Electronic Supplementary Information

1,2-Difunctionalization-Type (Hetero)arylation of Unactivated Alkenes Triggered by Radical Addition/Remote (Hetero)aryl Migration

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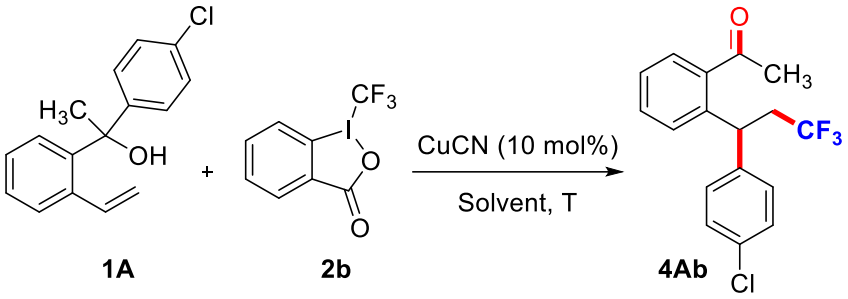
Table S1. Screening of reaction conditions for trifluoromethylation reaction of substrate **1A**.[a]

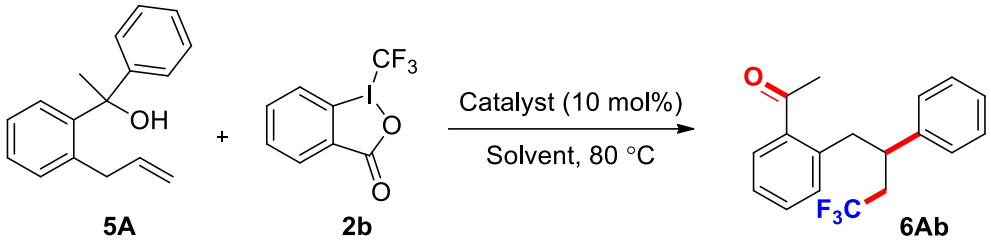


1A **2b** **4Ab**

Entry	Solvent	T (°C)	yield (%)[b]
1	1,4-dioxane	60	70
2	EtOAc	60	29
3	EtOAc	80	72
4	DCE	80	46
5	1,4-dioxane	80	82
6	CH_3CN	80	28
7	MeOH	80	49
8	DMSO	80	30

[a] Reaction conditions: **1A** (0.3 mmol), **2b** (0.6 mmol), and CuCN (10 mol%) in dried solvent (6 ml) at indicated temperatures; [b] Determined by ^{19}F-NMR with trifluoromethylbenzene as an internal standard.

Table S2. Screening of reaction conditions for trifluoromethylation reaction of substrate **6Ab**.[a]

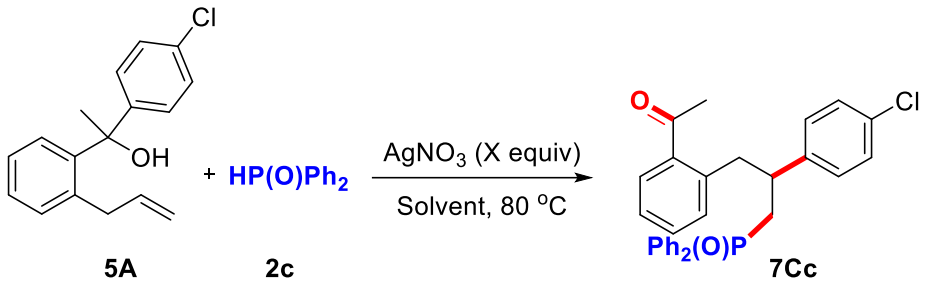


5A **2b** **6Ab**

Entry	Catalyst	Solvent	yield (%)[b]
1	CuI	EtOAc	68
2	CuBr	EtOAc	63
3	CuCl	EtOAc	61
4	CuCN	EtOAc	70
5	CuSCN	EtOAc	65
6	CuTc	EtOAc	64
7	$CuBr_2$	EtOAc	50
8	$Cu(OAc)_2$	EtOAc	38
9	$Cu(CH_3CN)_4BF_4$	EtOAc	53
10	CuCN	MeOH	17
11	CuCN	DCE	34
12	CuCN	1,4-dioxane	76
13	CuCN	NMP	31
14	CuCN	MeOAc	63
15	CuCN	CH_3CN	60
16	CuCN	DMSO	27

[a] Reaction conditions: **5A** (0.2 mmol), **2b** (0.4 mmol), and catalyst (10 mol%) in dried solvent (4 ml) at 80 °C; [b] Determined by ^{19}F-NMR with trifluoromethylbenzene as an internal standard.

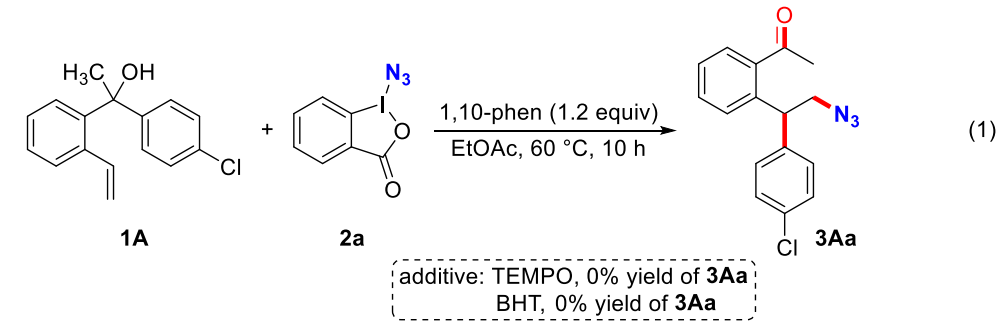
Table S3. Screening of reaction conditions for phosphonylation reaction of **7Cc**.[a]



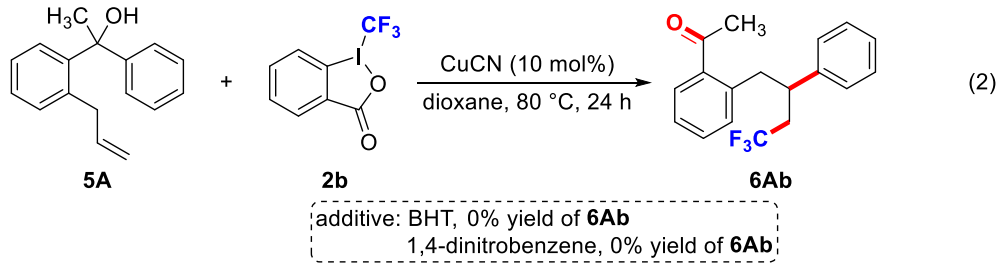
5A **2c** **7Cc**

Entry	$AgNO_3$ (X equiv)	Solvent	yield (%)[b]
1	0.5	CH_3CN	62
2	0.5	EtOAc	46
3	0.5	DMF	57
4	0.6	CH_3CN	77
5	1.0	CH_3CN	64

[a] Reaction conditions: **5A** (0.2 mmol), **2c** (0.4 mmol), and $AgNO_3$ (X equiv) in dried solvent (2 ml) at 80 °C; [b] Determined by ^{1}H-NMR with dibromomethane as an internal standard.



(1)



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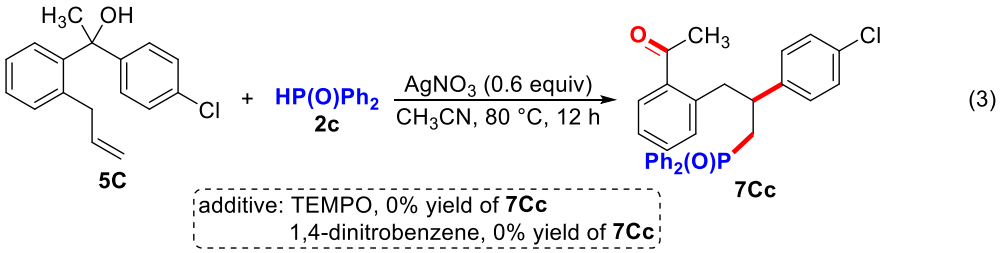

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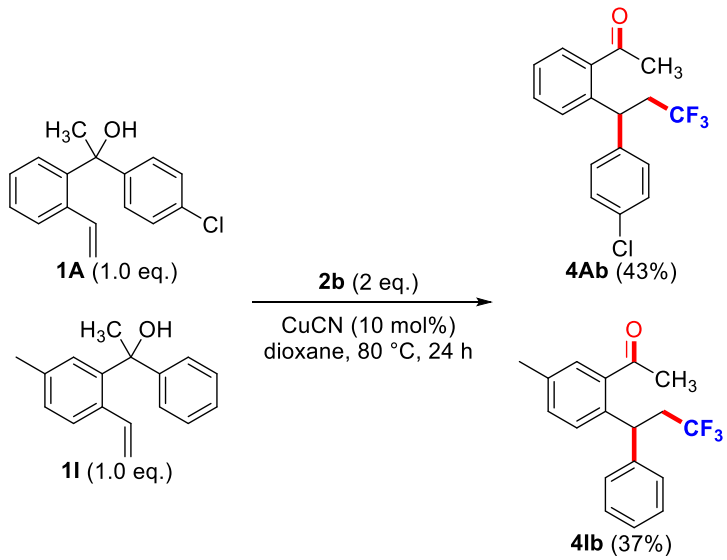


(4)

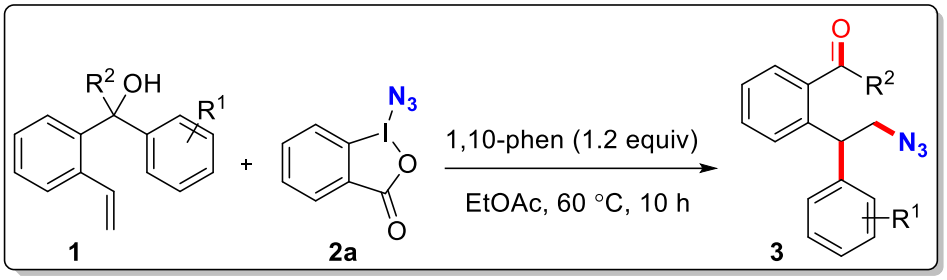
Scheme S1. Control and cross experiments.

General Information

All reactions were carried out under argon using Schlenk techniques. Reagents were purchased from commercial sources and used as received. 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 or a Bruker DPX 500 spectrometers at 400 MHz or 500 MHz for ^{1}H NMR, 100 MHz or 125 MHz for ^{13}C NMR, 376 MHz for ^{19}F NMR, and 162 MHz for ^{31}P NMR in $CDCl_3$ with tetramethylsilane (TMS) as an internal standard, [$CFCl_3$ as an external reference (0 ppm) for ^{19}F NMR, H_3PO_4 as an external reference (0 ppm) for ^{31}P NMR]. 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). Infrared absorption spectra were recorded as neat samples on a Shimadzu IRAffinity-1 Fourier Transform Infrared Spectrophotometer. Mass spectrometric data was obtained using Bruker Apex IV RTMS. All substrates were prepared according to literature.[1]

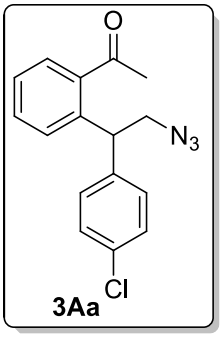
General Procedures for Azidation, Trifluoromethylation and Phosphonylation

General procedure for azidation reaction



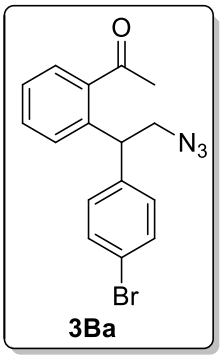
A 25 mL Schlenk tube equipped with a magnetic stir bar was charged with **1** (0.3 mmol, 1.0 equiv), **2a** (104.0 mg, 0.36 mmol, 1.2 equiv), 1,10-phen (64.8 mg, 0.36 mmol, 1.2 equiv), and EtOAc (3.0 mL) under argon atmosphere. The sealed tube was then stirred at 60 °C for 10 h. After completion of the reaction as monitored by TLC, EtOAc (30 mL) was added. The organic phase was washed with saturated $NaHCO_3$ solution (2 × 5 mL), dried over anhydrous Na_2SO_4, filtered, and concentrated to afford a crude product, which was purified by flash column chromatography to afford the corresponding product **3**.

1-(2-(2-azido-1-(4-chlorophenyl)ethyl)phenyl)ethanone



(66% yield), ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.67 (dd, *J* = 8.0, 1.2 Hz, 1H), 7.45 (td, *J* = 7.6, 1.2 Hz, 1H), 7.34 (td, *J* = 7.6, 1.2 Hz, 1H), 7.30 – 7.26 (m, 3H), 7.20 – 7.16 (m, 2H), 5.11 (t, *J* = 7.6 Hz, 1H), 3.90 (dd, *J* = 12.4, 7.2 Hz, 1H), 3.79 (dd, *J* = 12.4, 7.6 Hz, 1H), 2.51 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 202.51, 140.30, 139.69, 138.44, 132.63, 131.56, 129.84, 129.17, 128.88, 128.62, 126.86, 54.99, 44.44, 29.97. IR (neat) ν: 3028, 2987, 2098, 1685, 1492, 1357, 1244, 1093, 1014, 898 cm^{-1}. HRMS (APCI) m/z calcd. for $C_{16}H_{15}ON_3Cl$ $[M + H]^+$ 300.0898, found 300.0901.

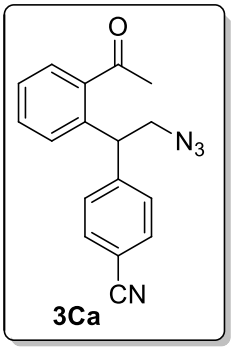
1-(2-(2-azido-1-(4-bromophenyl)ethyl)phenyl)ethanone



3Ba

(64% yield), ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.67 (dd, *J* = 7.6, 1.0 Hz, 1H), 7.48 – 7.39 (m, 3H), 7.34 (td, *J* = 7.6, 1.0 Hz, 1H), 7.27 (d, *J* = 8.0 Hz, 1H), 7.12 (d, *J* = 8.4 Hz, 2H), 5.10 (t, *J* = 7.2 Hz, 1H), 3.90 (dd, *J* = 12.4, 7.2 Hz, 1H), 3.79 (dd, *J* = 12.4, 7.6 Hz, 1H), 2.52 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 202.46, 140.23, 138.40, 131.57, 130.22, 129.21, 128.91, 126.88, 120.76, 54.92, 44.50, 29.98. IR (neat) ν: 3076, 2929, 2873, 2100, 1685, 1600, 1489, 1419, 1282, 958 cm^{-1}. HRMS (APCI) m/z calcd. for $C_{16}H_{14}ON_3BrNa$ $[M + Na]^+$ 366.0212, found 366.0208.

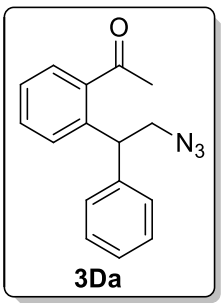
4-(1-(2-acetylphenyl)-2-azidoethyl)benzonitrile



3Ca

(73% yield), ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.73 (dd, *J* = 7.6, 1.2 Hz, 1H), 7.62 – 7.56 (m, 2H), 7.47 (td, *J* = 7.6, 1.6 Hz, 1H), 7.40 – 7.34 (m, 3H), 7.26 – 7.22 (m, 1H), 5.21 (t, *J* = 7.2 Hz, 1H), 3.93 (dd, *J* = 12.4, 7.6 Hz, 1H), 3.82 (dd, *J* = 12.4, 7.7 Hz, 1H), 2.54 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 202.09, 146.77, 139.51, 137.96, 132.18, 131.85, 129.65, 129.28, 129.01, 127.22, 118.67, 110.59, 54.62, 45.10, 29.80. IR (neat) ν: 30788, 2954, 2890, 2230, 2102, 1695, 1610, 1479, 1440, 1285, 960 cm^{-1}. HRMS (APCI) m/z calcd. for $C_{17}H_{15}ON_4$ $[M + H]^+$ 291.1240, found 291.1233.

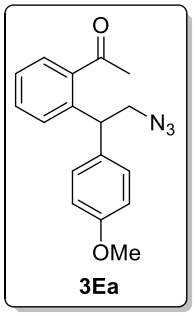
1-(2-(2-azido-1-phenylethyl)phenyl)ethanone



3Da

(62% yield), ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.65 – 7.61 (m, 1H), 7.47 – 7.41 (m, 1H), 7.36 – 7.30 (m, 4H), 7.26 – 7.20 (m, 3H), 5.12 (t, *J* = 7.6 Hz, 1H), 3.92 (dd, *J* = 12.4, 7.6 Hz, 1H), 3.84 (dd, *J* = 12.4, 7.6 Hz, 1H), 2.48 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 202.83, 141.11, 140.63, 138.91, 131.31, 128.93, 128.77, 128.50, 126.81, 126.61, 124.95, 55.14, 45.03, 30.05. IR (neat) ν: 3056, 2987, 2975, 2100, 1685, 1448, 1423, 1357, 958, 898 cm^{-1}. HRMS (APCI) m/z calcd. for $C_{16}H_{15}ON_3Na[M + Na]^+$ 288.1107, found 288.1100 .

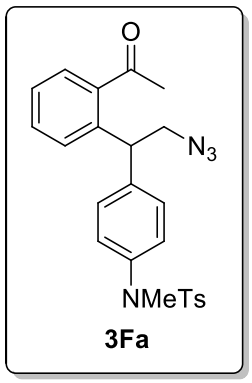
1-(2-(2-azido-1-(4-methoxyphenyl)ethyl)phenyl)ethanone



3Ea

(52% yield), ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.61 (d, *J* = 7.6 Hz, 1H), 7.46 – 7.40 (m, 1H), 7.34 – 7.28 (m, 2H), 7.15 (d, *J* = 8.4 Hz, 2H), 6.85 (d, *J* = 8.4 Hz, 2H), 5.05 (t, *J* = 7.6 Hz, 1H), 3.89 (dd, *J* = 12.4, 7.2 Hz, 1H), 3.82 – 3.77 (m, 4H), 2.47 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 203.00, 158.41, 141.02, 139.00, 133.27, 131.32, 129.58, 128.79, 126.60, 126.27, 113.96, 55.38, 55.24, 44.37, 30.15. IR (neat) ν: 3066, 2977, 2932, 2095, 1684, 1610, 1495, 1423, 1275, 962 cm^{-1}. HRMS (APCI) m/z calcd. for $C_{17}H_{17}O_2N_3Na$ $[M + Na]^+$ 318.1213, found 318.1205.

N-(4-(1-(2-acetylphenyl)-2-azidoethyl)phenyl)-N,4-dimethylbenzenesulfonamide

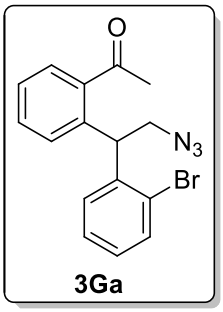


3Fa

(79% yield), ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.65 (d, *J* = 8.0 Hz, 1H), 7.48 – 7.43 (m, 1H), 7.40 (d, *J* = 8.0 Hz, 2H), 7.34 (t, *J* = 7.5 Hz, 1H), 7.29 (d, *J* = 8.0 Hz, 1H), 7.22 (d, *J* = 8.0 Hz, 2H), 7.16 (d, *J* = 8.5 Hz, 2H), 7.03 (d, *J* = 8.5 Hz, 2H), 5.09 (t, *J* = 7.0 Hz, 1H), 3.88 (dd, *J* = 12.5, 7.0 Hz, 1H), 3.81 (dd, *J* = 12.5, 7.5 Hz, 1H), 3.12 (s, 3H), 2.49 (s, 3H), 2.41 (s, 3H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 202.7, 143.5, 140.3, 140.2, 140.2, 138.7, 133.3, 131.5, 129.3, 129.0, 128.9, 128.9, 127.8, 126.8, 126.5, 55.1, 44.6, 37.9, 30.0, 21.5. IR (neat) ν: 3076, 3028, 2926, 2100, 1685, 1435, 1419, 1348, 1282,

908 cm^{-1}. HRMS (APCI) m/z calcd. for $C_{24}H_{25}N_4O_3S$ $[M + H]^+$ 449.1642, found 449.1630.

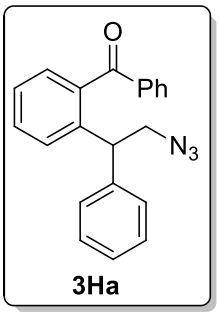
1-(2-(2-azido-1-(2-bromophenyl)ethyl)phenyl)ethanone



3Ga

(66% yield), ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.71 (dd, *J* = 7.6, 1.2 Hz, 1H), 7.56 – 7.52 (m, 1H), 7.41 – 7.31 (m, 4H), 7.16 – 7.08 (m, 2H), 5.32 (dd, *J* = 8.4, 5.6 Hz, 1H), 4.00 (dd, *J* = 12.8, 5.6 Hz, 1H), 3.81 (dd, *J* = 12.8, 8.4 Hz, 1H), 2.58 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 202.11, 140.04, 139.15, 138.65, 133.43, 131.41, 129.46, 129.06, 128.49, 127.27, 126.77, 125.93, 53.54, 45.60, 29.50. IR (neat) ν: 3051, 2929, 2872, 2098, 1683, 1598, 1571, 1469, 1280, 1232, 908 cm^{-1}. HRMS (APCI) m/z calcd. for $C_{16}H_{15}ON_3Br$ $[M + H]^+$ 344.0393, found 344.0405.

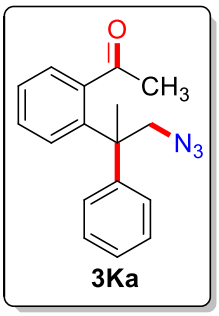
(2-(2-azido-1-phenylethyl)phenyl)(phenyl)methanone



3Ha

(44% yield), ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.70 – 7.66 (m, 2H), 7.58 – 7.53 (m, 1H), 7.50 – 7.46 (m, 2H), 7.40 (t, *J* = 7.5 Hz, 2H), 7.27 – 7.23 (m, 4H), 7.23 – 7.18 (m, 2H), 7.14 – 7.09 (m, 1H), 4.85 (t, *J* = 7.5 Hz, 1H), 3.05 – 2.95 (m, 1H), 2.94 – 2.83 (m, 1H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 198.32, 140.64, 140.35, 139.30, 137.49, 133.32, 130.37, 130.21, 128.72, 128.51, 128.32, 128.24, 128.22, 126.87, 126.10, 55.18, 45.92. IR (neat) ν: 3072, 3039, 2966, 2100, 1662, 1597, 1448, 1411, 1282, 927 cm^{-1}. HRMS (APCI) m/z calcd. for $C_{21}H_{18}ON_3$ $[M + H]^+$ 328.1444, found 328.1436.

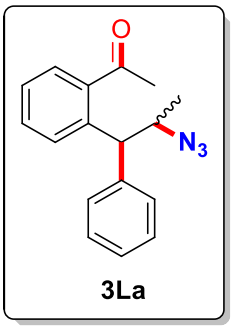
1-(2-(1-azido-2-phenylpropan-2-yl)phenyl)ethanone



3Ka

(75% yield), ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.63 (d, *J* = 8.0 Hz, 1H), 7.44 (td, *J* = 8.0, 1.5 Hz, 1H), 7.33 – 7.26 (m, 3H), 7.23 – 7.19 (m, 1H), 7.12 – 7.06 (m, 3H), 4.26 (d, *J* = 11.5 Hz, 1H), 3.97 (d, *J* = 11.5 Hz, 1H), 1.80 (s, 3H), 1.54 (s, 3H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 206.34, 146.15, 143.41, 143.39, 129.00, 128.21, 128.06, 127.86, 126.50, 126.46, 126.25, 61.56, 47.90, 29.66, 28.08. IR (neat) ν: 3072, 2981, 2933, 2105, 1693, 1419, 1415, 1305, 1244, 893 cm^{-1}. HRMS (APCI) m/z calcd. for $C_{17}H_{17}ON_3Na$ $[M + Na]^+$ 302.1264, found 302.1257.

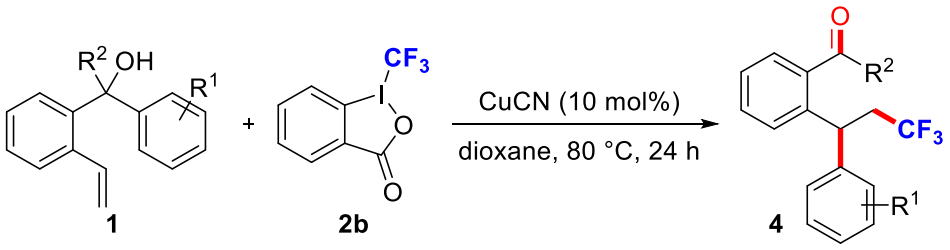
1-(2-(2-azido-1-phenylpropyl)phenyl)ethanone



3La

(52% yield), ^{1}H NMR (400 MHz, $CDCl_3$, a mixture of two diastereomers with a ratio of ca. 2:1) δ 7.70 – 7.16 (m, 9H), 4.85 (d, *J* = 9.8 Hz, 1H), 4.33 – 4.15 (m, 1H), 2.51 (s, 2H), 2.45 (s, 1H), 1.33 – 1.26 (m, 3H). ^{13}C NMR (101 MHz, $CDCl_3$, a mixture of two diastereomers with a ratio of ca. 2:1) δ 203.42, 203.32, 141.27, 140.94, 140.88, 140.54, 139.73, 139.30, 131.13, 130.98, 129.12, 128.8, 128.70, 128.54, 128.42, 128.34, 126.75, 126.32, 126.29, 60.83, 60.40, 50.73, 50.63, 30.40, 30.34, 18.55, 18.35. IR (neat) ν: 3072, 2927, 2854, 2108, 1687, 1419, 1357, 1244, 958, 893 cm^{-1}.

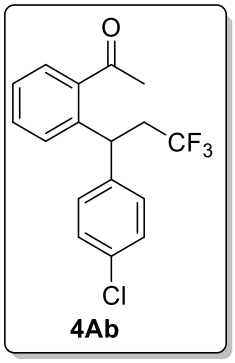
General procedure for trifluoromethylation reaction of 1 (method a)



1 **2b** **4**

A 25 mL Schlenk tube equipped with a magnetic stir bar was charged with **1** (0.3 mmol, 1.0 equiv), **2b** (189.0 mg, 0.6 mmol, 2.0 equiv), CuCN (2.7 mg, 0.03 mmol, 0.1 equiv), and dioxane (6.0 mL) under argon atmosphere. The sealed tube was then stirred at 80 °C for 24 h. After completion of the reaction as monitored by TLC, EtOAc (30 mL) was added and the reaction mixture was washed with saturated $NaHCO_3$ (2 × 5 mL) solution. The organic layer was dried over anhydrous Na_2SO_4, filtered and concentrated to afford a crude product, which was purified by flash column chromatography to afford product **4**.

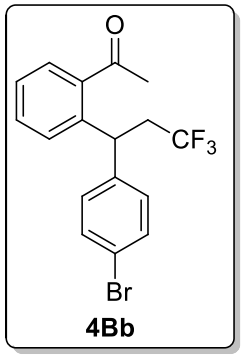
1-(2-(1-(4-chlorophenyl)-3,3,3-trifluoropropyl)phenyl)ethanone



4Ab

(80% yield), ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.59 (dd, *J* = 7.6, 1.2 Hz, 1H), 7.46 – 7.40 (m, 1H), 7.35 – 7.24 (m, 6H), 5.25 (t, *J* = 7.6 Hz, 1H), 2.93 – 2.78 (m, 2H), 2.48 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 202.93, 141.43, 140.95, 138.45, 132.50, 131.46, 129.31, 128.74, 128.61, 128.36, 126.64, 126.27 (q, *J* = 276.1 Hz), 39.38 (q, *J* = 27.2 Hz), 38.07 (q, *J* = 2.7 Hz), 29.99. ^{19}F NMR (376 MHz, $CDCl_3$) δ –63.44. HRMS (APCI) m/z calcd. for $C_{17}H_{15}OClF_3$ $[M + H]^+$ 327.0758, found 327.0751.

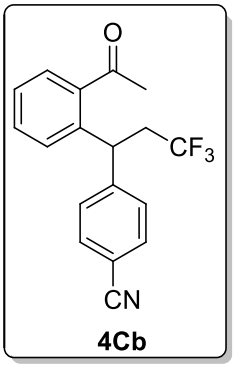
1-(2-(1-(4-bromophenyl)-3,3,3-trifluoropropyl)phenyl)ethanone



4Bb

(82% yield), ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.62 – 7.57 (m, 1H), 7.47 – 7.38 (m, 3H), 7.36 – 7.27 (m, 2H), 7.22 – 7.18 (m, 2H), 5.24 (t, *J* = 7.6 Hz, 1H), 2.93 – 2.78 (m, 2H), 2.49 (s, 3H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 202.90, 141.47, 141.34, 138.41, 131.56, 131.47, 129.68, 128.76, 128.37, 126.65, 126.25 (q, *J* = 276.1 Hz), 120.61, 39.31 (q, *J* = 27.3 Hz), 38.11 (q, *J* = 2.6 Hz), 29.98. ^{19}F NMR (376 MHz, $CDCl_3$) δ –63.43. HRMS (APCI) m/z calcd. for $C_{17}H_{15}OBrF_3$ $[M + Na]^+$ 371.0253, found 371.0245.

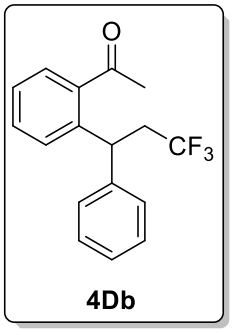
4-(1-(2-acetylphenyl)-3,3,3-trifluoropropyl)benzonitrile



4Cb

(88% yield), ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.65 (d, *J* = 7.2 Hz, 1H), 7.57 (d, *J* = 8.4 Hz, 2H), 7.46 (t, *J* = 8.0 Hz, 3H), 7.36 – 7.30 (m, 2H), 5.36 (t, *J* = 7.2 Hz, 1H), 2.96 – 2.79 (m, 2H), 2.51 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 202.53, 147.77, 140.56, 138.02, 132.23, 131.78, 129.22, 128.76, 128.47, 127.04, 126.07 (q, *J* = 276.0 Hz), 118.63, 110.57, 39.11 (q, *J* = 27.5 Hz), 38.70 (q, *J* = 2.1 Hz), 29.82. ^{19}F NMR (376 MHz, $CDCl_3$) δ –63.46. HRMS (APCI) m/z calcd. for $C_{18}H_{15}ONF_3$ $[M + H]^+$ 318.1100, found 318.1092.

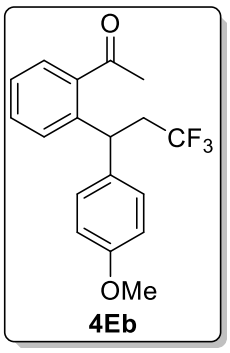
1-(2-(3,3,3-trifluoro-1-phenylpropyl)phenyl)ethanone



4Db

(79% yield), ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.55 (dd, *J* = 8.0, 1.2 Hz, 1H), 7.45 – 7.37 (m, 2H), 7.33 – 7.27 (m, 5H), 7.23 – 7.18 (m, 1H), 5.25 (t, *J* = 7.6 Hz, 1H), 2.96 – 2.83 (m, 2H), 2.45 (s, 3H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 203.23, 142.44, 141.79, 138.88, 131.19, 128.49, 128.35, 127.94, 126.67, 126.44 (q, *J* = 276.0 Hz), 126.38, 39.42 (q, *J* = 27.1 Hz), 38.64 (q, *J* = 2.6 Hz), 30.05. ^{19}F NMR (376 MHz, $CDCl_3$) δ –63.44. HRMS (APCI) m/z calcd. for $C_{17}H_{16}OF_3$ $[M + H]^+$ 293.1148, found 293.1141.

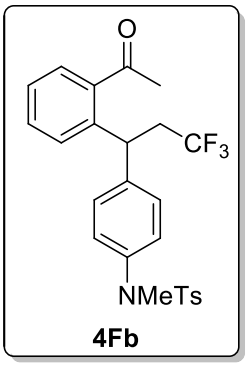
1-(2-(3,3,3-trifluoro-1-(4-methoxyphenyl)propyl)phenyl)ethanone



4Eb

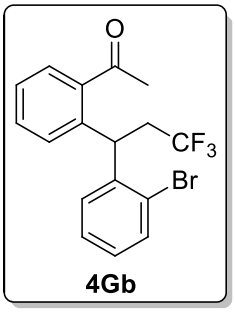
(69% yield), ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.52 – 7.48 (m, 1H), 7.41 – 7.33 (m, 2H), 7.25 – 7.18 (m, 3H), 6.83 – 6.78 (m, 2H), 5.18 (t, *J* = 7.6 Hz, 1H), 3.72 (s, 3H), 2.93 – 2.77 (m, 2H), 2.41 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 203.17, 158.18, 142.10, 138.77, 134.53, 131.07, 128.89, 128.22, 126.45 (q, *J* = 276.1 Hz), 126.22, 113.78, 55.02, 39.47 (q, *J* = 27.1 Hz), 37.90 (q, *J* = 2.6 Hz), 29.95. ^{19}F NMR (376 MHz, $CDCl_3$) δ –63.35. HRMS (APCI) m/z calcd. for $C_{18}H_{18}O_2F_3$ $[M + H]^+$ 323.1253, found 323.1246.

N-(4-(1-(2-acetylphenyl)-3,3,3-trifluoropropyl)phenyl)-N,4-dimethylbenzenesulfonamide



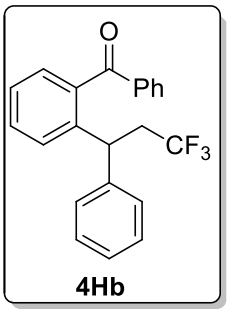
(72% yield), ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.57 (d, *J* = 7.5 Hz, 1H), 7.44 (t, *J* = 7.5 Hz, 1H), 7.36 (t, *J* = 8.0 Hz, 3H), 7.30 (t, *J* = 7.5 Hz, 1H), 7.22 (dd, *J* = 12.5, 8.5 Hz, 4H), 7.01 (d, *J* = 8.5 Hz, 2H), 5.23 (t, *J* = 7.5 Hz, 1H), 3.10 (s, 3H), 2.92 – 2.78 (m, 2H), 2.46 (s, 3H), 2.41 (s, 3H).^{13}C NMR (125 MHz, $CDCl_3$) δ 203.1, 143.6, 141.5, 141.4, 140.0, 138.6, 133.3, 131.4, 129.3, 128.6, 128.4, 128.4, 127.8, 126.6, 126.5, 126.3 (q, *J* = 276.1 Hz), 39.4 (q, *J* = 27.1 Hz), 38.2 (q, *J* = 2.5 Hz), 37.9, 30.0, 21.5. ^{19}F NMR (376 MHz, $CDCl_3$) δ –63.4. HRMS (APCI) m/z calcd. for $C_{25}H_{25}F_3NO_3S$ $[M + H]^+$ 476.1502, found 476.1489.

1-(2-(1-(2-bromophenyl)-3,3,3-trifluoropropyl)phenyl)ethanone



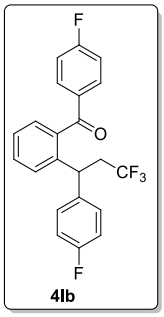
(74% yield), ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.65 (dd, *J* = 7.6, 1.2 Hz, 1H), 7.54 (dd, *J* = 8.0, 1.2 Hz, 1H), 7.42 – 7.29 (m, 4H), 7.24 (d, *J* = 7.6 Hz, 1H), 7.13 – 7.08 (m, 1H), 5.45 (t, *J* = 7.2 Hz, 1H), 2.97 – 2.87 (m, 2H), 2.56 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 202.29, 140.41, 139.99, 138.67, 133.51, 131.20, 129.32, 129.03, 128.77, 128.42, 127.08, 126.71, 125.91 (q, *J* = 276.7 Hz), 125.38, 39.98 (q, *J* = 2.7 Hz), 38.11 (q, *J* = 27.9 Hz), 29.56. ^{19}F NMR (376 MHz, $CDCl_3$) δ –63.09. HRMS (APCI) m/z calcd. for $C_{17}H_{15}OBr\ F_3$ $[M + H]^+$ 371.0253, found 371.0247.

phenyl(2-(3,3,3-trifluoro-1-phenylpropyl)phenyl)methanone



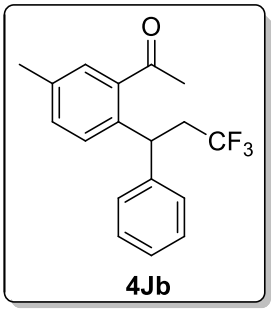
(70% yield), ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.69 – 7.64 (m, 2H), 7.56 – 7.51 (m, 1H), 7.48 – 7.44 (m, 2H), 7.40 – 7.35 (m, 2H), 7.26 – 7.21 (m, 4H), 7.20 – 7.16 (m, 2H), 7.12 – 7.07 (m, 1H), 4.83 (t, *J* = 7.5 Hz, 1H), 3.04 – 2.82 (m, 2H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 198.33, 141.97, 141.92, 138.67, 137.52, 133.20, 130.48, 130.22, 128.96, 128.47, 128.22, 127.81, 127.77, 126.69, 126.26 (q, *J* = 276.1 Hz), 125.81, 39.79 (q, *J* = 2.6 Hz), 39.30 (q, *J* = 27.4 Hz). ^{19}F NMR (376 MHz, $CDCl_3$) δ –63.41. HRMS (APCI) m/z calcd. for $C_{22}H_{18}OF_3$ $[M + H]^+$ 355.1304, found 355.1297.

(4-fluorophenyl)(2-(3,3,3-trifluoro-1-(4-fluorophenyl)propyl)phenyl)methanone



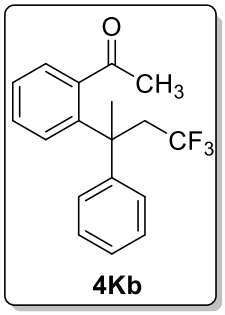
(71% yield), ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.69 – 7.64 (m, 2H), 7.51 – 7.45 (m, 2H), 7.28 (td, *J* = 7.5, 1.5 Hz, 1H), 7.23 (dd, *J* = 7.5, 1.5 Hz, 1H), 7.21 – 7.16 (m, 2H), 7.09 – 7.03 (m, 2H), 6.89 – 6.84 (m, 2H), 4.78 (t, *J* = 7.5 Hz, 1H), 3.01 – 2.89 (m, 1H), 2.89 – 2.77 (m, 1H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 196.68, 165.86 (d, *J* = 254.4 Hz), 161.50 (d, *J* = 244.4 Hz), 141.68, 138.40, 137.69 (d, *J* = 3.3 Hz), 133.71 (d, *J* = 2.9 Hz), 132.87 (d, *J* = 9.5 Hz), 130.64, 129.44 (d, *J* = 8.0 Hz), 128.77, 127.62, 126.16 (q, *J* = 276.1 Hz), 126.05, 115.47 (d, *J* = 19.9 Hz), 115.30 (d, *J* = 19.3 Hz), 39.37 (q, *J* = 27.4 Hz), 39.15 (q, *J* = 2.8 Hz). ^{19}F NMR (376 MHz, $CDCl_3$) δ –63.40 (s, 3F), –104.31 (s, 1F), –115.91 (s, 1F). HRMS (APCI) m/z calcd. for $C_{22}H_{16}OF_5$ $[M + H]^+$ 391.1116, found 391.1107.

1-(5-methyl-2-(3,3,3-trifluoro-1-phenylpropyl)phenyl)ethanone



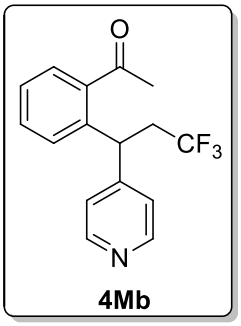
(62% yield), ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.32 (s, 1H), 7.30 – 7.26 (m, 4H), 7.25 – 7.20 (m, 2H), 7.19 – 7.15 (m, 1H), 5.18 (t, *J* = 7.5 Hz, 1H), 2.94 – 2.80 (m, 2H), 2.42 (s, 3H), 2.33 (s, 3H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 203.38, 142.70, 138.82, 138.76, 136.06, 131.89, 128.92, 128.45, 128.36, 127.87, 126.56, 126.48 (q, *J* = 276.9 Hz), 39.40 (q, *J* = 27.1 Hz), 38.38 (q, *J* = 2.6 Hz), 30.03, 20.87. ^{19}F NMR (376 MHz, $CDCl_3$) δ –63.42. HRMS (APCI) m/z calcd. for $C_{18}H_{18}OF_3$ $[M + H]^+$ 307.1304, found 307.1298.

1-(2-(4,4,4-trifluoro-2-phenylbutan-2-yl)phenyl)ethanone



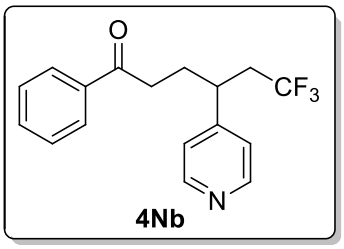
(72% yield), ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.70 (d, *J* = 8.0 Hz, 1H), 7.46 – 7.41 (m, 1H), 7.31 – 7.23 (m, 3H), 7.18 (t, *J* = 7.5 Hz, 1H), 7.13 (d, *J* = 7.5 Hz, 1H), 7.04 (d, *J* = 7.5 Hz, 2H), 3.79 – 3.67 (m, 1H), 2.93 – 2.82 (m, 1H), 1.85 (s, 3H), 1.50 (s, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 206.27, 148.37, 143.80, 143.04, 129.01, 128.21, 127.84, 127.35, 127.08 (q, *J* = 276.8 Hz), 126.56, 126.43, 126.33, 44.04 (q, *J* = 25.6 Hz), 43.91 (q, *J* = 1.6 Hz), 30.76 (q, *J* = 1.8 Hz), 29.63. ^{19}F NMR (376 MHz, $CDCl_3$) δ –58.56. HRMS (APCI) m/z calcd. for $C_{18}H_{18}OF_3$ $[M + H]^+$ 307.1304, found 307.1296.

1-(2-(3,3,3-trifluoro-1-(pyridin-4-yl)propyl)phenyl)ethanone



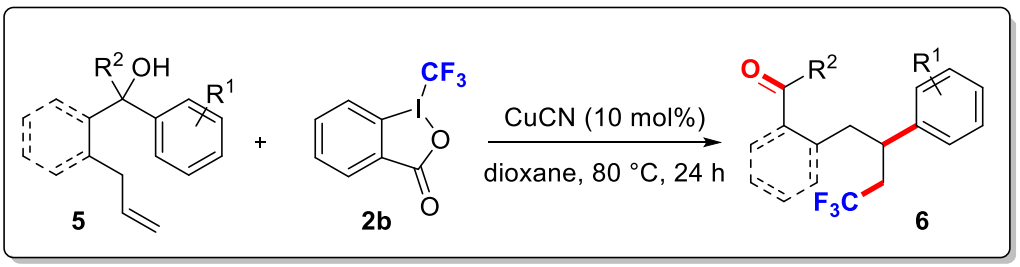
(65% yield), ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.50 (d, *J* = 5.5 Hz, 2H), 7.65 (dd, *J* = 7.5, 1.0 Hz, 1H), 7.45 (td, *J* = 7.5, 1.5 Hz, 1H), 7.35 – 7.29 (m, 2H), 7.24 (d, *J* = 6.0 Hz, 2H), 5.28 (t, *J* = 7.5 Hz, 1H), 2.92 – 2.83 (m, 2H), 2.52 (s, 3H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 202.46, 151.34, 149.84, 140.31, 138.14, 131.76, 129.16, 128.75, 127.07, 126.10 (q, *J* = 276.1 Hz), 123.09, 38.74 (q, *J* = 27.8 Hz), 38.16 (q, *J* = 2.7 Hz), 29.80. ^{19}F NMR (376 MHz, $CDCl_3$) δ –63.52. HRMS (APCI) m/z calcd. for $C_{16}H_{15}ONF_3$ $[M + H]^+$ 294.1100, found 294.1093.

6,6,6-trifluoro-1-phenyl-4-(pyridin-4-yl)hexan-1-one



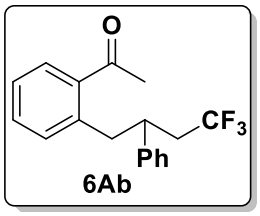
4Nb (36% yield), ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.58 (s, 2H), 7.84 – 7.78 (m, 2H), 7.57 – 7.51 (m, 1H), 7.42 (t, *J* = 8.0 Hz, 2H), 7.14 (s, 2H), 3.11 – 3.02 (m, 1H), 2.86 – 2.77 (m, 1H), 2.77 – 2.69 (m, 1H), 2.56 – 2.44 (m, 2H), 2.33 – 2.24 (m, 1H), 2.07 – 1.98 (m, 1H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 198.7, 151.3, 150.3, 136.5, 133.3 128.6, 127.8, 126.0 (q, *J* = 27.8 Hz), 122.9, 40.2 (q, *J* = 275.9 Hz), 38.7 (d, *J* = 2.4 Hz), 35.5, 29.8. ^{19}F NMR (376 MHz, $CDCl_3$) δ –63.6. HRMS (APCI) m/z calcd. for $C_{17}H_{17}F_3NO$ $[M + H]^+$ 308.1257 , found 308.1246.

General procedure for trifluoromethylation reaction (method b)



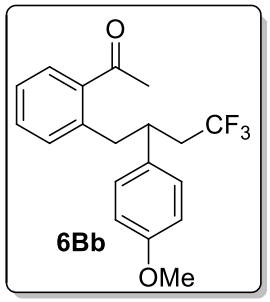
A 25 mL Schlenk tube equipped with a magnetic stir bar was charged with **5** (0.2 mmol, 1.0 equiv), **2b** (126.0 mg, 0.4 mmol, 2.0 equiv), CuCN (1.8 mg, 0.02 mmol, 0.1 equiv) and dioxane (4.0 mL) under argon atmosphere. The sealed tube was then stirred at 80 °C for 24 h. After completion of the reaction as monitored by TLC, EtOAc (30 mL) was added and the reaction mixture was washed with saturated $NaHCO_3$ solution (2 × 5 mL). The organic layer was dried over anhydrous Na_2SO_4, filtered and concentrated to afford a crude product, which was purified by flash column chromatography to afford product **6**.

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



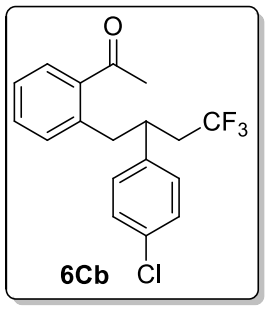
(73% yield), ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.63 (dd, *J* = 7.6, 1.6 Hz, 1H), 7.30 (td, *J* = 7.6, 1.6 Hz, 1H), 7.27 – 7.22 (m, 3H), 7.21 – 7.17 (m, 1H), 7.09 – 7.05 (m, 2H), 6.99 (dd, *J* = 7.6, 1.2 Hz, 1H), 3.32 – 3.15 (m, 3H), 2.62 – 2.47 (m, 2H), 2.43 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 201.87, 142.47, 139.19, 137.89, 132.11, 131.31, 129.44, 128.36, 127.61, 126.67, 126.61 (q, *J* = 276.0 Hz), 126.35, 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.

1-(2-(4,4,4-trifluoro-2-(4-methoxyphenyl)butyl)phenyl)ethanone



(67% yield), ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.64 (dd, *J* = 8.0, 1.5 Hz, 1H), 7.30 (td, *J* = 7.5, 1.5 Hz, 1H), 7.27 – 7.23 (m, 1H), 7.02 – 6.97 (m, 3H), 6.80 – 6.76 (m, 2H), 3.77 (s, 3H), 3.29 – 3.23 (m, 1H), 3.23 – 3.16 (m, 1H), 3.15 – 3.09 (m, 1H), 2.58 – 2.42 (m, 5H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 201.87, 158.22, 139.34, 137.86, 134.49, 132.13, 131.32, 129.43, 128.53, 126.64 (q, *J* = 275.8 Hz), 126.30, 113.71, 55.16, 41.08 (q, *J* = 2.4 Hz), 40.94, 39.2 (q, *J* = 26.8 Hz), 29.53. ^{19}F NMR (376 MHz, $CDCl_3$) δ –63.45. HRMS (APCI) m/z calcd. for $C_{19}H_{20}O_2F_3$ $[M + H]^+$ 337.1410, found 337.1404.

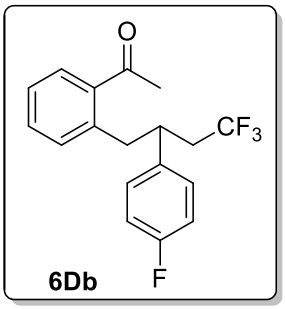
1-(2-(2-(4-chlorophenyl)-4,4,4-trifluorobutyl)phenyl)ethanone



(78% yield), ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.69 (dd, *J* = 7.6, 1.6 Hz, 1H), 7.34 – 7.26 (m, 2H), 7.25 – 7.19 (m, 2H), 7.06 – 7.02 (m, 2H), 6.96 (dd, *J* = 7.6, 1.6 Hz, 1H), 3.31 – 3.23 (m, 2H), 3.15 – 3.07 (m, 1H), 2.58 – 2.44 (m, 5H). ^{13}C NMR (100 MHz,

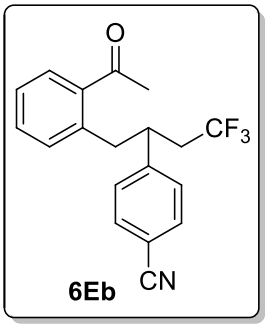
$CDCl_3$) δ 201.59, 141.03, 138.94, 137.47, 132.33, 132.14, 131.51, 129.84, 128.96, 128.48, 126.58, 126.44 (q, *J* = 275.9 Hz), 41.23 (q, *J* = 2.4 Hz), 41.02, 38.88 (q, *J* = 27.1 Hz), 29.41. ^{19}F NMR (376 MHz, $CDCl_3$) δ –63.40. HRMS (APCI) m/z calcd. for $C_{18}H_{17}OClF_3$ $[M + H]^+$ 341.0915, found 341.0912.

1-(2-(4,4,4-trifluoro-2-(4-fluorophenyl)butyl)phenyl)ethanone



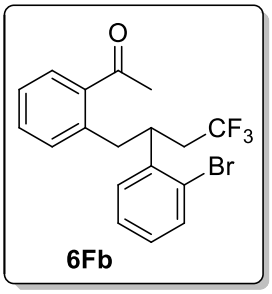
(72% yield), ^1H NMR (500 MHz, $CDCl_3$) δ 7.68 (dd, *J* = 7.5, 1.5 Hz, 1H), 7.33 – 7.25 (m, 2H), 7.07 – 7.03 (m, 2H), 6.97 – 6.90 (m, 3H), 3.30 – 3.22 (m, 2H), 3.14 – 3.08 (m, 1H), 2.57 – 2.44 (m, 5H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 201.67, 161.57 (d, *J* = 243.1Hz), 139.11, 138.17 (d, *J* = 3.3 Hz), 137.55, 132.16, 131.48, 129.79, 129.03 (d, *J* = 7.9 Hz), 126.53, 126.49 (q, *J* = 275.9 Hz), 115.18 (d, *J* = 21.1 Hz), 41.13, 39.10 (q, *J* = 27.0 Hz), 29.50. ^{19}F NMR (376 MHz, $CDCl_3$) δ –63.45 (s, 3F), –116.25 (s, 1F). HRMS (APCI) m/z calcd. for $C_{18}H_{17}OF_4$ $[M + Na]^+$ 325.1210, found 325.1207.

4-(1-(2-acetylphenyl)-4,4,4-trifluorobutan-2-yl)benzonitrile



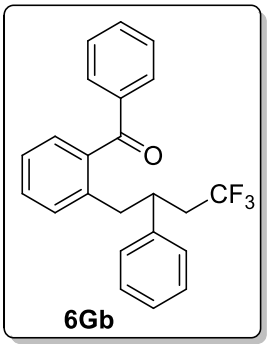
(90% yield), ^1H NMR (400 MHz, $CDCl_3$) δ 7.78 – 7.74 (m, 1H), 7.58 – 7.53 (m, 2H), 7.35 – 7.29 (m, 2H), 7.27 – 7.23 (m, 2H), 6.93 – 6.89 (m, 1H), 3.43 – 3.34 (m, 1H), 3.27 (dd, *J* = 12.8, 7.2 Hz, 1H), 3.11 (dd, *J* = 12.8, 8.0 Hz, 1H), 2.62 – 2.47 (m, 5H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 201.34, 148.25, 138.56, 137.03, 132.20, 132.16, 131.74, 130.34, 128.48, 126.93, 126.22 (q, *J* = 275.9 Hz), 118.76, 110.61, 41.79 (q, *J* = 2.4 Hz), 41.16, 38.45 (q, *J* = 27.5 Hz), 29.42. ^{19}F NMR (376 MHz, $CDCl_3$) δ –63.44. HRMS (APCI) m/z calcd. for $C_{19}H_{17}ONF_3$ $[M + H]^+$ 332.1257, found 332.1251.

1-(2-(2-(2-bromophenyl)-4,4,4-trifluorobutyl)phenyl)ethanone



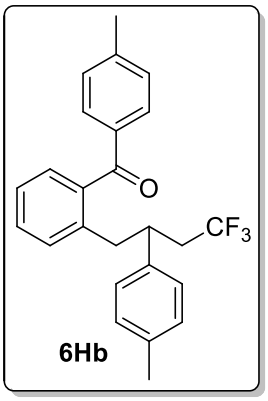
(70% yield), ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.67 (dd, *J* = 7.2, 1.6 Hz, 1H), 7.43 (d, *J* = 8.0 Hz, 1H), 7.0 – 7.22 (m, 4H), 7.06 – 7.00 (m, 2H), 4.01 (s, 1H), 3.51 (dd, *J* = 12.8, 6.8 Hz, 1H), 3.04 (s, 1H), 2.76 – 2.30 (m, 5H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 201.73, 141.52, 138.46, 137.80, 132.79, 131.96, 131.40, 129.51, 128.05, 127.46 (q, *J* = 275.9 Hz), 127.54, 126.49, 39.70 (s), 39.67, 39.39, 38.36, 29.49. ^{19}F NMR (376 MHz, $CDCl_3$) δ –63.59. HRMS (APCI) m/z calcd. for $C_{18}H_{17}OBrF_3$ $[M + H]^+$ 385.0409, found 385.0404.

phenyl(2-(4,4,4-trifluoro-2-phenylbutyl)phenyl)methanone



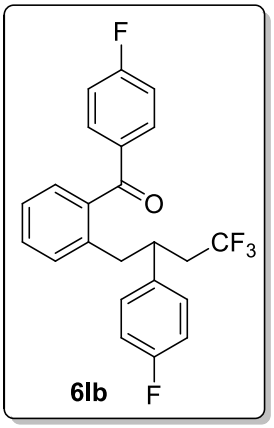
(62% yield), ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.68 – 7.64 (m, 2H), 7.60 – 7.56 (m, 1H), 7.43 (t, *J* = 8.0 Hz, 2H), 7.34 (td, *J* = 7.5, 2.0 Hz, 1H), 7.26 – 7.20 (m, 2H), 7.17 – 7.08 (m, 4H), 7.04 – 7.00 (m, 2H), 3.27 – 3.20 (m, 1H), 3.14 – 3.06 (m, 2H), 2.54 – 2.36 (m, 2H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 198.20, 142.20, 138.59, 138.46, 137.62, 133.14, 130.99, 130.24, 129.19, 128.42, 128.32, 127.86, 126.46 (q, *J* = 275.9 Hz), 127.39, 126.79, 125.63, 41.80 (q, *J* = 2.4 Hz), 39.94, 39.24 (q, *J* = 27.1 Hz). ^{19}F NMR (376 MHz, $CDCl_3$) δ –63.55. HRMS (APCI) m/z calcd. for $C_{23}H_{20}OF_3$ $[M + H]^+$ 369.1461, found 369.1460.

p-tolyl(2-(4,4,4-trifluoro-2-(p-tolyl)butyl)phenyl)methanone



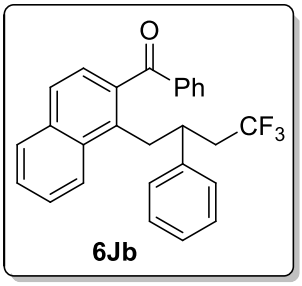
(60% yield), ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.54 (d, *J* = 8.5 Hz, 2H), 7.36 – 7.32 (m, 1H), 7.24 – 7.19 (m, 4H), 7.16 (d, *J* = 7.5 Hz, 1H), 6.93 (d, *J* = 8.0 Hz, 2H), 6.89 (d, *J* = 8.0 Hz, 2H), 3.19 – 3.13 (m, 1H), 3.11 – 3.03 (m, 2H), 2.43 (s, 3H), 2.41 – 2.31 (m, 2H), 2.22 (s, 3H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 197.87, 143.99, 139.14, 138.92, 138.43, 136.18, 135.00, 130.91, 130.42, 130.01, 129.09, 128.95, 128.92, 127.21, 126.51 (q, *J* = 276.0 Hz), 125.49, 41.45 (q, *J* = 2.4 Hz), 39.82, 39.35 (q, *J* = 26.9 Hz), 21.69, 20.97. ^{19}F NMR (376 MHz, $CDCl_3$) δ –63.48. HRMS (APCI) m/z calcd. for $C_{25}H_{24}OF_3$ $[M + H]^+$ 397.1774, found 397.1769.

(4-fluorophenyl)(2-(4,4,4-trifluoro-2-(4-fluorophenyl)butyl)phenyl)methanone



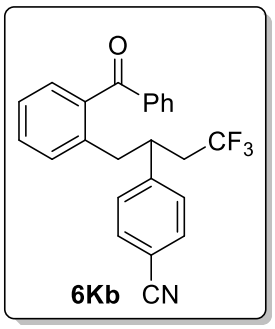
(59% yield), ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.68 – 7.61 (m, 2H), 7.39 – 7.34 (m, 1H), 7.24 –7.20 (m, 2H), 7.16 – 7.08 (m, 3H), 6.97 – 6.92 (m, 2H), 6.84 – 6.76 (m, 2H), 3.26 – 3.18 (m, 1H), 3.10 – 3.06 (m, 2H), 2.49 – 2.38 (m, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 196.42, 165.83 (d, *J* = 254.1 Hz), 161.60 (d, *J* = 243.5 Hz), 138.31, 138.21, 137.68 (d, *J* = 3.2 Hz), 133.83 (d, *J* = 2.9 Hz), 132.83 (d, *J* = 9.3 Hz), 131.11, 130.42, 129.03, 128.86 (d, *J* = 7.9 Hz), 126.33 (q, *J* = 278.0 Hz), 125.75, 115.50 (d, *J* = 18.9 Hz), 115.29 (d, *J* = 18.3 Hz), 41.32 (q, *J* = 2.2 Hz), 39.86, 39.55 (q, *J* = 27.1 Hz). ^{19}F NMR (376 MHz, $CDCl_3$) δ –63.56 (s, 3F), –104.57 (s, 1F), –115.88 (s, 1F). HRMS (APCI) m/z calcd. for $C_{23}H_{18}OF_5$ $[M + H]^+$ 405.1272, found 405.1266.

phenyl(1-(4,4,4-trifluoro-2-phenylbutyl)naphthalen-2-yl)methanone



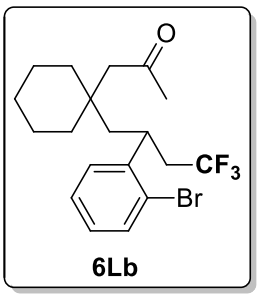
(64% yield), ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.14 (d, *J* = 8.4 Hz, 1H), 7.96 – 7.89 (m, 1H), 7.77 (d, *J* = 8.4 Hz, 1H), 7.69 – 7.52 (m, 5H), 7.39 (t, *J* = 8.0 Hz, 2H), 7.30 (d, *J* = 8.4 Hz, 1H), 7.14 – 7.00 (m, 5H), 3.67 – 3.59 (m, 1H), 3.55 – 3.42 (m, 2H), 2.62 – 2.39 (m, 2H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 198.64, 142.66, 137.57, 136.88, 134.90, 134.32, 133.15, 132.03, 130.24, 129.05, 128.52, 128.34, 127.20, 127.07, 126.99, 126.97, 126.60, 126.58 (q, *J* = 276.0 Hz), 125.24, 124.72, 41.27 (q, *J* = 2.3 Hz), 38.99 (q, *J* = 27.1 Hz), 36.15. ^{19}F NMR (376 MHz, $CDCl_3$) δ –63.46. HRMS (APCI) m/z calcd. for $C_{27}H_{22}OF_3$ $[M + H]^+$ 419.1617, found 419.1612.

4-(1-(2-benzoylphenyl)-4,4,4-trifluorobutan-2-yl)benzonitrile



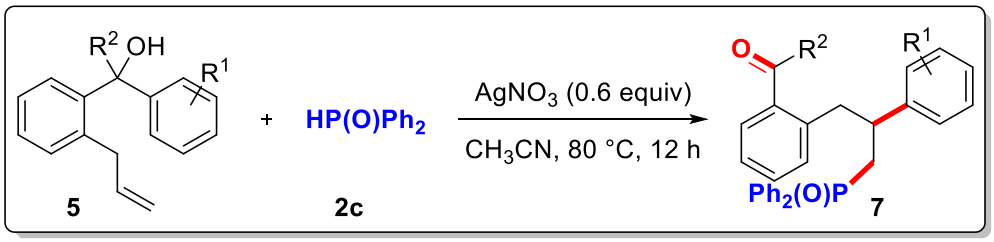
(85% yield), ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.65 – 7.56 (m, 3H), 7.47 – 7.35 (m, 5H), 7.30 – 7.23 (m, 2H), 7.16 – 7.11 (m, 3H), 3.40 – 3.30 (m, 1H), 3.18 – 3.06 (m, 2H), 2.55 – 2.43 (m, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 197.83, 147.60, 138.23, 137.71, 137.33, 133.41, 132.27, 130.99, 130.54, 130.15, 129.61, 128.39, 128.34, 126.09 (q, *J* = 275.8 Hz), 125.98, 118.61, 110.85, 42.20 (q, *J* = 2.3 Hz), 39.60, 39.00 (q, *J* = 27.5 Hz). ^{19}F NMR (376 MHz, $CDCl_3$) δ –63.53. HRMS (APCI) m/z calcd. for $C_{24}H_{19}ONF_3$ $[M + H]^+$ 394.1413, found 394.1408.

1-(1-(2-(2-bromophenyl)-4,4,4-trifluorobutyl)cyclohexyl)propan-2-one



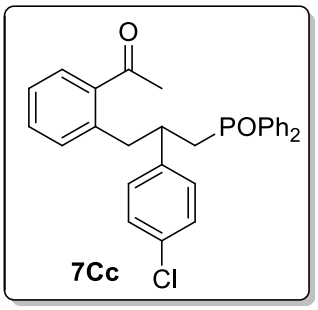
(72% yield), ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.28 (d, *J* = 7.5 Hz, 1H), 7.22 – 7.16 (m, 3H), 3.12 – 2.94 (m, 1H), 2.39 – 2.27 (m, 3H), 2.21 (d, *J* = 18.0 Hz, 1H), 2.04 (d, *J* = 17.5 Hz, 1H), 1.80 (dd, *J* = 14.0, 2.0 Hz, 1H), 1.71 (s, 3H), 1.43 – 1.33 (m, 8H), 1.30 – 1.22 (m, 2H). ^{13}C NMR (125 MHz, CDCl3) δ 208.42, 144.53, 128.65, 127.85, 127.76, 126.64, 126.42 (q, *J* = 276.3 Hz), 124.78, 48.78, 43.03 (q, *J* = 26.3 Hz), 41.87, 36.29, 36.21, 35.99, 35.71 (q, *J* = 2.3 Hz), 31.44, 26.05, 21.46, 21.32. ^{19}F NMR (376 MHz, $CDCl_3$) δ –63.56. HRMS (APCI) m/z calcd. for $C_{19}H_{25}OBrF_3$ $[M + H]^+$ 405.1035, found 405.1037.

General procedure for phosphonylation reaction



To a flame-dried Schlenk tube equipped with a magnetic stir bar were added **5** (0.2 mmol, 1.0 equiv), **2c** (80.8 mg, 0.4 mmol, 2.0 equiv), and $AgNO_3$ (20.4 mg, 0.12 mmol, 0.6 equiv). The tube was evacuated and backfilled with argon for three times, and then CH_3CN (2.0 mL) were added. The tube was stirred at 80 °C for 12 h and then H_2O (5 mL) was added. EtOAc was used to extract the product from the aqueous layer (3 × 10 mL). The combined organic layer was dried over anhydrous Na_2SO_4, filtered and concentrated to afford a crude product, which was purified by flash column chromatography to afford product **7**.

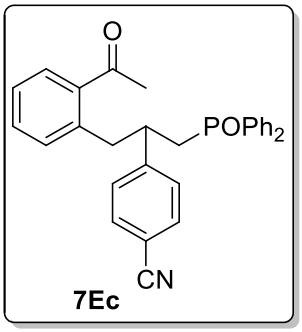
1-(2-(2-(4-chlorophenyl)-3-(diphenylphosphoryl)propyl)phenyl)ethanone



(75% yield), ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.65 – 7.58 (m, 2H), 7.51 (dd, *J* = 7.6, 1.2 Hz, 1H), 7.46 – 7.32 (m, 6H), 7.31 – 7.26 (m, 1H), 7.25 – 7.15 (m, 3H), 7.08 (dd, *J* = 7.6, 0.8 Hz, 1H), 6.94 – 6.89 (m, 2H), 6.86 – 6.81 (m, 2H), 3.47 – 3.36 (m, 1H), 3.35 – 3.24 (m, 2H), 2.77 – 2.61 (m, 2H), 2.30 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 202.03, 141.18 (d, *J* = 4.3 Hz), 138.97, 138.02, 134.33, 133.26 (d, *J* = 20.2 Hz), 132.18, 131.92, 131.43 (d, *J* = 2.6 Hz), 131.24, 130.88 (d, *J* = 2.8 Hz), 130.48 (d, *J* = 9.4 Hz), 130.36 (d, *J* = 9.1 Hz), 129.34, 128.99, 128.46 (d, *J* = 11.4 Hz), 128.09 (d, *J* = 11.7 Hz), 127.96, 126.13, 41.35 (d, *J* = 3.0 Hz), 41.25 (d, *J* = 11.5 Hz), 35.56 (d, *J* =

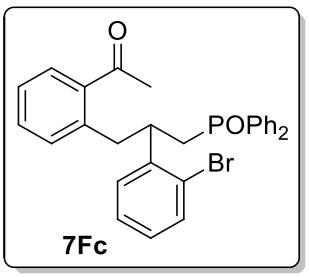
70.4 Hz), 29.46. ^{31}P NMR (162 MHz, $CDCl_3$) δ 29.40. HRMS (APCI) m/z calcd. for $C_{29}H_{27}O_2ClP$ $[M + H]^+$ 473.1432, found 473.1427.

4-(1-(2-acetylphenyl)-3-(diphenylphosphoryl)propan-2-yl)benzonitrile



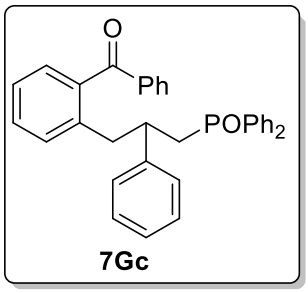
(87% yield), ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.62 – 7.54 (m, 3H), 7.48 – 7.29 (m, 7H), 7.28 – 7.19 (m, 5H), 7.12 – 6.97 (m, 3H), 3.58 – 3.44 (m, 1H), 3.29 (d, *J* = 7.2 Hz, 2H), 2.80 – 2.64 (m, 2H), 2.37 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 201.61, 148.40 (d, *J* = 3.3 Hz), 138.03 (d, *J* = 123.4 Hz), 133.37 (d, *J* = 79.8 Hz), 132.38 (d, *J* = 79.6 Hz), 131.96, 131.63, 131.60, 131.51, 131.15 (d, *J* = 2.5 Hz), 130.384, 130.381 (d, *J* = 17.1 Hz), 129.65, 128.87, 128.52 (d, *J* = 11.6 Hz), 128.16 (d, *J* = 11.7 Hz), 126.51, 118.79, 109.96, 41.87 (d, *J* = 3.1 Hz), 41.51 (d, *J* = 12.4 Hz), 34.78 (d, *J* = 70.4 Hz), 29.45. ^{31}P NMR (162 MHz, $CDCl_3$) δ 29.34. HRMS (APCI) m/z calcd. for $C_{30}H_{27}O_2NP$ $[M + H]^+$ 464.1774, found 464.1768.

1-(2-(2-(2-bromophenyl)-3-(diphenylphosphoryl)propyl)phenyl)ethanone



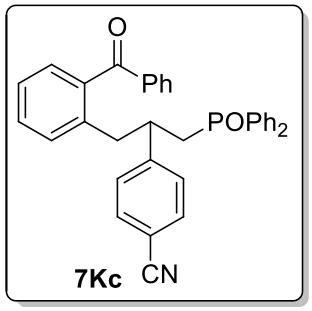
(77% yield), ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.71 – 7.54 (m, 4H), 7.51 – 7.28 (m, 7H), 7.25 – 7.13 (m, 4H), 7.07 (d, *J* = 7.6 Hz, 2H), 6.85 (t, *J* = 7.2 Hz, 1H), 3.98 (s, 1H), 3.62 – 3.50 (m, 1H), 3.26 (s, 1H), 2.72 (dd, *J* = 11.6, 5.2 Hz, 2H), 2.32 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 202.27, 142.02 (d, *J* = 4.1 Hz), 138.45, 133.87, 132.99 (d, *J* = 23.1 Hz), 132.42 (d, *J* = 5.7 Hz), 132.35 (d, *J* = 2.4 Hz), 132.07, 131.31 (d, *J* = 2.5 Hz), 131.22, 131.05, 130.68 (d, *J* = 9.3 Hz), 130.53 (d, *J* = 9.1 Hz), 128.62, 127.49, 128.38, 128.22 (d, *J* = 11.8 Hz), 127.75, 127.27, 126.05, 124.78, 39.96 (br, 2C), 35.20 (d, *J* = 71.5 Hz), 29.58. ^{31}P NMR (162 MHz, $CDCl_3$) δ 29.98. HRMS (APCI) m/z calcd. for $C_{29}H_{27}O_2BrP$ $[M + H]^+$ 517.0927, found 517.0923.

(2-(3-(diphenylphosphoryl)-2-phenylpropyl)phenyl)(phenyl)methanone



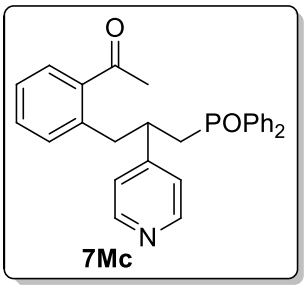
(50% yield), ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.40 (d, *J* = 7.6 Hz, 1H), 7.87 – 7.81 (m, 1H), 7.67 (d, *J* = 8.4 Hz, 1H), 7.62 – 7.50 (m, 6H), 7.50 – 7.45 (m, 2H), 7.39 – 7.27 (m, 7H), 7.19 (d, *J* = 8.4 Hz, 1H), 6.90 – 6.75 (m, 5H), 3.91 – 3.76 (m, 1H), 3.71 – 3.59 (m, 2H), 2.88 – 2.76 (m, 1H), 2.70 – 2.60 (m, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 198.58, 143.50 (d, *J* = 7.1 Hz), 137.12 (d, *J* = 104.2 Hz), 135.05 (d, *J* = 128.0 Hz), 134.21, 133.41 (d, *J* = 4.3 Hz), 132.76, 132.41, 132.10, 131.34 (d, *J* = 2.5 Hz), 131.12 (d, *J* = 2.5 Hz), 130.58 (d, *J* = 9.2 Hz), 130.23 (d, *J* = 9.1 Hz), 130.11, 128.54 (d, *J* = 9.0 Hz), 128.34 (d, *J* = 6.3 Hz), 128.19, 128.16, 127.39, 126.97, 126.87, 126.67, 126.24, 125.77, 125.10, 41.07 (d, *J* = 1.5 Hz), 37.30 (d, *J* = 7.8 Hz), 35.81 (d, *J* = 73.1 Hz). ^{31}P NMR (162 MHz, $CDCl_3$) δ 30.48. HRMS (APCI) m/z calcd. for $C_{34}H_{30}O_2P$ $[M+H]^+$ 501.1978, found 501.1972 .

4-(1-(2-benzoylphenyl)-3-(diphenylphosphoryl)propan-2-yl)benzonitrile



(60% yield), ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.64 – 7.53 (m, 3H), 7.47 – 7.42 (m, 3H), 7.42 – 7.30 (m, 8H), 7.28 – 7.24 (m, 1H), 7.24 – 7.14 (m, 4H), 7.04 (d, *J* = 8.4 Hz, 2H), 6.93 (d, *J* = 8.4 Hz, 2H), 3.65 – 3.53 (m, 1H), 3.31 – 3.17 (m, 2H), 2.80 – 2.70 (m, 1H), 2.65 – 2.55 (m, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 197.70, 147.91 (d, *J* = 4.4 Hz), 138.28, 138.09, 137.19, 134.03, 133.20, 132.96 (d, *J* = 15.6 Hz), 131.71, 131.66, 131.18 (d, *J* = 2.7 Hz), 130.79 (d, *J* = 50.1 Hz), 130.46 (d, *J* = 9.4 Hz), 130.30 (d, *J* = 9.2 Hz), 130.09, 129.16, 128.74, 128.62 (d, *J* = 11.6 Hz), 128.195 (t, *J* = 11.7 Hz), 128.192, 125.50, 118.62, 110.22, 42.31 (d, *J* = 2.9 Hz), 40.12 (d, *J* = 11.3 Hz), 35.71 (d, *J* = 70.0 Hz). ^{31}P NMR (162 MHz, $CDCl_3$) δ 28.84. HRMS (APCI) m/z calcd. for $C_{35}H_{29}O_2NP$ $[M + H]^+$ 526.1930, found 526.1925.

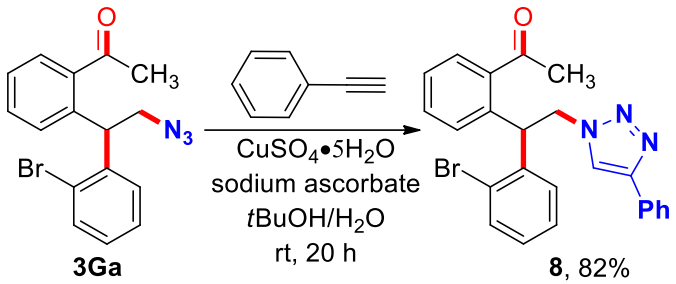
1-(2-(3-(diphenylphosphoryl)-2-(pyridin-4-yl)propyl)phenyl)ethanone



(55% yield), ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.17 (d, *J* = 6.0 Hz, 2H), 7.63 – 7.52 (m, 3H), 7.48 – 7.41 (m, 3H), 7.39 – 7.31 (m, 3H), 7.29 – 7.18 (m, 4H), 7.04 (d, *J* = 7.6 Hz, 1H), 6.84 (d, *J* = 5.6 Hz, 2H), 3.46 – 3.36 (m, 1H), 3.35 – 3.23 (m, 2H), 2.76 – 2.64 (m, 2H), 2.32 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 201.74, 151.87 (d, *J* = 4.1 Hz), 149.20, 138.51, 137.64, 133.89, 132.91 (d, *J* = 1.6 Hz), 131.94, 131.56 (d, *J* = 2.6 Hz), 131.41, 131.34 (d, *J* = 2.6 Hz), 130.46 (d, *J* = 9.0 Hz), 130.37 (d, *J* = 9.0 Hz), 129.39, 128.50 (d, *J* = 11.6 Hz), 128.19 (d, *J* = 11.7 Hz), 126.41, 123.29, 41.21 (d, *J* = 2.8 Hz), 41.08 (d, *J* = 11.5 Hz), 34.50 (d, *J* = 70.2 Hz), 29.41. ^{31}P NMR (162 MHz, $CDCl_3$) δ 29.19 (s). HRMS (APCI) m/z calcd. for $C_{28}H_{27}O_2NP$ $[M + H]^+$ 440.1774, found 440.1769.

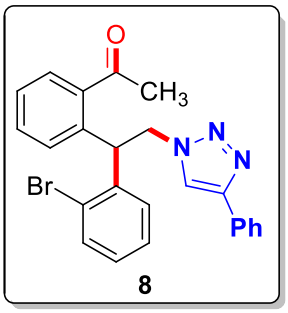
Procedures for Synthetic Applications

Experimental procedure for transformation of 3Ga to 8



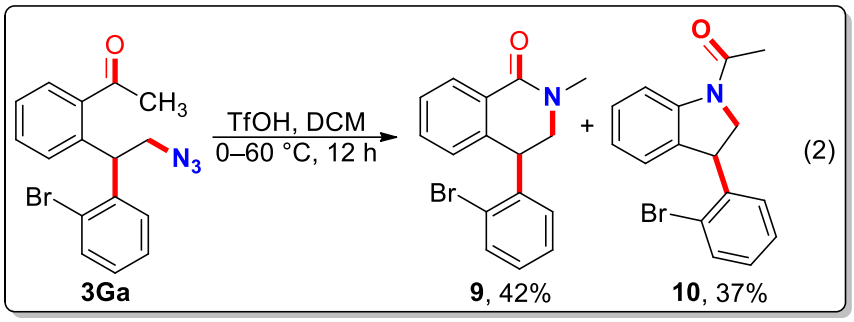
To a solution of **3Ga** (34.4 mg, 0.1 mmol, 1.0 equiv), phenylacetylene (18 mg, 0.15 mmol, 1.5 equiv) in H_2O/*t*-BuOH (1 mL/1 mL) were added $CuSO_4•5H_2O$ (12 mg, 0.05 mmol, 0.5 equiv) and sodium ascorbate (21 mg, 0.11 mmol, 1.1 equiv). The resulting mixture was stirred at room temperature for 20 h. Then the mixture was diluted with ethyl acetate (30 mL), saturated aqueous EDTA solution (0.2 mL) and water (5 mL). The aqueous layer was extracted with ethyl acetate (3 × 5 mL). The combined organic layer was dried over Na_2SO_4, filtered through a short silica gel plug, and concentrated to afford a crude product, which was purified by flash column chromatography to afford product **8**.

1-(2-(1-(2-bromophenyl)-2-(4-phenyl-1H-1,2,3-triazol-1-yl)ethyl)phenyl)ethanone



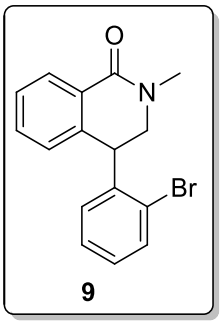
(82% yield), ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.10 (s, 1H), 7.81 (d, *J* = 13.0, 7.5 Hz, 2H), 7.79 (d, J = 13.0, 7.5 Hz, 2H), 7.46 (d, *J* = 8.0 Hz, 1H), 7.42 – 7.32 (m, 5H), 7.29 (t, *J* = 7.0 Hz, 1H), 7.15 (d, *J* = 7.5 Hz, 1H), 7.08 (t, *J* = 7.5 Hz, 1H), 5.72 (dd, *J* = 10.5, 5.0 Hz, 1H), 5.17 (dd, *J* = 14.0, 10.5 Hz, 1H), 4.92 (dd, *J* = 14.5, 5.0 Hz, 1H), 2.67 (s, 3H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 202.55, 147.83, 139.07, 138.18, 137.98, 133.43, 132.05, 130.56, 129.52, 129.47, 129.12, 128.81, 128.65, 127.93, 127.50, 127.13, 125.93, 125.62, 119.32, 52.41, 46.82, 29.51. HRMS (APCI) m/z calcd. for $C_{24}H_{21}ON_3Br$ $[M + H]^+$ 446.0863, found 446.0858.

Experimental procedure for transformation of 3Ga to 9 and 10



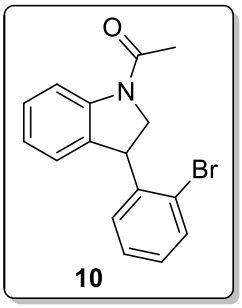
To a solution of **3Ga** (34.4 mg, 0.1 mmol, 1.0 equiv) in DCM (2.0 mL) was added TfOH (0.2 mmol, 2 equiv) at 0 °C and then the solution was stirred at room temperature for 12 h. After completion of the reaction as monitored by TLC, the reaction solution was diluted with DCM (30 mL) and washed with saturated $NaHCO_3$ (2 × 5 mL) and brine (5 mL). The organic layer was dried over anhydrous Na_2SO_4, filtered, and concentrated to afford a crude product, which was purified by flash column chromatography to afford products **9** and **10**.

4-(2-bromophenyl)-2-methyl-3,4-dihydroisoquinolin-1(2H)-one



(42% yield), ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.23 – 8.18 (m, 1H), 7.63 (dd, *J* = 7.5, 1.0 Hz, 1H), 7.44 – 7.39 (m, 2H), 7.19 – 7.10 (m, 2H), 7.01 – 6.96 (m, 1H), 6.82 (dd, *J* = 7.5, 1.5 Hz, 1H), 4.83 (t, *J* = 5.5 Hz, 1H), 3.90 (dd, *J* = 12.5, 5.5 Hz, 1H), 3.65 (dd, *J* = 12.5, 5.5Hz, 1H), 3.04 (s, 3H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 164.60, 139.79, 139.29, 133.15, 132.07, 130.16, 129.80, 128.80, 128.32, 127.70, 127.68, 127.42, 124.33, 53.33, 42.47, 35.33. HRMS (APCI) m/z calcd. for $C_{16}H_{15}ONBr$ $[M + H]^+$ 316.0332, found 316.0326.

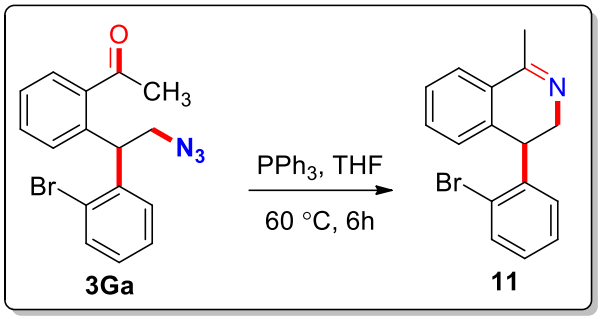
1-(3-(2-bromophenyl)indolin-1-yl)ethanone



(37% yield), ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.30 (d, *J* = 8.0 Hz, 1H), 7.62 (dd, *J* = 8.0, 1.0 Hz, 1H), 7.31 – 7.27 (m, 1H), 7.22 (t, *J* = 7.0 Hz, 1H), 7.13 (td, *J* = 8.0, 1.5 Hz,

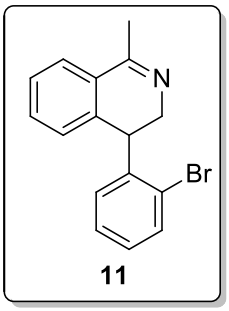
1H), 7.08 – 7.04 (m, 2H), 6.93 (d, *J* = 7.0 Hz, 1H), 5.11 (dd, *J* = 10.5, 6.0 Hz, 1H), 4.55 (t, *J* = 10.5 Hz, 1H), 3.82 (dd, *J* = 10.5, 6.0 Hz, 1H), 2.20 (s, 3H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 168.68, 143.50, 142.55, 132.89, 132.62, 129.05, 128.78, 128.49, 128.03, 125.25, 124.31, 123.98, 117.14, 56.79, 45.46, 24.23. HRMS (APCI) m/z calcd. for $C_{16}H_{15}ONBr$ $[M+H]^+$ 316.0332, found 316.0327.

Transformation of azido ketone 3Ga to 11



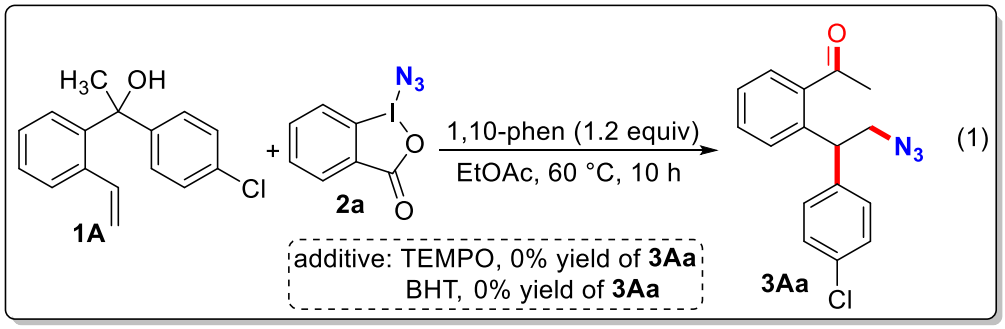
To a solution of **3Ga** (34.4 mg, 0.1 mmol, 1.0 equiv) in THF (2.0 mL) was added PPh_3 (31.4 mg, 0.12 mmol, 1.2 equiv). The resulting mixture was then stirred at 60 °C for 6 h. After completion of the reaction as monitored by TLC, the solvent were concentrated to afford a crude product, which was purified by flash column chromatography to give **11**.

4-(2-bromophenyl)-1-methyl-3,4-dihydroisoquinoline

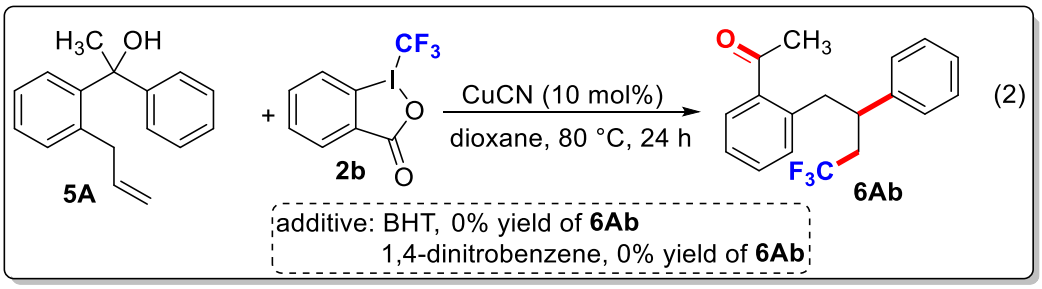


(89% yield), ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.63 (dd, *J* = 8.0, 1.2 Hz, 1H), 7.60 – 7.56 (m, 1H), 7.38 – 7.31 (m, 2H), 7.21 (td, *J* = 7.6, 1.2 Hz, 1H), 7.11 (td, *J* = 7.6, 1.6 Hz, 1H), 6.97 (dd, *J* = 7.6, 1.6 Hz, 1H), 6.93 – 6.88 (m, 1H), 4.65 (dd, *J* = 10.8, 6.4 Hz, 1H), 3.98 (ddd, *J* = 15.6, 6.4, 1.2 Hz, 1H), 3.88 – 3.79 (m, 1H), 2.47 (s, 3H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 164.76, 140.41, 138.80, 133.16, 131.17, 129.66, 129.35, 128.38, 127.58, 127.35, 127.27, 125.56, 125.29, 52.49, 40.89, 23.26. HRMS (APCI) m/z calcd. for $C_{16}H_{15}NBr$ $[M + H]^+$ 300.0382, found 300.0376.

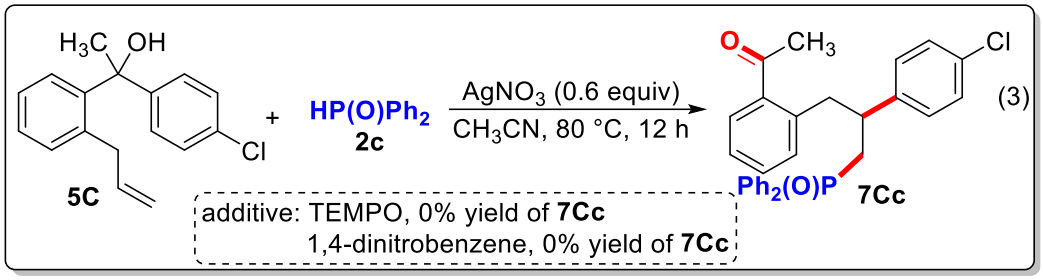
Mechanistic Study



A 25 mL Schlenk tube equipped with a magnetic stir bar was charged with **1A** (51.6 mg, 0.2 mmol, 1.0 equiv), **2a** (70 mg, 0.24 mmol, 1.2 equiv), 1,10-phen (43.2 mg, 0.24 mmol, 0.12 equiv), 2,6-di-*tert*-butyl-4-methylphenol (BHT, 52.8 mg, 0.24 mmol, 1.2 equiv) or 2,2,6,6-Tetramethylpiperidinooxy (TEMPO, 37.5 mg, 0.24 mmol, 1.2 equiv), and EtOAc (2.0 mL) under argon atmosphere. The sealed tube was then stirred at 60 °C for 12 h. Upon completion, the reaction solution was diluted with EtOAc (30 mL) and washed with saturated $NaHCO_3$ (2 × 5 mL) solution. The organic layer was dried over anhydrous Na_2SO_4, filtered and concentrated to afford a crude product. To a solution of this crude product in $CDCl_3$ was added mesitylene (24.0 mg, 0.2 mmol) as an internal standard. ^1H NMR analysis of this reaction mixture indicated that **3Aa** was not formed under either reaction conditions.

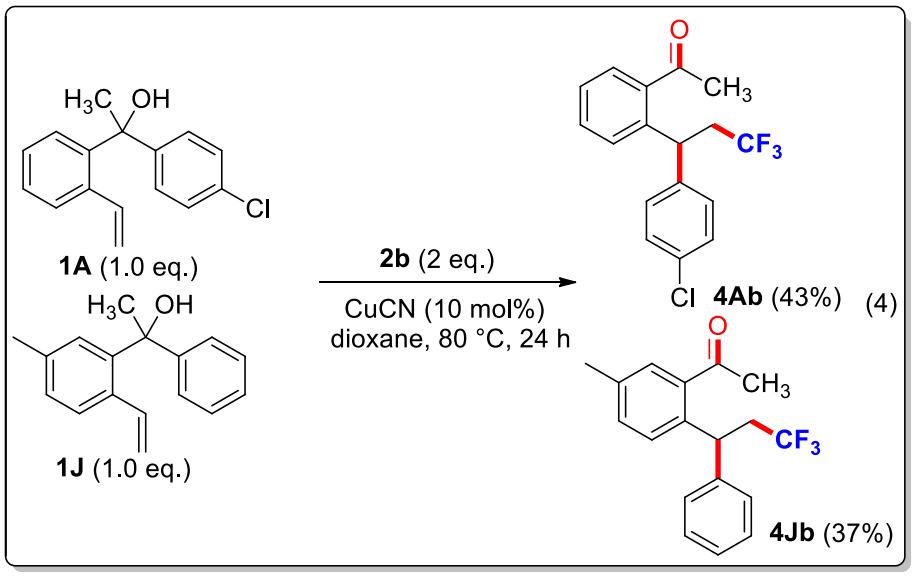


A 25 mL Schlenk tube equipped with a magnetic stir bar was charged with **5A** (47.6 mg, 0.2 mmol, 1.0 equiv), **2b** (126 mg, 0.4 mmol, 2.0 equiv), CuCN (1.8 mg, 0.02 mmol, 0.1 equiv), 2,2,6,6-Tetramethylpiperidinooxy (63 mg, 0.4 mmol, 2.0 equiv) or 1,4-dinitrobenzene (67 mg, 0.4 mmol, 2.0 equiv), and dioxane (4.0 mL) under argon atmosphere. The sealed tube was then stirred at 60 °C for 24 h. Upon completion, $PhCF_3$ (29.2 mg, 0.2 mmol) was added as an internal standard. ^{19}F NMR analysis of this reaction mixture indicated that **6Ab** was not formed under either conditions.



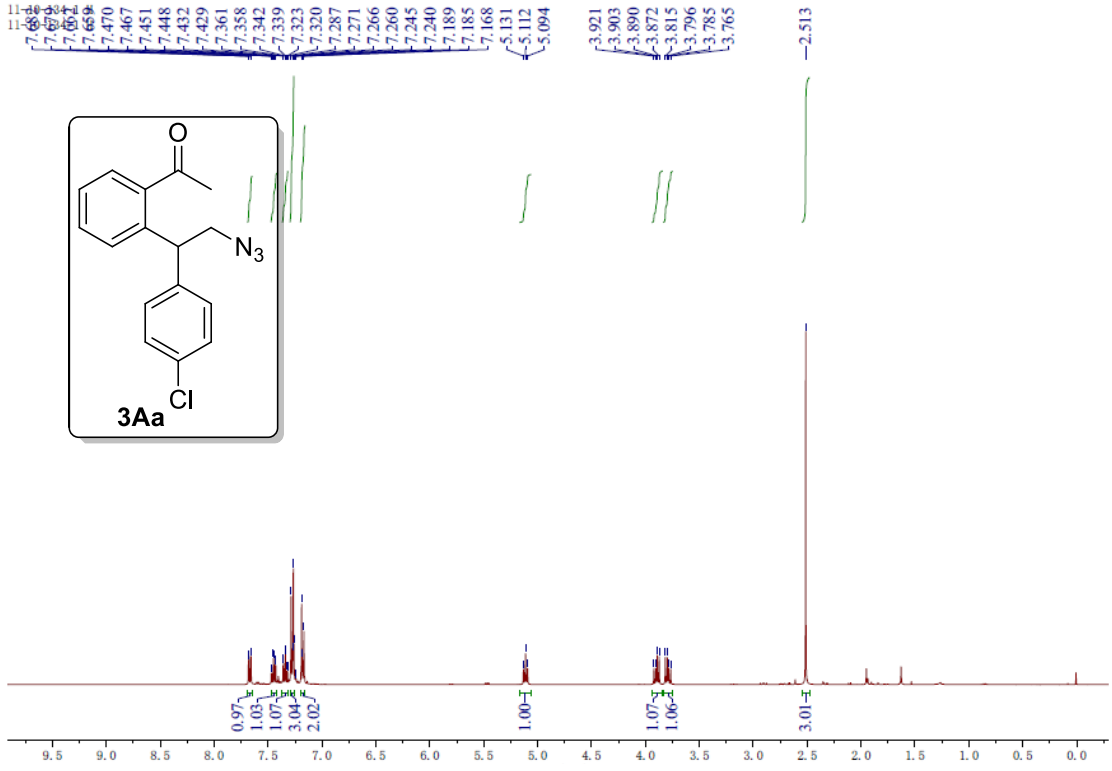
A 25 mL Schlenk tube equipped with a magnetic stir bar was charged with **5C** (54.4 mg, 0.2 mmol, 1.0 equiv), **2c** (80.8 mg, 0.4 mmol, 2.0 equiv), $AgNO_3$ (20.4 mg, 0.12 mmol, 0.6 equiv), 2,2,6,6-tetramethylpiperidinooxy (63 mg, 0.4 mmol, 2.0 equiv) or 1,4-dinitrobenzene (67 mg, 0.4 mmol, 2.0 equiv), and CH_3CN (2.0 mL) under argon atmosphere. The sealed tube was stirred at 80 °C for 12 h and then H_2O (5 mL) was added. EtOAc was used to extract the product from the aqueous layer (3 × 20 mL). The combined organic layer was dried over anhydrous Na_2SO_4, filtered and concentrated to afford a crude product. To a solution of this crude product in $CDCl_3$ was added mesitylene (24.0 mg, 0.2 mmol) as an internal standard. ^1H NMR analysis of this reaction mixture indicated that **7Cc** was not formed under either conditions.

Cross-experiment



A 50 mL Schlenk tube equipped with a magnetic stir bar was charged with **1A** (0.2 mmol, 1.0 equiv), **1J** (0.2 mmol, 1.0 equiv), **2b** (252 mg, 0.8 mmol, 2.0 equiv), CuCN (3.6 mg, 0.04 mmol, 0.1 equiv), and dioxane (8.0 mL) under argon atmosphere. The sealed tube was then stirred at 80 °C for 24 h. Upon completion, EtOAc (30 mL) was added and the reaction mixture was washed with saturated $NaHCO_3$ (2 × 5 mL) solution. The organic layer was dried over anhydrous Na_2SO_4, filtered and concentrated to afford a crude product. To a solution of this crude product in $CDCl_3$ was added mesitylene (24.0 mg, 0.2 mmol) as an internal standard. ^1H NMR analysis of this reaction mixture indicated that there were no cross products formed.

NMR Spectra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7.448
7.432
7.429
7.361
7.358
7.342
7.339
7.323
7.320
7.287
7.271
7.266
7.260
7.245
7.240
7.189
7.185
7.168
5.131
5.112
5.094
3.921
3.903
3.890
3.872
3.815
3.796
3.785
3.765
2.513
O
N3
Cl
3Aa
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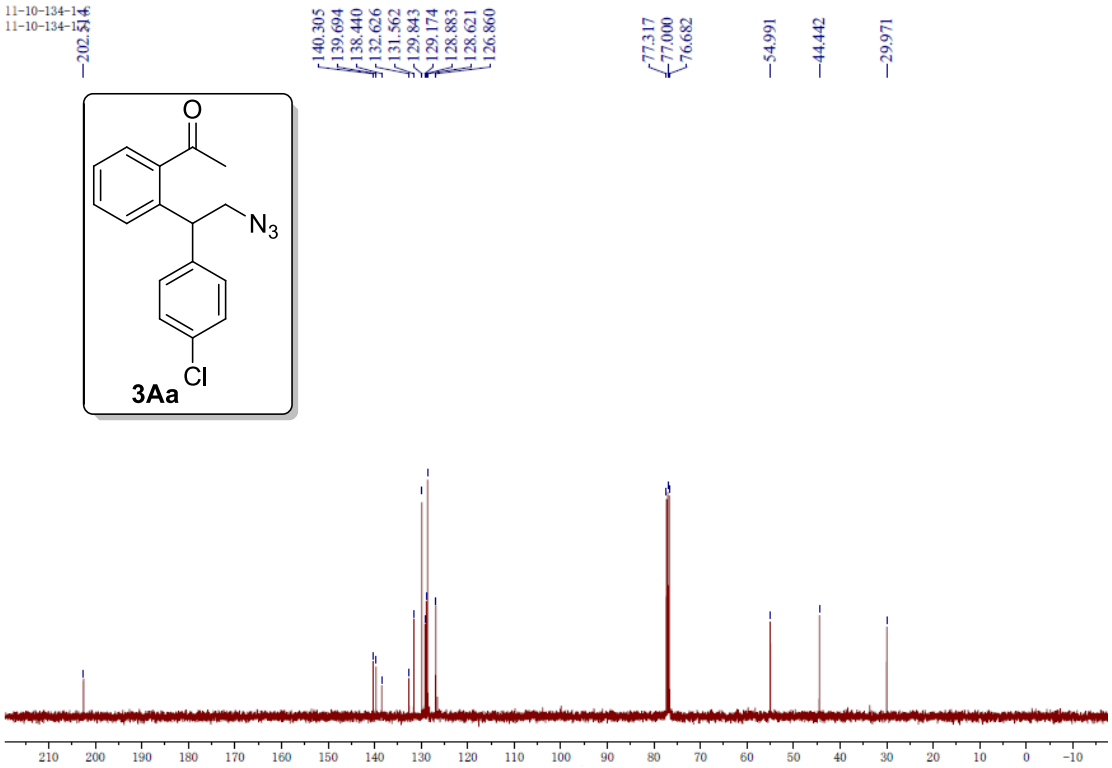
1.03
1.07
3.04
2.02
1.00
1.07
1.06
3.01


202.514
140.305
139.694
138.440
132.626
131.562
129.843
129.174
128.883
128.621
126.860
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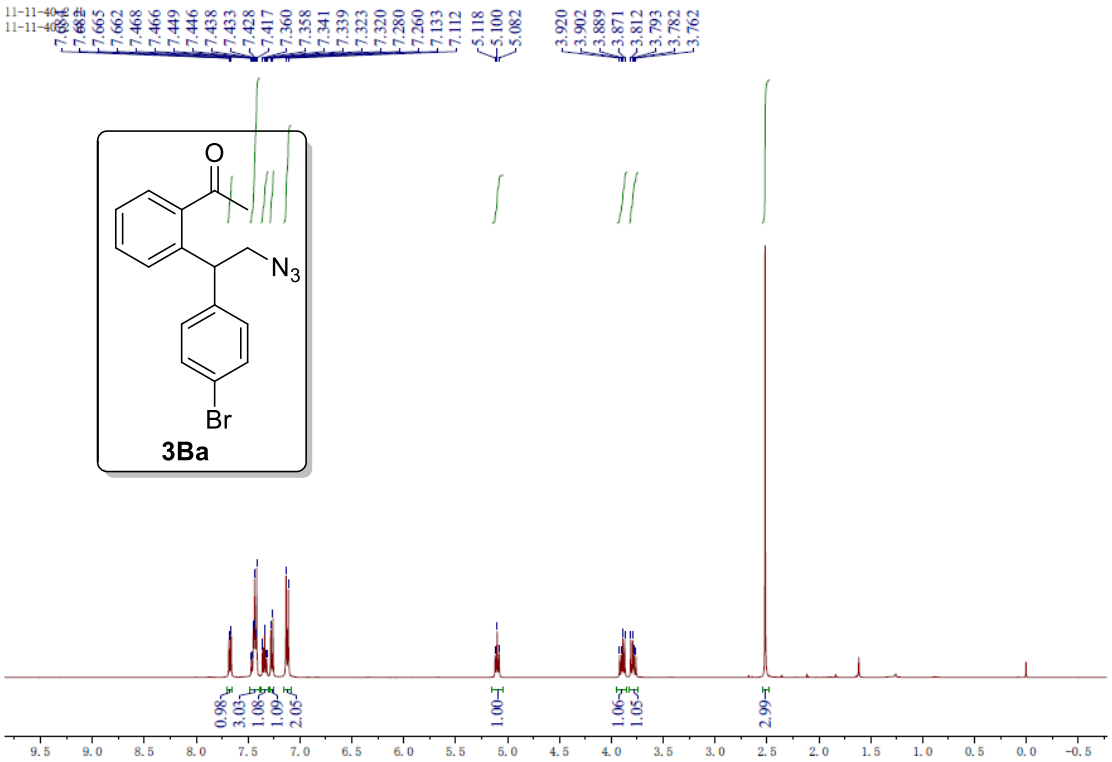
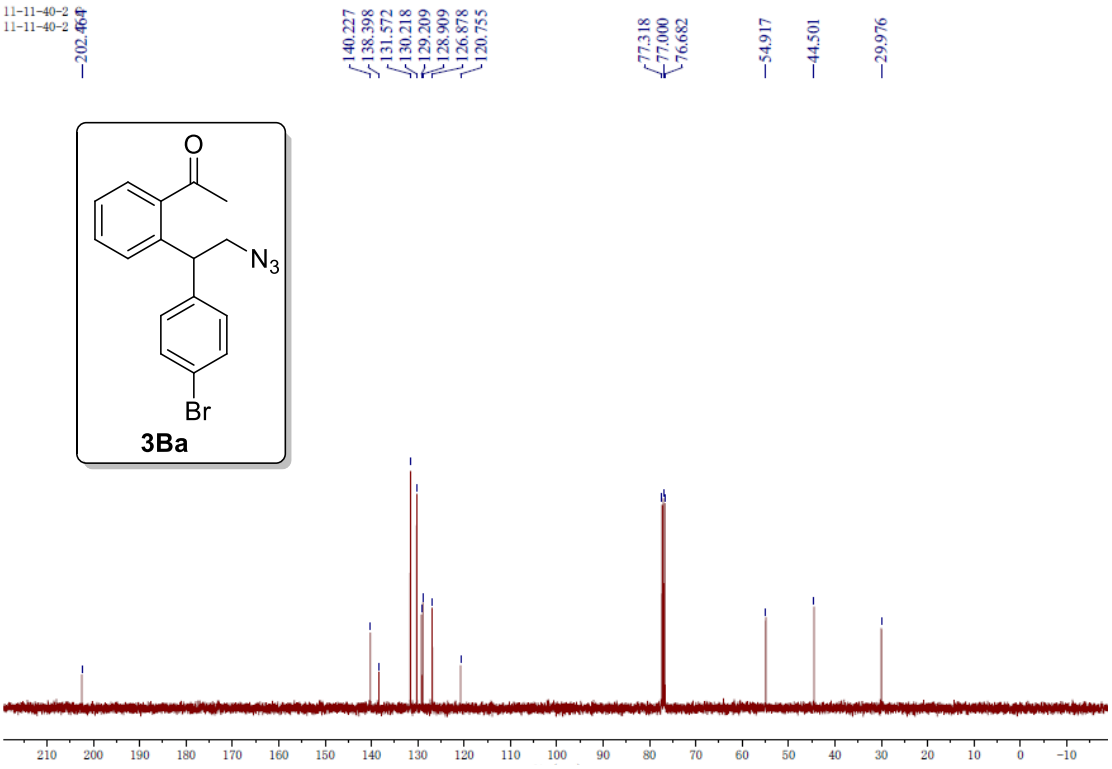
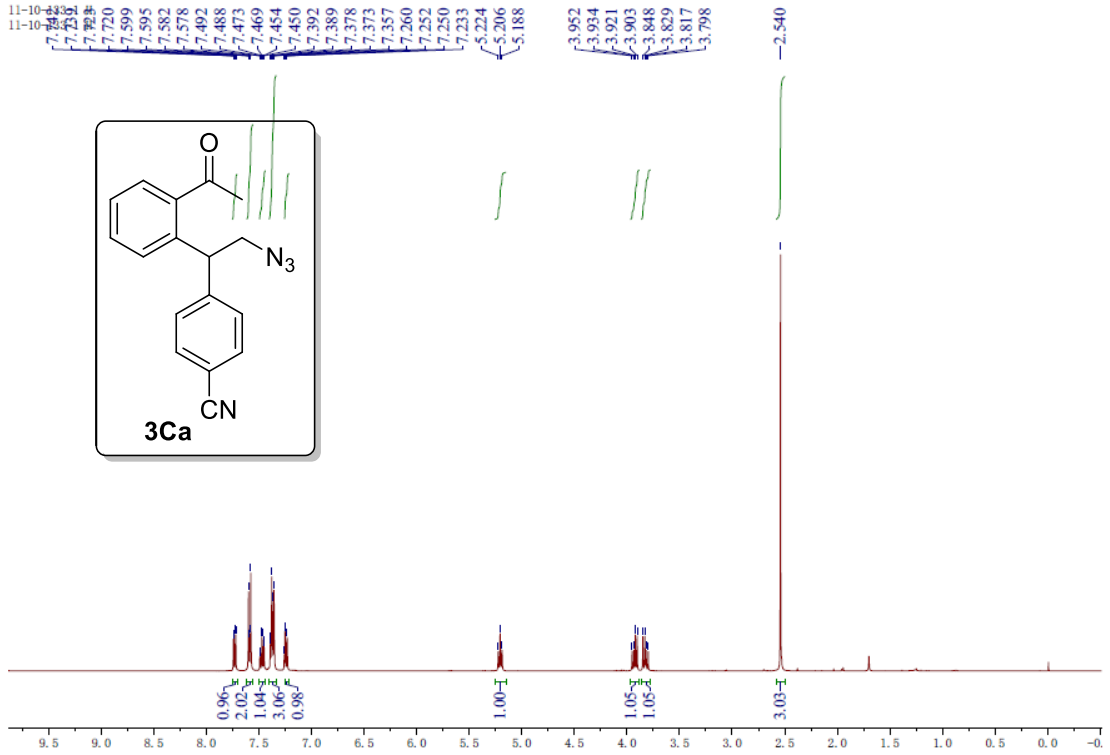
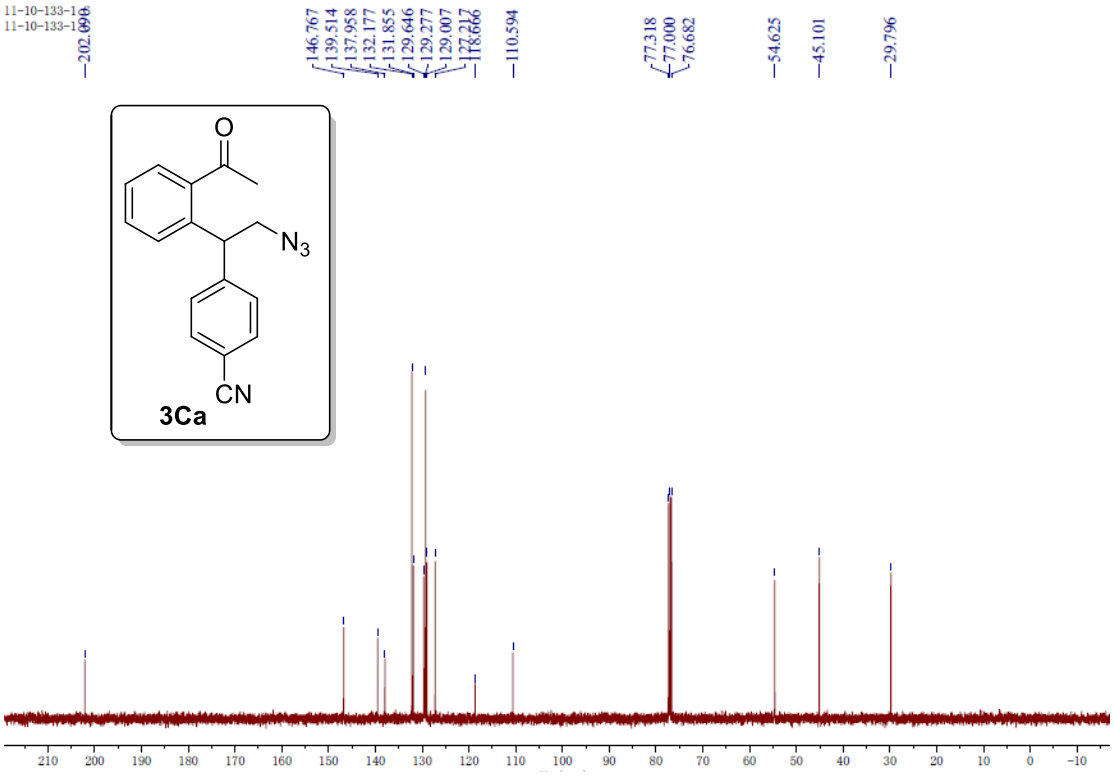
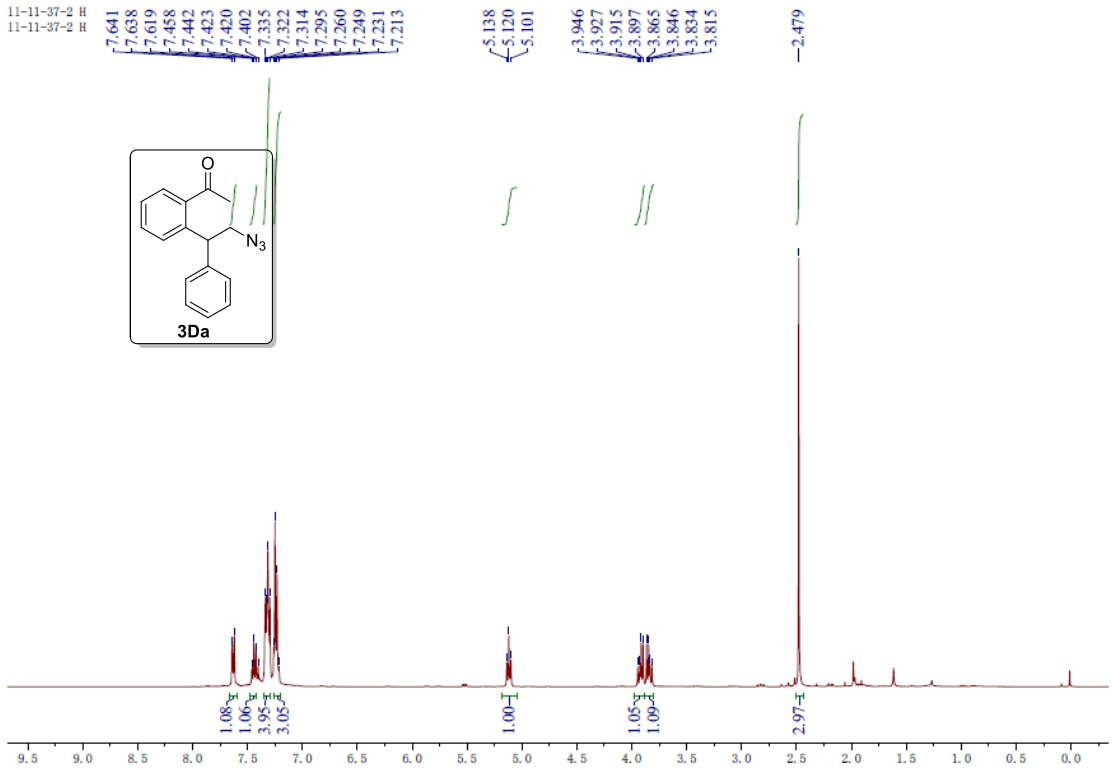
76.682
54.991
44.442
29.971
O
N3
Cl
3Aa


O
N3
Br
3Ba


O
N3
Br
3Ba


O
N3
CN
3Ca


O
N3
CN
3Ca


11-11-37-2 H
11-11-37-2 H
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7.638
7.619
7.458
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7.423
7.420
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7.322
7.314
7.295
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7.231
7.213
5.138
5.120
5.101
3.946
3.927
3.915
3.897
3.865
3.846
3.834
3.815
2.479
O
N3
3Da
1.08
1.06
3.95
3.05
1.00
1.05
1.09
2.97
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
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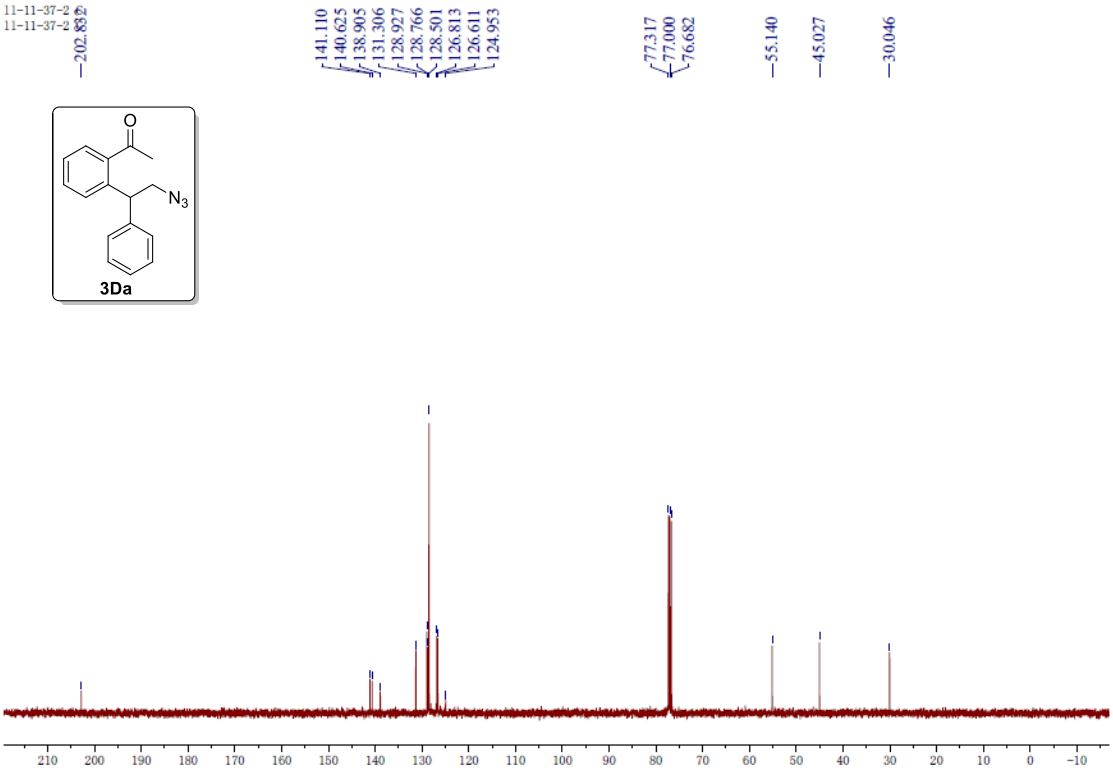
0.0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11-11-37-2 C
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128.766
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126.611
124.953
77.317
77.000
76.682
55.140
45.027
30.046
O
N3
3Da
210
200
190
180
170
160
150
140
130
120
110
100
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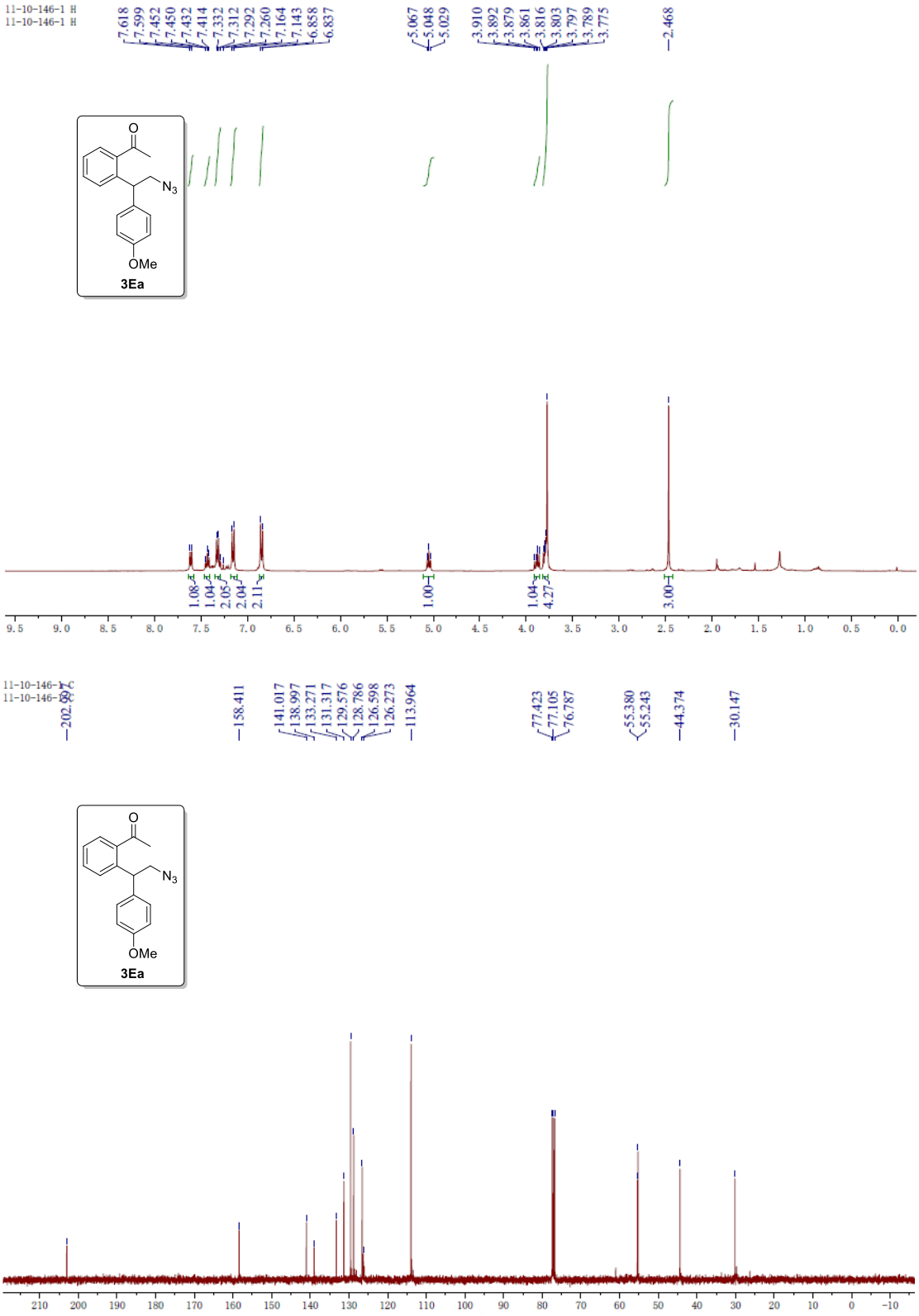
70
60
50
40
30
20
10
0
-10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11-10-146-1 H
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5.048
5.029
3.910
3.892
3.879
3.861
3.816
3.803
3.797
3.789
3.775
2.468
O
N3
OMe
3Ea
1.08
1.04
2.05
2.04
2.11
1.00
1.04
4.27
3.00
9.5 9.0 8.5 8.0 7.5 7.0 6.5 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
11-10-146-13C
11-10-146-13C
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133.271
131.317
129.576
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126.598
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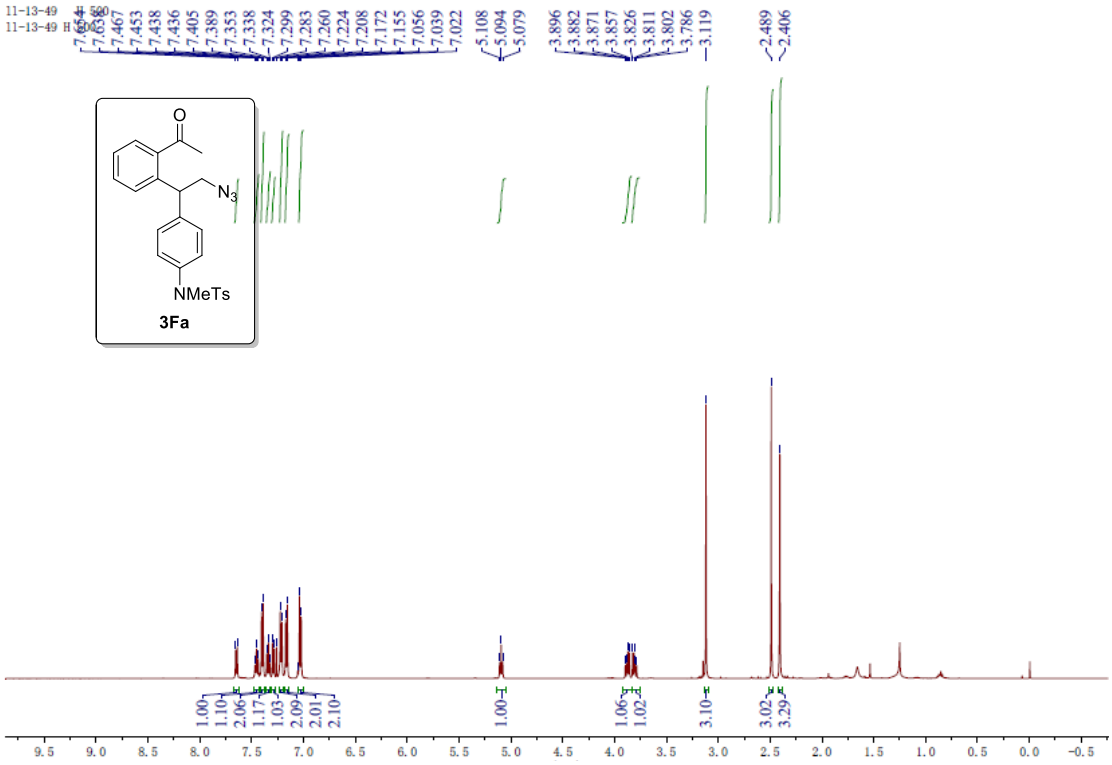
77.105
76.787
55.380
55.243
44.374
30.147
O
N3
OMe
3Ea
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10


11-13-49
11-13-49 H 500
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7.438
7.436
7.405
7.389
7.353
7.338
7.324
7.299
7.283
7.260
7.224
7.208
7.172
7.155
7.056
7.039
7.022
5.108
5.094
5.079
3.896
3.882
3.871
3.857
3.826
3.811
3.802
3.786
3.119
2.489
2.406
O
N3
NMeTs
3Fa
1.00
1.10
2.06
1.17
1.03
2.09
2.01
2.10
1.00
1.06
1.02
3.10
3.02
3.29
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
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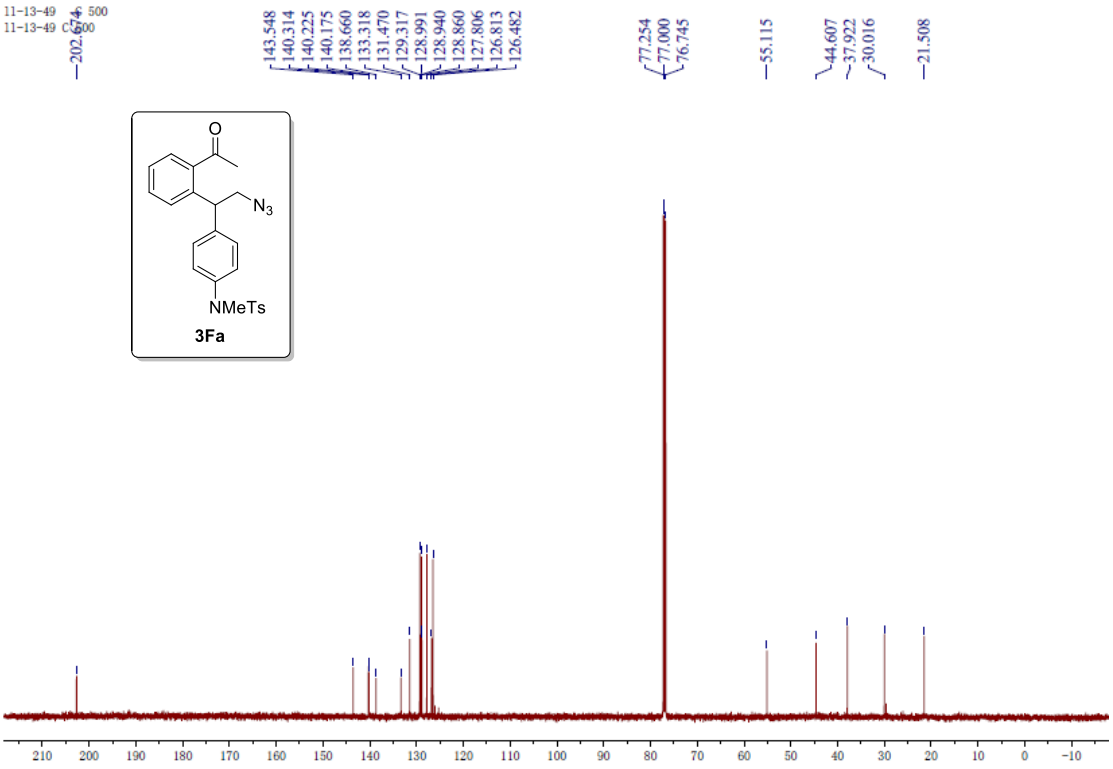
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5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11-13-49 C 500
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140.225
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131.470
129.317
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128.940
128.860
127.806
126.813
126.482
77.254
77.000
76.745
55.115
44.607
37.922
30.016
21.508
O
N3
NMeTs
3Fa
210
200
190
180
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100
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60
50
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0
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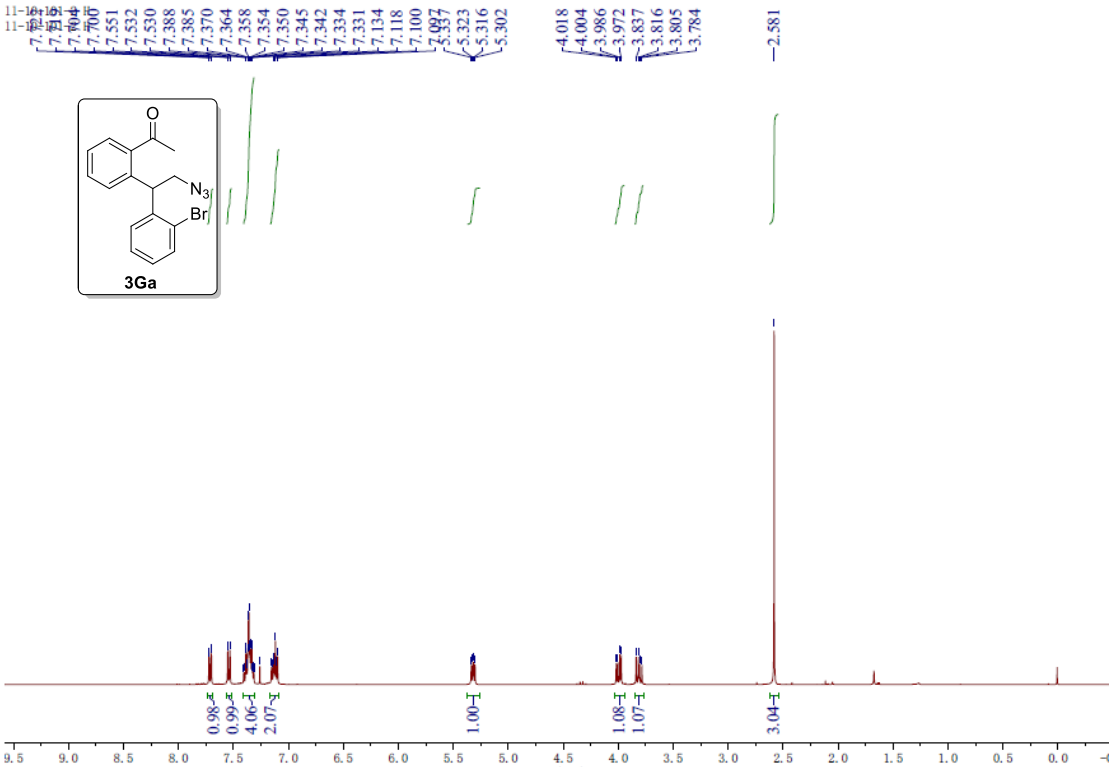
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7.530
7.388
7.385
7.370
7.364
7.358
7.354
7.350
7.345
7.342
7.334
7.331
7.134
7.118
7.100
5.323
5.316
5.302
4.018
4.004
3.986
3.972
3.837
3.816
3.805
3.784
2.581
O
N3
Br
3Ga
0.98
0.99
4.06
2.07
1.00
1.08
1.07
3.04
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
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3.0
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2.0
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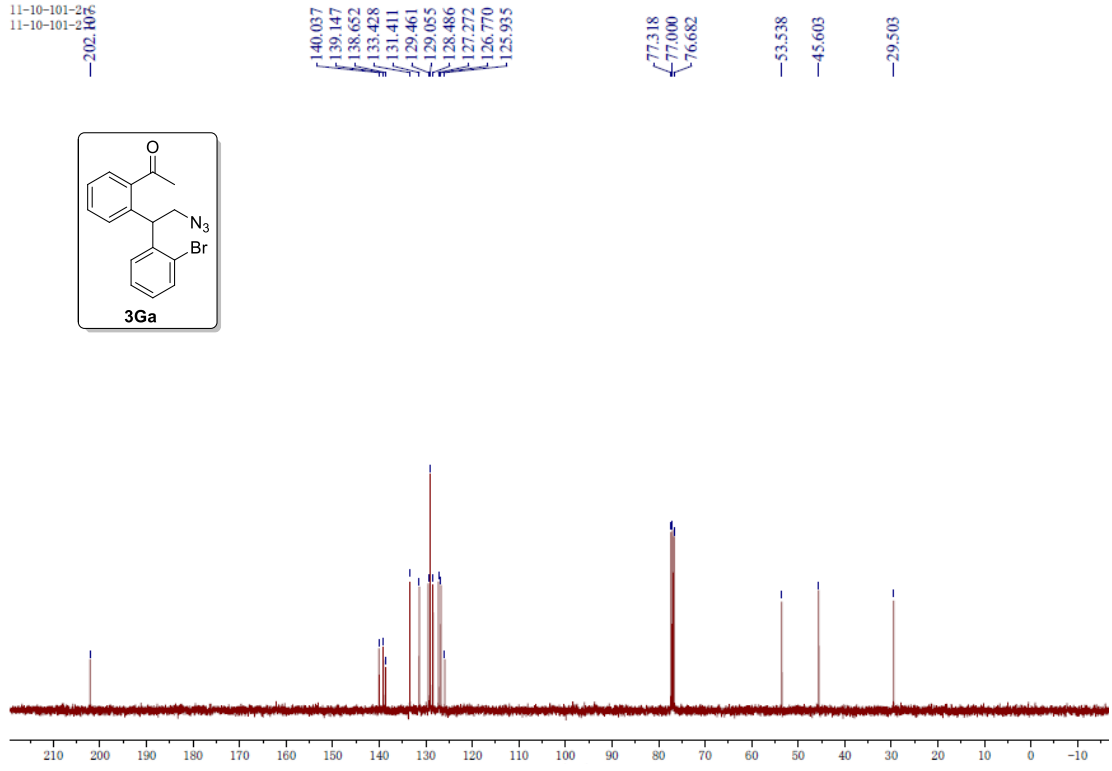
0.5
0.0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139.147
138.652
133.428
131.411
129.461
129.055
128.486
127.272
126.770
125.935
77.318
77.000
76.682
53.538
45.603
29.503
O
N3
Br
3Ga
210
200
190
180
170
160
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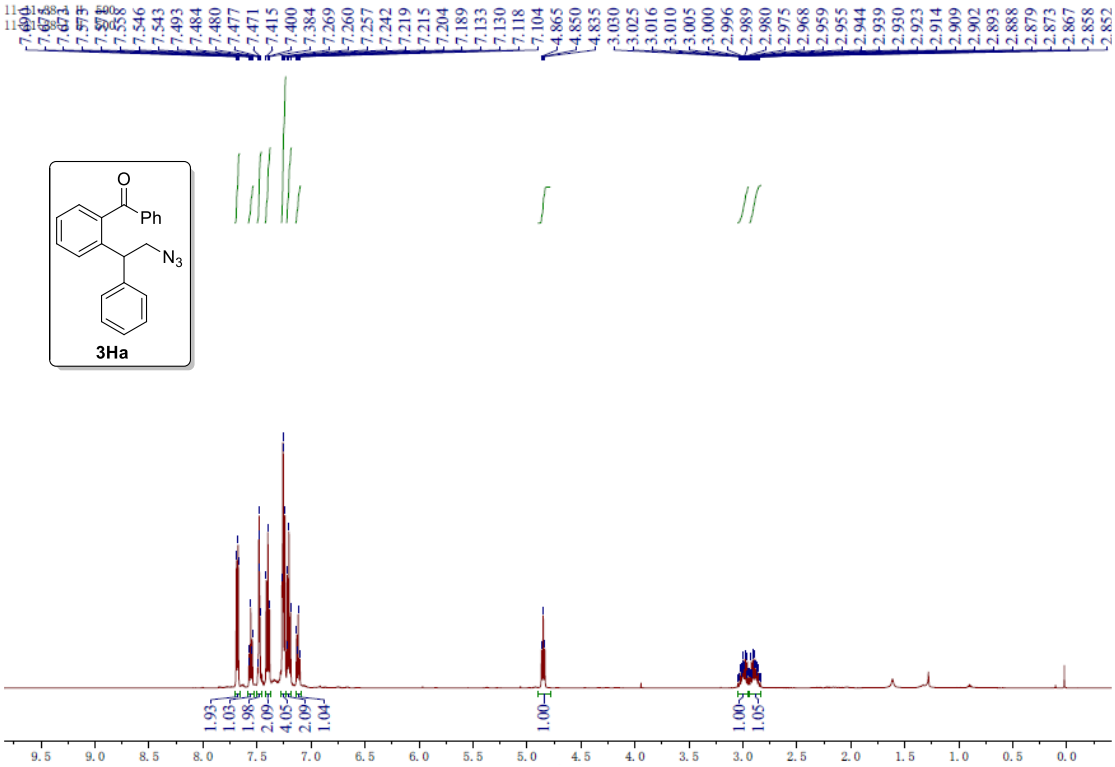
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10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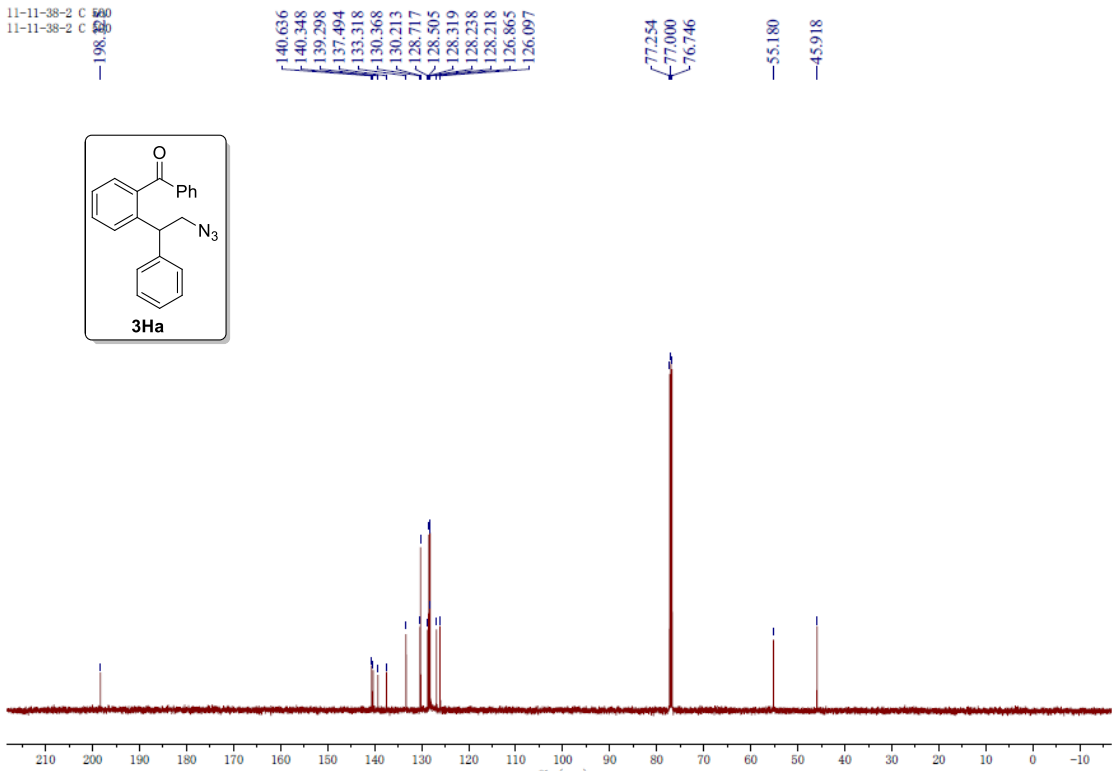
Ph
N3
3Ha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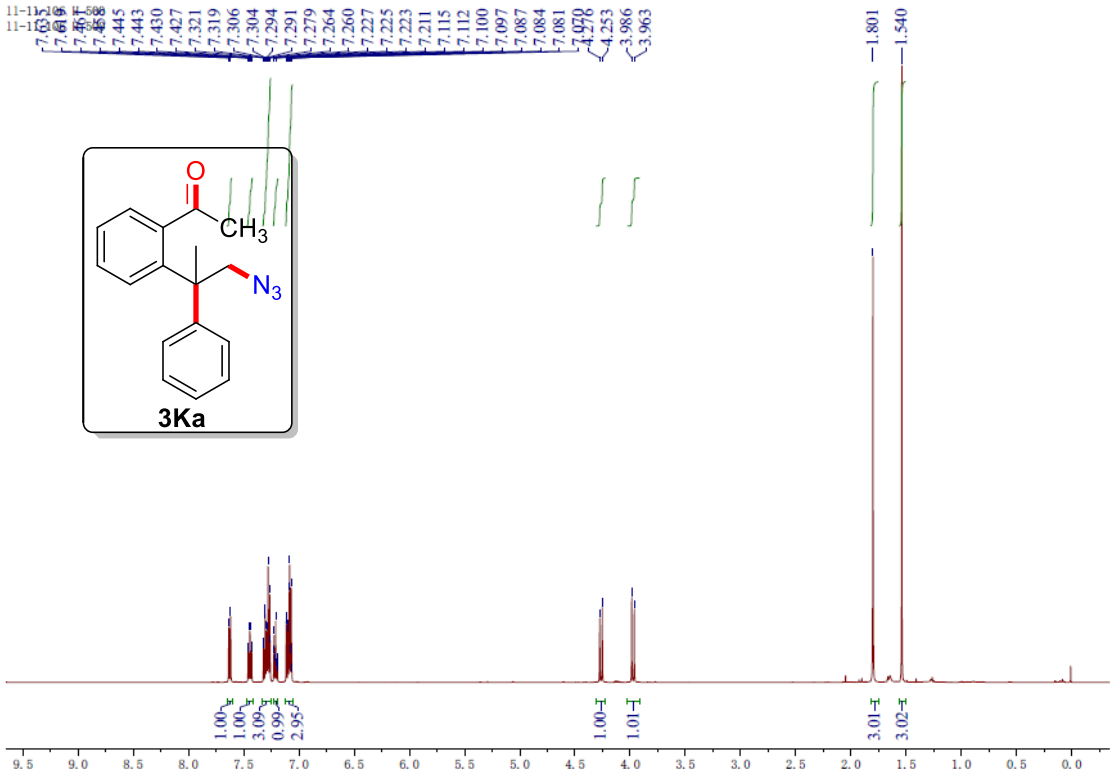
Ph
N3
3Ha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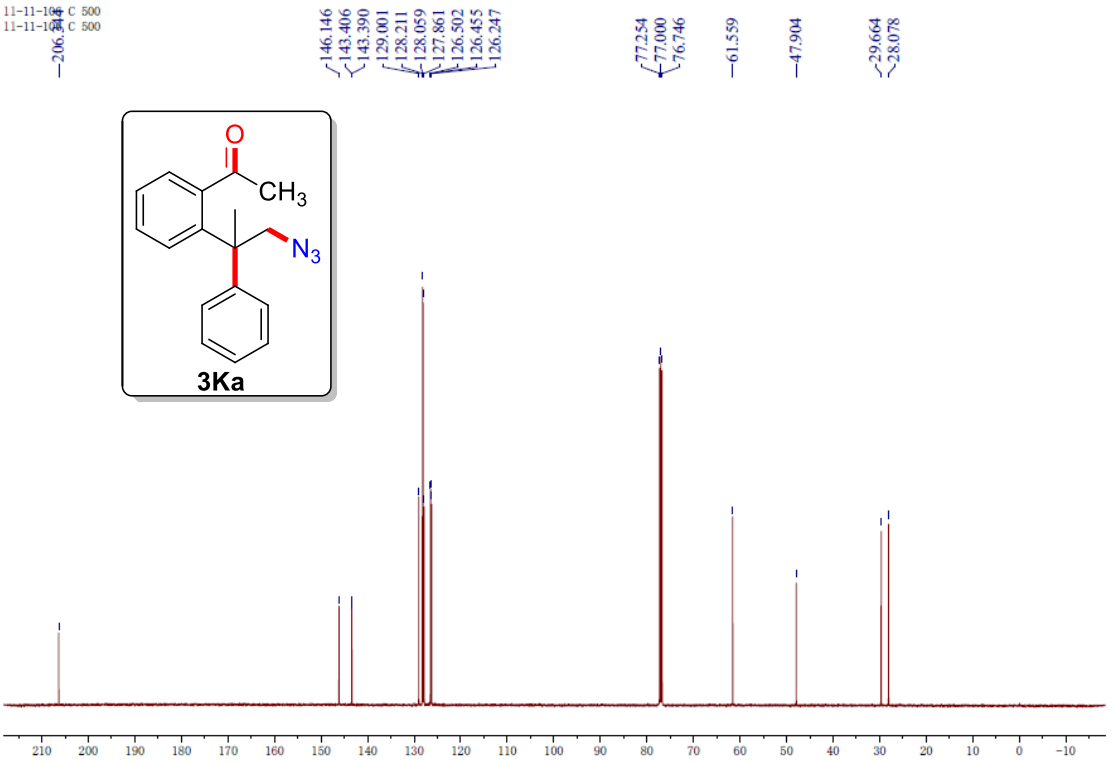
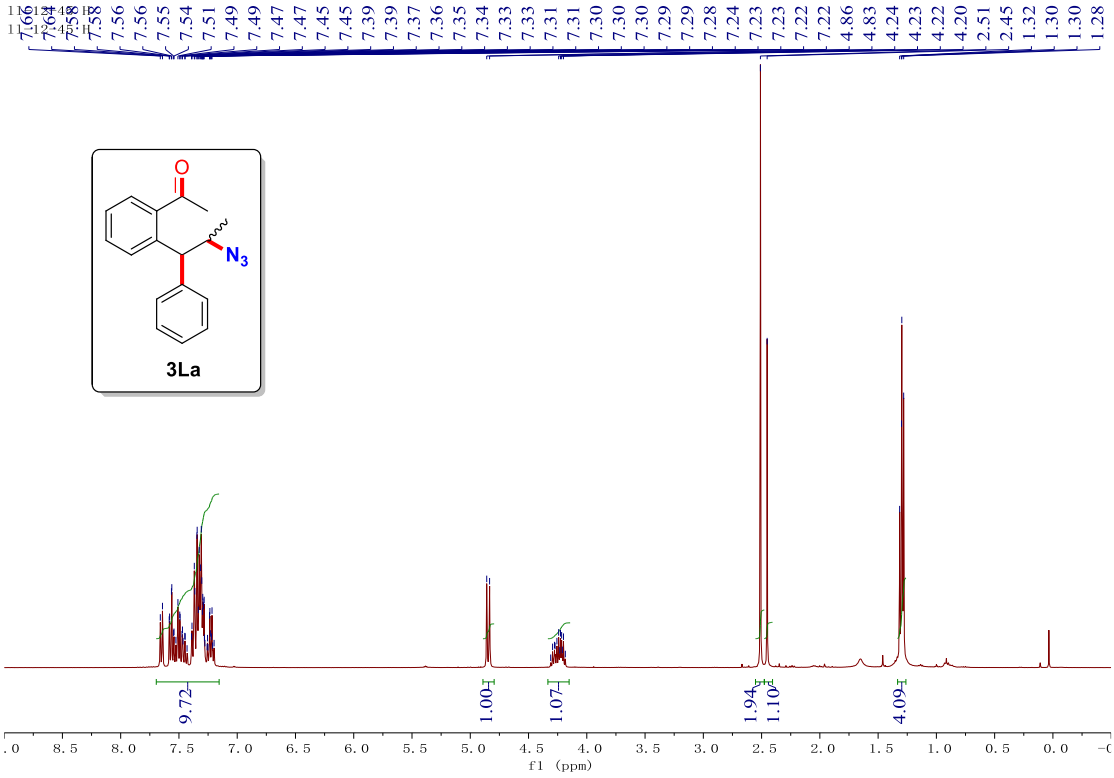
CH3
N3
3Ka


O
CH3
N3
3Ka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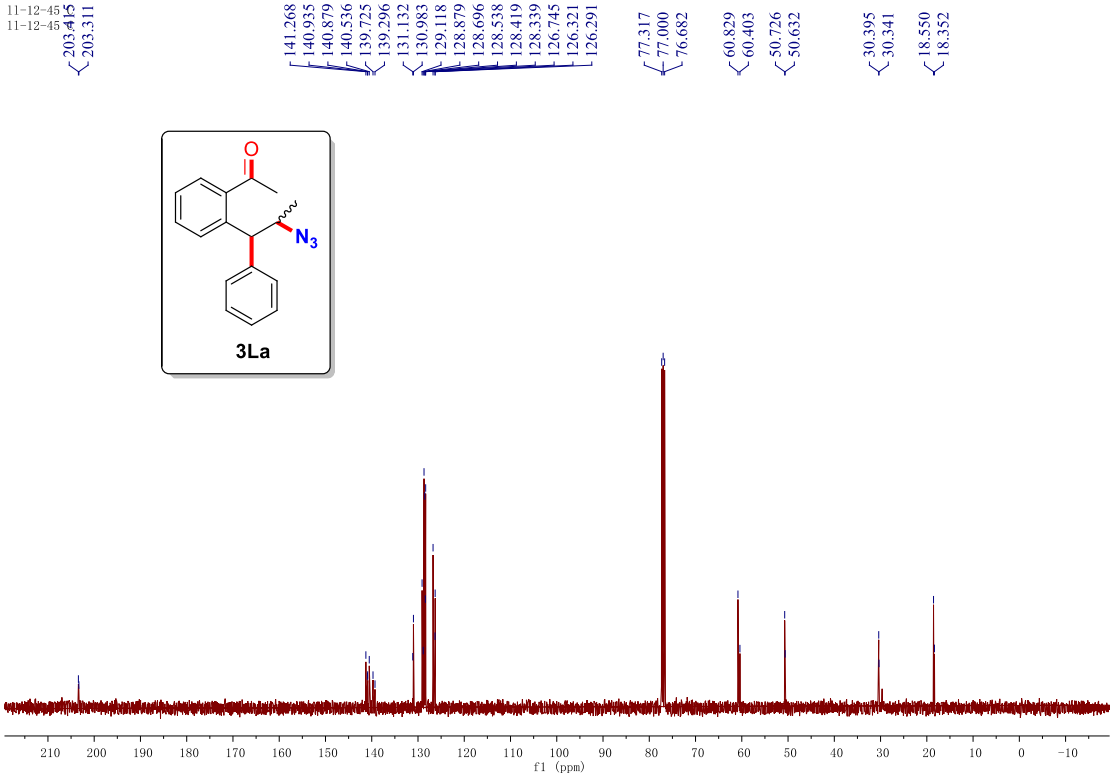
7.58
7.56
7.55
7.54
7.51
7.49
7.47
7.45
7.39
7.37
7.36
7.35
7.34
7.33
7.31
7.30
7.29
7.28
7.24
7.23
7.22
4.86
4.83
4.24
4.23
4.22
4.20
2.51
2.45
1.32
1.30
1.28
O
N3
3La
9.72
1.00
1.07
1.94
1.10
4.09
f1 (ppm)


11-12-45
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203.311
141.268
140.935
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140.536
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139.296
131.132
130.983
129.118
128.879
128.696
128.538
128.419
128.339
126.745
126.321
126.291
77.317
77.000
76.682
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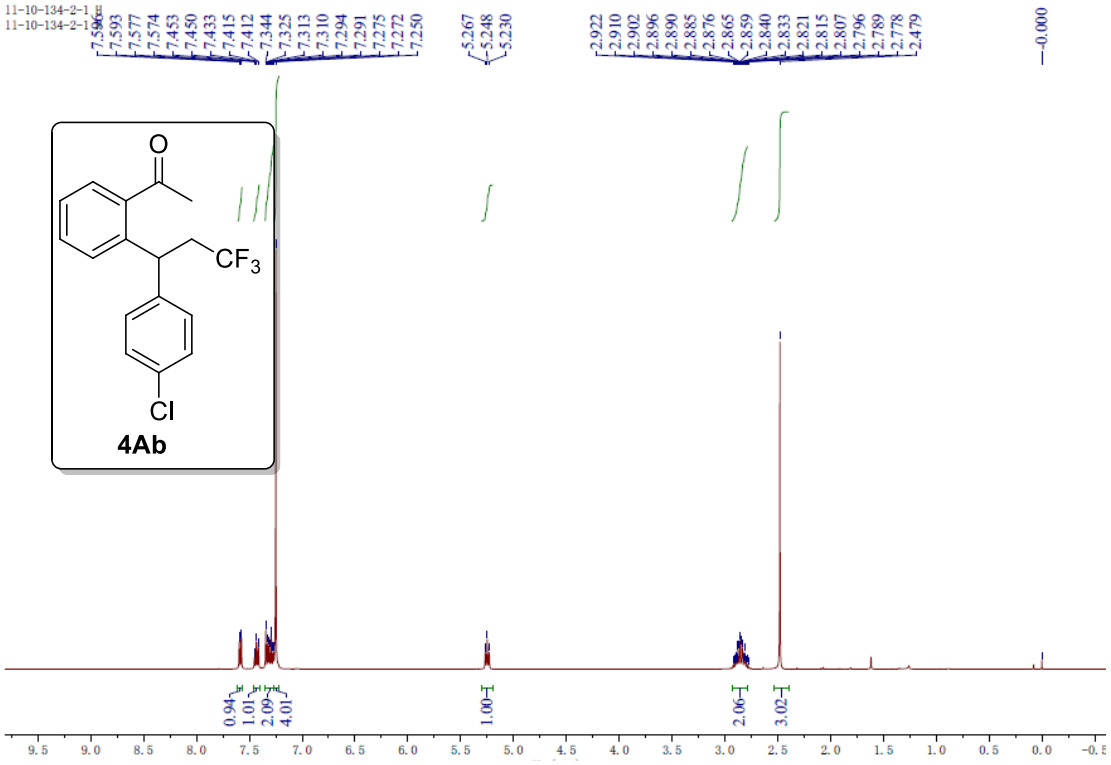
50.726
50.632
30.395
30.341
18.550
18.352
O
N3
3La
f1 (ppm)


11-10-134-2-1
11-10-134-2-1
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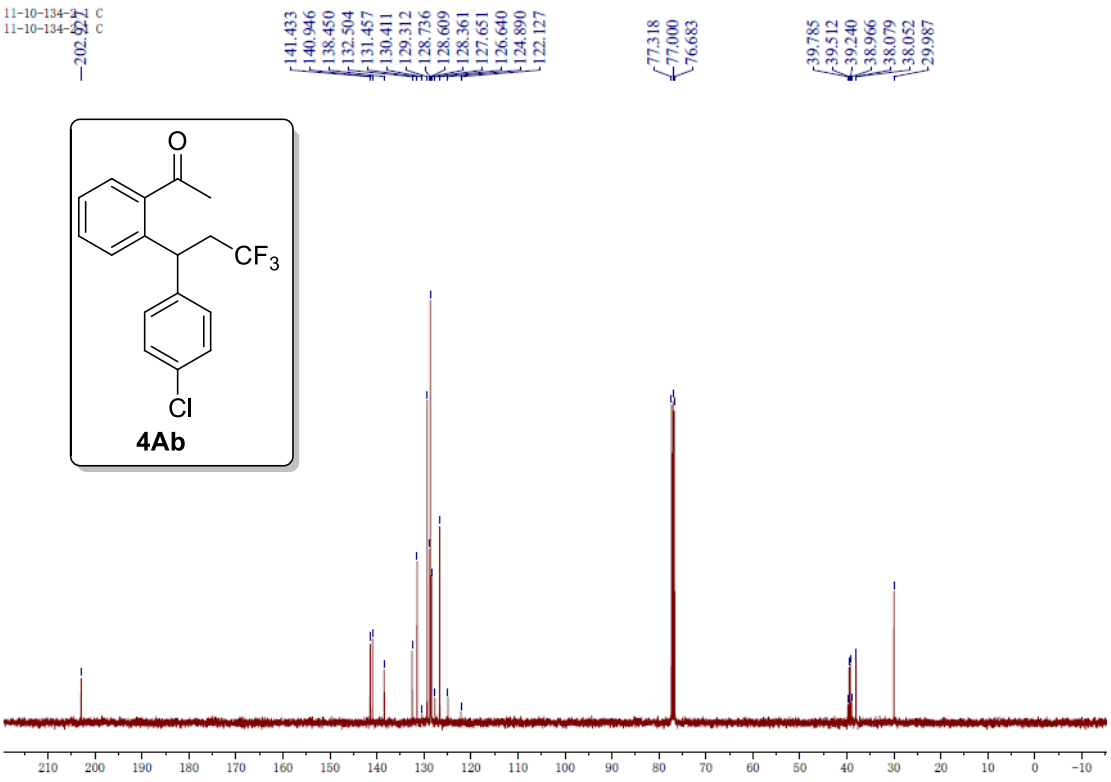
7.593
7.577
7.574
7.453
7.450
7.433
7.415
7.412
7.344
7.325
7.313
7.310
7.294
7.291
7.275
7.272
7.250
5.267
5.248
5.230
2.922
2.910
2.902
2.896
2.890
2.885
2.876
2.865
2.859
2.840
2.833
2.821
2.815
2.807
2.796
2.789
2.778
2.479
0.000
O
CF3
Cl
4Ab
0.94
1.01
2.09
4.01
1.00
2.06
3.02
9.5
9.0
8.5
8.0
7.5
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


11-10-134-2
11-10-134-2
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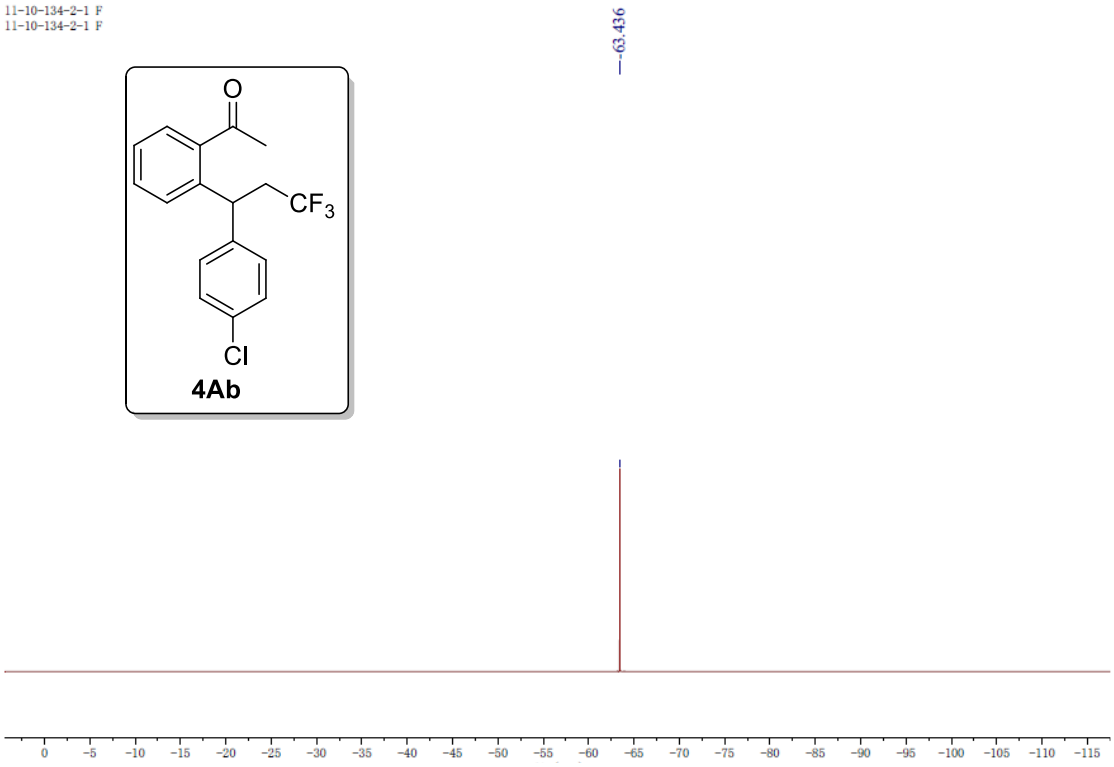
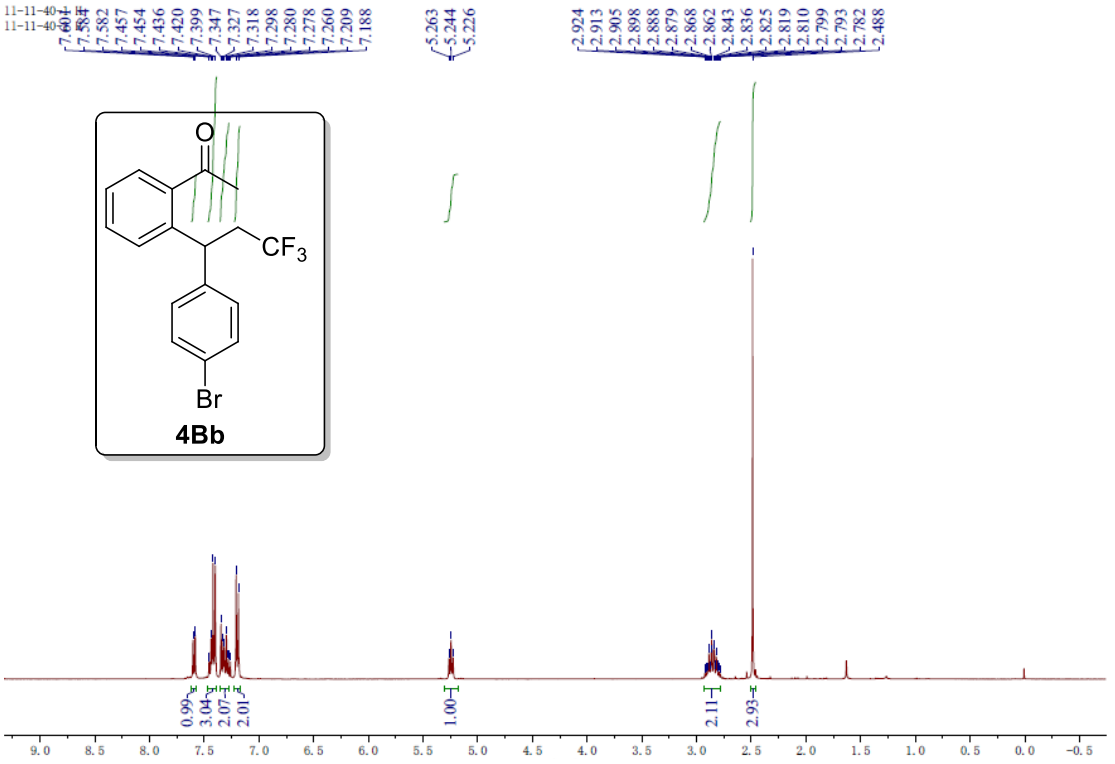
141.433
140.946
138.450
132.504
131.457
130.411
129.312
128.736
128.609
128.361
127.651
126.640
124.890
122.127
77.318
77.000
76.683
39.785
39.512
39.240
38.966
38.079
38.052
29.987
O
CF3
Cl
4Ab
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10


11-10-134-2-1 F
11-10-134-2-1 F
-63.436
O
CF3
Cl
4Ab


11-11-40-1
11-11-40-1
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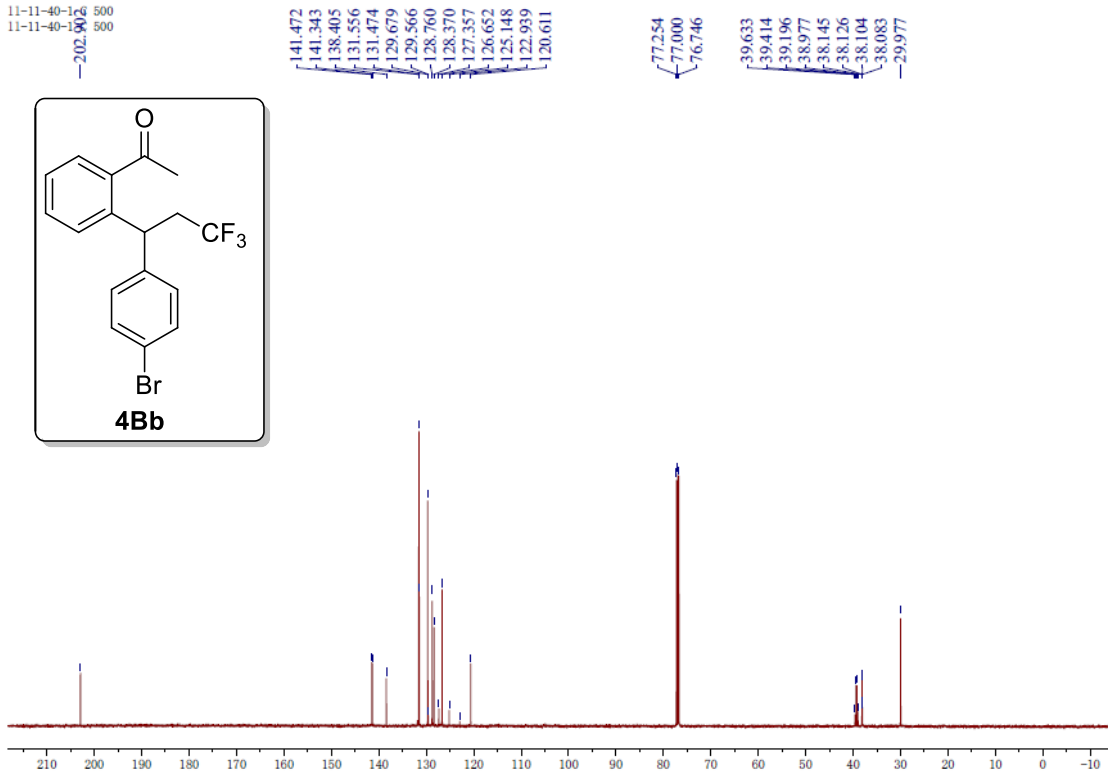
7.582
7.457
7.454
7.436
7.420
7.399
7.347
7.327
7.318
7.298
7.280
7.278
7.260
7.209
7.188
5.263
5.244
5.226
2.924
2.913
2.905
2.898
2.888
2.879
2.868
2.862
2.843
2.836
2.825
2.819
2.810
2.799
2.793
2.782
2.488
O
CF3
Br
4Bb
0.99
3.04
2.07
2.01
1.00
2.11
2.93


11-11-40-1c 500
11-11-40-1c 500
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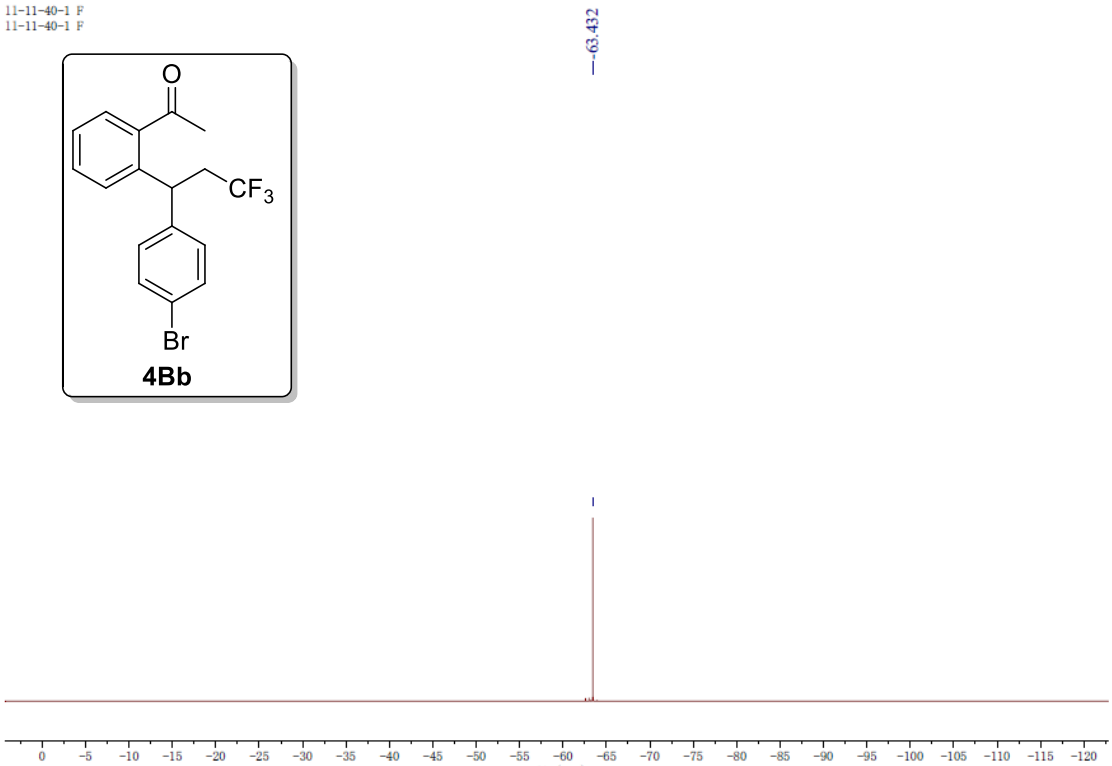
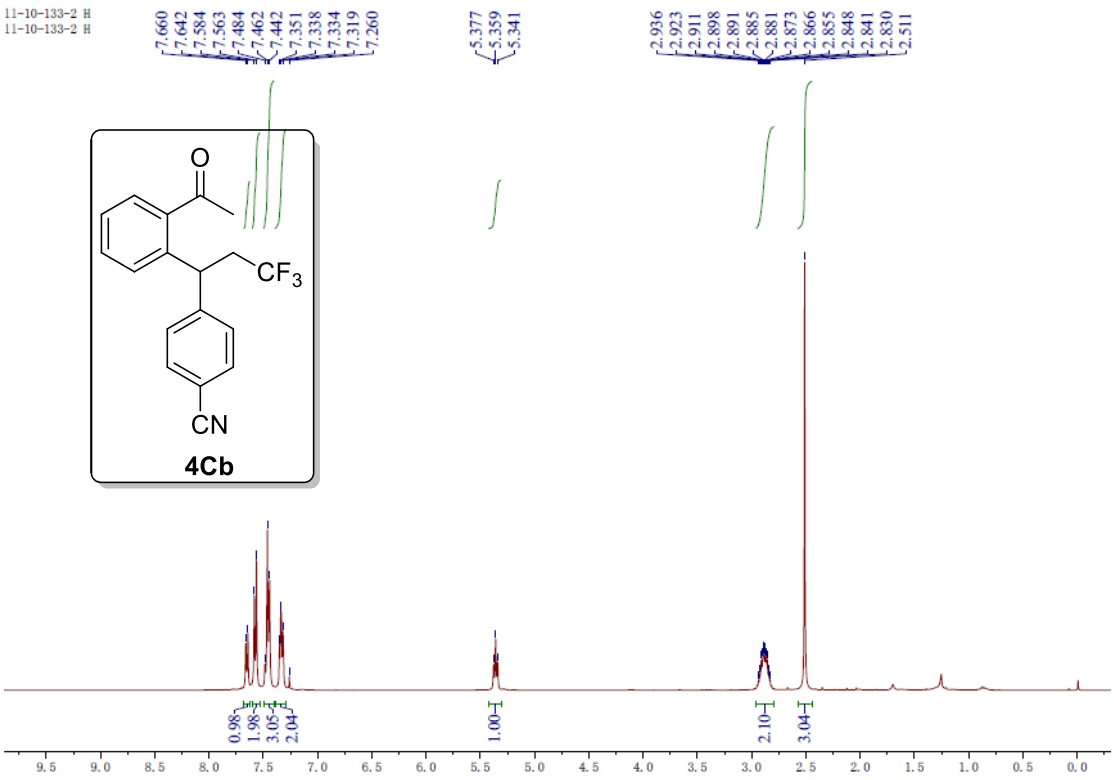
141.343
138.405
131.556
131.474
129.679
129.566
128.760
128.370
127.357
126.652
125.148
122.939
120.611
77.254
77.000
76.746
39.633
39.414
39.196
38.977
38.145
38.126
38.104
38.083
29.977
O
CF3
Br
4Bb
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10


11-11-40-1 F
11-11-40-1 F
-63.432
O
CF3
Br
4Bb
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


11-10-133-2 H
11-10-133-2 H
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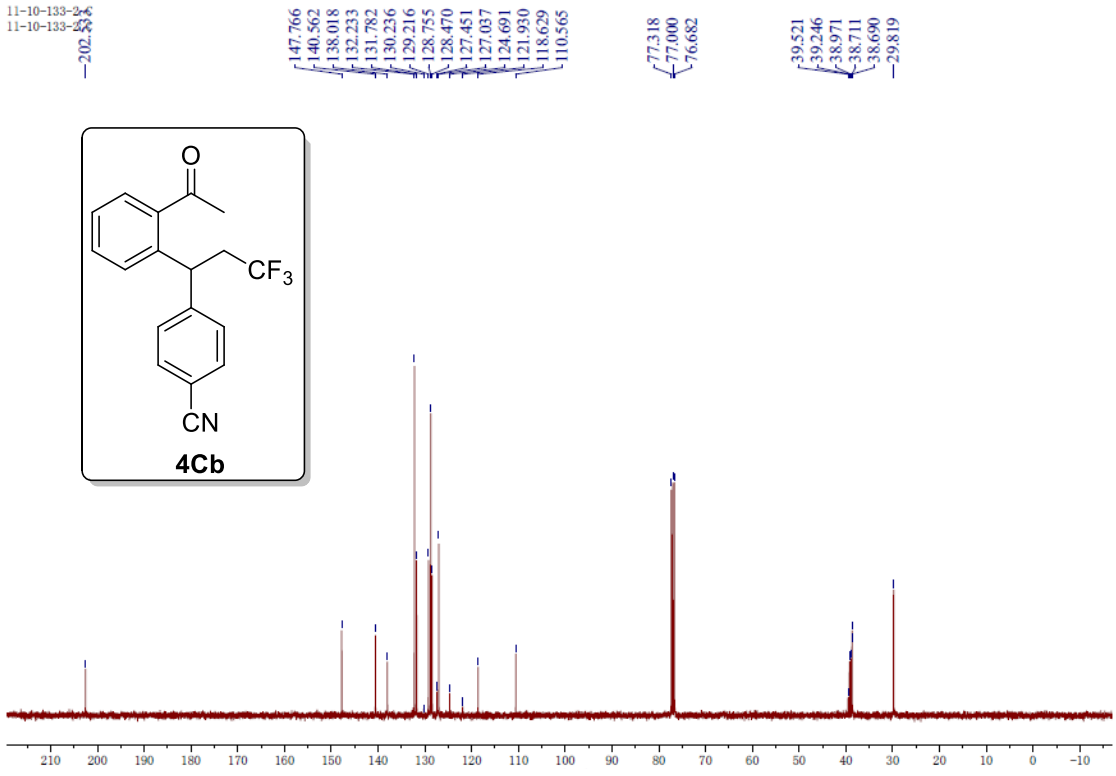
7.563
7.484
7.462
7.442
7.351
7.338
7.334
7.319
7.260
5.377
5.359
5.341
2.936
2.923
2.911
2.898
2.891
2.885
2.881
2.873
2.866
2.855
2.848
2.841
2.830
2.511
O
CF3
CN
4Cb
0.98
1.98
3.05
2.04
1.00
2.10
3.04
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0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11-10-133-2
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132.233
131.782
130.236
129.216
128.755
128.470
127.451
127.037
124.691
121.930
118.629
110.565
77.318
77.000
76.682
39.521
39.246
38.971
38.711
38.690
29.819
O
CF3
CN
4Cb
210
200
190
180
170
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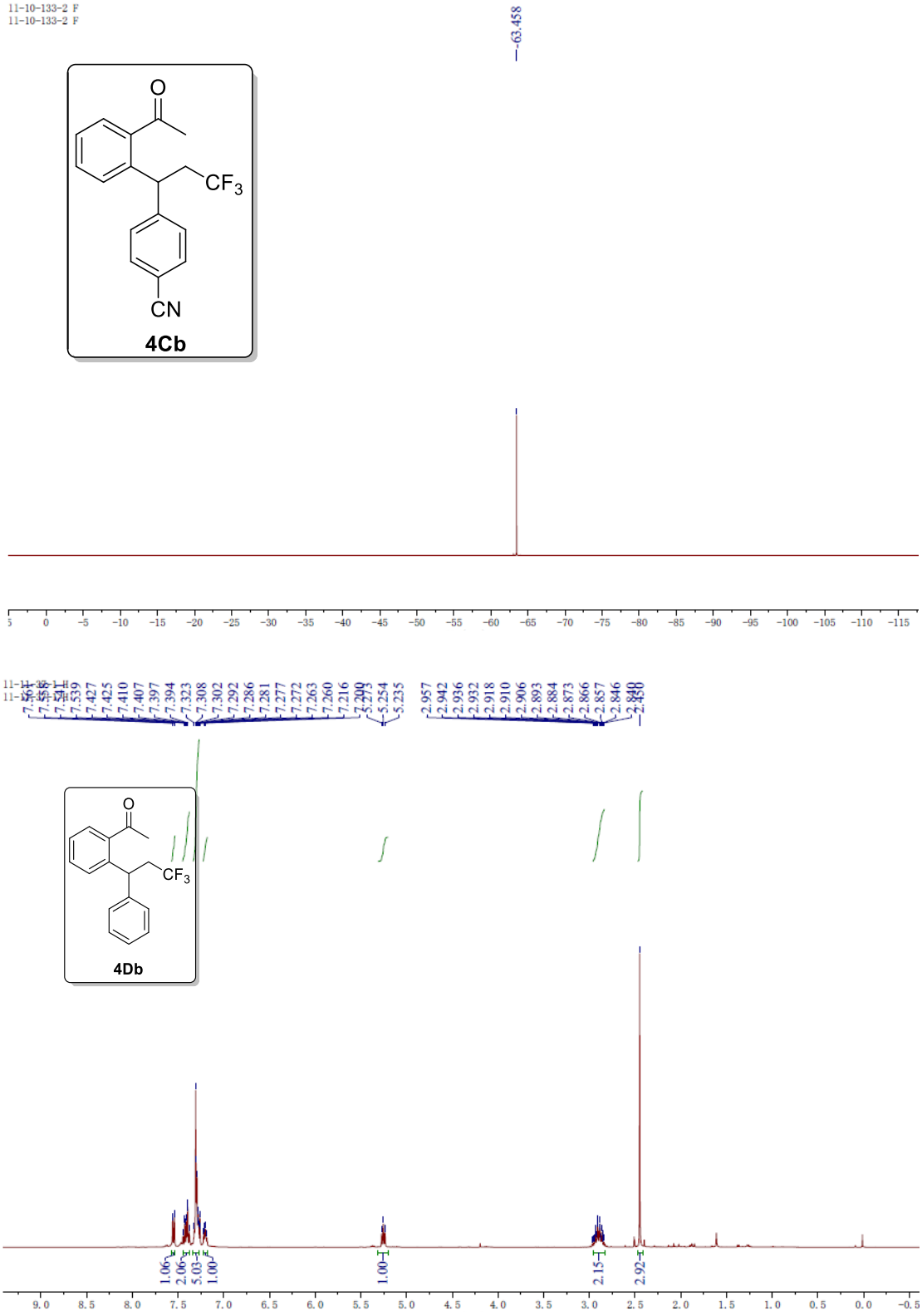
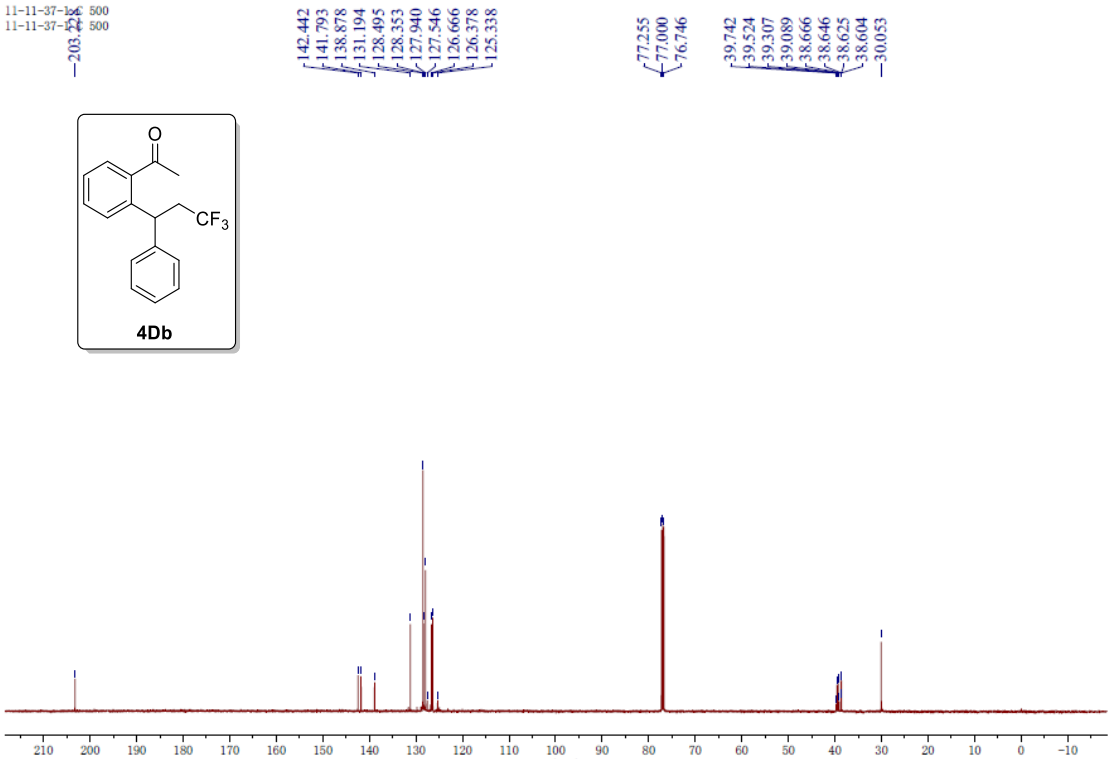
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10


11-10-133-2 F
11-10-133-2 F
-63.458
O
CF3
CN
4Cb
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
11-10-133-2 H
11-10-133-2 H
7.561
7.555
7.541
7.539
7.427
7.425
7.410
7.407
7.397
7.394
7.323
7.308
7.302
7.292
7.286
7.281
7.277
7.272
7.263
7.260
7.216
7.209
7.203
5.254
5.235
2.957
2.942
2.936
2.932
2.918
2.910
2.906
2.893
2.884
2.873
2.866
2.857
2.846
2.840
2.450
O
CF3
4Db
1.06
2.06
5.03
1.00
1.00
2.15
2.92
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


11-11-37-1a C 500
11-11-37-1a C 500
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141.793
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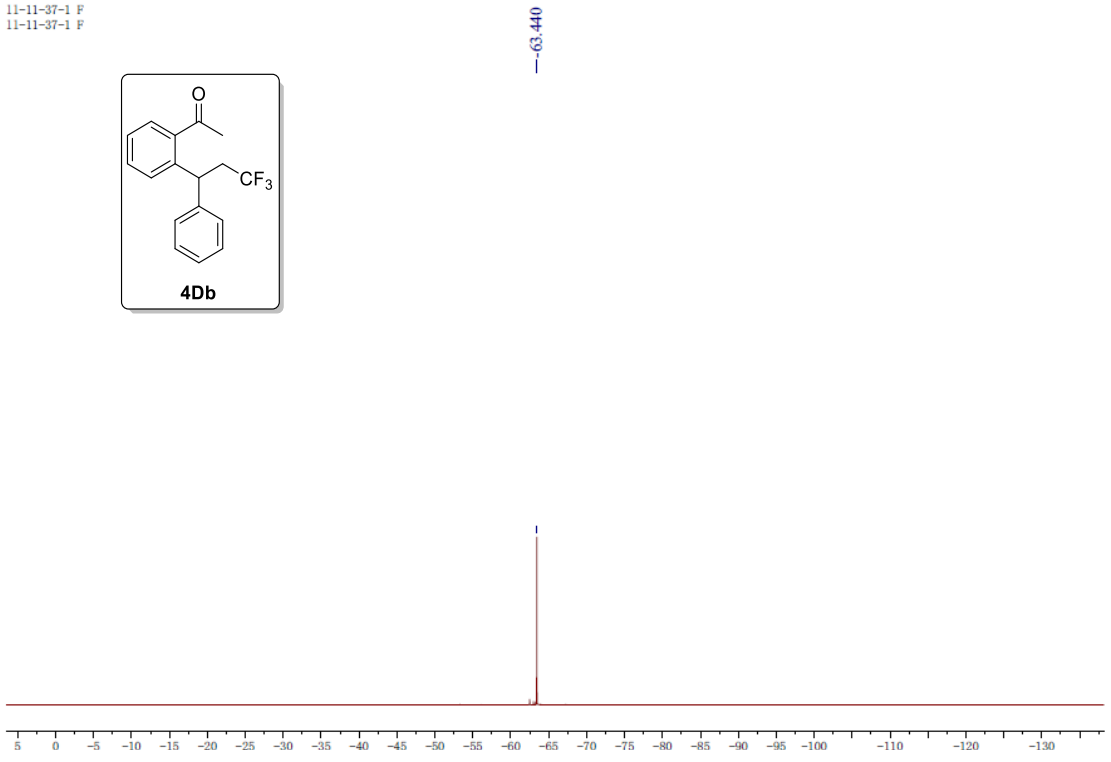
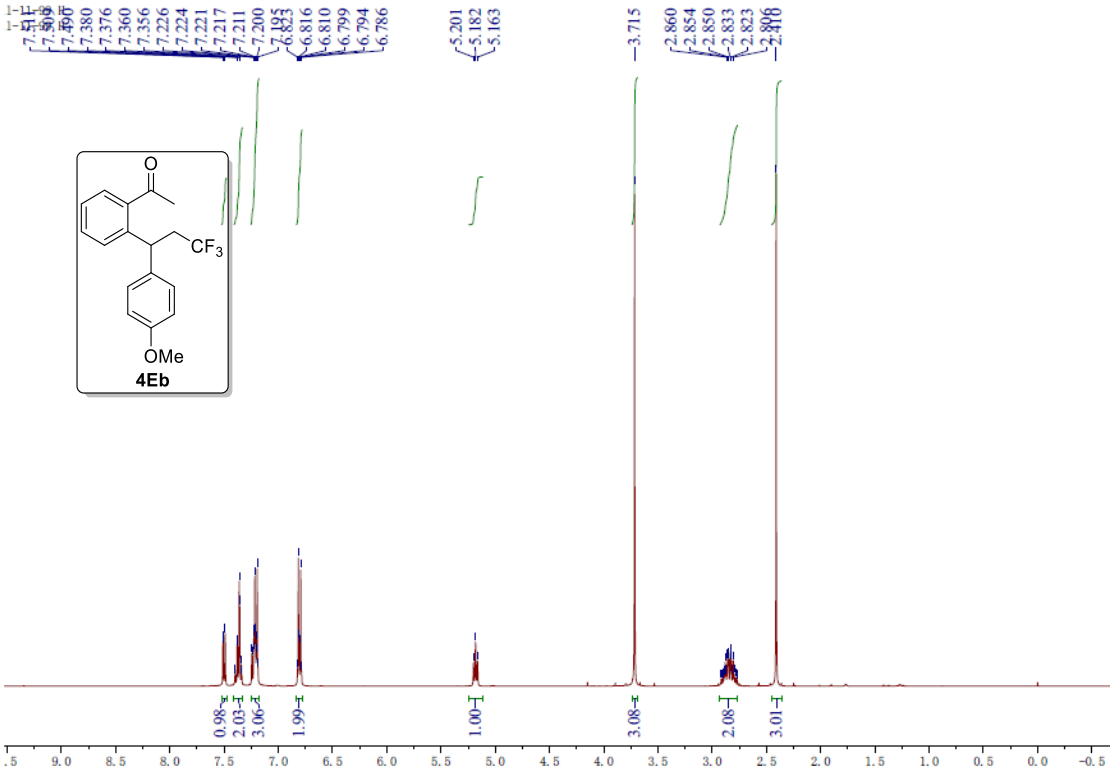
131.194
128.495
128.353
127.940
127.546
126.666
126.378
125.338
77.255
77.000
76.746
39.742
39.524
39.307
39.089
38.666
38.646
38.625
38.604
30.053
O
CF3
4Db
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10


11-11-37-1 F
11-11-37-1 F
-63.440
O
CF3
4Db
5 0 -5 -10 -15 -20 -25 -30 -35 -40 -45 -50 -55 -60 -65 -70 -75 -80 -85 -90 -95 -100 -110 -120 -130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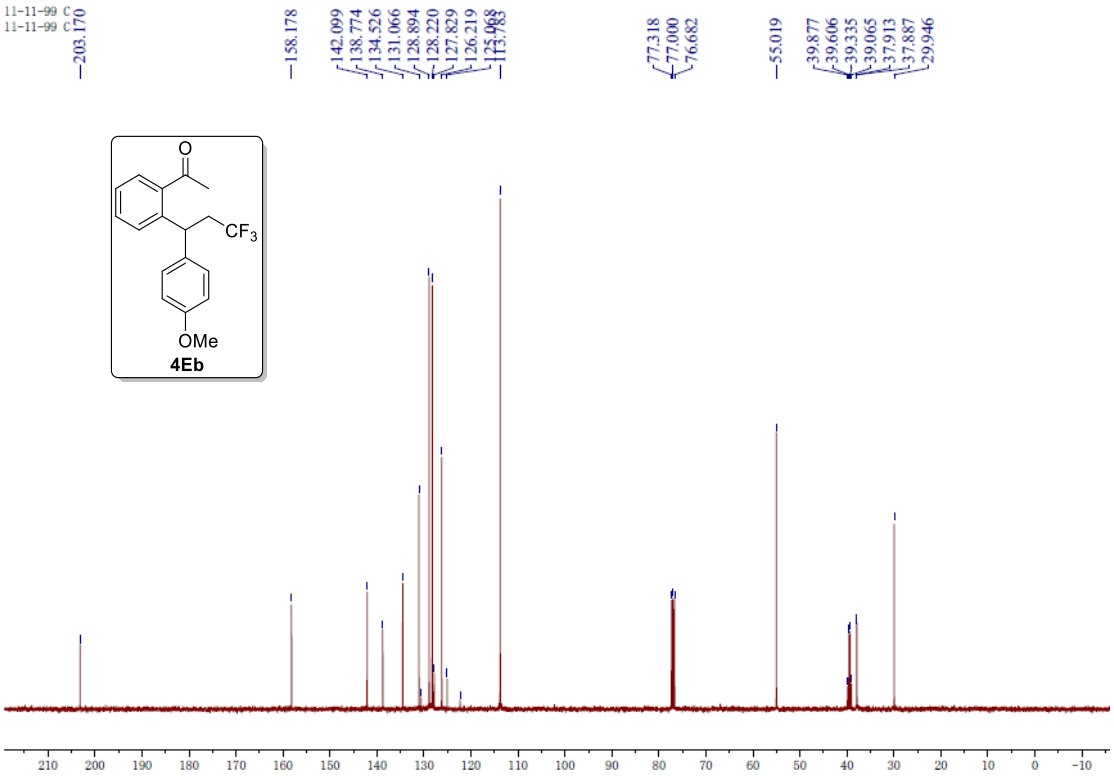
7.356
7.226
7.224
7.221
7.217
7.211
7.200
7.195
6.823
6.816
6.810
6.799
6.794
6.786
5.201
5.182
5.163
3.715
2.860
2.854
2.850
2.833
2.823
2.806
2.410
O
CF3
OMe
4Eb
0.98
2.03
3.06
1.99
1.00
3.08
2.08
3.01


11-11-99 C
11-11-99 C
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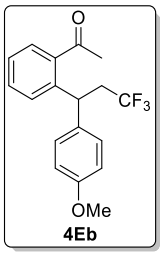
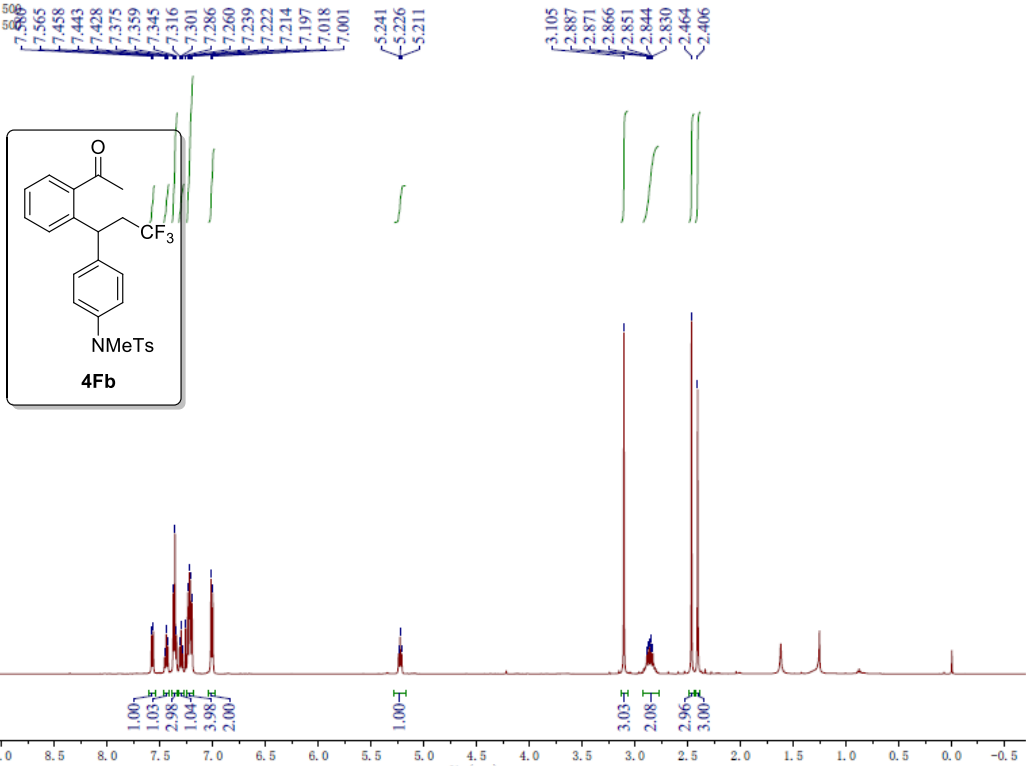
158.178
142.099
138.774
134.526
131.066
128.894
128.220
127.829
126.219
125.068
113.783
77.318
77.000
76.682
55.019
39.877
39.606
39.335
39.065
37.913
37.887
29.946
O
CF3
OMe
4Eb

11-11-99 F
11-11-99 F

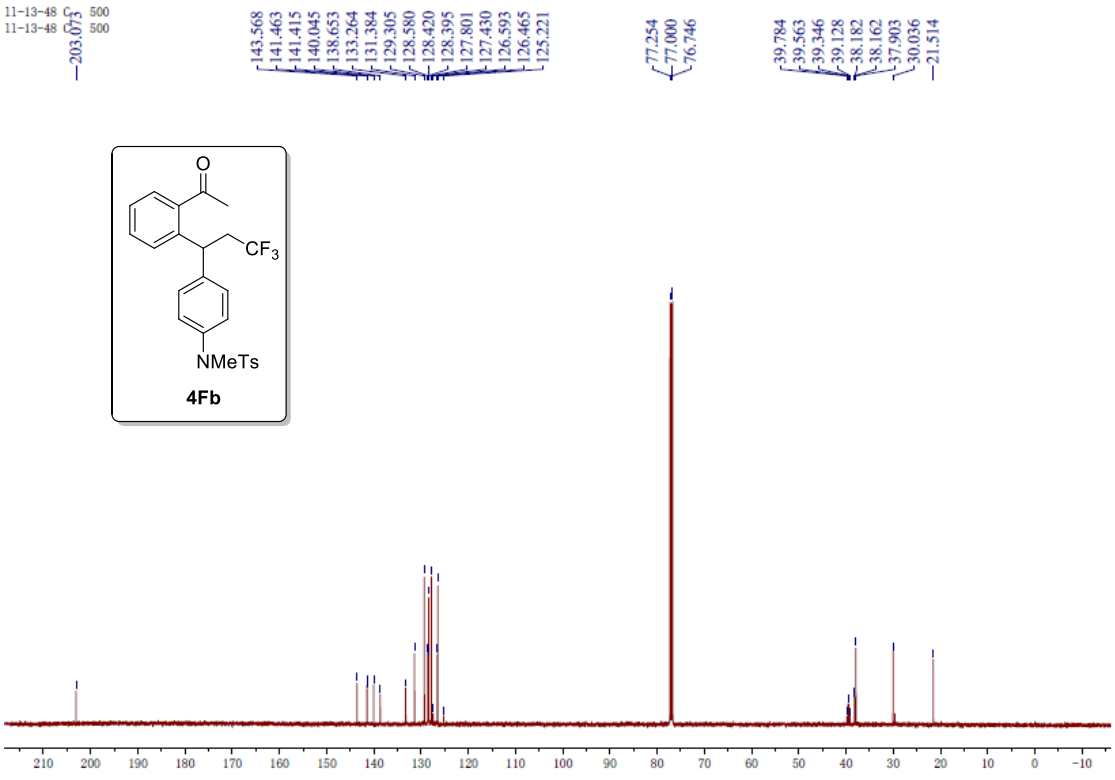


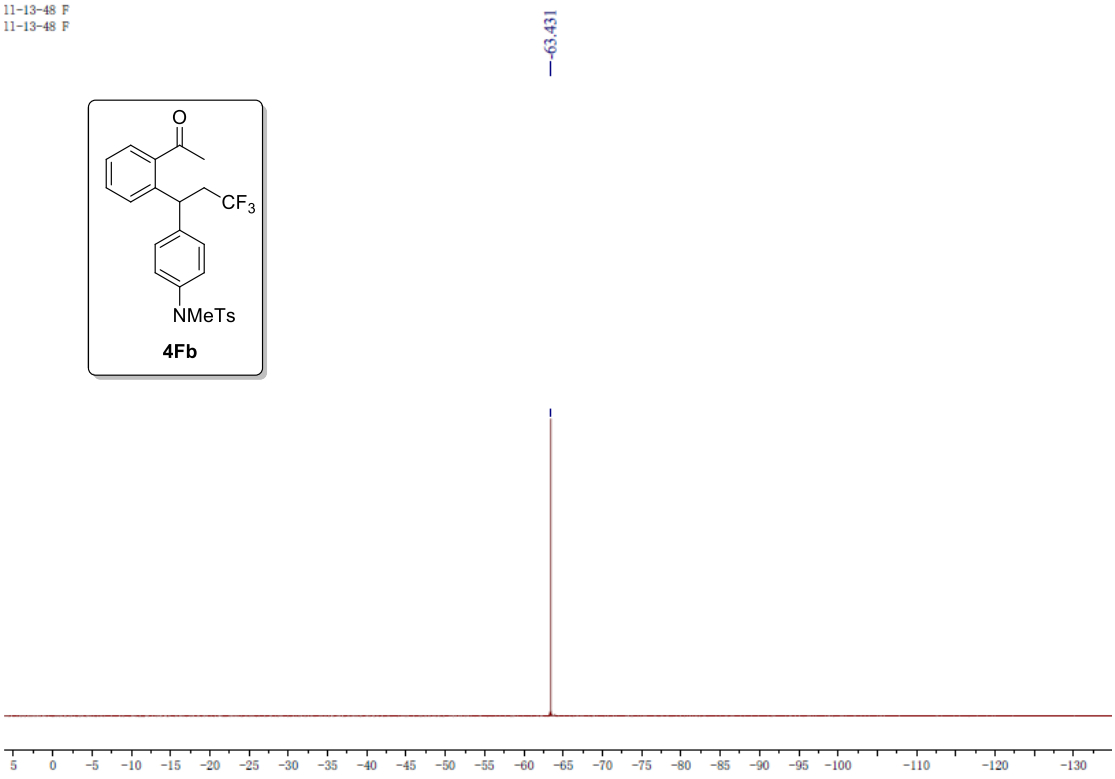
4Eb

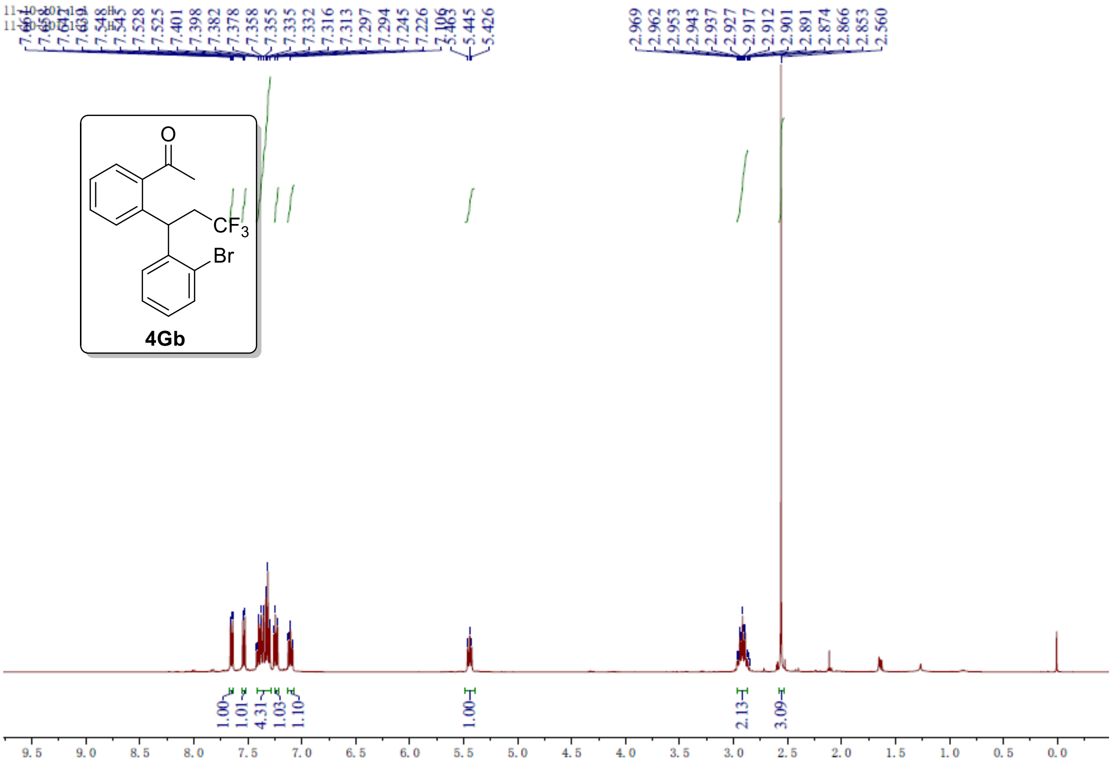
11-13-48 H
11-13-48 H

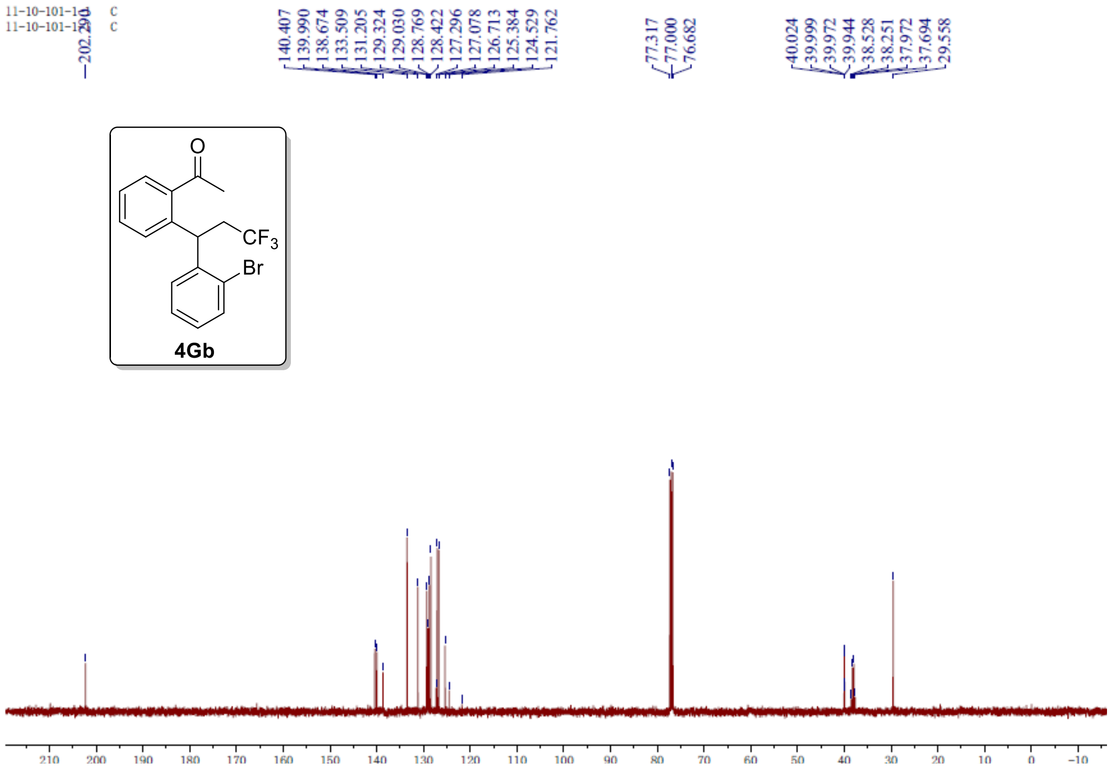


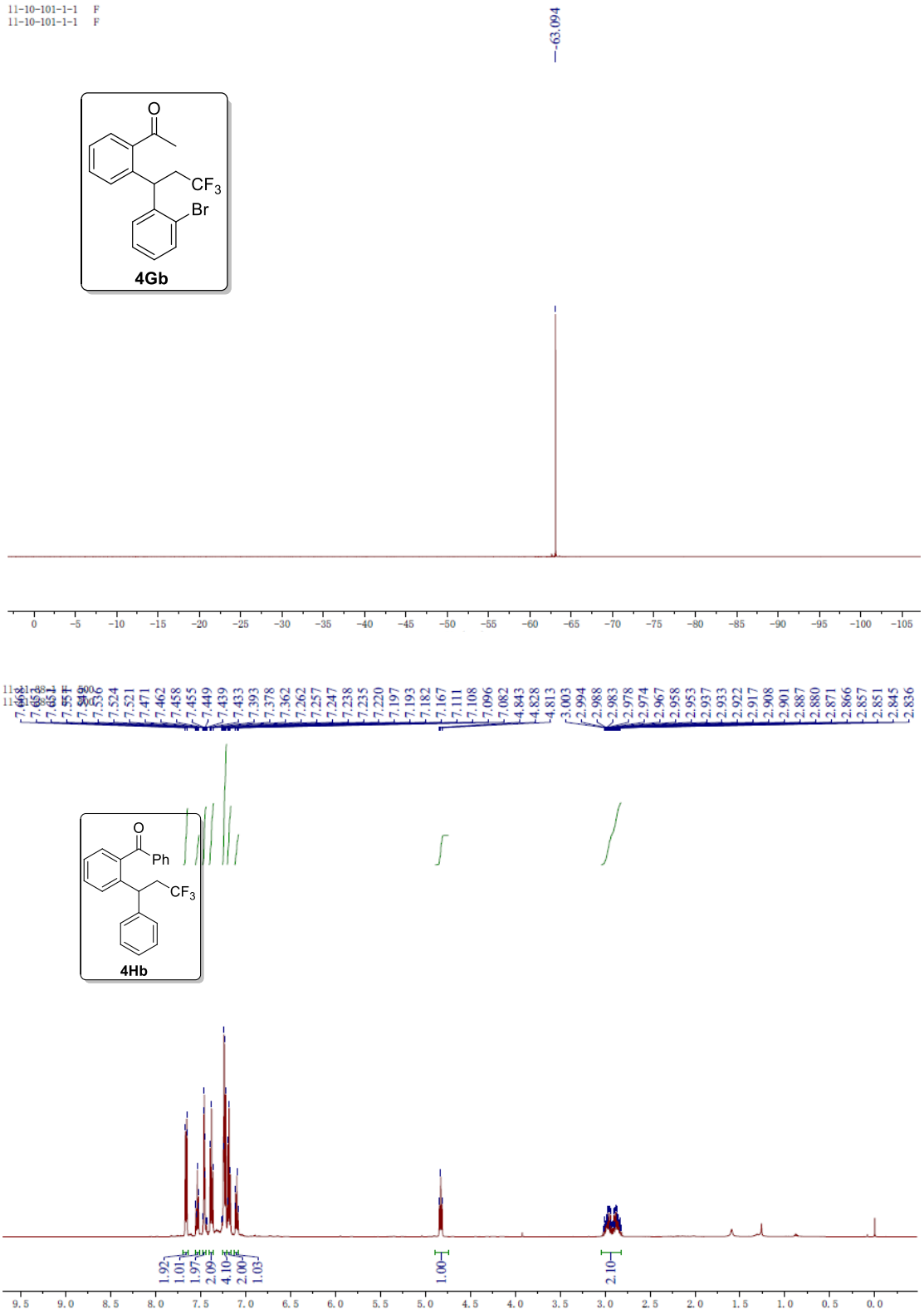
4Fb

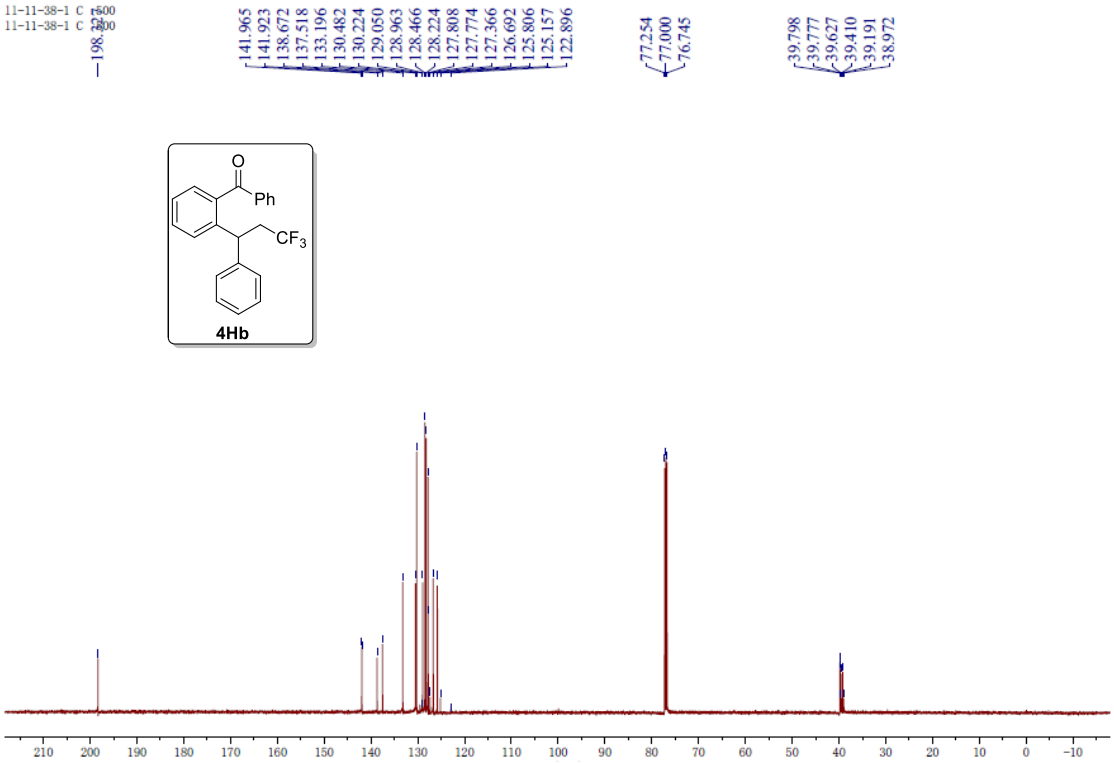

11-13-48 C 500
11-13-48 C 500
203.073
143.568
141.463
141.415
140.045
138.653
133.264
131.384
129.305
128.580
128.420
128.395
127.801
127.430
126.593
126.465
125.221
77.254
77.000
76.746
39.784
39.563
39.346
39.128
38.182
38.162
37.903
30.036
21.514
O
CF3
NMeTs
4Fb
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10

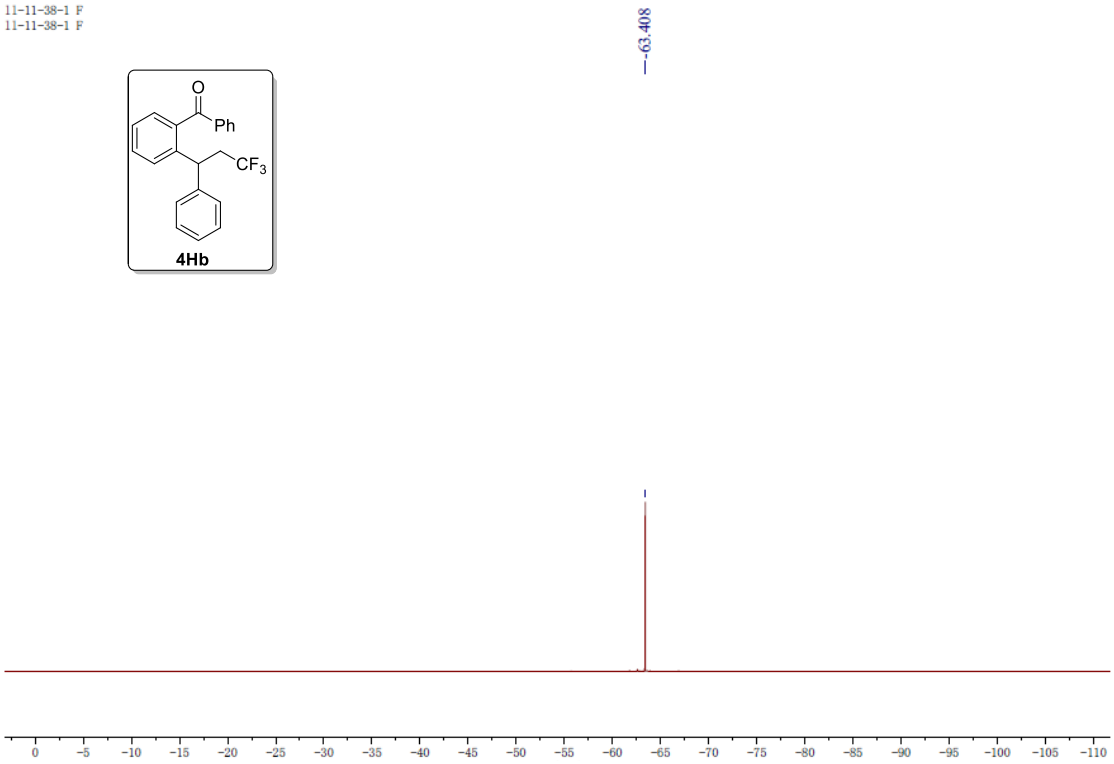

11-13-48 F
11-13-48 F
-63.431
O
CF3
NMeTs
4Fb
5 0 -5 -10 -15 -20 -25 -30 -35 -40 -45 -50 -55 -60 -65 -70 -75 -80 -85 -90 -95 -100 -110 -120 -130

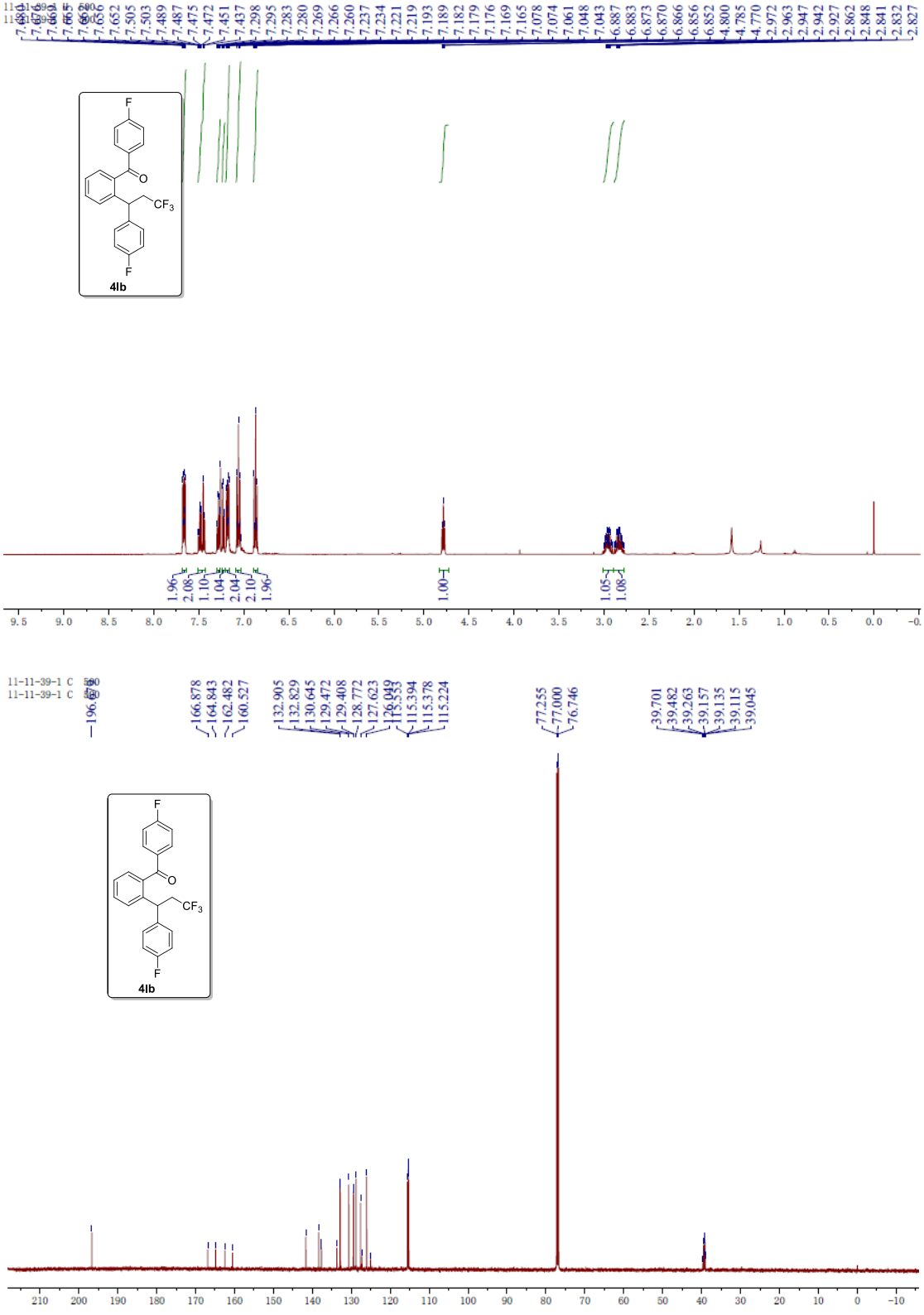

7.661 7.658 7.641 7.639 7.548 7.545 7.528 7.525 7.401 7.398 7.382 7.378 7.358 7.355 7.335 7.332 7.316 7.313 7.297 7.294 7.245 7.226 7.106 5.463 5.445 5.426
2.969 2.962 2.953 2.943 2.937 2.927 2.917 2.912 2.901 2.891 2.874 2.866 2.853 2.560
O
CF3
Br
4Gb
1.00 1.01 4.31 1.03 1.10 1.00 2.13 3.09
9.5 9.0 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

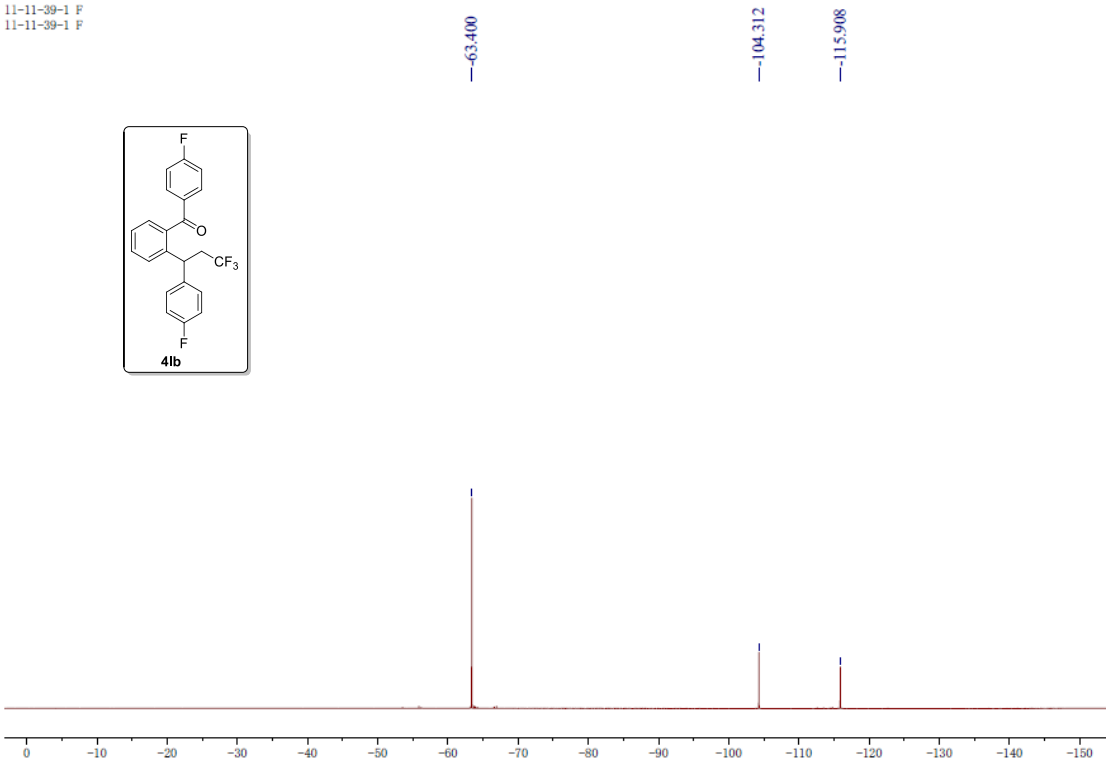

11-10-101-1 C
11-10-101-1 C
202.291
140.407 139.990 138.674 133.509 131.205 129.324 129.030 128.769 128.422 127.296 127.078 126.713 125.384 124.529 121.762
77.317 77.000 76.682
40.024 39.999 39.972 39.944 38.528 38.251 37.972 37.694 29.558
O
CF3
Br
4Gb
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10

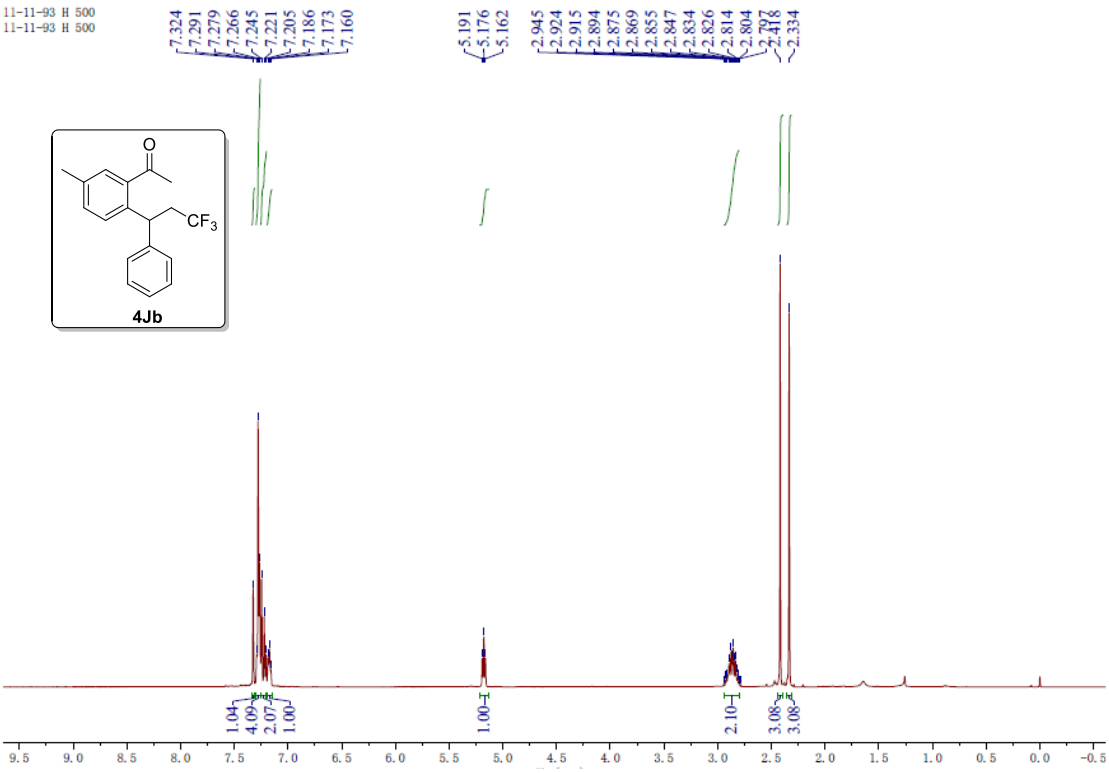

11-10-101-1-1 F
11-10-101-1-1 F
-63.094
4Gb
4Hb
1.92
1.01
1.97
2.09
4.10
2.00
1.03
1.00
2.10

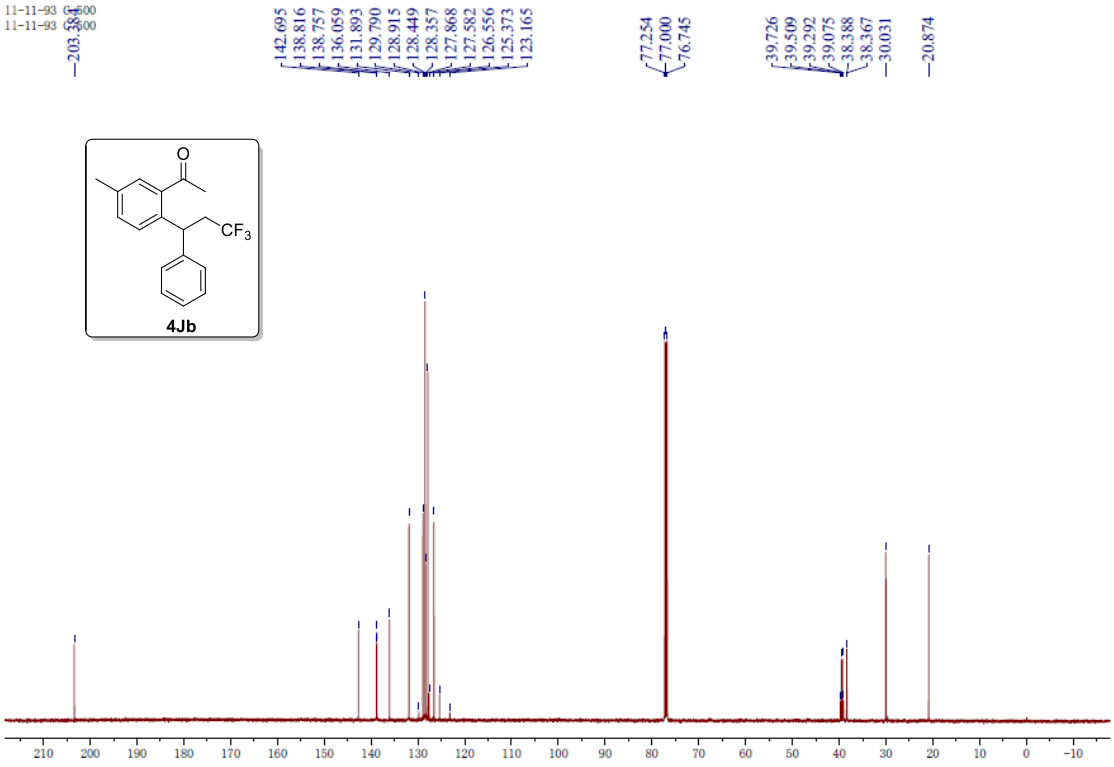

11-11-38-1 C
11-11-38-1 C
198.327
141.965
141.923
138.672
137.518
133.196
130.482
130.224
129.050
128.963
128.466
128.224
127.808
127.774
127.366
126.692
125.806
125.157
122.896
77.254
77.000
76.745
39.798
39.777
39.627
39.410
39.191
38.972
O
Ph
CF3
4Hb
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10

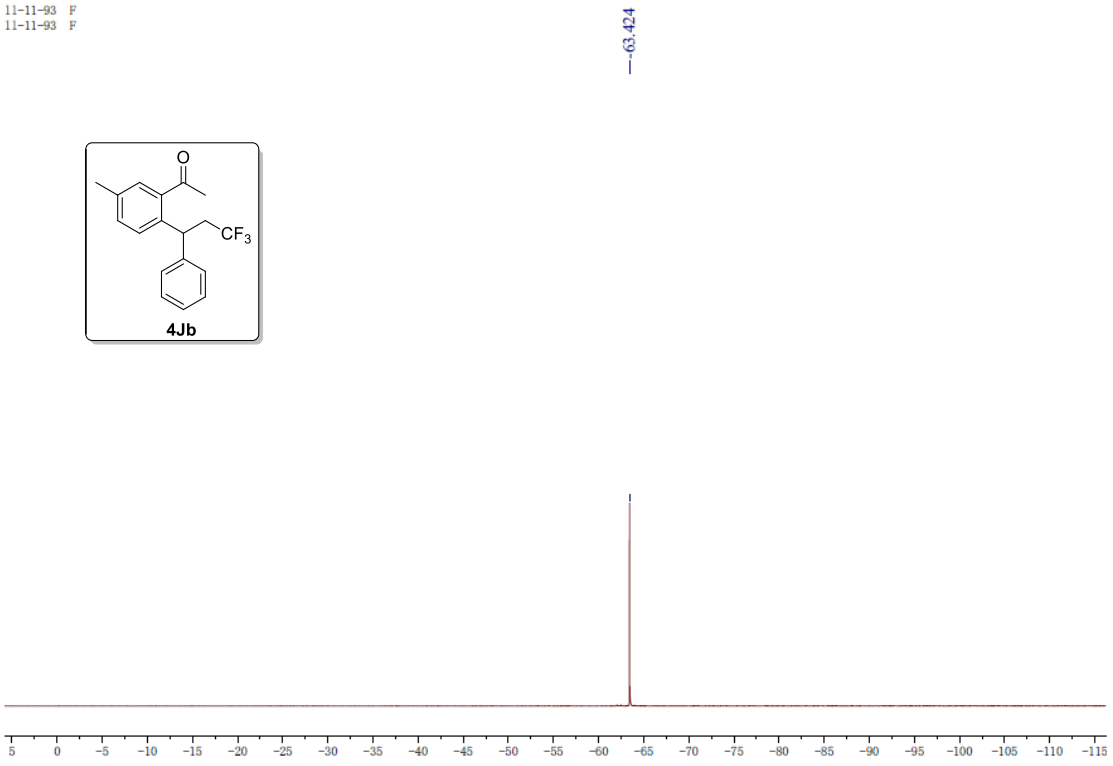

11-11-38-1 F
11-11-38-1 F
-63.408
O
Ph
CF3
4Hb
0
-5
-10
-15
-20
-25
-30
-35
-40
-45
-50
-55
-60
-65
-70
-75
-80
-85
-90
-95
-100
-105
-110


4lb
4lb


11-11-39-1 F
11-11-39-1 F
-63.400
-104.312
-115.908
F
O
CF3
F
4Ib


11-11-93 H 500
11-11-93 H 500
7.324
7.291
7.279
7.266
7.245
7.221
7.205
7.186
7.173
7.160
5.191
5.176
5.162
2.945
2.924
2.915
2.894
2.875
2.869
2.855
2.847
2.834
2.826
2.814
2.804
2.797
2.418
2.334
O
CF3
4Jb
1.04
4.09
2.07
1.00
1.00
2.10
3.08
3.08


11-11-93 C-600
11-11-93 C-600
203.388
142.695
138.816
138.757
136.059
131.893
129.790
128.915
128.449
128.357
127.868
127.582
126.556
125.373
123.165
77.254
77.000
76.745
39.726
39.509
39.292
39.075
38.388
38.367
30.031
20.874
O
CF3
4Jb
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10


11-11-93 F
11-11-93 F
-63.424
O
CF3
4Jb
5
0
-5
-10
-15
-20
-25
-30
-35
-40
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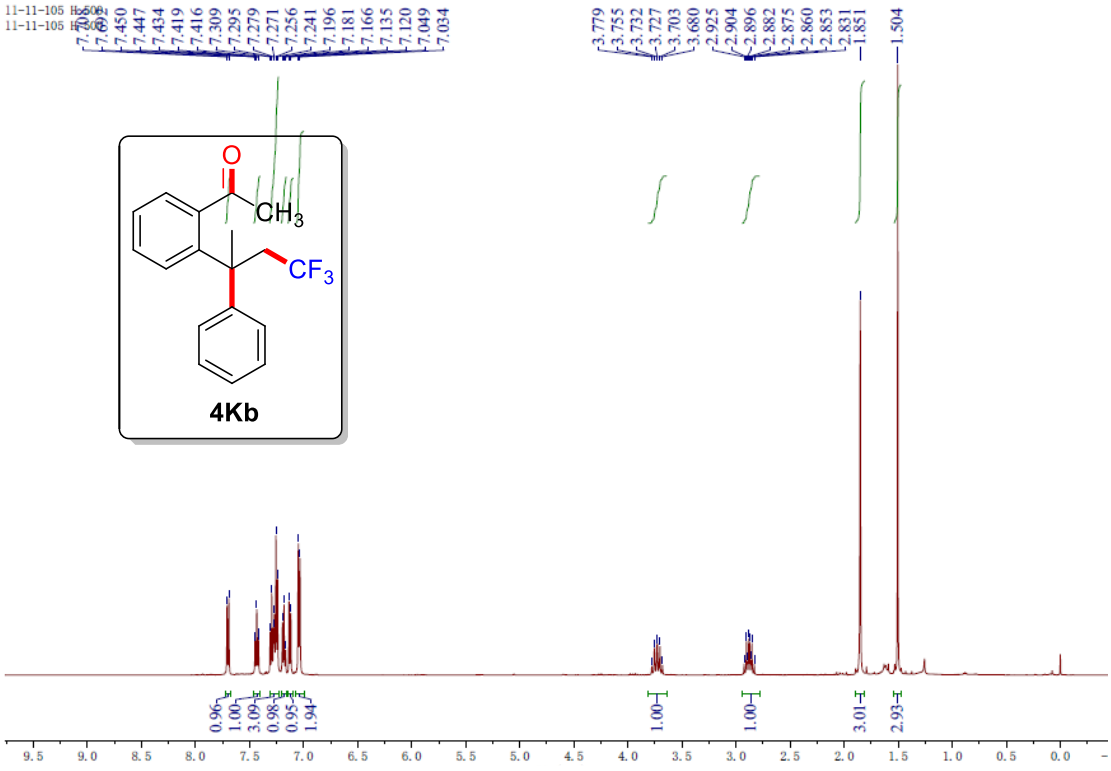
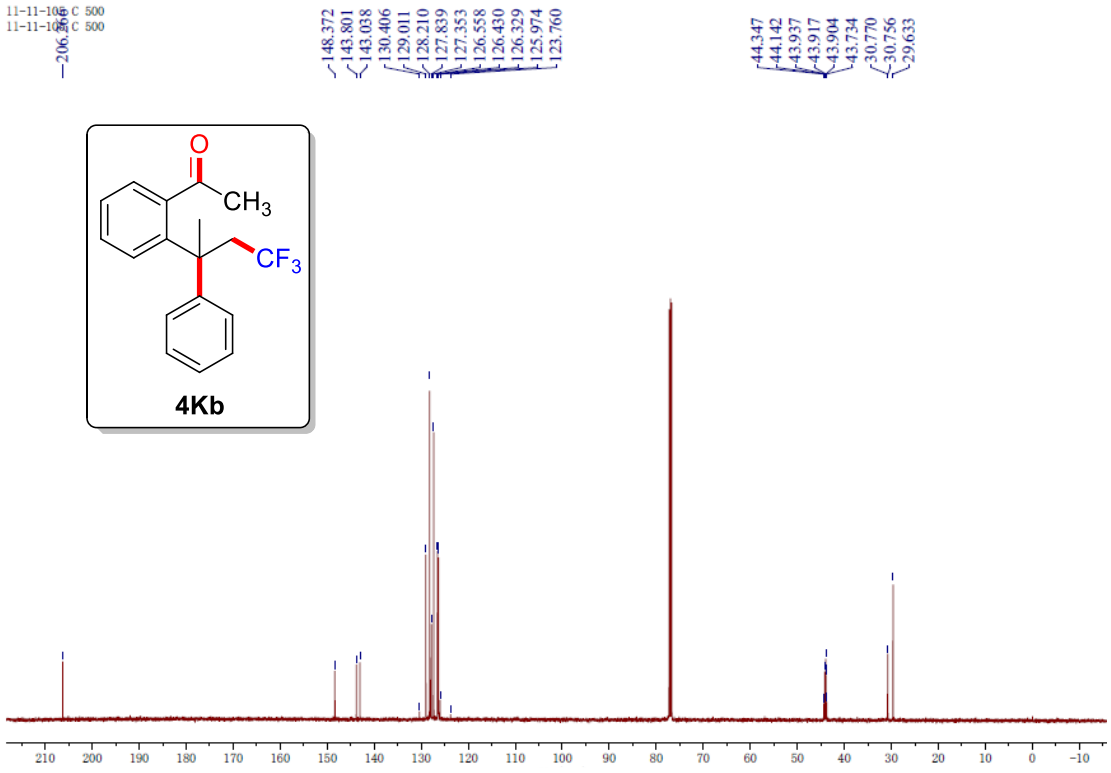
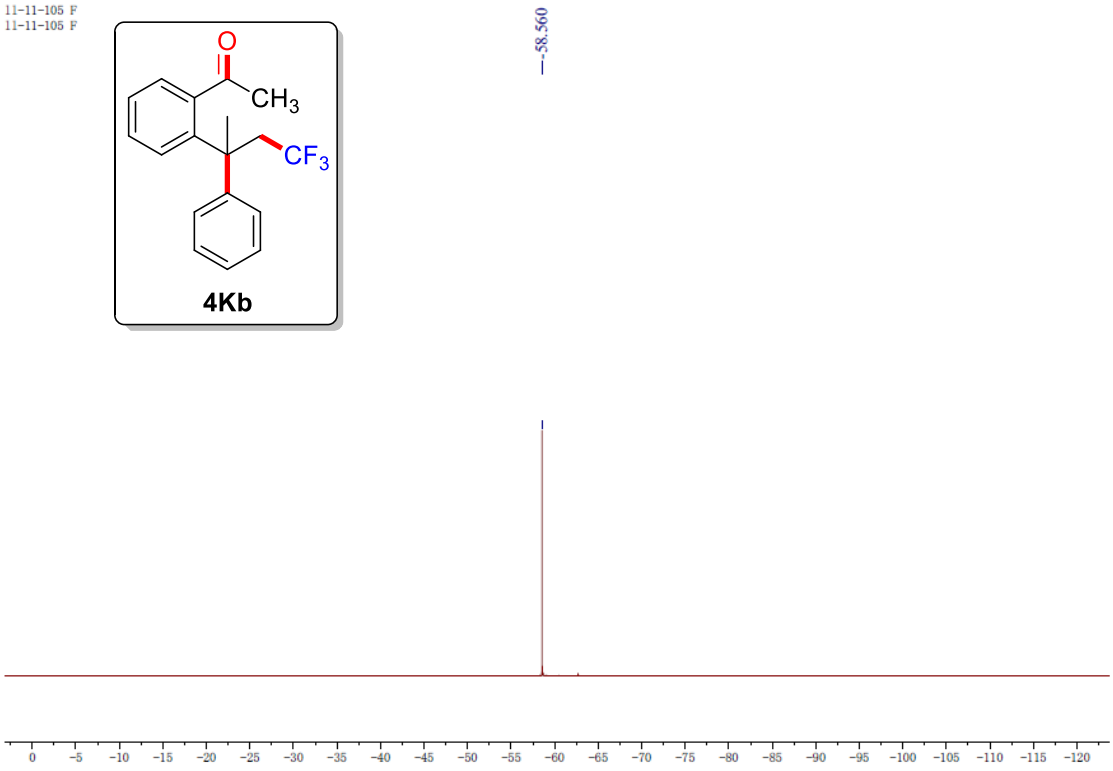
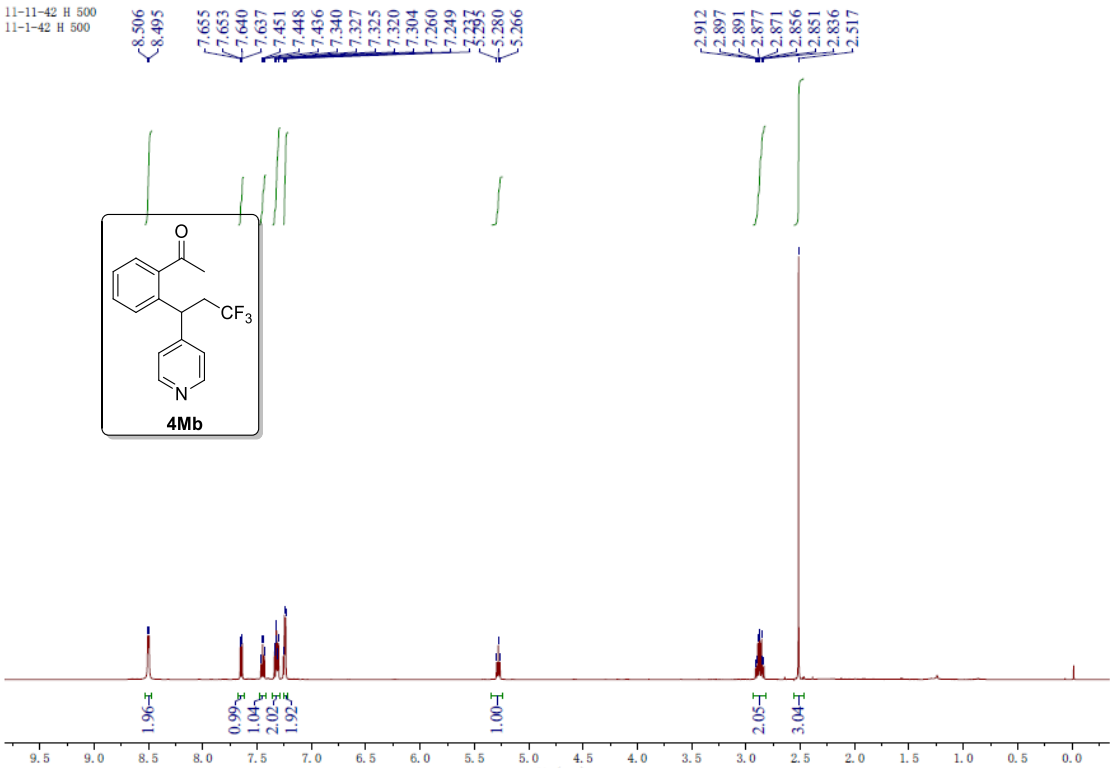
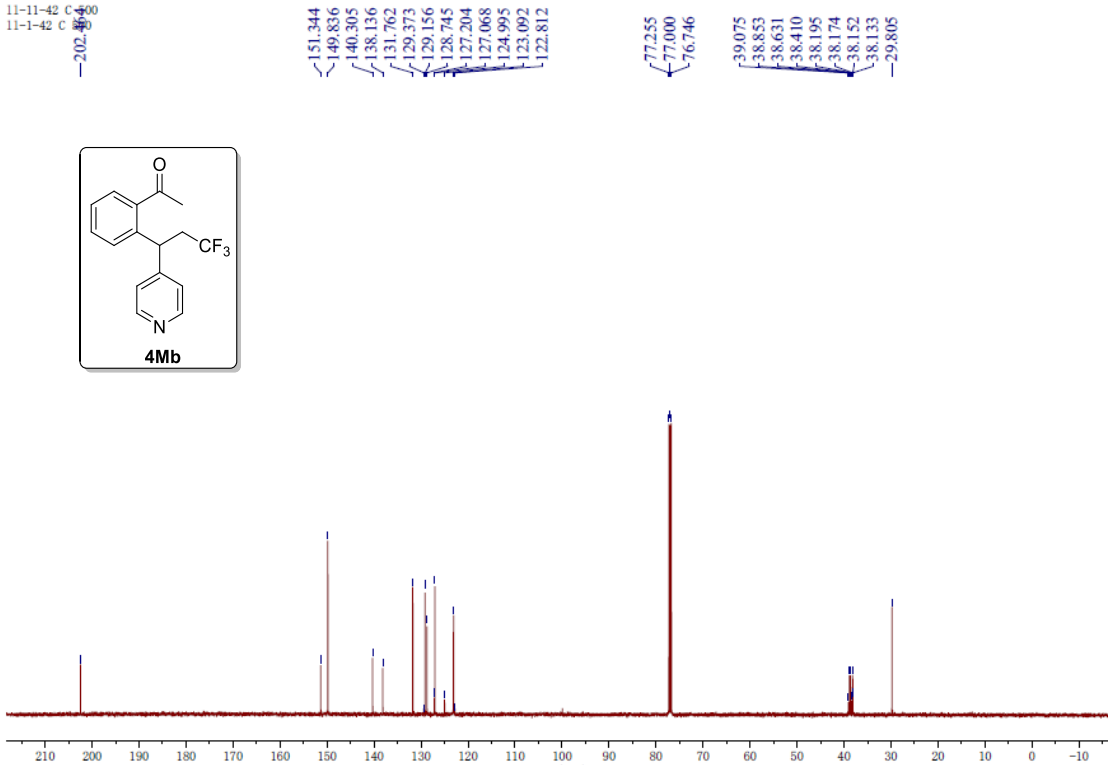
-60
-65
-70
-75
-80
-85
-90
-95
-100
-105
-110
-115

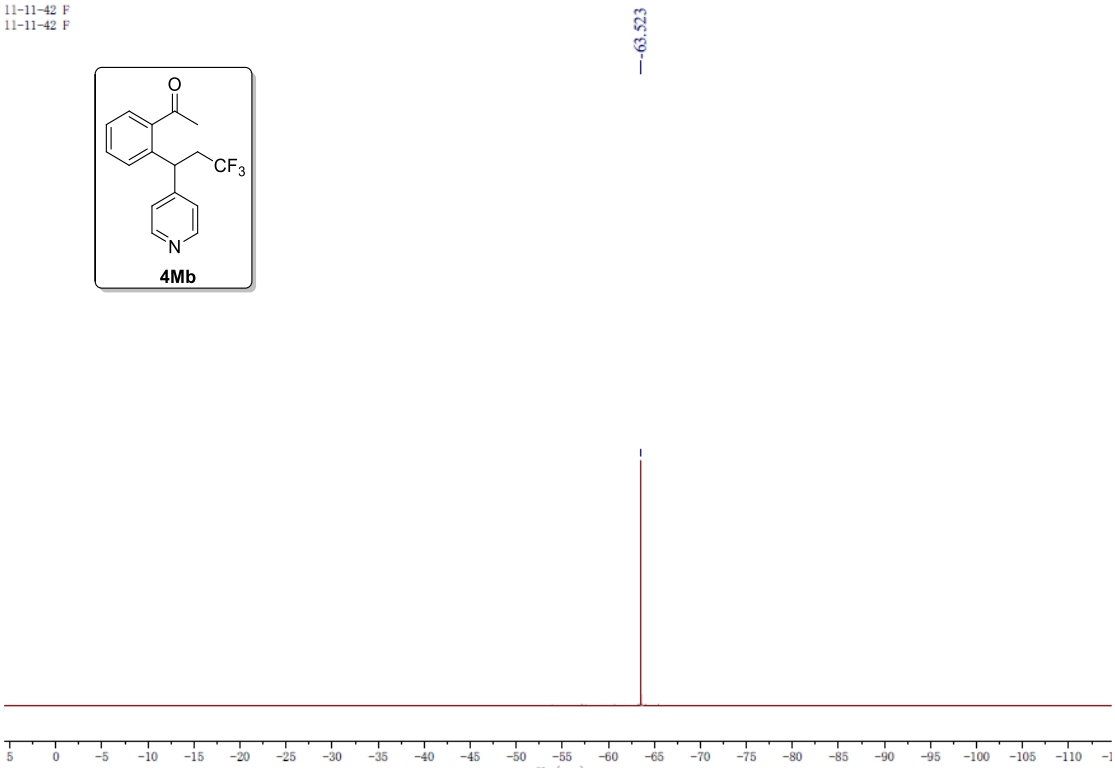

O
CH3
CF3
4Kb


O
CH3
CF3
4Kb


11-11-105 F
11-11-105 F
-58.560
O
CH3
CF3
4Kb
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


11-11-42 H 500
11-1-42 H 500
8.506
8.495
7.655
7.653
7.640
7.637
7.451
7.448
7.436
7.340
7.327
7.325
7.320
7.304
7.260
7.249
5.295
5.280
5.266
2.912
2.897
2.891
2.877
2.871
2.856
2.851
2.836
2.517
O
CF3
N
4Mb
1.96
0.99
1.04
2.02
1.92
1.00
2.05
3.04
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


11-11-42 C
11-1-42 C
202.450
151.344
149.836
140.305
138.136
131.762
129.373
129.156
128.745
127.204
127.068
124.995
123.092
122.812
77.255
77.000
76.746
39.075
38.853
38.631
38.410
38.195
38.174
38.152
38.133
29.805
O
CF3
N
4Mb
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10


11-11-42 F
11-11-42 F
-63.523
O
CF3
N
4Mb
5
0
-5
-10
-15
-20
-25
-30
-35
-40
-45
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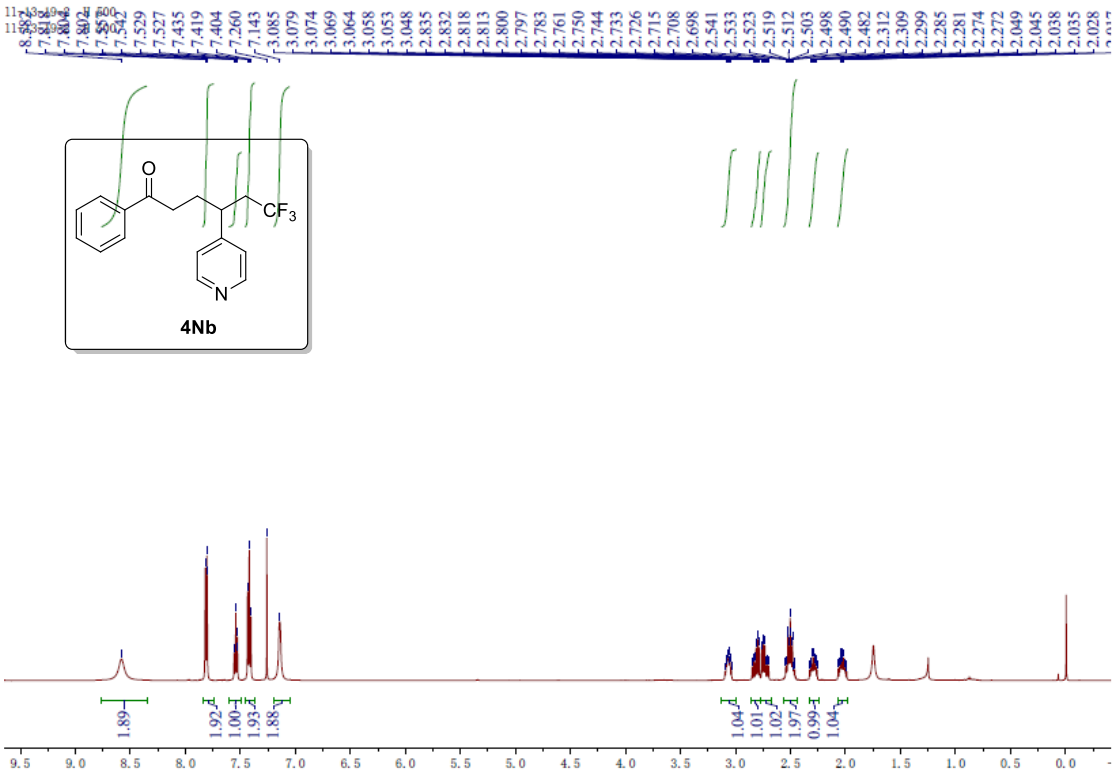
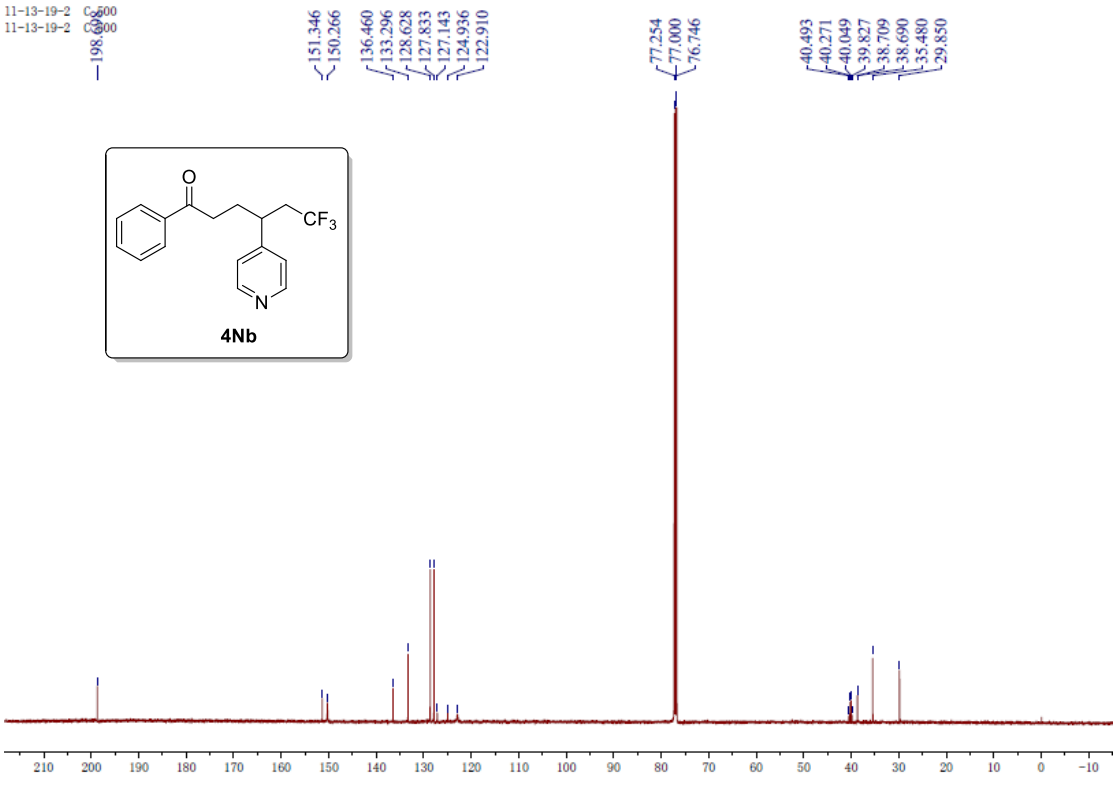
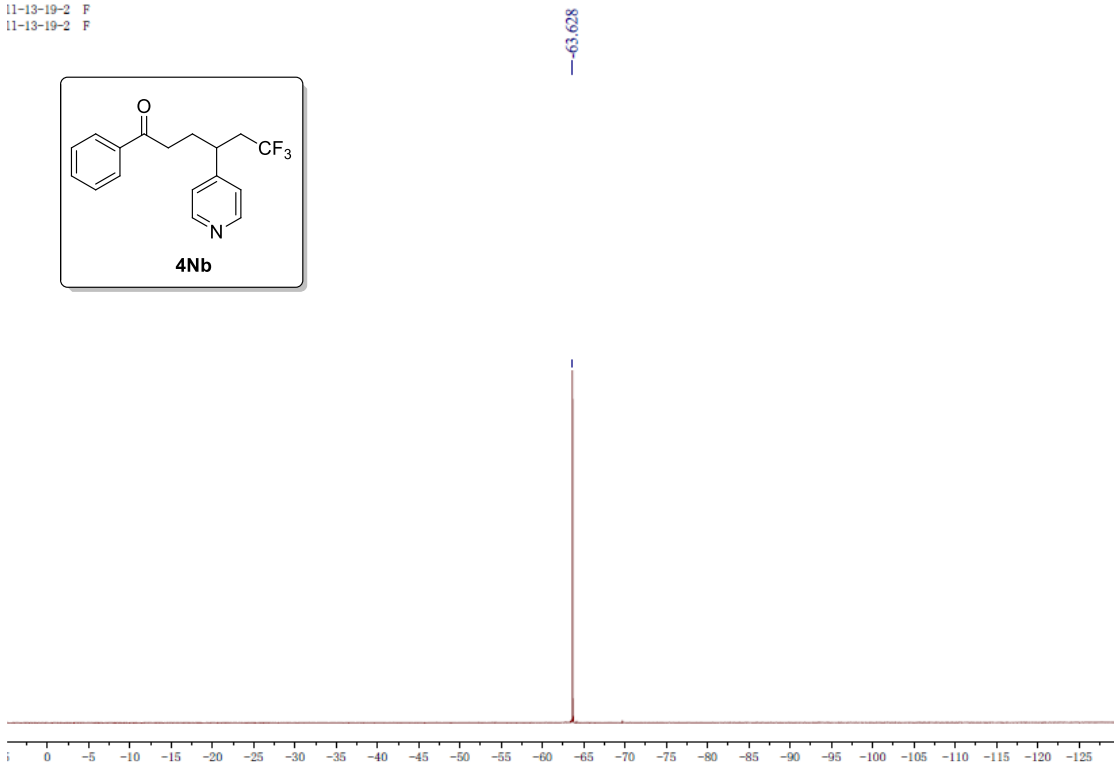
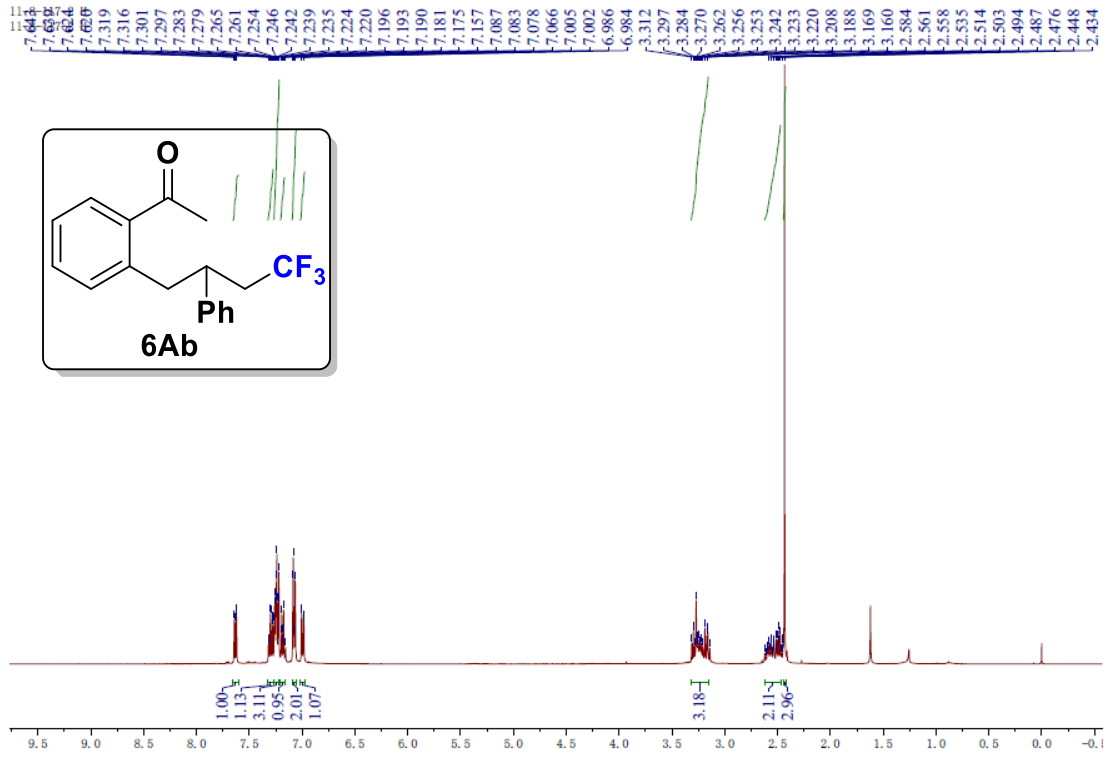
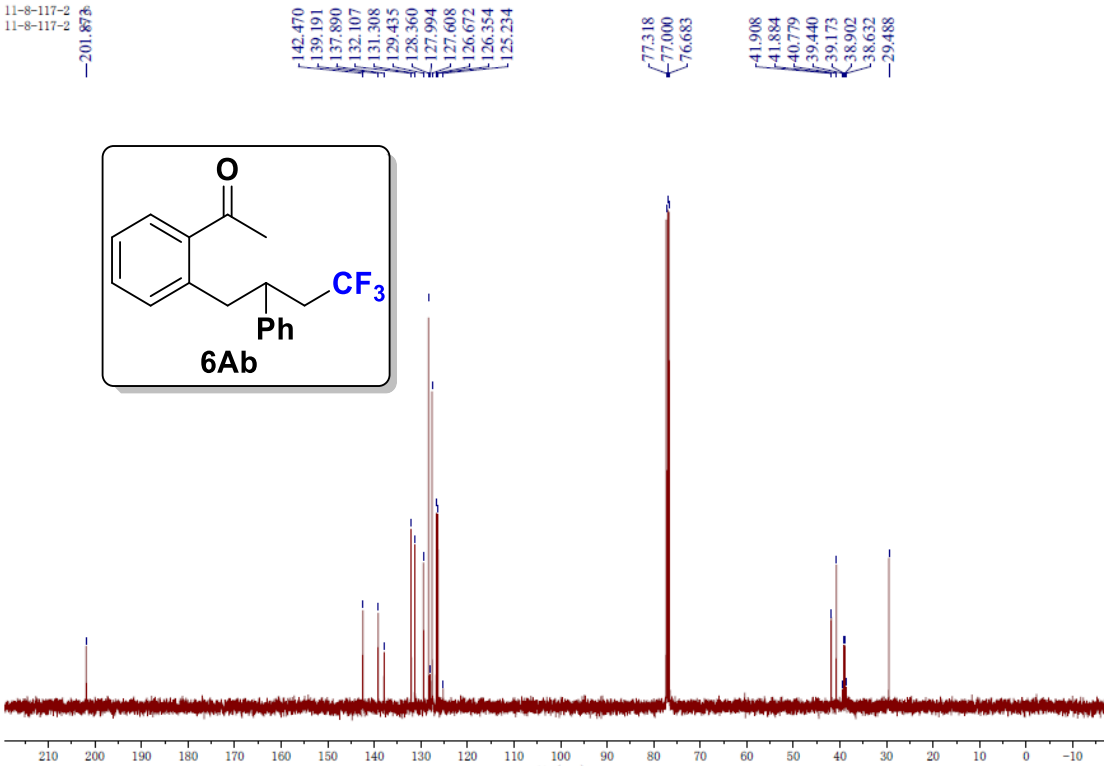
-55
-60
-65
-70
-75
-80
-85
-90
-95
-100
-105
-110

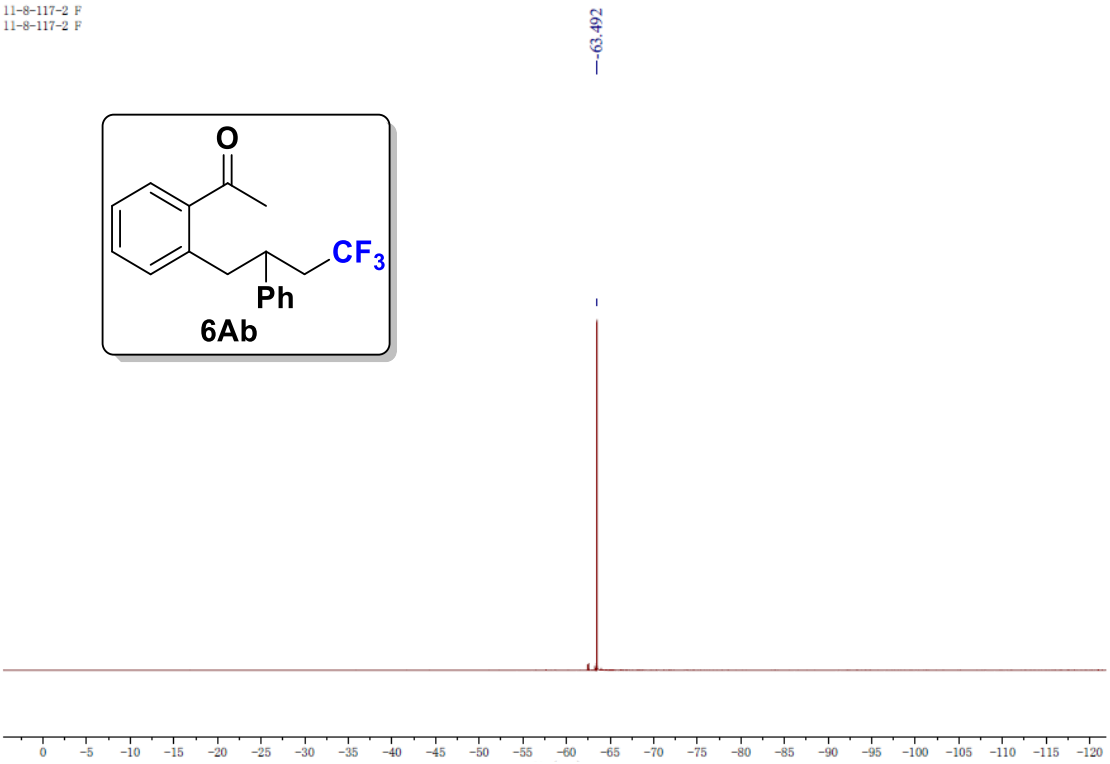

O
CF3
N
4Nb

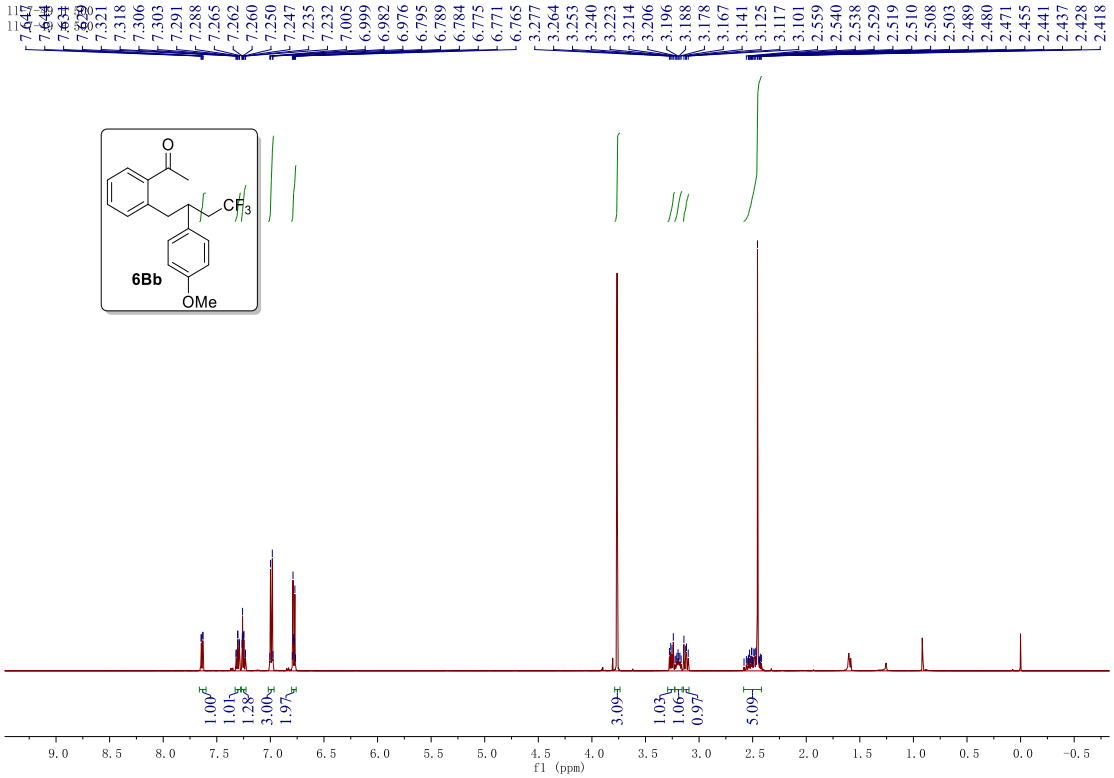

O
CF3
N
4Nb

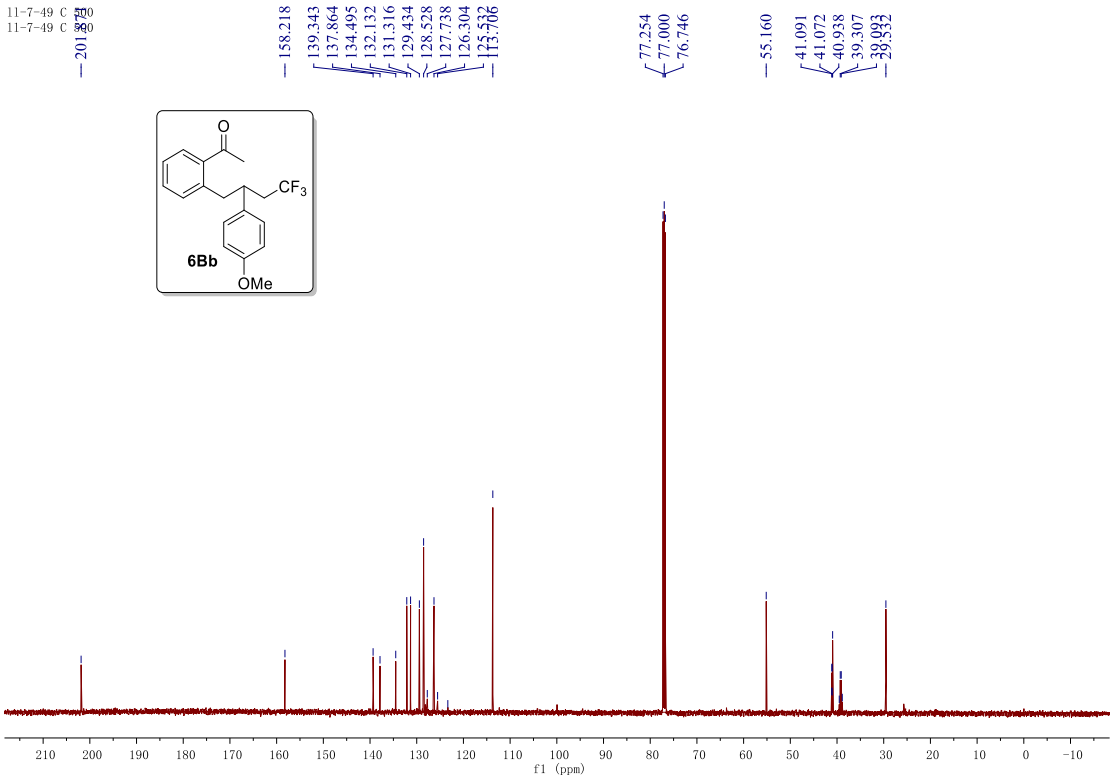

11-13-19-2 F
11-13-19-2 F
-63.628
O
CF3
N
4Nb

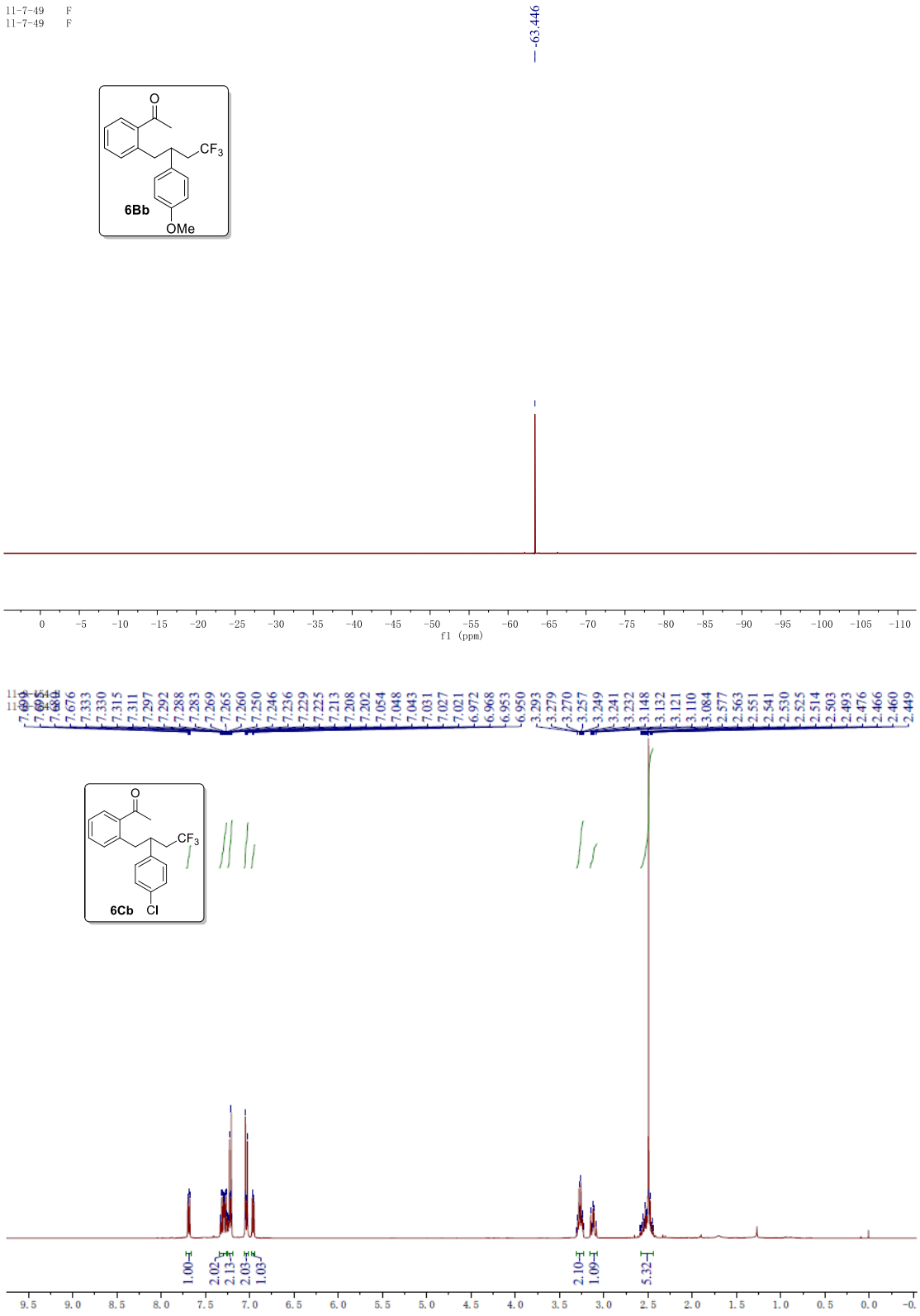

O
CF3
Ph
6Ab

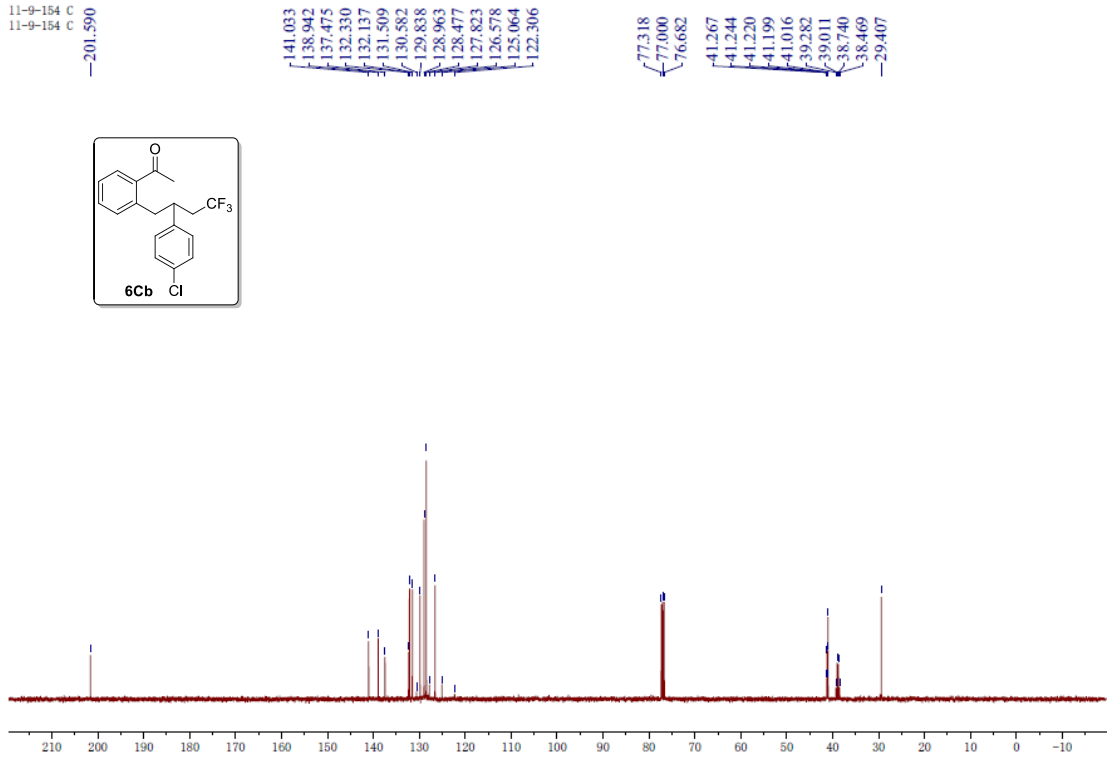

11-8-117-2
11-8-117-2
201.878
142.470
139.191
137.890
132.107
131.308
129.435
128.360
127.994
127.608
126.672
126.354
125.234
77.318
77.000
76.683
41.908
41.884
40.779
39.440
39.173
38.902
38.632
29.488
O
CF3
Ph
6Ab
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10

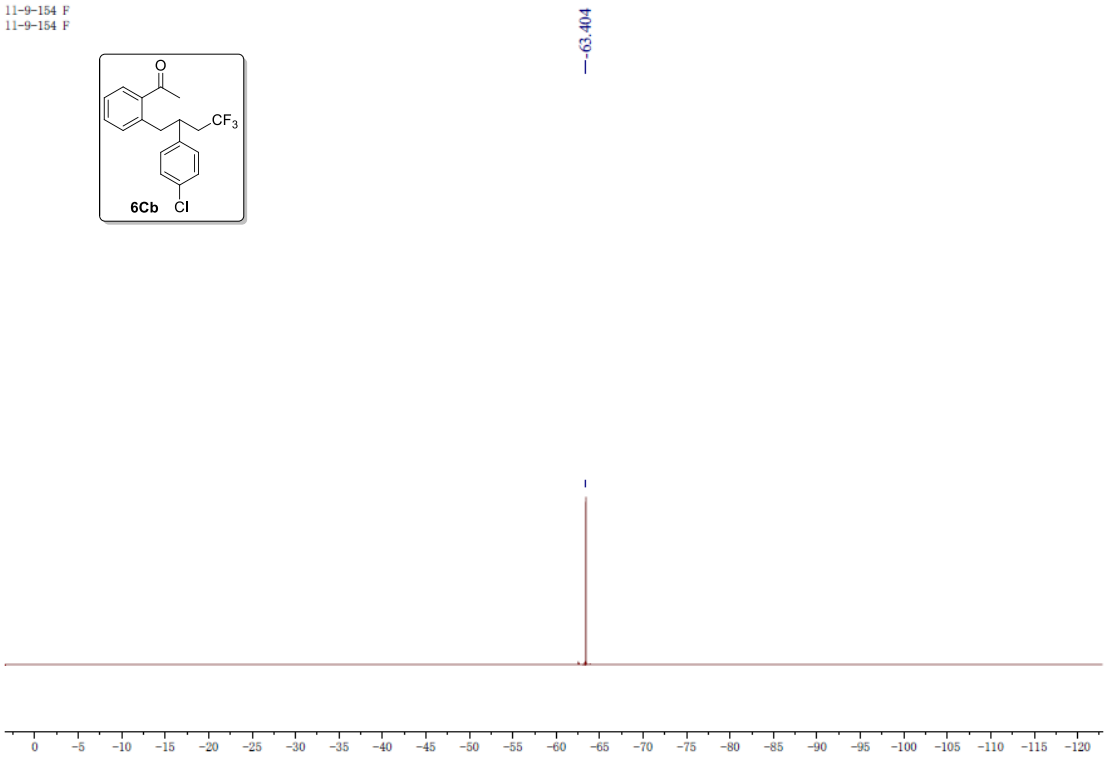

11-8-117-2 F
11-8-117-2 F
-63.492
O
CF3
Ph
6Ab
0 -5 -10 -15 -20 -25 -30 -35 -40 -45 -50 -55 -60 -65 -70 -75 -80 -85 -90 -95 -100 -105 -110 -115 -120

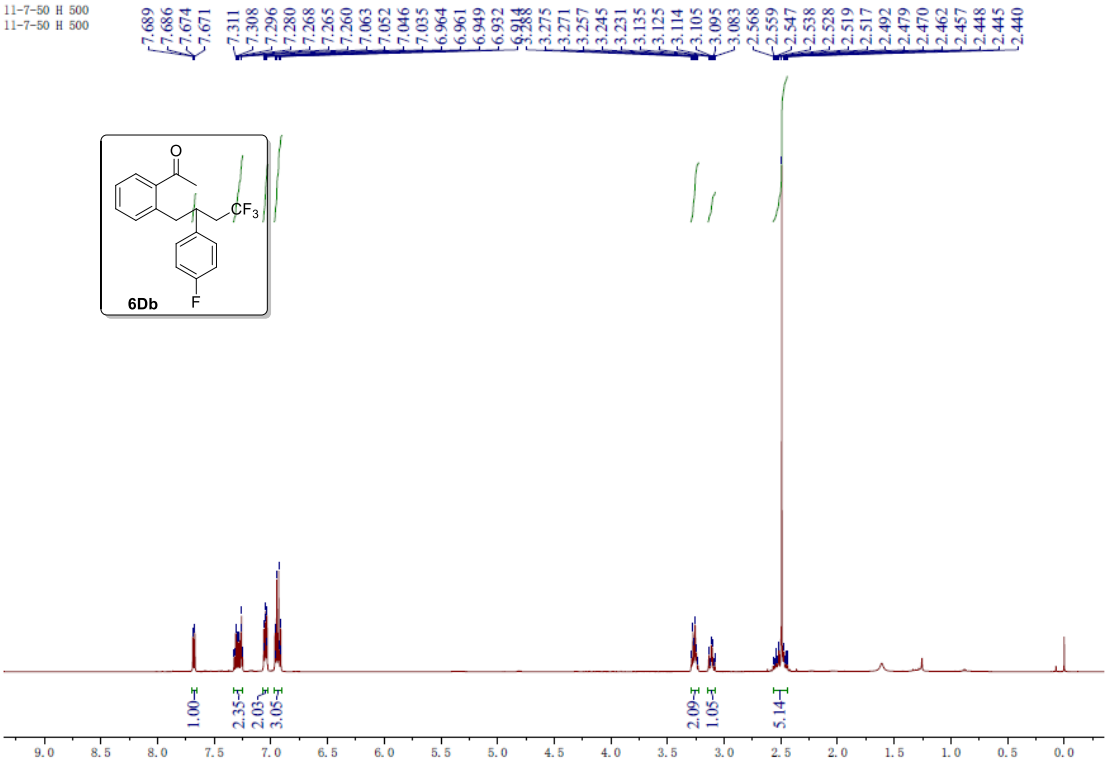

O
CF3
6Bb
OMe
1.00
1.01
1.28
3.00
1.97
3.09
1.03
1.06
0.97
5.09
f1 (ppm)

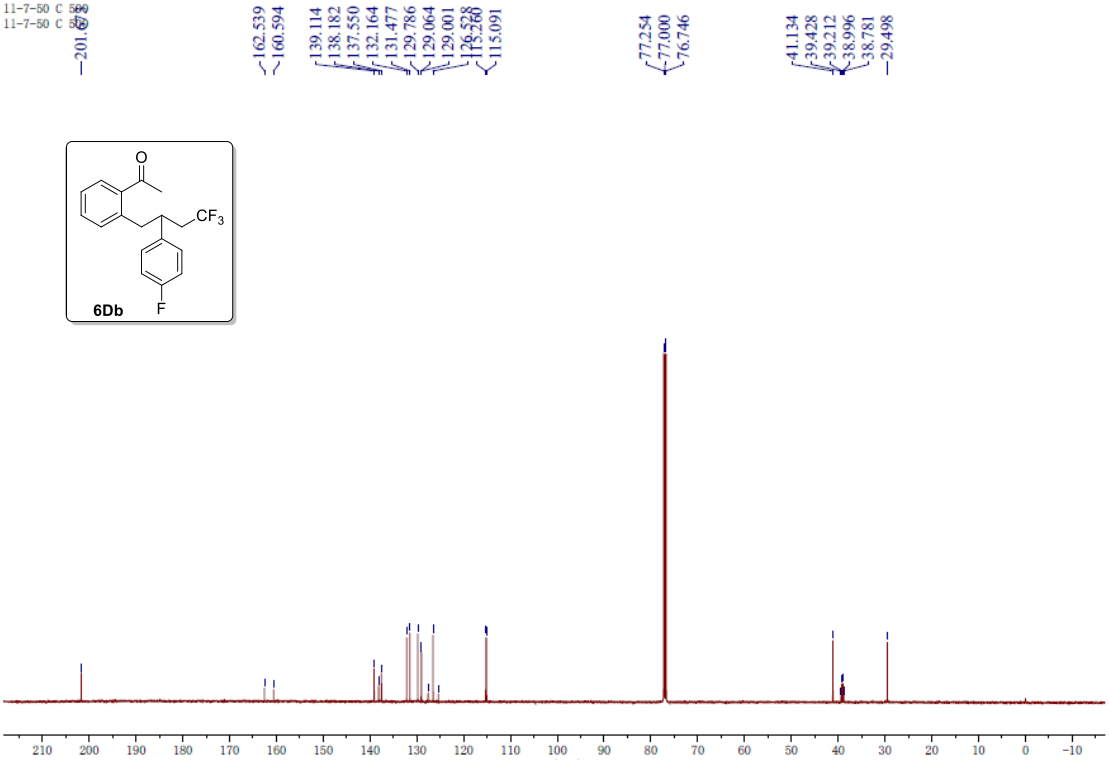

158.218
139.343
137.864
134.495
132.132
131.316
129.434
128.528
127.738
126.304
77.254
77.000
76.746
55.160
41.091
41.072
40.938
39.307
29.332
O
CF3
6Bb
OMe
f1 (ppm)

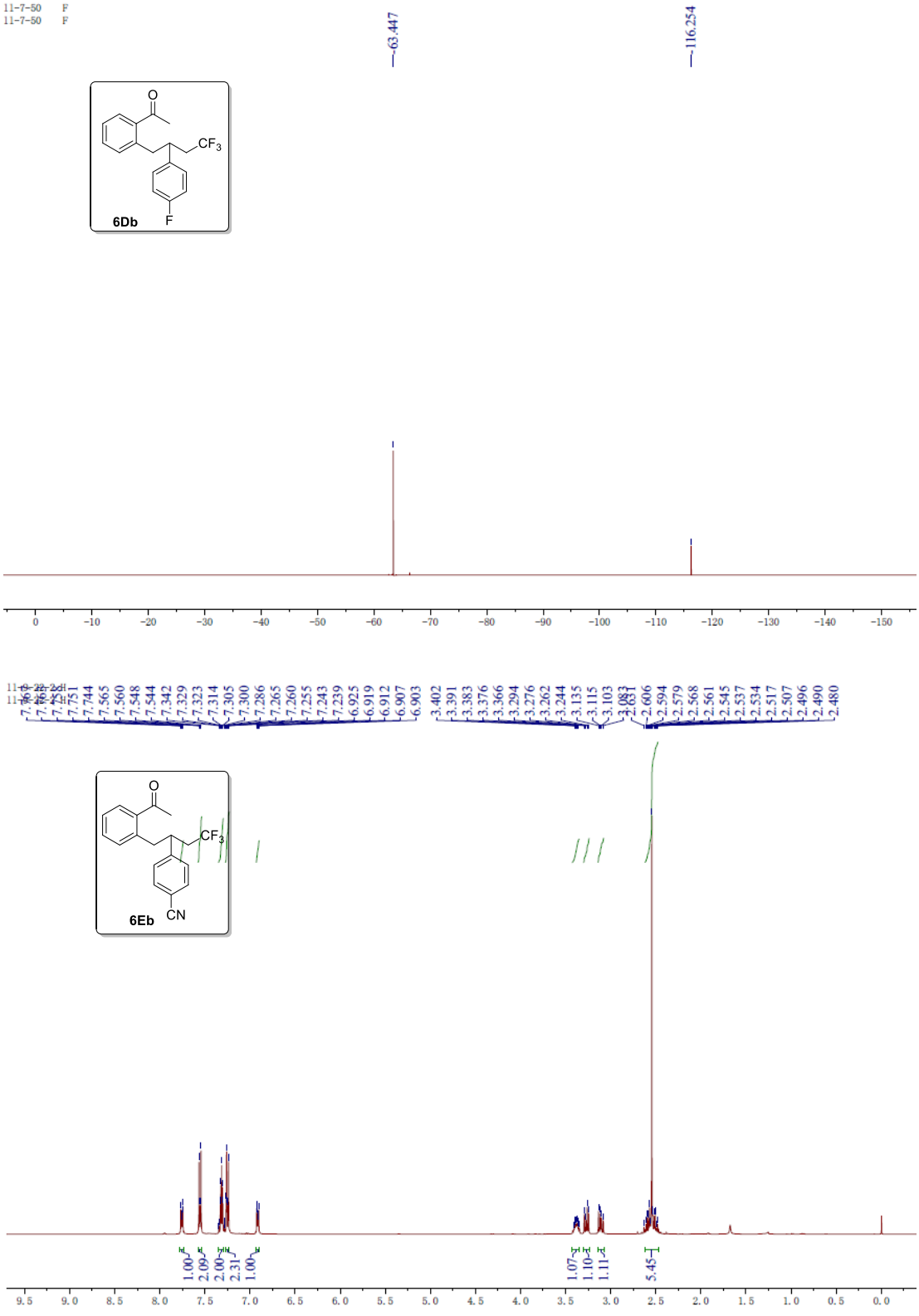

11-7-49 F
11-7-49 F
-63.446
O
CF3
6Bb
OMe
f1 (ppm)
O
CF3
6Cb
Cl


11-9-154 C
11-9-154 C
201.590
141.033
138.942
137.475
132.330
132.137
131.509
130.582
129.838
128.963
128.477
127.823
126.578
125.064
122.306
77.318
77.000
76.682
41.267
41.244
41.220
41.199
41.016
39.282
39.011
38.740
38.469
29.407
O
CF3
6Cb
Cl
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10


11-9-154 F
11-9-154 F
-63.404
O
CF3
6Cb
Cl
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

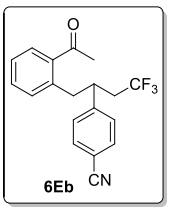

11-7-50 H 500
11-7-50 H 500
7.689
7.686
7.674
7.671
7.311
7.308
7.296
7.280
7.268
7.265
7.260
7.063
7.052
7.046
7.035
6.964
6.961
6.949
6.932
3.275
3.271
3.257
3.245
3.231
3.135
3.125
3.114
3.105
3.095
3.083
2.568
2.559
2.547
2.538
2.528
2.519
2.517
2.492
2.479
2.470
2.462
2.457
2.448
2.445
2.440
O
CF3
F
6Db
1.00
2.35
2.03
3.05
2.09
1.05
5.14
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


11-7-50 C 500
11-7-50 C 500
201.678
162.539
160.594
139.114
138.182
137.550
132.164
131.477
129.786
129.064
129.001
126.528
115.260
115.091
77.254
77.000
76.746
41.134
39.428
39.212
38.996
38.781
29.498
O
CF3
F
6Db
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10

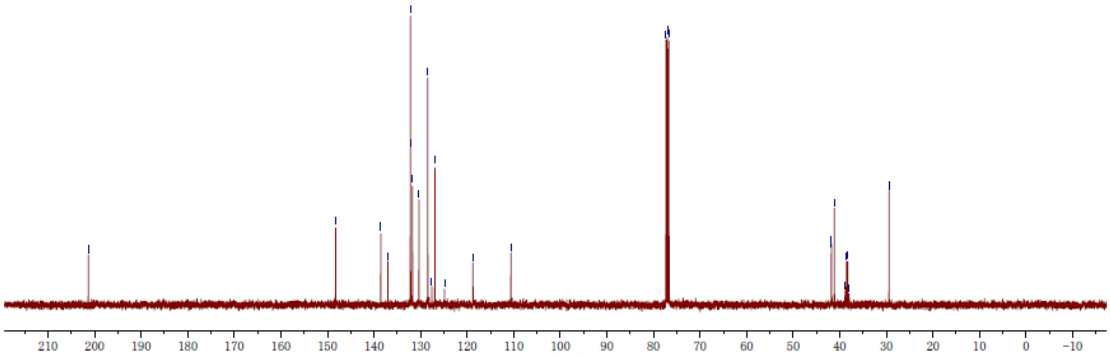

11-7-50 F
11-7-50 F
63.447
116.254
O
CF3
F
6Db
7.767
7.751
7.744
7.565
7.560
7.548
7.544
7.342
7.329
7.323
7.314
7.305
7.300
7.286
7.265
7.260
7.255
7.243
7.239
6.925
6.919
6.912
6.907
6.903
3.402
3.391
3.383
3.376
3.366
3.294
3.276
3.262
3.244
3.135
3.115
3.103
2.606
2.594
2.579
2.568
2.561
2.545
2.537
2.534
2.517
2.507
2.496
2.490
2.480
O
CF3
CN
6Eb
1.00
2.09
2.00
2.31
1.00
1.07
1.10
1.11
5.45

11-9-22-2 C
11-9-22-2 C

201.340
148.249
138.556
137.034
132.197
132.163
131.742
130.343
128.477
126.926
118.612
77.317
77.000
76.682
41.805
41.781
41.164
38.858
38.583
38.308
38.033
29.418

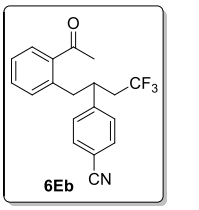


6Eb

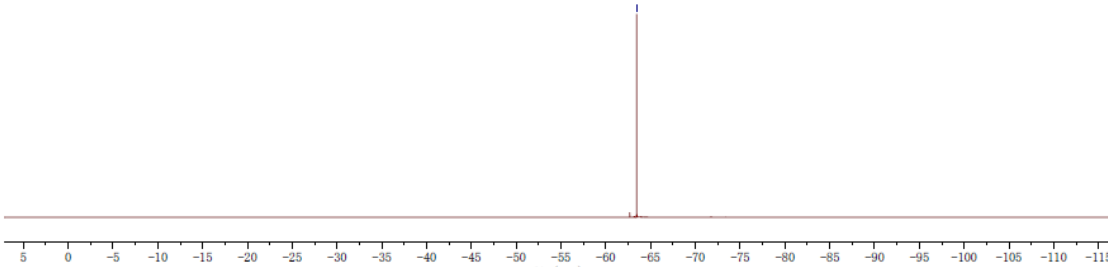


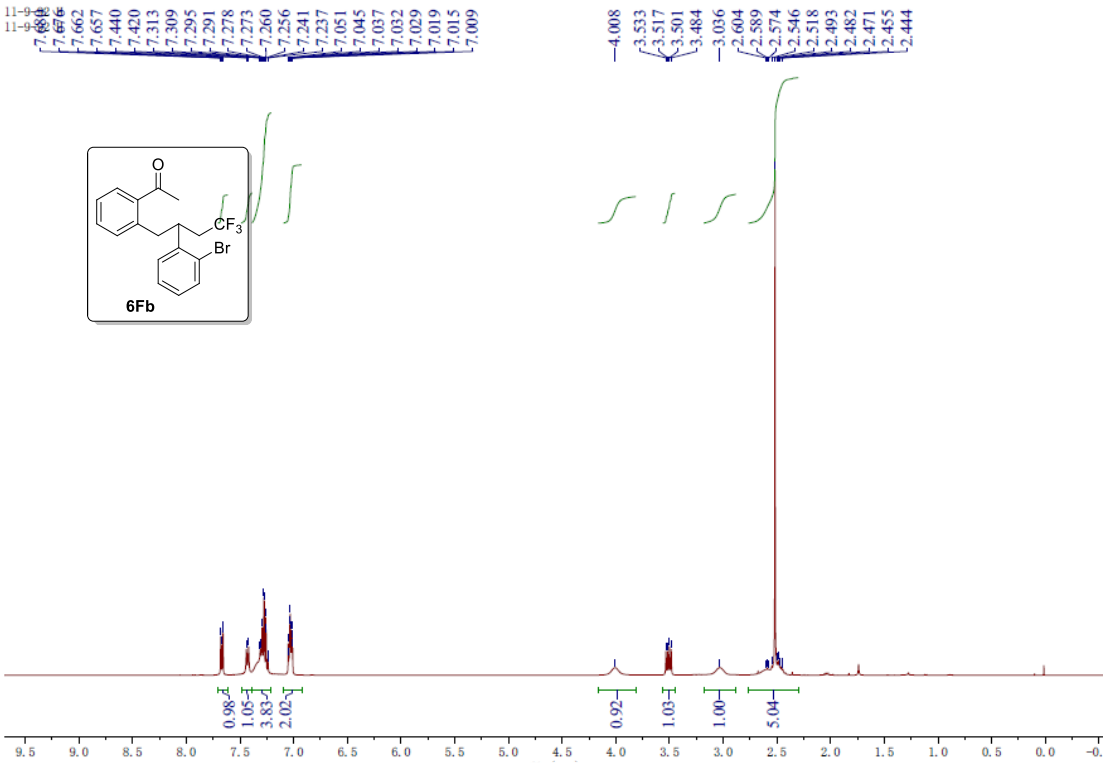
11-9-22-2 F
11-9-22-2 F

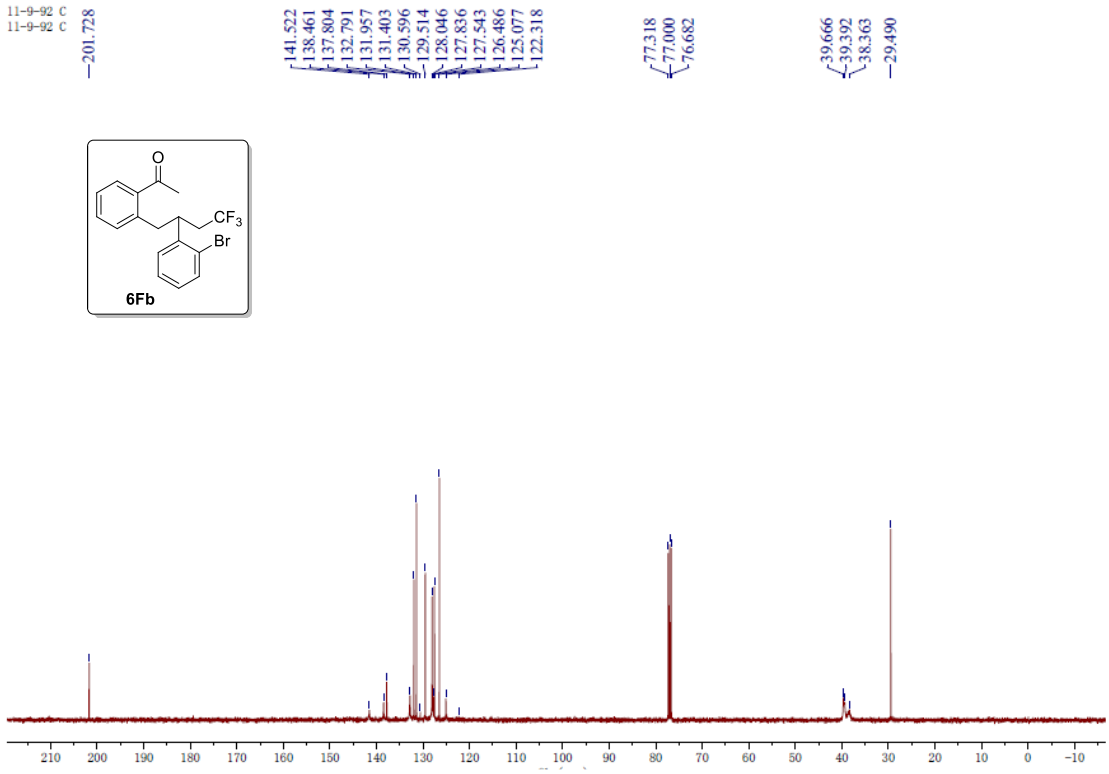
-63.445

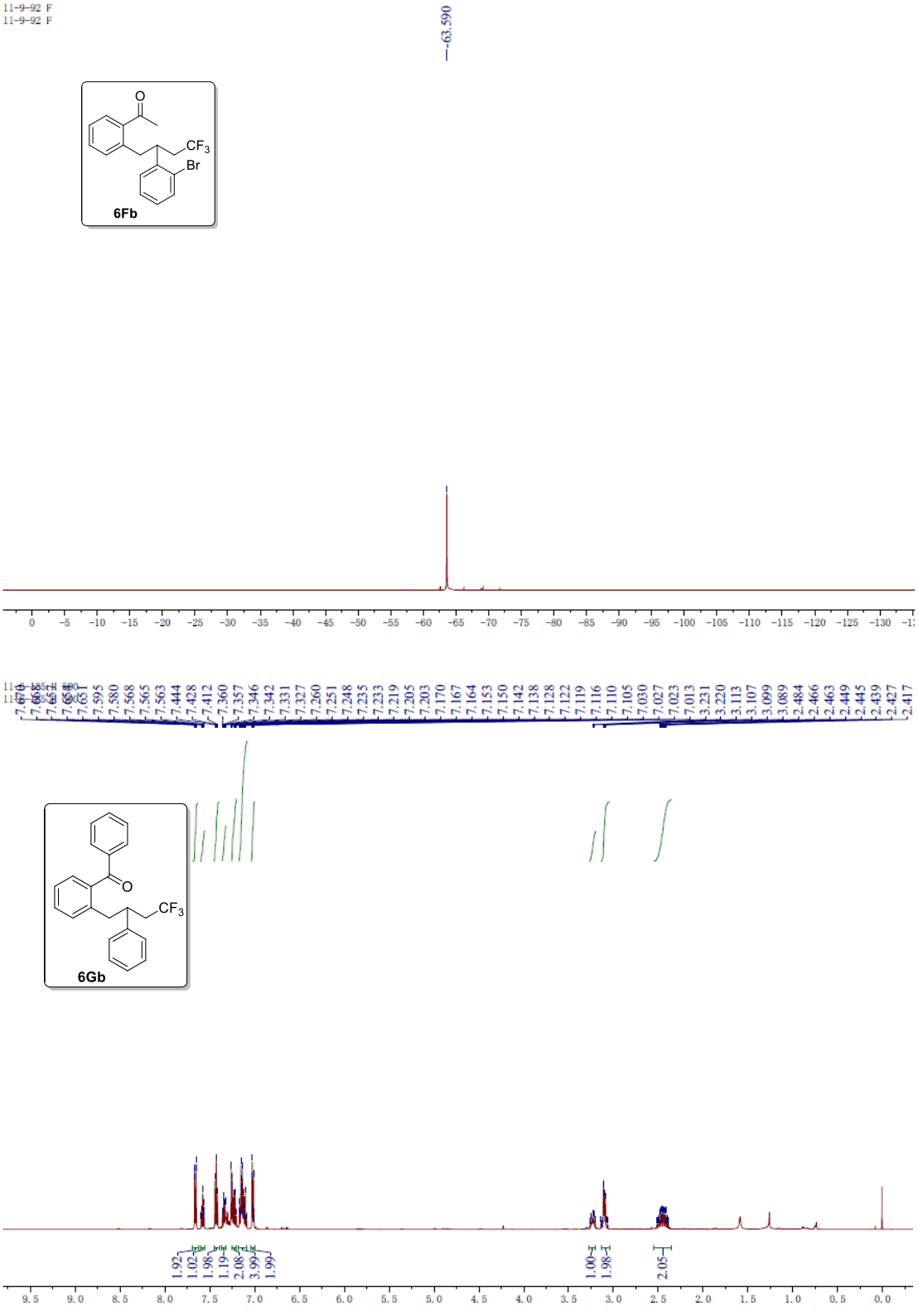


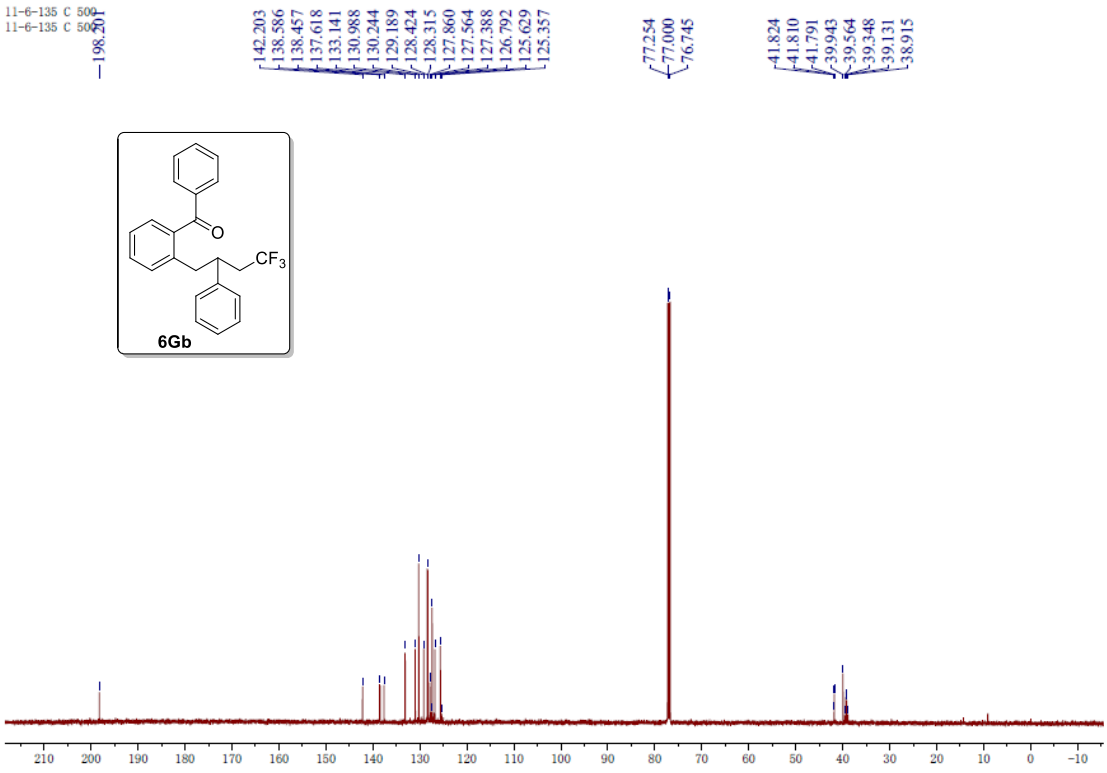
6Eb

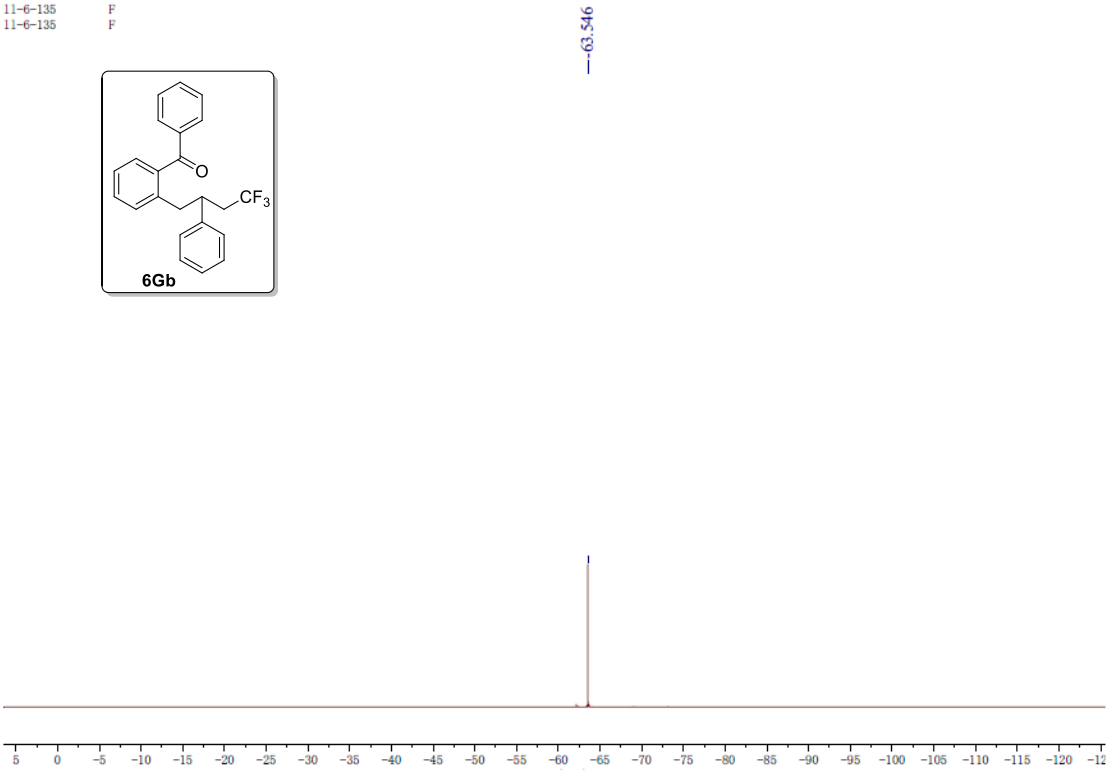


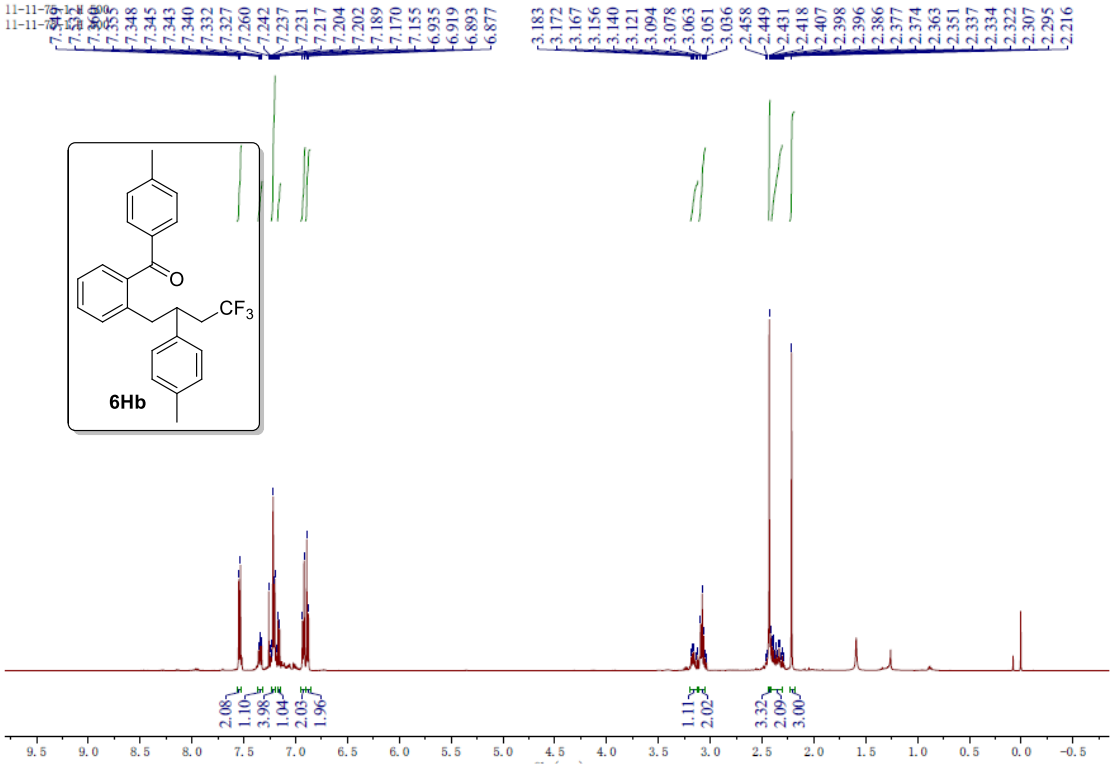

7.662
7.657
7.440
7.420
7.313
7.309
7.295
7.291
7.278
7.273
7.260
7.256
7.241
7.237
7.051
7.045
7.037
7.032
7.029
7.019
7.015
7.009
4.008
3.533
3.517
3.501
3.484
3.036
2.604
2.589
2.574
2.546
2.518
2.493
2.482
2.471
2.455
2.444
O
CF3
Br
6Fb
0.98
1.05
3.83
2.02
0.92
1.03
1.00
5.04

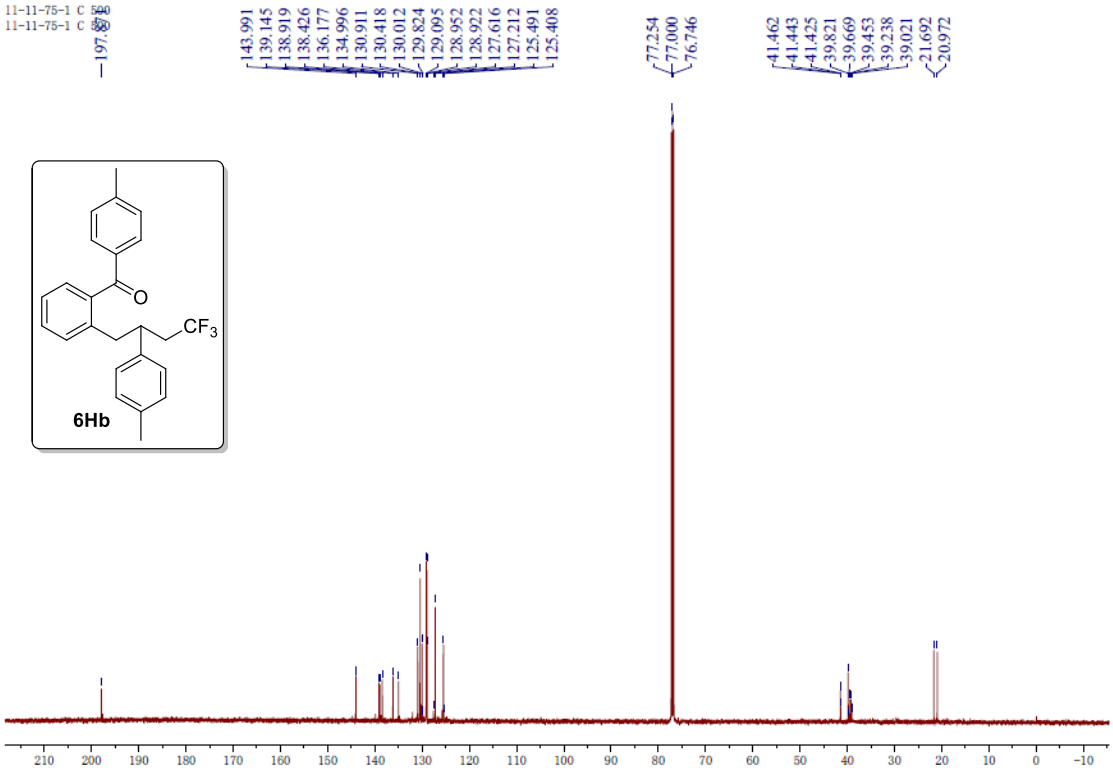

11-9-92 C
11-9-92 C
201.728
141.522
138.461
137.804
132.791
131.957
131.403
130.596
129.514
128.046
127.836
127.543
126.486
125.077
122.318
77.318
77.000
76.682
39.666
39.392
38.363
29.490
O
CF3
Br
6Fb

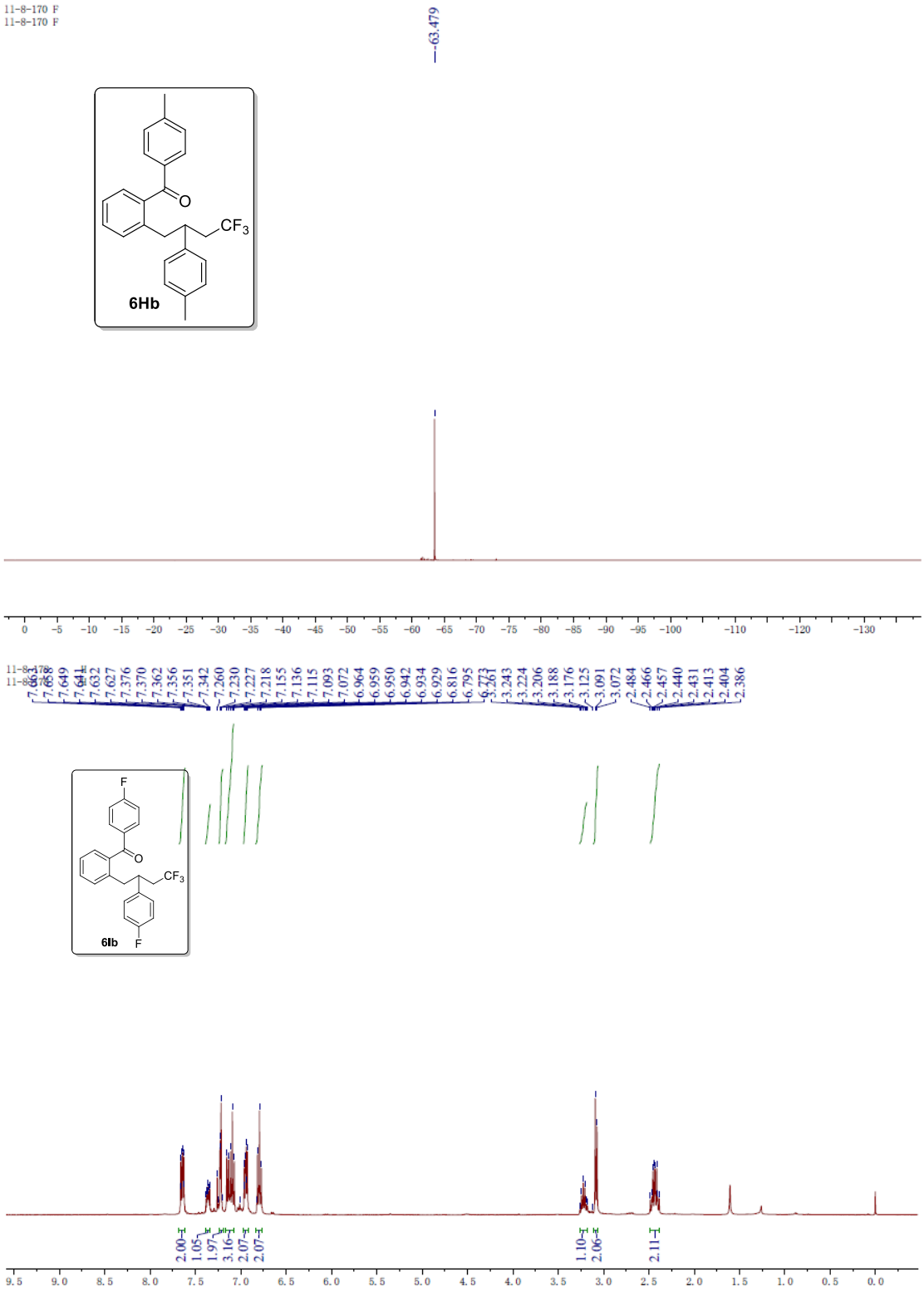

11-9-92 F
11-9-92 F
-63.590
6FB
6GB

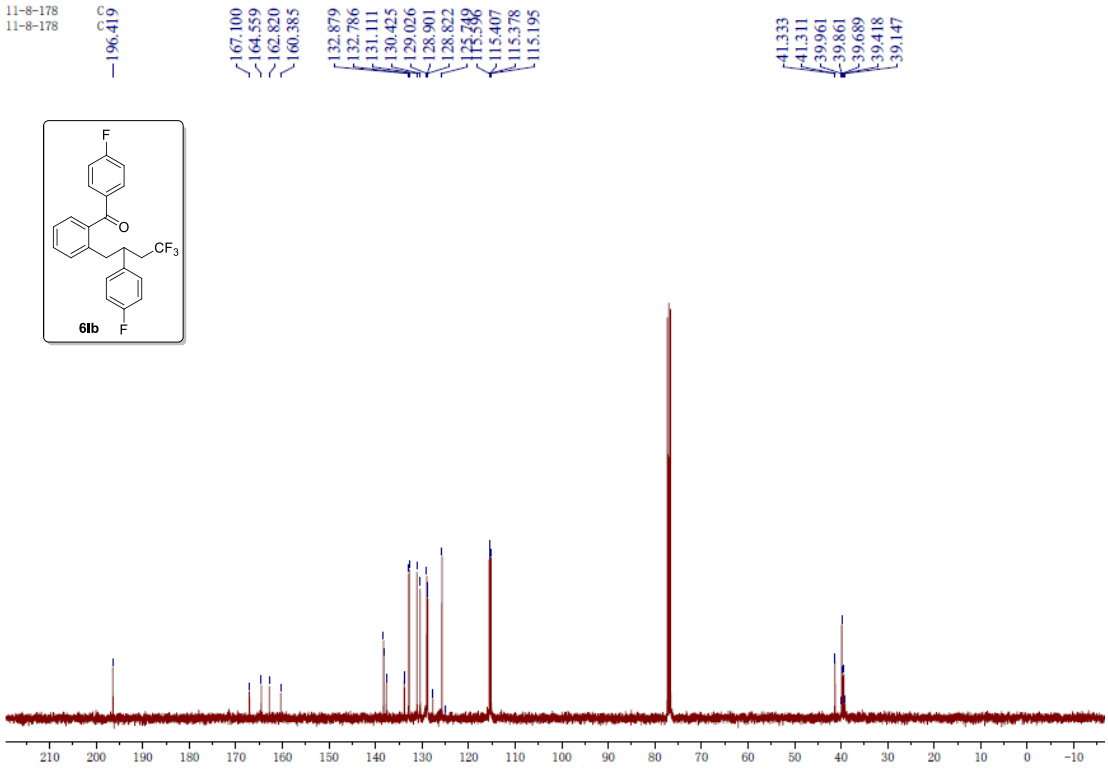

11-6-135 C 500
11-6-135 C 500
198.201
142.203
138.586
138.457
137.618
133.141
130.988
130.244
129.189
128.424
128.315
127.860
127.564
127.388
126.792
125.629
125.357
77.254
77.000
76.745
41.824
41.810
41.791
39.943
39.564
39.348
39.131
38.915
O
CF3
6Gb
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10

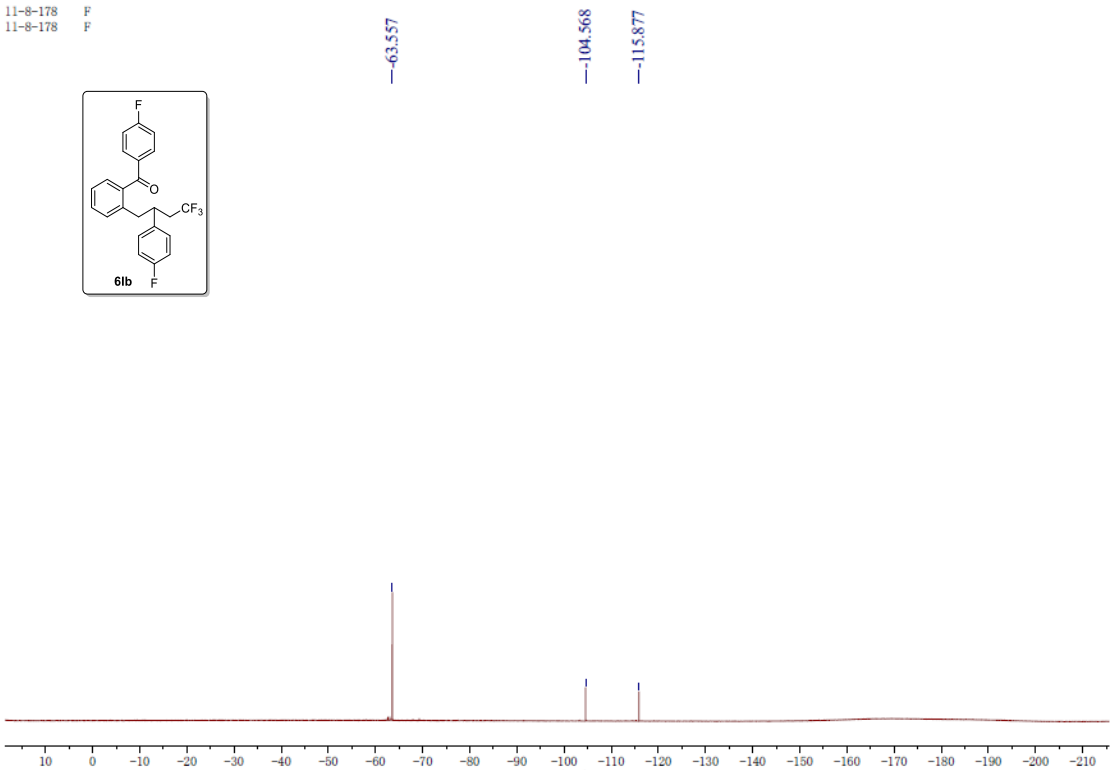

11-6-135 F
11-6-135 F
-63.546
O
CF3
6Gb
5 0 -5 -10 -15 -20 -25 -30 -35 -40 -45 -50 -55 -60 -65 -70 -75 -80 -85 -90 -95 -100 -105 -110 -115 -120 -12

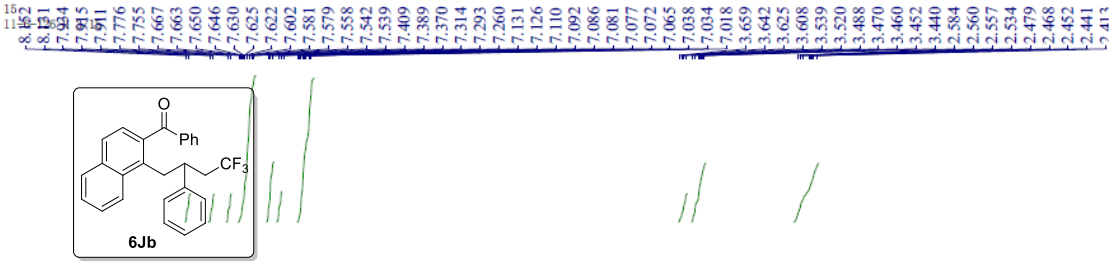

6Hb
O
CF3

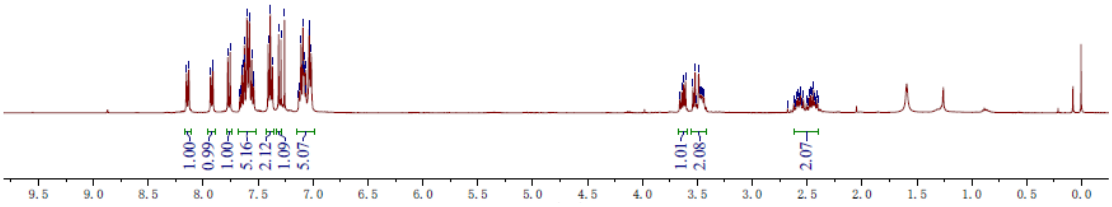

6Hb
O
CF3

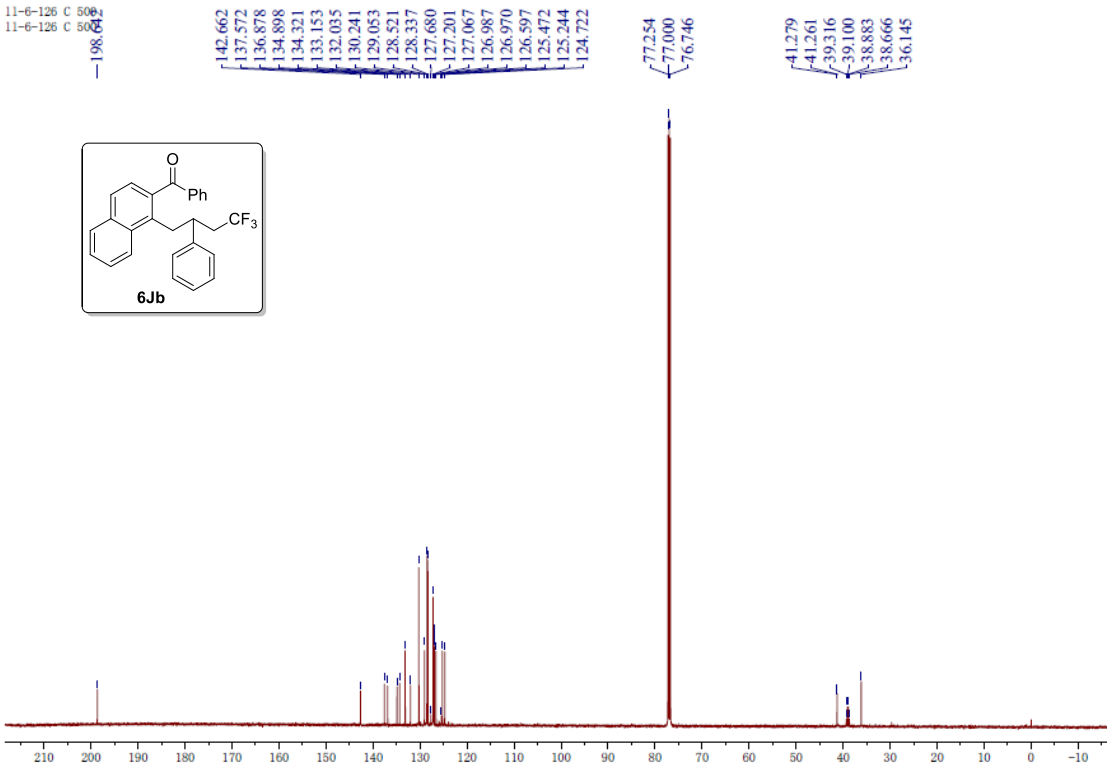

11-8-170 F
11-8-170 F
-63.479
O
CF3
6Hb
F
O
CF3
6Ib
F

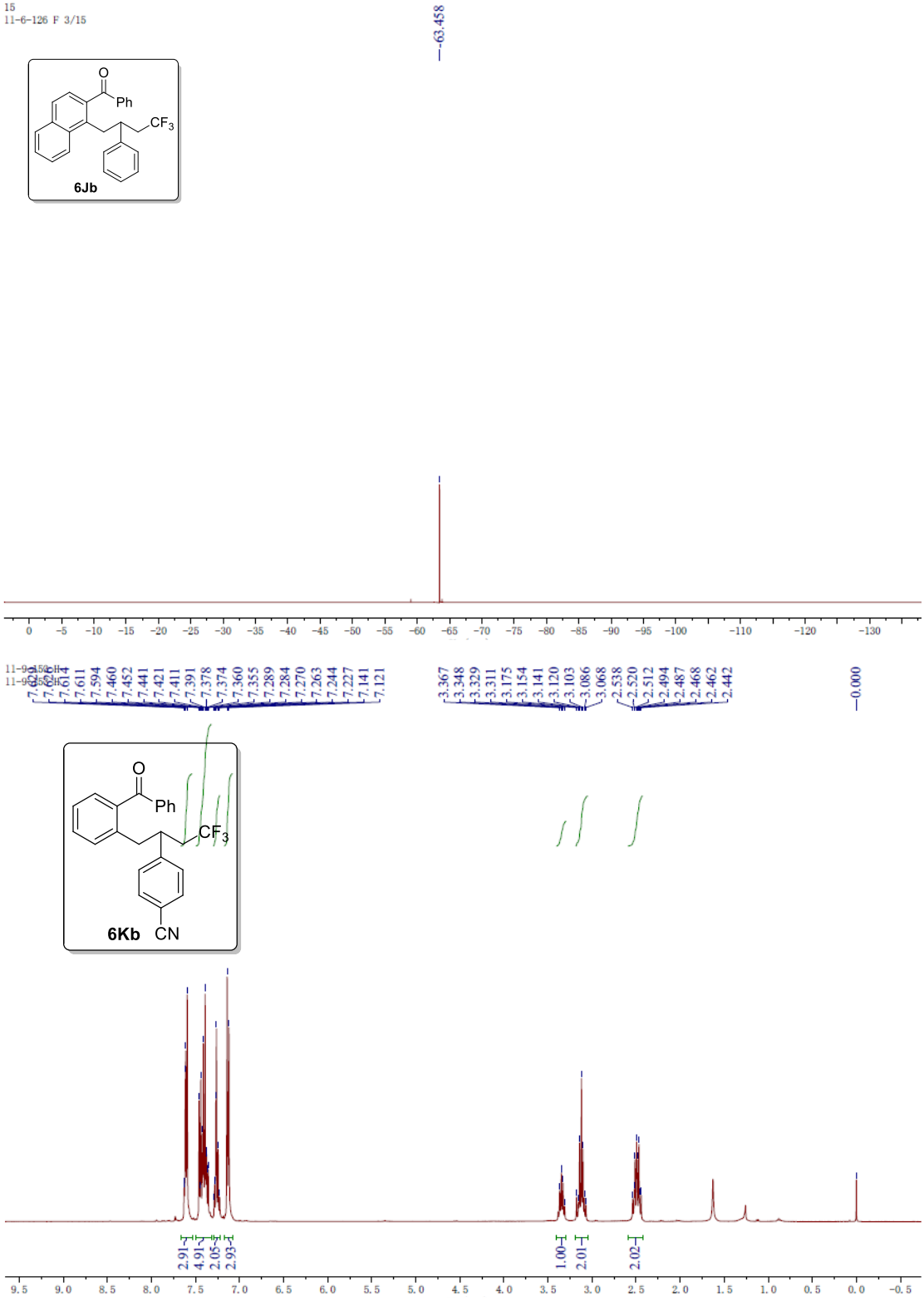

11-8-178 C
11-8-178 C
196.419
167.100
164.559
162.820
160.385
132.879
132.786
131.111
130.425
129.026
128.901
128.822
125.749
125.596
115.407
115.378
115.195
41.333
41.311
39.961
39.861
39.689
39.418
39.147
F
O
CF3
6lb
F
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10

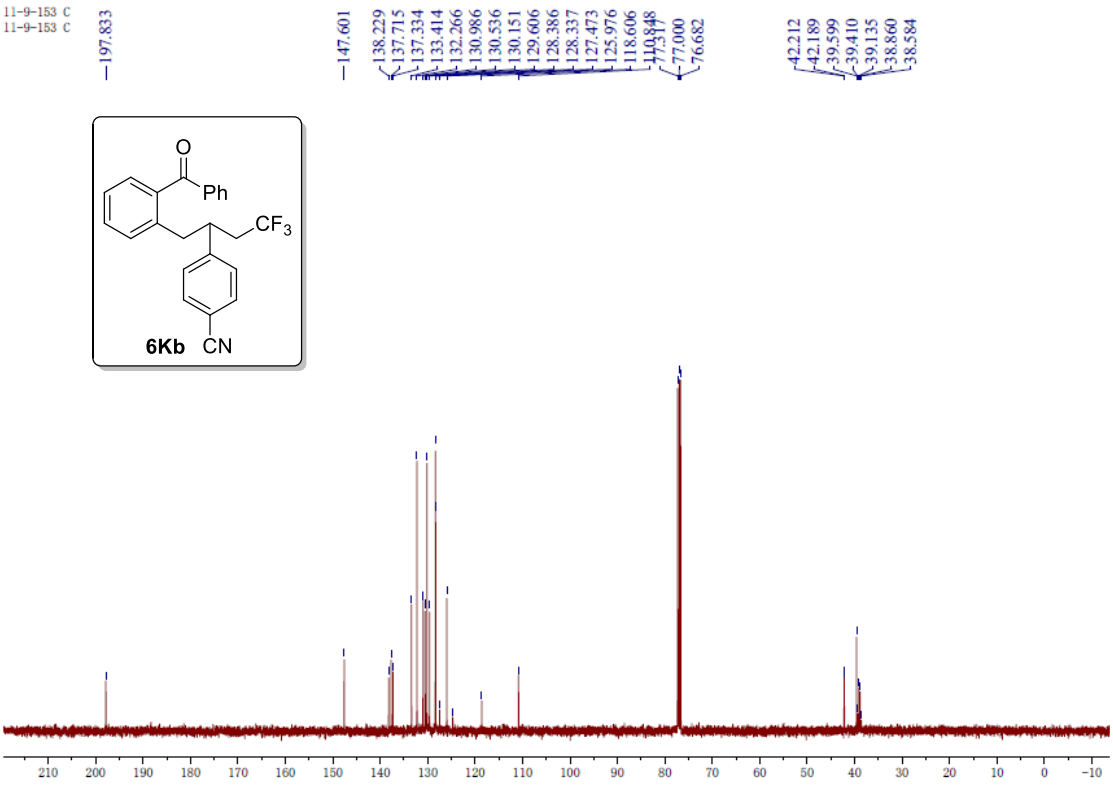

11-8-178 F
11-8-178 F
-63.557
-104.568
-115.877
F
O
CF3
6lb
F
10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210

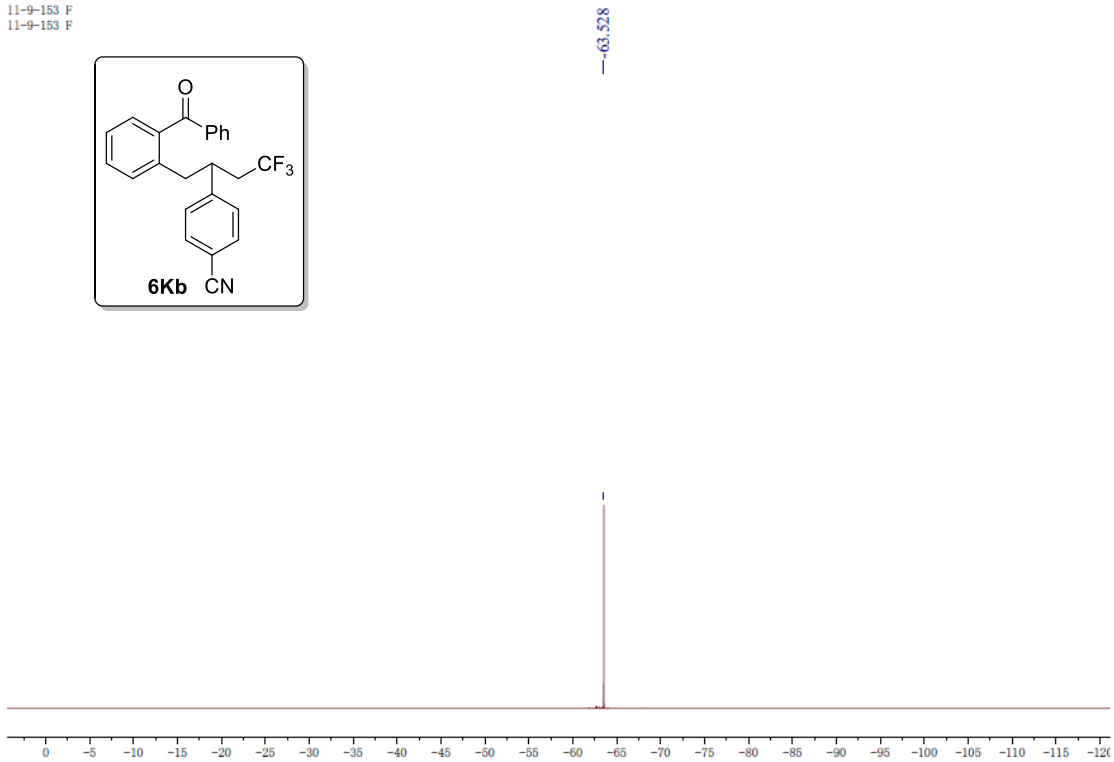

O
Ph
CF3
6Jb

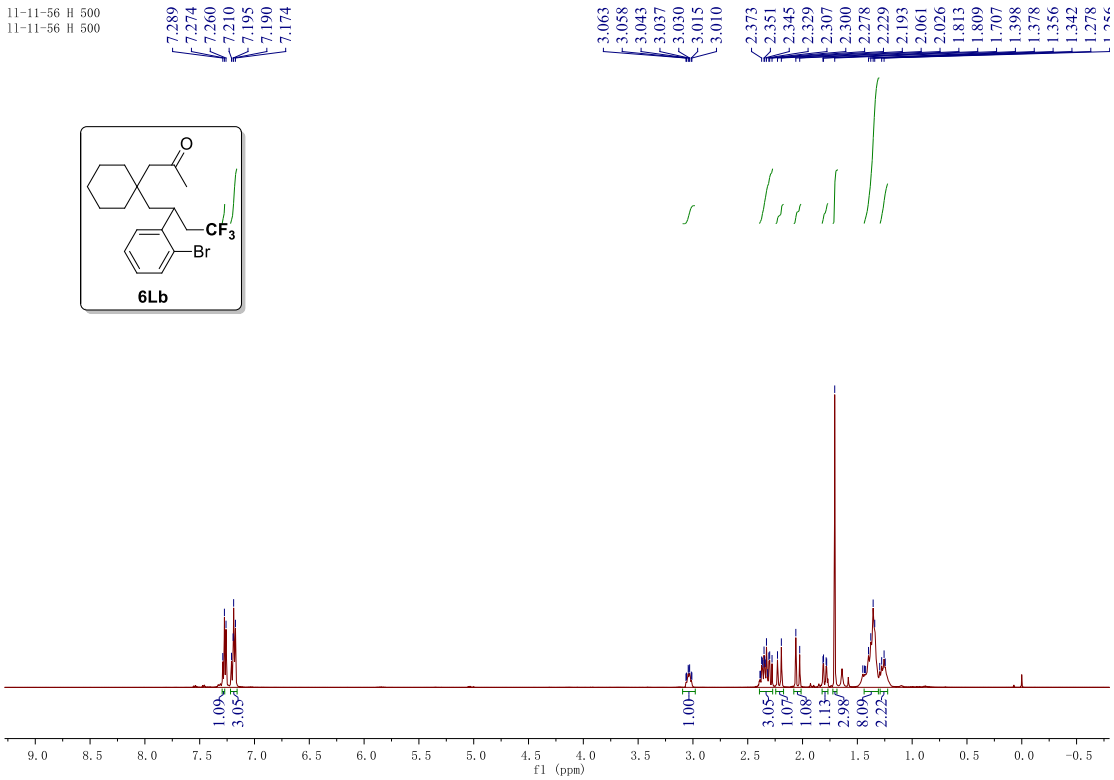

1.00
0.99
1.00
5.16
2.12
1.09
5.07
1.01
2.08
2.07

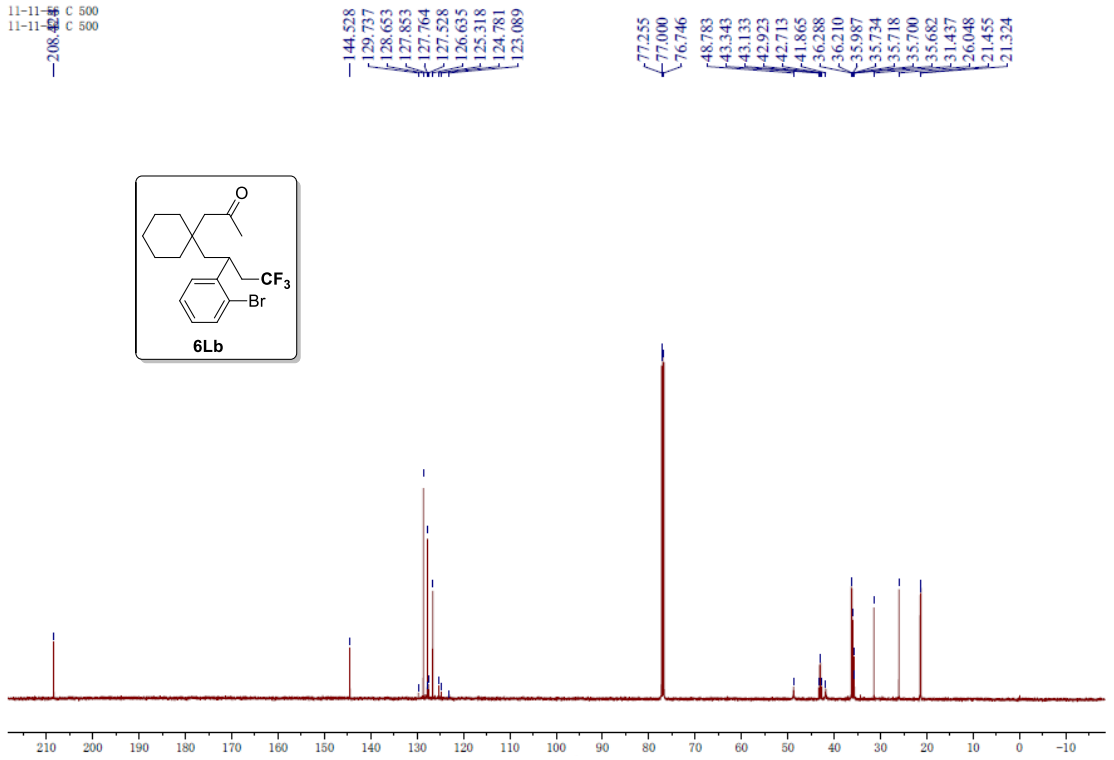

O
Ph
CF3
6Jb

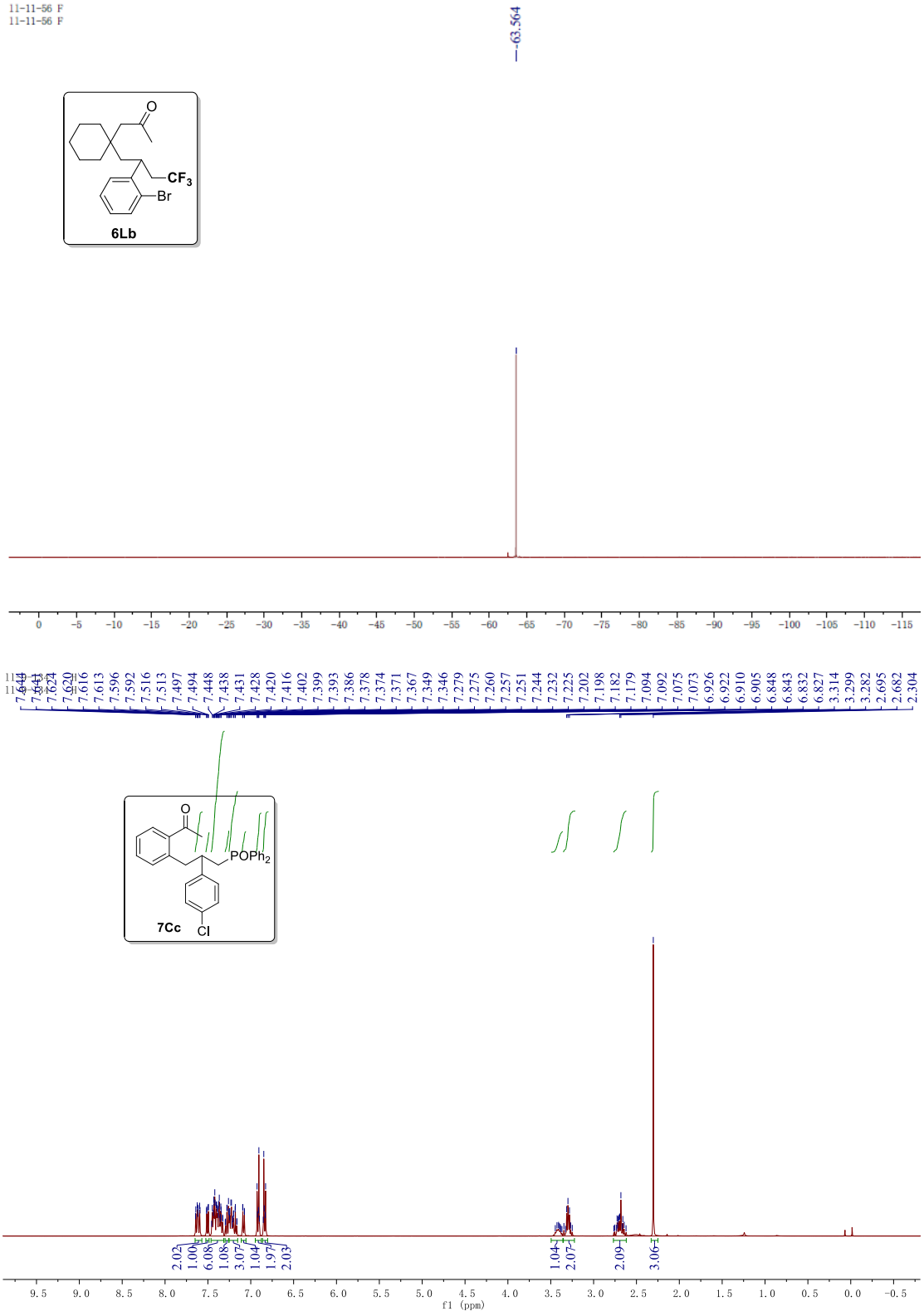

15
11-6-126 F 3/15
O
Ph
CF3
6Jb
-63.458
7.614
7.611
7.594
7.460
7.452
7.441
7.421
7.411
7.391
7.378
7.374
7.360
7.355
7.289
7.284
7.270
7.263
7.244
7.227
7.141
7.121
3.367
3.348
3.329
3.311
3.175
3.154
3.141
3.120
3.103
3.086
3.068
2.538
2.520
2.512
2.494
2.487
2.468
2.462
2.442
0.000
O
Ph
CF3
6Kb CN
2.91
4.91
2.05
2.93
1.00
2.01
2.02

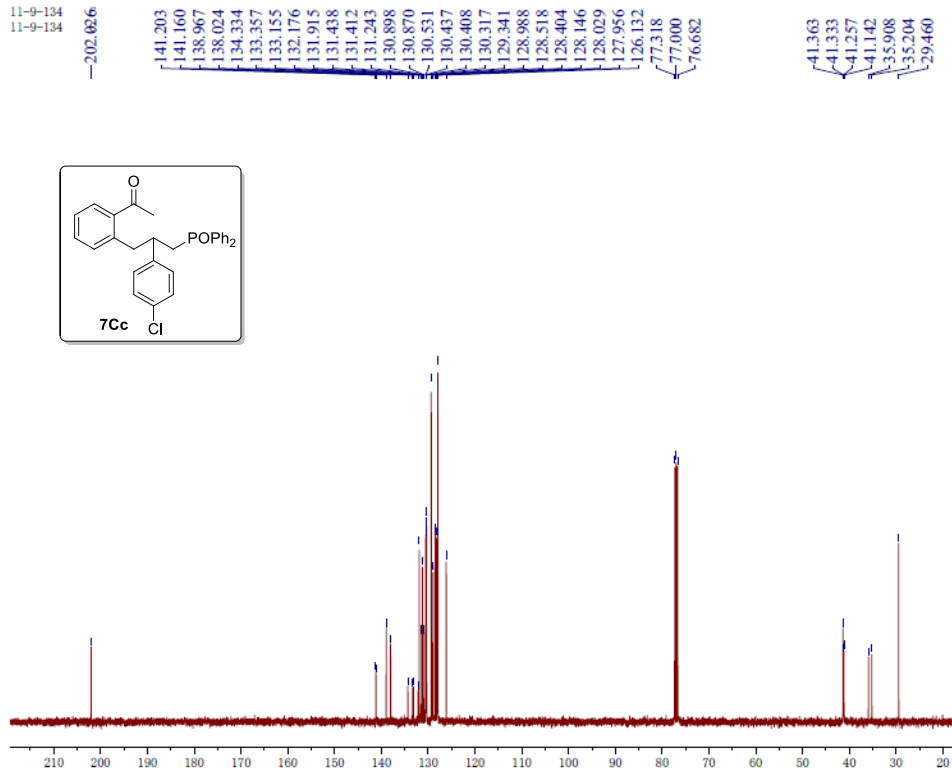

11-9-153 C
11-9-153 C
197.833
147.601
138.229
137.715
137.334
133.414
132.266
130.986
130.536
130.151
129.606
128.386
128.337
127.473
125.976
118.606
110.848
77.317
77.000
76.682
42.212
42.189
39.599
39.410
39.135
38.860
38.584
O
Ph
CF3
6Kb
CN
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10

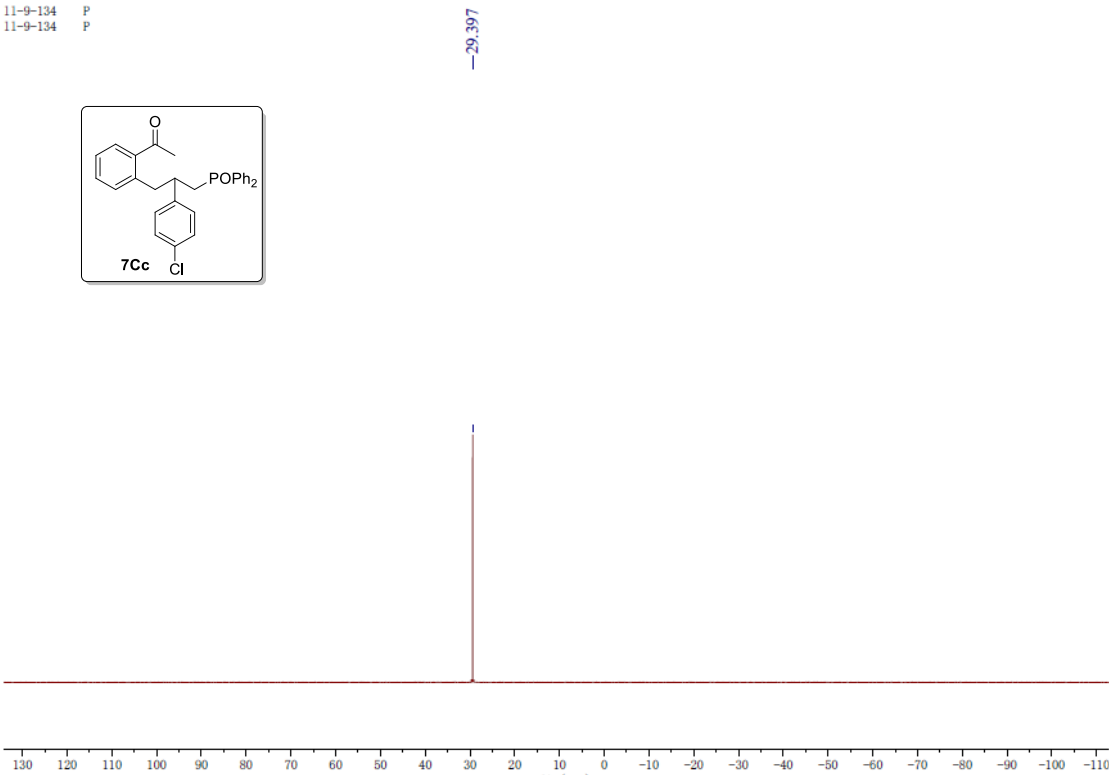

11-9-153 F
11-9-153 F
-63.528
O
Ph
CF3
6Kb
CN
0
-5
-10
-15
-20
-25
-30
-35
-40
-45
-50
-55
-60
-65
-70
-75
-80
-85
-90
-95
-100
-105
-110
-115
-120

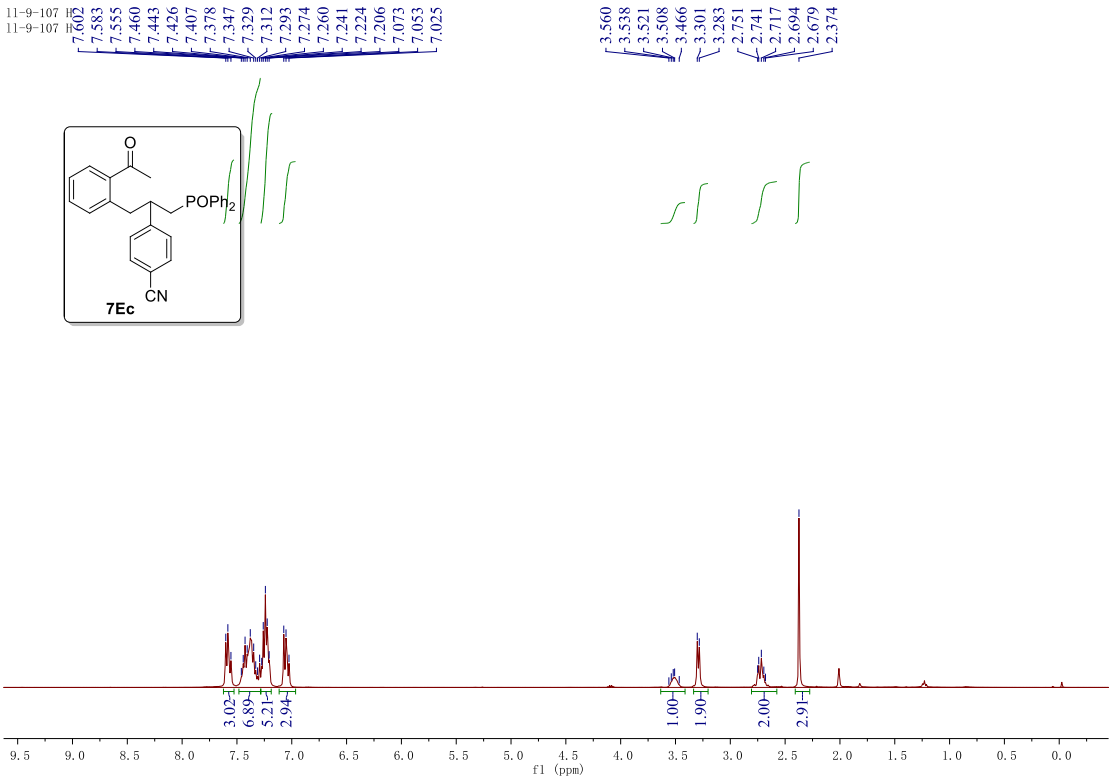

11-11-56 H 500
11-11-56 H 500
7.289
7.274
7.260
7.210
7.195
7.190
7.174
3.063
3.058
3.043
3.037
3.030
3.015
3.010
2.373
2.351
2.345
2.329
2.307
2.300
2.278
2.229
2.193
2.061
2.026
1.813
1.809
1.707
1.398
1.378
1.356
1.342
1.278
O
CF3
Br
6Lb
1.09
3.05
1.00
3.05
1.07
1.08
1.13
2.98
8.09
2.22
9.0
8.5
8.0
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
f1 (ppm)

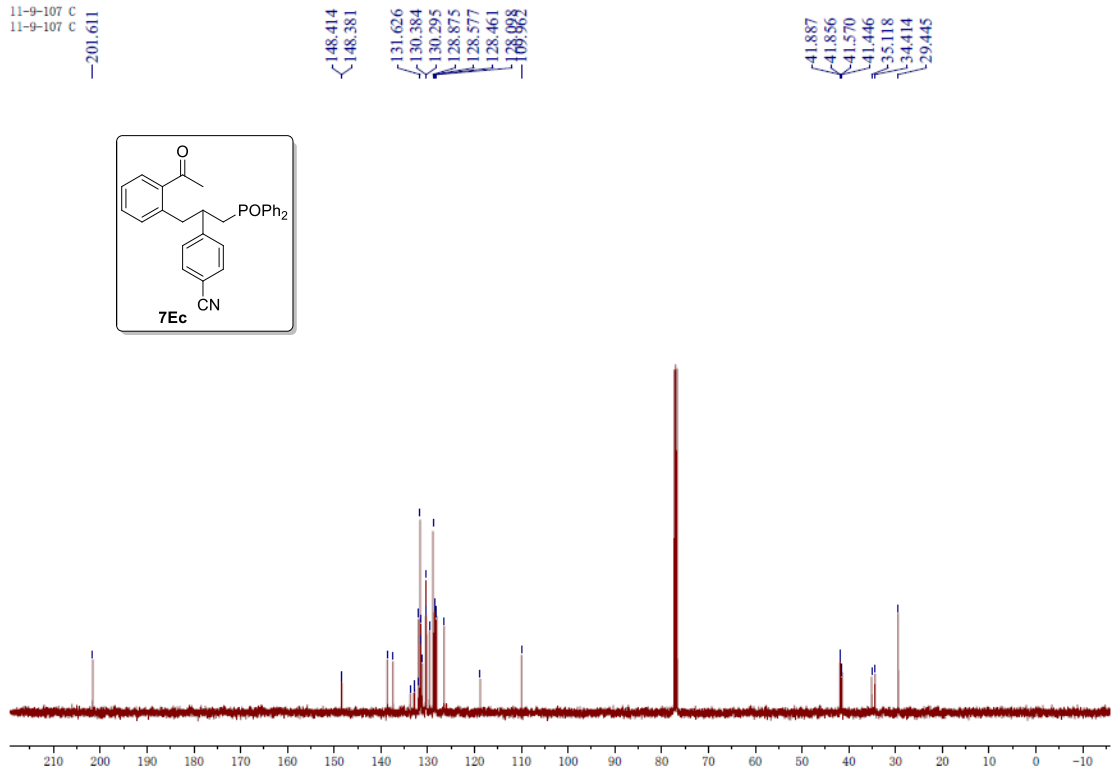

11-11-56 C 500
11-11-56 C 500
208.422
144.528
129.737
128.653
127.853
127.764
127.528
126.635
125.318
124.781
123.089
77.255
77.000
76.746
48.783
43.343
43.133
42.923
42.713
41.865
36.288
36.210
35.987
35.734
35.718
35.700
35.682
31.437
26.048
21.455
21.324
O
CF3
Br
6Lb
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10

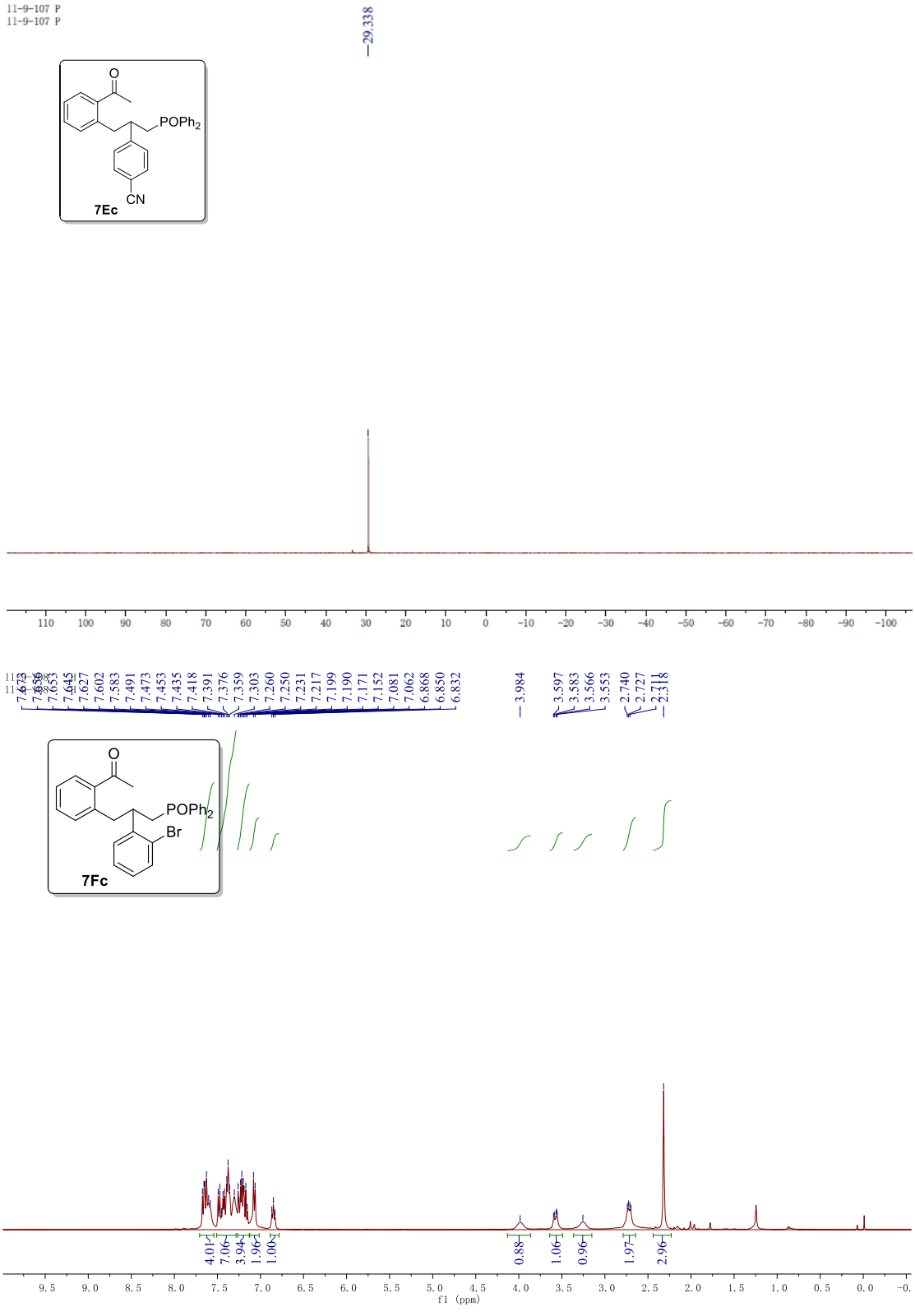

11-11-56 F
11-11-56 F
-63.564
O
CF3
Br
6Lb
POPh2
Cl
7Cc
f1 (ppm)


11-9-134
11-9-134
202.626
141.203
141.160
138.967
138.024
134.334
133.357
133.155
132.176
131.915
131.438
131.412
131.243
130.898
130.870
130.531
130.437
130.408
130.317
129.341
128.988
128.518
128.404
128.146
128.029
127.956
126.132
77.318
77.000
76.682
41.363
41.333
41.257
41.142
35.908
35.204
29.460
POPh2
7Cc
Cl
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10


11-9-134 P
11-9-134 P
29.397
POPh2
7Cc
Cl
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110

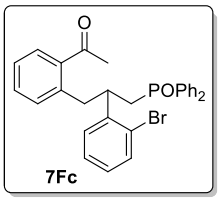

11-9-107 H
11-9-107 H
7.602
7.583
7.555
7.460
7.443
7.426
7.407
7.378
7.347
7.329
7.312
7.293
7.274
7.260
7.241
7.224
7.206
7.073
7.053
7.025
3.560
3.538
3.521
3.508
3.466
3.301
3.283
2.751
2.741
2.717
2.694
2.679
2.374
O
POPh2
CN
7Ec
3.02
6.89
5.21
2.94
1.00
1.90
2.00
2.91
f1 (ppm)

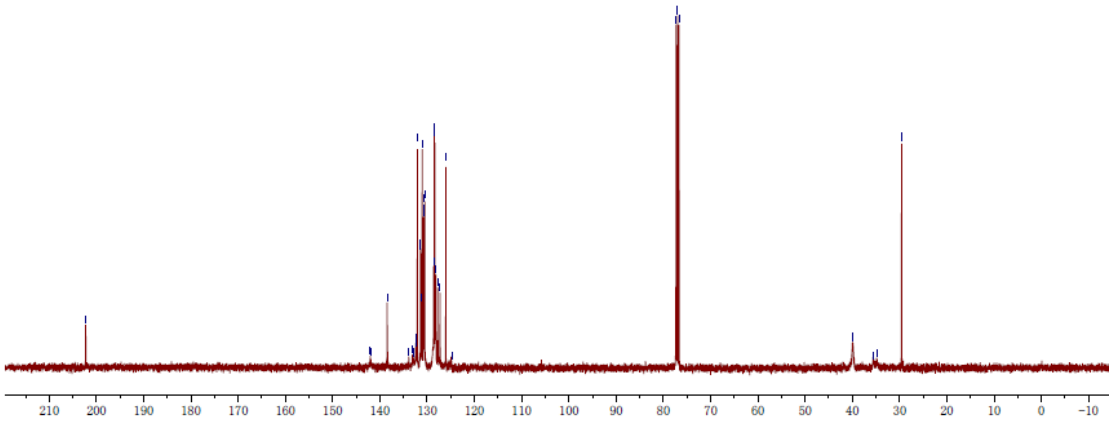

11-9-107 C
11-9-107 C
201.611
148.414
148.381
131.626
130.384
130.295
128.875
128.577
128.461
41.887
41.856
41.570
41.446
35.118
34.414
29.445
O
POPh2
CN
7Ec


11-9-107 P
11-9-107 P
29.338
O
POPh2
CN
7Ec
7.673
7.658
7.653
7.645
7.627
7.602
7.583
7.491
7.473
7.453
7.435
7.418
7.391
7.376
7.359
7.303
7.260
7.250
7.231
7.217
7.199
7.190
7.171
7.152
7.081
7.062
6.868
6.850
6.832
3.984
3.597
3.583
3.566
3.553
2.740
2.727
2.711
2.318
O
POPh2
Br
7Fc
4.01
7.06
3.94
1.96
1.00
0.88
1.06
0.96
1.97
2.96
f1 (ppm)

11-9-108
11-9-108

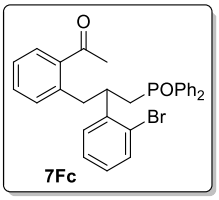
202.271
142.036
141.995
138.455
133.865
133.105
132.874
132.444
132.387
132.357
132.333
132.070
131.423
131.398
131.221
131.052
130.727
130.634
130.575
130.484
128.623
128.492
128.377
128.279
128.161
127.746
127.272
126.047
124.781
77.318
77.000
76.682
39.955
35.557
34.842
29.576

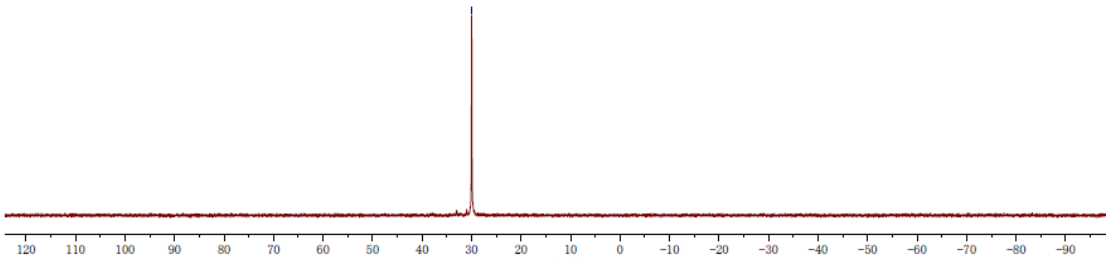


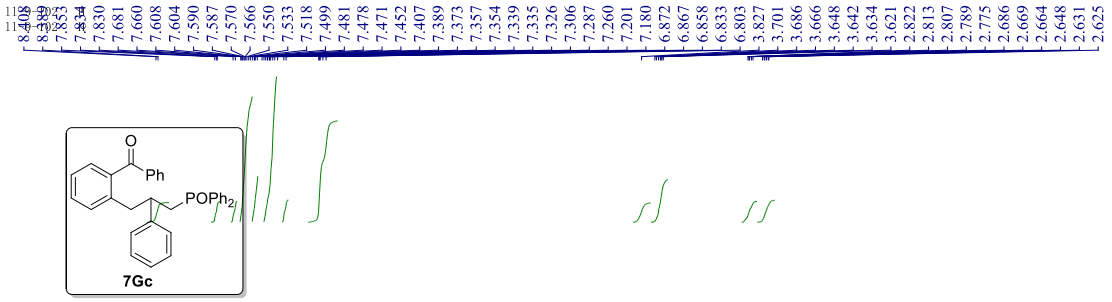


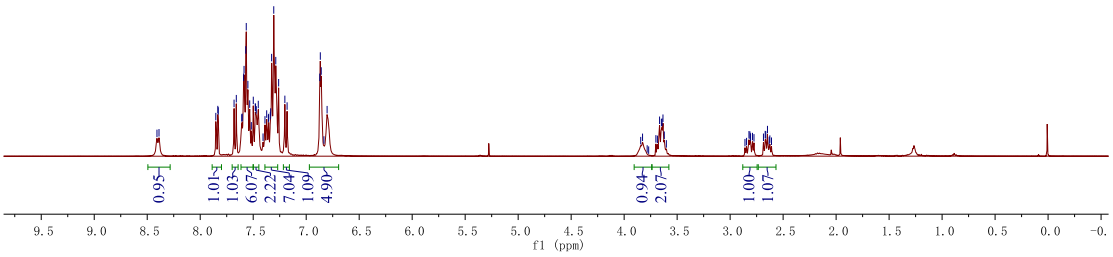
11-9-108 P
11-9-108 P

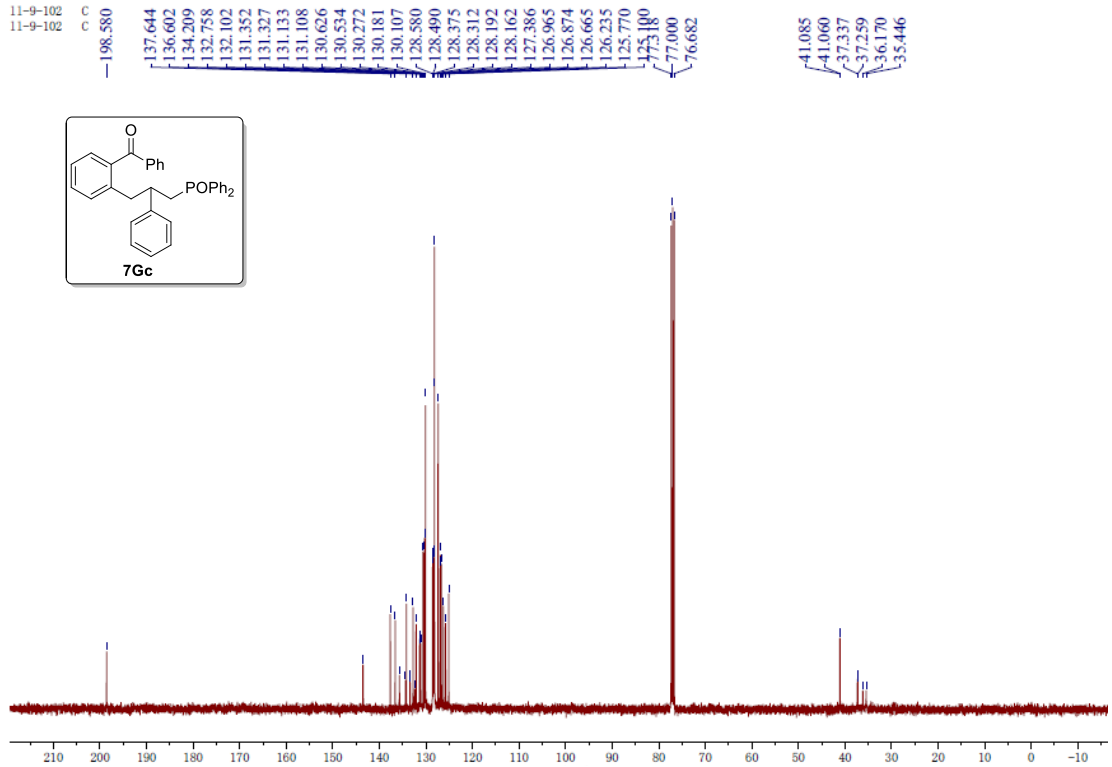
29.981

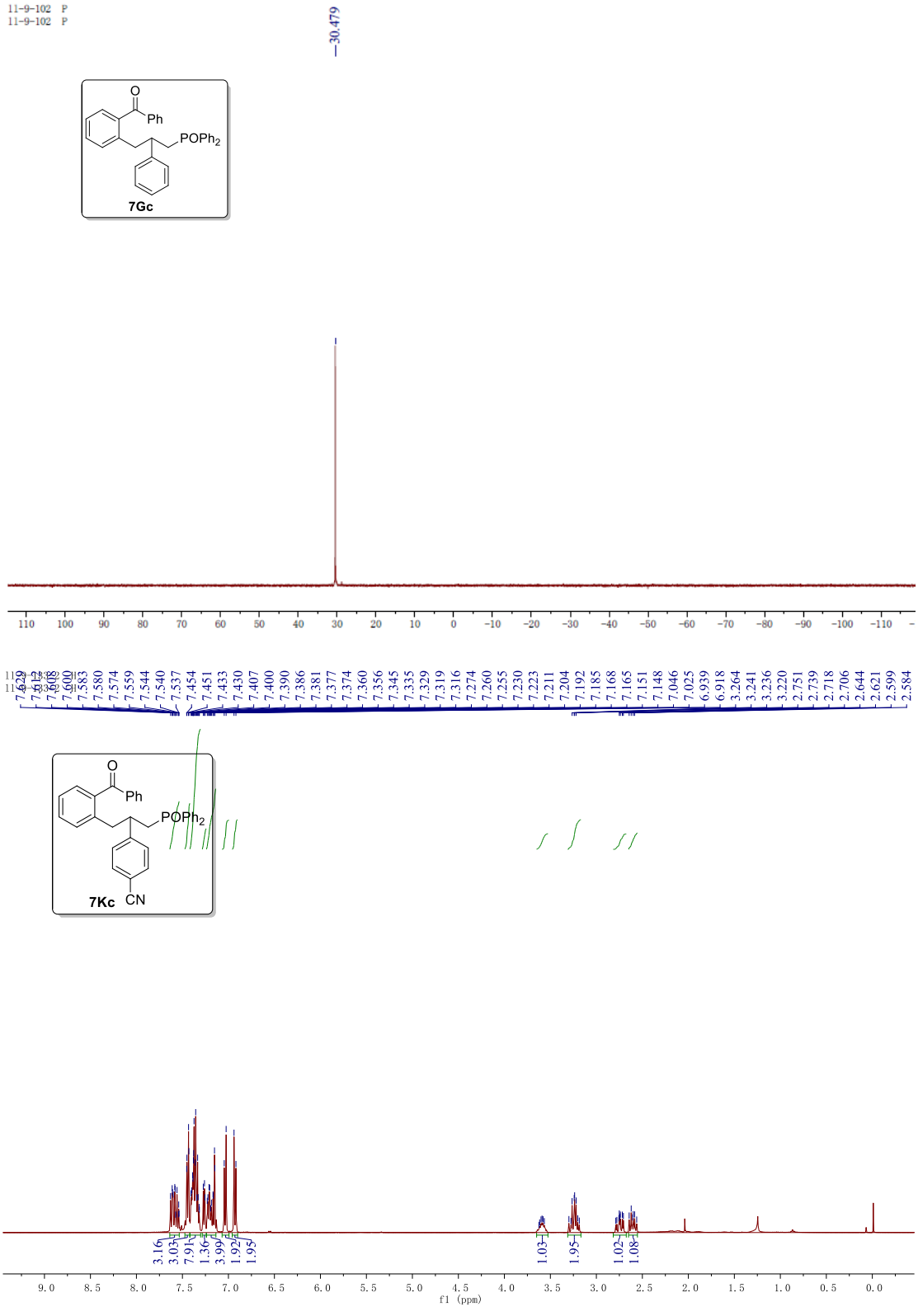


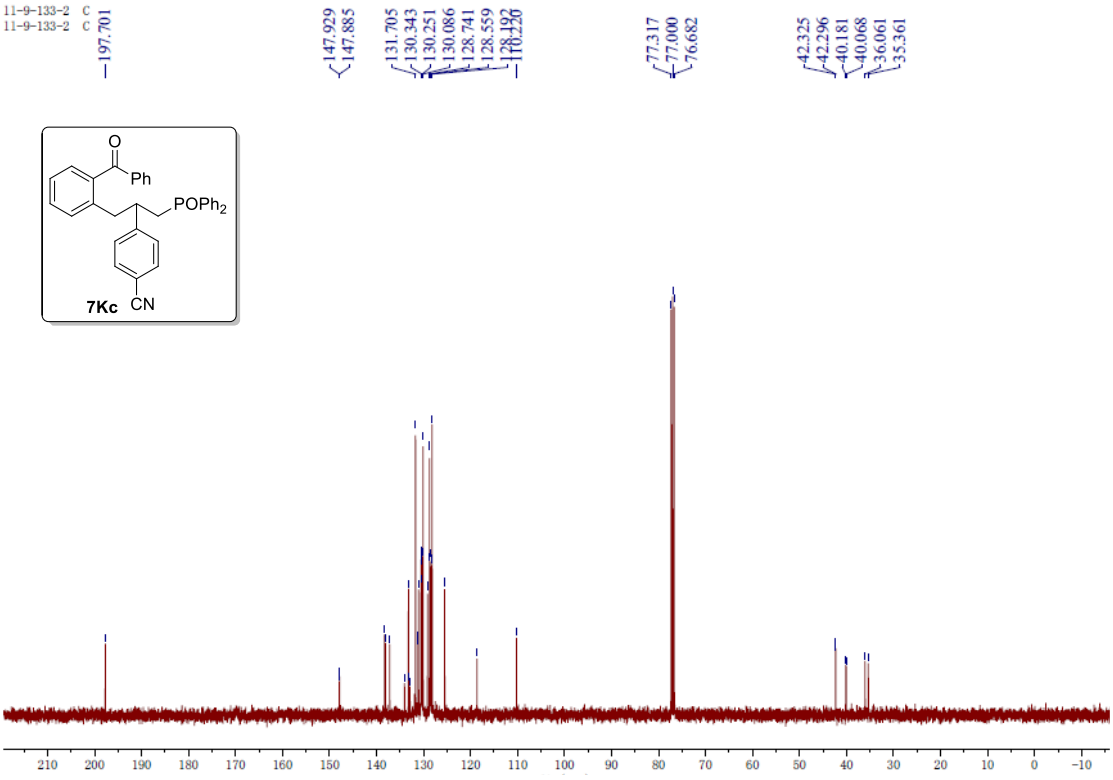


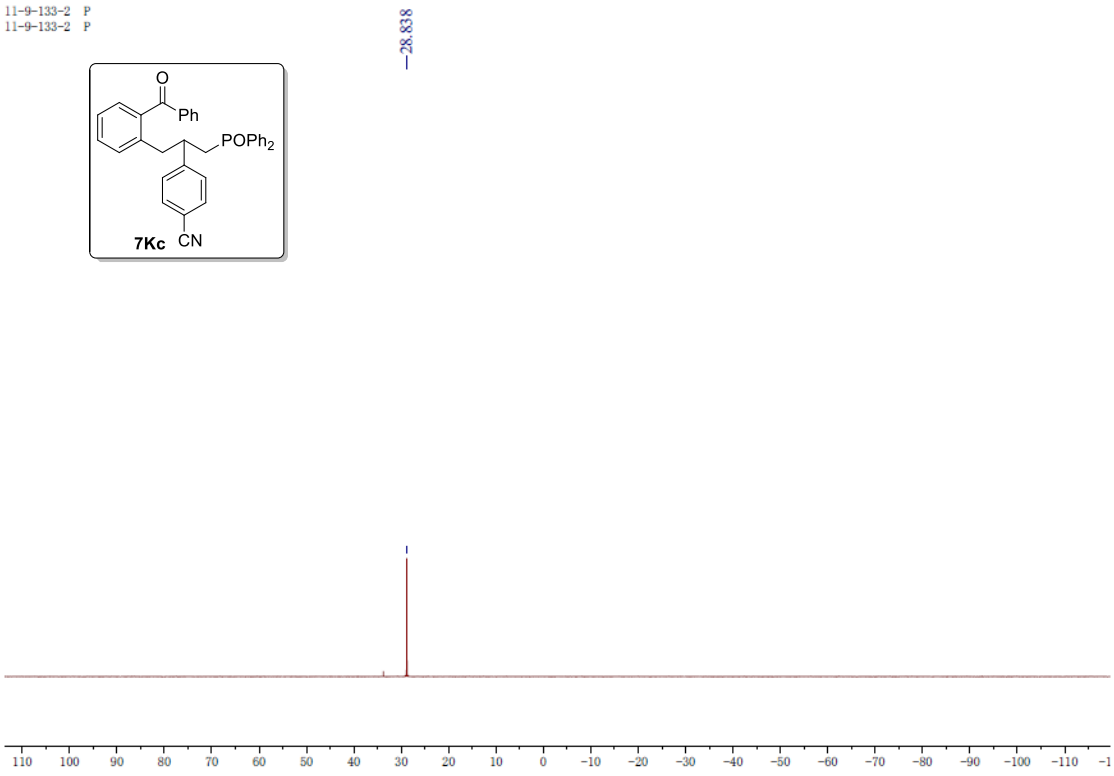

O
Ph
POPh2
7Gc

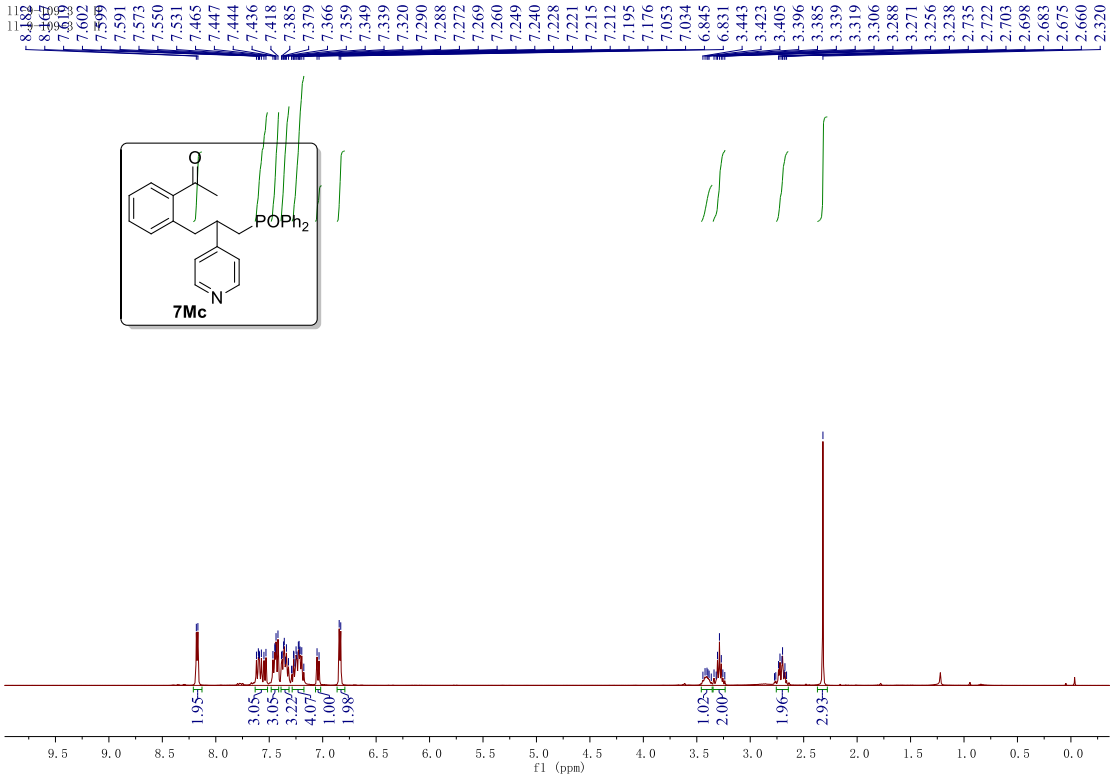

0.95
1.01
1.03
6.07
2.22
7.04
1.09
4.90
0.94
2.07
1.00
1.07
f1 (ppm)

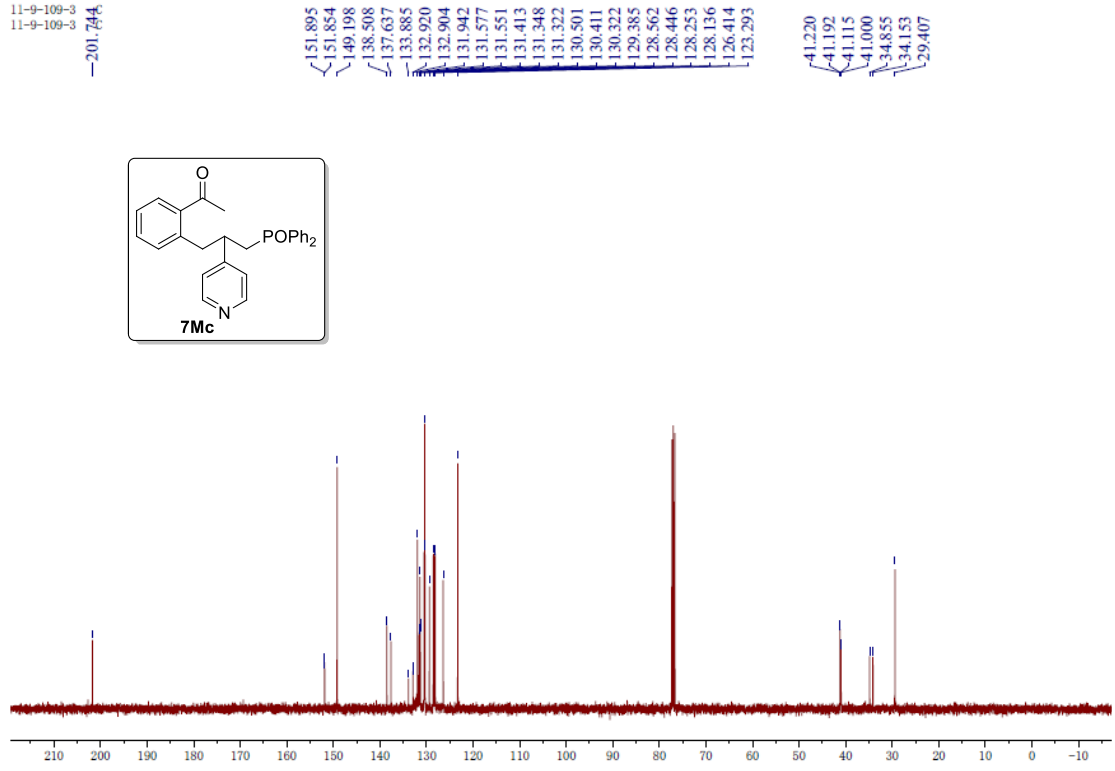

O
Ph
POPh2
7Gc

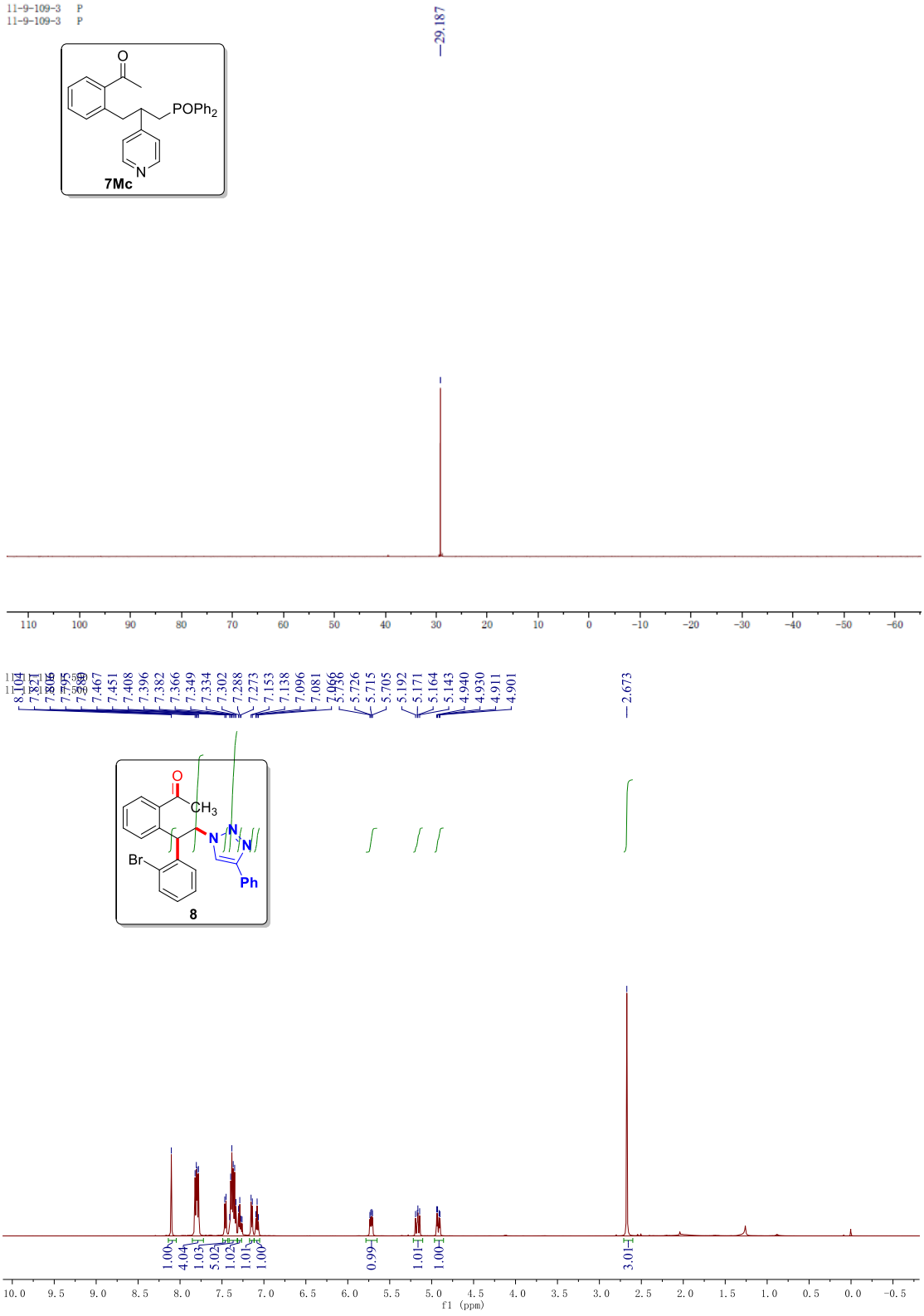

11-9-102 P
11-9-102 P
30.479
O
Ph
POPh2
7Gc
7.629
7.612
7.608
7.600
7.583
7.580
7.574
7.559
7.544
7.540
7.537
7.454
7.451
7.433
7.430
7.407
7.400
7.390
7.386
7.381
7.377
7.374
7.360
7.356
7.345
7.335
7.329
7.319
7.316
7.274
7.260
7.255
7.230
7.223
7.211
7.204
7.192
7.185
7.168
7.165
7.151
7.148
7.046
7.025
6.939
6.918
3.264
3.241
3.236
3.220
2.751
2.739
2.718
2.706
2.644
2.621
2.599
2.584
O
Ph
POPh2
7Kc
CN
3.16
3.03
7.91
1.36
3.99
1.92
1.95
1.03
1.95
1.02
1.08
f1 (ppm)

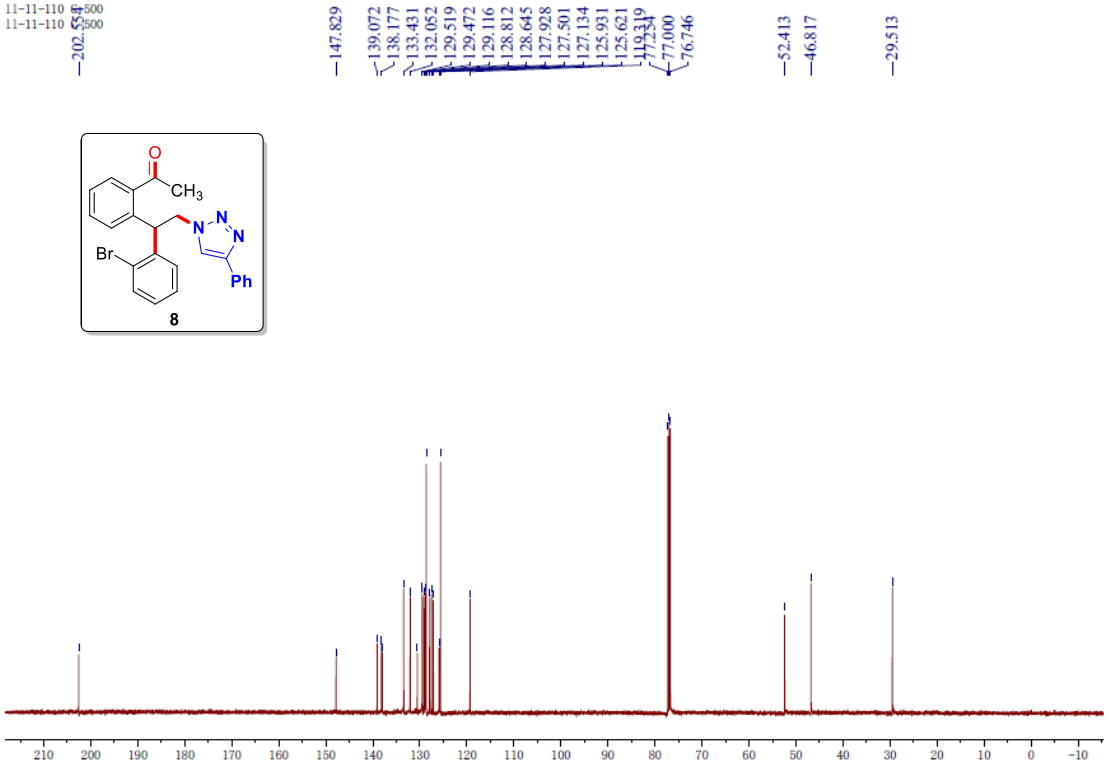

11-9-133-2 C
11-9-133-2 C
197.701
147.929
147.885
131.705
130.343
130.251
130.086
128.741
128.559
77.317
77.000
76.682
42.325
42.296
40.181
40.068
36.061
35.361
O
Ph
POPh2
7Kc
CN
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10

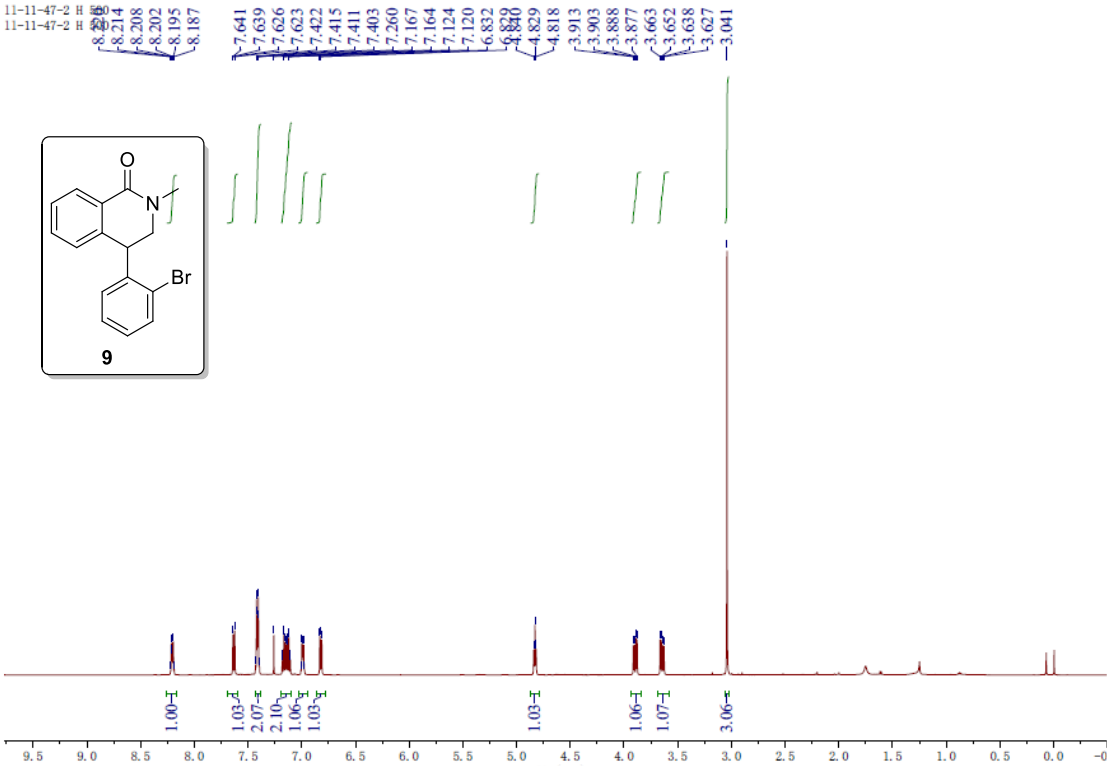

11-9-133-2 P
11-9-133-2 P
28.838
O
Ph
POPh2
7Kc
CN
110 100 90 80 70 60 50 40 30 20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -1

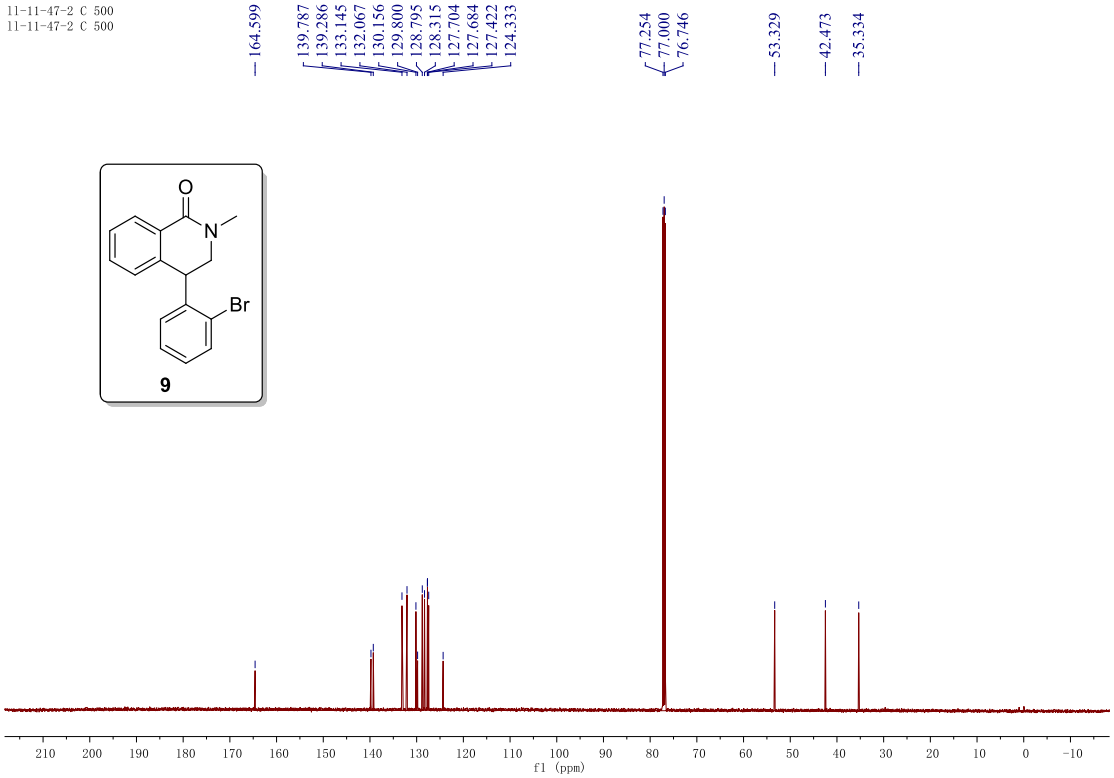

POPh2
7Mc
1.95
3.05
3.05
3.22
4.07
1.00
1.98
1.02
2.00
1.96
2.93
f1 (ppm)

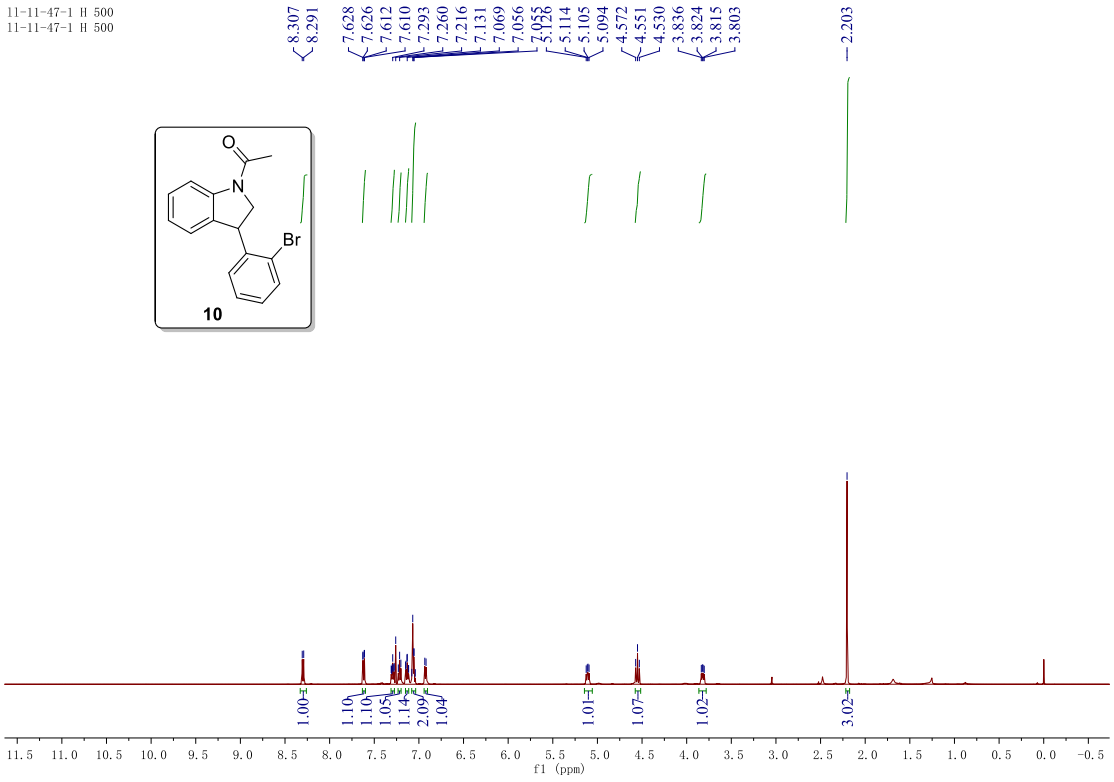

11-9-109-3
11-9-109-3
POPh2
7Mc
f1 (ppm)

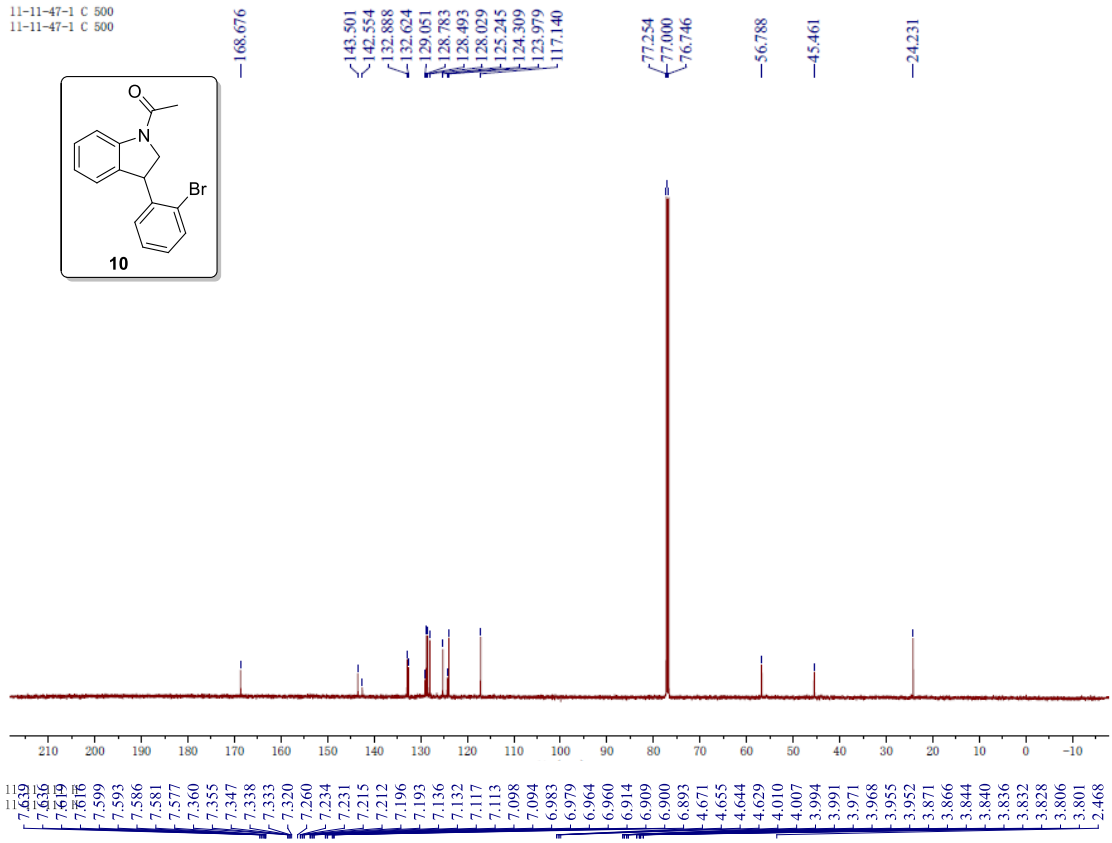

11-9-109-3 P
11-9-109-3 P
29.187
POPh2
7Mc
2.673
Br
Ph
8
f1 (ppm)

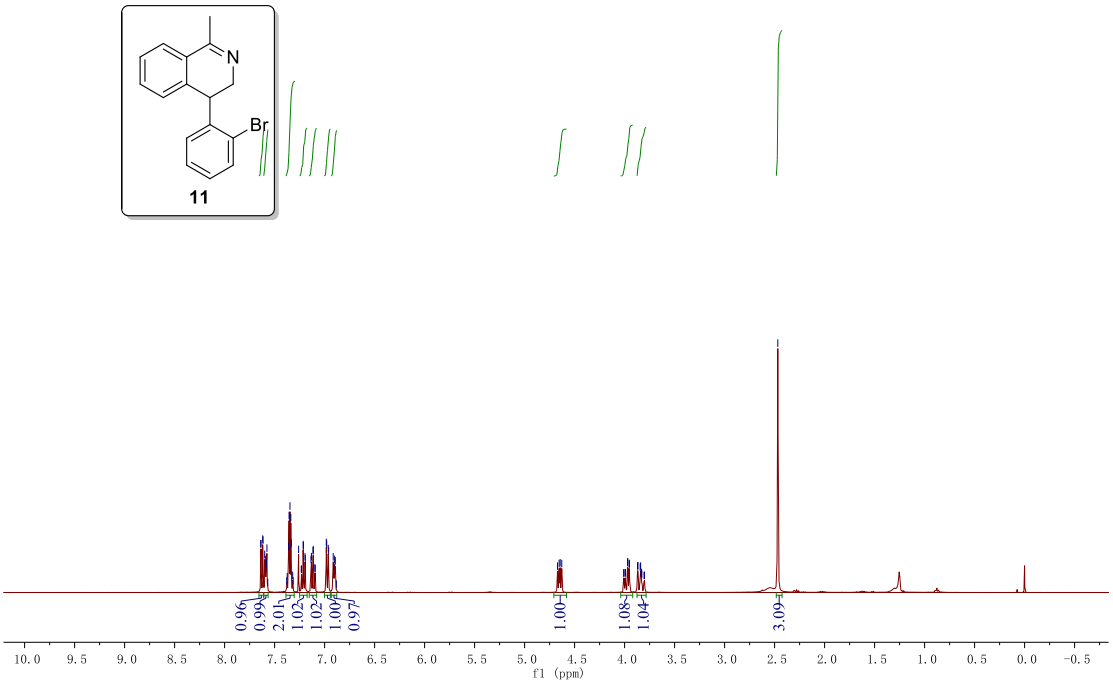

11-11-110
11-11-110
202.554
147.829
139.072
138.177
133.431
132.052
129.519
129.472
129.116
128.812
128.645
127.928
127.501
127.134
125.931
125.621
77.000
76.746
52.413
46.817
29.513
O
CH3
N
N
N
Br
Ph
8
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10


11-11-47-2 H
11-11-47-2 H
8.214
8.208
8.202
8.195
8.187
7.641
7.639
7.626
7.623
7.422
7.415
7.411
7.403
7.260
7.167
7.164
7.124
7.120
6.832
4.829
4.818
3.913
3.903
3.888
3.877
3.663
3.652
3.638
3.627
3.041
O
N
Br
9
1.00
1.03
2.07
2.10
1.06
1.03
1.03
1.06
1.07
3.06
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

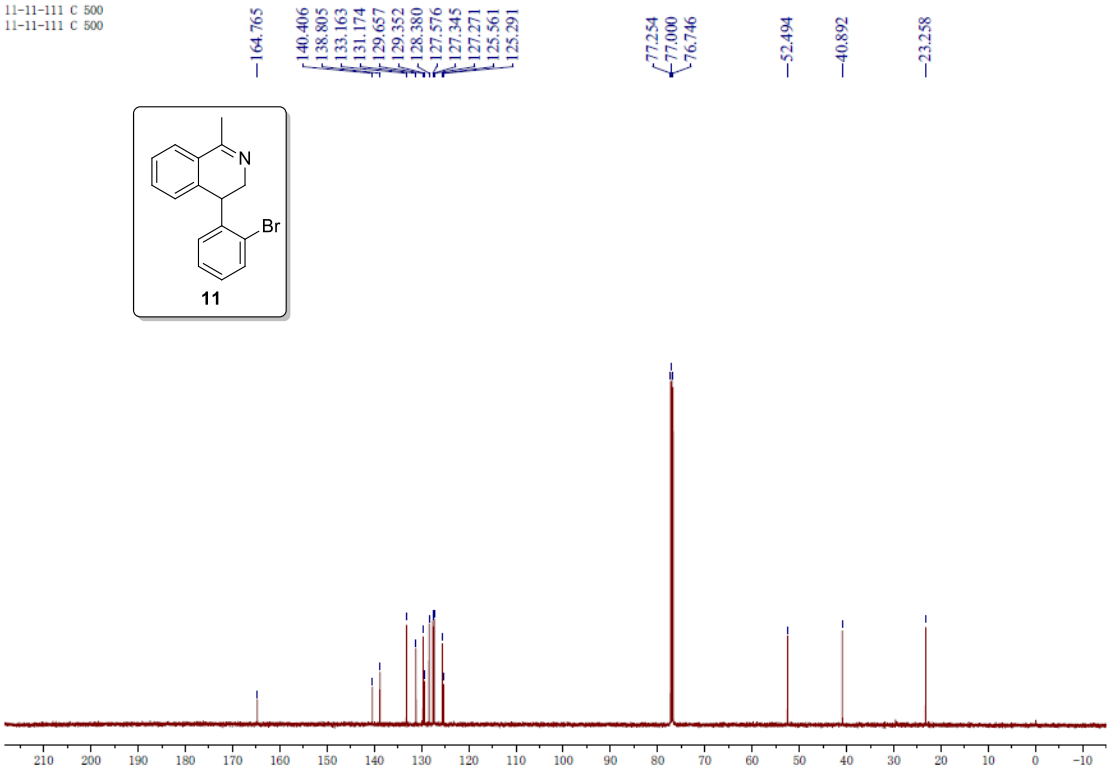

11-11-47-2 C 500
11-11-47-2 C 500
164.599
139.787
139.286
133.145
132.067
130.156
129.800
128.795
128.315
127.704
127.684
127.422
124.333
77.254
77.000
76.746
53.329
42.473
35.334
O
N
Br
9
f1 (ppm)


11-11-47-1 H 500
11-11-47-1 H 500
8.307
8.291
7.628
7.626
7.612
7.610
7.293
7.260
7.216
7.131
7.069
7.056
5.126
5.114
5.105
5.094
4.572
4.551
4.530
3.836
3.824
3.815
3.803
2.203
O
N
Br
10
1.00
1.10
1.10
1.05
1.14
2.09
1.04
1.01
1.07
1.02
3.02
f1 (ppm)


11-11-47-1 C 500
11-11-47-1 C 500
168.676
143.501
142.554
132.888
132.624
129.051
128.783
128.493
128.029
125.245
124.309
123.979
117.140
77.254
77.000
76.746
56.788
45.461
24.231
O
N
Br
10


N
Br
11
0.96
0.99
2.01
1.02
1.02
1.00
0.97
1.00
1.08
1.04
3.09
f1 (ppm)

11-11-111 C 500
11-11-111 C 500



References

1. L. Li, Z.-L. Li, F.-L. Wang, Z. Guo, Y.-F. Cheng, N. Wang, X.-W. Dong, C. Fang, J. Liu, C. Hou, B. Tan and X.-Y. Liu, *Nat. Commun.*, **7**, 13852.