2.0 mL). The sealed tube was then stirred at 80 °C for 16 hours, after reaction completion (monitored by TLC), concentrated *in vacuo*, and the residue was purified by silica gel column chromatography (petroleum ether/EtOAc) to give the product **E** in 21% yield along with other unidentified products.

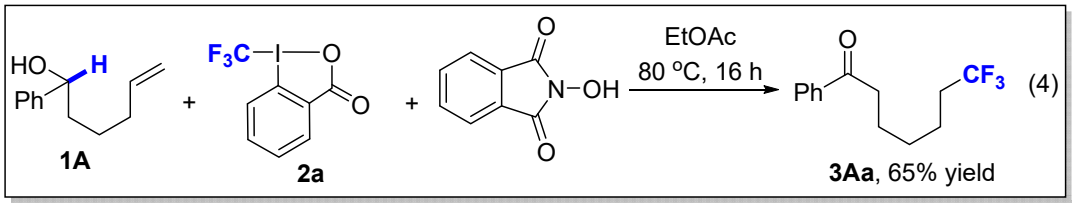
N-(7,7,7-trifluorohept-4-en-1-yl)benzamide (E)



^{1}H NMR (400 MHz, $CDCl_3$) δ 7.75 (d, *J* = 7.2 Hz, 2H), 7.49 (t, *J* = 7.2 Hz, 1H), 7.42 (t, *J* = 7.6 Hz, 2H), 6.22 (s, 1H), 5.78 - 5.68 (m, 1H), 5.48 – 5.38 (m, 1H), 3.47 (q, *J* = 6.8 Hz, 2H), 2.88 - 2.67 (m, 2H), 2.16 (q, *J* = 7.2 Hz, 2H), 1.76 - 1.68 (m, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 167.59, 137.03, 134.62, 131.37, 128.51, 126.79, 125.93 (q, *J* = 274.8 Hz), 118.53 (q, *J* = 3.5 Hz), 39.45, 37.25 (q, *J* = 29.4 Hz), 29.86, 28.84. ^{19}F NMR (376 MHz, $CDCl_3$) δ -66.64. HRMS (APCI) m/z calcd. for $C_{14}H_{17}F_3NO$ $[M+H]^+$ 272.1262, found 272.1253.

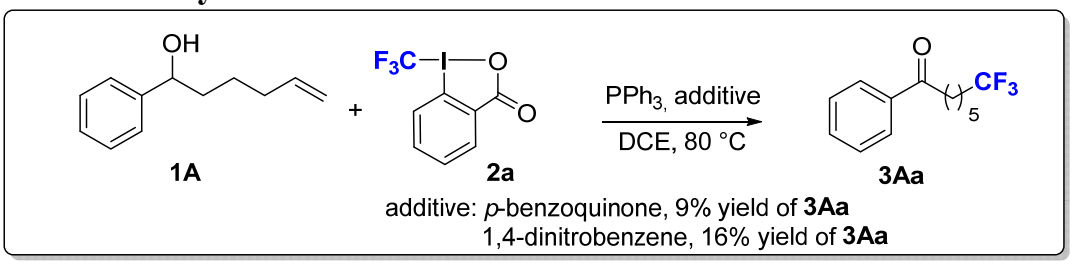


Procedure: Under argon, a 25 mL Schlenk tube equipped with a magnetic stir bar were charged with **1AB** (0.2 mmol, 1.0 equiv), Togni's reagent **2a** (0.4 mmol, 2.0 equiv), 2-hydroxyisoindoline-1,3-dione (0.4 mmol, 2.0 equiv) and EtOAc (super dry, 2.0 mL). The sealed tube was then stirred at 80 °C for 16 hours, after reaction completion (monitored by TLC), water was added and then extracted with EtOAc three times, dried with anhydrous Na_2SO_4, filtered and concentrated *in vacuo*. The residue was purified by silica gel column chromatography (petroleum ether/EtOAc) to give the **3Aa**.



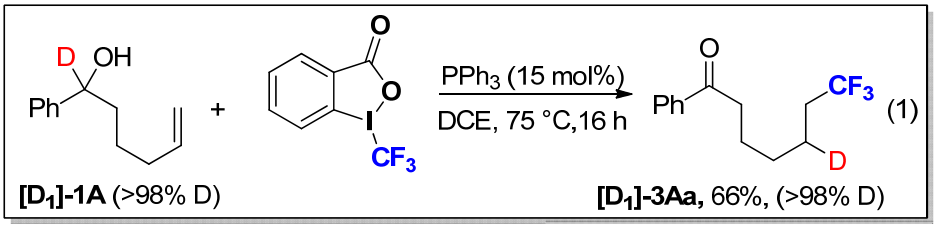
Procedure: Under argon, a 25 mL Schlenk tube equipped with a magnetic stir bar were charged with **1A** (0.2 mmol, 1.0 equiv), Togni's reagent **2a** (0.4 mmol, 2.0 equiv), 2-hydroxyisoindoline-1,3-dione (0.4 mmol, 2.0 equiv) and EtOAc (super dry, 2.0 mL). The sealed tube was then stirred at 80 °C for 16 hours, after reaction completion (monitored by TLC), concentrated *in vacuo*, and the residue was purified by silica gel column chromatography (petroleum ether/EtOAc) to give the **3Aa**.

Mechanistic Study



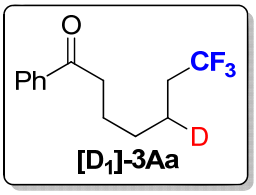
Reaction conditions: **1A** (0.2 mmol), Togni's reagent **2a** (1.5 equiv), benzoquinone (1.5 equiv) or 1, 4-dinitrobenzene (1.5 equiv), PPh_3 (15 mmol%), DCE (2.0 mL) at 80 ºC for 16 h under argon. Yield as determined by ^{19}F NMR spectroscopy using $PhCF_3$ as an internal standard.

Procedure: Under argon, a 25 mL Schlenk tube equipped with a magnetic stir bar were charged with **1A** (0.2 mmol, 1.0 equiv), Togni's reagent (0.3 mmol, 1.5 equiv), triphenylphosphine (0.03 mmol, 0.15 equiv)，benzoquinone (BQ, 0.3 mmol. 1.5 equiv) or 1,4-dinitrobenzene (0.5 mmol, 1.5 equiv) and 1,2-dichloroethane (DCE, super dry, 2.0 mL). The sealed tube was then stirred at 80 °C for 16 hours. After reaction completion (monitored by TLC), α,α,α-trifluorotoluene (internal standard, 29.2 mg, 0.2 mmol) was added. ^{19}F NMR analysis of this reaction mixture showed that **3Aa** was formed in 9% and 16% yield, respectively.

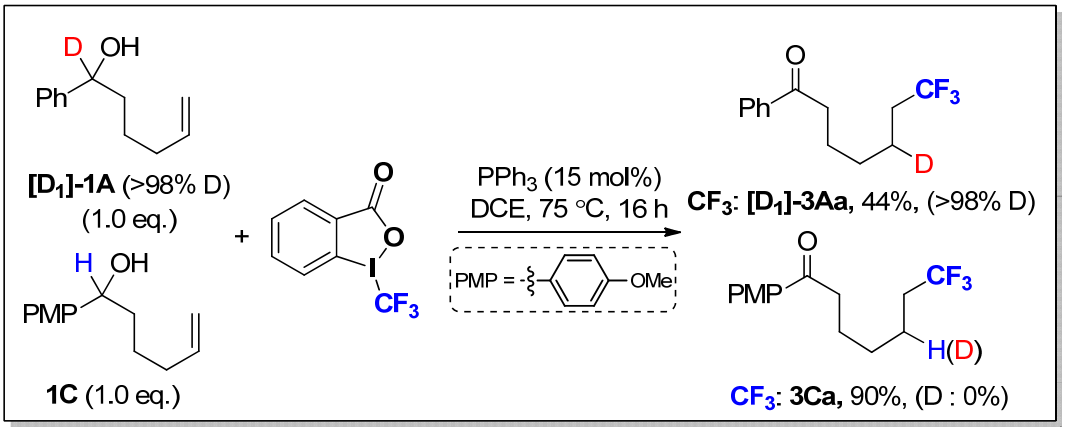


Procedure: Under argon, a 25 mL Schlenk tube equipped with a magnetic stir bar were charged with **[D_1]-1A** (0.2 mmol, 1.0 equiv), Togni's reagent (0.3 mmol, 1.5 equiv), PPh_3 (0.03 mmol, 0.15 equiv) and EtOAc (super dry, 2.0 mL). The sealed tube was then stirred at 80 °C for 16 hours, after completion (monitored by TLC), the reaction solution was concentrated *in vacuo*, and the residue was purified by silica gel column chromatography (petroleum ether/EtOAc) to give the **[D_1]-3Aa**.

[D_1]-7,7,7-trifluoro-1-phenylheptan-1-one (D_1-3Aa)

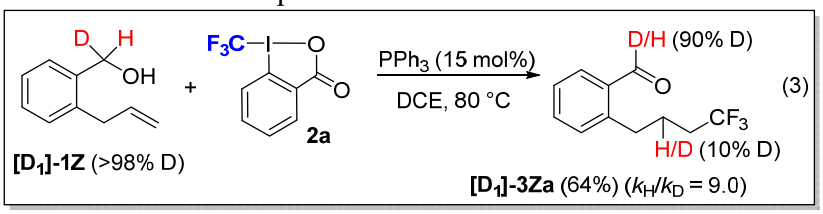


^1H NMR (400 MHz, $CDCl_3$) δ 7.98 - 7.93 (m, 2H), 7.60 - 7.53 (m, 1H), 7.49 - 7.43 (m, 2H), 2.99 (t, J = 7.2 Hz, 2H), 2.13 - 2.03 (m, 2H), 1.81 - 1.73 (m, 2H), 1.63 - 1.55 (m, 1H), 1.49 - 1.42 (m, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 199.92, 136.90, 133.01, 128.58, 127.97, 127.17 (q, J = 275.0 Hz), 38.09, 33.45 (q, J = 28.3 Hz), 28.22, 23.64, 21.44 (m). ^{19}F NMR (376 MHz, $CDCl_3$) δ -66.36. HRMS (APCI) m/z calcd. for $C_{13}H_{15}DF_3O$ $[M+H]^+$ 246.1216, found 246.1211.



Procedure: Under argon, a 25 mL Schlenk tube equipped with a magnetic stir bar were charged with **[D$_1$]-1A** (0.2 mmol, 1.0 equiv), **1C** (0.2 mmol, 1.0 equiv), Togni's reagent (0.6 mmol, 1.5 equiv), PPh_3 (0.06 mmol, 0.15 equiv) and DCE (super dry, 4.0 mL). The sealed tube was then stirred at 75 °C for 16 hours, after completion (monitored by TLC), the reaction solution was concentrated *in vacuo*, and the residue was purified by silica gel column chromatography (petroleum ether/EtOAc) to give the **[D$_1$]-3Aa** and **3Ca**.

Determination of Intramolecular Competition KIE



Procedure: Under argon, a 25 mL Schlenk tube equipped with a magnetic stir bar were charged with **[D$_1$]-1Z** (0.2 mmol, 16.3 mg.), Togni's reagent **2a** (0.3 mmol, 94.5 mg.), PPh_3 (0.03 mmol, 7.9 mg.) and DCE (super dry, 2.0 mL). The sealed tube was then stirred at 80 °C for 16 hours, after completion (monitored by TLC), the reaction solution was concentrated *in vacuo*, and the residue was purified by silica gel column chromatography (petroleum ether/EtOAc) to give the **[D$_1$]-3Za**, the ratio of deuterium product **[D$_1$]-3Za** was determined by ^{1}H NMR measurement.

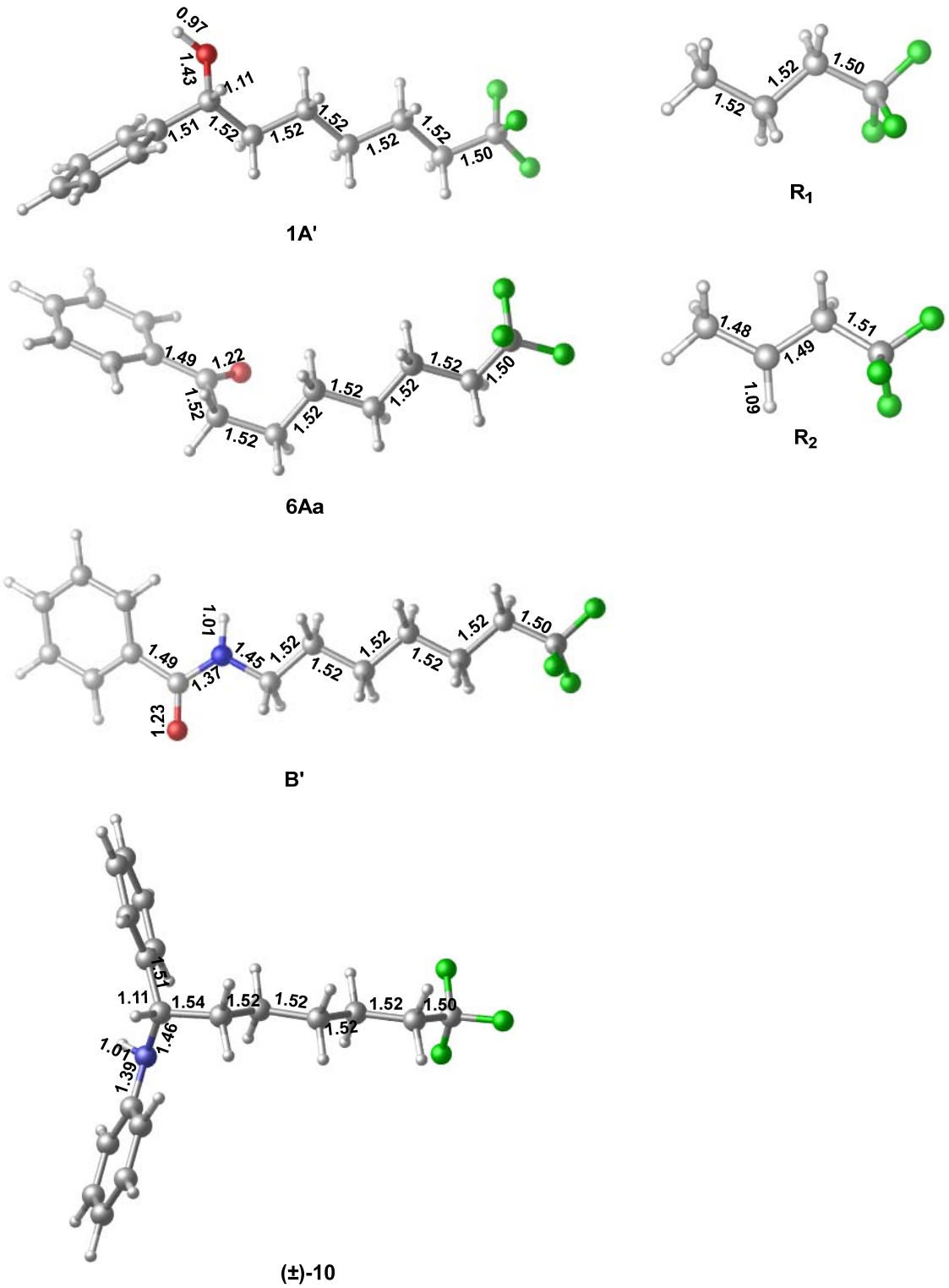
Computational Details

In this paper, our calculations were performed by using the Gaussian 09[1] with the M06L functional. The 6-31++G* basis set was used for all atoms.[2-4] The geometric structures of all species were optimized in the gas phase. Calculating the harmonic vibrational frequencies and noting the number of imaginary frequencies confirmed the nature of all intermediates (no imaginary frequency) and transition state structures (only one imaginary frequency). The latter were also confirmed to connect the appropriate intermediates by intrinsic reaction coordinate (IRC) calculations.[5,6] The gas-phase free energies, *G*, were calculated at $T = 298.15$ K within the harmonic potential approximation using the optimized structures. The solvation effects, with ethyl acetate as solvent, were included by utilizing the SMD solvent model[7] while retaining the gas-phase optimized geometries. We approximated the solution-phase free energy by adding solvation energies on the gas-phase relative free energies; experience has shown this to be very close to full optimization and frequency calculations in solvent. The solution phase free energies will be used in the discussions, unless otherwise specified. The 3D molecular structures of all the species shown in the Figures S1 and S2 were drawn by using the CYLview program.[8]

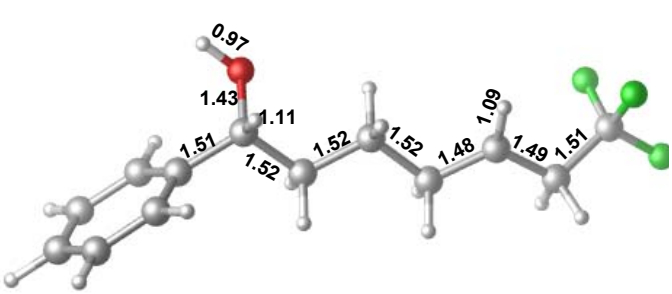
Here, the calculation of ΔGs_6, ΔGs_7, ΔGs_8 and ΔGs_9 is more practical than the calculation of ΔGs_2, ΔGs_3, ΔGs_4 and ΔGs_5, and the comparison of ΔGs_6, ΔGs_7, ΔGs_8 and ΔGs_9 represents the comparison of ΔGs_2, ΔGs_3, ΔGs_4 and ΔGs_5 which are the α-C-H bond dissociation energies of **1A'**, **(±)-10, 6Aa and B'**.

Supplementary Table S2. The ΔE_{gas}, ΔG_{gas}, and, ΔE_{sol} of the species involved in Equations S6-S9 and Figure 5

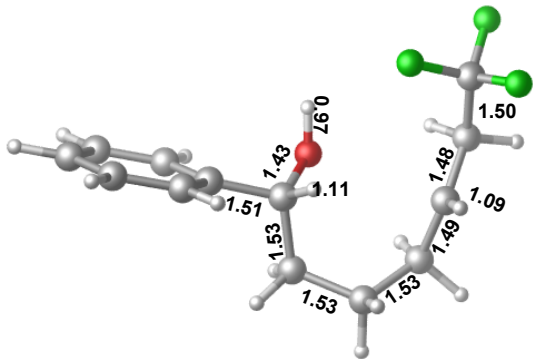
Species	ΔE_{gas}	ΔG_{gas}	ΔE_{sol}
1A'+R_2→1A_2+R_1	-19.1	-16.8	-19.7
6Aa+R_2→A_2+R_1	-9.1	-7.5	-9.8
B'+R_2→B_2+R_1	-8.7	-6.9	-9.2
(±)-10+R_2→1AB_2+R_1	-22.3	-19.6	-22.8
1A_1	0.0	0.0	0.0
1A_1′	-1.2	0.5	0.5
TS_{1A1}	11.1	11.6	11.8
1A_2′	-19.4	-15.7	-18.8
1A_2	-19.4	-17.7	-19.9
A_1	0.0	0.0	0.0
A_1′	-1.7	-0.5	-0.5
TS_{A1}	13.3	14.7	12.5
A_2′	-9.5	-7.9	-9.2
A_2	-9.4	-8.1	-9.7
B_1	0.0	0.0	0.0
B_1′	-1.1	1.6	-0.3
TS_{B1}	13.4	15.1	13.5
B_2′	-8.1	-6.3	-8.7
B_2	-9.0	-7.2	-9.5
1AB_1	0.0	0.0	0.0
1AB_1′	-1.9	1.3	-0.8
TS_{1AB1}	9.0	12.2	10.5
1AB_2′	-21.4	-16.8	-20.1
1AB_2	-21.1	-17.0	-21.3



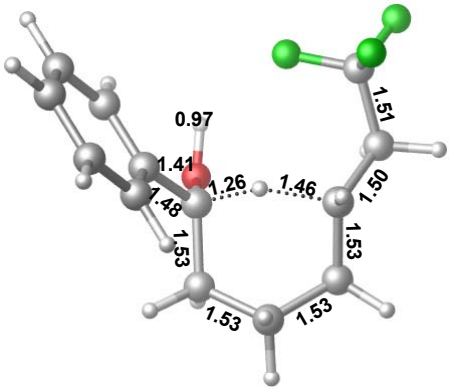
Supplementary Figure S2. Optimized geometries with selected structural parameters (distances in Å) for the species involved in Equations S6-S9.



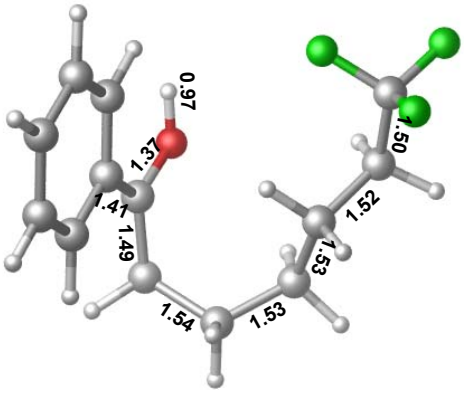
$1A_1$



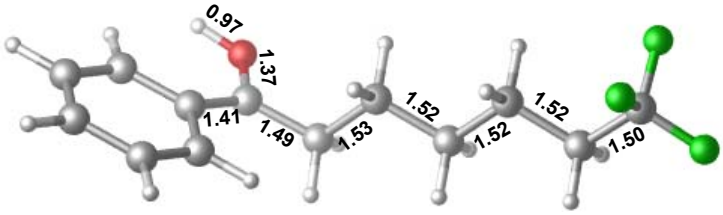
$1A_1'$



TS_{1A1}

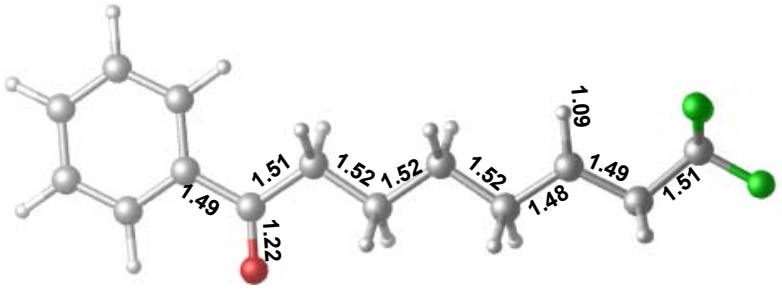


$1A_2'$

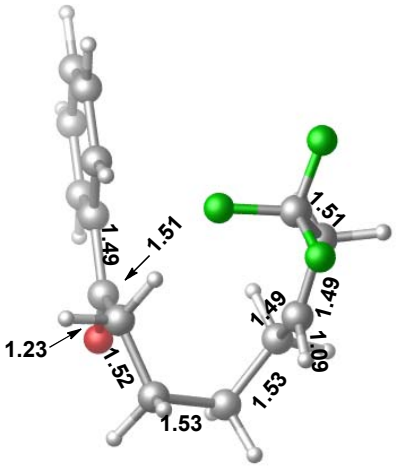


$1A_2$

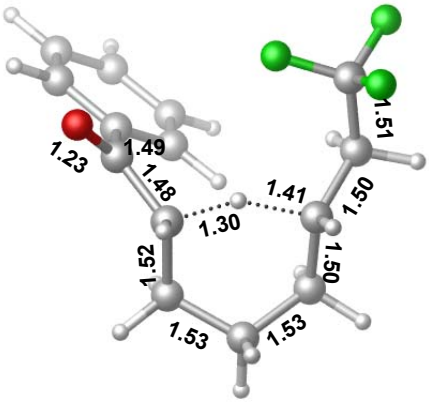
Supplementary Figure S3 continued



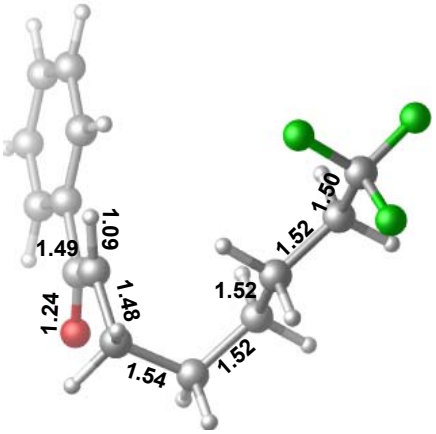
A_1



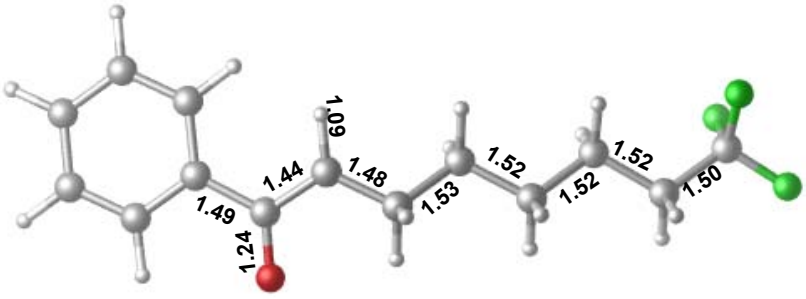
A_1'



TS_{A1}

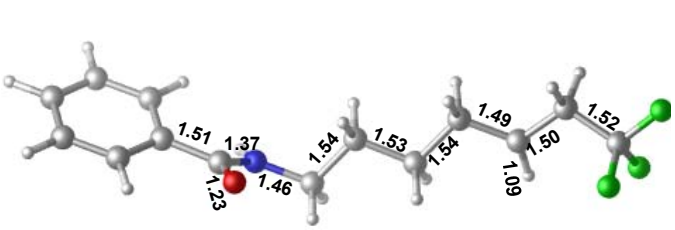


A_2'

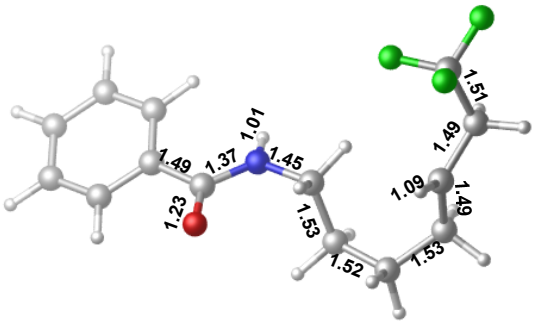


A_2

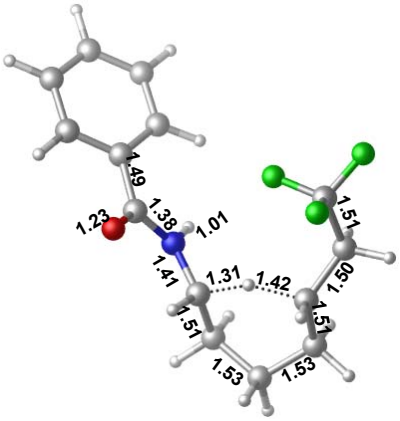
Supplementary Figure S3 continued



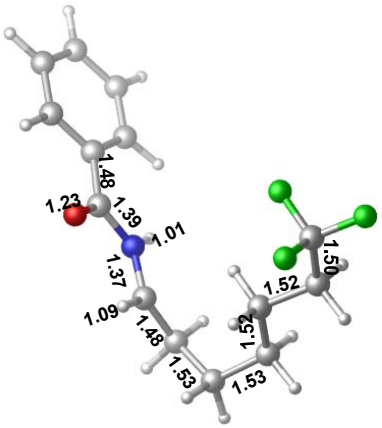
B_1



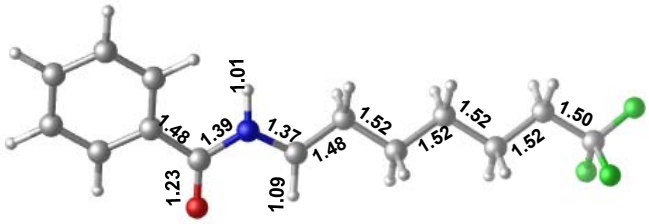
B_1'



TS_{B1}

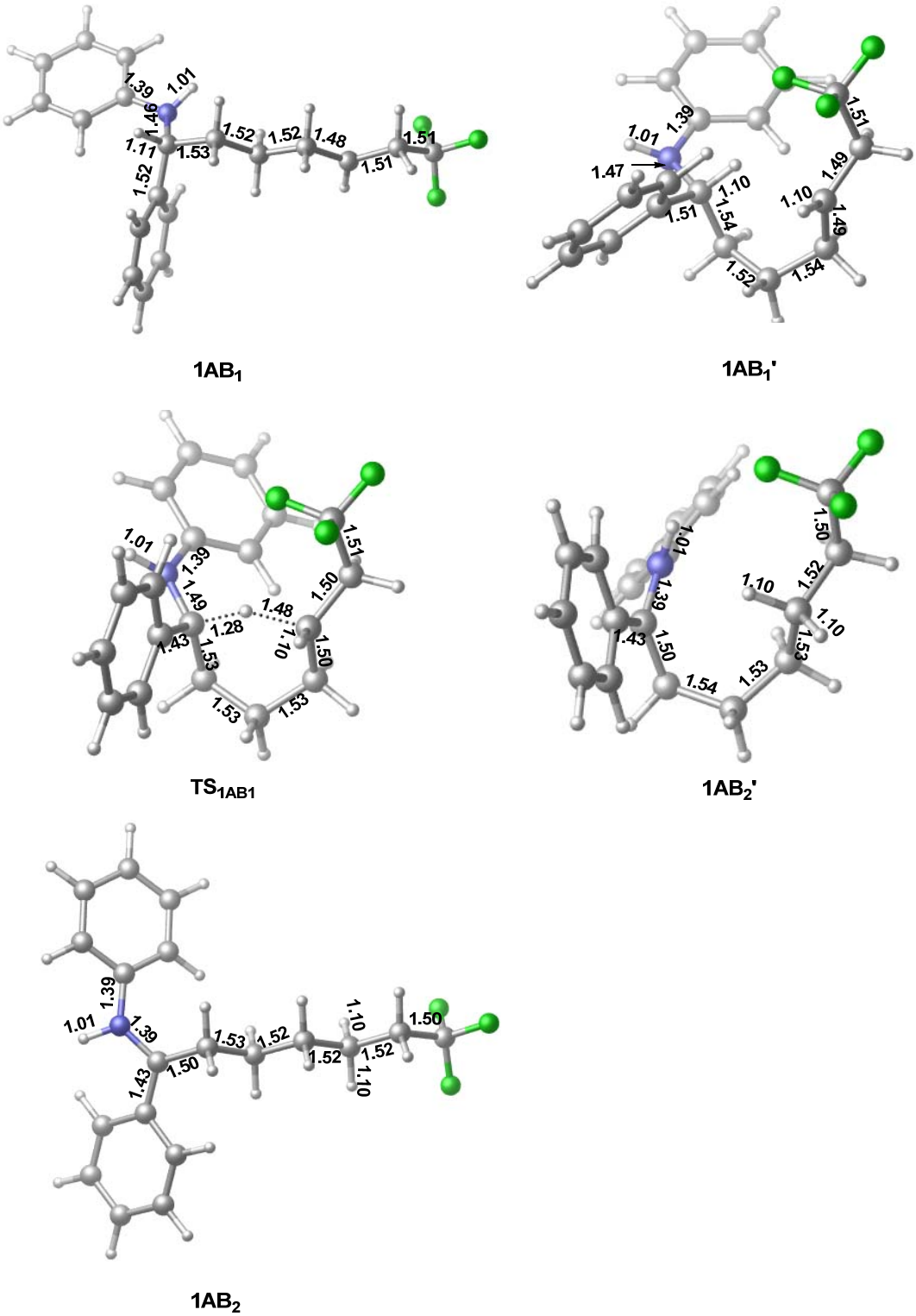


B_2'



B_2

Supplementary Figure S3 continued



Supplementary Figure S3. Optimized geometries with selected structural parameters (distances in Å) for the species involved in Figure 5 in the text.

Cartesian coordinates for all the complexes calculated in this study:

1A'

E= -880.29274429 a.u.

C	-0.20237400	0.48855500	-0.39468600
C	1.17476300	-0.01037300	0.01262400
C	2.31996100	0.76163000	-0.62759300
H	2.20752900	0.70491000	-1.72755500
C	-1.32625200	-0.30766200	0.25040200
H	-1.21612900	-1.37440000	-0.00540300
H	-1.22888800	-0.25488300	1.34685900
C	-2.71238800	0.16788600	-0.15825600
H	-2.81319900	0.12021800	-1.25176000
C	-3.81123500	-0.66236500	0.48836600
H	-3.71081100	-1.72075500	0.21652800
H	-3.75140800	-0.60828800	1.58270200
C	-5.19897400	-0.23826500	0.09985600
F	-5.46942100	1.03544500	0.47131900
F	-5.39829500	-0.30451700	-1.23879500
F	-6.14020700	-1.02155300	0.67662000
H	1.29100000	0.04953900	1.10612200
H	1.28716600	-1.07294700	-0.25045600
H	-0.29511500	1.55106600	-0.13190300
H	-0.30005300	0.43875400	-1.49153800
C	3.66259500	0.18226400	-0.25181100
C	4.20676800	0.41985800	1.01495800
C	4.36076400	-0.63448100	-1.14380900
C	5.42150700	-0.15250400	1.38100900
H	3.66701900	1.06571400	1.70768700
C	5.57519500	-1.21259800	-0.77887200
H	3.94560800	-0.81826500	-2.13645800
C	6.10823900	-0.97281700	0.48592000
H	5.83566800	0.04070000	2.36969800
H	6.10932400	-1.84616300	-1.48569400
H	7.05893000	-1.41966300	0.77269700
O	2.17840600	2.11764700	-0.20306600
H	2.92426300	2.61900200	-0.56293200
H	-2.83826100	1.22513700	0.11497600

6Aa

E= -918.41060908 a.u.

C	-0.51534100	0.82816100	0.07344300
C	0.50213500	1.84741700	-0.41949200
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H	1.91260300	1.37488900	1.15326400
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H	-2.22074500	2.10798500	-0.25739500
H	-1.90363300	0.97593900	-1.56387200
C	2.57258600	0.38861900	-0.63593100
C	3.90091900	-0.07711700	-0.14470900
C	4.55789800	0.52649700	0.93638100
C	4.51342500	-1.15909700	-0.79222400
C	5.79668700	0.05695300	1.36239000
H	4.10470800	1.36986200	1.45492500
C	5.74928700	-1.62859100	-0.36676700
H	3.99272200	-1.61721100	-1.63097000
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H	6.21595600	-2.46999700	-0.87646600
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C	-2.94408500	0.11443900	0.12169100
H	-2.99287500	0.25575200	1.21092600
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H	-4.65302800	1.35043300	-0.40031800
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F	-5.07417300	-1.84860500	0.19132600
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F	-6.59090400	-0.40501800	-0.39300500
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H	0.20287800	2.85140600	-0.08474900
H	-0.18574400	-0.18197700	-0.21016500
H	-0.54171000	0.84450600	1.17587800
H	2.56464300	2.43594600	-0.07014500

B'

E= -973.77263938 a.u.

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H	4.00748700	-1.00427800	-0.76071400
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F	6.65098300	-0.83501100	-0.85026200
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H	1.49686500	-1.10235700	0.94055900
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N	-2.38983900	-0.17312800	0.02473600
H	-2.43671500	0.75457600	-0.37569500
C	-3.54459500	-0.89657200	0.14681100
C	-4.82271200	-0.12985000	0.05273000
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H	-5.89477100	-1.92242700	-0.40853200
C	-7.29068900	1.17519200	-0.13680400
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H	-1.04646100	-1.47470000	0.90970700

(±)-10

E= -1091.44931153 a.u.

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C	-1.80013200	-0.30494300	-0.97977800
H	-2.01010000	0.22385500	-1.92403100
H	-1.63157100	-1.35743500	-1.25908100
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H	-4.51633600	-0.16013500	-1.62843500
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F	-5.33535800	-1.46646000	1.26620500
F	-5.74747100	0.56171400	0.60425600
F	-6.59656300	-1.12634800	-0.47191300
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H	-0.32433700	-0.26520500	0.59350600
H	-0.71029400	1.31529000	-0.07800800
N	2.35328300	-0.27521500	0.50729300
H	2.70813900	0.23620100	1.30640700
H	-2.81978900	-0.76931300	0.86141000
H	0.51869500	0.75427300	-2.16940000
H	2.78818300	0.49470000	-1.40083600
C	3.00950000	-1.49056700	0.32024600
C	3.55773700	-2.14188900	1.44116400
C	3.13622700	-2.11012300	-0.93341600
C	4.20520900	-3.36139000	1.31118900
H	3.46452900	-1.67439700	2.42225400
C	3.78558400	-3.33796700	-1.04996100
H	2.73820900	-1.63506500	-1.82706200
C	4.32469400	-3.97563900	0.06264800
H	4.62214500	-3.83825000	2.19757400
H	3.87261700	-3.79511100	-2.03498900
H	4.82979000	-4.93399600	-0.03767400
C	1.97009600	2.03293300	-0.19277900
C	2.40160100	3.02555200	-1.07734700
C	1.47067000	2.42416000	1.05485100
C	2.34119800	4.37223500	-0.72857800
H	2.79614800	2.73326200	-2.05181100
C	1.41521400	3.77022200	1.41038300
H	1.10405500	1.66901700	1.75102200
C	1.84978600	4.74923200	0.51970100
H	2.68925400	5.12842400	-1.43063000
H	1.02442000	4.05463400	2.38632000
H	1.80761000	5.80088900	0.79757900

R_1

E= -456.14103951 a.u.

C	2.93459800	0.18851000	-0.00012200
C	1.54930900	-0.43349100	0.00014000
H	3.71573000	-0.57924400	-0.00173100
H	3.09100300	0.81993400	-0.88389900
H	3.09239100	0.81766700	0.88500900

C	0.45401400	0.62431400	0.00027300
H	1.42866400	-1.08128200	-0.87805500
H	1.42898000	-1.08106500	0.87855100
C	-0.93383200	0.04739800	-0.00000600
H	0.53568000	1.27248700	0.88197200
H	0.53590400	1.27298300	-0.88104400
F	-1.16195200	-0.72861200	-1.08658100
F	-1.16219700	-0.72887500	1.08630700
F	-1.88172700	1.01283400	-0.00000500

R_2

E= -455.47664523 a.u.

C	-2.95996400	0.11251600	0.07238000
C	-1.56519900	-0.36125400	-0.07993400
H	-3.63465800	-0.69521500	0.37395300
H	-3.03786700	0.91434000	0.82115800
H	-3.36613800	0.53345100	-0.86495500
C	-0.45806900	0.61410800	-0.25971900
H	-1.36961700	-1.40929700	-0.30167800
C	0.90684100	0.03426700	0.00476400
H	-0.42750600	1.02782700	-1.28367000
H	-0.57958700	1.47969100	0.40666100
F	1.04328500	-0.39647900	1.27809100
F	1.17281200	-1.02340400	-0.79832200
F	1.88098300	0.94781400	-0.21048100

$1A_1$

E= -879.62800280 a.u.

C	0.26486100	0.14662500	0.51520600
C	-1.12711300	-0.12411200	-0.03142200
C	-2.23250300	0.56131000	0.76052200
H	-2.13627500	0.25321700	1.81985500
C	1.35261900	-0.58345900	-0.26176400
H	1.11231900	-1.66635000	-0.28762900
H	1.32136500	-0.27651300	-1.32280200
C	2.71848900	-0.37152400	0.27831700
H	2.84151300	-0.01782700	1.30265100
C	3.91653300	-0.87196500	-0.44422100
H	4.15996700	-1.91849300	-0.18858800
H	3.75683700	-0.85652300	-1.53095900
C	5.15979400	-0.06638200	-0.16742100
F	5.01975000	1.22635000	-0.53297600
F	5.48758000	-0.07011100	1.14647200
F	6.22708900	-0.55466400	-0.84095700
H	-1.19997200	0.20745900	-1.07902100
H	-1.32766000	-1.20624700	-0.03580400
H	0.46098600	1.22655100	0.50529900
H	0.30683300	-0.16078400	1.57262200
C	-3.60437000	0.15887600	0.27312900
C	-4.20616600	0.80857700	-0.80835600
C	-4.27406700	-0.90793800	0.87777000
C	-5.45299000	0.39670500	-1.27401700
H	-3.68739300	1.64391200	-1.27863900
C	-5.51706700	-1.32663400	0.40997800
H	-3.81220000	-1.41530400	1.72700600
C	-6.11108400	-0.67269500	-0.66787800
H	-5.91369200	0.91356900	-2.11493000
H	-6.02754200	-2.15857600	0.89304300
H	-7.08582300	-0.99269100	-1.03278300
O	-2.00020400	1.96339500	0.64975500
H	-2.69902100	2.41896100	1.14075500

$1A_1'$

E= -879.62989114 a.u.

C	0.31031800	2.81088500	-0.42920800
C	-0.92733400	2.05491300	0.04572100
C	-0.87238800	0.53152100	-0.05399800
H	-0.36016300	0.25599600	-0.99659700
C	1.63123300	2.43193200	0.24979500
H	2.32905000	3.28366900	0.14124300
H	1.47276100	2.31449200	1.33219300
C	2.25682800	1.20151900	-0.30100800
H	2.36331100	1.10825300	-1.38365400
C	3.00655800	0.25887200	0.56726400
H	4.02080700	0.61810900	0.81770000
H	2.48125300	0.12513500	1.52242300
C	3.18563400	-1.10193000	-0.04871000
F	2.00026000	-1.68263800	-0.37196900
F	3.91173300	-1.05510900	-1.18919500
F	3.81832100	-1.95301800	0.78989600
H	-1.14690700	2.30121500	1.09607300
H	-1.79022600	2.40615700	-0.53591300
H	0.42187600	2.67830400	-1.51721700
H	0.12400300	3.88334300	-0.27904200
C	-2.25669700	-0.07623000	-0.05877100
C	-2.93231100	-0.32064800	1.14034200
C	-2.89919700	-0.36254400	-1.26596200
C	-4.22365000	-0.84171800	1.13043900
H	-2.42785600	-0.10649000	2.08212400
C	-4.19175900	-0.88072500	-1.27916600
H	-2.37540700	-0.18192900	-2.20671600
C	-4.85798600	-1.12224300	-0.07886000
H	-4.73802400	-1.03035300	2.07203100
H	-4.67721800	-1.10468600	-2.22819300
H	-5.86699100	-1.53168700	-0.08593500
O	-0.10146200	0.07201200	1.05788000
H	0.03309600	-0.88036000	0.94058400

$1A_2'$

E= -879.65893383 a.u.

C	-0.40501200	2.78658400	-0.75920500
C	-1.29176900	2.50567400	0.46874700
C	-1.25335600	1.10362300	0.96638000
H	0.59047100	0.33615900	-0.40785600
C	1.06786900	2.44153800	-0.53958900
H	1.70108900	3.07000200	-1.18239300
H	1.34182900	2.70023000	0.49515500
C	1.39441200	0.97225300	-0.79642300
H	1.42531200	0.77884000	-1.87767300
C	2.70793600	0.54886400	-0.15424500
H	3.57443500	0.97770600	-0.67277900
H	2.75247600	0.89535200	0.88641700
C	2.88548500	-0.94177300	-0.11630700
F	1.91416900	-1.54099700	0.62190200
F	2.84004100	-1.50420300	-1.34556400
F	4.06779900	-1.29808600	0.43776700
H	-0.96718600	3.15864200	1.29069400
H	-2.32578300	2.79204400	0.23447900
H	-0.79016700	2.23059400	-1.62794500
H	-0.50991300	3.85189300	-1.00639400
C	-1.99587100	0.01968400	0.44175200
C	-1.82116500	-1.32098400	0.89065800
C	-2.95368600	0.22692000	-0.59318300
C	-2.55600600	-2.36342000	0.35181400
H	-1.09249000	-1.56378700	1.66637100
C	-3.68171800	-0.82371800	-1.12055300
H	-3.11535400	1.23218200	-0.97903700
C	-3.49623600	-2.13163300	-0.65633400
H	-2.39096700	-3.37525000	0.71959700
H	-4.40631600	-0.62606300	-1.90947700
H	-4.06879100	-2.95534600	-1.07763700
O	-0.30579800	0.93078600	1.93925000
H	-0.27564000	-0.00159200	2.20646500

$1A_2$

E= -879.65883492 a.u.

C	-0.07605200	0.80844600	-0.00363900
C	-1.22542000	1.32656000	-0.87630400
C	-2.53797200	1.33989100	-0.17850900
H	2.51952900	0.87104600	0.98856100
C	1.24809800	0.75020100	-0.74859600
H	1.13641800	0.11298000	-1.64119800
H	1.50328700	1.75256200	-1.12874400
C	2.38669200	0.22263400	0.11144100
H	2.12205000	-0.77007600	0.50195100
C	3.69694500	0.13052000	-0.65672000
H	3.59290200	-0.52583800	-1.52978400
H	4.00360600	1.11497700	-1.03213800
C	4.83381400	-0.40613100	0.16699800
F	5.09099400	0.36775200	1.24834200
F	4.58129800	-1.65286900	0.63175200
F	5.98050300	-0.47878500	-0.54641300
H	-0.99820500	2.35035200	-1.20416600
H	-1.28943800	0.71622400	-1.78863900
H	0.01773800	1.45077600	0.88431800
H	-0.33127700	-0.19375200	0.37452900
C	-3.41403300	0.23782400	-0.05924200
C	-4.67602700	0.32243700	0.59764900
C	-3.05903800	-1.03320200	-0.59963500
C	-5.50996000	-0.77787400	0.70156300
H	-5.02692600	1.26909900	1.01318000
C	-3.90083900	-2.12360900	-0.48616600
H	-2.10105600	-1.15071300	-1.10444600
C	-5.13616100	-2.01399300	0.16531900
H	-6.47050800	-0.67174400	1.20423800
H	-3.59291600	-3.07978100	-0.90754300
H	-5.79481100	-2.87556000	0.25175900
O	-2.79347200	2.54120300	0.41921800
H	-3.59806900	2.47270300	0.95627900

TS_{1A1}

E= -879.61039343 a.u.

C	0.25677500	3.04136000	-0.54400500
C	-0.65312300	2.51532000	0.57221000
C	-0.57067700	1.00337100	0.76997800
H	0.39352100	0.71309000	0.00916000
C	1.66654700	2.45105400	-0.46089000
H	2.33371500	2.97450400	-1.16671400
H	2.07982000	2.63629700	0.54388600
C	1.63045900	0.97293600	-0.72753600
H	1.33411300	0.69925200	-1.74628500
C	2.69810200	0.10672800	-0.13287300

H	3.66563300	0.20748800	-0.65351800
H	2.88199300	0.37911700	0.91524700
C	2.34712600	-1.35784200	-0.15595000
F	1.22386100	-1.62136000	0.56595400
F	2.11403300	-1.81131400	-1.40654500
F	3.33084900	-2.12279900	0.36759800
H	-0.35420100	2.97258600	1.52414500
H	-1.69074000	2.82343400	0.38474600
H	-0.17021700	2.79491900	-1.52924500
H	0.29445300	4.13675300	-0.49413300
C	-1.71029900	0.17039000	0.31914300
C	-2.16588900	-0.93280800	1.05523600
C	-2.31169200	0.42688600	-0.92576100
C	-3.18272100	-1.74808900	0.56782900
H	-1.74583000	-1.14543400	2.03789300
C	-3.32608800	-0.38849500	-1.41254300
H	-1.97243500	1.27642400	-1.52115200
C	-3.76647900	-1.48470200	-0.66929700
H	-3.52374300	-2.59415000	1.16284400
H	-3.77695700	-0.16831800	-2.37942400
H	-4.55895300	-2.12535400	-1.05216800
O	-0.09235000	0.74629300	2.06753700
H	0.05768500	-0.20834400	2.14810900

A_1

E= -917.74568063 a.u.

C	0.83696700	0.02733200	0.12273900
C	-0.42684200	-0.81400700	0.05076800
C	-1.69366800	0.02019300	0.03948500
H	-1.73781300	0.66889400	0.92941200
H	-1.69130300	0.71838700	-0.81328000
C	2.10538500	-0.81654300	0.13948600
H	2.04433500	-1.53460100	0.98227300
H	2.13257800	-1.45973500	-0.75834400
C	-2.95836400	-0.81138400	-0.01747000
C	-4.27367600	-0.10988700	-0.02403700
C	-4.38617700	1.28626700	0.01504300
C	-5.44023800	-0.88546700	-0.06813600
C	-5.63879900	1.89311800	0.01028400
H	-3.49268900	1.90790100	0.04858700
C	-6.69008600	-0.28071000	-0.07260100
H	-5.33350500	-1.96806100	-0.09771200
C	-6.79155600	1.11071400	-0.03282400
H	-5.71650300	2.97856600	0.04065300
H	-7.59039600	-0.89190200	-0.10587200
H	-7.77135800	1.58626500	-0.03599700
O	-2.90181900	-2.03349700	-0.05566000
C	3.35657600	-0.02397000	0.22855600
H	3.32031100	0.99574600	0.61294400
C	4.67934100	-0.68421900	0.08004200
H	4.92573700	-1.32576800	0.94461300
H	4.69567200	-1.35103900	-0.79467800
C	5.82234100	0.28341200	-0.07240500
F	5.68247500	1.07531300	-1.15897100
F	5.93612700	1.10509900	0.99764400
F	7.00393000	-0.36320000	-0.19949200
H	-0.40592700	-1.45113400	-0.84449500
H	-0.46372900	-1.51357100	0.89773600
H	0.87576300	0.72264900	-0.73036500
H	0.81337000	0.66137200	1.02360400

A_1'

E= -917.74844454 a.u.

C	-0.67085200	2.98350400	-0.47955200
C	-0.38352800	2.64920300	0.98701800
C	0.39264100	1.35579500	1.19202300
H	0.58755600	1.19498900	2.26439100
H	-0.22685300	0.50020100	0.89216500
C	-1.07654200	1.78072400	-1.33253000
H	-1.30051400	2.13921800	-2.35501500
H	-0.21215200	1.10668900	-1.46536700
C	1.72336800	1.31286800	0.47579900
C	2.36183600	-0.01185300	0.21891000
C	1.79972500	-1.22542600	0.64143100
C	3.58191300	-0.03315400	-0.47215900
C	2.44711900	-2.43030000	0.38091400
H	0.85656200	-1.23838100	1.18588100
C	4.22383800	-1.23520100	-0.73720200
H	4.00438400	0.91755700	-0.79197000
C	3.65759700	-2.43750800	-0.30957400
H	2.00501400	-3.36617800	0.71850900
H	5.16877300	-1.24016700	-1.27843100
H	4.16079800	-3.38127800	-0.51508800
O	2.27420300	2.34746300	0.11650900
C	-2.21822100	1.00229000	-0.78709300
H	-3.03393500	1.52965300	-0.28932000
C	-2.41993800	-0.43122300	-1.12639100
H	-3.10748200	-0.57320800	-1.97813800
H	-1.47087400	-0.90391500	-1.41531000
C	-2.98930900	-1.24169500	0.01128500
F	-2.15227100	-1.27918600	1.07751000
F	-4.16512600	-0.74426300	0.45458600
F	-3.21452500	-2.52300000	-0.35552300
H	0.16155100	3.48660100	1.43967000
H	-1.32895100	2.55437900	1.54001500
H	-1.46542300	3.74238500	-0.51986800
H	0.21733700	3.44165500	-0.93062800

A_2'

E= -917.76088509 a.u.

C	-0.53536700	2.74492600	-0.33291500
C	0.10383200	2.45005500	1.03967600
C	0.97497200	1.24768300	1.03274900
H	0.68722400	0.37865900	1.62563800
H	-1.86950300	0.57324500	0.82496200
C	-1.19087400	1.53590400	-0.98807400
H	-1.61159200	1.83816800	-1.95843500
H	-0.41708000	0.78537000	-1.22100700
C	2.18541700	1.20730400	0.24471100
C	2.95551600	-0.06518400	0.13210000
C	2.45327400	-1.30637300	0.54812800
C	4.23134600	-0.01287200	-0.44579900
C	3.21090900	-2.46406100	0.39699800
H	1.45539500	-1.38222700	0.97798000
C	4.99056200	-1.16662800	-0.59081500
H	4.60327000	0.95514600	-0.77548200
C	4.48285600	-2.39627400	-0.16808600
H	2.80631500	-3.42173700	0.72013800
H	5.98323100	-1.11093100	-1.03487800
H	5.07742000	-3.30146400	-0.28195700
O	2.58197400	2.23566700	-0.33288400
C	-2.27889000	0.88028000	-0.14835900
H	-3.07452600	1.60774600	0.06921000
C	-2.86682700	-0.33875800	-0.84261700
H	-3.29502700	-0.06989500	-1.81646400
H	-2.08682700	-1.08674600	-1.03426100
C	-3.94992700	-1.01942000	-0.05463100
F	-3.52503900	-1.40076600	1.17500200
F	-5.02493800	-0.21853600	0.13706800
F	-4.39586400	-2.13378800	-0.67822700
H	0.70455500	3.32822600	1.31827900
H	-0.67471800	2.33644700	1.80434100
H	-1.27548600	3.54731300	-0.20015100
H	0.24332700	3.13566000	-0.99782600

A_2

E= -917.76064075 a.u.

C	-0.70661900	0.01753200	-0.32643200
C	0.47568700	-0.87890000	-0.69122200
C	1.78361100	-0.19411600	-0.60810900
H	1.86099100	0.81718400	-1.01206300
H	-3.06527200	0.69006600	0.89773700
C	-2.03385000	-0.72440900	-0.36315300
H	-2.16804200	-1.19069100	-1.35242000
H	-2.00222700	-1.55815500	0.35615800
C	2.94857800	-0.84763700	-0.06035500
C	4.24404700	-0.11255000	0.02849200
C	4.36496200	1.26803600	-0.18207900
C	5.39119300	-0.84702100	0.35880600
C	5.60166000	1.89648900	-0.06675600
H	3.48979800	1.86924500	-0.42234400
C	6.62681300	-0.22209800	0.46603300
H	5.28105200	-1.91631400	0.52771200
C	6.73579200	1.15290100	0.25344000
H	5.67952300	2.97093600	-0.22489900
H	7.51034500	-0.80606500	0.71854500
H	7.70354400	1.64446300	0.34081100
O	2.87450800	-2.03158000	0.31674700
C	-3.22468000	0.17134200	-0.05796400
H	-3.30240000	0.95699700	-0.82305200
C	-4.52906500	-0.60987800	0.00633700
H	-4.68907800	-1.18454600	-0.91476100
H	-4.51236700	-1.33051900	0.83324100
C	-5.73852200	0.26225400	0.19519300
F	-5.64360900	1.03835500	1.30127800
F	-5.92799100	1.09969300	-0.85240600
F	-6.86832500	-0.47047100	0.32237700
H	0.50793200	-1.77669600	-0.05952500
H	0.32757800	-1.25142600	-1.72166900
H	-0.55101800	0.43815700	0.67862500
H	-0.74473200	0.88014600	-1.01069500

TS_{A1}

E= -917.72446483 a.u.

C	-1.12498300	3.15617300	-0.70471800
C	0.18905500	2.79048500	-0.01165700
C	-0.00875200	1.68010500	1.00286500
H	-0.54963700	2.02020100	1.89364000
H	-0.92930800	0.97040800	0.41584300
C	-1.74585400	1.94518900	-1.40336200
H	-2.65585700	2.25193700	-1.94593500
H	-1.05117100	1.57213300	-2.17446300
C	1.09663600	0.78859100	1.41950500

C	1.93168300	0.09315600	0.39725400
C	1.53935900	-0.04949900	-0.93986800
C	3.13333500	-0.49628800	0.81157800
C	2.32478200	-0.76145200	-1.84141800
H	0.59977100	0.38522400	-1.27898500
C	3.92700100	-1.19518000	-0.08945300
H	3.41759000	-0.39787500	1.85750900
C	3.52469900	-1.33089500	-1.41866600
H	2.00054800	-0.87324500	-2.87531700
H	4.86159000	-1.64294700	0.24472900
H	4.14334100	-1.88423400	-2.12367200
O	1.30250100	0.58994600	2.61923600
C	-2.05661400	0.84604800	-0.42512800
H	-2.84385400	1.10233100	0.29307200
C	-2.15168500	-0.55691300	-0.94792700
H	-3.03644300	-0.68562300	-1.59271000
H	-1.27977200	-0.81328500	-1.56443400
C	-2.25183700	-1.59272700	0.14238900
F	-1.17854000	-1.57337600	0.96060200
F	-3.34414600	-1.39976800	0.91956000
F	-2.34362100	-2.84052300	-0.36848300
H	0.93818000	2.50729500	-0.76373400
H	0.59396800	3.67858100	0.49581200
H	-1.83632400	3.54789000	0.03905600
H	-0.95682600	3.96388700	-1.42776700

B_1

E= -973.25499613 a.u.

C	-1.39296600	0.39096000	0.77331100
C	0.04857900	0.59076300	0.28969200
C	1.07961100	0.33471800	1.39867500
H	0.91531600	1.01936300	2.23925600
C	-2.43439700	0.64013100	-0.33042600
H	-2.28236100	1.66045400	-0.73618100
H	-2.23781200	-0.03377200	-1.17988700
C	-3.84741000	0.47694600	0.12663600
H	-4.09238000	0.65166900	1.17193600
C	-4.96610400	0.39524300	-0.86345000
H	-5.24850100	1.39026000	-1.25114400
H	-4.67857400	-0.20333200	-1.73769300
C	-6.23810100	-0.21372800	-0.30665100
F	-6.06223200	-1.49095800	0.11176000
F	-6.71940700	0.48698000	0.75388700
F	-7.22302400	-0.23583400	-1.24270600
H	0.26136200	-0.09036400	-0.54384900
H	0.17542100	1.61412800	-0.09280600
H	-1.51484200	-0.63179000	1.15571800
H	-1.59748200	1.06562500	1.61825500
N	2.45929300	0.50540300	0.95214900
H	2.92855900	1.37594700	1.15513300
C	3.17453800	-0.51738100	0.39304400
C	4.58818700	-0.20425300	-0.02059600
C	5.02852200	1.08629700	-0.35286400
C	5.49194200	-1.27411800	-0.09715600
C	6.35334400	1.30462100	-0.73869800
H	4.33729600	1.92577200	-0.34976600
C	6.81687300	-1.05454000	-0.47343300
H	5.13446700	-2.27137900	0.13937600
C	7.25185600	0.23584300	-0.79325200
H	6.67956600	2.30677000	-1.00485400
H	7.51023200	-1.89032400	-0.52102900
H	8.28316800	0.40624700	-1.09159500
O	2.69382800	-1.64187600	0.24444700
H	0.97602100	-0.68880200	1.77305600

B_1'

E= -973.10963235 a.u.

C	-1.68452900	2.87855800	-0.25472500
C	-0.38047600	2.17935900	-0.62256600
C	-0.26091900	0.74937300	-0.10492400
H	-0.99627600	0.08685900	-0.57676600
C	-2.95190500	2.19652900	-0.78202000
H	-3.76733500	2.94449300	-0.80613000
H	-2.80605200	1.90487000	-1.83628900
C	-3.37823100	1.01669900	0.01486700
H	-3.32007800	1.07739300	1.10296300
C	-4.16521300	-0.09615200	-0.57860700
H	-5.24774200	0.11994900	-0.61458400
H	-3.86165700	-0.28740200	-1.61737300
C	-4.01379500	-1.39014000	0.18083100
F	-2.72951200	-1.81516700	0.20283700
F	-4.40904100	-1.26839200	1.46803900
F	-4.74955200	-2.38460700	-0.36611600
H	-0.25956200	2.17992900	-1.71790900
H	0.46119900	2.75480400	-0.21613000
H	-1.75585700	2.96813200	0.84026900
H	-1.64510300	3.90694400	-0.63765300
N	1.05389500	0.17383100	-0.32275800
H	1.23984500	-0.26776900	-1.21186200
C	2.10055800	0.47749200	0.50140900
O	1.95974700	1.20484800	1.48362400
C	3.42108000	-0.13154400	0.15537300
C	4.55891500	0.43105700	0.74307700
C	3.57131600	-1.23095900	-0.69834800
C	5.82226200	-0.07941300	0.46790800
H	4.42116500	1.27088500	1.42126200
C	4.83571700	-1.74721500	-0.96873800
H	2.69986400	-1.72083300	-1.13297900
C	5.96422600	-1.16895600	-0.39091000
H	6.70083400	0.37056100	0.92763600
H	4.93838800	-2.60965100	-1.62544300
H	6.95275000	-1.57354800	-0.60285700
H	-0.45071900	0.72414500	0.97556000

B_2'

E= -973.12085238 a.u.

C	-2.16944000	3.13755100	-0.08482700
C	-0.65305900	3.08818400	-0.29549000
C	0.04052000	2.07742700	0.53644000
H	-1.66490300	0.33217200	-0.12758700
C	-2.94735800	1.98182800	-0.70673700
H	-4.02111900	2.21993900	-0.66186900
H	-2.70394100	1.91929600	-1.78042100
C	-2.72144000	0.62272600	-0.05662700
H	-2.94405500	0.68602600	1.01839100
C	-3.58658800	-0.45528700	-0.69402500
H	-4.65066300	-0.19190300	-0.63820400
H	-3.34270200	-0.57489300	-1.75741100
C	-3.42961500	-1.80258100	-0.04616000
F	-2.15062700	-2.24107600	-0.08281200
F	-3.80107300	-1.78520800	1.25504500
F	-4.18728100	-2.74430500	-0.65759000
H	-0.44242400	2.90594100	-1.36391000
H	-0.24528500	4.09688600	-0.09254900
H	-2.38116200	3.18792400	0.99446800
H	-2.54447500	4.07922400	-0.50758000
N	1.16529200	1.44389300	0.08721900
H	1.46802600	1.63519100	-0.86014900
C	1.91967900	0.57501300	0.86538200
O	1.61256000	0.37051200	2.04009300
C	3.08777300	-0.05667200	0.20830800
C	3.97807200	-0.75372000	1.03856500
C	3.34891400	-0.01715400	-1.17023500
C	5.10093500	-1.37719400	0.50998500
H	3.75768900	-0.78837800	2.10331100
C	4.47269500	-0.64281700	-1.69855300
H	2.66729000	0.48034900	-1.86124700
C	5.35531800	-1.32296000	-0.86031900
H	5.78247100	-1.91185200	1.16979200
H	4.65514500	-0.60705200	-2.77141200
H	6.23413300	-1.81316600	-1.27606400
H	-0.20916100	1.88219400	1.57514700

B_2

E= -973.12218400 a.u.

C	-1.37353200	-0.37484900	-0.09510400
C	-0.04477000	0.24093700	0.32651400
C	1.11725400	-0.61339000	-0.01026600
H	1.05790400	-1.68983800	-0.13812200
C	-2.56853700	0.48859900	0.27556000
H	-2.55089000	0.69330200	1.35834600
H	-2.47671600	1.47196100	-0.21390200
C	-3.90195600	-0.14240700	-0.09623000
H	-4.01047900	-1.10687800	0.41991800
C	-5.07565200	0.75952000	0.25475300
H	-5.06041800	1.02604900	1.31908800
H	-5.02967800	1.69928700	-0.30954200
C	-6.41658200	0.13999200	-0.02209600
F	-6.55678100	-0.22096600	-1.31991100
F	-6.62486700	-0.97489500	0.71767900
F	-7.42659100	0.99402100	0.26127000
H	0.06245600	1.23587800	-0.14299000
H	-1.36511100	-0.55458300	-1.18047300
H	-1.47626700	-1.36626500	0.37220000
N	2.38717200	-0.10791400	0.02709000
H	2.49682500	0.88464300	0.19690800
C	3.53042600	-0.88720100	-0.09495600
C	4.82215800	-0.16252100	-0.06055100
C	4.95977600	1.22072000	-0.25236000
C	5.97565300	-0.92811100	0.16334100
C	6.21289000	1.82237000	-0.20137700
H	4.09514700	1.84463700	-0.48122300
C	7.22597100	-0.32528900	0.21874500
H	5.85745100	-2.00201300	0.29115100
C	7.35002500	1.05264000	0.04051400
H	6.30300000	2.89575000	-0.36026000
H	8.11097000	-0.93263100	0.40172700
H	8.33007700	1.52505000	0.08218400
O	3.44287800	-2.10972800	-0.20731100
H	-3.92135200	-0.36743600	-1.17183900
H	-0.08075700	0.44680900	1.41543800

TS_{B1}

E= -973.08652857 a.u.

C	3.12965700	-2.65258400	-0.40956000
C	1.61778000	-2.74157200	-0.61163700
C	0.90207900	-1.75439600	0.27929700
H	1.74911900	-0.75587400	0.24997500
C	3.66137500	-1.26327400	-0.77562100
H	4.76037200	-1.25061800	-0.68539200
H	3.44736600	-1.07490800	-1.84082200
C	3.02934300	-0.18049000	0.06238400
H	3.38396400	-0.15708700	1.09874100
C	2.90703700	1.18067100	-0.55998700
H	3.88100100	1.69389500	-0.62694400
H	2.52754900	1.11057900	-1.58863800
C	1.98132900	2.10509000	0.18802300
F	0.69665400	1.67656500	0.15206300
F	2.32308200	2.22223700	1.48922000
F	1.99037500	3.35334700	-0.33799800
H	1.38572600	-2.52390200	-1.66815600
H	1.25989300	-3.76597500	-0.42722100
H	3.37233400	-2.87489300	0.64126900
H	3.63542800	-3.41799400	-1.01099600
N	-0.38875700	-1.36031500	-0.12650700
H	-0.55395700	-1.21327800	-1.11416000
C	-1.37013000	-0.98533200	0.76501200
O	-1.24403900	-1.16193100	1.97460200
C	-2.59578700	-0.39178500	0.16573000
C	-3.79100500	-0.50913100	0.88541000
C	-2.60109800	0.29881900	-1.05294300
C	-4.97225700	0.02038200	0.38054700
H	-3.76549900	-1.02359000	1.84410700
C	-3.78291700	0.83847200	-1.55299100
H	-1.67048000	0.46480000	-1.59747900
C	-4.97268600	0.69219500	-0.84215200
H	-5.89809800	-0.08563200	0.94389200
H	-3.77192700	1.38730800	-2.49339900
H	-5.89739100	1.11156200	-1.23521700
H	0.88089700	-2.01846300	1.34054800

1AB$_1$

E= -1090.78680793 a.u.

C	-0.97102000	0.13533800	0.64546900
C	0.16207300	0.12171500	1.66106900
C	1.57317800	0.18255500	1.06268600
C	-2.34070400	0.03586900	1.30672900
H	-2.39085100	-0.87646000	1.92779700
H	-2.44537300	0.86592600	2.03511900
C	-3.46849900	0.04528100	0.34262900
C	-4.84291100	-0.31930000	0.77305300
H	-4.83268600	-1.19815900	1.43346800
H	-5.32978500	0.48427400	1.35382000
C	-5.76505600	-0.63085500	-0.37638100
F	-5.90691700	0.42767300	-1.20786100
F	-5.31757800	-1.66196300	-1.12684600
F	-7.00300000	-0.96140300	0.05668600
H	0.04766100	0.97607500	2.34421800
H	-0.91763300	1.05733800	0.04791400
H	-0.85708300	-0.68962100	-0.07437000
N	1.80566400	-1.00375000	0.25265200
H	1.14432700	-1.74889600	0.43344000
H	0.09032900	-0.77983300	2.29159600
H	2.28338500	0.19047000	1.91279300
C	3.09857600	-1.47399000	0.02934700
C	3.28562500	-2.80952700	-0.36855300
C	4.22782000	-0.65126400	0.16437600
C	4.55774600	-3.30403800	-0.61912800
H	2.41564000	-3.45909000	-0.47711500
C	5.49906100	-1.16034600	-0.09248200
H	4.11552700	0.39060200	0.45837400
C	5.67926100	-2.48412900	-0.48345900
H	4.67393900	-4.34441800	-0.92078600
H	6.36065300	-0.50282900	0.01775400
H	6.67626500	-2.87380100	-0.67845200
H	-3.33610300	0.52676600	-0.62673500
C	1.78163000	1.47161300	0.28905300
C	2.07195900	2.64409100	0.99263800
C	1.64990000	1.53446800	-1.09934100
C	2.21738600	3.85849500	0.32772600
H	2.19290300	2.59982400	2.07731300
C	1.79580400	2.74820000	-1.76846300
H	1.44225600	0.61703100	-1.64934200
C	2.07735100	3.91380000	-1.05836600
H	2.44855300	4.76174500	0.89068800
H	1.69504500	2.78201900	-2.85247100
H	2.19576000	4.86066000	-1.58300200

1AB$_1$'

E= -1090.78984173 a.u.

C	-1.19109700	0.14719500	2.73092400
C	-0.61196000	-1.07967000	2.03607500
C	-0.56090600	-0.99395500	0.50388900
H	-0.09429600	-0.03718100	0.21775200
C	-0.31016600	1.40103800	2.63852700
H	-0.60064600	2.08775000	3.45635800
H	0.73716100	1.13025900	2.85493100
C	-0.39167600	2.11710800	1.33815900
H	-1.38341000	2.31625900	0.92760500
C	0.75815700	2.87182000	0.77293200
H	0.82987500	3.89790000	1.17607000
H	1.71299100	2.38415700	1.01485500
C	0.69906100	3.01231400	-0.72796600
F	0.74614400	1.81673400	-1.35794400
F	-0.44387400	3.61937100	-1.13318400
F	1.72729500	3.74938200	-1.19951700
H	0.40402500	-1.26790200	2.41284200
H	-1.19564500	-1.97036600	2.30925300
H	-2.19045500	0.37340600	2.32613900
H	-1.34328100	-0.09558100	3.79091900
N	0.25130100	-2.09065100	-0.03196100
H	-0.17656700	-2.56668900	-0.81680800
C	1.62987100	-1.94927200	-0.15885700
C	2.34760200	-2.86751400	-0.94736500
C	2.35053000	-0.93572600	0.49624200
C	3.72615300	-2.77440700	-1.07223400
H	1.80446400	-3.66062800	-1.46249300
C	3.73490000	-0.85497900	0.36543500
H	1.83100600	-0.20272000	1.11073900
C	4.43724200	-1.76798500	-0.41509200
H	4.25292100	-3.49832500	-1.69299700
H	4.26761400	-0.05765800	0.88350400
H	5.51833300	-1.69763800	-0.51372800
C	-1.93620700	-1.02327000	-0.11773300
C	-2.80298400	-2.09933200	0.10841000
C	-2.36513600	0.02133400	-0.94135600
C	-4.06825500	-2.12726500	-0.47252000
H	-2.47995400	-2.92452100	0.74454700
C	-3.63376000	0.00006000	-1.51800100
H	-1.69078700	0.85590400	-1.13647200
C	-4.48909500	-1.07417300	-1.28391000
H	-4.73042300	-2.97203800	-0.28783500
H	-3.95128000	0.82424600	-2.15503100
H	-5.48048200	-1.09337800	-1.73397600

1AB$_2$'

E= -1090.82091511 a.u.

C	0.39828900	0.82549600	2.68949800
C	0.07591900	1.90219200	1.63369700
C	0.41246600	1.50882900	0.22540900
H	0.87749000	-0.91901400	0.70866400
C	-0.33023700	-0.49776300	2.44937900
H	-0.54340000	-0.99114600	3.40895900
H	-1.31476100	-0.28827100	1.99938500
C	0.44064800	-1.46365000	1.55382100
H	1.29711700	-1.88003600	2.10164000
C	-0.43582700	-2.59260400	1.02566900
H	-0.61533300	-3.36219000	1.78619200
H	-1.41989300	-2.20684700	0.72675800
C	0.14590300	-3.26589700	-0.18378900
F	0.22257400	-2.40711600	-1.24165900
F	1.39735700	-3.72688200	0.02531400
F	-0.60178300	-4.31425700	-0.59536500
H	-0.99459600	2.12289900	1.71719200
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H	0.11810700	1.23540000	3.66978400
N	-0.55341300	0.86193500	-0.53785200
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C	-4.14899700	0.20496700	-1.00438500
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H	-4.30401600	3.44959700	-0.01806500
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C	2.08132700	1.08861600	-1.57997400
C	4.14789900	1.86682200	0.11356400
H	2.64508400	2.24239400	1.58447100
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H	1.28685200	0.83128100	-2.27949700
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$1AB_2$

E= -1090.82046824 a.u.

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C	4.32122900	0.25774500	0.70832600
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H	4.48262200	-0.37696500	1.58863700
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F	5.45265300	0.90560300	-1.27134800
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H	-1.26925800	1.80222700	1.16879400
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F	0.92763700	1.52179100	-1.24859900
F	-0.37527900	3.21383600	-0.85102000
F	1.78293000	3.48081800	-0.85473200
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H	-1.35024900	-2.39908700	2.03069200
H	-2.13395200	-0.12703300	2.73894100
H	-1.04697800	-0.82604100	3.93118500
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H	-0.18253700	-1.98685600	-1.29426700
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C	2.29030200	-0.92293200	0.62640900
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C	3.68015400	-0.85837200	0.59637100
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C	4.40607300	-1.46364900	-0.42613800
H	4.25648600	-2.61910300	-2.24385800
H	4.19965200	-0.32000900	1.38893200
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C	-4.47279000	-1.01321100	-0.18707500
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C	-3.32980100	-0.09969100	-2.09656600
H	-1.18833900	0.01200600	-1.94928700
C	-4.52012600	-0.45590500	-1.46234700
H	-5.39462300	-1.29739500	0.31895400
H	-3.35174600	0.35052800	-3.08799600
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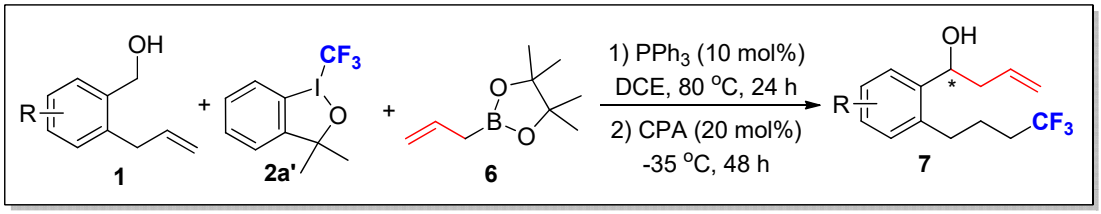
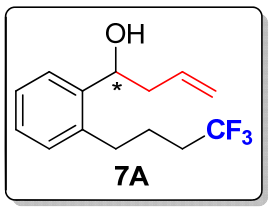
Versatile transformations

Typical procedure for synthesis of 7A-7C



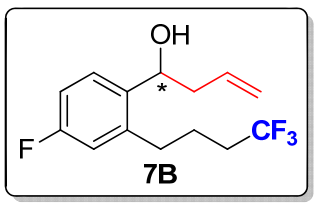
Procedure: Under argon, a 25 mL Schlenk tube equipped with a magnetic stir bar were charged with **1** (0.1 mmol, 1.0 equiv), Togni's reagent **2a'** (0.13 mmol, 1.3 equiv), triphenylphosphine (0.01 mmol, 0.1 equiv) and 1,2-dichloroethane (DCE, super dry, 1.0 mL). The sealed tube was then stirred at 80 °C for 24 hours. After completion, the reaction temperature was directly decreased to -35 °C and allylboronic acid pinacol ester **6** and (*R*)-2,4,6-triisopropylphenyl-SPINOL-derived chiral phosphoric acid (20 mol%) were added to this reaction mixture, and then the reaction mixture was stirred for 48 hours. After completion (monitored by TLC), the reaction solution was concentrated *in vacuo*, and the residue was purified by silica gel column chromatography (petroleum ether/EtOAc) to give the desired products **7**.

1-(2-(4,4,4-trifluorobutyl)phenyl)but-3-en-1-ol (7A)



^{1}H NMR (400 MHz, $CDCl_3$) δ 7.51 (dd, *J* = 7.6, 1.6 Hz, 1H), 7.29 - 7.20 (m, 2H), 7.14 (dd, *J* = 7.6, 1.6 Hz, 1H), 5.78 - 5.90 (m, 1H), 5.23 - 5.12 (m, 2H), 4.94 (t, *J* = 6.4 Hz, 1H), 2.68 - 2.80 (m, 2H), 2.46 - 2.52 (m, 2H), 2.23 - 1.95 (m, 3H), 1.82 - 1.92 (m, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 141.36, 137.38, 134.51, 129.26, 127.61, 127.06 (q, *J* = 274.7 Hz), 126.86, 125.93, 118.47, 69.22, 43.35, 33.39 (q, *J* = 28.4 Hz), 31.08, 23.57 (q, *J* = 2.8 Hz). ^{19}F NMR (376 MHz, $CDCl_3$) δ -66.09 (s). HRMS (ESI) m/z calcd. for $C_{14}H_{17}F_3NaO$ $[M+Na]^+$ 281.1129, found 281.1124. 89% ee, HPLC analysis [Daicel Chiralpak AD-H, isopropanol/hexane = 5/95, 0.5 mL/min, λ = 214 nm, t_R (major) = 21.9 min, t_R (minor) = 17.2 min].

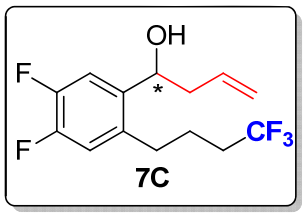
1-(4-fluoro-2-(4,4,4-trifluorobutyl)phenyl)but-3-en-1-ol (7B)



^{1}H NMR (400 MHz, $CDCl_3$) δ 7.47 (dd, *J* = 8.4, 6.0 Hz, 1H), 6.95 (td, *J* = 8.4, 2.4 Hz,

1H), 6.85 (dd, J = 10.0, 2.8 Hz, 1H), 5.75 - 5.85 (m, 1H), 5.24 - 5.12 (m, 2H), 4.90 (t, J = 6.8 Hz, 1H), 2.65 - 2.78 (m, 2H), 2.47 (t, J = 7.2 Hz, 2H), 2.22 - 1.99 (m, 3H), 1.82 - 1.91 (m, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 161.98 (d, J = 234.4 Hz), 139.89 (d, J = 7.0 Hz), 137.11 (d, J = 3.1 Hz), 134.22, 127.92 (d, J = 8.3 Hz), 126.97 (q, J = 274.8 Hz), 118.77, 115.62 (d, J = 21.0 Hz), 113.65 (d, J = 20.8 Hz), 68.80, 43.42, 33.29 (q, J = 28.5 Hz), 30.94, 23.29 (q, J = 2.8 Hz). ^{19}F NMR (376 MHz, $CDCl_3$) δ -66.08 (s, 3F), -115.12 (s, 1 F). HRMS (APCI) m/z calcd. for $C_{14}H_{15}F_4$ $[M\text{-}OH]^+$ 259.1110, found 259.1103. 90% ee, HPLC analysis [Daicel Chiralpak AD-H, isopropanol/hexane = 5/95, 0.5 mL/min, λ = 254 nm, t_R (major) = 16.6 min, t_R (minor) = 14.3 min].

1-(4,5-difluoro-2-(4,4,4-trifluorobutyl)phenyl)but-3-en-1-ol (7C)

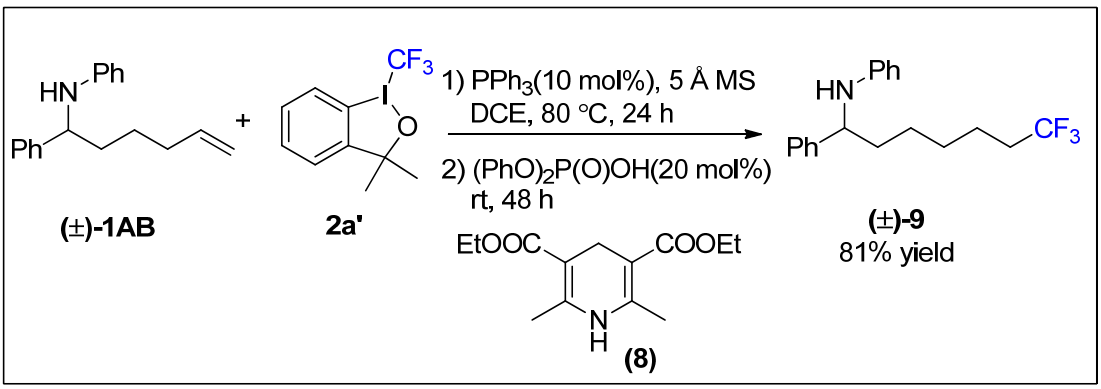


7C

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.32 (dd, J = 12.0, 8.0 Hz, 1H), 6.93 (dd, J = 11.6, 8.0 Hz, 1H), 5.74 - 5.86 (m, 1H), 5.24 - 5.12 (m, 2H), 4.91 - 4.80 (m, 1H), 2.60 - 2.74 (m, 2H), 2.35 - 2.47 (m, 2H), 2.26 - 2.02 (m, 3H), 1.89 - 1.79 (m, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 150.32 (dd, J = 17.7, 10.7 Hz), 147.88 (dd, J = 17.6, 10.7 Hz), 138.31 (t, J = 44.0 Hz), 134.00 (t, J = 49.0 Hz), 133.73, 126.92 (q, J = 274.8 Hz), 119.21, 117.54 (d, J = 16.7 Hz), 115.18 (d, J = 17.5 Hz), 68.45, 43.46, 33.22 (q, J = 28.6 Hz), 30.28, 23.36 (q, J = 2.2 Hz). ^{19}F NMR (376 MHz, $CDCl_3$) δ -66.07 (s, 3F), -139.67 (d, J = 21.8 Hz, 1F), -140.19 (d, J = 21.8 Hz, 1F). HRMS (APCI) m/z calcd. for $C_{14}H_{14}F_5$ $[M\text{-}OH]^+$ 277.1016, found 277.1008. 91% ee, HPLC analysis [Daicel Chiralpak AD-H, isopropanol/hexane = 5/95, 0.5 mL/min, λ = 214 nm, t_R (major) = 16.2 min, t_R (minor) = 12.3 min].

Typical procedure for synthesis of (±)-9

Synthesis of racemic trifluoromethyl amine (±)-9



(±)-1AB

2a'

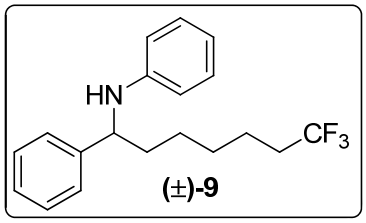
(8)

(±)-9
81% yield

Procedure: Under argon, a 25 mL Schlenk tube equipped with a magnetic stir bar

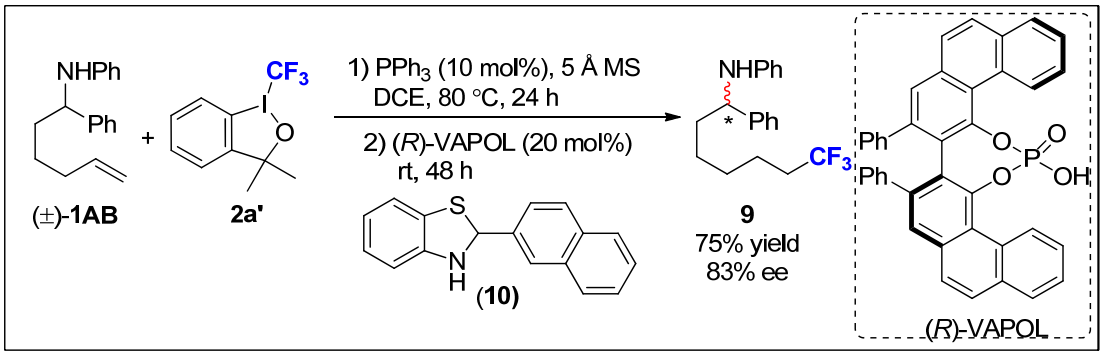
were charged with **(±)-1AB** (0.2 mmol, 1.0 equiv), Togni's reagent **2a'** (0.26 mmol, 1.3 equiv), triphenylphosphine (0.02 mmol, 0.1 equiv) 5 Å molecular sieves (200 mg) and 1, 2-dichloroethane (DCE, super dry, 2.0 mL). The sealed tube was then stirred at 80 °C for 24 hours. After completion, the reaction temperature was directly decreased to room temperature and diethyl 2,6-dimethyl-1,4-dihydropyridine-3,5-dicarboxylate (**8**, 1.5 equiv) and diphenyl hydrogen phosphate (20 mol%) were added to this reaction mixture, and then the reaction mixture was stirred for 48 hours. After completion (monitored by TLC), the reaction solution was concentrated *in vacuo*, and the residue was purified by silica gel column chromatography (petroleum ether/EtOAc) to give the desired products **(±)-9**.

N-(7,7,7-trifluoro-1-phenylheptyl)aniline ((±)-9)



^{1}H NMR (400 MHz, $CDCl_3$) δ 7.36 - 7.29 (m, 4H), 7.26 – 7.21 (m, 1H), 7.13 - 7.06 (m, 2H), 6.65 (t, *J* = 7.2 Hz, 1H), 6.55 – 6.50 (m, 2H), 4.31 (t, *J* = 6.8 Hz, 1H), 4.06 (s, 1H), 2.11 – 1.97 (m, 2H), 1.86 - 1.75 (m, 2H), 1.59 - 1.50 (m, 2H), 1.48 - 1.32 (m, 4H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 147.30, 143.94, 129.08, 128.56, 127.14 (q, *J* = 274.5 Hz), 126.96, 126.31, 117.21, 113.21, 58.05, 38.54, 33.57 (q, *J* = 28.2 Hz), 28.53, 25.91, 21.72 (q, J = 3.0 Hz). ^{19}F NMR (376 MHz, $CDCl_3$) δ -66.36 (s). HRMS (APCI) m/z calcd. for $C_{19}H_{23}F_3N$ $[M+H]^+$ 322.1777, found 322.1775.

Deracemization of racemic amine 9



Procedure: Under argon, a 25 mL Schlenk tube equipped with a magnetic stir bar were charged with **(±)-1AB** (0.1 mmol, 1.0 equiv), Togni's reagent **2a'** (0.13 mmol, 1.3 equiv), triphenylphosphine (0.01 mmol, 0.1 equiv) 5 Å molecular sieves (100 mg) and 1, 2-dichloroethane (DCE, super dry, 1.0 mL). The sealed tube was then stirred at 80 °C for 24 hours. After completion, the reaction temperature was directly decreased to room temperature and 2-(naphthalen-2-yl)-2,3-dihydrobenzo[d]thiazole (**10**, 1.5 equiv) and (*R*)-VAPOL phosphoric acid (20 mol%) were added to this reaction mixture, and then the reaction mixture was stirred for 48 hours. After completion

(monitored by TLC), the reaction solution was concentrated *in vacuo*, and the residue was purified by silica gel column chromatography (petroleum ether/EtOAc) to give the desired product **9**. 83% ee, HPLC analysis [Daicel Chiralpak AD-H, isopropanol/hexane = 2/98, 0.5 mL/min, λ = 254 nm, t_R (major) = 37.7 min, t_R (minor) = 24.5 min].

Reference:

(1) Gaussian 09, 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. Jr. Vreven, J. A. Montgomery, J. E. Peralta, F. Ogliaro, M. Heyd, J. J. Bearpark, 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, N. J. 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, Ö. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, Fox, D. J. Gaussian, Inc., Wallingford CT, **2009**.

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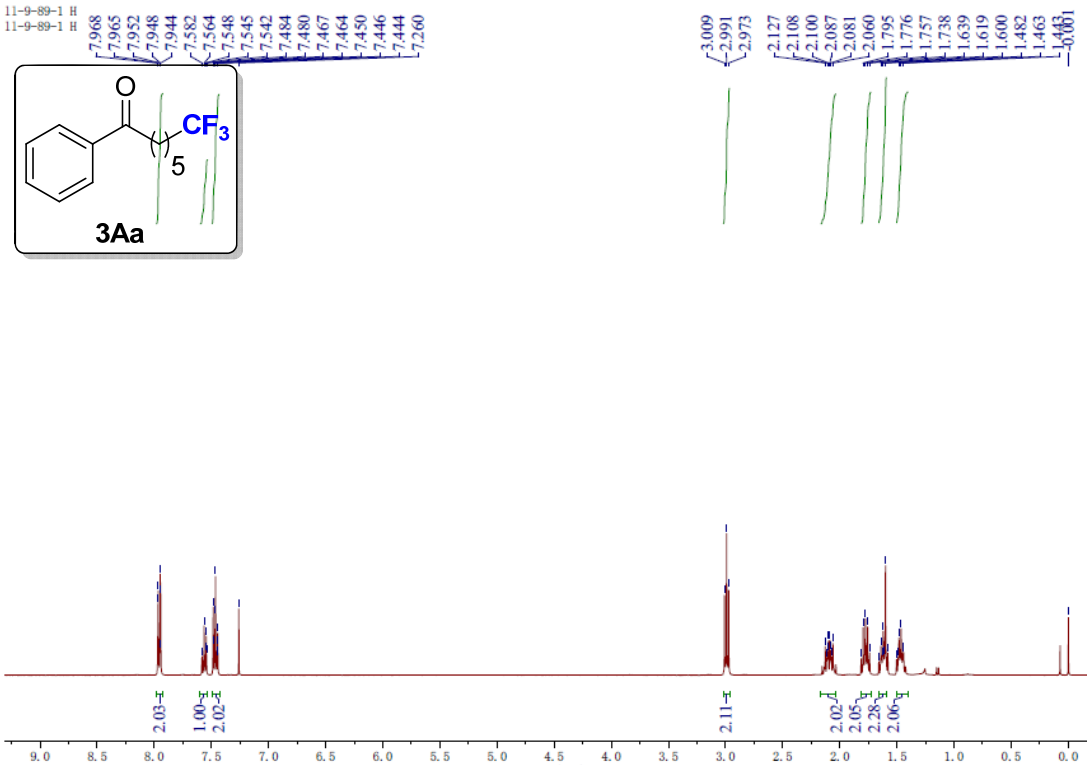
(8) CYLview, 1.0b, C. Y. Legault, Université de Sherbrooke, **2009** (http://www.cylview.org).

NMR Spectra: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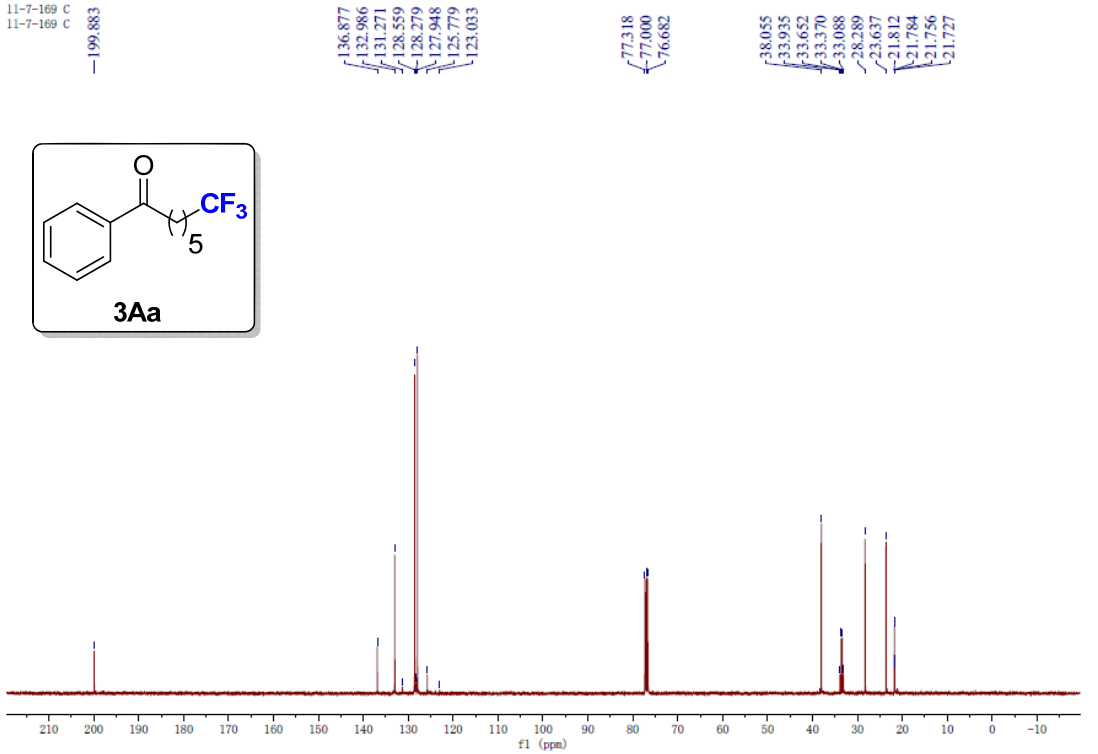
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20
10
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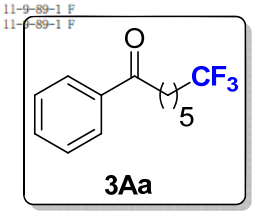
-10
f1 (ppm)


11-9-89-1 F
11-9-89-1 F
O
CF3
5
3Aa

-66.378
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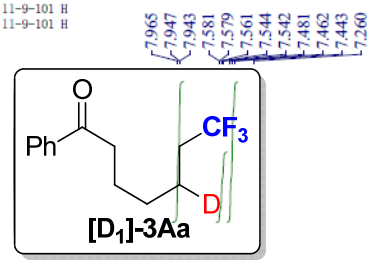
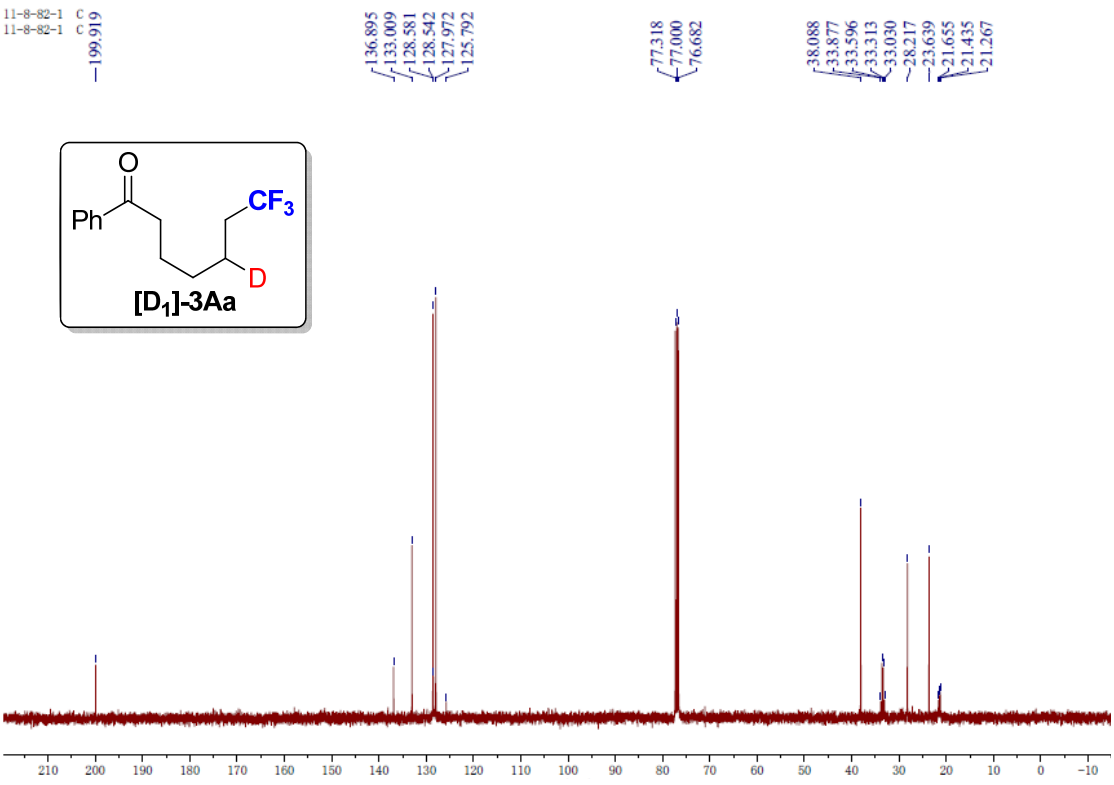

11-9-101 H
11-9-101 H
O
Ph
CF3
D
[D1]-3Aa

7.965
7.947
7.943
7.581
7.579
7.561
7.544
7.542
7.481
7.462
7.443
7.260
3.006
2.988
2.970
2.107
2.086
2.081
2.060
1.790
1.782
1.770
1.751
1.733
1.597
1.577
1.482
1.462
1.443
0.002
1.99
1.00
1.99
2.08
2.03
2.08
1.03
2.05
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


11-8-82-1 C
11-8-82-1 C
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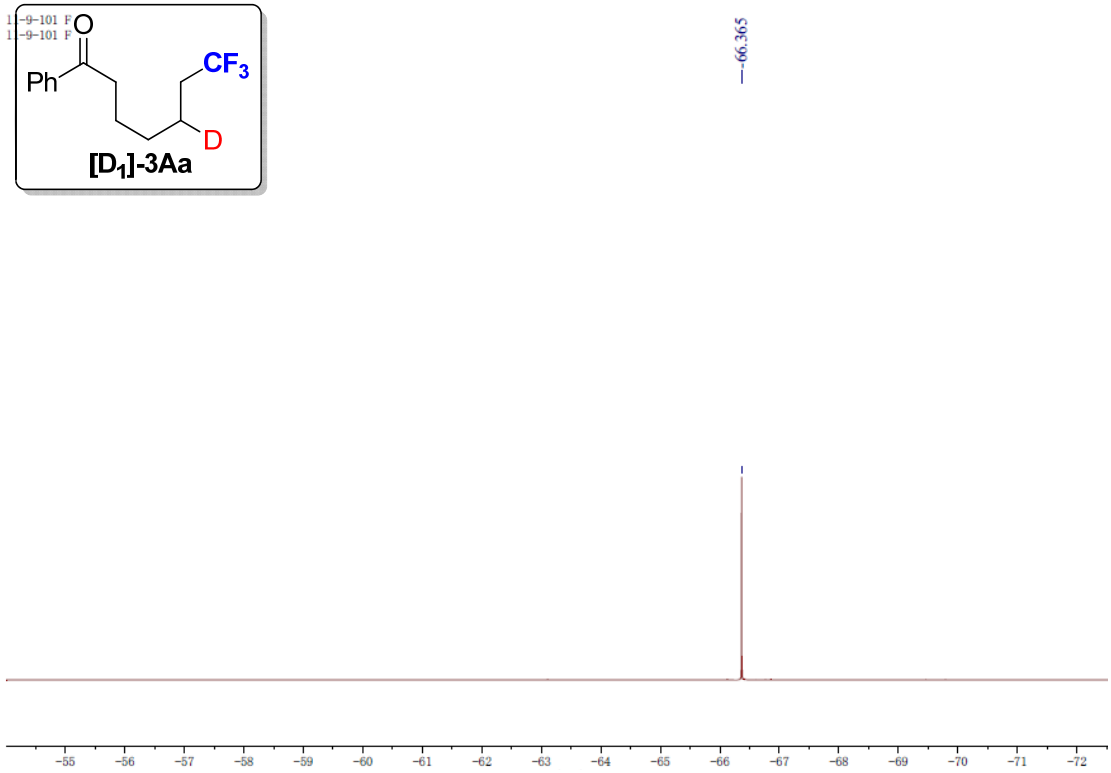
133.009
128.581
128.542
127.972
125.792
77.318
77.000
76.682
38.088
33.877
33.596
33.313
33.030
28.217
23.639
21.655
21.435
21.267
O
Ph
CF3
D
[D1]-3Aa
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10


1-9-101 F
1-9-101 F
-66.365
O
Ph
CF3
D
[D1]-3Aa
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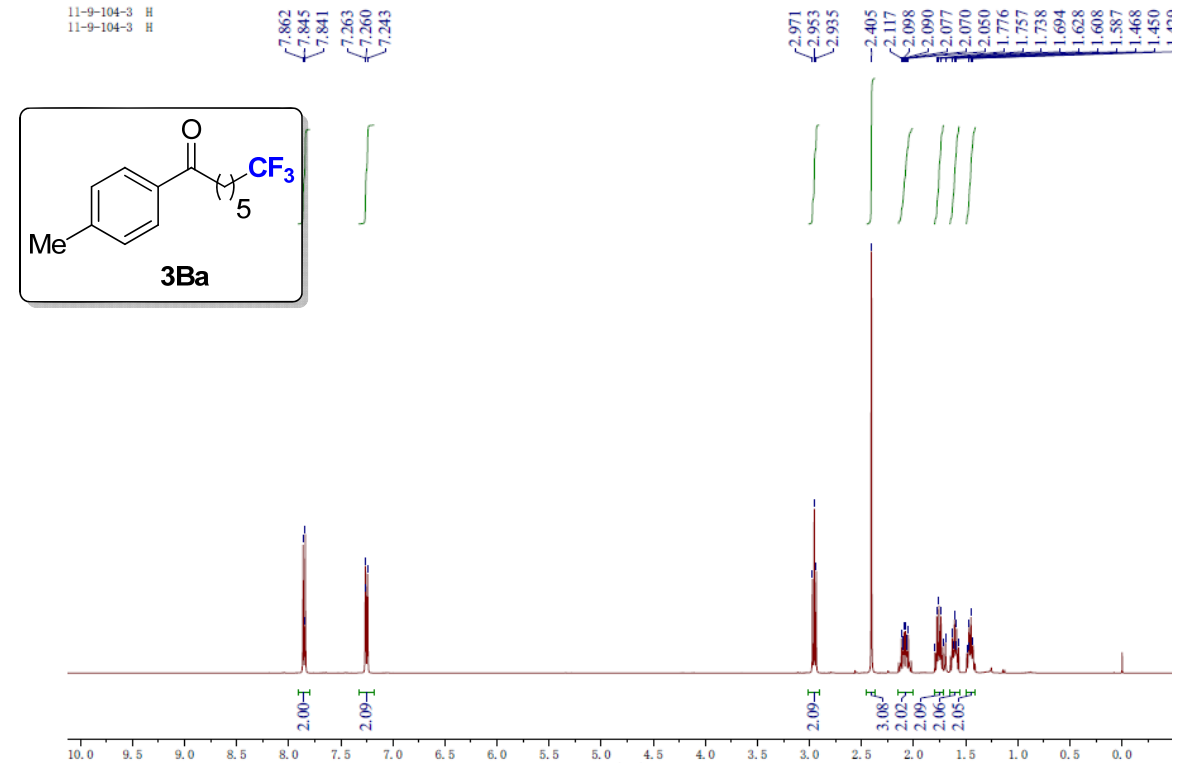
11-9-104-3 H
11-9-104-3 H
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7.845
7.841
7.263
7.260
7.243
2.971
2.953
2.935
2.405
2.117
2.098
2.090
2.077
2.070
2.050
1.776
1.757
1.738
1.694
1.628
1.608
1.587
1.468
1.450
O
CF3
5
Me
3Ba
2.00
2.09
2.09
3.08
2.02
2.09
2.06
2.05
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
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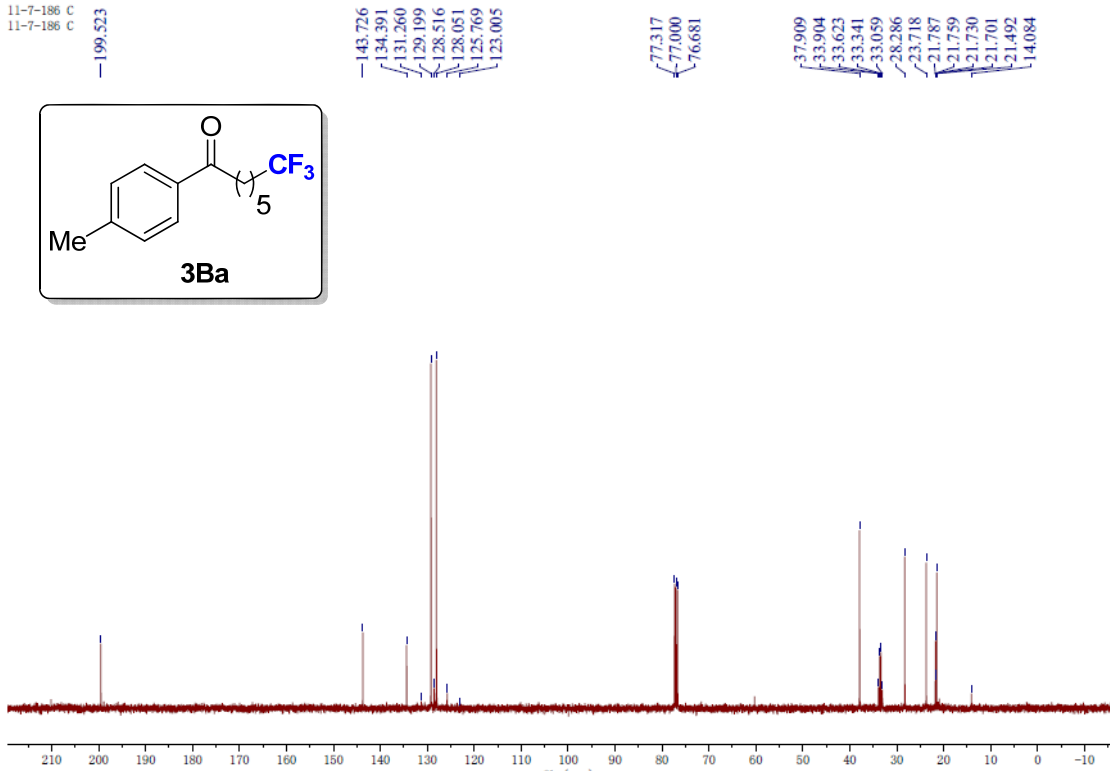
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0


11-7-186 C
11-7-186 C
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143.726
134.391
131.260
129.199
128.516
128.051
125.769
123.005
77.317
77.000
76.681
37.909
33.904
33.623
33.341
33.059
28.286
23.718
21.787
21.759
21.730
21.701
21.492
14.084
O
CF3
5
Me
3Ba
210
200
190
180
170
160
150
140
130
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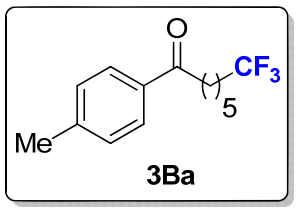
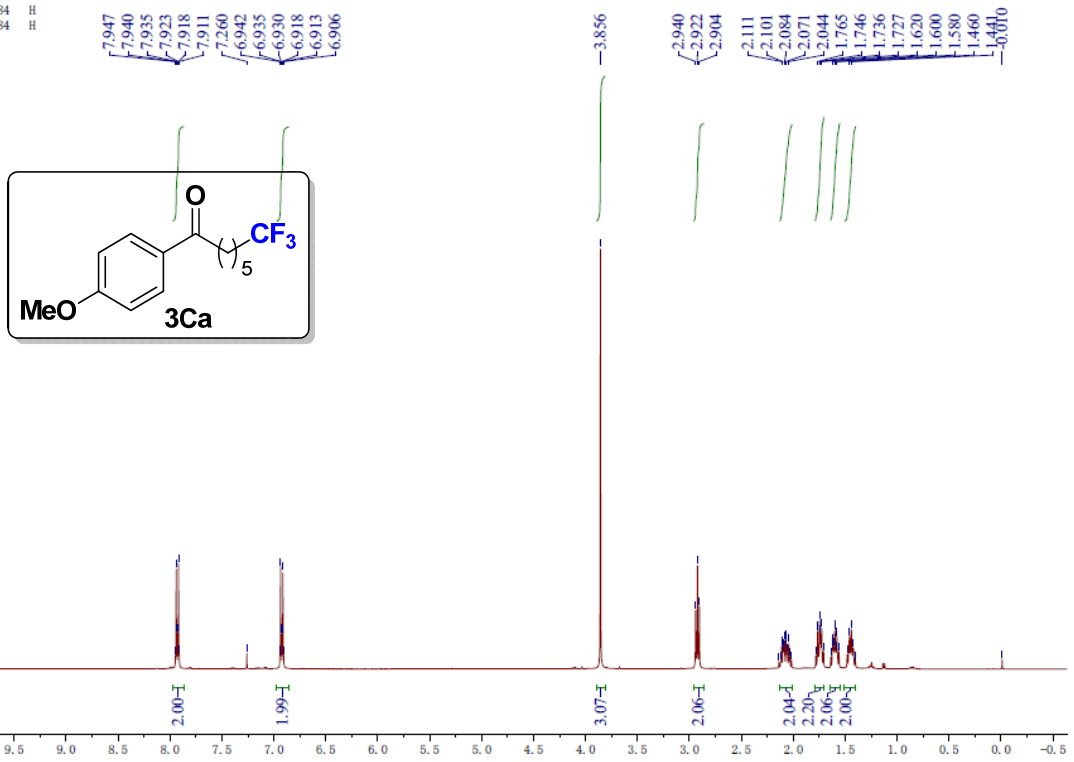
50
40
30
20
10
0
-10

11-9-104-3 F
11-9-104-3 F

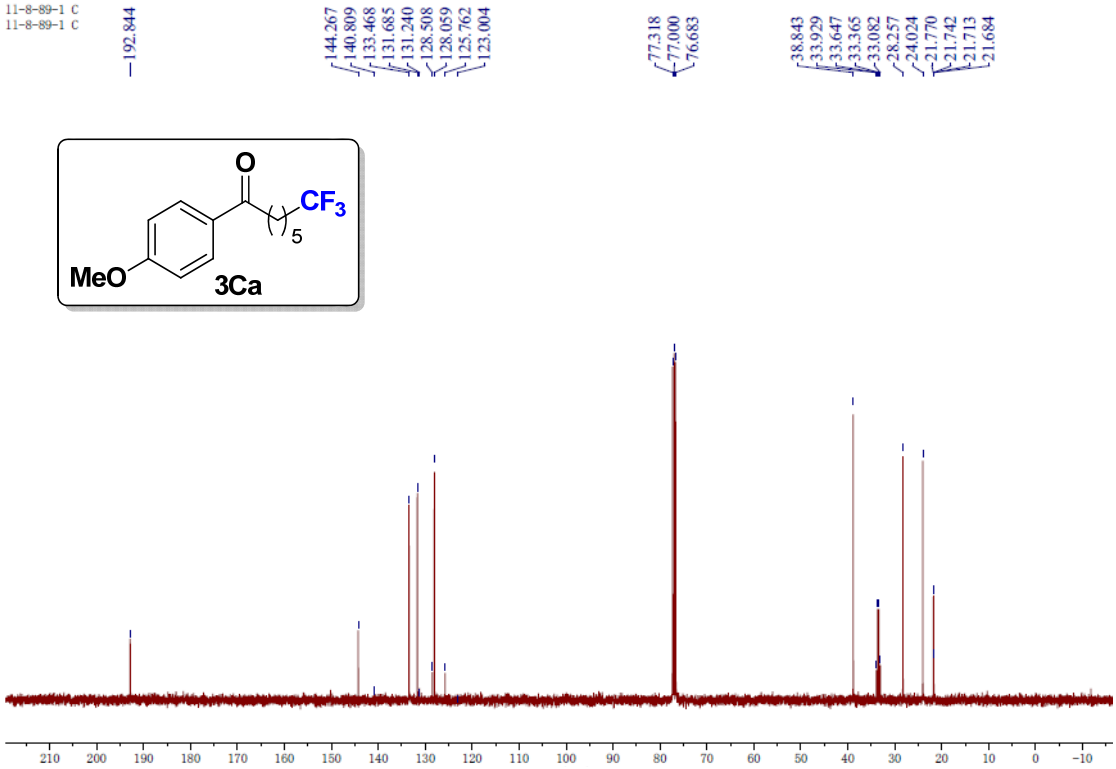


3Ba

11-8-84 H
11-8-84 H



3Ca


11-8-89-1 C
11-8-89-1 C
192.844
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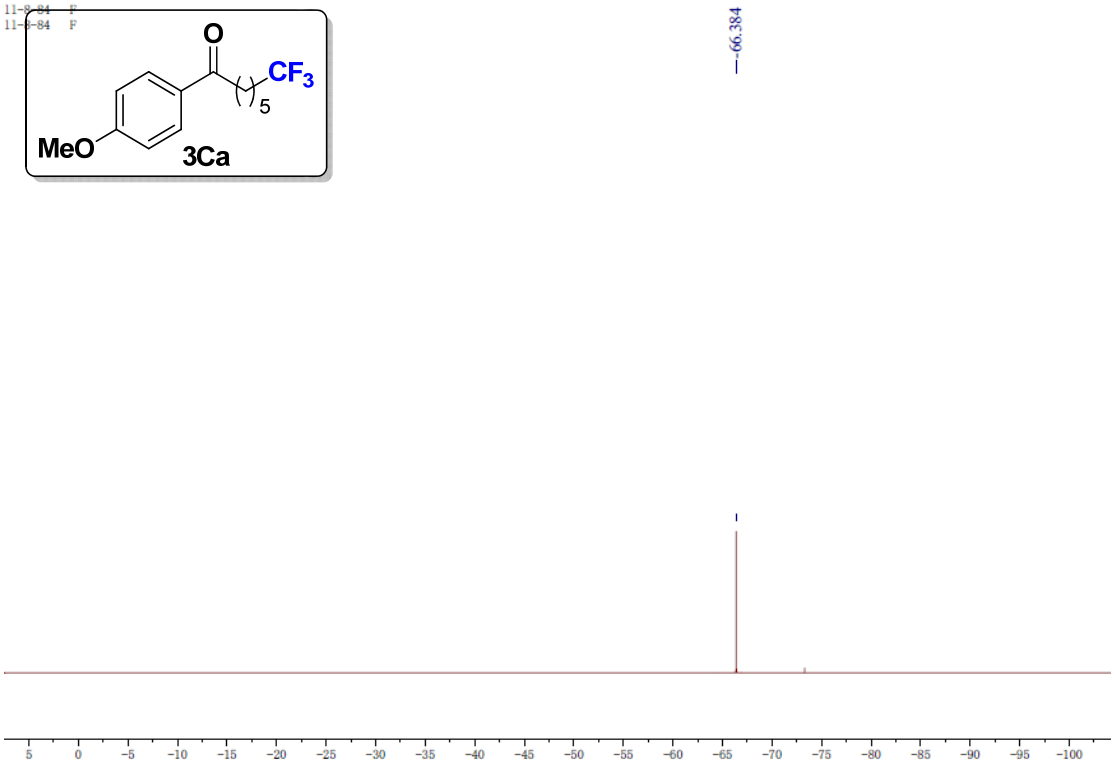
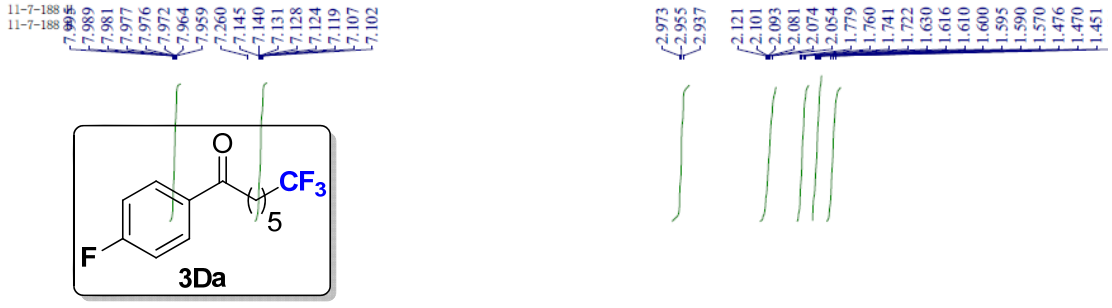
140.809
133.468
131.685
131.240
128.508
128.059
125.762
123.004
77.318
77.000
76.683
38.843
33.929
33.647
33.365
33.082
28.257
24.024
21.770
21.742
21.713
21.684
O
CF3
5
MeO
3Ca
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10


11-8-84 F
11-8-84 F
-66.384
O
CF3
5
MeO
3Ca
5 0 -5 -10 -15 -20 -25 -30 -35 -40 -45 -50 -55 -60 -65 -70 -75 -80 -85 -90 -95 -100


11-7-188
11-7-188
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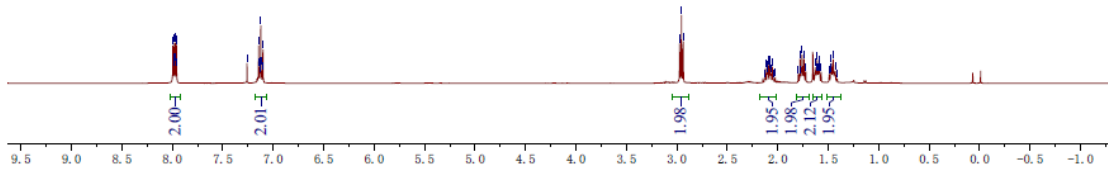
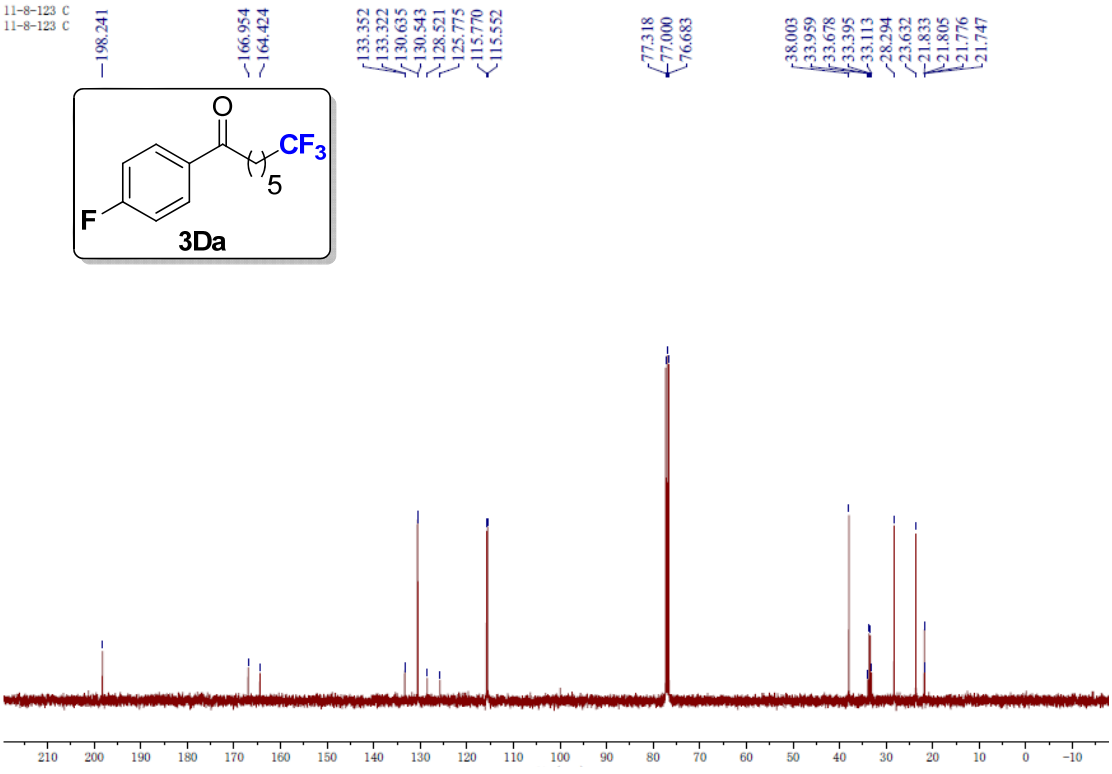
7.989
7.981
7.977
7.976
7.972
7.964
7.959
7.260
7.145
7.140
7.131
7.128
7.124
7.119
7.107
7.102
2.973
2.955
2.937
2.121
2.101
2.093
2.081
2.074
2.054
1.779
1.760
1.741
1.722
1.630
1.616
1.610
1.600
1.595
1.590
1.570
1.476
1.470
1.451
O
CF3
5
F
3Da


2.00
2.01
1.98
1.95
1.98
2.12
1.95
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
-0.5
-1.0


11-8-123 C
11-8-123 C
198.241
166.954
164.424
133.352
133.322
130.635
130.543
128.521
125.775
115.770
115.552
77.318
77.000
76.683
38.003
33.959
33.678
33.395
33.113
28.294
23.632
21.833
21.805
21.776
21.747
O
CF3
5
F
3Da
210
200
190
180
170
160
150
140
130
120
110
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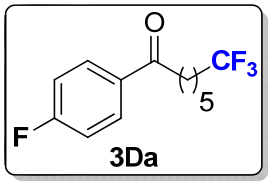
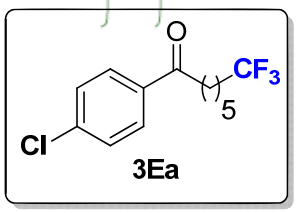
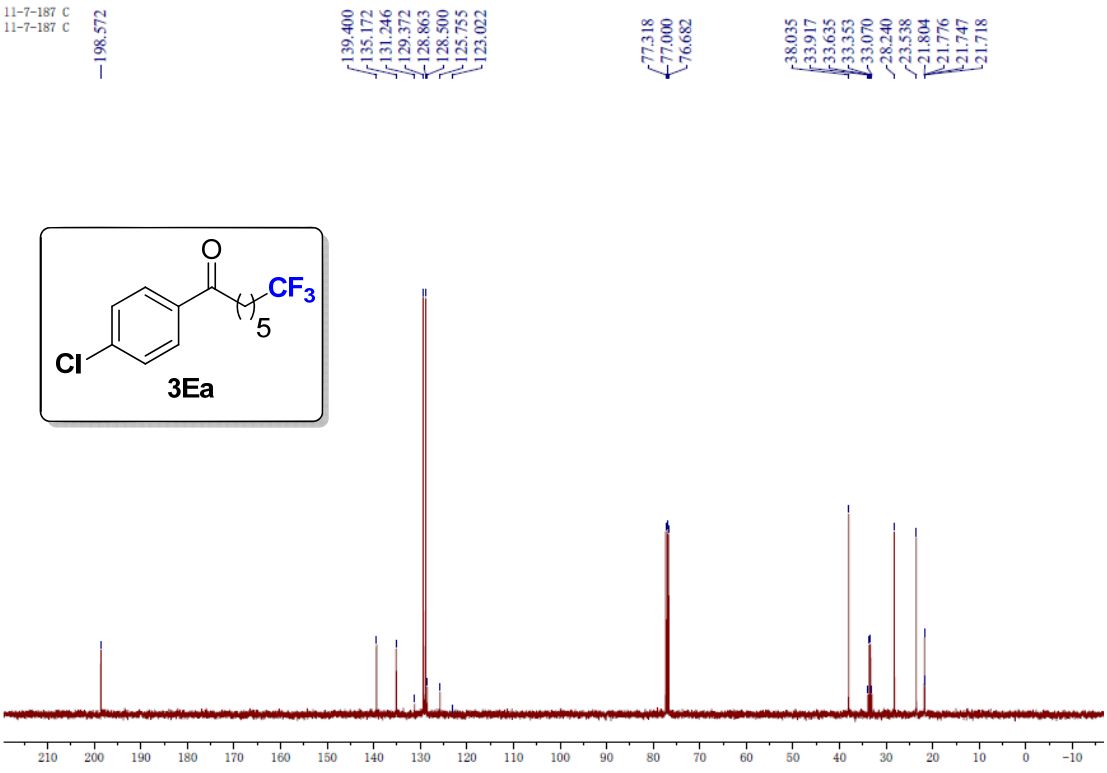
90
80
70
60
50
40
30
20
10
0
-10

11-7-188 F
11-7-188 F



11-7-187 H
11-7-187 H




11-7-187 C
11-7-187 C
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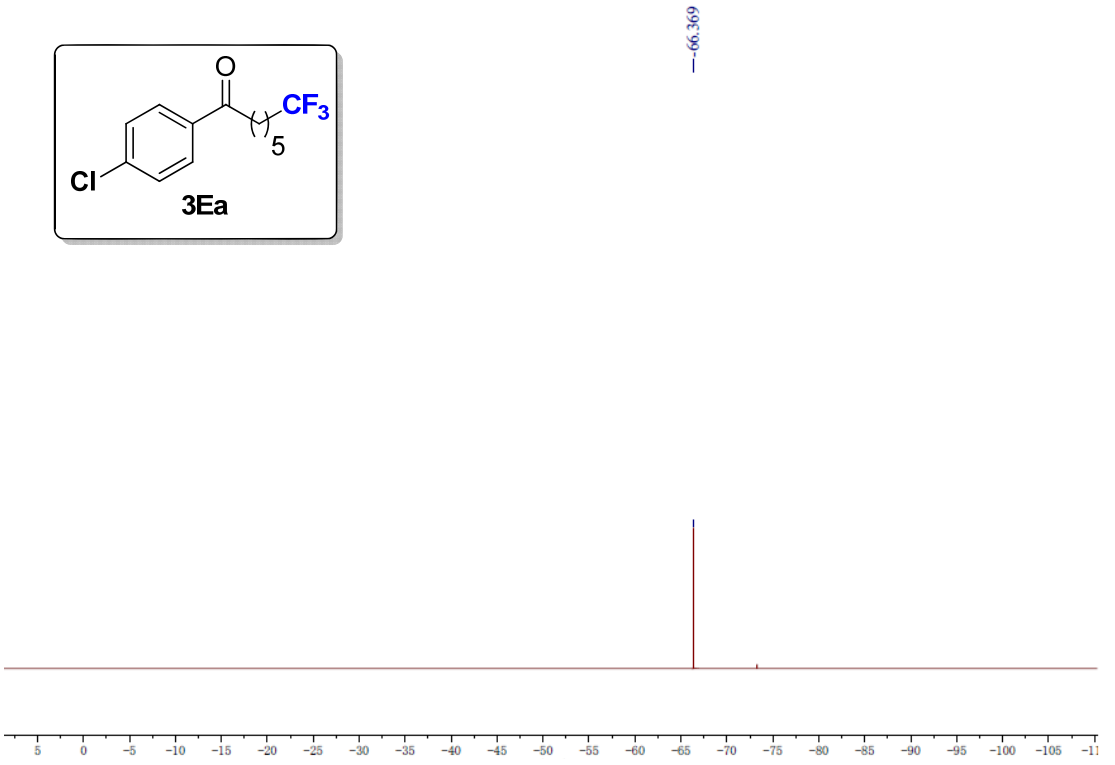
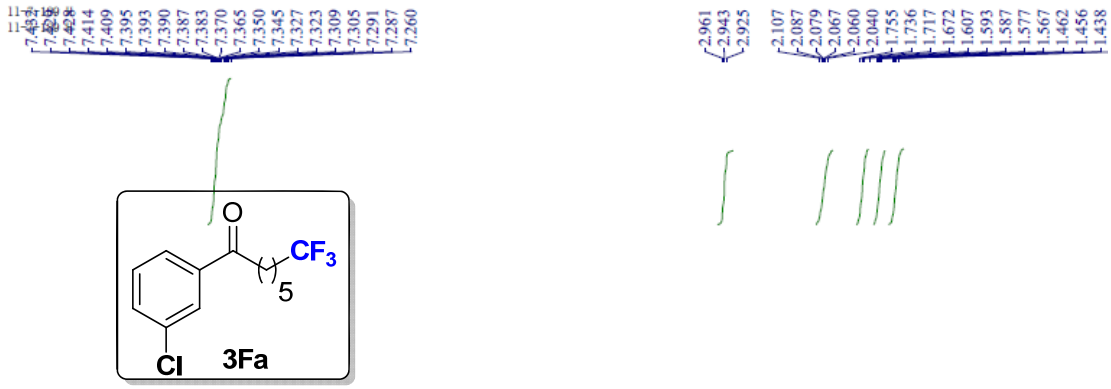
135.172
131.246
129.372
128.863
128.500
125.755
123.022
77.318
77.000
76.682
38.035
33.917
33.635
33.353
33.070
28.240
23.538
21.804
21.776
21.747
21.718
O
CF3
5
Cl
3Ea


-66.369
O
CF3
5
Cl
3Ea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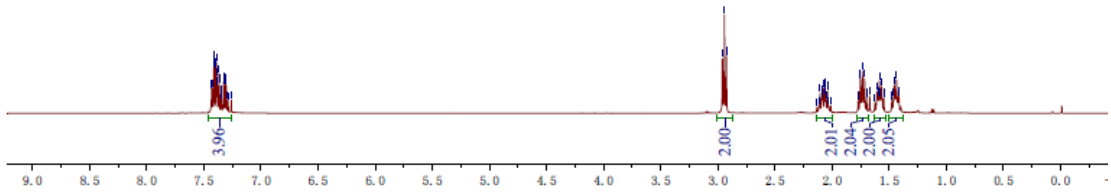
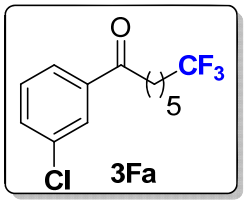
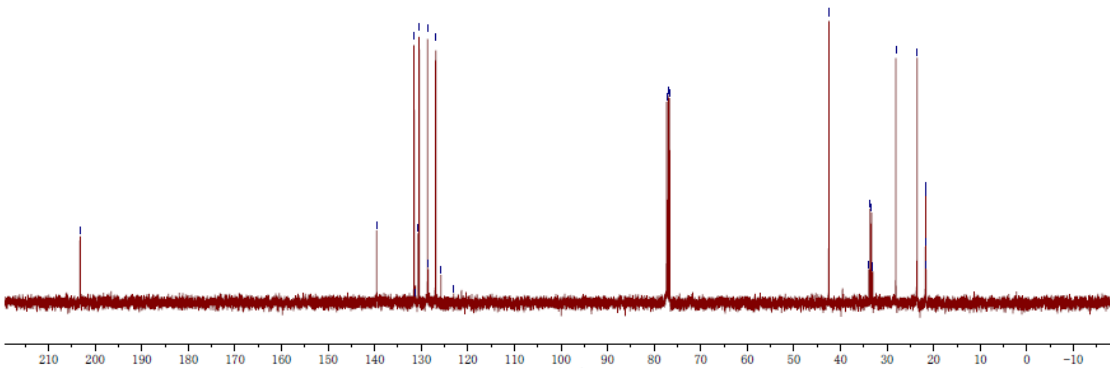
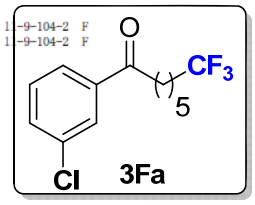
CF3
5
Cl
3Fa




O
CF3
5
Cl
3Fa




O
CF3
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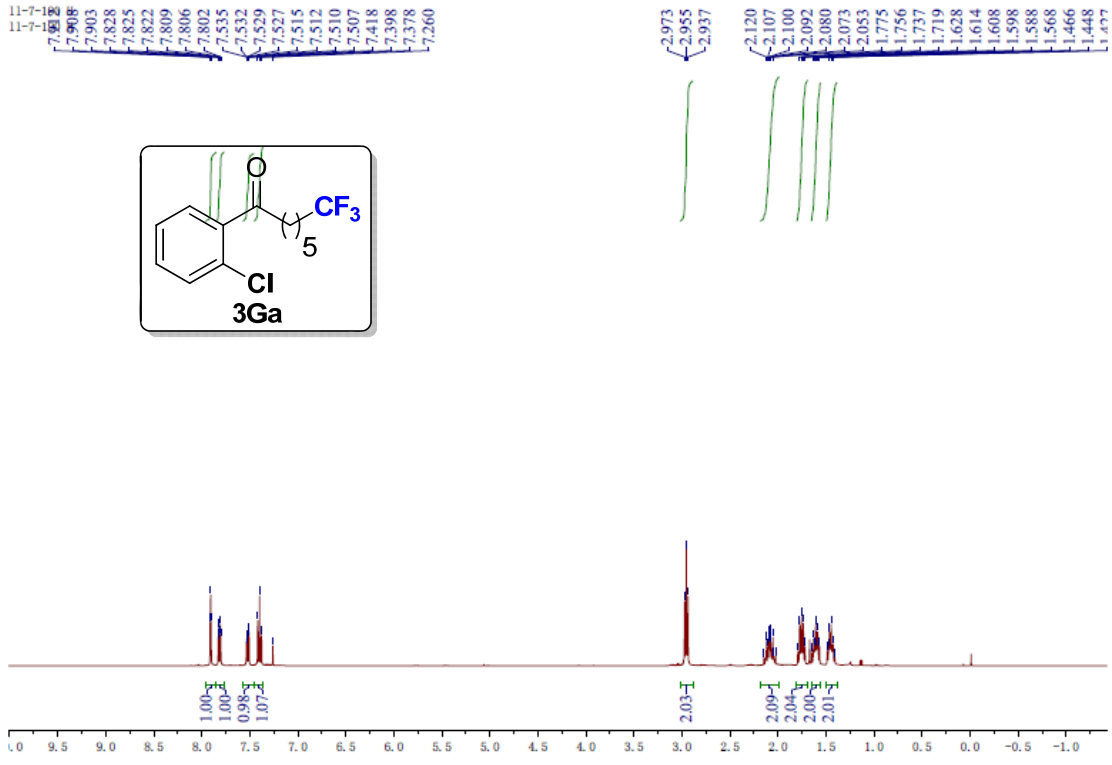
Cl
3Fa

-66.386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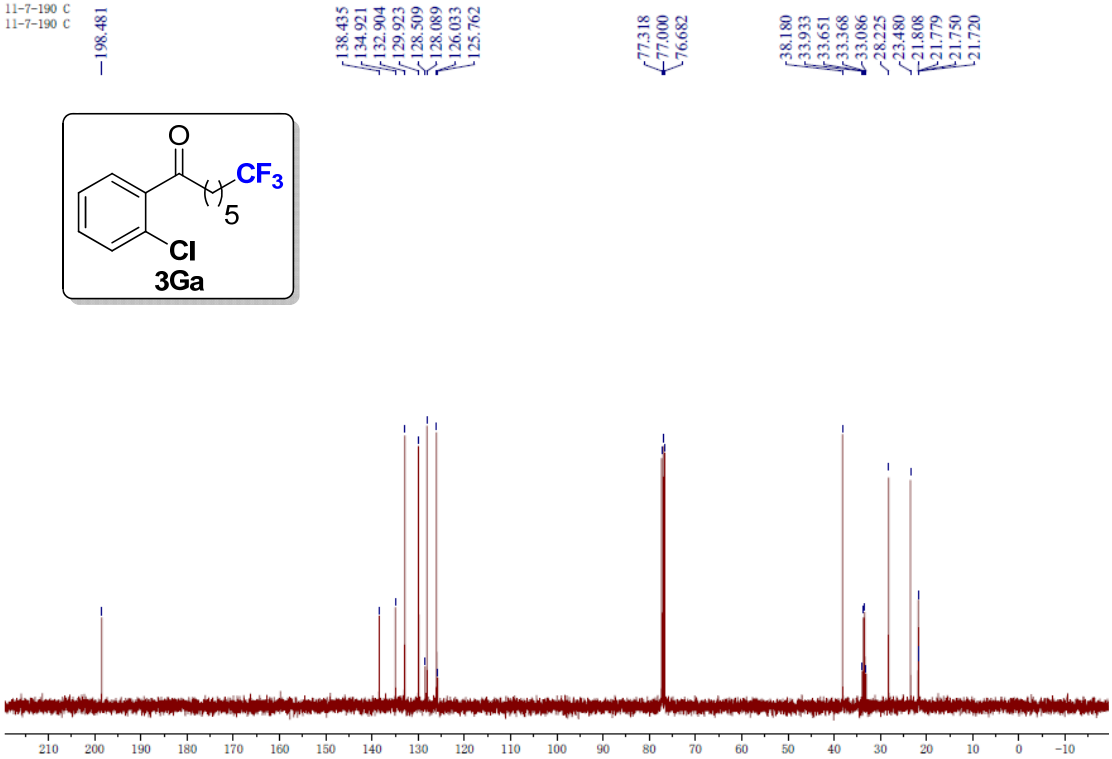
7.825
7.822
7.809
7.806
7.802
7.535
7.532
7.529
7.527
7.515
7.512
7.510
7.507
7.418
7.398
7.378
7.260
2.973
2.955
2.937
2.120
2.107
2.100
2.092
2.080
2.073
2.053
1.775
1.756
1.737
1.719
1.628
1.614
1.608
1.598
1.588
1.568
1.466
1.448
1.00
1.00
0.98
1.07
2.03
2.09
2.04
2.00
2.01

O
CF3
5
Cl
3Ga


11-7-190 C
11-7-190 C
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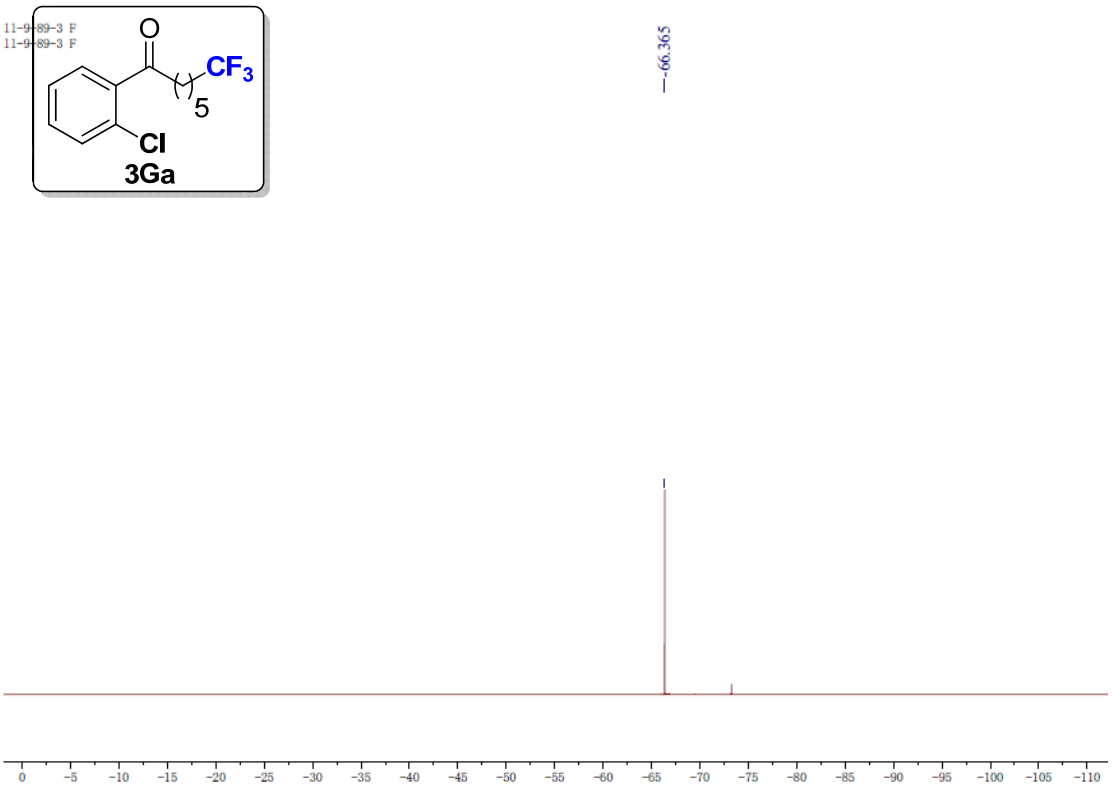
134.921
132.904
129.923
128.509
128.089
126.033
125.762
77.318
77.000
76.682
38.180
33.933
33.651
33.368
33.086
28.225
23.480
21.808
21.779
21.750
21.720
O
CF3
5
Cl
3Ga
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10


11-9-89-3 F
11-9-89-3 F
-66.365
O
CF3
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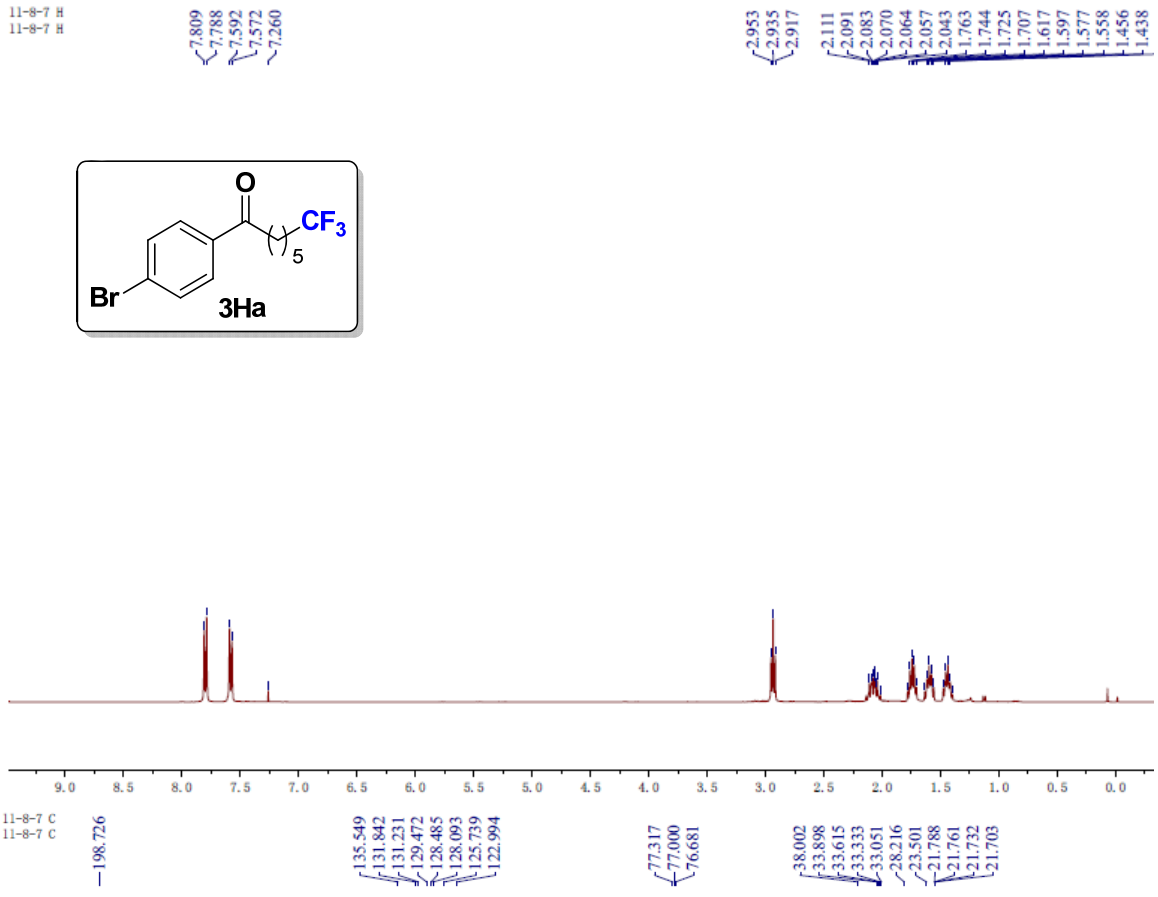
Cl
3Ga
0 -5 -10 -15 -20 -25 -30 -35 -40 -45 -50 -55 -60 -65 -70 -75 -80 -85 -90 -95 -100 -105 -110


11-8-7 H
11-8-7 H
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7.788
7.592
7.572
7.260
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2.935
2.917
2.111
2.091
2.083
2.070
2.064
2.057
2.043
1.763
1.744
1.725
1.707
1.617
1.597
1.577
1.558
1.456
1.438
O
CF3
5
Br
3Ha
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
11-8-7 C
11-8-7 C
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135.549
131.842
131.231
129.472
128.485
128.093
125.739
122.994
77.317
77.000
76.681
38.002
33.898
33.615
33.333
33.051
28.216
23.501
21.788
21.761
21.732
21.703
O
CF3
5
Br
3Ha
210
200
190
180
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140
130
120
110
100
90
80
70
60
50
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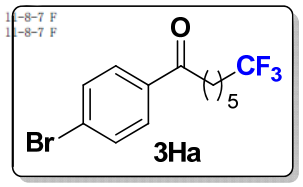
30
20
10
0
-10


O
CF3
5
Br
3Ha

-66.356
11-8-64 H
11-8-64 H
8.464
8.042
8.038
8.021
8.017
7.977
7.957
7.906
7.885
7.866
7.622
7.619
7.605
7.602
7.586
7.582
7.576
7.572
7.555
7.552
7.538
7.535
7.260
3.135
3.117
3.099
2.144
2.124
2.116
2.104
2.097
2.076
1.848
1.828
1.809
1.791
1.669
1.665
1.650
1.644
1.634
1.624
1.605
1.524
1.517
1.499
O
CF3
5
3Ia
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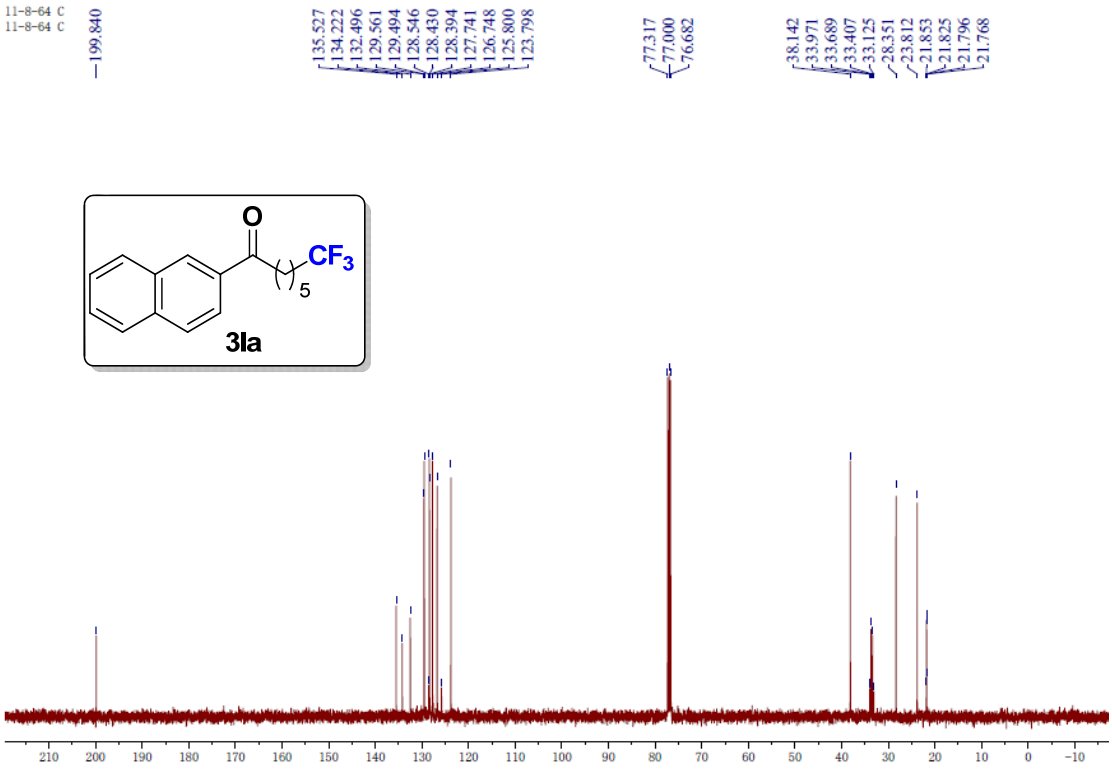
1.00
1.06
2.01
0.96
1.05
2.07
2.02
2.10
2.20
2.03


11-8-64 C
11-8-64 C
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134.222
132.496
129.561
129.494
128.546
128.430
128.394
127.741
126.748
125.800
123.798
77.317
77.000
76.682
38.142
33.971
33.689
33.407
33.125
28.351
23.812
21.853
21.825
21.796
21.768
O
CF3
5
3la
210
200
190
180
170
160
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140
130
120
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100
90
80
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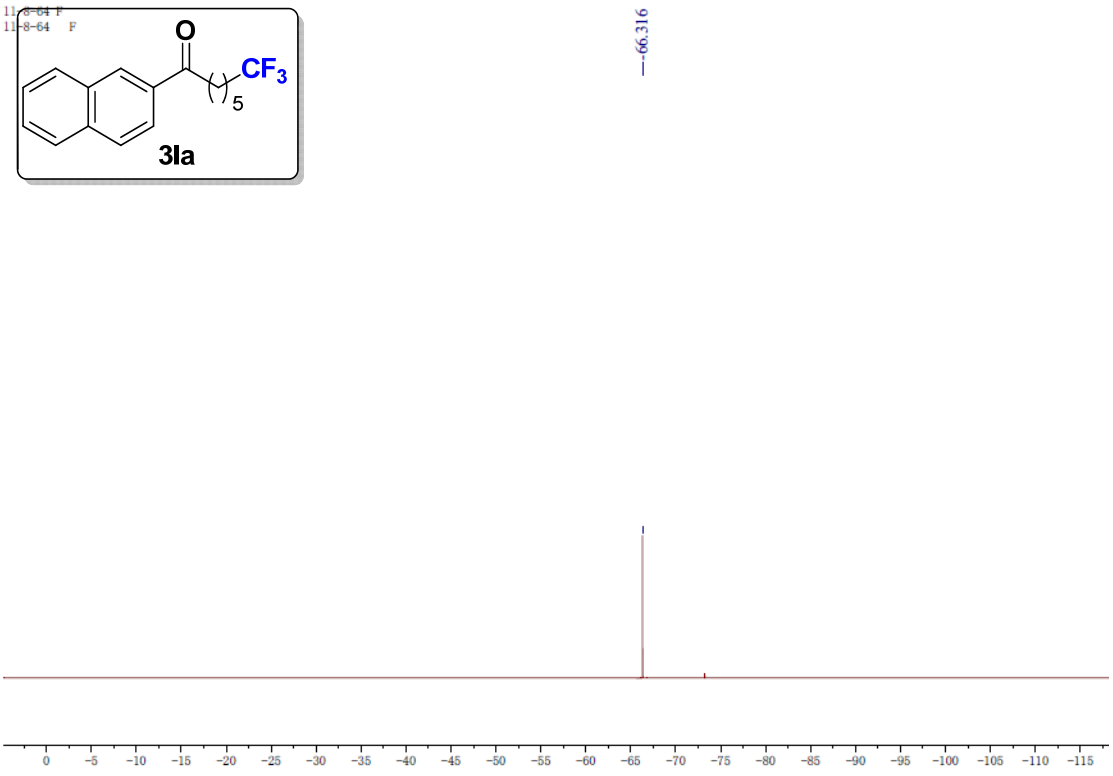
60
50
40
30
20
10
0
-10


11-8-64 F
11-8-64 F
-66.316
O
CF3
5
3la
0
-5
-10
-15
-20
-25
-30
-35
-40
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-50
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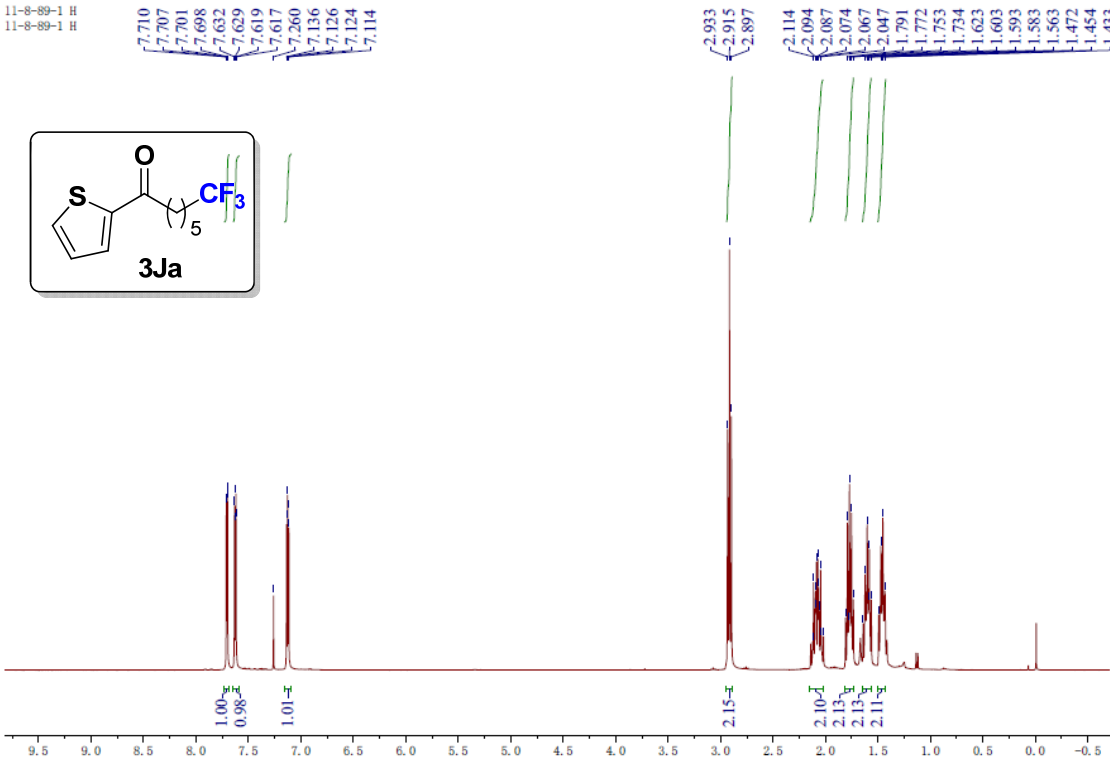
-60
-65
-70
-75
-80
-85
-90
-95
-100
-105
-110
-115


11-8-89-1 H
11-8-89-1 H
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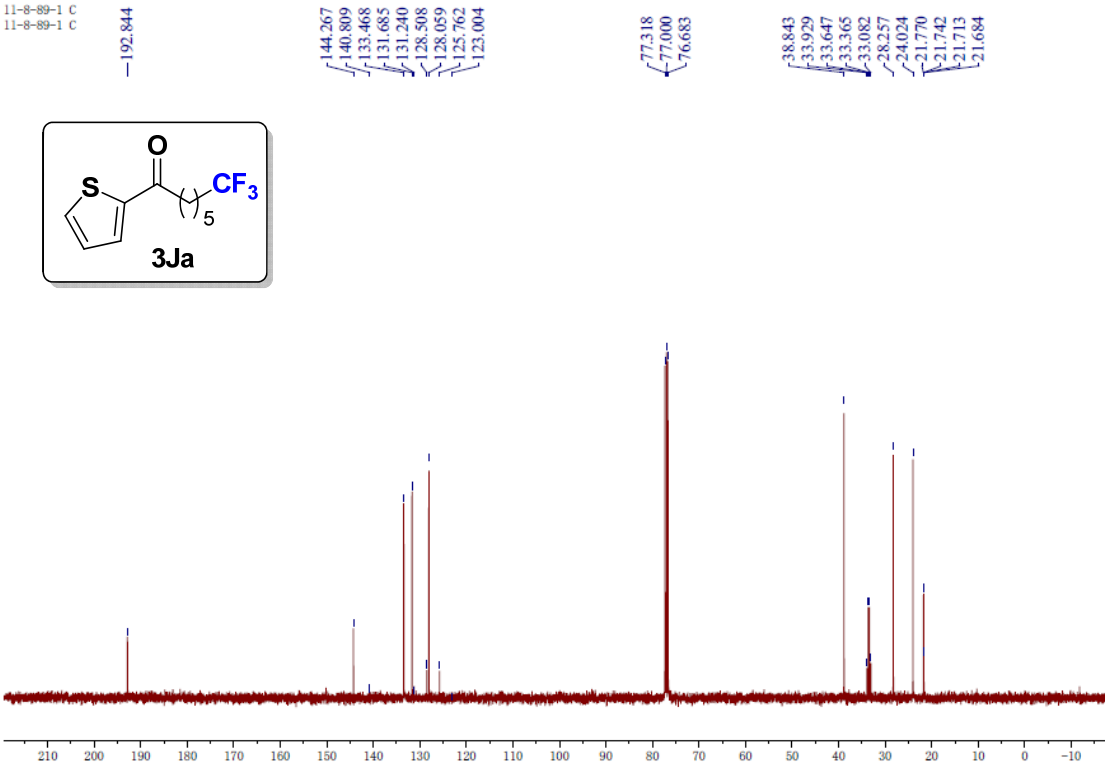
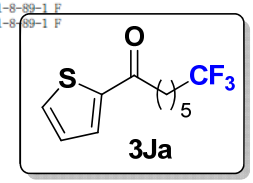
7.707
7.701
7.698
7.632
7.629
7.619
7.617
7.260
7.136
7.126
7.124
7.114
2.933
2.915
2.897
2.114
2.094
2.087
2.074
2.067
2.047
1.791
1.772
1.753
1.734
1.623
1.603
1.593
1.583
1.563
1.472
1.454
O
S
CF3
5
3Ja
1.00
0.98
1.01
2.15
2.10
2.13
2.13
2.11
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5

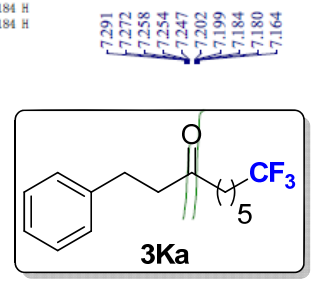

11-8-89-1 C
11-8-89-1 C
192.844
144.267
140.809
133.468
131.685
131.240
128.508
128.059
125.762
123.004
77.318
77.000
76.683
38.843
33.929
33.647
33.365
33.082
28.257
24.024
21.770
21.742
21.713
21.684
O
S
CF3
5
3Ja
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10

11-8-89-1 F
11-8-89-1 F

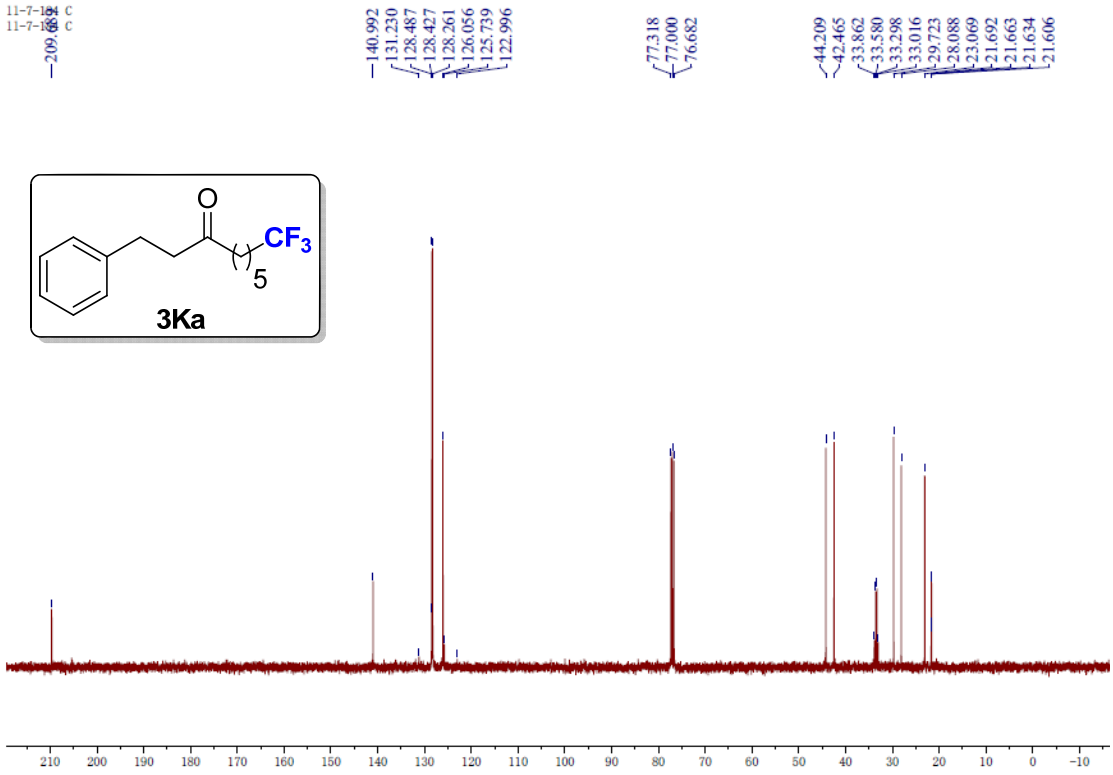


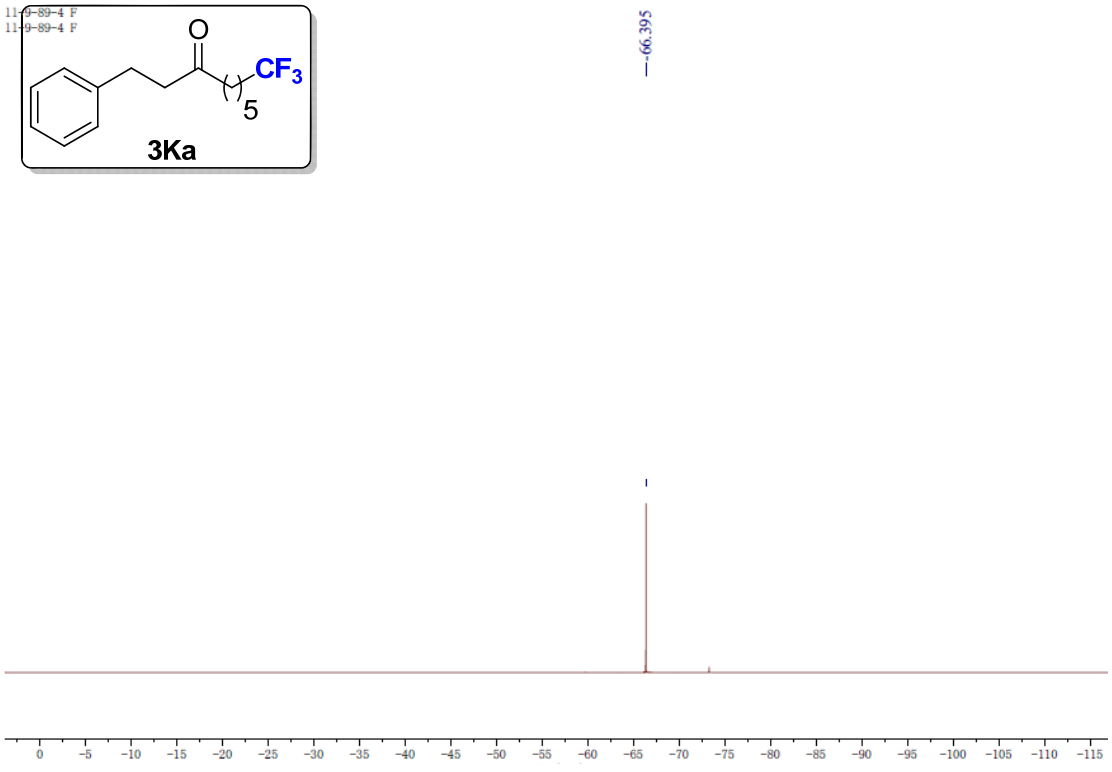
3Ja

11-7-184 H
11-7-184 H

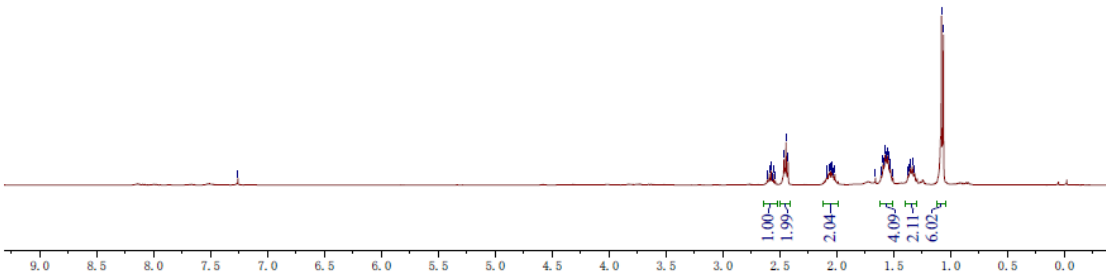


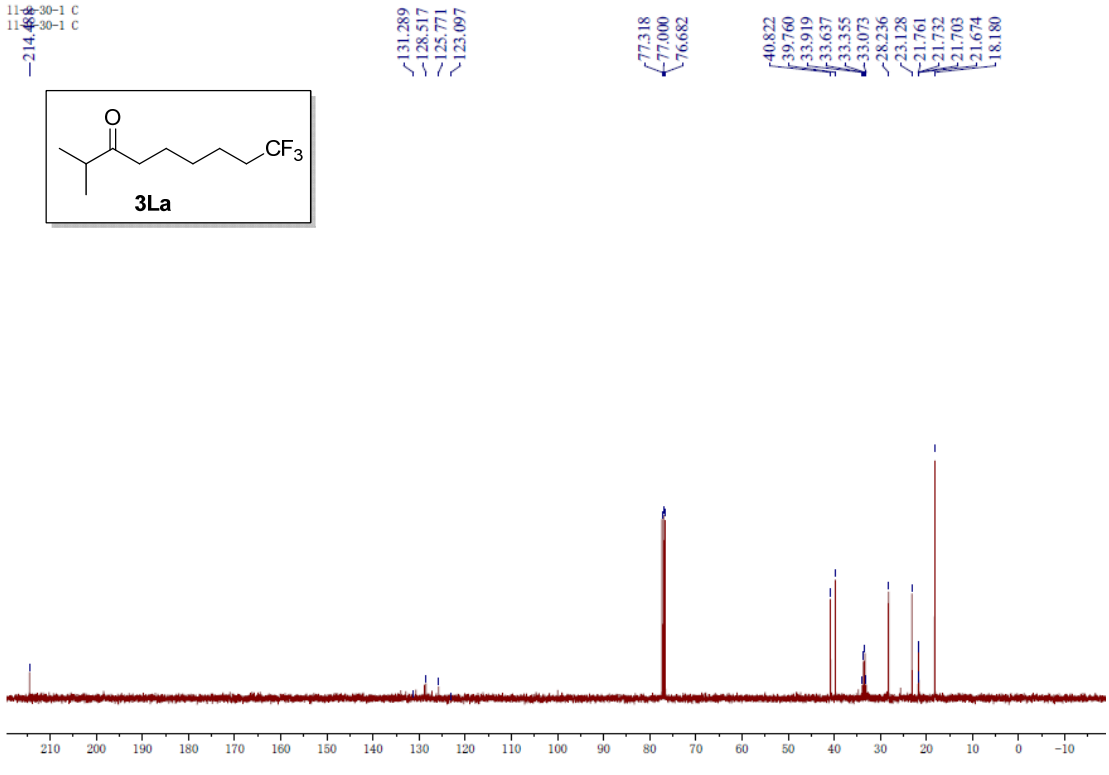
3Ka


11-7-184 C
11-7-184 C
209.686
140.992
131.230
128.487
128.427
128.261
126.056
125.739
122.996
77.318
77.000
76.682
44.209
42.465
33.862
33.580
33.298
33.016
29.723
28.088
23.069
21.692
21.663
21.634
21.606
O
CF3
5
3Ka
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10

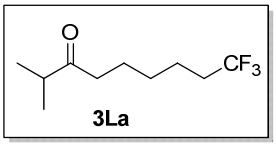

11-9-89-4 F
11-9-89-4 F
-66.395
O
CF3
5
3Ka
0
-5
-10
-15
-20
-25
-30
-35
-40
-45
-50
-55
-60
-65
-70
-75
-80
-85
-90
-95
-100
-105
-110
-115


11-9-30-2 H
11-9-30-2 H
7.260
2.610
2.592
2.575
2.568
2.558
2.540
2.464
2.446
2.428
2.057
2.044
1.594
1.586
1.574
1.568
1.555
1.547
1.537
1.527
1.361
1.354
1.336
1.081
O
CF3
3La


1.00
1.99
2.04
4.09
2.11
6.02
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

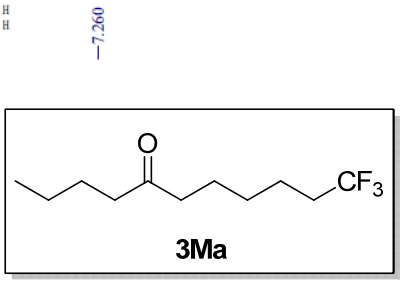

11-9-30-1 C
11-9-30-1 C
214.468
131.289
128.517
125.771
123.097
77.318
77.000
76.682
40.822
39.760
33.919
33.637
33.355
33.073
28.236
23.128
21.761
21.732
21.703
21.674
18.180
O
CF3
3La
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10

11-9-30-1 F
11-9-30-1 F

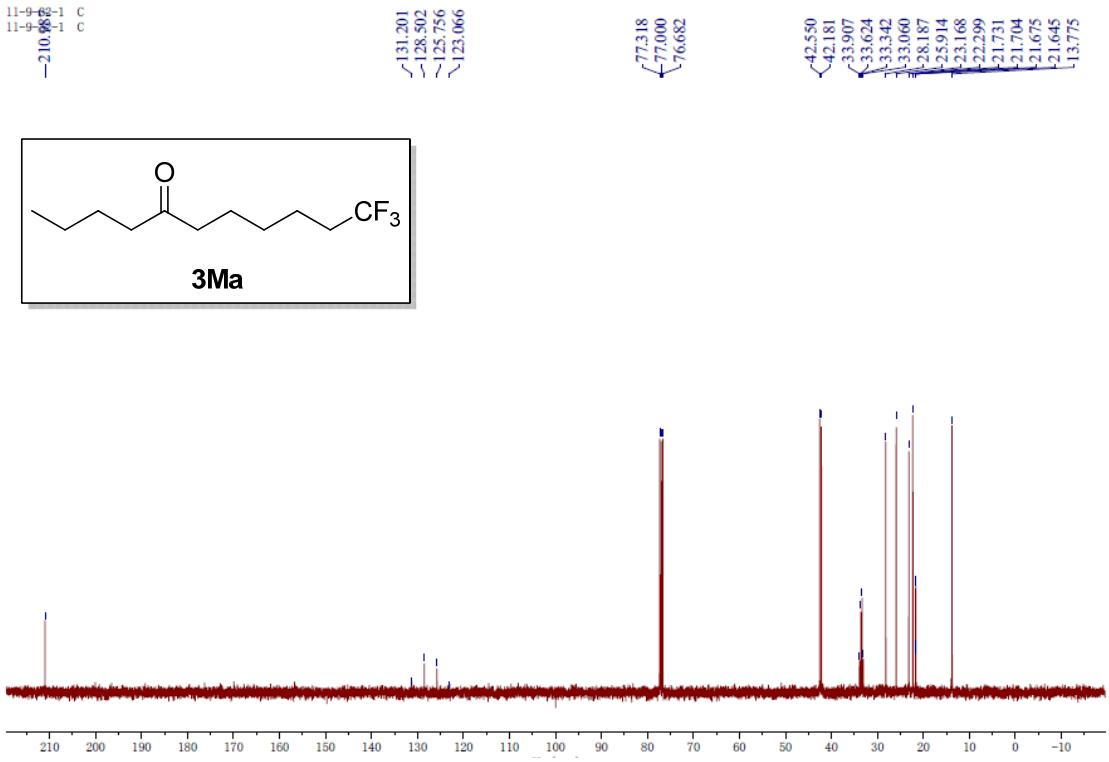


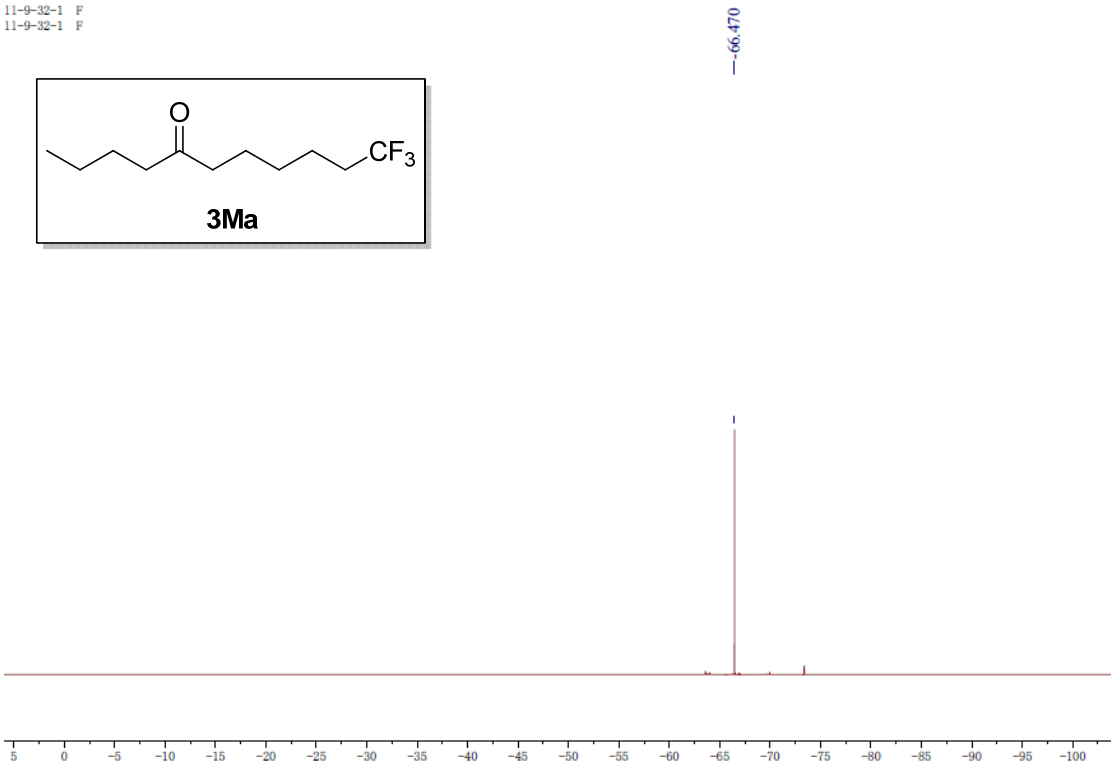
3La

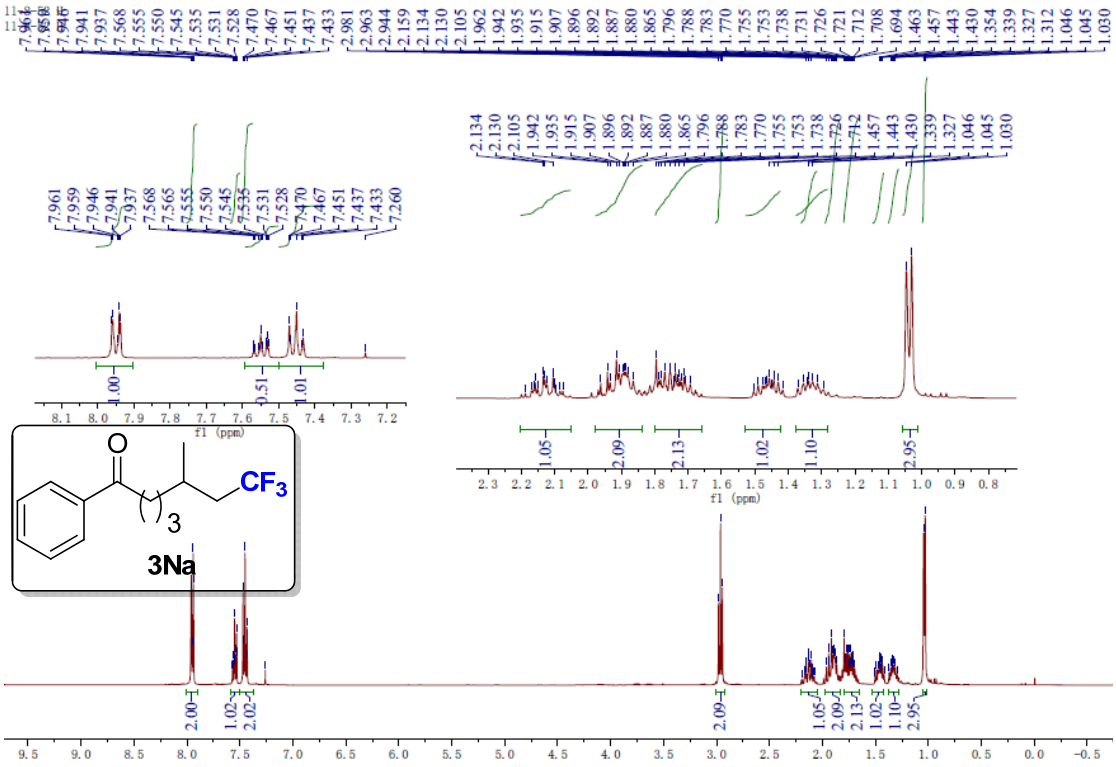
11-9-32-2 H
11-9-32-2 H

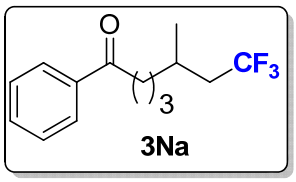


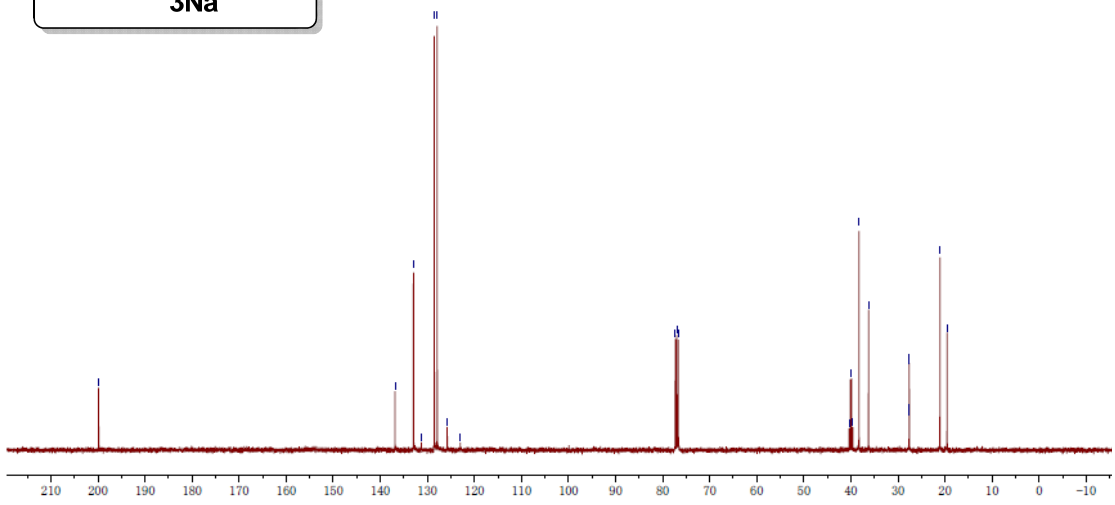
3Ma


11-9-32-1 C
11-9-32-1 C
210.688
131.201
128.502
125.756
123.066
77.318
77.000
76.682
42.550
42.181
33.907
33.624
33.342
33.060
28.187
25.914
23.168
22.299
21.731
21.704
21.675
21.645
13.775
O
CF3
3Ma
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10

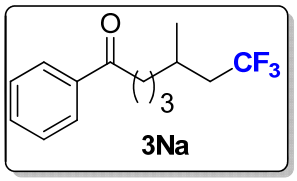

11-9-32-1 F
11-9-32-1 F
-66.470
O
CF3
3Ma
5 0 -5 -10 -15 -20 -25 -30 -35 -40 -45 -50 -55 -60 -65 -70 -75 -80 -85 -90 -95 -100


3Na
f1 (ppm)

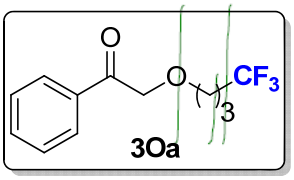

3Na

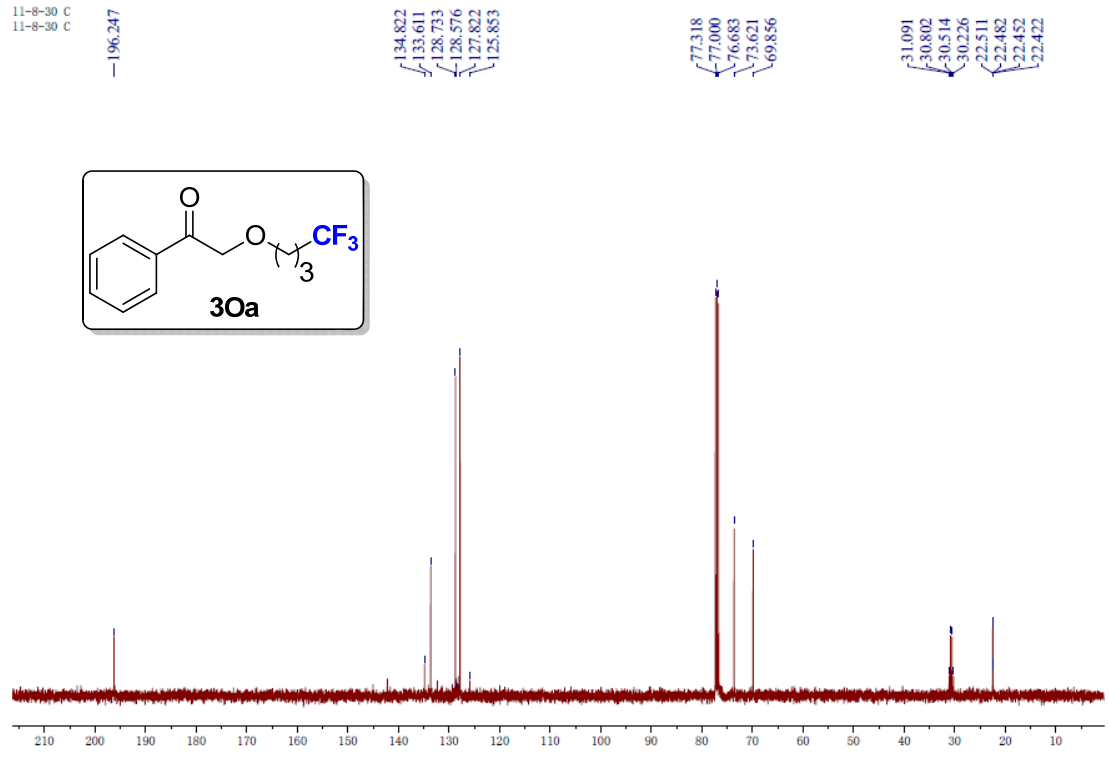


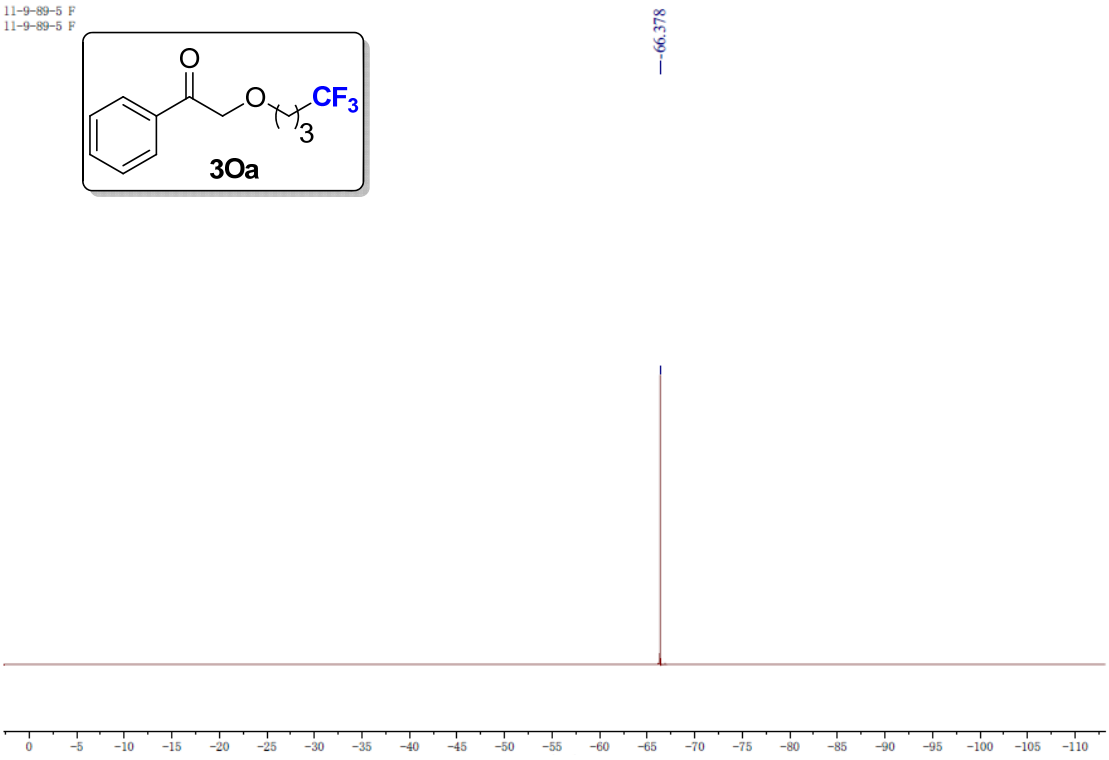
11-8-52 F
11-8-52 F

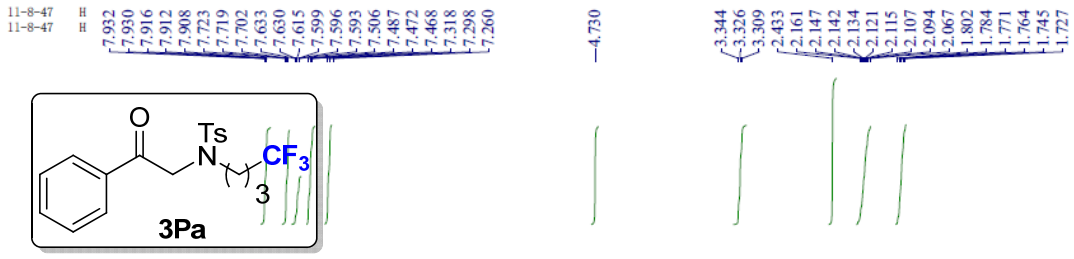


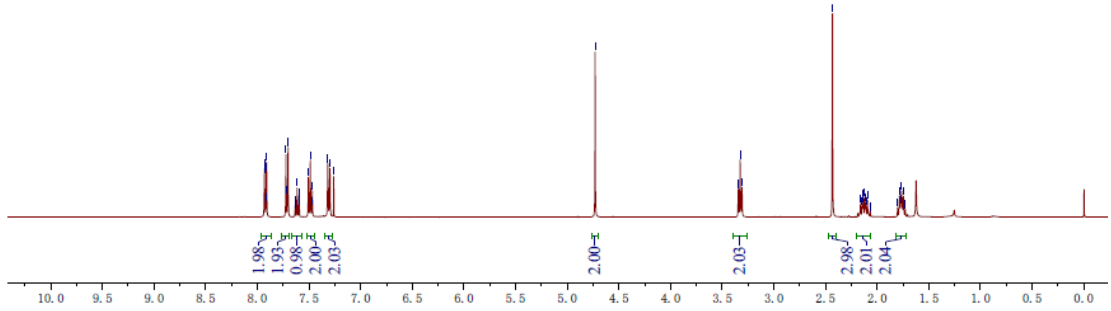
11-9-89-5
11-9-89-5



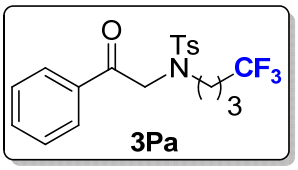

11-8-30 C
11-8-30 C
196.247
134.822
133.611
128.733
128.576
127.822
125.853
77.318
77.000
76.683
73.621
69.856
31.091
30.802
30.514
30.226
22.511
22.482
22.452
22.422
O
O
CF3
3
3Oa
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10

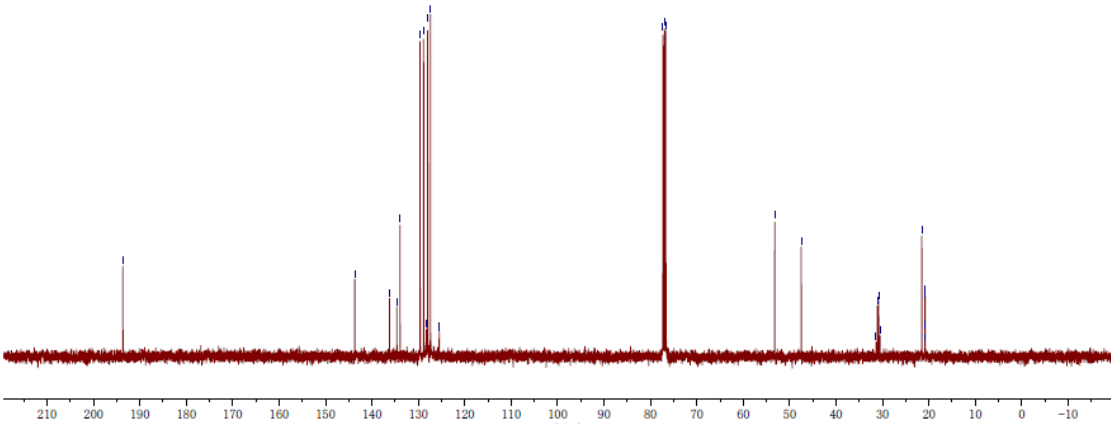

11-9-89-5 F
11-9-89-5 F
-66.378
O
O
CF3
3
3Oa
0
-5
-10
-15
-20
-25
-30
-35
-40
-45
-50
-55
-60
-65
-70
-75
-80
-85
-90
-95
-100
-105
-110

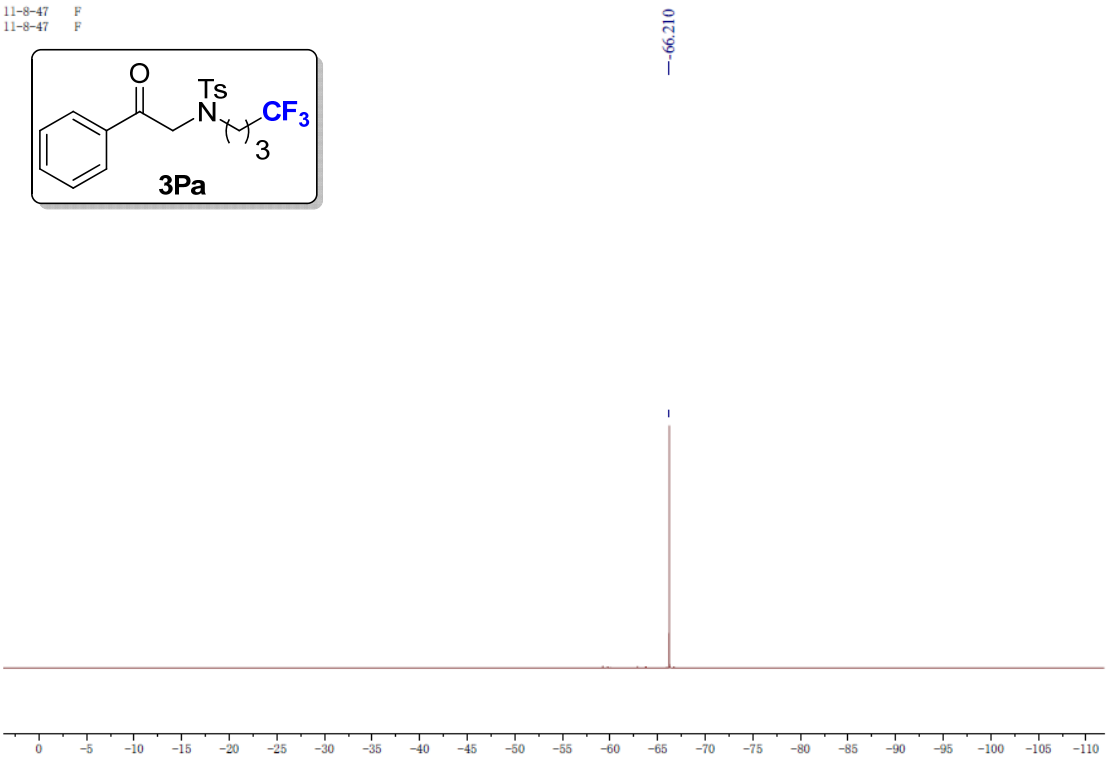

11-8-47 H
11-8-47 H
7.932
7.930
7.916
7.912
7.908
7.723
7.719
7.702
7.633
7.630
7.615
7.599
7.596
7.593
7.506
7.487
7.472
7.468
7.318
7.298
7.260
4.730
3.344
3.326
3.309
2.433
2.161
2.147
2.142
2.134
2.121
2.115
2.107
2.094
2.067
1.802
1.784
1.771
1.764
1.745
1.727
O
Ts
N
CF3
3
3Pa

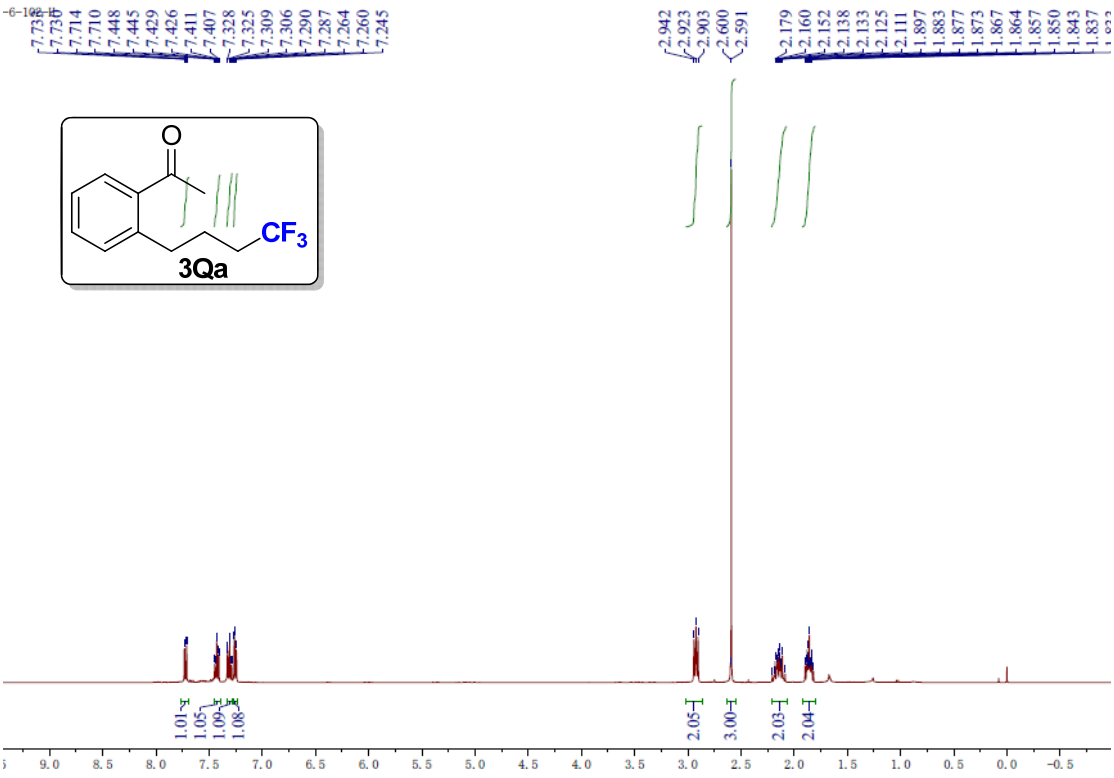

1.98
1.93
0.98
2.00
2.03
2.00
2.03
2.98
2.01
2.04
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0

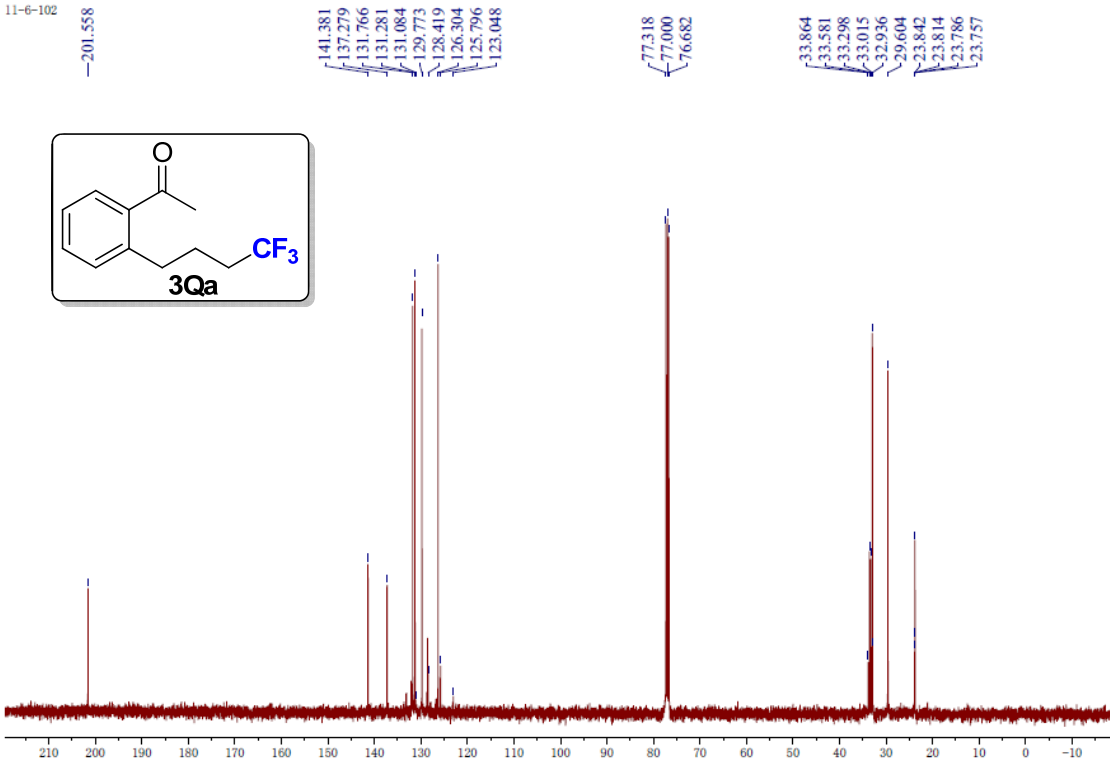

11-8-47 C
11-8-47 C
193.655
143.691
136.221
134.626
133.937
129.635
128.866
128.259
127.984
127.395
125.511
77.317
77.000
76.681
53.216
47.490
31.392
31.102
30.813
30.525
21.517
20.858
20.828
20.802
20.773

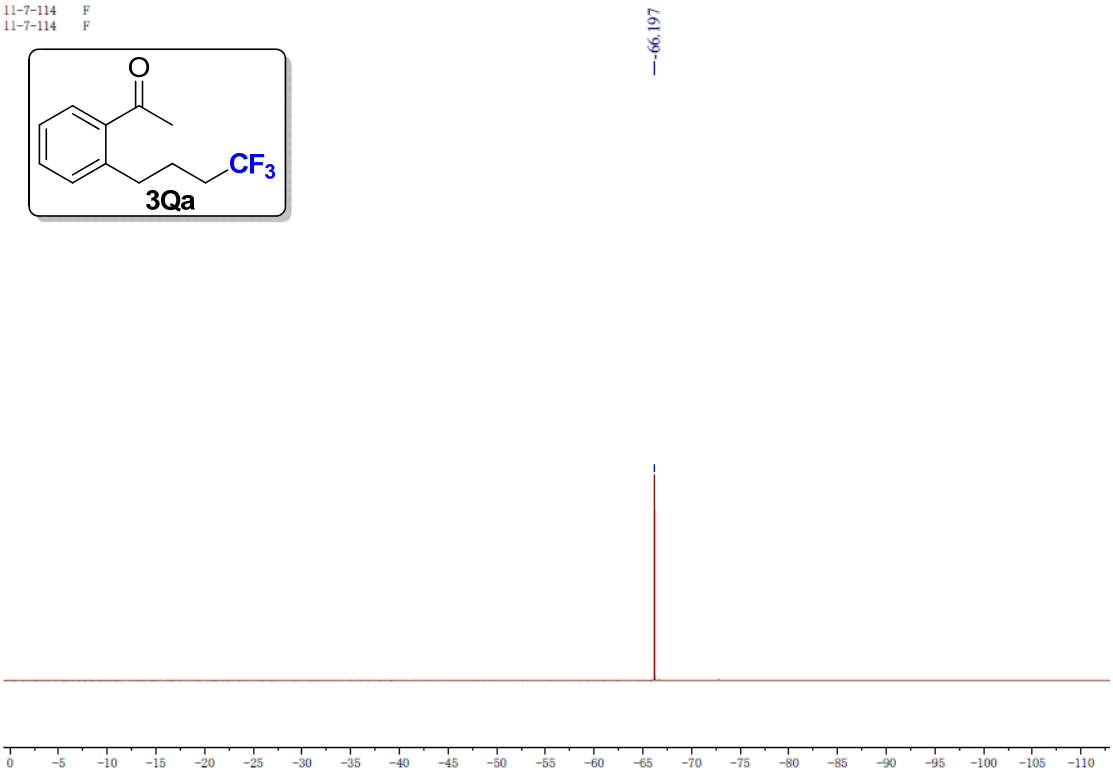

O
Ts
N
CF3
3
3Pa

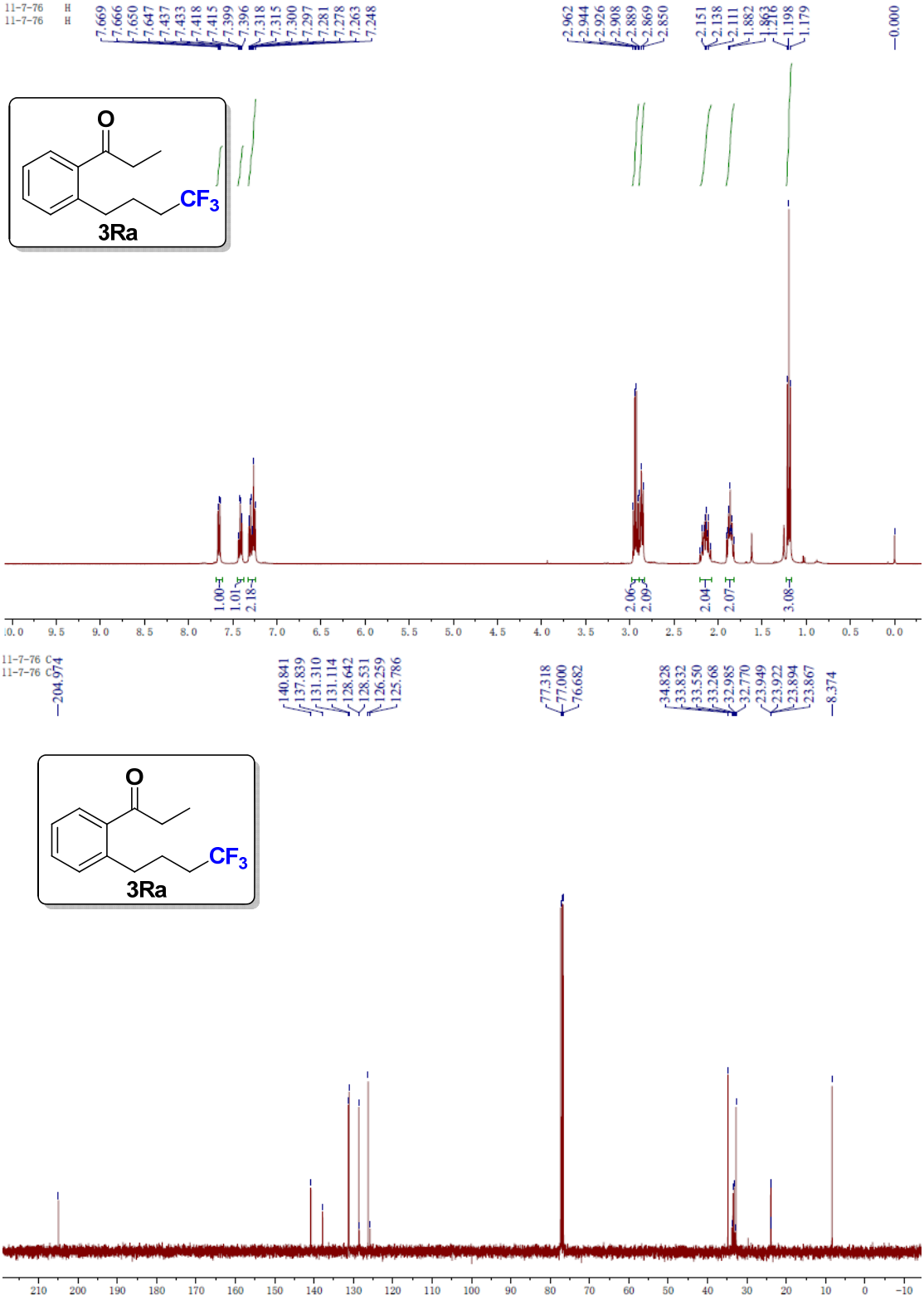

210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10


11-8-47 F
11-8-47 F
O
Ts
N
CF3
3
3Pa
-66.210
0 -5 -10 -15 -20 -25 -30 -35 -40 -45 -50 -55 -60 -65 -70 -75 -80 -85 -90 -95 -100 -105 -110

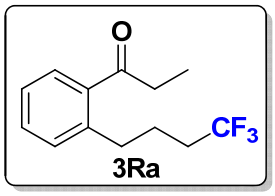

7.738
7.730
7.714
7.710
7.448
7.445
7.429
7.426
7.411
7.407
7.328
7.325
7.309
7.306
7.290
7.287
7.264
7.260
7.245
2.942
2.923
2.903
2.600
2.591
2.179
2.160
2.152
2.138
2.133
2.125
2.111
1.897
1.883
1.877
1.873
1.867
1.864
1.857
1.850
1.843
1.837
O
CF3
3Qa
1.01
1.05
1.09
1.08
2.05
3.00
2.03
2.04
9.0 8.5 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 -0.5


11-6-102
201.558
141.381
137.279
131.766
131.281
131.084
129.773
128.419
126.304
125.796
123.048
77.318
77.000
76.682
33.864
33.581
33.298
33.015
32.936
29.604
23.842
23.814
23.786
23.757
O
CF3
3Qa
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10

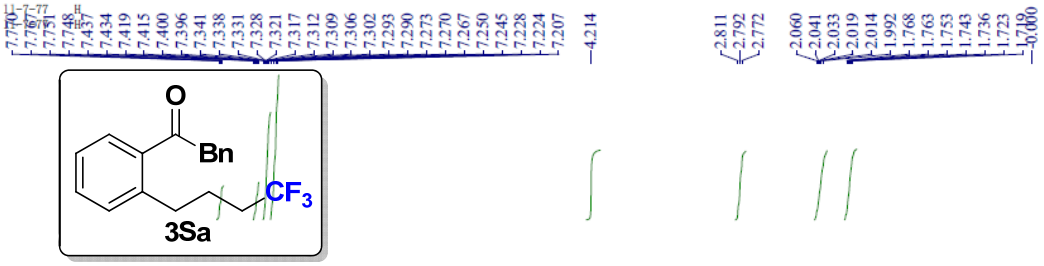

11-7-114 F
11-7-114 F
-66.197
O
CF3
3Qa
0 -5 -10 -15 -20 -25 -30 -35 -40 -45 -50 -55 -60 -65 -70 -75 -80 -85 -90 -95 -100 -105 -110


11-7-76 H
11-7-76 H
7.669
7.666
7.650
7.647
7.437
7.433
7.418
7.415
7.399
7.396
7.318
7.315
7.300
7.297
7.281
7.278
7.263
7.248
2.962
2.944
2.926
2.908
2.889
2.869
2.850
2.151
2.138
2.111
1.882
1.863
1.216
1.198
1.179
0.000
O
CF3
3Ra
1.00
1.01
2.18
2.06
2.09
2.04
2.07
3.08
11-7-76 C
11-7-76 C
204.974
140.841
137.839
131.310
131.114
128.642
128.531
126.259
125.786
77.318
77.000
76.682
34.828
33.832
33.550
33.268
32.985
32.770
23.949
23.922
23.894
23.867
8.374
O
CF3
3Ra

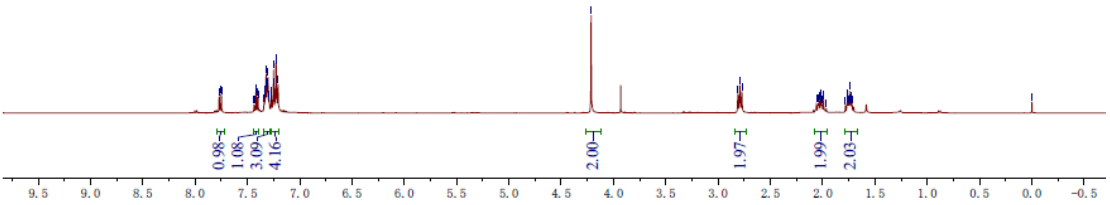
11-7-76 F
11-7-76 F

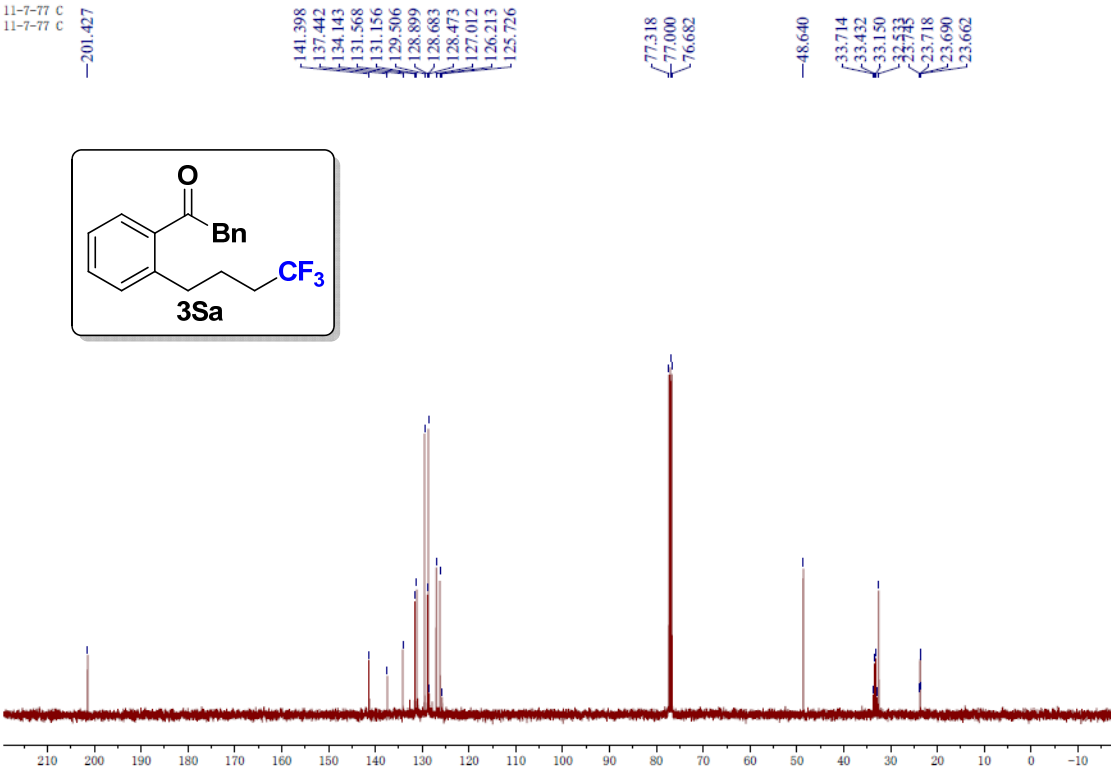


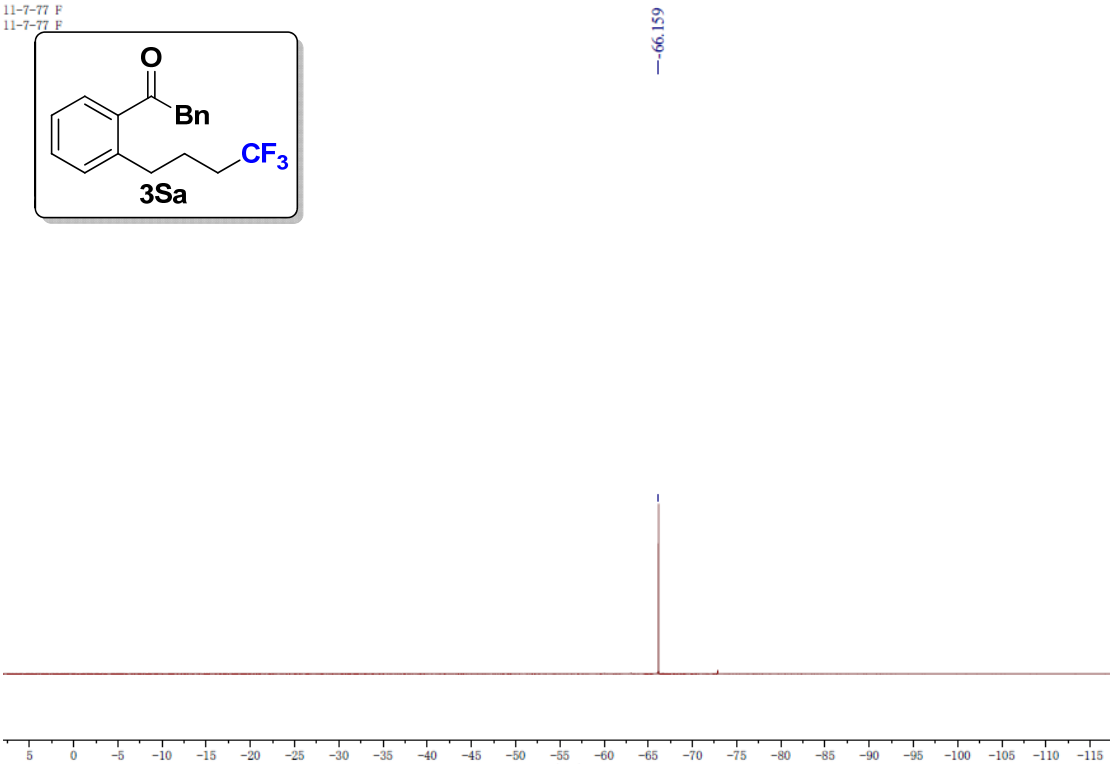
3Ra



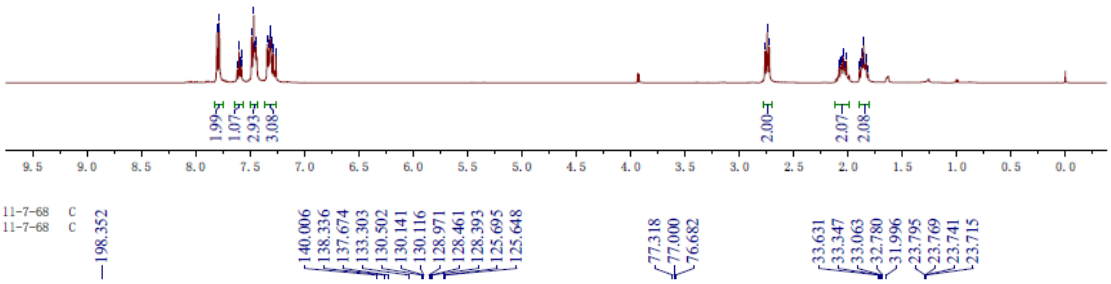
3Sa

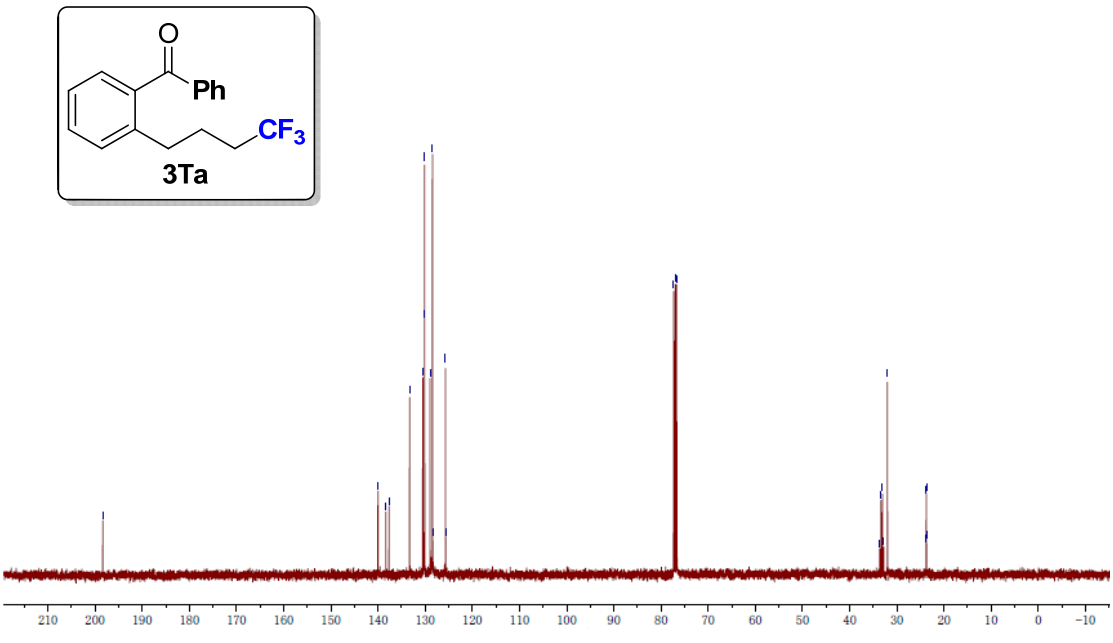



11-7-77 C
11-7-77 C
201.427
141.398
137.442
134.143
131.568
131.156
129.506
128.899
128.683
128.473
127.012
126.213
125.726
77.318
77.000
76.682
48.640
33.714
33.432
33.150
23.718
23.690
23.662
O
Bn
CF3
3Sa
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10


11-7-77 F
11-7-77 F
-66.159
O
Bn
CF3
3Sa
5 0 -5 -10 -15 -20 -25 -30 -35 -40 -45 -50 -55 -60 -65 -70 -75 -80 -85 -90 -95 -100 -105 -110 -115


O
Ph
CF3
3Ta

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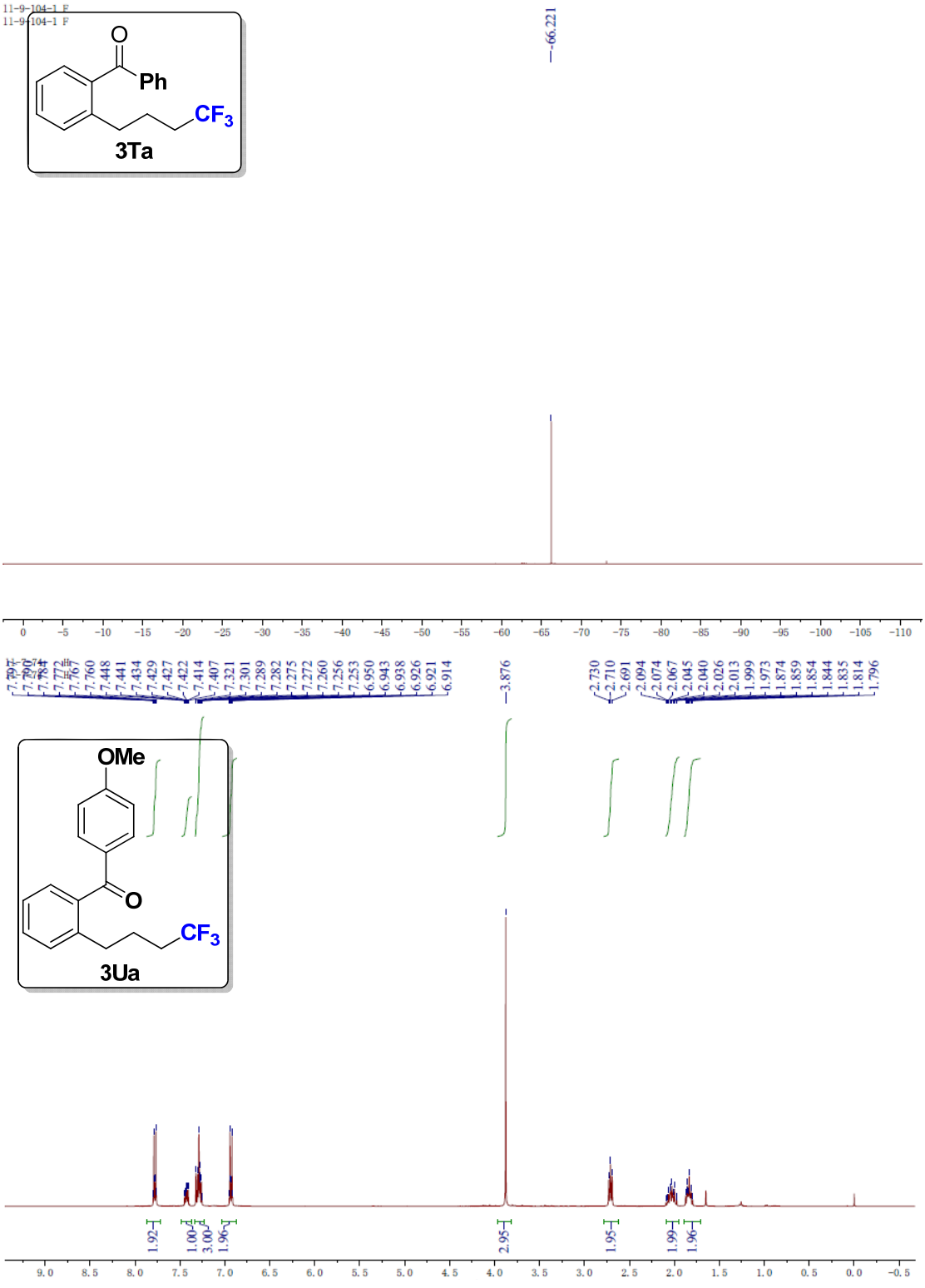
Ph
CF3
3Ta


11-9-104-1 F
11-9-104-1 F
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Ph
CF3
3Ta
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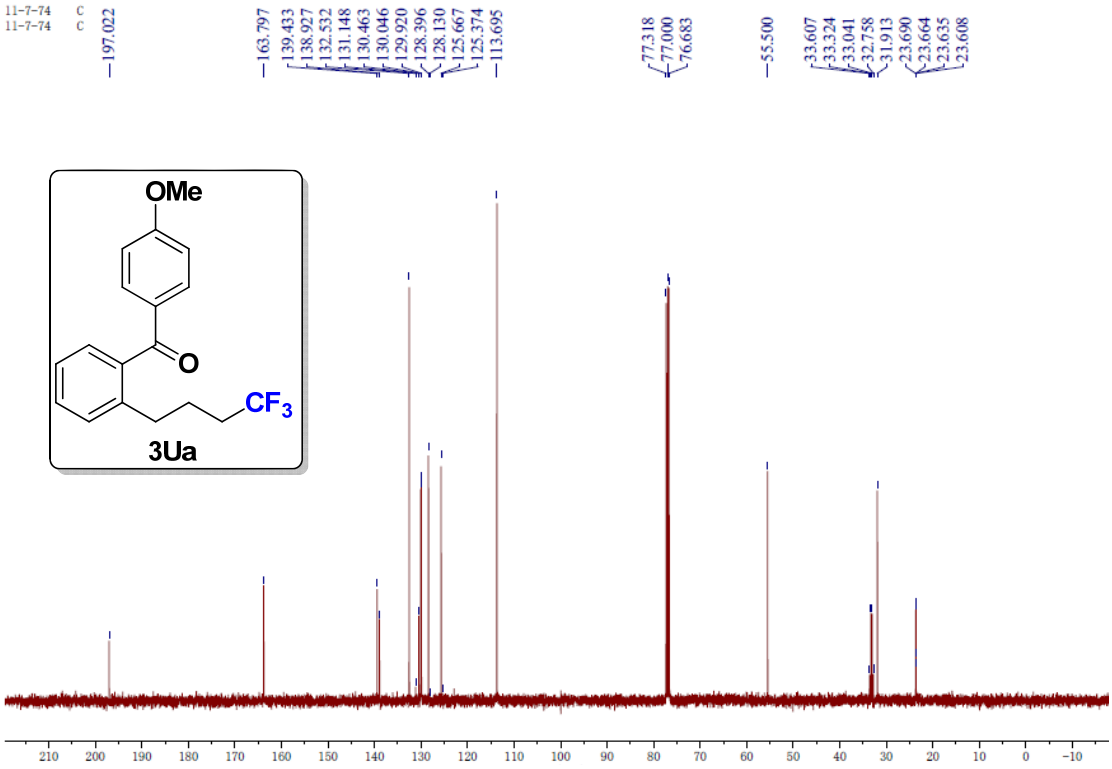
OMe
O
CF3
3Ua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11-7-74 C
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139.433
138.927
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130.463
130.046
129.920
128.396
128.130
125.667
125.374
113.695
77.318
77.000
76.683
55.500
33.607
33.324
33.041
32.758
31.913
23.690
23.664
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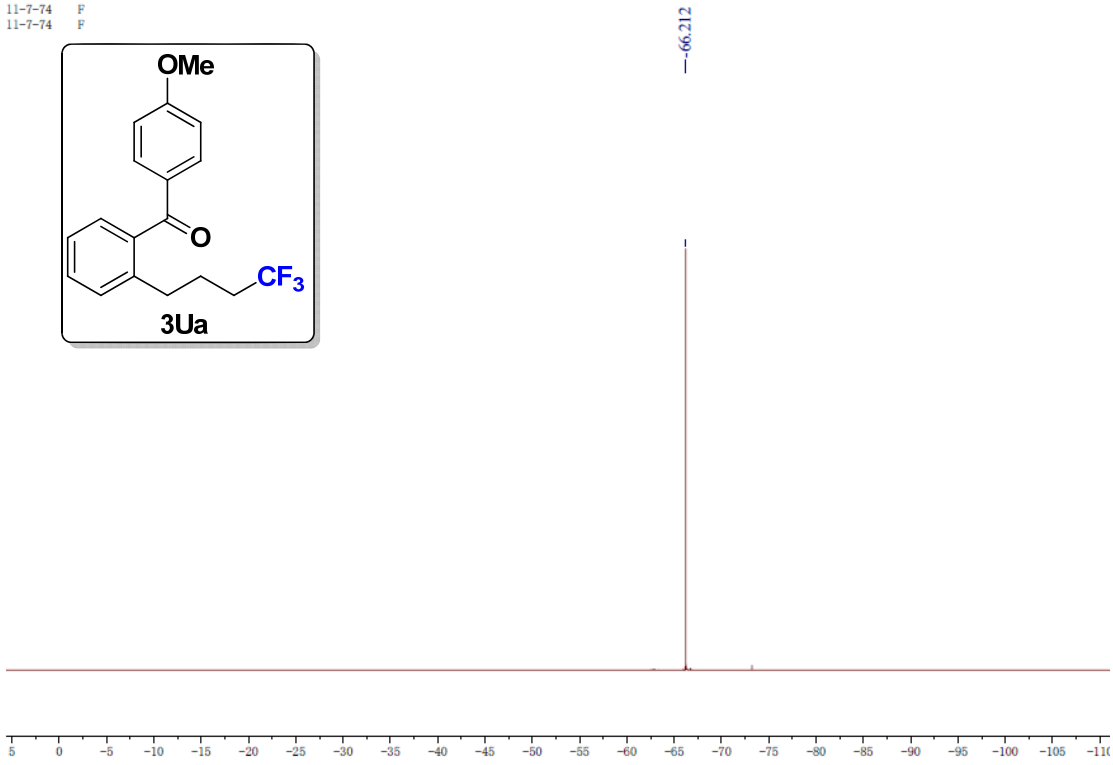
23.608
OMe
O
CF3
3Ua
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10


11-7-74 F
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OMe
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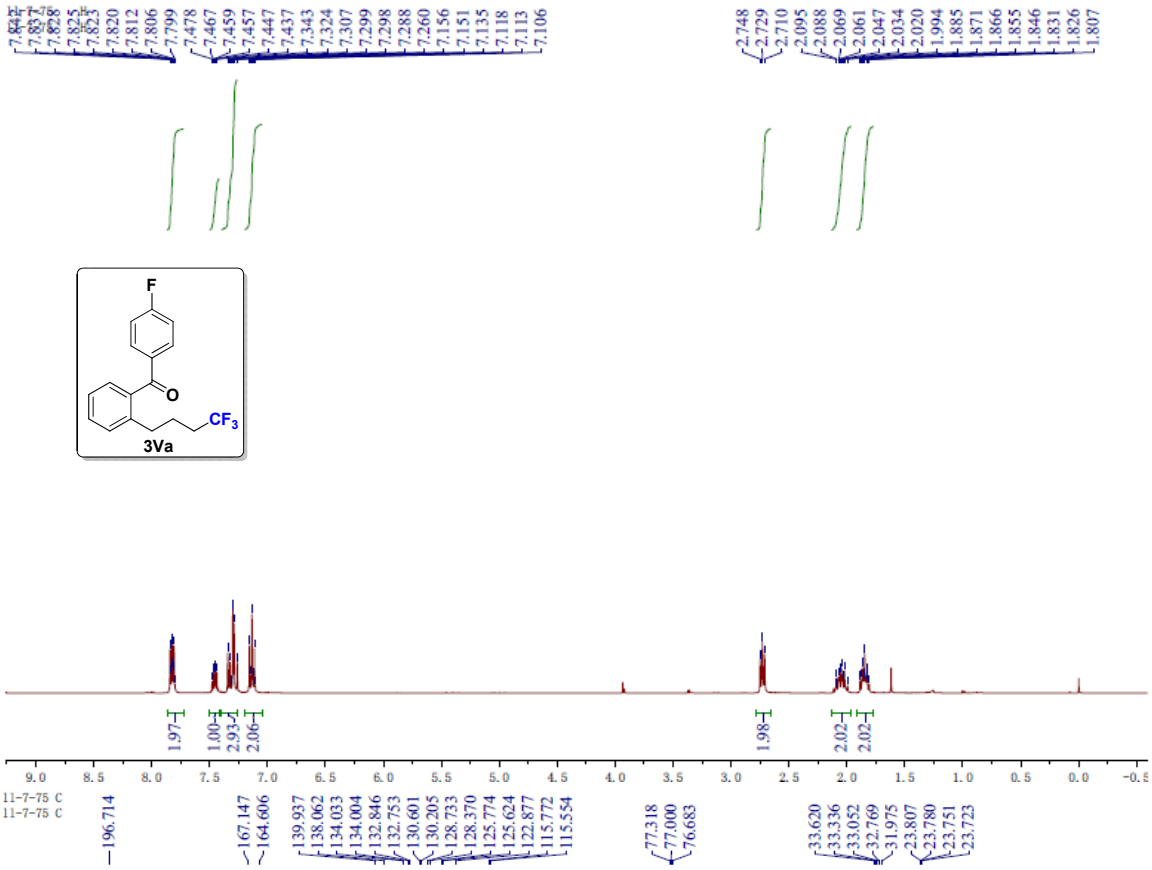
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7.806
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7.459
7.457
7.447
7.437
7.343
7.324
7.307
7.299
7.298
7.288
7.260
7.156
7.151
7.135
7.118
7.113
7.106
2.748
2.729
2.710
2.095
2.088
2.069
2.061
2.047
2.034
2.020
1.994
1.885
1.871
1.866
1.855
1.846
1.831
1.826
1.807
F
O
CF3
3Va
1.97
1.00
2.93
2.06
1.98
2.02
2.02
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
11-7-75 C
11-7-75 C
196.714
167.147
164.606
139.937
138.062
134.033
134.004
132.846
132.753
130.601
130.205
128.733
128.370
125.774
125.624
122.877
115.772
115.554
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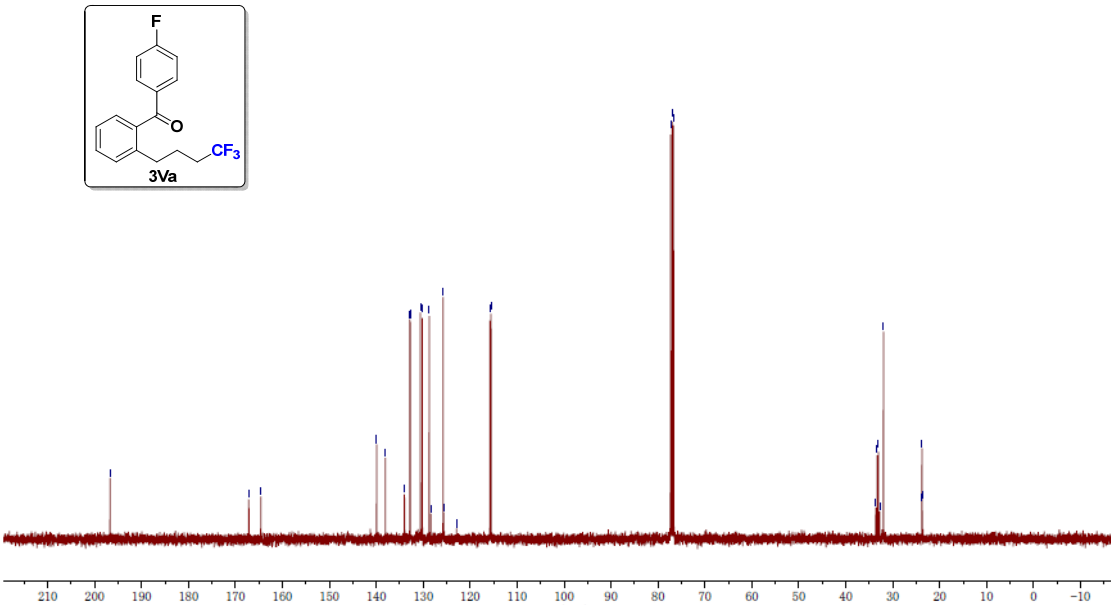
33.620
33.336
33.052
32.769
31.975
23.807
23.780
23.751
23.723


F
O
CF3
3Va
210
200
190
180
170
160
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140
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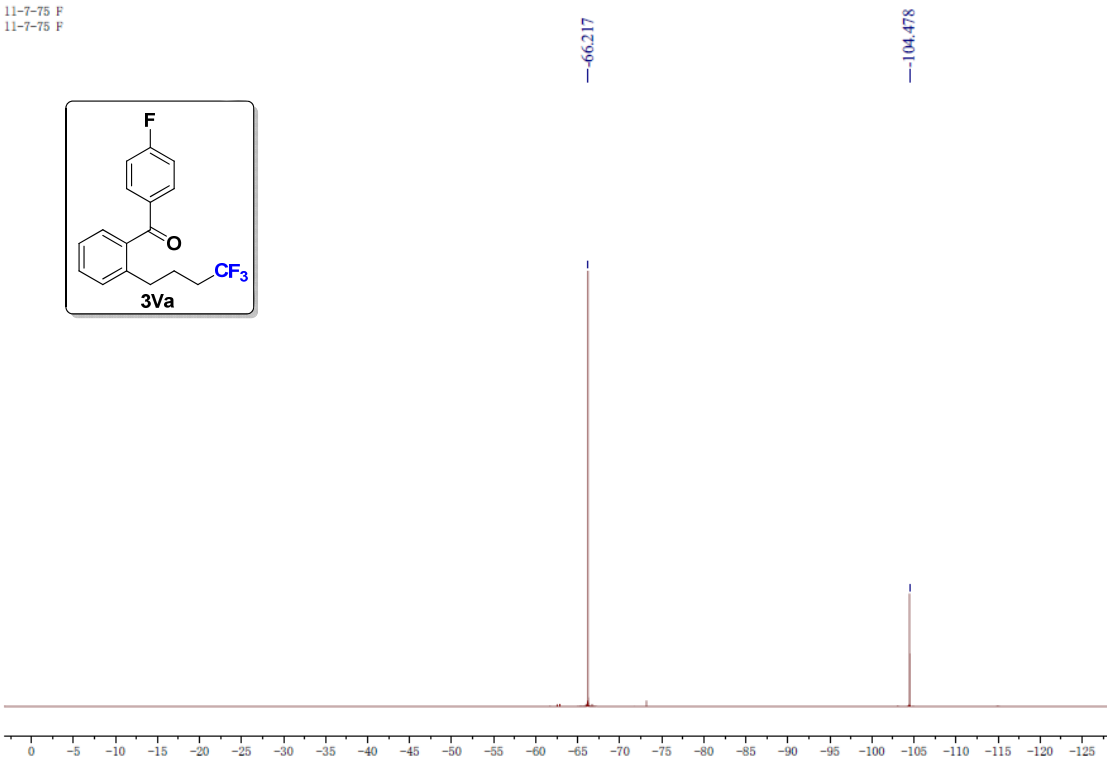
120
110
100
90
80
70
60
50
40
30
20
10
0
-10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11-7-75 F
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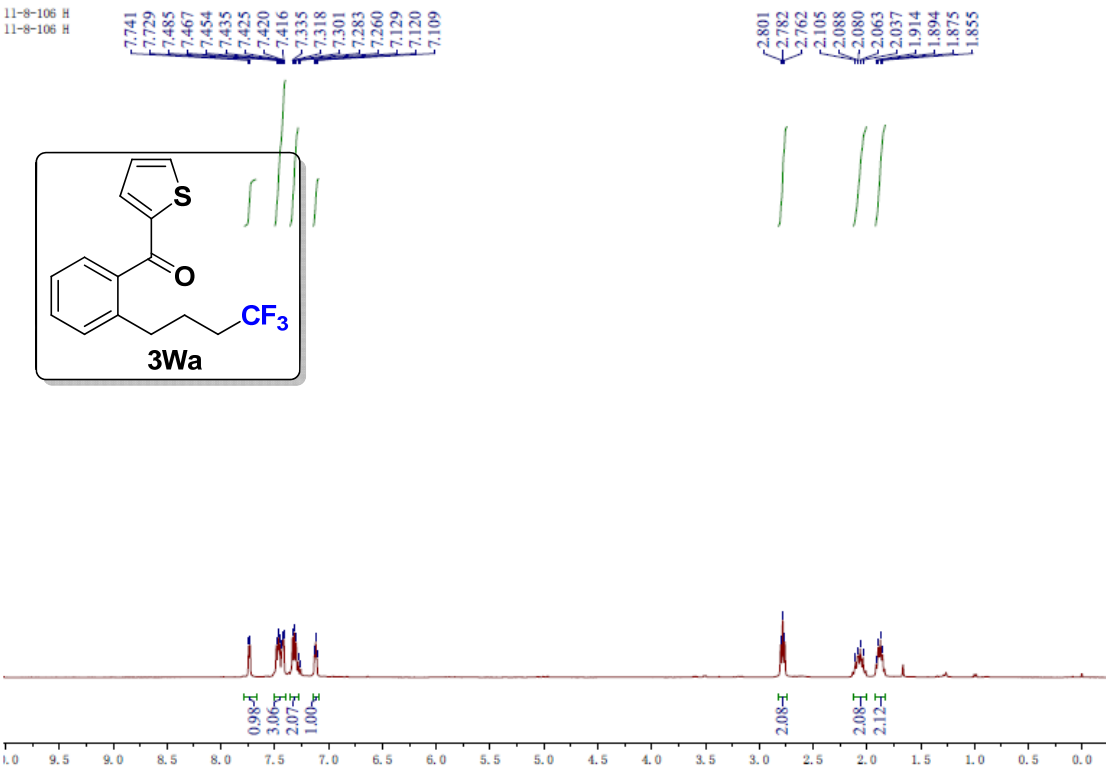
-104.478
F
O
CF3
3Va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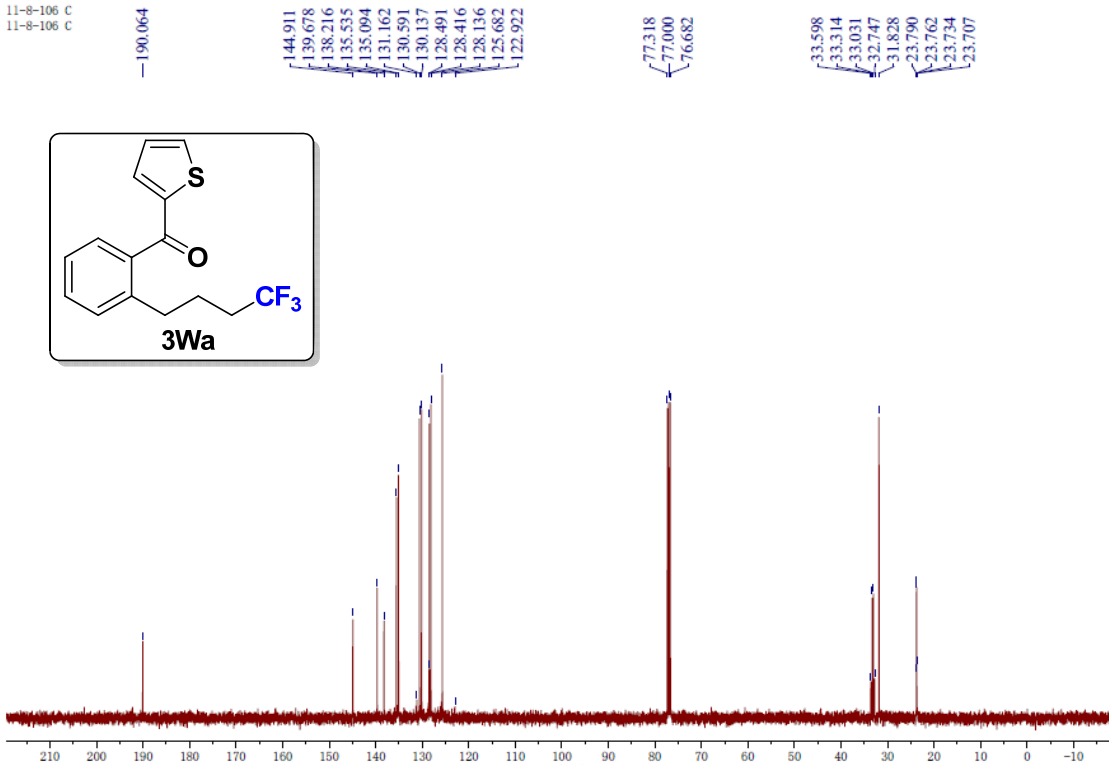
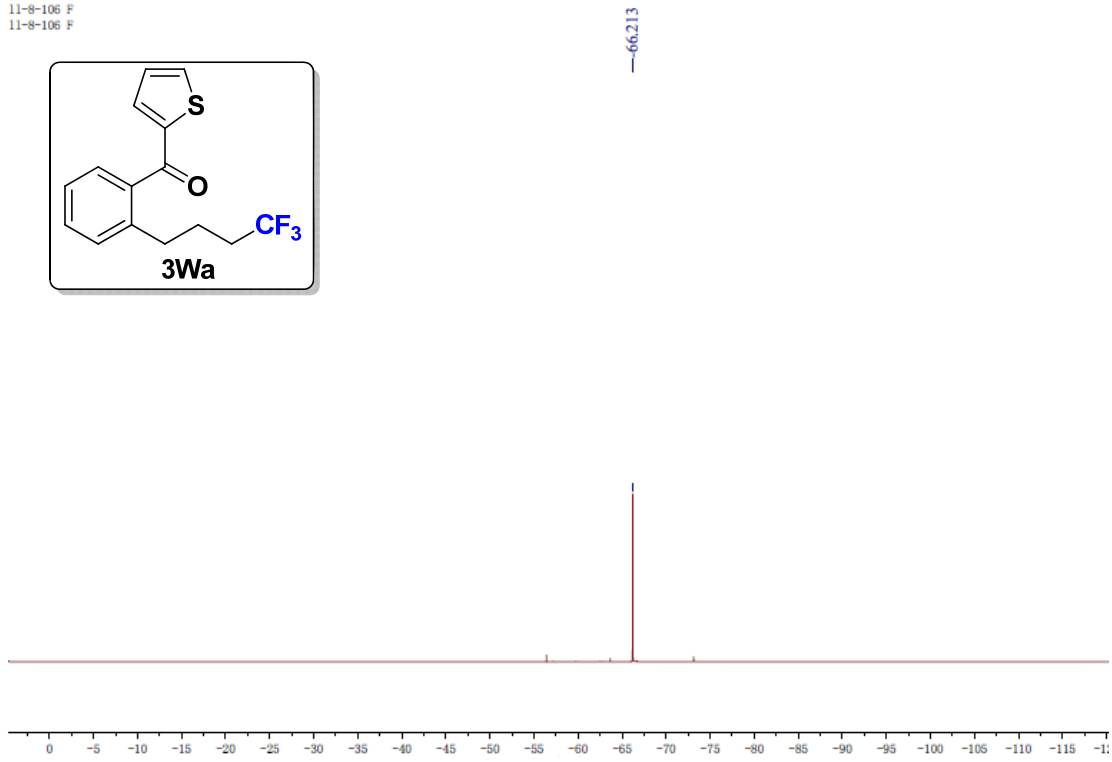
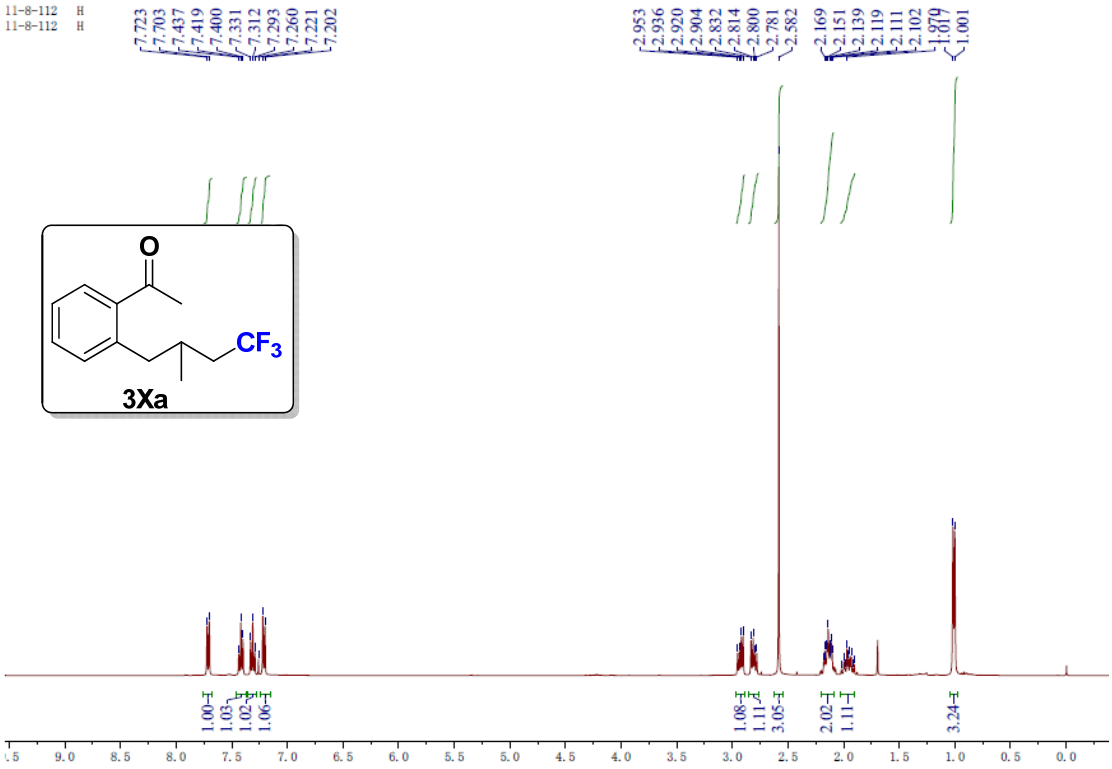
7.729
7.485
7.467
7.454
7.435
7.425
7.420
7.416
7.335
7.318
7.301
7.283
7.260
7.129
7.120
7.109
2.801
2.782
2.762
2.105
2.088
2.080
2.063
2.037
1.914
1.894
1.875
1.855
S
O
CF3
3Wa
0.98
3.06
2.07
1.00
2.08
2.08
2.12

11-8-106 C
11-8-106 C



11-8-106 F
11-8-106 F




11-8-112 H
11-8-112 H
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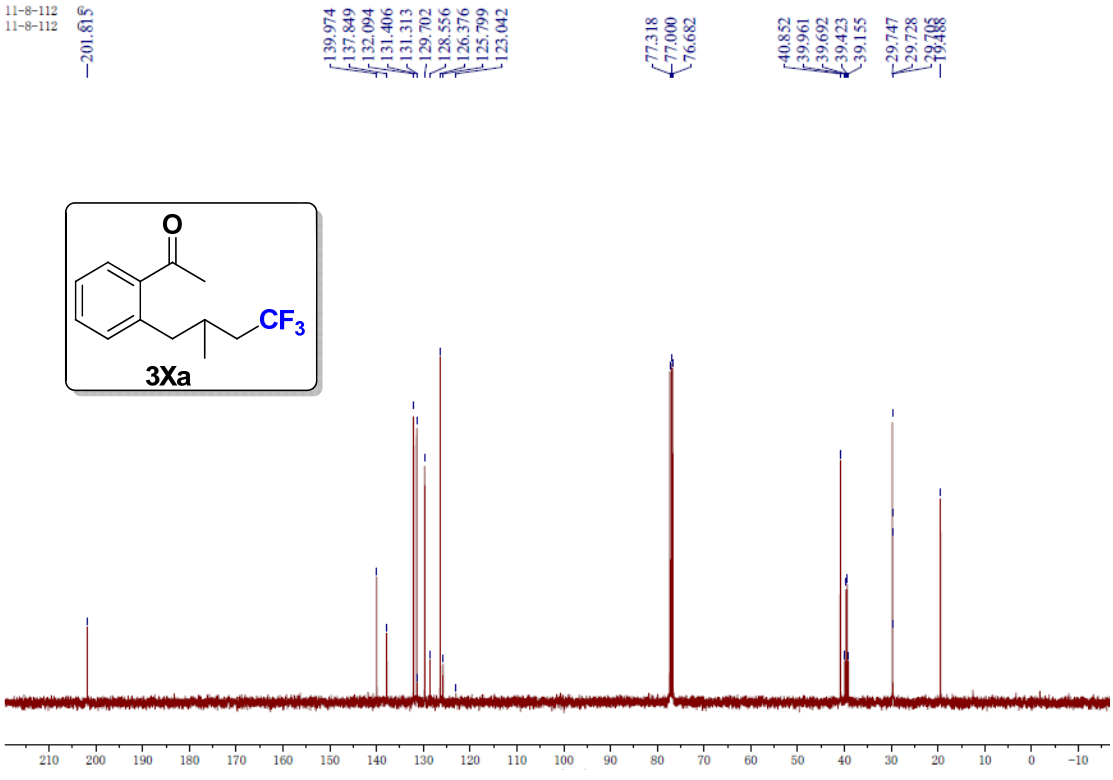
7.703
7.437
7.419
7.400
7.331
7.312
7.293
7.260
7.221
7.202
2.953
2.936
2.920
2.904
2.832
2.814
2.800
2.781
2.582
2.169
2.151
2.139
2.119
2.111
2.102
1.979
1.017
1.001
O
CF3
3Xa
1.00
1.03
1.02
1.06
1.08
1.11
3.05
2.02
1.11
3.24


11-8-112 C
11-8-112 C
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132.094
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131.313
129.702
128.556
126.376
125.799
123.042
77.318
77.000
76.682
40.852
39.961
39.692
39.423
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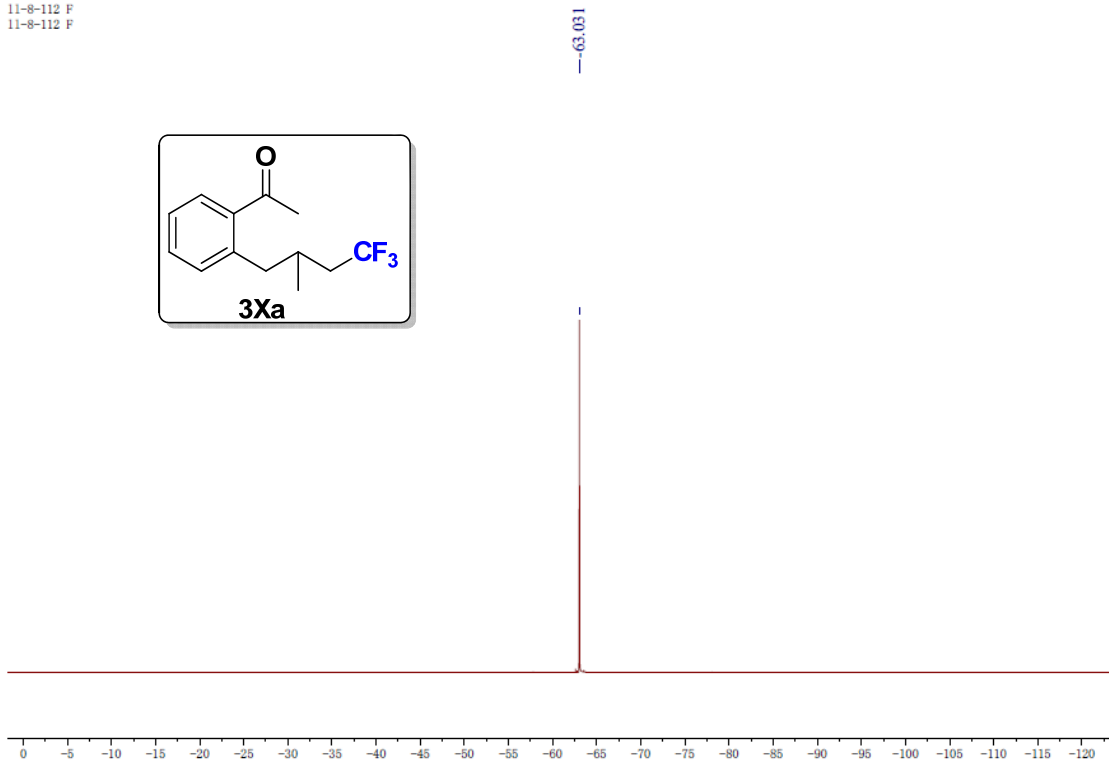
29.747
29.728
O
CF3
3Xa


11-8-112 F
11-8-112 F
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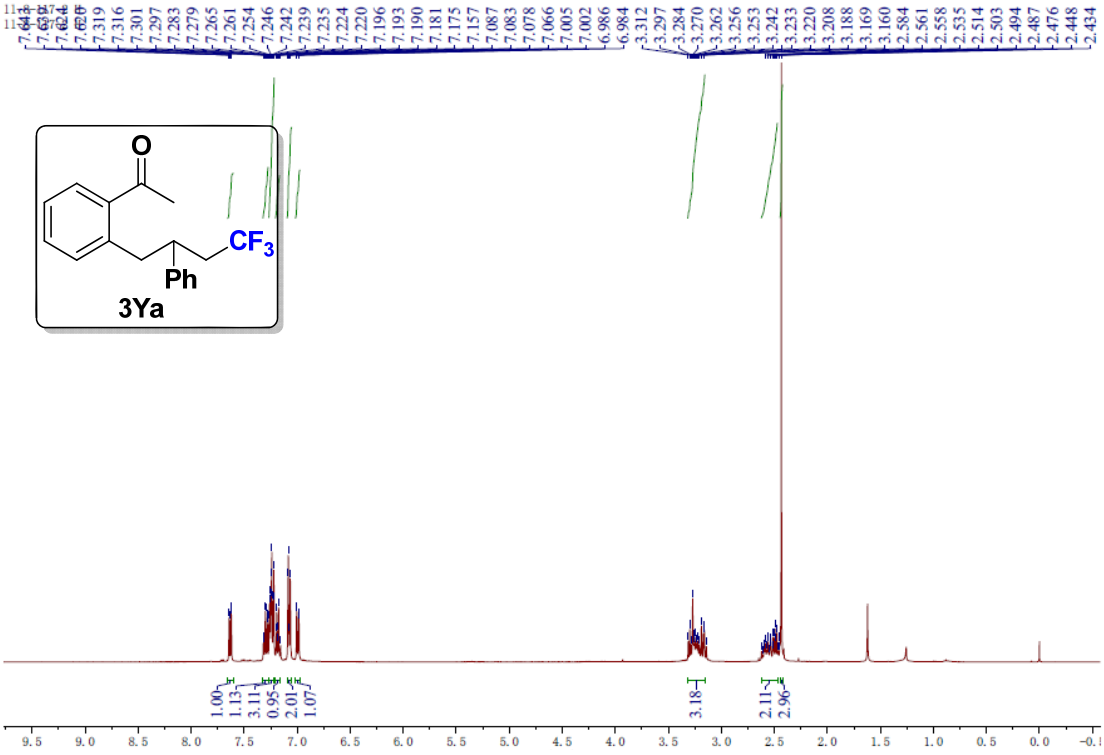
CF3
3Xa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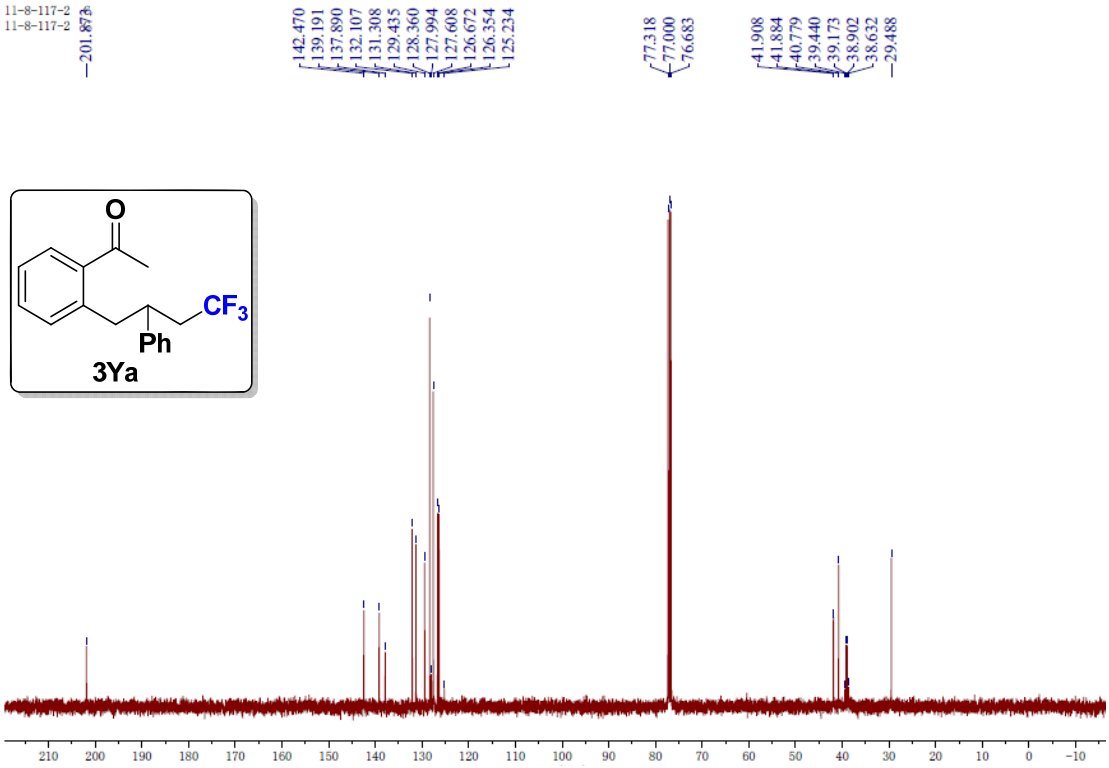
CF3
Ph
3Ya


11-8-117-2
11-8-117-2
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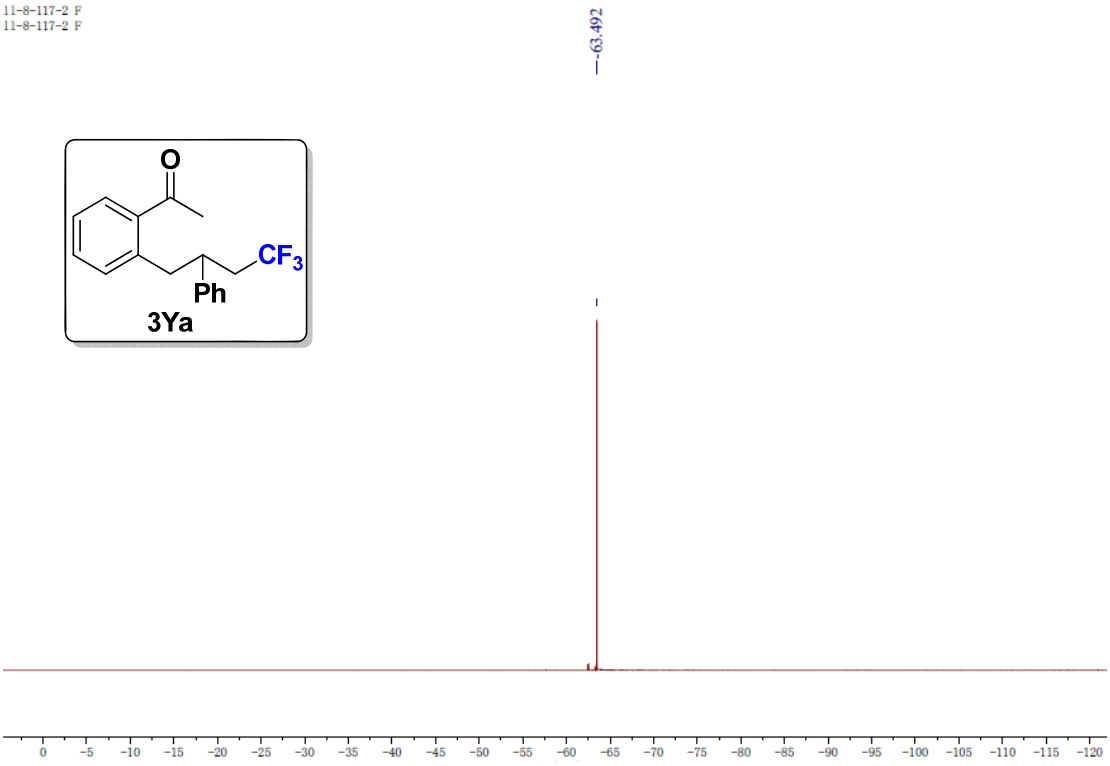
139.191
137.890
132.107
131.308
129.435
128.360
127.994
127.608
126.672
126.354
125.234
77.318
77.000
76.683
41.908
41.884
40.779
39.440
39.173
38.902
38.632
29.488
O
CF3
Ph
3Ya
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10


11-8-117-2 F
11-8-117-2 F
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O
CF3
Ph
3Ya
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-30
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-40
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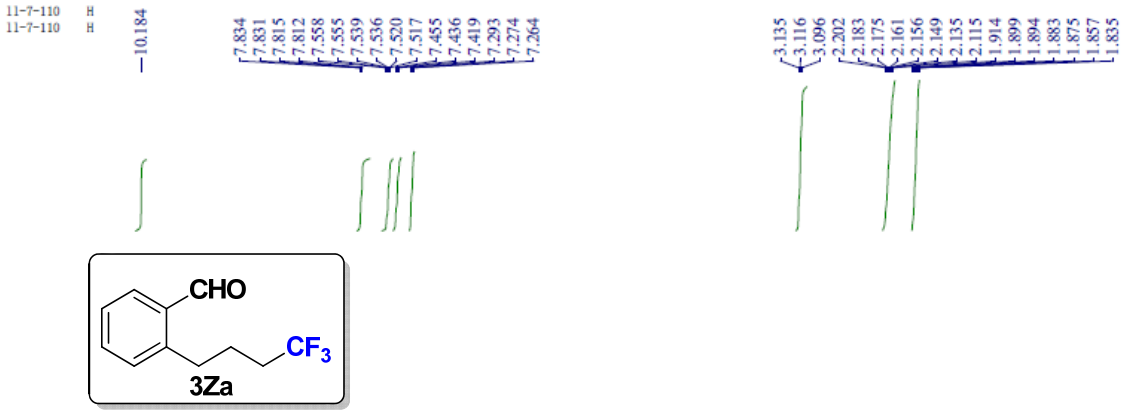
-110
-115
-120


11-7-110 H
11-7-110 H
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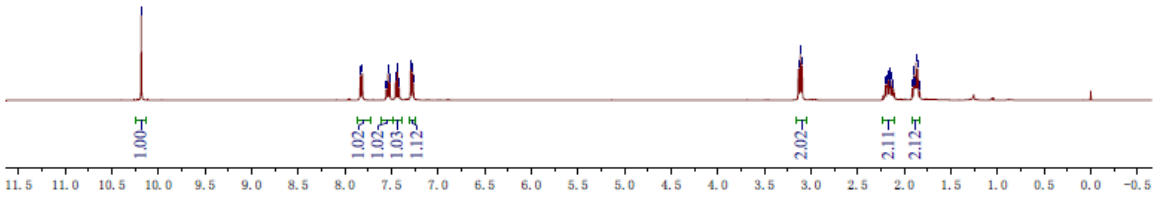
7.558
7.555
7.539
7.536
7.520
7.517
7.455
7.436
7.419
7.293
7.274
7.264
3.135
3.116
3.096
2.202
2.183
2.175
2.161
2.156
2.149
2.135
2.115
1.914
1.899
1.894
1.883
1.875
1.857
1.835
CHO
CF3
3Za


1.00
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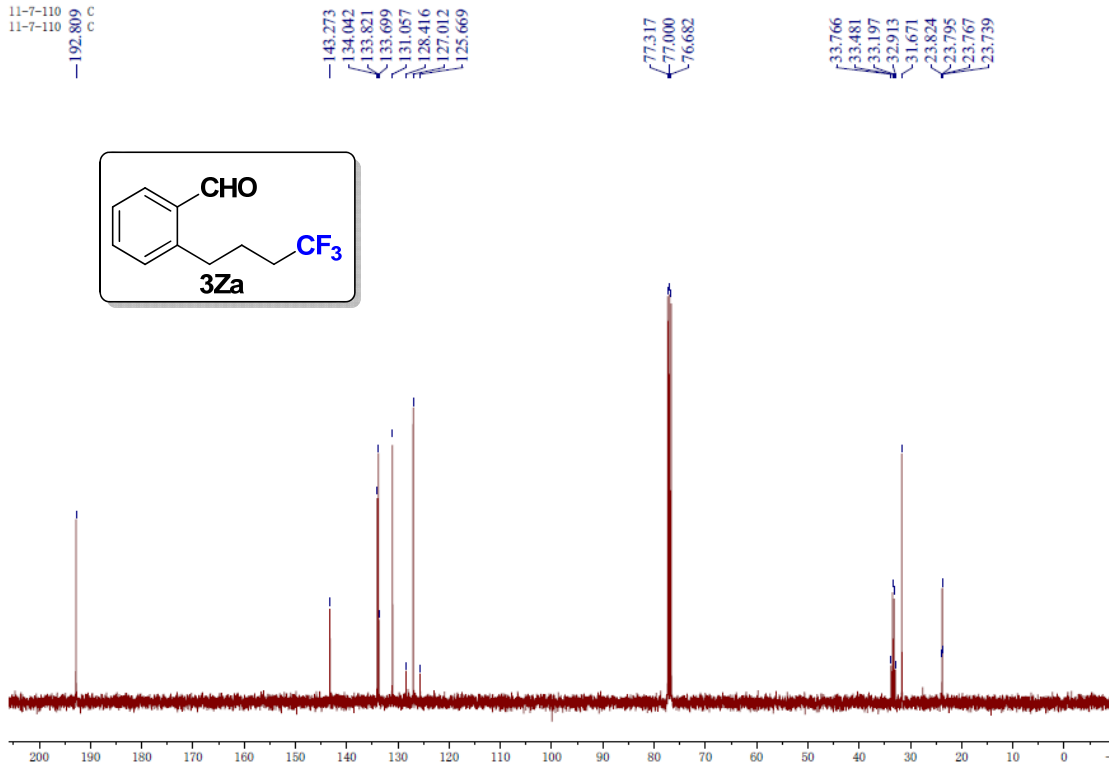
1.02
1.03
1.12
2.02
2.11
2.12


11-7-110 C
11-7-110 C
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133.821
133.699
131.057
128.416
127.012
125.669
77.317
77.000
76.682
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33.197
32.913
31.671
23.824
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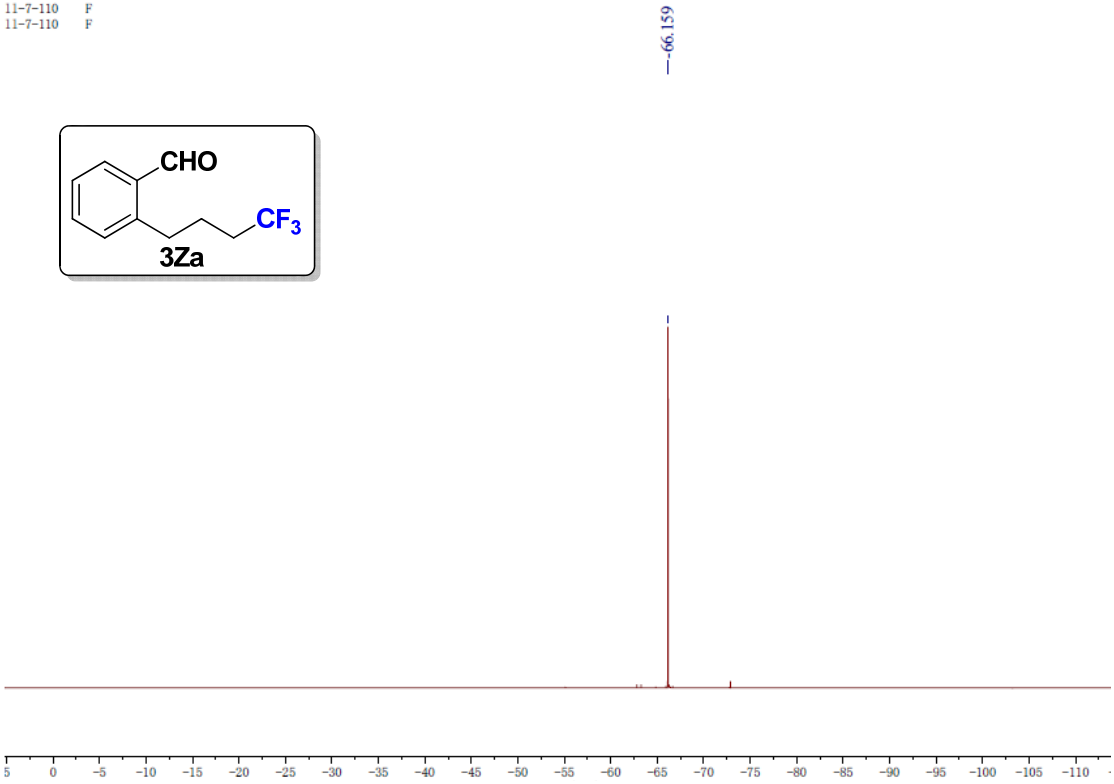
23.767
23.739
CHO
CF3
3Za


11-7-110 F
11-7-110 F
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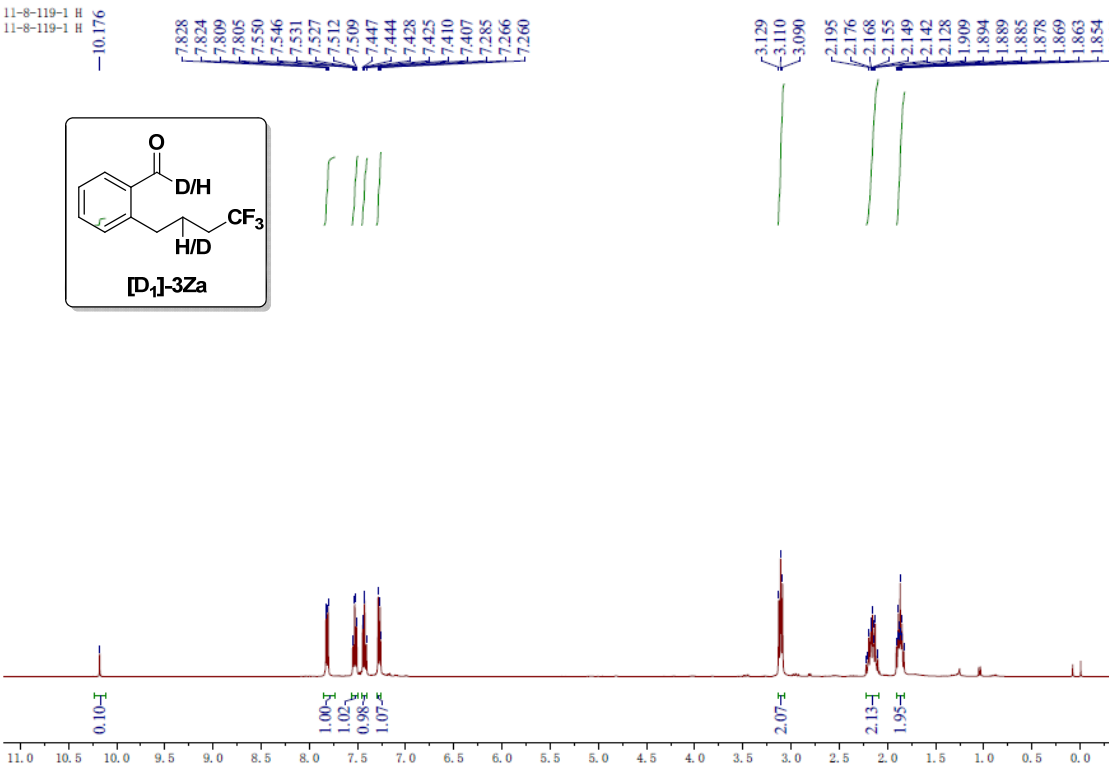
CHO
CF3
3Za


11-8-119-1 H
11-8-119-1 H
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7.824
7.809
7.805
7.550
7.546
7.531
7.527
7.512
7.509
7.447
7.444
7.428
7.425
7.410
7.407
7.285
7.266
7.260
3.129
3.110
3.090
2.195
2.176
2.168
2.155
2.149
2.142
2.128
1.909
1.894
1.889
1.885
1.878
1.869
1.863
1.854
O
D/H
CF3
H/D
[D1]-3Za
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1.02
0.98
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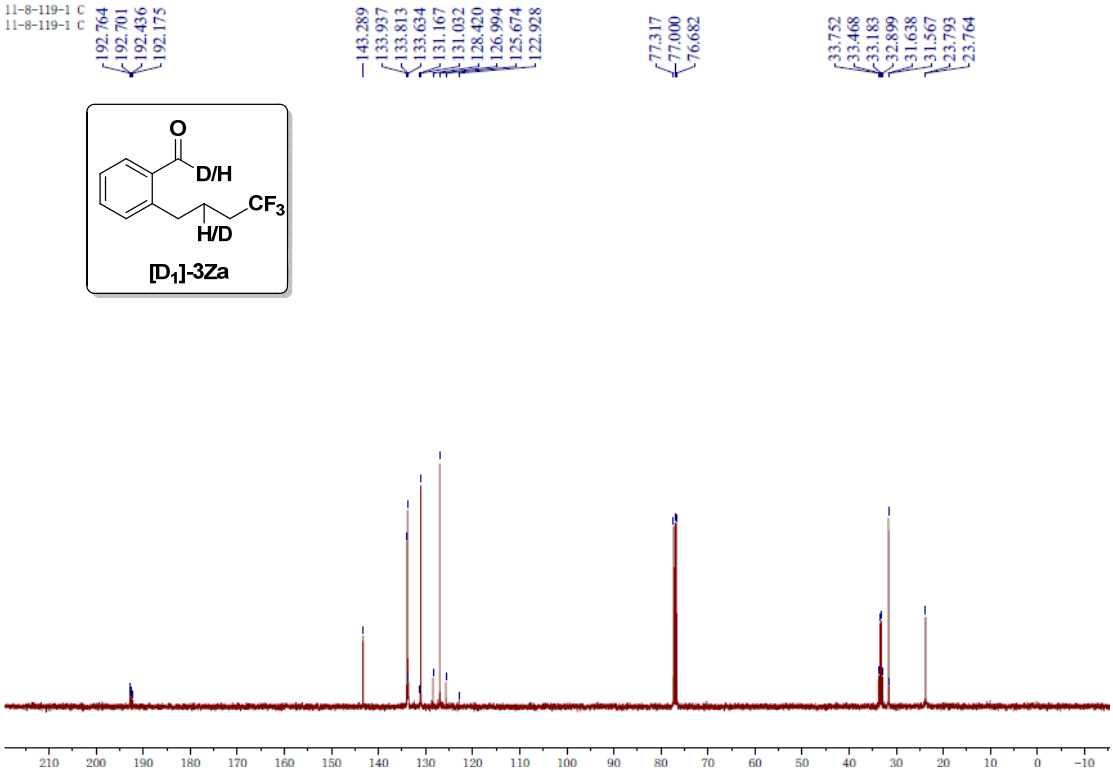
2.13
1.95


11-8-119-1 C
11-8-119-1 C
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192.175
143.289
133.937
133.813
133.634
131.167
131.032
128.420
126.994
125.674
122.928
77.317
77.000
76.682
33.752
33.468
33.183
32.899
31.638
31.567
23.793
23.764
O
D/H
CF3
H/D
[D1]-3Za
210
200
190
180
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120
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100
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80
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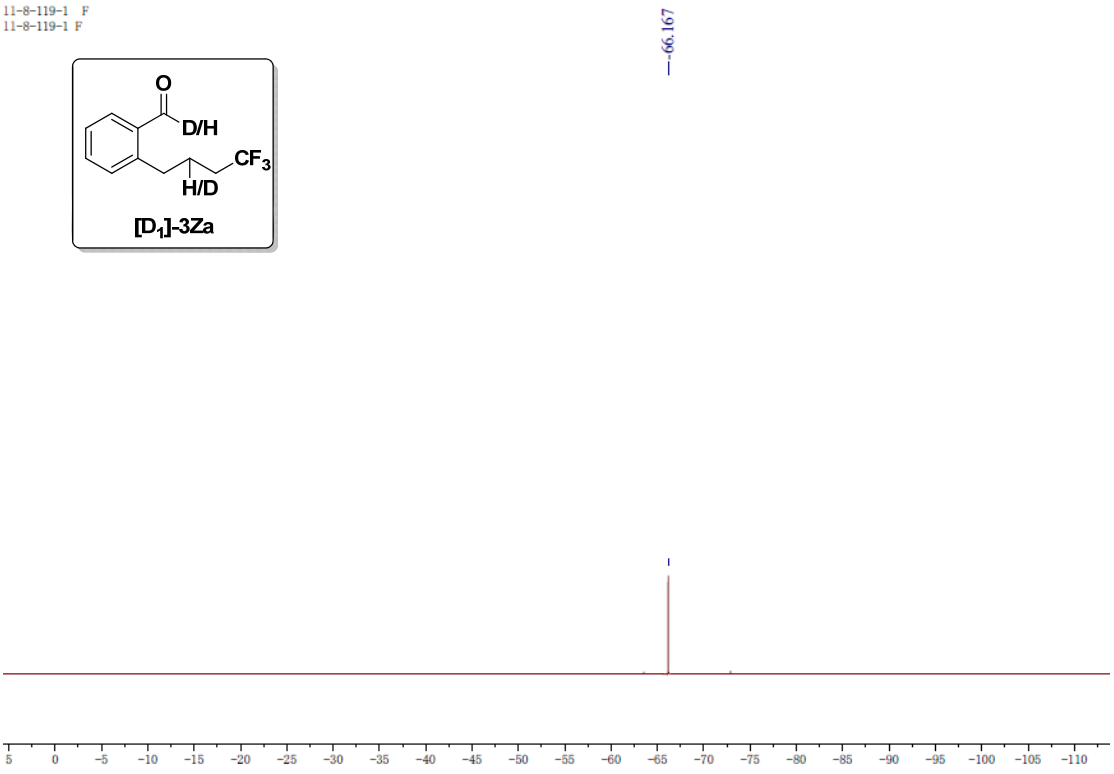
10
0
-10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11-8-119-1 F
-66.167
O
D/H
CF3
H/D
[D1]-3Za
5
0
-5
-10
-15
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-25
-30
-35
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-55
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-70
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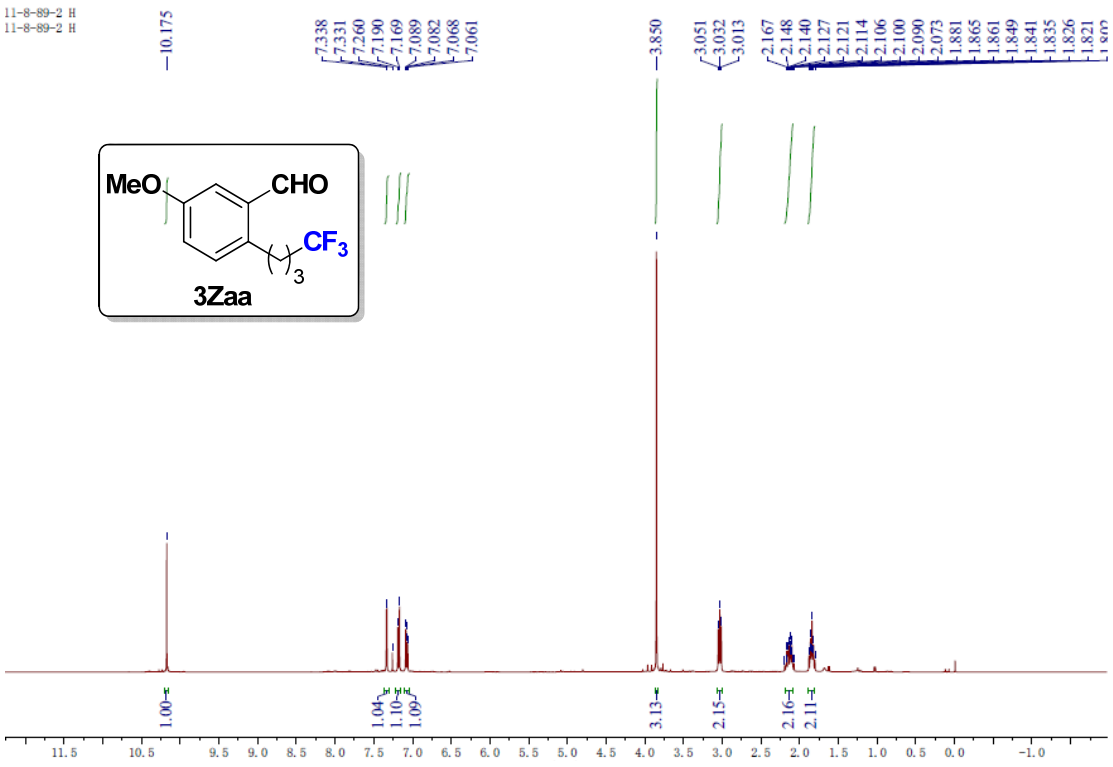
-85
-90
-95
-100
-105
-110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11-8-89-2 H
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7.169
7.089
7.082
7.068
7.061
3.850
3.051
3.032
3.013
2.167
2.148
2.140
2.127
2.121
2.114
2.106
2.100
2.090
2.073
1.881
1.865
1.861
1.849
1.841
1.835
1.826
1.821
MeO
CHO
CF3
3
3Zaa
1.00
1.04
1.10
1.09
3.13
2.15
2.16
2.11
11.5
10.5
9.5
9.0
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8.0
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6.5
6.0
5.5
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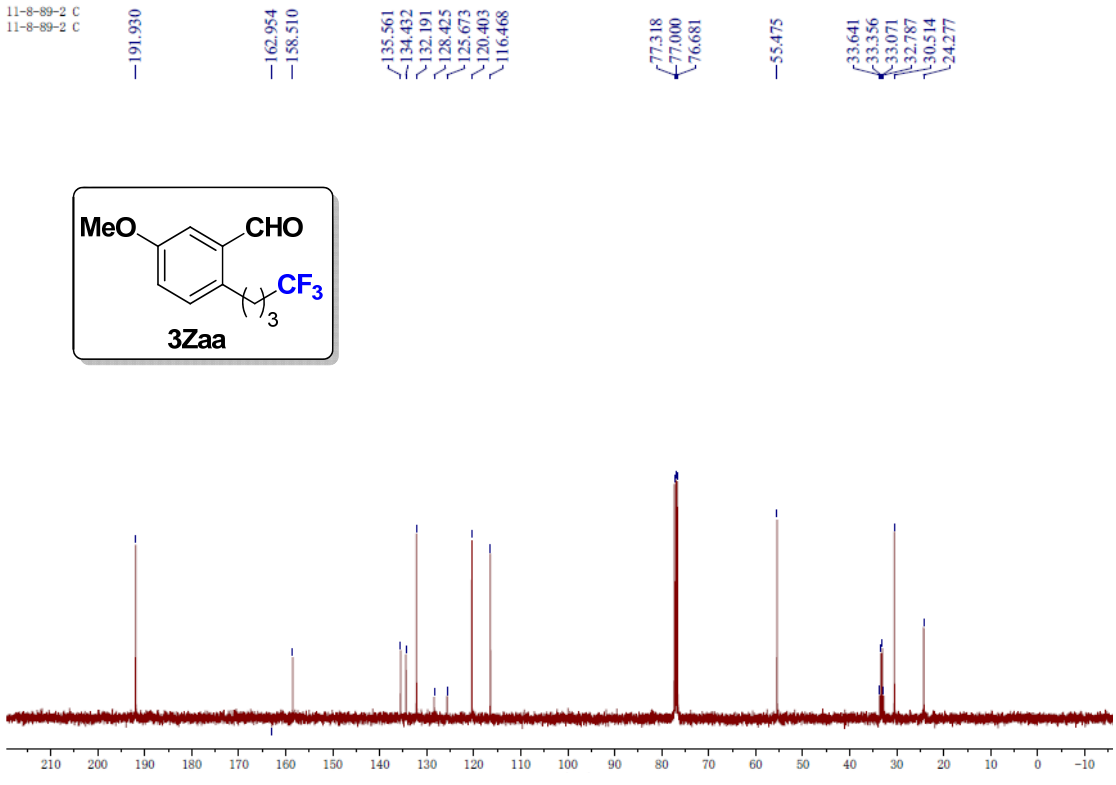
0.0
-1.0


11-8-89-2 C
11-8-89-2 C
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134.432
132.191
128.425
125.673
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116.468
77.318
77.000
76.681
55.475
33.641
33.356
33.071
32.787
30.514
24.277
MeO
CHO
CF3
3
3Zaa
210
200
190
180
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130
120
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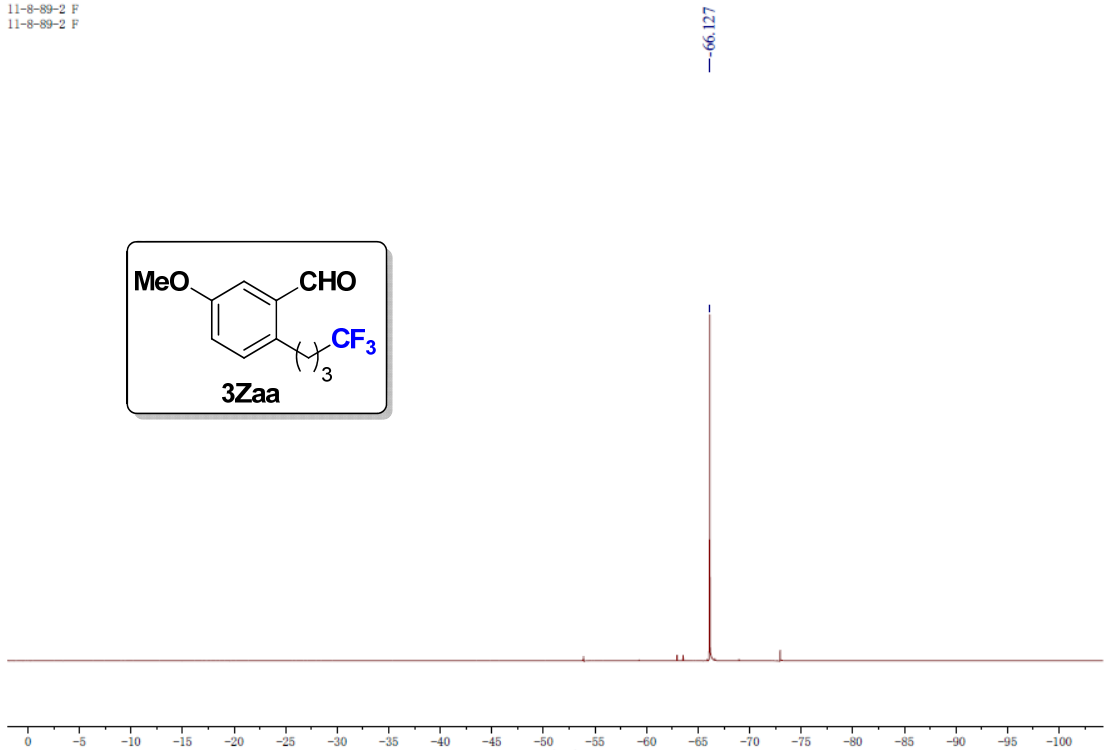
100
90
80
70
60
50
40
30
20
10
0
-10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11-8-89-2 F
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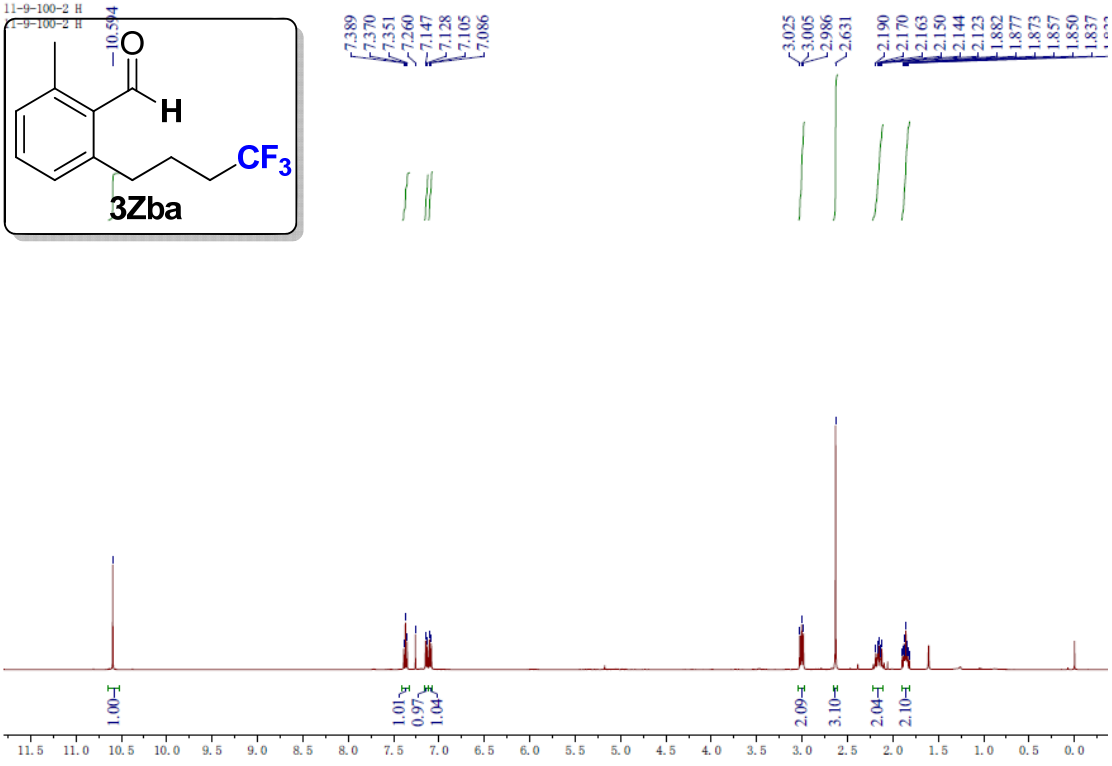
CHO
CF3
3
3Zaa


11-9-100-2 H
11-9-100-2 H
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O
H
CF3
3Zba
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7.351
7.260
7.147
7.128
7.105
7.086
3.025
3.005
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2.631
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2.123
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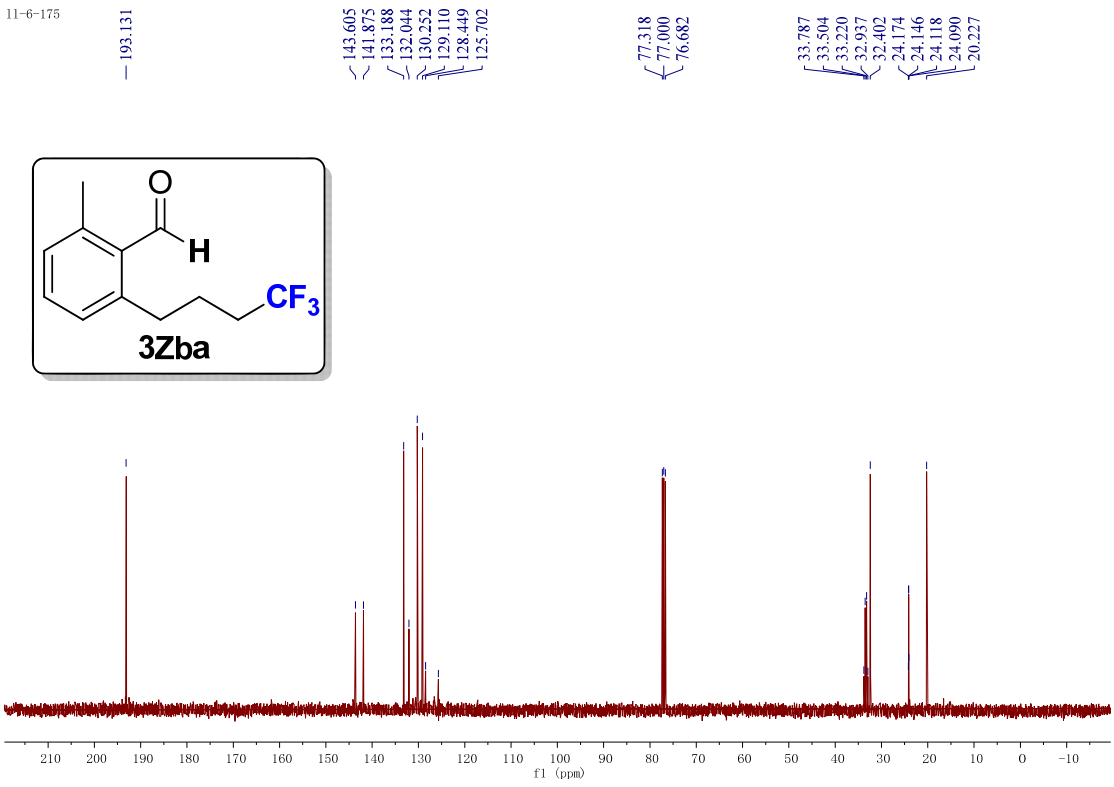
1.01
0.97
1.04
2.09
3.10
2.04
2.10


11-6-175
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141.875
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130.252
129.110
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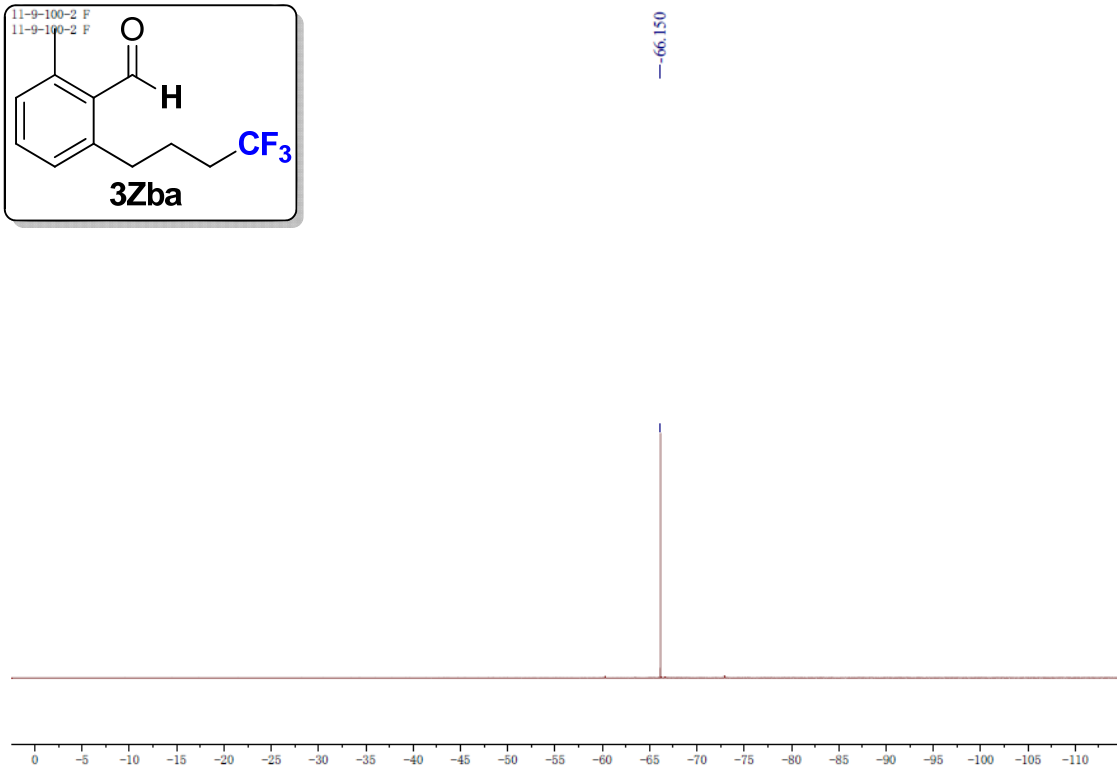
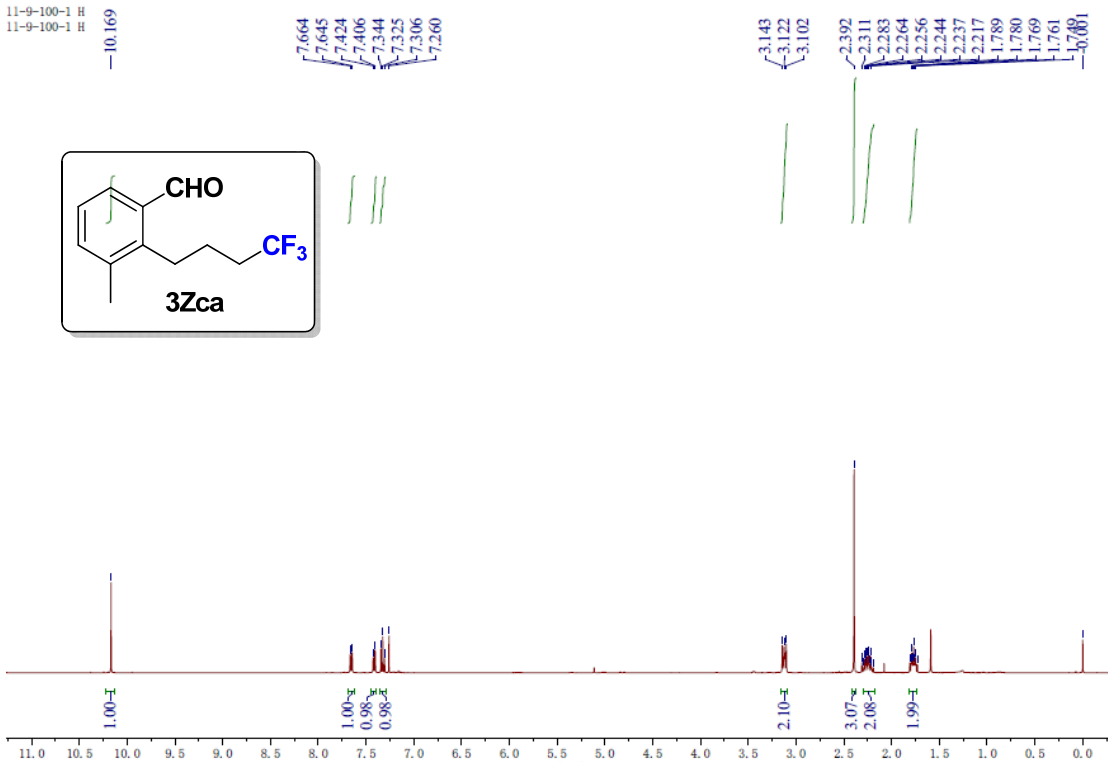
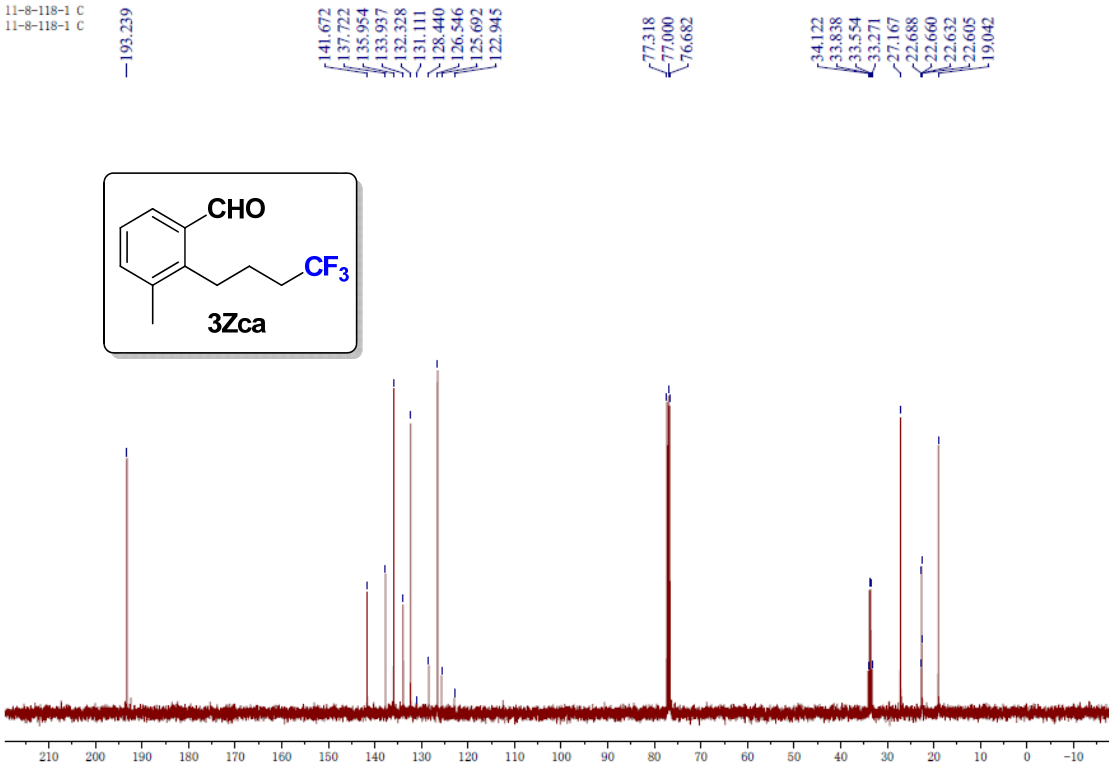
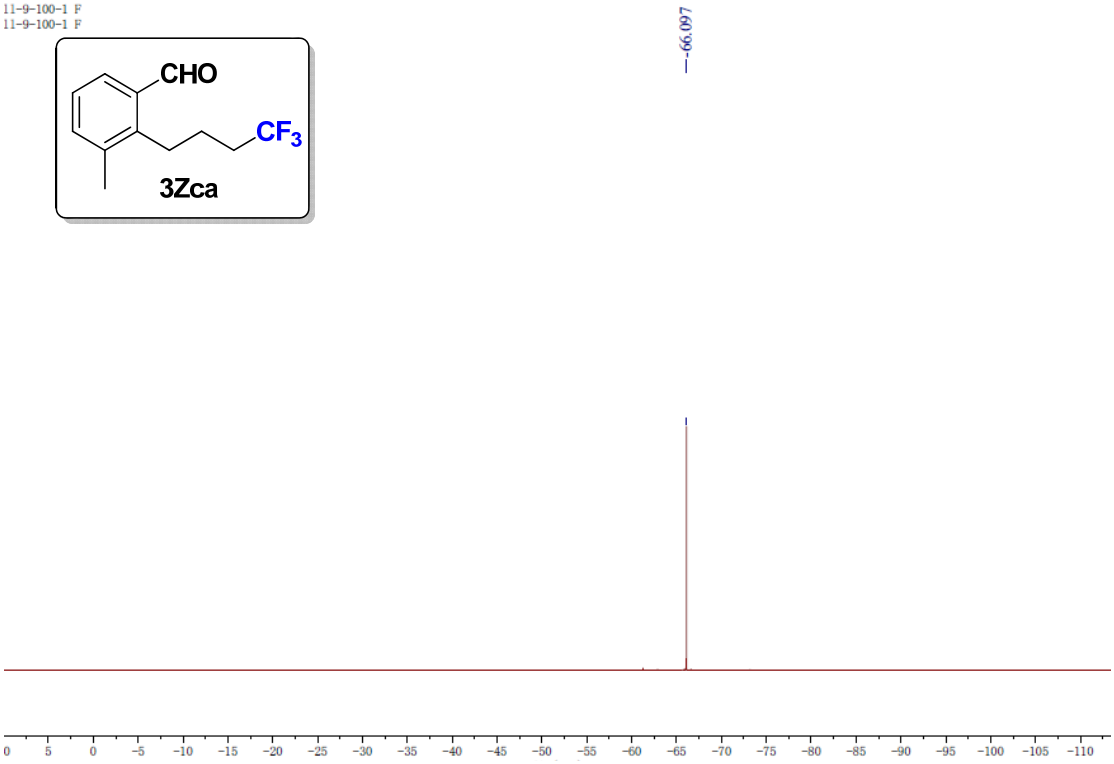
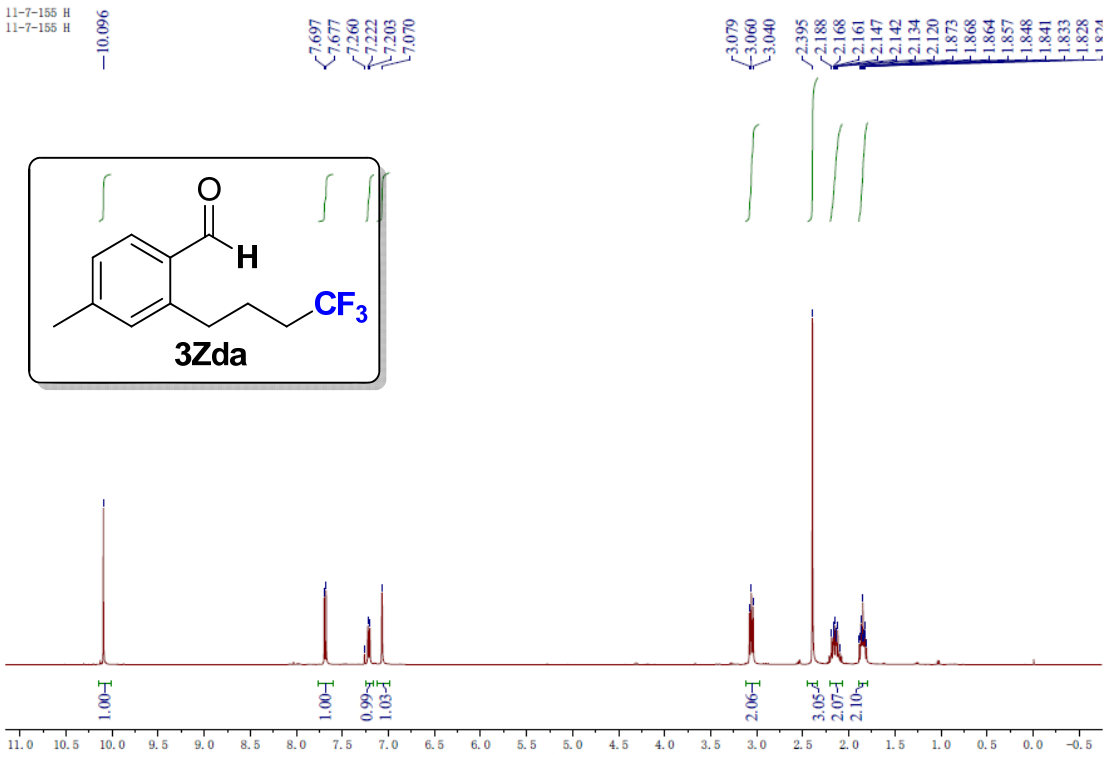
77.000
76.682
33.787
33.504
33.220
32.937
32.402
24.174
24.146
24.118
24.090
20.227
O
H
CF3
3Zba
f1 (ppm)

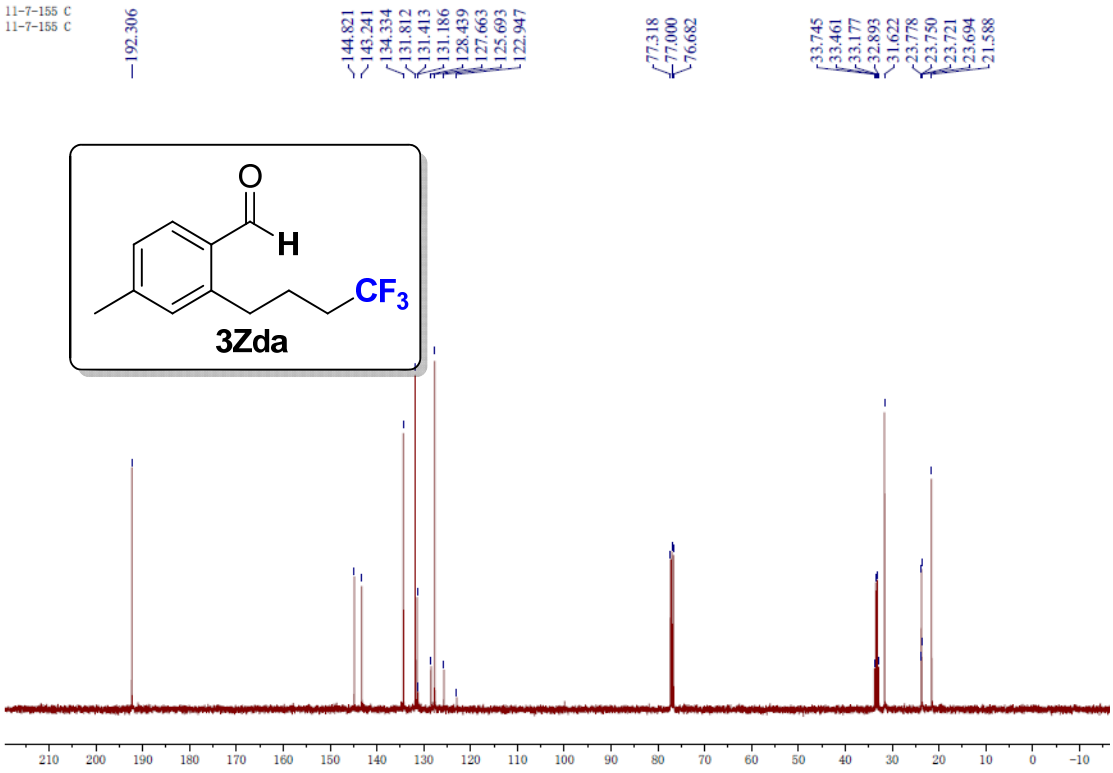

11-9-100-2 F
11-9-100-2 F
-66.150
O
H
CF3
3Zba

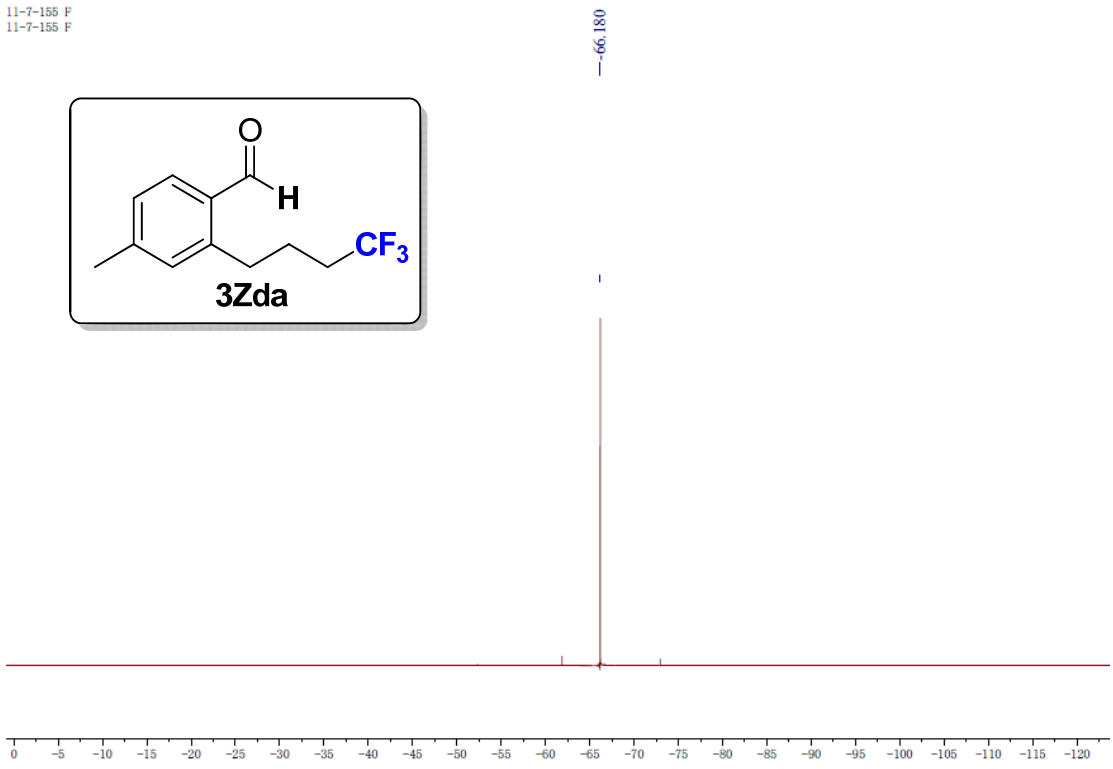

11-9-100-1 H
11-9-100-1 H
10.169
7.664
7.645
7.424
7.406
7.344
7.325
7.306
7.260
3.143
3.122
3.102
2.392
2.311
2.283
2.264
2.256
2.244
2.237
2.217
1.789
1.780
1.769
1.761
1.749
0.001
CHO
CF3
3Zca
1.00
1.00
0.98
0.98
2.10
3.07
2.08
1.99
11.0
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0

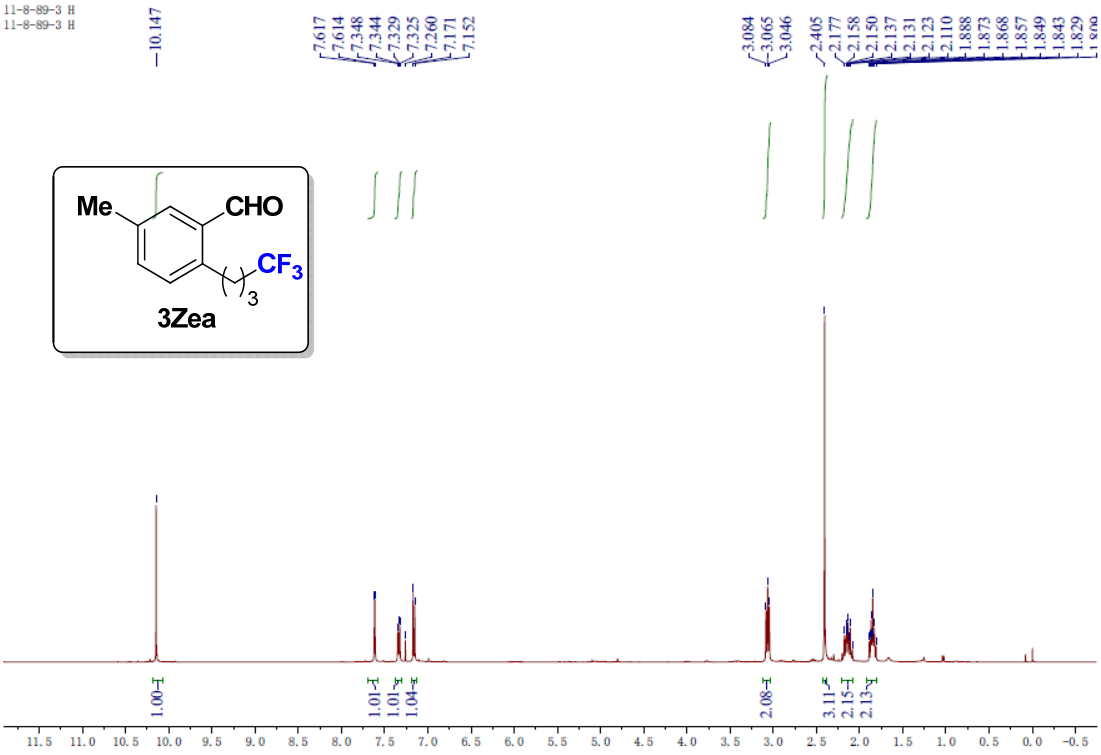

11-8-118-1 C
11-8-118-1 C
193.239
141.672
137.722
135.954
133.937
132.328
131.111
128.440
126.546
125.692
122.945
77.318
77.000
76.682
34.122
33.838
33.554
33.271
27.167
22.688
22.660
22.632
22.605
19.042
CHO
CF3
3Zca
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10

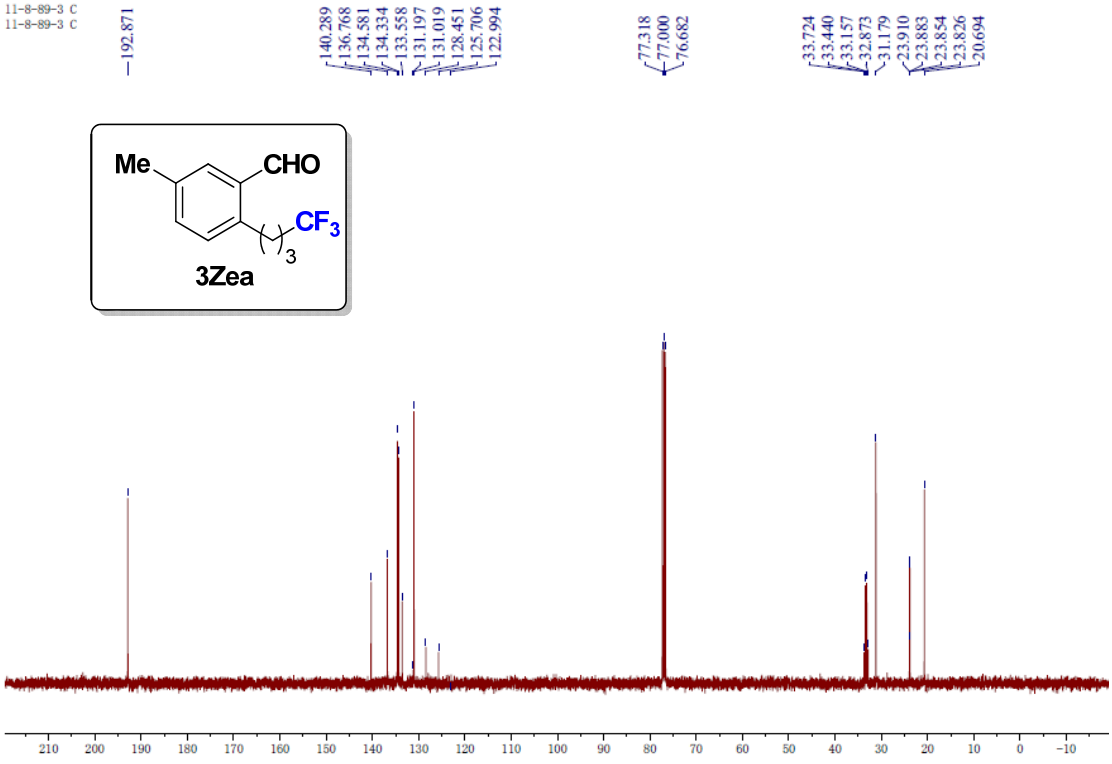

11-9-100-1 F
11-9-100-1 F
CHO
CF3
3Zca
-66.097


11-7-155 H
11-7-155 H
10.096
7.697
7.677
7.260
7.222
7.203
7.070
3.079
3.060
3.040
2.395
2.188
2.168
2.161
2.147
2.142
2.134
2.120
1.873
1.868
1.864
1.857
1.848
1.841
1.833
1.828
O
H
CF3
3Zda
1.00
1.00
0.99
1.03
2.06
3.05
2.07
2.10

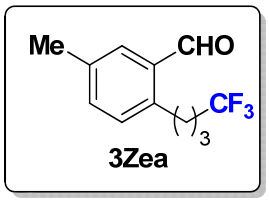

11-7-155 C
11-7-155 C
192.306
144.821
143.241
134.334
131.812
131.413
131.186
128.439
127.663
125.693
122.947
77.318
77.000
76.682
33.745
33.461
33.177
32.893
31.622
23.778
23.750
23.721
23.694
21.588
O
H
CF3
3Zda
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10


11-7-155 F
11-7-155 F
-66.180
O
H
CF3
3Zda
0 -5 -10 -15 -20 -25 -30 -35 -40 -45 -50 -55 -60 -65 -70 -75 -80 -85 -90 -95 -100 -105 -110 -115 -120

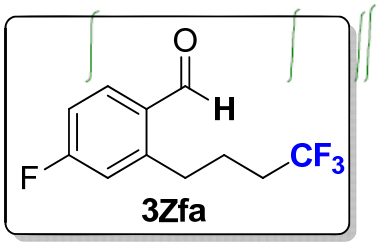

11-8-89-3 H
11-8-89-3 H
10.147
7.617
7.614
7.348
7.344
7.329
7.325
7.260
7.171
7.152
3.084
3.065
3.046
2.405
2.177
2.158
2.150
2.137
2.131
2.123
2.110
1.888
1.873
1.868
1.857
1.849
1.843
1.829
Me
CHO
CF3
3
3Zea
1.00
1.01
1.01
1.04
2.08
3.11
2.15
2.13
11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5

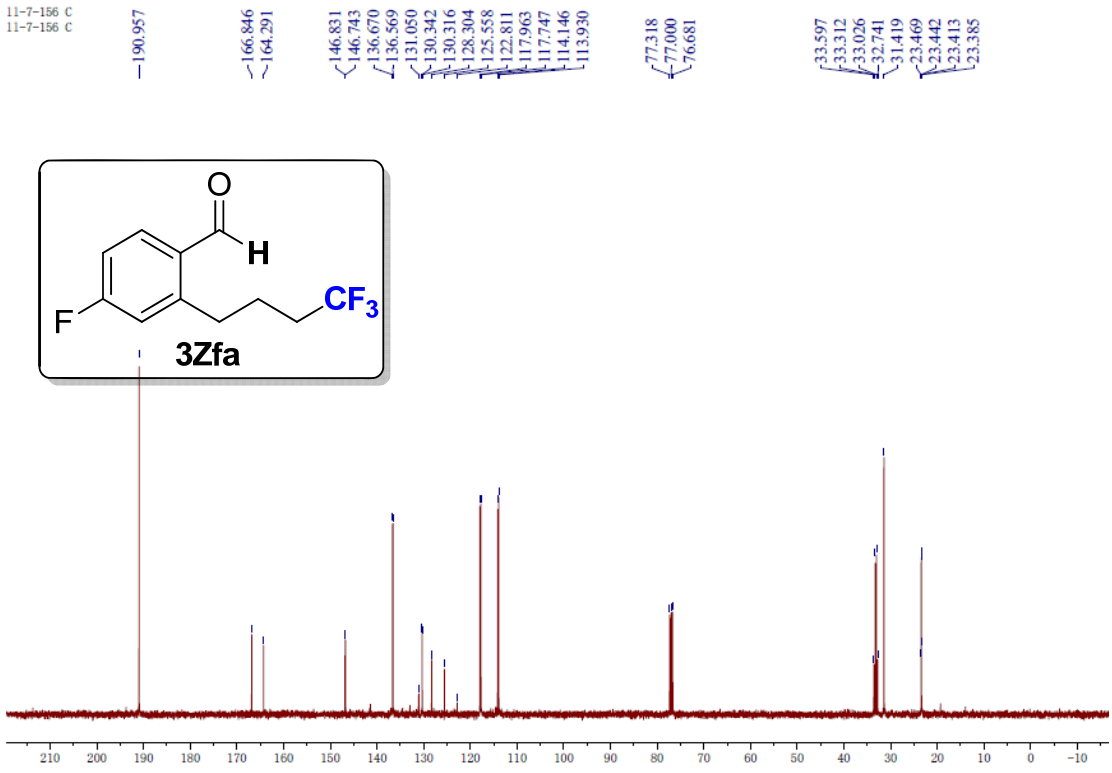

11-8-89-3 C
11-8-89-3 C
192.871
140.289
136.768
134.581
134.334
133.558
131.197
131.019
128.451
125.706
122.994
77.318
77.000
76.682
33.724
33.440
33.157
32.873
31.179
23.910
23.883
23.854
23.826
20.694
Me
CHO
CF3
3
3Zea
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10

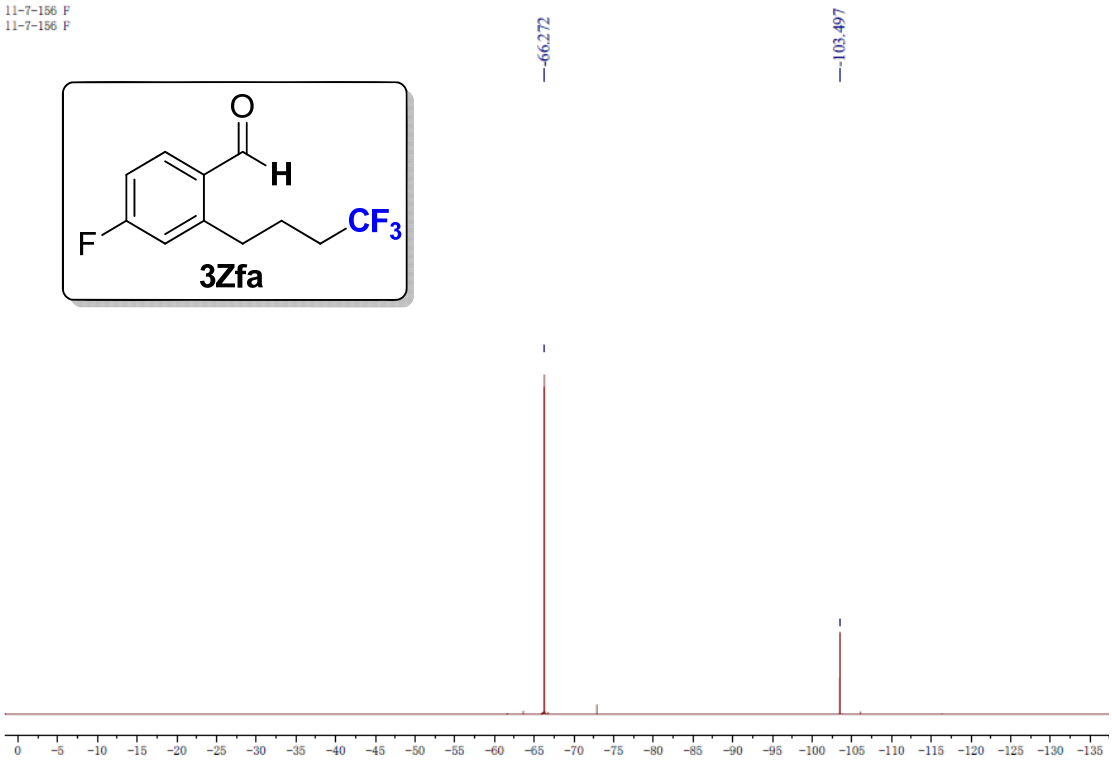
11-8-89-3 F
11-8-89-3 F

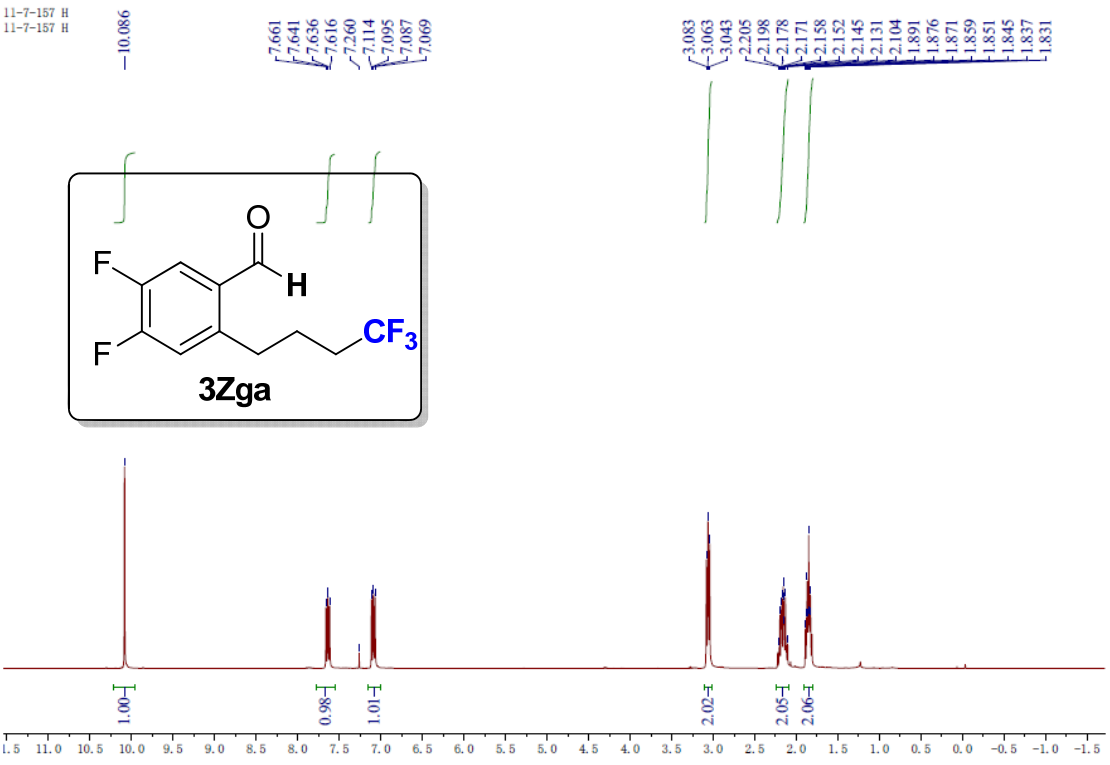


11-7-156 H
11-7-156 H




11-7-156 C
11-7-156 C
190.957
166.846
164.291
146.831
146.743
136.670
136.569
131.050
130.342
130.316
128.304
125.558
122.811
117.963
117.747
114.146
113.930
77.318
77.000
76.681
33.597
33.312
33.026
32.741
31.419
23.469
23.442
23.413
23.385
O
H
F
CF3
3Zfa
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10


11-7-156 F
11-7-156 F
-66.272
-103.497
O
H
F
CF3
3Zfa
0 -5 -10 -15 -20 -25 -30 -35 -40 -45 -50 -55 -60 -65 -70 -75 -80 -85 -90 -95 -100 -105 -110 -115 -120 -125 -130 -135


11-7-157 H
11-7-157 H
10.086
7.661
7.641
7.636
7.616
7.260
7.114
7.095
7.087
7.069
3.083
3.063
3.043
2.205
2.198
2.178
2.171
2.158
2.152
2.145
2.131
2.104
1.891
1.876
1.871
1.859
1.851
1.845
1.837
1.831
O
H
F
F
CF3
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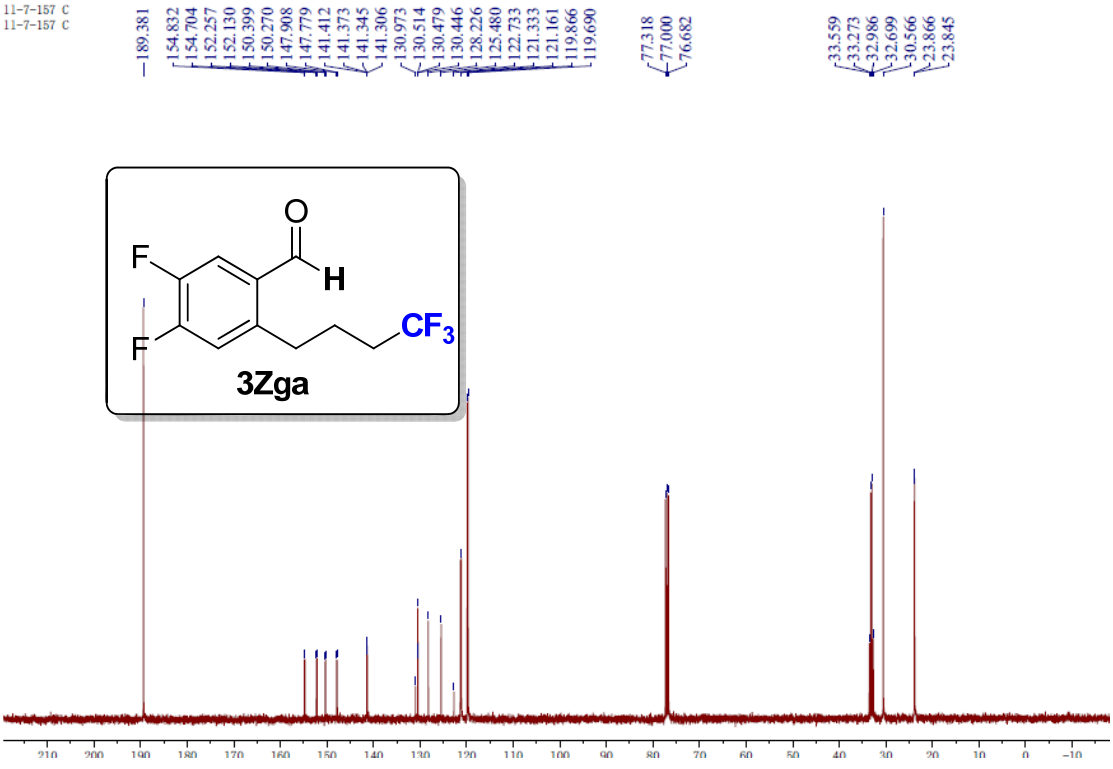
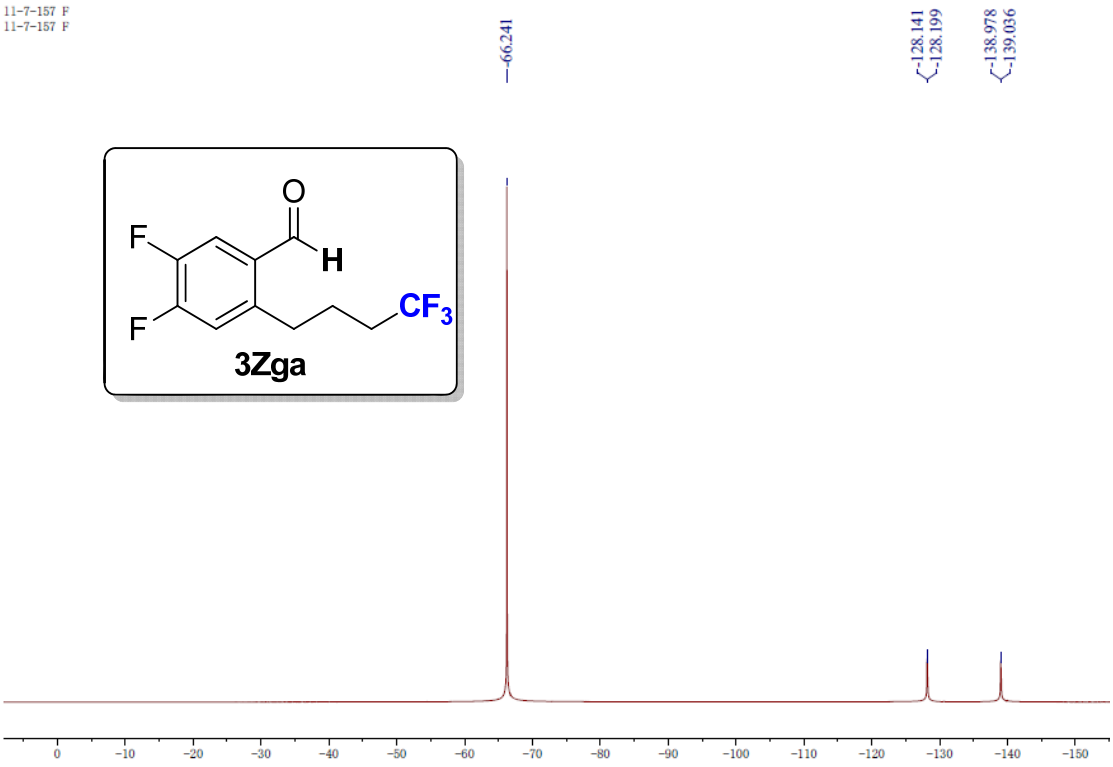
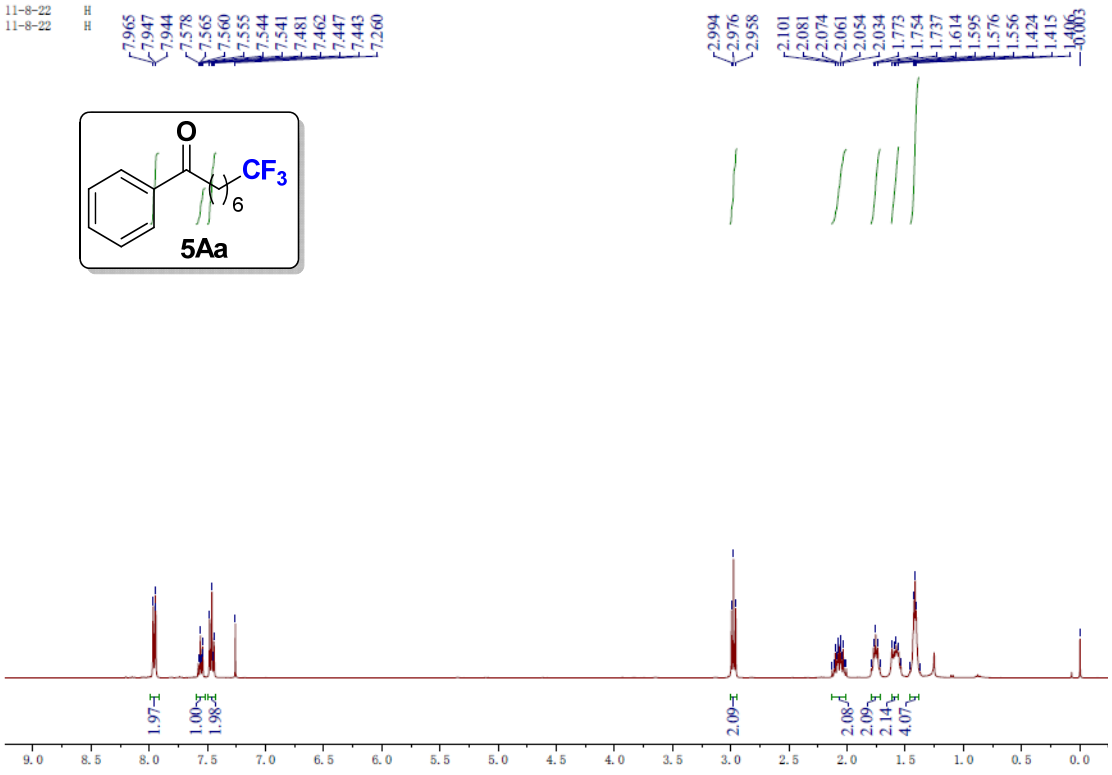
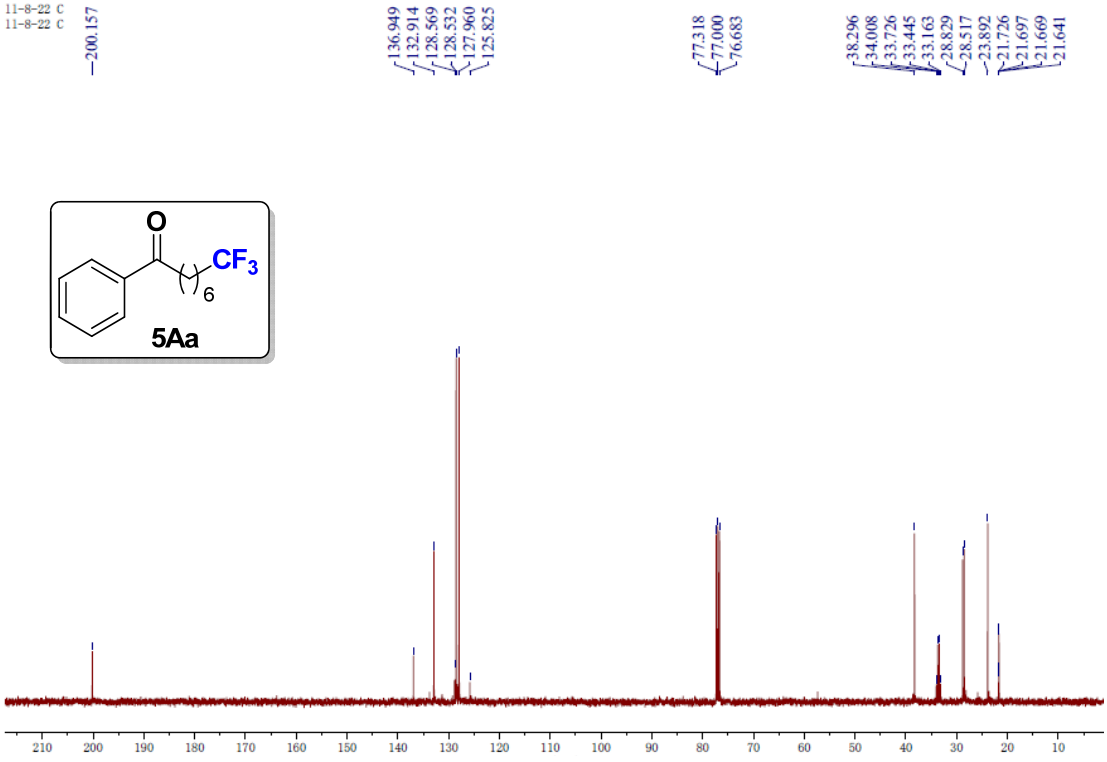
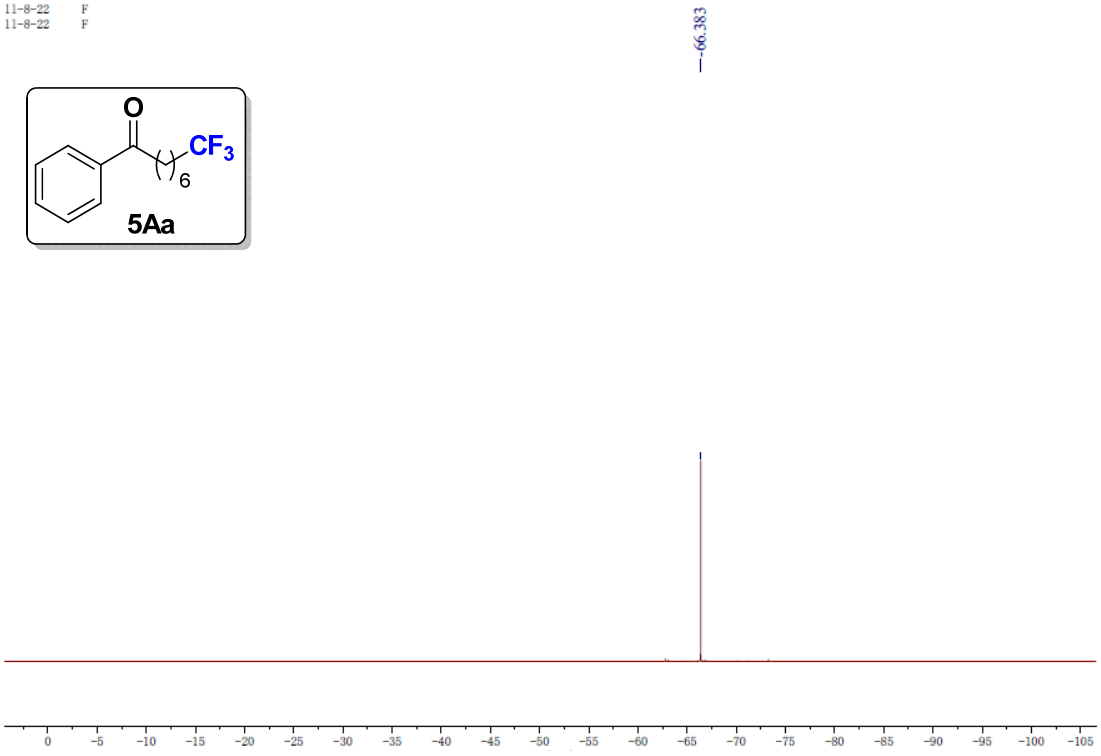
1.00
0.98
1.01
2.02
2.05
2.06


11-7-157 C
11-7-157 C
189.381
154.832
154.704
152.257
152.130
150.399
150.270
147.908
147.779
141.412
141.373
141.345
141.306
130.973
130.514
130.479
130.446
128.226
125.480
122.733
121.333
121.161
119.866
119.690
77.318
77.000
76.682
33.559
33.273
32.986
32.699
30.566
23.866
23.845
O
H
F
F
CF3
3Zga


11-7-157 F
11-7-157 F
-66.241
-128.141
-128.199
-138.978
-139.036
O
H
F
F
CF3
3Zga


11-8-22 H
11-8-22 H
7.965
7.947
7.944
7.578
7.565
7.560
7.555
7.544
7.541
7.481
7.462
7.447
7.443
7.260
2.994
2.976
2.958
2.101
2.081
2.074
2.061
2.054
2.034
1.773
1.754
1.737
1.614
1.595
1.576
1.556
1.424
1.415
0.003
O
CF3
6
5Aa
1.97
1.00
1.98
2.09
2.08
2.09
2.14
4.07


11-8-22 C
11-8-22 C
200.157
136.949
132.914
128.569
128.532
127.960
125.825
77.318
77.000
76.683
38.296
34.008
33.726
33.445
33.163
28.829
28.517
23.892
21.726
21.697
21.669
21.641
O
CF3
6
5Aa
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10


11-8-22 F
11-8-22 F
-66.383
O
CF3
6
5Aa
0
-5
-10
-15
-20
-25
-30
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-40
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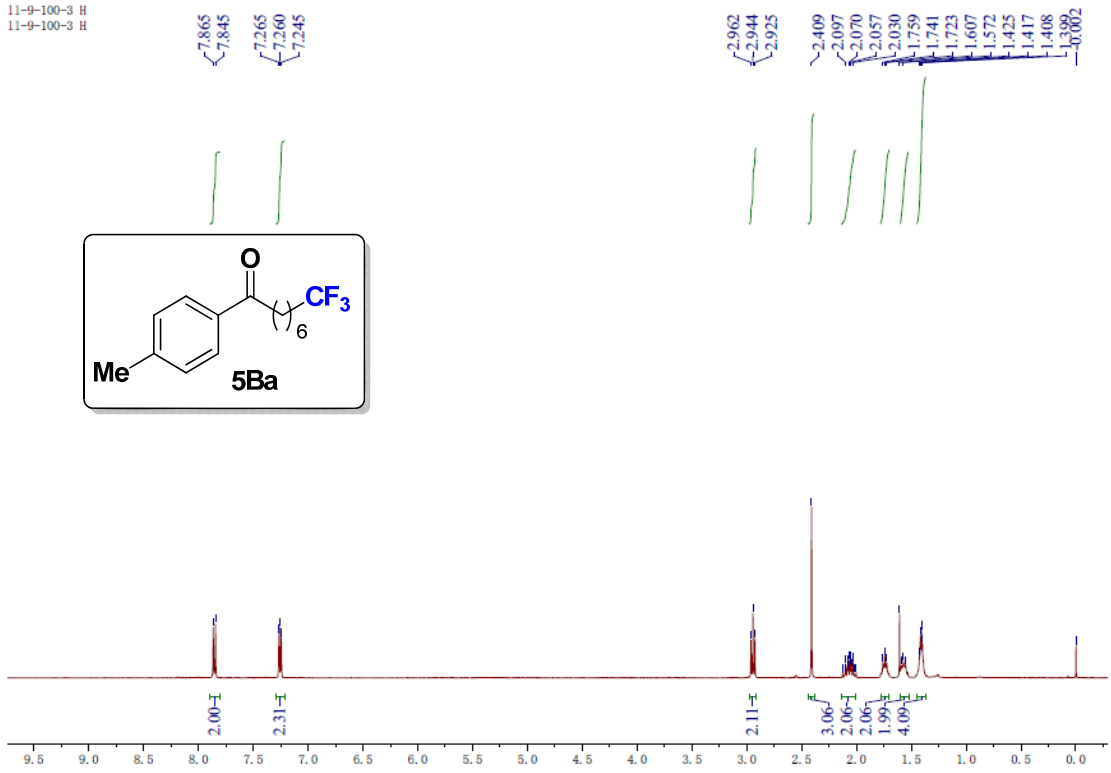
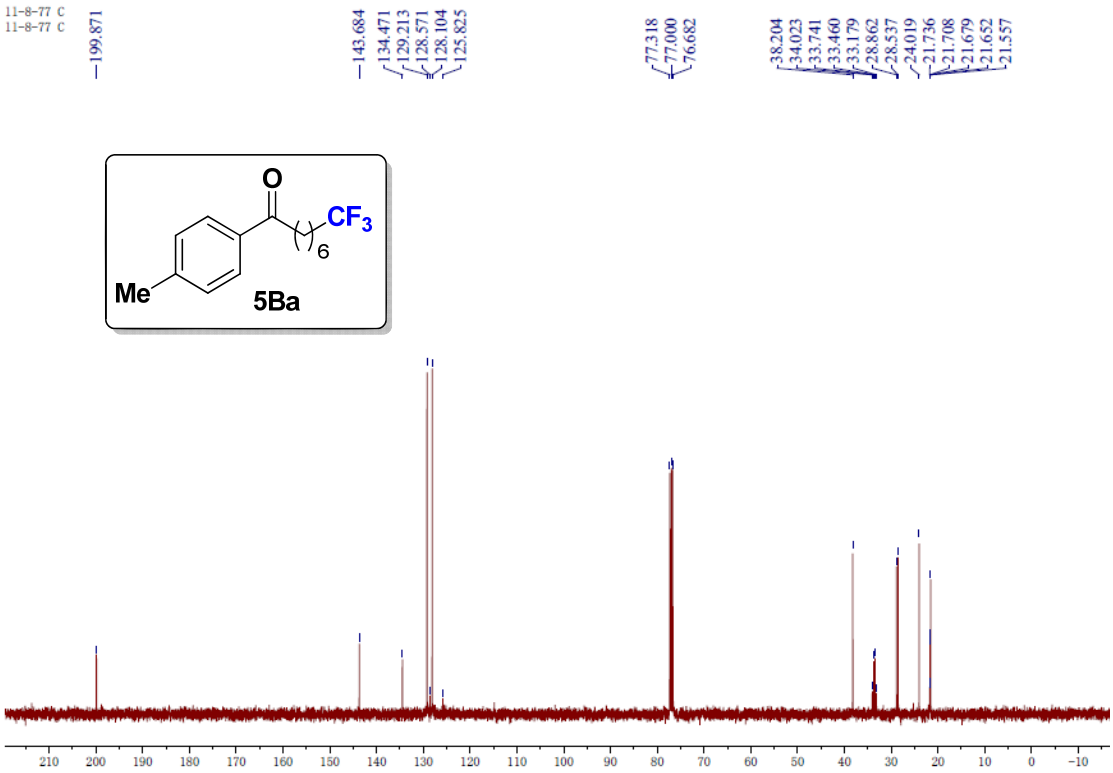
-50
-55
-60
-65
-70
-75
-80
-85
-90
-95
-100
-105


11-9-100-3 H
11-9-100-3 H
7.865
7.845
7.265
7.260
7.245
2.962
2.944
2.925
2.409
2.097
2.070
2.057
2.030
1.759
1.741
1.723
1.607
1.572
1.425
1.417
1.408
1.390
0.002
O
CF3
6
Me
5Ba
2.00
2.31
2.11
3.06
2.06
2.06
1.99
4.09
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


11-8-77 C
11-8-77 C
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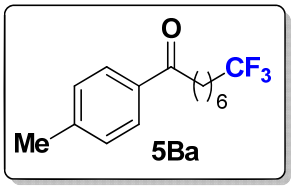
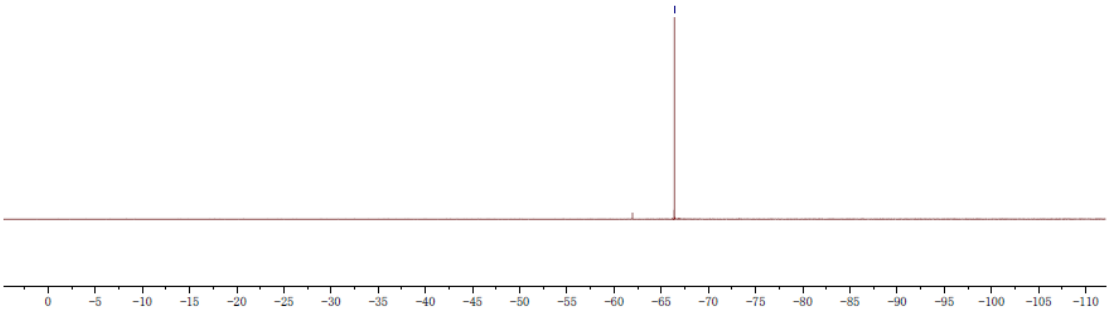
143.684
134.471
129.213
128.571
128.104
125.825
77.318
77.000
76.682
38.204
34.023
33.741
33.460
33.179
28.862
28.537
24.019
21.736
21.708
21.679
21.652
21.557
O
CF3
6
Me
5Ba
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10

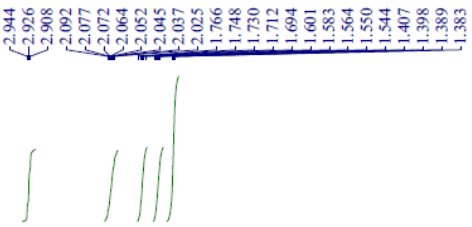
11-9-100-3 F
11-9-100-3 F

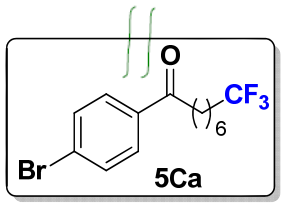


5Ba

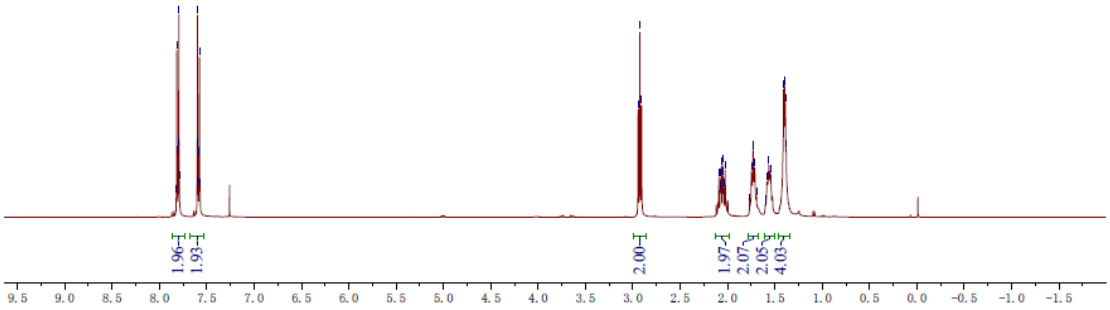


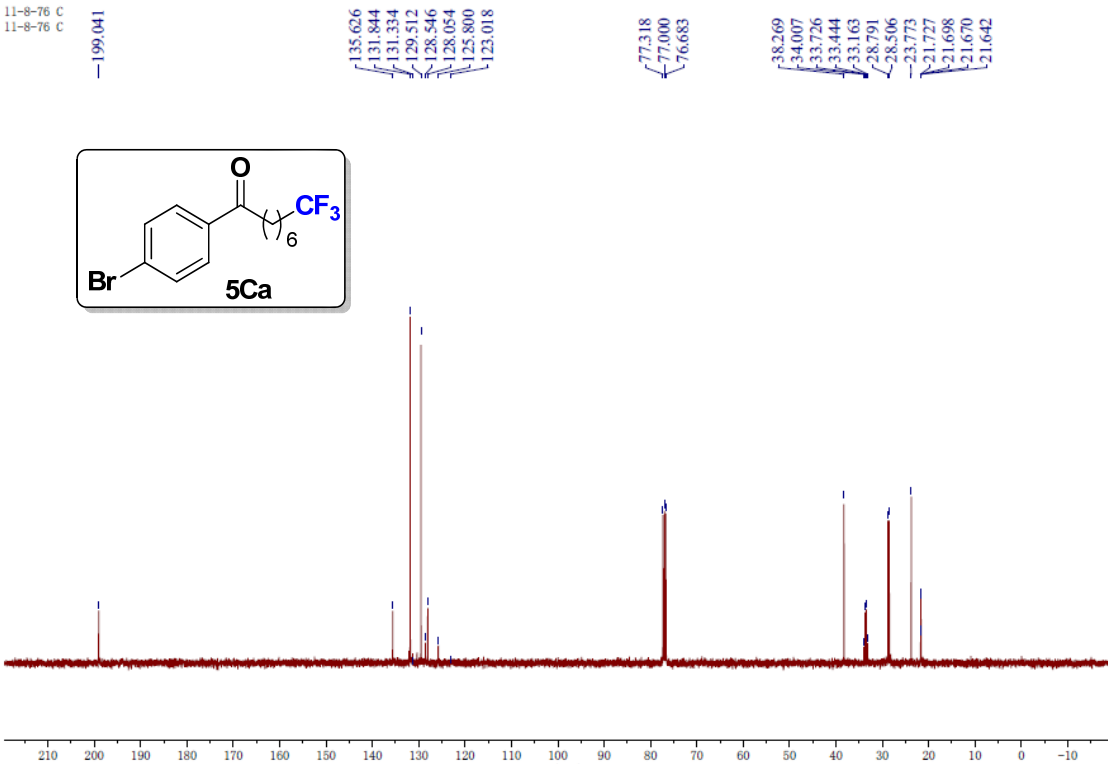
11-8-76 H
11-8-76 H

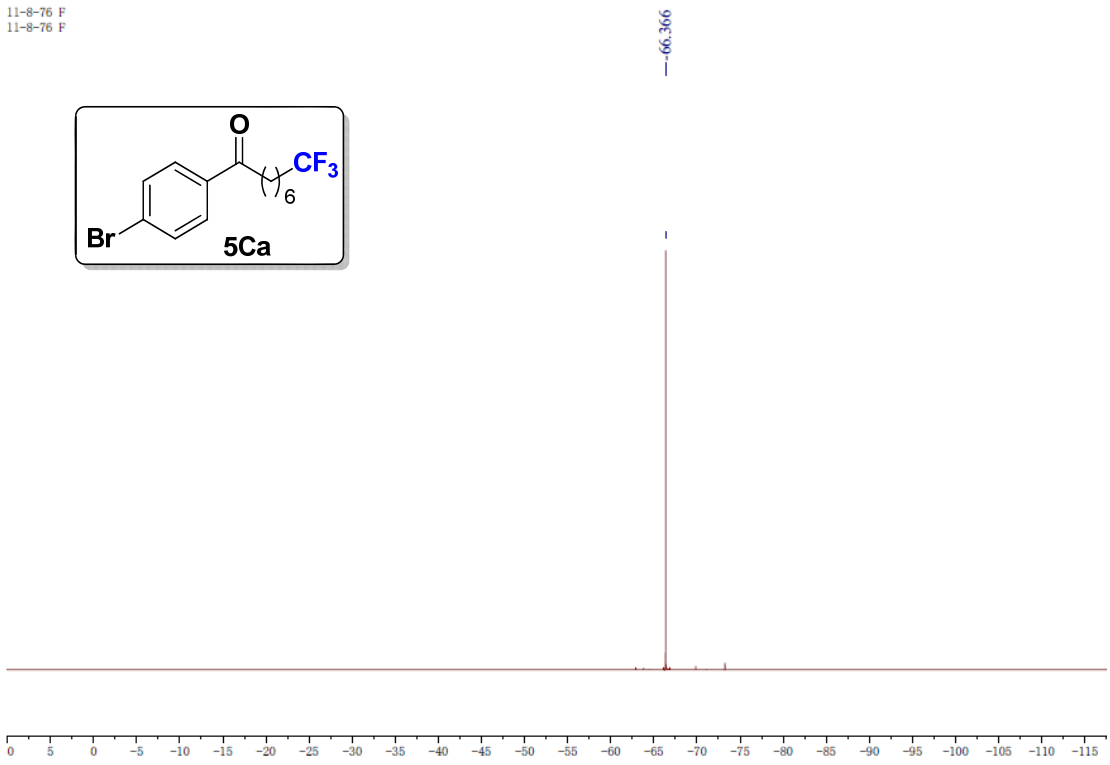


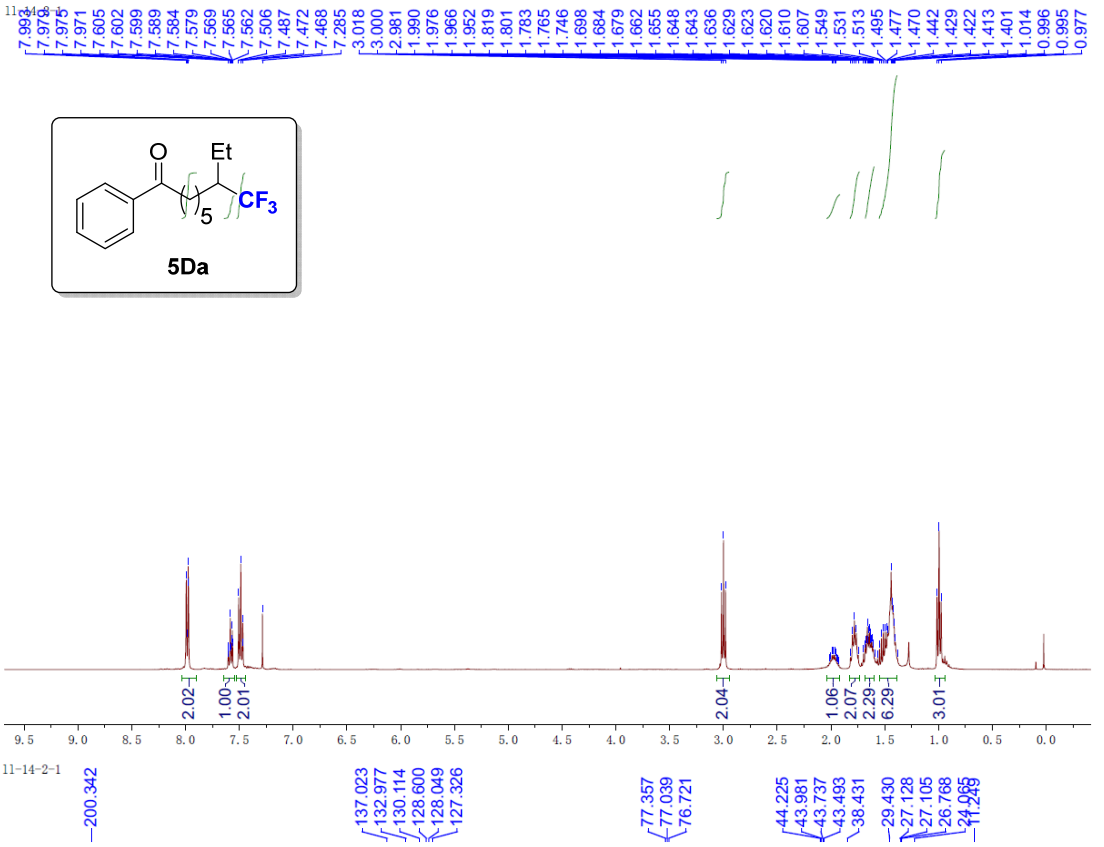


5Ca




11-8-76 C
11-8-76 C
199.041
135.626
131.844
131.334
129.512
128.546
128.054
125.800
123.018
77.318
77.000
76.683
38.269
34.007
33.726
33.444
33.163
28.791
28.506
23.773
21.727
21.698
21.670
21.642
O
CF3
6
Br
5Ca


11-8-76 F
11-8-76 F
66.366
O
CF3
6
Br
5Ca


11-14-1
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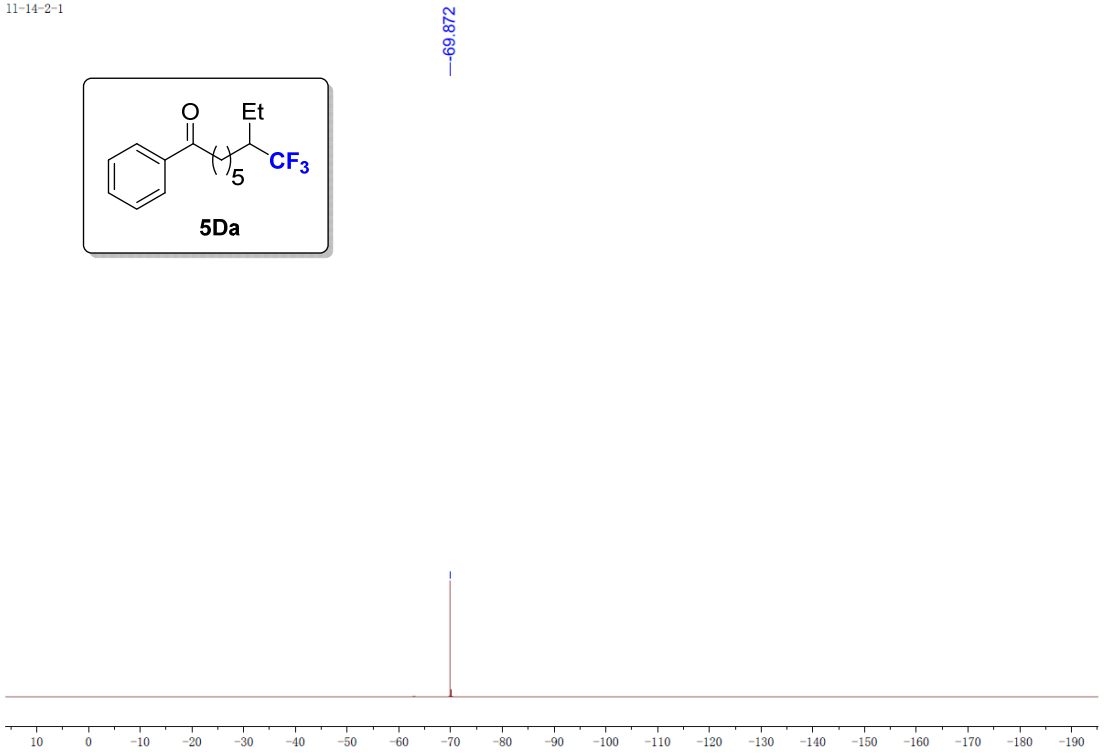
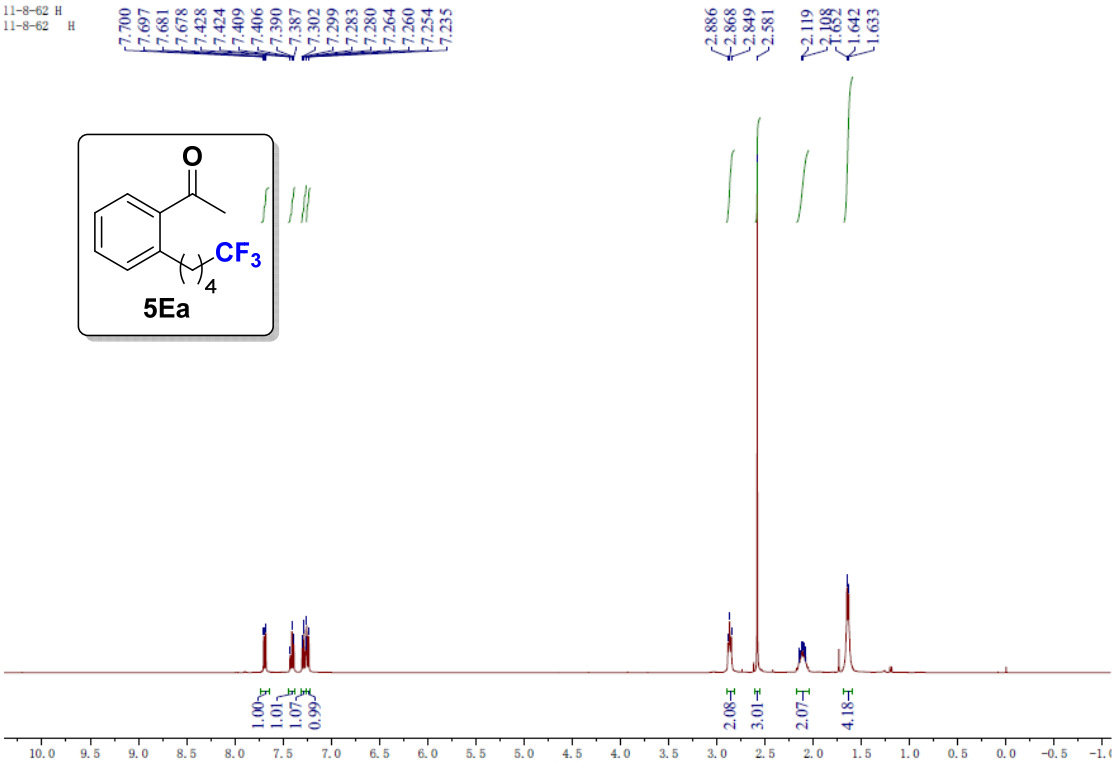
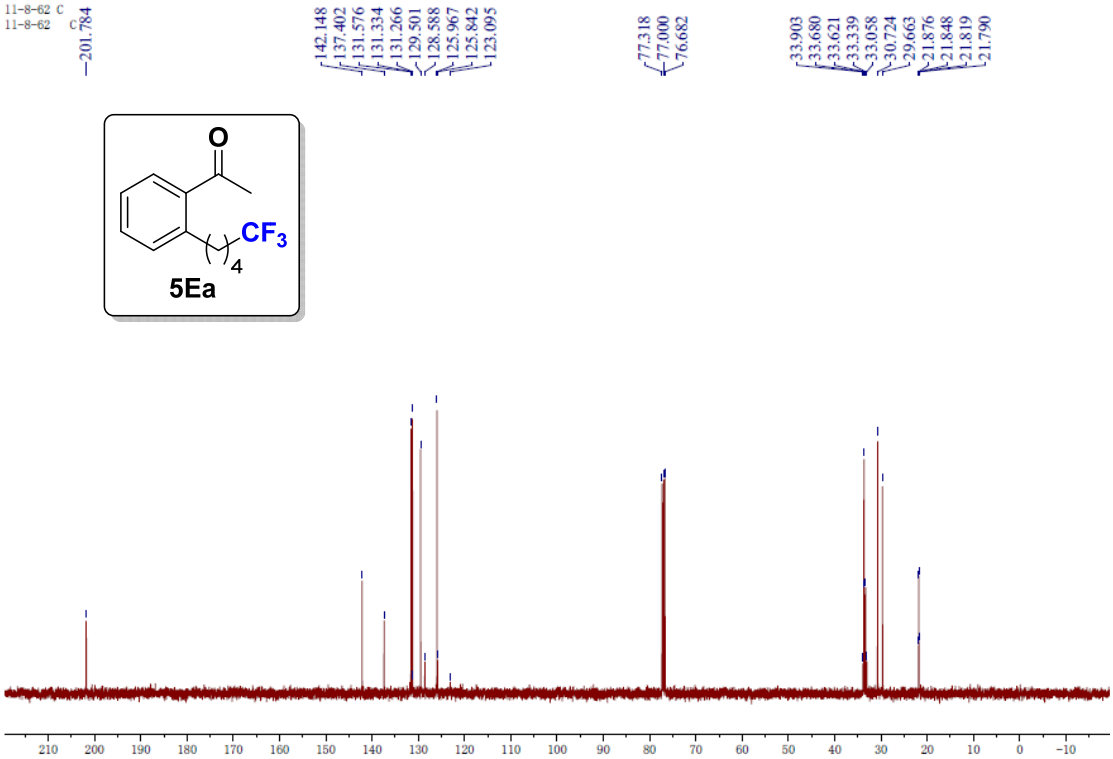
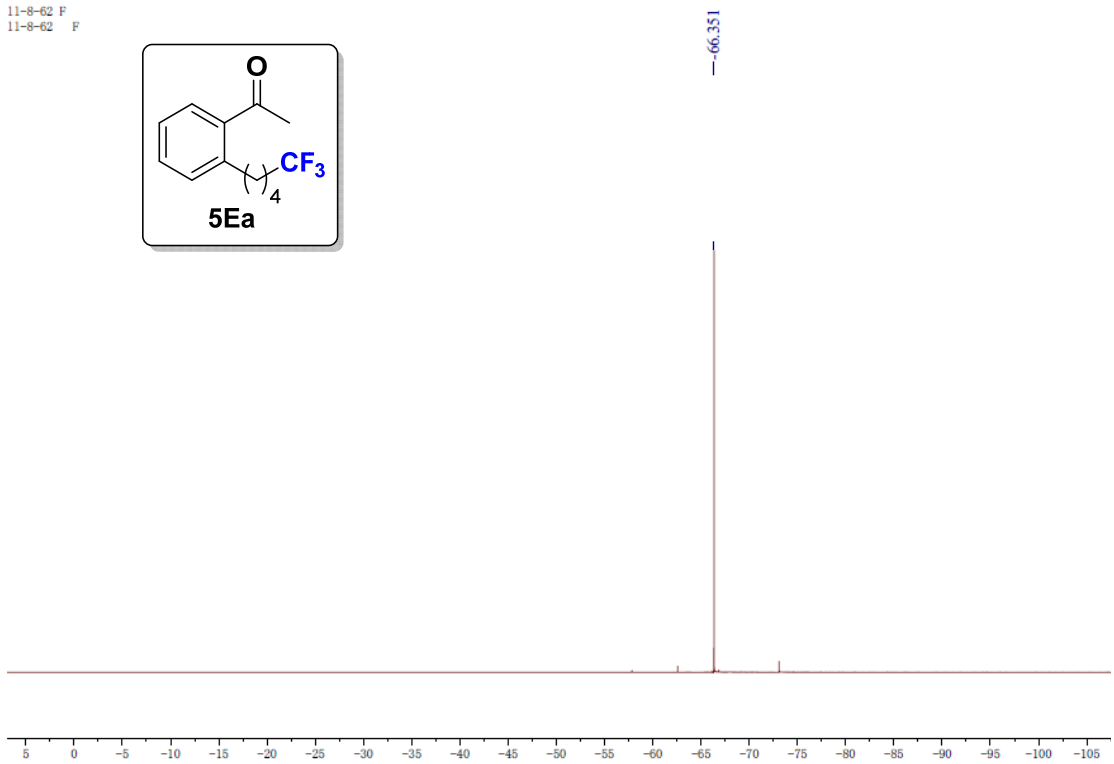
7.975
7.971
7.605
7.602
7.599
7.589
7.584
7.579
7.569
7.565
7.562
7.506
7.487
7.472
7.468
7.285
3.018
3.000
2.981
1.990
1.976
1.966
1.952
1.819
1.801
1.783
1.765
1.746
1.698
1.684
1.679
1.662
1.655
1.648
1.643
1.636
1.629
1.623
1.620
1.610
1.607
1.549
1.531
1.513
1.495
1.477
1.470
1.442
1.429
1.422
1.413
1.401
1.014
0.996
0.995
0.977
O
Et
CF3
5
5Da
2.02
1.00
2.01
2.04
1.06
2.07
2.29
6.29
3.01
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
11-14-2-1
200.342
137.023
132.977
130.114
128.600
128.049
127.326
77.357
77.039
76.721
44.225
43.981
43.737
43.493
38.431
29.430
27.128
27.105
26.768
24.065
11.249
O
Et
CF3
5
5Da
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10

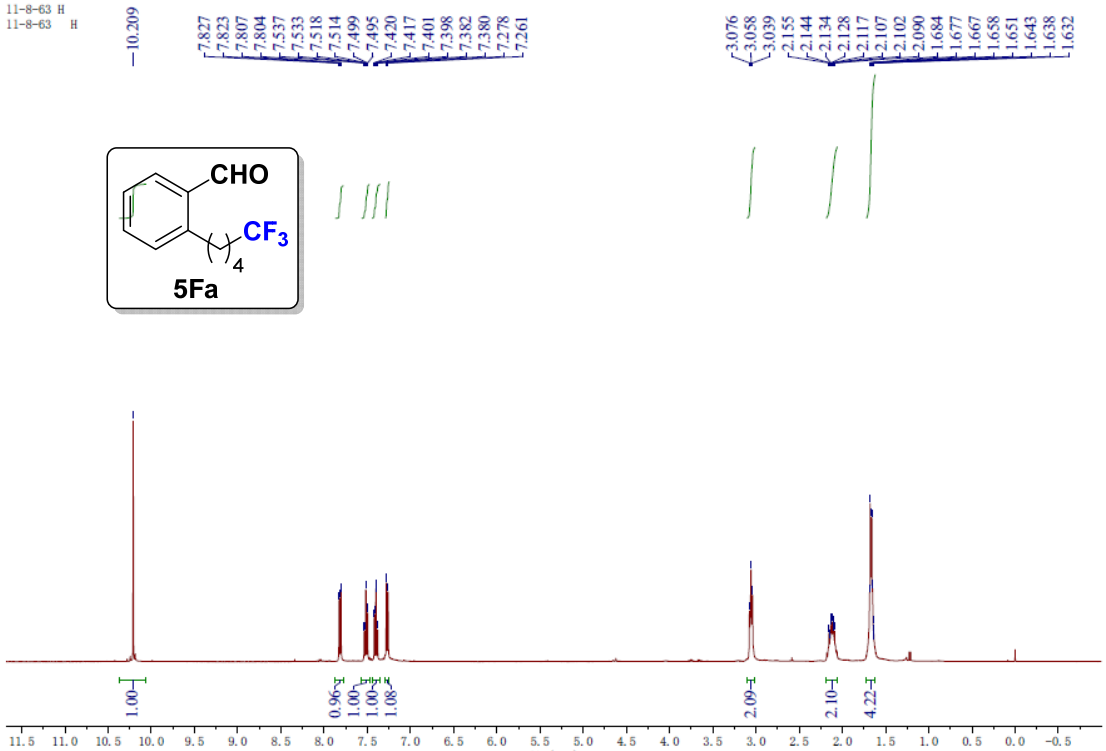
11-14-2-1

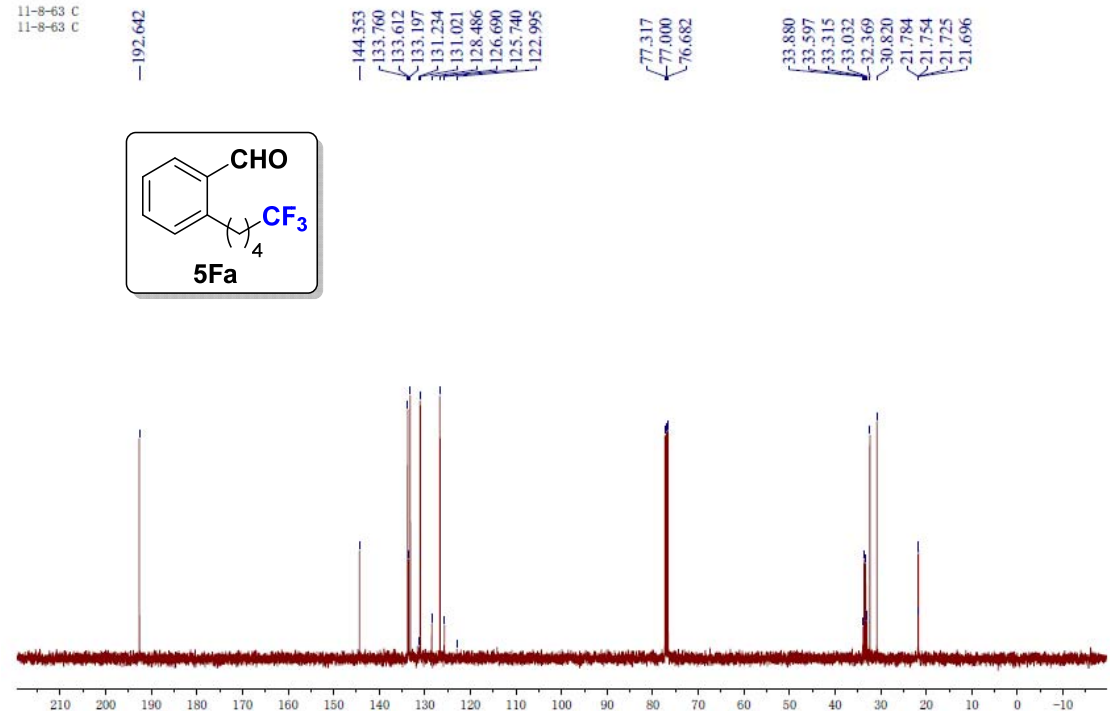

-69.872
O
Et
CF3
5
5Da
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190

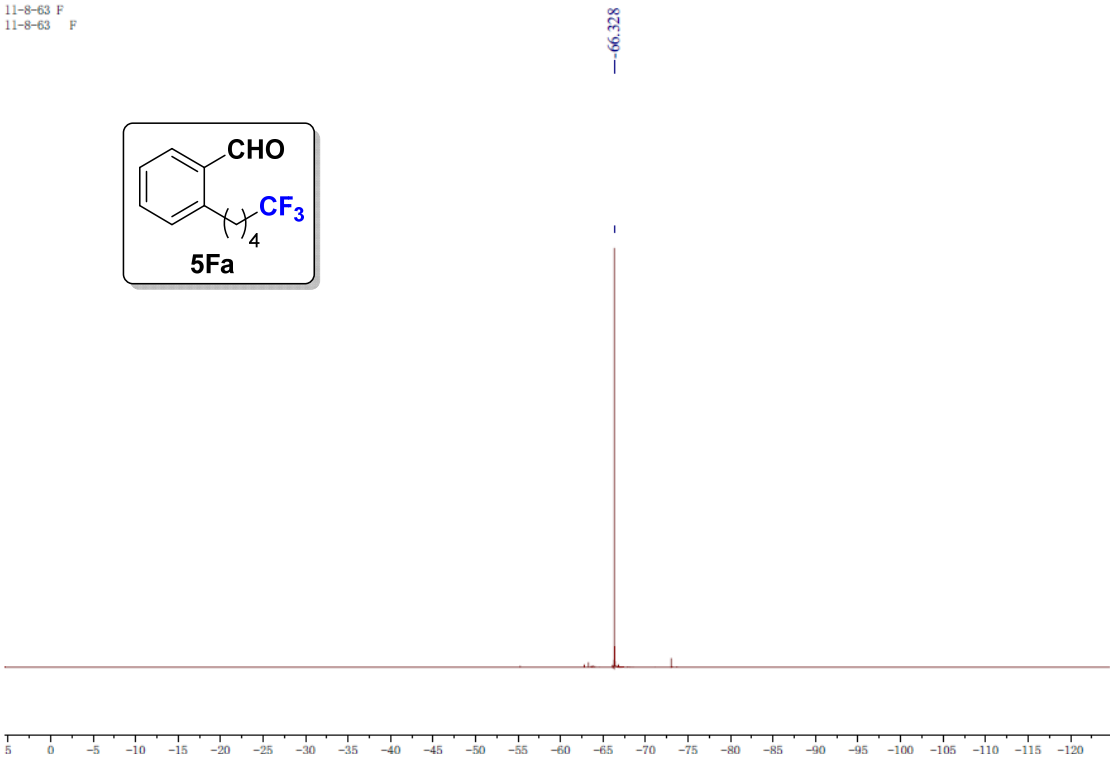

11-8-62 H
11-8-62 H
7.700
7.697
7.681
7.678
7.428
7.424
7.409
7.406
7.390
7.387
7.302
7.299
7.283
7.280
7.264
7.260
7.254
7.235
2.886
2.868
2.849
2.581
2.119
2.108
1.652
1.642
1.633
O
CF3
4
5Ea
1.00
1.01
1.07
0.99
2.08
3.01
2.07
4.18
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5

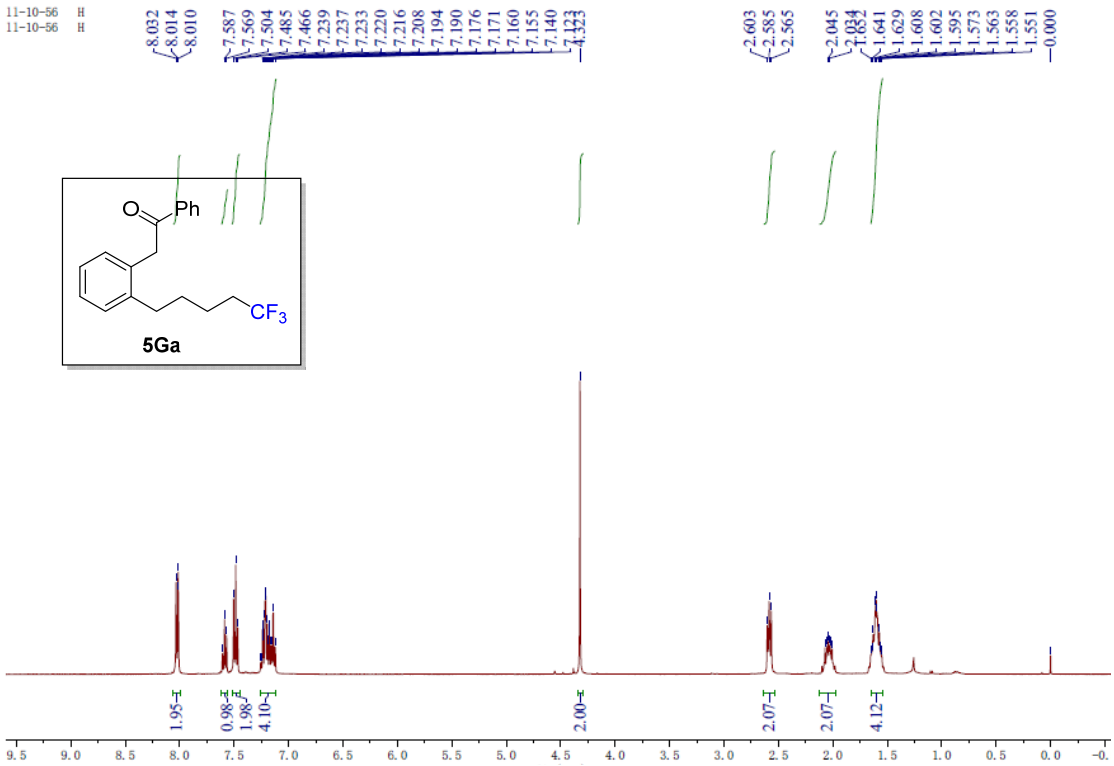

11-8-62 C
11-8-62 C
201.784
142.148
137.402
131.576
131.334
131.266
129.501
128.588
125.967
125.842
123.095
77.318
77.000
76.682
33.903
33.680
33.621
33.339
33.058
30.724
29.663
21.876
21.848
21.819
21.790
O
CF3
4
5Ea
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10

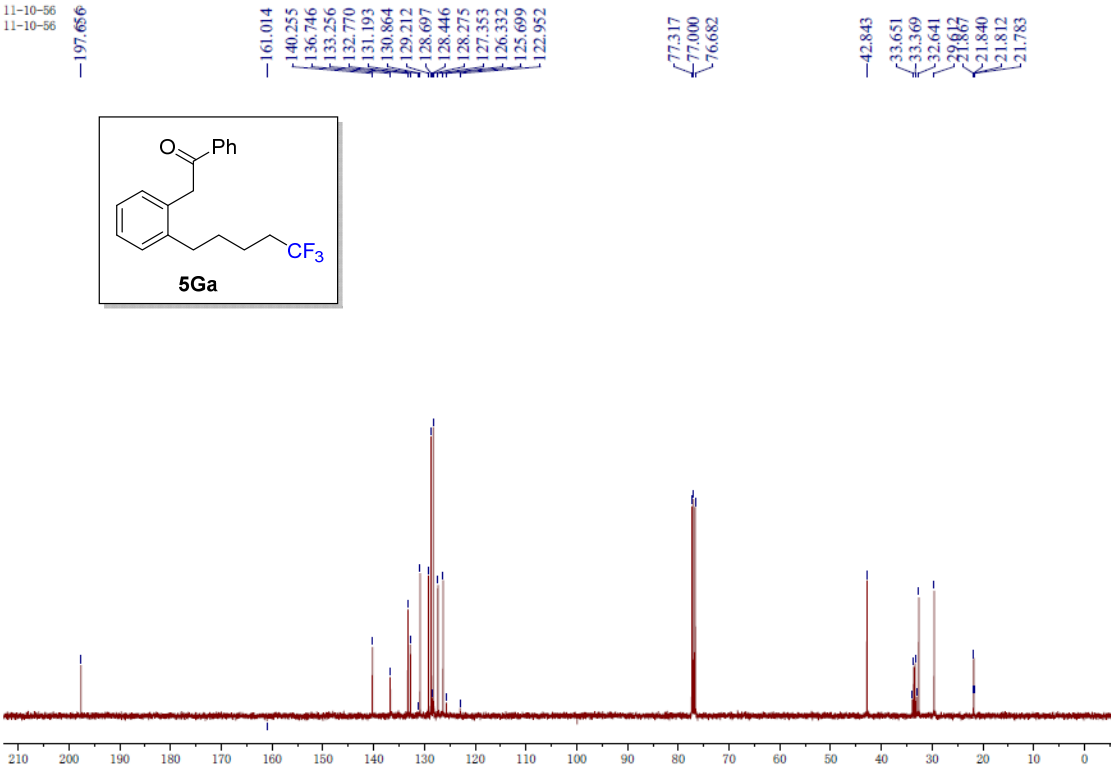

11-8-62 F
11-8-62 F
-66.351
O
CF3
4
5Ea
5 0 -5 -10 -15 -20 -25 -30 -35 -40 -45 -50 -55 -60 -65 -70 -75 -80 -85 -90 -95 -100 -105

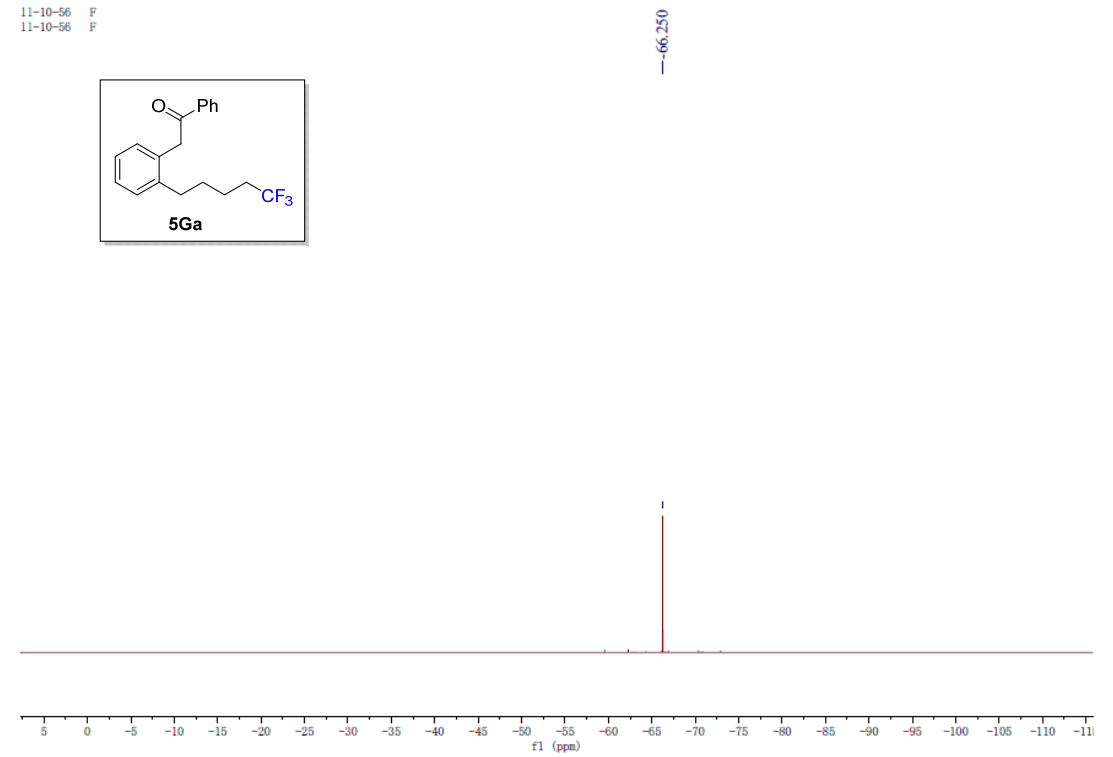

11-8-63 H
11-8-63 H
10.209
7.827
7.823
7.807
7.804
7.537
7.533
7.518
7.514
7.499
7.495
7.420
7.417
7.401
7.398
7.382
7.380
7.278
7.261
3.076
3.058
3.039
2.155
2.144
2.134
2.128
2.117
2.107
2.102
2.090
1.684
1.677
1.667
1.658
1.651
1.643
1.638
1.632
CHO
CF3
4
5Fa
1.00
0.96
1.00
1.00
1.08
2.09
2.10
4.22
11.5 11.0 10.5 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 -0.5

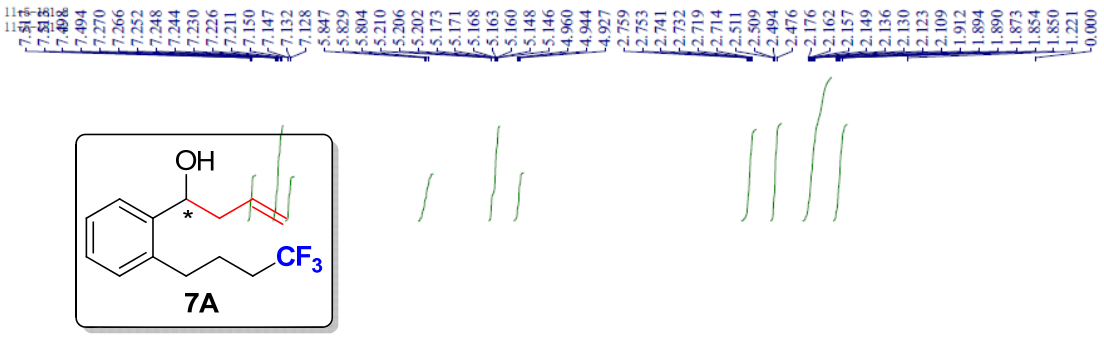

11-8-63 C
11-8-63 C
192.642
144.353
133.760
133.612
133.197
131.234
131.021
128.486
126.690
125.740
122.995
77.317
77.000
76.682
33.880
33.597
33.315
33.032
32.369
30.820
21.784
21.754
21.725
21.696
CHO
CF3
4
5Fa
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10

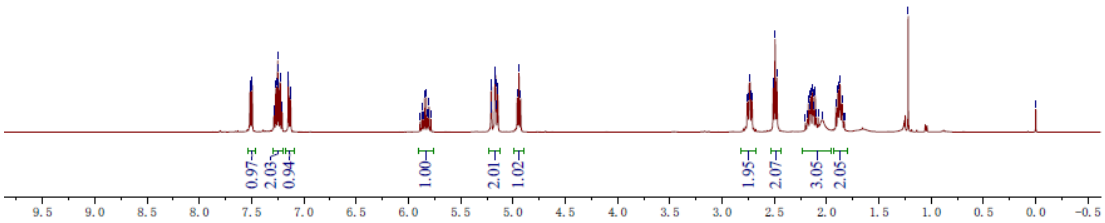

11-8-63 F
11-8-63 F
-66.328
CHO
CF3
4
5Fa


11-10-56 H
11-10-56 H
8.032
8.014
8.010
7.587
7.569
7.504
7.485
7.466
7.239
7.237
7.233
7.220
7.216
7.208
7.194
7.190
7.176
7.171
7.160
7.155
7.140
7.123
4.323
2.603
2.585
2.565
2.045
2.034
1.852
1.641
1.629
1.608
1.602
1.595
1.573
1.563
1.558
1.551
0.000
O
Ph
CF3
5Ga
1.95
0.98
1.98
4.10
2.00
2.07
2.07
4.12

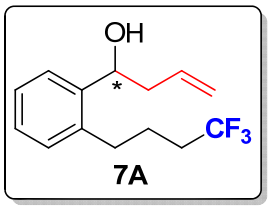

11-10-56
11-10-56
197.656
161.014
140.255
136.746
133.256
132.770
131.193
130.864
129.212
128.697
128.446
128.275
127.353
126.332
125.699
122.952
77.317
77.000
76.682
42.843
33.651
33.369
32.641
29.612
21.867
21.840
21.812
21.783
O
Ph
CF3
5Ga
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0

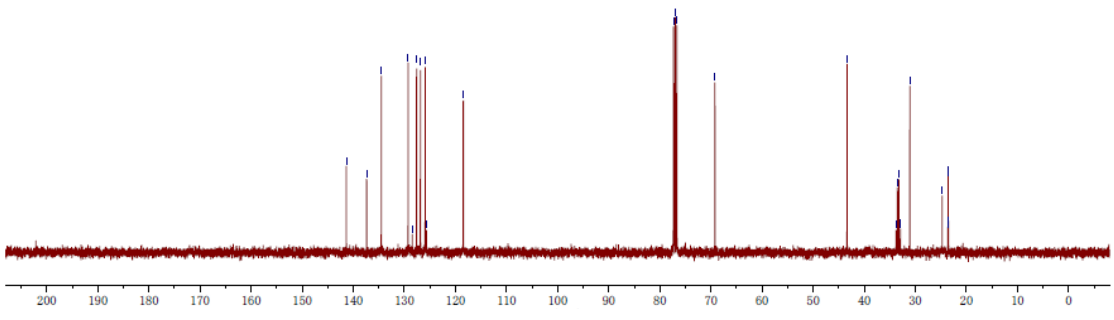

11-10-56 F
11-10-56 F
-66.250
O
Ph
CF3
5Ga
5
0
-5
-10
-15
-20
-25
-30
-35
-40
-45
-50
-55
-60
-65
-70
-75
-80
-85
-90
-95
-100
-105
-110
f1 (ppm)

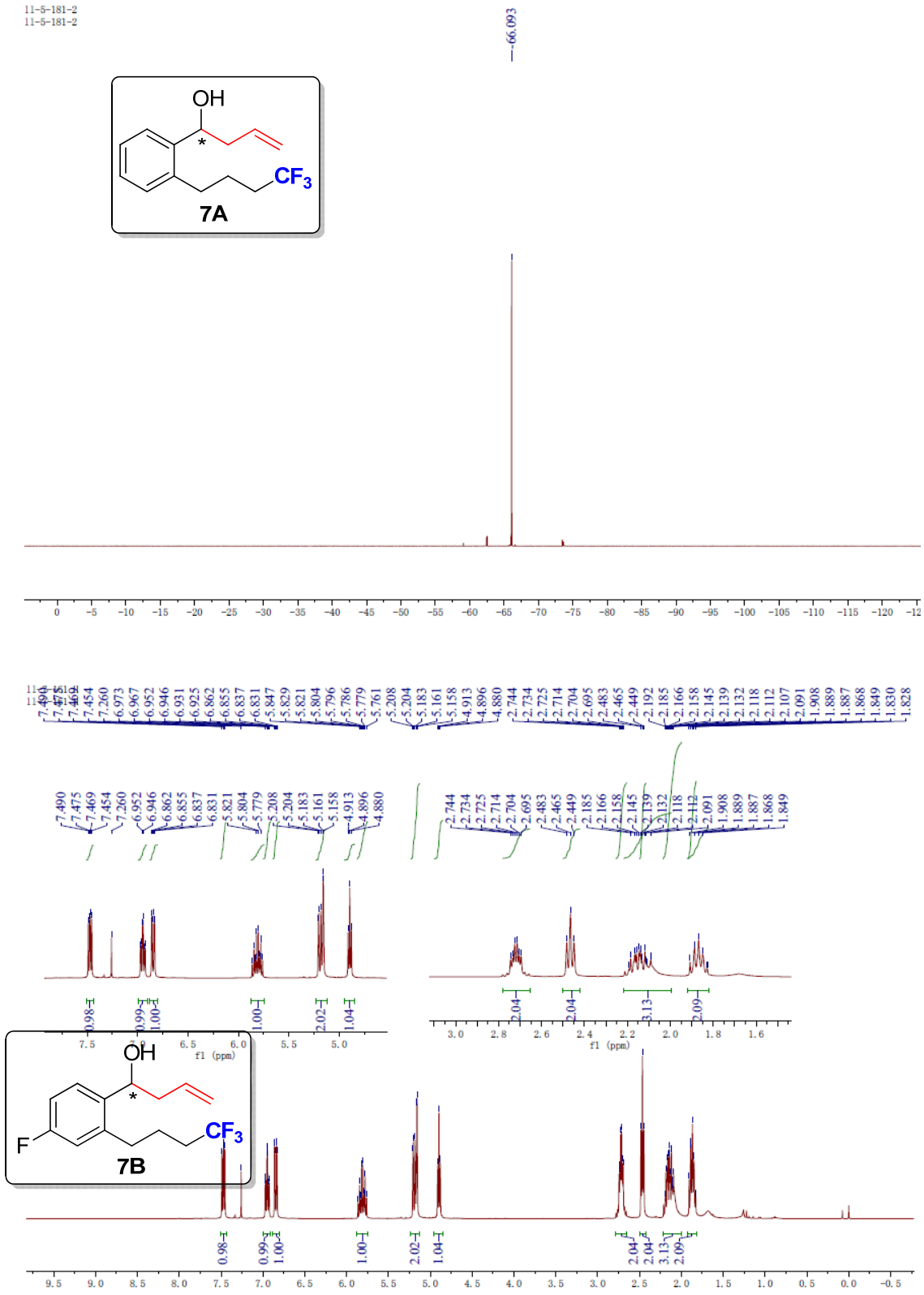

OH
*
CF3
7A

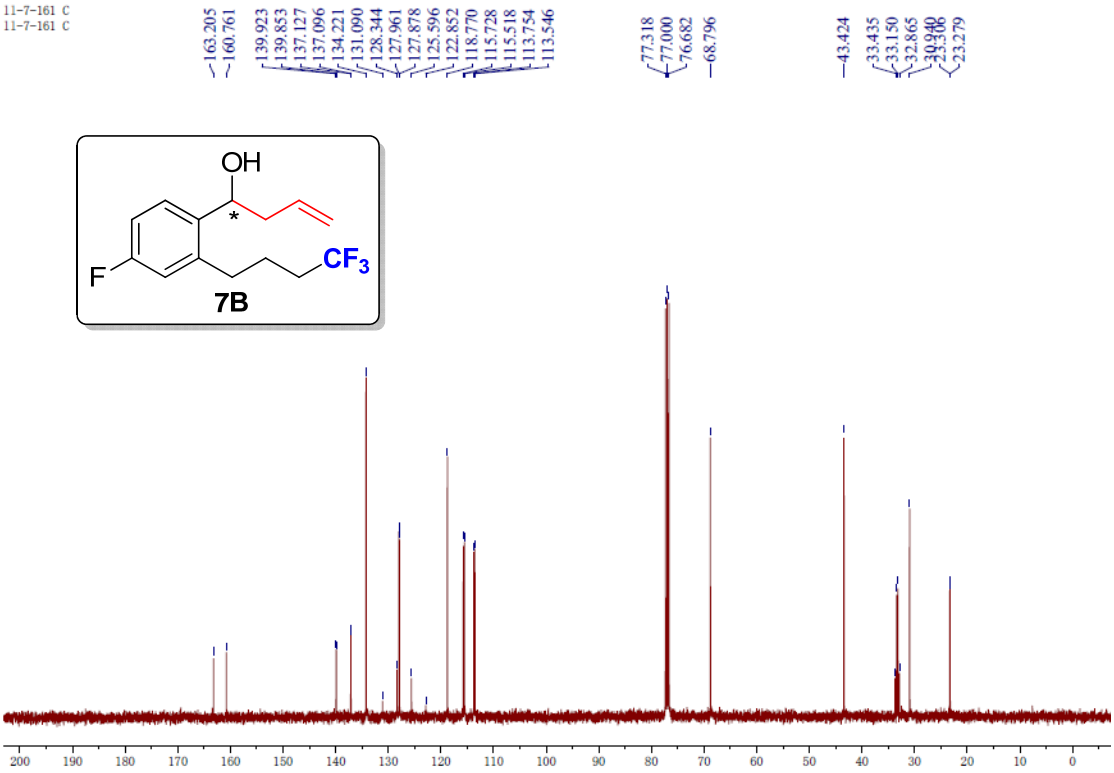

0.97
2.03
0.94
1.00
2.01
1.02
1.95
2.07
3.05
2.05

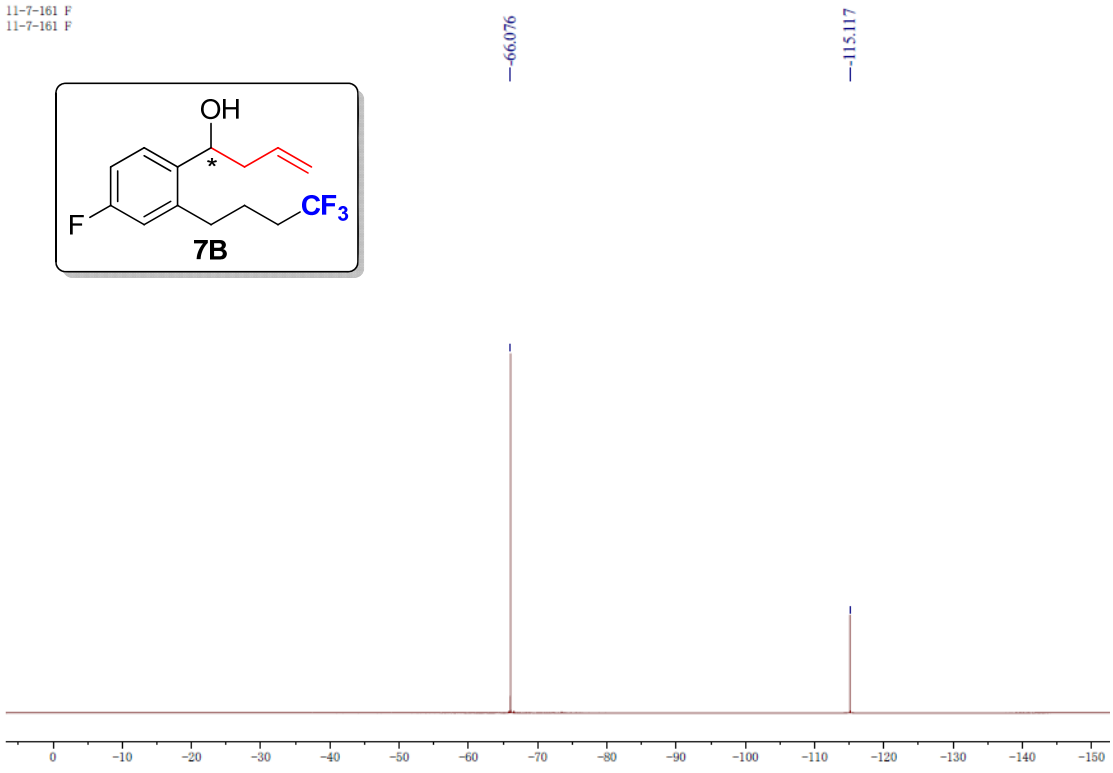

11-7-117 C
11-7-R(OH)CH2CHCH2 C

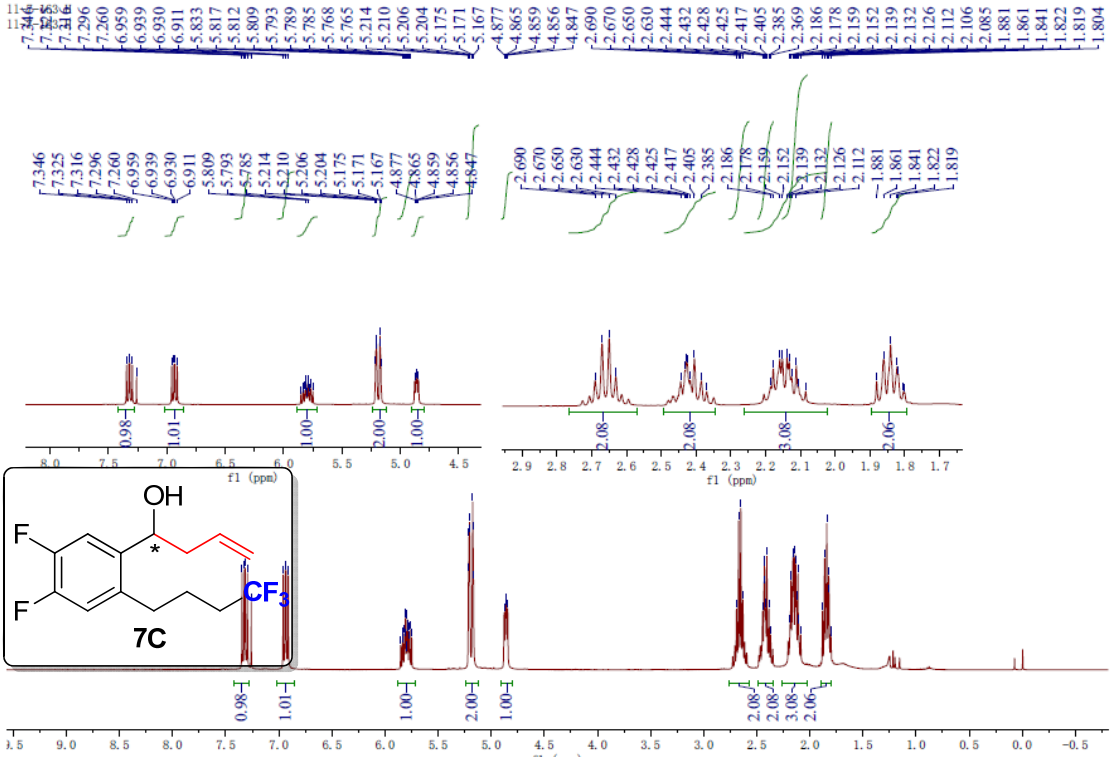

OH
*
CF3
7A

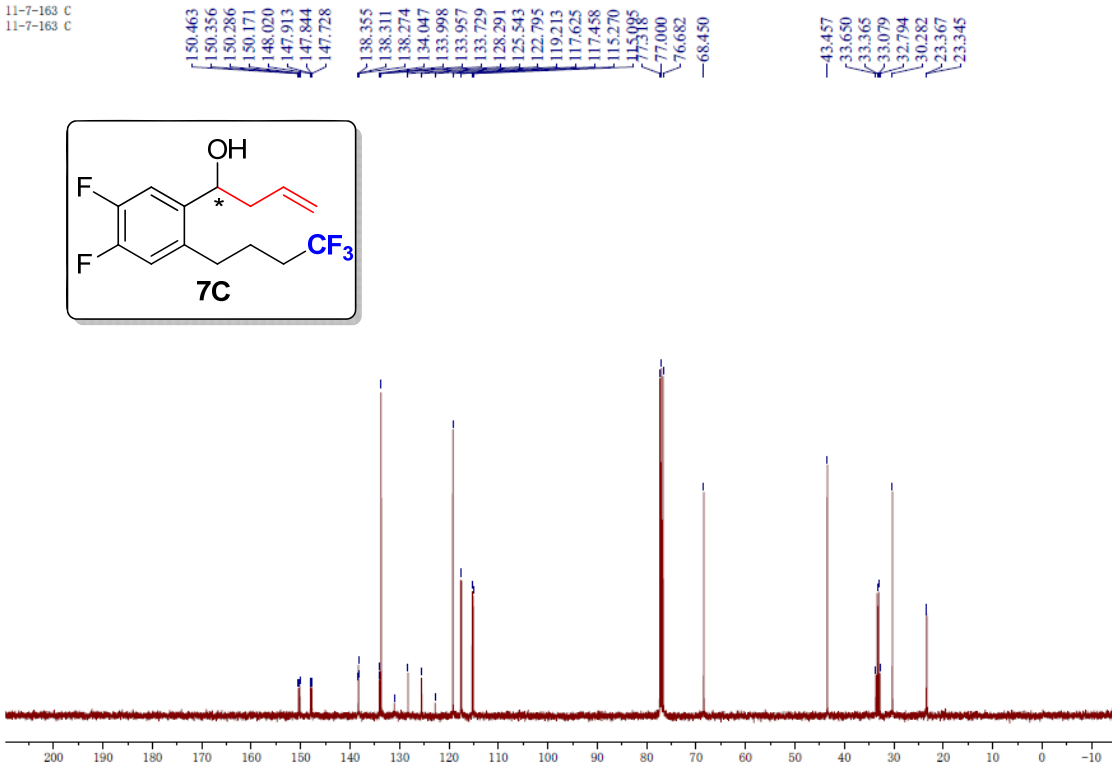


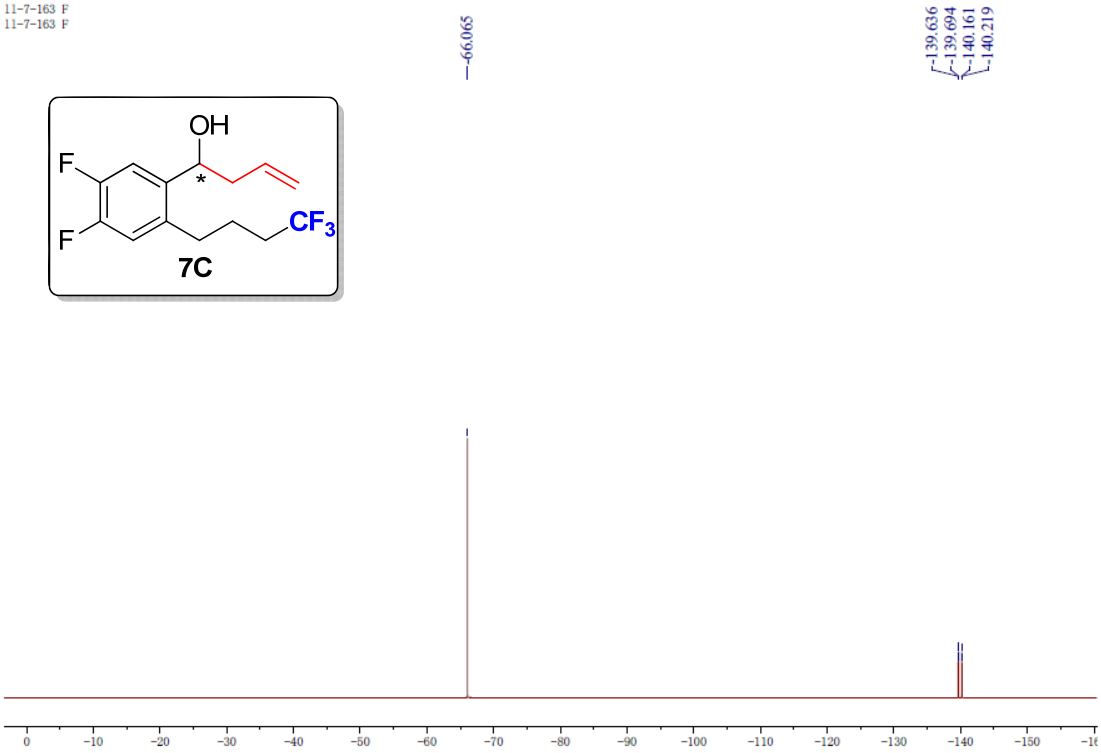

11-5-181-2
11-5-181-2
-66.093
OH
*
CF3
7A
7.490
7.475
7.469
7.454
7.260
6.952
6.946
6.862
6.855
6.837
6.831
5.821
5.804
5.779
5.208
5.204
5.183
5.161
5.158
4.913
4.896
4.880
2.744
2.734
2.725
2.714
2.704
2.695
2.483
2.465
2.449
2.185
2.166
2.158
2.145
2.139
2.132
2.118
2.112
2.091
1.908
1.889
1.887
1.868
1.849
0.98
0.99
1.00
1.00
2.02
1.04
2.04
2.04
3.13
2.09
f1 (ppm)
OH
*
F
CF3
7B

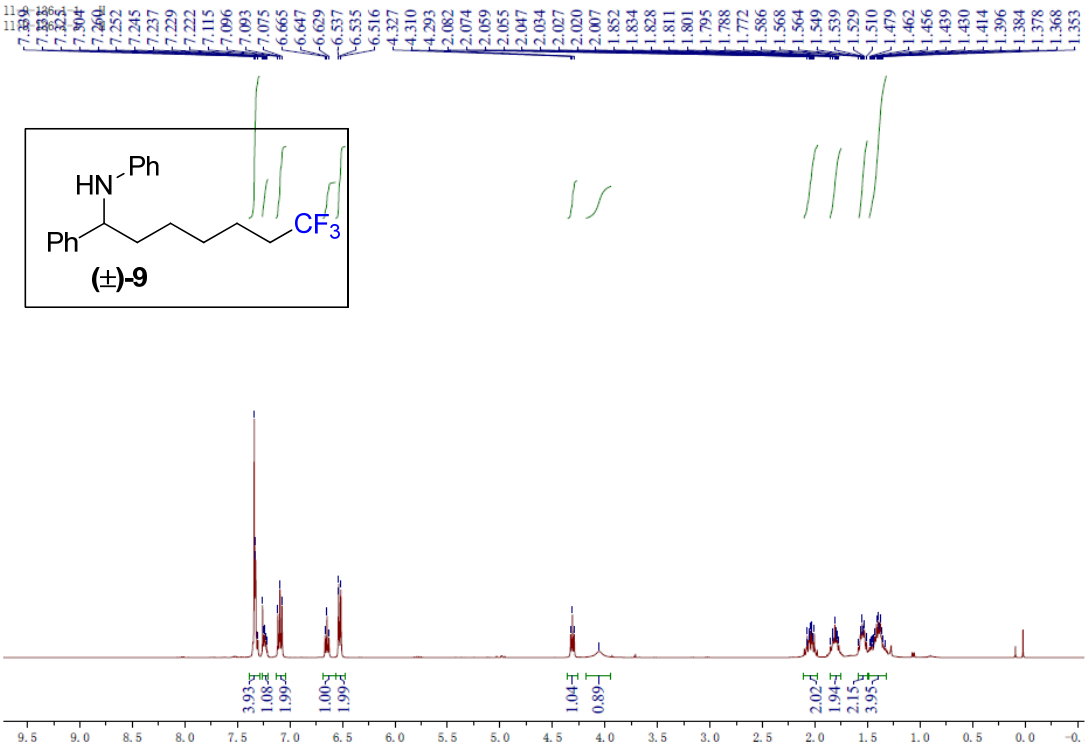

11-7-161 C
11-7-161 C
163.205
160.761
139.923
139.853
137.127
137.096
134.221
131.090
128.344
127.961
127.878
125.596
122.852
118.770
115.728
115.518
113.754
113.546
77.318
77.000
76.682
68.796
43.424
33.435
33.150
32.865
23.279
OH
*
F
CF3
7B
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0


11-7-161 F
11-7-161 F
-66.076
-115.117
OH
*
F
CF3
7B
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150


OH
F
F
CF3
7C
f1 (ppm)

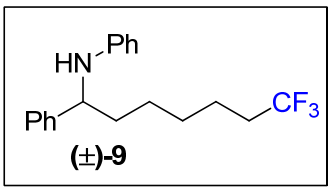

OH
F
F
CF3
7C


11-7-163 F
11-7-163 F
-66.065
-139.636
-139.694
-140.161
-140.219
OH
F
F
CF3
7C

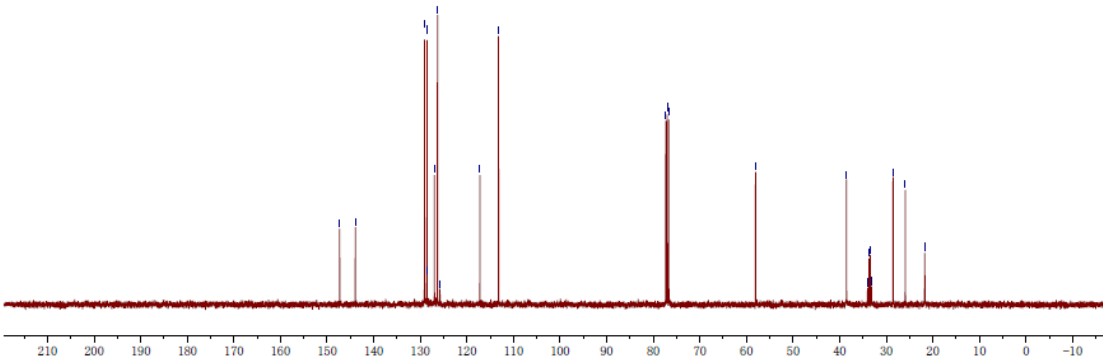

HN
Ph
Ph
CF3
(±)-9

11-9-124-1 C
11-9-124-1 C

147.300
143.939
129.077
128.560
128.521
126.955
126.312
117.210
113.205
77.317
77.000
76.682
58.051
38.536
33.996
33.714
33.432
33.150
28.532
25.912
21.739
21.709

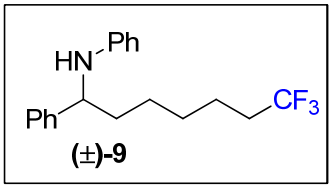


(±)-9

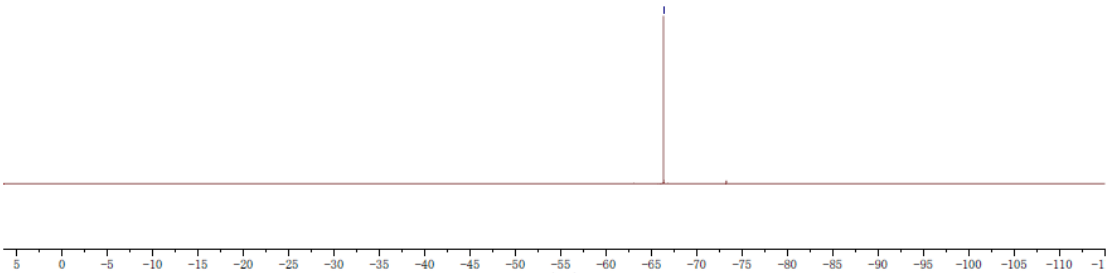


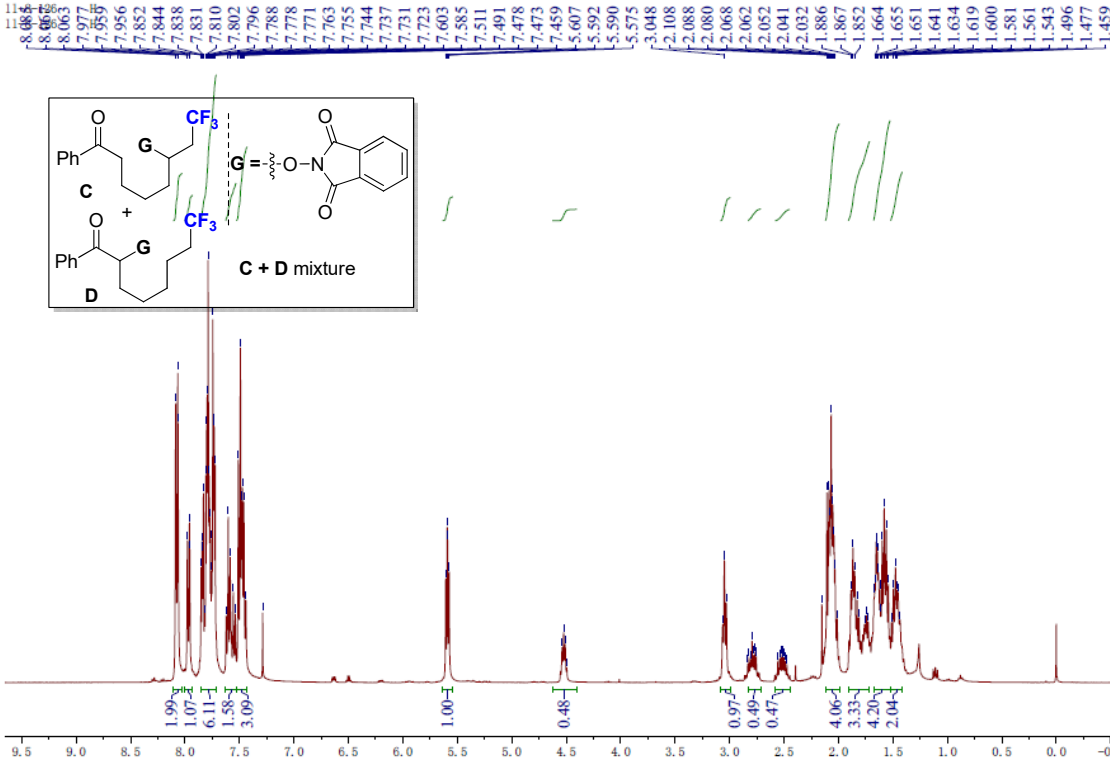
11-9-136-1 F
11-9-136-1 F

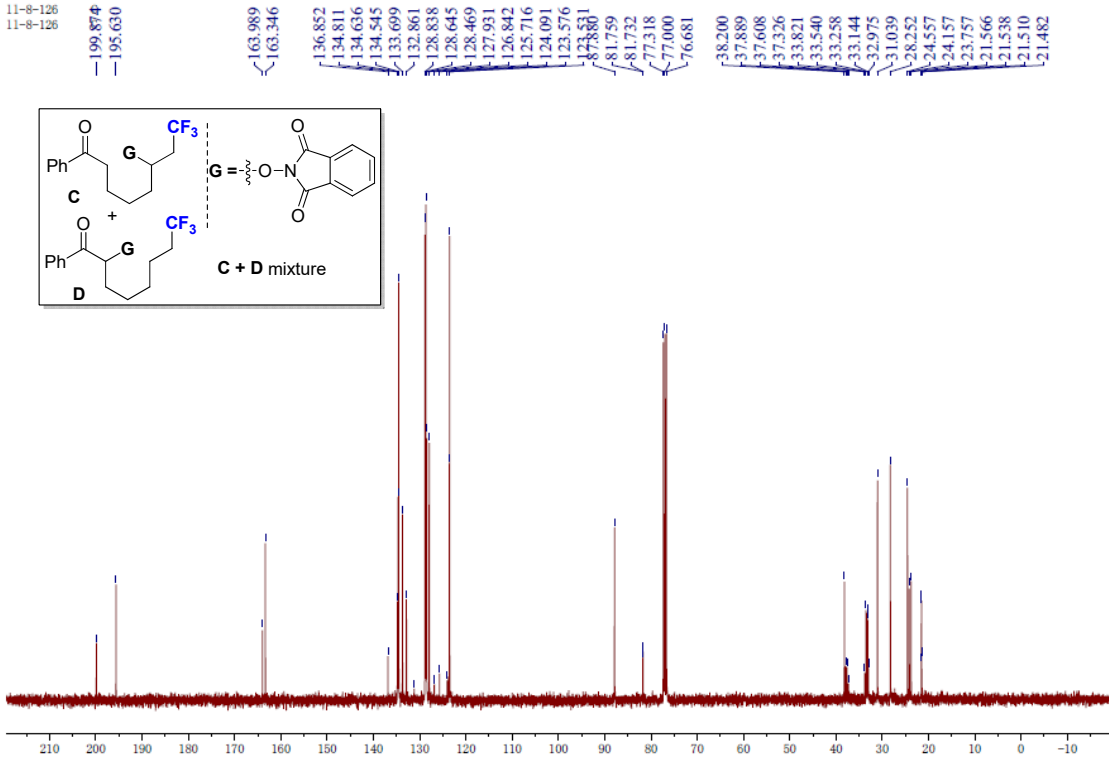
-66.356

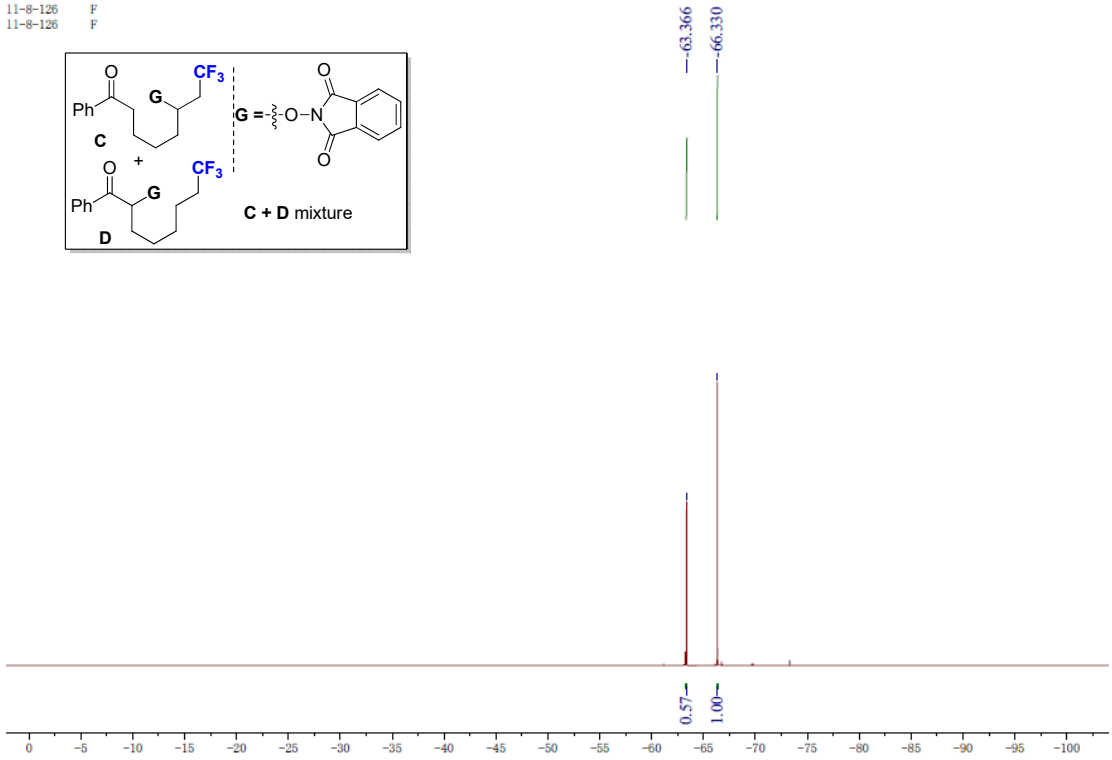


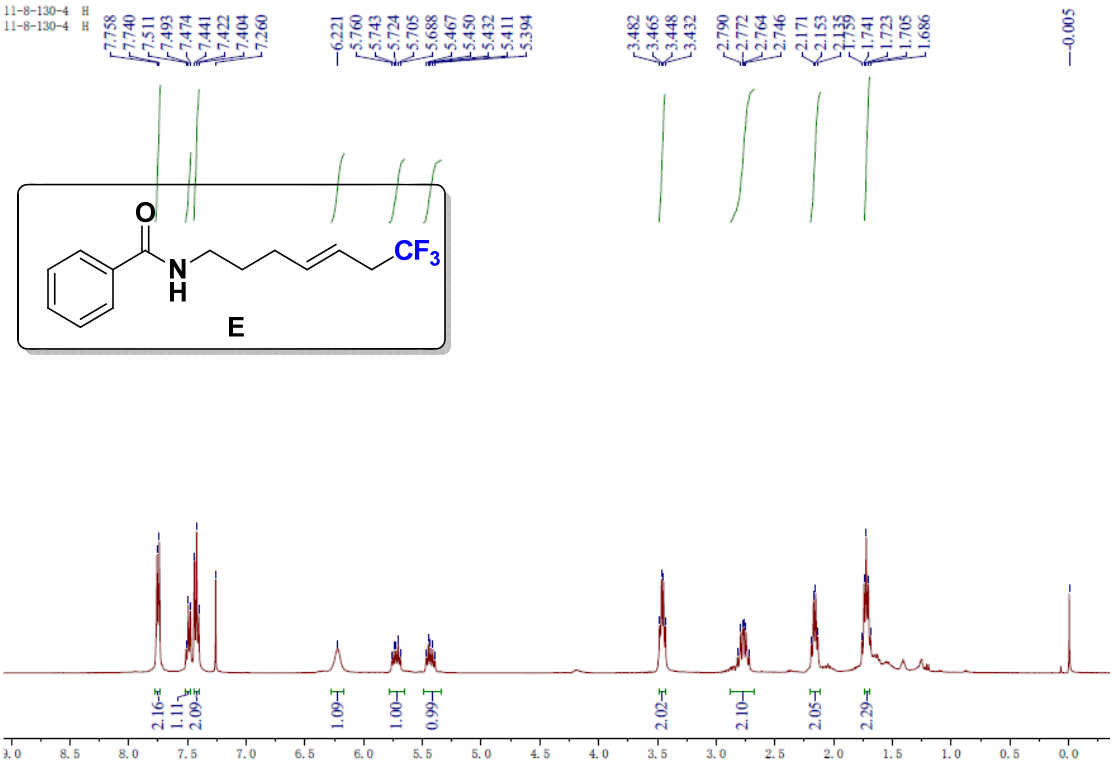
(±)-9

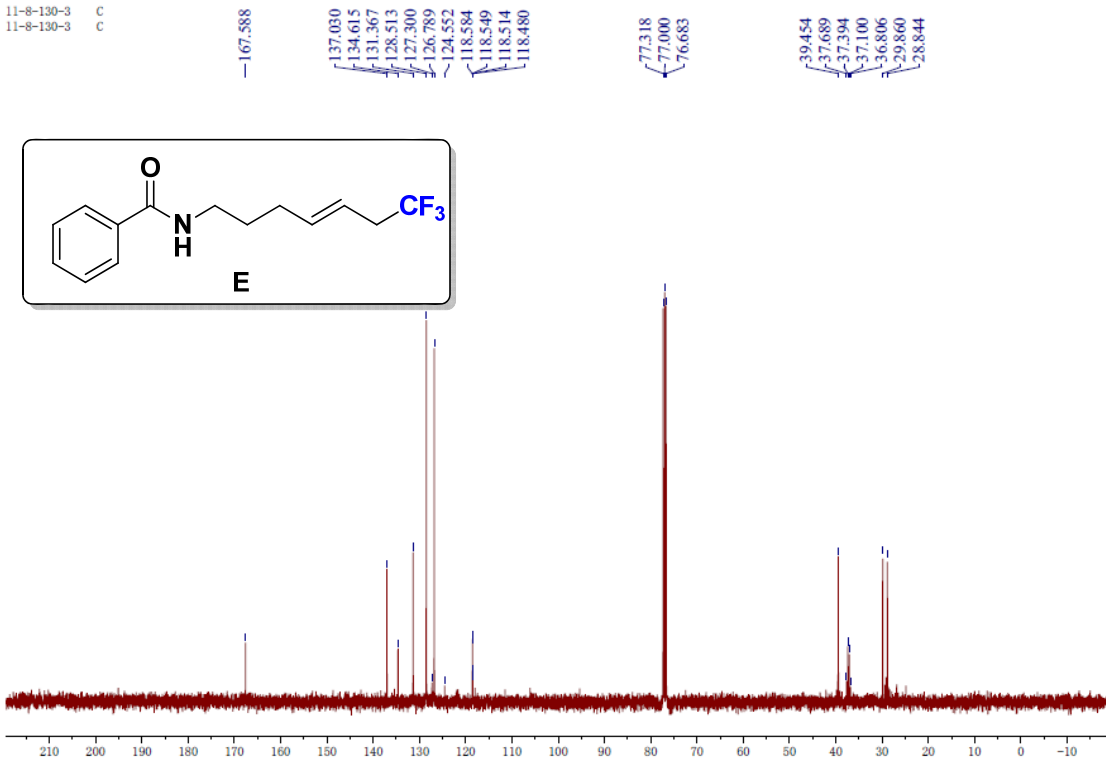


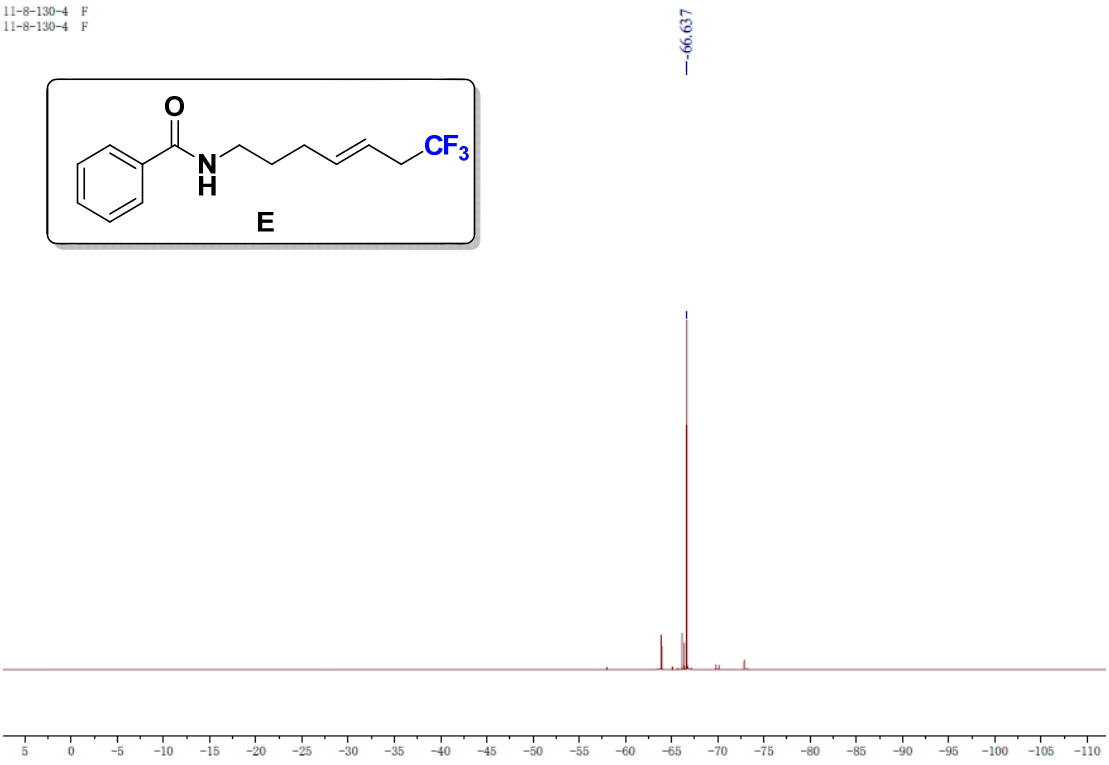

C + D mixture


C + D mixture

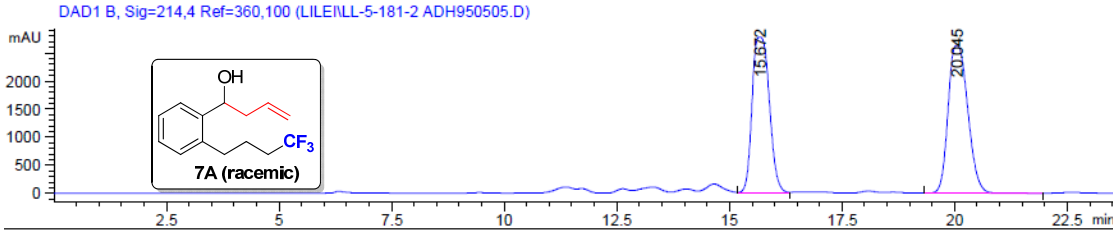

11-8-126 F
11-8-126 F
-63.366
-66.330
C + D mixture
0.57
1.00


11-8-130-4 H
11-8-130-4 H
E

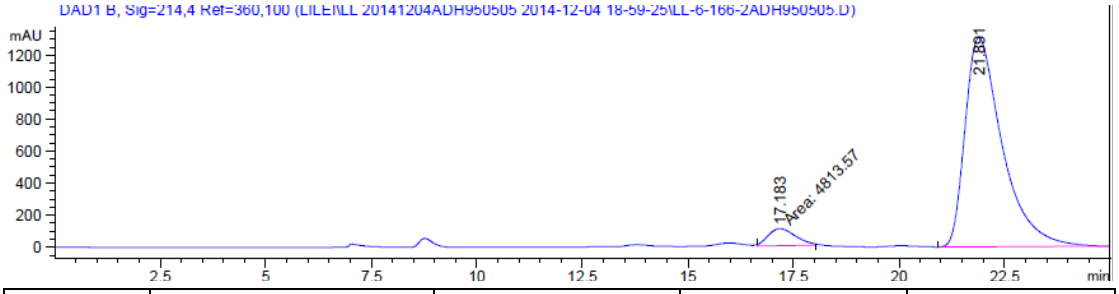

11-8-130-3 C
11-8-130-3 C
167.588
137.030
134.615
131.367
128.513
127.300
126.789
124.552
118.584
118.549
118.514
118.480
77.318
77.000
76.683
39.454
37.689
37.394
37.100
36.806
29.860
28.844
O
N
H
CF3
E
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10


11-8-130-4 F
11-8-130-4 F
-66.637
O
N
H
CF3
E
5 0 -5 -10 -15 -20 -25 -30 -35 -40 -45 -50 -55 -60 -65 -70 -75 -80 -85 -90 -95 -100 -105 -110

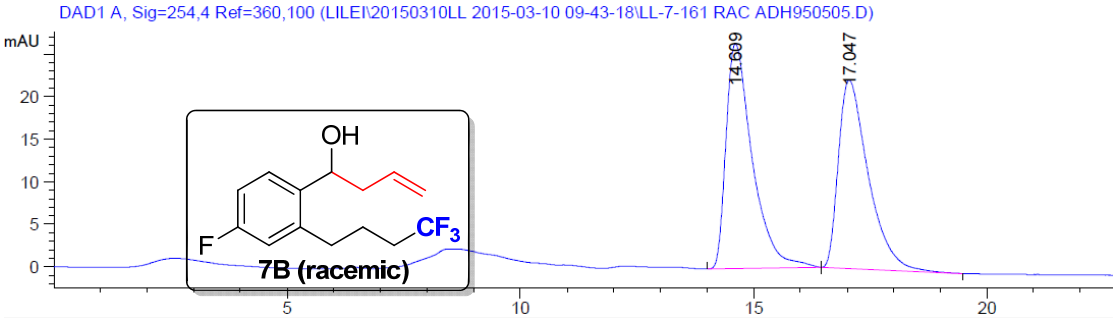
HPLC Spectra



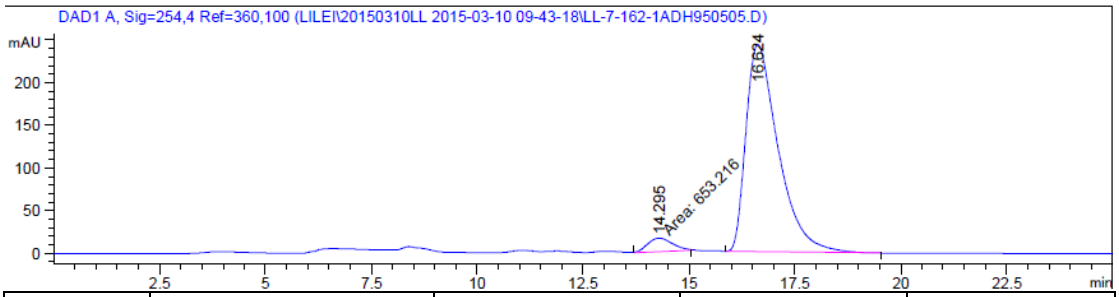
Peak	Retention time	Area	Height	Area%
1	15.672	7.30228e4	2767.75732	47.8575
2	20.045	7.95611e4	2634.24268	52.1425



Peak	Retention time	Area	Height	Area%
1	17.183	4813.57275	107.51881	5.6695
2	21.891	8.00895e4	1306.89050	94.3305

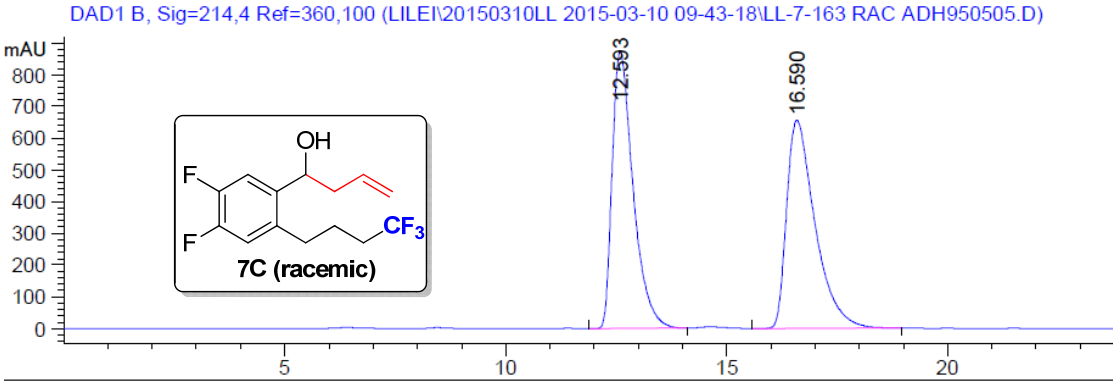


Peak	Retention time	Area	Height	Area%
1	14.609	1039.36011	26.43161	51.2926
2	17.047	986.97406	22.14137	48.7074

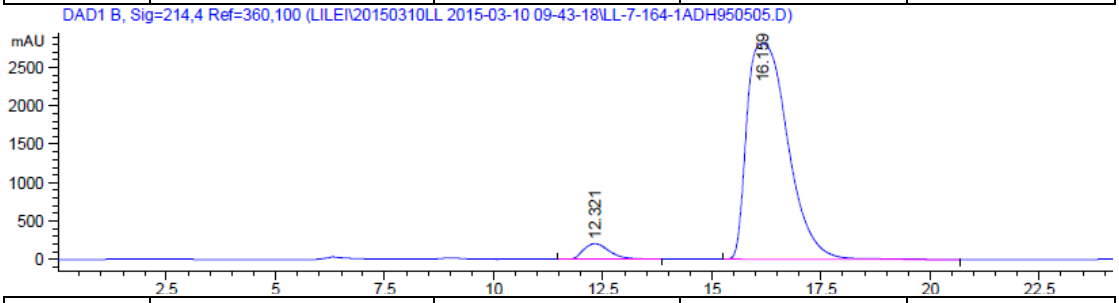


Peak	Retention time	Area	Height	Area%

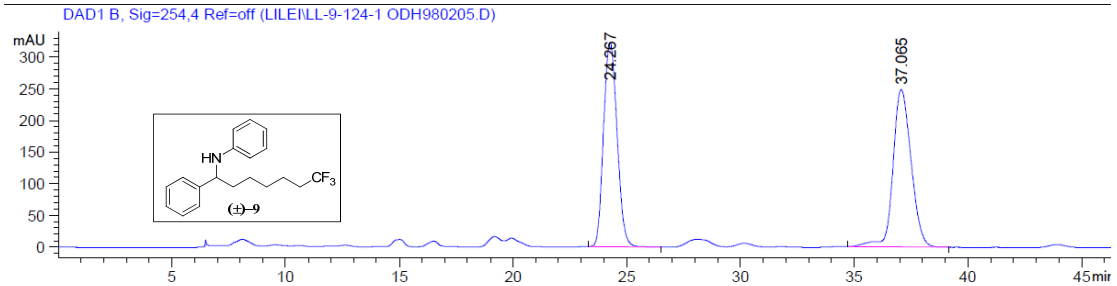
1	14.295	653.21625	15.89834	4.8432
2	16.624	1.28341e4	242.46364	95.1568



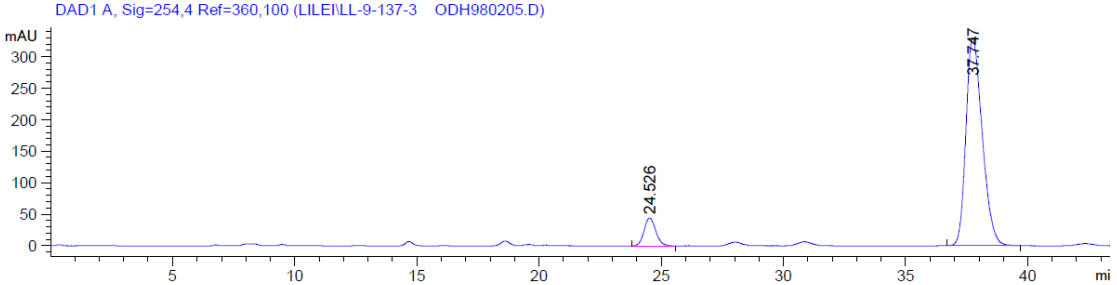
Peak	Retention time	Area	Height	Area%
1	12.593	2.87143e4	872.92535	49.4764
2	16.590	2.93220e4	656.12183	50.5236



Peak	Retention time	Area	Height	Area%
1	12.321	8375.90234	201.55574	4.3716
2	16.159	1.83221e5	2809.68359	95.6284



Peak	Retention time	Area	Height	Area%
1	24.267	1.33679e4	323.42657	49.2055
2	37.065	1.37996e4	248.97102	50.7945



Peak	Retention time	Area	Height	Area%
1	24.526	1436.38123	44.15376	8.6009
2	37.747	1.52639e4	329.56754	91.3991