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Supporting Information

For

Pd(II)-Catalyzed C-H Arylation of Aryl and Benzyl Weinreb Amides

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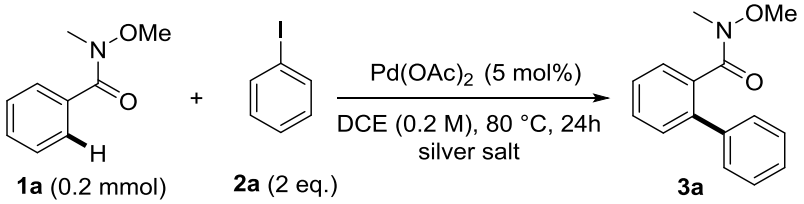
General Information:

Unless otherwise noted, all the reagents were commercially available, and used as received. NMR spectra were recorded on Bruker-400 (400 MHz for ^{1}H; 100 MHz for ^{13}C) instruments internally referenced to $SiMe_4$ signal. Chemical shifts are reported in δ ppm, High resolution mass spectra were recorded on P-SIMS-Gly of Bruker Daltonics Inc. using ESI-TOF (electrospray ionization-time of flight) or Micromass GCT using EI (electron impact).

Tables of the Optimization of Reaction Conditions

Table S1. Silver Salts Screening:

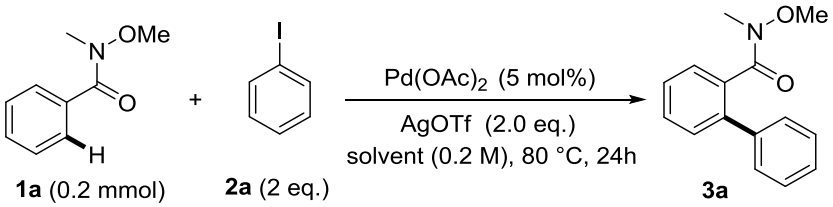


1a (0.2 mmol) **2a** (2 eq.) **3a**

entry	silver salt (equiv)	yield (%)[a]
1	Ag_2O (1)	N. R.
2	Ag_2CO_3 (1)	N. R.
3	AgTFA (2)	N. R.
4	AgOAc (2)	N. R.
5	AgOTf (2)	69 (4)

[a]GC yield using dodecane as the internal standard, yield of diarylation product was given in the parentheses.

Table S2. Solvent Screening:

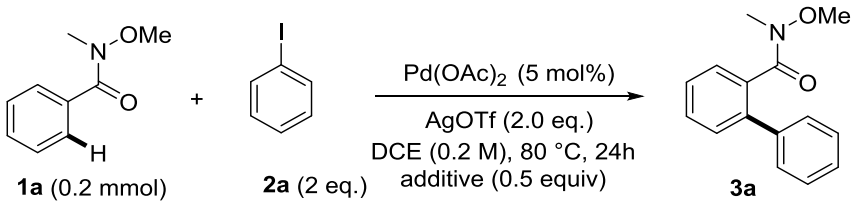


1a (0.2 mmol) **2a** (2 eq.) **3a**

entry	solvent	yield (%)[a]
1	PhMe	67 (6)
2	t-AmlyOH	0
3	dioxane	50 (3)
4	DMF	N. R.
5	CH_3CN	N. R.
6	DMSO	N. R.
7	acetone	complex
8	DCE	69 (4)

[a]GC yield using dodecane as the internal standard, yield of diarylation product was given in the parentheses.

Table S3. Additive Screening:

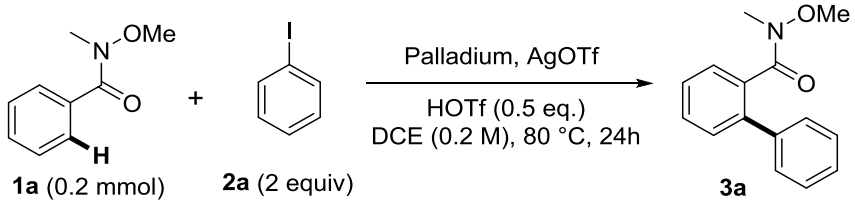


1a (0.2 mmol) **2a** (2 eq.) **3a**

entry	additive	yield (%)[a]
1	HOTf	89 (5), 91[b]
2	HOAc	66 (19)
3	TFA	75 (21)
4	PivOH	70 (20)
5	TsOH	74 (17)
6	HBF_4	62 (18)

[a]GC yield using dodecane as the internal standard, yield of diarylation product was given in the parentheses. [b]Isolated yield.

Table S4. Other conditions:



1a (0.2 mmol) **2a** (2 equiv) **3a**

entry	Pd (mol %)	AgOTf (equiv)	yield(%)[a]
1	$Pd(OAc)_2$ (5)	AgOTf (1.0)	77 (3)
2[b]	$Pd(OAc)_2$ (5)	AgOTf (2)	80 (6)
3[c]	$Pd(OAc)_2$ (5)	AgOTf (2)	76 (3)
4	$Pd(Ph_3P)_4$ (5)	AgOTf (2)	90 (6)
5	$Pd_2(dba)_3$ (2.5)	AgOTf (2)	56 (1)
6	-	AgOTf (2)	N. R.
7	$Pd(OAc)_2$ (1)	AgOTf (2)	81 (4)

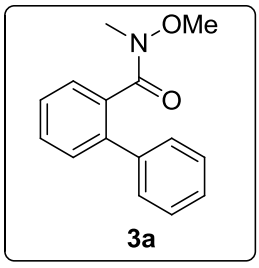
[a]GC yield using dodecane as the internal standard, yield of diarylation product was given in the parentheses. [b]PhI (1.1 equiv). [c]60 °C.

Preparation of Substrates:

Weinreb amides **1a-1g**,[1] **1o-1p**[1] and **4a-4l**[2] were prepared according to the known methods, respectively. [D_5]-N-methoxy-N-methylbenzamide (**[D_5]-1a**) was prepared from D_6-Benzene according to the literature.[1,3] All the aryl iodides were commercially available and used as received.

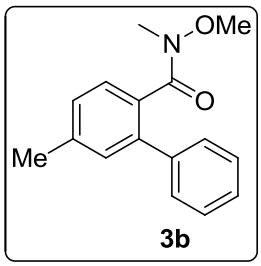
General Procedure for Pd(II)-Catalyzed C–H Arylation of Aryl and Benzyl Weinreb Amides:

1a (33.0 mg, 0.2 mmol), $Pd(OAc)_2$ (2.2 mg, 5 mol%), AgOTf (102.8 mg, 2 equiv), PhI (40.8 mg, 2 equiv), DCE (1 mL) and HOTf (15 mg, 0.5 equiv) were sequentially added to a 35 mL sealed tube. The reaction mixture was then placed into a preheated oil bath at 80 ℃ for 24 h. After cooling to room temperature, the mixture was diluted with ethyl acetate, filtered through a plug of silica. The filtrate was concentrated under vacuum, and the residue was purified by flash column chromatography on silica gel (petroleum ether : EtOAc = 5 : 1) to give monoarylation product **3a** (91% yield) as a white solid with minor diarylation product (5% yield) (determined by ^{1}H NMR and GC-MS) (Note: Arylation products **3a-3l** were showed as mixture in the NMR spectra because of the C-N bond rotation of the amide bond.[4] Substrates **1a-1h**, **1j**, **1k**, **1m** affroded monoarylation product majorly along with minor diarylation product which were detected by crude ^{1}H NMR, ^{13}C NMR and GC-MS.)



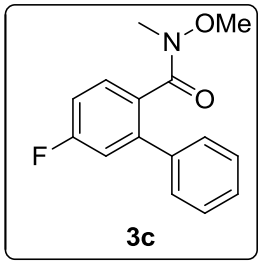
3a

3a: Purification by flash chromatography (petroleum ether/ EtOAc = 5:1) on silica gel to give **3a** (91% yield) as a white solid and minor diarylation product (5% yield) (The yields were determined by ^{1}H NMR and GC). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.49-7.26 (m, 9H), 3.49 (br s, 1.2H), 3.26 (br s, 1.8H), 3.09 (br s, 1.8H), 2.66 (br s, 1.2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 171.90, 167.05, 140.49, 139.45, 139.18, 134.85, 134.28, 129.90, 129.35, 128.41, 128.29, 127.68, 127.57, 127.36, 126.84, 61.00, 59.74, 35.76, 32.37. HRMS EI (*m/z*): $[M + Na]^+$ calcd. for $C_{15}H_{15}NO_2Na$: 264.1000, found: 264.1001.



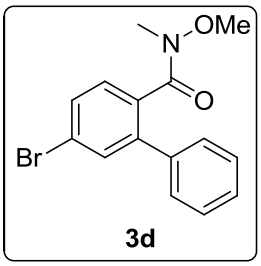
3b

3b: Purification by flash chromatography (petroleum ether/ EtOAc = 5:1) on silica gel to give **3b** (93% yield) as a yellow oil and minor diarylation product (6% yield) (determined by ^{1}H NMR). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.31 (m, 2H), 7.24-7.21 (m, 4H), 7.09-7.05 (m, 2H), 3.34 (br s, 1.3H), 3.12 (br s, 1.9H), 2.94 (br s, 1.9H), 2.54 (br s, 1.3H), 2.27 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 171.86, 167.06, 140.42, 139.67, 139.08, 131.74, 131.35, 129.87, 128.07, 127.35, 127.16, 126.73, 60.76, 59.43, 35.55, 32.17, 21.11. HRMS EI (m/z): $[M+Na]^+$ calcd. for $C_{16}H_{17}NO_2Na$: 278.1157, found: 278.1159.



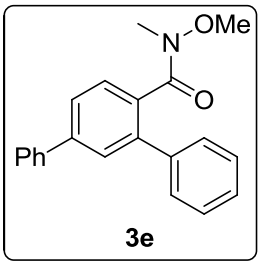
3c

3c: Purification by flash chromatography (petroleum ether/ EtOAc = 5:1) on silica gel to give **3c** (71% yield) as a yellow oil and minor diarylation product (8% yield) (determined by ^{1}H NMR and GC). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.31-7.10 (m, 6H), 7.08-6.94 (m, 2H), 3.38 (br s, 1.2H), 3.12 (br s, 2H), 2.95 (br s, 1.9H), 2.53 (br s, 0.9H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 170.86, 166.12, 162.84 (d, J = 251.0 Hz), 142.06, 141.67, 139.28, 138.16, 128.84, 128.33, 127.81, 116.22, 116.01, 114.55, 113.78, 113.57, 60.87, 59.77, 35.66, 32.27. HRMS ESI (m/z): $[M+Na]^+$ calcd. for $C_{15}H_{14}NO_2NaF$: 282.0926, found: 282.0916.



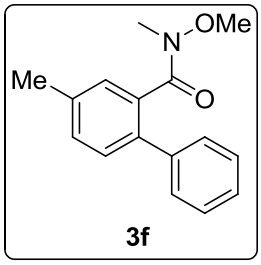
3d

3d: Purification by flash chromatography (petroleum ether/ EtOAc = 5:1) on silica gel to give **3d** (88% yield) as a yellow oil and minor diarylation product (9% yield) (determined by ^{1}H NMR and GC). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.50 (d, *J* = 2.0 Hz, 1H), 7.45 (d, *J* = 8.4 Hz, 1H), 7.33-7.11(m, 6H), 3.41 (br s, 1.2H), 3.18 (br s, 1.8H), 2.99 (br s, 2H), 2.58 (br s, 0.8H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 170.95, 141.69, 140.79, 139.19, 134.73, 133.83, 132.38, 130.81, 130.66, 129.98, 129.81, 129.39, 128.52, 128.42, 128.03, 127.10, 126.89, 123.39, 61.23, 59.95, 35.91, 32.50. HRMS ESI (m/z): [M+Na]+ calcd. for $C_{15}H_{14}NO_2NaBr$: 342.0104, found: 342.0106.



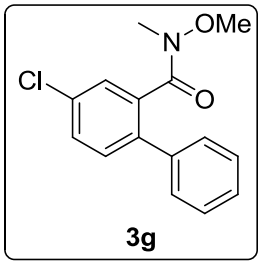
3e

3e: Purification by flash chromatography (petroleum ether/ EtOAc = 5:1) on silica gel to give **3e** (91% yield) as a white solid and minor diarylation product (4% yield) (determined by ^{1}H NMR and GC). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.51-7.49 (m, 4H), 7.41-7.39 (m, 3H), 7.33-7.21 (m, 6H), 3.37 (br s, 1.2H), 3.16 (br s, 1.8H), 2.98 (br s, 1.8H), 2.58 (br s, 1.2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ171.76, 166.95, 142.73, 142.21, 140.48, 140.06, 133.70, 133.14, 130.98, 130.53, 129.90, 128.85, 128.48, 128.38, 128.19, 127.79, 127.52, 127.12, 126.95, 126.81, 126.55, 126.21, 125.50, 61.08, 59.80, 35.92, 32.41. HRMS ESI (m/z): $[M+Na]^+$ calcd. for $C_{21}H_{19}NO_2Na$: 340.1313, found: 340.1314.



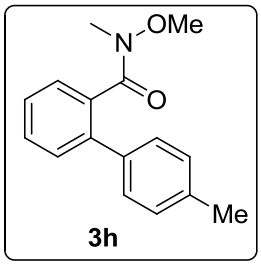
3f

3f: Purification by flash chromatography (petroleum ether/ EtOAc = 5:1) on silica gel to give **3f** (93% yield) as a yellow oil and minor diarylation product (4% yield) (determined by ^{1}H NMR). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.49-7.40 (m, 2H), 7.39-7.25 (m, 6H), 3.49 (br s, 1.7H), 3.22 (br s, 1.9H), 3.08 (br s, 1.8H), 2.65 (br s, 1.5H), 2.39 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 172.11, 167.29, 140.51, 139.41, 137.66, 136.73, 136.33, 134.64, 134.09, 130.78, 130.17, 129.46, 129.28, 128.64, 128.39, 127.62, 127.44, 127.31, 127.15, 61.05, 59.80, 35.68, 32.39, 20.98. HRMS ESI (m/z): $[M+Na]^+$ calcd. for $C_{16}H_{17}NO_2Na$: 278.1157, found: 278.1166.



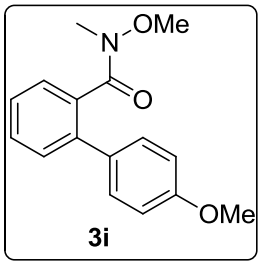
3g

3g: Purification by flash chromatography (petroleum ether/ EtOAc = 5:1) on silica gel to give **3g** (92% yield) as a yellow oil and minor diarylation product (3% yield) (determined by ^{1}H NMR and GC). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.52-7.27 (m, 8H), 3.49 (br s, 1.1H), 3.27 (br s, 1.8H), 3.08 (br s, 1.9H), 2.67 (br s, 0.9H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 170.31, 165.60, 135.75, 133.88, 133.17, 132.96, 131.06, 130.81, 130.73, 130.13, 129.91, 129.79, 129.46, 128.45, 128.37, 128.22, 127.97, 127.76, 127.06, 126.88, 126.72, 126.53, 61.23, 59.91, 35.88, 32.44. HRMS ESI (m/z): $[M+Na]^+$ calcd. for $C_{15}H_{14}NO_2NaCl$: 298.0611, found: 298.0616.



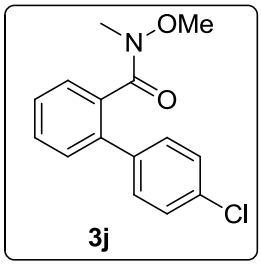
3h

3h: Purification by flash chromatography (petroleum ether/ EtOAc = 5:1) on silica gel to give **3h** (88% yield) as a yellow oil and minor diarylation product (8% yield) (determined by ^{1}H NMR). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.29-7.17 (m, 6H), 7.06 (m, 2H), 3.40 (br s, 1.2H), 3.11 (br s, 1.8H), 2.97 (br s, 1.9H), 2.52 (br s, 1.2H), 2.22 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 171.79, 166.83, 139.11, 138.87, 137.35, 136.69, 136.27, 134.57, 134.00, 129.61, 129.05, 128.80, 128.01, 127.25, 127.17, 126.46, 126.33, 60.70, 59.82, 35.49, 32.09, 20.86. HRMS ESI (m/z): $[M+Na]^+$ calcd. for $C_{16}H_{17}NO_2Na$: 278.1157, found: 278.1160.



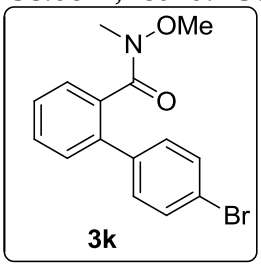
3i

3i: Purification by flash chromatography (petroleum ether/ EtOAc = 2:1) on silica gel to give **3i** (39.1 mg, 72%) as a yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.24-7.14(m, 6H), 6.76 (d, *J* =8.4, 2H), 3.60 (s, 3H), 3.38 (br s, 1.2H), 3.07 (br s, 1.7H), 2.94 (br s, 1.7H), 2.49 (br s, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 171.56, 166.68, 158.87, 158.60, 138.51, 138.27, 134.41, 133.73, 132.43, 131.32, 129.25, 129.05, 128.78, 127.04, 126.72, 126.19, 125.90, 113.30, 60.44, 59.33, 54.62, 35.18, 31.80. HRMS ESI (*m/z*): $[M+Na]^+$ calcd. for $C_{16}H_{17}NO_3Na$: 294.1106, found: 294.1113.



3j

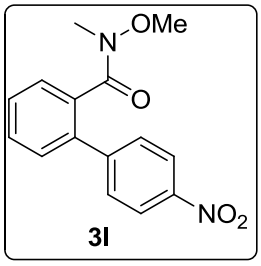
3j: Purification by flash chromatography (petroleum ether/ EtOAc = 5:1) on silica gel to give **3j** (51.8 mg, 94%) as a yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.28-7.17 (m, 8H), 3.37 (br s, 0.9H), 3.09 (br s, 2H), 2.93(br s, 2H), 2.53 (br s, 0.9H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 171.05, 166.20, 138.63, 137.68, 134.47, 132.99, 129.42, 129.03, 128.81, 128.04, 127.65, 126.81, 126.41, 60.57, 59.42, 35.46, 31.90. HRMS ESI (m/z): $[M+Na]^+$ calcd. for $C_{15}H_{14}NO_2NaCl$: 298.0611, found: 298.0617.



3k

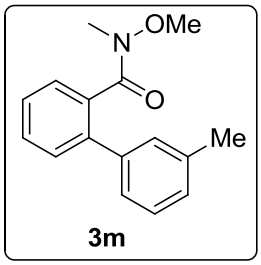
3k: Purification by flash chromatography (petroleum ether/ EtOAc = 5:1) on silica gel to give **3k** (90% yield) as a yellow oil and minor diarylation product (4% yield) (determined by ^{1}H

NMR and GC). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.40 (d, *J* = 7.6 Hz, 2H), 7.34-7.31 (m, 2H), 7.28-7.27 (m, 1H), 7.24-7.19 (m, 3H), 3.42 (br s, 0.9H), 3.15(br s, 2H), 2.98 (br s, 2H), 2.59 (br, 0.8H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 171.23, 166.50, 139.23, 137.91, 134.52, 131.19, 129.91, 129.25, 128.95, 127.80, 127.04, 126.63, 121.80, 121.49, 60.81, 59.61, 35.56, 32.16. HRMS ESI (m/z): $[M+Na]^+$ calcd. for $C_{15}H_{14}NO_2NaBr$: 342.0106, found: 342.0104.



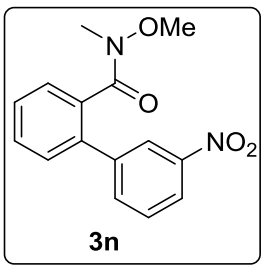
3l

3l: Purification by flash chromatography (petroleum ether/ EtOAc = 4:1) on silica gel to give **3l** (51.2 mg, 89%) as a yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.26 (d, *J* = 8.4 Hz, 2H), 7.61-7.56 (m, 2H), 7.56-7.47 (m,3H), 7.43 (d, *J* = 7.2 Hz, 1H), 7.27 (s, 1H), 3.69-3.33 (br, 3H), 3.11-2.67 (br, 3H). ^{13}C NMR (101 MHz, CDCl3) δ 170.98, 147.42, 137.41, 135.01, 129.85, 129.42, 129.28, 128.42, 127.32, 123.68, 61.25, 32.47, 29.83. HRMS ESI (*m/z*): $[M+Na]^+$ calcd. for $C_{15}H_{14}N_2O_4Na$: 309.0851, found:309.0852.



3m

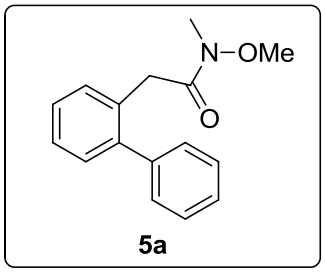
3m: Purification by flash chromatography (petroleum ether/ EtOAc = 5:1) on silica gel to give **3m** (89% yield) as a yellow oil and minor diarylation product (9% yield) (determined by ^{1}H NMR). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.26-7.20 (m, 4H), 7.12-7.10 (m, 3H), 6.98 (s, 1H), 3.32 (br s, 1.3H), 3.09 (br s, 1.8H), 2.93(br s, 1.7H), 2.48 (br, 1.2H), 2.20 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 171.69, 166.50, 140.05, 139.09, 137.33, 134.58, 133.93, 129.46, 128.93, 127.76, 127.14, 126.27, 125.09, 60.53, 59.13, 35.35, 31.99, 21.00. HRMS ESI (*m/z*): $[M+Na]^+$ calcd. for $C_{16}H_{17}NO_2Na$: 278.1157, found:278.1165.



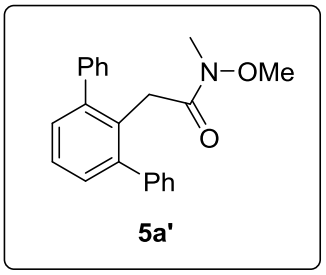
3n

3n: Purification by flash chromatography (petroleum ether/ EtOAc = 3:1) on silica gel to give **3n** (55.0 mg, 96%) as a yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.08 (s, 1H), 7.93 (d, *J* = 7.2, 1H), 7.55 (d, *J* = 4.4 Hz, 1H), 7.35 (t, *J* = 7.6 Hz, 1H), 7.27-7.20 (m, 4H), 3.33-3.16 (br, 3H), 2.90-2.66 (br, 3H) . ^{13}C NMR (101 MHz, $CDCl_3$) δ 170.53, 165.69, 147.60, 141.50, 136.36, 134.61, 134.08, 129.20, 128.94, 128.81, 127.50, 126.44, 122.58, 121.71, 60.56, 59.42, 35.40, 31.73.

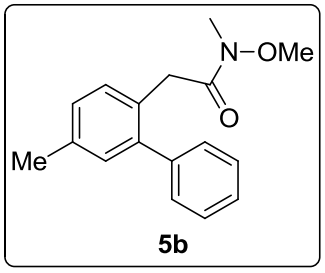
HRMS ESI (*m/z*): $[M+Na]^+$ calcd. for $C_{15}H_{14}N2O_4Na$: 309.0851, found: 309.0853.



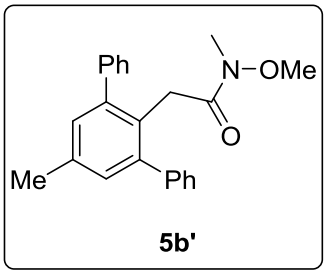
5a: Purification by flash chromatography (petroleum ether/ EtOAc = 8:1) on silica gel to give **5a** (27.2 mg, 43%) as a yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.38-7.29 (m, 8H), 7.28-7.25 (m, 1H), 3.71 (s, 2H), 3.34(s, 3H), 3.12 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ142.44, 141.59, 132.68, 130.35, 130.12, 129.43, 128.24, 127.62, 127.13, 126.93, 60.99, 37.02, 32.41. HRMS ESI (*m/z*): $[M+Na]^+$ calcd. for $C_{16}H_{17}NO_2Na$: 278.1157, found: 278.1168.



5a': Purification by flash chromatography (petroleum ether/ EtOAc =8:1) on silica gel to give **5a'** (18.1 mg, 27%) as a white solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.31-7.28 (m, 8H), 7.28-7.22 (m, 3H), 7.19 (s, 1H), 7.18-7.17 (m, 1H), 3.45 (s, 2H), 3.02 (s, 3H), 2.91 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ173.18, 143.70, 142.18, 130.93, 129.45, 129.30, 128.14, 127.10, 126.57, 60.56, 35.12, 32.32. HRMS ESI (*m/z*): $[M+Na]^+$ calcd. for $C_{22}H_{21}NO_2Na$: 354.1470, found: 354.1458.

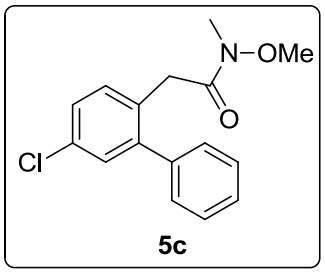


5b: Purification by flash chromatography (petroleum ether/ EtOAc =10:1) on silica gel to give **5b** (21.0 mg, 39%) as a yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.41-7.37 (m, 2H), 7.34-7.29 (m, 3H), 7.26-7.23 (m, 1H), 7.16-7.10 (m, 1H), 7.09 (s, 1H), 3.66 (s, 2H), 3.34 (s, 3H), 3.11 (s, 3H), 2.36 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ142.26, 141.75, 136.49, 130.88, 130.24, 129.58, 129.41, 128.42, 128.20, 127.05, 36.47, 32.07, 21.18. HRMS ESI (*m/z*): $[M+Na]^+$ calcd. for $C_{17}H_{19}NO_2Na$: 292.1313, found: 292.1324.



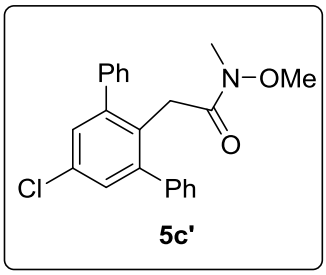
5b': Purification by flash chromatography (petroleum ether/ EtOAc = 10:1) on silica gel to give **5b'** (19.5 mg, 28%) as a white solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.37-7.28 (m, 10H), 7.08 (s, 2H), 3.48 (s, 2H), 3.09 (s, 3H), 2.95 (s, 3H), 2.38 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ143.56, 142.33, 136.04, 130.14, 129.43, 128.11, 127.87, 127.01, 60.50, 34.68, 32.33,

21.14. HRMS ESI (*m/z*): $[M+Na]^+$ calcd. for $C_{23}H_{23}NO_2Na$: 368.1626, found: 368.1626.



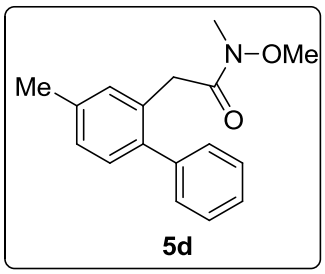
5c

5c: Purification by flash chromatography (petroleum ether/ EtOAc = 10:1) on silica gel to give **5c** (26.3 mg, 45%) as a yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.35-7.25 (m, 3H), 7.24-7.19 (m, 5H), 3.58 (s, 2H), 3.28 (s, 3H), 3.05 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ172.56, 143.99, 140.26, 132.53, 131.85, 131.24, 129.97, 129.21, 128.39, 127.64, 61.04, 36.37, 32.41. HRMS ESI (*m/z*): $[M+Na]^+$ calcd. for $C_{16}H_{16}NO_2NaCl$: 312.0767, found: 312.0764.



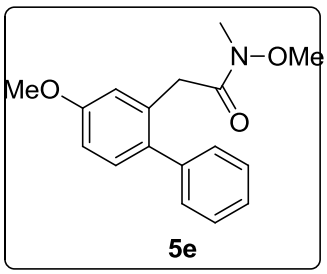
5c'

5c': Purification by flash chromatography (petroleum ether/ EtOAc = 10:1) on silica gel to give **5c'** (17.9 mg, 24%) as a white solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ7.33-7.24 (m, 10H), 7.19 (s, 2H), 3.39 (s, 2H), 3.01 (s, 3H), 2.91 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ172.86, 145.14, 140.85, 132.01, 129.72, 129.19, 129.06, 128.27, 127.55, 60.55, 34.66, 32.22. HRMS ESI (*m/z*): $[M+Na]^+$ calcd. for $C_{22}H_{20}NO_2NaCl$: 388.1080, found: 388.1083.



5d

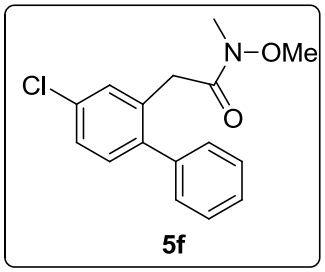
5d: Purification by flash chromatography (petroleum ether/ EtOAc = 10:1) on silica gel to give **5d** (43.8 mg, 81%) as a yellow solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.29-7.28 (m, 2H), 7.23-7.22 (m, 3H), 7.16-7.12 (m, 2H), 7.03 (m, 1H), 3.60(s, 2H), 3.35 (s, 3H), 3.09 (s, 3H), 2.82 (s, 2H).^{13}C NMR (101 MHz, $CDCl_3$) δ172.76, 143.35, 142.36, 138.00, 131.55, 129.48, 129.31, 128.15, 127.71, 126.97, 126.72, 60.99, 34.45, 32.56, 20.35. HRMS ESI (*m/z*): $[M+Na]^+$ calcd. for $C_{17}H_{19}NO_2Na$: 292.1313, found: 292.1311.



5e

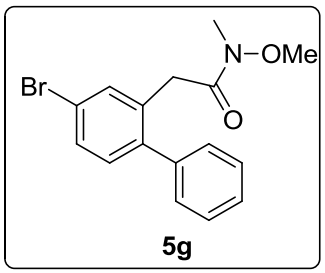
5e: Purification by flash chromatography (petroleum ether/ EtOAc = 5:1) on silica gel to give **5e** (35.6mg, 61%) as a yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.32-7.29 (m, 2H), 7.25-7.21 (m, 3H), 7.12 (d, *J* = 8.4Hz, 1H), 6.84 (d, *J* = 2.4Hz, 1H), 6.78 (dd, *J* =8.4, 2.8Hz, 1H), 3,76 (s, 3H), 3.61 (s, 2H), 3.27 (s, 3H), 3.04 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ172.74, 158.95,

141.30, 135.08, 133.86, 131.13, 129.67, 128.21, 126.87, 115.41, 112.76, 60.89, 55.36, 37.21, 32.46. HRMS ESI (*m/z*): $[M+Na]^+$ calcd. for $C_{17}H_{19}NO_3Na$: 308.1263, found: 308.1259.



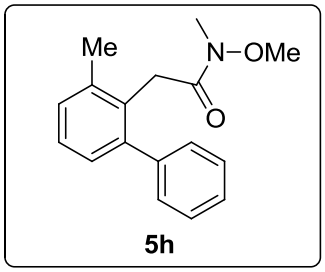
5f

5f: Purification by flash chromatography (petroleum ether/ EtOAc = 10:1) on silica gel to give **5f** (48.6 mg, 84%) as a yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.42-7.38 (m, 2H), 7.36-7.32 (m, 2H), 7.29-7.27 (m, 3H), 7.19 (d, *J* =8.0 Hz, 1H), 3.67(s, 2H), 3.36 (s, 3H), 3.13 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) 172.25, 140.94, 140.37, 134.52, 133.28, 131.28, 130.37, 129.30, 128.34, 127.44, 127.10, 61.04, 36.75, 32.38. HRMS ESI (*m/z*): $[M+Na]^+$ calcd. for $C_{16}H_{16}NO_2NaCl$: 312.0767, found: 312.0767.



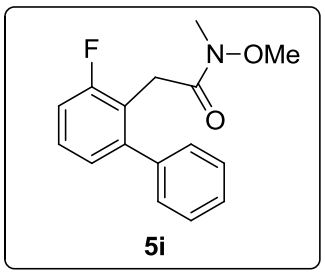
5g

5g: Purification by flash chromatography (petroleum ether/ EtOAc = 5:1) on silica gel to give **5g** (47.9 mg, 72%) as a yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.42 (d, *J*=2.0 Hz, 1H), 7.36-7.32 (m, 2H), 7.31-7.25 (m, 2H), 7.21-7.18 (m, 2H), 7.05 (d, *J* =8.4 Hz, 1H), 3.58 (s, 2H), 3.28 (s, 3H), 3.05 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ172.16, 141.37, 140.32, 134.85, 133.27, 131.56, 130.03, 129.21, 128.34, 127.46, 121.44, 61.03, 36.69, 32.42. HRMS ESI (*m/z*): $[M+Na]^+$ calcd. for $C_{16}H_{16}NO_2NaBr$: 356.0262, found:356.0259.



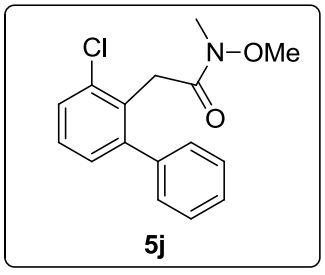
5h

5h: Purification by flash chromatography (petroleum ether/ EtOAc =10:1) on silica gel to give **5h** (39.4 mg, 73%) as a yellow solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.33-7.27 (m, 2H), 7.24-7.22 (m, 3H), 7.16-7.09 (m, 2H), 7.05-7.01 (m, 1H), 3.60 (s, 2H), 3.35(s, 3H), 3.08 (s, 3H), 2.23 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 172.74, 143.34, 142.36, 137.99, 131.55, 129.48, 129.31, 128.15, 127.71, 126.96, 126.71, 60.89, 34.45, 32.53, 20.28. HRMS ESI (*m/z*): $[M+Na]^+$ calcd. for $C_{17}H_{19}NO_2Na$: 292.1313, found: 292.1317.



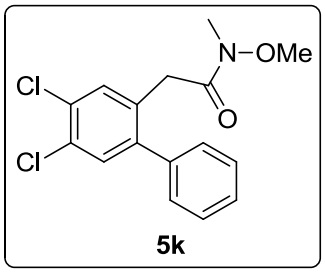
5i

5i: Purification by flash chromatography (petroleum ether/ EtOAc = 5:1) on silica gel to give **5i** (36.5 mg, 67%) as a yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.34-7.31 (m, 1H), 7.30-7.29 (m, 1H), 7.28-7.26 (m, 1H), 7.26-7.24 (m, 1H), 7.24-7.22 (m, 1H), 7.21-7.17 (m, 1H), 3.64 (s, 2H), 3.01(s, 3H), 3.00 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ171.75, 161.86 (d, *J* = 246.44 Hz), 144.91 (d, *J* = 4.14 Hz), 140.28 (d, *J* = 2.63 Hz), 129.25, 128.34, 128.12 (d, *J* = 9.09 Hz), 127.53, 125.55 (d, *J* =9.80 Hz), 120.86 (d, *J* =16.16 Hz), 114.07 (d, *J* =16.16 Hz), 61.07, 32.47, 30.63. HRMS ESI (*m/z*): $[M+Na]^+$ calcd. for $C_{16}H_{16}NO_2NaF$: 296.1063, found: 296.1068.



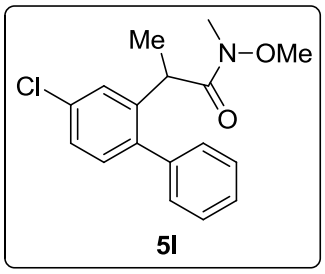
5j

5j: Purification by flash chromatography (petroleum ether/ EtOAc = 5:1) on silica gel to give **5j** (36.3 mg, 63%) as a yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.33-7.31 (m, 2H), 7.29-7.26 (m, 2H), 7.25-7.23 (m, 2H), 7.19-7.15 (m, 1H), 7.11-7.09 (dd, *J* =7.6, 0.8 Hz, 1H), 3.74 (s, 2H), 3.48 (s, 3H), 3.11 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) 171.70, 145.13, 141.08, 135.82, 131.53, 129.13, 128.53, 128.34, 127.87, 127.53, 61.09, 35.35, 32.52. HRMS ESI (*m/z*): $[M+Na]^+$ calcd. for $C_{16}H_{16}NO_2NaCl$: 312.0767, found: 312.0766.



5k

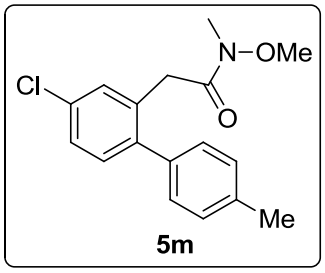
5k: Purification by flash chromatography (petroleum ether/ EtOAc = 5:1) on silica gel to give **5k** (38.1mg, 59%) as a yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.37 (s, 1H), 7.35-7.33 (m, 1H), 7.32-7.26 (m, 3H), 7.20-7.19 (m, 1H), 7.18-7.17 (m, 1H), 3.56 (s, 2H), 3.30 (s, 3H), 3.05 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 171.77, 142.42, 139.29, 132.90, 132.32, 131.60, 131.39, 130.77, 129.13, 128.48, 127.89, 61.27，36.18, 32.40. HRMS ESI (*m/z*): $[M+Na]^+$ calcd. for $C_{16}H_{15}NO_2NaCl_2$: 346.0378, found: 346.0376.



5l

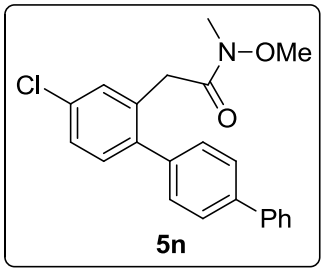
5l: Purification by flash chromatography (petroleum ether/ EtOAc = 5:1) on silica gel to give **5l** (27.2 mg, 45%) as a yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.45-7.40 (m,

3H), 7.39-7.36 (m, 1H), 7.36-7.29 (m, 2H), 7.26-7.23 (m, 1H), 7.17 (d, *J* =8.4 Hz, 1H), 4.08 (m, 1H), 3.06 (br, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) δ174.71, 141.29, 140.53, 139.80, 133.80, 131.48, 129.33, 128.37, 127.49, 127.29, 126.86, 60.16, 38.05, 32.36, 19.92. HRMS ESI (*m/z*): $[M+Na]^+$ calcd. for $C_{17}H_{18}NO_2NaCl$: 326.0924, found: 326.0923.



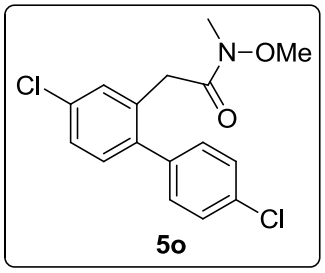
5m

5m: Purification by flash chromatography (petroleum ether/ EtOAc = 5:1) on silica gel to give **5m** (48.0 mg, 79%) as a yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.25 (t, *J* =2.0 Hz, 1H), 7.17 (dd, *J* =8.0, 2.0 Hz, 1H), 7.20 (d, *J* =8.0 Hz, 2H), 7.11-7.06 (m, 3H), 3.60 (s, 2H), 3.31 (s, 3H), 3.05(s, 3H), 2.30(s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ172.35, 140.90, 137.38, 137.11, 134.54, 133.05, 131.36, 130.22, 129.14, 129.01, 127.04, 61.04, 36.78, 32.36, 21.25. HRMS ESI (*m/z*): $[M+Na]^+$ calcd. for $C_{17}H_{18}NO_2NaCl$: 326.0924, found: 326.0921.



5n

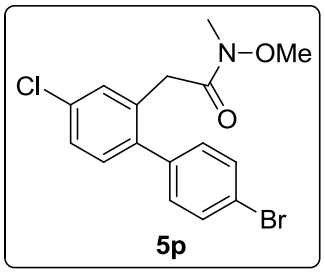
5n: Purification by flash chromatography (petroleum ether/ EtOAc = 5:1) on silica gel to give **5n** (52.2 mg, 71%) as a yellow solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.65-7.61 (m, 4H), 7.48-7.44 (m, 2H), 7.38-7.35 (m, 4H), 7.29 (dd, *J* =8.4, 2.4 Hz, 1H), 7.24-7.22 (m, 1H), 3.72 (s, 2H), 3.39 (s, 3H), 3.14 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 172.25, 140.65, 140.56, 140.27, 139.36, 134.60, 133.38, 131.32, 130.46, 129.77, 128.98, 127.58, 127.20, 127.13, 127.03, 61.09, 36.78, 32.41. HRMS ESI (*m/z*): $[M+Na]^+$ calcd. for $C_{22}H_{20}NO_2NaCl$: 388.1080, found: 388.1083.



5o

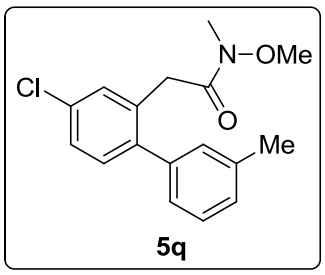
5o: Purification by flash chromatography (petroleum ether/ EtOAc = 5:1) on silica gel to give **5o** (44.7 mg, 69%) as a yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.30 (t, *J* =2.4 Hz, 1H), 7.28 (t, *J* =2.4 Hz, 1H), 7.25 (d, *J* =2.0 Hz, 1H), 7.20 (dd, *J* =6.0, 2.0 Hz, 1H), 7.16 (t, *J* = 2.4 Hz, 1H), 7.14 (t, *J* = 2.0 Hz, 1H), 7.07 (d, *J* = 8.4 Hz, 1H), 3.57 (s, 2H), 3.37 (s, 3H), 3.06 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ171.98, 139.74, 138.78, 134.52, 133.64, 133.57,

131.20, 130.66, 130.54, 128.51, 127.25, 61.14, 36.61, 32.40. HRMS ESI (*m/z*): $[M+Na]^+$ calcd. for $C_{16}H_{15}NO_2NaCl_2$: 346.0378, found: 346.0374.



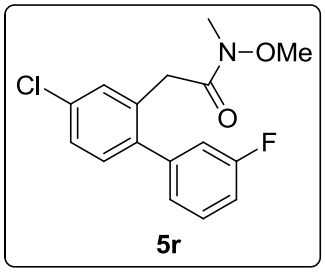
5p

5p: Purification by flash chromatography (petroleum ether/ EtOAc = 5:1) on silica gel to give **5p** (52.9 mg,72%) as a yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.45 (d, *J* = 8.4 Hz, 2H), 7.25 (d, *J* = 1.0 Hz, 1H), 7.20 (dd, *J* = 8.0, 1.6 Hz, 1H), 7.08 (t, *J* = 8.4 Hz, 3H), 3.57 (s, 2H), 3.37 (s, 3H), 3.06 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 172.05, 139.76, 139.29, 134.47, 133.70, 131.49, 131.15, 131.02, 130.57, 127.29, 121.76, 61.17, 36.62, 32.46. HRMS ESI (*m/z*): $[M+Na]^+$ calcd. for $C_{16}H_{15}NO_2NaClBr$: 389.9872, found: 389.9872.



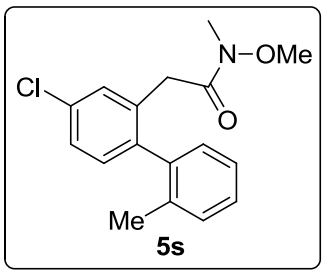
5q

5q: Purification by flash chromatography (petroleum ether/ EtOAc = 5:1) on silica gel to give **5q** (41.9 mg, 69%) as a white solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.26 (d, *J* = 2.4 Hz, 1H), 7.22-7.17 (m, 2H), 7.11-7.00 (m, 3H), 6.99 (d, *J* = 8.0 Hz, 2H), 3.59 (s, 2H), 3.29 (s, 3H), 3.06 (s, 3H), 2.30 (s, 3H) . ^{13}C NMR (101 MHz, $CDCl_3$) δ 172.30, 141.03, 140.28, 137.94, 134.50, 133.13, 131.22, 130.35, 129.98, 128.31, 128.14, 127.03, 126.25, 60.98, 36.80, 32.37, 21.51. HRMS ESI (*m/z*): $[M+Na]^+$ calcd. for $C_{17}H_{18}NO_2NaCl$: 326.0924, found: 326.0925.



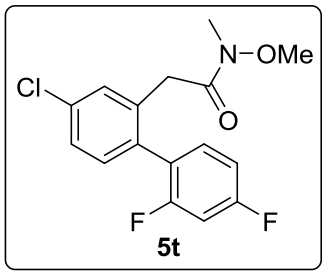
5r

5r: Purification by flash chromatography (petroleum ether/ EtOAc = 5:1) on silica gel to give **5r** (46.3 mg, 75%) as a yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.31-7.25 (m, 2H), 7.21-7.18 (m, 1H), 7.09 (d, *J* = 8.0 Hz, 1H), 7.00-6.91 (m, 3H), 3.58 (s, 2H), 3.35 (s, 3H), 3.06 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ171.97, 162.56 (d, *J* =251.5 Hz), 142.52 (d, *J* =7.7 Hz), 139.66, 134.50, 133.75, 131.10, 130.60, 129.90(d, *J* =8.1 Hz), 127.23, 125.13(d, *J* =3.0 Hz), 116.35 (d, *J* =21.6 Hz), 114.38 (d, *J* =10.9 Hz), 61.09, 36.63, 32.39. HRMS ESI (*m/z*): $[M+Na]^+$ calcd. for $C_{16}H_{15}NO_2NaClF$: 330.0673, found: 330.0677.



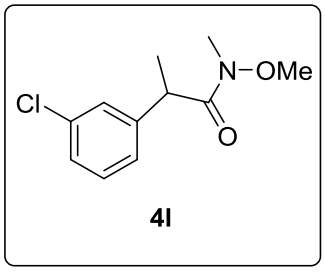
5s

5s: Purification by flash chromatography (petroleum ether/ EtOAc = 5:1) on silica gel to give **5s** (39.9 mg, 66%) as a yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.30-7.29 (d, *J* = 2.0 Hz, 2H), 7.22-7.16 (m, 3H), 7.15-7.10 (m, 1H), 7.02-6.99 (m, 2H), 3.42 (d, *J* = 8.0 Hz, 1H), 3.35 (d, *J* = 8.0 Hz, 1H), 3.21 (s, 3H), 3.00 (s, 3H), 1.20 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ171.72, 140.17, 139.65, 136.21, 135.07, 133.13, 130.92, 130.22, 130.09, 129.79, 127.82, 127.03, 125.68, 60.93, 36.40, 32.13, 20.02. HRMS ESI (*m/z*): $[M+Na]^+$ calcd. for $C_{17}H_{18}NO_2NaCl$: 326.0924, found: 326.0920.



5t

5t: Purification by flash chromatography (petroleum ether/ EtOAc = 5:1) on silica gel to give **5t** (35.5 mg, 54%) as a yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.31 (d, *J* = 2.0 Hz, 1H), 7.22 (dd, J = 10.4, 2.4 Hz, 1H), 7.19-7.13 (m, 1H), 7.08 (d, J = 8.0 Hz, 1H), 6.88-6.84 (m, 1H) , 6.84-6.80 (m, 1H), 3.53 (s, 2H), 3.35 (s, 3H), 3.02 (s, 3H). ^{13}C NMR (101 MHz, CDCl3) δ 171.65, 162.73 (dd, *J* =250.5, 12.1 Hz), 159.60 (dd, *J* =249.5, 12.1 Hz), 135.83, 134.32, 133.56, 132.75 (dd, *J* =9.1, 5.1 Hz), 131.85, 130.36, 127.26, 123.63 (dd, *J* =16.2, 4.4 Hz), 123.63 (dd, *J* =16.2, 4.0 Hz), 104.06 (t, *J* =25.3 Hz), 61.15, 36.65, 32.36. HRMS ESI (*m/z*): $[M+Na]^+$ calcd. for $C_{16}H_{14}NO_2NaClF_2$: 348.0579, found: 348.0581.

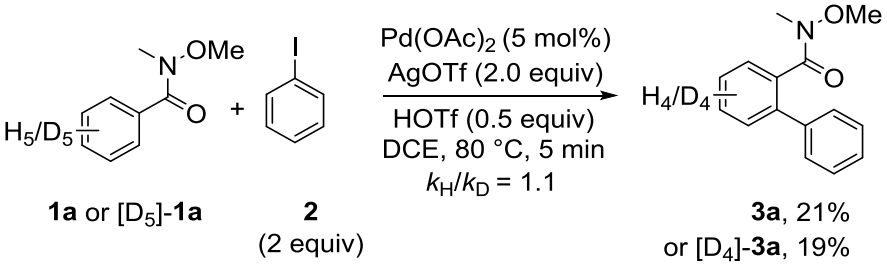


4l

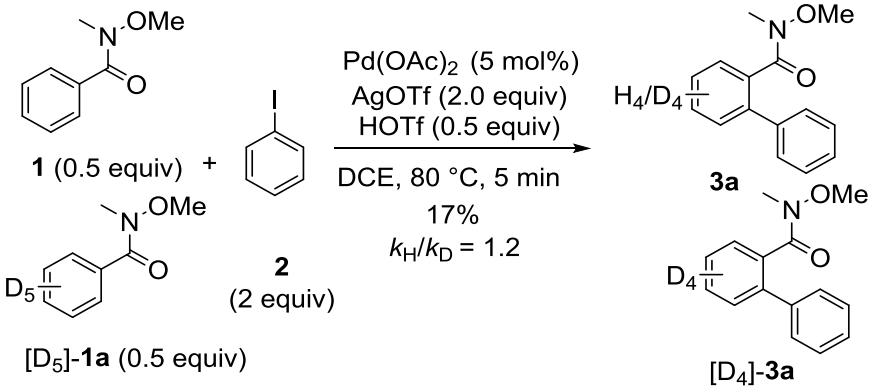
4l: ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.33 (s, 1H), 7.23-7.13 (m, 3H), 4.14 (m, 1H), 3.34 (s, 3H), 3.12 (s, 3H), 1.41 (d, *J* = 8.0Hz, 3H). ^{13}C NMR (101 MHz, CDCl3) δ 173.90, 143.47, 133.74, 129.43, 127.29, 126.45, 125.53, 60.69, 41.01, 31.77, 18.96. HRMS ESI (*m/z*): $[M+Na]^+$ calcd. for $C_{11}H_{14}NO_2NaCl$: 250.0611, found: 250.0619.

Mechanistic Investigation:

Deuterium Kinetic Iisotope Effect Experiment (KIE)



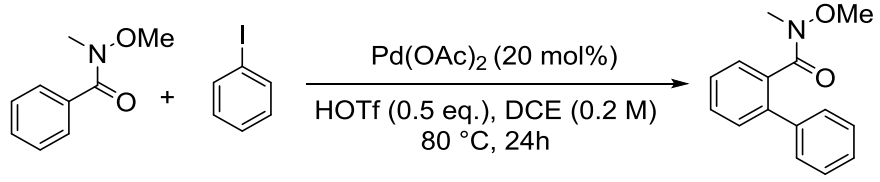
1a or [D_5]-**1a** **2** (2 equiv) **3a**, 21% or [D_4]-**3a**, 19%



1 (0.5 equiv) + **2** (2 equiv) → **3a**

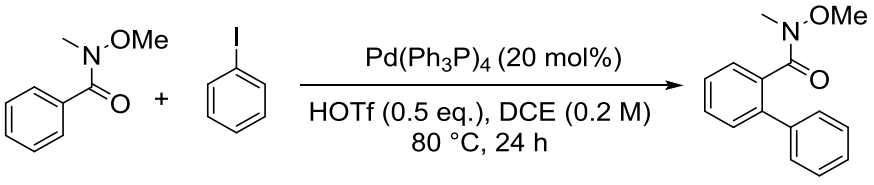
[D_5]-**1a** (0.5 equiv) → [D_4]-**3a**

Control Experiments



1a (0.2 mmol**) 2** (2 equiv) → **3a**

no AgOTf	27%
20 mol% AgOTf	51%
2.0 equiv AgOTf	91%



1a (0.2 mmol**) 2** (2 equiv) → **3a**

no AgOTf	N.R.
20 mol% AgOTf	14%
40 mol% AgOTf	31%
1.0 equiv AgOTf	81%
2.0 equiv AgOTf	91%

References:

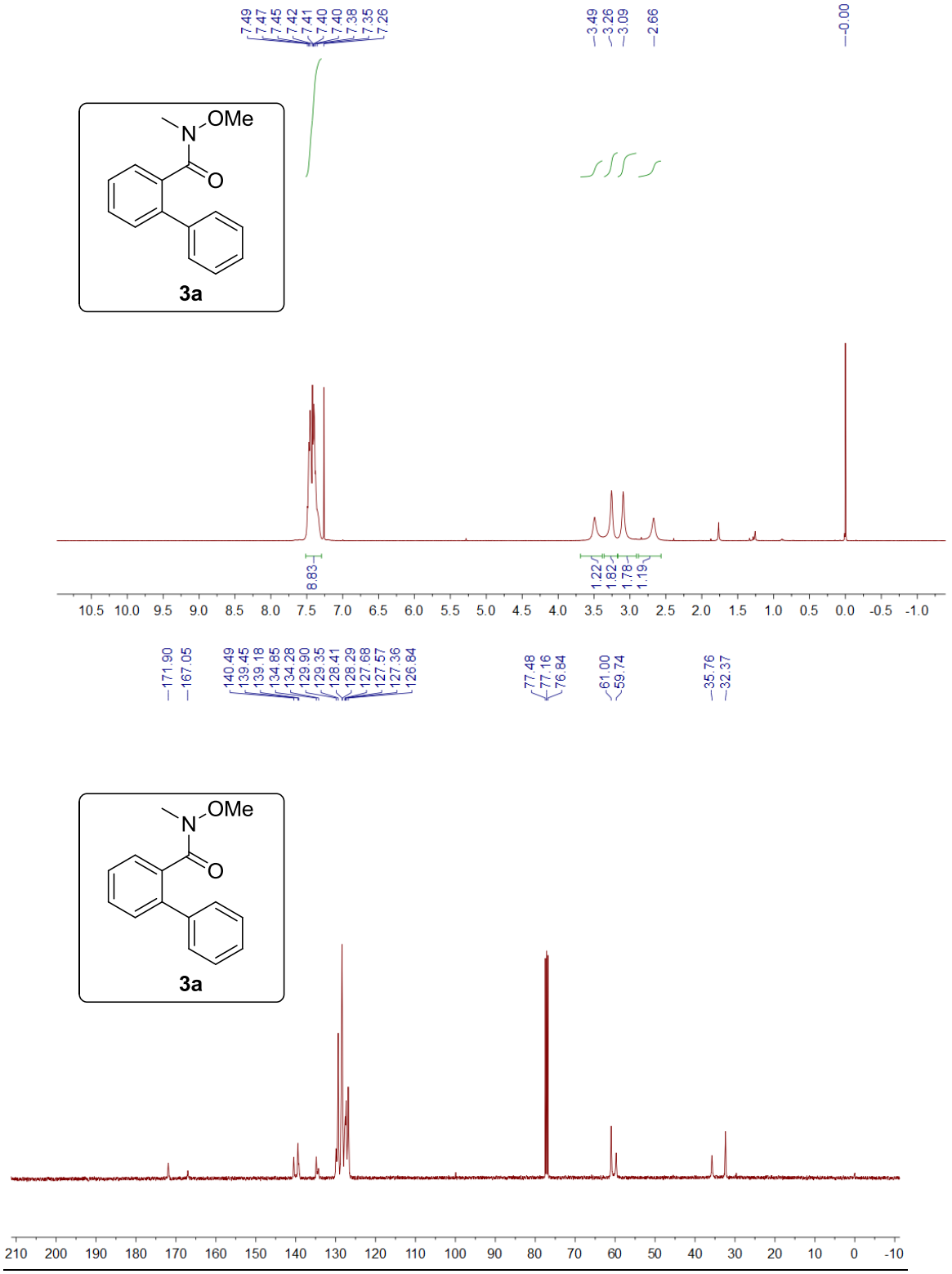
[1] K.-J. Hana, M. Kim, *Lett. Org. Chem.* **2007**, *4*, 20.

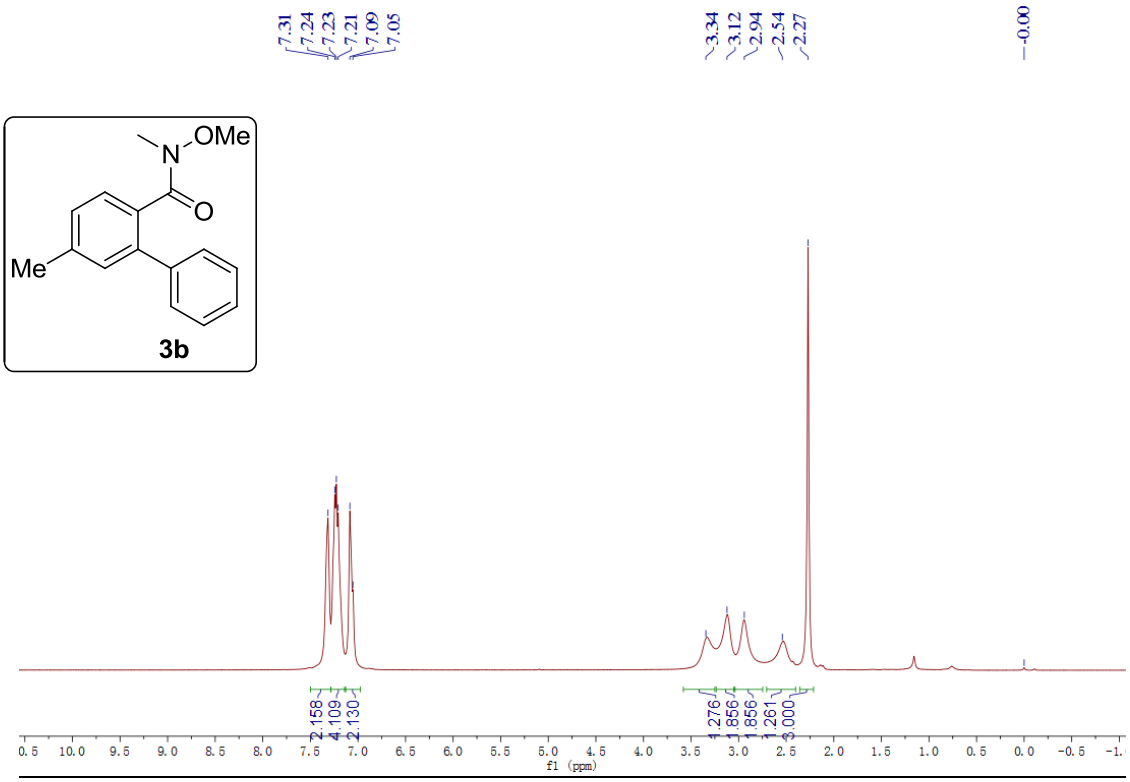
[2] H. A. Duong, R. E. Gilligan, M. L. Cooke, R. J. Phipps, M. J.Gaunt, *Angew. Chem. Int.Ed.* **2011**, *50*, 463.

[3] M. Schlosser, J. H. Choi, S. Takagishi, *Tetrahedron* **1990**, *46*, 5633.

[4] (a) M. Jithunsa, M. Ueda, O. Miyata, *Org. Lett*. **2011**, *13*, 518. (b) J. R. Martinelli, D. M. M. Freckmann, S. L. Buchwald, *Org. Lett*., **2006**, *8*, 4795.

Copies of ^{1}H and ^{13}C Spectra

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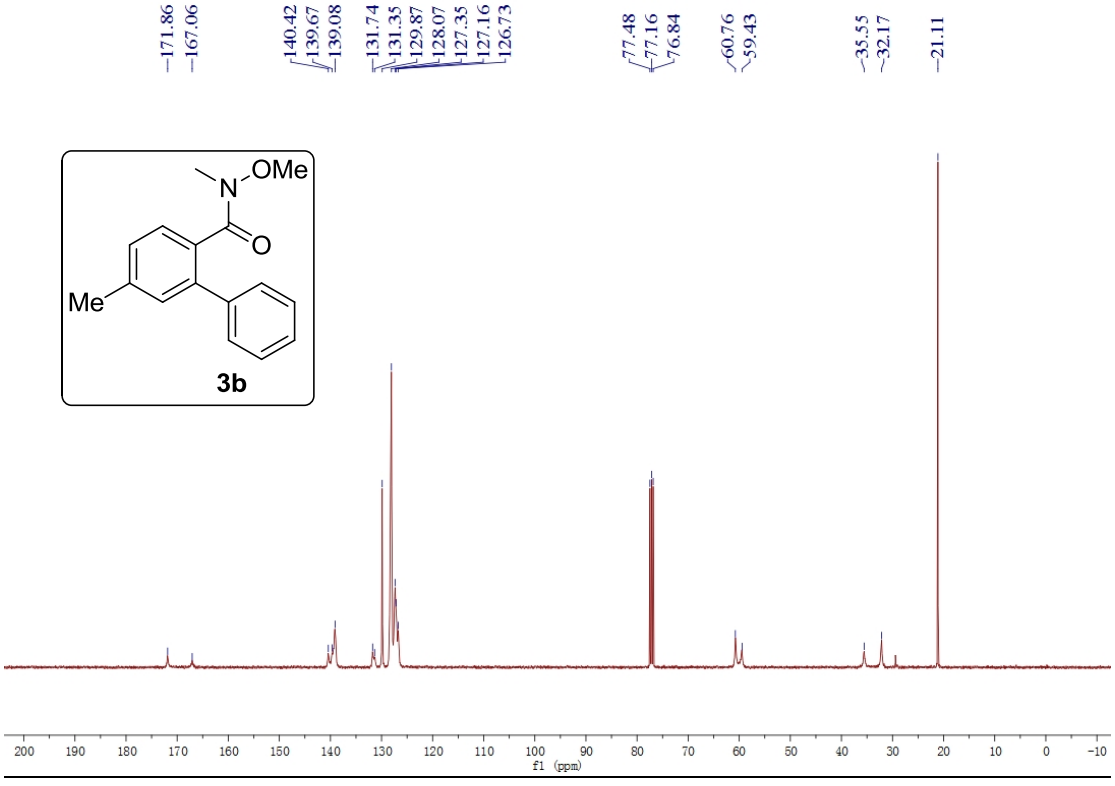
7.24
7.23
7.21
7.09
7.05
3.34
3.12
2.94
2.54
2.27
0.00
OMe
N
O
Me
3b
2.158
4.109
2.130
1.276
1.856
1.856
1.261
3.000
f1 (ppm)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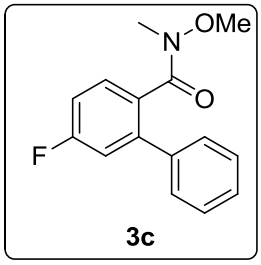
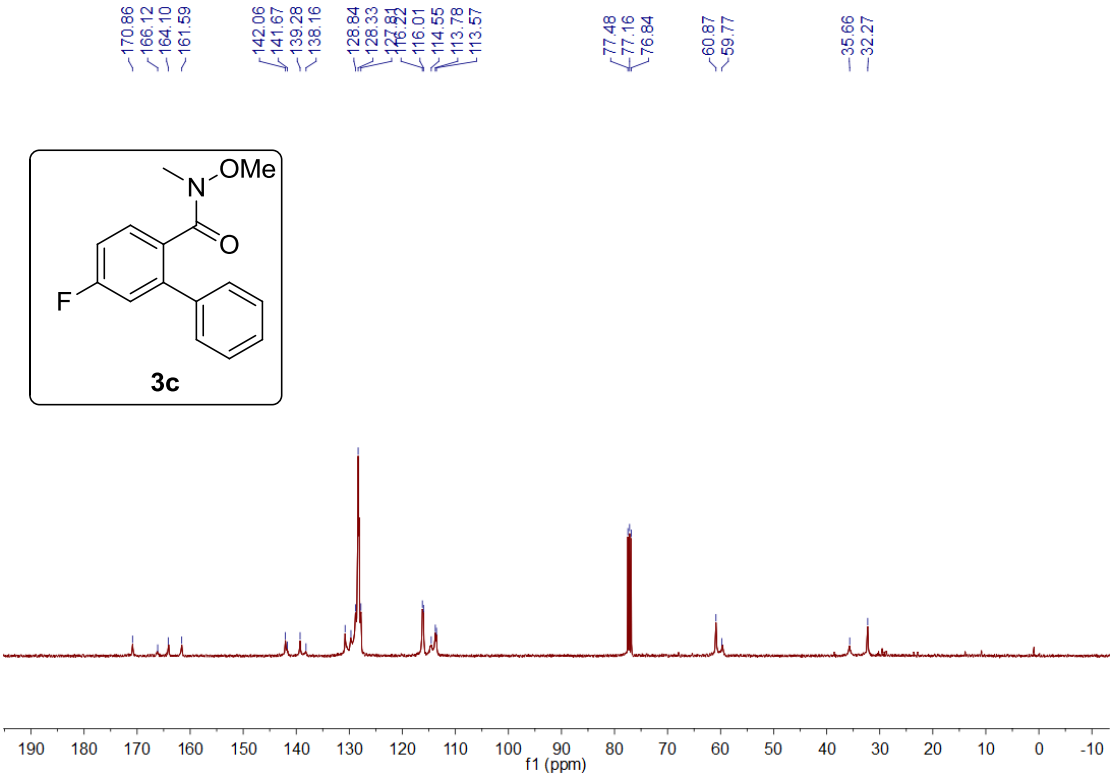
167.06
140.42
139.67
139.08
131.74
131.35
129.87
128.07
127.35
127.16
126.73
77.48
77.16
76.84
60.76
59.43
35.55
32.17
21.11
OMe
N
O
Me
3b
f1 (ppm)


OMe
N
O
F

3c

7.31
7.29
7.27
7.25
7.19
7.18
7.16
7.10
7.08
7.06
7.04
7.00
7.00
6.98
6.97
6.96
6.94
3.38
3.12
2.95
2.53
0.00
6.24
2.16
1.22
2.03
1.94
0.89
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5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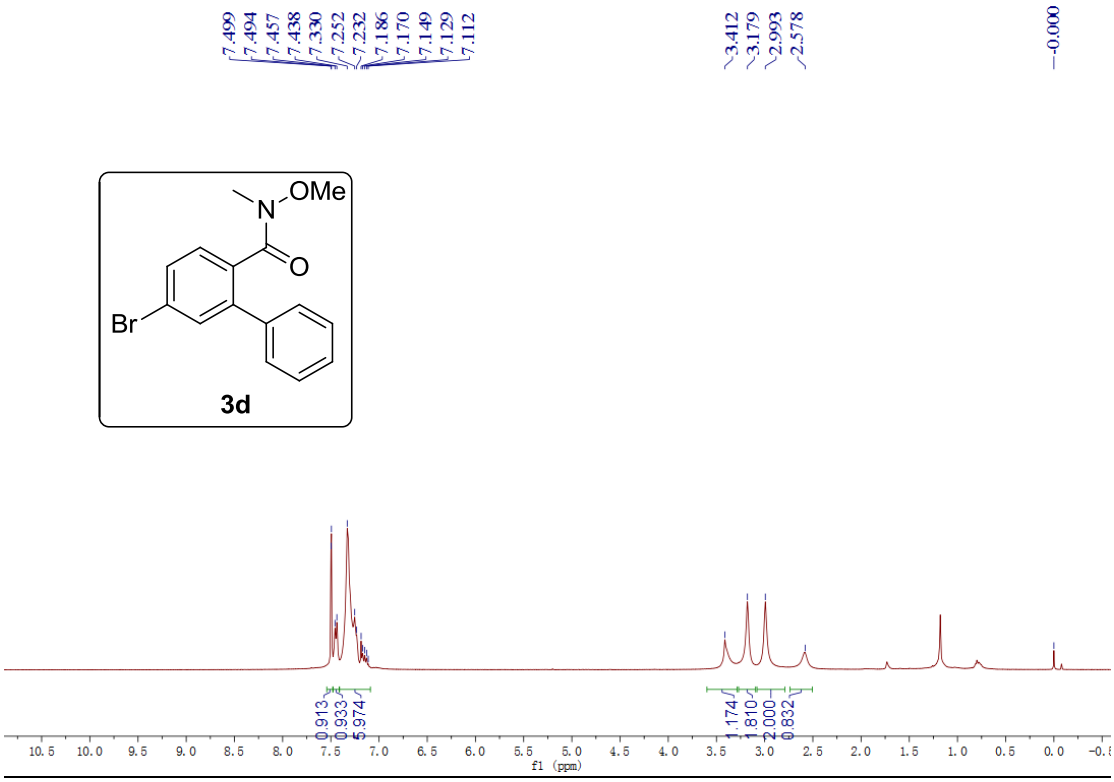
166.12
164.10
161.59
142.06
141.67
139.28
138.16
128.84
128.33
127.81
116.22
116.01
114.55
113.78
113.57
77.48
77.16
76.84
60.87
59.77
35.66
32.27
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

OMe
N
O
F

3c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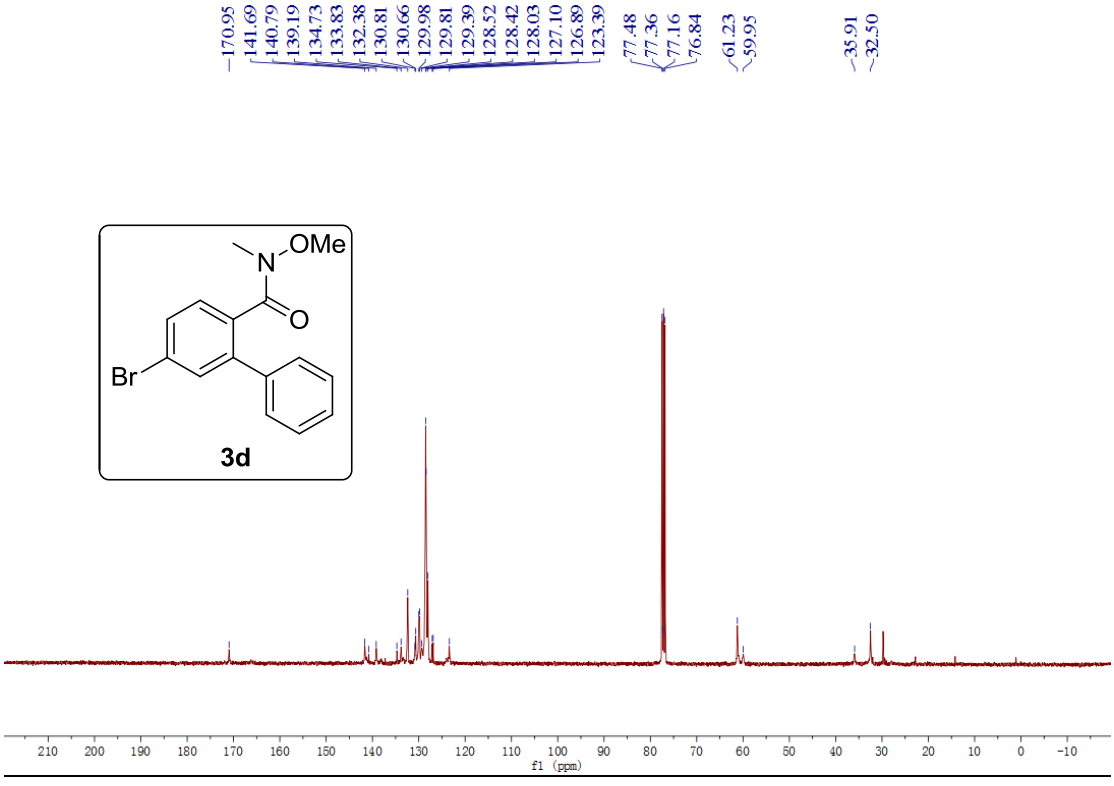
7.129
7.112
3.412
3.179
2.993
2.578
0.000
OMe
N
O
Br
3d
0.913
0.933
5.974
1.174
1.810
2.000
0.832
f1 (ppm)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129.98
129.81
129.39
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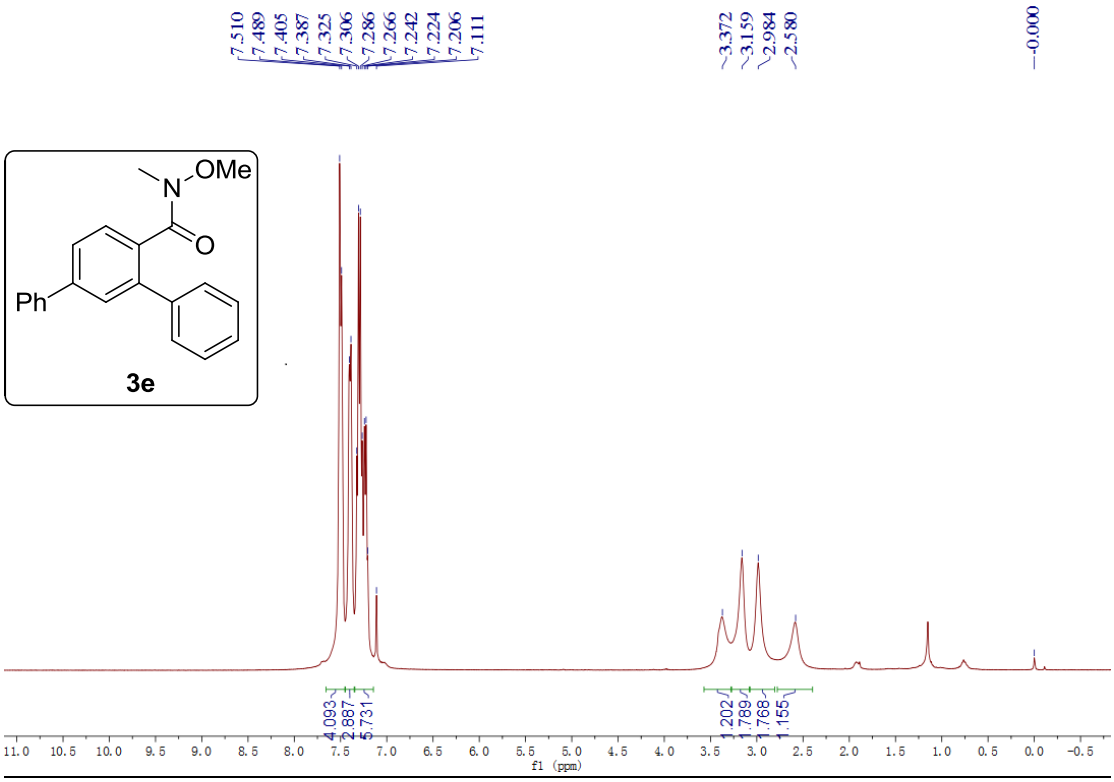
128.03
127.10
126.89
123.39
77.48
77.36
77.16
76.84
61.23
59.95
35.91
32.50
OMe
N
O
Br
3d
f1 (ppm)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7.224
7.206
7.111
3.372
3.159
2.984
2.580
0.000
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N
O
Ph
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4.093
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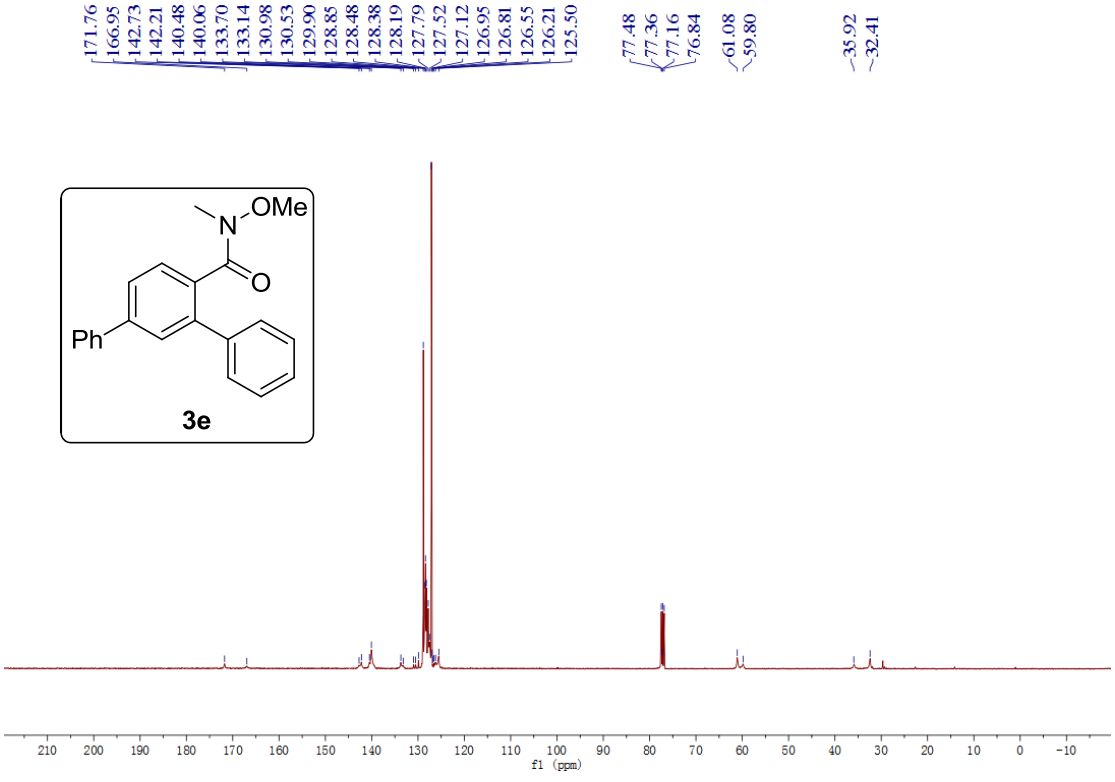
1.768
1.155
f1 (ppm)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128.48
128.38
128.19
127.79
127.52
127.12
126.95
126.81
126.55
126.21
125.50
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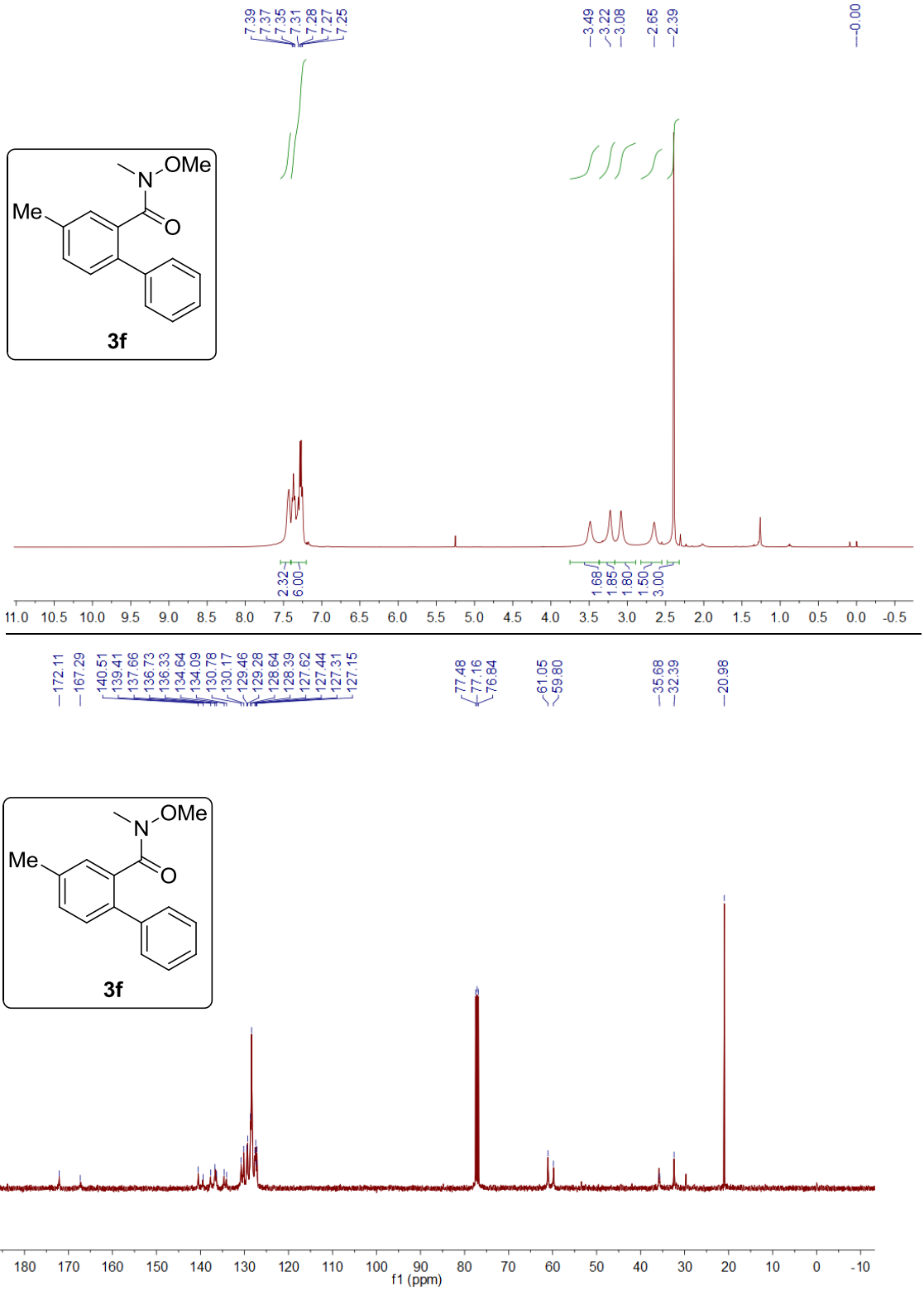
32.41
OMe
N
O
Ph
3e
f1 (ppm)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7.25
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2.39
0.00
OMe
N
Me
O
3f
2.32
6.00
1.68
1.85
1.80
1.50
3.00
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
172.11
167.29
140.51
139.41
137.66
136.73
136.33
134.64
134.09
130.78
130.17
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129.28
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127.31
127.15
77.48
77.16
76.84
61.05
59.80
35.68
32.39
20.98
OMe
N
Me
O
3f
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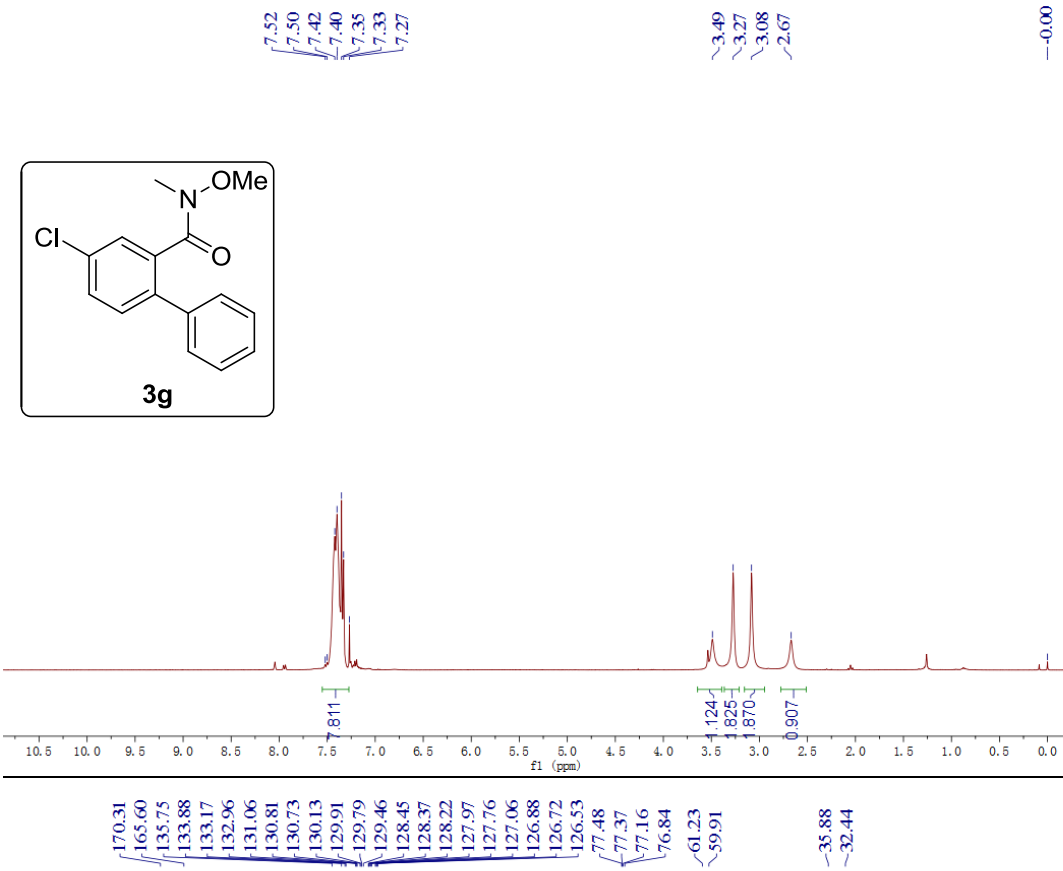
f1 (ppm)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3.27
3.08
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OMe
N
Cl
O
3g
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1.825
1.870
0.907
f1 (ppm)
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133.17
132.96
131.06
130.81
130.73
130.13
129.91
129.79
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128.45
128.37
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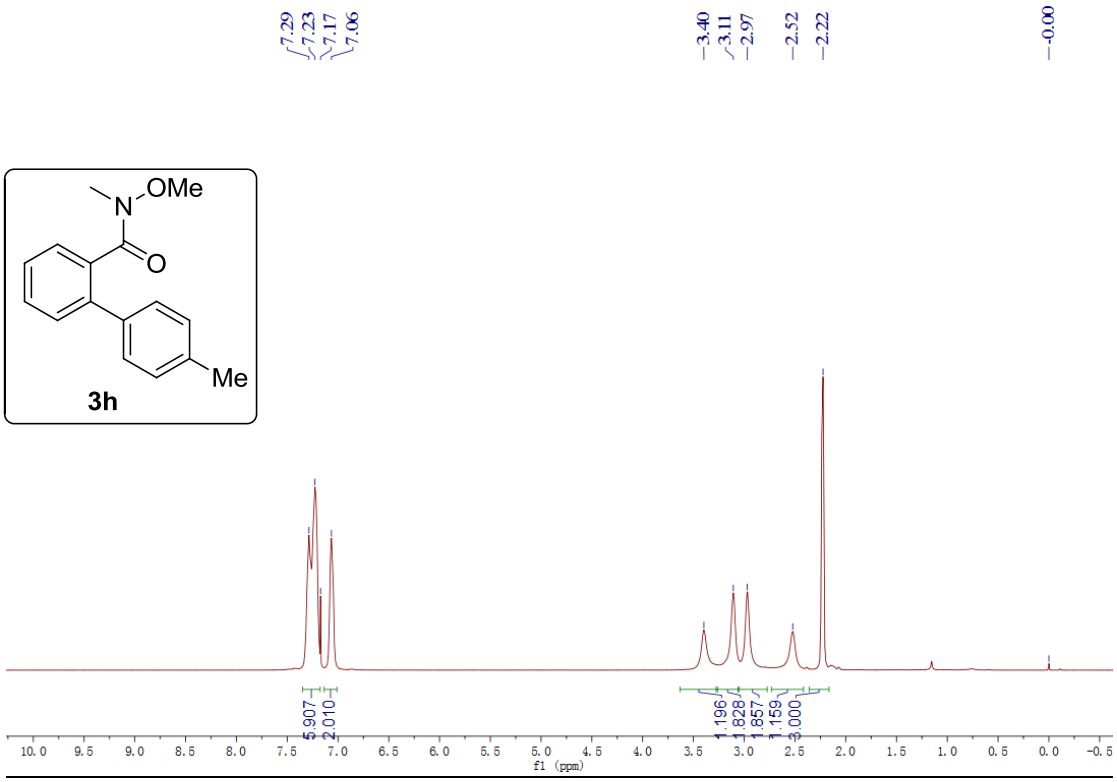
32.44
OMe
N
Cl
O
3g
f1 (ppm)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7.06
3.40
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2.52
2.22
0.00
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O
Me
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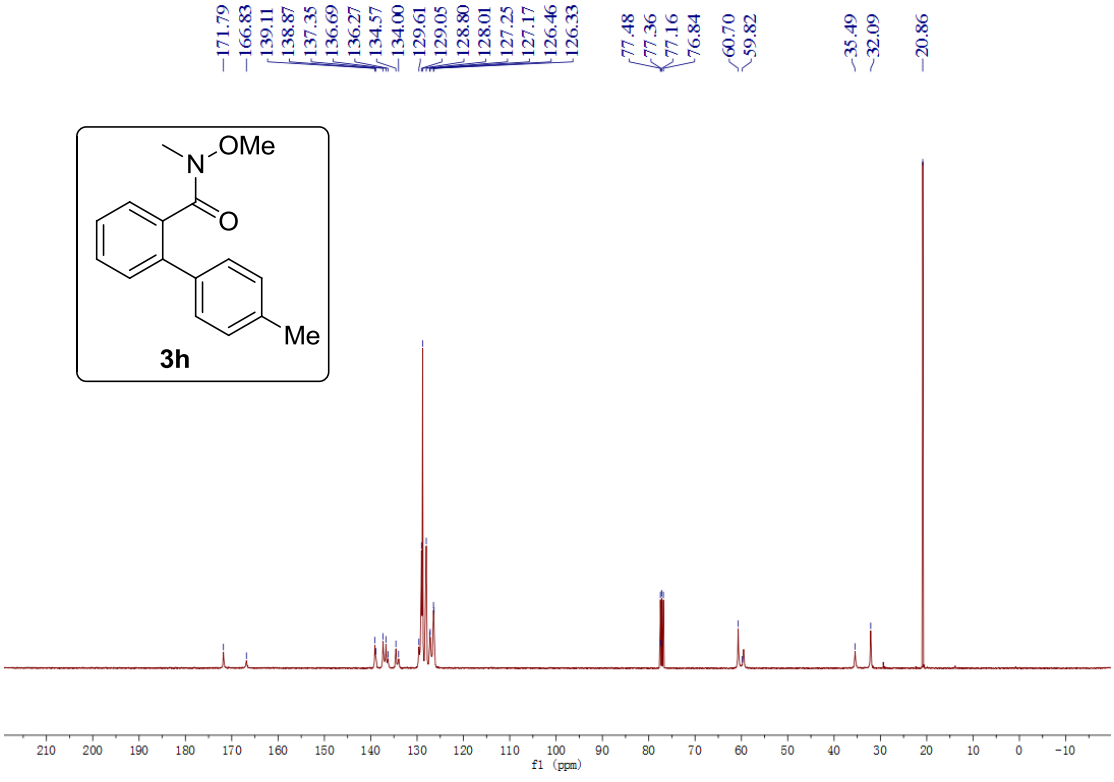
3.000
f1 (ppm)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128.01
127.25
127.17
126.46
126.33
77.48
77.36
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59.82
35.49
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N
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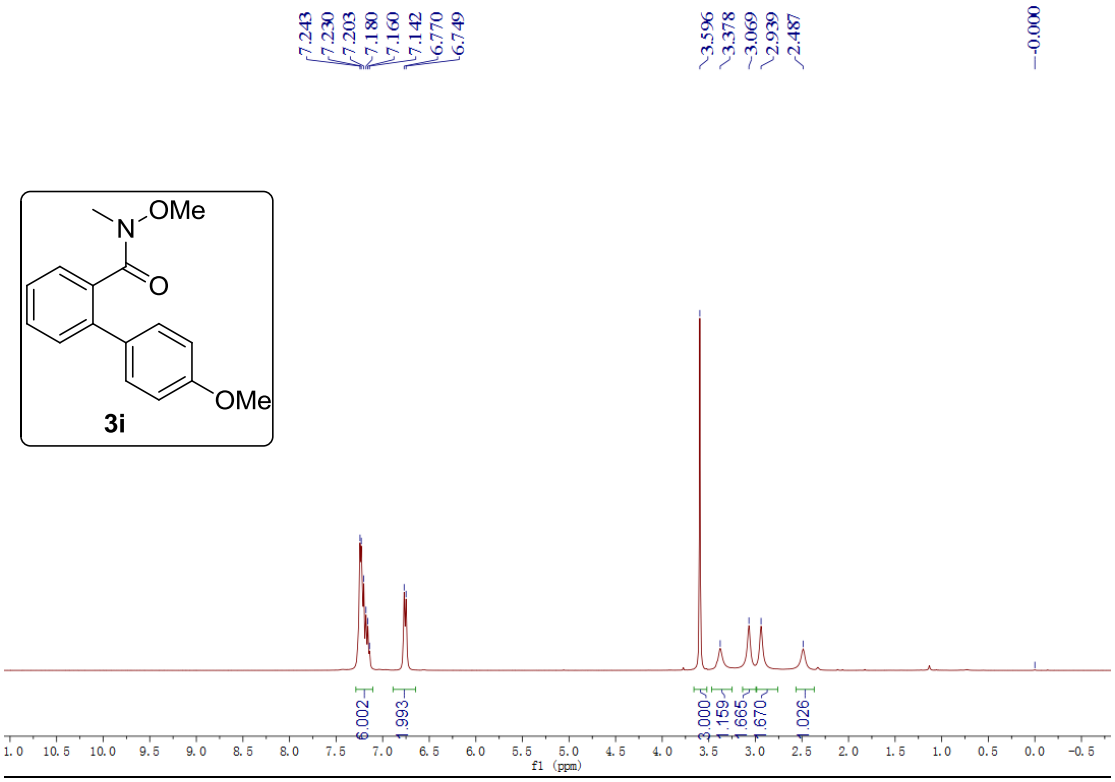
Me
3h
f1 (ppm)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2.487
-0.000
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N
O
OMe
3i
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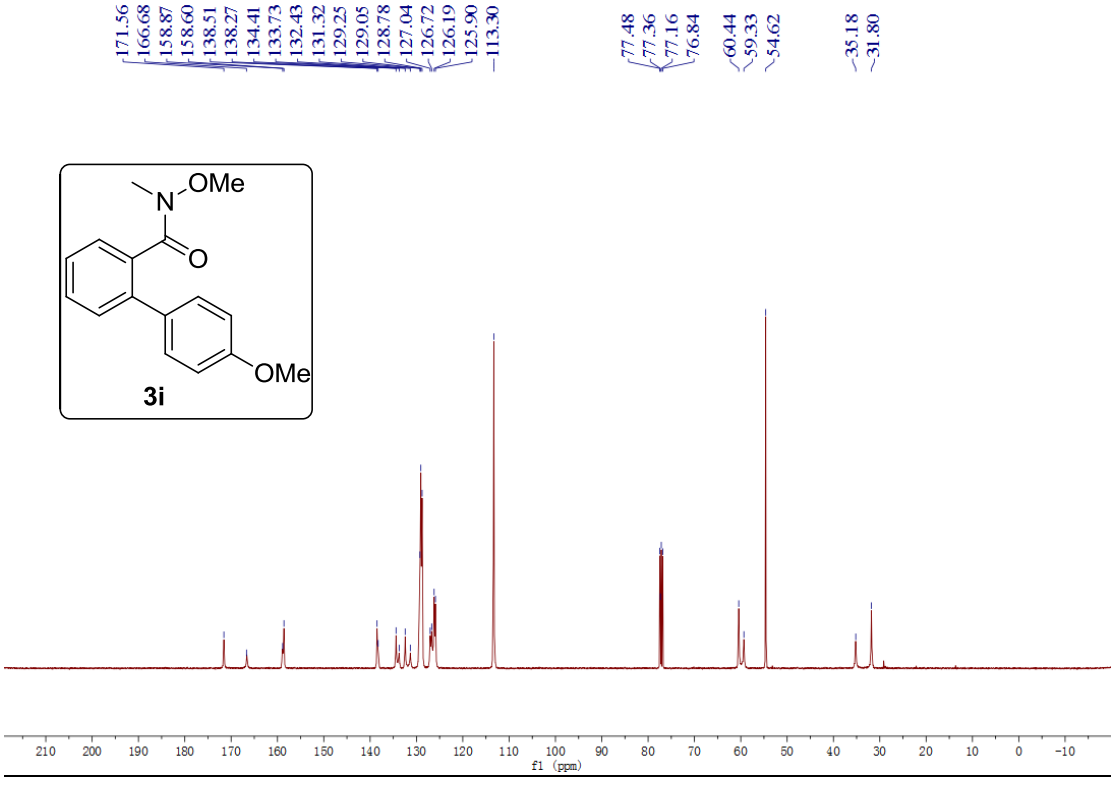
f1 (ppm)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128.78
127.04
126.72
126.19
125.90
113.30
77.48
77.36
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59.33
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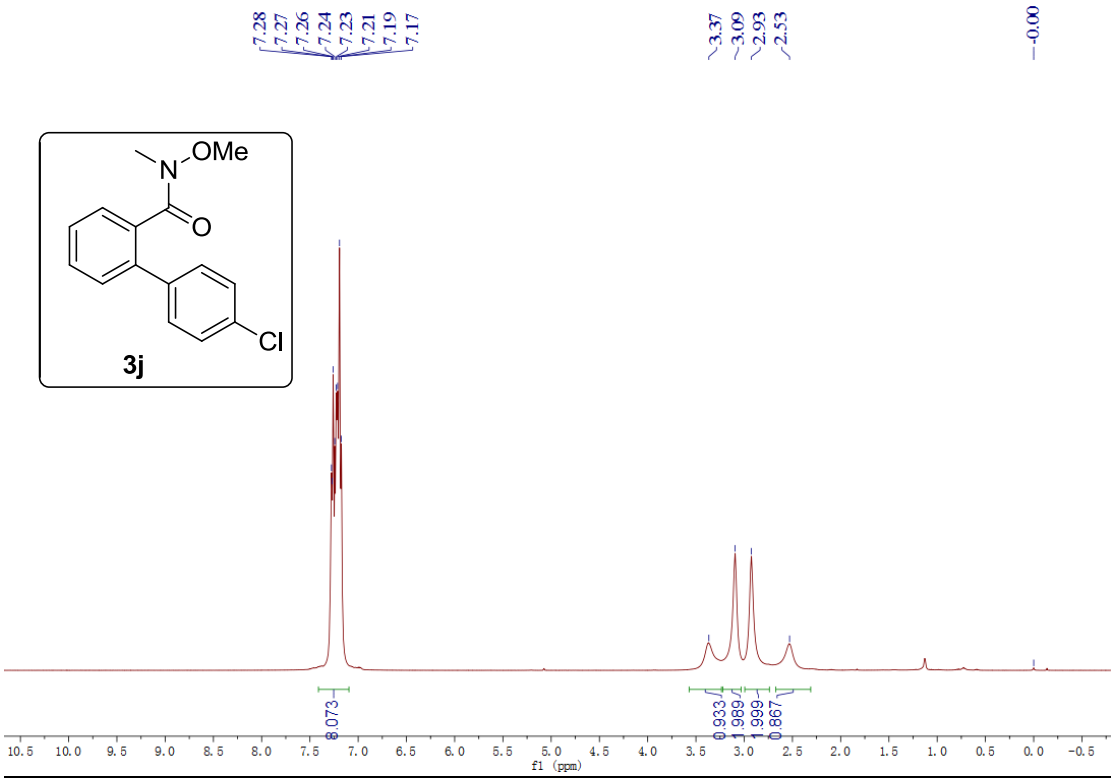
35.18
31.80
OMe
N
O
OMe
3i
f1 (ppm)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7.26
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7.17
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N
O
Cl
3j
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1.989
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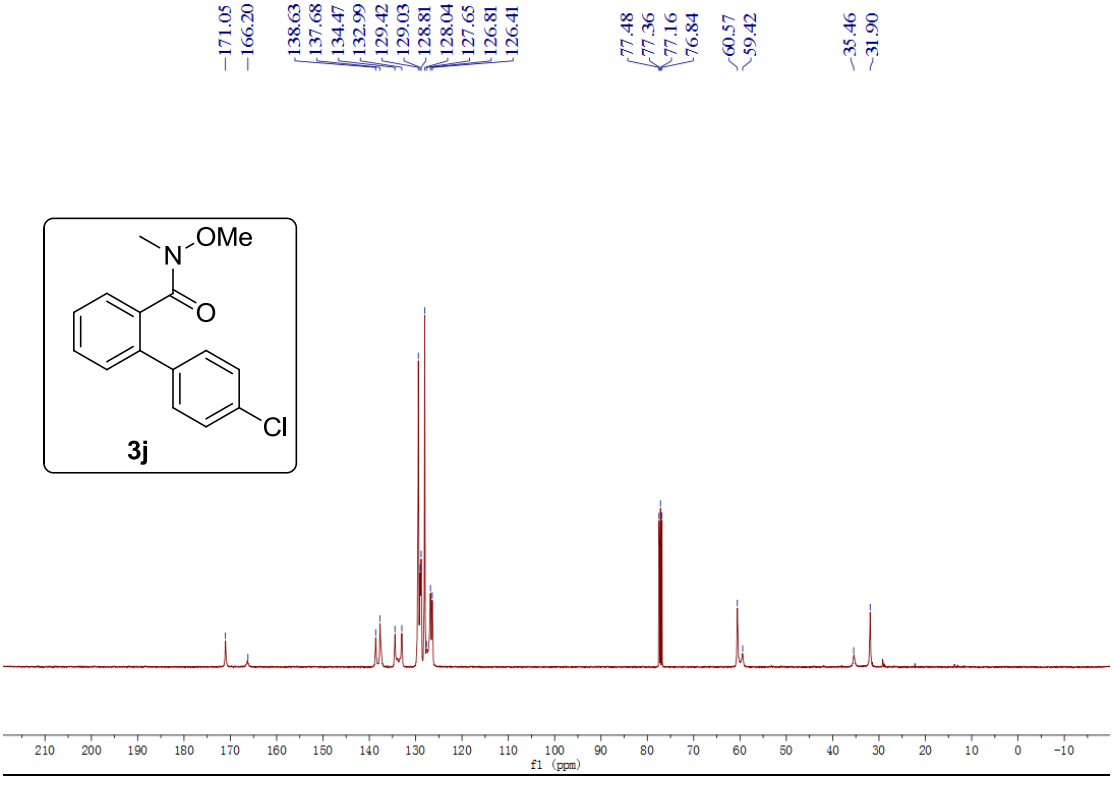
0.867
f1 (ppm)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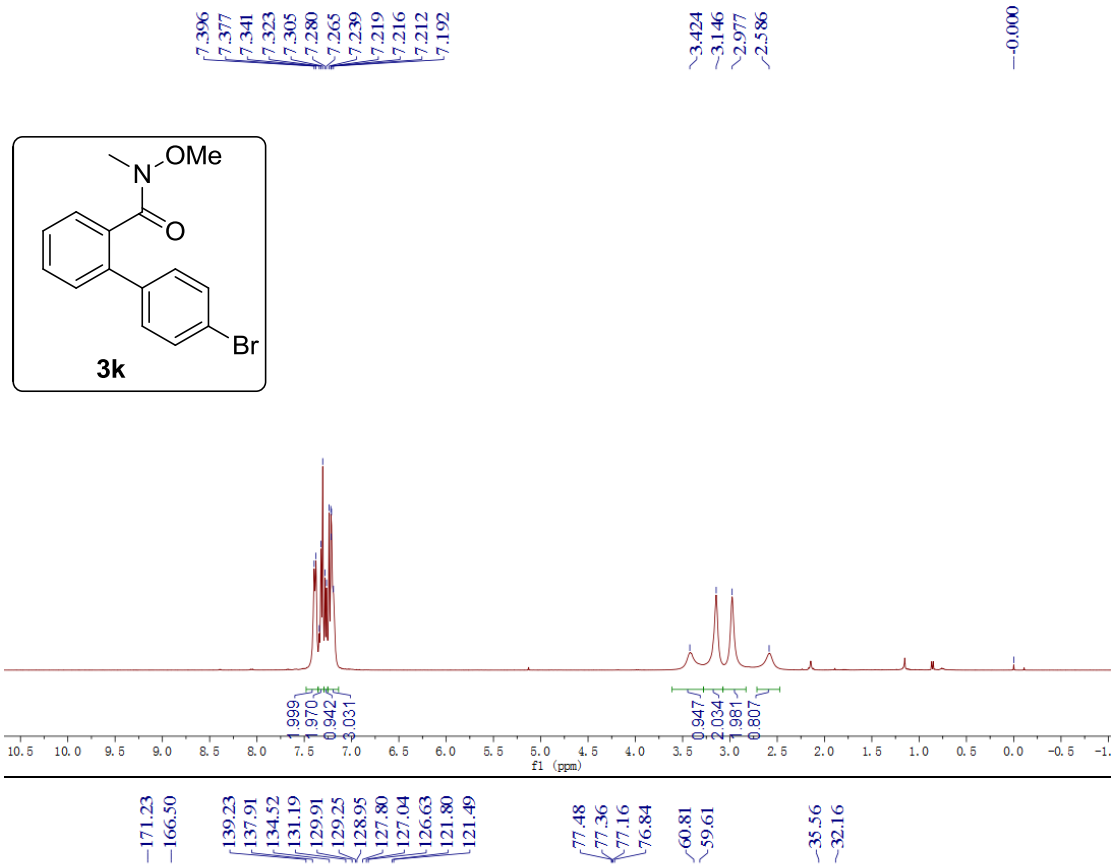
77.48
77.36
77.16
76.84
60.57
59.42
35.46
31.90
OMe
N
O
Cl
3j
f1 (ppm)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7.280
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7.216
7.212
7.192
3.424
3.146
2.977
2.586
0.000
OMe
N
O
Br
3k
1.999
1.970
0.942
3.031
0.947
2.034
1.981
0.807
f1 (ppm)
171.23
166.50
139.23
137.91
134.52
131.19
129.91
129.25
128.95
127.80
127.04
126.63
121.80
121.49
77.48
77.36
77.16
76.84
60.81
59.61
35.56
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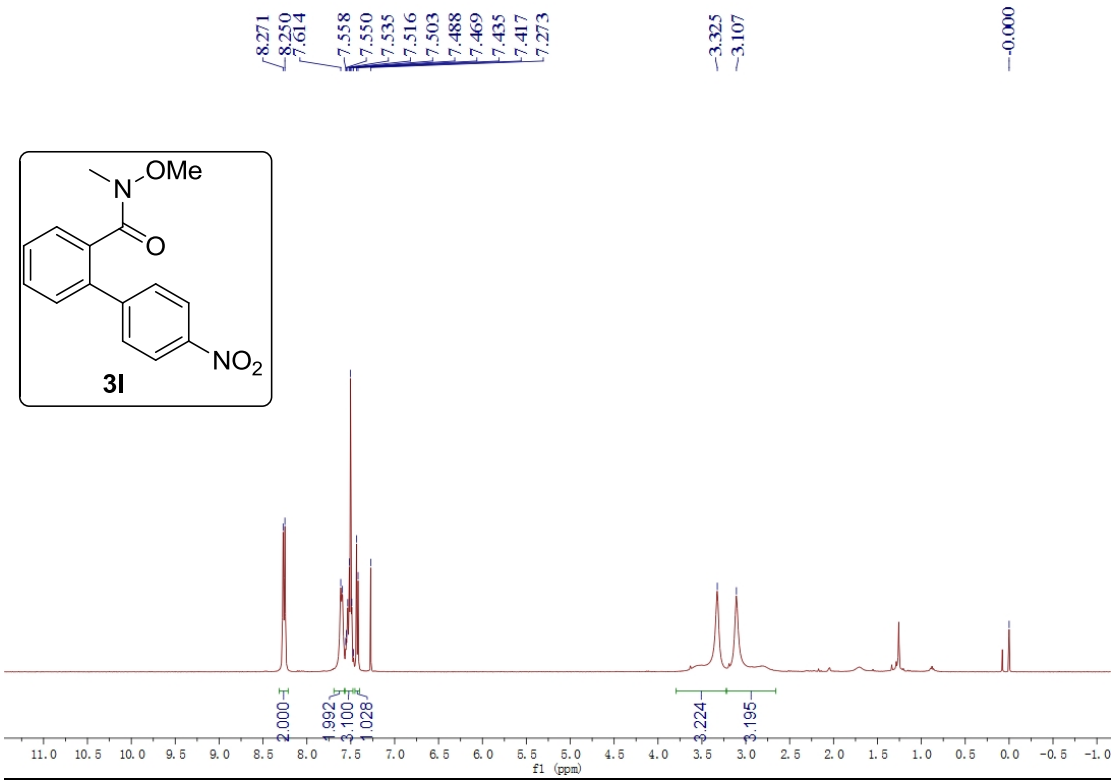
OMe
N
O
Br
3k
f1 (ppm)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7.469
7.435
7.417
7.273
3.325
3.107
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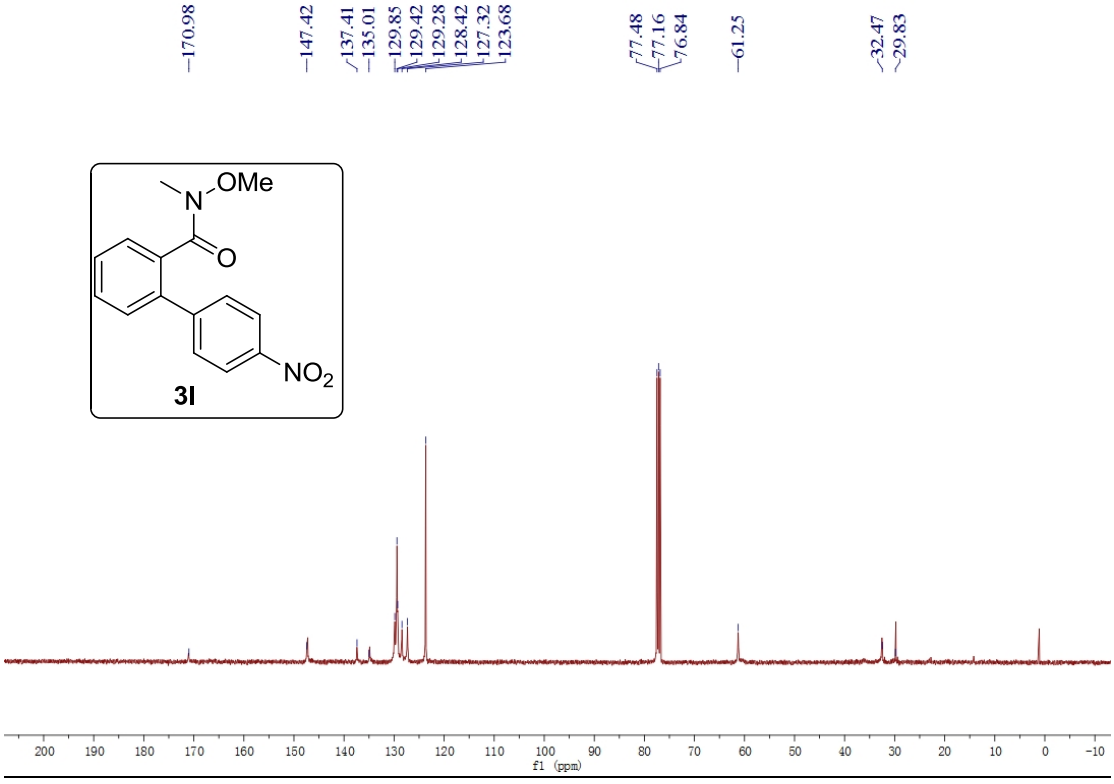
N
O
NO2
3l
2.000
1.992
3.100
1.028
3.224
3.195
f1 (ppm)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76.84
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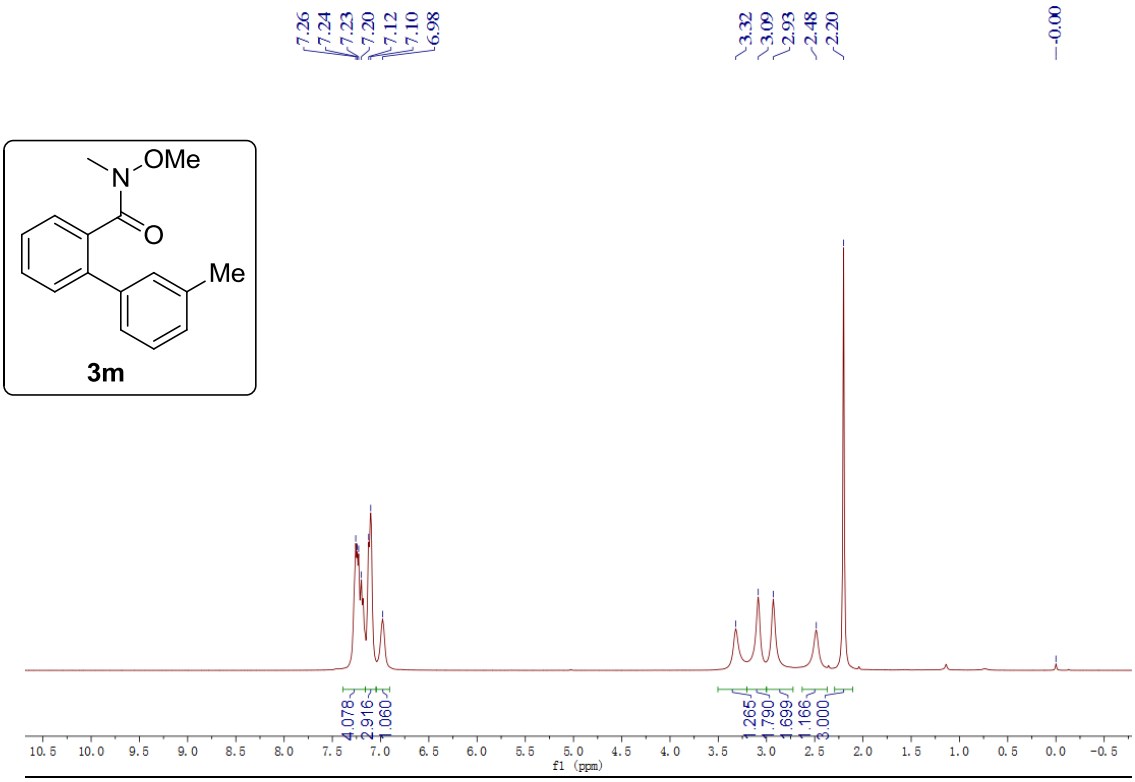
32.47
29.83
OMe
N
O
NO2
3l
f1 (ppm)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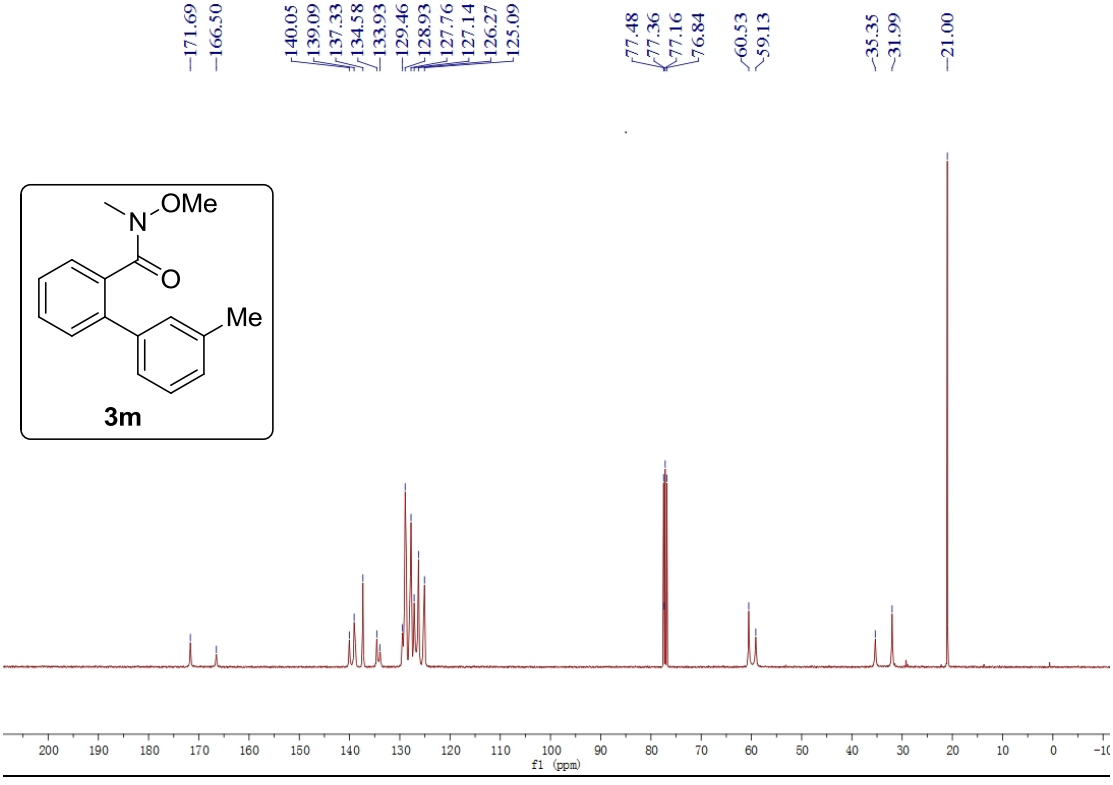
7.10
6.98
3.32
3.09
2.93
2.48
2.20
0.00
OMe
N
O
Me
3m
4.078
2.916
1.060
1.265
1.790
1.699
1.166
3.000
f1 (ppm)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126.27
125.09
77.48
77.36
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59.13
35.35
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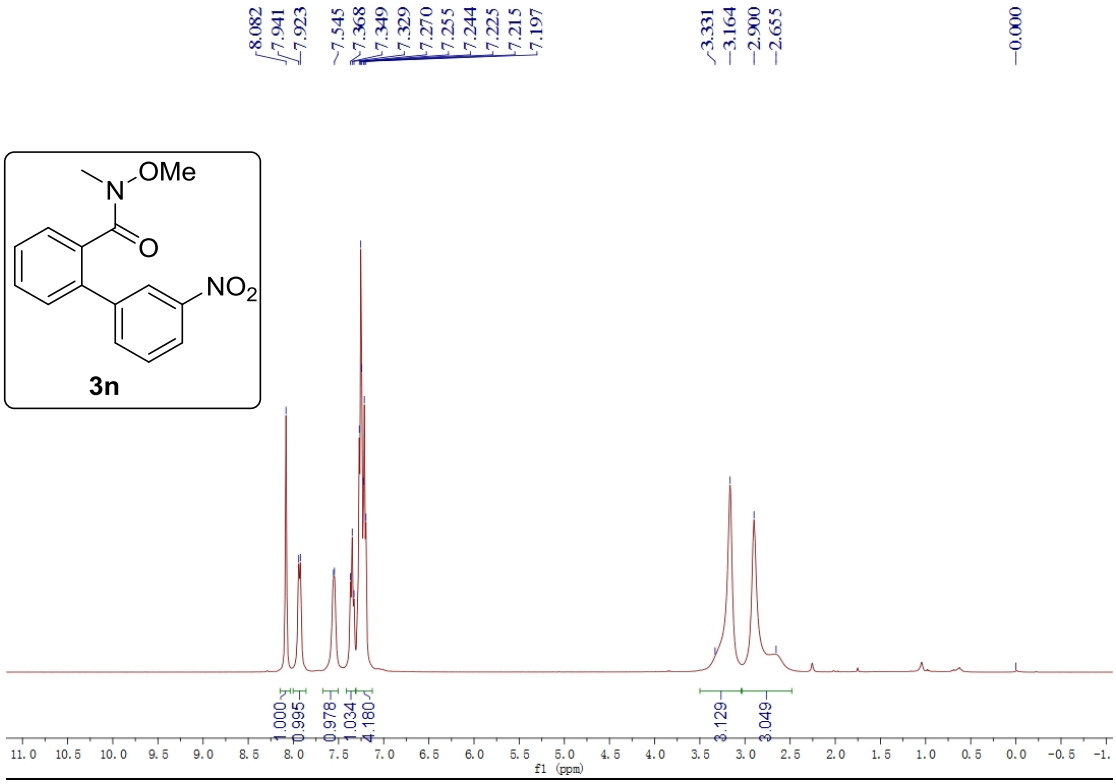
21.00
OMe
N
O
Me
3m
f1 (ppm)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7.225
7.215
7.197
3.331
3.164
2.900
2.655
0.000
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NO2
3n
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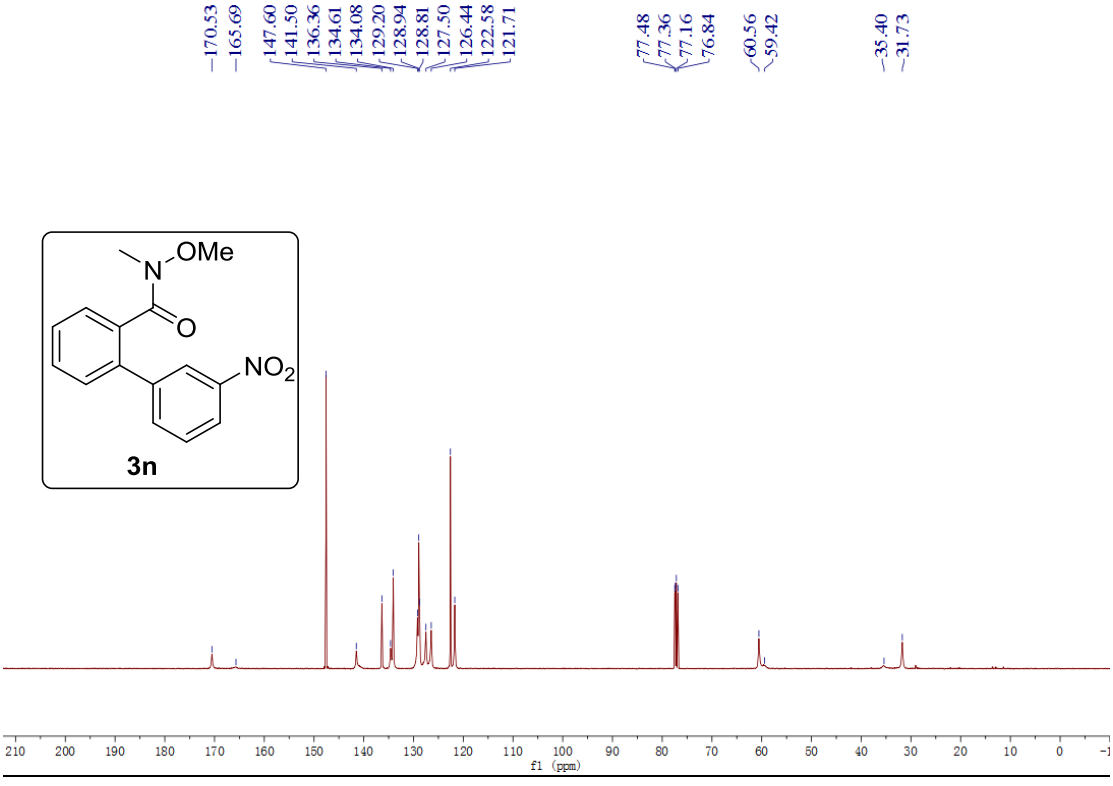
3.049
f1 (ppm)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128.81
127.50
126.44
122.58
121.71
77.48
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60.56
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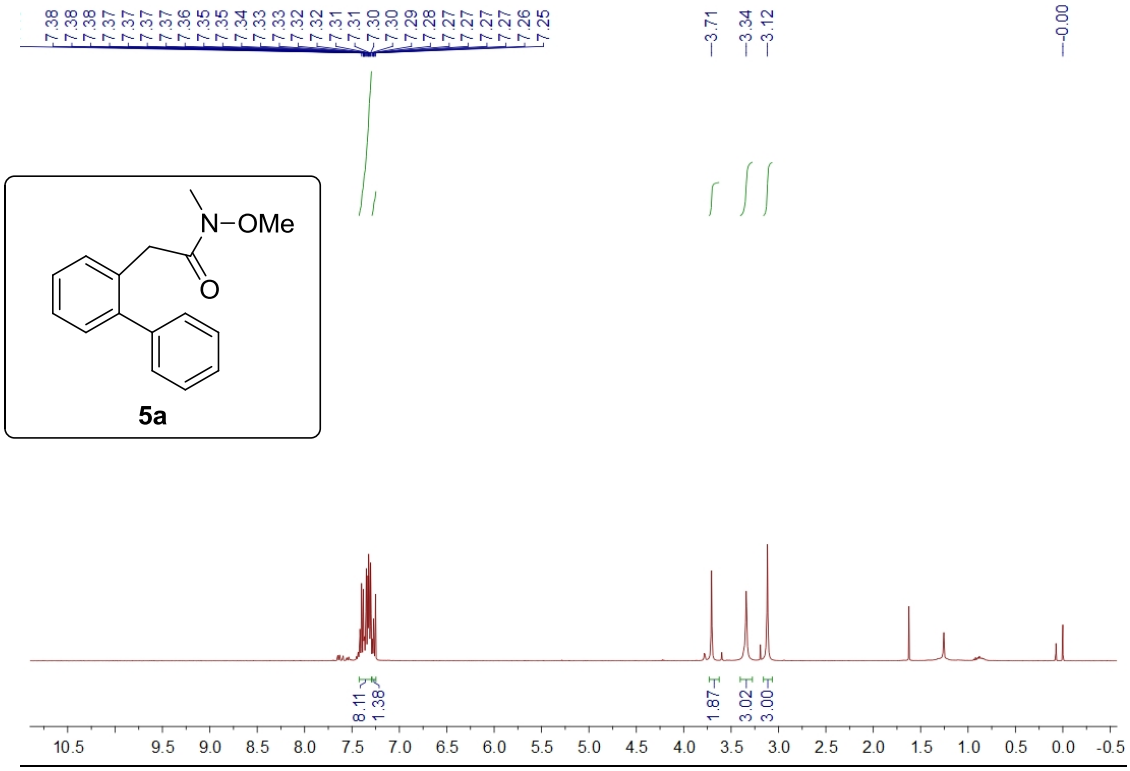
31.73
OMe
N
O
NO2
3n
f1 (ppm)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7.31
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7.30
7.30
7.29
7.28
7.27
7.27
7.27
7.27
7.26
7.25
3.71
3.34
3.12
0.00
N–OMe
O
5a
8.11
1.38
1.87
3.02
3.00
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
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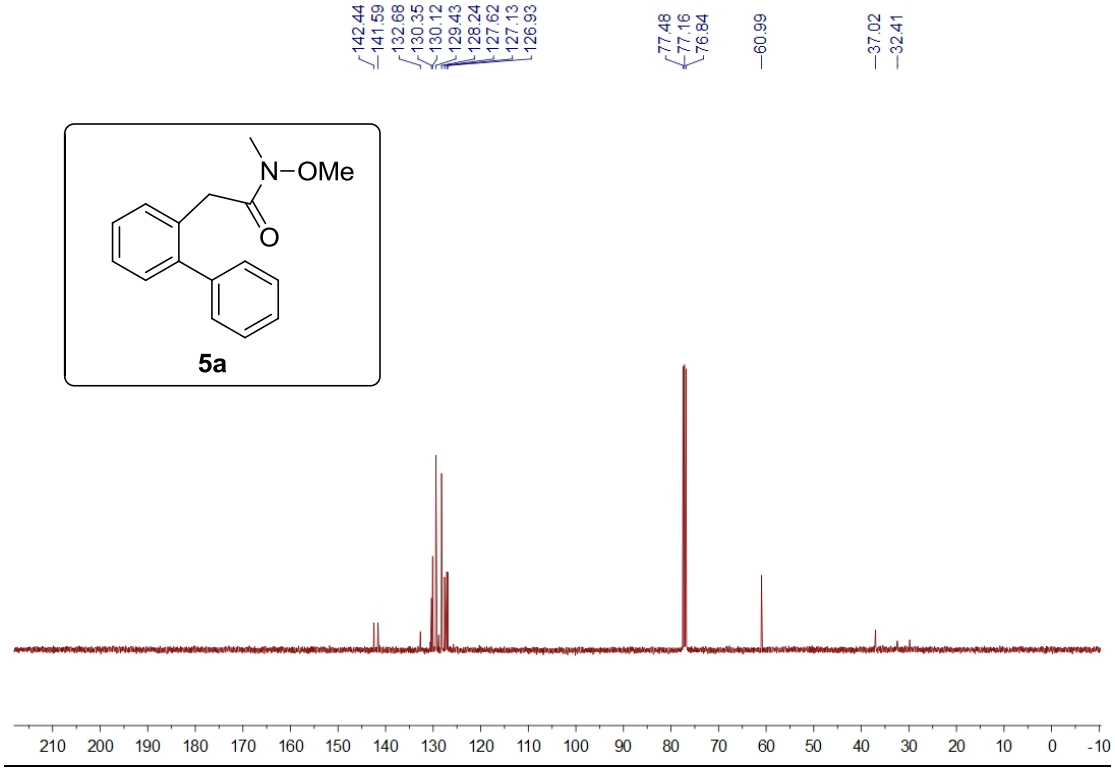
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77.16
76.84
60.99
37.02
32.41
N–OMe
O
5a
210
200
190
180
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140
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120
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100
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80
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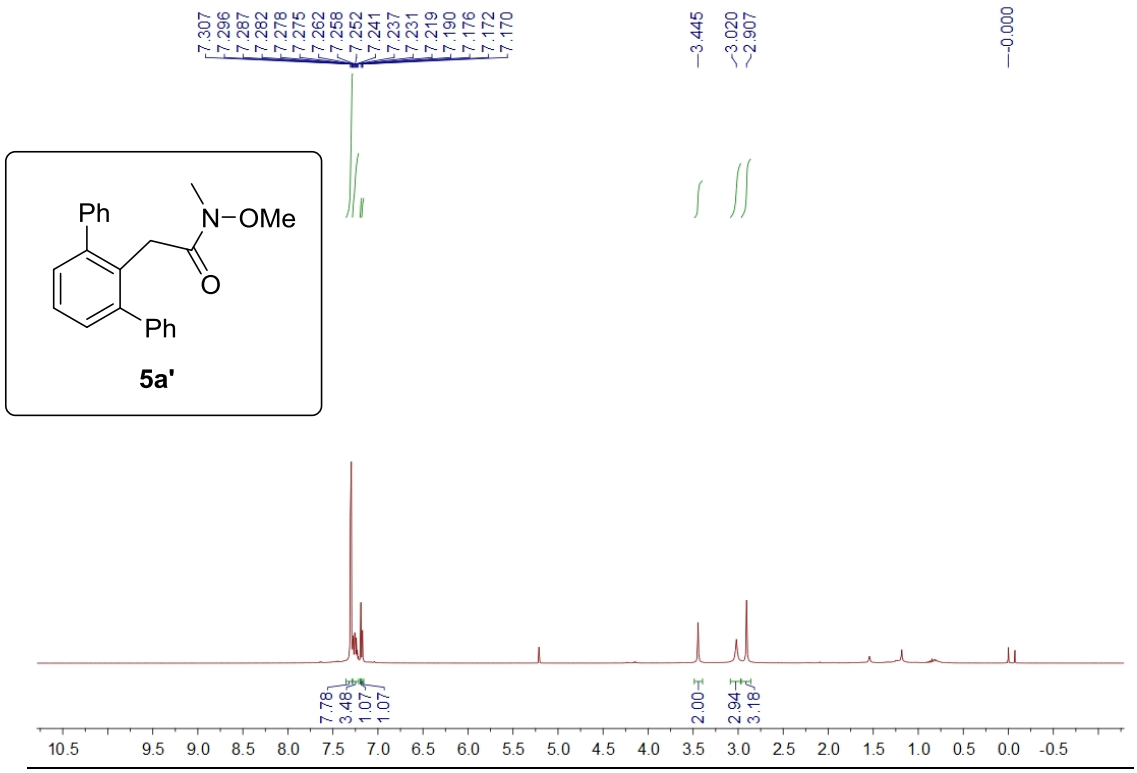
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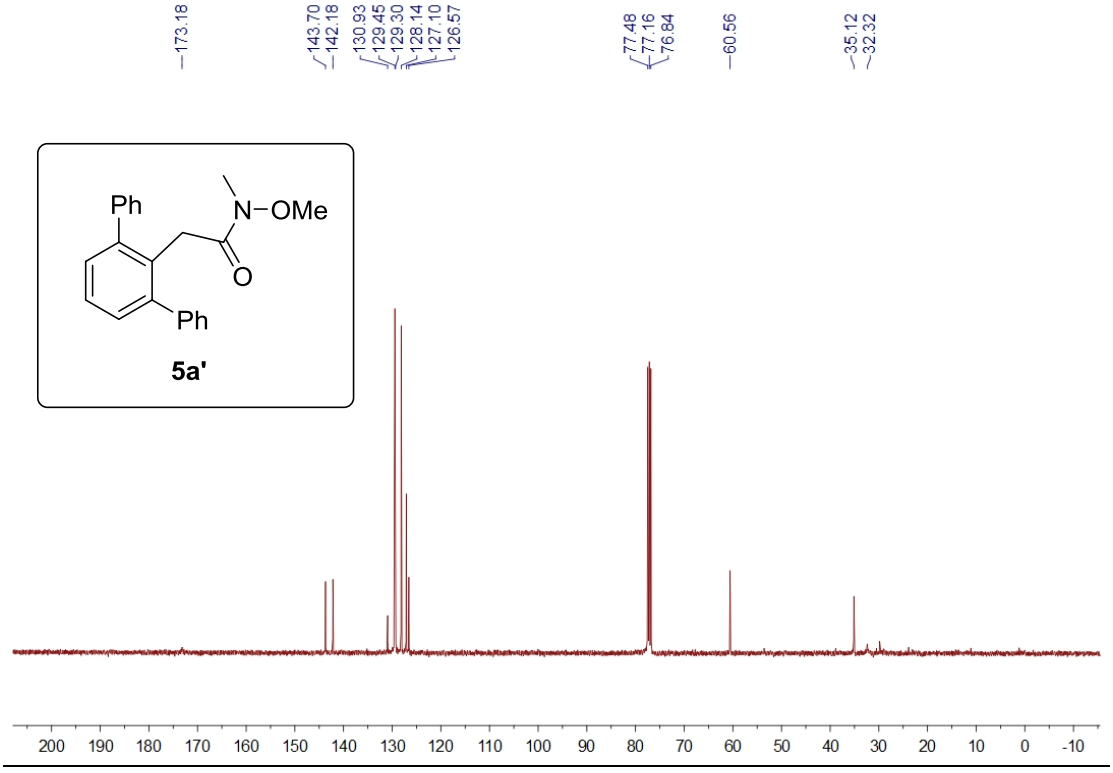
7.190
7.176
7.172
7.170
3.445
3.020
2.907
0.000
Ph
N−OMe
O
Ph
5a'
7.78
3.48
1.07
1.07
2.00
2.94
3.18
10.5 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5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127.10
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77.48
77.16
76.84
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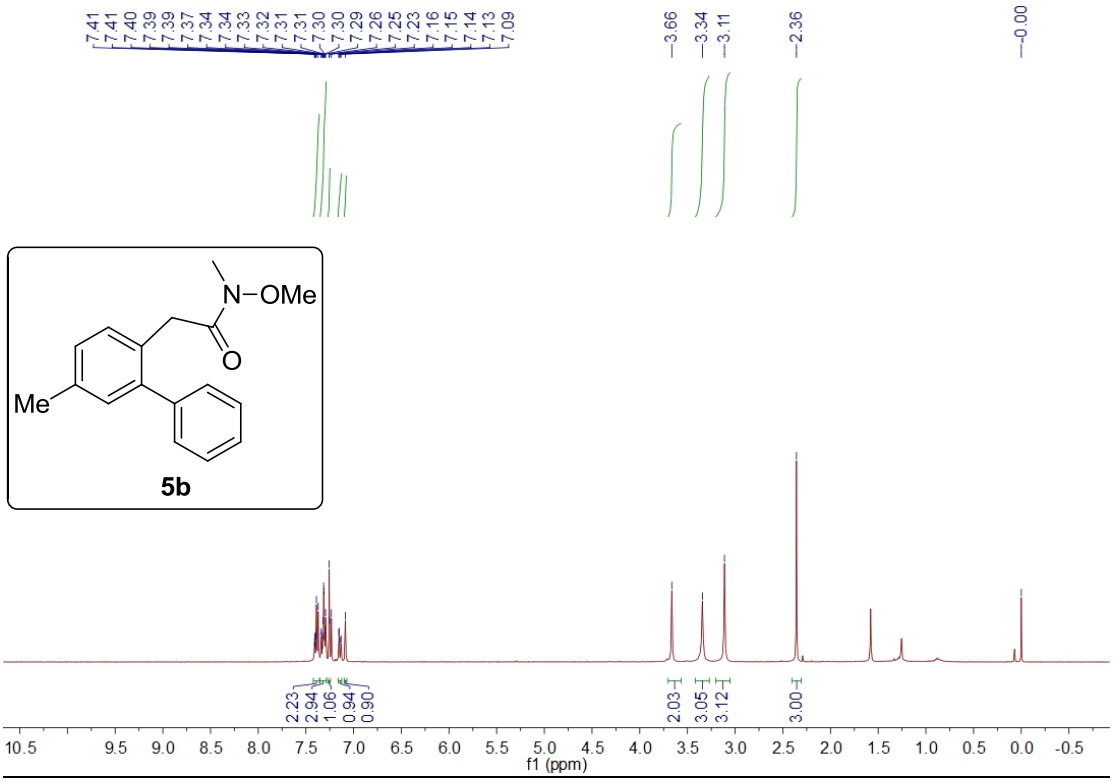
35.12
32.32
Ph
N−OMe
O
Ph
5a'
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10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7.31
7.30
7.30
7.29
7.26
7.25
7.23
7.16
7.15
7.14
7.13
7.09
3.66
3.34
3.11
2.36
0.00
N−OMe
O
Me
5b
2.23
2.94
1.06
0.94
0.90
2.03
3.05
3.12
3.00
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
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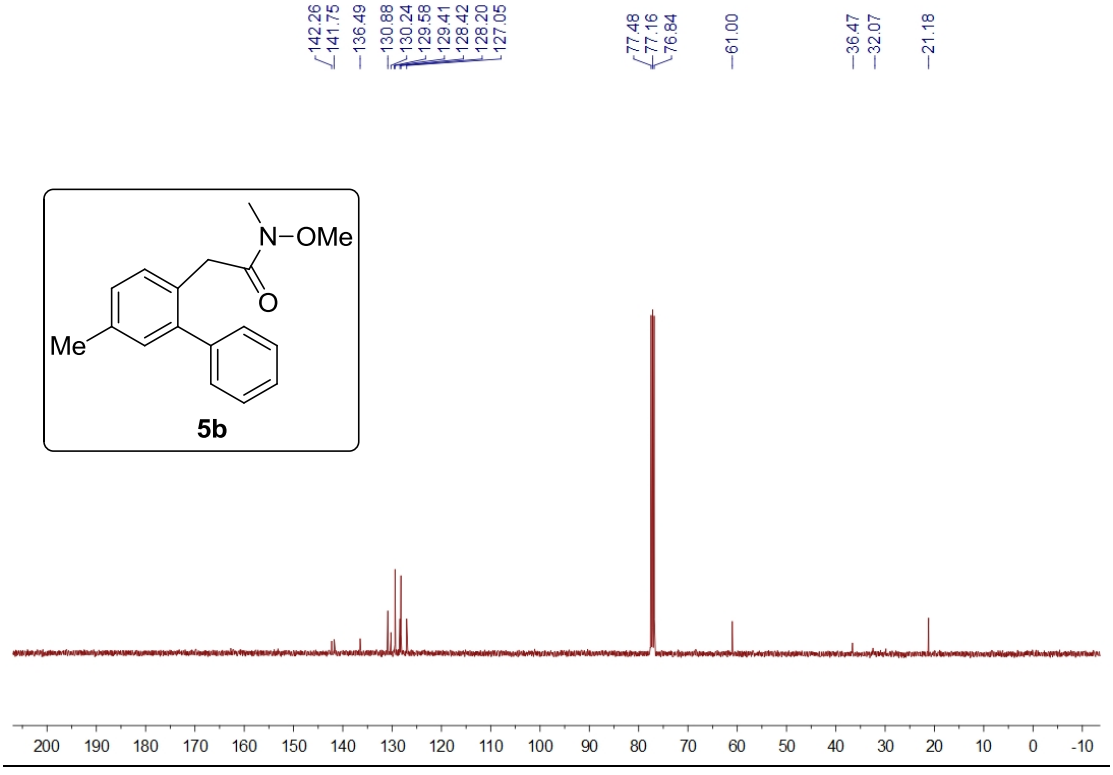
0.5
0.0
-0.5
f1 (ppm)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77.16
76.84
61.00
36.47
32.07
21.18
N−OMe
O
Me
5b
200
190
180
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100
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50
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20
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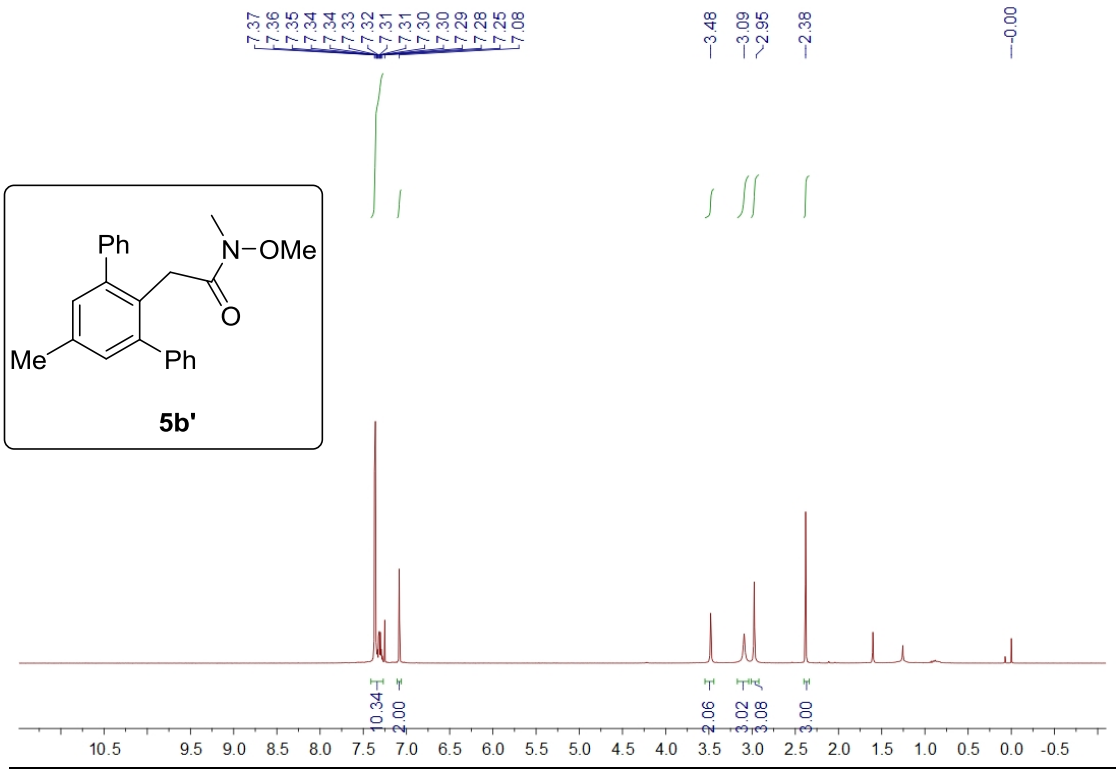
0
-10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7.28
7.25
7.08
3.48
3.09
2.95
2.38
0.00
Ph
N−OMe
O
Me
Ph
5b'
10.34
2.00
2.06
3.02
3.08
3.00
10.5
9.5
9.0
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8.0
7.5
7.0
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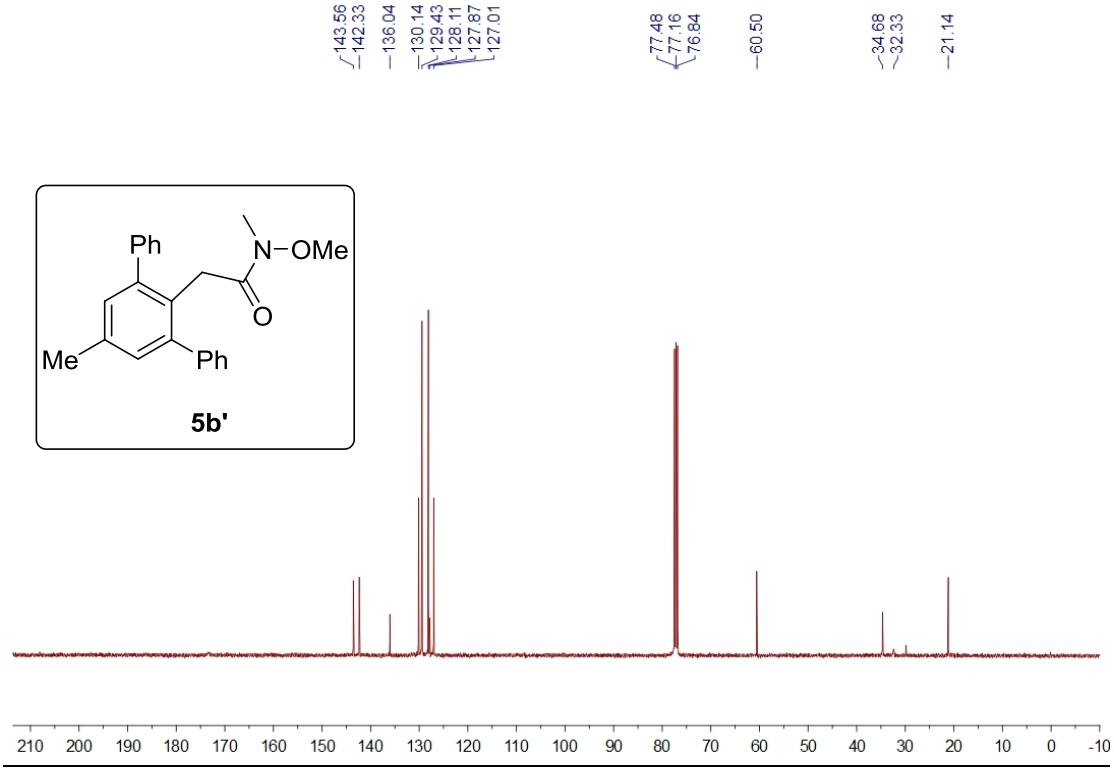
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32.33
21.14
Ph
N−OMe
O
Me
Ph
5b'
210
200
190
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100
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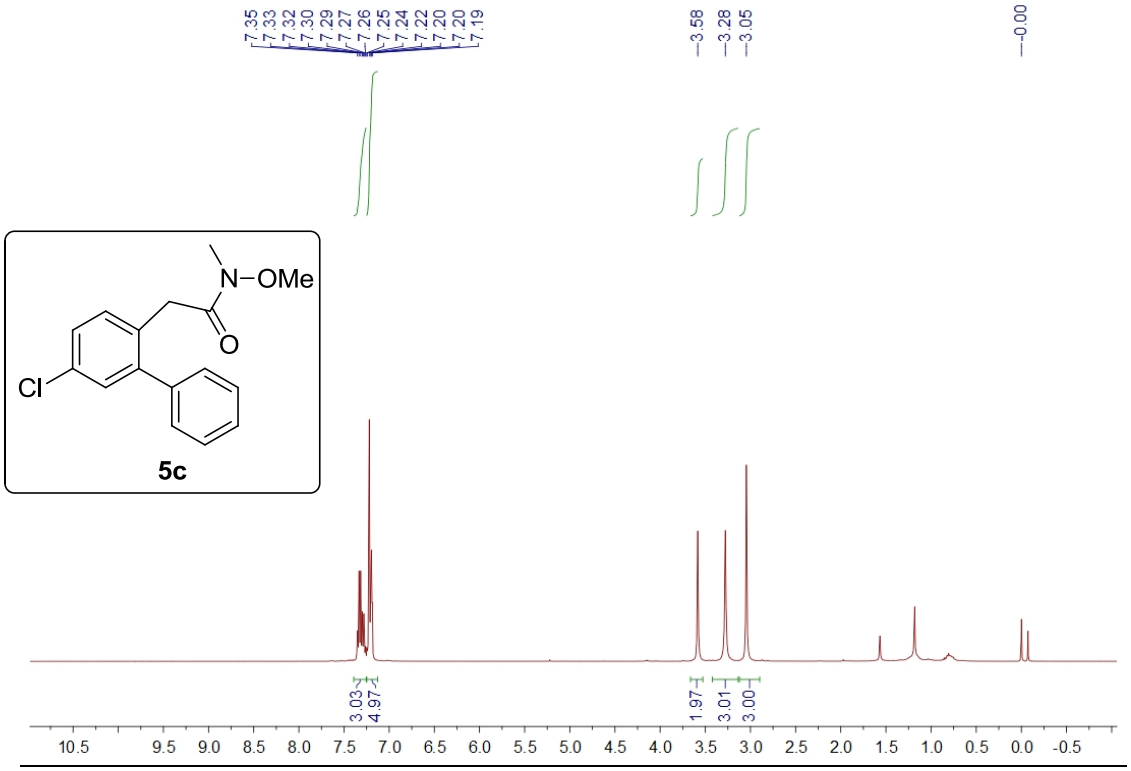
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7.20
7.19
3.58
3.28
3.05
0.00
N−OMe
O
Cl
5c
3.03
4.97
1.97
3.01
3.00
10.5
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9.0
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8.0
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6.0
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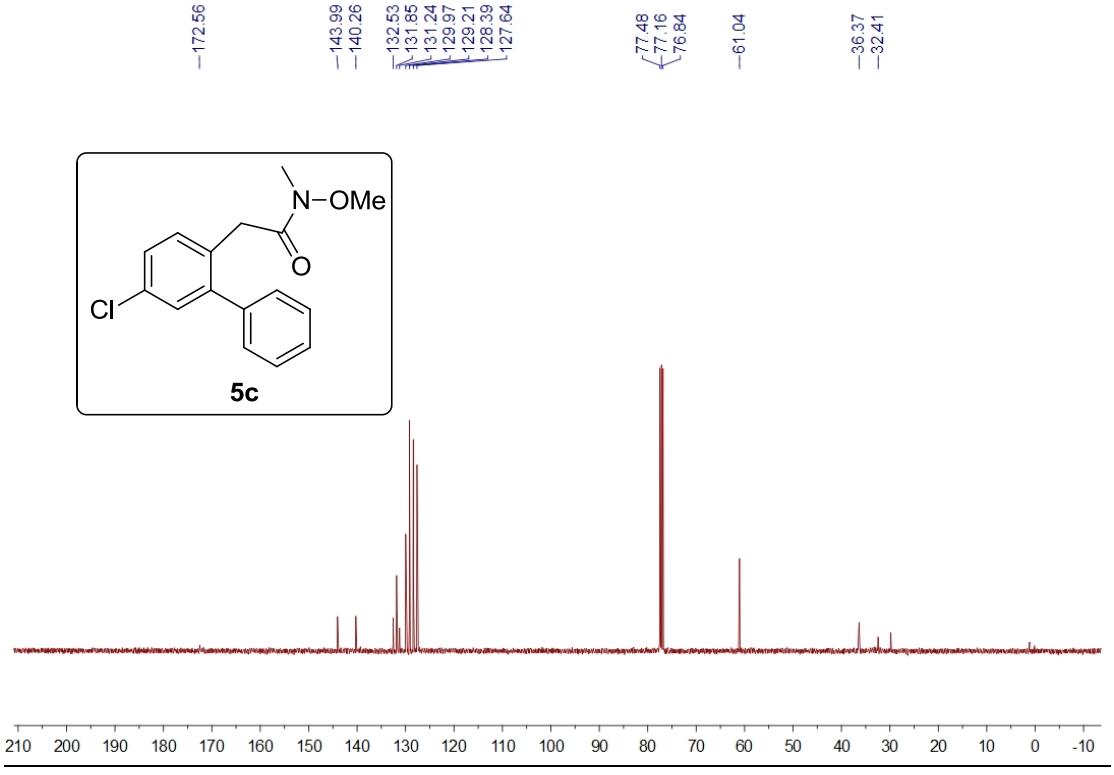
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61.04
36.37
32.41
N−OMe
O
Cl
5c
210
200
190
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50
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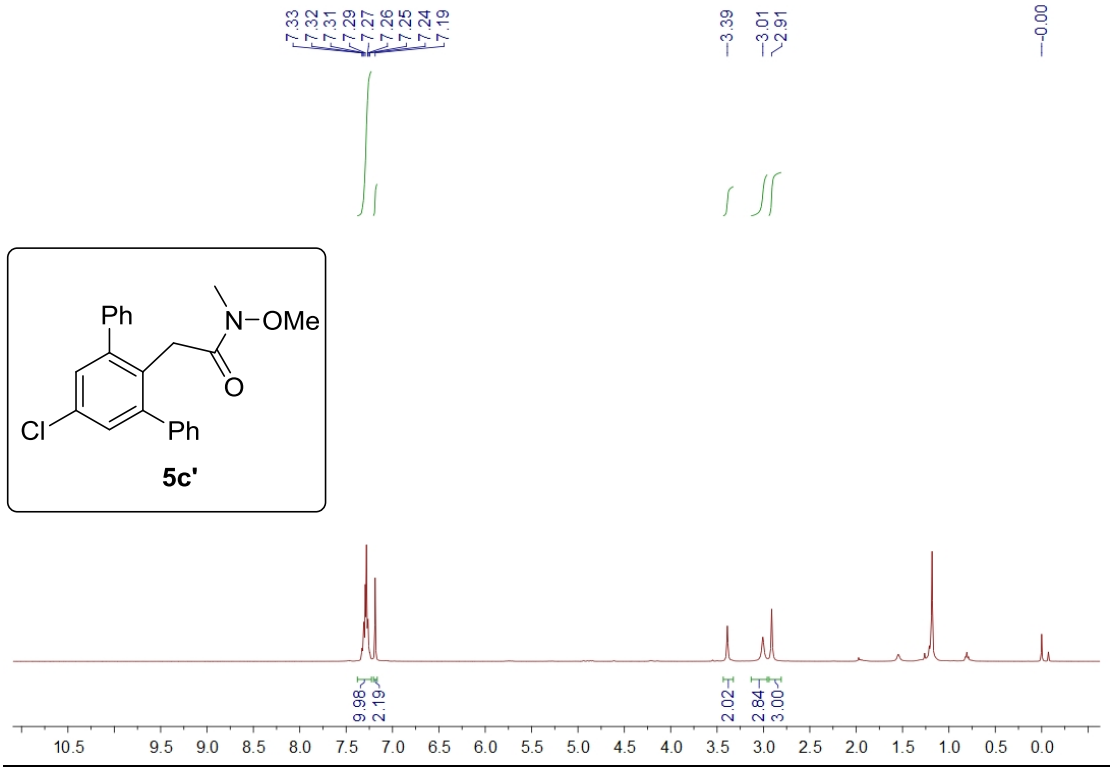
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Ph
N−OMe
O
Cl
Ph
5c'
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2.02
2.84
3.00
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8.0
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7.0
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6.0
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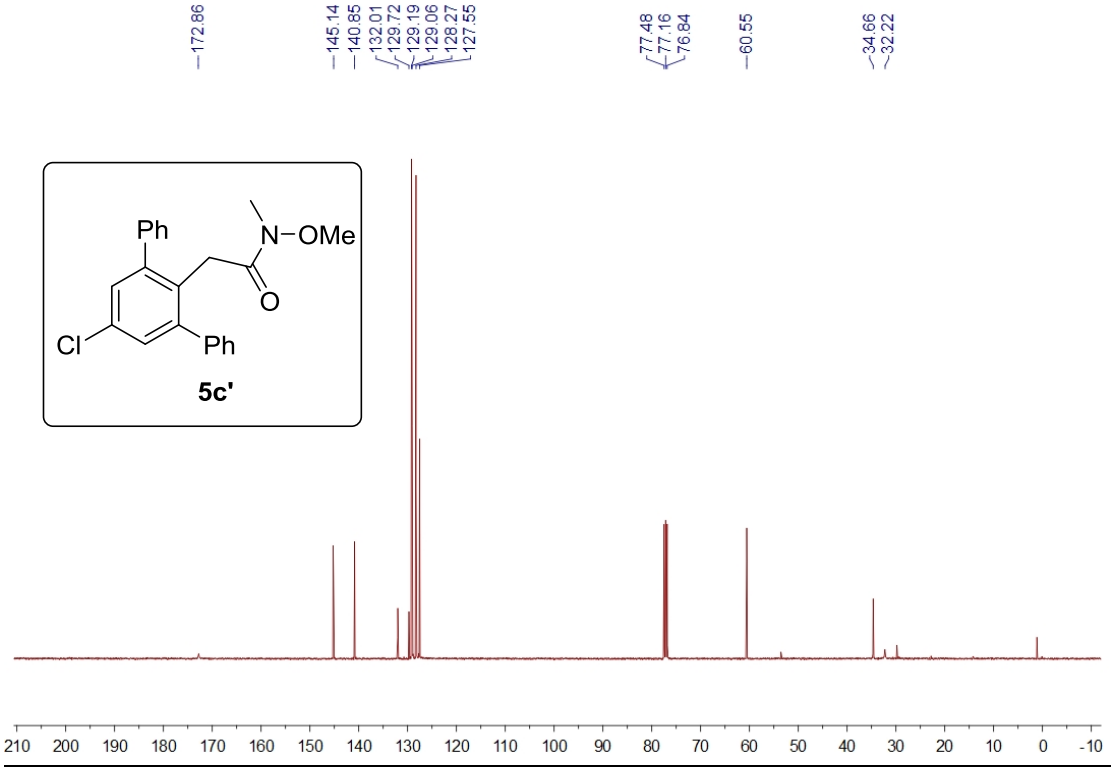
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34.66
32.22
Ph
N−OMe
O
Cl
Ph
5c'
210
200
190
180
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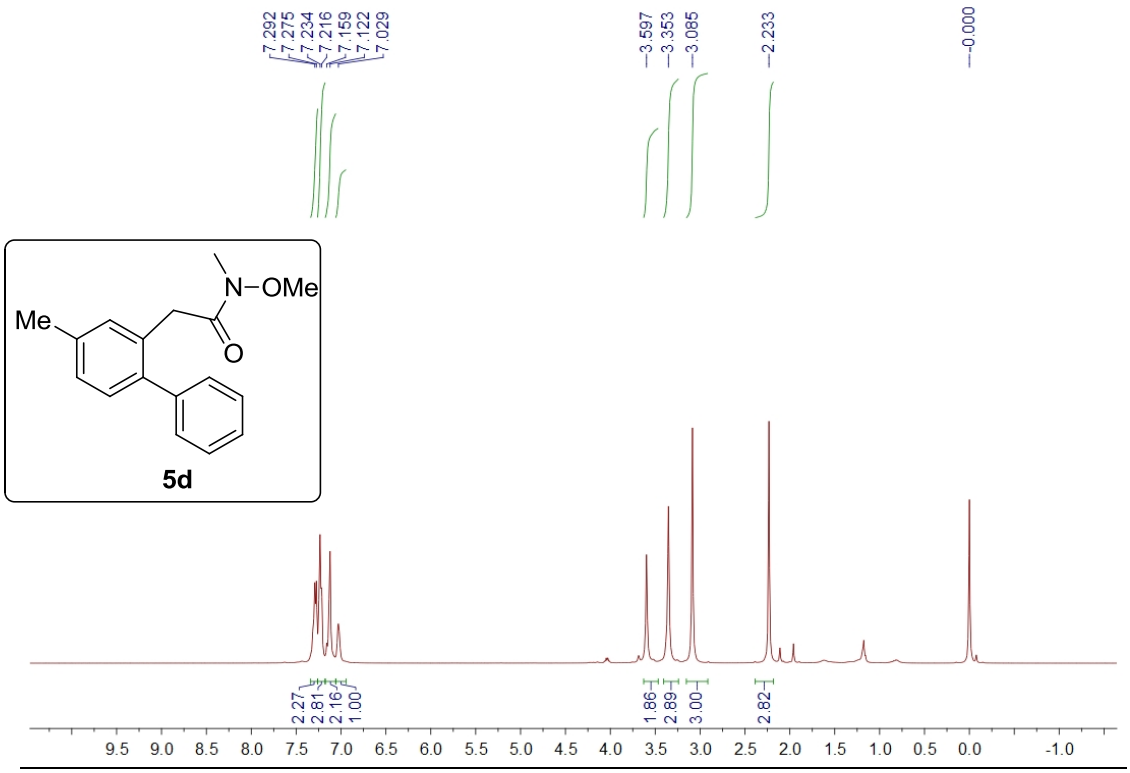
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Me
O
5d
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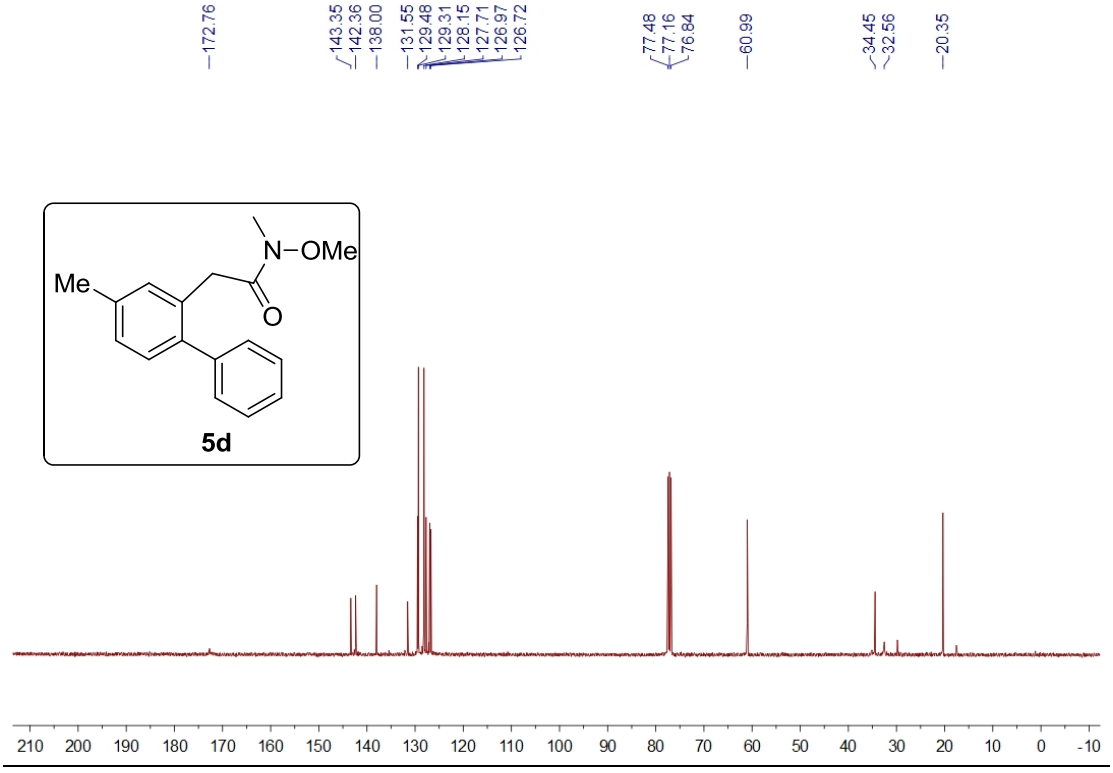
2.81
2.16
1.00
1.86
2.89
3.00
2.82
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -1.0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77.16
76.84
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34.45
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20.35
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Me
O
5d
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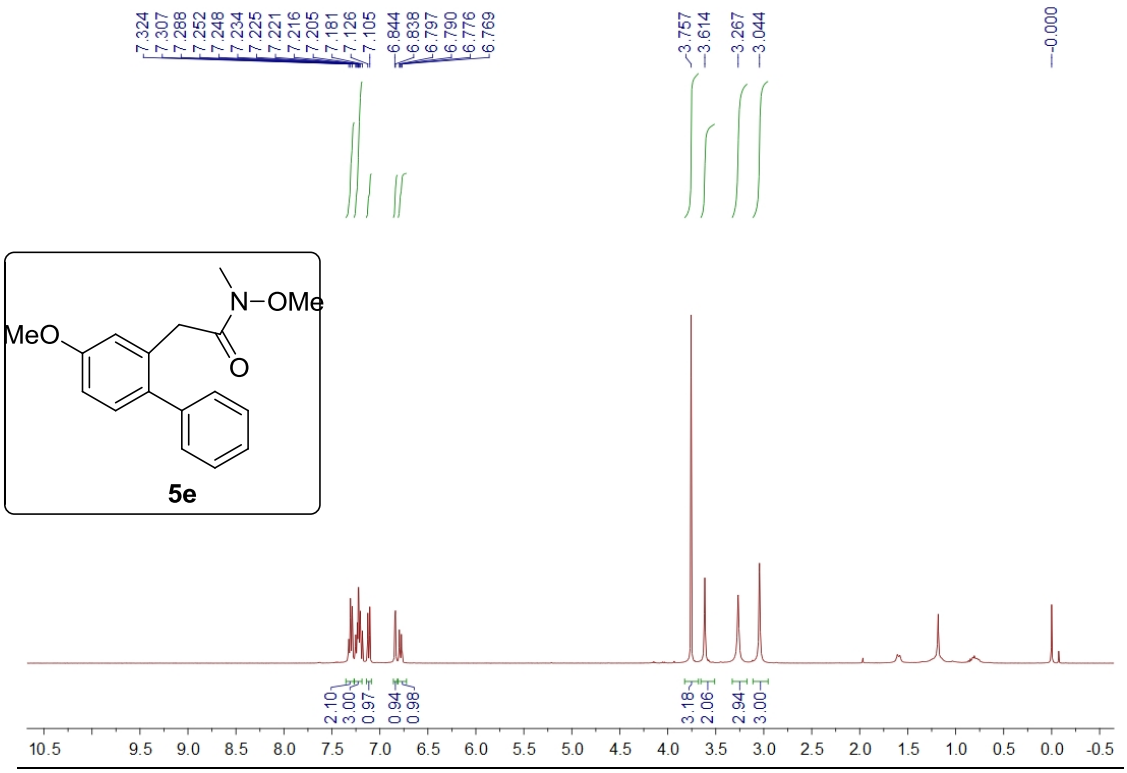
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3.267
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MeO
O
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3.00
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0.94
0.98
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2.94
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9.5
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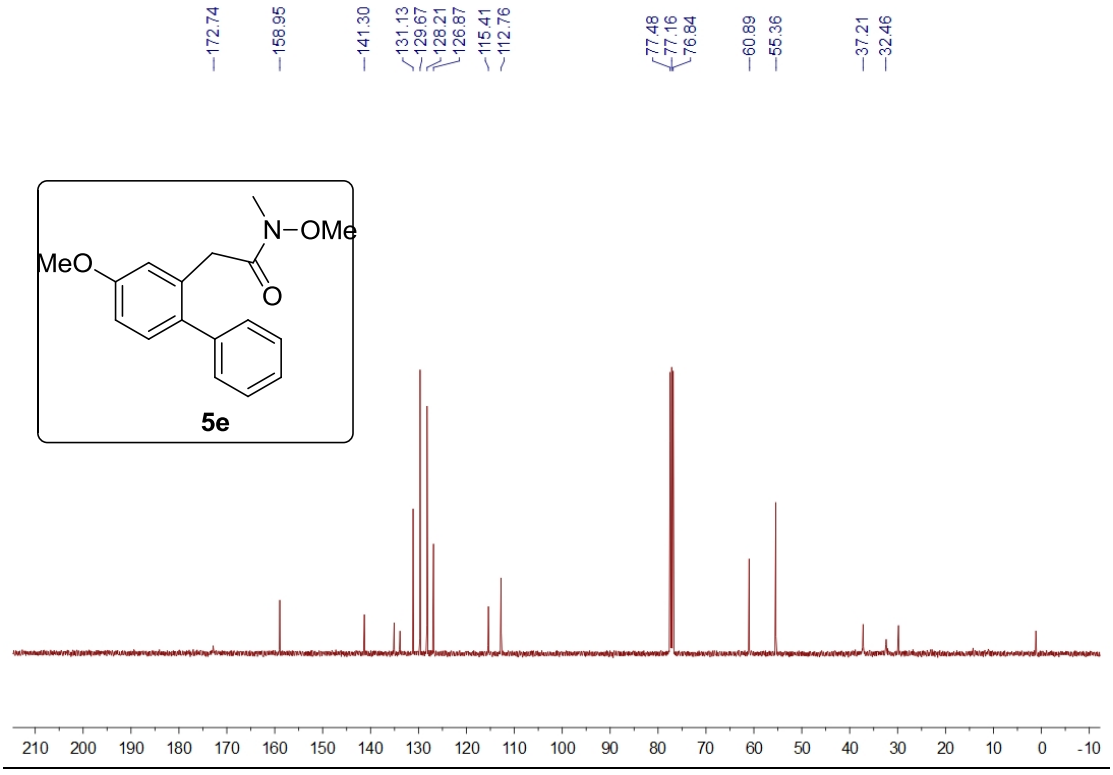
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37.21
32.46
N−OMe
MeO
O
5e
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200
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100
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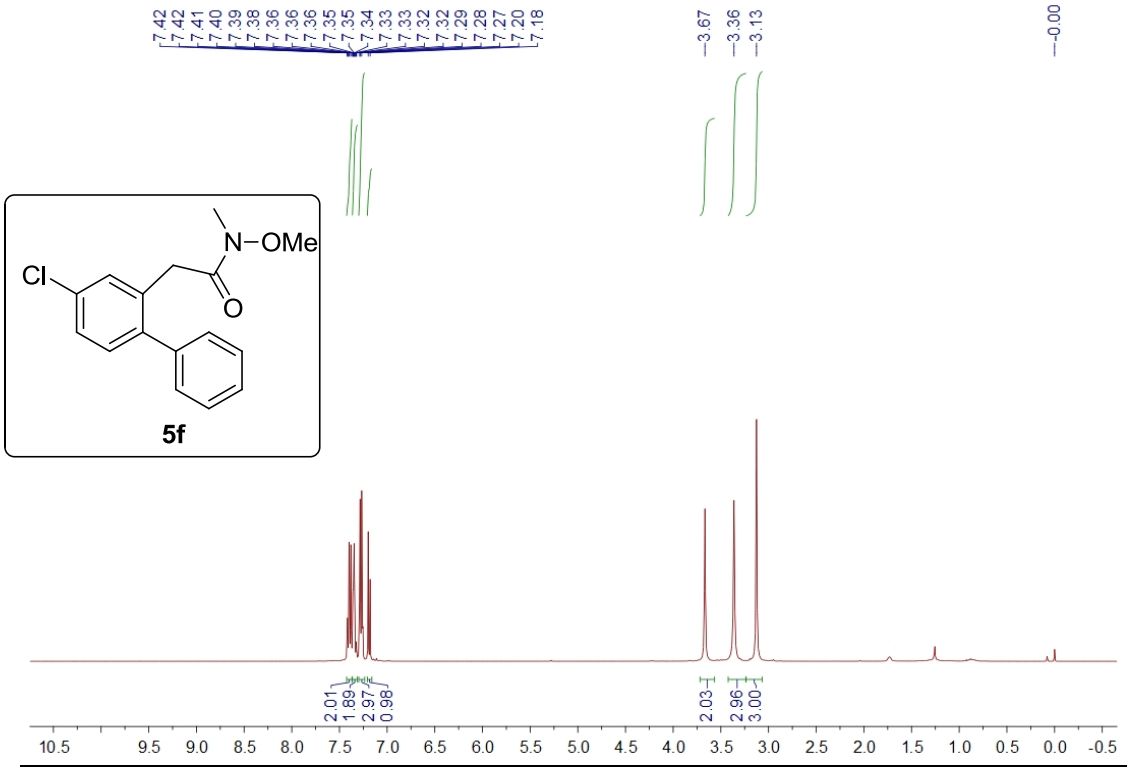
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7.29
7.28
7.27
7.20
7.18
3.67
3.36
3.13
0.00
N−OMe
Cl
O
5f
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1.89
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0.98
2.03
2.96
3.00
10.5
9.5
9.0
8.5
8.0
7.5
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6.5
6.0
5.5
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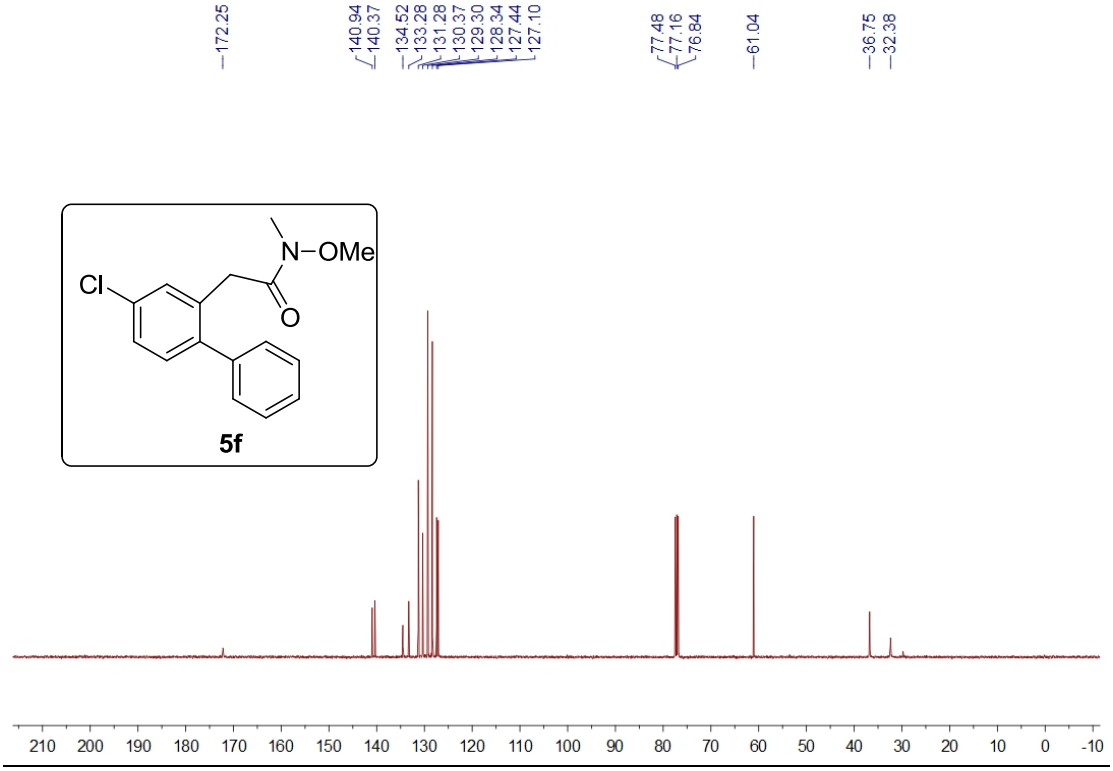
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76.84
61.04
36.75
32.38
N−OMe
Cl
O
5f
210
200
190
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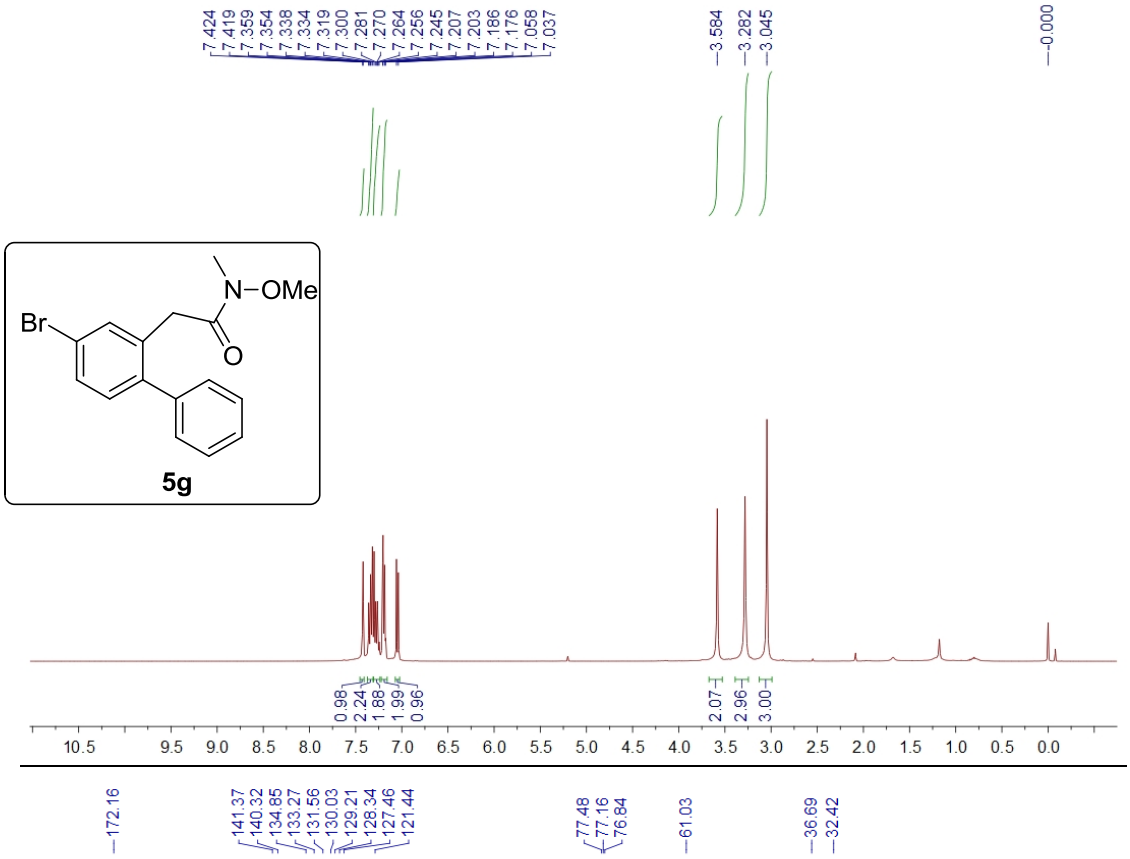
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7.245
7.207
7.203
7.186
7.176
7.058
7.037
3.584
3.282
3.045
0.000
N−OMe
Br
O
5g
0.98
2.24
1.88
1.99
0.96
2.07
2.96
3.00
10.5
9.5
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8.5
8.0
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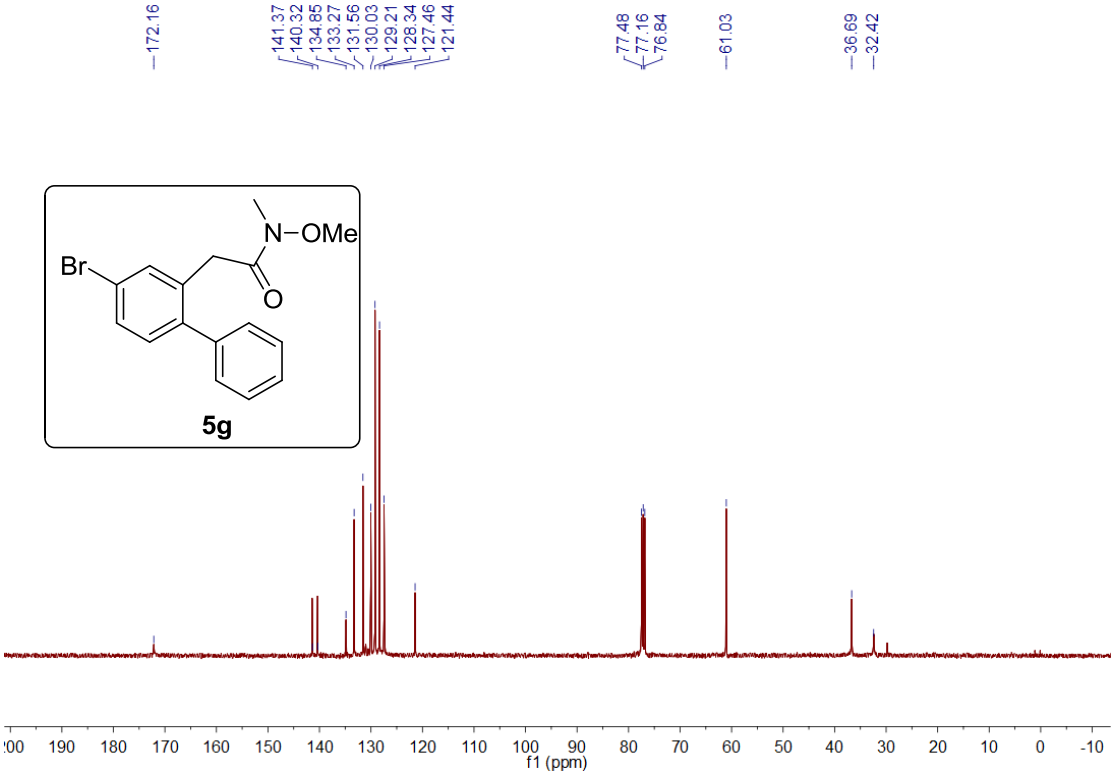
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77.16
76.84
61.03
36.69
32.42
N−OMe
Br
O
5g
200
190
180
170
160
150
140
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120
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100
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80
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40
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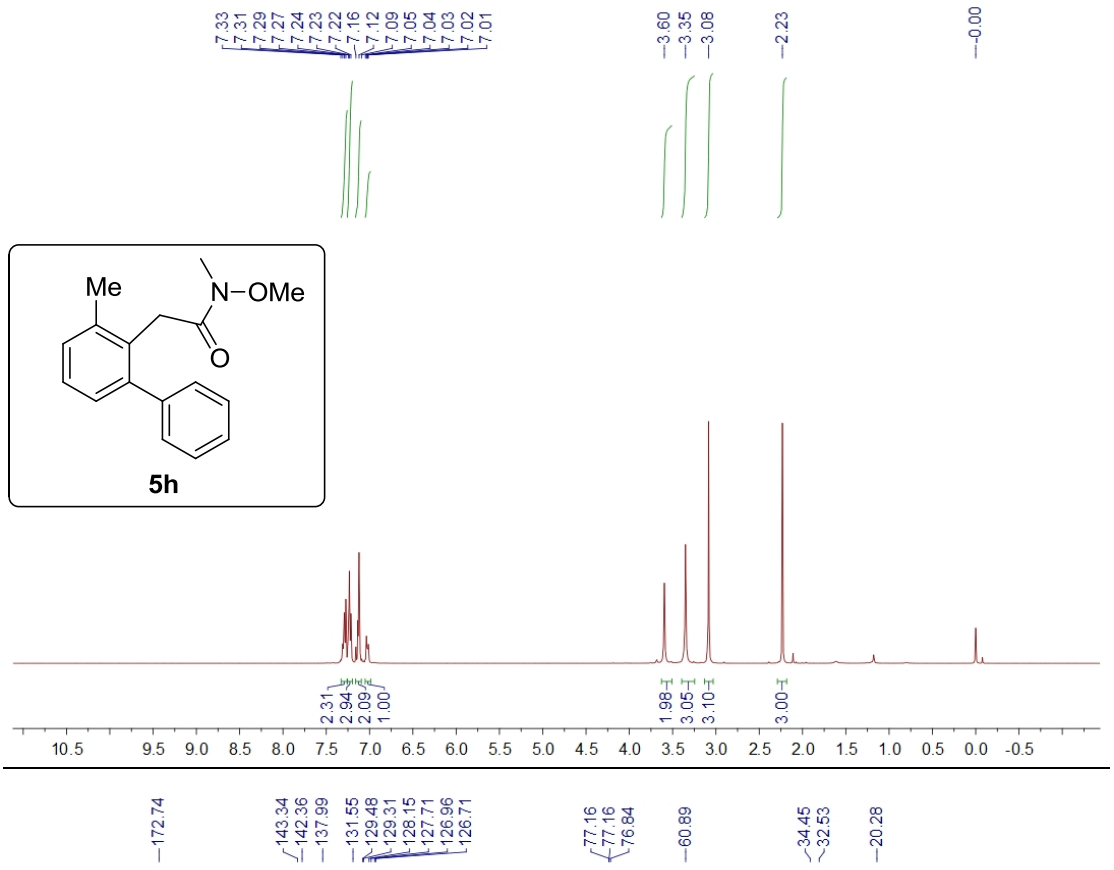
-10
f1 (ppm)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7.03
7.02
7.01
3.60
3.35
3.08
2.23
0.00
Me
N−OMe
O
5h
2.31
2.94
2.09
1.00
1.98
3.05
3.10
3.00
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
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5.5
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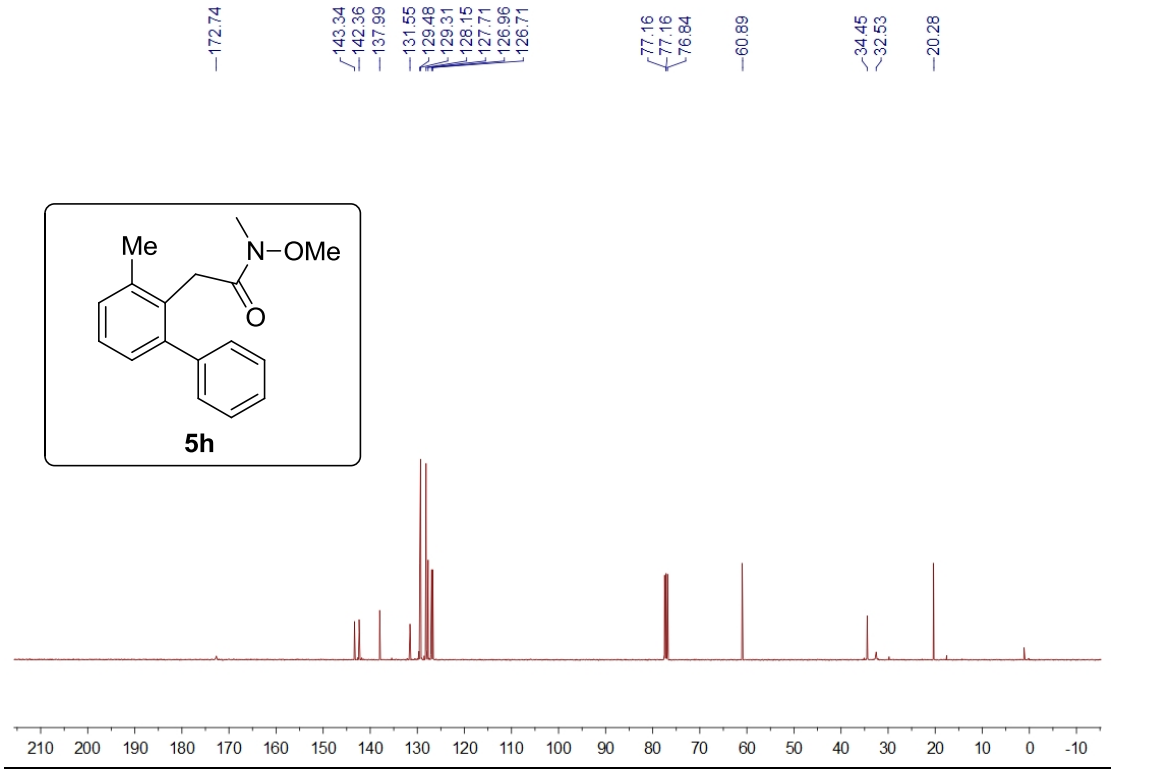
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126.71
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77.16
76.84
60.89
34.45
32.53
20.28
Me
N−OMe
O
5h
210
200
190
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100
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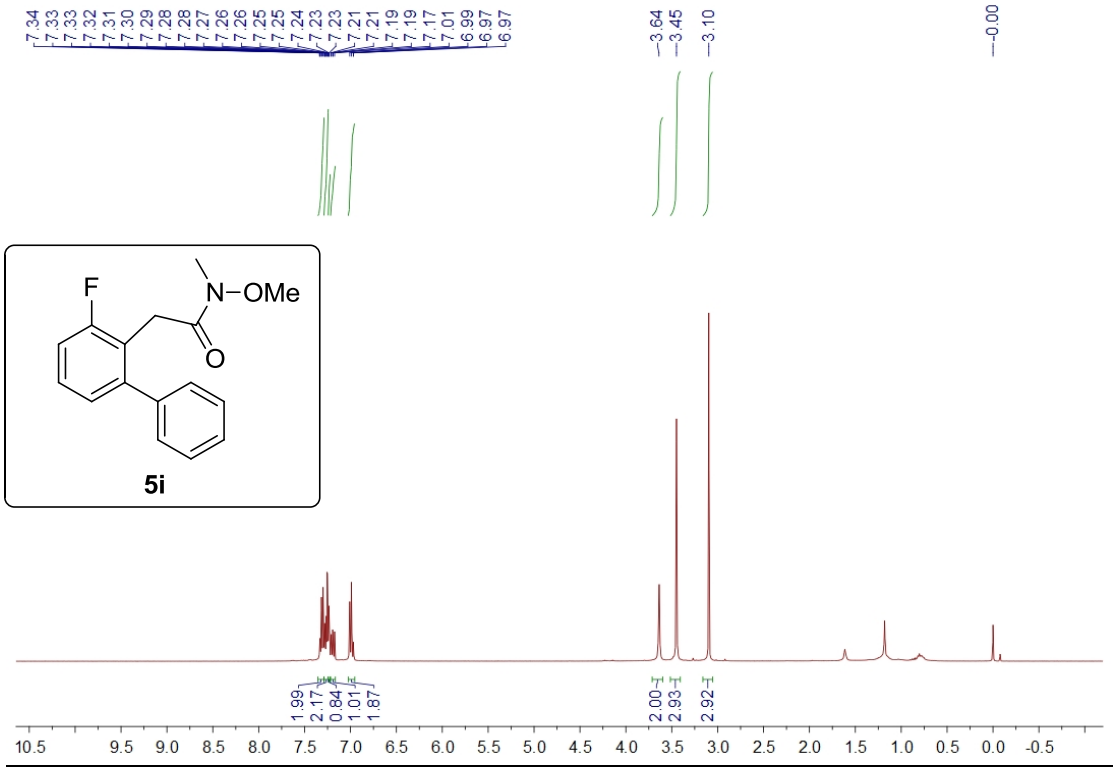
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7.24
7.23
7.23
7.21
7.21
7.19
7.19
7.17
7.01
6.99
6.97
6.97
3.64
3.45
3.10
0.00
F
N−OMe
O
5i
1.99
2.17
0.84
1.01
1.87
2.00
2.93
2.92
10.5
9.5
9.0
8.5
8.0
7.5
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6.0
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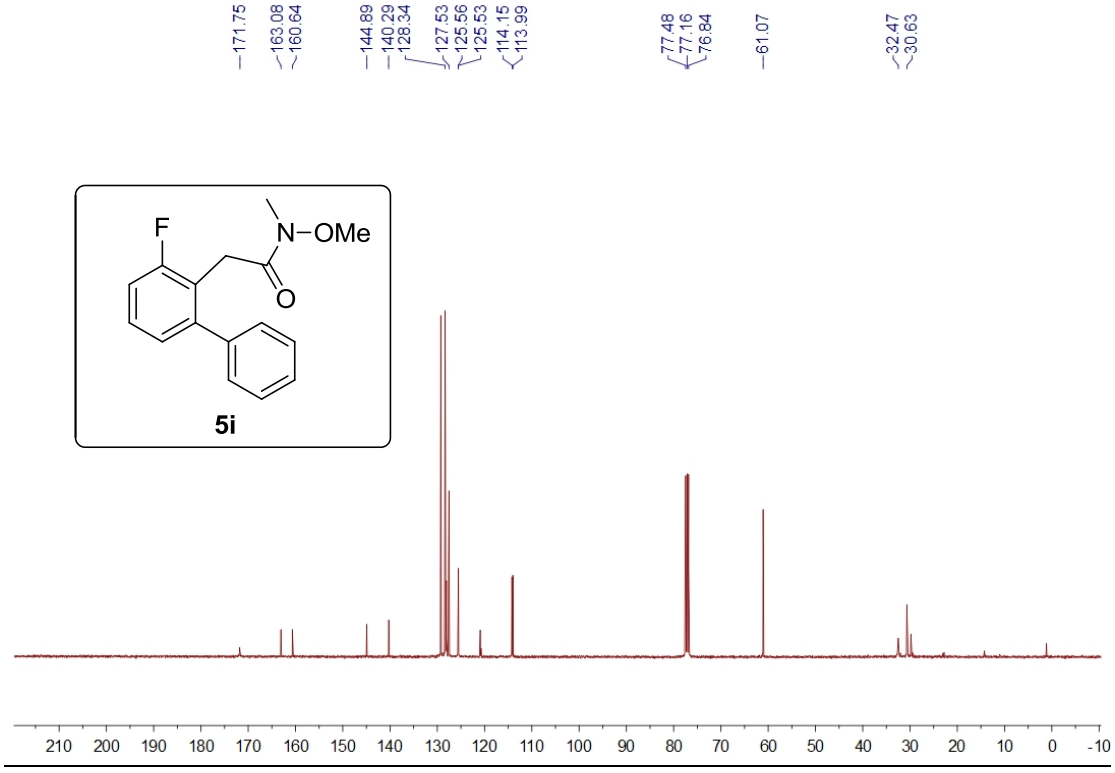
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125.56
125.53
114.15
113.99
77.48
77.16
76.84
61.07
32.47
30.63
F
N−OMe
O
5i
210
200
190
180
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140
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120
110
100
90
80
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60
50
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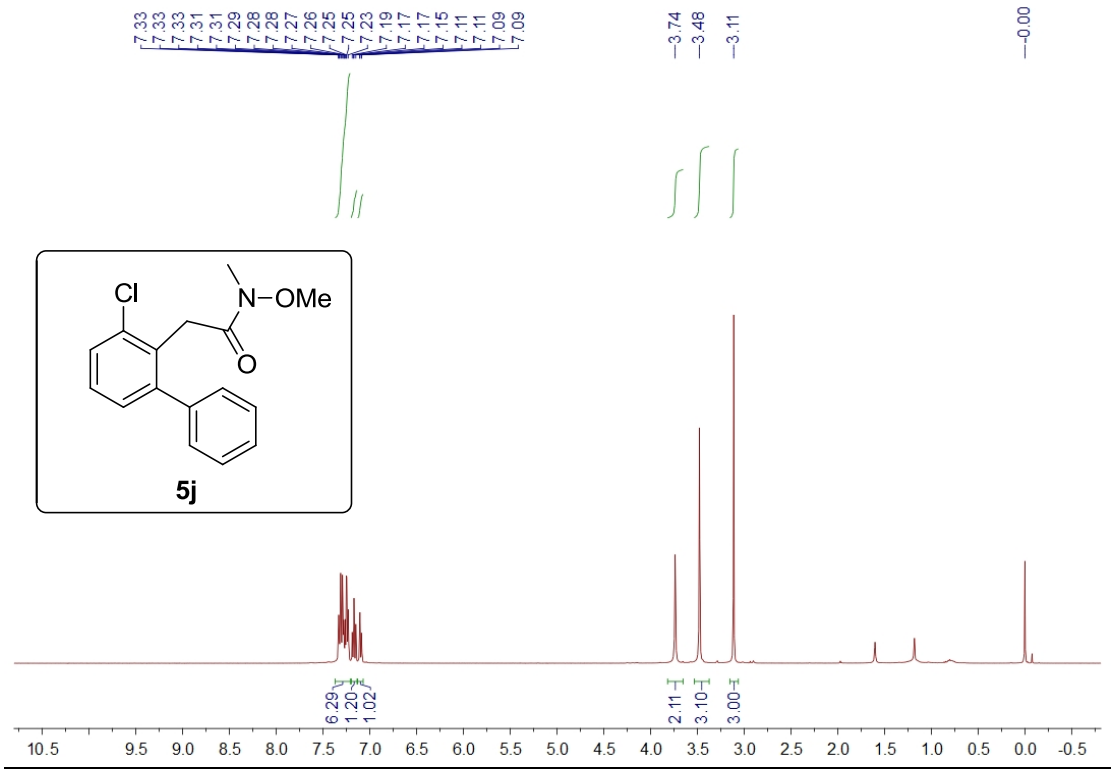
0
-10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7.23
7.19
7.17
7.17
7.15
7.11
7.11
7.09
7.09
3.74
3.48
3.11
0.00
Cl
N−OMe
O
5j
6.29
1.20
1.02
2.11
3.10
3.00
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
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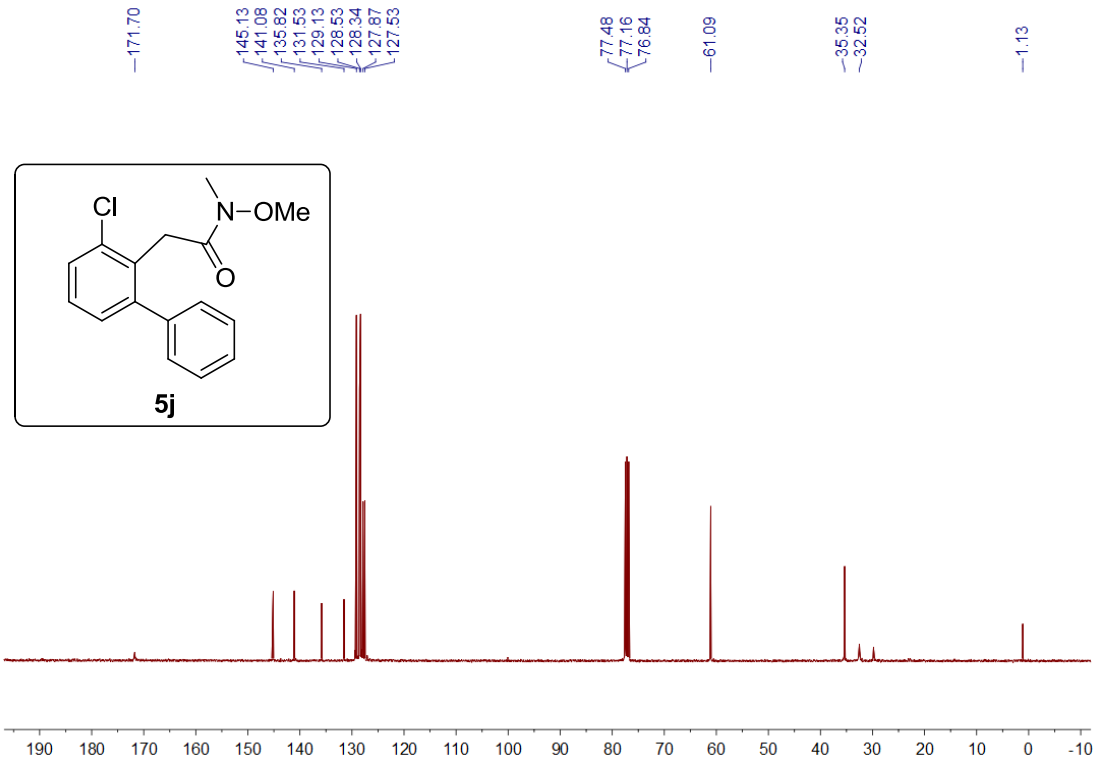
2.5
2.0
1.5
1.0
0.5
0.0
-0.5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128.34
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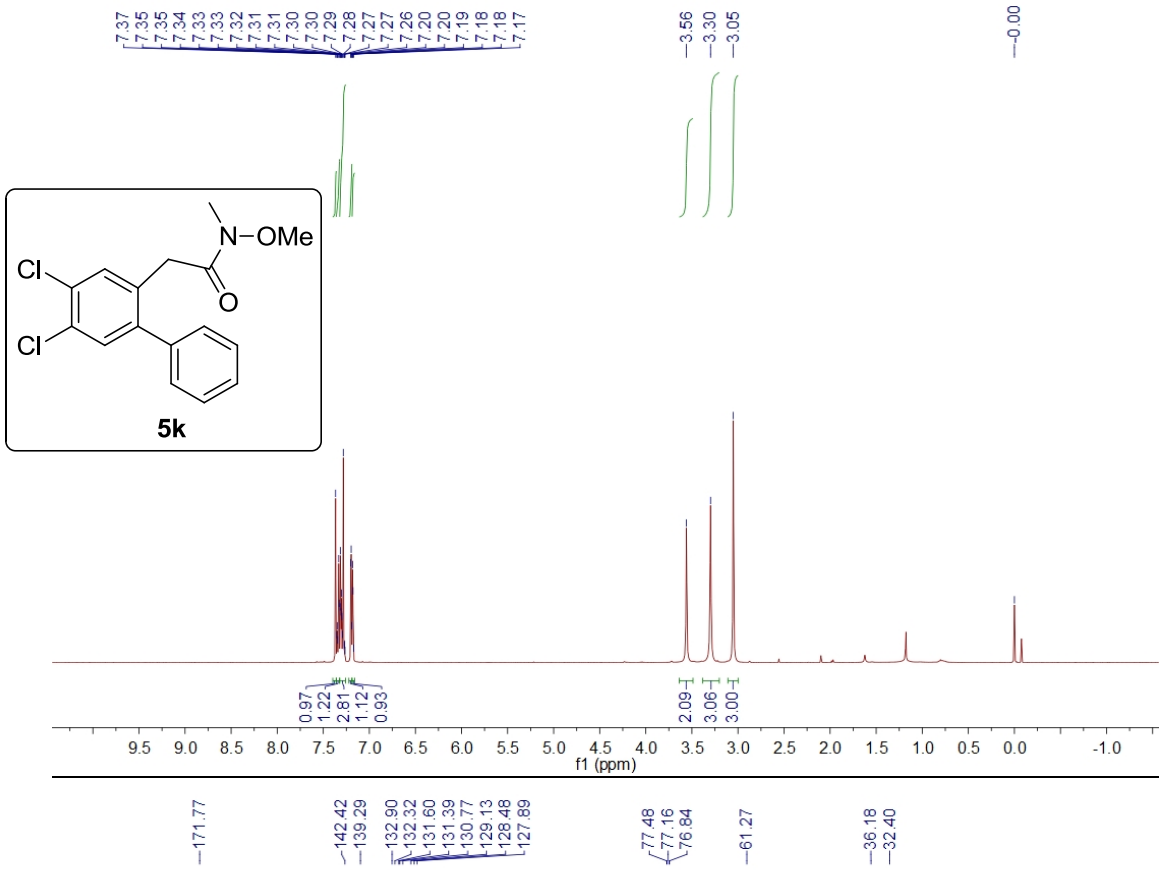
127.53
77.48
77.16
76.84
61.09
35.35
32.52
1.13
Cl
N−OMe
O
5j
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10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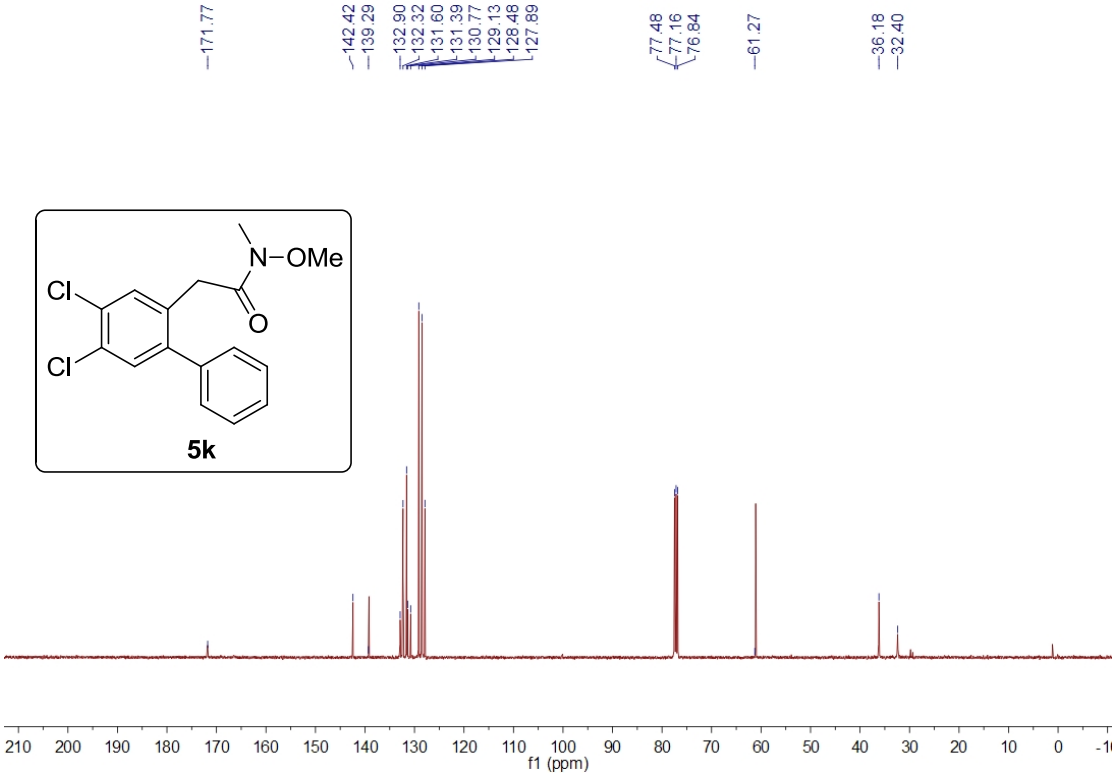
7.28
7.27
7.27
7.26
7.20
7.20
7.19
7.18
7.16
7.17
3.56
3.30
3.05
0.00
N−OMe
Cl
Cl
O
5k
0.97
1.22
2.81
1.12
0.93
2.09
3.06
3.00
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -1.0
f1 (ppm)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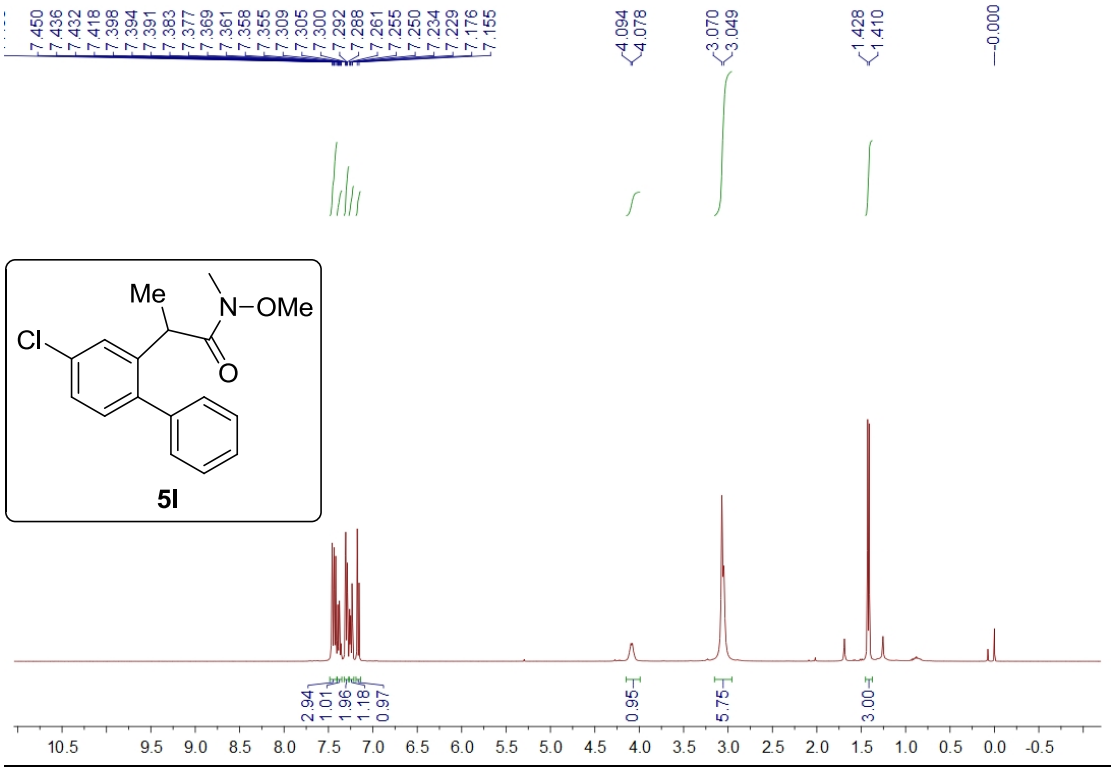
129.13
128.48
127.89
77.48
77.16
76.84
61.27
36.18
32.40
N−OMe
Cl
Cl
O
5k
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -1
f1 (ppm)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7.369
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7.358
7.355
7.309
7.305
7.300
7.292
7.288
7.261
7.255
7.250
7.234
7.229
7.176
7.155
4.094
4.078
3.070
3.049
1.428
1.410
0.000
Me
N–OMe
Cl
O
5l
2.94
1.01
1.96
1.18
0.97
0.95
5.75
3.00
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
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3.5
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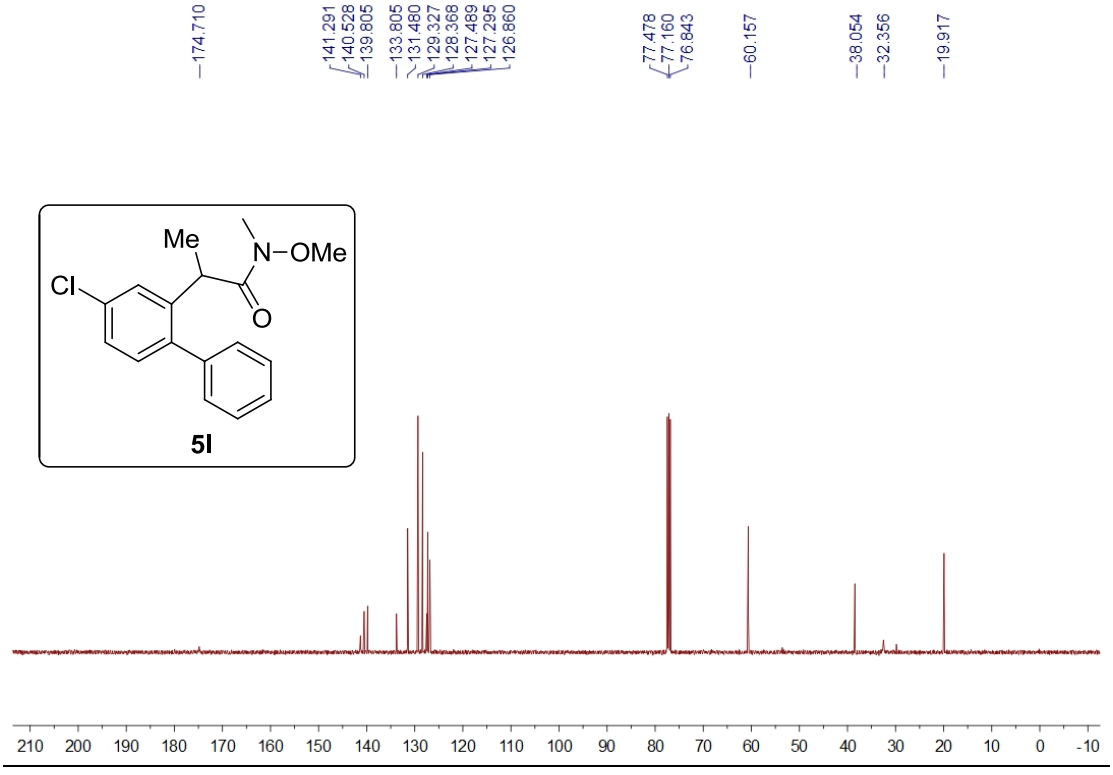
2.5
2.0
1.5
1.0
0.5
0.0
-0.5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127.295
126.860
77.478
77.160
76.843
60.157
38.054
32.356
19.917
Me
N–OMe
Cl
O
5l
210
200
190
180
170
160
150
140
130
120
110
100
90
80
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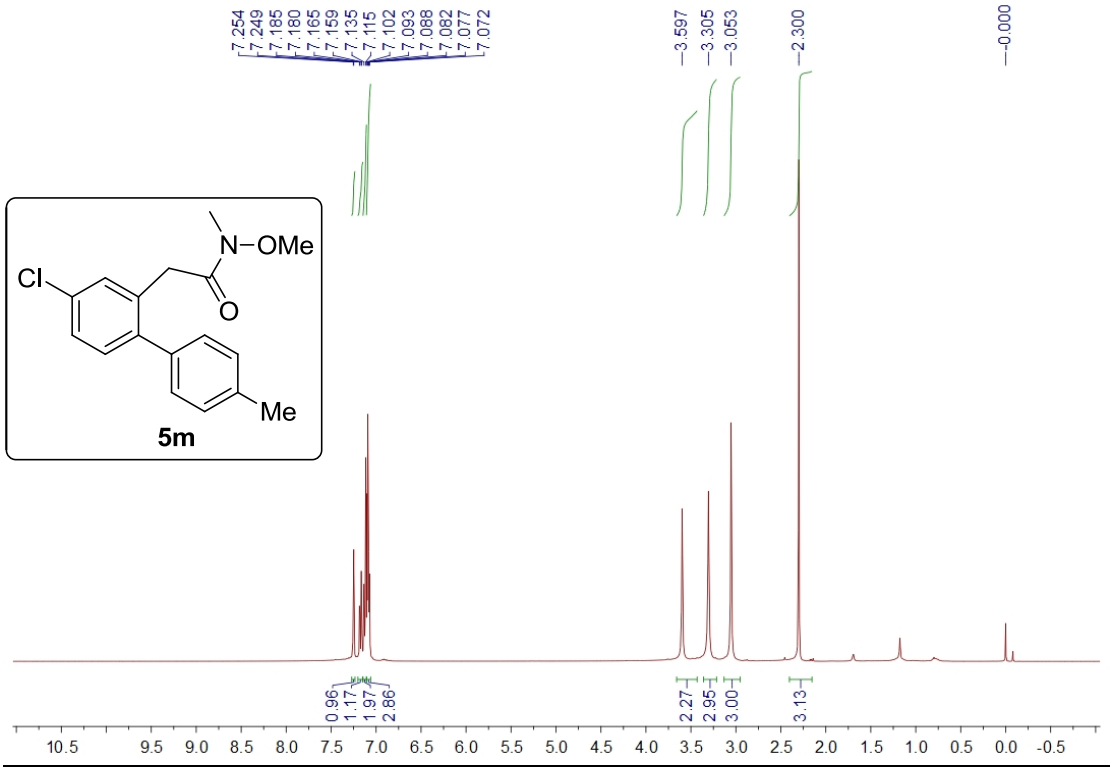
60
50
40
30
20
10
0
-10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7.135
7.115
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7.088
7.082
7.077
7.072
3.597
3.305
3.053
2.300
0.000
N−OMe
Cl
O
Me
5m
0.96
1.17
1.97
2.86
2.27
2.95
3.00
3.13
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
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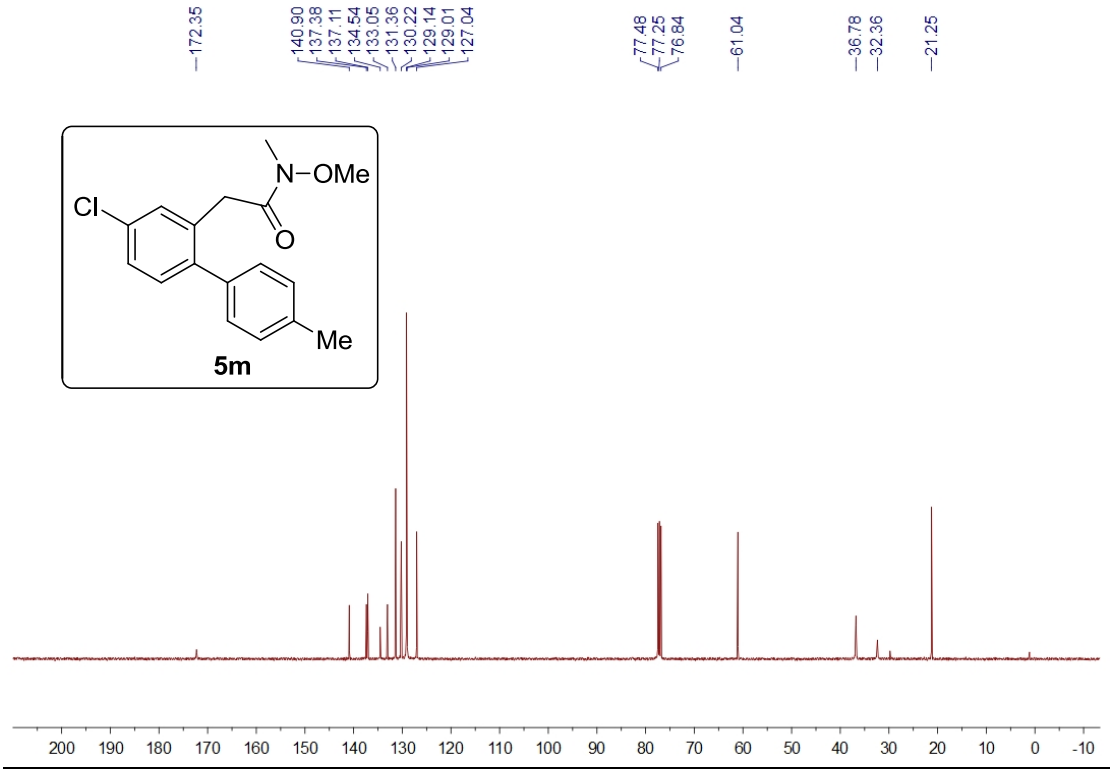
2.5
2.0
1.5
1.0
0.5
0.0
-0.5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129.14
129.01
127.04
77.48
77.25
76.84
61.04
36.78
32.36
21.25
N−OMe
Cl
O
Me
5m
200
190
180
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140
130
120
110
100
90
80
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60
50
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20
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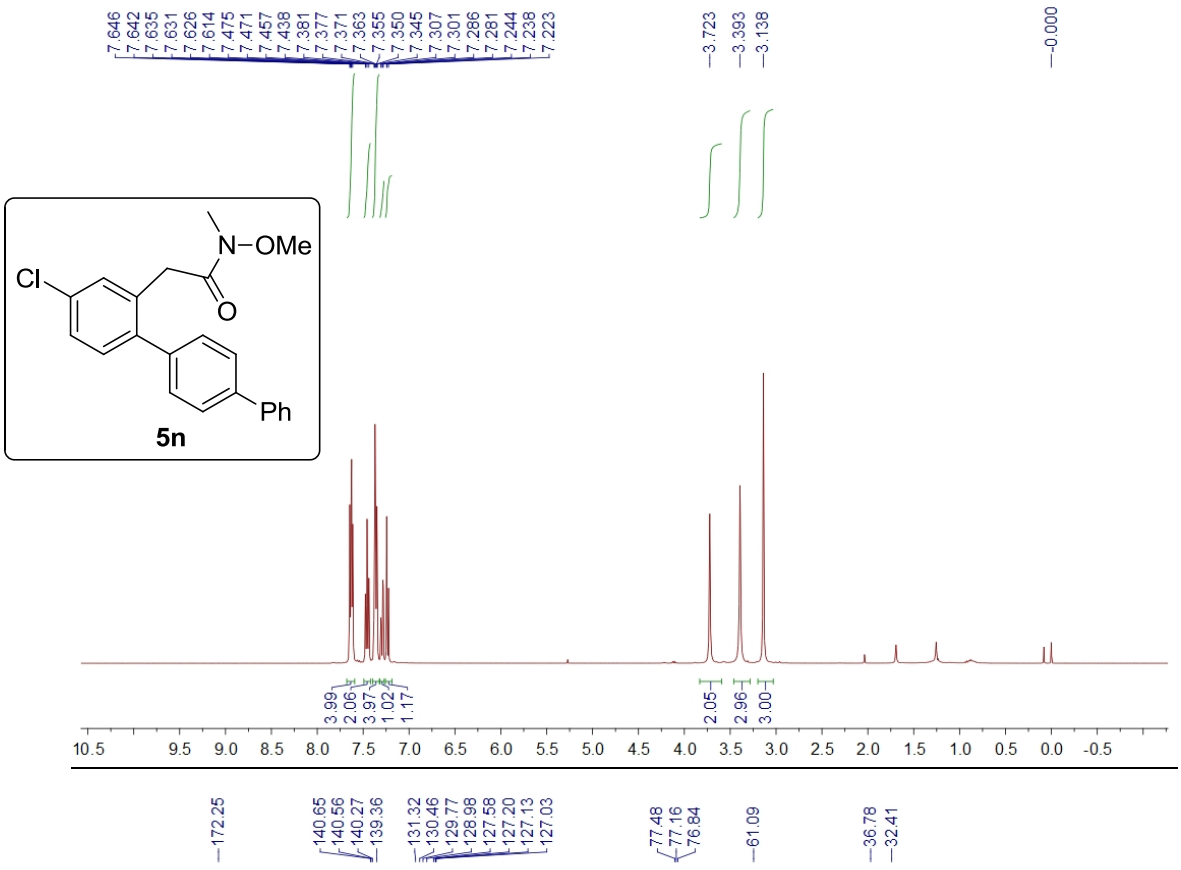
0
-10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7.371
7.363
7.355
7.350
7.345
7.307
7.301
7.286
7.281
7.244
7.238
7.223
3.723
3.393
3.138
0.000
N−OMe
Cl
O
Ph
5n
3.99
2.06
3.97
1.02
1.17
2.05
2.96
3.00
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
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2.5
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1.5
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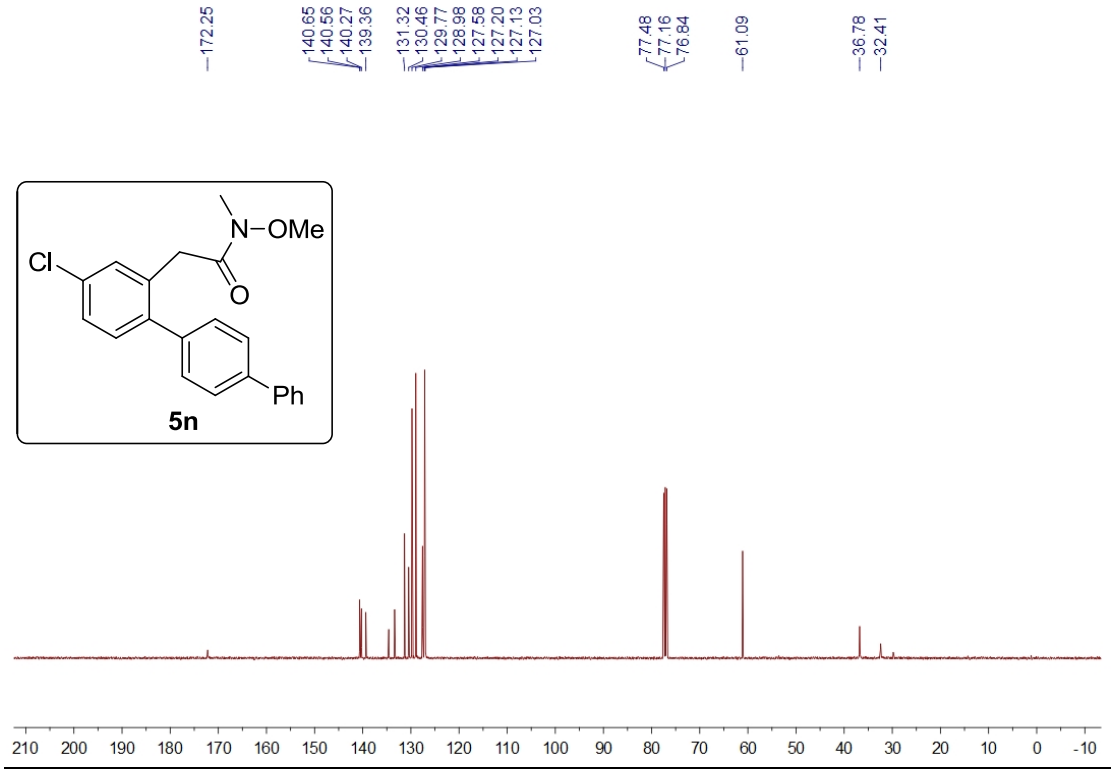
0.0
-0.5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127.20
127.13
127.03
77.48
77.16
76.84
61.09
36.78
32.41
N−OMe
Cl
O
Ph
5n
210
200
190
180
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120
110
100
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80
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60
50
40
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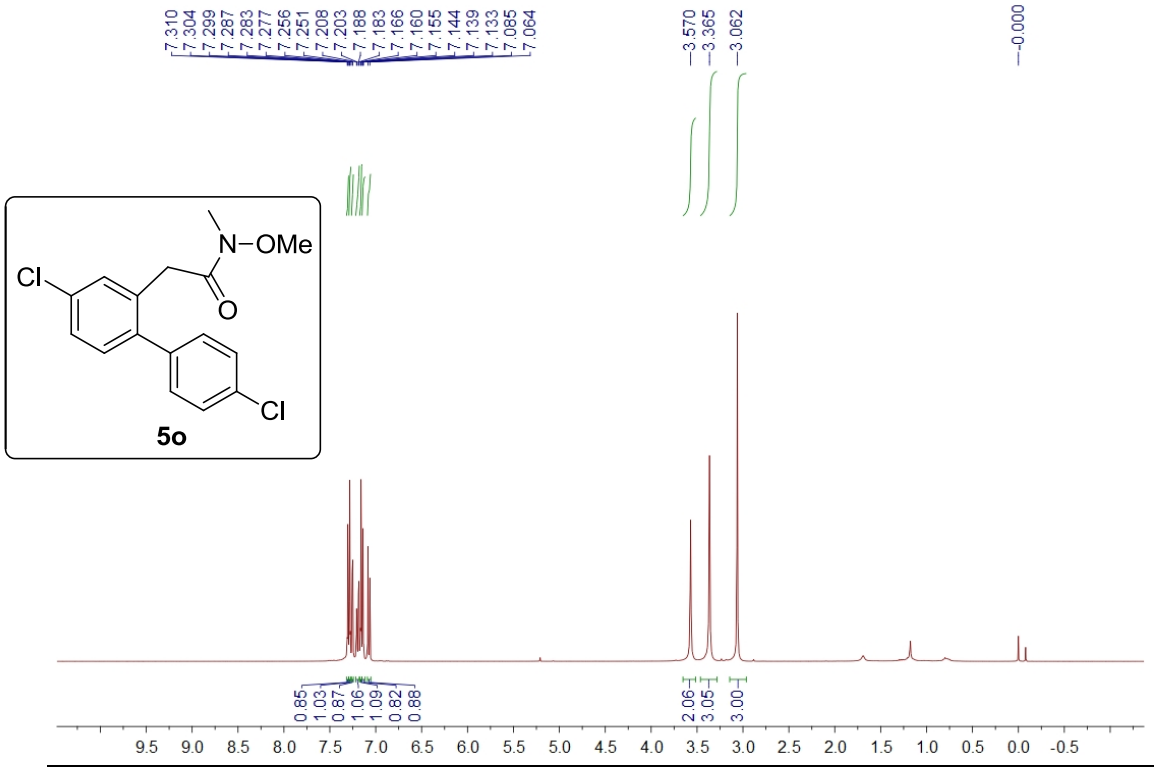
-10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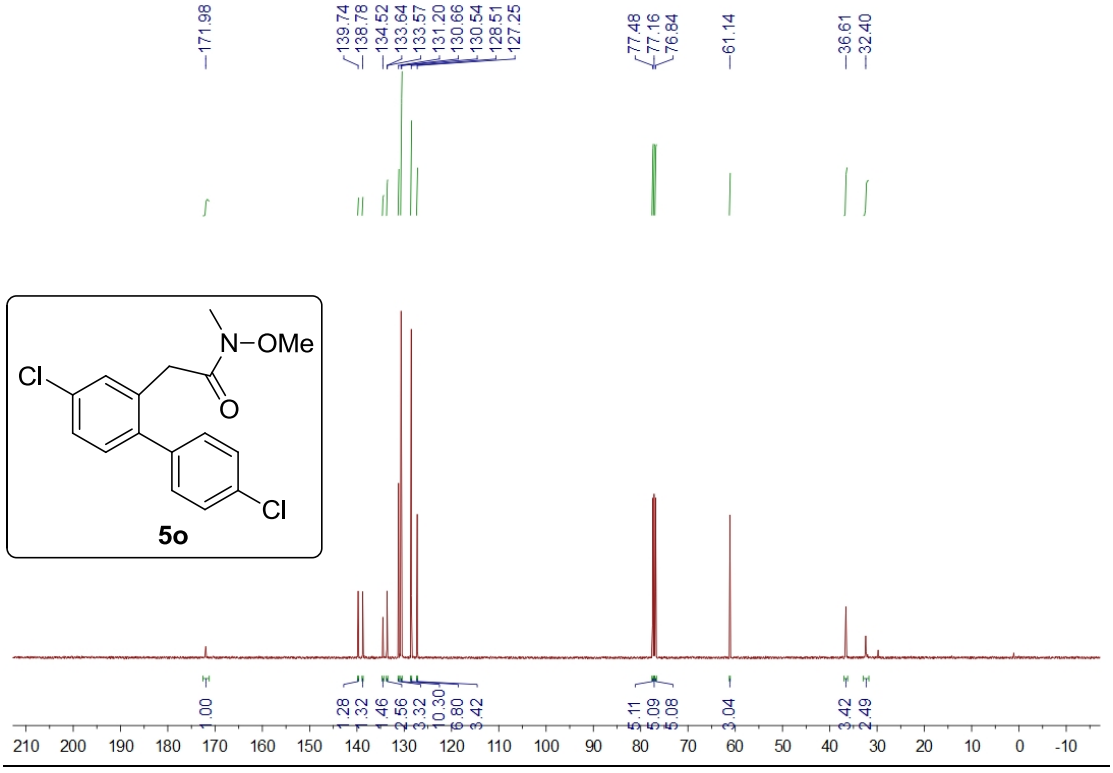
7.160
7.155
7.144
7.139
7.133
7.085
7.064
3.570
3.365
3.062
0.000
N−OMe
Cl
O
Cl
5o
0.85
1.03
0.87
1.06
1.09
0.82
0.88
2.06
3.05
3.00
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5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128.51
127.25
77.48
77.16
76.84
61.14
36.61
32.40
N−OMe
Cl
O
Cl
5o
1.00
1.28
1.32
1.46
2.56
3.32
10.30
6.80
3.42
5.11
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5.08
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3.42
2.49
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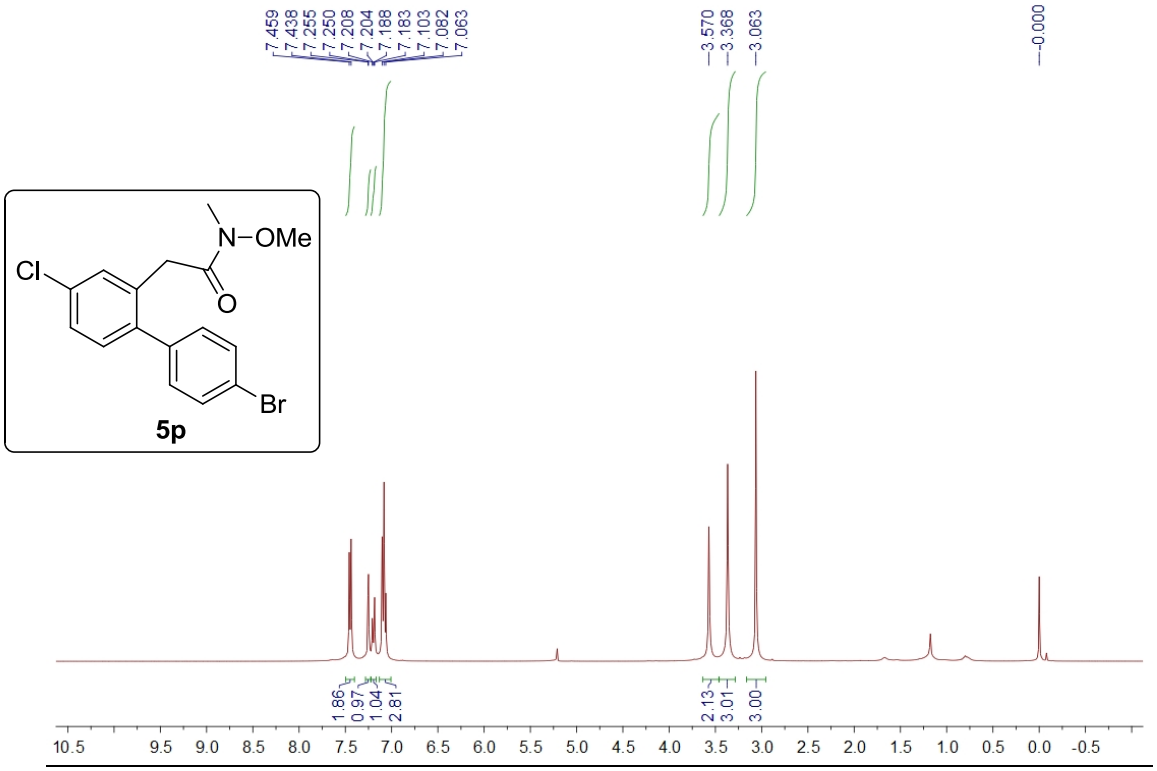
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7.204
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7.183
7.103
7.082
7.063
3.570
3.368
3.063
0.000
N–OMe
Cl
O
Br
5p
1.86
0.97
1.04
2.81
2.13
3.01
3.00
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
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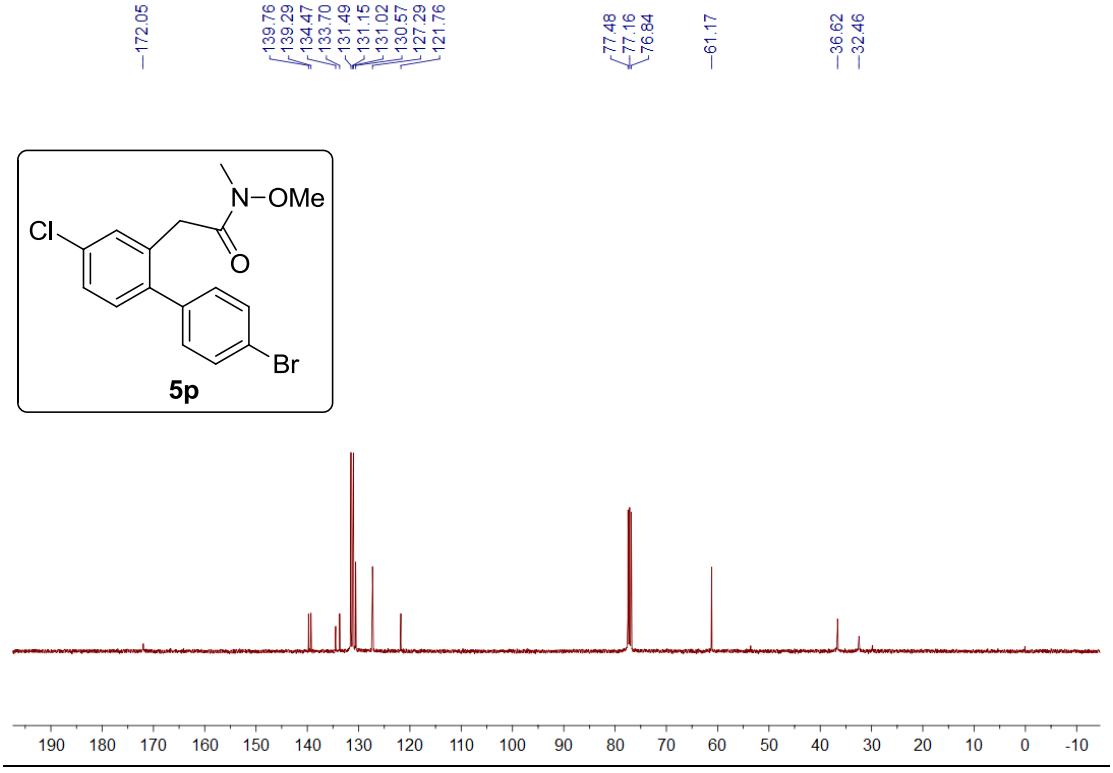
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5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131.02
130.57
127.29
121.76
77.48
77.16
76.84
61.17
36.62
32.46
N–OMe
Cl
O
Br
5p
190
180
170
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140
130
120
110
100
90
80
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60
50
40
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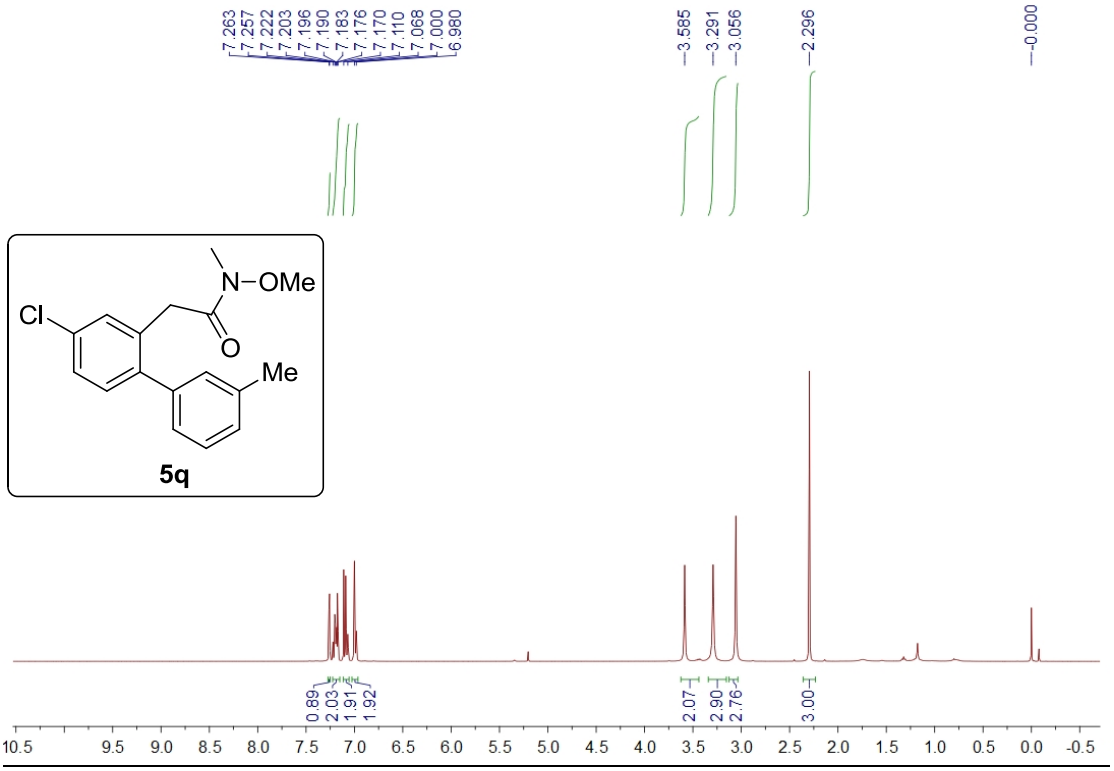
10
0
-10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7.183
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7.000
6.980
3.585
3.291
3.056
2.296
-0.000
N−OMe
Cl
O
Me
5q
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2.03
1.91
1.92
2.07
2.90
2.76
3.00
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9.5
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1.5
1.0
0.5
0.0
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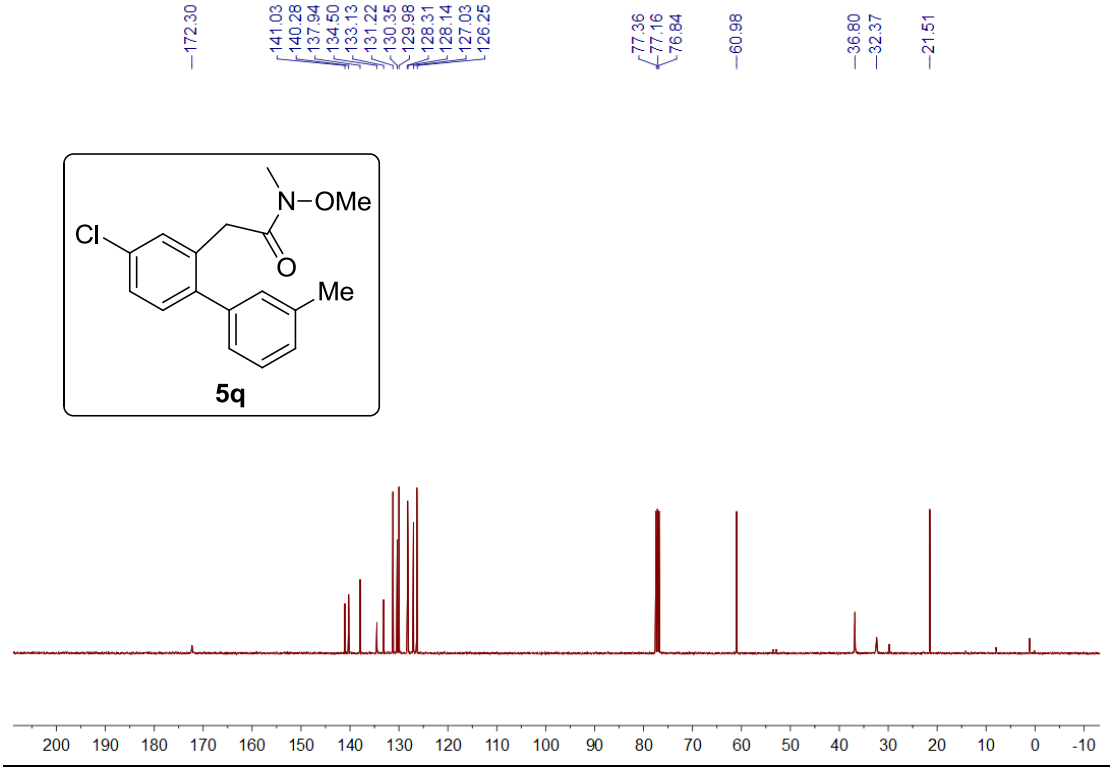
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128.31
128.14
127.03
126.25
77.36
77.16
76.84
60.98
36.80
32.37
21.51
N−OMe
Cl
O
Me
5q
200
190
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140
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120
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100
90
80
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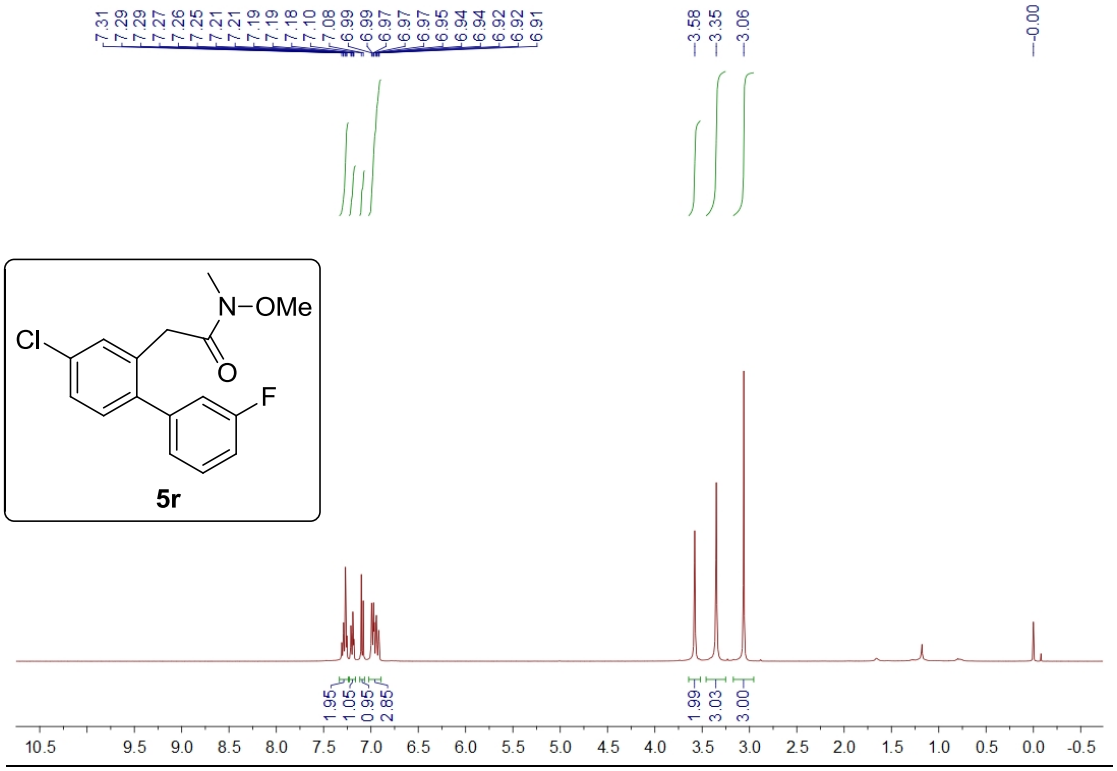
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7.27
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7.25
7.21
7.21
7.19
7.19
7.18
7.10
7.08
6.99
6.99
6.97
6.97
6.97
6.95
6.94
6.94
6.92
6.92
6.91
3.58
3.35
3.06
0.00
N−OMe
Cl
O
F
5r
1.95
1.05
0.95
2.85
1.99
3.03
3.00
10.5
9.5
9.0
8.5
8.0
7.5
7.0
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6.0
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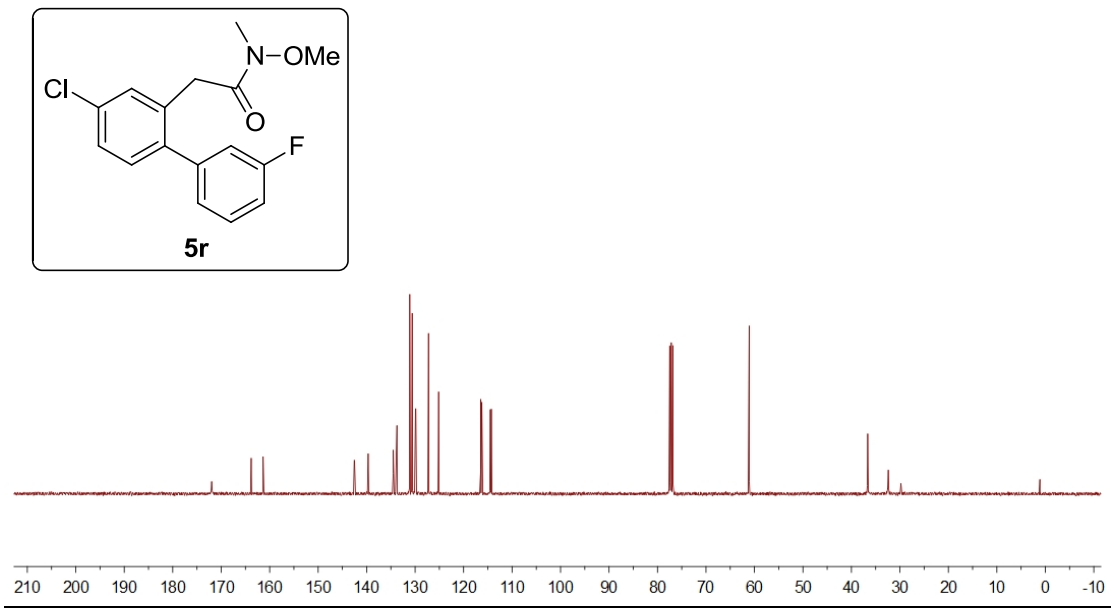
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114.276
77.478
77.160
76.843
61.089
36.634
32.394
N−OMe
Cl
O
F
5r
210
200
190
180
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160
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100
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80
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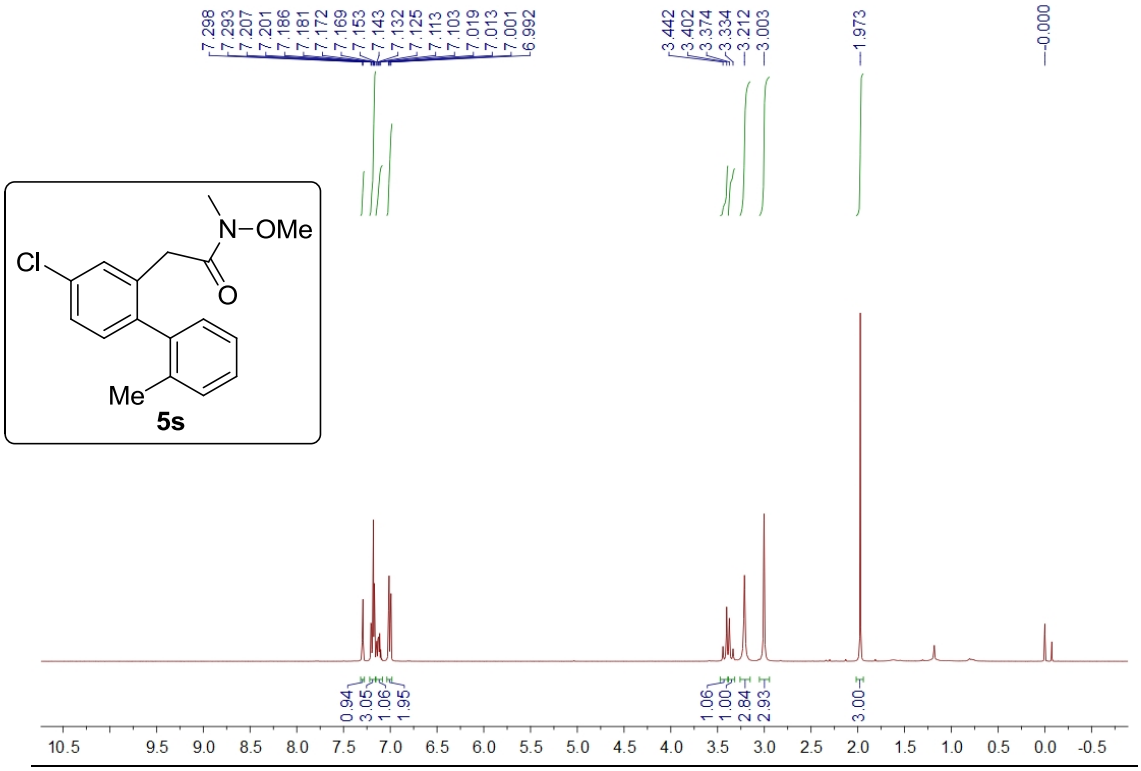
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7.169
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7.103
7.019
7.013
7.001
6.992
3.442
3.402
3.374
3.334
3.212
3.003
1.973
0.000
N−OMe
Cl
O
Me
5s
0.94
3.05
1.06
1.95
1.06
1.00
2.84
2.93
3.00
10.5
9.5
9.0
8.5
8.0
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5.5
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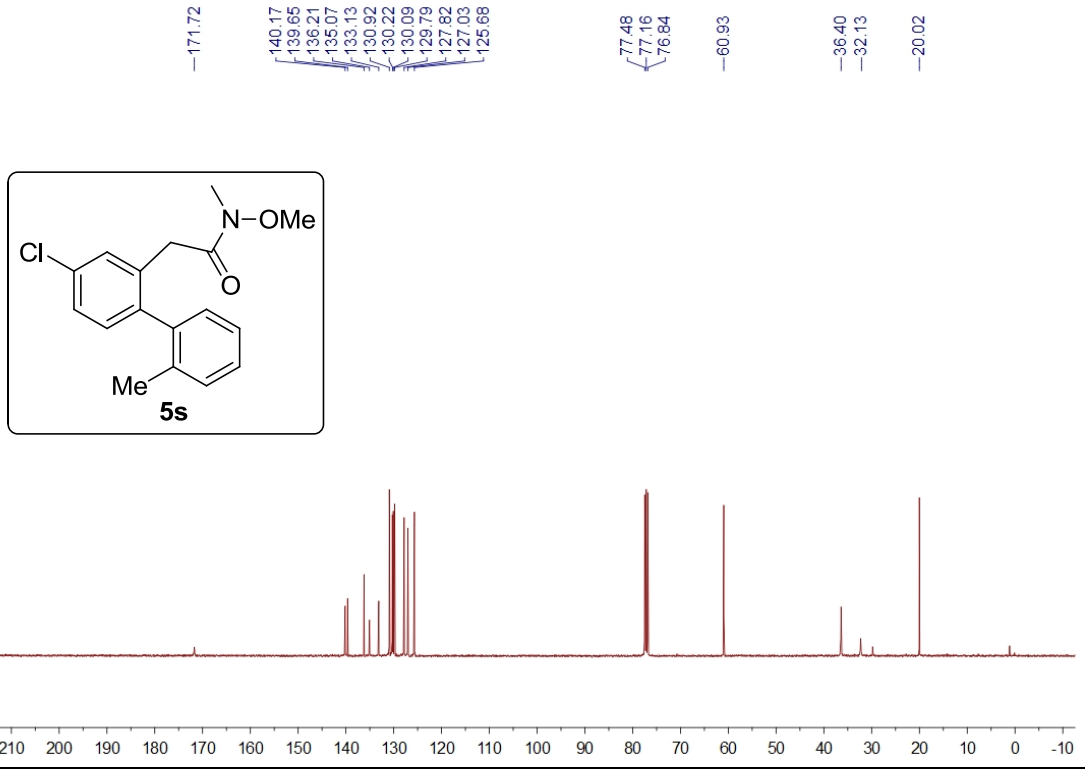
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130.22
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125.68
77.48
77.16
76.84
60.93
36.40
32.13
20.02
N−OMe
Cl
O
Me
5s
210
200
190
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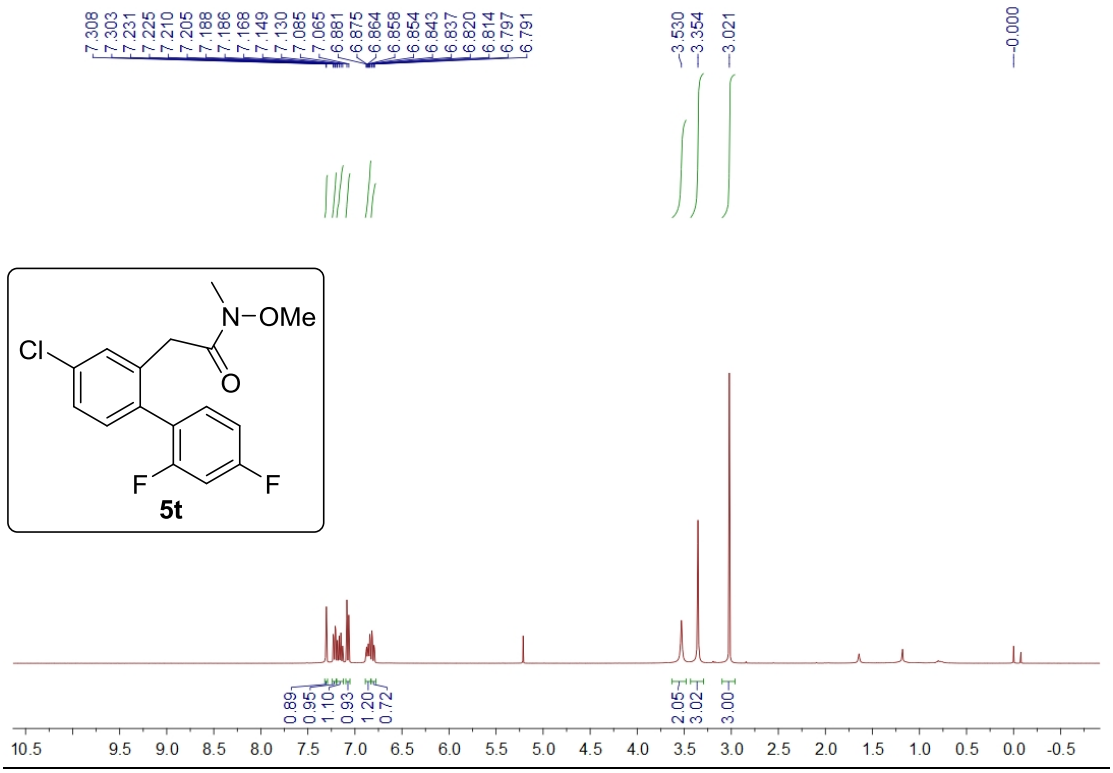
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7.130
7.085
7.065
6.881
6.875
6.864
6.858
6.854
6.843
6.837
6.820
6.814
6.797
6.791
3.530
3.354
3.021
0.000
N−OMe
Cl
O
F
F
5t
0.89
0.95
1.10
0.93
1.20
0.72
2.05
3.02
3.00
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
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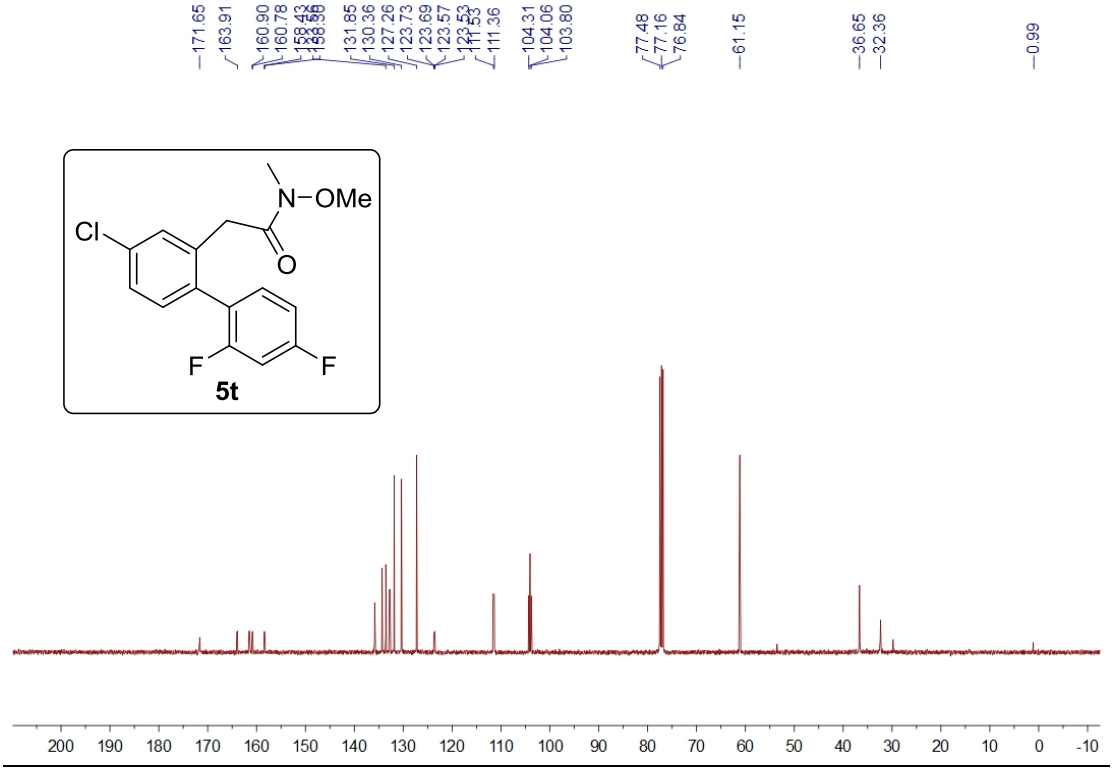
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103.80
77.48
77.16
76.84
61.15
36.65
32.36
0.99
N−OMe
Cl
O
F
F
5t
200
190
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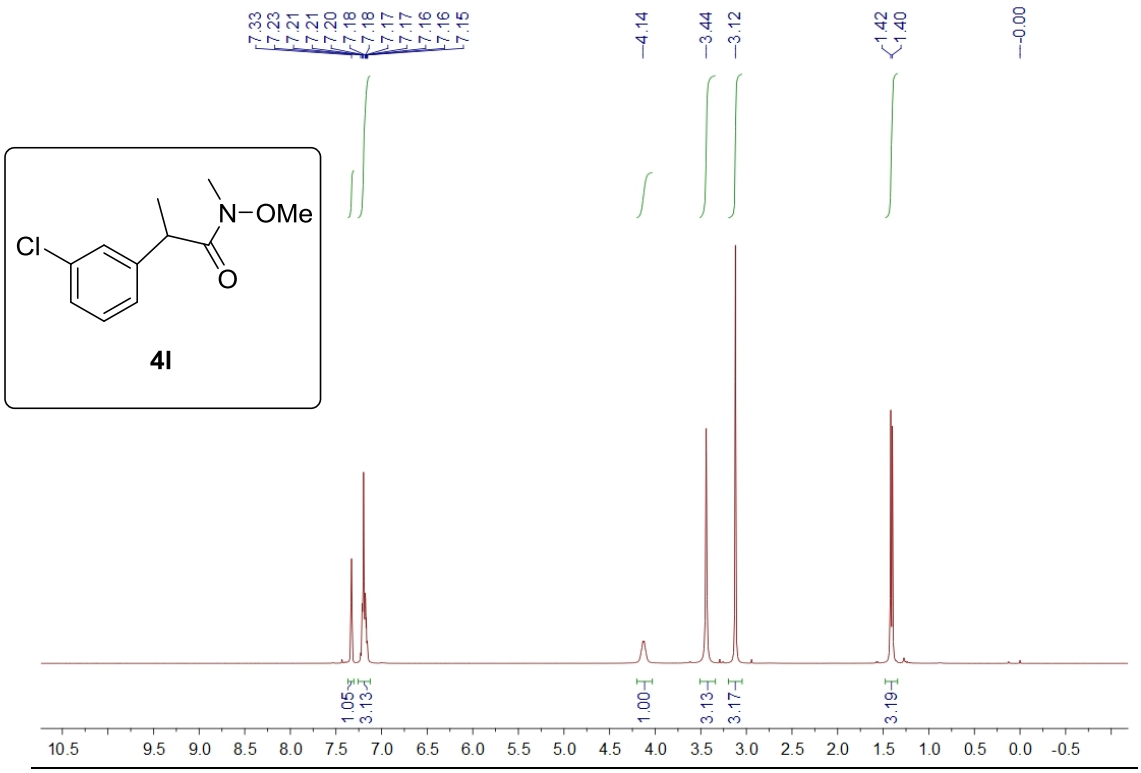
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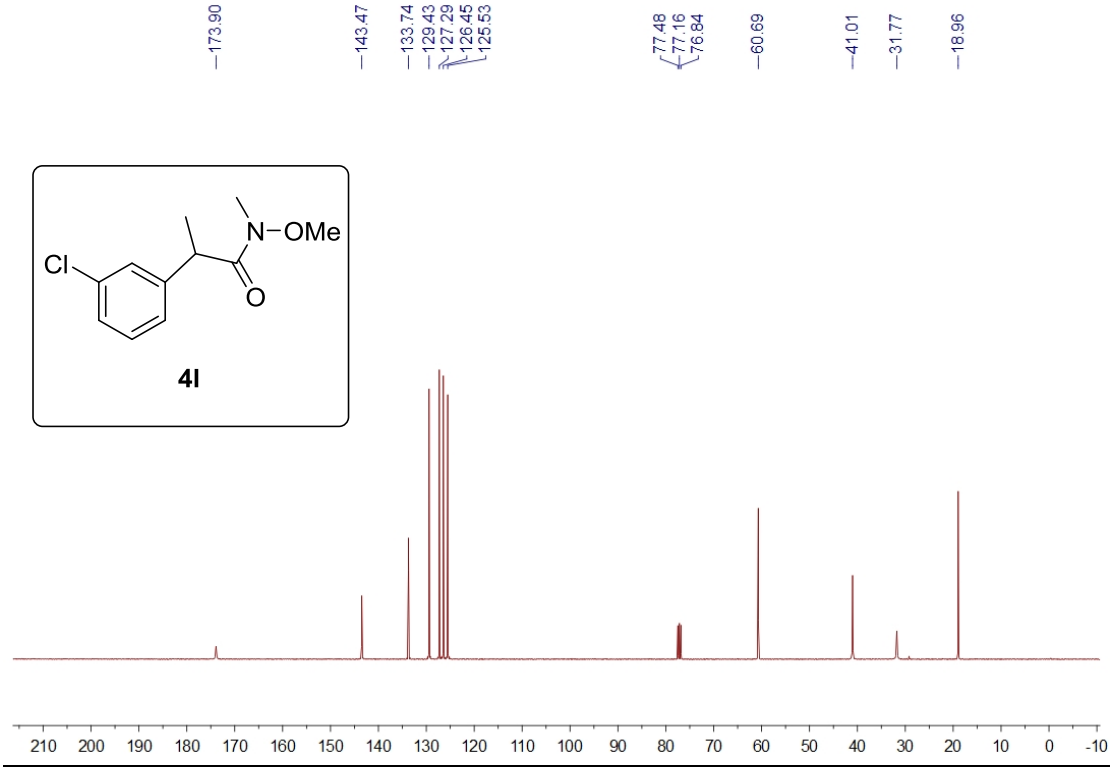
3.44
3.12
1.42
1.40
0.00
Cl
N−OMe
O
4l
1.05
3.13
1.00
3.13
3.17
3.19
10.5 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5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76.84
60.69
41.01
31.77
18.96
Cl
N−OMe
O
4l
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10

Kinetic isotope effect (KIE)