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Supporting Information

Nickel-Catalyzed Cross-Coupling of Epoxides with Aryltriflates: Rapid and Regioselective Construction of Aryl Ketones

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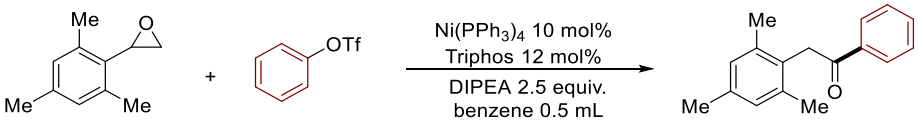
Table of Contents

1. General Information

Unless noted otherwise, all solvents were dried by filtration through a Pure–Solv MD–5 Solvent Purification System (Innovative Technology). Reaction temperatures were reported as the temperatures of the bath surrounding the flasks or cylindrical pressure vessel. Sensitive reagents and solvents were transferred under nitrogen into a nitrogen–filled glovebox with standard techniques. Analytical thin–layer chromatography (TLC) was carried out using 0.2 mm commercial silica gel plates (silica gel 60, F254, Leyan chemical). Cylindrical pressure vessel (26 x 109 mm (15 mL) with PTFE lined cap attached) were purchased from Synthware. Nuclear magnetic resonance spectra (^{1}H NMR, ^{13}C NMR and ^{19}F NMR) were recorded with a Bruker Model DMX 500 (500 MHz, ^{1}H at 500 MHz, ^{13}C at 126 MHz,). Chemical shifts were reported in parts per million (ppm, δ), downfield from tetramethylsilane (TMS, δ=0.00ppm) and were referenced to residual solvent ($CDCl_3$, δ=7.26 ppm (^{1}H) and 77.00 ppm (^{13}C)). All the ^{19}F chemical shifts were not referenced. Coupling constants were reported in Hertz (Hz). Data for ^{1}H NMR spectra were reported as follows: chemical shift (ppm, referenced to protium, s = singlet, d = doublet, t = triplet, q = quartet, dd = doublet of doublets, td = triplet of doublets, ddd = doublet of doublet of doublets, m = multiplet, coupling constant (Hz), and integration). All other materials were obtained from Rhawn Corporation, Aladdin Bio–Chem Technology or Energy chemical and were used as received.

2. The screening of different reaction conditions.

The screening of different nickel precursors.

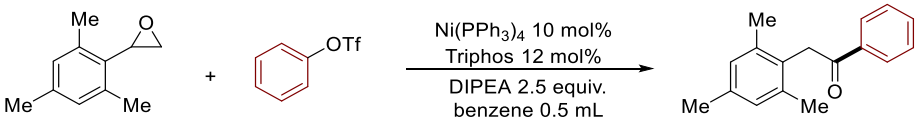


1.0 equiv.
0.1 mmol

2.0 equiv.

entry	variation	yield (%)
1	none	90
2	$Ni(cod)_2$ instead of $Ni(PPh_3)_4$	14
3	$Ni(OTf)_2$ instead of $Ni(PPh_3)_4$	29
4	$Ni(acac)_2$ instead of $Ni(PPh_3)_4$	6
5	5 mol% $Ni(PPh_3)_4$ and 6 mol% Triphos instead of 10 mol% $Ni(PPh_3)_4$ and 12 mol% Triphos	13
6	without nickel catalyst	trace

The screening of different base.



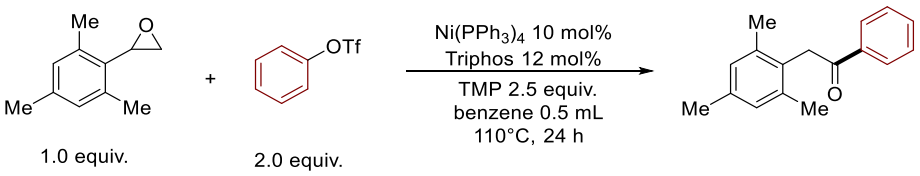
1.0 equiv.
0.1 mmol

2.0 equiv.

entry	variation	yield (%)

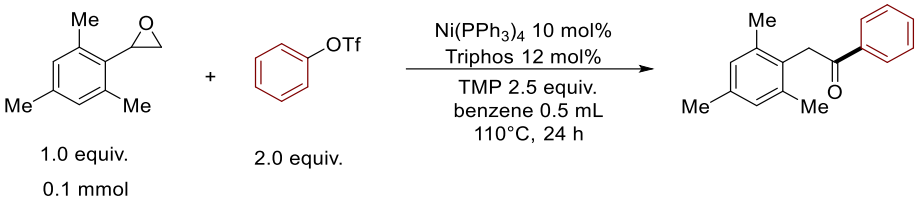
1	none	90
2	TMP instead of DIPEA	**92**
3	Et_3N instead of DIPEA	89
4	dipropylamine instead of DIPEA	13
5	4-methyipiperdine instead of DIPEA	85
6	K_2CO_3 instead of DIPEA	85
7	DBU instead of DIPEA	trace
8	Ag_2CO_3 instead of DIPEA	trace
9	Cs_2CO_3 instead of DIPEA	trace
10	DABCO instead of DIPEA	trace
11	Na^tOBu instead of DIPEA	trace
12	1.0 equiv. TMP instead of 2.5 equiv. TMP	84
13	1.5 equiv. TMP instead of 2.5 equiv. TMP	85
14	2.0 equiv. TMP instead of 2.5 equiv. TMP	87
15	without base	7

The screening of different liagnds.



entry	variation	yield (%)
1	none	92
2	Bis(2-diphenylphosphinoethyl)phenylphosphine instead of Triphos	11
3	Sphos instead of Triphos	trace
4	Davephos instead of Triphos	trace
5	dppp instead of Triphos	14
6	IPr instead of Triphos	trace
7	PCy_3 instead of Triphos	trace
8	Sphos instead of Triphos	trace
9	IMes instead of Triphos	trace
10	dppe instead of Triphos	6
11	Amphos instead of Triphos	trace
12	without ligand	trace

The screening of other reaction conditions.



entry	variation	yield (%)
1	none	92
2	1.0 equiv. B instead of 2.0 equiv. B	43
3	toluene instead of benzene	84
4	1,3,5-trimethylbenzene instead of benzene	77
5	THF instead of benzene	61
6	DMA instead of benzene	trace
7	NMP instead of benzene	trace
8	DMF instead of benzene	21
9	r.t. instead of 110 ˚C	trace
10	70 ˚C instead of 110 ˚C	trace
11	100 ˚C instead of 110 ˚C	88
12	120 ˚C instead of 110 ˚C	84

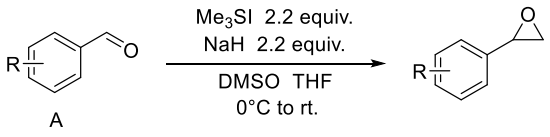
3. General procedure for substrates synthesis

General procedure for triflate derivatives synthesis. Aryl triflates were prepared according to previous literature procedures. [1]

General procedure for epoxide derivatives synthesis.

Synthesis of compound 1a-1o (procedure A)

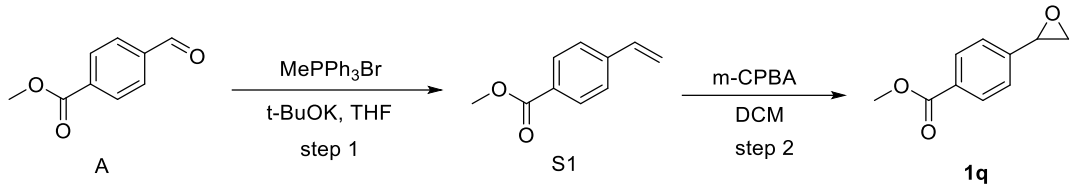
A solution of NaH (33 mol, 2.2 equiv.) and Me_3SI (33 mol, 2.2 equiv.) in DMSO (23 mL) and THF (17 mL) stirred for 30 min at room temperature in a 200mL flask under N_2 atmosphere. Then a solution of A (15 mmol, 1.0 equiv.) in THF was added dropwise at 0 ˚C. After complete addition, the mixture was warmed to room temperature and allowed to stir for 12 hours. The mixture was quenched with sat. NH_4Cl and diluted with EtOAc. Then the mixture was separated and the aqueous layer was back-extracted with EtOAc. The organic layer was washed with brine and dried over Na_2SO_4. The solvent was removed under reduced pressure and the residue was purified by column chromatography with Et_3N to give the desired epoxides.



Synthesis of compound 1p (procedure B)

1p was prepared according to previous literature procedures. [2]

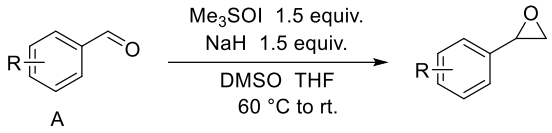
Synthesis of compound 1q (procedure C)



Step 1: To a solution of methyltriphenylphosphonium bromide (30 mmol) in dry THF (25 mL) was added potassium tertiary-butoxide (20 mmol) at 0 °C under N_2 atmosphere. The reaction mixture was stirred for 30 min at room temperature, after which the solution was cooled to 0 °C and the aldehyde A(10 mmol) was added dropwise to it as a solution in dry THF (5 mL). The reaction mixture was further stirred at room temperature for overnight. Upon dilution with diethyl ether, the reaction mixture was poured into ice-water and extracted twice. The combined organic layers were dried over anhydrous Na_2SO_4 and evaporated under reduced pressure. The crude product was purified by silica gel column chromatography (eluent: Petroleum ether : EtOAc).

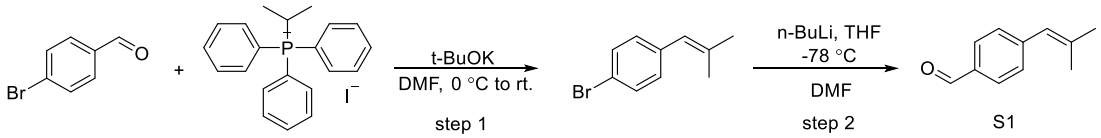
Step 2: To a solution of S1(5 mmol, 1 equiv.) in DCM (15 mL) was added *m*-CPBA(10 mmol, 2 equiv.) in portions at 0 °C and the mixture was stirred for 12 hours until the starting materiel was fully consumed by TLC. The reaction was quenched with saturated aqueous $NaHCO_3$ and extracted three times with DCM. The combined organic layers were washed with water, saturated aqueous $NaHCO_3$, then brine, dried with $MgSO_4$, filtered, and concentrated under reduced pressure, then it was purified by column chromatography with Et_3N to give the desired epoxides.

Synthesis of compound 1r, 1t-1y (procedure D)

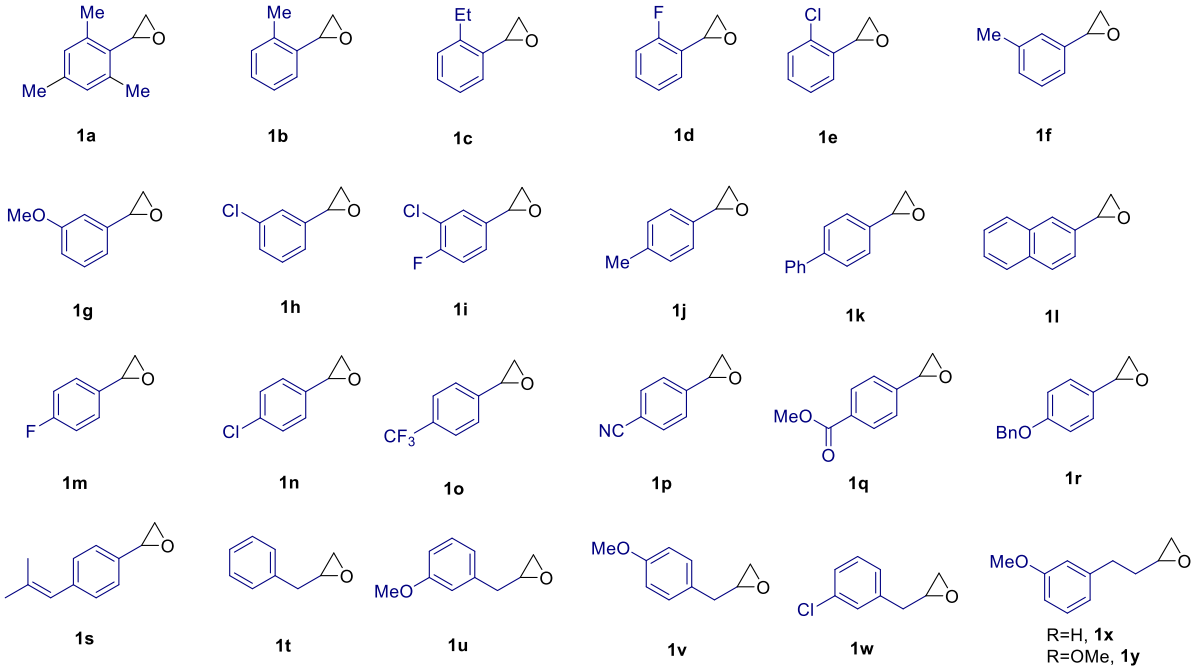


A solution of NaH (15 mol, 1.5 equiv.) and Me_3SOI (15 mol, 1.5 equiv.) in DMSO (15 mL) and THF (10 mL) stirred for 30 min at 60 ˚C in a 200mL flask under N_2 atmosphere. Then a solution of A (10 mmol, 1.0 equiv.) in THF was added dropwise at room temperature and allowed to stir for 12 hours. After complete addition, the mixture was quenched with sat. NH_4Cl and diluted with EtOAc. Then the mixture was separated and the aqueous layer was back-extracted with EtOAc. The organic layer was washed with brine and dried over Na_2SO_4. The solvent was removed under reduced pressure and the residue was purified by column chromatography with Et_3N to give the desired epoxides.

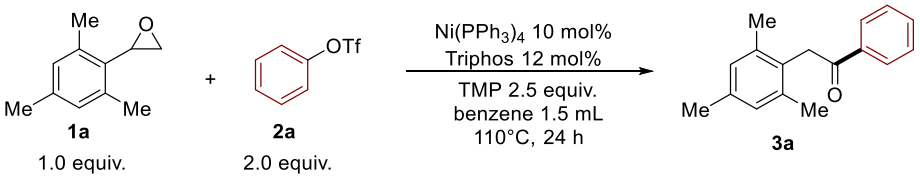
Synthesis of compound 1s (procedure E)



S1 was prepared according to previous literature procedures,[3] and then **1s** prepared according to procedure D.

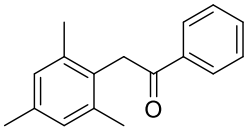


4. General procedures for the nickel–catalyzed cross–coupling reactions

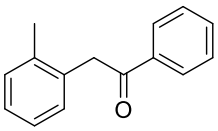


A flame–dried 15 mL cylindrical pressure vessel was charged with 2-mesityloxirane **1a** (0.3 mmol, 1.0 equiv.) and phenyl trifluoromethanesulfonate **2a** (0.6 mmol, 2.0 equiv.). The cylindrical pressure vessel was directly transferred into a nitrogen-filled glovebox without caps. Then, $Ni(PPh_3)_4$ (33.2 mg, 0.03 mmol, 10 mol%), Triphos (22.5 mg, 0.036 mmol, 12 mol%), TMP (105.9 mg, 0.75 mmol, 2.5 equiv.) and 1.5 mL dry benzene were added. Then the cylindrical pressure vessel was tightly sealed, transferred out of the glovebox and stirred at 110 °C or 130 °C with corresponding reaction time. After the completion of the reaction, the solvent was removed in vacuo and the residue was purified by flash column chromatography on silica gel to give the desired ketone product **3a**.

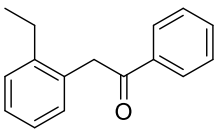
5. Characterization data for the products



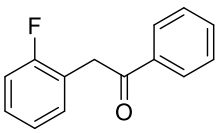
3a (CAS: 5350-76-5): ^{1}**H NMR** (500 MHz, $CDCl_3$) δ 8.12 – 8.02 (m, 2H), 7.63 – 7.53 (m, 1H), 7.47 – 7.51 (m, 2H), 6.89 (s, 2H), 4.33 (s, 2H), 2.28 (s, 3H), 2.18 (s, 6H). ^{13}**C NMR** (126 MHz, $CDCl_3$) δ 197.2, 137.2, 136.9, 136.4, 133.2, 129.3, 128.9, 128.7, 128.1, 39.4, 21.0, 20.4. All spectral data was in accord with the literature.[7]



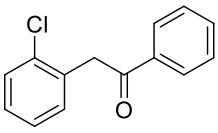
3b (CAS: 6332-83-8): ^{1}**H NMR** (500 MHz, $CDCl_3$) δ 8.09 – 8.03 (m, 2H), 7.64 – 7.58 (m, 1H), 7.54 – 7.59 (m, 2H), 7.30 – 7.22 (m, 2H), 7.21 – 7.13 (m, 2H), 4.34 (s, 2H), 2.30 (s, 3H). ^{13}**C NMR** (126 MHz, $CDCl_3$) δ 197.5, 136.9, 133.5, 133.2, 130.4, 130.3, 128.7, 128.36, 127.3, 126.1, 43.5, 19.8. All spectral data was in accord with the literature.[9]



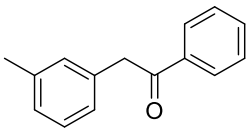
3c (CAS: 133145-62-7):^{1}**H NMR** (500 MHz, $CDCl_3$) δ 8.09-8.04 (m, 2H), 7.64 – 7.58 (m, 1H), 7.54 – 7.48 (m 2H), 7.31 – 7.25 (m, 2H), 7.24 – 7.17 (m, 1H), 7.15 (d, J = 7.4 Hz, 1H), 4.37 (s, 2H), 2.64 (q, J = 7.5 Hz, 2H), 1.24 (t, J = 7.5 Hz, 3H). ^{13}**C NMR** (126 MHz, $CDCl_3$) δ 197.8, 142.6, 136.9, 133.2, 132.7, 130.6, 128.7, 128.5, 128.4, 127.4, 126.0, 42.9, 26.0, 14.8. All spectral data was in accord with the literature.[13]



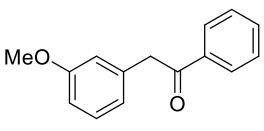
3d (CAS: 3826-47-9):^{1}**H NMR** (500 MHz, $CDCl_3$) δ 8.10 – 8.03 (m, 2H), 7.64 – 7.58 (m, 1H), 7.53 – 7.43 (m, 2H), 7.34 – 7.02 (m, 5H), 4.36 (s, 2H). ^{13}**C NMR** (126 MHz, $CDCl_3$) δ 196.3, 161.0 (d, J = 246.1 Hz), 136.4, 133.3, 131.7(d, J = 4.5 Hz), 128.9 (d, J = 8.3 Hz), 128.7, 128.4, 124.2(d, J = 3.7 Hz), 121.9 (d, J = 16.2 Hz), 115.4(d, J = 22.0 Hz), 38.6. ^{19}**F NMR** (471 MHz, $CDCl_3$) δ -117.14. All spectral data was in accord with the literature.[10]



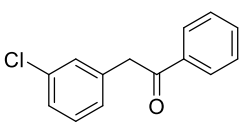
3e (CAS: 57479-60-4): ^{1}**H NMR** (500 MHz, $CDCl_3$) δ 8.09-8.03 (m, 2H), 7.64 – 7.60 (m, 1H), 7.54 – 7.49 (m, 2H), 7.50-7.43 (m, 1H), 7.28-7.24 (m, 3H), 4.47 (s, 2H). ^{13}**C NMR** (126 MHz, $CDCl_3$) δ 196.4, 136.6, 134.5, 133.3, 133.2, 131.7, 129.5, 128.7, 128.6, 128.4, 126.9, 43.2. All spectral data was in accord with the literature.[10]



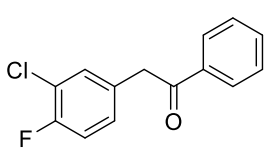
3f (CAS: 34403-03-7): ^{1}**H NMR** (500 MHz, $CDCl_3$) δ 8.09 – 8.03 (m, 2H), 7.62 – 7.55 (m, 1H), 7.52 – 7.46 (m, 2H), 7.30 – 7.22 (m, 1H), 7.12 (dd, J = 9.3, 6.2 Hz, 3H), 4.28 (s, 2H), 2.37 (s, 3H). ^{13}**C NMR** (126 MHz, $CDCl_3$) δ 197.8, 138.3, 136.7, 134.5, 133.2, 130.2, 128.7, 128.6, 127.7, 126.5, 45.5, 21.4. All spectral data was in accord with the literature.[8]



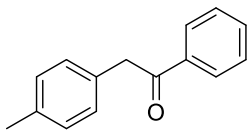
3g (CAS: 29955-26-8): ^{1}**H NMR** (500 MHz, $CDCl_3$) δ 8.08 – 8.00 (m, 2H), 7.60 – 7.56 (m, 1H), 7.50 – 7.45 (m, 2H), 7.29 – 7.25 (m, 1H), 6.89 (d, J = 7.8 Hz, 1H), 6.87 – 6.79 (m, 2H), 4.28 (s, 2H), 3.81 (s, 3H). ^{13}**C NMR** (126 MHz, $CDCl_3$) δ 197.5, 159.8, 136.6, 136.0, 133.2, 129.7, 128.7, 121.8, 115.1, 112.4, 55.2, 45.6. All spectral data was in accord with the literature.[11]



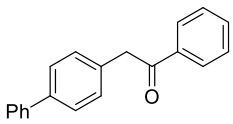
3h (CAS: 27798-43-2): ^{1}**H NMR** (500 MHz, $CDCl_3$) δ 8.06 – 7.99 (m, 2H), 7.64 – 7.57 (m, 1H), 7.53 – 7.47 (m, 2H), 7.34 – 7.22 (m, 3H), 7.20-7.15 (m, 1H), 4.29 (s, 2H). ^{13}**C NMR** (126 MHz, $CDCl_3$) δ 196.8, 136.4, 136.4, 134.4, 133.4, 129.9, 129.7, 128.8, 128.6, 127.8, 127.2, 44.9. All spectral data was in accord with the literature.[10]



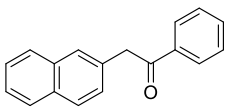
3i (CAS: 1914649-83-4): ^{1}**H NMR** (500 MHz, $CDCl_3$) δ 8.07 – 7.97 (m, 2H), 7.68 – 7.58 (m, 1H), 7.54 – 7.48(m, 2H), 7.33 (dd, *J* = 7.0, 2.0 Hz, 1H), 7.28 – 7.04 (m, 2H), 4.27 (s, 2H). ^{13}**C NMR** (126 MHz, $CDCl_3$) δ 196.7, 157.3 (d, *J* = 248.2 Hz), 136.3, 133.5, 131.7, 131.4 (d, *J* = 3.9 Hz), 129.3 (d, *J* = 7.2 Hz), 128.8, 128.5, 116.7 (d, *J* = 21.2 Hz), 44.1. ^{19}**F NMR** (471 MHz, $CDCl_3$) δ -118.2. All spectral data was in accord with the literature.[8]



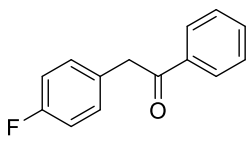
3j (CAS: 2430-99-1): ^{1}**H NMR** (500 MHz, $CDCl_3$) δ 8.10 – 8.00 (m, 2H), 7.62 – 7.54 (m, 1H), 7.51 – 7.46 (m, 2H), 7.31 – 7.15 (m, 4H), 4.28 (s, 2H), 2.36 (s, 3H). ^{13}**C NMR** (126 MHz, $CDCl_3$) δ 197.9, 136.7, 136.5, 133.1, 131.5, 129.4, 129.3, 128.7, 45.2, 21.1. All spectral data was in accord with the literature.[9]



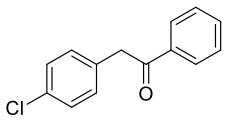
3k (CAS: 27644-00-4): ^{1}**H NMR** (500 MHz, $CDCl_3$) δ 8.11-8.07 (m, 2H), 7.59 – 7.50 (m, 5H), 7.47 – 7.40 (m, 4H), 7.38-7.30 (m, 3H), 4.31 (s, 2H). ^{13}**C NMR** (126 MHz, $CDCl_3$) δ 197.6, 140.7, 139.9, 136.7, 133.6, 133.3, 130.0, 128.8, 128.7, 128.7, 127.5, 127.3, 127.1, 45.2. All spectral data was in accord with the literature.[8]



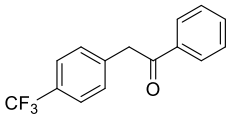
3l (CAS: 83015-77-4): ^{1}**H NMR** (500 MHz, $CDCl_3$) δ 8.09 – 7.98 (m, 2H), 7.81-7.76(m, 3H), 7.70 (s, 1H), 7.55 – 7.49 (m, 1H), 7.47 – 7.39 (m, 4H), 7.46 – 7.28 (m, 1H), 4.42 (s, 2H). ^{13}**C NMR** (126 MHz, $CDCl_3$) δ 197.7, 136.6, 133.6, 133.3, 132.4, 132.2, 128.7, 128.7, 128.4, 128.2, 127.7, 127.7, 127.6, 126.2, 125.8, 45.7. All spectral data was in accord with the literature.[9]



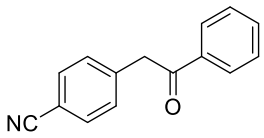
3m (CAS: 347-91-1): ^{1}**H NMR** (500 MHz, $CDCl_3$) δ 8.05-8.01 (m, 2H), 7.64 – 7.56 (m, 1H), 7.52 – 7.47 (m, 2H), 7.29 – 7.25 (m, 1H), 7.25 – 7.23 (m, 1H), 7.10 – 7.01 (m, 2H), 4.29 (s, 2H). ^{13}**C NMR** (126 MHz, $CDCl_3$) δ 197.4, 161.9 (d, *J* = 245.4 Hz), 136.5, 133.3, 131.1 (d, *J* = 8.0 Hz), 130.2 (d, *J* = 2.9 Hz), 128.7, 115.5 (d, *J* = 21.2 Hz), 115.4, 44.5. ^{19}**F NMR** (471 MHz, $CDCl_3$) δ -116.1. All spectral data was in accord with the literature.[8]



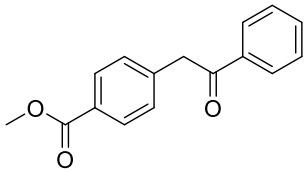
3n (CAS: 6332-83-8): ^{1}**H NMR** (500 MHz, $CDCl_3$) δ 8.13 – 7.93 (m, 2H), 7.63 – 7.57 (m, 1H), 7.52 – 7.47(m, 2H), 7.36 – 7.30 (m, 2H), 7.26 – 7.16 (m, 2H), 4.29 (s, 2H). ^{13}**C NMR** (126 MHz, $CDCl_3$) δ 197.1, 136.4, 133.4, 132.9, 132.9, 130.9, 128.8, 128.7, 128.5, 44.7. All spectral data was in accord with the literature.[10]



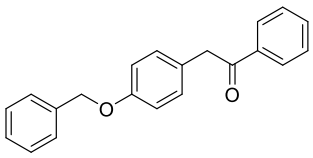
3o (CAS: 30934-68-0): ^{1}**H NMR** (500 MHz, $CDCl_3$) δ 8.09 – 7.98 (m, 2H), 7.68 – 7.58 (m, 3H), 7.53 – 7.49 (m, 2H), 7.36 – 7.43(m, 2H), 4.38 (s, 2H). ^{13}**C NMR** (126 MHz, $CDCl_3$) δ 196.7, 138.5, 136.4, 130.0, 129.3 (q, *J* = 32.4 Hz), 128.8, 128.5, 125.6 (q, *J* = 3.7 Hz), 124.2 (q, *J* = 270.4 Hz), 45.1. ^{19}**F NMR** (471 MHz, $CDCl_3$) δ -62.5. All spectral data was in accord with the literature.[8]



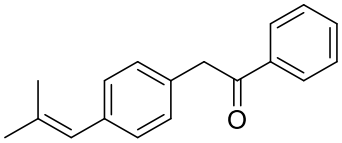
3p (CAS: 59824-23-6): ^{1}**H NMR** (500 MHz, $CDCl_3$) δ 8.08 – 7.98 (m, 1H), 7.64 (t, *J* = 7.8 Hz, 2H), 7.52 (t, *J* = 7.7 Hz, 1H), 7.40 (d, *J* = 8.0 Hz, 1H), 4.39 (s, 1H). ^{13}**C NMR** (126 MHz, $CDCl_3$) δ 196.14, 139.98, 136.22, 133.69, 132.34, 130.54, 128.87, 128.46, 118.80, 110.99, 45.22, 29.72. All spectral data was in accord with the literature.[11]



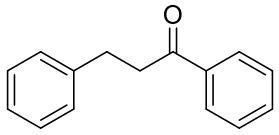
3q (CAS: 94161-45-2): **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.00 (d, *J* = 7.8 Hz, 4H), 7.57 (t, *J* = 7.4 Hz, 1H), 7.46 (t, *J* = 7.6 Hz, 2H), 7.33 (d, *J* = 7.9 Hz, 2H), 4.34 (s, 2H), 3.89 (s, 3H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 196.80, 166.90, 139.84, 136.41, 133.43, 129.93, 129.65, 128.87, 128.76, 128.55, 52.09, 45.38. All spectral data was in accord with the literature.[8]



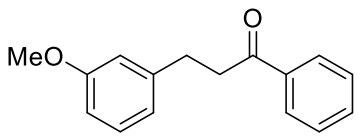
3r **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.05 – 7.95 (m, 2H), 7.54 (t, *J* = 7.4 Hz, 1H), 7.48 – 7.39 (m, 4H), 7.37 (t, *J* = 7.6 Hz, 2H), 7.33 – 7.29 (m, 1H), 7.18 (d, *J* = 8.6 Hz, 2H), 6.93 (d, *J* = 8.6 Hz, 2H), 5.03 (s, 2H), 4.22 (s, 2H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 197.92, 157.83, 137.05, 136.65, 133.13, 130.53, 128.65, 128.62, 128.60, 127.97, 127.50, 126.82, 115.11, 70.05, 44.65. **HRMS** (ESI): Calculated for $C_{21}H_{19}O_2$ ($M + H^+$): 303.1380, found: 303.1385.



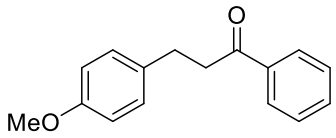
3s (CAS: 934236-52-9): **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.06 – 7.99 (m, 2H), 7.58 – 7.53 (m, 1H), 7.48 – 7.42 (m, 2H), 7.20 (q, *J* = 8.3 Hz, 4H), 6.22 (t, *J* = 1.8 Hz, 1H), 4.26 (s, 2H), 1.89 (d, *J* = 1.4 Hz, 3H), 1.85 (d, *J* = 1.3 Hz, 3H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 197.75, 137.35, 136.68, 135.54, 133.13, 131.88, 129.13, 129.03, 128.66, 124.73, 45.23, 26.92, 19.43. All spectral data was in accord with the literature.[12]



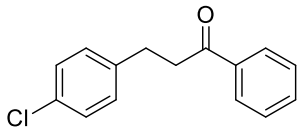
3t (CAS: 1083-30-3): **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.07 – 7.96 (m, 2H), 7.64 – 7.57 (m, 1H), 7.51 (dd, *J* = 8.4, 7.1 Hz, 2H), 7.40 – 7.32 (m, 4H), 7.30 – 7.26 (m, 1H), 3.35 (t, *J* = 7.7 Hz, 2H), 3.14 (t, *J* = 7.7 Hz, 2H).**^{13}C NMR** (126 MHz, $CDCl_3$) δ 199.0, 141.2, 136.7, 132.9, 128.5, 128.4, 128.3, 128.3, 127.9, 126.0, 40.3, 30.0. All spectral data was in accord with the literature.[14]



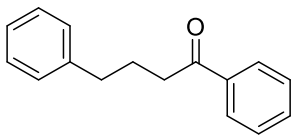
3u (CAS: 15101-68-5): **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.96 (d, *J* = 7.0 Hz, 2H), 7.56 (d, *J* = 14.8 Hz, 1H), 7.46 (t, *J* = 7.6 Hz, 2H), 7.22 (t, *J* = 7.8 Hz, 1H), 6.85 (d, *J* = 7.5 Hz, 1H), 6.80 (s, 1H), 6.76 (dd, *J* = 8.2, 2.5 Hz, 1H), 3.80 (s, 3H), 3.30 (t, *J* = 7.7 Hz, 2H), 3.05 (t, *J* = 7.7 Hz, 2H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 199.2, 159.7, 142.9, 136.8, 133.1, 129.5, 128.6, 128.0, 120.8, 114.2, 111.4, 55.2, 40.4, 30.2. All spectral data was in accord with the literature.[14]



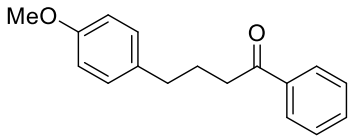
3v (CAS: 1669-49-4): **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.00 – 7.96 (m, 2H), 7.36 – 7.31 (m, 2H), 7.30-7.28 (m, 2H), 7.27 – 7.21 (m, 1H), 6.98 – 6.93 (m, 2H), 3.90 (s, 3H), 3.30 (t, 7.8Hz, 2H), 3.09(t, 7.8Hz, 2H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 197.8, 163.4, 141.4, 130.3, 129.9, 128.5, 128.4, 126.0, 113.7, 55.4, 40.1, 30.3. All spectral data was in accord with the literature.[14]



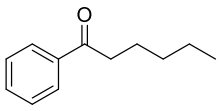
3w (CAS: 5739-39-9): **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.95 – 7.89 (m, 2H), 7.51 – 7.42 (m, 2H), 7.36 – 7.29 (m, 2H), 7.29 – 7.22 (m, 3H), 3.30 (t, *J* = 7.7 Hz, 2H), 3.09 (t, *J* = 7.7 Hz, 2H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 198.0, 141.0, 139.5, 135.1, 129.4, 128.9, 128.5, 128.4, 126.2, 40.4, 30.0. All spectral data was in accord with the literature.[14]



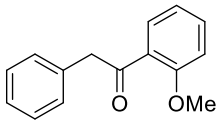
3x (CAS: 5407-91-0): **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.04 – 7.86 (m, 2H), 7.57 – 7.51 (m, 1H), 7.43 (d, *J* = 7.7 Hz, 2H), 7.29 (t, *J* = 7.6 Hz, 2H), 7.25 – 7.15 (m, 3H), 2.97 (t, *J* = 7.3 Hz, 2H), 2.72 (t, *J* = 7.6 Hz, 2H), 2.11-2.05 (m, 2H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 200.1, 141.7, 137.0, 132.9, 128.5, 128.5, 128.4, 128.0, 125.9, 37.7, 35.2, 25.7. All spectral data was in accord with the literature.[1c]



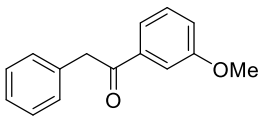
3y (CAS: 153389-13-0): **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.95 (dd, *J* = 8.0, 1.5 Hz, 2H), 7.62 – 7.53 (m, 1H), 7.47 (t, *J* = 7.6 Hz, 2H), 7.15 (d, *J* = 8.4 Hz, 2H), 6.86 (d, *J* = 8.6 Hz, 2H), 3.82 (s, 3H), 2.99 (t, *J* = 7.3 Hz, 2H), 2.69 (t, *J* = 7.5 Hz, 2H), 2.10-2.04 (m, 2H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 200.2, 157.8, 137.0, 133.7, 132.9, 129.4, 128.5, 128.0, 113.8, 55.2, 37.6, 34.3, 25.9. All spectral data was in accord with the literature.[1c]



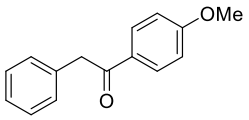
3z (CAS: 942-92-7): **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.99 – 7.92 (m, 2H), 7.58 – 7.50 (m, 1H), 7.47 – 7.43(m, 2H), 2.95 (t, *J* = 7.4 Hz, 2H), 1.79 – 1.69 (m, 2H), 1.39-1.33 (m, 4H), 0.99 – 0.82 (m, 3H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 200.6, 137.1, 132.9, 128.6, 128.1, 38.6, 31.6, 24.1, 22.6, 14.0. All spectral data was in accord with the literature.[15]



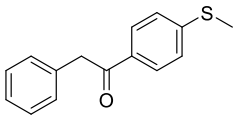
4a (CAS: 33470-10-9): **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.73 – 7.69 (m, 1H), 7.49 – 7.45 (m, 1H), 7.30 – 7.37(m, 2H), 7.28 – 7.23 (m, 3H), 7.04 – 6.97 (m, 2H), 4.34 (s, 2H), 3.94 (s, 3H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 200.2, 158.4, 135.3, 133.5, 130.7, 129.7, 128.4, 128.3, 126.6, 120.7, 111.5, 55.5, 50.2. All spectral data was in accord with the literature.[18]



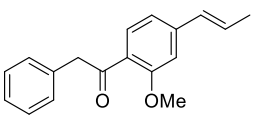
4b (CAS: 62381-24-2): **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.64 (d, *J* = 7.6, 1H), 7.57 (t, *J* = 2.1 Hz, 1H), 7.41 – 7.34 (m, 3H), 7.32 – 7.26 (m, 3H), 7.13 (dd, *J* = 8.2, 2.7 Hz, 1H), 4.30 (s, 2H), 3.86 (s, 3H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 197.5, 159.9, 138.0, 134.6, 129.6, 129.5, 128.7, 126.9, 121.3, 119.7, 112.9, 55.4, 45.7. All spectral data was in accord with the literature.[8]



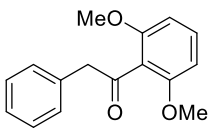
4c (CAS: 1023-17-2): **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.10 – 7.84 (m, 2H), 7.33-7.29 (m, 2H), 7.29 – 7.21 (m, 3H), 7.01 – 6.81 (m, 2H), 4.22 (s, 2H), 3.84 (s, 3H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 196.3, 163.6, 135.0, 131.0, 129.7, 129.4, 128.7, 126.8, 113.8, 55.5, 45.3. All spectral data was in accord with the literature.[9]



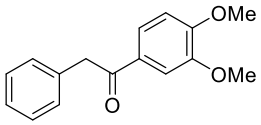
4d (CAS: 73242-07-6): **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.98 – 7.84 (m, 2H), 7.33 – 7.29 (m, 2H), 7.27 – 7.23 (m, 5H), 4.23 (s, 2H), 2.50 (s, 3H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 196.7, 146.1, 134.7, 132.9, 129.4, 129.1, 128.7, 126.9, 125.0, 45.4, 14.8. All spectral data was in accord with the literature.[16]



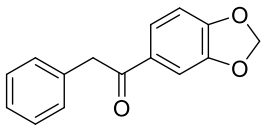
4e (CAS: 2725744-92-1): **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.71 (d, *J* = 8.0 Hz, 1H), 7.35 – 7.30 (m, 2H), 7.28 – 7.22 (m, 3H), 6.99 (dd, *J* = 8.1, 1.5 Hz, 1H), 6.90 (d, *J* = 1.5 Hz, 1H), 6.48 – 6.33 (m, 2H), 4.33 (s, 2H), 3.94 (s, 3H), 1.94 (d, *J* = 5.4 Hz, 3H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 199.1, 159.0, 143.6, 135.5, 131.3, 130.5, 129.7, 128.9, 128.3, 126.5, 126.2, 118.3, 108.9, 55.4, 50.1, 18.6.



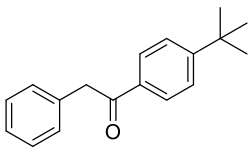
4f (CAS: 52856-19-6): ^{1}**H NMR** (500 MHz, $CDCl_3$) δ 7.29 – 7.25 (m, 2H), 7.25 – 7.17 (m, 4H), 6.51 (d, *J* = 8.4 Hz, 2H), 4.04 (s, 2H), 3.73 (s, 6H). ^{13}**C NMR** (126 MHz, $CDCl_3$) δ 202.3, 156.7, 134.4, 130.8, 130.0, 128.2, 126.7, 120.0, 104.0, 55.8, 51.5. All spectral data was in accord with the literature.[18]



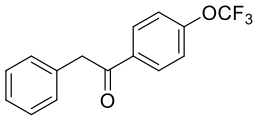
4g (CAS: 3141-93-3): ^{1}**H NMR** (500 MHz, $CDCl_3$) δ 7.66 (dd, *J* = 8.4, 2.1 Hz, 1H), 7.55 (d, *J* = 2.1 Hz, 1H), 7.42 – 7.13 (m, 5H), 6.87 (d, *J* = 8.4 Hz, 1H), 4.24 (s, 2H), 3.93 (s, 3H), 3.90 (s, 3H). ^{13}**C NMR** (126 MHz, $CDCl_3$) δ 196.3, 153.4, 149.1, 135.1, 129.8, 129.3, 128.7, 126.8, 123.5, 110.7, 110.0, 56.1, 56.0, 45.2. All spectral data was in accord with the literature.[18]



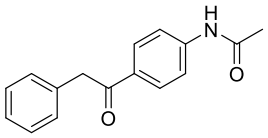
4h (CAS: 126266-77-1): ^{1}**H NMR** (500 MHz, $CDCl_3$) δ 7.65 (dd, *J* = 8.1, 1.8 Hz, 1H), 7.50 (d, *J* = 1.8 Hz, 1H), 7.38 – 7.32 (m, 2H), 7.30 – 7.24 (m, 3H), 6.86 (d, *J* = 8.1 Hz, 1H), 6.05 (s, 2H), 4.23 (s, 2H). ^{13}**C NMR** (126 MHz, $CDCl_3$) δ 195.8, 151.9, 148.3, 134.8, 131.4, 129.4, 128.7, 126.9, 125.0, 108.4, 107.9, 101.9, 45.4. All spectral data was in accord with the literature.[9]



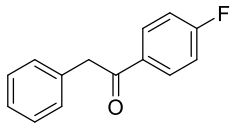
4i (CAS: 121149-70-0): ^{1}**H NMR** (500 MHz, $CDCl_3$) δ 8.02 – 7.98 (m, 2H), 7.52 – 7.49 (m, 2H), 7.38 – 7.34 (m, 2H), 7.32 – 7.28 (m, 3H), 4.30 (s, 2H), 1.37 (s, 9H). ^{13}**C NMR** (126 MHz, $CDCl_3$) δ 197.3, 156.9, 134.8, 134.1, 129.5, 128.7, 128.7, 126.8, 125.6, 45.5, 35.1, 31.1. All spectral data was in accord with the literature.[17]



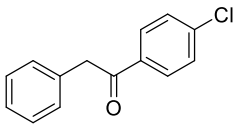
4j (CAS: 83882-93-3): ^{1}**H NMR** (500 MHz, $CDCl_3$) δ 8.06 (d, *J* = 8.1 Hz, 2H), 7.37 – 7.32 (m, 2H), 7.31 – 7.22 (m, 5H), 4.27 (s, 2H). ^{13}**C NMR** (126 MHz, $CDCl_3$) δ 196.0, 152.7, 134.8, 134.1, 130.7, 129.4, 128.8, 127.1, 120.4, 118.2 (q, *J* = 257.7 Hz), 45.6. ^{19}F NMR (471 MHz, $CDCl_3$) δ -57.6. All spectral data was in accord with the literature.[20]



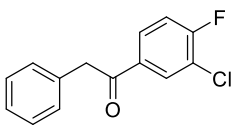
4k (CAS:63596-28-1): ^{1}**H NMR** (500 MHz, $CDCl_3$) δ 7.98 (d, *J* = 8.6 Hz, 2H), 7.64 – 7.52 (m, 3H), 7.31 (t, *J* = 7.5 Hz, 2H), 7.24 (m, *J* = 3.6 Hz, 2H), 4.25 (s, 2H), 2.19 (s, 3H), 1.64 (s, 1H). ^{13}**C NMR** (126 MHz, $CDCl_3$) δ 196.6, 168.6, 142.4, 134.6, 132.2, 130.1, 129.4, 128.7, 126.9, 118.9, 45.4, 24.8. All spectral data was in accord with the literature.[19]



4l (CAS: 347-84-2): ^{1}**H NMR** (500 MHz, $CDCl_3$) δ 8.15 – 7.91 (m, 2H), 7.33 (t, *J* = 7.5 Hz, 2H), 7.34 – 7.25 (m, 3H), 7.12 (t, *J* = 8.4 Hz, 2H), 4.25 (s, 2H). ^{13}**C NMR** (126 MHz, $CDCl_3$) δ 196.1, 165.8, (d, *J* = 255.4 Hz), 134.4, 133.0(d, *J* = 2.8 Hz), 131.3(d, *J* = 9.3 Hz), 129.4, 128.8, 127.0, 115.8 (d, *J* = 21.4 Hz), 45.5. ^{19}**F NMR** (471 MHz, $CDCl_3$) δ -105.0. All spectral data was in accord with the literature.[8]

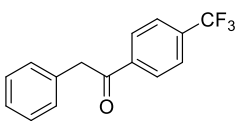


4m (CAS: 1889-71-0): ^{1}**H NMR** (500 MHz, $CDCl_3$) δ 8.00 – 7.94 (m, 2H), 7.48 – 7.42 (m, 2H), 7.36 (dd, *J* = 8.6, 6.5 Hz, 2H), 7.30 – 7.27 (m, 3H), 4.28 (s, 2H). ^{13}**C NMR** (126 MHz, $CDCl_3$) δ 196.4, 139.7, 134.9, 134.2, 130.1, 129.4, 129.0, 128.8, 127.1, 45.6. All spectral data was in accord with the literature.[8]

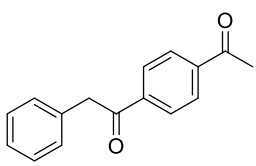


4n (CAS: 845781-19-3): ^{1}**H NMR** (500 MHz, $CDCl_3$) δ 8.07 (dd, *J* = 7.1, 2.2 Hz, 1H), 7.92 – 7.88 (m, 1H), 7.35-7.30 (m, 2H), 7.29 – 7.22 (m, 3H), 7.20 (t, *J* = 8.6 Hz, 1H), 4.23 (s, 2H). ^{13}**C NMR** (126 MHz, $CDCl_3$) δ 195.0, 161.0 (d, *J* = 257.3 Hz), 133.8, 133.7 (d, *J* = 3.7 Hz), 131.6, 129.4, 129.0 (d, *J* = 8.3 Hz), 128.9, 127.2, 122.0

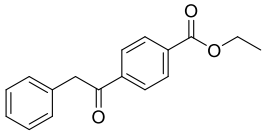
(d, *J* = 18.5 Hz), 116.9 (d, *J* = 21.3 Hz), 45.5. **^{19}F NMR** (471 MHz, $CDCl_3$) δ -107.4.



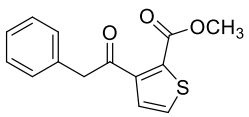
4o (CAS: 61062-55-3): **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.10 (d, *J* = 8.1 Hz, 2H), 7.72 (d, *J* = 8.1 Hz, 2H), 7.36 – 7.31 (m, 2H), 7.29 – 7.23 (m, 3H), 4.31 (s, 2H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 196.6, 139.2, 134.5 (q, *J* = 33.0 Hz), 133.8, 129.4, 129.0, 128.9, 127.2, 125.7(q, *J* = 3.8 Hz), 123.6 (q, *J* = 272.9 Hz), 122.5, 120.3, 45.9. **^{19}F NMR** (471 MHz, $CDCl_3$) δ -63.2. All spectral data was in accord with the literature.[17]



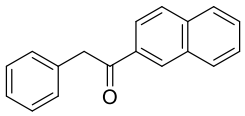
4p (CAS: 6420-94-6): **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.14 – 8.08 (m, 2H), 8.07 – 8.01 (m, 2H), 7.38 – 7.34 (m, 2H), 7.32 – 7.26 (m, 3H), 4.33 (s, 2H), 2.65 (s, 3H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 197.4, 197.1, 140.2, 139.7, 134.0, 129.4, 128.8, 128.5, 127.1, 45.9, 26.9. All spectral data was in accord with the literature.[17]



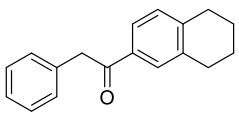
4q (CAS: 898776-56-2): **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.11 (d, *J* = 8.0, 2H), 8.05 (d, *J* = 7.6 Hz, 2H), 7.33 (t, *J* = 7.8 Hz, 2H), 7.30 – 7.24 (m, 3H), 4.40 (q, *J* = 7.1, 2H), 4.31 (s, 2H), 1.40 (t, *J* = 7.2, 3H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 197.2, 165.7, 139.7, 134.3, 134.0, 129.8, 129.5, 128.8, 128.5, 127.1, 61.5, 45.9, 14.3. All spectral data was in accord with the literature.[18]



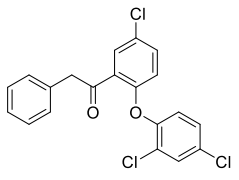
4r : yellow oil. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.43 (d, *J* = 5.0 Hz, 1H), 7.31 (t, *J* = 7.4 Hz, 2H), 7.26 – 7.21 (m, 3H), 6.93 (d, *J* = 5.1 Hz, 1H), 4.19 (s, 2H), 3.90 (s, 3H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 199.7, 161.8, 147.6, 133.6, 131.4, 130.4, 129.8, 128.6, 128.0, 127.1, 52.7, 50.3. **HRMS** (ESI): Calculated for $C_{14}H_{13}O_3S$ ($M + H^+$): 261.0585, found: 261.0584.



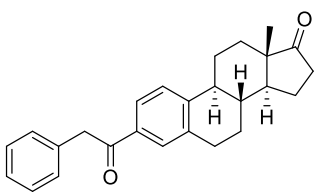
4s (CAS: 1762-15-8): **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.55 (s, 1H), 8.06 (dd, *J* = 8.7, 1.8 Hz, 1H), 7.96 (d, *J* = 8.1 Hz, 1H), 7.92 – 7.82 (m, 2H), 7.61 – 7.53 (m, 2H), 7.39 – 7.27 (m, 4H), 7.27 – 7.23 (m, 1H), 4.42 (s, 2H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 197.6, 135.6, 134.7, 134.0, 132.5, 130.4, 129.6, 129.5, 128.7, 128.6, 128.5, 127.8, 126.9, 126.8, 124.3, 45.6. All spectral data was in accord with the literature.[8]



4t (CAS: 6976-03-0): **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.74 – 7.71 (m,2H), 7.71 (t, *J* = 2.0 Hz, 2H), 7.35 – 7.28 (m, 2H), 7.28 – 7.22 (m, 4H), 7.12 (d, *J* = 8.4 Hz, 1H), 4.24 (s, 2H), 2.84-2.75 (m, 4H), 1.84-1.78 (m, 4H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 197.6, 143.4, 137.6, 134.9, 134.1, 129.6, 129.5, 129.4, 128.6, 126.8, 125.8, 45.4, 29.7, 29.4, 23.0, 22.8. All spectral data was in accord with the literature.[8]

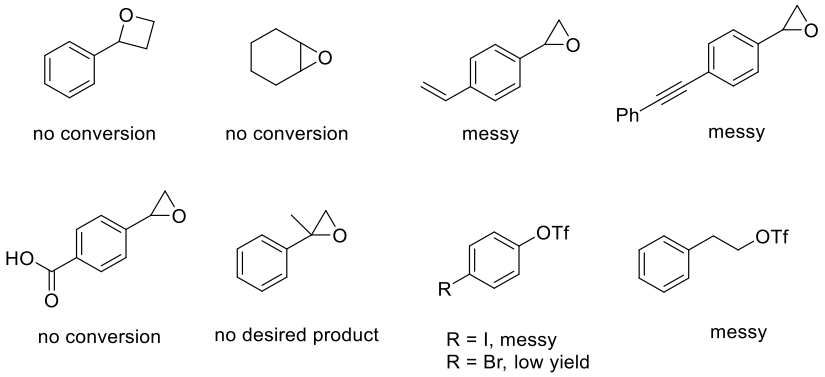


4u: colorless oil. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.77 (d, J = 2.7 Hz, 1H), 7.55 (d, J = 2.5 Hz, 1H), 7.36 (dd, J = 8.8, 2.7 Hz, 1H), 7.33 – 7.21 (m, 6H), 6.87 (d, J = 8.7 Hz, 1H), 6.67 (d, J = 8.8 Hz, 1H), 4.39 (s, 2H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 197.7, 153.7, 149.8, 134.0, 133.2, 130.9, 130.7, 130.6, 129.7, 129.2, 128.6, 128.5, 127.0, 127.0, 122.0, 118.3, 50.0. **HRMS** (ESI): Calculated for $C_{20}H_{14}O_2Cl_3$ ($M + H^+$): 391.0059, found: 391.0060.



4v: White solid. Melting point: 164 °C. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.85 – 7.68 (m, 2H), 7.37 (d, *J* = 8.1 Hz, 1H), 7.35 – 7.29 (m, 2H), 7.29 – 7.19 (m, 3H), 4.25 (s, 2H), 2.99-2.92 (m, 2H), 2.51 (dd, *J* = 19.0, 8.8 Hz, 1H), 2.47 – 2.39 (m, 1H), 2.32 (td, *J* = 10.9, 4.0 Hz, 1H), 2.19-2.11 (m 1H), 2.09-2.02 (m, 2H), 2.01 – 1.93 (m, 1H), 1.69 – 1.58 (m, 2H), 1.58 – 1.42 (m, 4H), 0.91 (s, 3H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 220.5, 197.5, 145.6, 137.0, 134.8, 134.3, 129.5, 129.3, 128.7, 126.8, 126.2, 125.7, 50.5, 47.9, 45.4, 44.7, 37.8, 35.8, 31.6, 29.4, 26.3, 25.6, 21.6, 13.8. **HRMS** (ESI): Calculated for $C_{26}H_{29}O_2$ ($M + H^+$): 373.2168, found: 373.2171.

6. Unsuccessful examples



7. DFT calculation for the mechanistic study

7.1 Computational details

All calculations were performed using Gaussian 16, Revision A.03 package.[4] All of the reactants, intermediates, transition states, products were optimized by the DFT with the B3LYP-D3(BJ) functional.[5] For geometry optimizations and frequency calculations, BS-I basis set system was employed. In BSI, we employed LANL2DZ basis set for Ni with effective core potentials, 6-31G(d) basis sets for H, C and O. All the stationary structures were characterized with no imaginary frequency and the transition state structures (TSs) were characterized with a single imaginary frequency. Intrinsic reaction coordinate (IRC) calculations were performed on all the TSs. The solvent effect of benzene was evaluated through the SMD method,[6] in which a better basis system BS-II was used. In BS-II, we employed SDD basis sets for Ni, 6-311++G(2d,2p) basis sets for the other atoms. All reported energies are free energies at a concentration of 1 M and a temperature of 298.15 K

7.2 Energy profiles of nickel insertion to epoxide

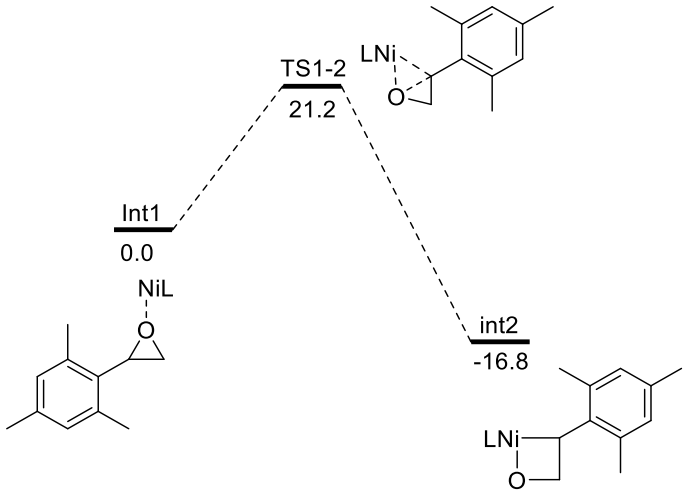


Figure S5.2.1 Nickel insertion to epoxide

The formation of intermediate 1 via TS1-2 is estimated to be exothermic about 17 kcal/mol by DFT calculations, and the needed free energy barrier is 21.2 kcal/mol, which is affordable under the current conditions

Cartesian coordinates of the optimized structures:

Int1

E = -3282.346029 a.u.

0 1

Ni	-0.84303400	1.96469300	0.01846500
O	-2.44406000	1.48231900	1.51275800

C	0.54630700	2.87651800	-2.75488600
C	1.24362100	3.28072300	-4.07337700
H	0.83695800	2.71647800	-4.92132500
H	1.10488100	4.34868300	-4.28052100
H	2.32129100	3.08427900	-4.02359500
C	1.28358100	3.63909200	-1.61855800
H	2.28744800	3.21788800	-1.51270700
H	1.42789800	4.68203900	-1.92302300
C	-0.93754900	3.31428800	-2.89665500
H	-0.98377200	4.40783100	-2.91071900
H	-1.31010000	2.98528600	-3.87280500
C	0.67824000	1.32749400	-2.64768900
H	1.65565600	1.01194000	-3.02996700
H	-0.05870500	0.87524800	-3.32004900
P	0.37173200	0.51644600	-0.97532200
P	0.53868500	3.59158100	0.11518400
P	-2.11172500	2.73723600	-1.54893400
C	2.07035000	0.09099800	-0.39042800
C	2.16301900	-0.76528900	0.72016800
C	3.25318500	0.64246200	-0.89833600
C	3.39540000	-1.07714400	1.28499800
H	1.25888800	-1.18405700	1.14912700
C	4.48946900	0.35317700	-0.31556000
H	3.22694500	1.30997500	-1.75199200
C	4.56753400	-0.51181500	0.77343600
H	3.44038100	-1.75628000	2.13063600
H	5.39113600	0.80648000	-0.71839900
H	5.52930700	-0.74038400	1.22413900
C	-0.20823300	-1.15325500	-1.54454400
C	0.62568800	-2.26304200	-1.74439000
C	-1.58365100	-1.29964000	-1.78500200
C	0.09372200	-3.48542700	-2.15939100
H	1.69233800	-2.17503500	-1.56789400
C	-2.11461300	-2.51440000	-2.21751100
H	-2.23745000	-0.44754400	-1.64296800
C	-1.27616600	-3.61640700	-2.39754500
H	0.75385700	-4.33709500	-2.30302800
H	-3.18103600	-2.59323500	-2.41080000
H	-1.68548100	-4.56934700	-2.72185800
C	-3.39154900	1.78056700	-2.47423500
C	-4.66356700	1.64471600	-1.88664700
C	-3.11363700	1.02638000	-3.62378100
C	-5.61758500	0.78837400	-2.42993500
H	-4.90304500	2.22429000	-0.99904200

C	-4.06955000	0.16761400	-4.17025700
H	-2.13760000	1.08577900	-4.09437800
C	-5.32446100	0.04114600	-3.57557000
H	-6.59540900	0.70588400	-1.96222400
H	-3.82655700	-0.40732600	-5.05989900
H	-6.06770300	-0.62853400	-3.99887900
C	-3.07284900	4.26658200	-1.17599200
C	-3.65045100	5.06791300	-2.17083800
C	-3.19462400	4.64891800	0.16538600
C	-4.32024900	6.24228700	-1.83033500
H	-3.57973700	4.76840300	-3.21358200
C	-3.87365200	5.81837600	0.50811900
H	-2.72871300	4.03137100	0.92662600
C	-4.43088800	6.61919000	-0.48884100
H	-4.75937900	6.86197500	-2.60801800
H	-3.94344900	6.11607500	1.55012700
H	-4.94845000	7.53742400	-0.22419700
C	0.02116200	5.34072400	0.40524500
C	-0.14940800	5.75597100	1.73761800
C	-0.35563500	6.22434500	-0.61429700
C	-0.67121600	7.01152700	2.03646300
H	0.13775800	5.08751100	2.54503100
C	-0.88588100	7.48080900	-0.31750400
H	-0.25219100	5.93623900	-1.65417400
C	-1.04582100	7.88075300	1.00767300
H	-0.78634000	7.31393600	3.07426900
H	-1.18446900	8.14099200	-1.12700800
H	-1.46270000	8.85685600	1.23930600
C	2.08683900	3.56001000	1.12448200
C	3.03458600	4.59418900	1.09707300
C	2.33399300	2.43225400	1.91302200
C	4.21147700	4.49189200	1.83747100
H	2.84320300	5.48445900	0.50393700
C	3.51153700	2.32716700	2.65396300
H	1.60370800	1.63294500	1.92835200
C	4.45290600	3.35552500	2.61605500
H	4.94063200	5.29768400	1.81052000
H	3.69362900	1.43512600	3.24581100
H	5.37240000	3.27631000	3.19020800
C	-3.07587200	0.22873700	1.20885900
H	-4.15694500	0.28180100	1.09103300
H	-2.54916600	-0.36097300	0.46906700
C	-2.47397700	0.43949500	2.53165400
H	-3.16141100	0.71126100	3.33581200

C	-1.17575200	-0.13245300	2.99212800
C	-0.87607600	-1.50088300	2.87111700
C	-0.28621400	0.73272300	3.66522600
C	0.30776700	-1.98359400	3.44595500
C	0.88790900	0.21322900	4.20834000
C	1.19739500	-1.14762600	4.12066200
H	0.53562800	-3.04382300	3.36049300
H	1.57432300	0.88701500	4.71540200
C	-1.77429900	-2.47107800	2.13631100
H	-2.83401100	-2.30060700	2.34868600
H	-1.63997300	-2.39428100	1.05005500
H	-1.53678500	-3.50061700	2.42046900
C	-0.59387900	2.20465200	3.79440500
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Int2

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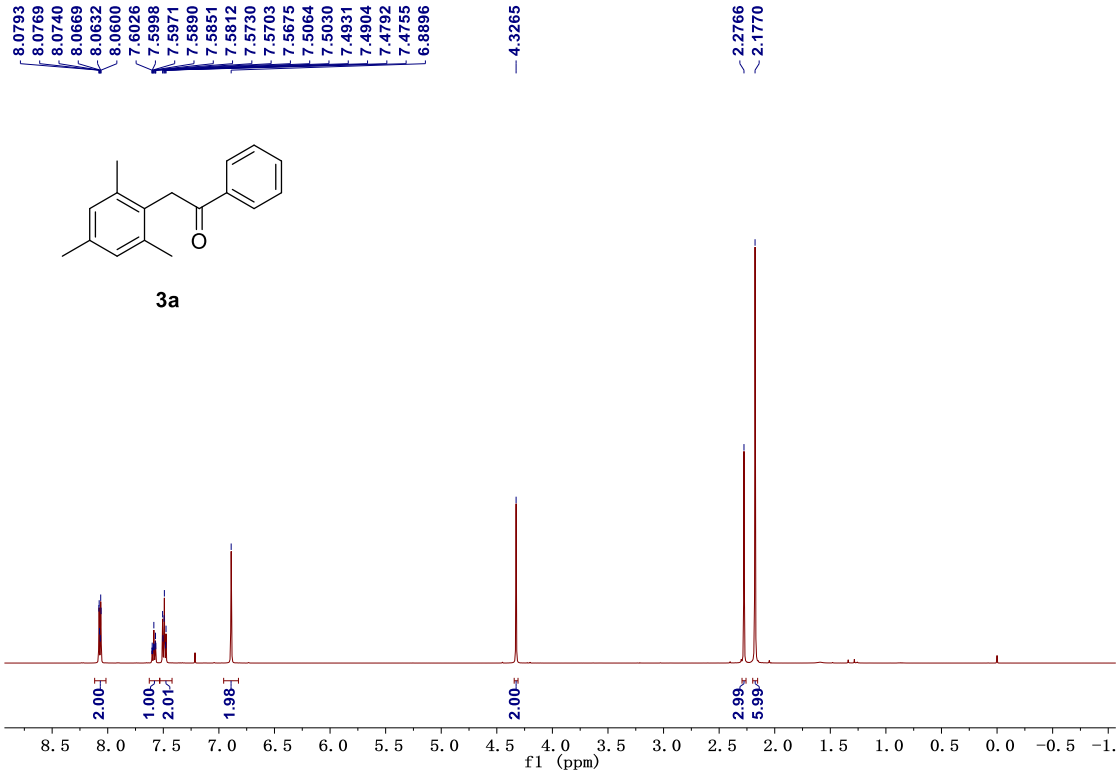
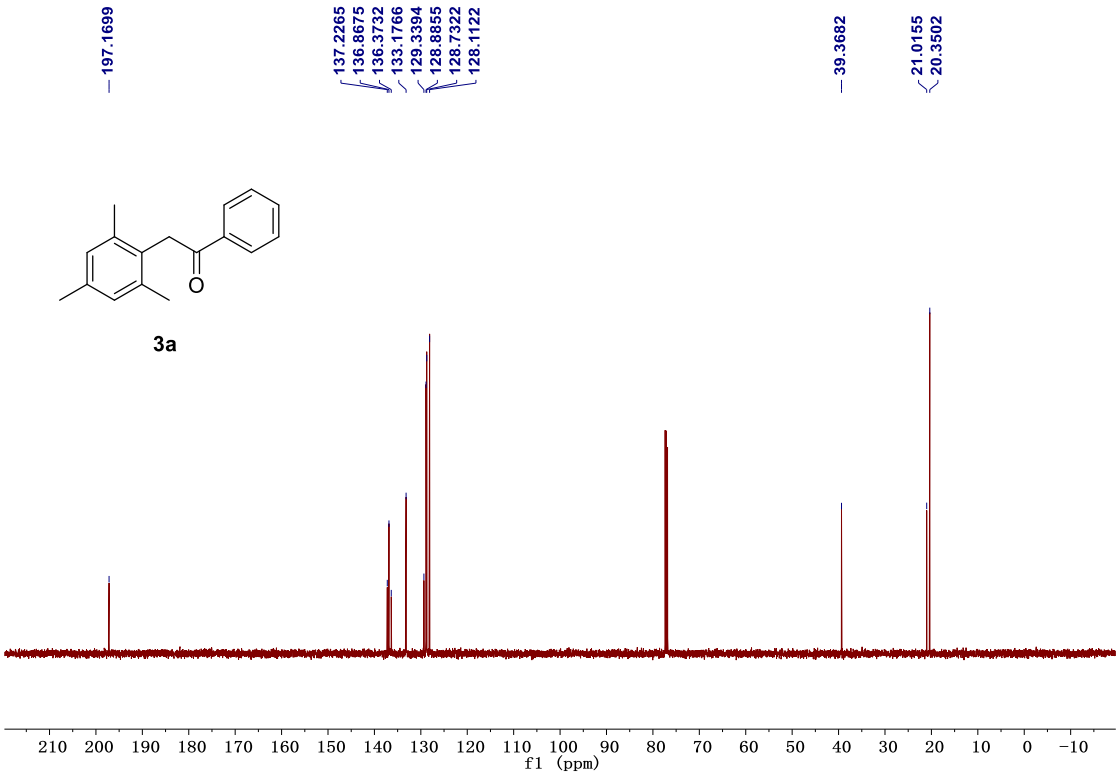
9. ^{1}H NMR, ^{13}C NMR, and ^{19}F NMR spectra



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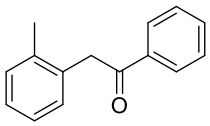

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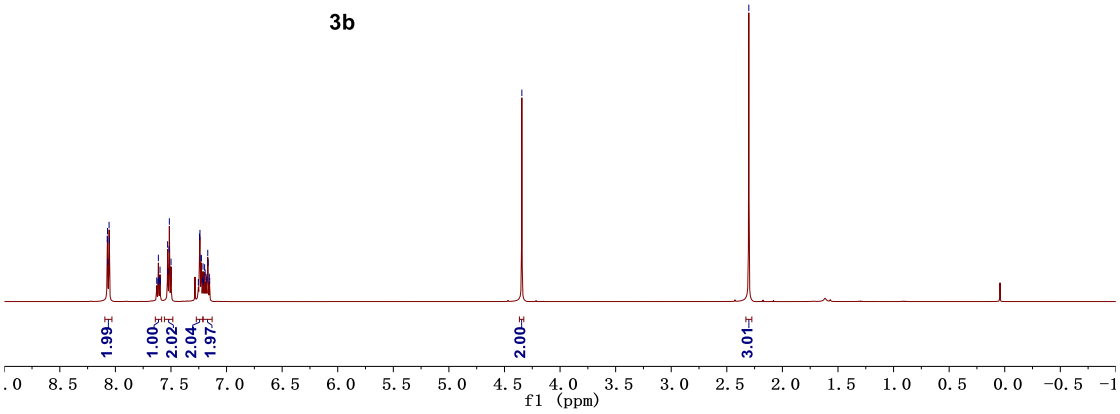
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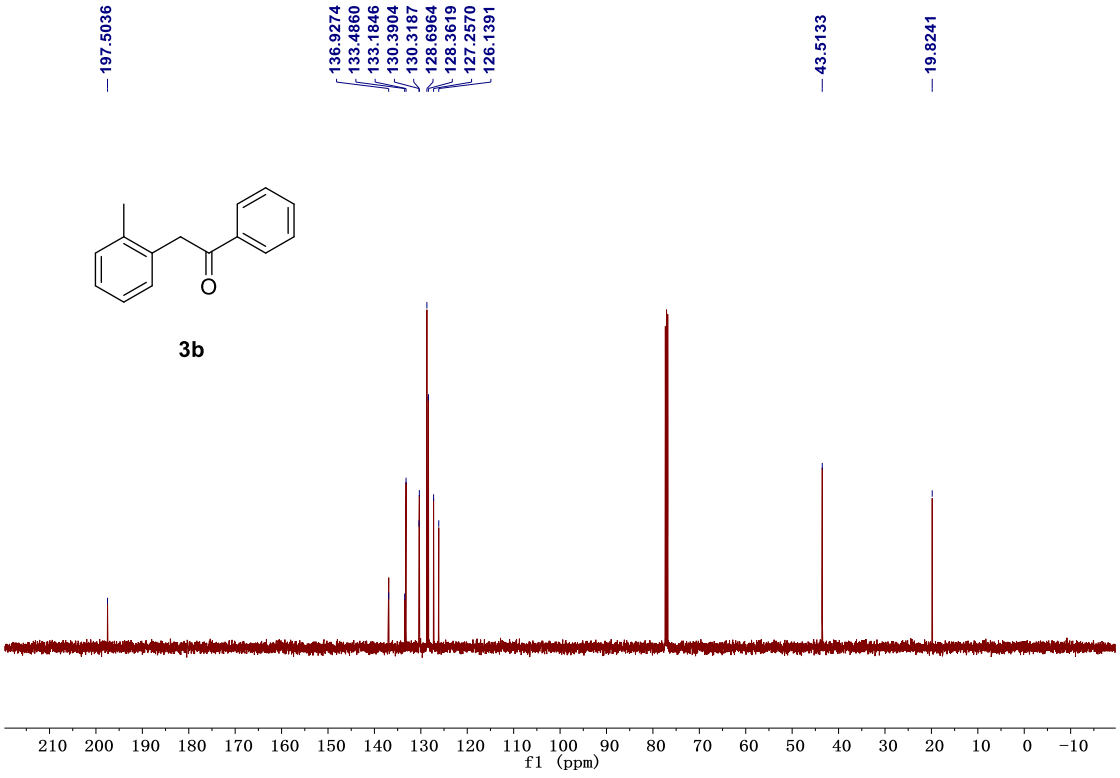
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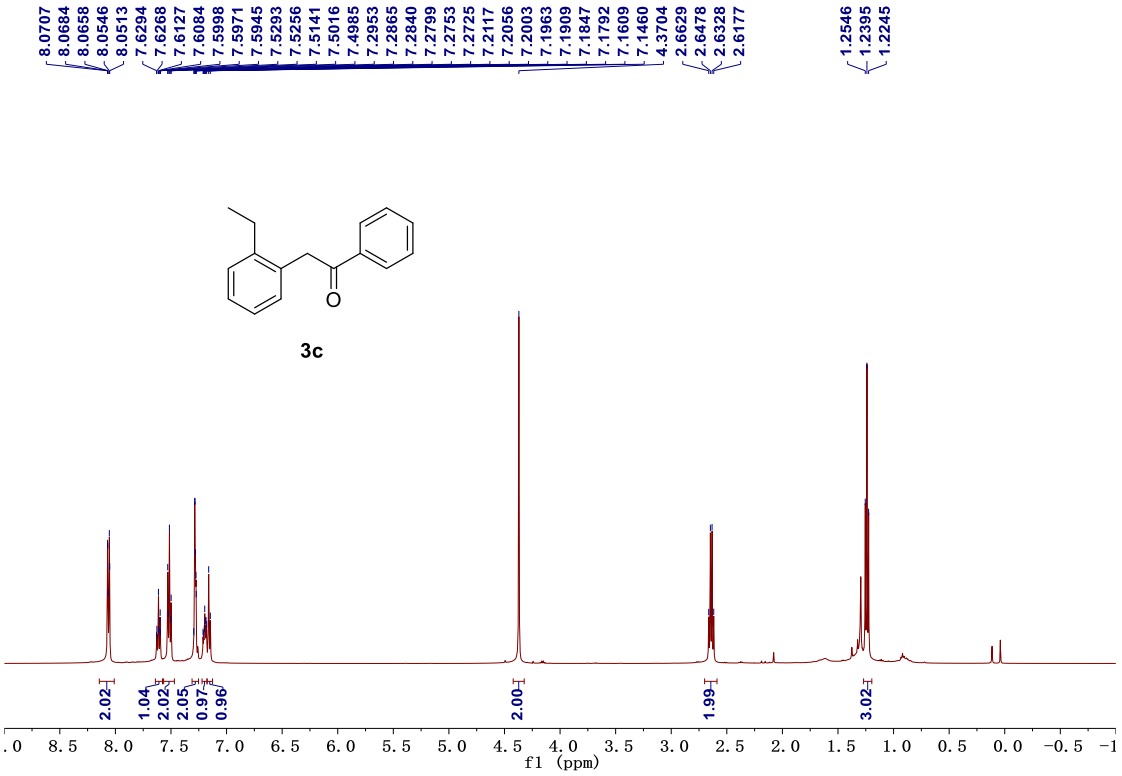
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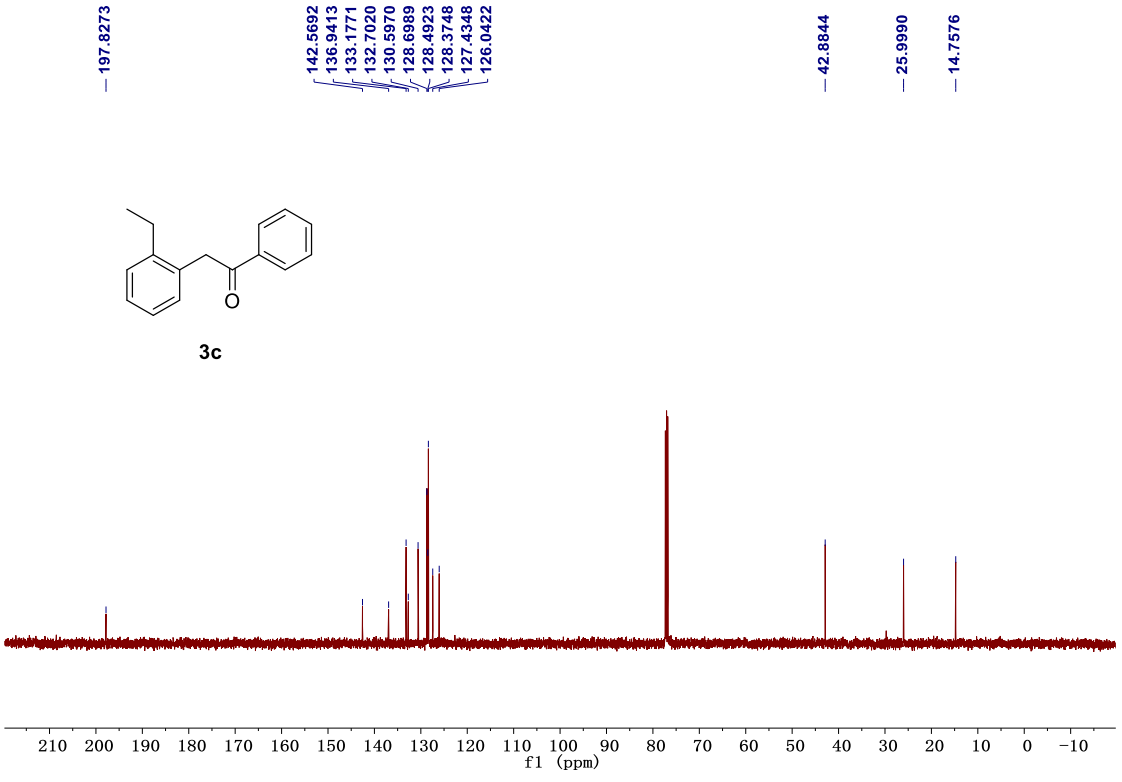
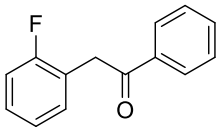
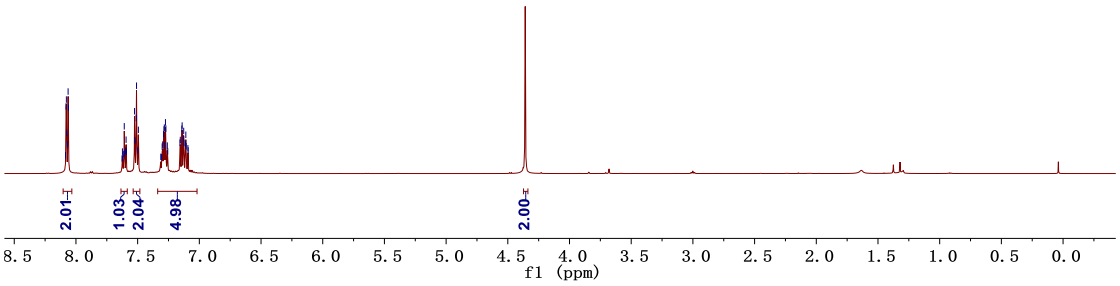
7.6268
7.6127
7.6084
7.5998
7.5971
7.5945
7.5293
7.5256
7.5141
7.5016
7.4985
7.2953
7.2865
7.2840
7.2799
7.2753
7.2725
7.2117
7.2056
7.2003
7.1963
7.1909
7.1847
7.1792
7.1609
7.1460
4.3704
2.6629
2.6478
2.6328
2.6177
1.2546
1.2395
1.2245
O
3c
2.02
1.04
2.02
2.05
0.97
0.96
2.00
1.99
3.02
f1 (ppm)

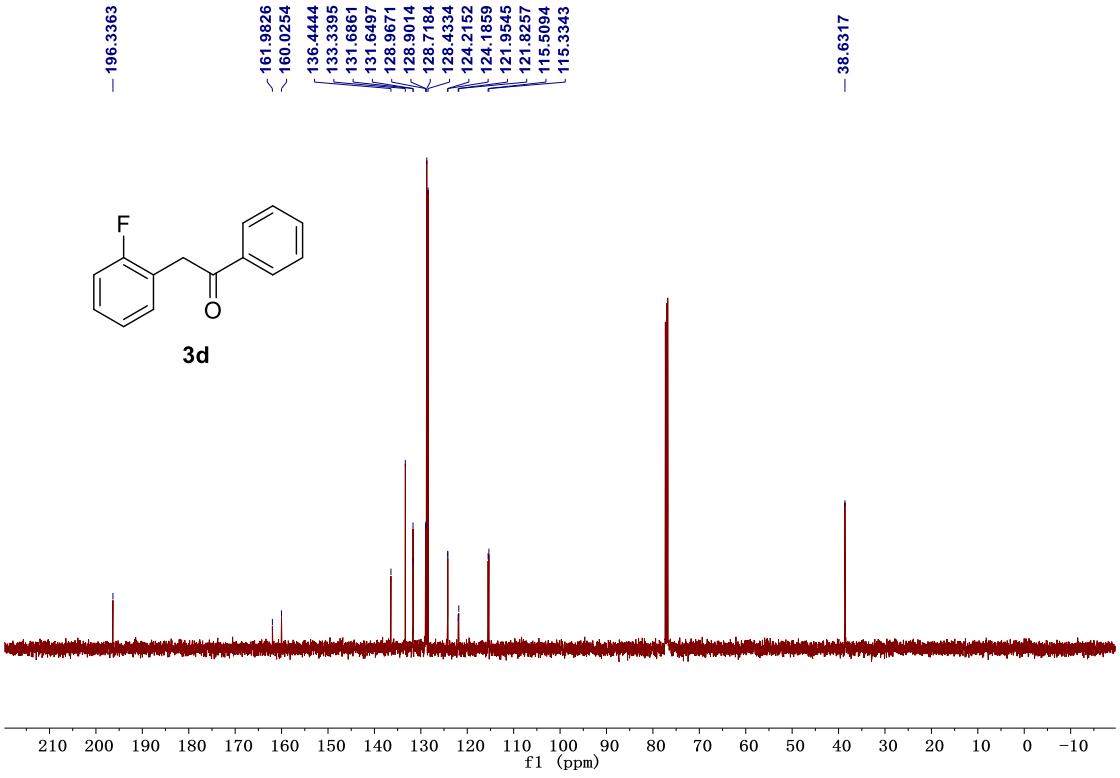

197.8273
142.5692
136.9413
133.1771
132.7020
130.5970
128.6989
128.4923
128.3748
127.4348
126.0422
42.8844
25.9990
14.7576
O
3c
f1 (ppm)


8.0840
8.0800
8.0776
8.0747
8.0676
8.0635
8.0605
7.6260
7.6233
7.6205
7.6125
7.6084
7.6046
7.5964
7.5937
7.5910
7.5251
7.5217
7.5117
7.5090
7.4976
7.4939
7.3125
7.3055
7.3013
7.2971
7.2899
7.2864
7.2837
7.2810
7.2745
7.2710
7.2595
7.2560
7.1568
7.1543
7.1418
7.1393
7.1290
7.1267
7.1243
7.1128
7.1095
7.1065
7.0927
7.0904


F
O

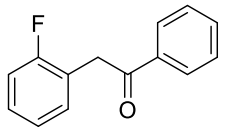
3d


2.01
1.03
2.04
4.98
2.00
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
f1 (ppm)


196.3363
161.9826
160.0254
136.4444
133.3395
131.6861
131.6497
128.9671
128.9014
128.7184
128.4334
124.2152
124.1859
121.9545
121.8257
115.5094
115.3343
38.6317
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 −10
f1 (ppm)

F
O

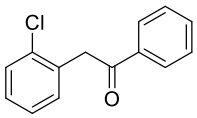
3d


F
O

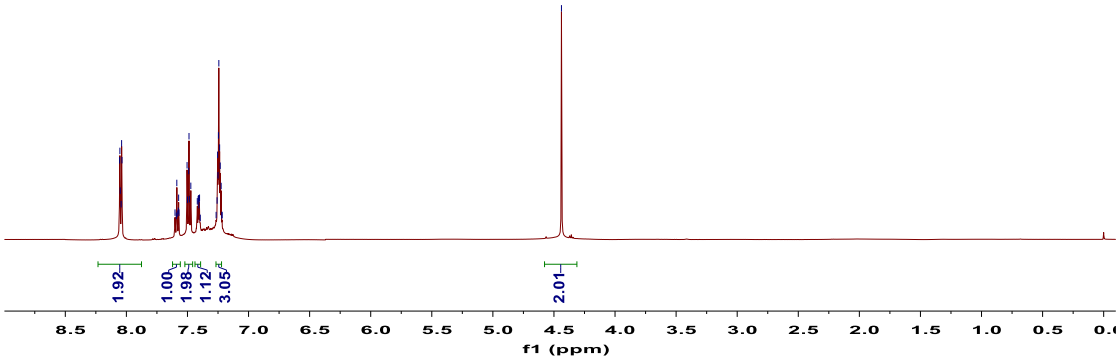
3d

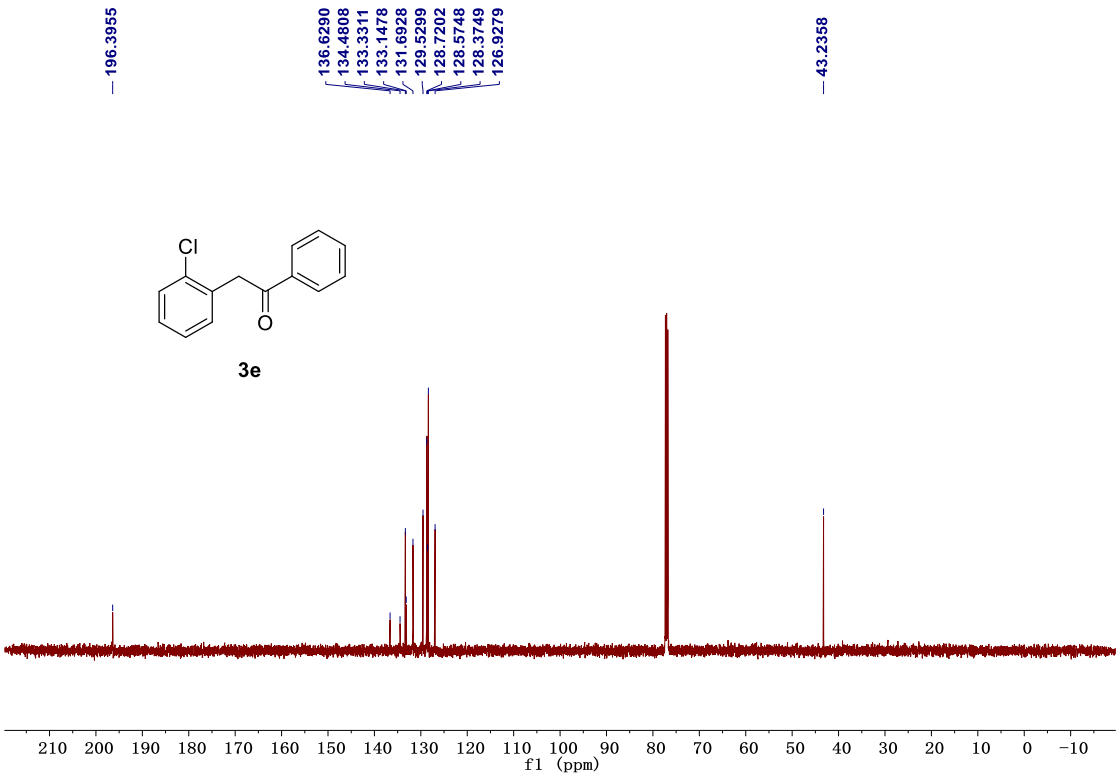
-117.1408
20
0
−20
−40
−60
−80
−100
−120
−140
−160
−180
−200
−2
f1 (ppm)

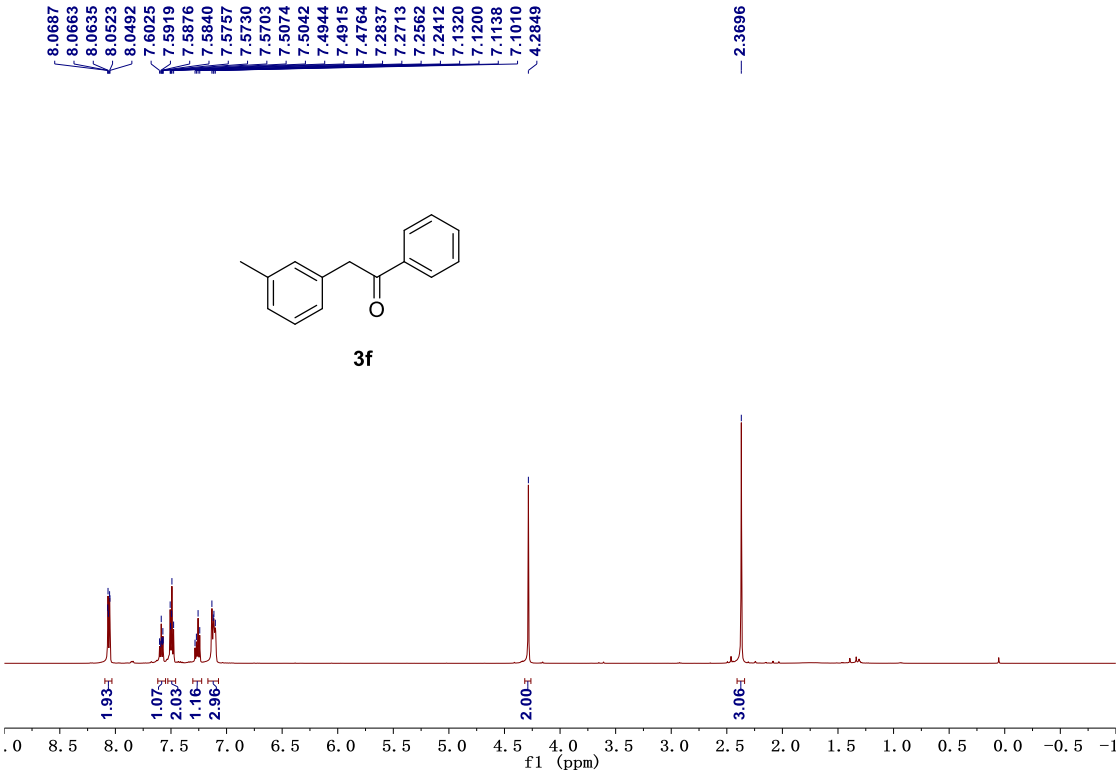

8.0555
8.0532
8.0503
8.0431
8.0391
8.0361
7.6019
7.5911
7.5873
7.5833
7.5750
7.5723
7.5696
7.5034
7.4999
7.4900
7.4874
7.4841
7.4726
7.4196
7.4123
7.4095
7.4075
7.4030
7.4011
7.3951
7.2655
7.2574
7.2536
7.2501
7.2464
7.2432
7.2368
7.2319
7.2242
7.2184
7.2166
4.4386

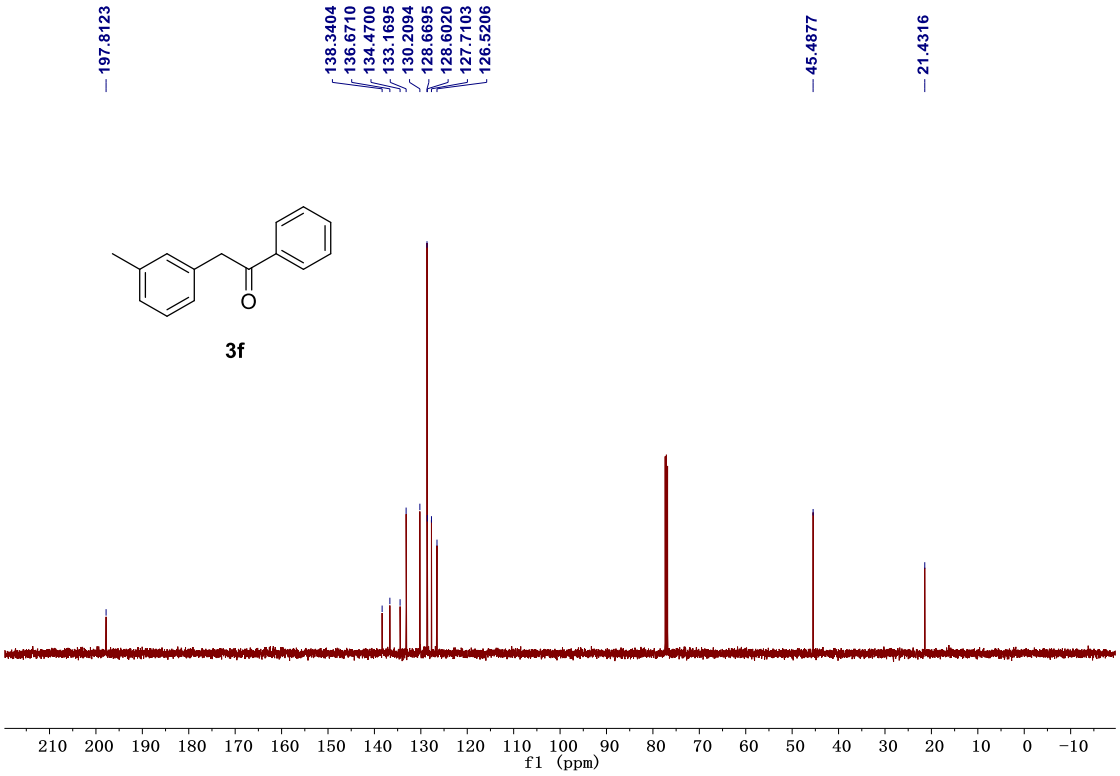

Cl
O

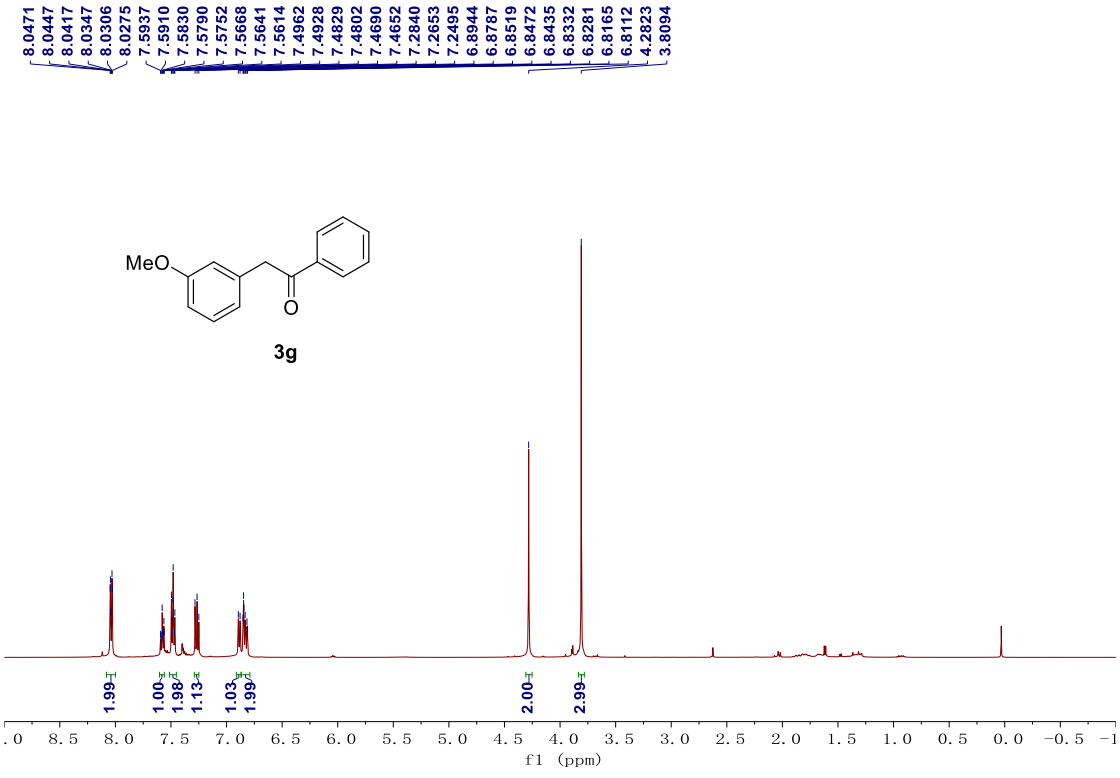
3e

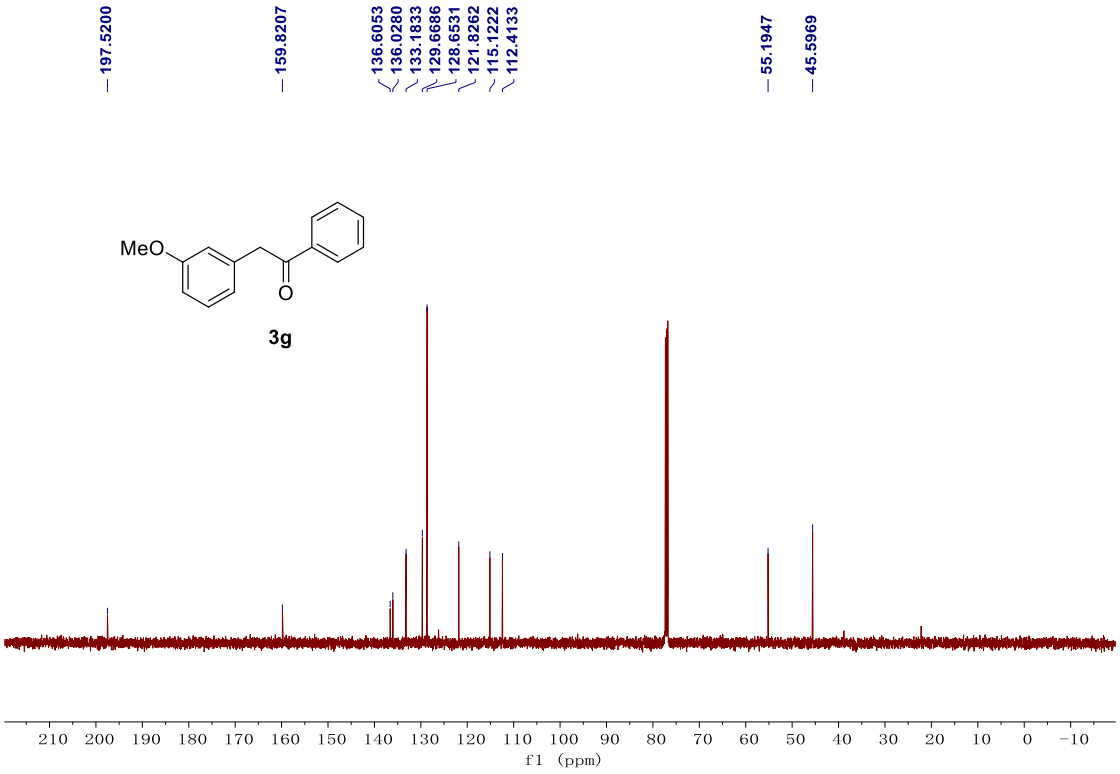

1.92
1.00
1.98
1.12
3.05
2.01
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
f1 (ppm)

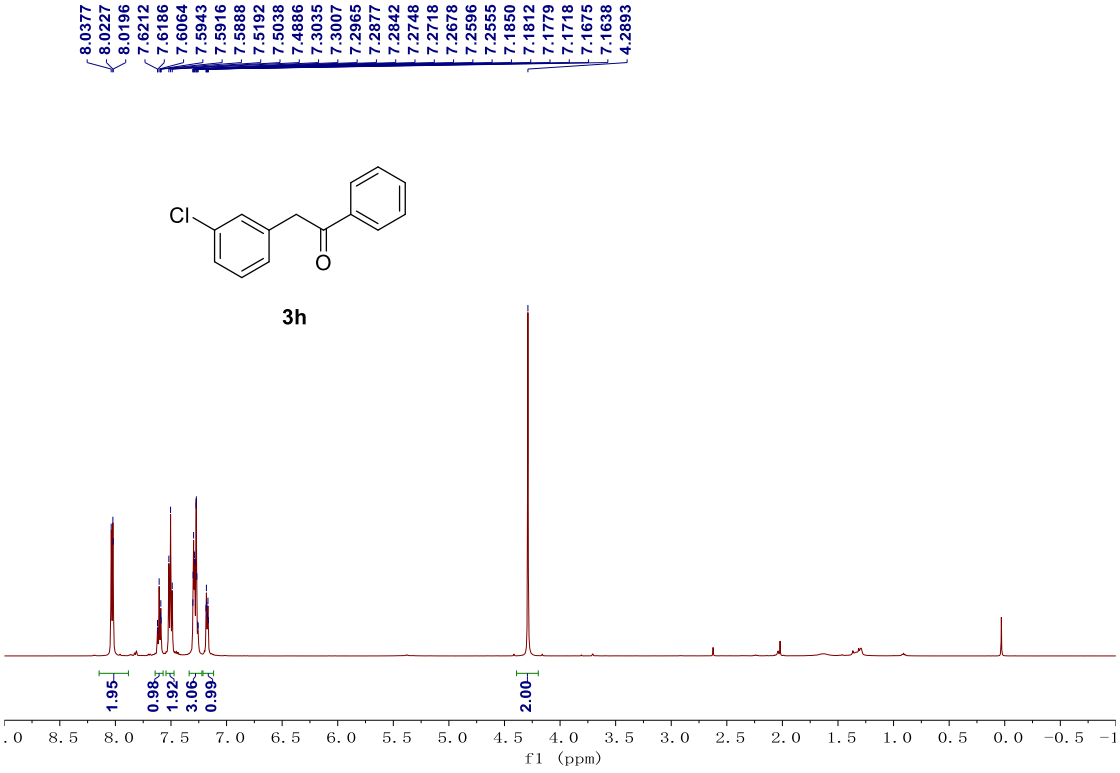

196.3955
136.6290
134.4808
133.3311
133.1478
131.6928
129.5299
128.7202
128.5748
128.3749
126.9279
43.2358
Cl
O
3e
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 −10
f1 (ppm)

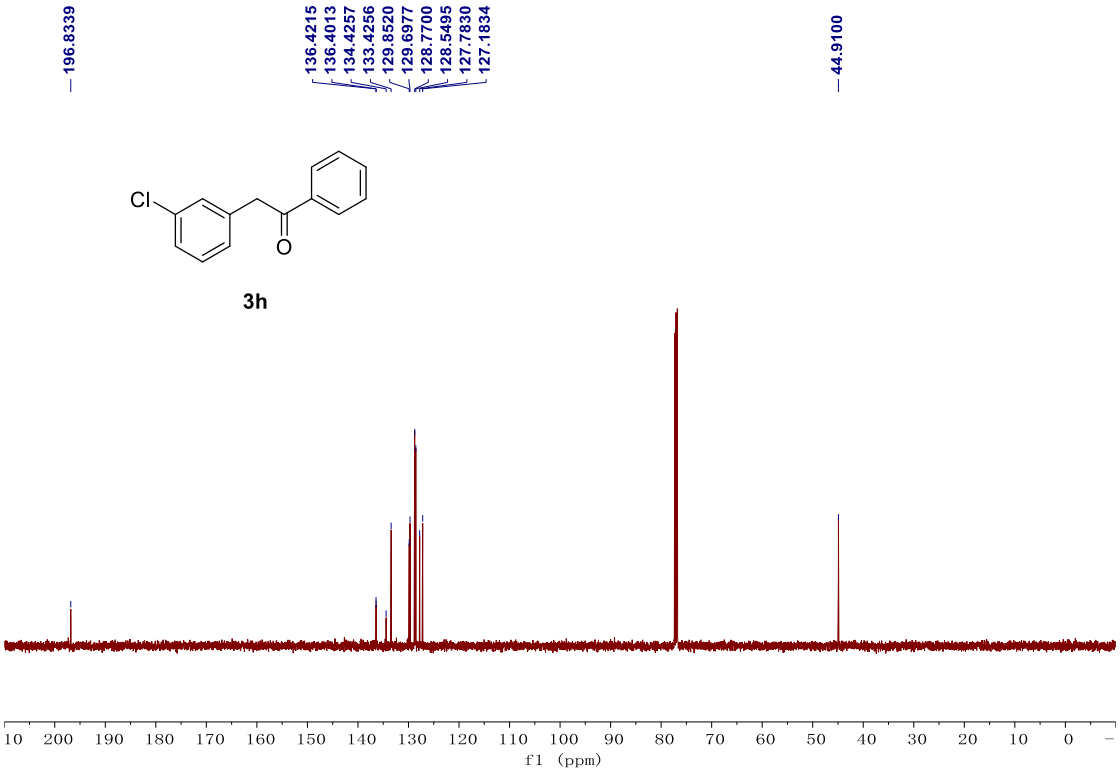

8.0687
8.0663
8.0635
8.0523
8.0492
7.6025
7.5919
7.5876
7.5840
7.5757
7.5730
7.5703
7.5074
7.5042
7.4944
7.4915
7.4764
7.2837
7.2713
7.2562
7.2412
7.1320
7.1200
7.1138
7.1010
4.2849
2.3696
O
3f
1.93
1.07
2.03
1.16
2.96
2.00
3.06
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 −0.5 −1
f1 (ppm)

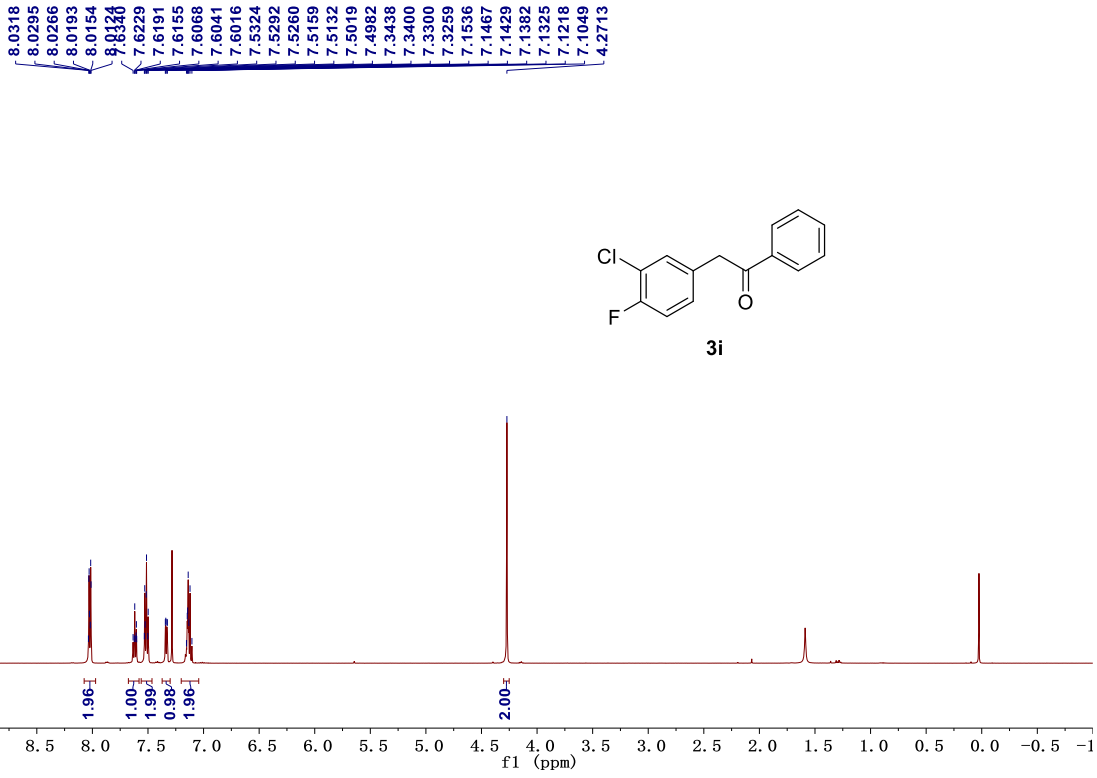

197.8123
138.3404
136.6710
134.4700
133.1695
130.2094
128.6695
128.6020
127.7103
126.5206
45.4877
21.4316
O
3f
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 −10
f1 (ppm)

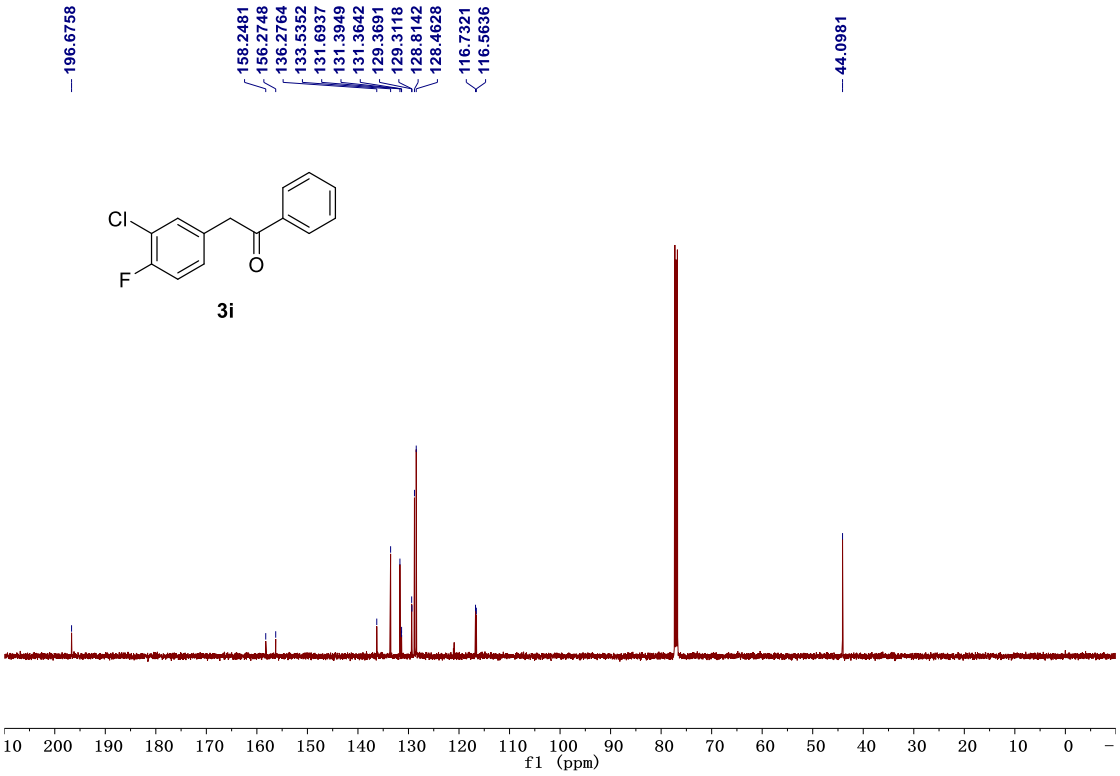

8.0471
8.0447
8.0417
8.0347
8.0306
8.0275
7.5937
7.5910
7.5830
7.5790
7.5752
7.5668
7.5641
7.5614
7.4962
7.4928
7.4829
7.4802
7.4690
7.4652
7.2840
7.2653
7.2495
6.8944
6.8787
6.8519
6.8472
6.8435
6.8332
6.8281
6.8165
6.8112
4.2823
3.8094
MeO
O
3g
1.99
1.00
1.98
1.13
1.03
1.99
2.00
2.99
.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 −0.5 −1
f1 (ppm)

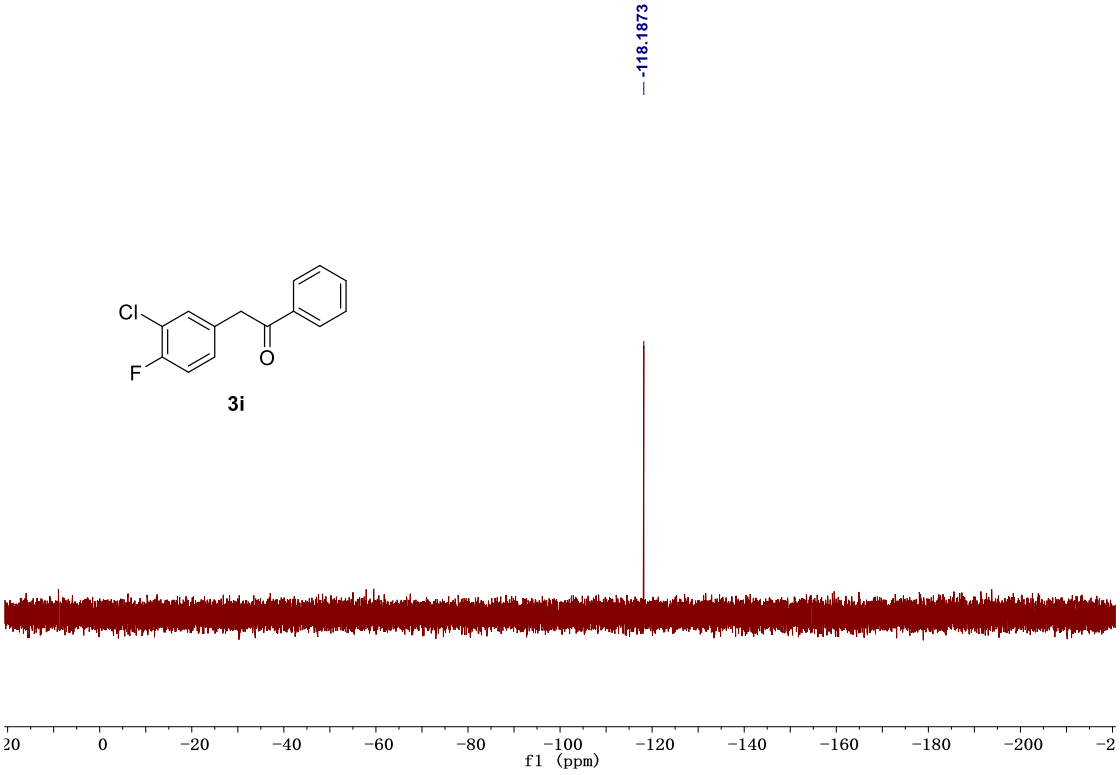

197.5200
159.8207
136.6053
136.0280
133.1833
129.6686
128.6531
121.8262
115.1222
112.4133
55.1947
45.5969
MeO
O
3g
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 −10
f1 (ppm)


8.0377
8.0227
8.0196
7.6212
7.6186
7.6064
7.5943
7.5916
7.5888
7.5192
7.5038
7.4886
7.3035
7.3007
7.2965
7.2877
7.2842
7.2748
7.2718
7.2678
7.2596
7.2555
7.1850
7.1812
7.1779
7.1718
7.1675
7.1638
4.2893
Cl
O
3h
1.95
0.98
1.92
3.06
0.99
2.00
.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 −0.5 −1
f1 (ppm)

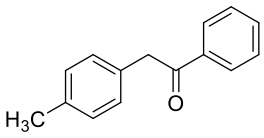

196.8339
136.4215
136.4013
134.4257
133.4256
129.8520
129.6977
128.7700
128.5495
127.7830
127.1834
44.9100
Cl
O
3h
f1 (ppm)


8.0318
8.0295
8.0266
8.0193
8.0154
7.6229
7.6191
7.6155
7.6068
7.6041
7.6016
7.5324
7.5292
7.5260
7.5159
7.5132
7.5019
7.4982
7.3438
7.3400
7.3300
7.3259
7.1536
7.1467
7.1429
7.1382
7.1325
7.1218
7.1049
4.2713
Cl
F
O
3i
1.96
1.00
1.99
0.98
1.96
2.00
f1 (ppm)

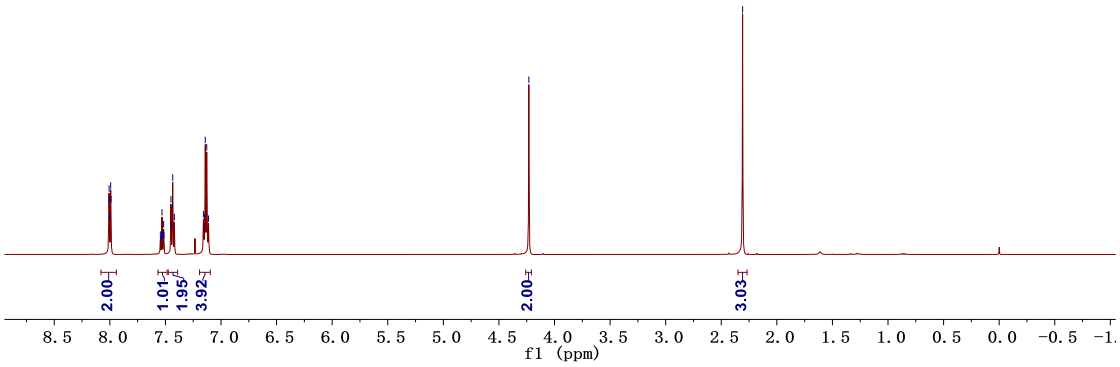

196.6758
158.2481
156.2748
136.2764
133.5352
131.6937
131.3949
131.3642
129.3691
129.3118
128.8142
128.4628
116.7321
116.5636
44.0981
Cl
F
O
3i
f1 (ppm)


-118.1873
Cl
F
O
3i
f1 (ppm)

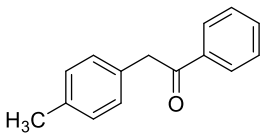

8.0089
8.0066
8.0034
7.9924
7.9893
7.5455
7.5429
7.5348
7.5309
7.5272
7.5187
7.5160
7.5132
7.4503
7.4469
7.4371
7.4344
7.4195
7.1580
7.1540
7.1468
7.1417
7.1284
7.1124
4.2310
2.3081


H3C
O

3j


2.00
1.01
1.95
3.92
2.00
3.03
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 −0.5 −1.
f1 (ppm)

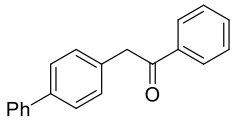

197.8499
136.6704
136.5039
133.1184
131.4669
129.4282
129.3396
128.6500
45.1724
21.1032


H3C
O

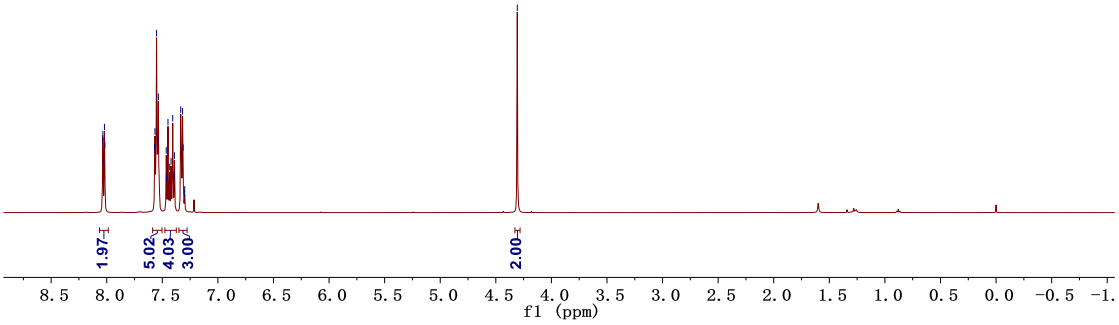
3j

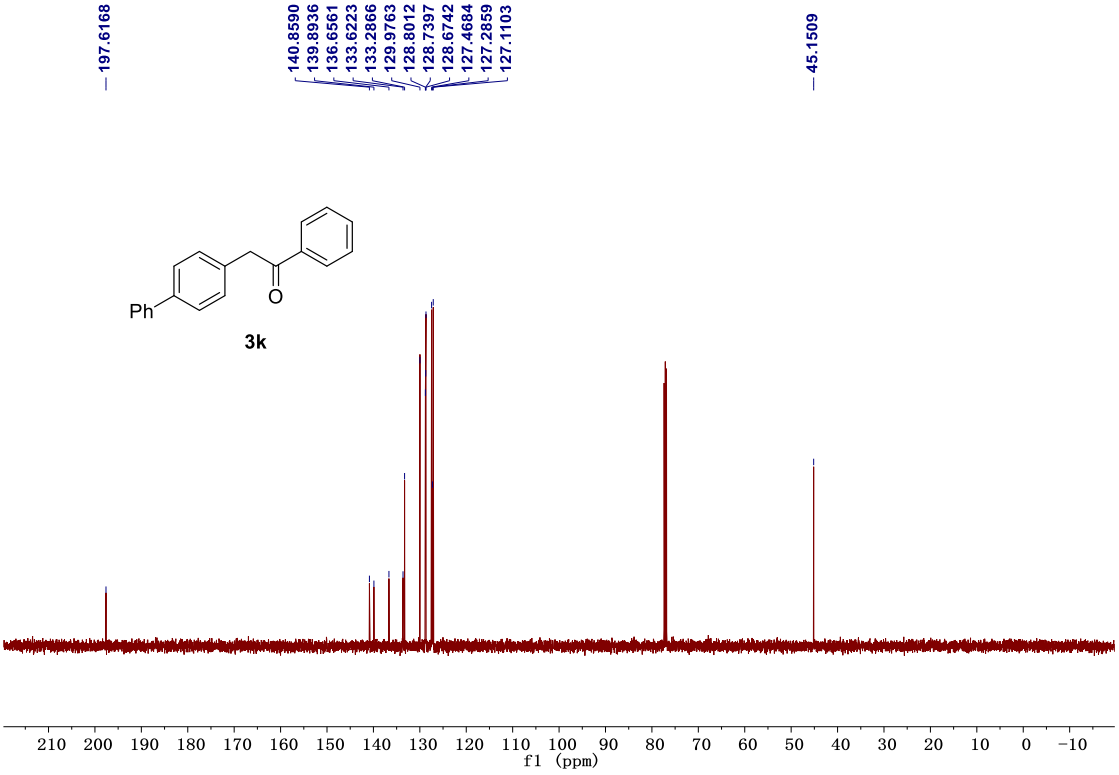
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 −10
f1 (ppm)


8.0366
8.0344
8.0320
8.0205
8.0172
7.5691
7.5659
7.5517
7.5430
7.5394
7.5355
7.4646
7.4612
7.4490
7.4336
7.4215
7.4064
7.3939
7.3907
7.3343
7.3288
7.3178
7.3130
7.3014
7.2986
4.3069


Ph
O

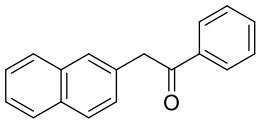
3k


1.97
5.02
4.03
3.00
2.00
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 −0.5 −1.
f1 (ppm)

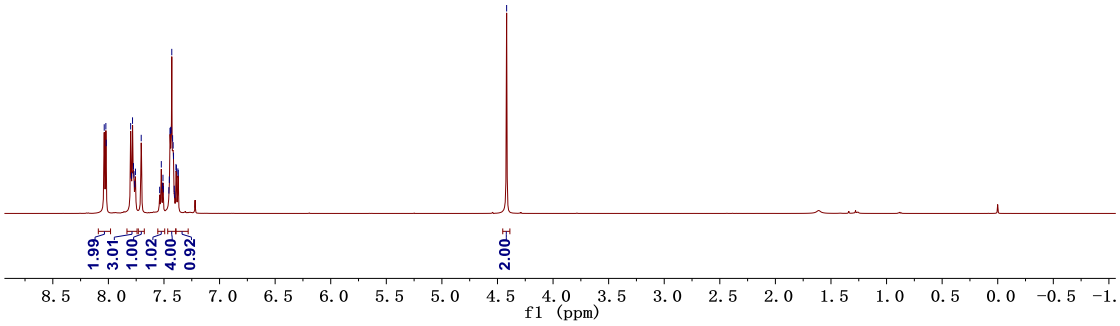

197.6168
140.8590
139.8936
136.6561
133.6223
133.2866
129.9763
128.8012
128.7397
128.6742
127.4684
127.2859
127.1103
45.1509
Ph
O
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 −10
f1 (ppm)

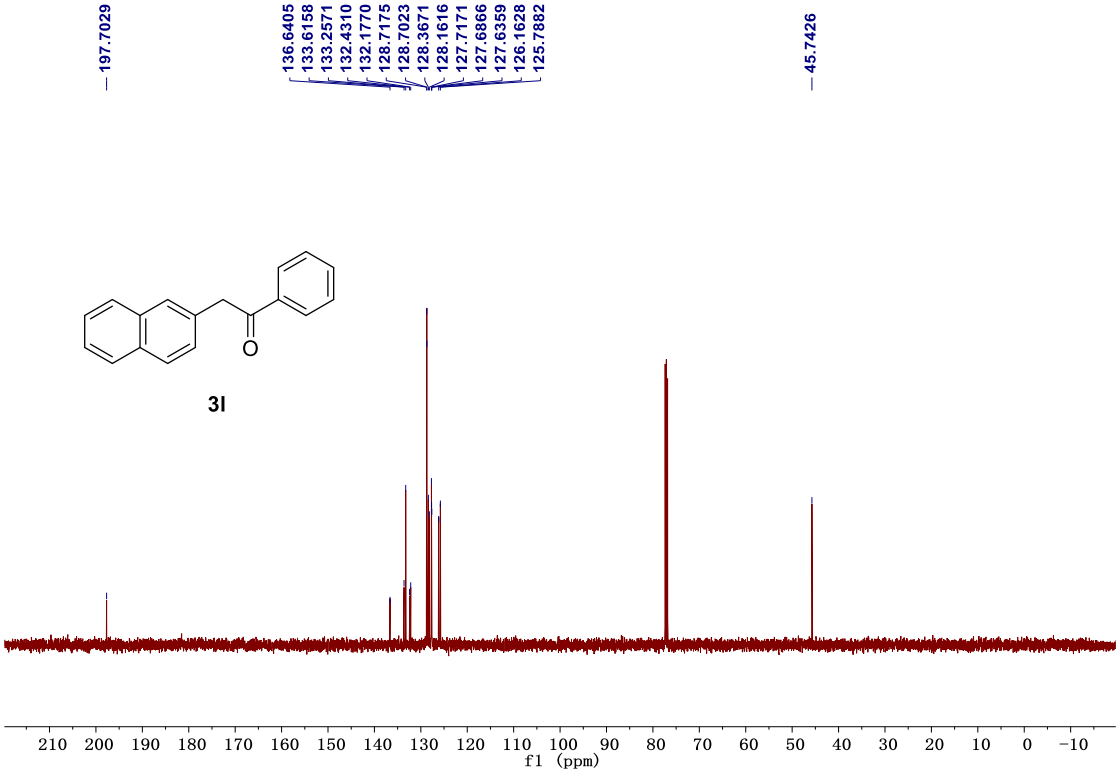
3k


8.0375
8.0228
8.0197
7.7997
7.7921
7.7829
7.7743
7.7696
7.7629
7.7566
7.7048
7.5387
7.5240
7.5119
7.5090
7.5062
7.4559
7.4520
7.4456
7.4422
7.4370
7.4298
7.4224
7.4175
7.4142
7.4073
7.4037
7.3918
7.3882
7.3750
7.3715
4.4176


O

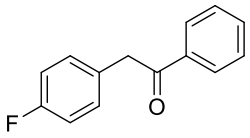
3l


1.99
3.01
1.00
1.02
4.00
0.92
2.00
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 −0.5 −1.
f1 (ppm)

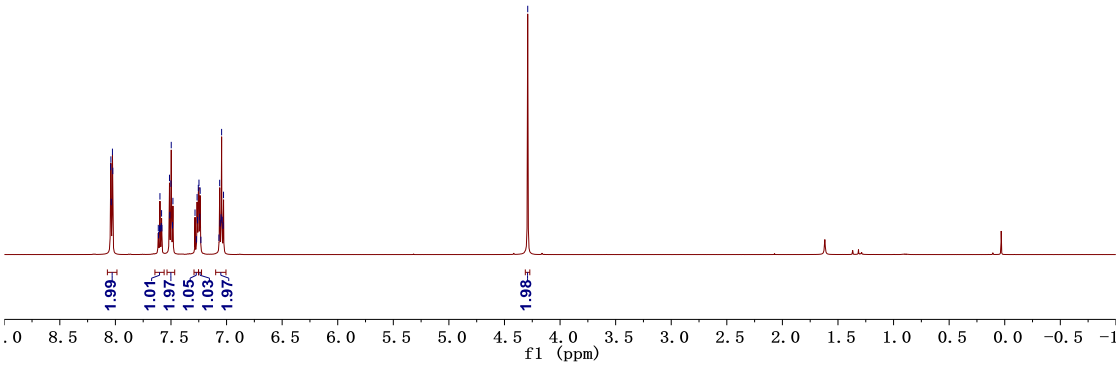

197.7029
136.6405
133.6158
133.2571
132.4310
132.1770
128.7175
128.7023
128.3671
128.1616
127.7171
127.6866
127.6359
126.1628
125.7882
45.7426
O
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 −10
f1 (ppm)

3l

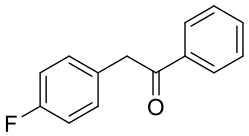

8.0428
8.0404
8.0375
8.0266
8.0234
7.6141
7.6115
7.6032
7.5993
7.5955
7.5873
7.5845
7.5818
7.5135
7.5100
7.5004
7.4977
7.4863
7.4826
7.2838
7.2717
7.2652
7.2608
7.2543
7.2483
7.2416
7.2373
7.2308
7.0683
7.0620
7.0576
7.0494
7.0446
7.0398
7.0317
7.0273
4.2910


F
O

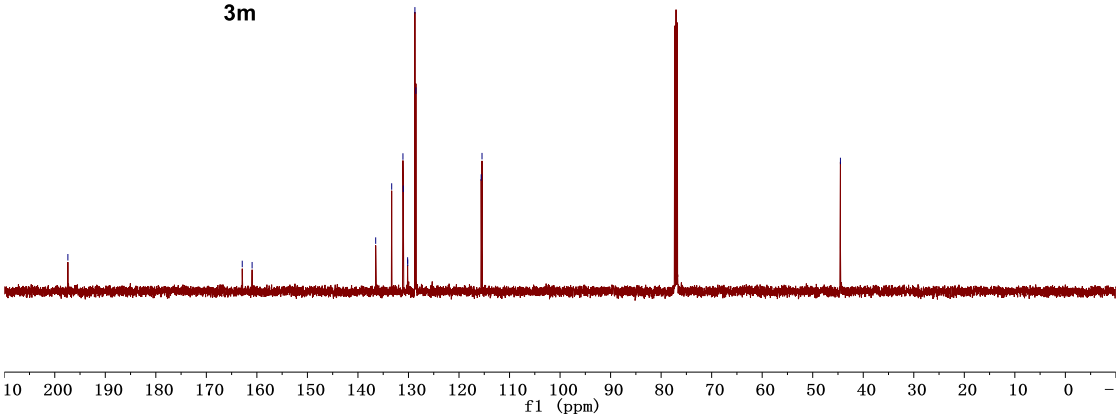
3m

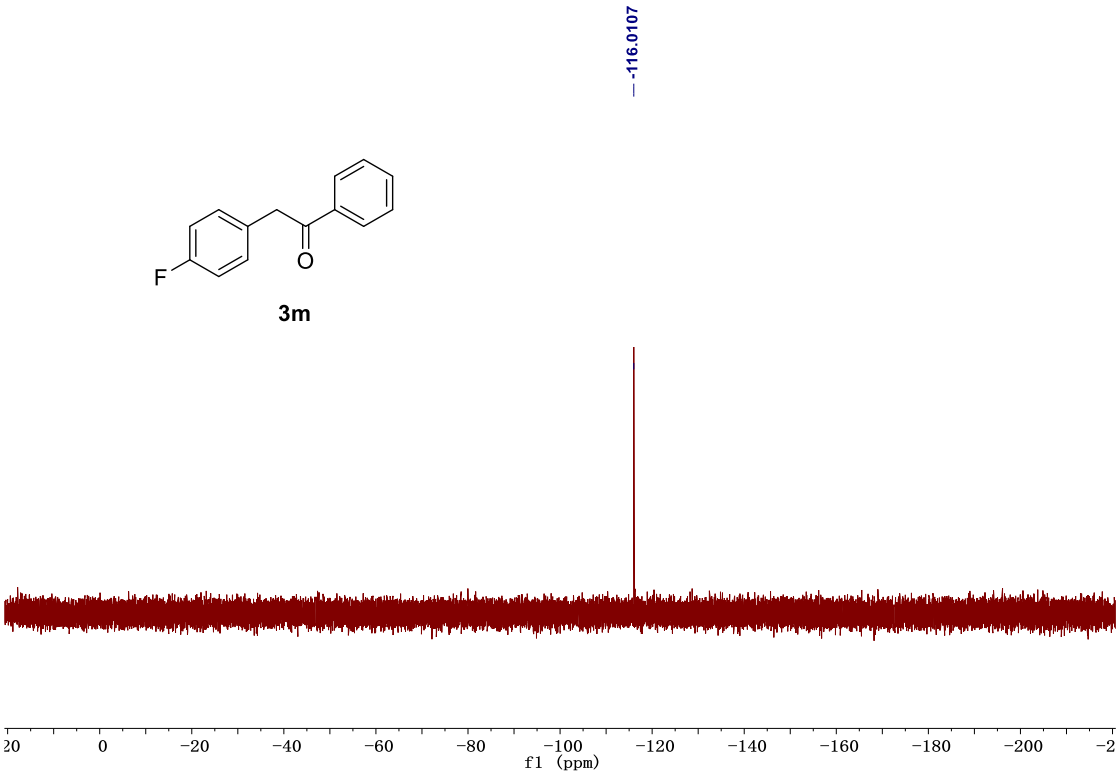

1.99
1.01
1.97
1.05
1.03
1.97
1.98
f1 (ppm)


197.4029
162.8968
160.9454
136.4881
133.3213
131.0939
131.0304
130.1731
130.1502
128.7255
128.5322
115.6133
115.4446
44.5157


F
O

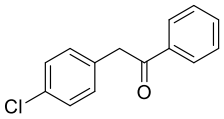
3m


f1 (ppm)

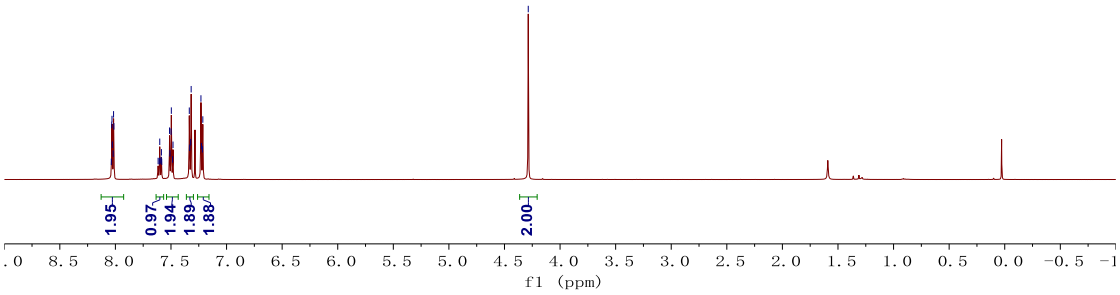

-116.0107
F
O
f1 (ppm)

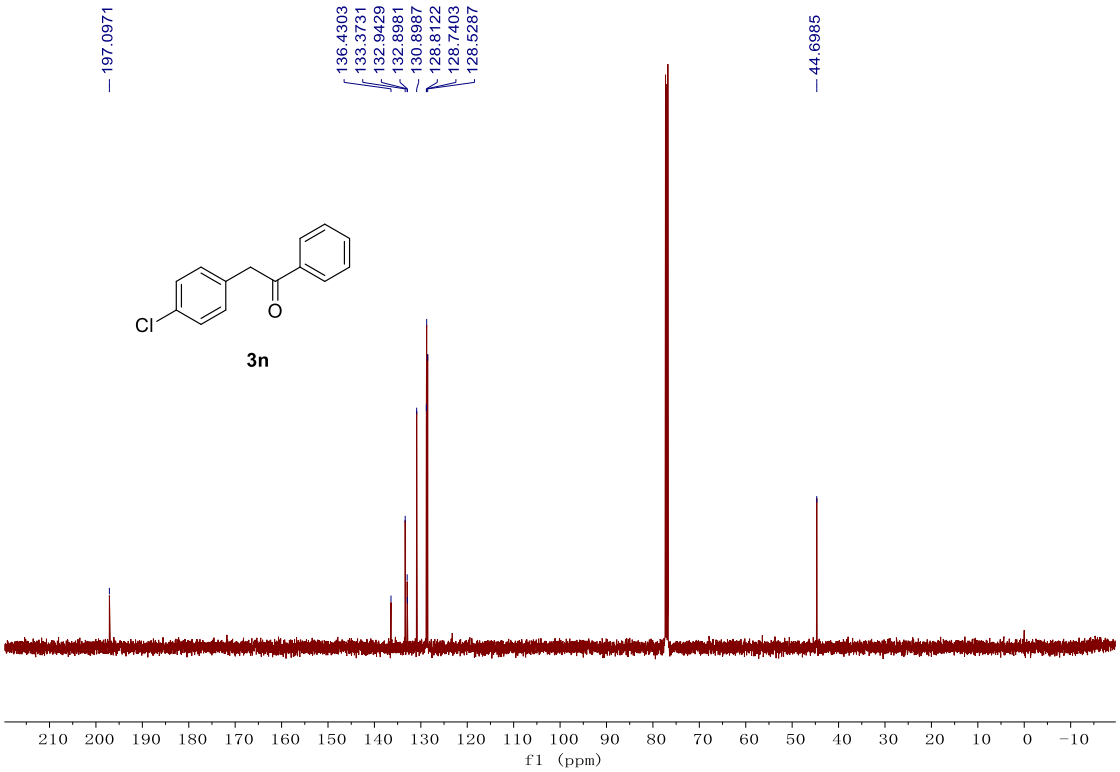
3m


8.0330
8.0306
8.0278
8.0205
8.0166
7.6047
7.6010
7.5975
7.5888
7.5861
7.5834
7.5128
7.5094
7.4994
7.4968
7.4854
7.4818
7.3353
7.3313
7.3226
7.3185
7.2305
7.2262
7.2175
7.2136
4.2861

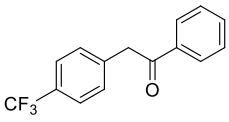

Cl
O

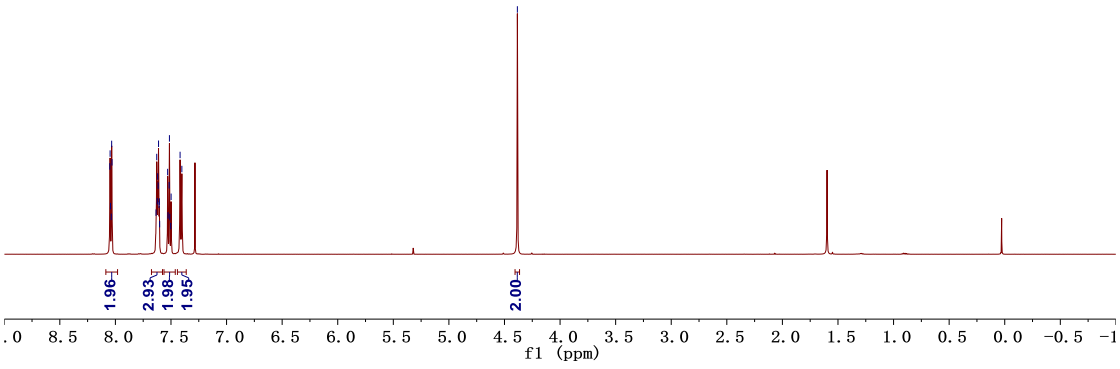
3n

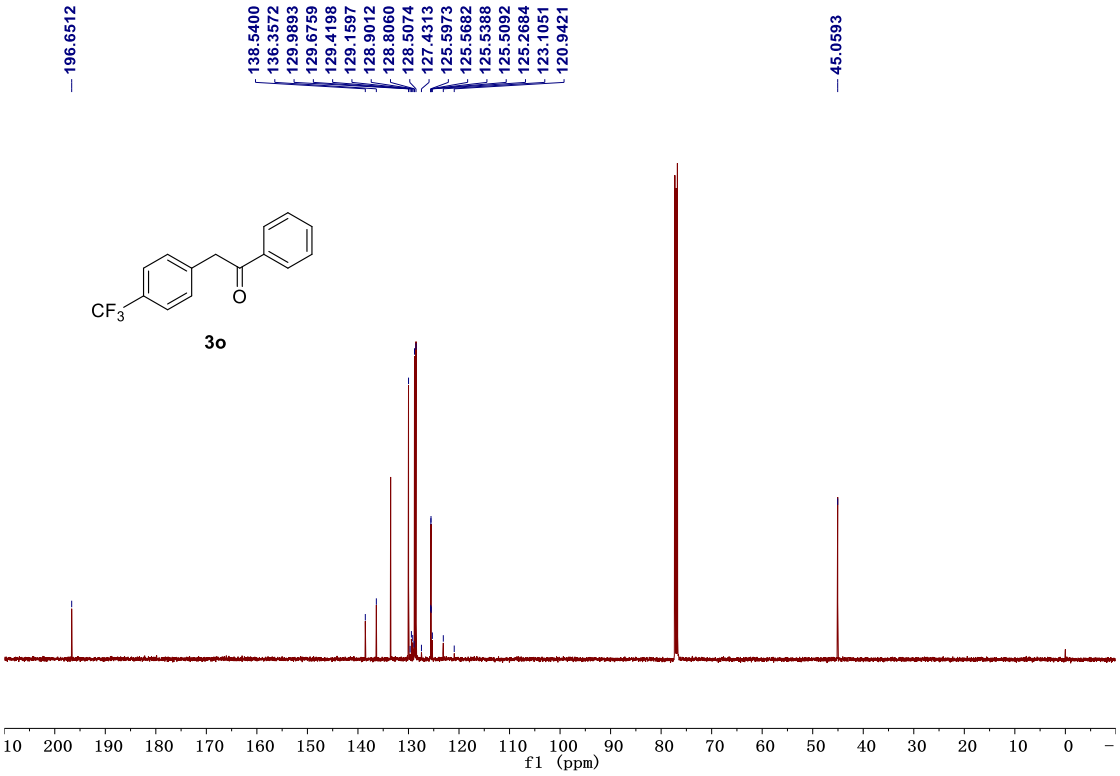

1.95
0.97
1.94
1.89
1.88
2.00
f1 (ppm)

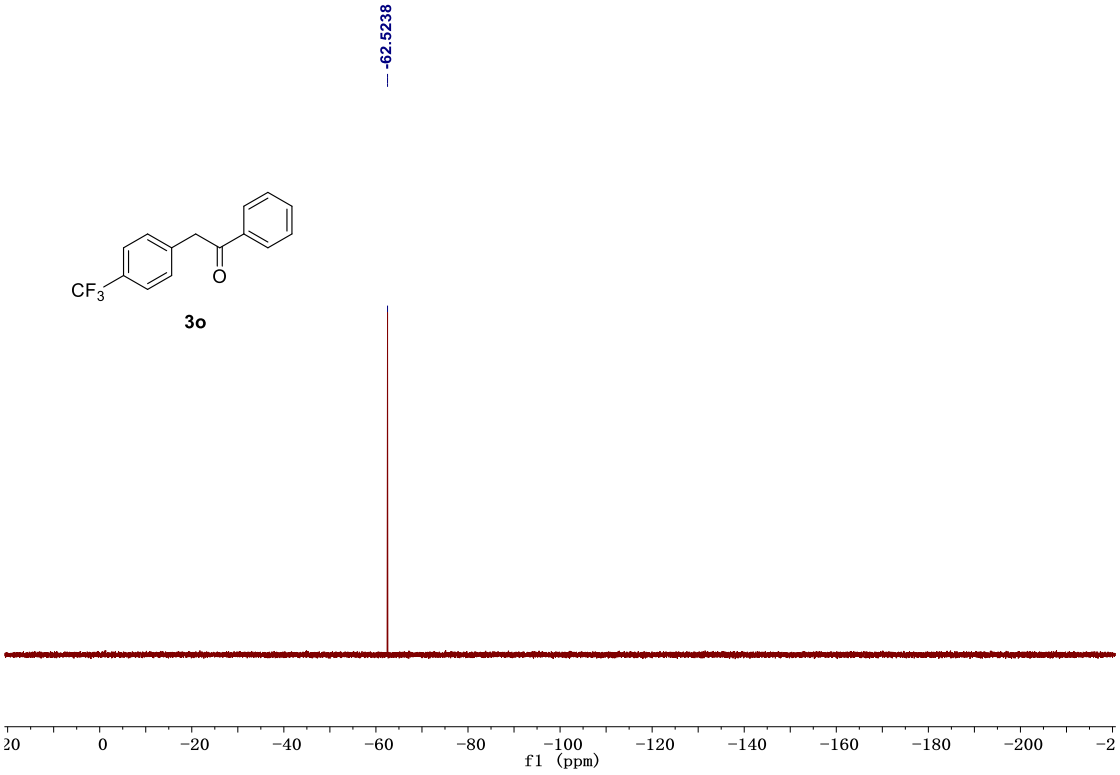

197.0971
136.4303
133.3731
132.9429
132.8981
130.8987
128.8122
128.7403
128.5287
44.6985
Cl
O
3n
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 −10
f1 (ppm)

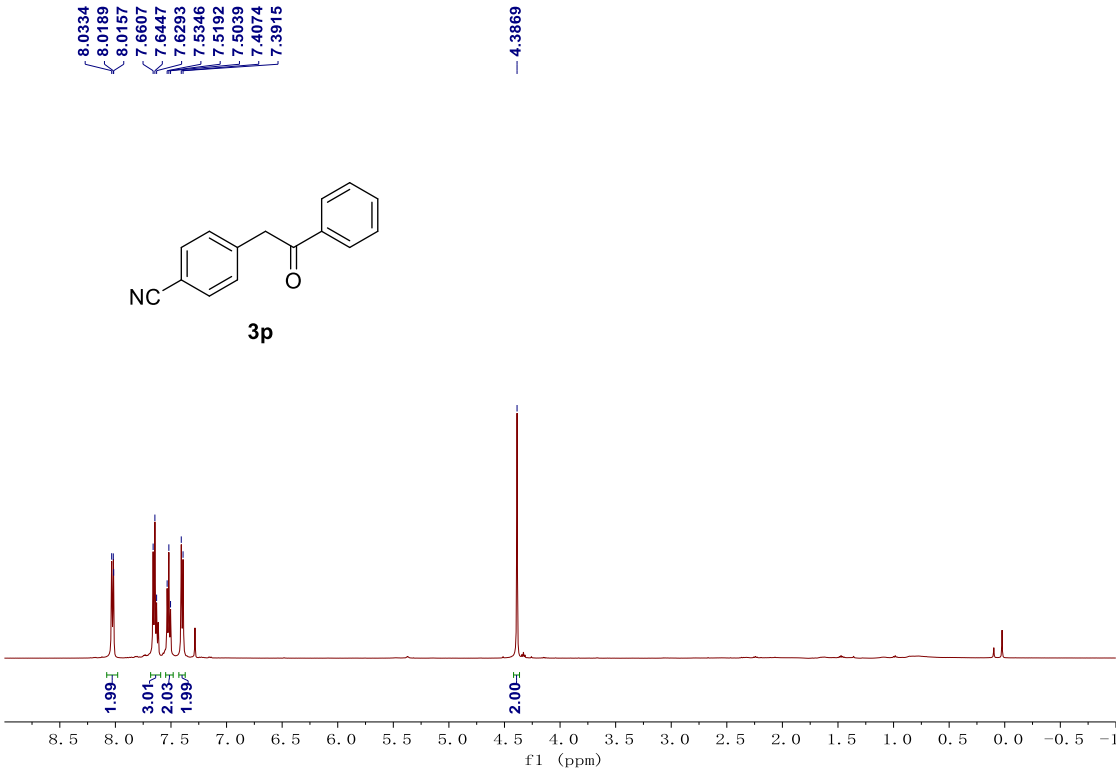

8.0500
8.0476
8.0445
8.0374
8.0336
8.0306
7.6343
7.6282
7.6236
7.6196
7.6157
7.6119
7.6073
7.6047
7.6020
7.5300
7.5265
7.5166
7.5139
7.5106
7.5025
7.4989
7.4182
7.4022
4.3841

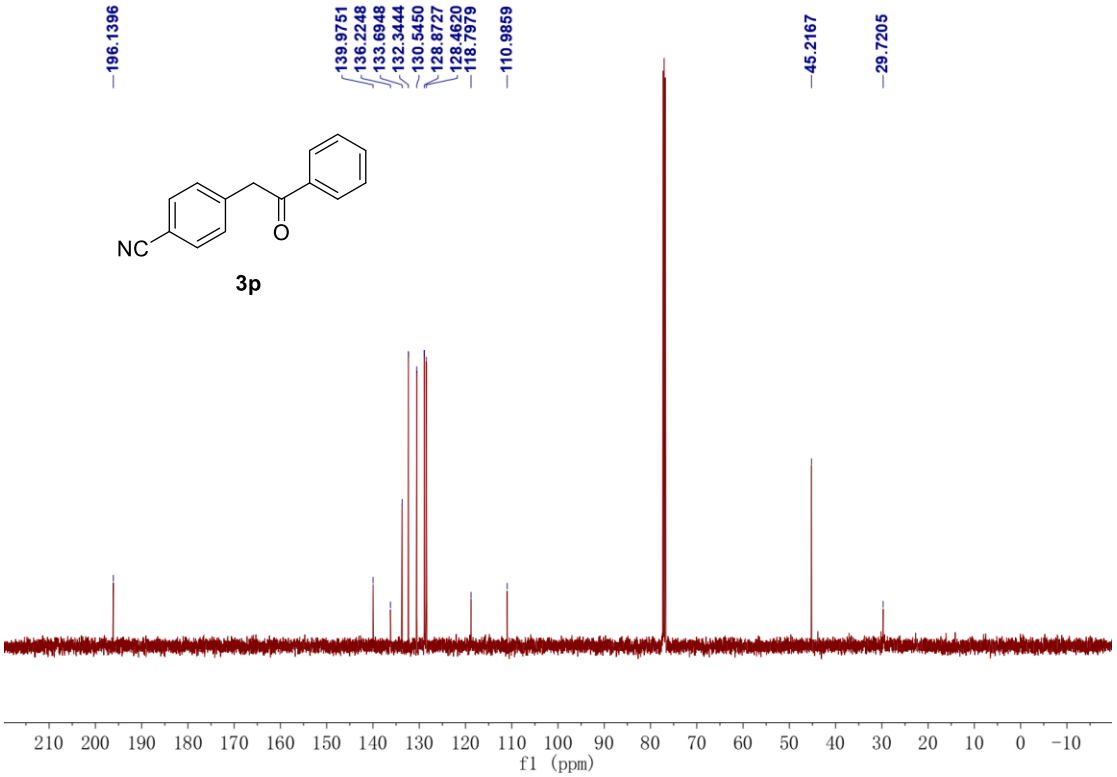

CF3
O
3o

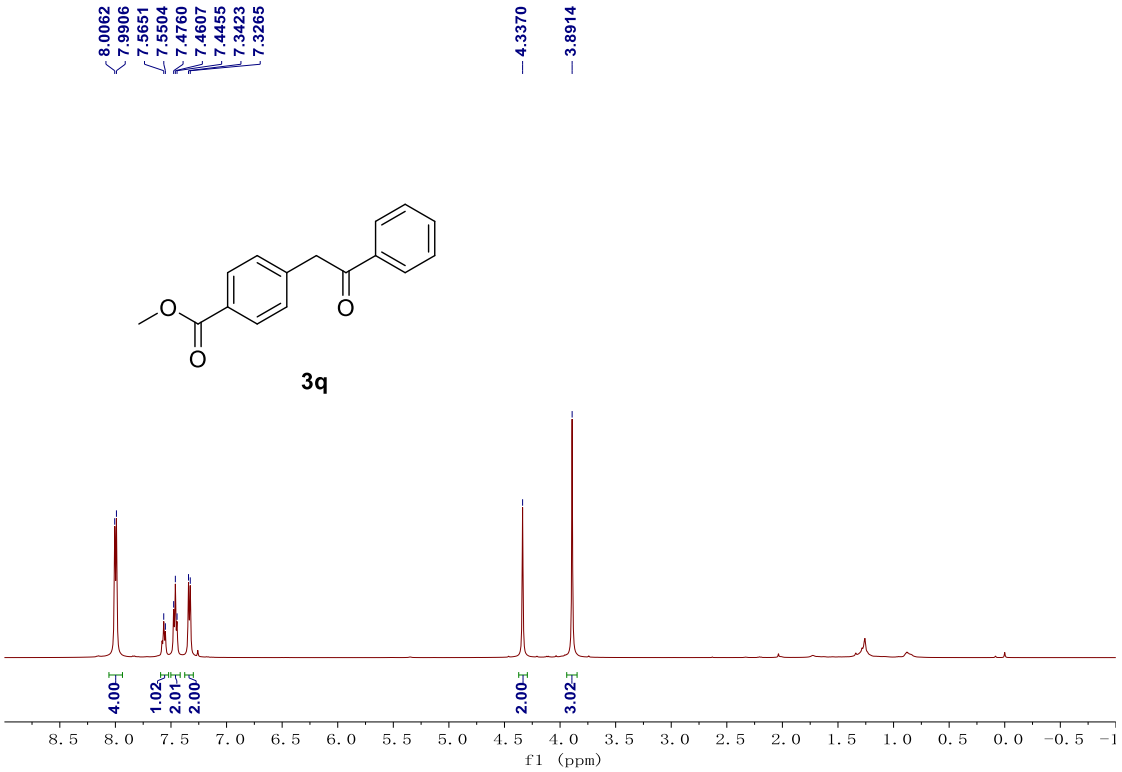

1.96
2.93
1.98
1.95
2.00
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 −0.5 −1
f1 (ppm)

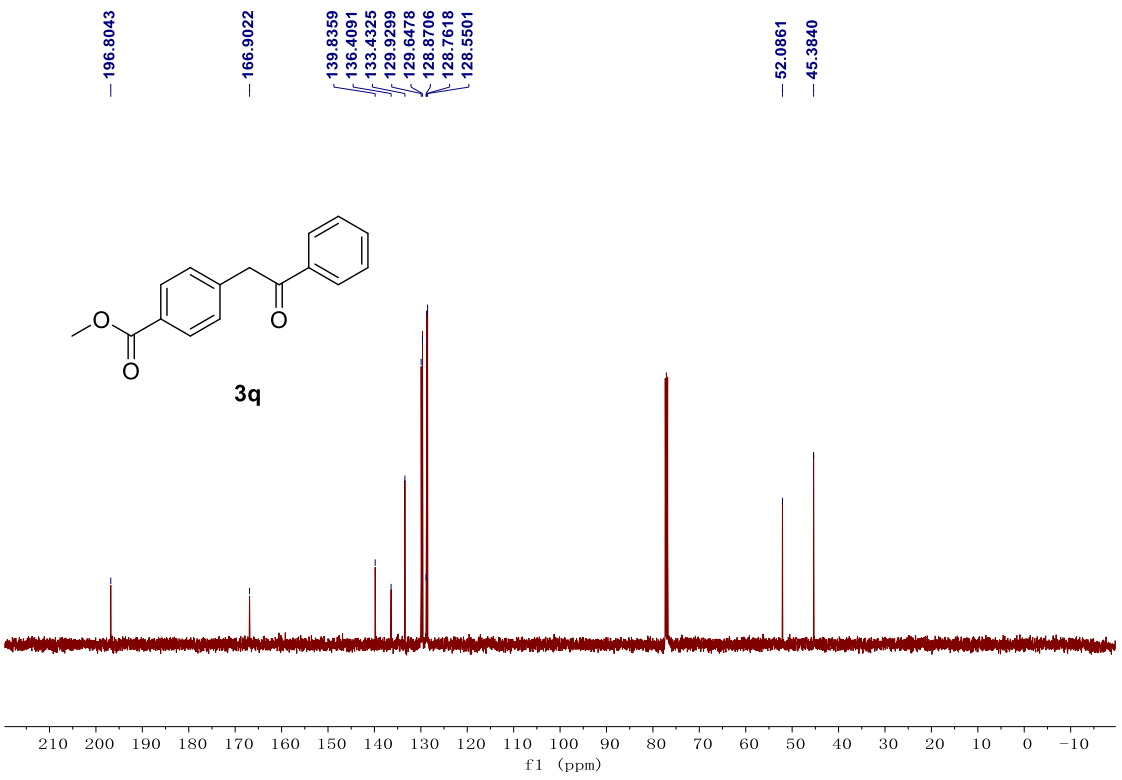

196.6512
138.5400
136.3572
129.9893
129.6759
129.4198
129.1597
128.9012
128.8060
128.5074
127.4313
125.5973
125.5682
125.5388
125.5092
125.2684
123.1051
120.9421
45.0593
CF3
O
3o
f1 (ppm)


-62.5238
CF3
O
3o
f1 (ppm)


8.0334
8.0189
8.0157
7.6607
7.6447
7.6293
7.5346
7.5192
7.5039
7.4074
7.3915
4.3869
NC
O
3p
1.99
3.01
2.03
1.99
2.00
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 −0.5 −1
f1 (ppm)


196.1396
139.9751
136.2248
133.6948
132.3444
130.5450
128.8727
128.4620
118.7979
110.9859
45.2167
29.7205
NC
O
3p
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 −10
f1 (ppm)


8.0062
7.9906
7.5651
7.5504
7.4760
7.4607
7.4455
7.3423
7.3265
4.3370
3.8914
3q
4.00
1.02
2.01
2.00
2.00
3.02
f1 (ppm)


196.8043
166.9022
139.8359
136.4091
133.4325
129.9299
129.6478
128.8706
128.7618
128.5501
52.0861
45.3840
3q
f1 (ppm)


8.0098
7.9952
7.9921
7.5587
7.5440
7.5320
7.5291
7.5263
7.4627
7.4474
7.4356
7.4320
7.4239
7.4204
7.4063
7.3844
7.3795
7.3696
7.3568
7.3540
7.3272
7.3240
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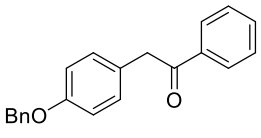
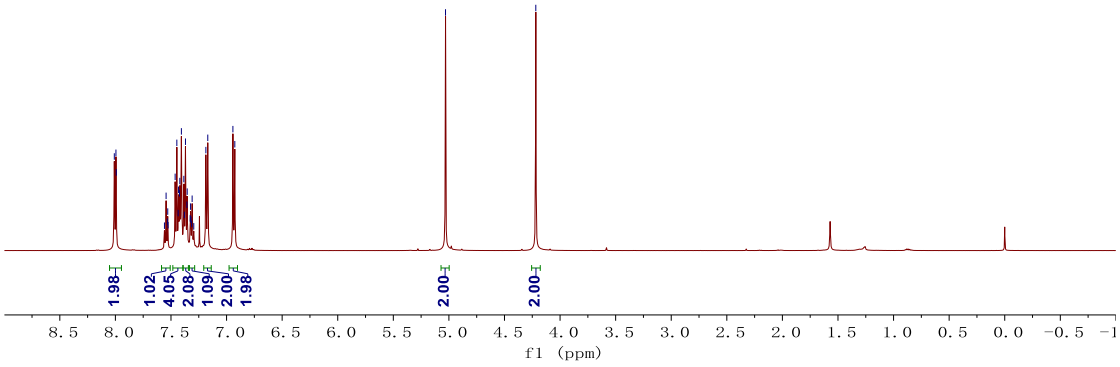
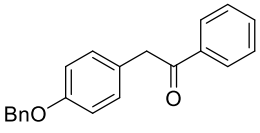
7.1690
6.9430
6.9258
5.0304
4.2182


BnO
O

3r

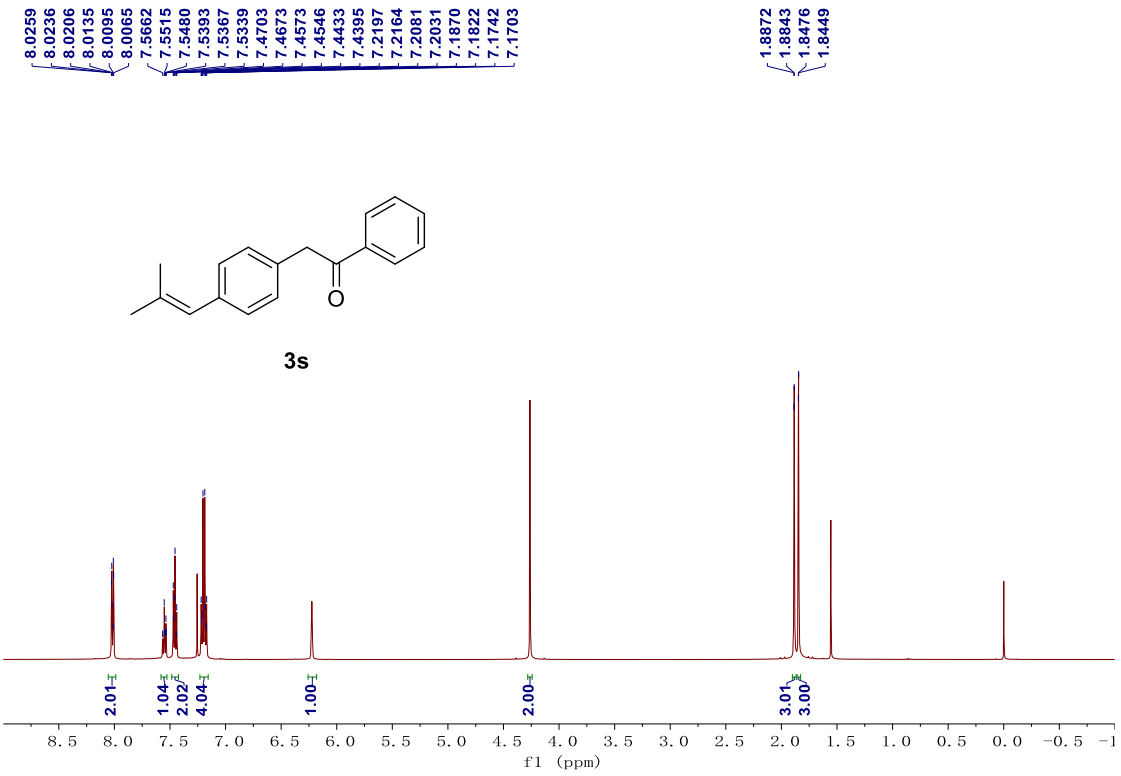

1.98
1.02
4.05
2.08
1.09
2.00
1.98
2.00
2.00
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 −0.5 −1
f1 (ppm)

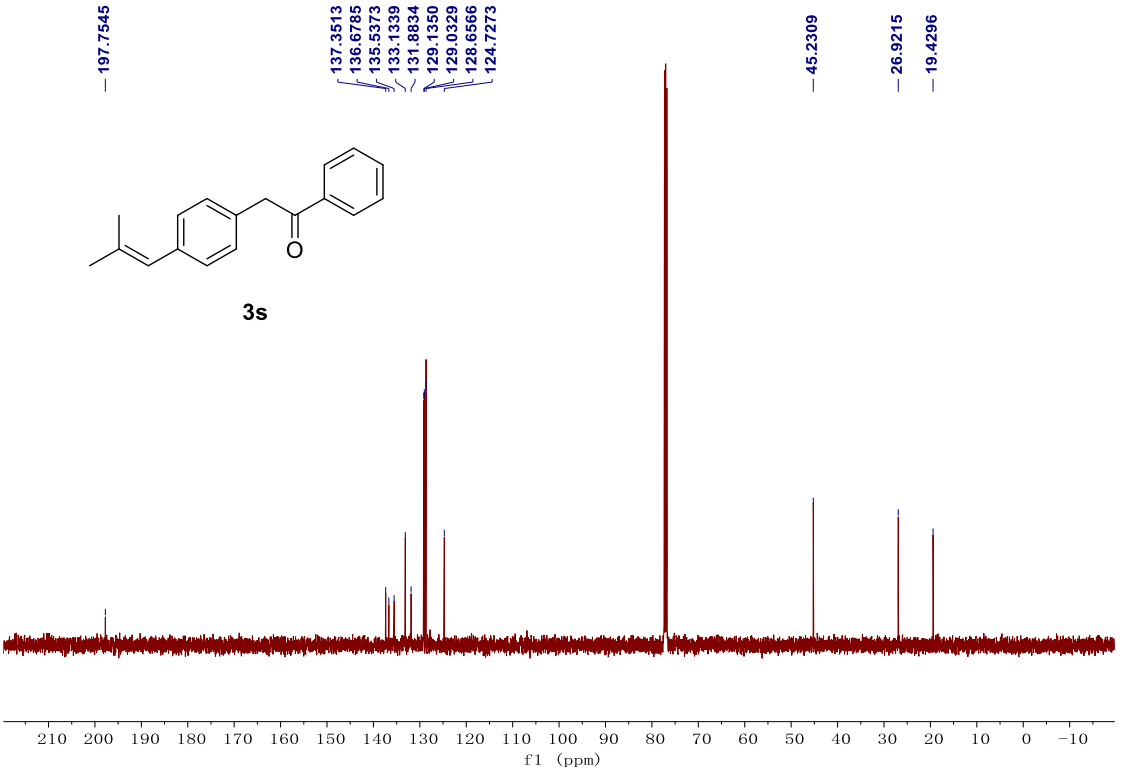

197.9152
157.8314
137.0506
136.6493
133.1331
130.5299
128.6528
128.6231
128.6018
127.9723
127.4976
126.8244
115.1083
70.0540
44.6466

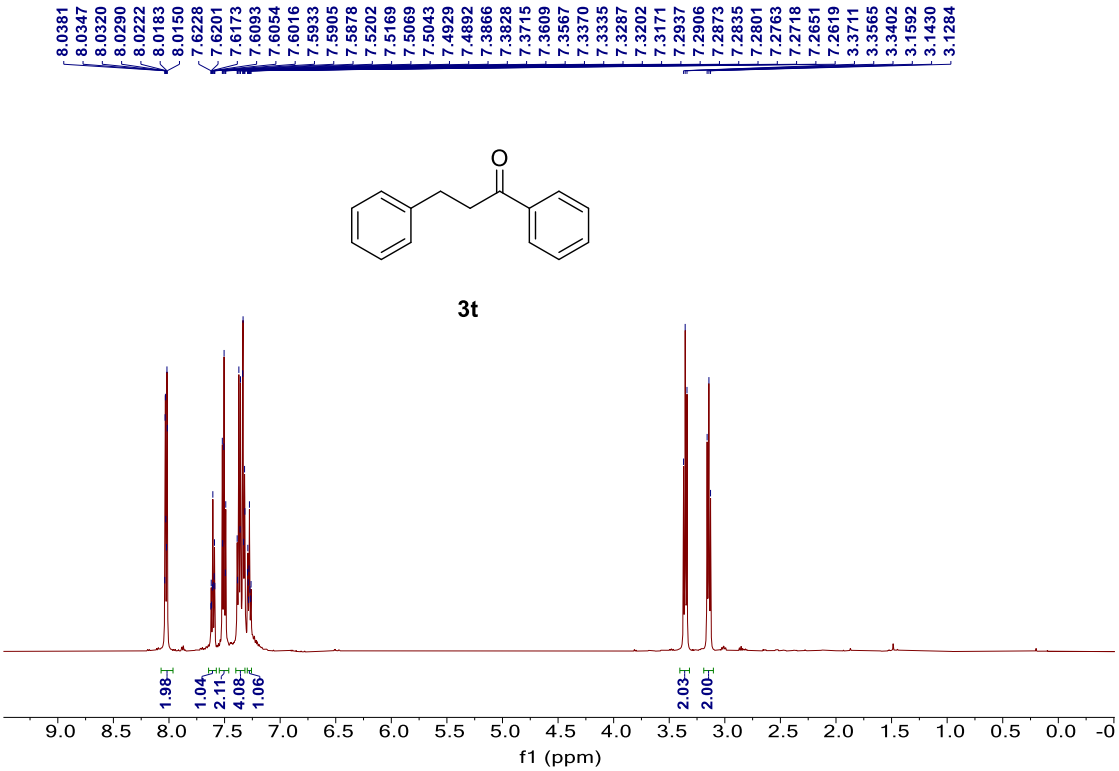

BnO
O

3r

210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 −10
f1 (ppm)


8.0259
8.0236
8.0206
8.0135
8.0095
8.0065
7.5662
7.5515
7.5480
7.5393
7.5367
7.5339
7.4703
7.4673
7.4573
7.4546
7.4433
7.4395
7.2197
7.2164
7.2081
7.2031
7.1870
7.1822
7.1742
7.1703
1.8872
1.8843
1.8476
1.8449
O
3s
2.01
1.04
2.02
4.04
1.00
2.00
3.01
3.00
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 −0.5 −1
f1 (ppm)


197.7545
137.3513
136.6785
135.5373
133.1339
131.8834
129.1350
129.0329
128.6566
124.7273
45.2309
26.9215
19.4296
O
3s
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 −10
f1 (ppm)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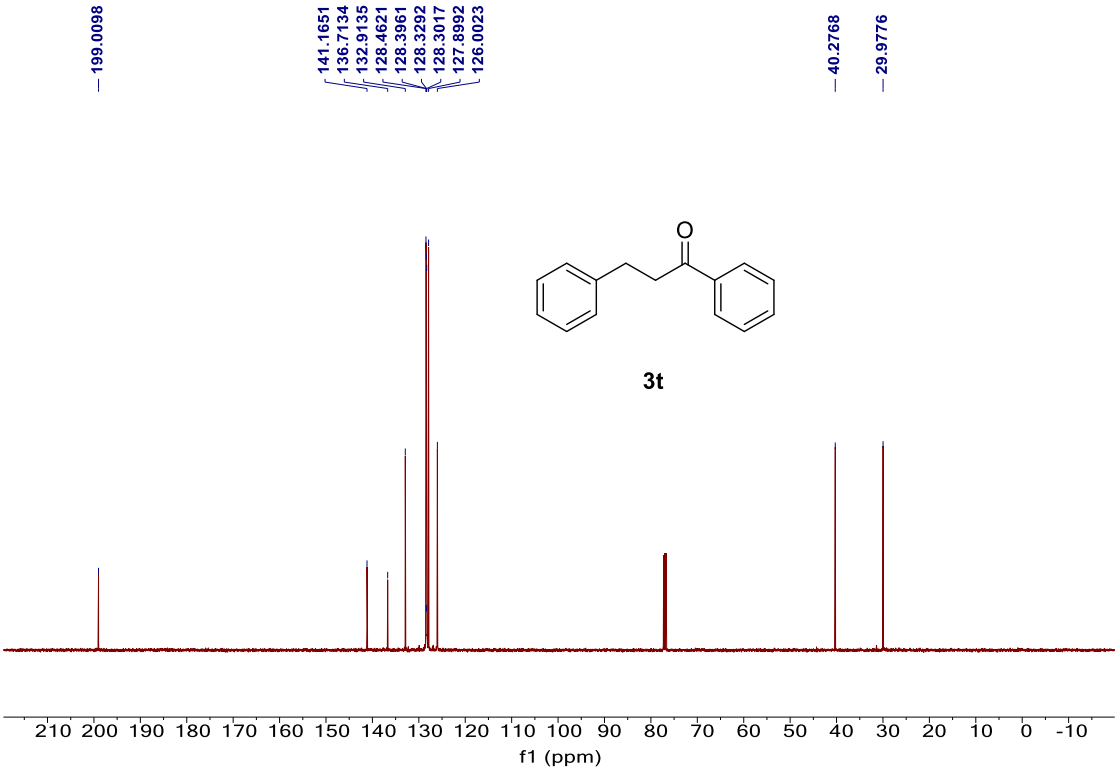
8.0347
8.0320
8.0290
8.0222
8.0183
8.0150
7.6228
7.6201
7.6173
7.6093
7.6054
7.6016
7.5933
7.5905
7.5878
7.5202
7.5169
7.5069
7.5043
7.4929
7.4892
7.3866
7.3828
7.3715
7.3609
7.3567
7.3370
7.3335
7.3287
7.3202
7.3171
7.2937
7.2906
7.2873
7.2835
7.2801
7.2763
7.2718
7.2651
7.2619
3.3711
3.3565
3.3402
3.1592
3.1430
3.1284
O
3t
1.98
1.04
2.11
4.08
1.06
2.03
2.00
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
f1 (ppm)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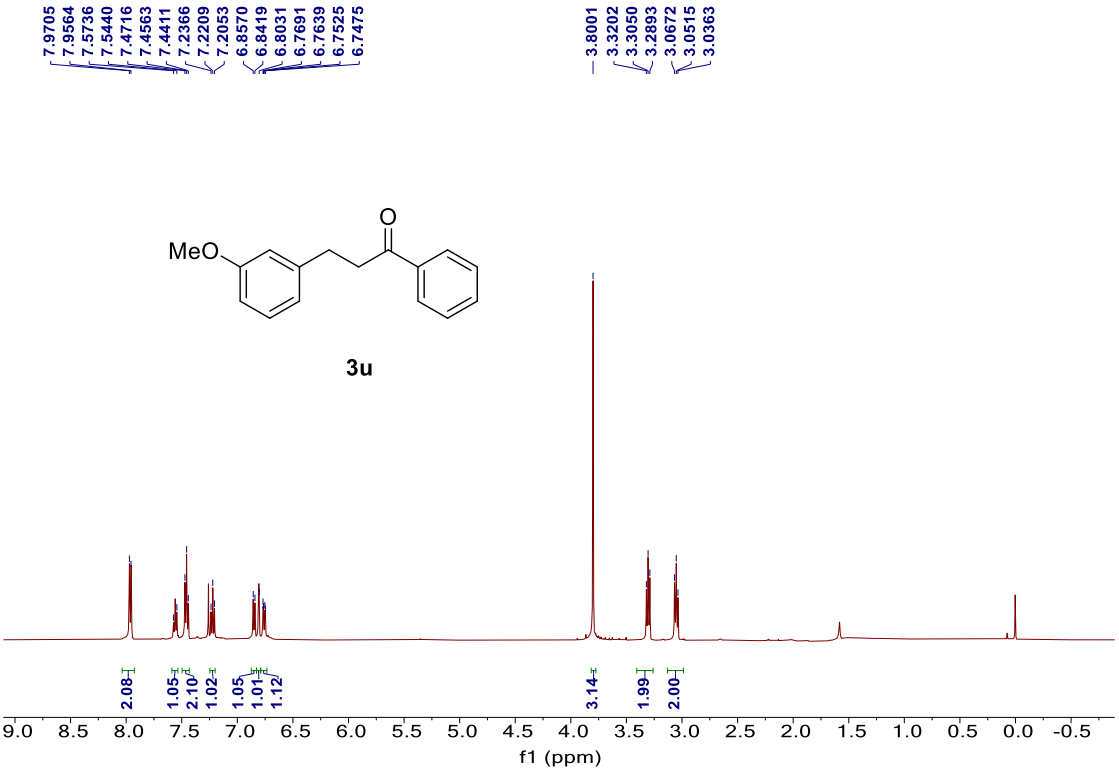
141.1651
136.7134
132.9135
128.4621
128.3961
128.3292
128.3017
127.8992
126.0023
40.2768
29.9776
O
3t
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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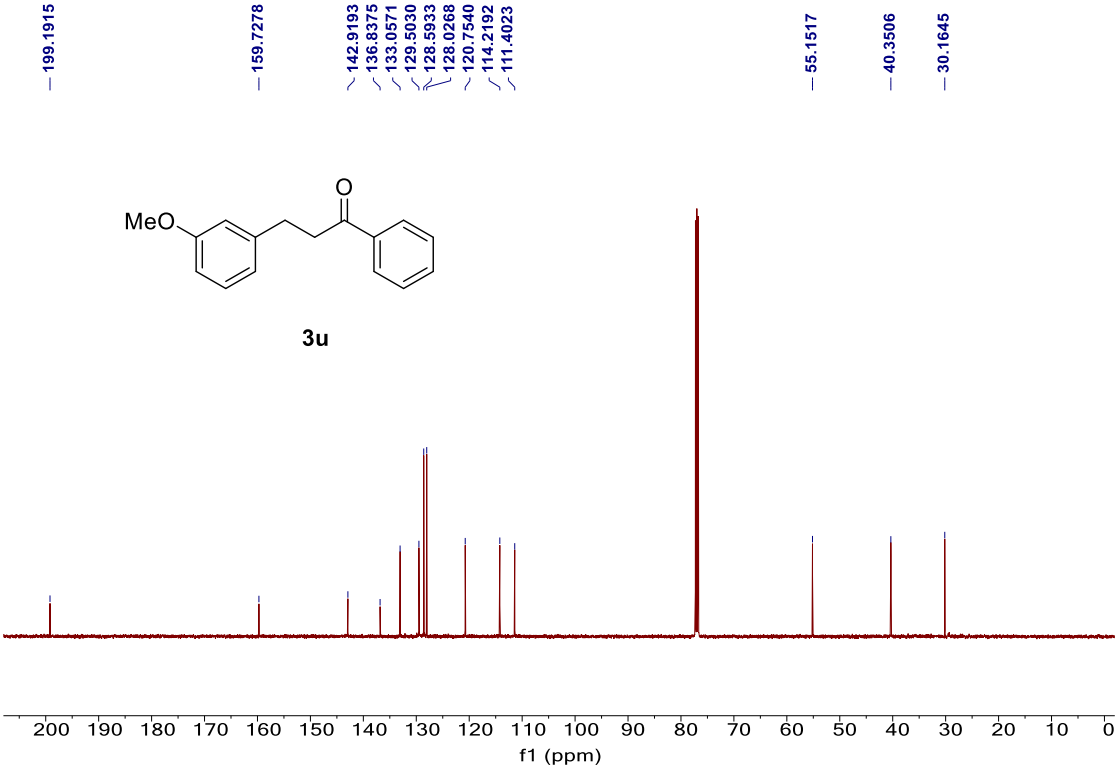
7.9564
7.5736
7.5440
7.4716
7.4563
7.4411
7.2366
7.2209
7.2053
6.8570
6.8419
6.8031
6.7691
6.7639
6.7525
6.7475
3.8001
3.3202
3.3050
3.2893
3.0672
3.0515
3.0363
MeO
O
3u
2.08
1.05
2.10
1.02
1.05
1.01
1.12
3.14
1.99
2.00
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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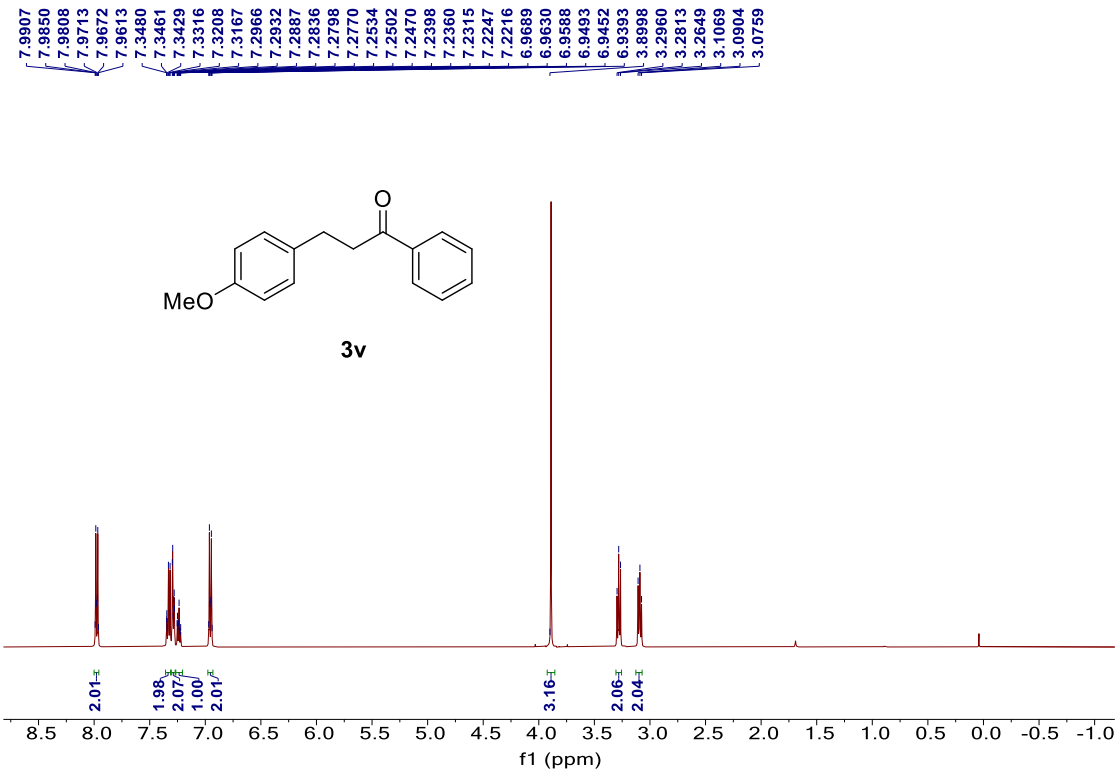
159.7278
142.9193
136.8375
133.0571
129.5030
128.5933
128.0268
120.7540
114.2192
111.4023
55.1517
40.3506
30.1645
MeO
O
3u
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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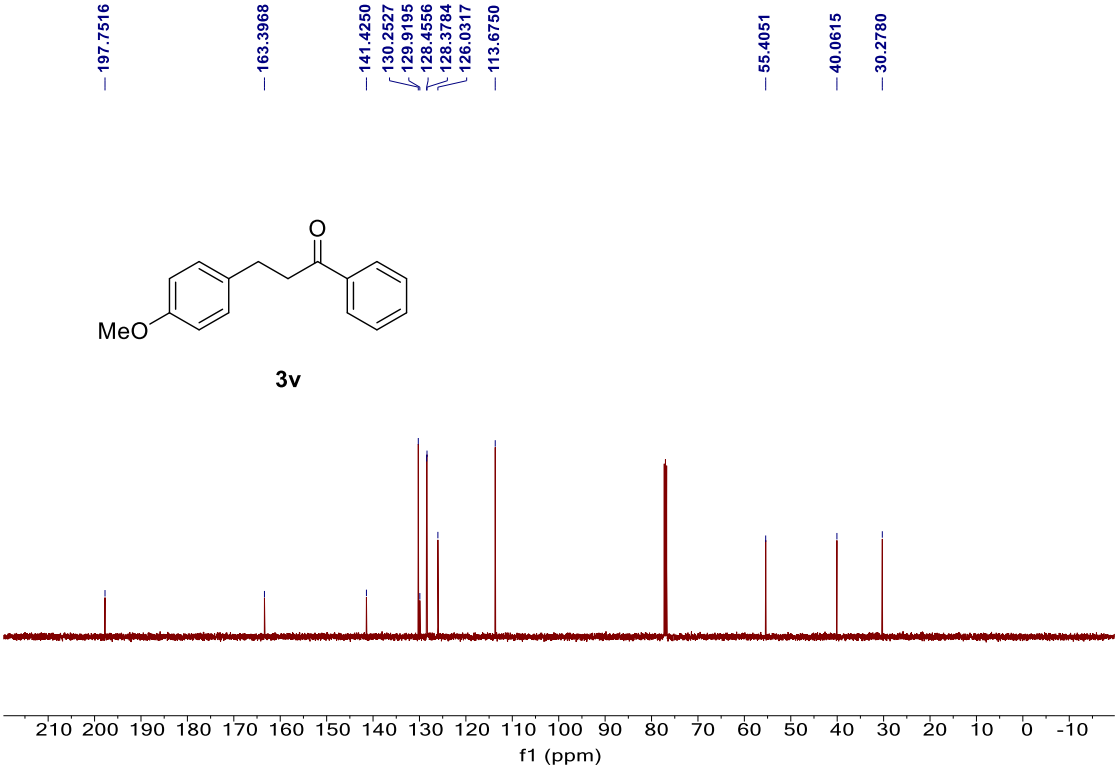
7.9850
7.9808
7.9713
7.9672
7.9613
7.3480
7.3461
7.3429
7.3316
7.3208
7.3167
7.2966
7.2932
7.2887
7.2836
7.2798
7.2770
7.2534
7.2502
7.2470
7.2398
7.2360
7.2315
7.2247
7.2216
6.9689
6.9630
6.9588
6.9493
6.9452
6.9393
3.8998
3.2960
3.2813
3.2649
3.1069
3.0904
3.0759
O
MeO
3v
2.01
1.98
2.07
1.00
2.01
3.16
2.06
2.04
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0
f1 (ppm)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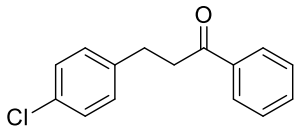
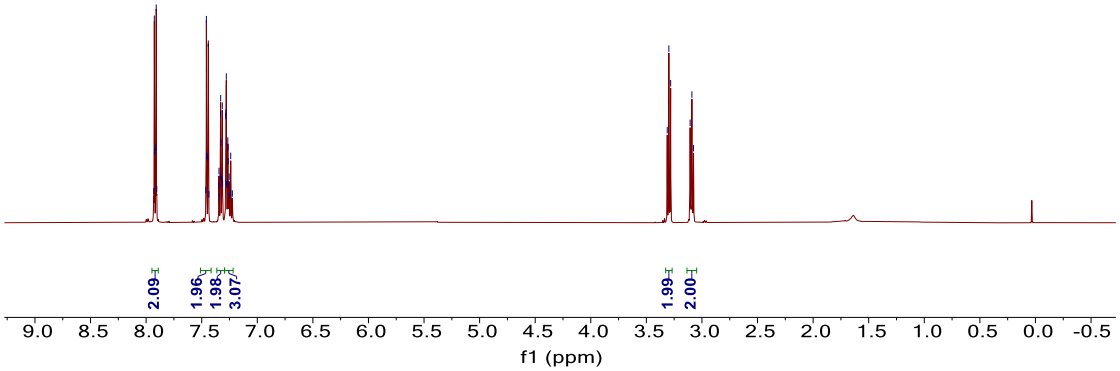
141.4250
130.2527
129.9195
128.4556
128.3784
126.0317
113.6750
55.4051
40.0615
30.2780
O
MeO
3v
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

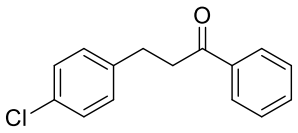

7.9313
7.9263
7.9225
7.9130
7.9091
7.9042
7.4630
7.4580
7.4541
7.4447
7.4409
7.4358
7.3463
7.3444
7.3411
7.3330
7.3307
7.3293
7.3275
7.3187
7.3148
7.3121
7.2842
7.2821
7.2788
7.2743
7.2686
7.2654
7.2636
7.2623
7.2562
7.2534
7.2504
7.2428
7.2390
7.2244
3.3125
3.2978
3.2817
3.1065
3.0905
3.0758


O
Cl

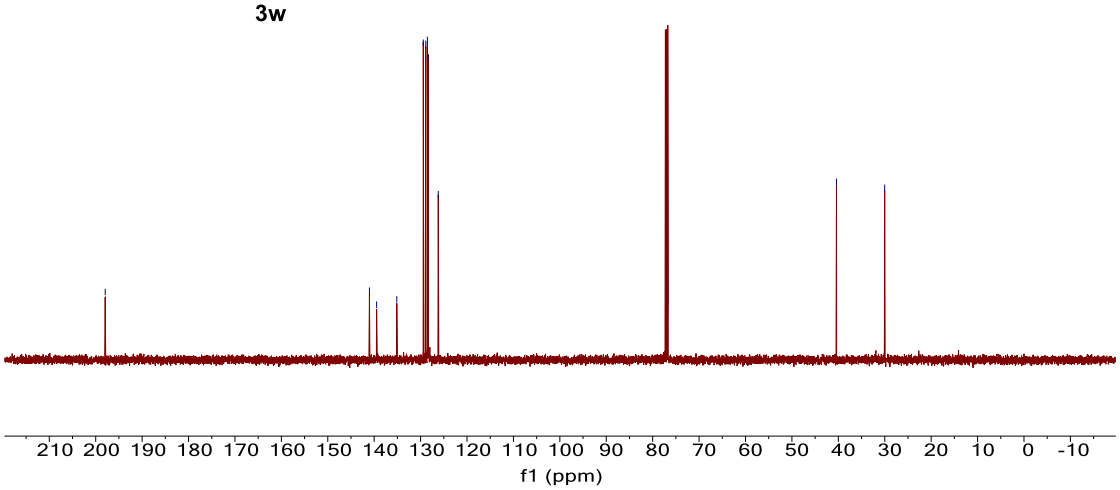
3w


2.09
1.96
1.98
3.07
1.99
2.00
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)


197.9528
141.0230
139.4779
135.1317
129.4260
128.8923
128.5389
128.3773
126.1954
40.3948
30.0168


O
Cl

3w


210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


7.9235
7.9092
7.9061
7.5535
7.5507
7.5386
7.5268
7.5239
7.5211
7.4367
7.4252
7.4213
7.3009
7.2969
7.2856
7.2751
7.2707
7.2120
7.2069
7.1965
7.1909
7.1797
7.1765
2.9889
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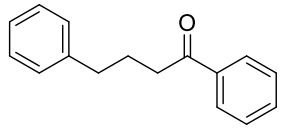
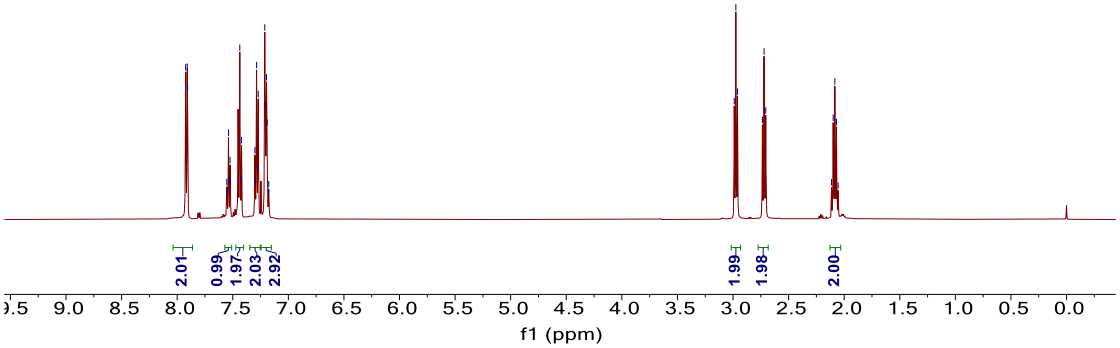
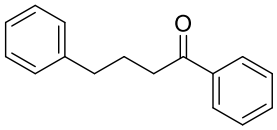
2.9598
2.7356
2.7206
2.7054
2.1139
2.0990
2.0840
2.0691
2.0545


O

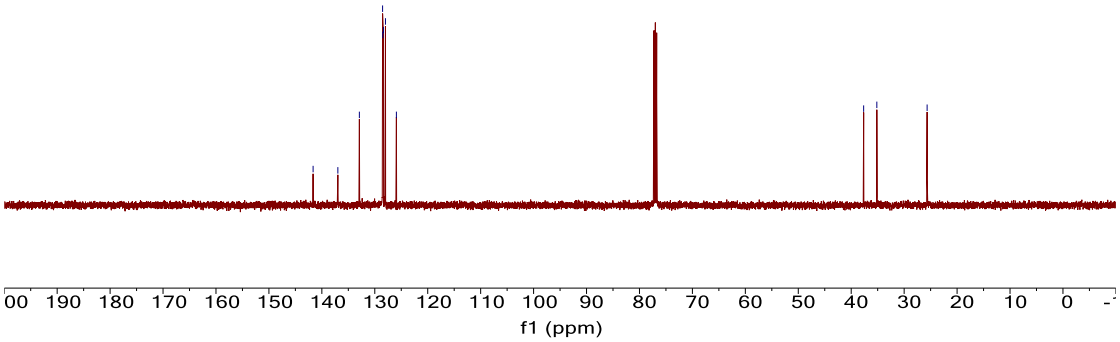
3x


2.01
0.99
1.97
2.03
2.92
1.99
1.98
2.00
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
f1 (ppm)

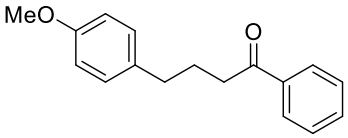

141.6537
136.9778
132.9120
128.5242
128.4873
128.3671
127.9833
125.9190
37.6508
35.1608
25.6621


O

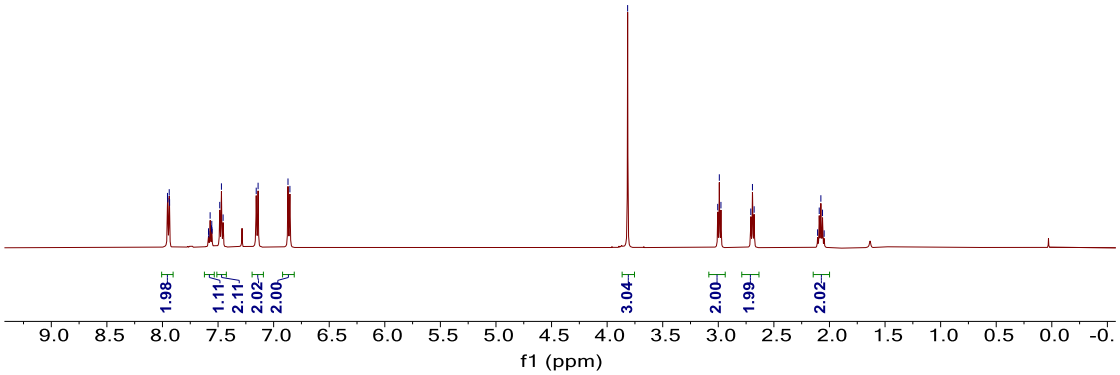
3x


00 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

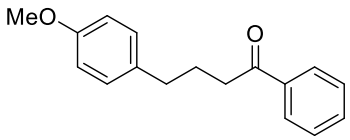

7.9549
7.9522
7.9392
7.9359
7.5859
7.5834
7.5712
7.5589
7.5563
7.5537
7.4849
7.4696
7.4544
7.1566
7.1399
6.8709
6.8537
3.8156
3.0053
2.9908
2.9762
2.7077
2.6927
2.6776
2.1070
2.0921
2.0773
2.0625
2.0477


MeO
O

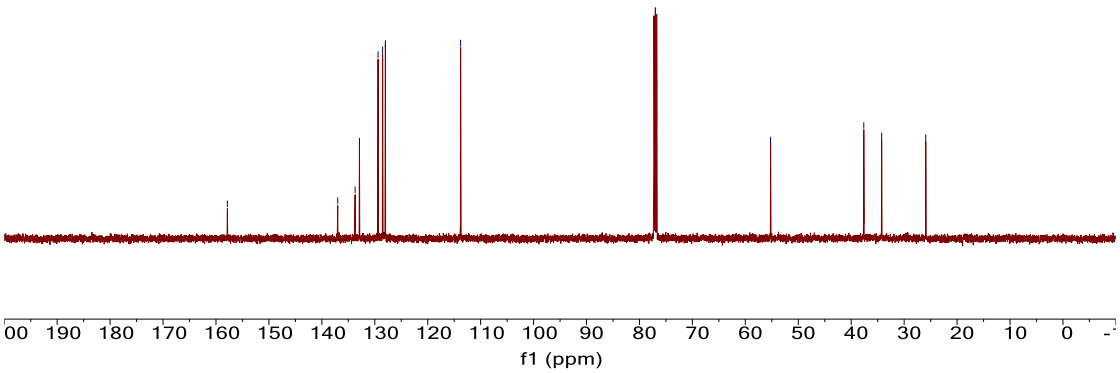
3y

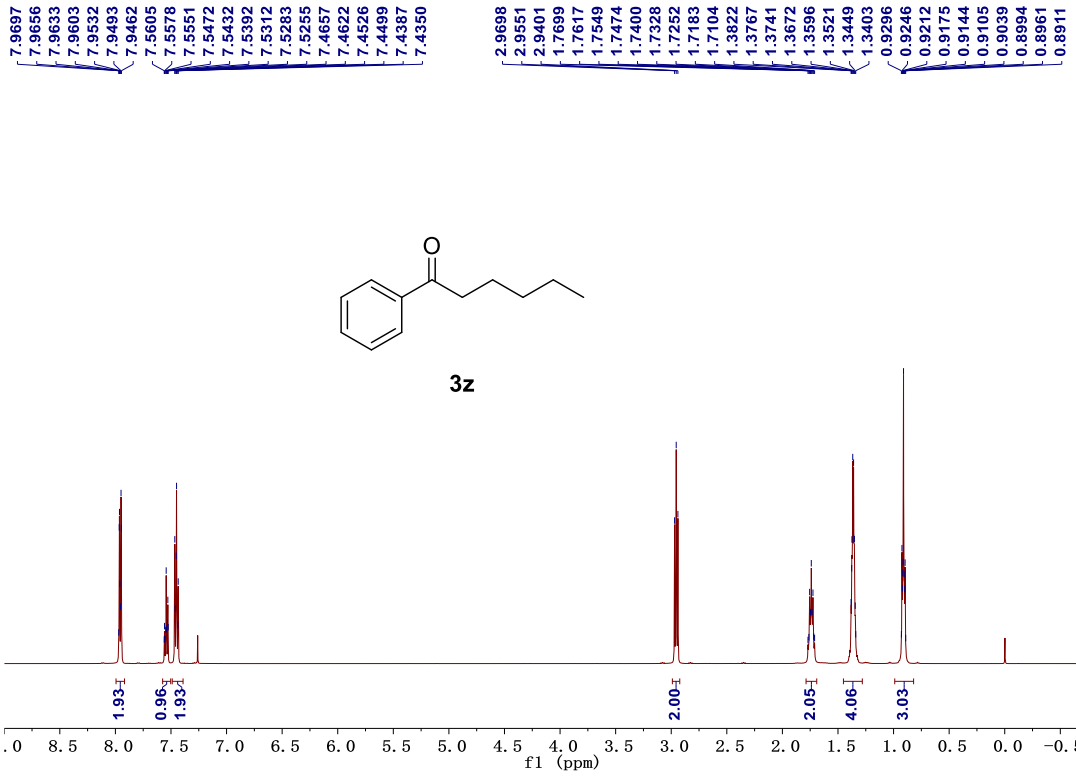

1.98
1.11
2.11
2.02
2.00
3.04
2.00
1.99
2.02
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.
f1 (ppm)

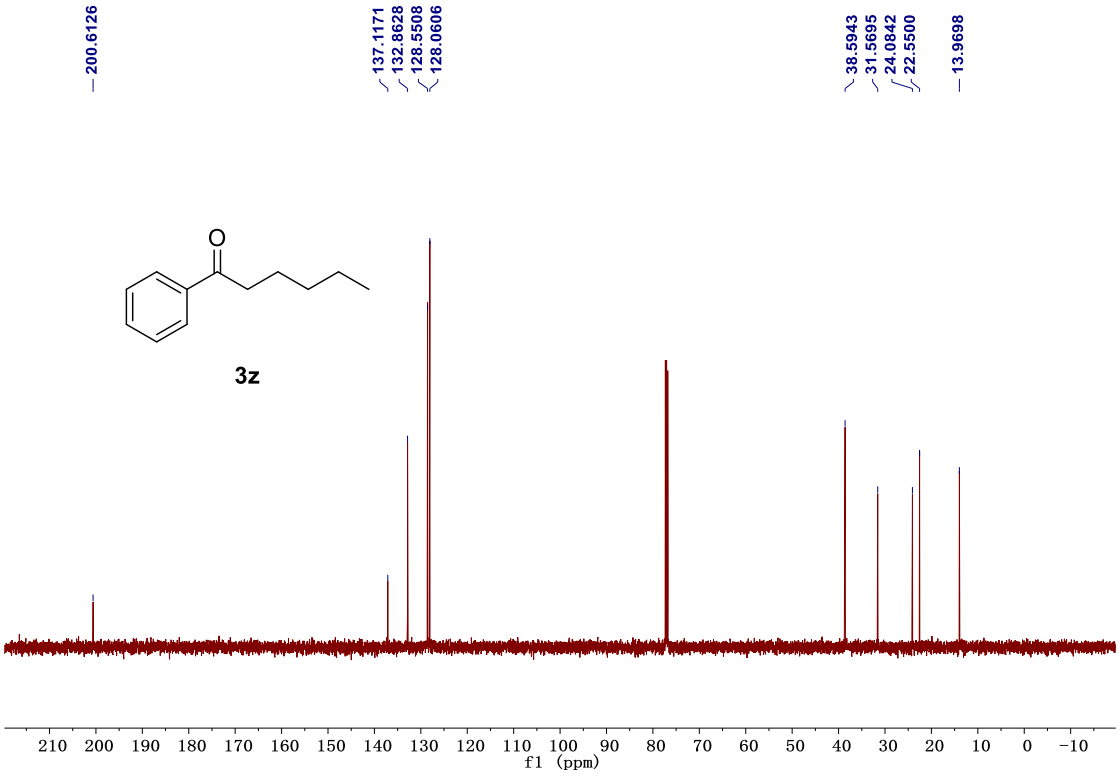

157.8446
137.0029
133.7172
132.8999
129.3819
128.5234
127.9943
113.7880
55.2332
37.6237
34.2499
25.9224


MeO
O

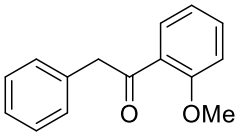
3y


00 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -
f1 (ppm)

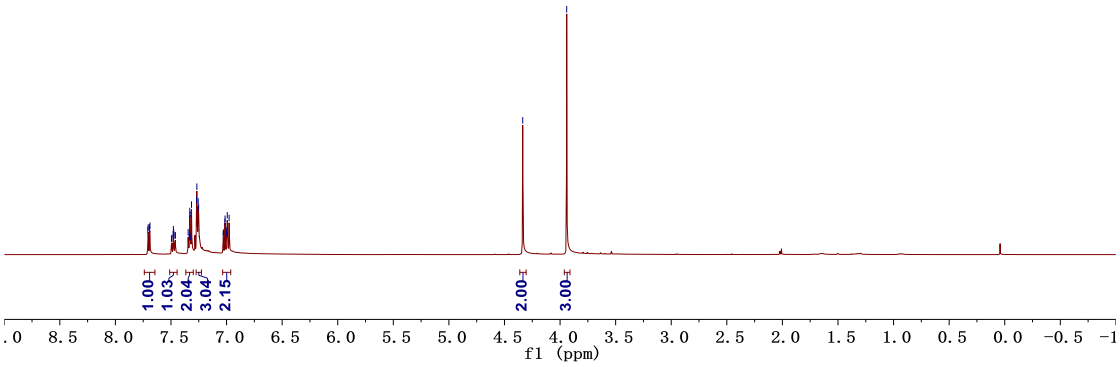

7.9697
7.9656
7.9633
7.9603
7.9532
7.9493
7.9462
7.5605
7.5578
7.5551
7.5472
7.5432
7.5392
7.5312
7.5283
7.5255
7.4657
7.4622
7.4526
7.4499
7.4387
7.4350
2.9698
2.9551
2.9401
1.7699
1.7617
1.7549
1.7474
1.7400
1.7328
1.7252
1.7183
1.7104
1.3822
1.3767
1.3741
1.3672
1.3596
1.3521
1.3449
1.3403
0.9296
0.9246
0.9212
0.9175
0.9144
0.9105
0.9039
0.8994
0.8961
0.8911
O
3z
1.93
0.96
1.93
2.00
2.05
4.06
3.03
f1 (ppm)

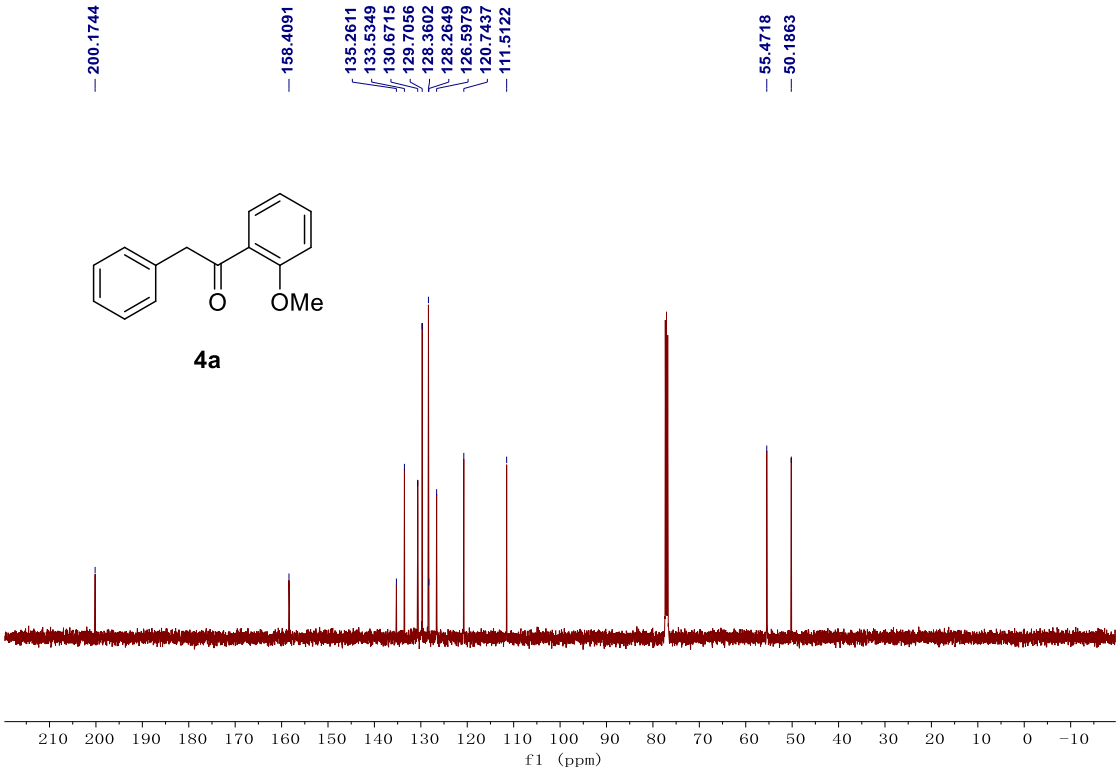

200.6126
137.1171
132.8628
128.5508
128.0606
38.5943
31.5695
24.0842
22.5500
13.9698
O
3z
f1 (ppm)


7.7084
7.7048
7.6931
7.6893
7.4810
7.4783
7.4754
7.4643
7.4607
7.3454
7.3304
7.3280
7.3227
7.3155
7.2701
7.2673
7.2613
7.2557
7.2514
7.0302
7.0283
7.0152
7.0134
7.0003
6.9986
6.9938
6.9770
4.3358
4.3403
3.9403


O
OMe

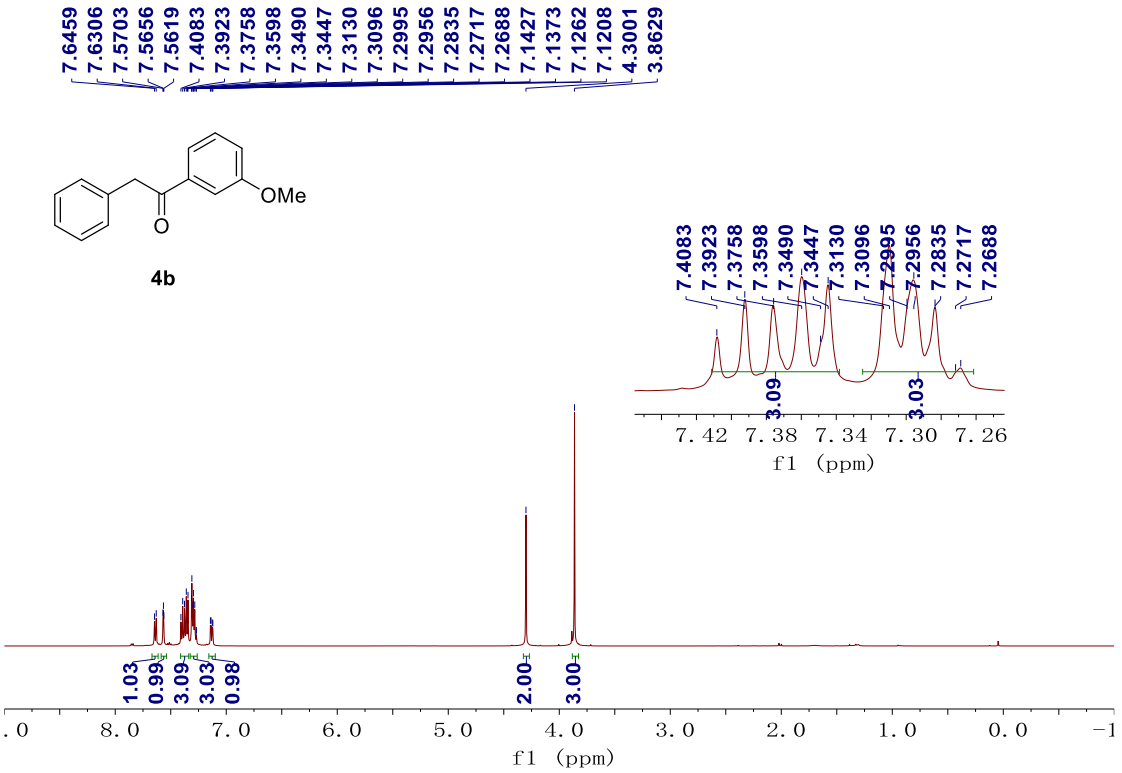
4a

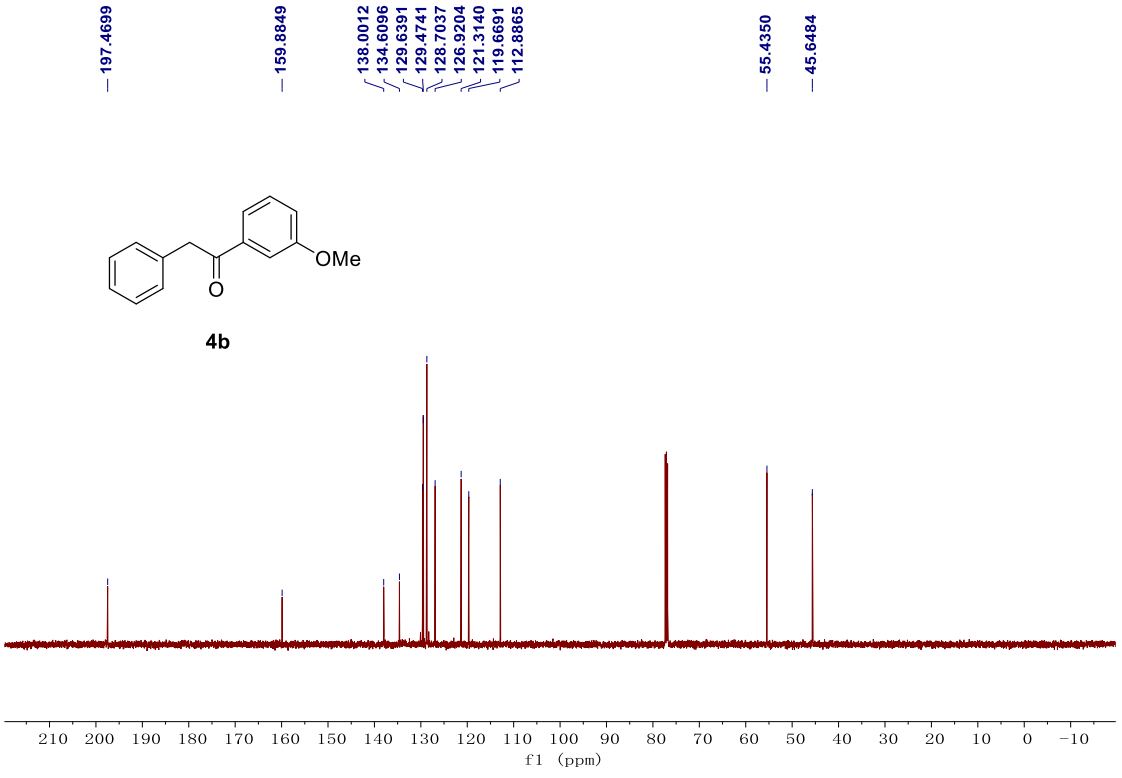

1.00
1.03
2.04
3.04
2.15
2.00
3.00
f1 (ppm)

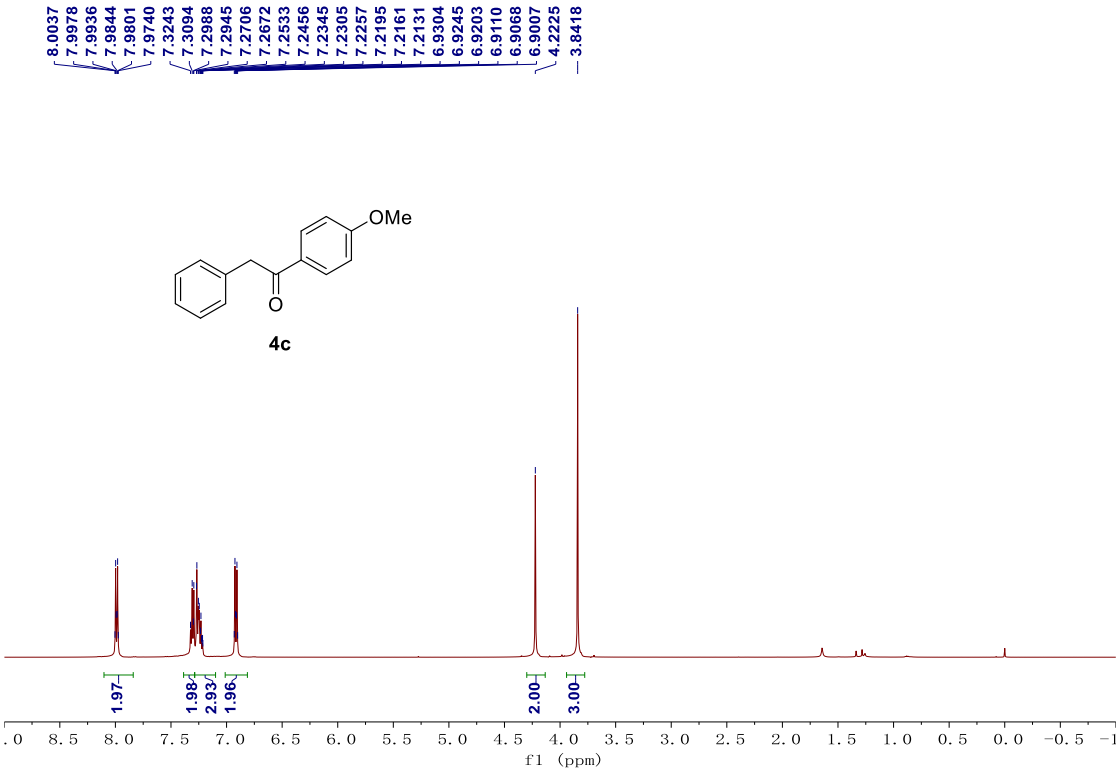

200.1744
158.4091
135.2611
133.5349
130.6715
129.7056
128.3602
128.2649
126.5979
120.7437
111.5122
55.4718
50.1863
f1 (ppm)

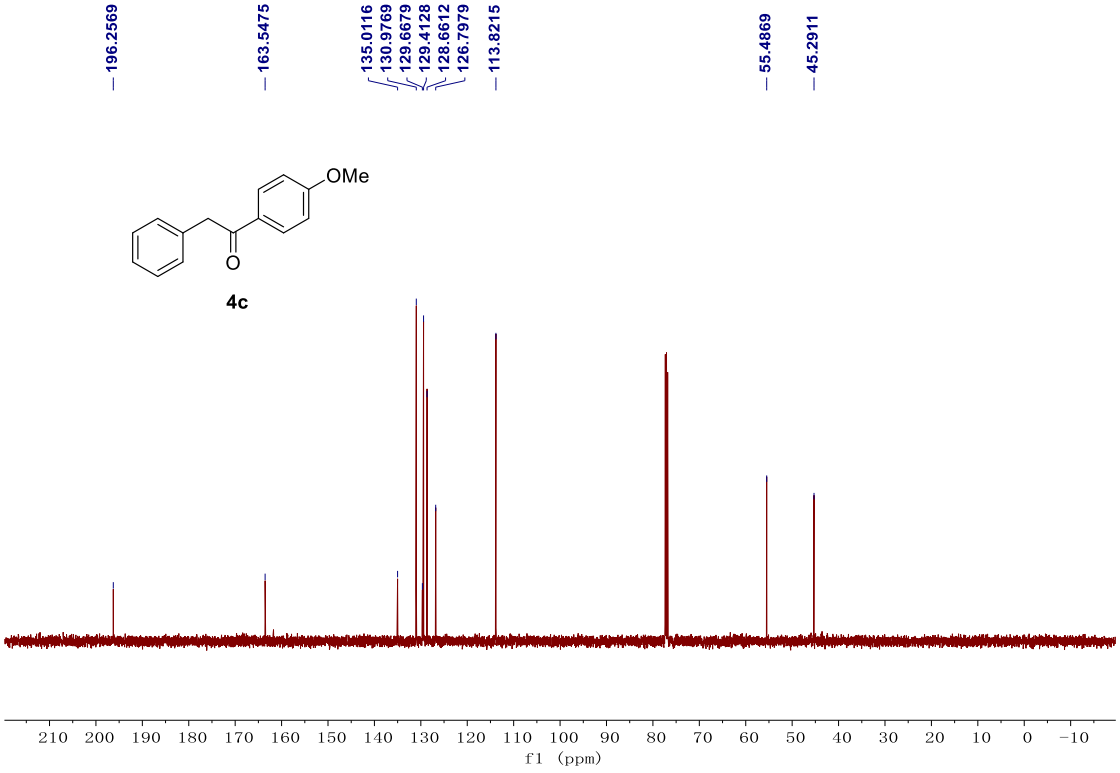
O
OMe

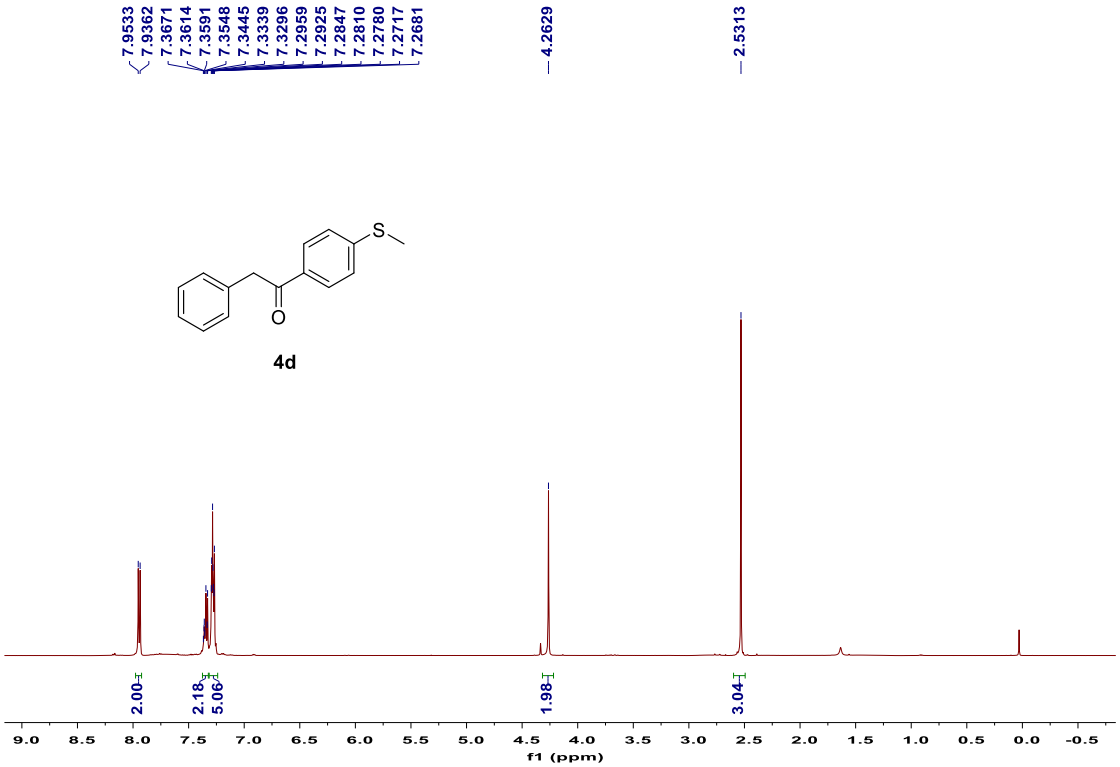
4a

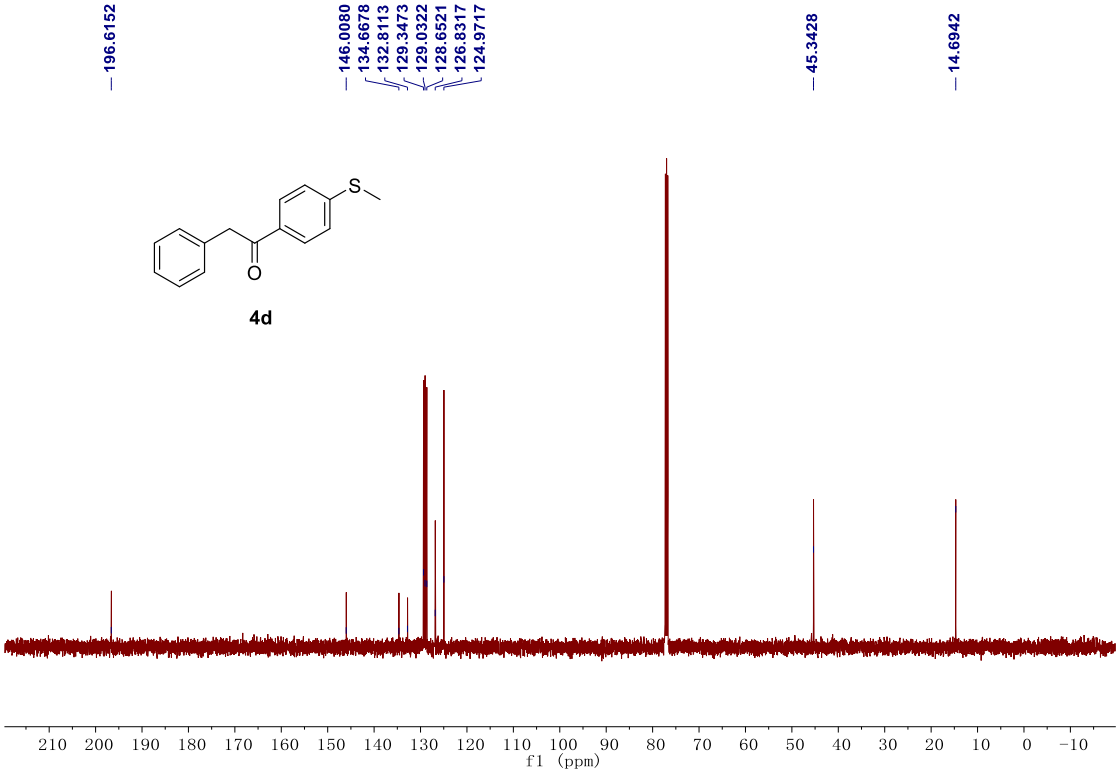

7.6459
7.6306
7.5703
7.5656
7.5619
7.4083
7.3923
7.3758
7.3598
7.3490
7.3447
7.3130
7.3096
7.2995
7.2956
7.2835
7.2717
7.2688
7.1427
7.1373
7.1262
7.1208
4.3001
3.8629
OMe
O
4b
3.09
3.03
7.42 7.38 7.34 7.30 7.26
f1 (ppm)
1.03
0.99
3.09
3.03
0.98
2.00
3.00
8.0 7.0 6.0 5.0 4.0 3.0 2.0 1.0 0.0
f1 (ppm)


197.4699
159.8849
138.0012
134.6096
129.6391
129.4741
128.7037
126.9204
121.3140
119.6691
112.8865
55.4350
45.6484
OMe
O
4b
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 −10
f1 (ppm)

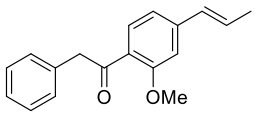

8.0037
7.9978
7.9936
7.9844
7.9801
7.9740
7.3243
7.3094
7.2988
7.2945
7.2706
7.2672
7.2533
7.2456
7.2345
7.2305
7.2257
7.2195
7.2161
7.2131
6.9304
6.9245
6.9203
6.9110
6.9068
6.9007
4.2225
3.8418
OMe
O
4c
1.97
1.98
2.93
1.96
2.00
3.00
f1 (ppm)


196.2569
163.5475
135.0116
130.9769
129.6679
129.4128
128.6612
126.7979
113.8215
55.4869
45.2911
OMe
O
4c
f1 (ppm)

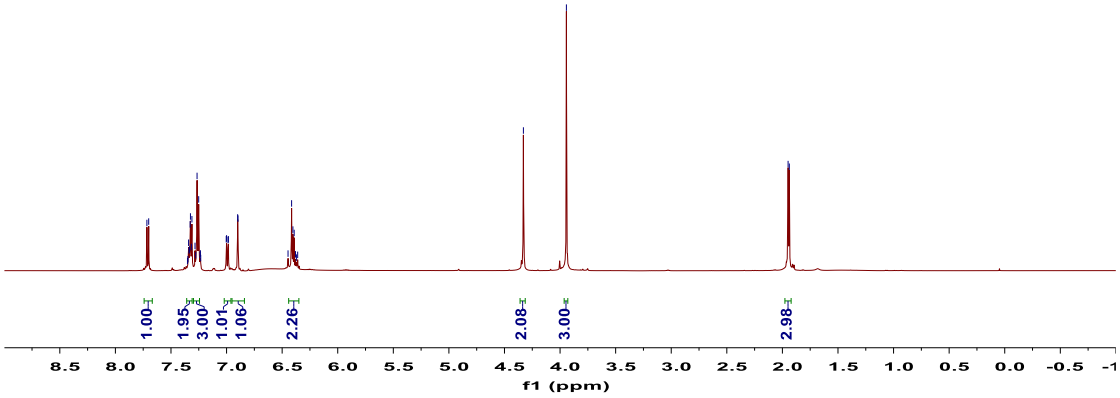

7.9533
7.9362
7.3671
7.3614
7.3591
7.3548
7.3445
7.3339
7.3296
7.2959
7.2925
7.2847
7.2810
7.2780
7.2717
7.2681
4.2629
2.5313
S
O
4d
2.00
2.18
5.06
1.98
3.04
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)


196.6152
146.0080
134.6678
132.8113
129.3473
129.0322
128.6521
126.8317
124.9717
45.3428
14.6942
S
O
4d
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

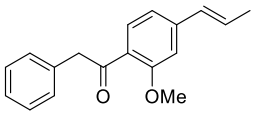

7.7166
7.7005
7.3516
7.3471
7.3416
7.3379
7.3330
7.3275
7.3248
7.3168
7.3116
7.2839
7.2776
7.2655
7.2508
7.2384
7.2354
7.2325
7.0029
6.9998
6.9867
6.9837
6.9004
6.8973
6.4470
6.4150
6.4032
6.3918
6.3796
6.3717
6.3603
4.3298
3.9430
1.9488
1.9378


O
OMe

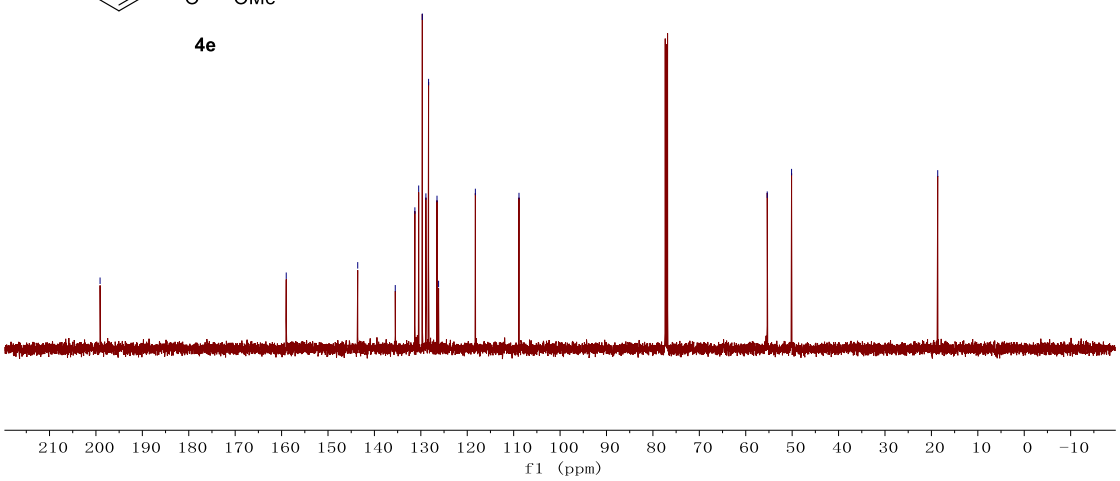
4e

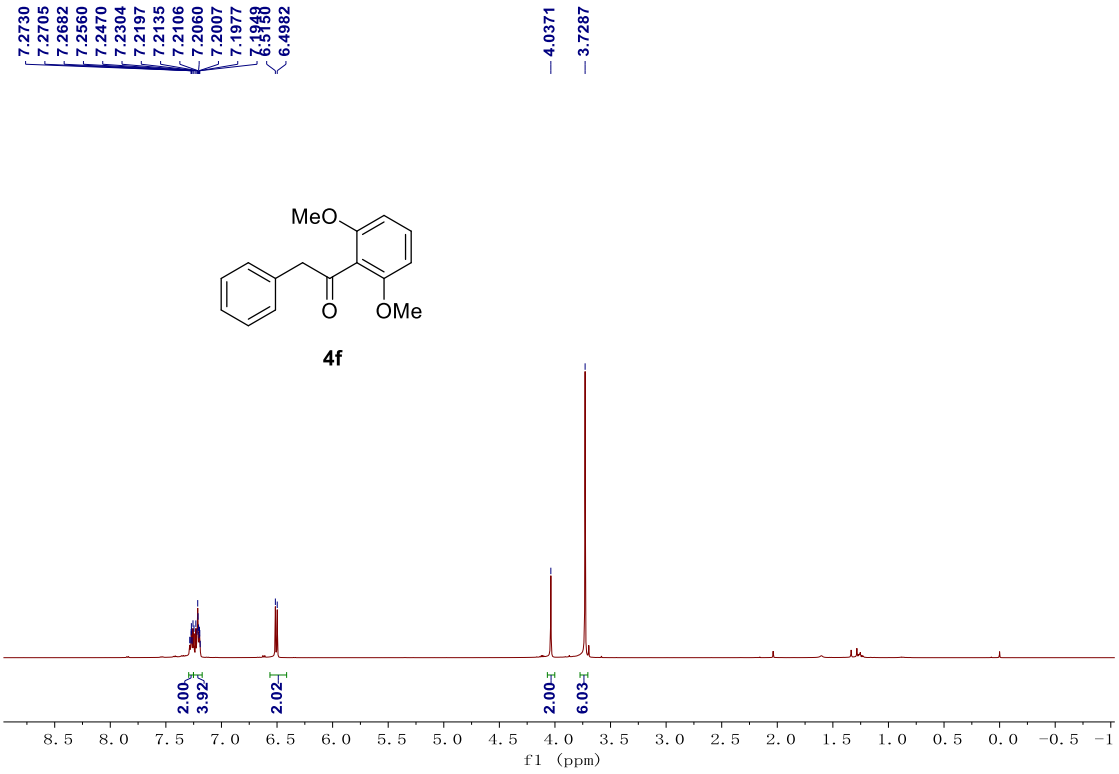

1.00
1.95
3.00
1.01
1.06
2.26
2.08
3.00
2.98
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1
f1 (ppm)

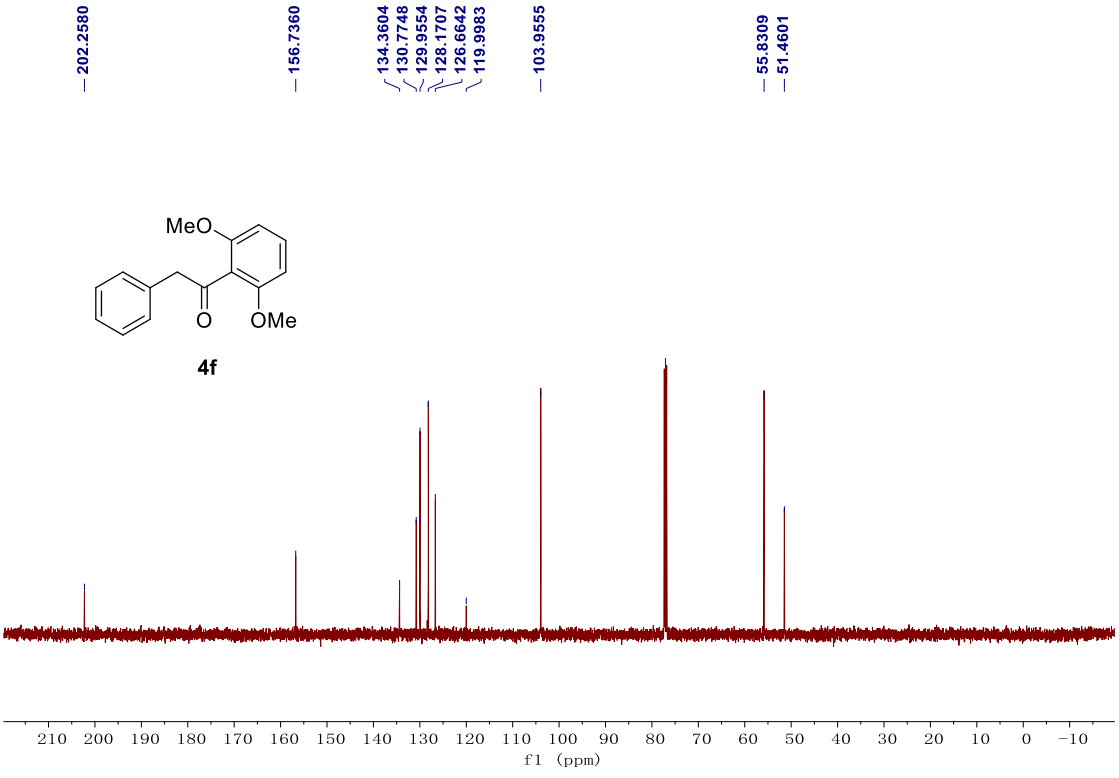

199.1071
159.0006
143.6001
135.5096
131.2827
130.4654
129.6828
128.9078
128.3317
126.5176
126.1748
118.2510
108.8520
55.3703
50.1288
18.6401


O
OMe

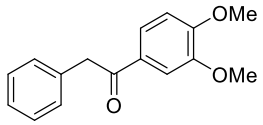
4e


210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

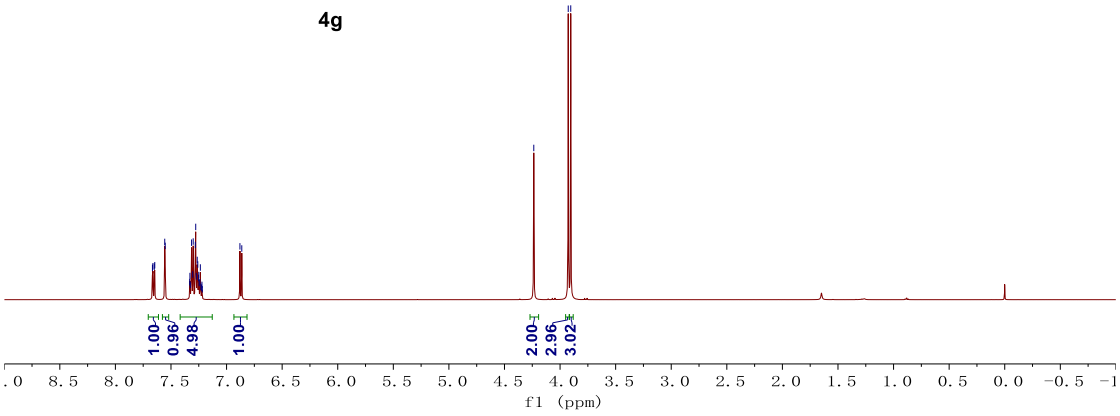

7.2730
7.2705
7.2682
7.2560
7.2470
7.2304
7.2197
7.2135
7.2106
7.2060
7.2007
7.1977
6.4982
4.0371
3.7287
MeO
O
OMe
4f
2.00
3.92
2.02
2.00
6.03
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 −0.5 −1
f1 (ppm)


202.2580
156.7360
134.3604
130.7748
129.9554
128.1707
126.6642
119.9983
103.9555
55.8309
51.4601
MeO
O
OMe
4f
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 −10
f1 (ppm)

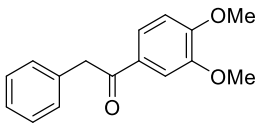

7.6668
7.6627
7.6500
7.6459
7.5561
7.5519
7.3319
7.3296
7.3263
7.3148
7.3042
7.3001
7.2809
7.2775
7.2725
7.2638
7.2588
7.2529
7.2499
7.2468
7.2400
7.2358
7.2308
7.2248
7.2215
7.2183
6.8798
6.8631
4.2364
3.9265
3.9039


OMe
OMe
O

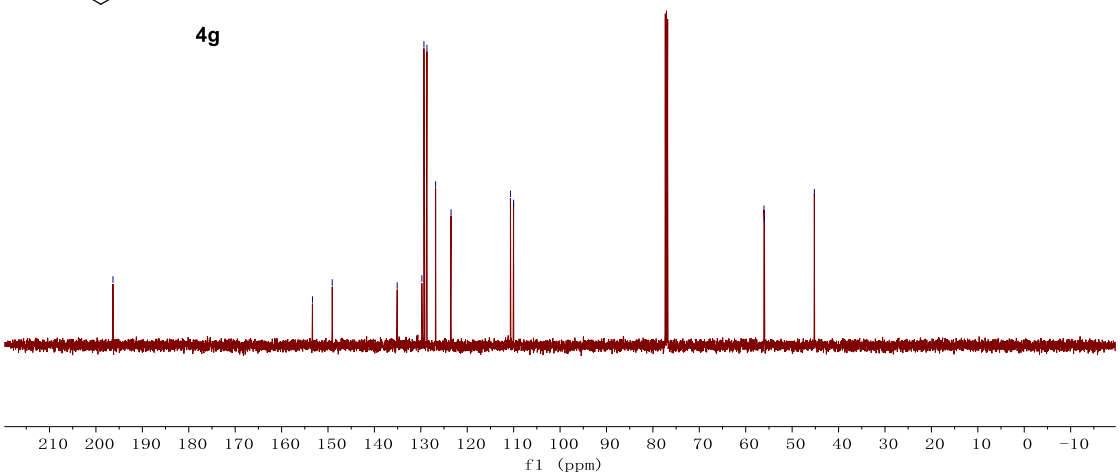
4g

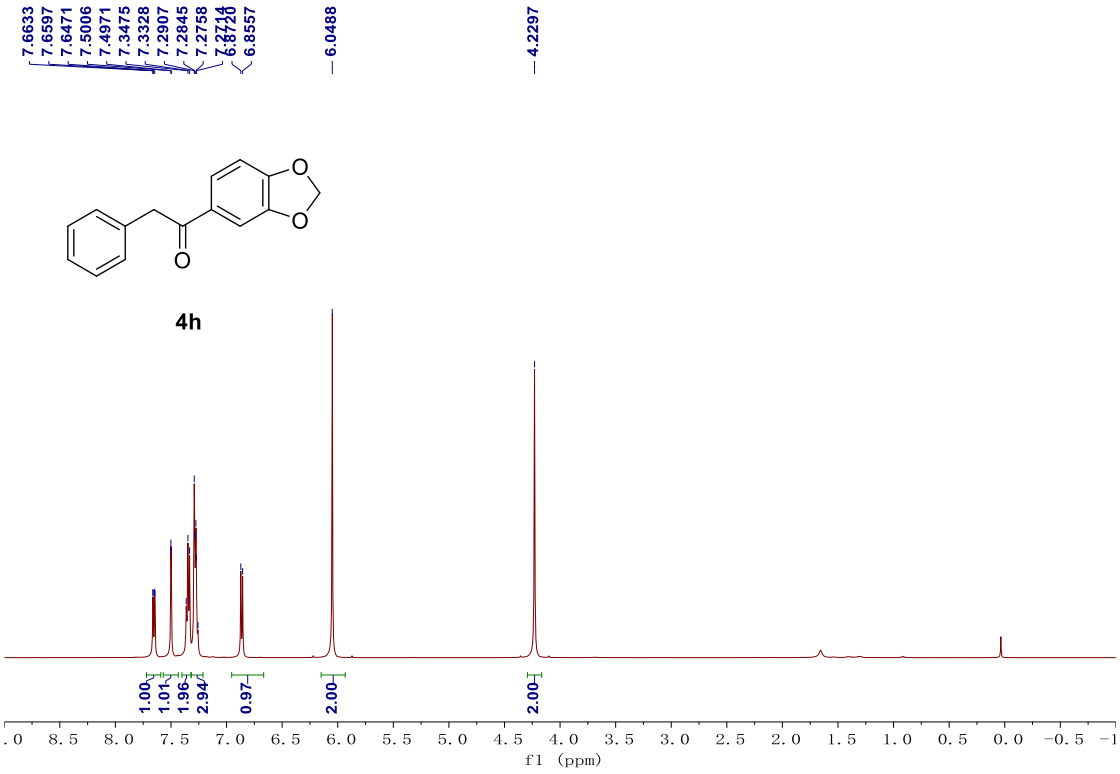

1.00
0.96
4.98
1.00
2.00
2.96
3.02
f1 (ppm)

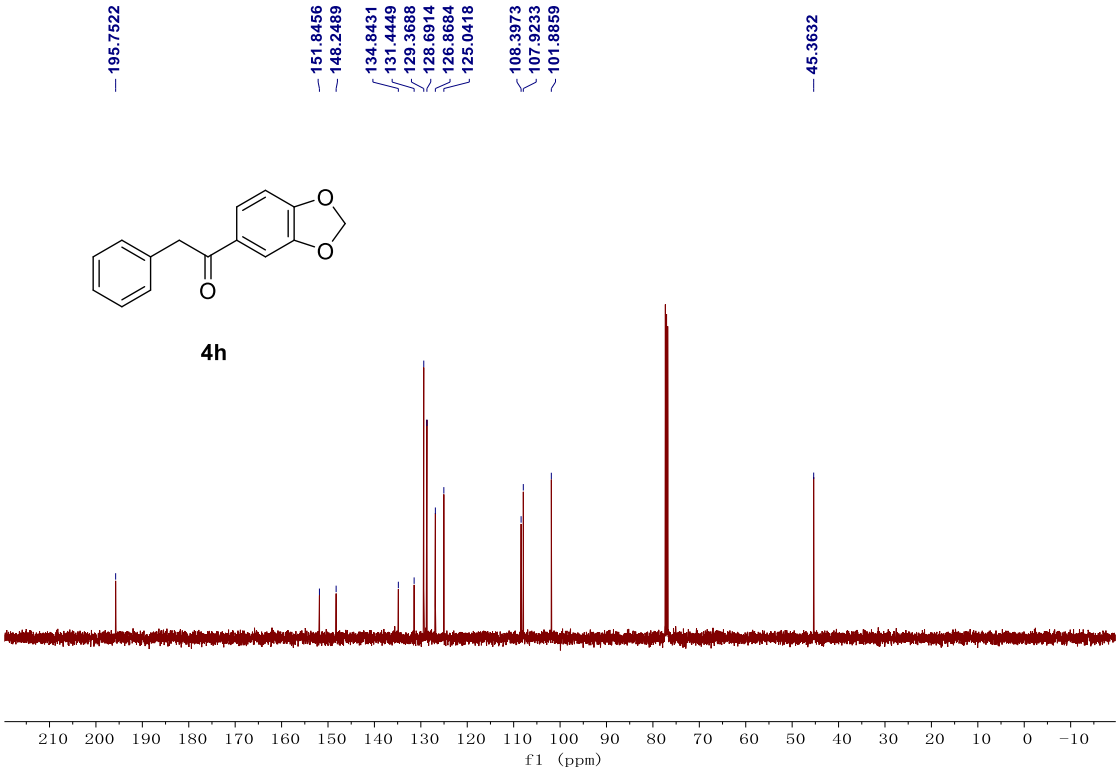

196.3295
153.3497
149.0893
135.0919
129.7855
129.3323
128.6818
126.8180
123.4916
110.6935
110.0216
56.0771
55.9575
45.2242

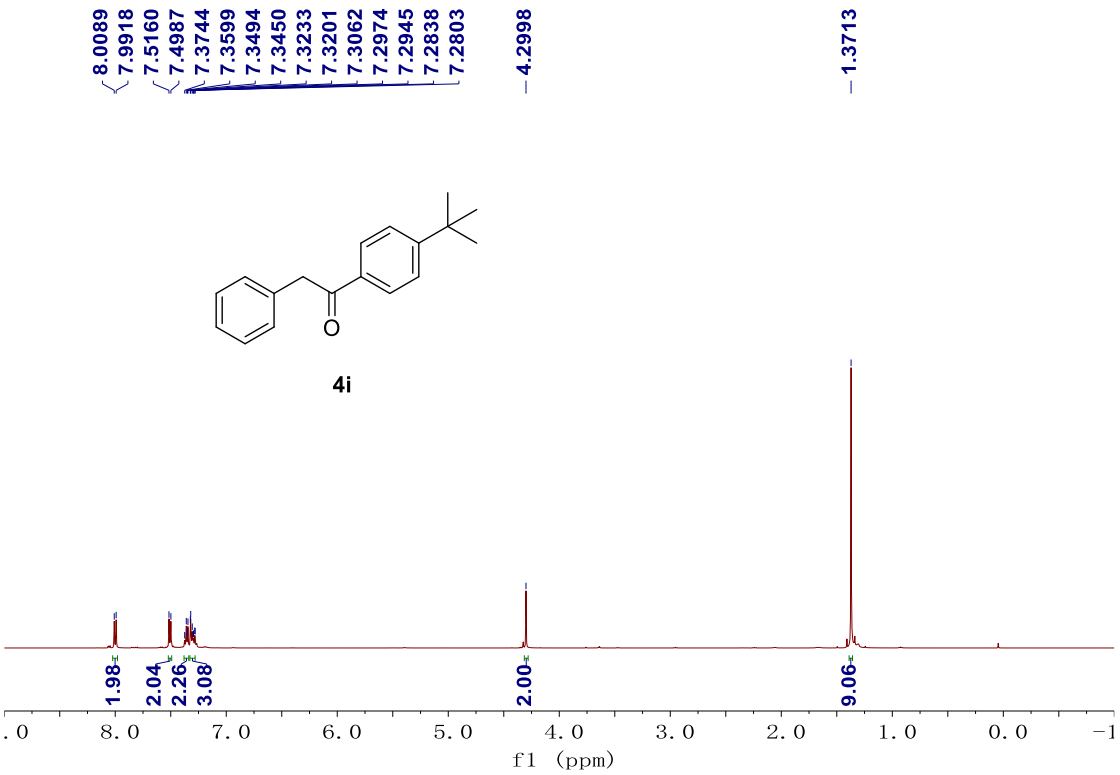

OMe
OMe
O

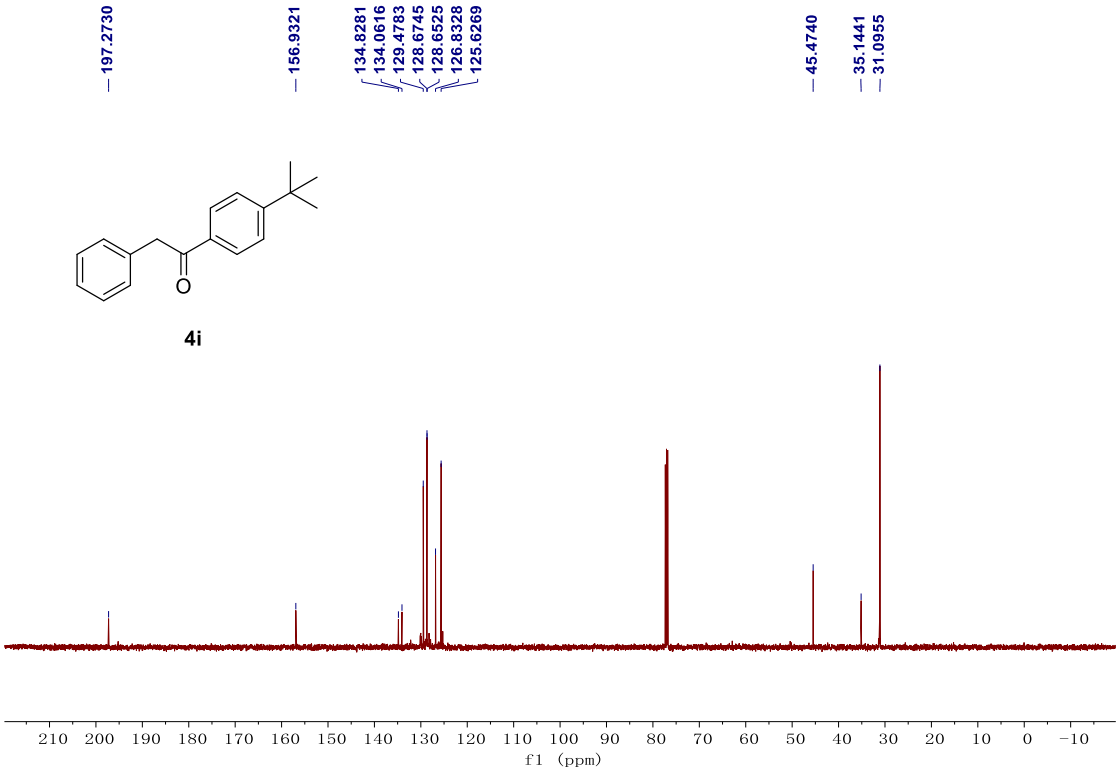
4g

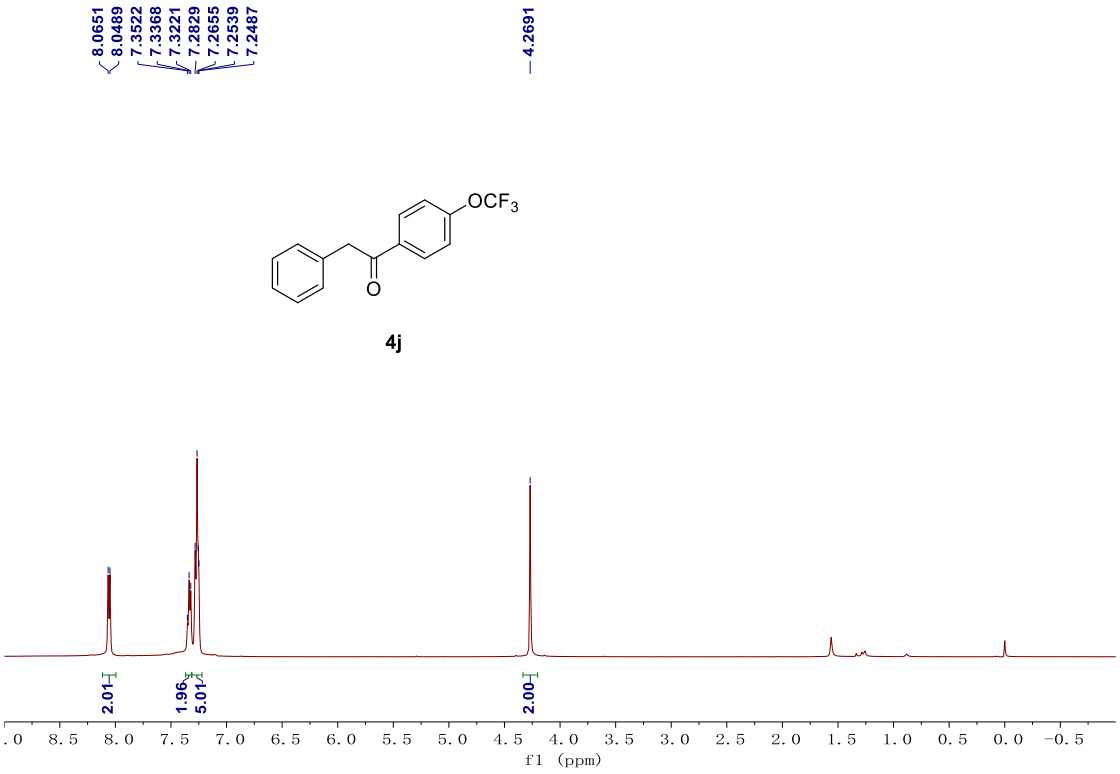

f1 (ppm)

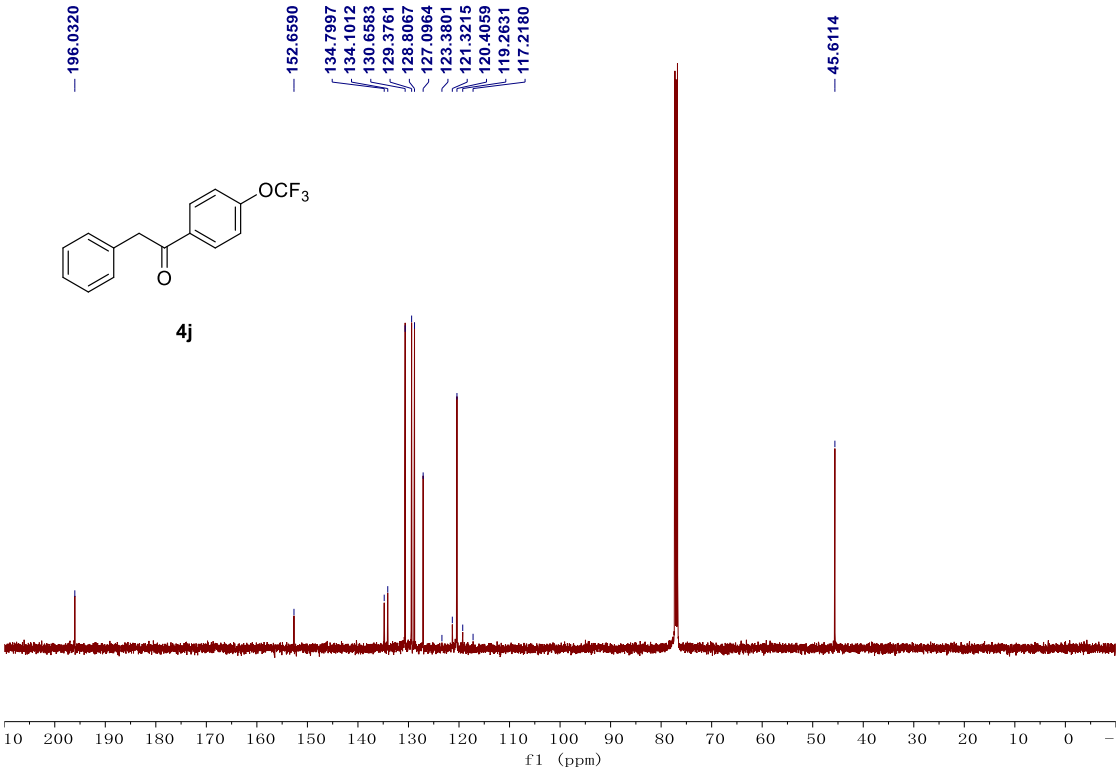

7.6633
7.6597
7.6471
7.5006
7.4971
7.3475
7.3328
7.2907
7.2845
7.2758
7.2714
6.8720
6.8557
6.0488
4.2297
4h
1.00
1.01
1.96
2.94
0.97
2.00
2.00
f1 (ppm)

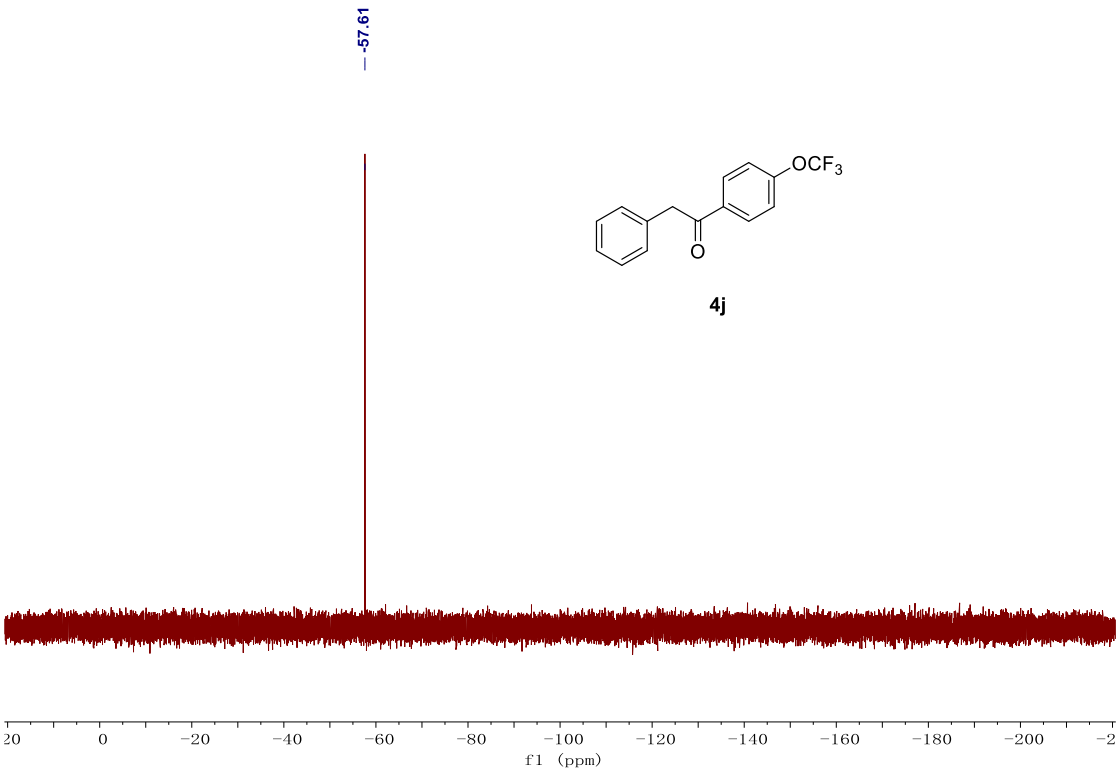

195.7522
151.8456
148.2489
134.8431
131.4449
129.3688
128.6914
126.8684
125.0418
108.3973
107.9233
101.8859
45.3632
4h
f1 (ppm)


8.0089
7.9918
7.5160
7.4987
7.3744
7.3599
7.3494
7.3450
7.3233
7.3201
7.3062
7.2974
7.2945
7.2838
7.2803
4.2998
1.3713
O
4i
1.98
2.04
2.26
3.08
2.00
9.06
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
f1 (ppm)


197.2730
156.9321
134.8281
134.0616
129.4783
128.6745
128.6525
126.8328
125.6269
45.4740
35.1441
31.0955
O
4i
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
−10
f1 (ppm)

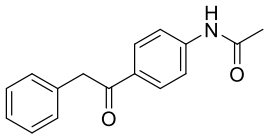

8.0651
8.0489
7.3522
7.3368
7.3221
7.2829
7.2655
7.2539
7.2487
4.2691
OCF3
O
4j
2.01
1.96
5.01
2.00
f1 (ppm)


196.0320
152.6590
134.7997
134.1012
130.6583
129.3761
128.8067
127.0964
123.3801
121.3215
120.4059
119.2631
117.2180
45.6114
OCF3
O
4j
f1 (ppm)

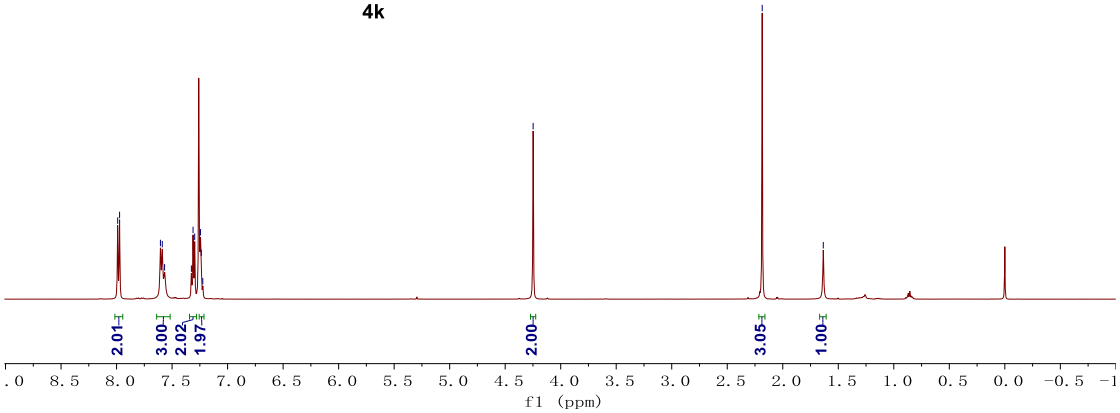

-57.61
OCF3
O
f1 (ppm)

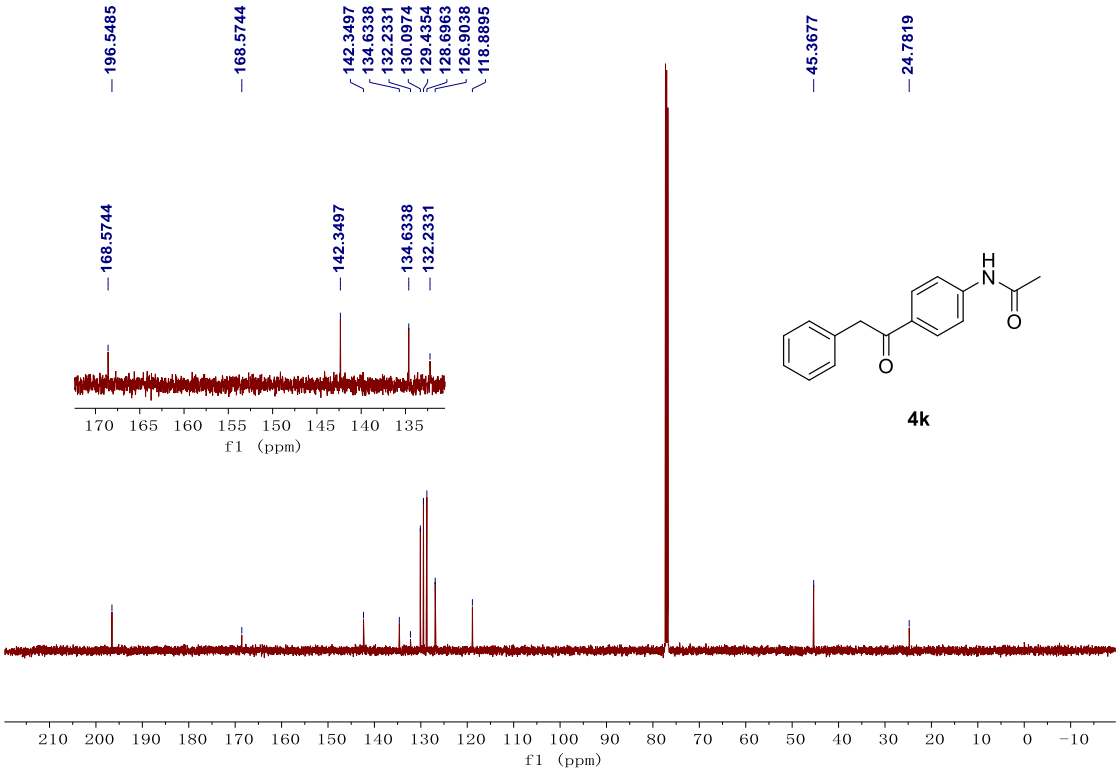
4j


7.9899
7.9727
7.6049
7.5882
7.5675
7.3261
7.3111
7.2963
7.2444
7.2372
7.2233
4.2481
2.1851
1.6351

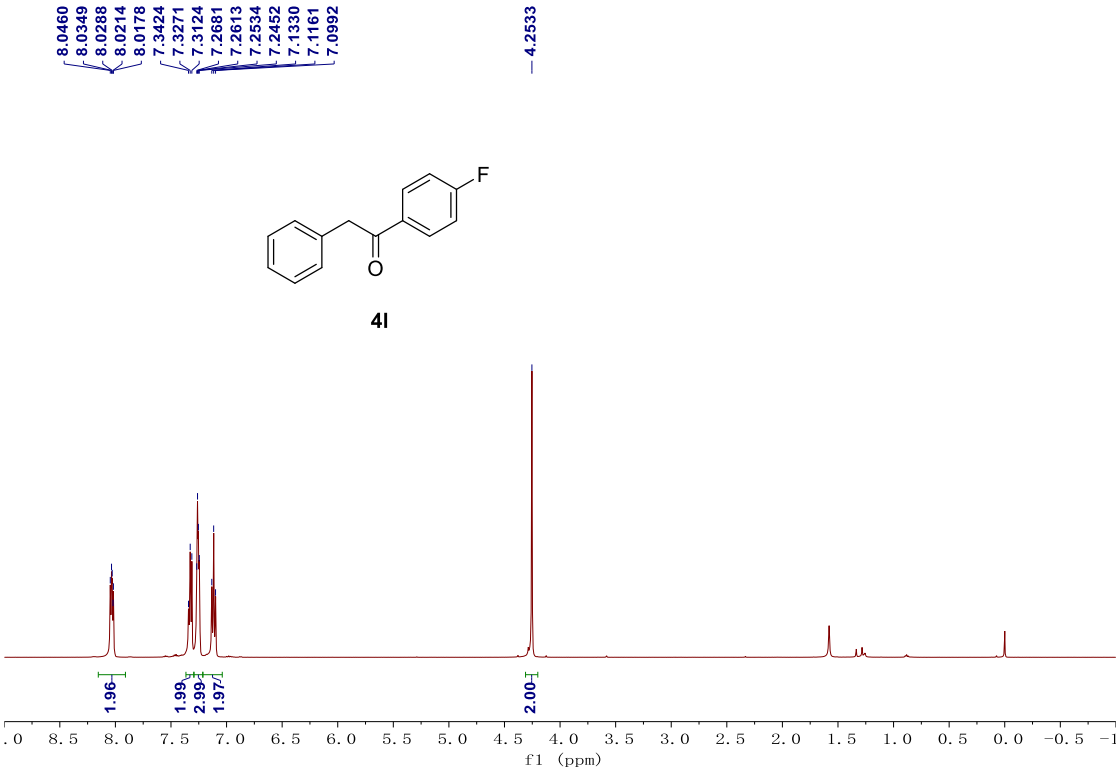

H
N
O
O

4k

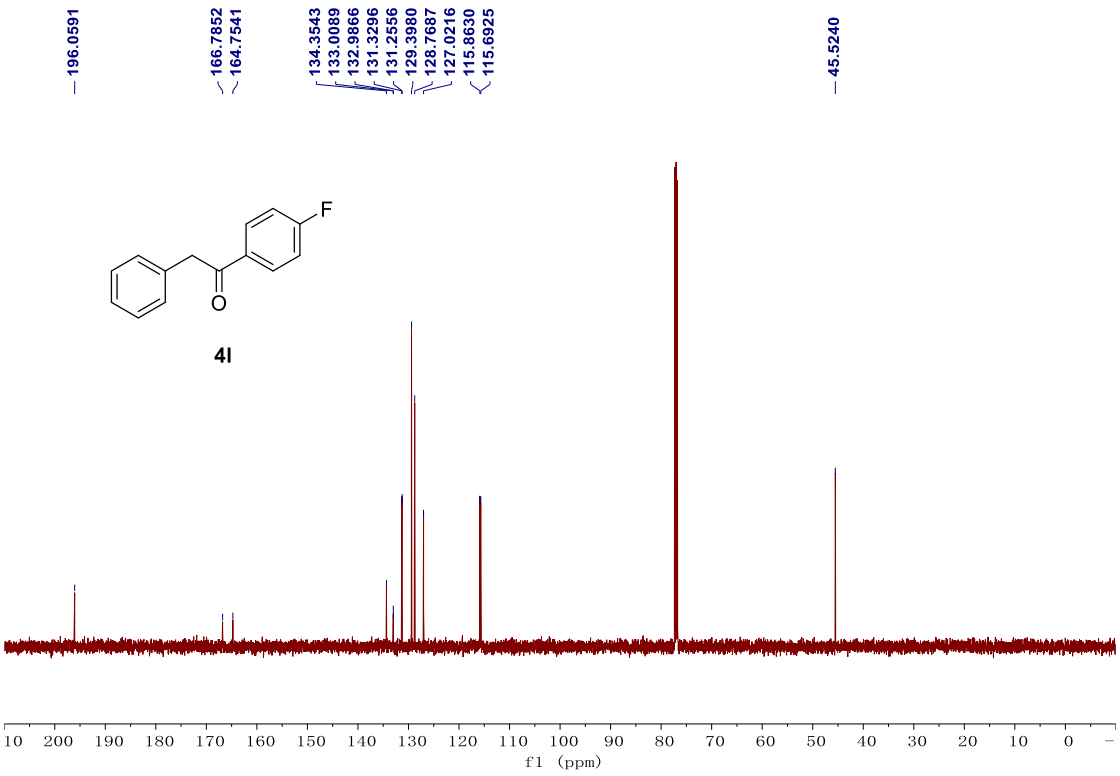

2.01
3.00
2.02
1.97
2.00
3.05
1.00
f1 (ppm)

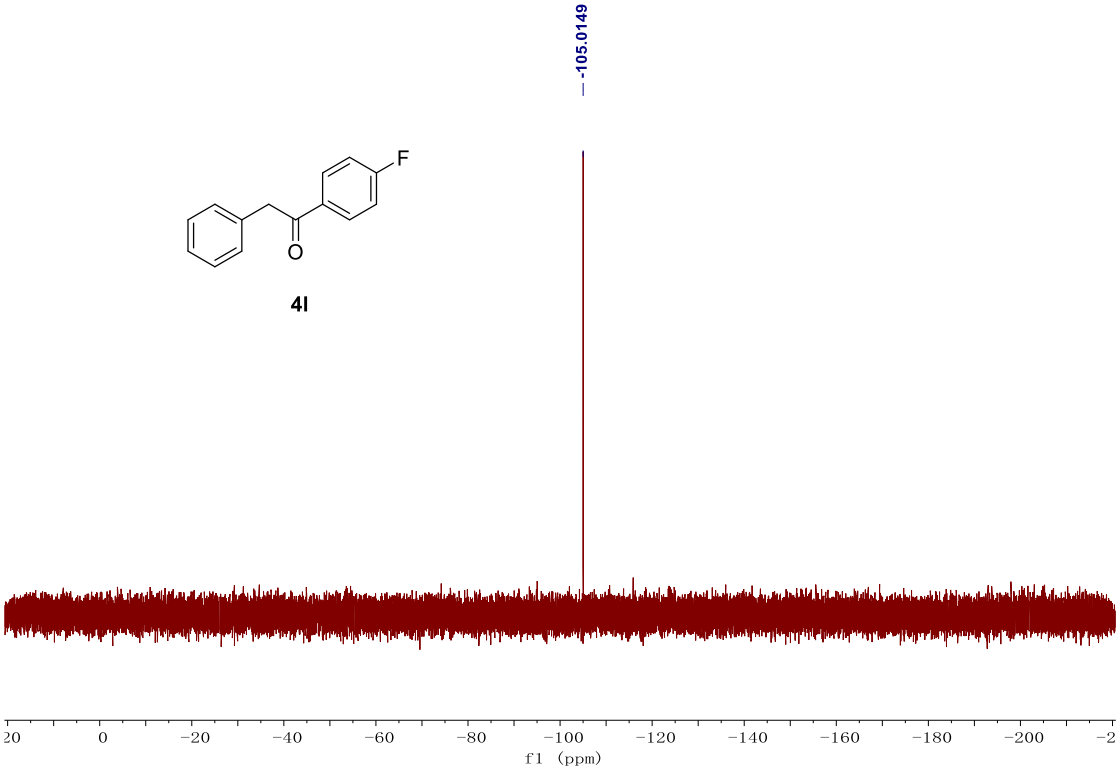

196.5485
168.5744
142.3497
134.6338
132.2331
130.0974
129.4354
128.6963
126.9038
118.8895
45.3677
24.7819
168.5744
142.3497
134.6338
132.2331
170 165 160 155 150 145 140 135
f1 (ppm)
H
N
O
O
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 −10
f1 (ppm)

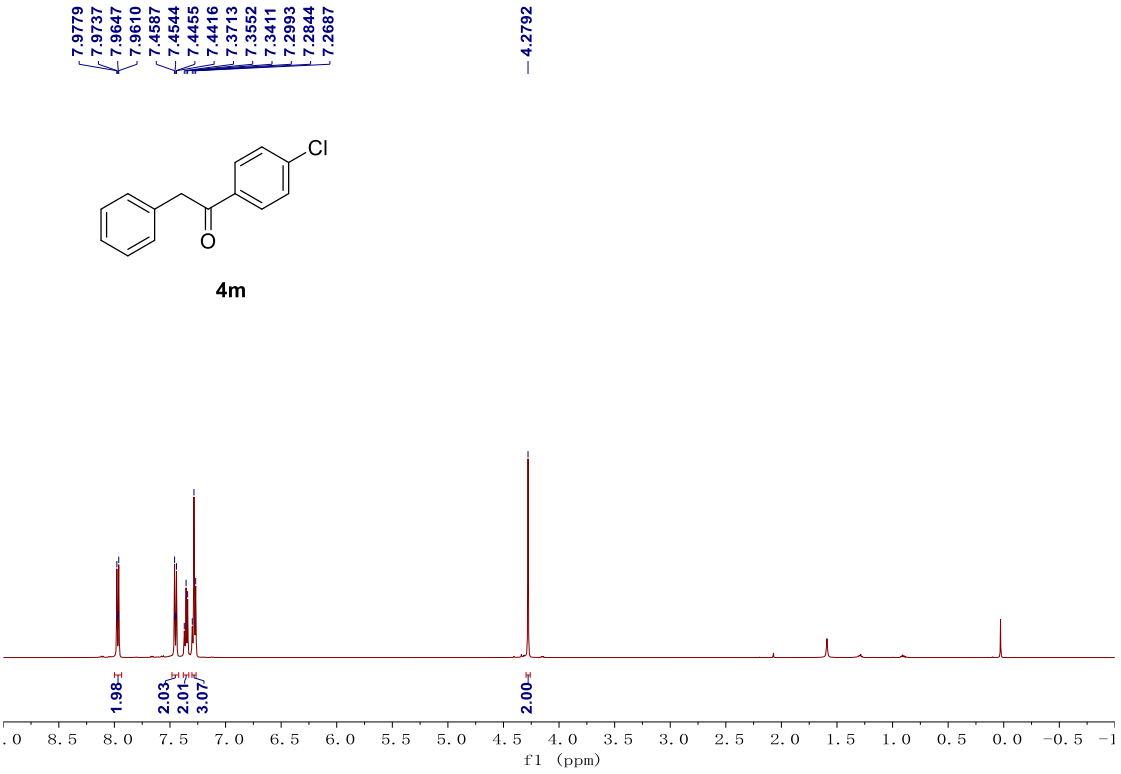
4k

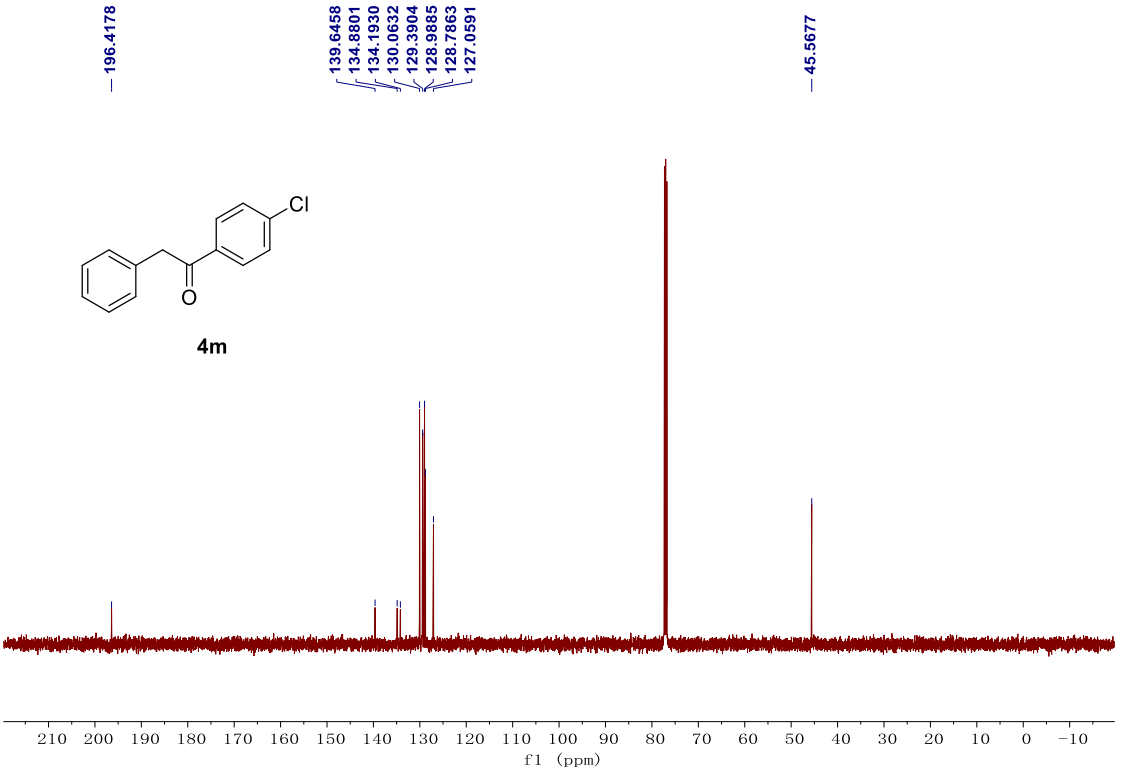

8.0460
8.0349
8.0288
8.0214
8.0178
7.3424
7.3271
7.3124
7.2681
7.2613
7.2534
7.2452
7.1330
7.1161
7.0992
4.2533
F
O
1.96
1.99
2.99
1.97
2.00
.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 −0.5 −1
f1 (ppm)

4l

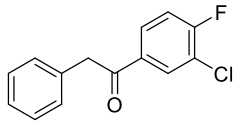

196.0591
166.7852
164.7541
134.3543
133.0089
132.9866
131.3296
131.2556
129.3980
128.7687
127.0216
115.8630
115.6925
45.5240
F
O
4l
10 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


-105.0149
F
O
4l
20 0 -20 -40 -60 -80 -100 -120 -140 -160 -180 -200 -2
f1 (ppm)

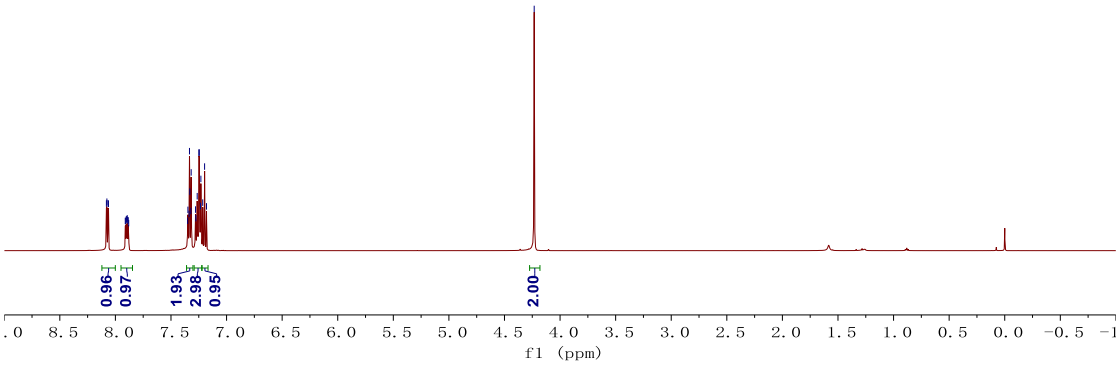

7.9779
7.9737
7.9647
7.9610
7.4587
7.4544
7.4455
7.4416
7.3713
7.3552
7.3411
7.2993
7.2844
7.2687
4.2792
Cl
O
4m
1.98
2.03
2.01
3.07
2.00
f1 (ppm)


196.4178
139.6458
134.8801
134.1930
130.0632
129.3904
128.9885
128.7863
127.0591
45.5677
Cl
O
4m
f1 (ppm)

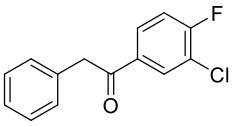

8.0809
8.0765
8.0668
8.0623
7.9112
7.9067
7.9020
7.8975
7.8939
7.8895
7.8847
7.8804
7.3501
7.3477
7.3373
7.3336
7.3306
7.3216
7.3183
7.2790
7.2762
7.2642
7.2494
7.2453
7.2345
7.2310
7.2148
7.1976
7.1805
4.2327


F
Cl
O

4n

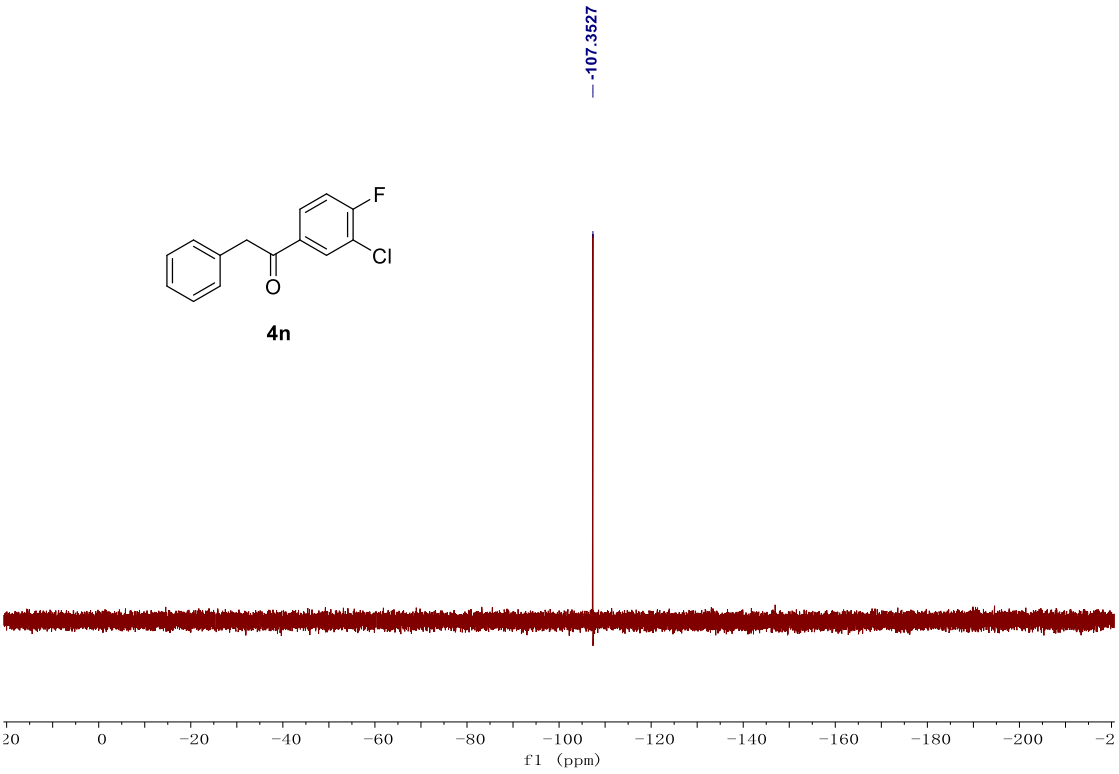

0.96
0.97
1.93
2.98
0.95
2.00
f1 (ppm)


195.0212
162.0855
160.0393
133.8505
133.7401
133.7107
131.5569
129.3829
129.0911
129.0254
128.8634
127.1980
122.0298
121.8831
116.9576
116.7880
45.4878

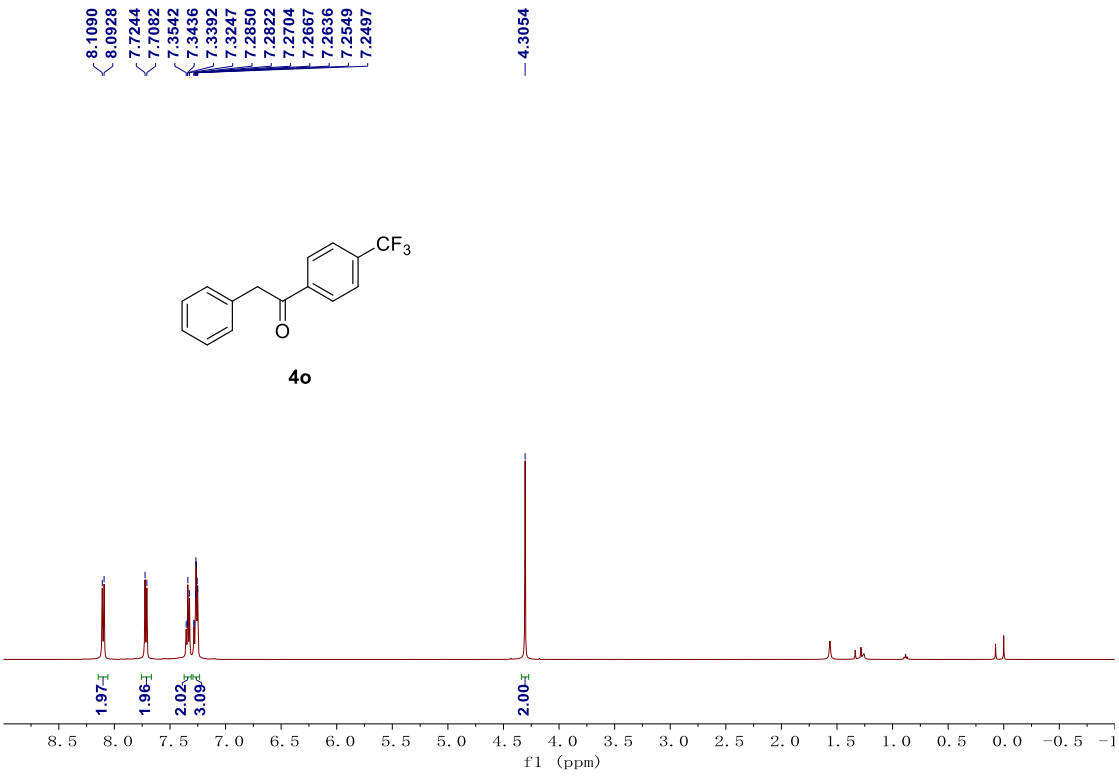

F
Cl
O

4n

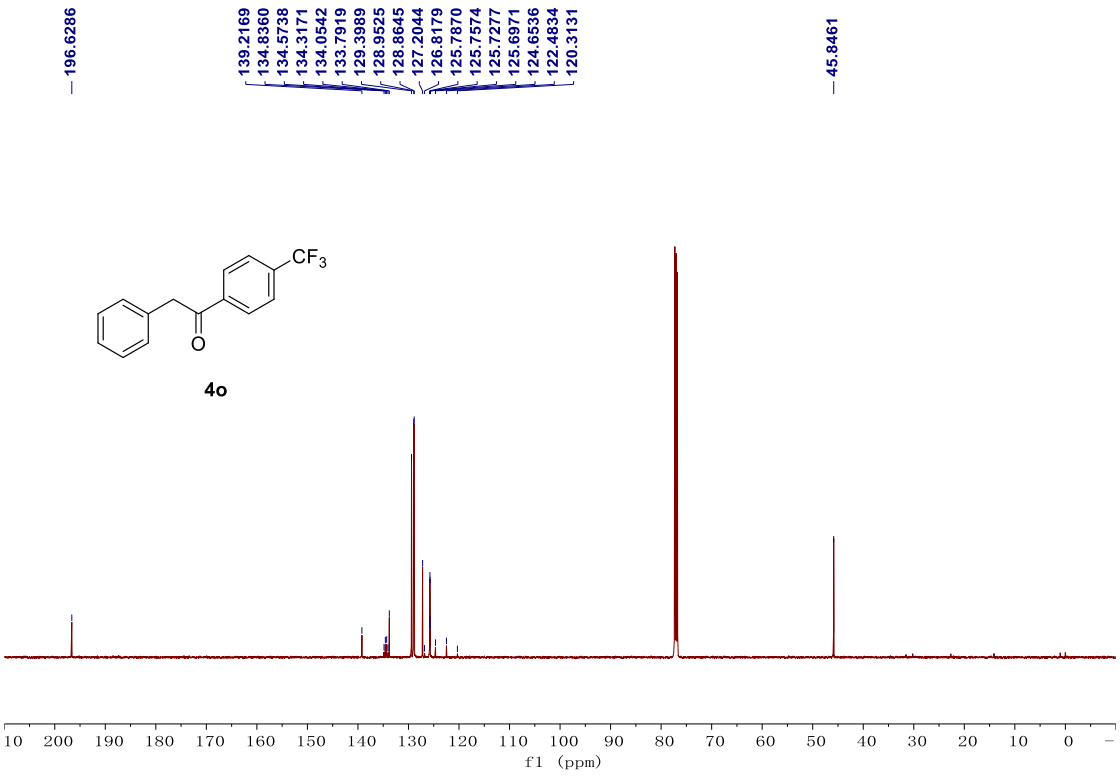
f1 (ppm)

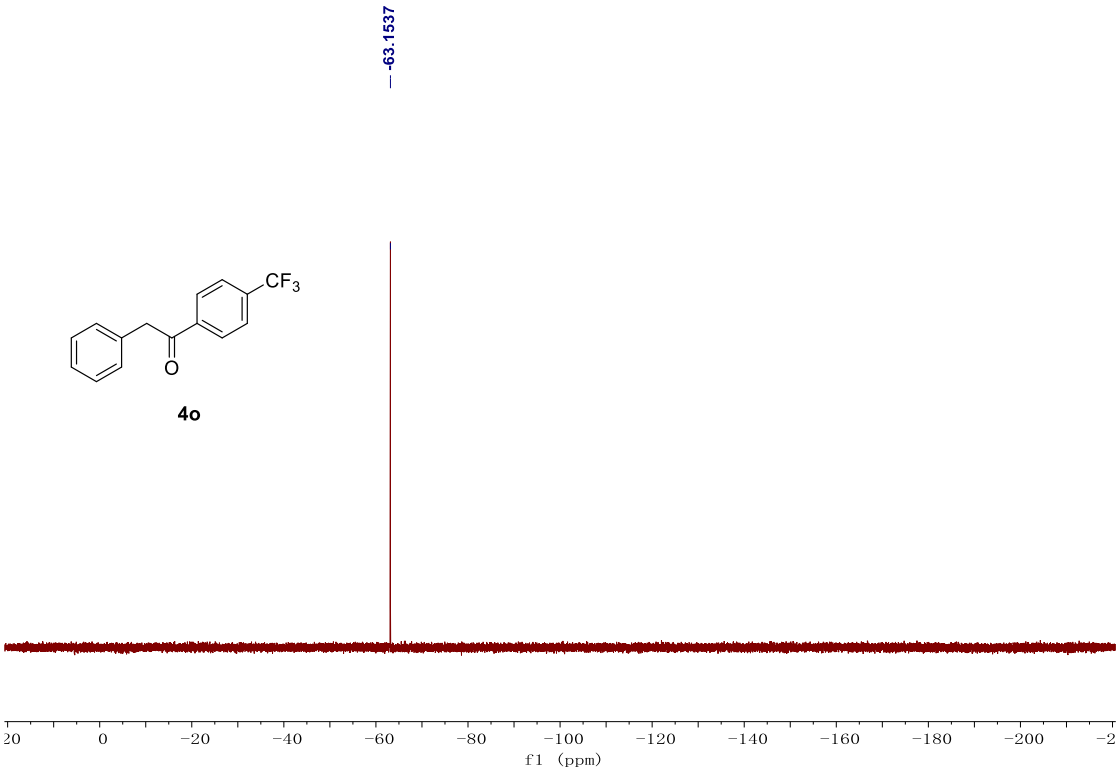

-107.3527
F
Cl
O
20
0
−20
−40
−60
−80
−100
−120
−140
−160
−180
−200
−2
f1 (ppm)

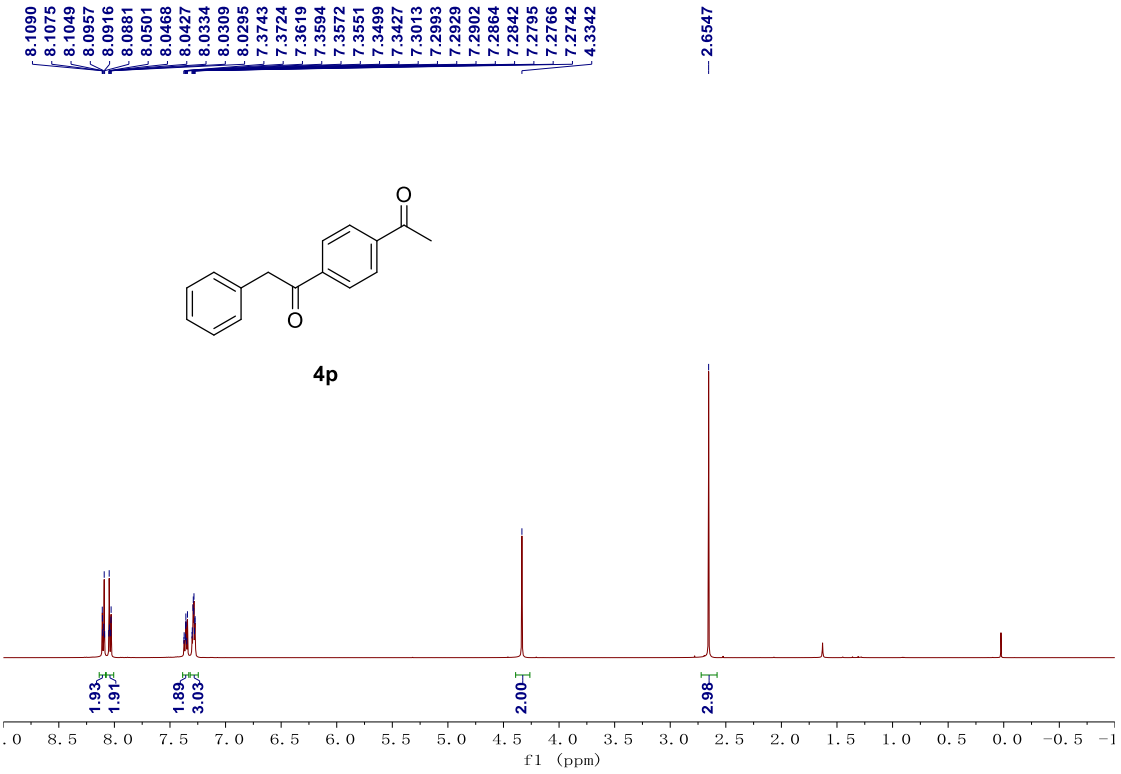
4n

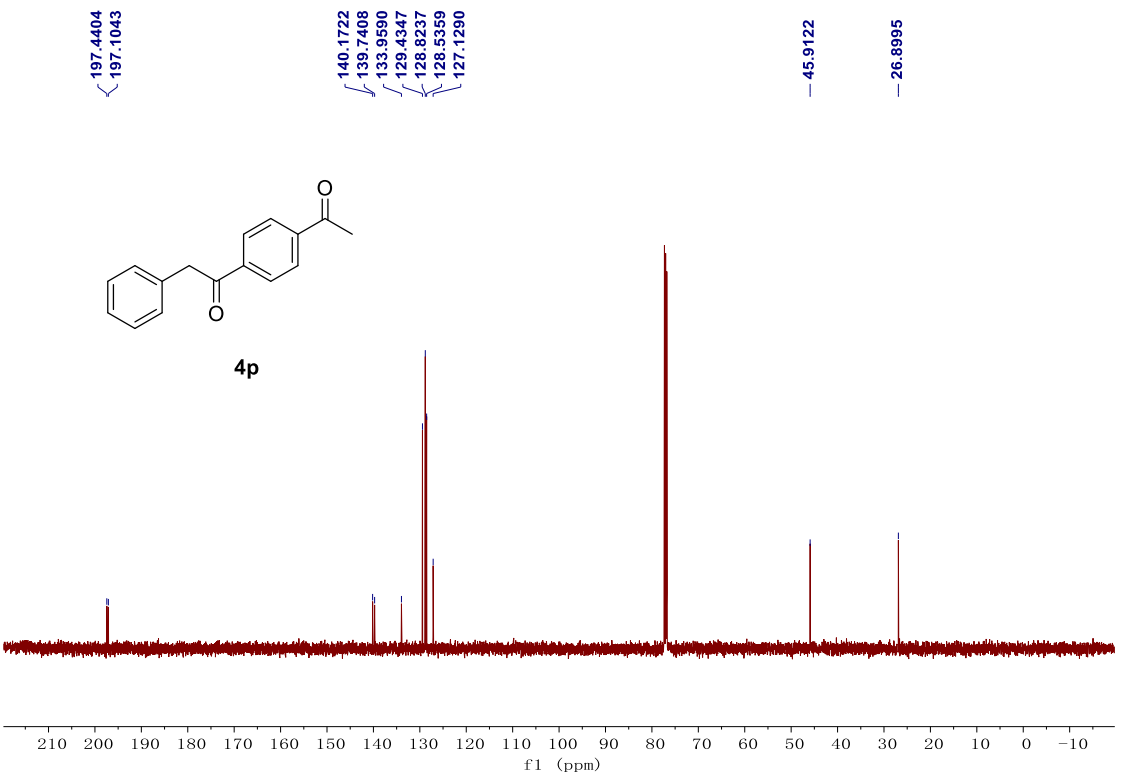

8.1090
8.0928
7.7244
7.7082
7.3542
7.3436
7.3392
7.3247
7.2850
7.2822
7.2704
7.2667
7.2636
7.2549
7.2497
4.3054
CF3
O
1.97
1.96
2.02
3.09
2.00
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
−0.5
−1
f1 (ppm)

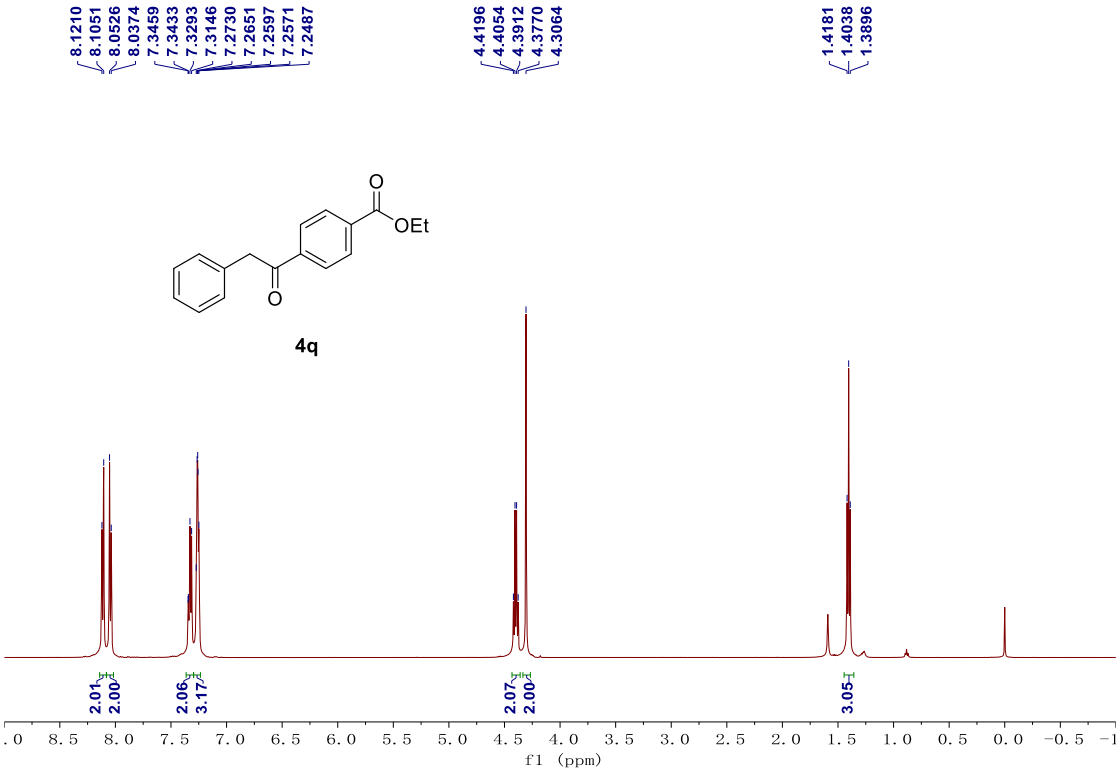
4o

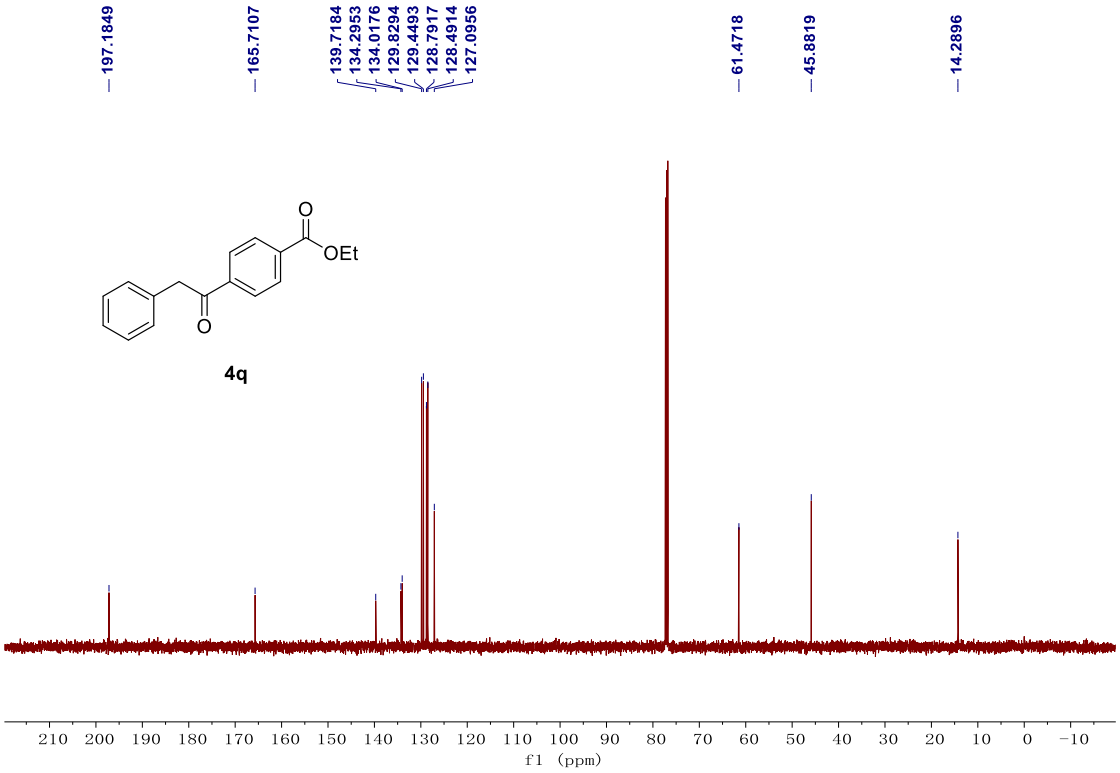

196.6286
139.2169
134.8360
134.5738
134.3171
134.0542
133.7919
129.3989
128.9525
128.8645
127.2044
126.8179
125.7870
125.7574
125.7277
125.6971
124.6536
122.4834
120.3131
45.8461
CF3
O
4o
f1 (ppm)

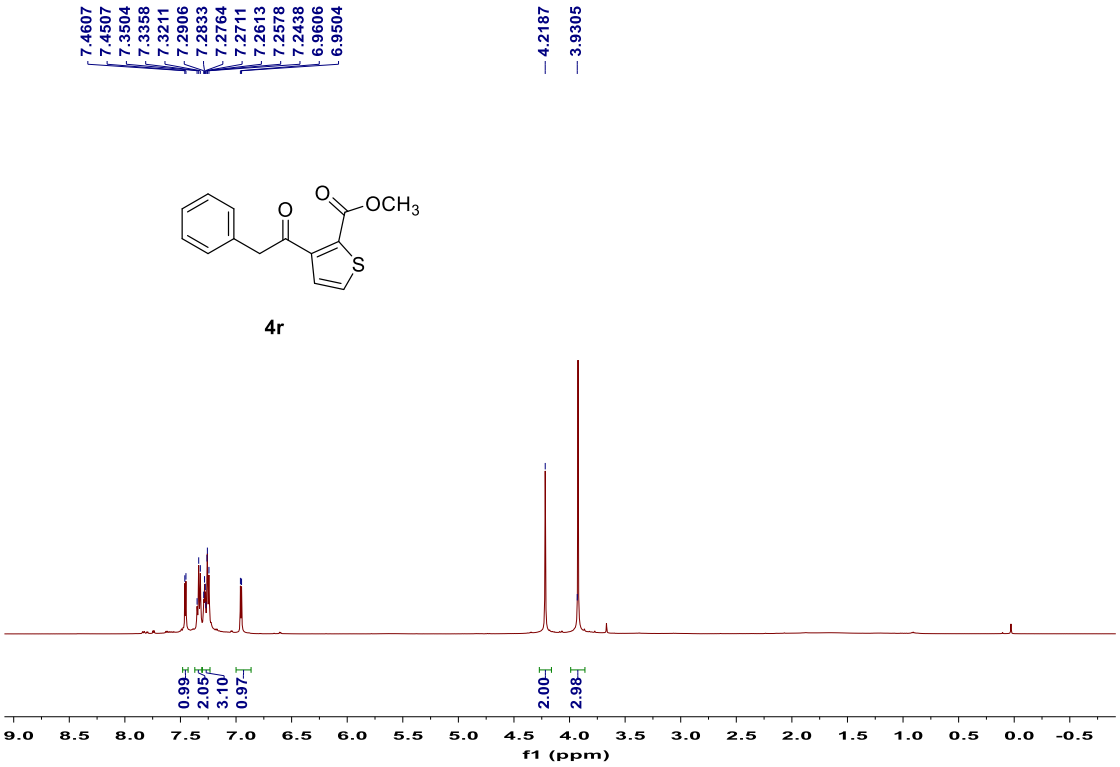

-63.1537
CF3
O
4o
f1 (ppm)


8.1090
8.1075
8.1049
8.0957
8.0916
8.0881
8.0501
8.0468
8.0427
8.0334
8.0309
8.0295
7.3743
7.3724
7.3619
7.3594
7.3572
7.3551
7.3499
7.3427
7.3013
7.2993
7.2929
7.2902
7.2864
7.2842
7.2795
7.2766
7.2742
4.3342
2.6547
O
O
4p
1.93
1.91
1.89
3.03
2.00
2.98
f1 (ppm)


197.4404
197.1043
140.1722
139.7408
133.9590
129.4347
128.8237
128.5359
127.1290
45.9122
26.8995
O
O
4p
f1 (ppm)


8.1210
8.1051
8.0526
8.0374
7.3459
7.3433
7.3293
7.3146
7.2730
7.2651
7.2597
7.2571
7.2487
4.4196
4.4054
4.3912
4.3770
4.3064
1.4181
1.4038
1.3896
O
OEt
O
4q
2.01
2.00
2.06
3.17
2.07
2.00
3.05
f1 (ppm)


197.1849
165.7107
139.7184
134.2953
134.0176
129.8294
129.4493
128.7917
128.4914
127.0956
61.4718
45.8819
14.2896
O
OEt
O
4q
f1 (ppm)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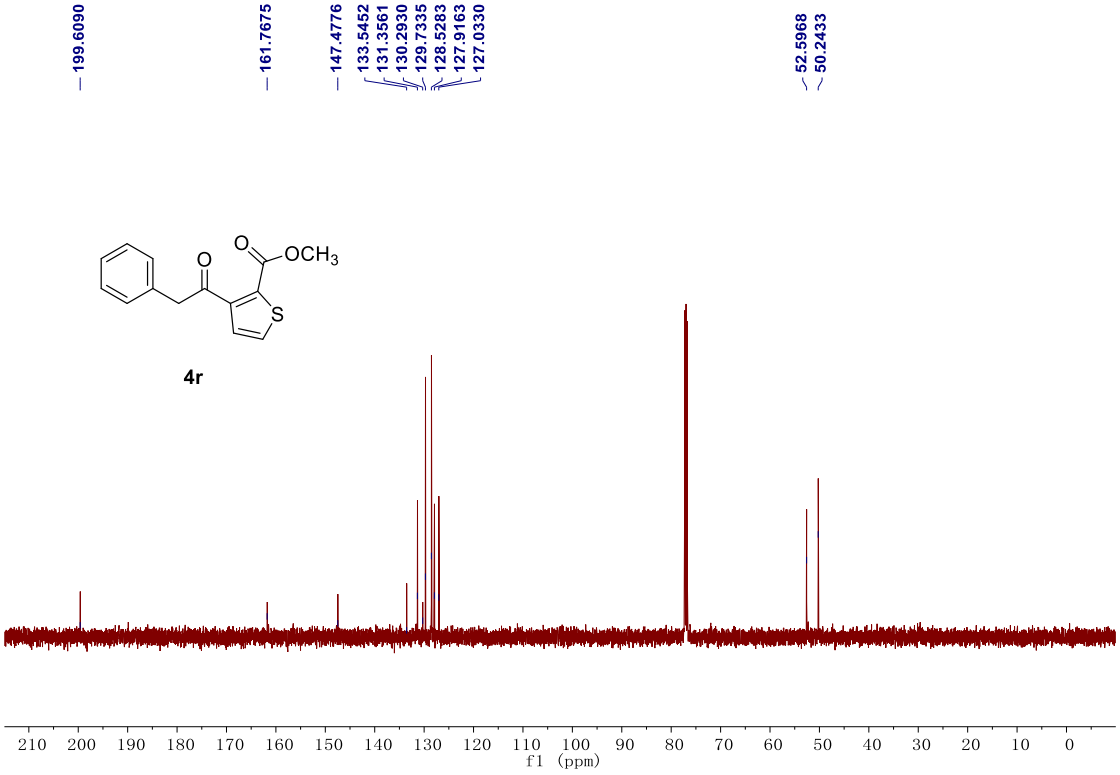
7.4507
7.3504
7.3358
7.3211
7.2906
7.2833
7.2764
7.2711
7.2613
7.2578
7.2438
6.9606
6.9504
4.2187
3.9305
O
OCH3
S
4r
0.99
2.05
3.10
0.97
2.00
2.98
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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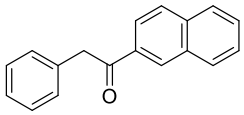
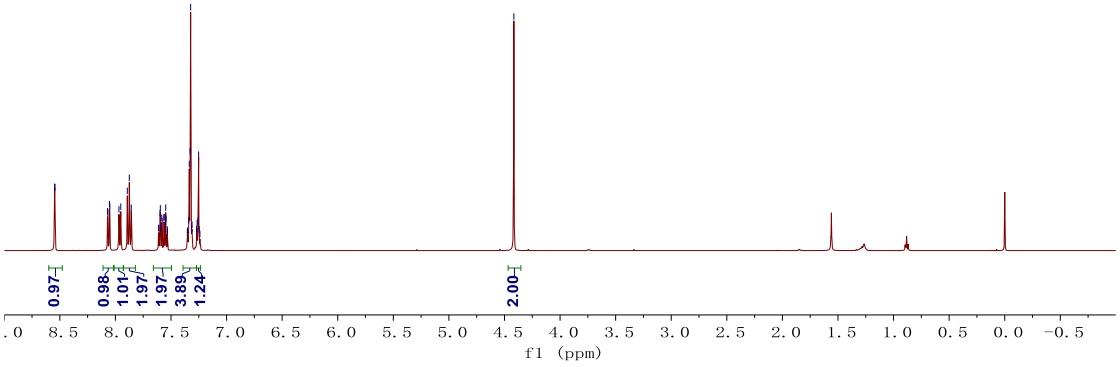
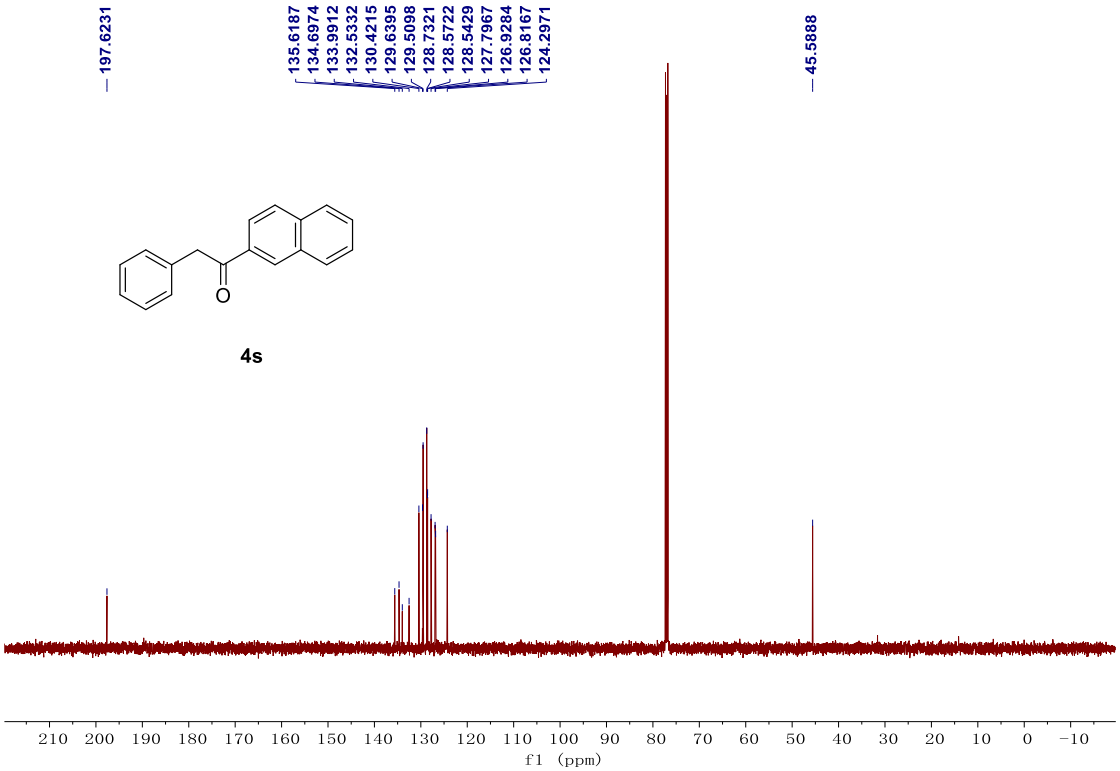
161.7675
147.4776
133.5452
131.3561
130.2930
129.7335
128.5283
127.9163
127.0330
52.5968
50.2433
O
OCH3
S
4r
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


8.5469
8.5436
8.0708
8.0672
8.0535
8.0499
7.9678
7.9516
7.8929
7.8751
7.8574
7.6123
7.6096
7.5985
7.5958
7.5931
7.5824
7.5796
7.5637
7.5609
7.5500
7.5473
7.5447
7.5335
7.5310
7.3529
7.3509
7.3403
7.3355
7.3277
7.3230
7.3137
7.3106
7.2694
7.2646
7.2578
7.2512
7.2454
7.2397
4.4156


O

4s


0.97
0.98
1.01
1.97
1.97
3.89
1.24
2.00
f1 (ppm)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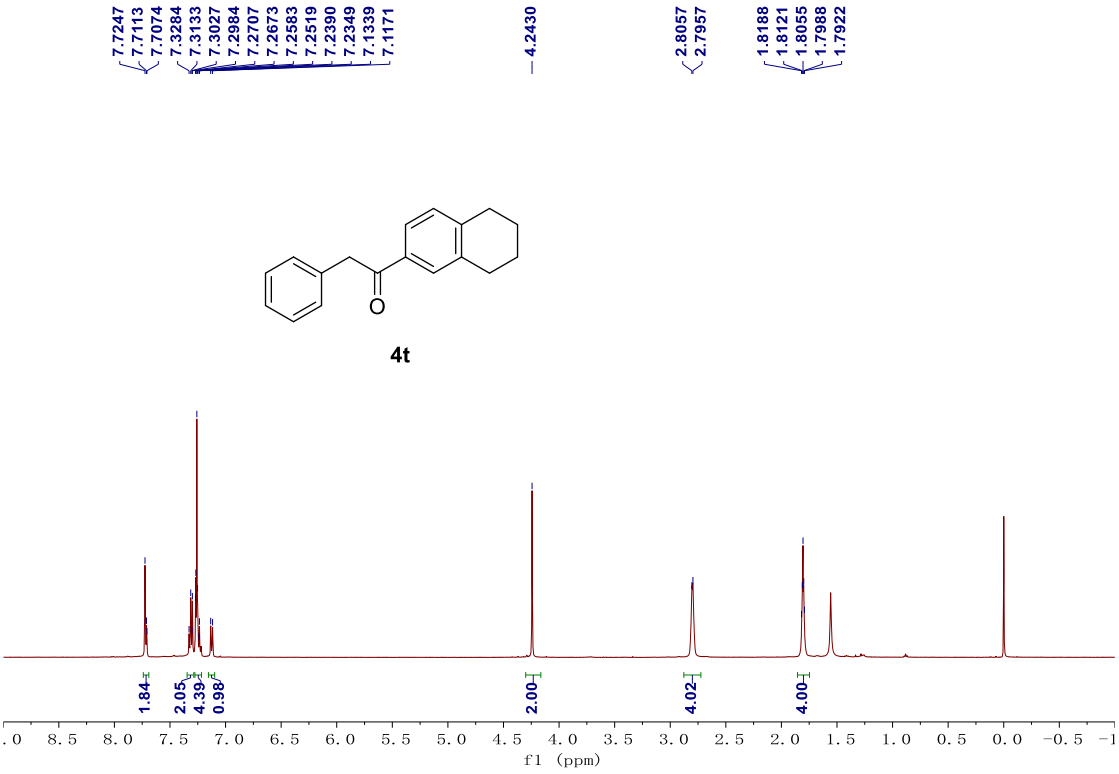
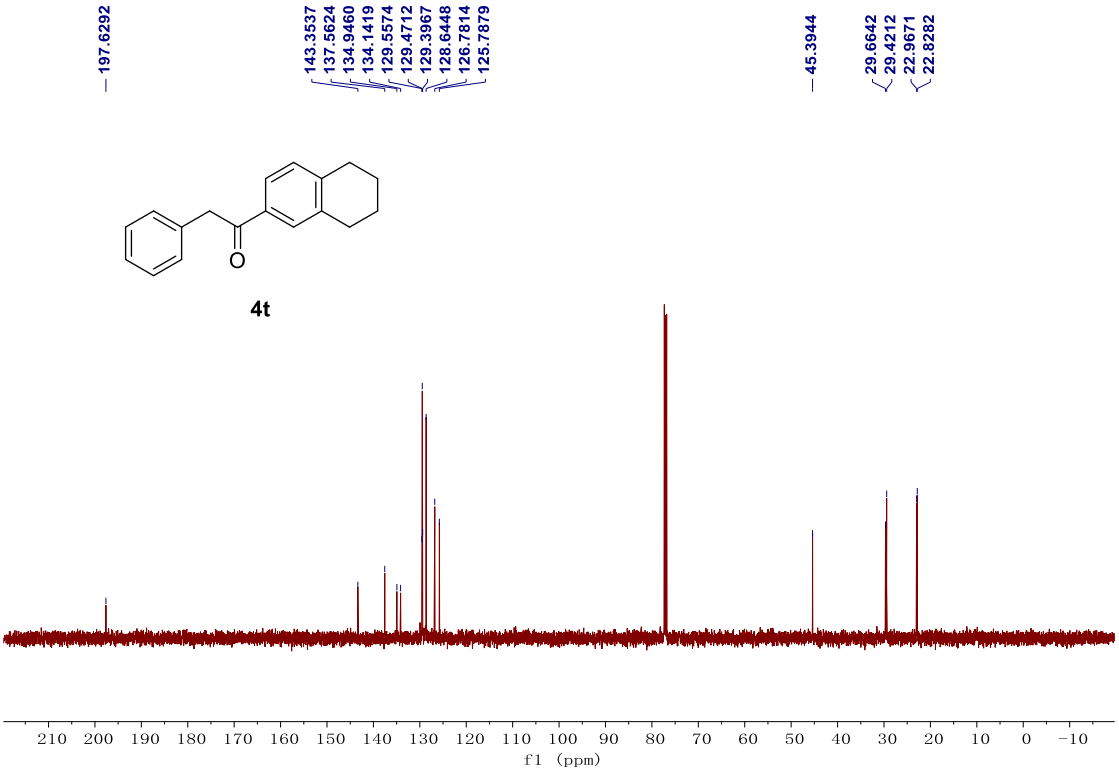
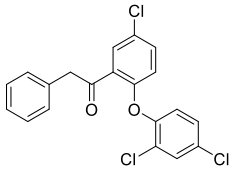
135.6187
134.6974
133.9912
132.5332
130.4215
129.6395
129.5098
128.7321
128.5722
128.5429
127.7967
126.9284
126.8167
124.2971
45.5888
O
f1 (ppm)

4s

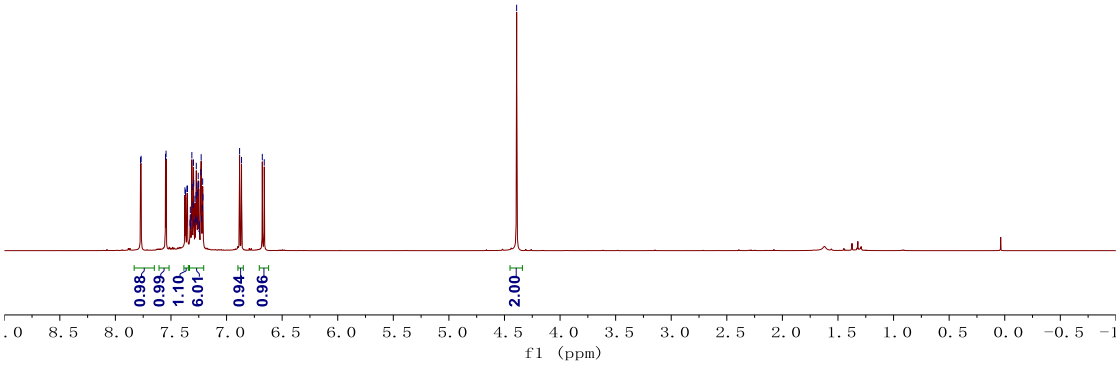

7.7247
7.7113
7.7074
7.3284
7.3133
7.3027
7.2984
7.2707
7.2673
7.2583
7.2519
7.2390
7.2349
7.1339
7.1171
4.2430
2.8057
2.7957
1.8188
1.8121
1.8055
1.7988
1.7922
O
4t
1.84
2.05
4.39
0.98
2.00
4.02
4.00
f1 (ppm)


197.6292
143.3537
137.5624
134.9460
134.1419
129.5574
129.4712
129.3967
128.6448
126.7814
125.7879
45.3944
29.6642
29.4212
22.9671
22.8282
O
4t
f1 (ppm)


7.7738
7.7685
7.5492
7.5443
7.3744
7.3690
7.3567
7.3514
7.3289
7.3259
7.3226
7.3161
7.3123
7.3090
7.3002
7.2974
7.2957
7.2927
7.2841
7.2776
7.2746
7.2722
7.2672
7.2649
7.2600
7.2547
7.2498
7.2453
7.2423
7.2318
7.2284
7.2239
7.2182
7.2149
7.2125
6.8829
6.8655
6.6784
6.6609
4.3907


Cl
O
O
Cl
Cl

4u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0.99
1.10
6.01
0.94
0.96
2.00
f1 (ppm)


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134.0320
133.2051
130.9186
130.7361
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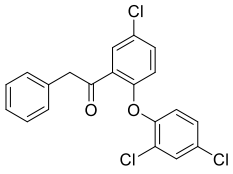
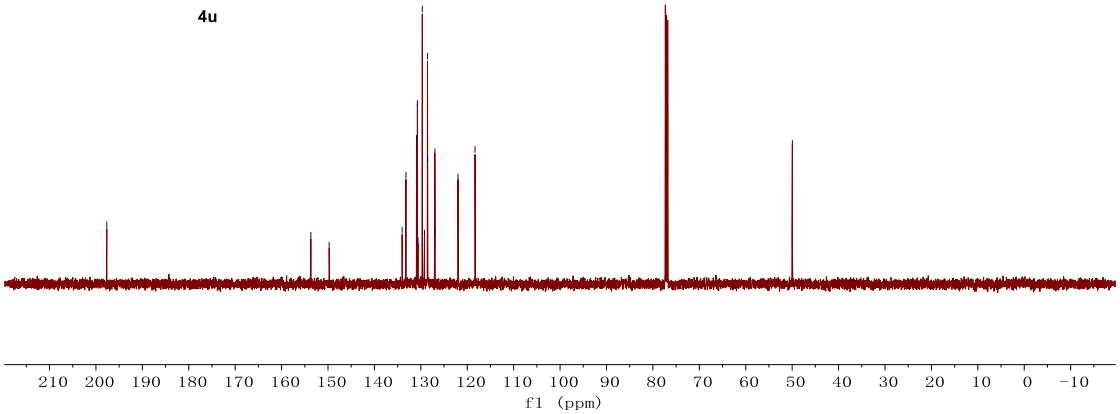
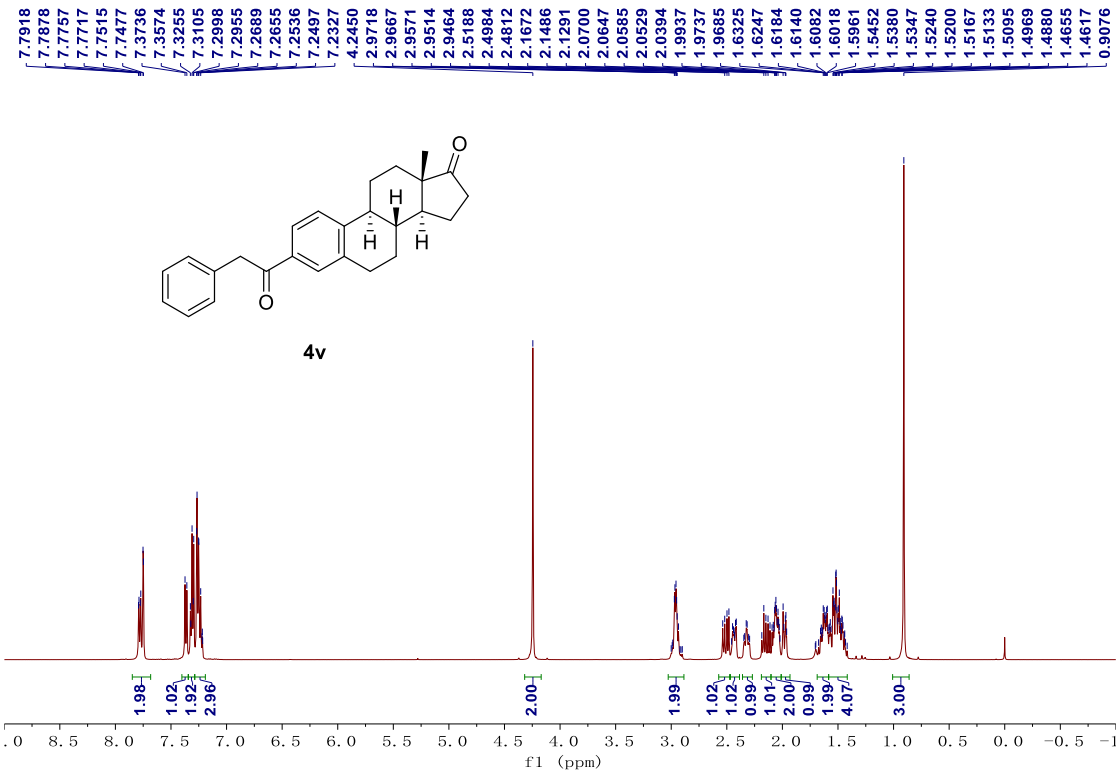
129.2160
128.5648
128.5426
127.0101
126.9784
121.9958
118.3245
49.9607


Cl
O
O
Cl
Cl

4u


f1 (ppm)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7.7515
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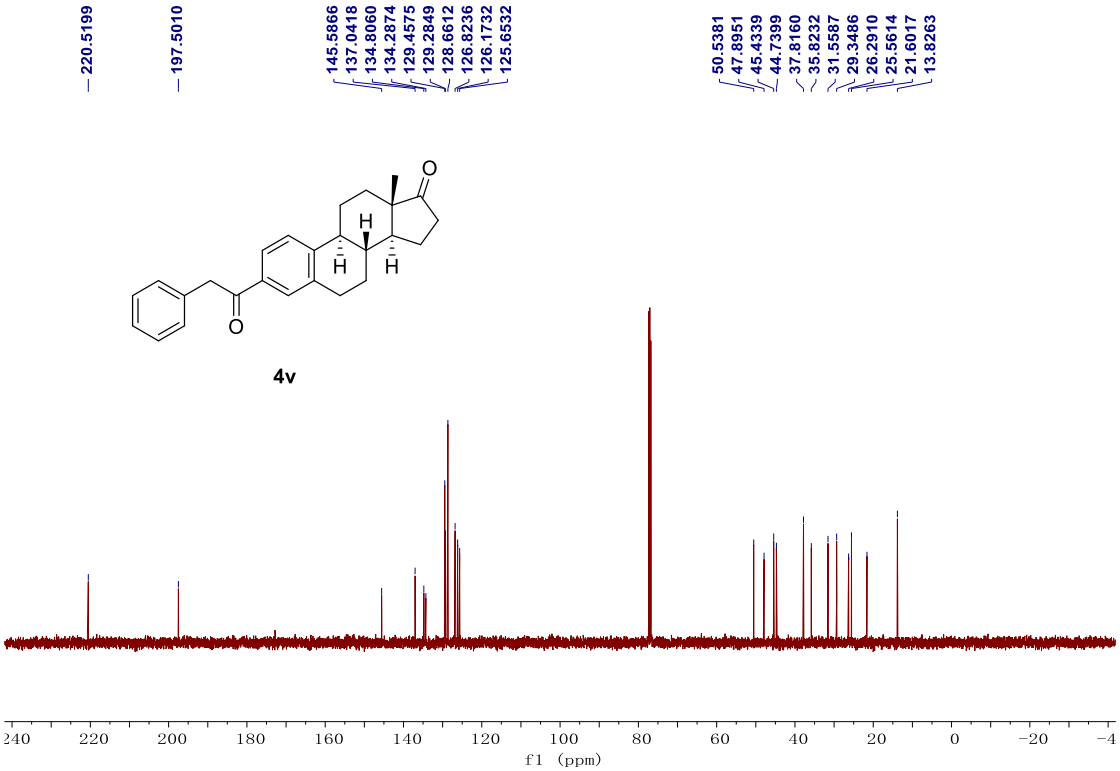
7.3105
7.2998
7.2955
7.2689
7.2655
7.2536
7.2497
7.2327
4.2450
2.9718
2.9667
2.9571
2.9514
2.9464
2.5188
2.4984
2.4812
2.1672
2.1486
2.1291
2.0700
2.0647
2.0585
2.0529
2.0394
1.9937
1.9737
1.9685
1.6325
1.6247
1.6184
1.6140
1.6082
1.6018
1.5961
1.5452
1.5380
1.5347
1.5240
1.5200
1.5167
1.5133
1.5095
1.4969
1.4880
1.4655
1.4617
0.9076
O
H
H
H
O
4v
1.98
1.02
1.92
2.96
2.00
1.99
1.02
1.02
0.99
1.01
2.00
0.99
1.99
4.07
3.00
f1 (ppm)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126.1732
125.6532
50.5381
47.8951
45.4339
44.7399
37.8160
35.8232
31.5587
29.3486
26.2910
25.5614
21.6017
13.8263
O
H
H
H
O
4v
f1 (ppm)