Supporting Information

Unmasked Acyl Anion Equivalent from Acid Chloride with Indium: Reversed-Polarity Synthesis of Unsymmetric Aryl Aryl and Alkenyl Aryl Ketone through Palladium-Catalyzed Cross-Coupling Reaction

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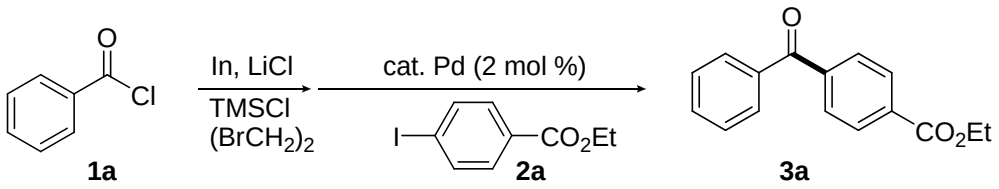
Contents

Experimental Section

General: Reactions were carried out in oven-dried glassware under a nitrogen atmosphere. Indium and pd_2dba_3 were purchased from Aldrich Chemical Co. and were used as received. Commercial available reagents were used without purification. NMP was dried by distilling the benzene-water azeotrope from an NMP-benzene mixture. THF was purified by distillation from sodium-benzophenone ketyl under nitrogen. DMSO was purified by distillation from CaH_2 under nitrogen. DMF was purified by distillation from CaH_2 under nitrogen. All reaction mixtures were stirred magnetically and were monitored by thin-layer chromatography using silica gel pre-coated glass plates, which were visualized with UV light and then, developed using either iodine or a solution of anisaldehyde. Flash column chromatography was carried out using silica gel (230-400 mesh). ^{1}H NMR (400 MHz), ^{13}C NMR (100 MHz), spectra were recorded on NMR spectrometer. Deuterated chloroform was used as the solvent, and chemical shift values (δ) are reported in parts per million relative to the residual signals of this solvent (δ 7.26 for ^{1}H and δ 77.0 for ^{13}C). Infrared spectra were recorded on FT-IR spectrometer as either a thin film pressed between two sodium chloride plates or as a solid suspended in a potassium bromide disk. Mass spectra were obtained from the KBSI on high resolution mass spectrometer. Melting points were determined in open capillary tube using Electrothermal 9100 apparatus.

Additional Data for Optimization of Reaction Conditions

Table 1. Optimization of Solvent[a]

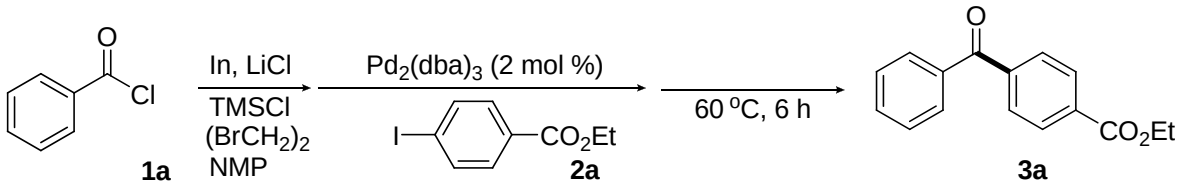


1a **2a** **3a**

entry	cat.	solvent	*T* (°C)	*t* (h)	yield (%)
1	$Pd(OAc)_2$ / SPhos	THF	70	18	21 (18)[b] (18)[c]
2	$Pd_2(dba)_3$	THF:NMP (2:1)	70	12	67 (16)[b] (16)[c]
3	$Pd_2(dba)_3$	THF:DMF (2:1)	25	12	41 (8)[b] (36)[c]
4	$Pd_2(dba)_3$	THF:DMSO (2:1)	25	12	45 (25)[b] (16)[c]
5	$Pd_2(dba)_3$	DMF	90	5	31 (27)[b]
6	$Pd_2(dba)_3$	DMSO	90	12	0
7	$Pd_2(dba)_3$	NMP	25	3	86

[a] **1a** (1.5 equiv) and **2a** (1 equiv) were used in the presence of In (3 equiv), LiCl (3 equiv), TMSCl (6 mol %), and $(BrCH_2)_2$ (15 mol %). [b] Numbers in parenthesis are isolated yield of 4,4'-diethoxycarbonyl-1,1'-biphenyl (**4**). [c] Benzil (**3m**).

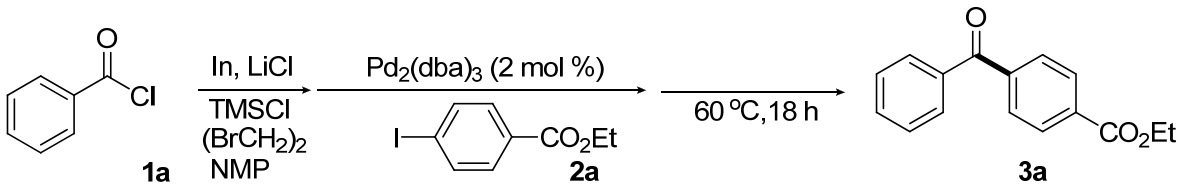
Table 2. Optimization of Ligand[a]



entry	ligand (mol %)	yield (%)[b]
1	Xantphos (8)	0
2	DPEphos (8)	0 (48)
3	PPh_3 (16)	0 (44)
4	PCy_3 (16)	56
5	P(Biphenyl)Cy_2 (16)	53
6	P(furyl)$_3$ (16)	20 (12)
7	P(*o*-tolyl)3 (16)	0

[a] **1a** (1.5 equiv) and **2a** (1 equiv) were used in the presence of In (3 equiv), LiCl (3 equiv), TMSCl (6 mol %), and $(BrCH_2)_2$ (15 mol %) in NMP (1 mL). [b] Numbers in parenthesis are isolated yield of 4,4'-diethoxycarbonyl-1,1'-biphenyl (**4**).

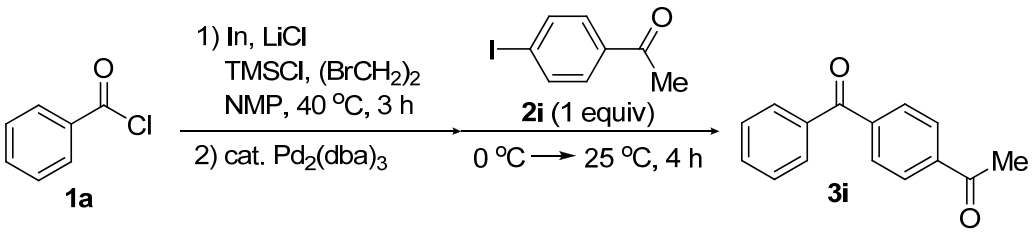
Table 3. Optimization of Additive[a]



entry	additive (equiv)	yield (%)[b]
1	-	0 (55)
2	LiCl (1)	53 (15)
3	LiCl (2)	30 (13)
4	LiCl (3)	86
5	LiCl (4)	61 (33)
6	LiBr (3)	64 (21)
7	LiI (3)	68 (19)
8	KBr (3)	0
9	KI (3)	0

[a] **1a** (1.5 equiv) and **2a** (1 equiv) were used in the presence of In (3 equiv) TMSCl (6 mol %), and $(CH_2Br)_2$ (15 mol %) in NMP (1 mL). [b] Numbers in parenthesis are isolated yield of 4,4'-diethoxycarbonyl-1,1'-biphenyl (**4**).

Table 4. Control Experiment Using Benzoyl Chloride



entry	**1a** (equiv)	In (equiv)	LiCl (equiv)	TMSCl (mol %)	$(BrCH_2)_2$ (mol %)	yield (%)[a]
1	2.0	3.0	3.0	-	15	39 (26)
2	2.0	3.0	3.0	6	-	42 (19)
3	2.0	3.0	3.0	-	-	37 (22)

[a] Numbers in parenthesis are isolated yield of 4,4'-dimthoxycarbonyl-1,1'-biphenyl (**4**).

General procedure for indium insertion : First, LiCl must be dried as follows: LiCl was placed in a nitrogen-flushed flask and dried for additionally 5-10 min with a heat gun under high vacuum. NMP (1 mL) was added to In (104.0 mg, 0.9 mmol) and LiCl (38.0 mg, 0.9 mmol) in test tube and then, TMSCl (2.0 mg, 15 mol %) and 1,2-dibromoethane (8.5 mg, 6 mol %) were successively added at 25 °C.

Preparation of acylindium from benzoyl chloride (1a) : Benzoyl chloride **1a** (84.0 mg, 0.6 mmol) was added to above mixture at 25 °C and then, it was stirred at 40 °C for 3 h, producing acylindium reagent.

Preparation of acylindium from *m*-methylbenzoyl chloride (1b) : *m*-Methylbenzoyl chloride **1b** (93.0 mg, 0.6 mmol) was added to above mixture at 25 °C and then, it was stirred at 40 °C for 3 h, producing acylindium reagent.

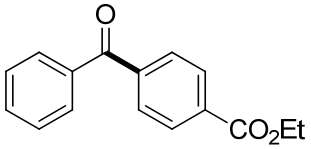
Preparation of acylindium from *tert*-butylbenzoyl chloride (1c) : *tert*-Butylbenzoyl chloride **1b** (118.0 mg, 0.6 mmol) was added to above mixture at 25 °C and then, it was stirred at 80 °C for 3 h, producing acylindium reagent.

Preparation of acylindium from *p*-methoxybenzoyl chloride (1d) : *p*-Methoxybenzoyl chloride **1d** (102.0 mg, 0.6 mmol) was added to above mixture at 25 °C and then, it was stirred at 80 °C for 3 h, producing acylindium reagent.

Preparation of acylindium from *p*-chlorobenzoyl chloride (1e) : *p*-Chlorobenzoyl chloride **1e** (105.0 mg, 0.6 mmol) was added to above mixture at 25 °C and then, it was stirred at 80 °C for 3 h, producing acylindium reagent.

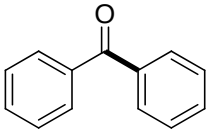
General procedure for cross-coupling reaction of acylindium reagent generated in situ from benzoyl chloride with ethyl 4-iodobenzoate (Table 1-3) : Above pre-preapred organoindium reagent in NMP was carefully transferred to solution of $Pd_2(dba)_3$ (2 mol %) in NMP (0.3 mL) using syringe at 0 ^oC. After ehtyl 4-iodobenzoate (82.8 mg, 0.3 mmol) was added, the reaction mixture was stirred at 25 ^oC. After the completion of the reaction (checked by TLC), the reaction mixture was quenched with NH_4Cl (2 mL) and water (2 mL). The aqueous layer was extracted with ethyl acetate. The combined organic extracts were dried over $MgSO_4$, filtered, and concentrated under reduced pressure. Silica gel fresh column chromatography (ethyl acetate:hexane = 1:10) gave ethyl 4-benzoylbenzoate (65.6 mg, 0.26 mmol, 86%) as white solid.

Ethyl 4-benzoylbenzoate (3a)[1] : R_f = 0.3 (EtOAc: hexane = 1:20); Yellow oil; ^1H NMR (400 MHz, $CDCl_3$) δ 8.15 (dt, J = 8.22 Hz, 1.73 Hz, 2H), 7.84 (dt, J = 8.34 Hz, 1.72 Hz, 2H), 7.81-7.79 (m, 2H), 7.65-7.60 (m, 1H), 7.52-7.48 (m, 2H), 4.42 (q, J = 7.12 Hz, 2H), 1.42 (t, J = 7.12 Hz, 3H); ^{13}C NMR (100 MHz) δ = 196.1, 165.8, 141.2, 136.9, 133.5, 132.9, 130.1, 129.7, 129.4, 128.4, 61.4, 14.3; IR (film): 1729, 1714, 1660, 1597, 1447, 1367, 1276, 1104, 1020, 768 cm^{-1}; HRMS (EI): *m/z* calcd for $C_{16}H_{14}O_3$: 254.0943; found : 254.0943



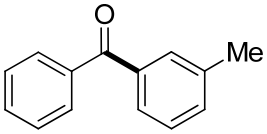
3a

Benzophenone (**3b**)[2] : R_f = 0.3 (EtOAc: hexane = 1:15); White solid. Melting point: 48-50 ^oC; ^1H NMR (400 MHz, $CDCl_3$) δ 7.99-7.96 (m, 4H), 7.70-7.65 (m, 2H), 7.54-7.50 (m, 4H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 194.5, 134.9, 132.9, 129.9, 129.0; IR (film): 1681, 1671, 1595, 1449, 1211, 1175, 873, 684 cm^{-1}; HRMS (EI): *m/z* calcd for $C_{13}H_{10}O$: 182.0732; found : 183.0732



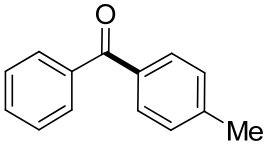
3b

3-Methylbenzophenone (**3c**)[3] : R_f = 0.3 (EtOAc: hexane = 1:15); Pale yellow oil; ^1H NMR (400 MHz, $CDCl_3$) δ 7.81-7.79 (m, 2H), 7.63-7.62 (m, 1H), 7.61-7.56 (m, 2H), 7.51-7.46 (m, 2H), 7.42-7.34 (m, 2H), 2.42 (s, 3H); ^{13}C NMR (400 MHz, $CDCl_3$) δ 197.0, 138.1, 137.7, 137.6, 133.1, 132.3, 130.4, 130.0, 128.2, 128.0, 127.3, 21.3; IR (film): 3060, 2923, 1660, 1598, 1447, 1316, 1280, 1178, 719 cm^{-1}; HRMS (EI): *m/z* calcd for $C_{14}H_{12}O$: 196.0888; found : 196.0888



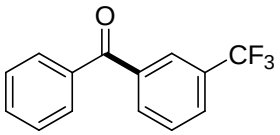
3c

4-Methylbenzophenone (**3d**)[3] : R_f = 0.3 (EtOAc: hexane = 1:30); Pale yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.80-7.71 (m, 2H), 7.72 (dt, *J* = 8.17 Hz, 1.72 Hz, 2H), 7.60-7.56 (m, 1H), 7.49-7.45 (m, 2H), 7.30-7.26 (m, 2H), 2.44 (s, 3H); ^{13}C NMR (400 MHz, $CDCl_3$) δ 196.5, 143.2, 137.9, 134.8, 132.1, 130.3, 129.9, 128.9, 128.2, 21.6; IR (film): 3058, 2921, 1657, 1605, 1446, 1314, 1277, 1177, 922, 700 cm^{-1}; HRMS (EI): *m/z* calcd for $C_{14}H_{12}O$: 196.0888; found : 196.0890



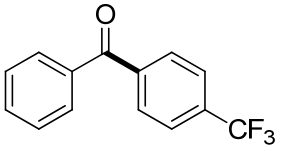
3d

3-Trifluoromethylbenzophenone (3e)[4] : R_f = 0.3 (EtOAc: hexane = 1:30); White solid. Melting point: 51-53 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.06 (s, 1H), 7.98 (d, *J* = 7.76 Hz, 1H), 7.87-7.83 (m, 1H), 7.81-7.78 (m, 2H), 7.66-7.61 (m, 2H), 7.54-7.50 (m, 2H); ^{13}C NMR (100 MHz) δ 195.2, 138.3, 136.7, 133.1, 133.0, 131.0 (q, *J* = 32.9 Hz), 130.0, 128.9, 128.85 (q, *J* = 3.6 Hz), 128.6, 126.7 (q, *J* = 3.7 Hz), 123.7 (q, *J* = 272.5 Hz); IR (film): 1665, 1336, 1267, 1127, 1073, 713, 692, 659 cm^{-1}; HRMS (EI): *m/z* calcd for $C_{14}H_9F_3O$: 250.0605; found : 250.0604



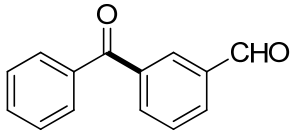
3e

4-Trifluoromethylbenzophenone (3f)[3] : R_f = 0.3 (EtOAc: hexane = 1:30); White solid. Melting point: 107-110 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.89 (d, *J* = 8.00, 2H), 7.82-7.79 (m, 2H), 7.76 (d, *J* = 8.03, 2H), 7.66-7.61 (m, 1H), 7.53-7.48 (m, 2H), ; ^{13}C NMR (100 MHz) δ 195.6, 140.7, 136.7, 133.7 (q, *J* = 32.8 Hz), 133.1, 130.15, 130.1, 128.5, 125.4 (q, *J* = 3.7 Hz), 123.6 (q, *J* = 271.1 Hz); IR (film): 1650, 1576, 1447, 1407, 1335, 1168, 1115, 857, 695 cm^{-1}; HRMS (EI): *m/z* calcd for $C_{14}H_9F_3O$: 250.0605; found : 250.0602



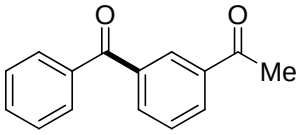
3f

3-Benzoylbenzaldehyde (3g)[5] : R_f = 0.3 (EtOAc: hexane = 1:15); Pale yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.09 (s, 1H), 8.28(t, *J* = 1.46 Hz, 1H), 8.12 (dt, *J* = 7.64 Hz, 1.44 Hz, 1H), 8.08 (dt, *J* = 7.70 Hz, 1.49 Hz, 1H), 7.83-7.80 (m, 2H), 7.68 (t, *J* = 7.66 Hz, 1H), 7.66-7.62 (m, 1H), 7.54-7.50 (m, 2H); ^{13}C NMR (100 MHz) δ 195.5, 191.4, 138.5, 136.8, 136.3, 135.4, 133.0, 132.6, 131.3, 130.0, 129.2, 128.5; IR (film): 1700, 1659, 1596, 1447, 1278, 1200, 972, 712 cm^{-1}; HRMS (EI): *m/z* calcd for $C_{14}H_{10}O_2$: 210.0681; found : 210.0683



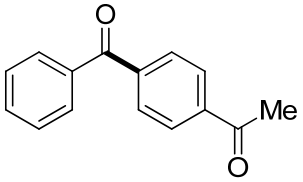
3g

3-Acetobenzophenone (3h)[4] : R_f = 0.3 (EtOAc: hexane = 1:5); Pale yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.37 (t, *J* = 1.54 Hz, 1H), 8.19 (dt, *J* = 7.83 Hz, 1.46 Hz, 1H), 7.99 (dt, *J* = 7.66 Hz, 1.45 Hz, 1H), 7.82-7.79 (m, 2H), 7.65-7.58 (m, 2H), 7.53-7.48 (m, 2H), 2.65 (s, 3H); ^{13}C NMR (100 MHz) δ 197.3, 195.8, 138.0, 137.1, 137.0, 134.2, 132.9, 131.7, 130.0, 129.7, 128.7, 128.5, 26.7; IR (film): 1692, 1661, 1597, 1578, 1447, 1425, 1358, 1240, 968, 719 cm^{-1}; HRMS (EI): *m/z* calcd for $C_{15}H_{12}O_2$: 224.0837, found : 224.0841



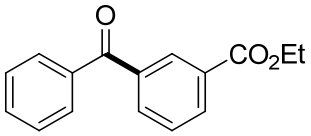
3h

4-Acetobenzophenone (3i)[6] **:** R_f = 0.3 (EtOAc: hexane = 1:7); White solid. Melting point: 83-85 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.06 (dt, *J* = 8.26 Hz, 1.75 Hz, 2H), 7.87 (dt, *J* = 8.26 Hz, 1.75 Hz, 2H) 7.82-7.79 (m, 2H), 7.65-7.61 (m, 1H), 7.52-7.49 (m, 2H), 2.67 (s, 3H); ^{13}C NMR (100 MHz,) δ 197.5, 195.9, 141.3, 139.5, 136.9, 133.0, 130.1, 130.0, 128.4, 128.1, 26.9; IR (film): 1687, 1660, 1596, 1578, 1402, 1357, 1316, 1276, 925, 700 cm^{-1}; HRMS (EI): *m/z* calcd for $C_{15}H_{12}O_2$: 224.0837; found : 224.0837



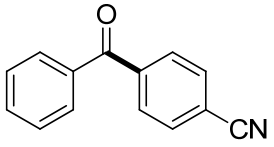
3i

Ethyl 3-benzoylbenzoate (3j)[7] : R_f = 0.3 (EtOAc: hexane = 1:15); Pale yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.45 (t, *J* = 1.70 Hz, 1H), 8.27 (dt, *J* = 7.75 Hz, 1.49 Hz, 1H), 7.99 (dt, *J* = 7.72 Hz, 1.50 Hz, 1H), 7.82-7.79 (m, 2H), 7.64-7.58 (m, 2H), 7.56-7.48 (m, 2H), 4.40 (q, *J* = 7.16 Hz, 2H), 1.40 (t, *J* = 7.21 Hz, 3H); ^{13}C NMR (100 MHz) δ 195.8, 165.8, 137.9, 137.0, 133.9, 133.1, 132.8, 130.9, 130.0, 128.4, 61.3, 14.3; IR (film): 2358, 1719, 1661, 1600, 1247, 1103, 798, 711 cm^{-1}; HRMS (EI): *m/z* calcd for $C_{16}H_{14}O_3$: 254.0943; found : 254.0943



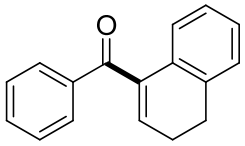
3j

4-Benzoylbenzonitrile (3k)[7] : R_f = 0.2 (EtOAc: hexane = 1:15); Pale yellow solid. Melting point: 110-113 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.89-8.86 (m, 2H), 7.81-7.77 (m, 4H), 7.67-7.63 (m, 1H), 7.54-7.49 (m, 2H); ^{13}C NMR (100 MHz) δ 195.0, 141.2, 136.3, 133.3, 132.1, 130.2, 130.0, 128.6, 118.0, 115.6; IR (film): 2228, 1697, 1649, 1596, 1447, 1279, 1251, 1112, 857, 695 cm^{-1}; HRMS (EI): *m/z* calcd for $C_{14}H_9NO$: 207.0684; found : 207.0685



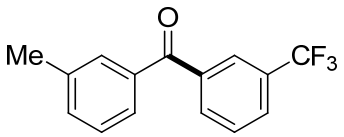
3k

3,4-Dihydronaphthalen-1-yl(phenyl)methanone (3l) : R_f = 0.3 (EtOAc: hexane = 1:20); Pale yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.88-7.86 (m, 2H), 7.57-7.49 (m, 1H), 7.43 (t, *J* = 7.7 Hz, 2H), 7.27-7.25 (m, 1H), 7.20-7.12 (m, 3H), 6.49 (t, *J* = 4.7 Hz, 1H), 2.88 (t, *J* = 8.01 Hz, 2H), 2.52-2.47 (m, 2H); ^{13}C NMR (100 MHz) δ 197.1, 138.8, 138.0, 136.5, 135.8, 132.9, 132.0, 130.0, 128.4, 127.85, 127.8, 126.7, 125.8, 27.6, 23.3; IR (film): 2359, 1665, 1603, 1434, 1335, 1205, 1168, 1073 cm^{-1}; HRMS (EI): *m/z* calcd for $C_{17}H_{14}O$: 234.1045; found : 234.1045



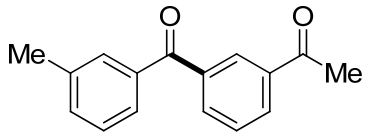
3l

3'-Methyl-3-trifluoromethylbenzophenone (3m) : R_f = 0.3 (EtOAc: hexane = 1:50); Pale yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.06 (s, 1H), 7.97 (d, *J* = 7.7 Hz, 1H), 7.84 (d, *J* = 7.84 Hz, 1H), 7.62 (t, *J* = 7.84 Hz, 2H), 7.55 (d, *J* = 7.44 Hz, 1H), 7.46-7.37 (m, 2H), 2.43 (s, 3H); ^{13}C NMR (100 MHz) δ 195.4, 138.5, 138.4, 136.8, 133.8, 133.1, 131.0 (q, *J* = 32.7 Hz), 130.4, 128.8, 128.7 (q, *J* = 3.6 Hz), 128.3, 127.3, 126.7 (q, *J* = 3.9 Hz), 123.7 (q, *J* = 272.6 Hz), 21.3; IR (film): 3064, 2925, 1721, 1666, 1434, 1335, 1275, 1204, 1168, 1130, 798, 742 cm^{-1}; HRMS (EI): *m/z* calcd for $C_{15}H_{11}F_3O$: 264.0762; found : 264.0762



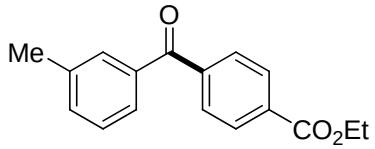
3m

3-(3-Methylbenzoyl)acetophenone (3n) : R_f = 0.3 (EtOAc: hexane = 1:10); Pale yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.36 (td, *J* = 2.5 Hz, 0.4 Hz, 1H), 8.19 (ddd, *J* = 7.8 Hz, 1.7 Hz, 1.3 Hz, 1H), 7.98 (dt, *J* = 7.66 Hz, 1.45 Hz, 1H), 7.63-7.55 (m, 3H), 7.45-7.36 (m, 2H), 2.65 (s, 3H), 2.43 (s, 3H); ^{13}C NMR (100 MHz) δ 197.3, 196.1, 138.4, 138.2, 137.1, 137.0, 134.2, 133.6, 131.6, 130.4, 129.7, 128.7, 128.3, 127.3, 26.7, 21.3; IR (film): 3062, 2922, 1688, 1660, 1597, 1424, 1305, 1254, 798, 739 cm^{-1}; HRMS (EI): *m/z* calcd for $C_{16}H_{14}O_2$: 238.0994; found : 238.0994



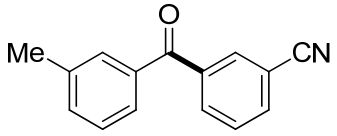
3n

Ethyl 4-(3-methylbenzoyl)benzoate (3o) : R_f = 0.3 (EtOAc: hexane = 1:15); Pale yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.15 (dt, *J* = 8.24 Hz, 1.74 Hz, 2H), 7.83 (dt, *J* = 8.24 Hz, 1.74 Hz, 2H), 7.63-7.55 (m, 2H), 7.44-7.35 (m, 2H), 4.42 (q, *J* = 7.29 Hz, 2H), 2.42 (s, 3H), 1.42 (t, *J* = 7.14 Hz, 3H); ^{13}C NMR (100 MHz) δ 196.3, 165.8, 141.4, 138.3, 137.0, 133.7, 133.5, 130.5, 129.7, 129.4, 128.2, 127.4, 61.4, 21.3, 14.3; IR (film): 3048, 2981, 1720, 1662, 1367, 1273, 1104, 730 cm^{-1}; HRMS (EI): *m/z* calcd for $C_{17}H_{16}O_3$: 268.1099; found : 268.1097



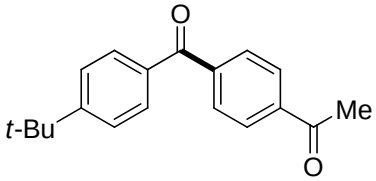
3o

3-(3-Methylbenzoyl)benzonitrile (3p) : R_f = 0.3 (EtOAc: hexane = 1:15); White solid. Melting point: 108-110 ^oC; ^1H NMR (400 MHz, $CDCl_3$) δ 8.06 (td, *J* = 2.5 Hz, 0.6 Hz, 1H), 8.04 (dt, *J* = 7.8 Hz, 1.5 Hz, 1H), 7.86 (dt, *J* = 7.74 Hz, 1.43 Hz, 1H), 7.62 (td, *J* = 11.7 Hz, 0.6 Hz, 1H), 7.61-7.59 (m, 1H), 7.55-7.52 (m, 1H), 7.47-7.45 (m, 1H), 7.42-7.38 (m, 1H), 2.44 (s, 3H); ^{13}C NMR (100 MHz) δ 194.6, 138.8, 138.7, 136.4, 135.3, 134.1, 133.8, 133.5, 130.4, 129.4, 128.5, 127.3, 117.9, 112.8, 21.4; IR (film): 3064, 2922, 2231, 1663, 1600, 1426, 1294, 1173, 821 cm^{-1}; HRMS (EI): *m/z* calcd for $C_{15}H_{11}NO$: 221.0841; found : 221.0838



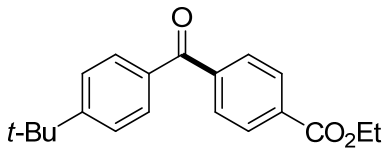
3p

1-(4-(4-*tert*-Butyl benzoyl)phenyl)ethanone (3q) : R_f = 0.2 (EtOAc: hexane = 1:15); Pale yellow oil; ^1H NMR (400 MHz, $CDCl_3$) δ 8.05 (d, *J* = 7.9 Hz, 2H), 7.86 (d, *J* = 7.9 Hz, 2H), 7.76 (d, *J* = 8.0 Hz, 2H), 7.51 (d, *J* = 8.0 Hz, 2H), 2.67 (s, 3H), 1.37 (s, 9H); ^{13}C NMR (100 MHz) δ 197.9, 196.0, 157.3, 142.2, 139.8, 134.6, 130.6, 130.3, 128.5,125.8, 35.6, 31.5, 27.3; IR (film): 2964, 1687, 1660, 1402, 1266, 931 cm^{-1}; HRMS (EI): *m/z* calcd for $C_{19}H_{20}O_2$: 280.1463; found : 280.1464



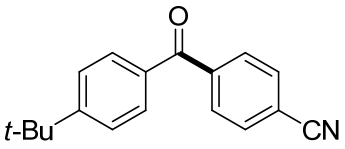
3q

Ethyl 4-(4-*tert*-butylbenzoyl)benzoate (3r) : R_f = 0.3 (EtOAc: hexane = 1:10); Pale yellow oil; ^1H NMR (400 MHz, $CDCl_3$) δ 8.15 (d, *J* = 8.2 Hz, 2H), 7.83 (d, *J* = 8.3 Hz, 2H), 7.76 (d, *J* = 8.4 Hz, 2H), 7.51 (d, *J* = 8.4 Hz, 2H), 4.43 (q, *J* = 7.1 Hz, 2H), 1.42 (t, *J* = 7.11 Hz, 3H), 1.37 (s, 9H); ^{13}C NMR (100 MHz) δ 196.2, 166.3, 157.2, 142.0, 134.9, 133.8, 130.6, 129.8, 125.8, 124.5, 81.8, 35.6, 31.5, 14.7; IR (film): 2360, 1683, 1652, 1540, 1473 cm^{-1}; HRMS (EI): *m/z* calcd for $C_{20}H_{22}O_3$: 310.1569; found : 310.1569



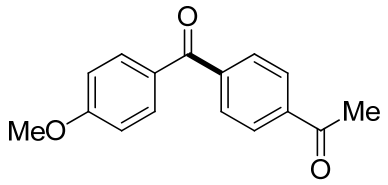
3r

3-(4-*tert*-Butylbenzoyl)benzonitrile (3s) : R_f = 0.2 (EtOAc: hexane = 1:15); Pale yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.87 (dt, *J* = 8.38 Hz, 1.61 Hz, 2H), 7.79 (dt, *J* = 8.2 Hz, 1.7 Hz, 2H), 7.73 (dt, *J* = 8.5 Hz, 1.95 Hz, 2H), 7.52 (dt, *J* = 8.48 Hz, 1.94 Hz, 2H), 1.37 (s, 9H); ^{13}C NMR (100 MHz) δ 195.1, 157.7, 142.1, 134.0, 132.5, 130.5, 126.0, 118.5, 115.8, 35.6, 31.5; IR (film) 2231, 1661, 1604, 1277, 932, 771 cm^{-1}; HRMS (EI): *m/z* calcd for $C_{18}H_{17}NO$: 263.1310, found : 263.1307



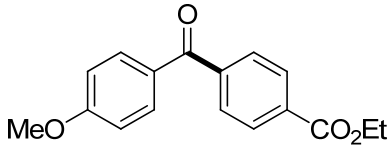
3s

1-(4-(4-Methoxybenzoyl)phenyl)ethanone (3t)[8] : R_f = 0.2 (EtOAc: hexane = 1:10); White solid. Melting point: 110-112 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.05 (d, *J* = 8.0 Hz, 2H), 7.84-7.77 (m, 4H), 6.98 (d, *J* = 8.6 Hz, 2H), 3.90 (s, 3H), 2.67 (s, 3H); ^{13}C NMR (100 MHz) δ 197.6, 194.7, 163.7, 142.2, 139.3, 132.6, 129.7, 129.5, 128.1, 113.8, 55.6, 26.9; IR (film): 2460, 1684, 1644, 1600, 1508, 1261, 1025 cm^{-1}; HRMS (EI): *m/z* calcd for $C_{16}H_{14}O_3$: 254.0943; found : 254.0943



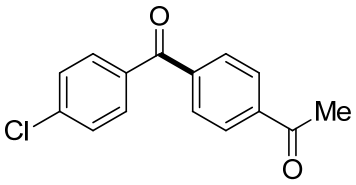
3t

Ethyl 4-(4-methoxy benzoyl)benzoate (3u)[9] **:** R_f = 0.2 (EtOAc: hexane = 1:15); White solid. Melting point: 86-88 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.15 (dd, *J* = 6.8 Hz, 1.6 Hz, 2H), 7.84-7.77 (m, 4H), 6.97 (dd, *J* = 6.8 Hz, 2.0 Hz, 2H), 4.42 (q, *J* = 7.1 Hz, 2H), 3.90 (s, 3H),1.42 (t, *J* = 7.19 Hz, 3H); ^{13}C NMR (100 MHz) δ 195.2, 166.3, 164.0, 142.4, 133.5, 133.0, 130.0, 129.9, 114.1, 61.8, 55.9, 14.7; IR (film): 1711, 1601, 1279, 1105, 843 cm^{-1}; HRMS (EI): *m/z* calcd for $C_{17}H_{16}O_4$: 284.1049; found : 284.1050



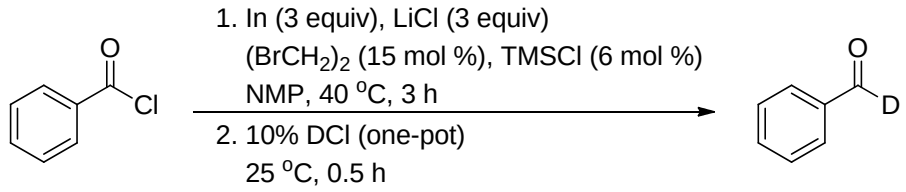
3u

1-(4-(4-Chlorobenzoyl)phenyl)ethanone (3v)[10] : R_f = 0.3 (EtOAc: hexane = 1:5); Yellow solid. Melting point: 125-127 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.07 (dt, *J* = 8.26 Hz, 1.77 Hz, 2H), 7.84 (dt, *J* = 8.30 Hz, 1.79 Hz, 2H), 7.76 (dt, *J* = 8.88 Hz, 2.21 Hz, 2H), 7.48 (dt, *J* = 9.00 Hz, 2.16 Hz, 2H), 2.67 (s, 3H); ^{13}C NMR (100 MHz) δ 197.4, 194.7, , 140.9, 139.7, 139.6, 135.2, 131.4, 129.9, 128.8, 128.2, 26.9; IR (film): 3055, 2913, 1658, 1311, 1263, 974, 754 cm^{-1}; HRMS (EI): *m/z* calcd for $C_{15}H_{11}ClO_2$: 258.0448; found : 258.0448



3v

Experiments with isotopically-labeled substrates



1a **5a**

The general procedure was followed using indium powder (104.0 mg, 0.9 mmol), LiCl (38.0 mg, 0.9 mmol), TMSCl (6 mol %), 1,2-dibromoethane (15 mol %) in NMP (1 mL). Benzoyl chloride **1a** (84.0 mg, 0.6 mmol) was added. The mixture was stirred at 40 °C for 3 h and provided the indium reagent**.** Then, 10% DCl was added. The resulting mixture was stirred under N_2 at 25 °C for 0.5 h. After the completion of the reaction (checked by TLC), the aqueous layer was extracted with ethyl acetate. The combined organic extracts were dried over $MgSO_4$, filtered, and concentrated under reduced pressure. Silica gel fresh column chromatography (ethyl acetate:hexane = 1:10) gave benzaldehyde-d_1 (64.2 mg, 60%) as colorless oil. R_f = 0.3 (EtOAc:hexane = 1:3); Colorless oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.02 (s, 0.01H), 7.90-7.88 (m, 2H), 7.66-7.62 (m, 1H), 7.56-7.51 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 192.0 (t, *J* = 26.7 Hz), 136.3 (t, *J* = 3.54 Hz), 134.4, 129.7, 129.0; IR (film): 3061, 2942, 2242, 1843 cm^{-1}; HRMS (EI): *m/z* calcd for C_7H_5DO : 107.0481; found : 107.0480

References

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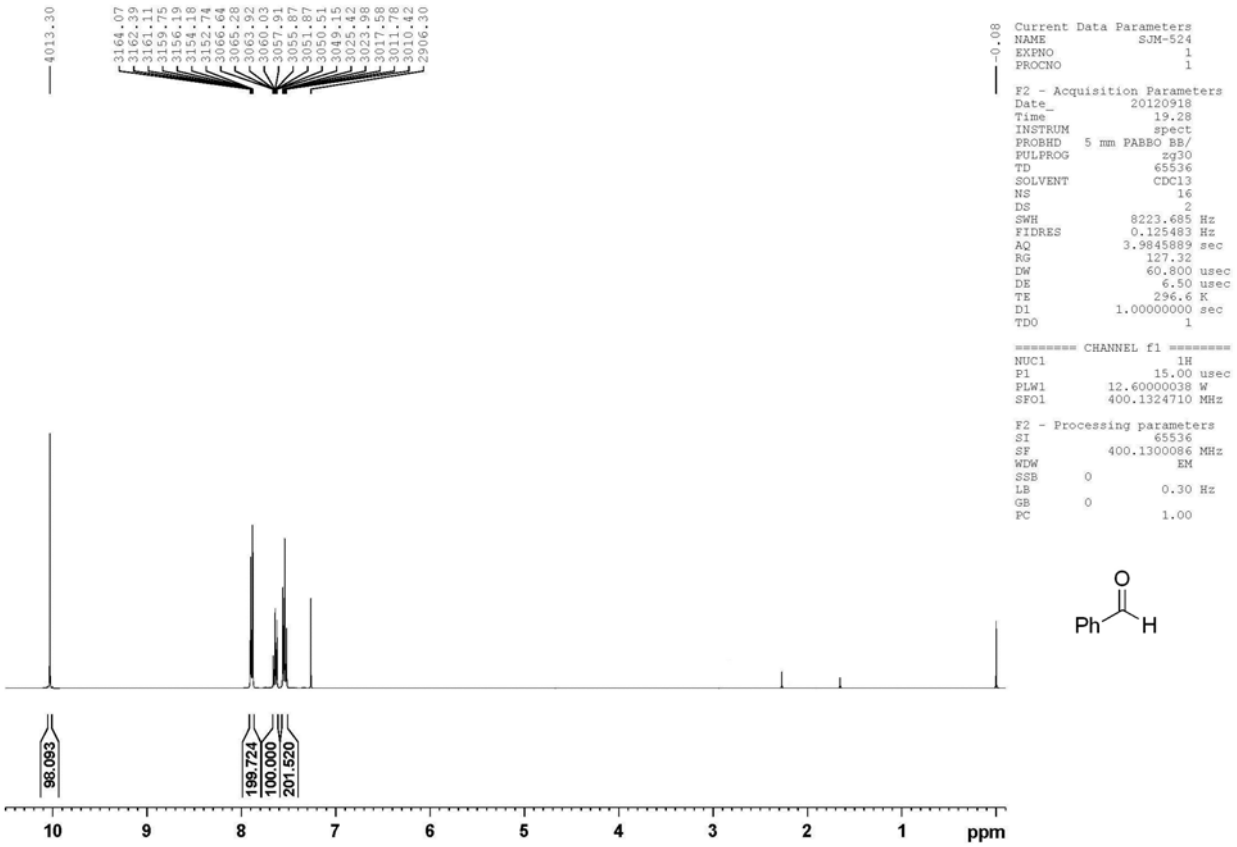


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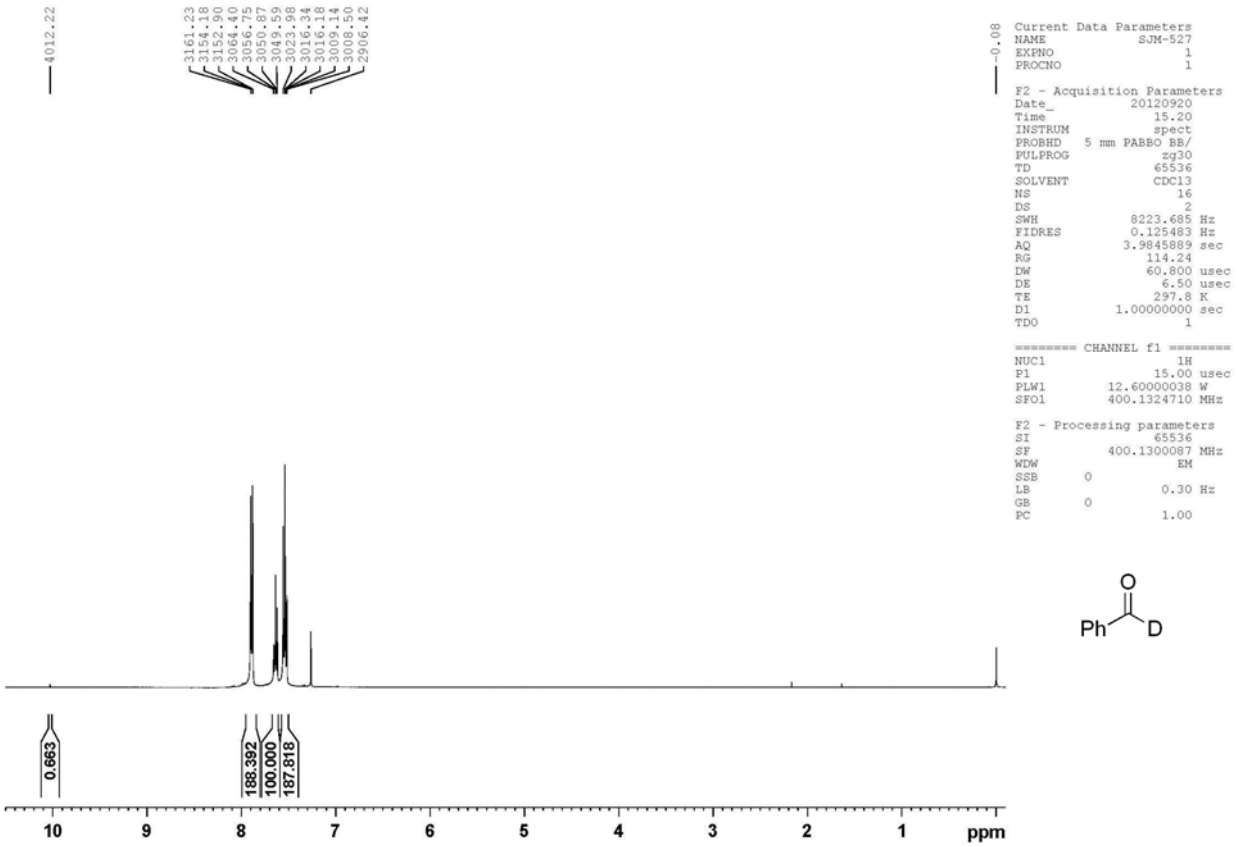


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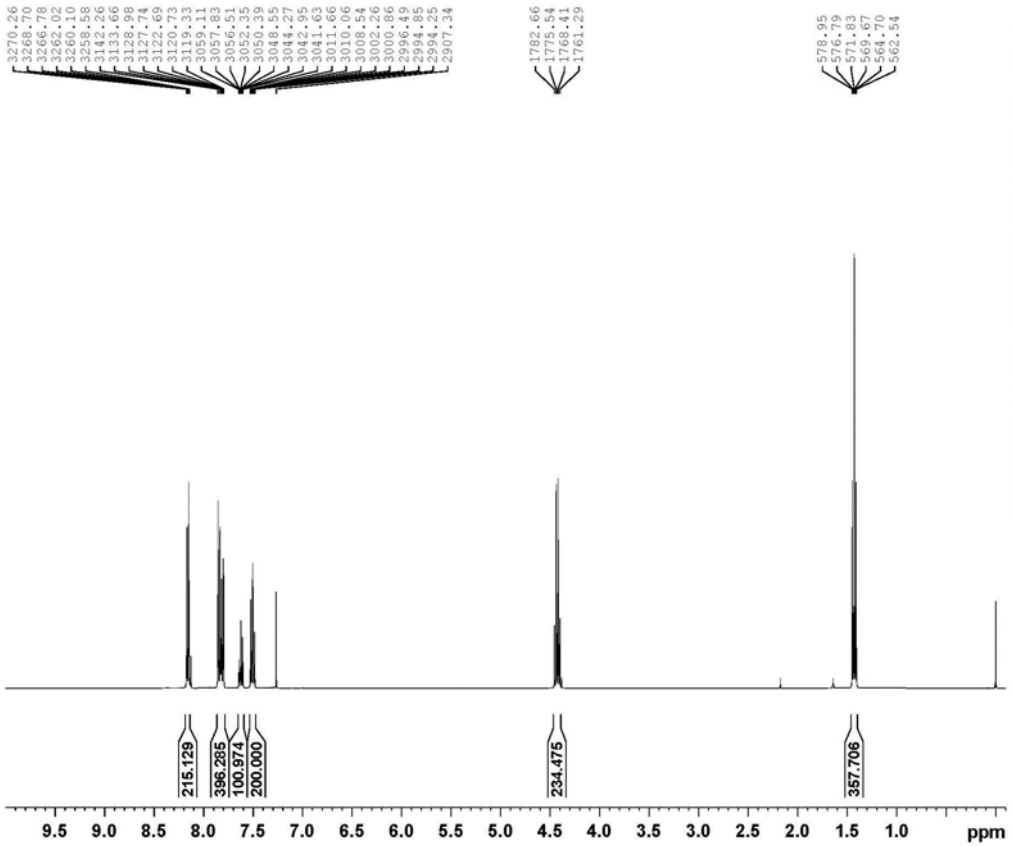


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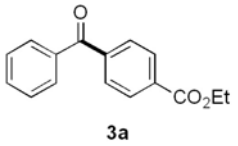
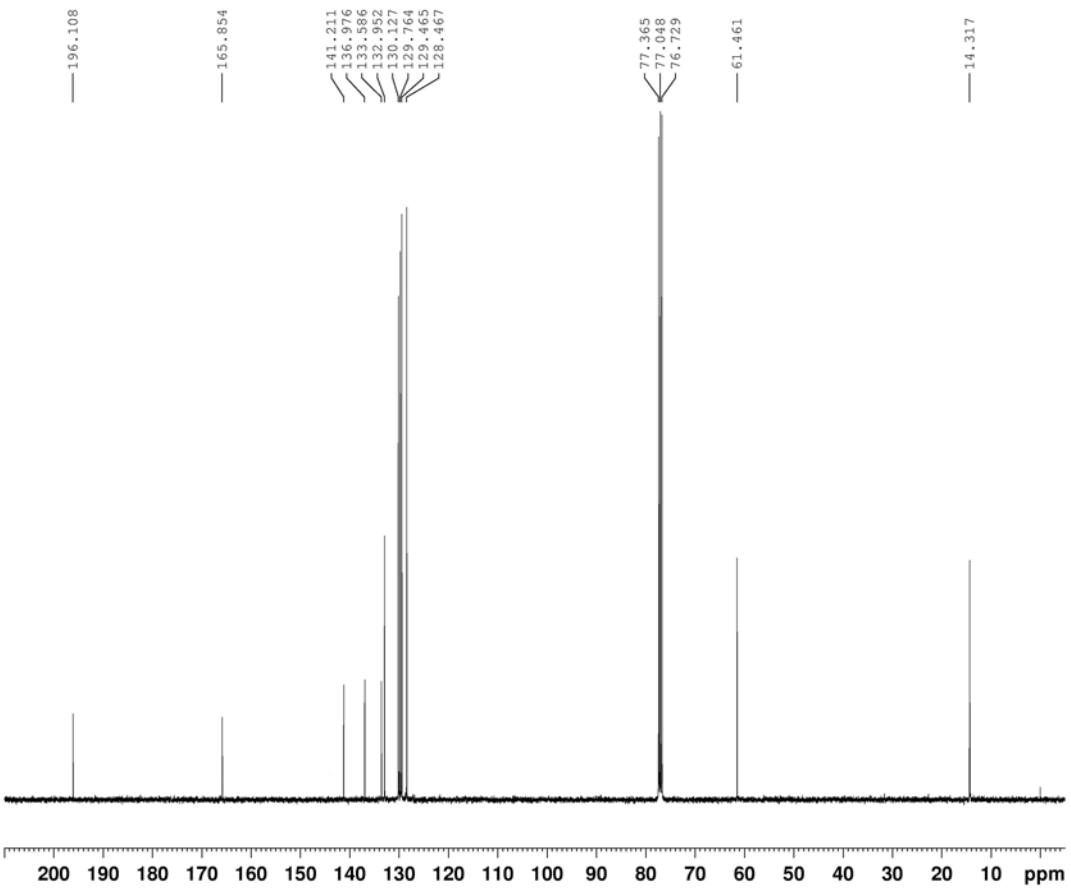


3a

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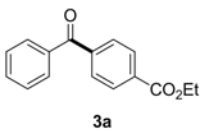
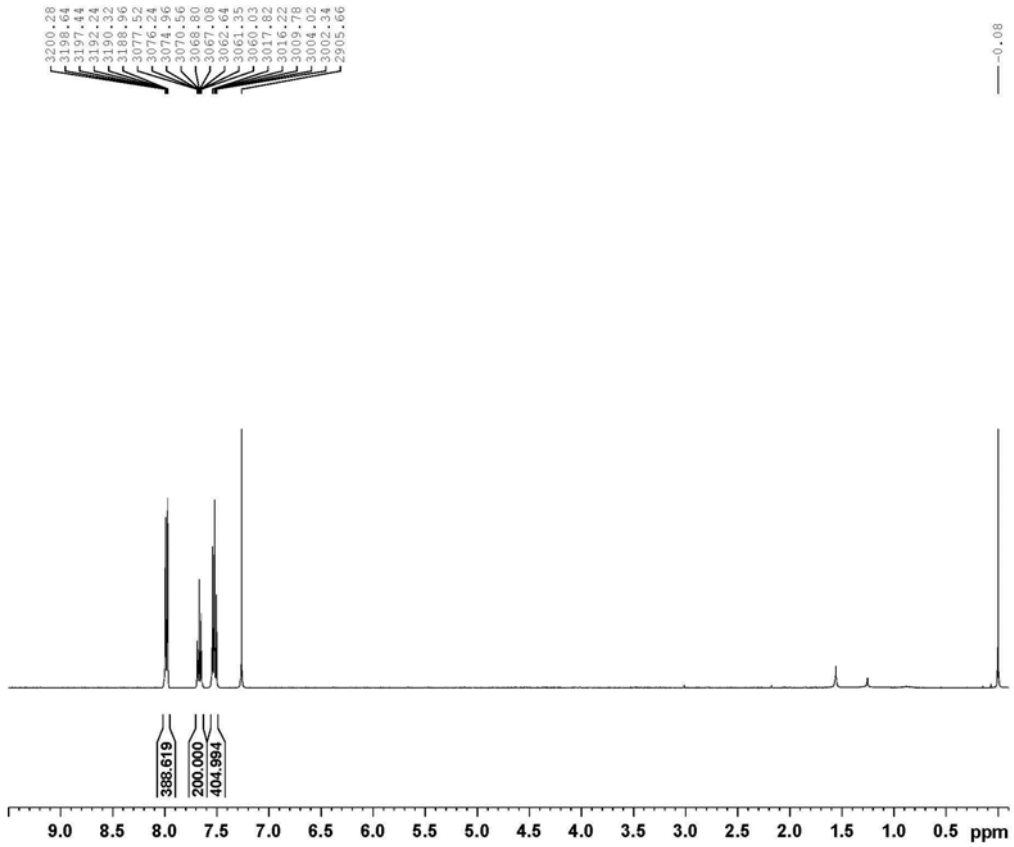


3a

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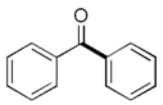
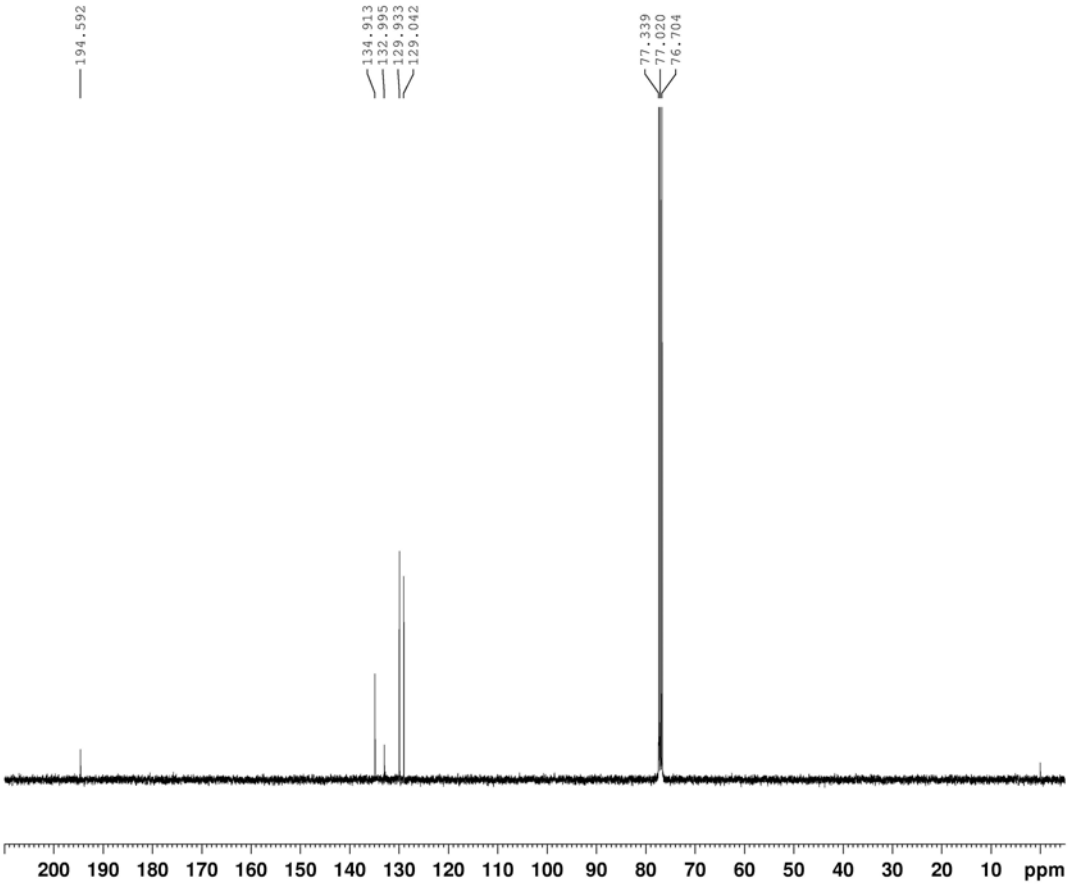
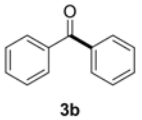


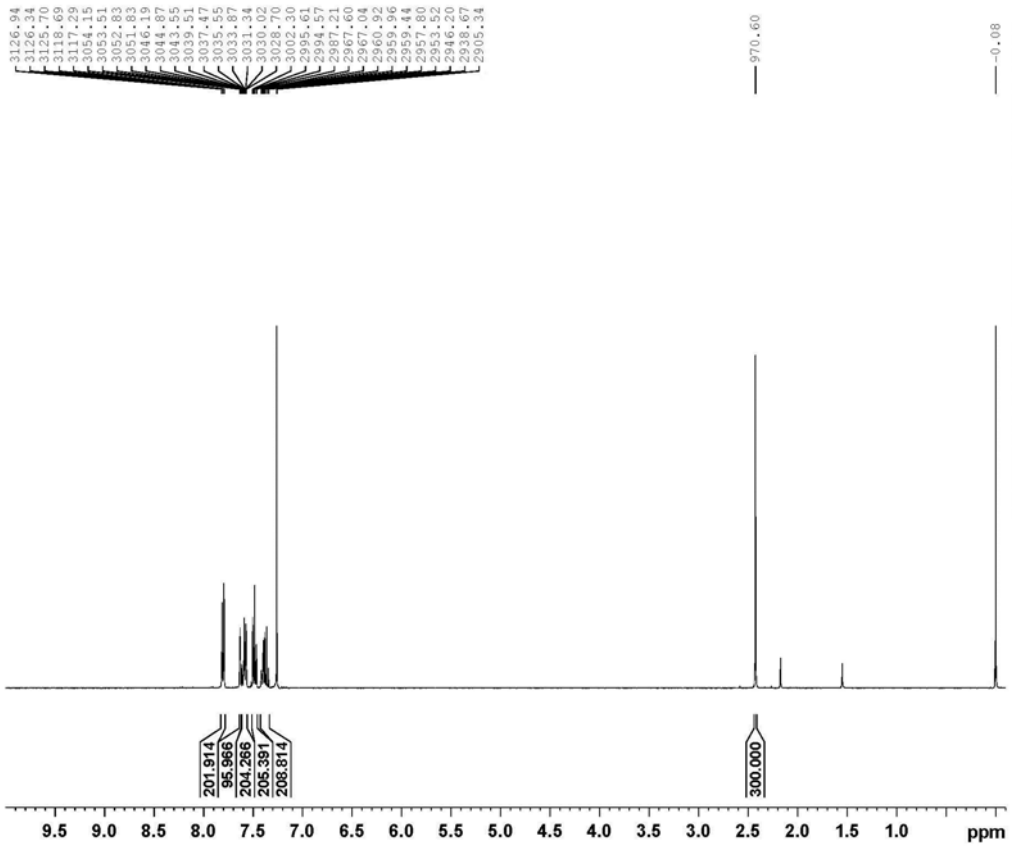
3b



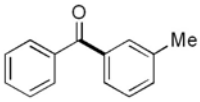

```
Current Data Parameters
NAME                 SJM-388
EXPNO                      2
PROCNO                     1

F2 - Acquisition Parameters
Date_               20120622
Time                    1.06
INSTRUM                spect
PROBHD   5 mm PABBO BB/
PULPROG              zgpg30
TD                    65536
SOLVENT               CDCl3
NS                     1024
DS                        4
SWH               24038.461 Hz
FIDRES             0.366798 Hz
AQ                 1.3631488 sec
RG                    186.53
DW                   20.800 usec
DE                    6.50 usec
TE                   295.4 K
D1                2.00000000 sec
d11               0.03000000 sec
DELTA             1.89999998 sec
TD0                        1
SFO1            100.6228293 MHz
NUC1                      13C
P1                     9.98 usec
PLW1             52.09999847 W
SFO2            400.1316005 MHz
NUC2                      1H
CPDPRG[2              waltz16
PCPD2                 90.00 usec
PLW2             12.60000038 W
PLW12             0.34999999 W
PLW13             0.28349999 W

F2 - Processing parameters
SI                        32768
SF              100.6127690 MHz
WDW                        EM
SSB          0
LB                     1.00 Hz
GB           0
PC                     1.40
```



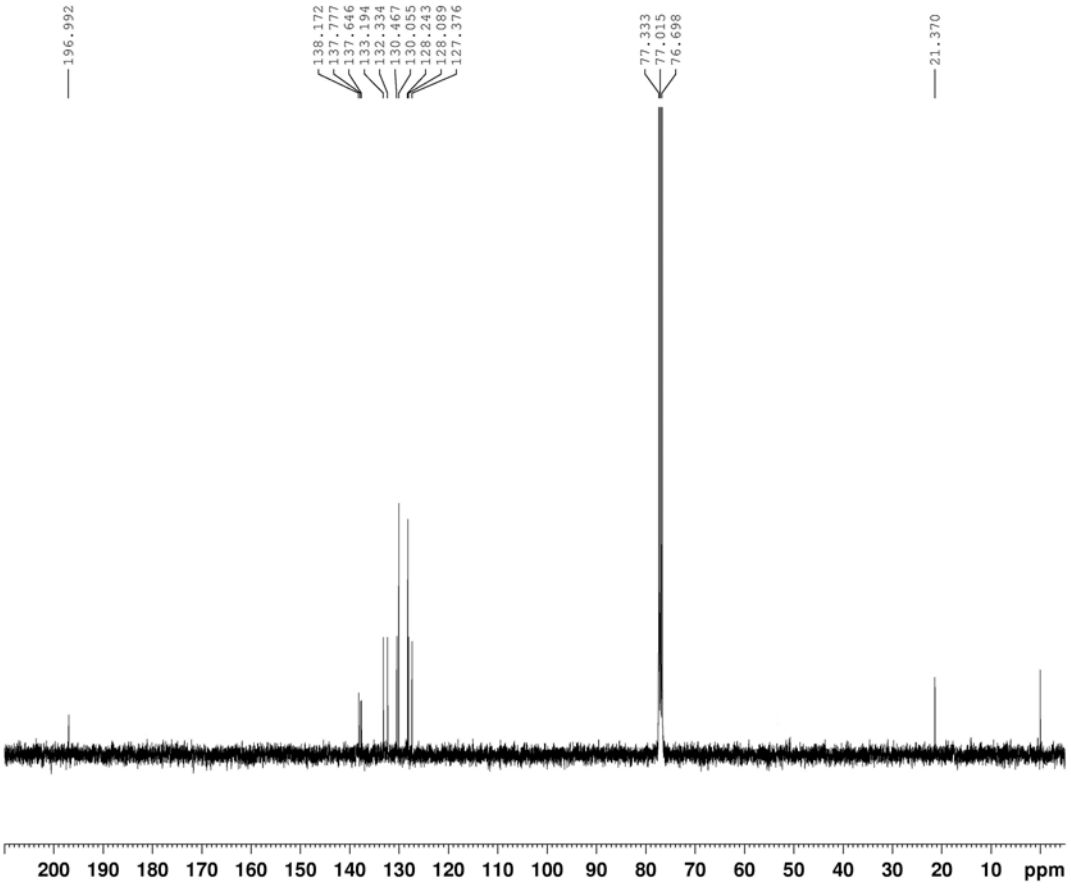
3b



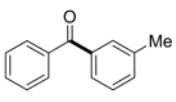

```
Current Data Parameters
NAME                  SJM-464
EXPNO                       1
PROCNO                      1

F2 - Acquisition Parameters
Date_               20120814
Time                   14.21
INSTRUM                spect
PROBHD   5 mm PABBO BB/
PULPROG                zg30
TD                    65536
SOLVENT               CDCl3
NS                       16
DS                        2
SWH                8223.685 Hz
FIDRES            0.125483 Hz
AQ                3.9845889 sec
RG                   186.53
DW                   60.800 usec
DE                    6.50 usec
TE                   295.4 K
D1                1.00000000 sec
TD0                         1

======== CHANNEL f1 ========
NUC1                       1H
P1                      15.00 usec
PLW1              12.60000038 W
SFO1             400.1324710 MHz

F2 - Processing parameters
SI                         65536
SF                400.1300096 MHz
WDW                           EM
SSB          0
LB                       0.30 Hz
GB           0
PC                       1.00
```



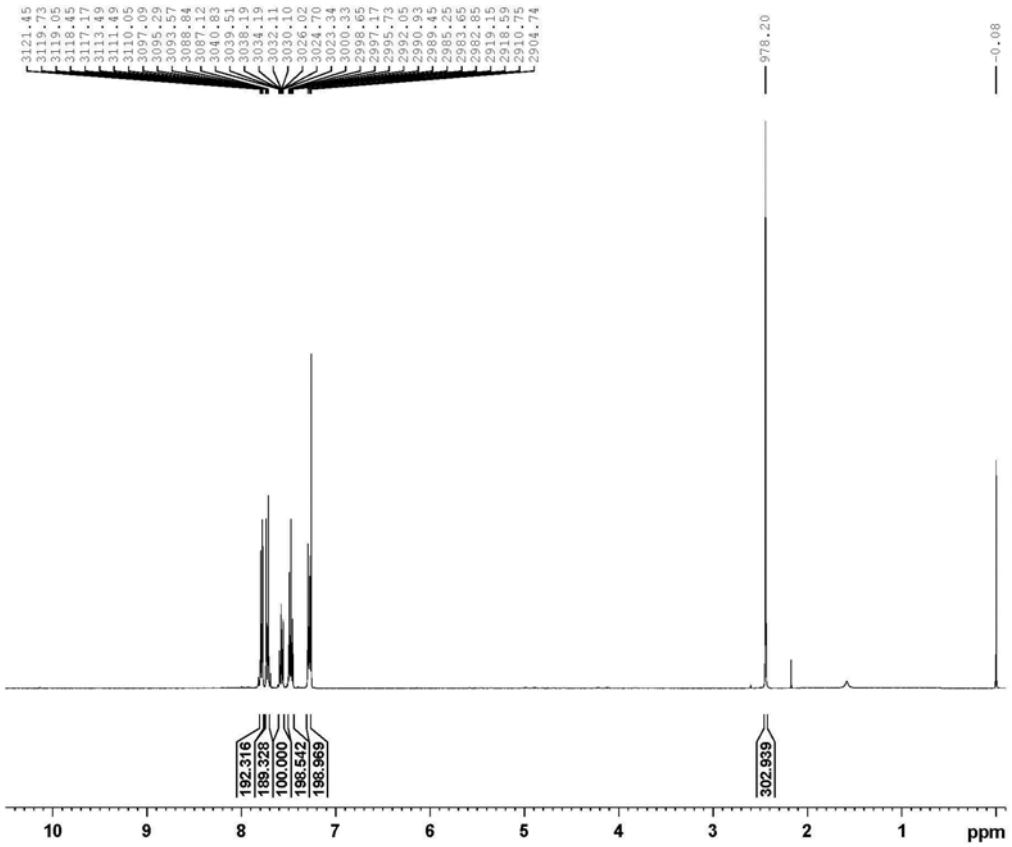
3c



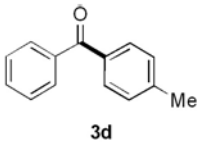

```
Current Data Parameters
NAME                  SJM-464
EXPNO                       2
PROCNO                      1

F2 - Acquisition Parameters
Date_               20120815
Time                    1.00
INSTRUM                spect
PROBHD   5 mm PABBO BB/
PULPROG              zgpg30
TD                    65536
SOLVENT               CDCl3
NS                     2048
DS                        4
SWH               24038.461 Hz
FIDRES            0.366798 Hz
AQ                1.3631488 sec
RG                   186.53
DW                   20.800 usec
DE                    6.50 usec
TE                   296.9 K
D1                2.00000000 sec
d11               0.03000000 sec
DELTA             1.89999998 sec
TD0                         1
SFO1             100.6228293 MHz
NUC1                       13C
P1                       9.98 usec
PLW1              52.09999847 W
SFO2             400.1316005 MHz
NUC2                       1H
CPDPRG[2              waltz16
PCPD2                   90.00 usec
PLW2              12.60000038 W
PLW12              0.34999999 W
PLW13              0.28349999 W

F2 - Processing parameters
SI                         32768
SF               100.6127690 MHz
WDW                           EM
SSB          0
LB                       1.00 Hz
GB           0
PC                       1.40
```



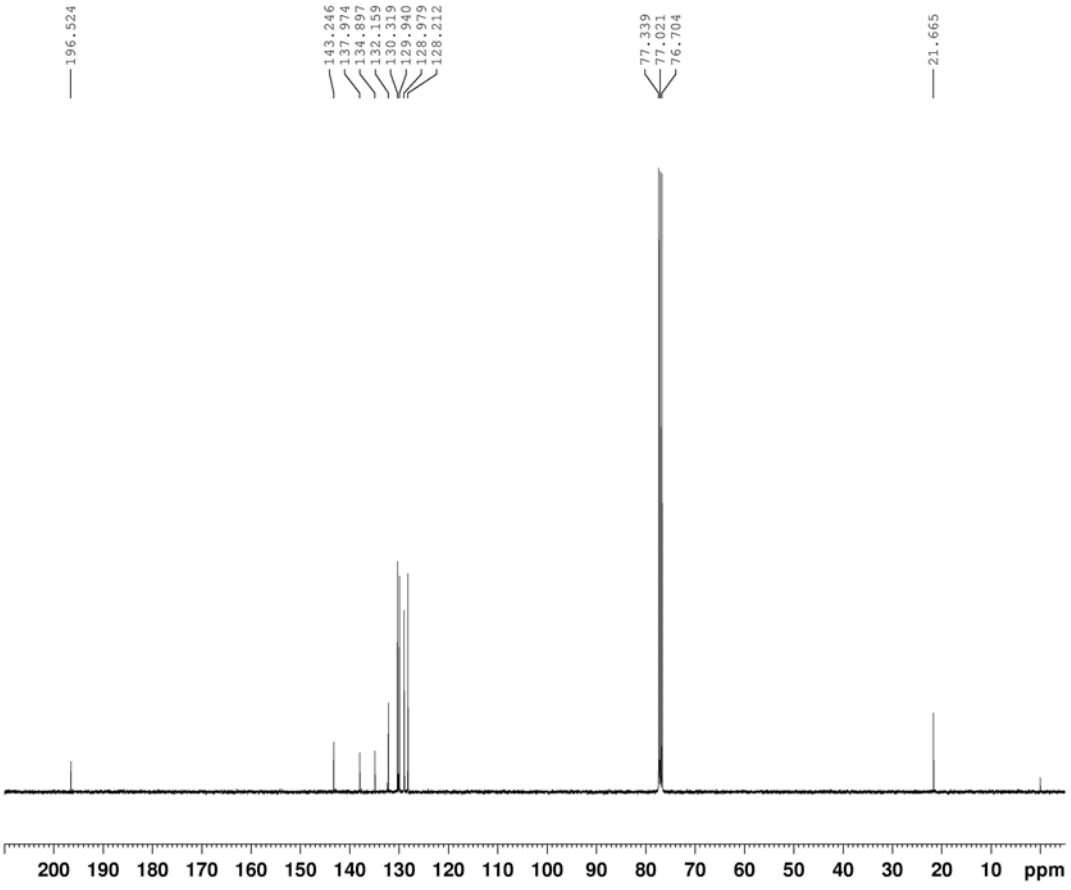
3c



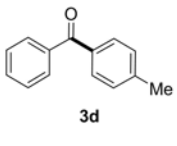

```
Current Data Parameters
NAME                  SJM-469
EXPNO                       1
PROCNO                      1

F2 - Acquisition Parameters
Date_               20120819
Time                   18.16
INSTRUM                spect
PROBHD    5 mm PABBO BB/
PULPROG                zg30
TD                    65536
SOLVENT               CDCl3
NS                       16
DS                        2
SWH                8223.685 Hz
FIDRES            0.125483 Hz
AQ                3.9845889 sec
RG                    127.32
DW                  60.800 usec
DE                   6.50 usec
TE                   295.9 K
D1              1.00000000 sec
TD0                         1

======== CHANNEL f1 ========
NUC1                       1H
P1                    15.00 usec
PLW1           12.60000038 W
SFO1           400.1324710 MHz

F2 - Processing parameters
SI                        65536
SF              400.1300102 MHz
WDW                         EM
SSB          0
LB                     0.30 Hz
GB           0
PC                     1.00
```



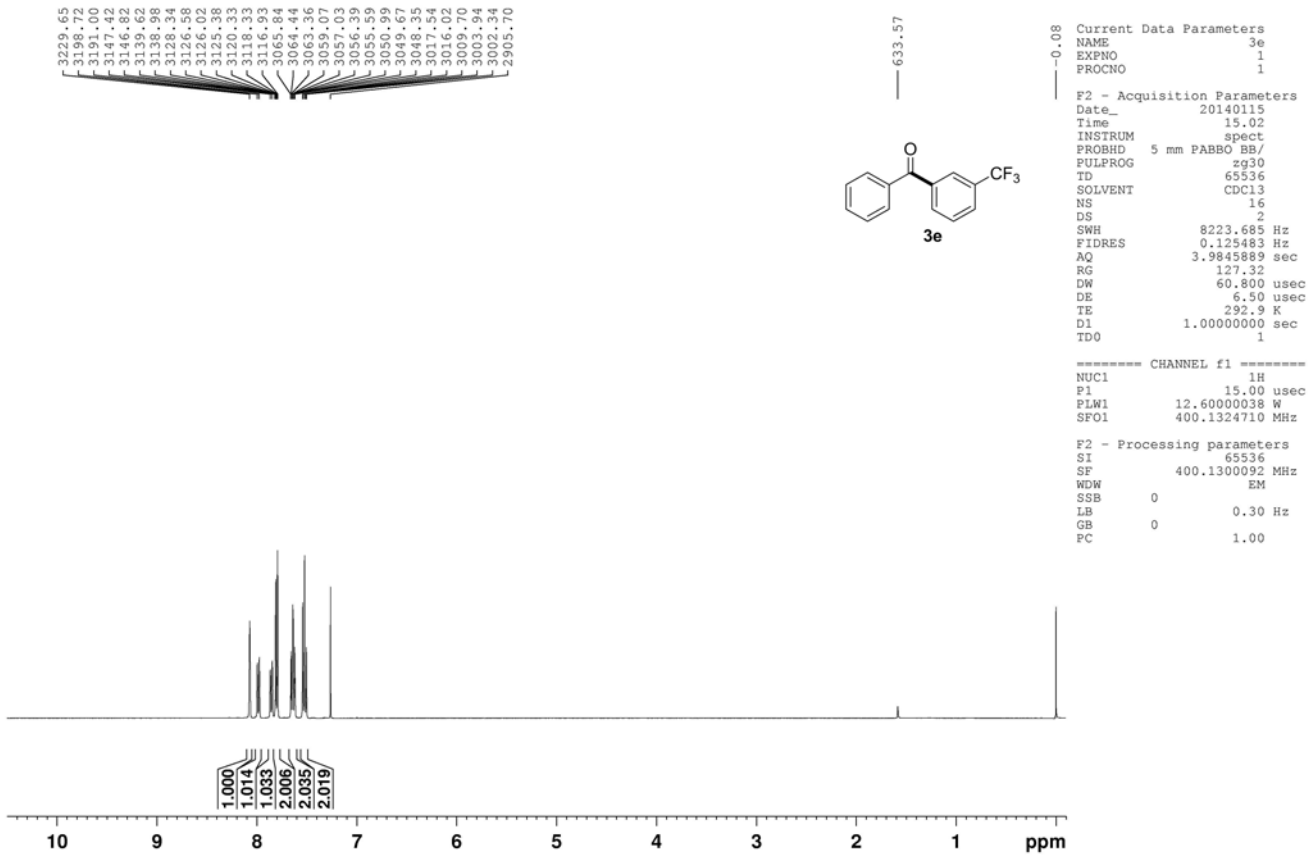
3d



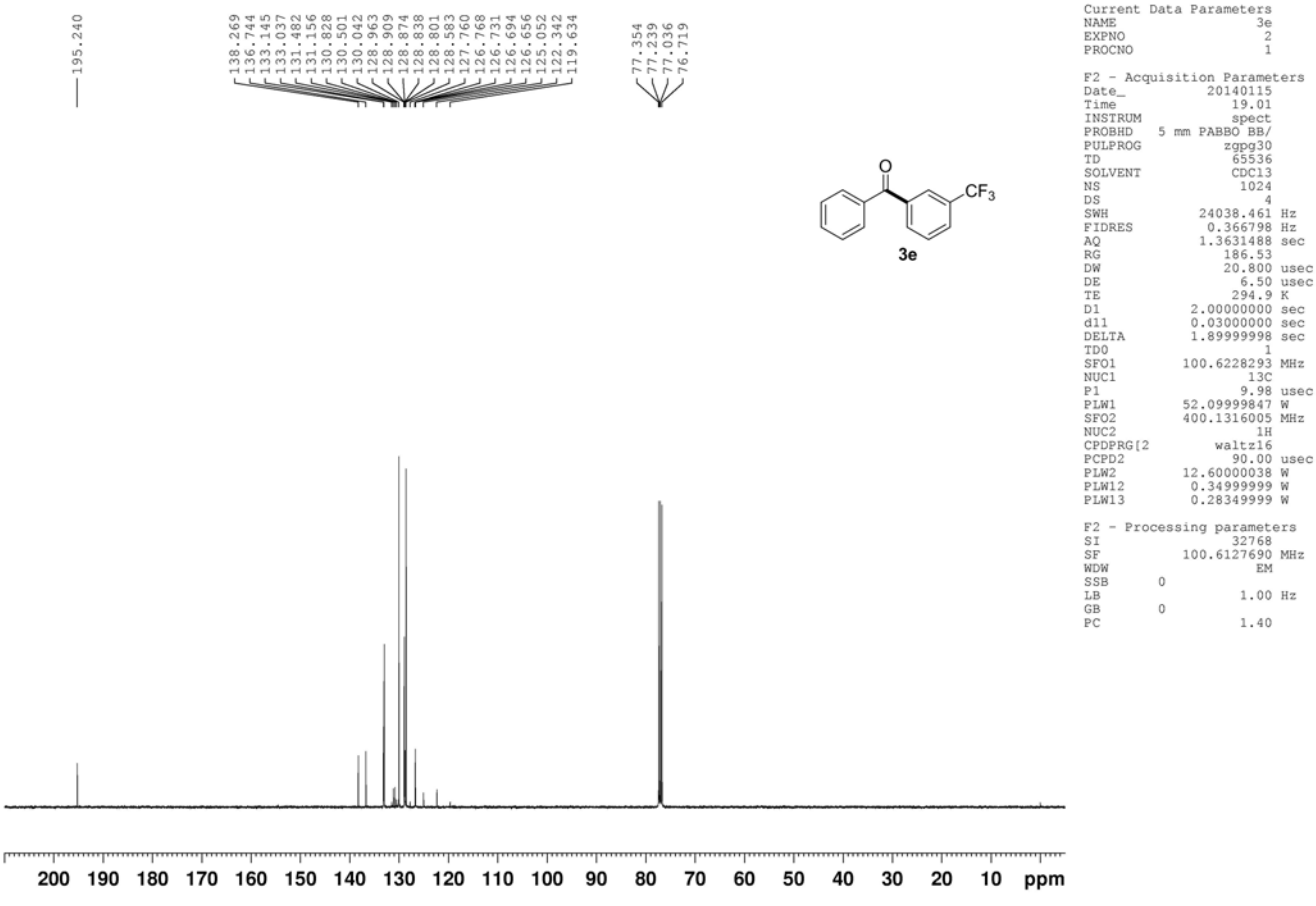

```
Current Data Parameters
NAME                  SJM-469
EXPNO                       2
PROCNO                      1

F2 - Acquisition Parameters
Date_               20120820
Time                    4.04
INSTRUM                spect
PROBHD    5 mm PABBO BB/
PULPROG             zgpg30
TD                    65536
SOLVENT               CDCl3
NS                     2048
DS                        4
SWH               24038.461 Hz
FIDRES            0.366798 Hz
AQ                1.3631488 sec
RG                    186.53
DW                  20.800 usec
DE                   6.50 usec
TE                   297.5 K
D1              2.00000000 sec
d11             0.03000000 sec
DELTA           1.89999998 sec
TD0                         1
SFO1           100.6228293 MHz
NUC1                      13C
P1                    9.98 usec
PLW1           52.09999847 W
SFO2           400.1316005 MHz
NUC2                       1H
CPDPRG[2           waltz16
PCPD2                90.00 usec
PLW2           12.60000038 W
PLW12           0.34999999 W
PLW13           0.28349999 W

F2 - Processing parameters
SI                        32768
SF             100.6127690 MHz
WDW                         EM
SSB          0
LB                     1.00 Hz
GB           0
PC                     1.40
```



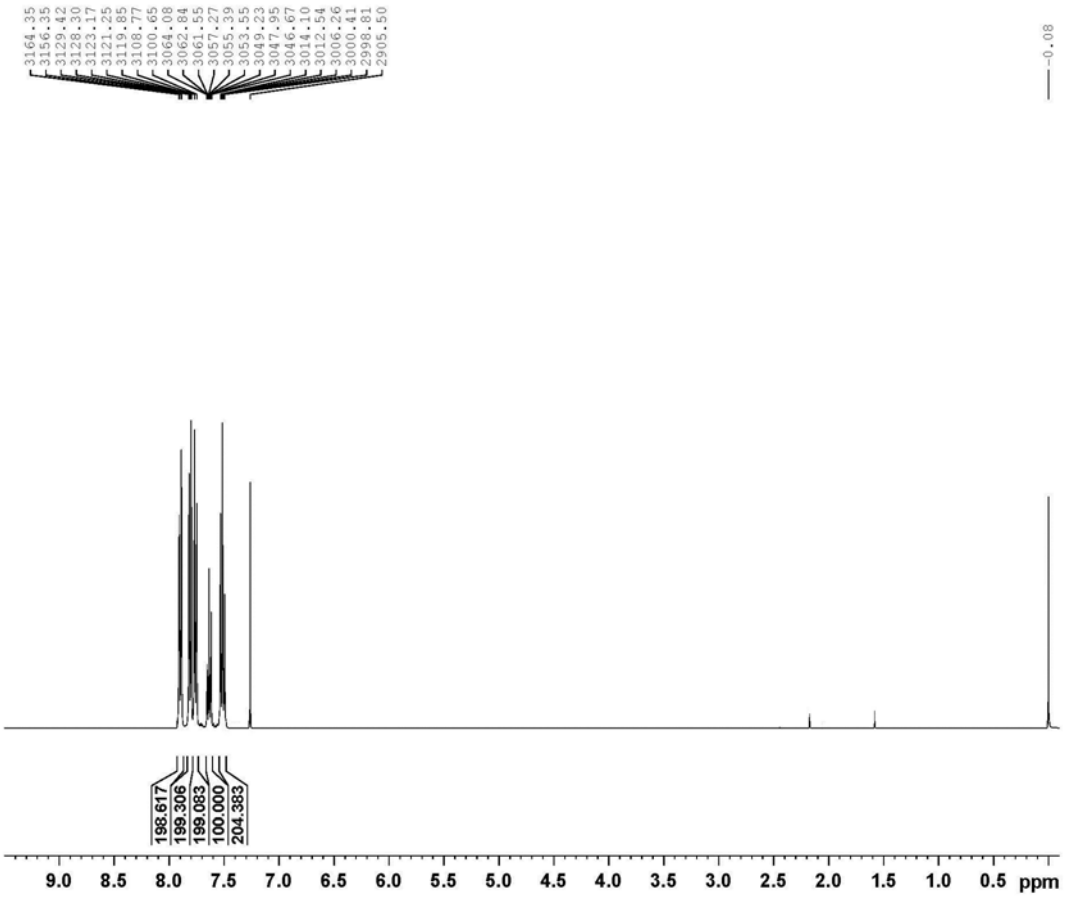
3d



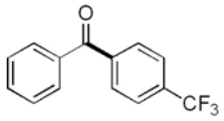

```
Current Data Parameters
NAME                  3e
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20140115
Time               15.02
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH             8223.685 Hz
FIDRES          0.125483 Hz
AQ              3.9845889 sec
RG                127.32
DW                60.800 usec
DE                 6.50 usec
TE                292.9 K
D1             1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                 15.00 usec
PLW1          12.60000038 W
SFO1          400.1324710 MHz

F2 - Processing parameters
SI                 65536
SF            400.1300092 MHz
WDW                   EM
SSB       0
LB                 0.30 Hz
GB        0
PC                 1.00
```



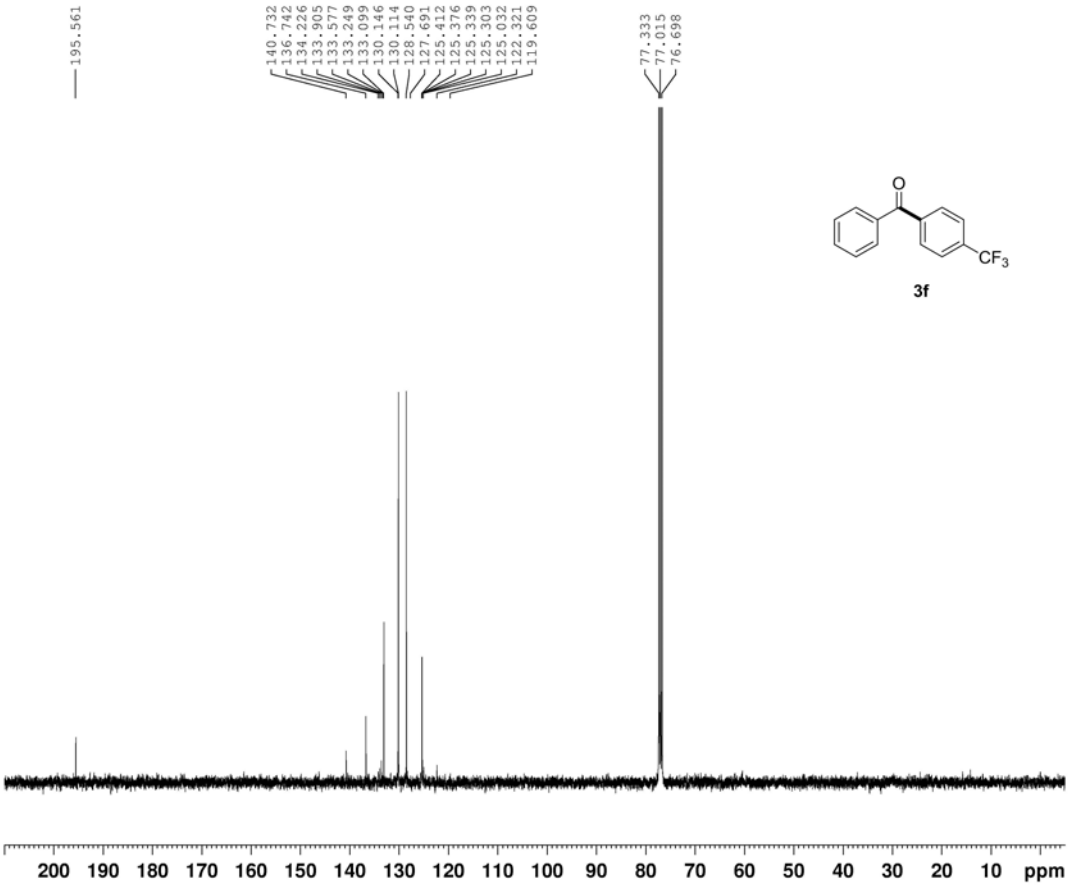

```
Current Data Parameters
NAME                  3e
EXPNO                  2
PROCNO                 1

F2 - Acquisition Parameters
Date_           20140115
Time               19.01
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG            zgpg30
TD                 65536
SOLVENT            CDCl3
NS                  1024
DS                     4
SWH            24038.461 Hz
FIDRES          0.366798 Hz
AQ              1.3631488 sec
RG                186.53
DW                20.800 usec
DE                 6.50 usec
TE                294.9 K
D1             2.00000000 sec
d11            0.03000000 sec
DELTA          1.89999998 sec
TD0                    1
SFO1          100.6228293 MHz
NUC1                  13C
P1                 9.98 usec
PLW1          52.09999847 W
SFO2          400.1316005 MHz
NUC2                  1H
CPDPRG[2          waltz16
PCPD2             90.00 usec
PLW2          12.60000038 W
PLW12          0.34999999 W
PLW13          0.28349999 W

F2 - Processing parameters
SI                 32768
SF            100.6127690 MHz
WDW                   EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
```




```
Current Data Parameters
NAME            SJM-394-1
EXPNO                   1
PROCNO                  1

F2 - Acquisition Parameters
Date_            20120627
Time                20.24
INSTRUM             spect
PROBHD    5 mm PABBO BB/
PULPROG              zg30
TD                  65536
SOLVENT             CDCl3
NS                     16
DS                      2
SWH              8223.685 Hz
FIDRES           0.125483 Hz
AQ               3.9845889 sec
RG                 127.32
DW                 60.800 usec
DE                  6.50 usec
TE                 294.6 K
D1              1.00000000 sec
TD0                     1

======== CHANNEL f1 ========
NUC1                   1H
P1                  15.00 usec
PLW1          12.60000038 W
SFO1         400.1324710 MHz

F2 - Processing parameters
SI                  65536
SF           400.1300094 MHz
WDW                    EM
SSB       0
LB                  0.30 Hz
GB        0
PC                  1.00
```

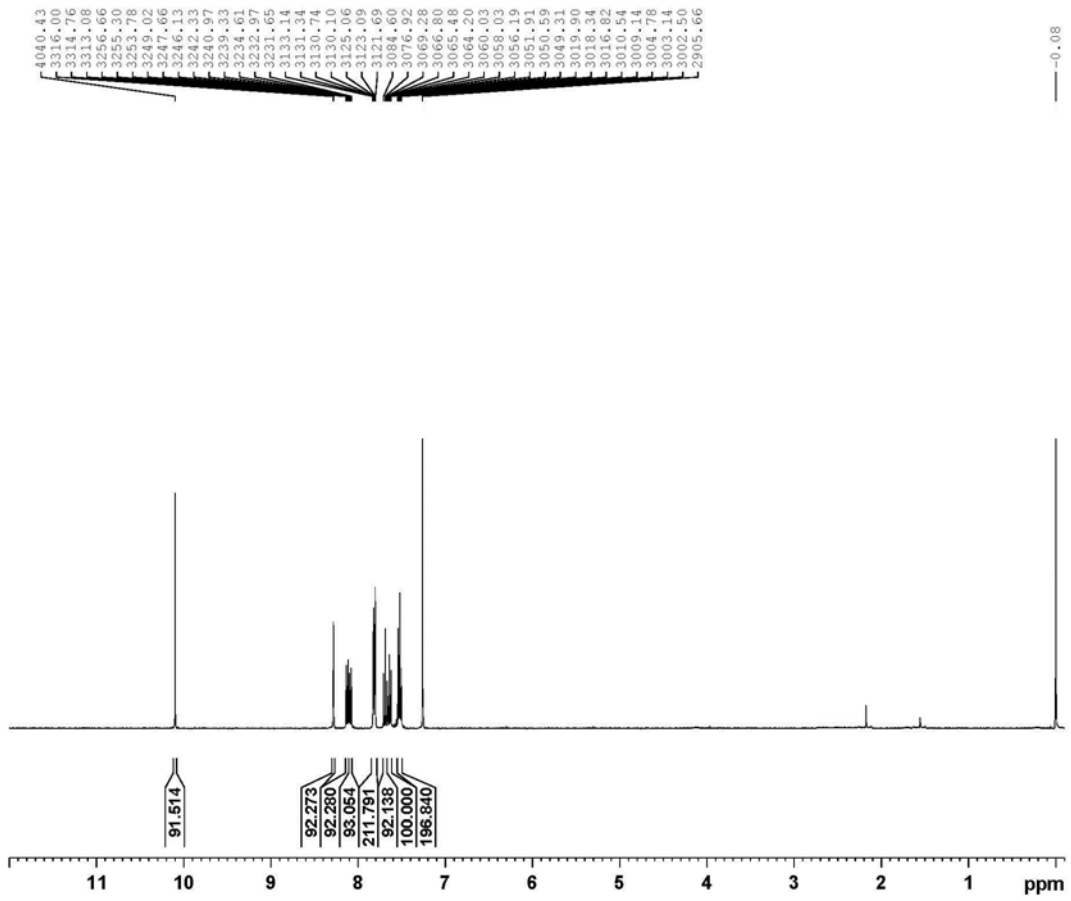


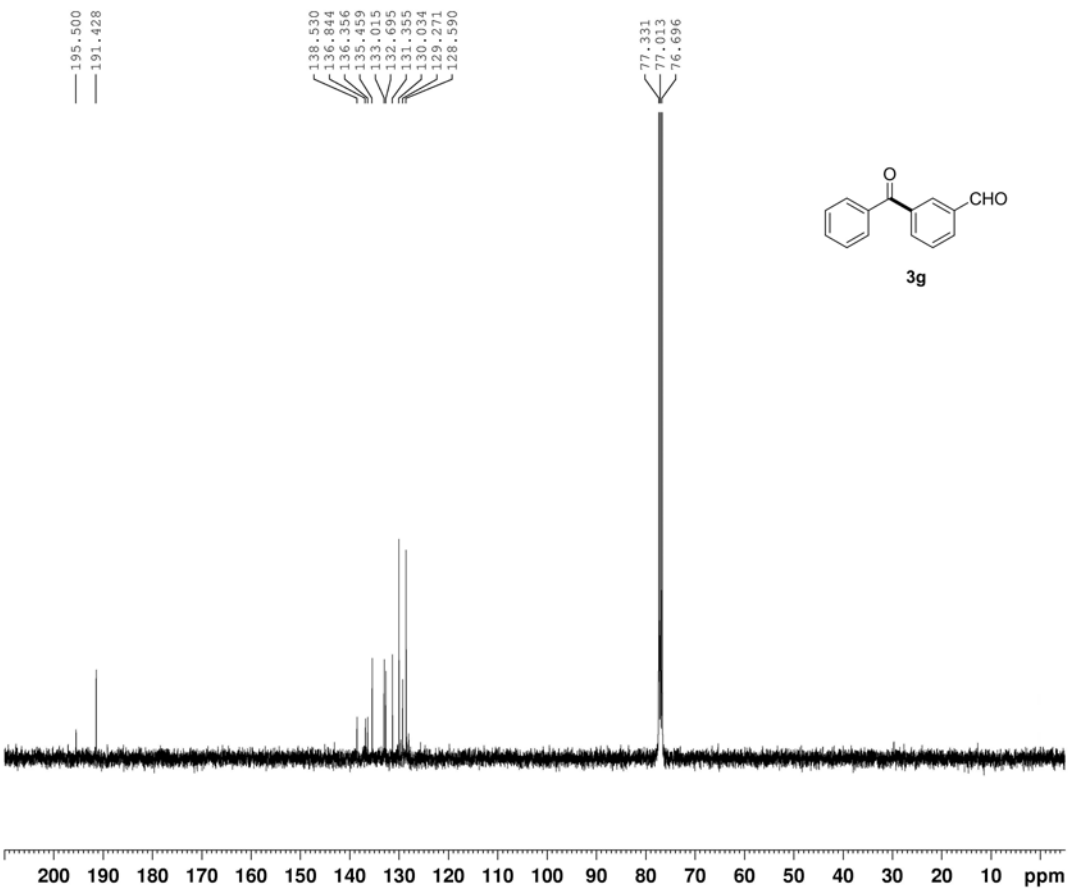
3f

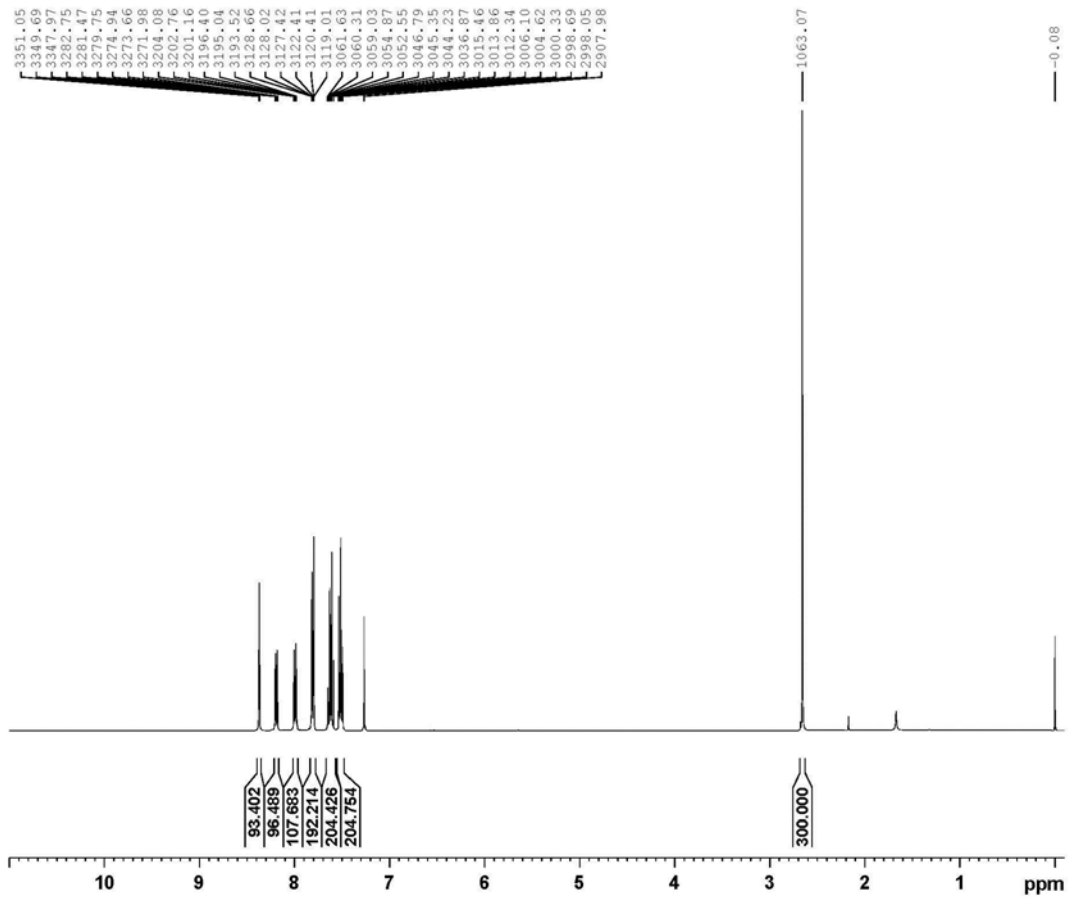


3f

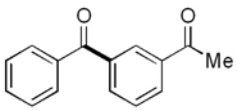
```
Current Data Parameters
NAME            SJM-480
EXPNO                 2
PROCNO                1

F2 - Acquisition Parameters
Date_            20120821
Time                23.01
INSTRUM             spect
PROBHD    5 mm PABBO BB/
PULPROG           zgpg30
TD                  65536
SOLVENT             CDCl3
NS                   1024
DS                      4
SWH             24038.461 Hz
FIDRES           0.366798 Hz
AQ               1.3631488 sec
RG                 186.53
DW                 20.800 usec
DE                  6.50 usec
TE                 297.3 K
D1              2.00000000 sec
d11             0.03000000 sec
DELTA           1.89999998 sec
TD0                     1
SFO1         100.6228293 MHz
NUC1                  13C
P1                  9.98 usec
PLW1          52.09999847 W
SFO2         400.1316005 MHz
NUC2                   1H
CPDPRG[2          waltz16
PCPD2              90.00 usec
PLW2          12.60000038 W
PLW12          0.34999999 W
PLW13          0.28349999 W

F2 - Processing parameters
SI                  32768
SF           100.6127690 MHz
WDW                    EM
SSB       0
LB                  1.00 Hz
GB        0
PC                  1.40
```


4040.43
3316.00
3314.76
3313.08
3256.66
3255.30
3253.78
3249.02
3247.66
3246.13
3242.33
3240.97
3239.33
3234.61
3232.97
3231.65
3133.14
3131.34
3130.74
3130.10
3125.06
3123.09
3121.69
3084.60
3076.92
3069.28
3066.80
3065.48
3064.20
3060.03
3058.03
3056.19
3051.91
3050.59
3049.31
3019.90
3018.34
3016.82
3010.54
3009.14
3004.78
3003.14
3002.50
2905.66
-0.08
Current Data Parameters
NAME SJM-483
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20120829
Time 16.36
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9845889 sec
RG 186.53
DW 60.800 usec
DE 6.50 usec
TE 296.2 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 15.00 usec
PLW1 12.60000038 W
SFO1 400.1324710 MHz
F2 - Processing parameters
SI 65536
SF 400.1300091 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
O
CHO
3g
91.514
92.273
92.280
93.054
211.791
92.138
100.000
196.840
11
10
9
8
7
6
5
4
3
2
1
ppm

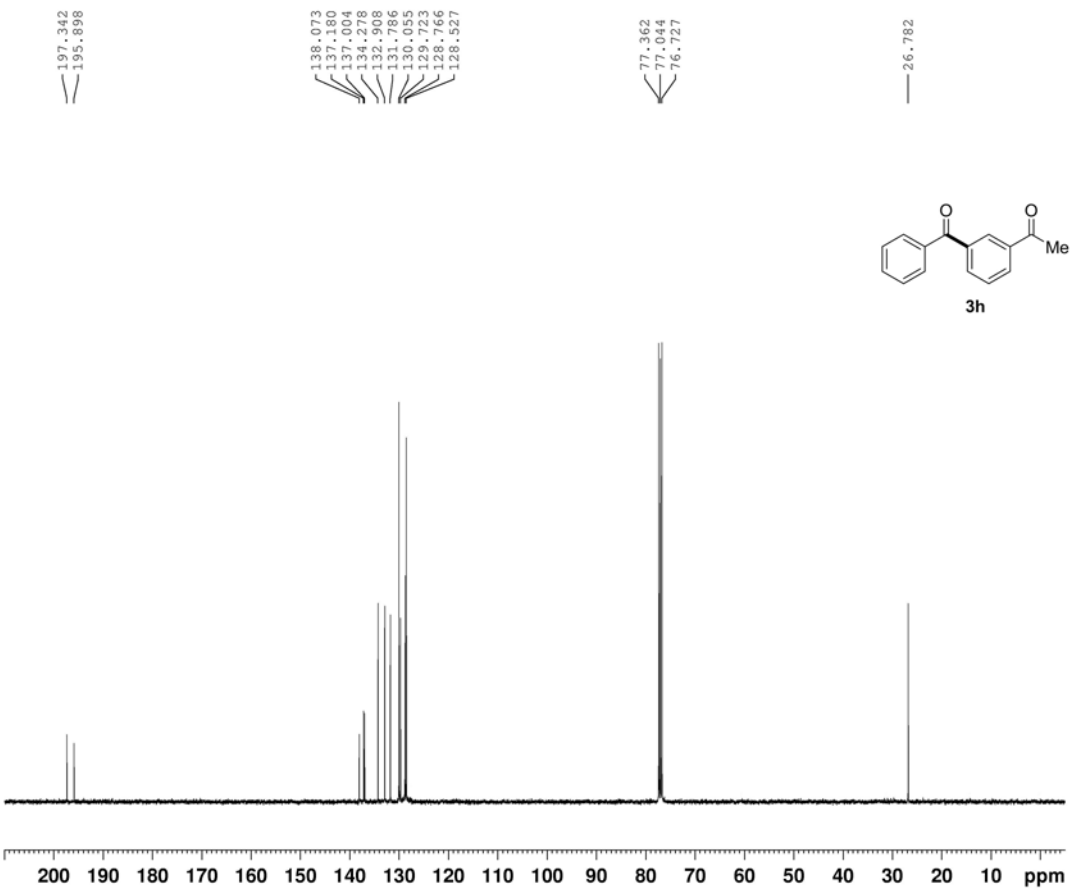

195.500
191.428
138.530
136.844
136.356
135.459
133.015
132.695
131.355
130.034
129.271
128.590
77.331
77.013
76.696
Current Data Parameters
NAME SJM-483
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20120830
Time 3.04
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 2048
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 186.53
DW 20.800 usec
DE 6.50 usec
TE 297.6 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1
SFO1 100.6228293 MHz
NUC1 13C
P1 9.98 usec
PLW1 52.09999847 W
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 90.00 usec
PLW2 12.60000038 W
PLW12 0.34999999 W
PLW13 0.28349999 W
F2 - Processing parameters
SI 32768
SF 100.6127690 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
O
CHO
3g
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm




```
Current Data Parameters
NAME                 SJM-424
EXPNO                      1
PROCNO                     1

F2 - Acquisition Parameters
Date_               20120711
Time                   20.48
INSTRUM                spect
PROBHD    5 mm PABBO BB/
PULPROG                zg30
TD                    65536
SOLVENT               CDCl3
NS                       16
DS                        2
SWH                8223.685 Hz
FIDRES             0.125483 Hz
AQ                 3.9845889 sec
RG                     87.66
DW                   60.800 usec
DE                    6.50 usec
TE                   294.6 K
D1                1.00000000 sec
TD0                        1

======== CHANNEL f1 ========
NUC1                      1H
P1                     15.00 usec
PLW1             12.60000038 W
SFO1            400.1324710 MHz

F2 - Processing parameters
SI                        65536
SF               400.1300067 MHz
WDW                        EM
SSB          0
LB                     0.30 Hz
GB           0
PC                     1.00
```

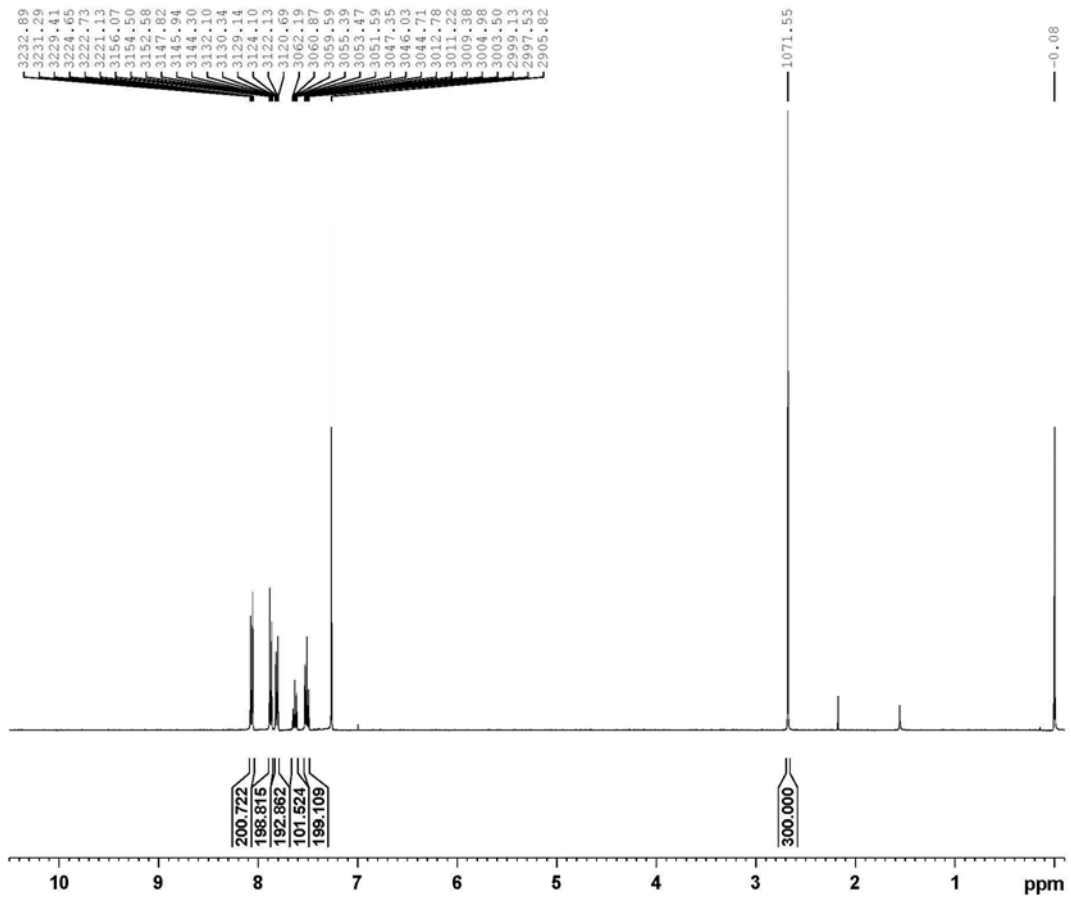


3h

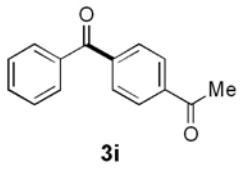


3h

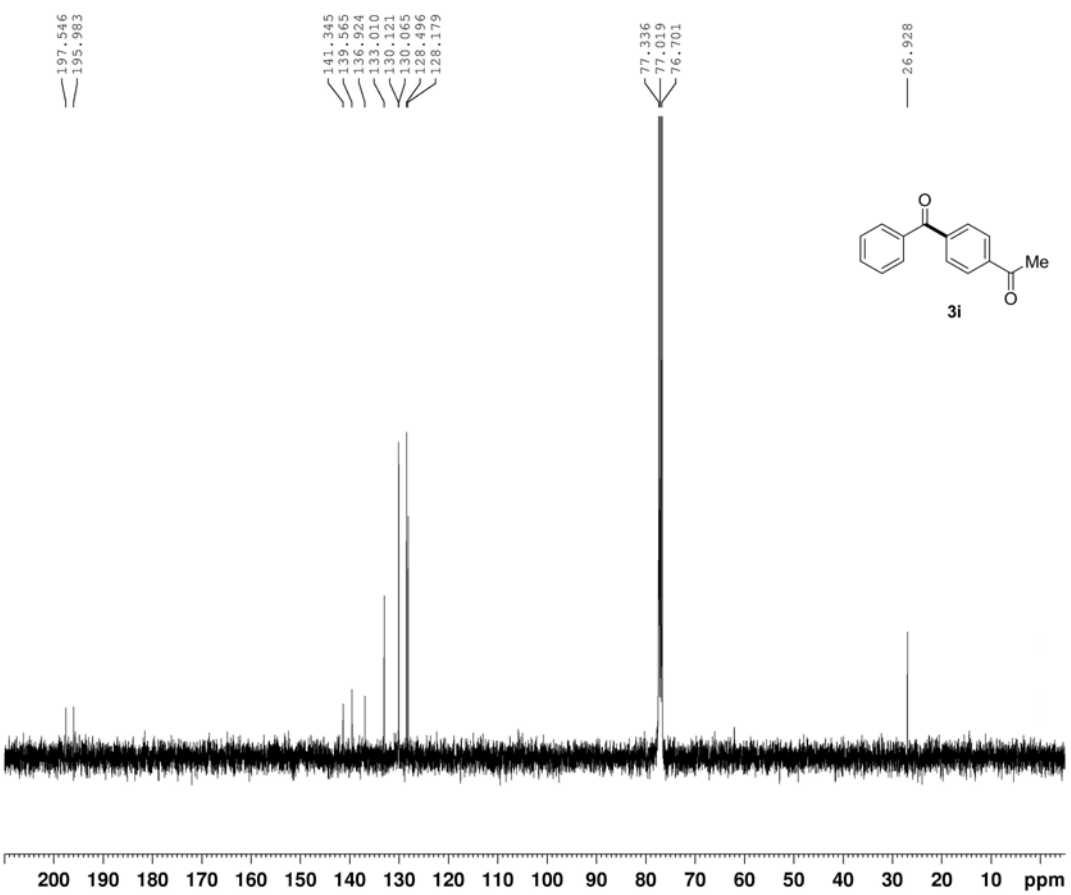
```
Current Data Parameters
NAME                 SJM-424
EXPNO                      2
PROCNO                     1

F2 - Acquisition Parameters
Date_               20120712
Time                    2.02
INSTRUM                spect
PROBHD    5 mm PABBO BB/
PULPROG             zgpg30
TD                    65536
SOLVENT               CDCl3
NS                      1024
DS                         4
SWH               24038.461 Hz
FIDRES             0.366798 Hz
AQ                 1.3631488 sec
RG                    186.53
DW                   20.800 usec
DE                    6.50 usec
TE                   295.1 K
D1                2.00000000 sec
d11               0.03000000 sec
DELTA             1.89999998 sec
TD0                        1
SFO1            100.6228293 MHz
NUC1                     13C
P1                     9.98 usec
PLW1             52.09999847 W
SFO2            400.1316005 MHz
NUC2                      1H
CPDPRG[2             waltz16
PCPD2                 90.00 usec
PLW2             12.60000038 W
PLW12             0.34999999 W
PLW13             0.28349999 W

F2 - Processing parameters
SI                        32768
SF              100.6127690 MHz
WDW                        EM
SSB          0
LB                     1.00 Hz
GB           0
PC                     1.40
```




```
Current Data Parameters
NAME                  SJM-347
EXPNO                       1
PROCNO                      1

F2 - Acquisition Parameters
Date_              20120710
Time                   2.08
INSTRUM               spect
PROBHD    5 mm PABBO BB/
PULPROG                zg30
TD                    65536
SOLVENT               CDCl3
NS                       16
DS                        2
SWH                8223.685 Hz
FIDRES             0.125483 Hz
AQ                 3.9845889 sec
RG                    186.53
DW                    60.800 usec
DE                     6.50 usec
TE                    294.2 K
D1                1.00000000 sec
TD0                         1

======== CHANNEL f1 ========
NUC1                       1H
P1                     15.00 usec
PLW1             12.60000038 W
SFO1            400.1324710 MHz

F2 - Processing parameters
SI                        65536
SF               400.1300091 MHz
WDW                         EM
SSB          0
LB                      0.30 Hz
GB           0
PC                      1.00
```

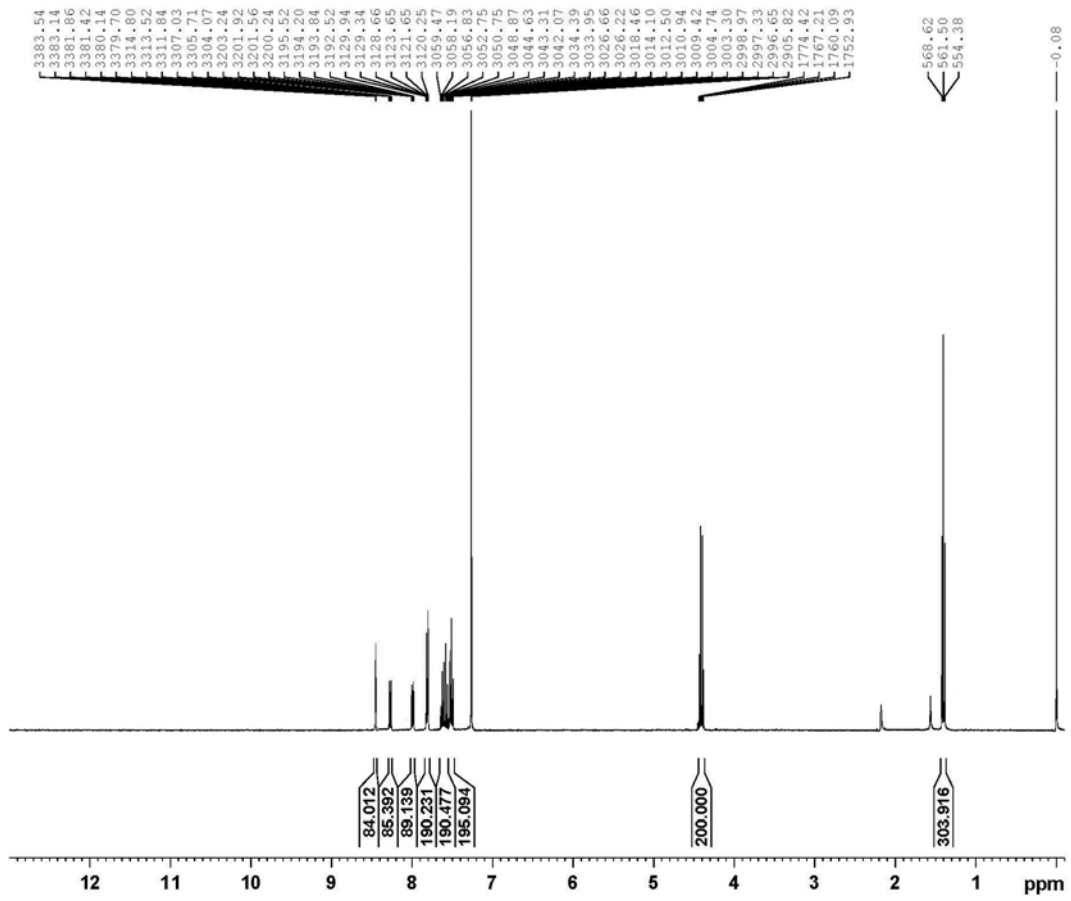


3i

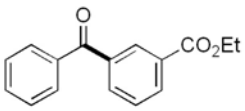



```
Current Data Parameters
NAME                  SJM-347
EXPNO                       2
PROCNO                      1

F2 - Acquisition Parameters
Date_              20120710
Time                   1.59
INSTRUM               spect
PROBHD    5 mm PABBO BB/
PULPROG             zgpg30
TD                    65536
SOLVENT               CDCl3
NS                     2048
DS                        4
SWH               24038.461 Hz
FIDRES             0.366798 Hz
AQ                 1.3631488 sec
RG                    186.53
DW                    20.800 usec
DE                     6.50 usec
TE                    295.4 K
D1                2.00000000 sec
d11               0.03000000 sec
DELTA             1.89999998 sec
TD0                         1
SFO1             100.6228293 MHz
NUC1                       13C
P1                     9.98 usec
PLW1             52.09999847 W
SFO2             400.1316005 MHz
NUC2                       1H
CPDPRG[2            waltz16
PCPD2                 90.00 usec
PLW2             12.60000038 W
PLW12             0.34999999 W
PLW13             0.28349999 W

F2 - Processing parameters
SI                        32768
SF               100.6127690 MHz
WDW                         EM
SSB          0
LB                      1.00 Hz
GB           0
PC                      1.40
```

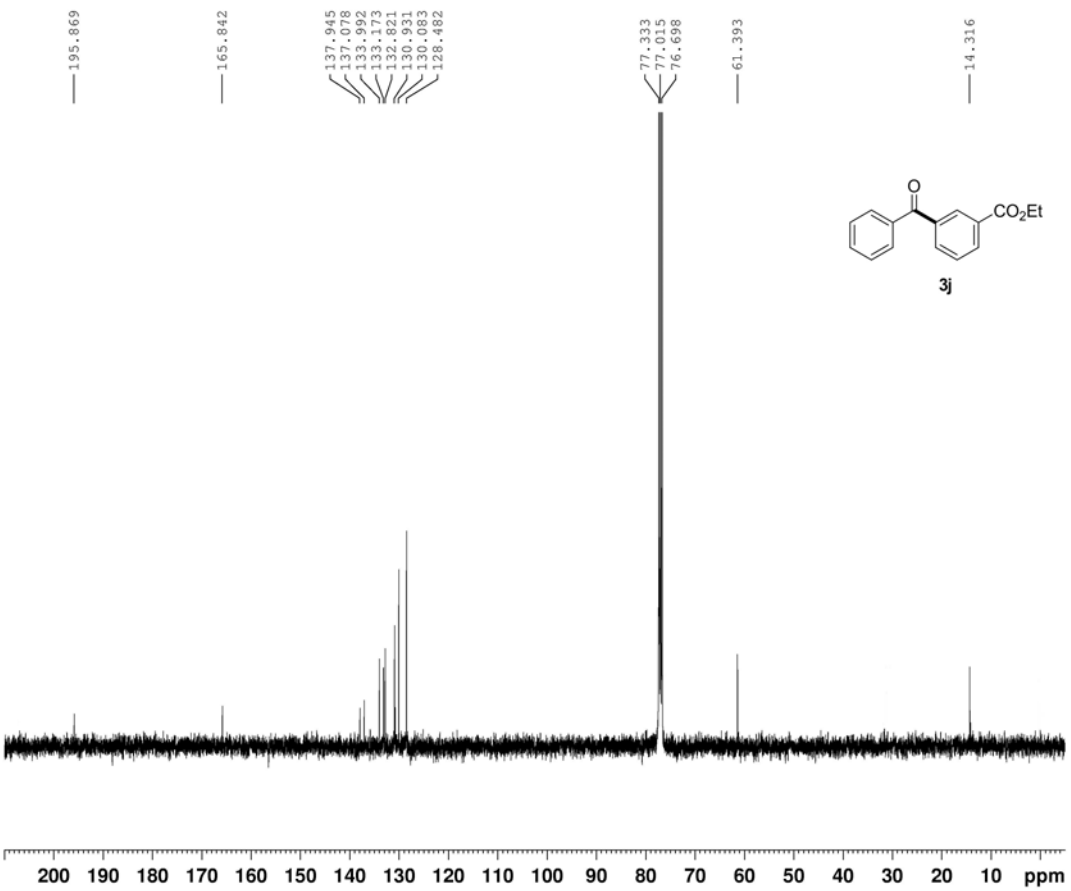

3i




```
Current Data Parameters
NAME                  SJM-463
EXPNO                       1
PROCNO                      1

F2 - Acquisition Parameters
Date_              20120814
Time                  14.17
INSTRUM               spect
PROBHD    5 mm PABBO BB/
PULPROG               zg30
TD                   65536
SOLVENT              CDCl3
NS                      16
DS                       2
SWH                8223.685 Hz
FIDRES            0.125483 Hz
AQ                3.9845889 sec
RG                   186.53
DW                   60.800 usec
DE                    6.50 usec
TE                   295.4 K
D1                1.00000000 sec
TD0                         1

======== CHANNEL f1 ========
NUC1                       1H
P1                    15.00 usec
PLW1             12.60000038 W
SFO1            400.1324710 MHz

F2 - Processing parameters
SI                       65536
SF                400.1300091 MHz
WDW                         EM
SSB          0
LB                     0.30 Hz
GB           0
PC                     1.00
```

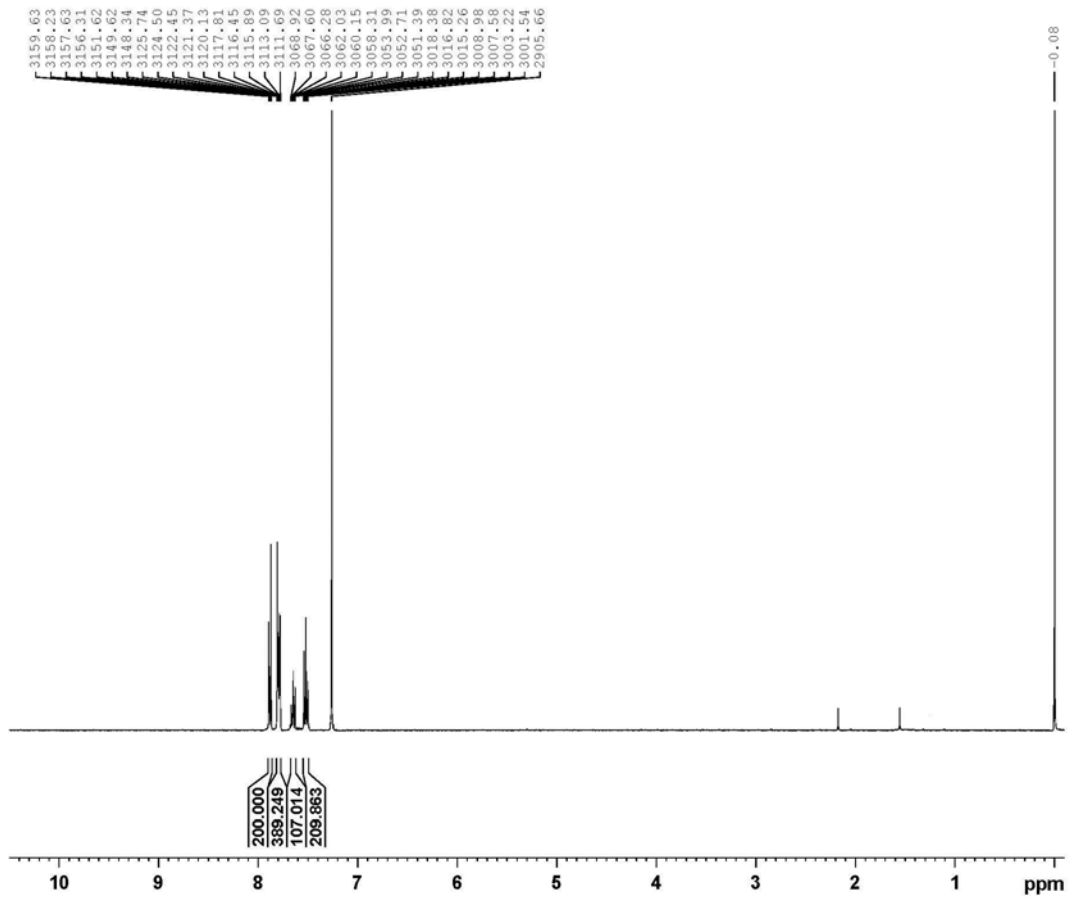


3j

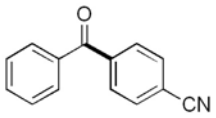



```
Current Data Parameters
NAME                  SJM-463
EXPNO                       2
PROCNO                      1

F2 - Acquisition Parameters
Date_              20120815
Time                   9.04
INSTRUM               spect
PROBHD    5 mm PABBO BB/
PULPROG            zgpg30
TD                   65536
SOLVENT              CDCl3
NS                    3072
DS                       4
SWH               24038.461 Hz
FIDRES            0.366798 Hz
AQ                1.3631488 sec
RG                   186.53
DW                   20.800 usec
DE                    6.50 usec
TE                   296.9 K
D1                2.00000000 sec
d11               0.03000000 sec
DELTA             1.89999998 sec
TD0                         1
SFO1            100.6228293 MHz
NUC1                      13C
P1                    9.98 usec
PLW1             52.09999847 W
SFO2            400.1316005 MHz
NUC2                       1H
CPDPRG[2             waltz16
PCPD2                 90.00 usec
PLW2             12.60000038 W
PLW12             0.34999999 W
PLW13             0.28349999 W

F2 - Processing parameters
SI                       32768
SF                100.6127690 MHz
WDW                         EM
SSB          0
LB                     1.00 Hz
GB           0
PC                     1.40
```

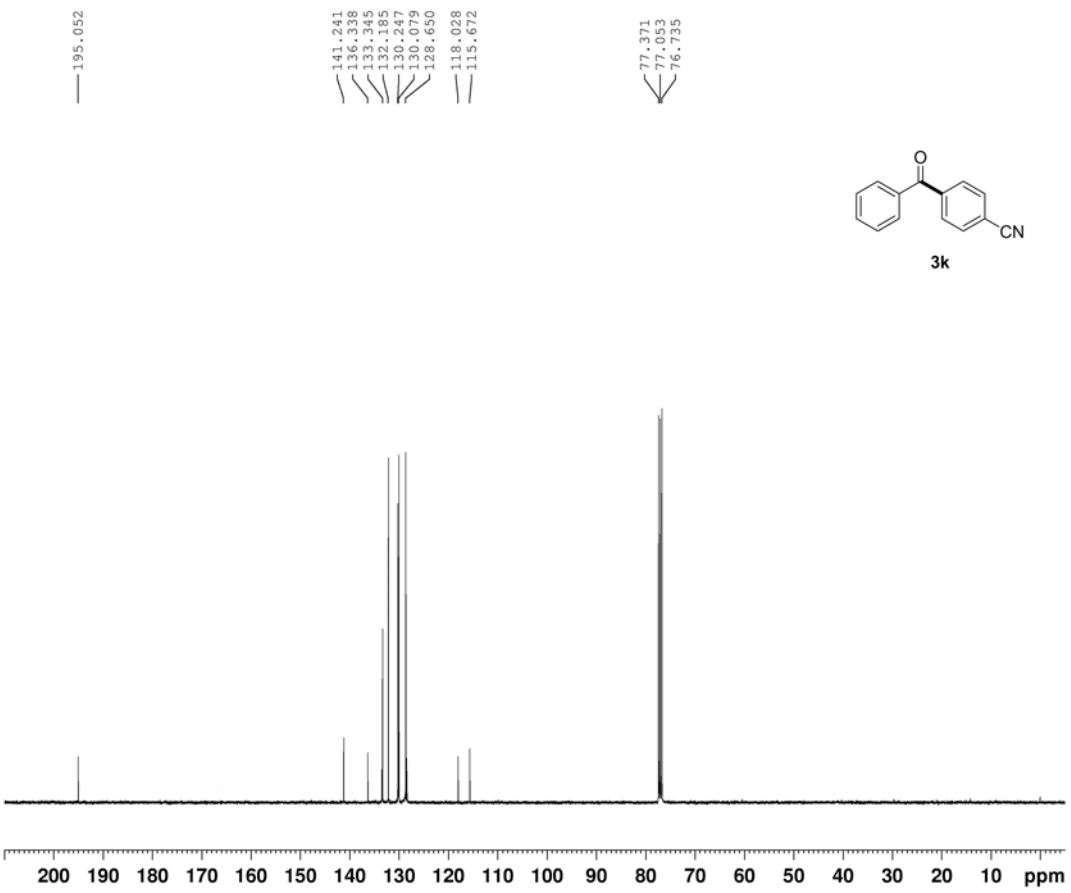

3j




```
Current Data Parameters
NAME                  SJM-468
EXPNO                       1
PROCNO                      1

F2 - Acquisition Parameters
Date_              20120816
Time                  21.12
INSTRUM               spect
PROBHD    5 mm PABBO BB/
PULPROG                zg30
TD                    65536
SOLVENT               CDCl3
NS                       16
DS                        2
SWH                8223.685 Hz
FIDRES             0.125483 Hz
AQ                 3.9845889 sec
RG                    186.53
DW                    60.800 usec
DE                     6.50 usec
TE                    296.1 K
D1                 1.00000000 sec
TD0                         1

======== CHANNEL f1 ========
NUC1                       1H
P1                      15.00 usec
PLW1              12.60000038 W
SFO1             400.1324710 MHz

F2 - Processing parameters
SI                        65536
SF               400.1300092 MHz
WDW                         EM
SSB          0
LB                       0.30 Hz
GB           0
PC                       1.00
```

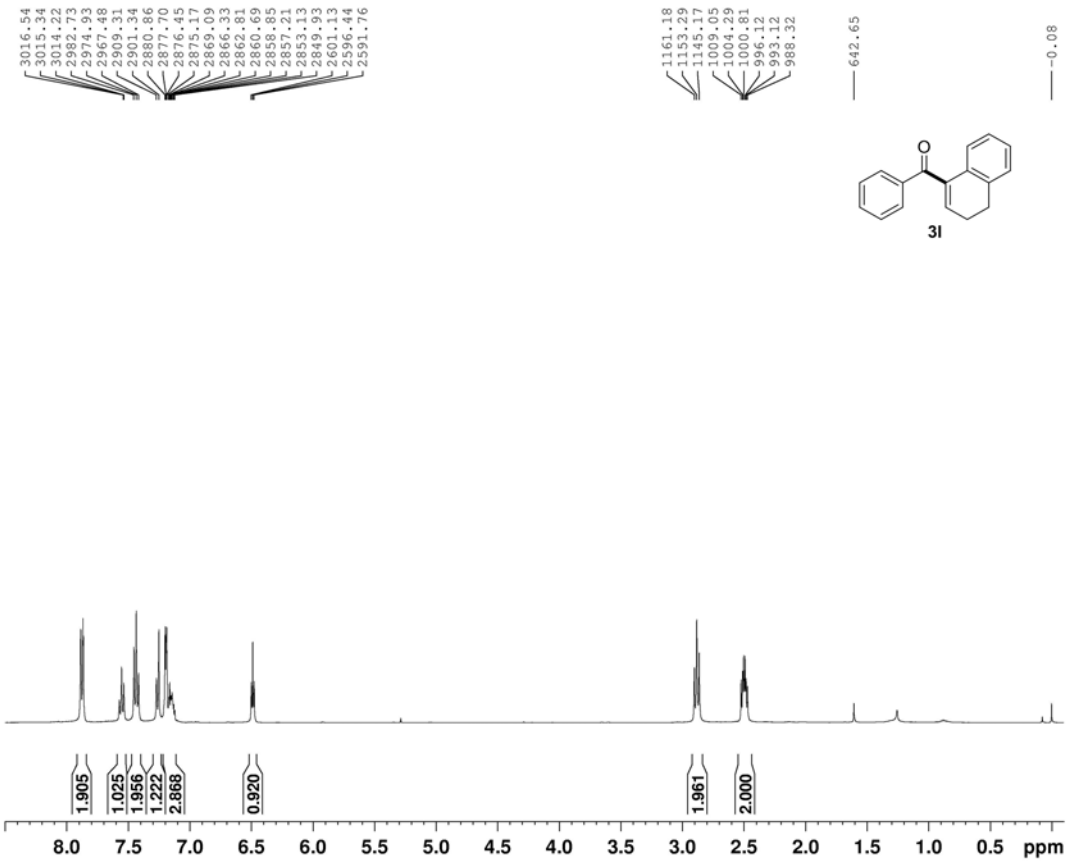


3k

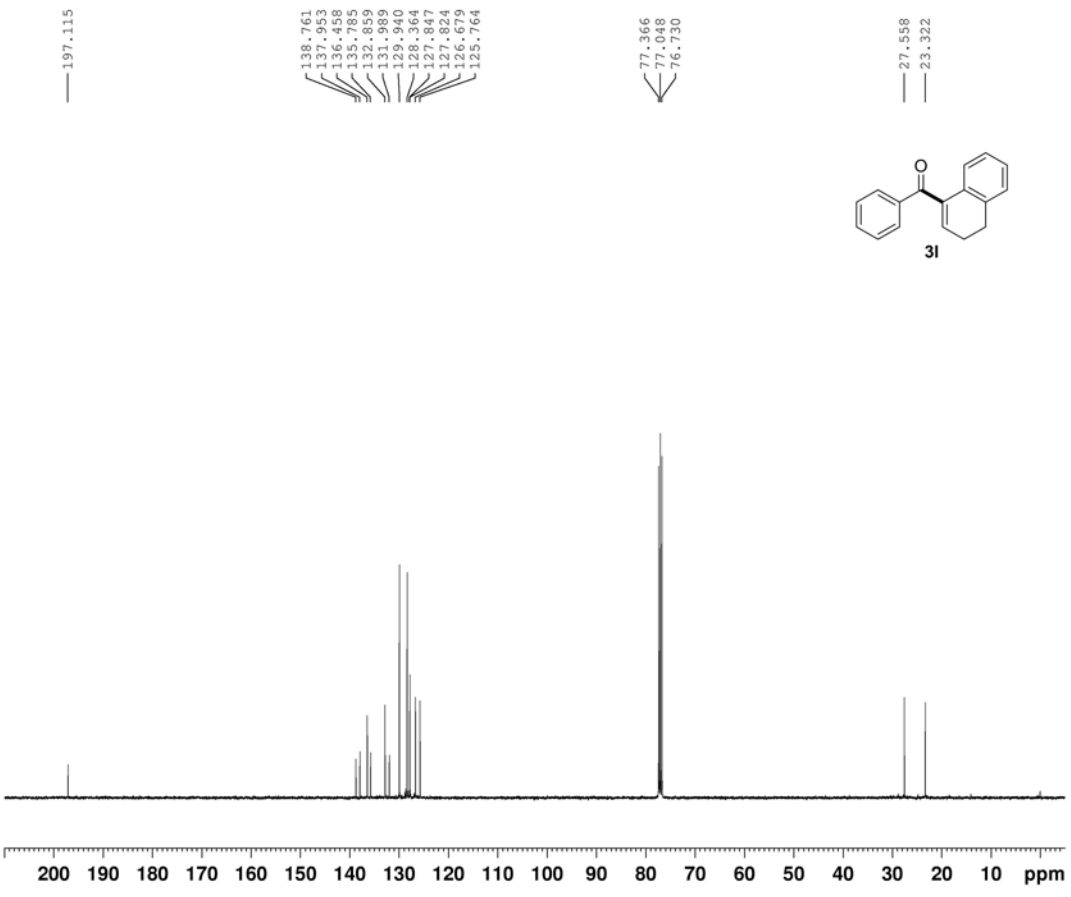


3k

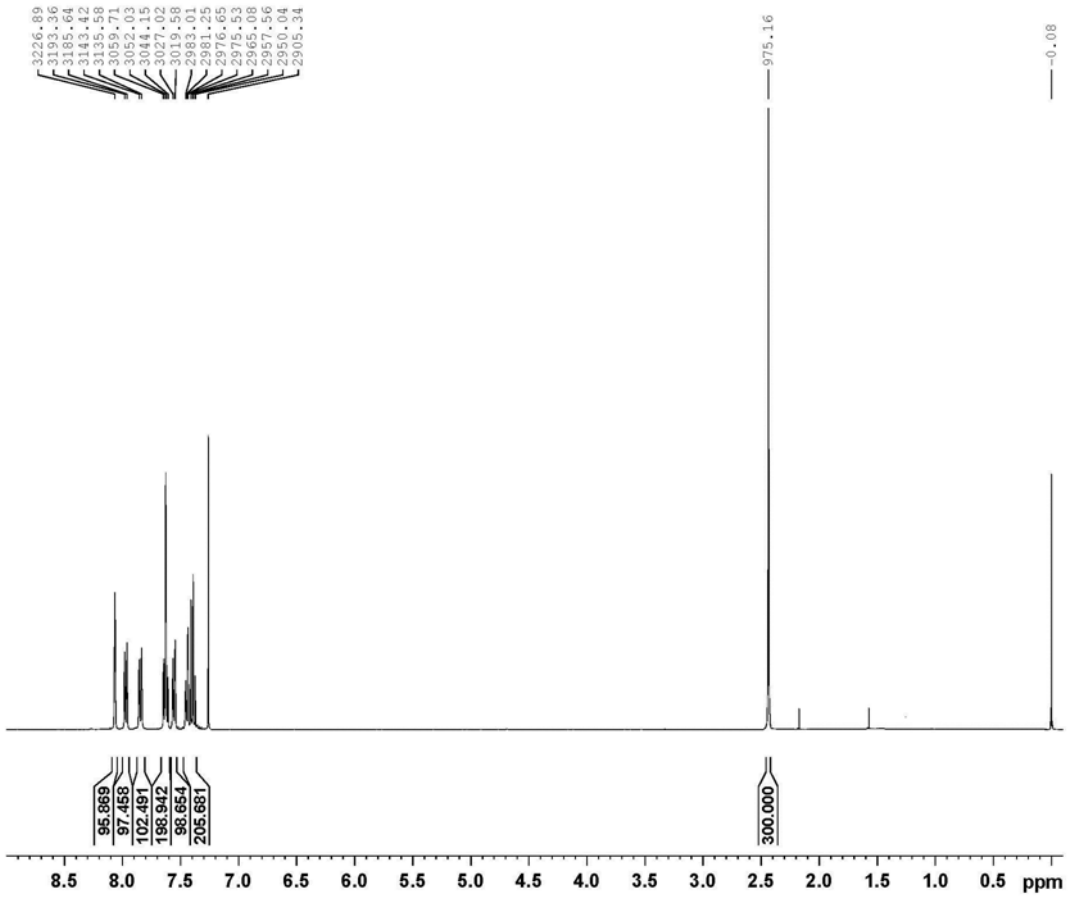
```
Current Data Parameters
NAME                  SJM-468
EXPNO                       2
PROCNO                      1

F2 - Acquisition Parameters
Date_              20120821
Time                   1.06
INSTRUM               spect
PROBHD    5 mm PABBO BB/
PULPROG             zgpg30
TD                    65536
SOLVENT               CDCl3
NS                     1024
DS                        4
SWH               24038.461 Hz
FIDRES             0.366798 Hz
AQ                 1.3631488 sec
RG                    186.53
DW                    20.800 usec
DE                     6.50 usec
TE                    296.8 K
D1                 2.00000000 sec
d11                0.03000000 sec
DELTA              1.89999998 sec
TD0                         1
SFO1             100.6228293 MHz
NUC1                      13C
P1                      9.98 usec
PLW1              52.09999847 W
SFO2             400.1316005 MHz
NUC2                       1H
CPDPRG[2             waltz16
PCPD2                  90.00 usec
PLW2              12.60000038 W
PLW12              0.34999999 W
PLW13              0.28349999 W

F2 - Processing parameters
SI                        32768
SF               100.6127690 MHz
WDW                         EM
SSB          0
LB                       1.00 Hz
GB           0
PC                       1.40
```



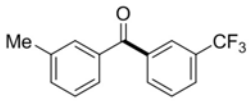

```
Current Data Parameters
NAME                   31
EXPNO                   1
PROCNO                  1

F2 - Acquisition Parameters
Date_           20140127
Time               15.53
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH             8223.685 Hz
FIDRES          0.125483 Hz
AQ              3.9845889 sec
RG                 83.43
DW                 60.800 usec
DE                  6.50 usec
TE                 294.0 K
D1              1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                 15.00 usec
PLW1          12.60000038 W
SFO1         400.1324710 MHz

F2 - Processing parameters
SI                 65536
SF           400.1300137 MHz
WDW                   EM
SSB       0
LB                 0.30 Hz
GB        0
PC                 1.00
```



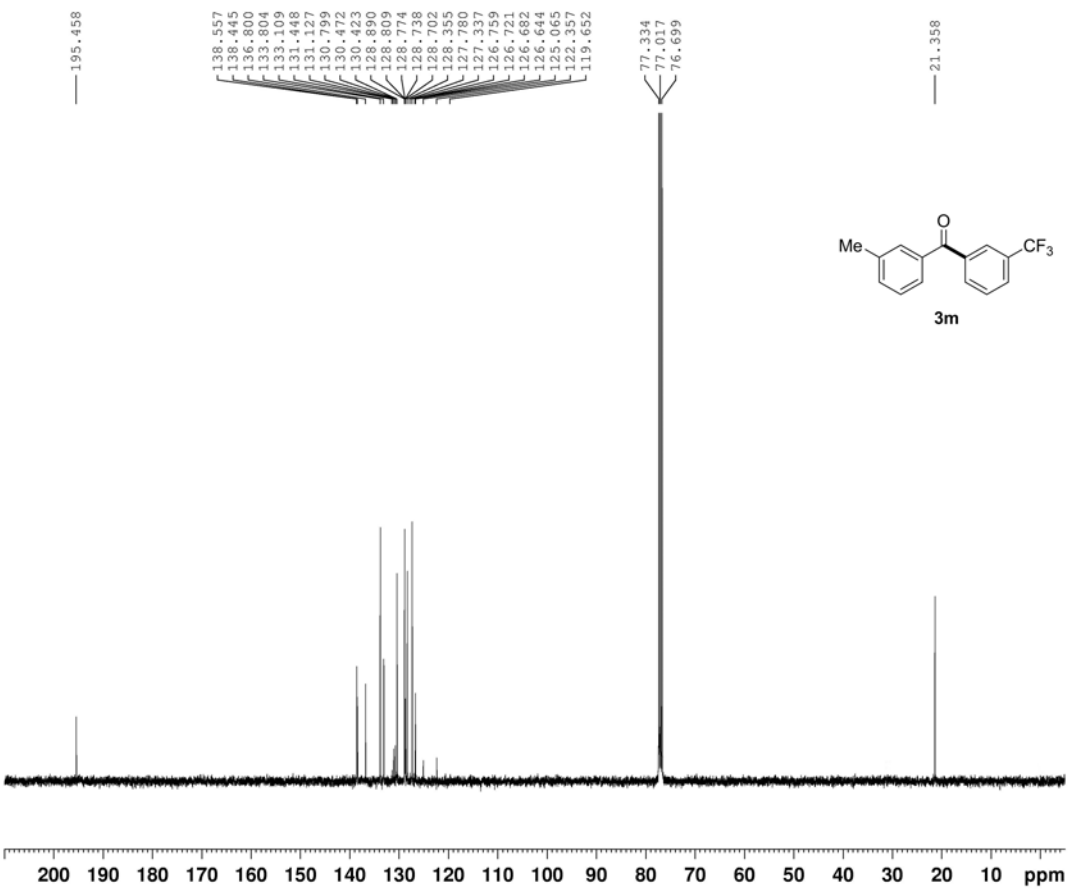

```
Current Data Parameters
NAME                   31
EXPNO                   2
PROCNO                  1

F2 - Acquisition Parameters
Date_           20140126
Time               2.11
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG          zgpg30
TD                 65536
SOLVENT            CDCl3
NS                  1024
DS                     4
SWH            24038.461 Hz
FIDRES          0.366798 Hz
AQ              1.3631488 sec
RG                186.53
DW                 20.800 usec
DE                  6.50 usec
TE                 294.9 K
D1              2.00000000 sec
d11             0.03000000 sec
DELTA           1.89999998 sec
TD0                    1
SFO1         100.6228293 MHz
NUC1                  13C
P1                  9.98 usec
PLW1          52.09999847 W
SFO2         400.1316005 MHz
NUC2                  1H
CPDPRG[2          waltz16
PCPD2              90.00 usec
PLW2          12.60000038 W
PLW12          0.34999999 W
PLW13          0.28349999 W

F2 - Processing parameters
SI                 32768
SF           100.6127690 MHz
WDW                   EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
```




```
Current Data Parameters
NAME                 SJM-486
EXPNO                      1
PROCNO                     1

F2 - Acquisition Parameters
Date_               20120829
Time                   16.48
INSTRUM                spect
PROBHD    5 mm PABBO BB/
PULPROG                zg30
TD                    65536
SOLVENT               CDCl3
NS                        16
DS                         2
SWH                 8223.685 Hz
FIDRES              0.125483 Hz
AQ                  3.9845889 sec
RG                     127.32
DW                     60.800 usec
DE                      6.50 usec
TE                     296.1 K
D1                1.00000000 sec
TD0                        1

======== CHANNEL f1 ========
NUC1                       1H
P1                     15.00 usec
PLW1             12.60000038 W
SFO1            400.1324710 MHz

F2 - Processing parameters
SI                        65536
SF               400.1300094 MHz
WDW                          EM
SSB          0
LB                      0.30 Hz
GB           0
PC                      1.00
```

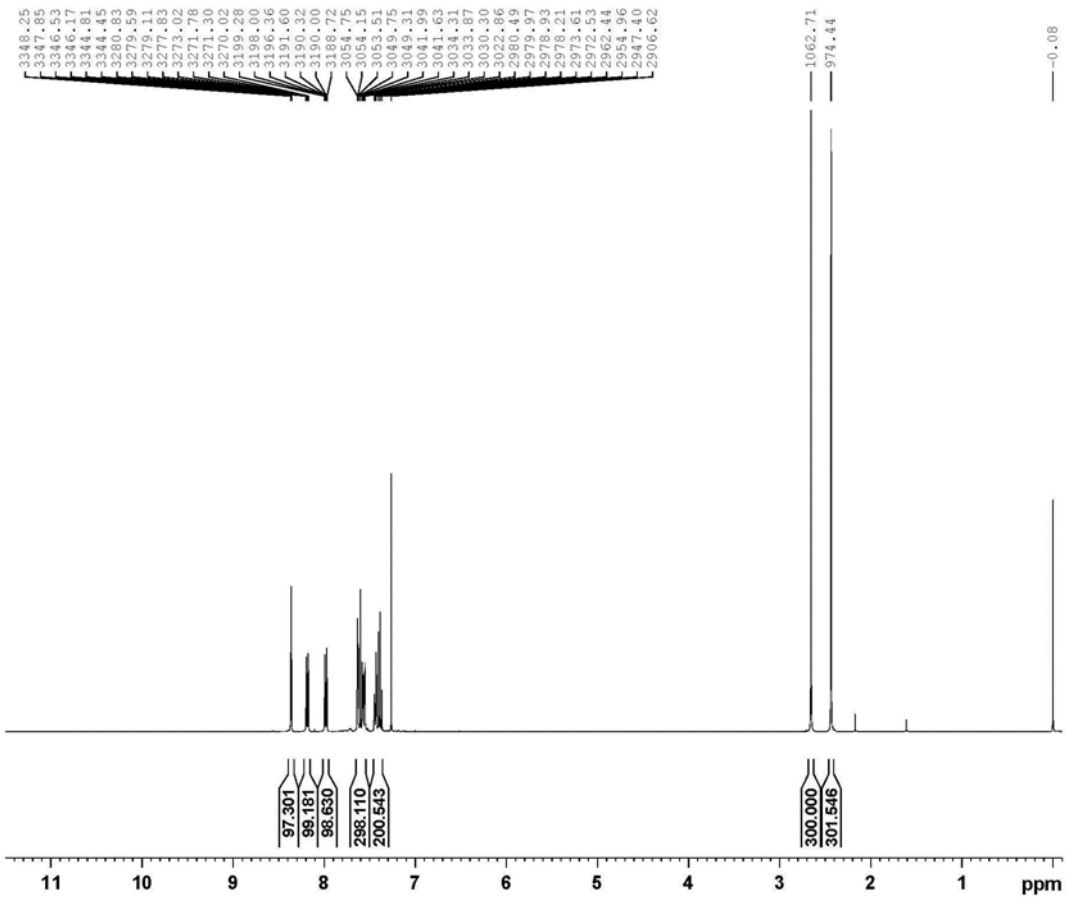


3m

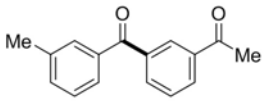



```
Current Data Parameters
NAME                 SJM-486
EXPNO                      2
PROCNO                     1

F2 - Acquisition Parameters
Date_               20120830
Time                    4.06
INSTRUM                spect
PROBHD    5 mm PABBO BB/
PULPROG             zgpg30
TD                    65536
SOLVENT               CDCl3
NS                      1024
DS                         4
SWH                24038.461 Hz
FIDRES              0.366798 Hz
AQ                  1.3631488 sec
RG                     186.53
DW                     20.800 usec
DE                      6.50 usec
TE                     297.6 K
D1                2.00000000 sec
d11               0.03000000 sec
DELTA             1.89999998 sec
TD0                        1
SFO1            100.6228293 MHz
NUC1                      13C
P1                      9.98 usec
PLW1             52.09999847 W
SFO2            400.1316005 MHz
NUC2                       1H
CPDPRG[2             waltz16
PCPD2                  90.00 usec
PLW2             12.60000038 W
PLW12             0.34999999 W
PLW13             0.28349999 W

F2 - Processing parameters
SI                        32768
SF               100.6127690 MHz
WDW                          EM
SSB          0
LB                      1.00 Hz
GB           0
PC                      1.40
```

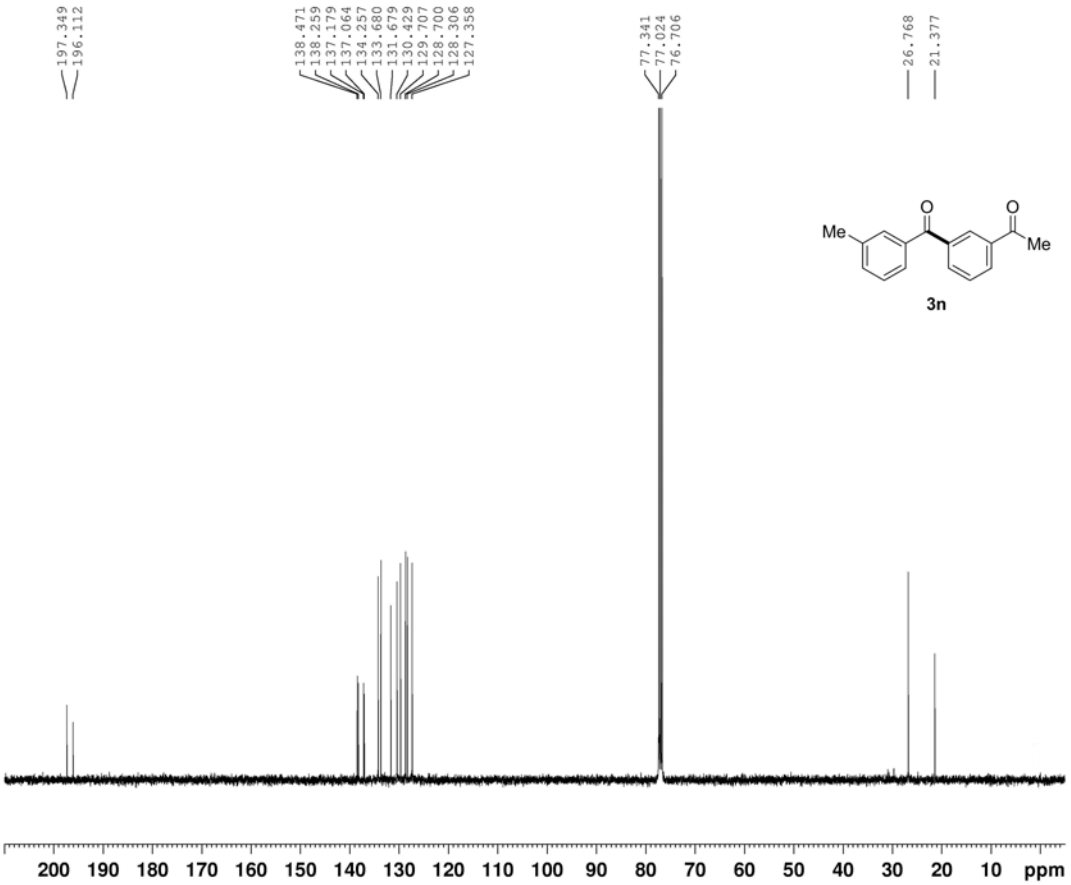

3m




```
Current Data Parameters
NAME                  SJM-484
EXPNO                       1
PROCNO                      1

F2 - Acquisition Parameters
Date_              20120829
Time                   16.40
INSTRUM                spect
PROBHD    5 mm PABBO BB/
PULPROG                zg30
TD                    65536
SOLVENT               CDCl3
NS                       16
DS                        2
SWH                8223.685 Hz
FIDRES            0.125483 Hz
AQ                3.9845889 sec
RG                    114.24
DW                  60.800 usec
DE                   6.50 usec
TE                   296.2 K
D1                1.00000000 sec
TD0                         1

======== CHANNEL f1 ========
NUC1                       1H
P1                      15.00 usec
PLW1             12.60000038 W
SFO1            400.1324710 MHz

F2 - Processing parameters
SI                         65536
SF                400.1300081 MHz
WDW                           EM
SSB          0
LB                       0.30 Hz
GB           0
PC                       1.00
```

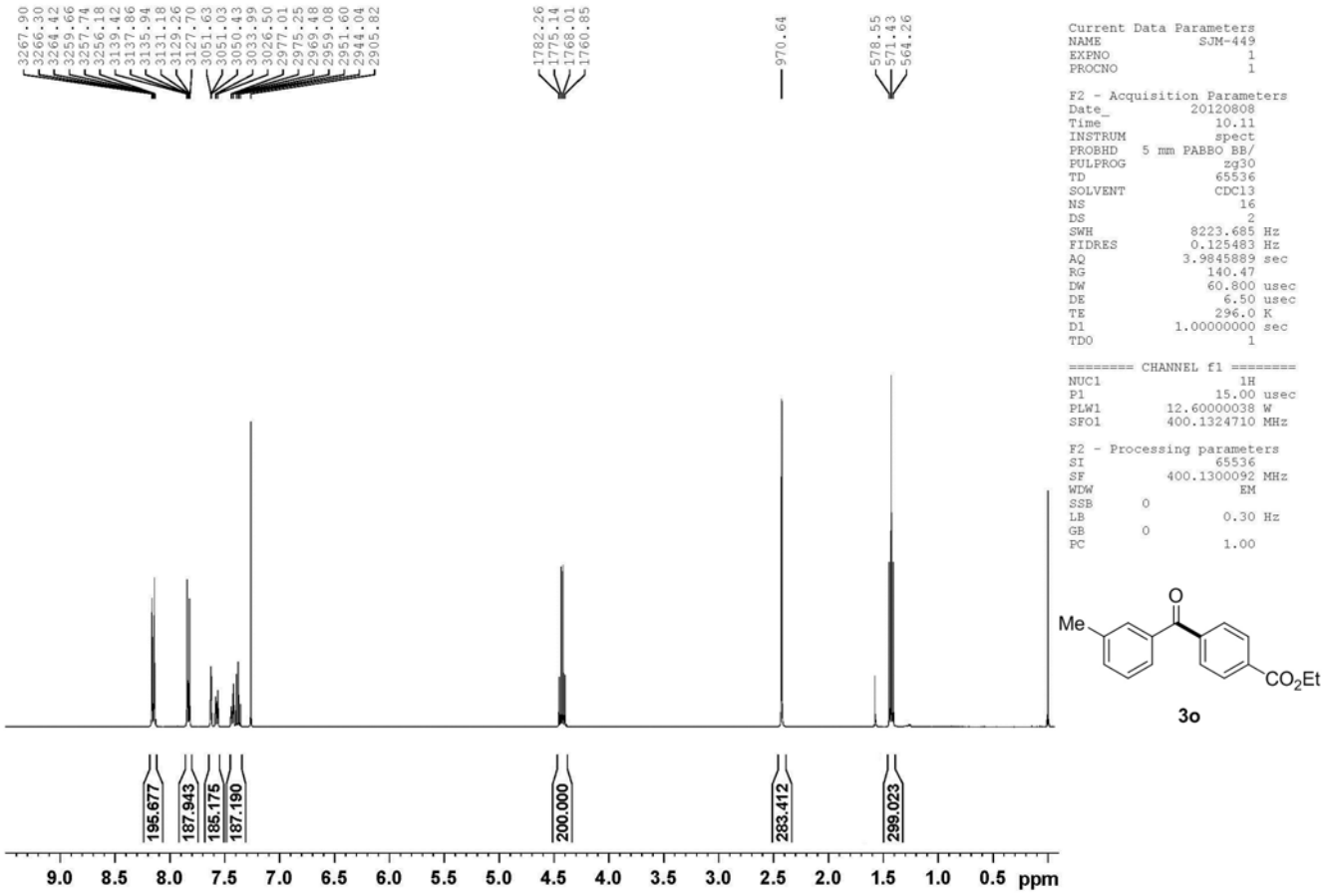


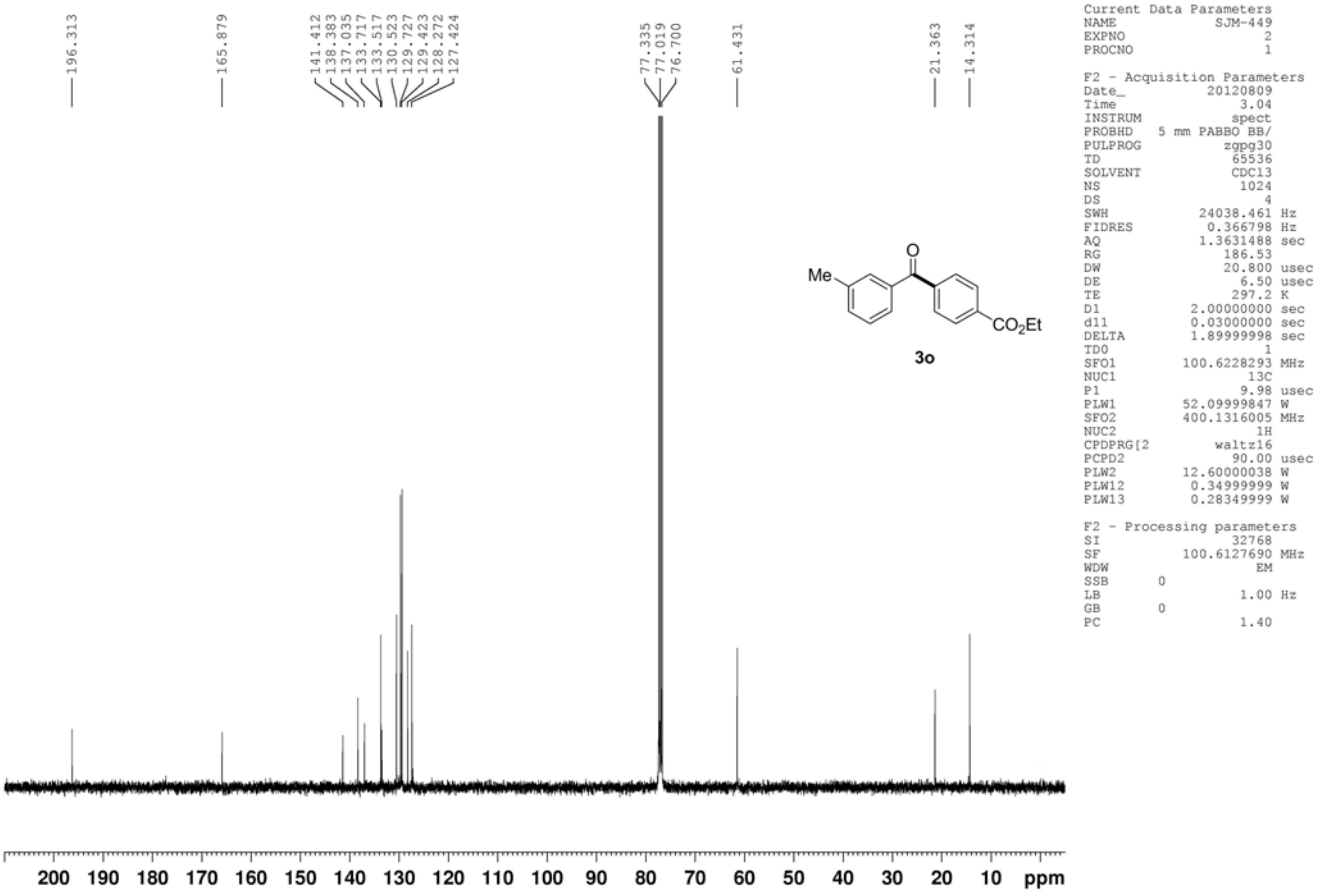
3n

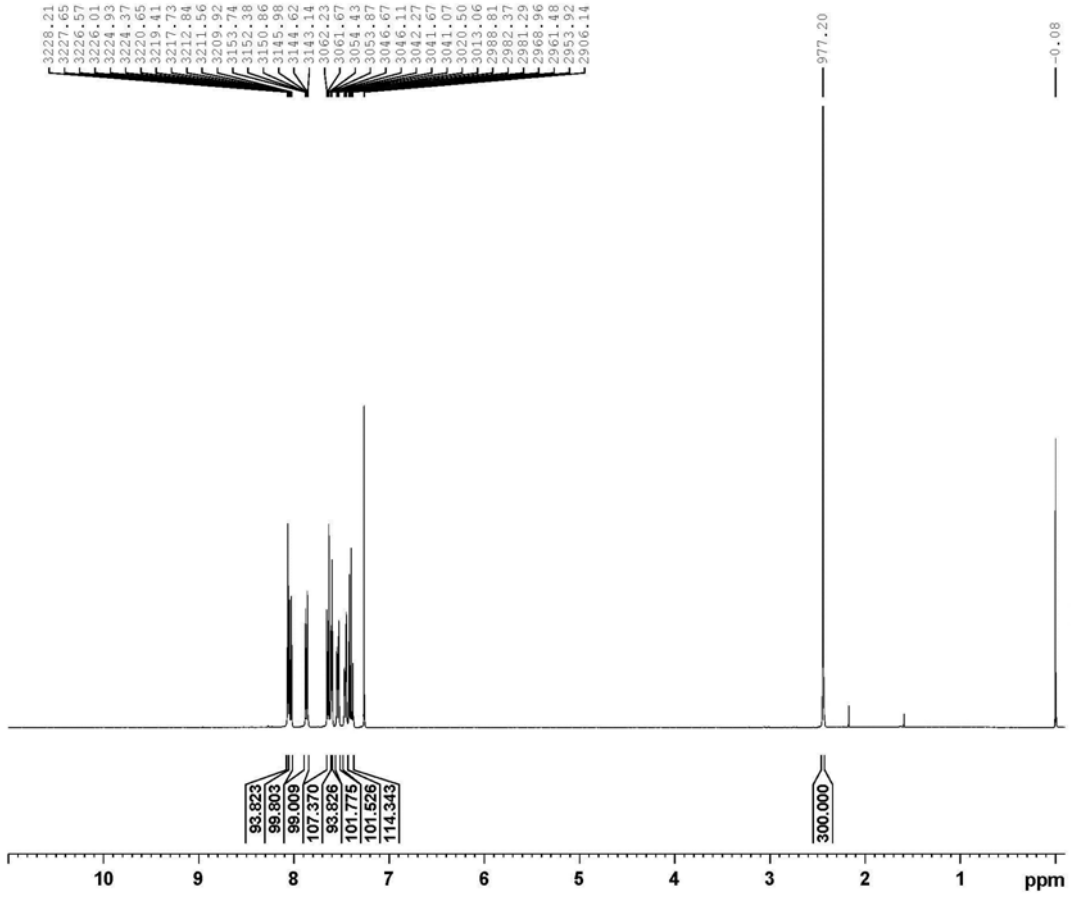


3n

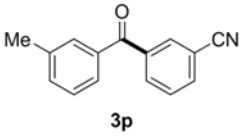
```
Current Data Parameters
NAME                  SJM-484
EXPNO                       2
PROCNO                      1

F2 - Acquisition Parameters
Date_              20120830
Time                    5.08
INSTRUM                spect
PROBHD    5 mm PABBO BB/
PULPROG             zgpg30
TD                    65536
SOLVENT               CDCl3
NS                     1024
DS                        4
SWH               24038.461 Hz
FIDRES            0.366798 Hz
AQ                1.3631488 sec
RG                    186.53
DW                  20.800 usec
DE                   6.50 usec
TE                   297.6 K
D1                2.00000000 sec
d11               0.03000000 sec
DELTA             1.89999998 sec
TD0                         1
SFO1            100.6228293 MHz
NUC1                      13C
P1                       9.98 usec
PLW1             52.09999847 W
SFO2            400.1316005 MHz
NUC2                       1H
CPDPRG[2              waltz16
PCPD2                   90.00 usec
PLW2             12.60000038 W
PLW12             0.34999999 W
PLW13             0.28349999 W

F2 - Processing parameters
SI                         32768
SF                100.6127690 MHz
WDW                           EM
SSB          0
LB                       1.00 Hz
GB           0
PC                       1.40
```


3267.90
3266.30
3264.42
3259.66
3257.74
3256.18
3139.42
3137.86
3135.94
3131.18
3129.26
3127.70
3051.63
3051.03
3050.43
3033.99
3026.50
2977.01
2975.25
2969.48
2959.08
2951.60
2944.04
2905.82
1782.26
1775.14
1768.01
1760.85
970.64
578.55
571.43
564.26
Current Data Parameters
NAME SJM-449
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20120808
Time 10.11
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9845889 sec
RG 140.47
DW 60.800 usec
DE 6.50 usec
TE 296.0 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 15.00 usec
PLW1 12.60000038 W
SFO1 400.1324710 MHz
F2 - Processing parameters
SI 65536
SF 400.1300092 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
Me
O
CO2Et
3o
195.677
187.943
185.175
187.190
200.000
283.412
299.023
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 ppm

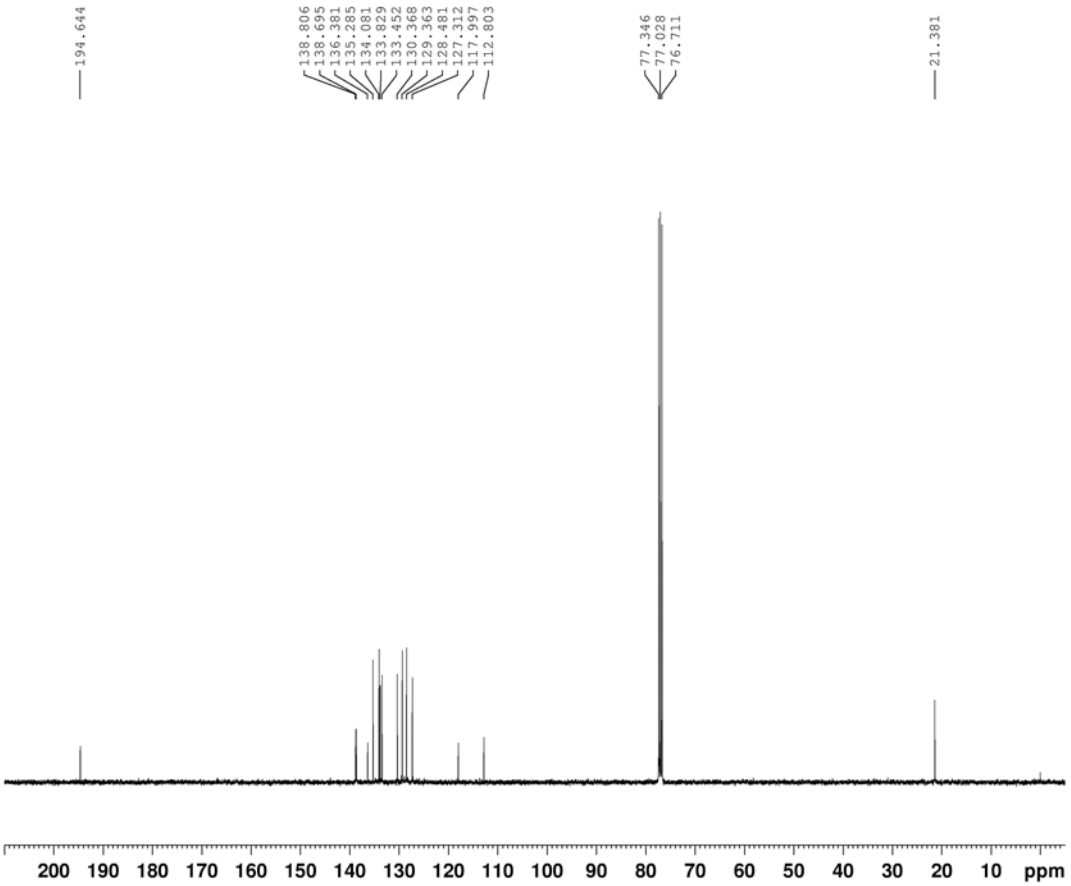

196.313
165.879
141.412
138.383
137.035
133.717
133.517
130.523
129.727
129.423
128.272
127.424
77.335
77.019
76.700
61.431
21.363
14.314
Current Data Parameters
NAME SJM-449
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20120809
Time 3.04
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1024
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 186.53
DW 20.800 usec
DE 6.50 usec
TE 297.2 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1
SFO1 100.6228293 MHz
NUC1 13C
P1 9.98 usec
PLW1 52.09999847 W
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 90.00 usec
PLW2 12.60000038 W
PLW12 0.34999999 W
PLW13 0.28349999 W
F2 - Processing parameters
SI 32768
SF 100.6127690 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
Me
O
CO2Et
3o
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm



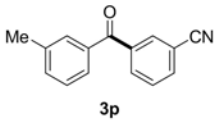

```
Current Data Parameters
NAME                  SJM-485
EXPNO                       1
PROCNO                      1

F2 - Acquisition Parameters
Date_              20120829
Time                   16.44
INSTRUM                spect
PROBHD    5 mm PABBO BB/
PULPROG                zg30
TD                    65536
SOLVENT               CDCl3
NS                       16
DS                        2
SWH                8223.685 Hz
FIDRES             0.125483 Hz
AQ                 3.9845889 sec
RG                    127.32
DW                    60.800 usec
DE                     6.50 usec
TE                    296.2 K
D1                 1.00000000 sec
TD0                         1

======== CHANNEL f1 ========
NUC1                       1H
P1                      15.00 usec
PLW1              12.60000038 W
SFO1             400.1324710 MHz

F2 - Processing parameters
SI                         65536
SF                400.1300086 MHz
WDW                           EM
SSB          0
LB                       0.30 Hz
GB           0
PC                       1.00
```



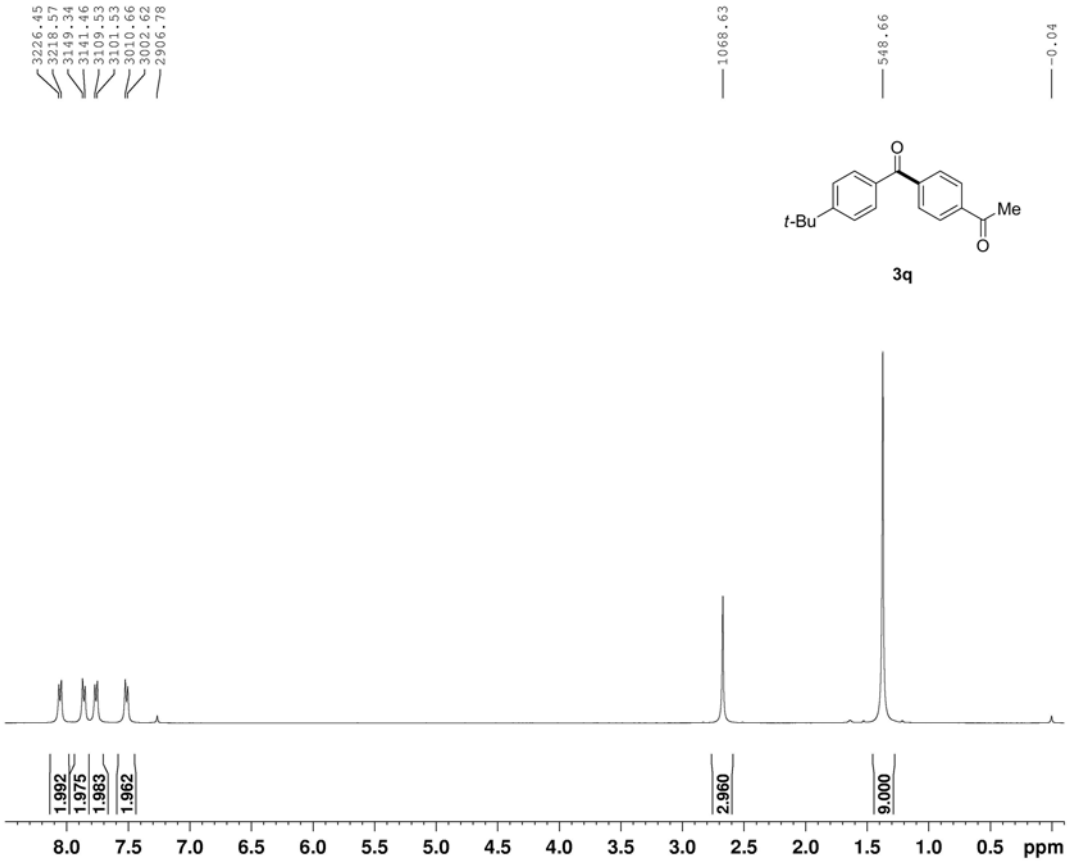
3p



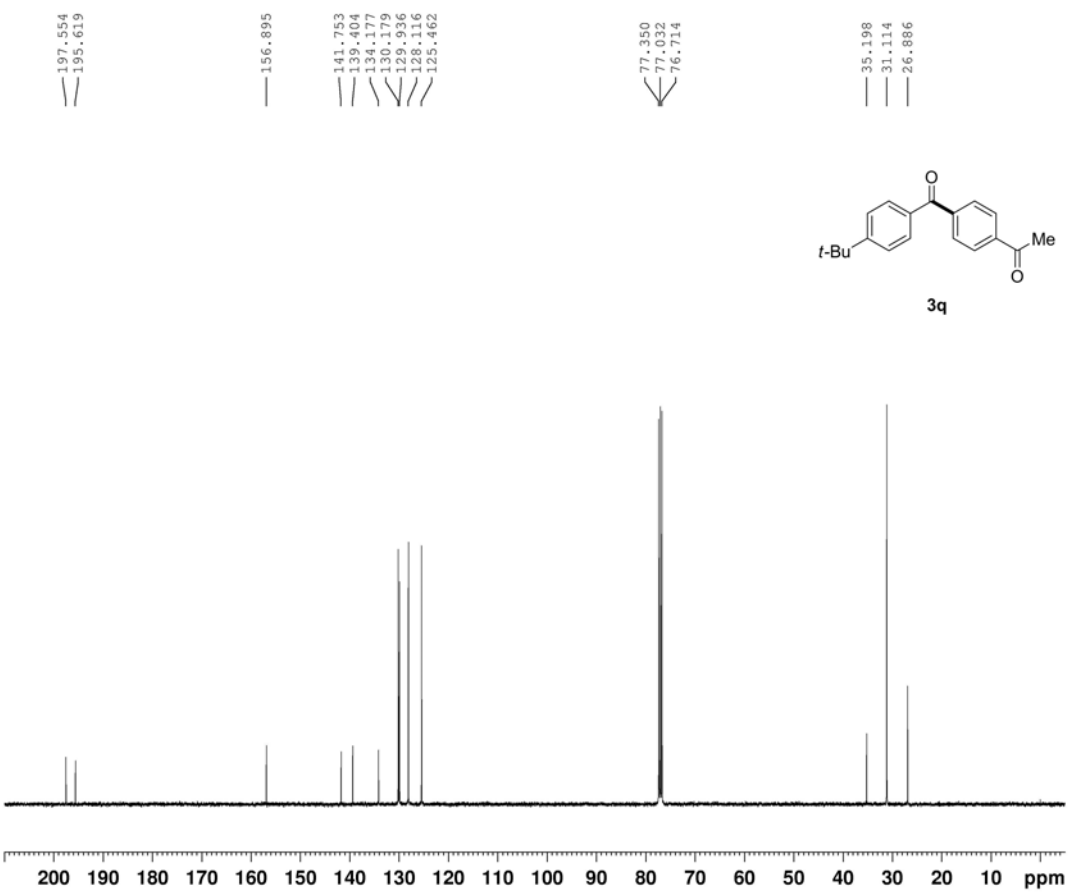

```
Current Data Parameters
NAME                  SJM-485
EXPNO                       2
PROCNO                      1

F2 - Acquisition Parameters
Date_              20120830
Time                    6.09
INSTRUM                spect
PROBHD    5 mm PABBO BB/
PULPROG             zgpg30
TD                    65536
SOLVENT               CDCl3
NS                     1024
DS                        4
SWH               24038.461 Hz
FIDRES             0.366798 Hz
AQ                 1.3631488 sec
RG                    186.53
DW                    20.800 usec
DE                     6.50 usec
TE                    297.6 K
D1                 2.00000000 sec
d11                0.03000000 sec
DELTA              1.89999998 sec
TD0                         1
SFO1              100.6228293 MHz
NUC1                       13C
P1                      9.98 usec
PLW1              52.09999847 W
SFO2              400.1316005 MHz
NUC2                       1H
CPDPRG[2              waltz16
PCPD2                  90.00 usec
PLW2              12.60000038 W
PLW12              0.34999999 W
PLW13              0.28349999 W

F2 - Processing parameters
SI                         32768
SF                100.6127690 MHz
WDW                           EM
SSB          0
LB                       1.00 Hz
GB           0
PC                       1.40
```



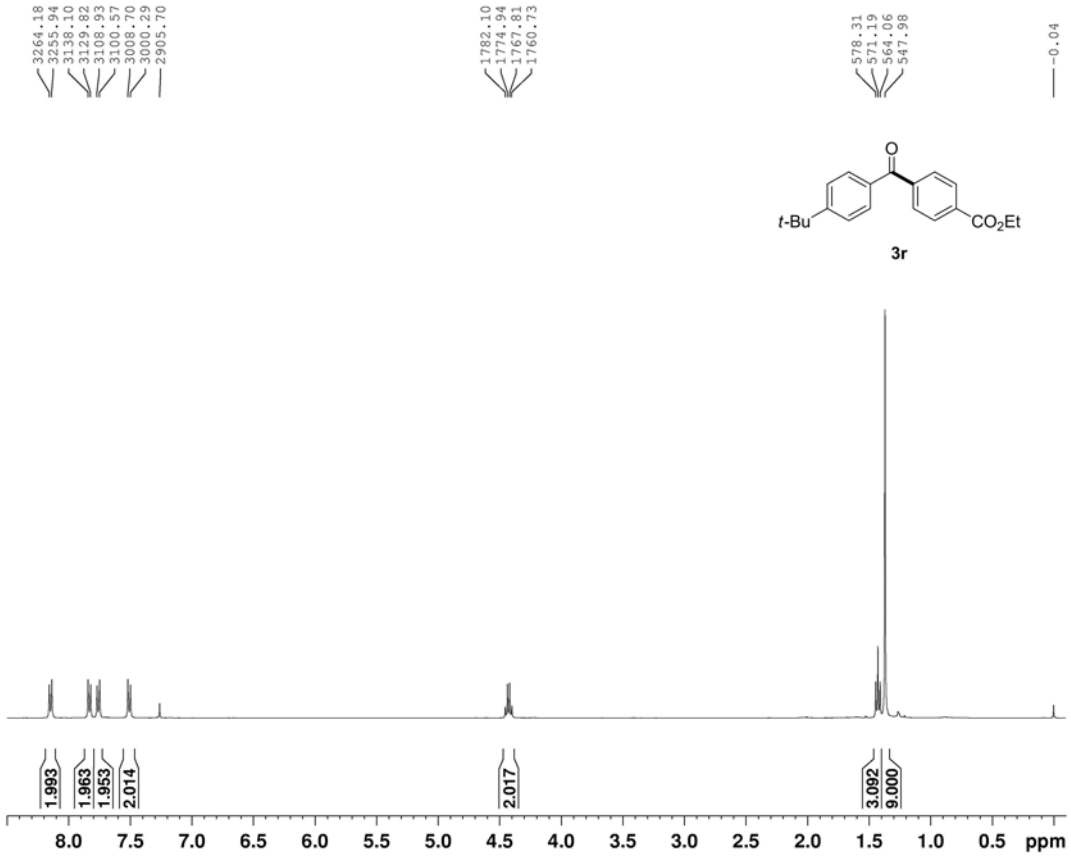
3p



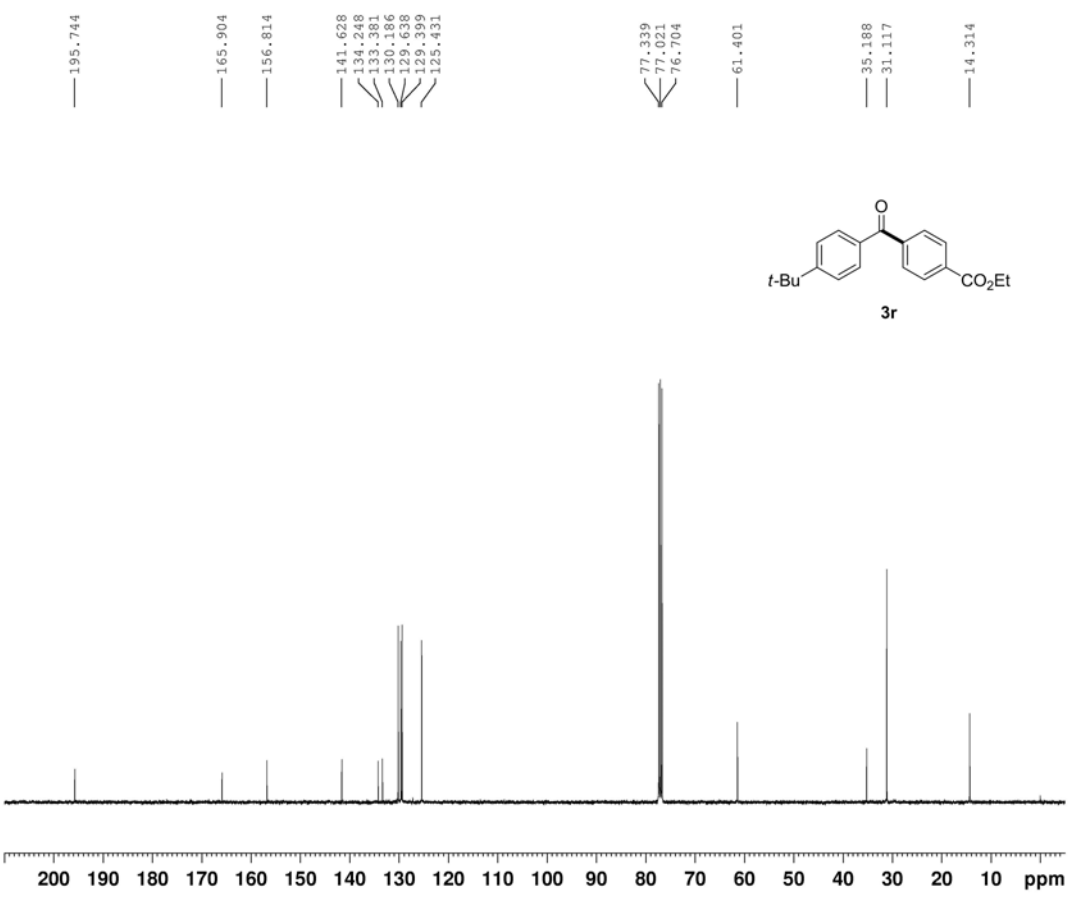

```
Current Data Parameters
NAME                   3r
EXPNO                   1
PROCNO                  1

F2 - Acquisition Parameters
Date_           20140119
Time               18.11
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH             8012.820 Hz
FIDRES             0.122266 Hz
AQ              4.0894465 sec
RG                 113.82
DW                 62.400 usec
DE                  6.50 usec
TE                 298.0 K
D1              1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                   1H
P1                  15.00 usec
PLW1           12.58899975 W
SFO1          400.1316005 MHz

F2 - Processing parameters
SI                  131072
SF            400.1300094 MHz
WDW                    EM
SSB       0
LB                  0.30 Hz
GB        0
PC                  1.00
```



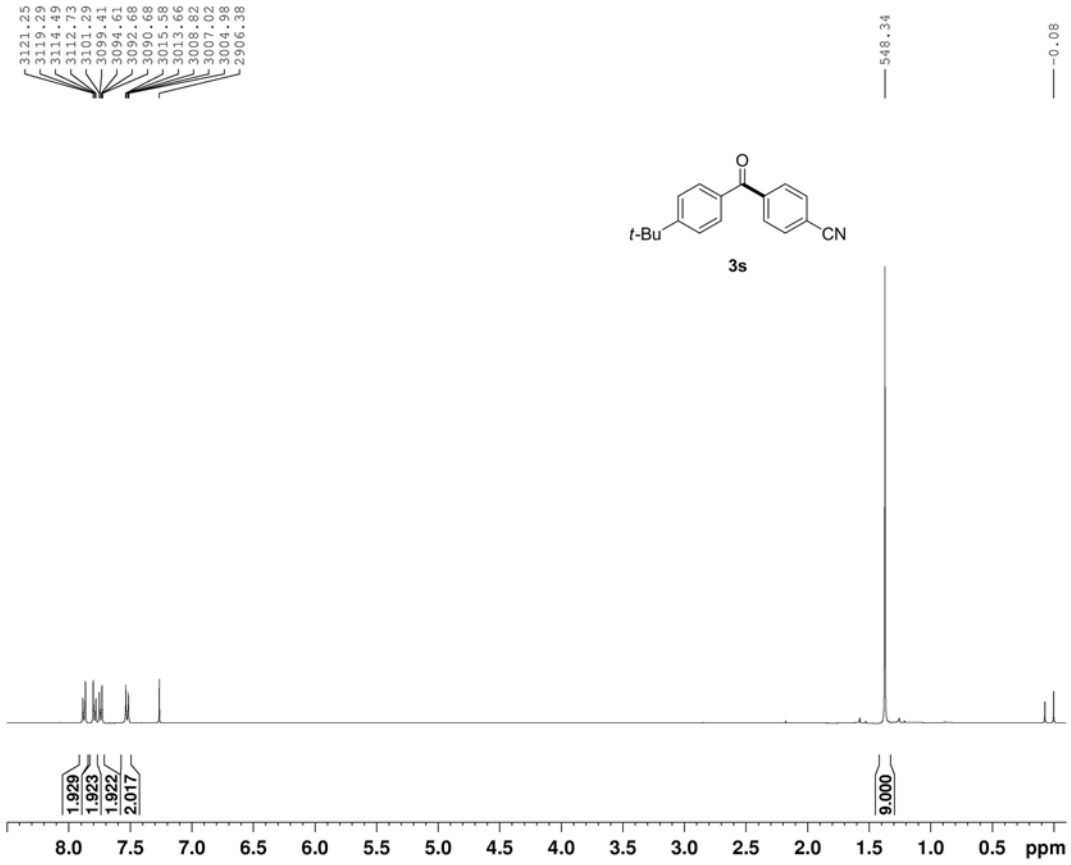

```
Current Data Parameters
NAME                   3r
EXPNO                   2
PROCNO                  1

F2 - Acquisition Parameters
Date_           20140119
Time               19.13
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG           zgpg30
TD                 65536
SOLVENT            CDCl3
NS                  1024
DS                     4
SWH            24038.461 Hz
FIDRES             0.366798 Hz
AQ              1.3631488 sec
RG                 201.85
DW                 20.800 usec
DE                  6.50 usec
TE                 298.0 K
D1              2.00000000 sec
d11             0.03000000 sec
DELTA           1.89999998 sec
TD0                    1
SFO1          100.6228293 MHz
NUC1                  13C
P1                  10.80 usec
PLW1           50.11899948 W
SFO2          400.1316005 MHz
NUC2                   1H
CPDPRG[2           waltz16
PCPD2               90.00 usec
PLW2           12.58899975 W
PLW12           0.34968999 W
PLW13           0.28325000 W

F2 - Processing parameters
SI                  32768
SF            100.6127690 MHz
WDW                    EM
SSB       0
LB                  1.00 Hz
GB        0
PC                  1.40
```



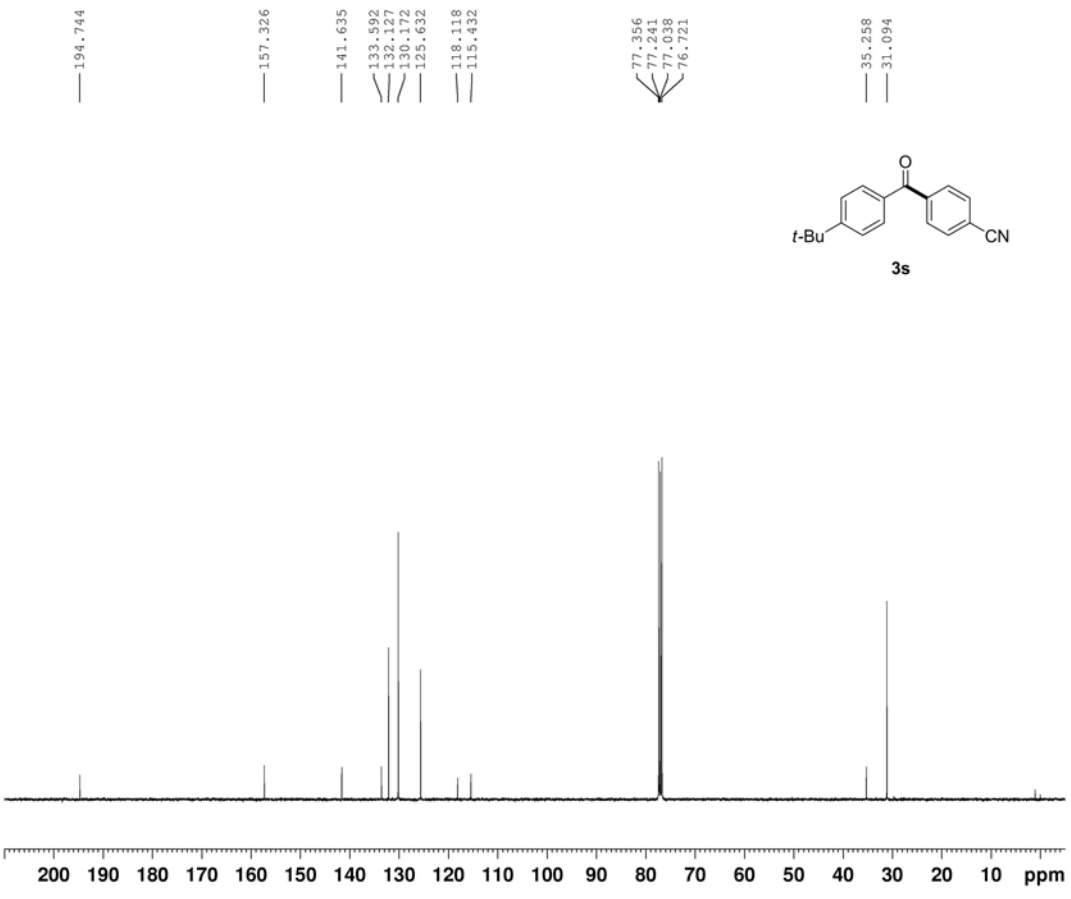

```
Current Data Parameters
NAME                  3s
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20140117
Time               14.01
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH             8012.820 Hz
FIDRES             0.122266 Hz
AQ              4.0894465 sec
RG                123.33
DW                62.400 usec
DE                 6.50 usec
TE                298.0 K
D1             1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                 15.00 usec
PLW1          12.58899975 W
SFO1         400.1316005 MHz

F2 - Processing parameters
SI                131072
SF           400.1300099 MHz
WDW                   EM
SSB       0
LB                 0.30 Hz
GB        0
PC                 1.00
```



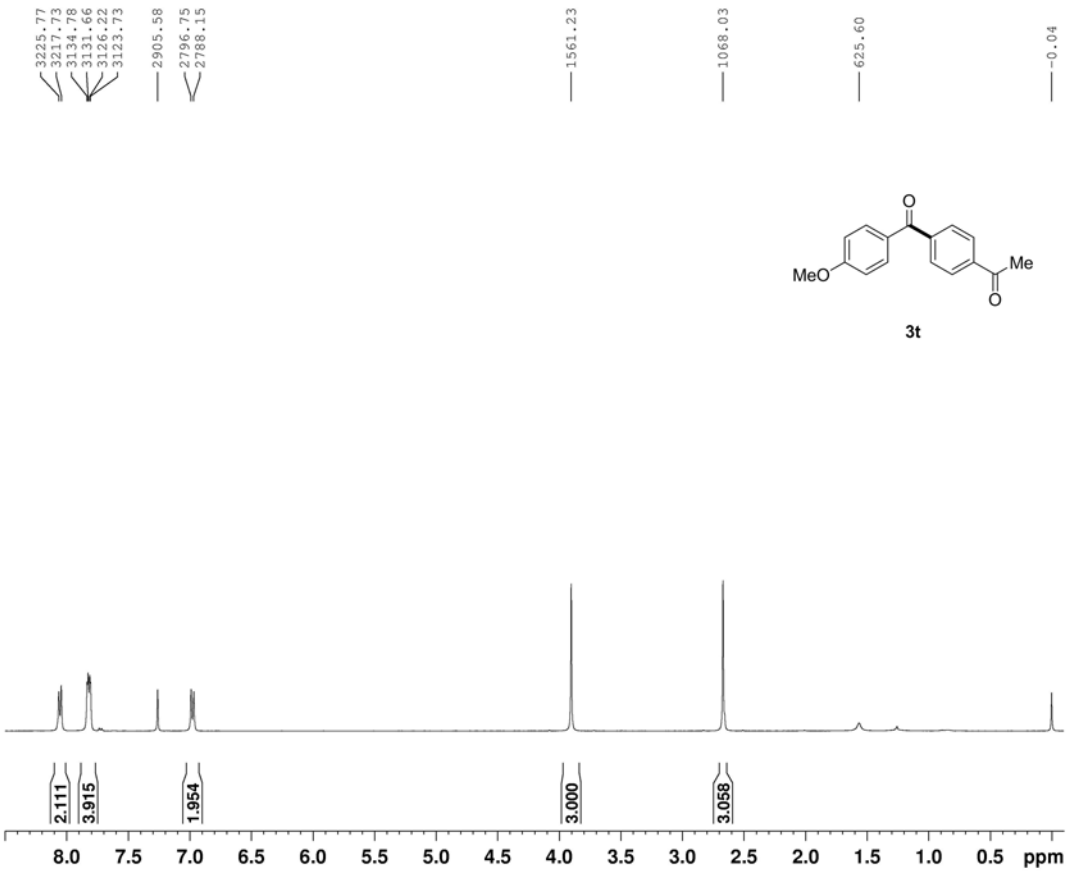

```
Current Data Parameters
NAME                  3s
EXPNO                  2
PROCNO                 1

F2 - Acquisition Parameters
Date_           20140117
Time               20.57
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG           zgpg30
TD                 65536
SOLVENT            CDCl3
NS                  1024
DS                     4
SWH            24038.461 Hz
FIDRES             0.366798 Hz
AQ              1.3631488 sec
RG                201.85
DW                20.800 usec
DE                 6.50 usec
TE                298.0 K
D1             2.00000000 sec
d11            0.03000000 sec
DELTA          1.89999998 sec
TD0                    1
SFO1         100.6228293 MHz
NUC1                  13C
P1                 10.80 usec
PLW1          50.11899948 W
SFO2         400.1316005 MHz
NUC2                  1H
CPDPRG[2          waltz16
PCPD2              90.00 usec
PLW2          12.58899975 W
PLW12          0.34968999 W
PLW13          0.28325000 W

F2 - Processing parameters
SI                 32768
SF           100.6127690 MHz
WDW                   EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
```



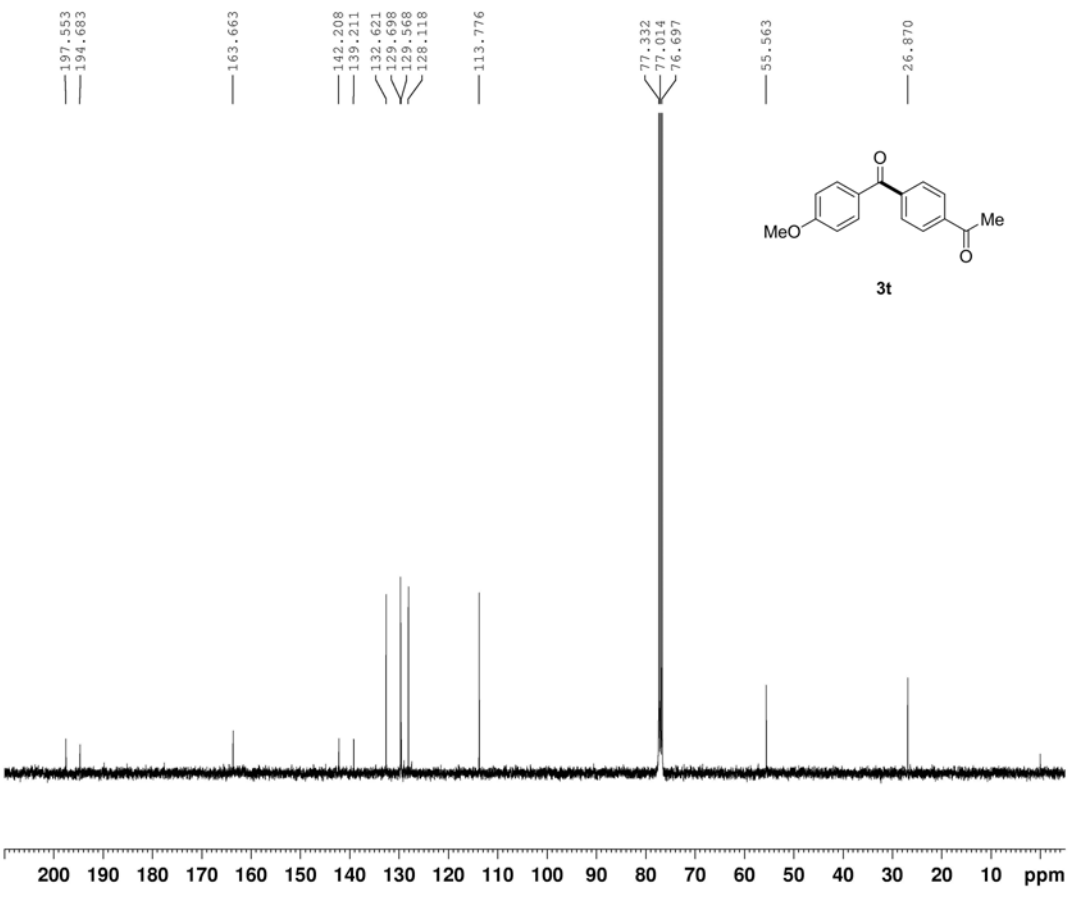

```
Current Data Parameters
NAME                  3t
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20140112
Time               14.38
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH             8223.685 Hz
FIDRES          0.125483 Hz
AQ              3.9845889 sec
RG                127.32
DW                60.800 usec
DE                 6.50 usec
TE                292.5 K
D1             1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                15.00 usec
PLW1         12.60000038 W
SFO1         400.1324710 MHz

F2 - Processing parameters
SI                 65536
SF           400.1300085 MHz
WDW                   EM
SSB       0
LB                0.30 Hz
GB        0
PC                1.00
```



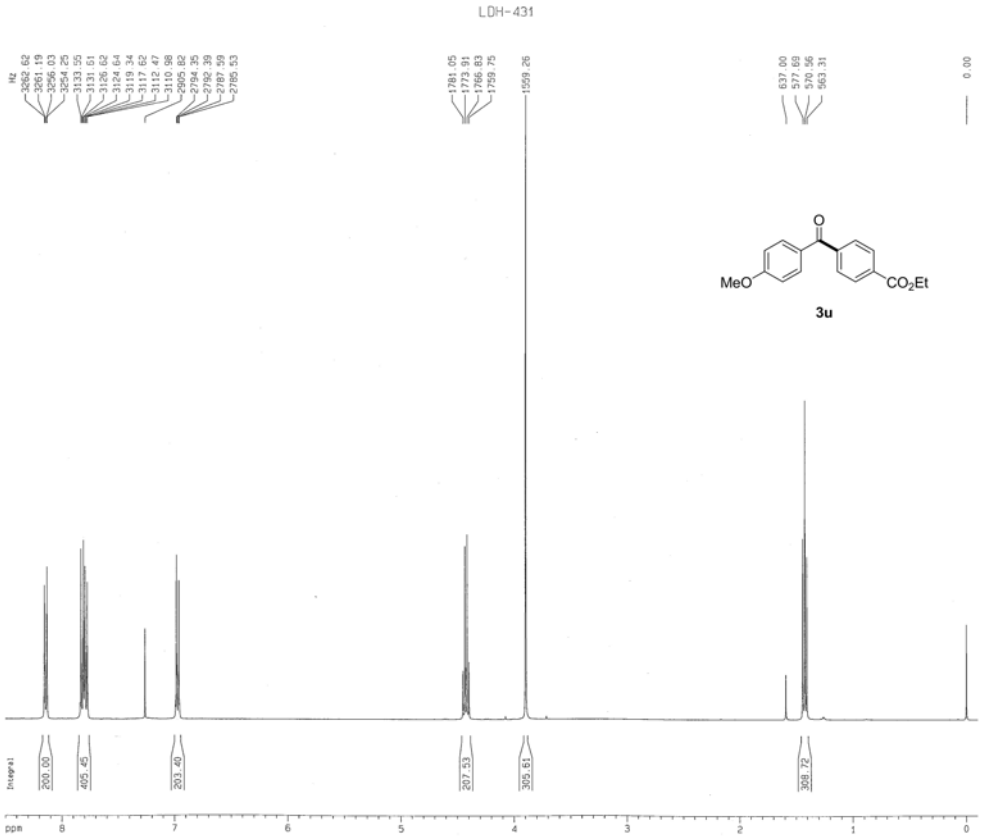

```
Current Data Parameters
NAME                  3t
EXPNO                  2
PROCNO                 1

F2 - Acquisition Parameters
Date_           20140113
Time               0.03
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG           zgpg30
TD                 65536
SOLVENT            CDCl3
NS                  1024
DS                     4
SWH            24038.461 Hz
FIDRES          0.366798 Hz
AQ              1.3631488 sec
RG                186.53
DW                20.800 usec
DE                 6.50 usec
TE                294.2 K
D1             2.00000000 sec
d11            0.03000000 sec
DELTA          1.89999998 sec
TD0                    1
SFO1         100.6228293 MHz
NUC1                  13C
P1                 9.98 usec
PLW1         52.09999847 W
SFO2         400.1316005 MHz
NUC2                  1H
CPDPRG[2          waltz16
PCPD2             90.00 usec
PLW2         12.60000038 W
PLW12         0.34999999 W
PLW13         0.28349999 W

F2 - Processing parameters
SI                 32768
SF           100.6127690 MHz
WDW                   EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.40
```

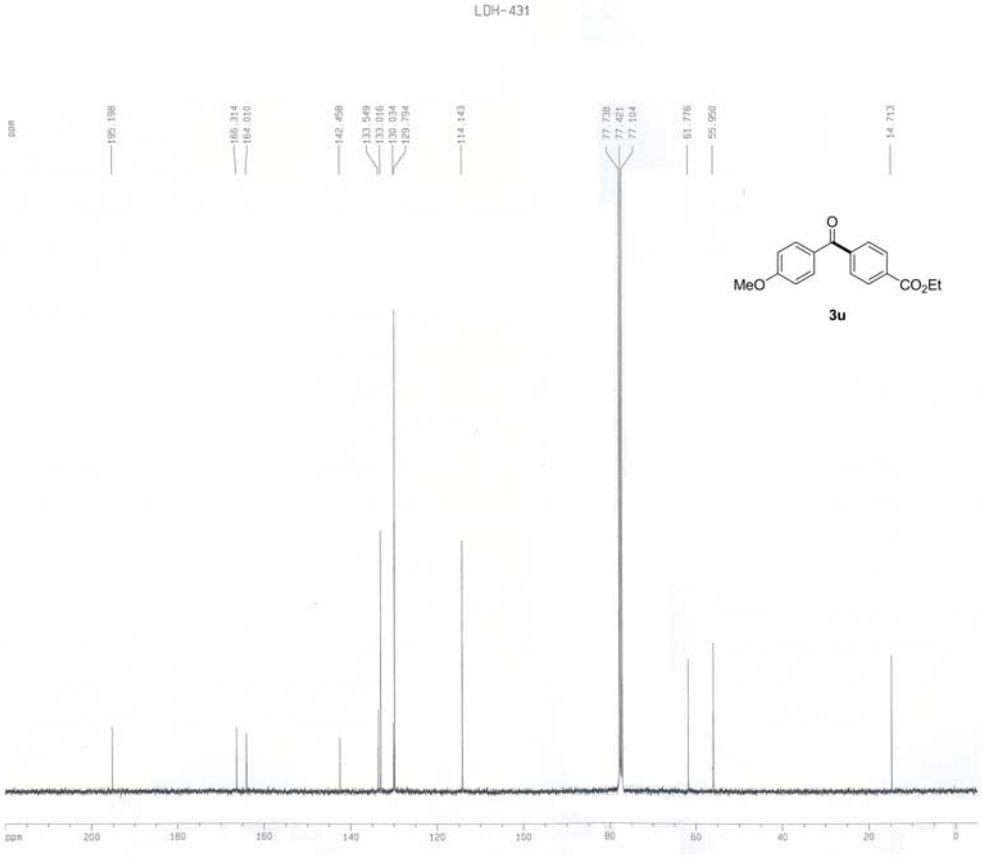


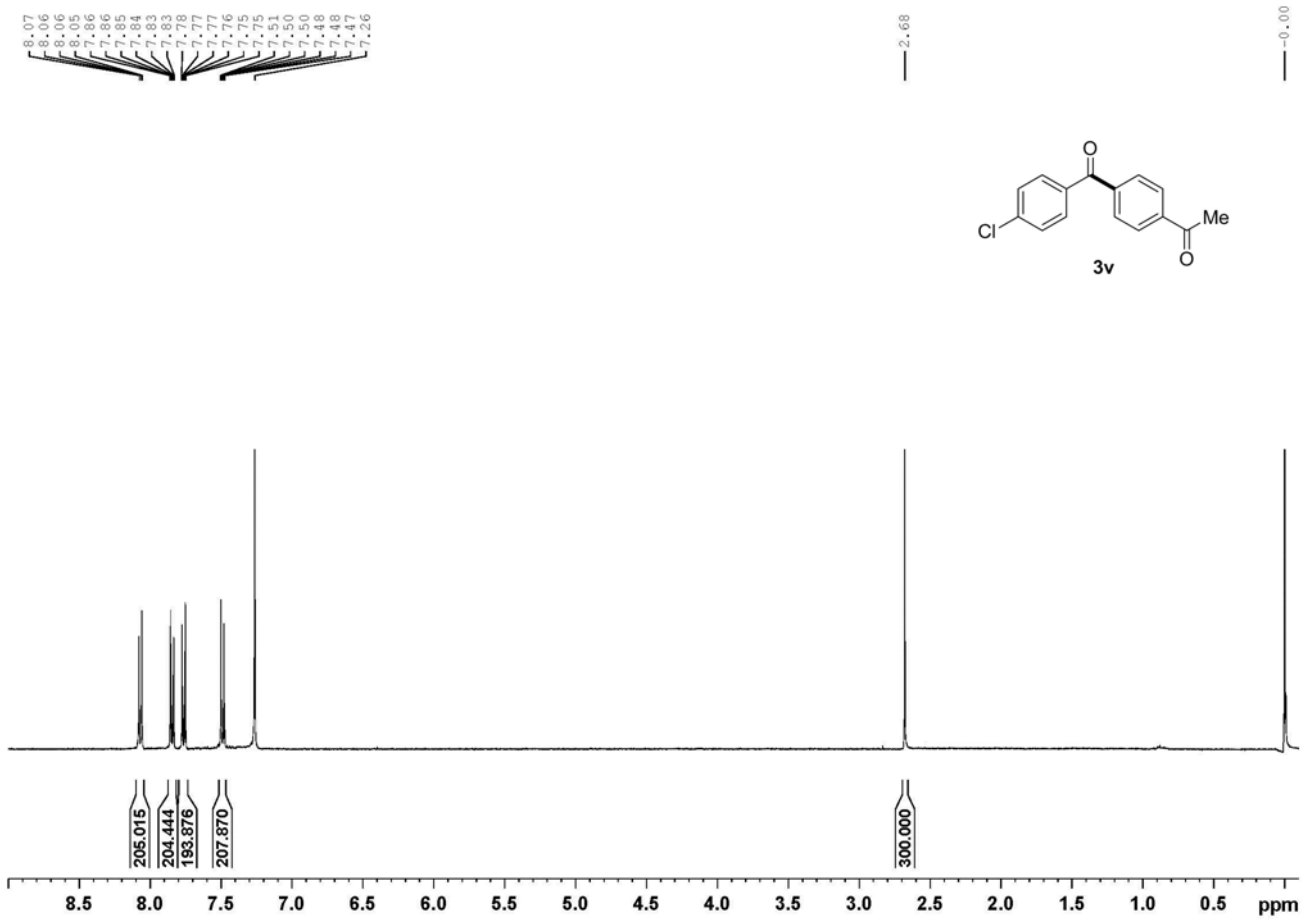

```
Current Data Parameters
NAME                  3u
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20140120
Time               10.52
INSTRUM            spect
PROBHD    5 mm PABBO BB/
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH             8012.820 Hz
FIDRES             0.122266 Hz
AQ              4.0894465 sec
RG                 177.8
DW                62.400 usec
DE                 6.50 usec
TE                298.0 K
D1             1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                   1H
P1                 15.00 usec
PLW1          12.58899975 W
SFO1         400.1316005 MHz

F2 - Processing parameters
SI                131072
SF           400.1300102 MHz
WDW                   EM
SSB       0
LB                0.30 Hz
GB        0
PC                1.00
```

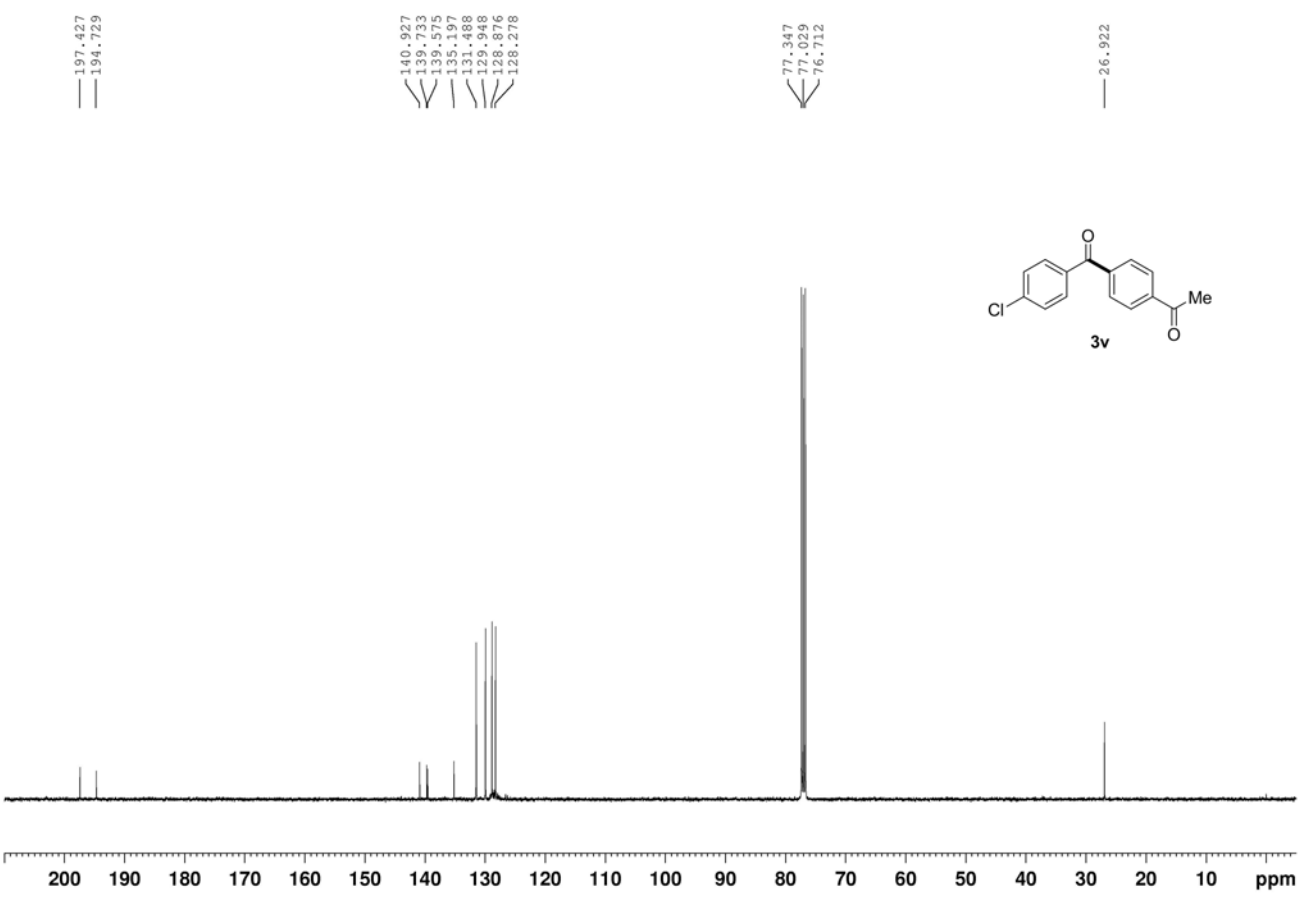



```
Current Data Parameters
NAME                  3u
EXPNO                  2
PROCNO                 1

F2 - Acquisition Parameters
Date_           20140120
Time               13.10
INSTRUM            spect
PROBHD    5 mm PABBO BB/
PULPROG          zgpg30
TD                 65536
SOLVENT            CDCl3
NS                  1024
DS                     4
SWH            24038.461 Hz
FIDRES             0.366798 Hz
AQ              1.3631488 sec
RG                 201.85
DW                20.800 usec
DE                 6.50 usec
TE                298.0 K
D1             2.00000000 sec
d11            0.03000000 sec
DELTA          1.89999998 sec
TD0                    1
SFO1          100.6228293 MHz
NUC1                  13C
P1                10.80 usec
PLW1          50.11899948 W
SFO2         400.1316005 MHz
NUC2                   1H
CPDPRG[2         waltz16
PCPD2             90.00 usec
PLW2          12.58899975 W
PLW12          0.34968999 W
PLW13          0.28325000 W

F2 - Processing parameters
SI                 32768
SF           100.6127690 MHz
WDW                   EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.40
```


LDH-431
Hz
3262.62
3261.19
3256.03
3244.25
3133.55
3131.61
3126.62
3124.64
3119.34
3117.62
3112.47
3110.98
2805.82
2794.35
2792.39
2787.59
2785.53
1781.05
1773.91
1766.83
1759.75
1559.26
637.00
577.68
570.56
563.31
0.00
MeO
CO2Et
3u
Current Data Parameters
NAME jan-12
EXPNO 15
PROCNO 1
F2 - Acquisition Parameters
Date_ 20120109
Time 21.22
INSTRUM spect
PROBHD 5 mm Dual 13C/
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 32
DS 0
SWH 8223.685 Hz
FIDRES 0.250967 Hz
AQ 1.9923444 sec
RG 287.4
DW 60.800 usec
DE 6.00 usec
TE 298.2 K
D1 1.00000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 11.00 usec
PL1 -2.00 dB
SFO1 400.1324710 MHz
F2 - Processing parameters
SI 16384
SF 400.1300084 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
1D NMR plot parameters
CX 30.00 cm
CY 20.00 cm
F1P 8.500 ppm
F1 3401.10 Hz
F2P -0.100 ppm
F2 -40.01 Hz
PPMCM 0.28667 ppm/cm
HZCM 114.70393 Hz/cm
Integral
200.00
405.45
203.40
207.53
305.61
308.72
ppm
8
7
6
5
4
3
2
1
0


LDH-431
ppm
195.198
166.314
164.010
142.458
133.549
133.016
130.034
129.794
114.143
77.738
77.421
77.104
61.776
55.960
14.713
MeO
CO2Et
3u
Current Data Parameters
NAME jan-12
EXPNO 16
PROCNO 1
F2 - Acquisition Parameters
Date_ 20120109
Time 23.11
INSTRUM spect
PROBHD 5 mm Dual 13C/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 2048
DS 2
SWH 31847.133 Hz
FIDRES 0.485949 Hz
AQ 1.0289652 sec
RG 3649.1
DW 15.700 usec
DE 6.00 usec
TE 298.2 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 10.50 usec
PL1 -1.00 dB
SFO1 100.6254358 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 105.00 usec
PL2 -2.00 dB
PL12 18.00 dB
PL13 20.00 dB
SFO2 400.1324708 MHz
F2 - Processing parameters
SI 32768
SF 100.6127290 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
1D NMR plot parameters
CX 30.00 cm
CY 23.00 cm
F1P 220.000 ppm
F1 22134.80 Hz
F2P -5.000 ppm
F2 -503.06 Hz
PPMCM 7.50000 ppm/cm
HZCM 754.59546 Hz/cm
ppm
200
180
160
140
120
100
80
60
40
20
0


8.07
8.06
8.06
8.05
7.86
7.86
7.85
7.84
7.83
7.83
7.78
7.77
7.77
7.77
7.76
7.75
7.75
7.51
7.50
7.50
7.48
7.48
7.47
7.26
2.68
0.00
Cl
O
Me
O
3v
205.015
204.444
193.876
207.870
300.000
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
ppm


197.427
194.729
140.927
139.733
139.575
135.197
131.488
129.948
128.876
128.278
77.347
77.029
76.712
26.922
Cl
O
Me
O
3v
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm