Electronic Supplementary Material (ESI) for Organic Chemistry Frontiers.

Supporting Information
For

Formates Plus Triazabicyclodecene(TBD): An Efficient Platform for Non-Gaseous Carbonylation and Unexepcted Hydrogenation

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Table of contents

1. General information

All reactions were carried out in oven-dried glassware sealed with rubber septa. All solvents were distilled under nitrogen atmosphere prior to use. THF was dried over sodium; toluene and acetonitrile was dried over CaH_2. Purification of products was conducted by flash chromatography on silica gel (200-300 mesh). NMR spectra were measured on a Varian 400 (^1H at 400 MHz, ^{13}C at 100 MHz) magnetic resonance spectrometer. Chemical shifts are reported in ppm using tetramethylsilane as internal standard (s = singlet, d = doublet, t = triplet, q = quartet, dd = doublet of doublets, m = multiplet). Infrared spectra were recorded on a Nicolet Avatar 330 Fourier transform spectrometer (FT-IR) and are reported in wave numbers (cm^{-1}). MS data were obtained on an Agilent 5975C inert 350 EI mass spectrometer (GC-MS). HRMS data were obtained on a VG ZAB-HS mass spectrometer, Brucker Apex IV FTMS spectrometer. Compounds described in the literature were characterized by comparison of their ^1H, and/or ^{13}C NMR spectra to the previously reported data.

2. General procedure of the reaction

Typical procedure for the synthesis of 3.

A solution of aryl halides **1** (0.5 mmol, 1.0 eq), $Pd_2(dba)_3$ (0.025 mmol, 5 mol%), TBD (0.0125 mmol, 2.5 mol%), DBU (0.6 mmol, 1.2 eq) and formate **2** (1.5 mmol, 3.0 eq) in toluene (5 mL) was charged in a tube. The tube was sealed with a cap, placed in an oil bath and stirred for 12 hours at 80 °C. Then the reaction was quenched with water (20 mL), extracted with DCM (3×10 mL), dried with anhydrous Na_2SO_4. After evaporation, chromatography on silica gel of the reaction mixture afforded desired product **3**.

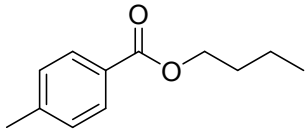
Typical procedure for the synthesis of 5.

A solution of aryl halides **1** (0.5 mmol, 1.0 eq), $Pd_2(dba)_3$ (0.025 mmol, 5 mol%), TBD (0.0125 mmol, 2.5 mol%), DBU (0.6 mmol, 1.2 eq), formate **2a** (1.5 mmol, 3.0 eq) and **4** (0.5 mmol, 1.5 eq.) in toluene (5 mL) was charged in a tube. The tube was sealed with a cap, placed in an oil bath and stirred for 12 hours at 80 °C. Then the reaction was quenched with water (20 mL), extracted with DCM (3×10 mL), dried with anhydrous Na_2SO_4. After evaporation, chromatography on silica gel of the reaction mixture afforded desired product **5**.

Typical procedure for the synthesis of 7.

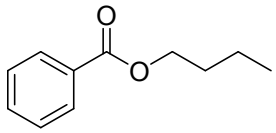
A solution of 2-iodoanilines **6** (0.5 mmol, 1.0 eq), $Pd_2(dba)_3$ (0.025 mmol, 5 mol%), TBD (0.0125 mmol, 2.5 mol%), DBU (0.6 mmol, 1.2 eq) and formate **2a** (1.5 mmol, 3.0 eq) in aqueous toluene (5 mL) was charged in a tube. The tube was sealed with a cap, placed in an oil bath and stirred for 12 hours at 80 °C. Then the reaction was quenched with water (20 mL), extracted with DCM (3×10 mL), dried with anhydrous Na_2SO_4. After evaporation, chromatography on silica gel of the reaction mixture afforded desired product **7**.

3. Characterization data



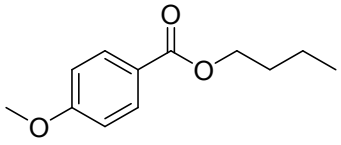
3a

butyl 4-methylbenzoate (3a): Colorless oil, 75mg, 78% yield; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.92 (d, *J* = 8.0 Hz, 2H), 7.21 (d, *J* = 8.0 Hz, 2H), 4.29 (t, *J* = 6.0 Hz, 2H), 2.39 (s, 3H), 1.73 (dd, *J* = 1.0, 5.0 Hz, 2H), 1.50–1.43 (m, 2H), 0.96 (t, *J* = 7.0 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 166.8, 143.4, 129.5, 129.0, 127.8, 64.6, 30.8, 21.6, 19.3, 13.8; IR (neat) 3480, 1641, 740cm^{-1}; HRMS (EI-TOF) calcd for $C_{12}H_{16}O_2$ 192.1150, found 192.1152.



3b

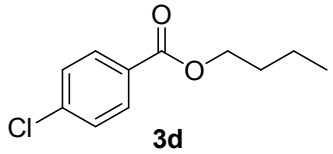
butyl benzoate (3b): Colorless oil, 71mg, 80% yield; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.08–7.97 (m, 2H), 7.57–7.50 (m, 1H), 7.42 (dd, *J* = 10.0, 5.0 Hz, 2H), 4.31 (t, *J* = 6.0 Hz, 2H), 1.78–1.71 (m, 2H), 1.47 (dd, *J* = 15.0, 7.0 Hz, 2H), 0.97 (t, *J* = 7.0 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 166.7, 132.8, 130.5, 129.5, 128.3, 64.8, 30.7, 19.3, 13.8; IR (neat) 3477, 1640, 740cm^{-1}; HRMS (EI-TOF) calcd for $C_{11}H_{14}O_2$ 178.0994, found 178.0995.



3c

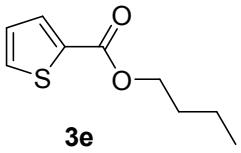
butyl 4-methoxybenzoate (3c): Colorless oil, 88mg, 85% yield; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.98 (d, *J* = 9.0 Hz, 2H), 6.90 (d, *J* = 9.0 Hz, 2H), 4.27 (t, *J* = 7.0 Hz, 2H), 3.84 (s, 3H), 1.72 (dd, *J* = 10.0, 5.0 Hz, 2H), 1.49–1.42 (m, 2H), 0.96 (t, *J* = 7.0Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 166.4, 163.2, 131.5, 122.9, 113.5, 64.5, 55.4, 30.8, 19.3, 13.8; IR (neat) 3465, 1639, 1264cm^{-1}; HRMS (EI-TOF) calcd for

$C_{12}H_{16}O_3$ 208.1099, found 208.1099.



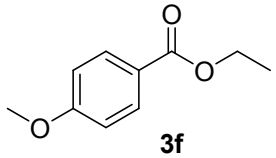
3d

butyl 4-chlorobenzoate (3d): Colorless oil, 78mg, 74% yield; ^{1}H NMR (400 MHz, $CDCl_3$) δ7.96 (d, *J* = 9.0 Hz, 2H), 7.39 (d, *J* = 9.0 Hz, 2H), 4.30 (t, *J* = 7.0 Hz, 2H), 1.73 (dd, *J* = 10.0, 5.0 Hz, 2H), 1.48–1.42 (m, 2H), 0.96 (t, *J* = 7.0 Hz, 3H).; ^{13}C NMR (100 MHz, $CDCl_3$) δ 165.8, 139.2, 130.9, 128.9, 128.6, 65.1, 30.7, 19.3, 13.7; IR (neat) 3465, 1640, 741cm^{-1}; HRMS (EI-TOF) calcd for $C_{11}H_{13}ClO_2$ 212.0604, found 212.0607.



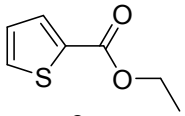
3e

butyl thiophene-2-carboxylate (3e): Colorless oil, 75mg, 81% yield; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.78 (dd, *J* = 4.0, 1.0 Hz, 1H), 7.52 (dd, *J* = 5.0, 1.0 Hz, 1H), 7.08 (dd, *J* = 5.0, 3.0 Hz, 1H), 4.29 (d, *J* = 7.0 Hz, 2H), 1.71 (dd, *J* = 5.0, 3.0 Hz, 2H), 1.44 (m, 2H), 0.95 (t, *J* = 7.0 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 162.3, 134.1, 133.2, 132.1, 127.7, 65.0, 30.7, 19.2, 13.7; IR (neat) 3478, 1641, 740cm^{-1}; HRMS (EI-TOF) calcd for $C_9H_{12}O_2S$ 184.0558, found 184.0554.



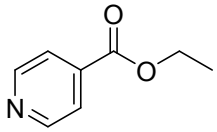
3f

ethyl 4-methoxybenzoate (3f): Colorless oil, 69mg, 77% yield; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.98 (d, *J* = 9.0 Hz, 2H), 6.89 (d, *J* = 9.0 Hz, 2H), 4.32 (q, *J* = 7.0 Hz, 2H), 3.83 (s, 3H), 1.36 (t, *J* = 7.0 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 166.4, 163.2, 131.5, 122.9, 113.5, 60.6, 55.4, 14.4; IR (neat) 3466, 1611, 740cm^{-1}; HRMS (EI-TOF) calcd for $C_{10}H_{12}O_3$ 180.0786, found 180.0788.



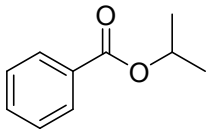
3g

ethyl thiophene-2-carboxylate (3g): Colorless oil, 59mg, 75% yield; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.78 (dd, *J* = 4.0, 1.0 Hz, 1H), 7.53 (dd, *J* = 5.0, 1.0 Hz, 1H), 7.08 (dd, *J* = 5.0, 4.0 Hz, 1H), 4.33 (q, *J* = 7.0 Hz, 2H), 1.36 (t, *J* = 7.0 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 162.3, 134.1, 133.2, 132.2, 127.7, 61.1, 14.3; IR (neat) 3474, 1642, 742cm^{-1}; HRMS (EI-TOF) calcd for $C_7H_8O_2S$ 156.0245, found 156.0251.



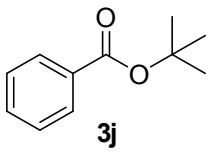
3h

ethyl isonicotinate (3h): Colorless oil, 52mg, 69% yield; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.75 (d, *J* = 6.0 Hz, 2H), 7.83 (d, *J* = 6.0 Hz, 2H), 4.39 (q, *J* = 7.0 Hz, 2H), 1.38 (t, *J* = 7.1 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 165.1, 150.5, 137.6, 122.8, 61.8, 14.2; IR (neat) 3476, 1642, 741cm^{-1}; HRMS (EI-TOF) calcd for $C_8H_9NO_2$ 151.0633, found 151.0635.



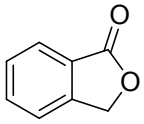
3i

isopropyl benzoate (3i): Colorless oil, 51mg, 62% yield; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.03 (d, *J* = 8.0 Hz, 2H), 7.55–7.49 (m, 1H), 7.41 (t, *J* = 8.0 Hz, 2H), 5.24 (m, 1H), 1.36–1.34 (m, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 166.1, 132.6, 130.9, 129.5, 128.2, 68.3, 21.9; IR (neat) 3459, 1638, 712cm^{-1}; HRMS (EI-TOF) calcd for $C_{10}H_{12}O_2$ 164.0837, found 164.0836.



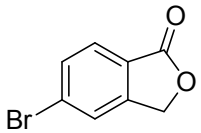
3j

***tert*-butyl benzoate (3j):** Colorless oil, 41mg, 46% yield; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.00–7.95 (m, 2H), 7.53–7.48 (m, 1H), 7.42–7.38 (m, 2H), 1.58 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 165.8, 132.4, 132.0, 129.4, 128.1, 80.9, 28.2; IR (neat) 3476, 1643, 740cm^{-1}; HRMS (EI-TOF) calcd for $C_{11}H_{14}O_2$ 178.0994, found 178.0996.



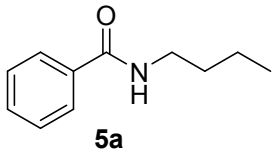
3k

isobenzofuran-1(3*H*)-one (3k): White powder, 51mg, 76% yield; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.90 (d, *J* = 8.0 Hz, 1H), 7.67 (t, *J* = 8.0 Hz, 1H), 7.50 (dd, *J* = 17.0, 8.0 Hz, 2H), 5.31 (s, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 171.1, 146.5, 134.0, 129.0, 125.7, 125.6, 122.1, 69.6; IR (neat) 3475, 1636, 737cm^{-1}; HRMS (EI-TOF) calcd for $C_8H_6O_2$ 134.0368, found 134.0366.



3l

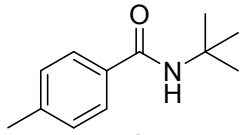
5-bromoisobenzofuran-1(3*H*)-one (3l): White powder, 74mg, 70% yield; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.75 (dd, *J* = 7.0, 2.0 Hz, 1H), 7.65 (s, 2H), 5.28 (s, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 170.0, 148.2, 132.7, 129.3, 127.0, 125.6, 124.7, 68.9; IR (neat) 3463, 1640, 763cm^{-1}; HRMS (EI-TOF) calcd for $C_8H_5BrO_2$ 211.9473, found 211.9474.



5a

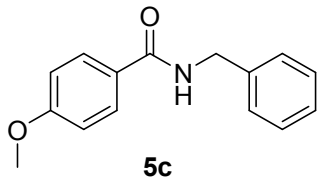
***N*-butylbenzamide (5a):** White powder, 76mg, 86% yield; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.75–7.71 (m, 2H), 7.49–7.43 (m, 1H), 7.39 (t, *J* = 7.0 Hz, 2H), 6.27 (br, 1H), 3.46–3.40 (m, 2H), 1.60–1.55 (m, 2H), 1.38 (dd, *J* = 15.0, 7.0 Hz, 2H), 0.93 (t, *J* = 7.0 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 167.6, 134.7, 131.3, 128.5, 126.8, 39.8,

31.7, 20.1, 13.8; IR (neat) 3462, 1640, 701cm^{-1}; HRMS (EI-TOF) calcd for $C_{11}H_{15}NO$ 177.1154, found 177.1152.



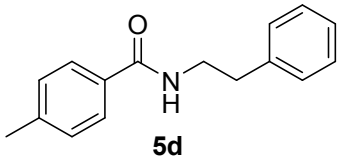
5b

***N-tert*-butyl-4-methylbenzamide (5b):** White powder, 74mg, 78% yield; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.60 (d, *J* = 8.0 Hz, 2H), 7.19 (d, *J* = 8.0 Hz, 2H), 5.91 (br, 1H), 2.36 (s, 3H), 1.45 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 166.8, 141.4, 132.9, 129.1, 126.7, 51.5, 28.9, 21.4; IR (neat) 3460, 1639, 691cm^{-1}; HRMS (EI-TOF) calcd for $C_{12}H_{17}NO$ 191.1310, found 191.1312.



5c

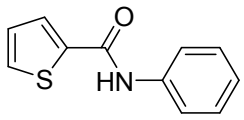
***N*-benzyl-4-methoxybenzamide (5c):** White powder, 100mg, 83% yield; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.76–7.73 (d, *J* = 9.0 Hz, 2H), 7.33 (d, *J* = 5.0 Hz, 4H), 7.28 (d, *J* = 5.0 Hz, 1H), 6.90 (d, *J* = 9.0 Hz, 2H), 6.39 (br, 1H), 4.61 (d, *J* = 5.0 Hz, 2H), 3.82 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 166.9, 162.2, 138.3, 128.8, 128.7, 127.9, 127.5, 126.5, 113.7, 55.4, 44.1; IR (neat) 3468, 1632, 724cm^{-1}; HRMS (EI-TOF) calcd for $C_{15}H_{15}NO_2$ 241.1103, found 241.1102.



5d

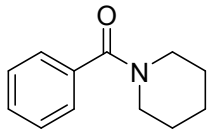
4-methyl-N-phenethylbenzamide (5d): White powder, 96mg, 80% yield; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.58 (d, *J* = 8.0 Hz, 2H), 7.31 (t, *J* = 7.0 Hz, 2H), 7.25–7.17 (m, 5H), 6.18 (br, 1H), 3.69 (dd, *J* = 13.0, 7.0 Hz, 2H), 2.91 (t, *J* = 7.0 Hz, 2H), 2.36 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 167.4, 141.8, 138.9, 131.7, 129.2, 128.8, 128.7, 126.8, 126.5, 41.1, 35.7, 21.4; IR (neat) 3463, 1636, 742cm^{-1}; HRMS (EI-TOF)

calcd for $C_{16}H_{17}NO$ 239.1310, found 239.1314.



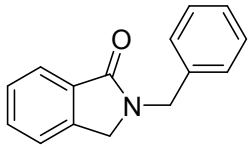
5e

***N*-phenylthiophene-2-carboxamide (5e):** White powder, 78mg, 77% yield; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.88 (br, 1H), 7.63 (dd, *J* = 4.0, 1.0 Hz, 1H), 7.61–7.58 (m, 2H), 7.51 (d, *J* = 5.0 Hz, 1H), 7.32 (t, *J* = 8.0 Hz, 2H), 7.13 (d, *J* = 7.0 Hz, 1H), 7.08 (dd, *J* = 5.0, 4.0 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 160.0, 139.3, 137.6, 130.8, 129.1, 128.5, 127.8, 124.6, 120.3; IR (neat) 3475, 1637, 747cm^{-1}; HRMS (EI-TOF) calcd for $C_{11}H_9NOS$ 203.0405, found 203.0406.



5f

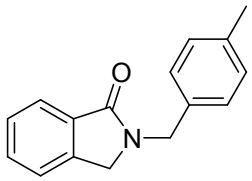
phenyl(piperidin-1-yl)methanone (5f): Colorless oil, 64mg, 68% yield; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.35 (s, 5H), 3.67 (s, 2H), 3.31 (s, 2H), 1.64 (s, 4H), 1.49 (s, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 170.3, 136.5, 129.3, 128.4, 126.7, 45.9, 26.1, 24.6; IR (neat) 3475, 1668, 766cm^{-1}; HRMS (EI-TOF) calcd for $C_{12}H_{15}NO$ 189.1154, found 189.1157.



5g

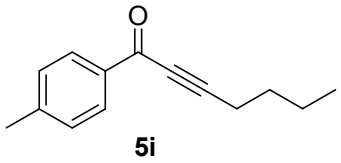
2-benzylisoindolin-1-one (5g): White powder, 84mg, 75% yield; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.87 (d, *J* = 7.0 Hz, 1H), 7.48 (dd, *J* = 11.0, 4.0 Hz, 1H), 7.43 (t, *J* = 7.0 Hz, 1H), 7.35 (d, *J* = 7.0 Hz, 1H), 7.33–7.30 (m, 1H), 7.29 (d, *J* = 3.0 Hz, 3H), 7.26 (d, *J* = 7.0 Hz, 1H), 4.78 (s, 2H), 4.23 (s, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 168.4, 141.2, 137.0, 132.6, 131.3, 128.8, 128.1, 128.0, 127.6, 123.8, 122.8, 49.4, 46.3; IR (neat) 3466, 1679, 737cm^{-1}; HRMS (EI-TOF) calcd for $C_{15}H_{13}NO$ 223.0997, found

223.1000.



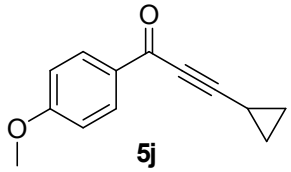
5h

2-(4-methylbenzyl)isoindolin-1-one (5h): White powder, 92mg, 78% yield; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.86 (d, *J* = 7.0 Hz, 1H), 7.47 (dd, *J* = 7.0, 1.0 Hz, 1H), 7.43 (d, *J* = 7.0 Hz, 1H), 7.34 (d, *J* = 7.0 Hz, 1H), 7.18 (d, *J* = 8.0 Hz, 2H), 7.11 (d, *J* = 8.0 Hz, 2H), 4.74 (s, 2H), 4.21 (s, 2H), 2.30 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 168.4, 141.2, 137.3, 134.0, 132.7, 131.3, 129.4, 128.2, 128.0, 123.8, 122.7, 49.3, 46.1, 21.1; IR (neat) 3465, 1682, 739cm^{-1}; HRMS (EI-TOF) calcd for $C_{16}H_{15}NO$ 237.1154, found 237.1156.



5i

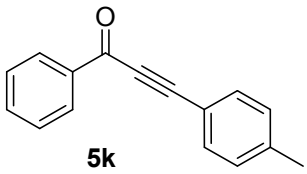
1-*p*-tolylhept-2-yn-1-one (5i): Light yellow oil, 75mg, 75% yield; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.01 (d, *J* = 8.0 Hz, 2H), 7.25 (d, *J* = 8.0 Hz, 2H), 2.48 (t, *J* = 7.0 Hz, 2H), 2.41 (s, 3H), 1.67–1.62 (m, 2H), 1.52–1.46 (m, 2H), 0.94 (t, *J* = 7.0 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 178.0, 144.9, 134.6, 129.7, 129.2, 96.3, 79.7, 29.8, 22.1, 21.8, 18.9, 13.5; IR (neat) 3466, 1642, 740cm^{-1}; HRMS (EI-TOF) calcd for $C_{14}H_{16}O$ 200.1201, found 200.1203.



5j

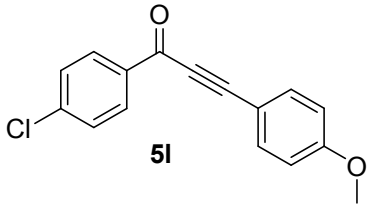
3-cyclopropyl-1-(4-methoxyphenyl)prop-2-yn-1-one (5j): Light yellow oil, 73mg, 73% yield; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.05 (d, *J* = 9.0 Hz, 2H), 6.91 (d, *J* = 9.0 Hz, 2H), 3.85 (s, 3H), 1.55–1.45 (m, 1H), 1.02–0.97 (m, 4H); ^{13}C NMR (100 MHz,

$CDCl_3$) δ 176.7, 164.1, 131.8, 130.3, 113.6, 100.0, 75.4, 55.5, 9.8, 0.04; IR (neat) 3463, 1634, 755cm^{-1}; HRMS (EI-TOF) calcd for $C_{13}H_{12}O_2$ 200.0837, found 200.0839.



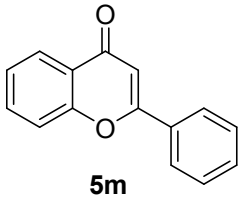
5k

1-phenyl-3-*p*-tolylprop-2-yn-1-one (5k): White powder, 90mg, 82% yield; ^1H NMR (400 MHz, $CDCl_3$) δ 8.24–8.19 (m, 2H), 7.62 (s, 2H), 7.58 (d, *J* = 8.0 Hz, 1H), 7.51 (t, *J* = 8.0 Hz, 2H), 7.22 (d, *J* = 8.0 Hz, 2H), 2.40 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 178.1, 141.6, 136.9, 134.0, 133.1, 129.5, 129.5, 128.6, 117.0, 93.8, 86.8, 21.8; IR (neat) 3467, 1640, 740cm^{-1}; HRMS (EI-TOF) calcd for $C_{16}H_{12}O$ 220.0888, found 220.0890.



5l

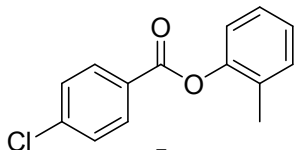
1-(4-chlorophenyl)-3-(4-methoxyphenyl)prop-2-yn-1-one (5l): White powder, 109mg, 81% yield; ^1H NMR (400 MHz, $CDCl_3$) δ 8.13 (d, *J* = 9.0 Hz, 2H), 7.63 (d, *J* = 9.0 Hz, 2H), 7.47 (d, *J* = 9.0 Hz, 2H), 6.93 (d, *J* = 9.0 Hz, 2H), 3.85 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 176.7, 161.8, 140.4, 138.4, 135.2, 130.8, 128.9, 114.5, 111.6, 105.0, 86.6, 55.5; IR (neat) 3456, 1633, 739cm^{-1}; HRMS (EI-TOF) calcd for $C_{16}H_{11}ClO_2$ 270.0448, found 270.0446.



5m

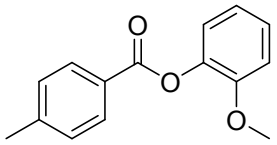
2-phenyl-4*H*-chromen-4-one (5m): White powder, 84mg, 76% yield; ^1H NMR (400 MHz, $CDCl_3$) δ 8.21 (dd, *J* = 8.0, 2.0 Hz, 1H), 7.92–7.89 (m, 2H), 7.68 (m, 1H),

7.55 (d, J = 8.0 Hz, 1H), 7.52–7.47 (m, 3H), 7.43–7.37 (m, 1H), 6.81 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 178.4, 163.4, 156.2, 133.8, 131.7, 131.6, 129.0, 126.3, 125.7, 125.2, 123.9, 118.1, 107.5; IR (neat) 3461, 1640, 768cm^{-1}; HRMS (EI-TOF) calcd for $C_{15}H_{10}O_2$ 222.0681, found 222.0684.



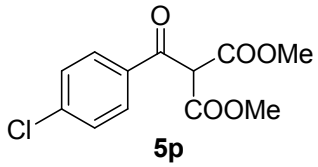
5n

***o*-tolyl 4-chlorobenzoate (5n):** Colorless oil, 89mg, 72% yield; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.18–8.12 (m, 2H), 7.51–7.46 (m, 2H), 7.28–7.23 (m, 2H), 7.19 (dd, J = 7.0, 1.0 Hz, 1H), 7.14–7.09 (m, 1H), 2.21 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 164.0, 149.3, 140.1, 131.5, 131.2, 130.2, 129.0, 127.9, 127.0, 126.2, 121.9, 16.2; IR (neat) 3463, 1639, 747cm^{-1}; HRMS (EI-TOF) calcd for $C_{14}H_{11}ClO_2$ 246.0448, found 246.0447.



5o

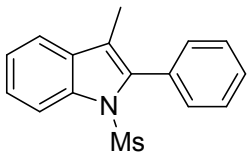
2-methoxyphenyl 4-methylbenzoate (5o): Colorless oil, 93mg, 77% yield; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.10 (d, J = 8.0 Hz, 2H), 7.29 (d, J = 8.0 Hz, 2H), 7.24–7.20 (m, 1H), 7.14 (dd, J = 8.0, 2.0 Hz, 1H), 7.01–6.96 (m, 2H), 3.80 (s, 3H), 2.44 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 164.8, 151.4, 144.2, 140.0, 130.3, 129.2, 126.8, 126.7, 123.0, 120.8, 112.5, 55.9, 21.6; IR (neat) 3476, 1639, 744cm^{-1}; HRMS (EI-TOF) calcd for $C_{15}H_{14}O_3$ 242.0943, found 242.0946.



5p

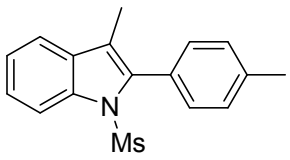
dimethyl 2-(4-chlorobenzoyl)malonate (5p): Light yellow oil, 84mg, 62% yield; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.82 (d, J = 9.0 Hz, 2H), 7.44 (d, J = 9.0 Hz, 2H),

5.25 (s, 1H), 3.78 (s, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 187.5, 165.0, 140.8, 133.5, 129.6, 128.8, 61.4, 53.4; IR (neat) 3478, 1690, 740cm^{-1}; HRMS (EI-TOF) calcd for $C_{12}H_{11}ClO_5$ 270.0295, found 270.0298.



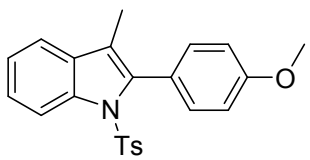
7a

3-methyl-1-(methylsulfonyl)-2-phenyl-1*H*-indole (7a): White powder, 114mg, 80% yield; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.14–8.09 (m, 1H), 7.57–7.53 (m, 1H), 7.44 (d, *J* = 3.0 Hz, 5H), 7.39–7.36 (m, 2H), 2.72 (s, 3H), 2.15 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 136.9, 136.6, 131.6, 131.3, 131.0, 128.6, 127.8, 125.2, 124.2, 119.5, 119.3, 115.5, 39.5, 9.5; IR (neat) 3486, 1678, 762cm^{-1}; HRMS (EI-TOF) calcd for $C_{16}H_{15}NO_2S$ 285.0823, found 285.0827.



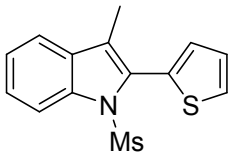
7b

3-methyl-1-(methylsulfonyl)-2-*p*-tolyl-1*H*-indole (7b): White powder, 117mg, 78% yield; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.13–8.08 (m, 1H), 7.56–7.51 (m, 1H), 7.38–7.34 (m, 2H), 7.32 (dd, *J* = 8.0, 2.0 Hz, 2H), 7.25 (d, *J* = 8.0 Hz, 2H), 2.71 (s, 3H), 2.42 (s, 3H), 2.14 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 138.5, 136.9, 136.7, 131.6, 130.9, 128.5, 128.2, 125.1, 124.1, 119.2, 119.2, 115.5, 39.5, 21.5, 9.5; IR (neat) 3484, 1672, 761cm^{-1}; HRMS (EI-TOF) calcd for $C_{17}H_{17}NO_2S$ 299.0980, found 299.0981.



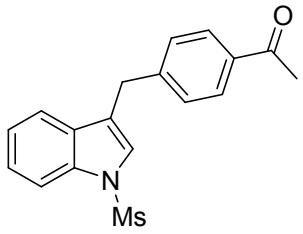
7c

2-(4-methoxyphenyl)-3-methyl-1-tosyl-1*H*-indole (7c): White powder, 139mg, 71% yield; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.30 (d, *J* = 8.0 Hz, 1H), 7.39 (d, *J* = 8.0 Hz, 2H), 7.34 (d, *J* = 8.0 Hz, 1H), 7.28 (s, 2H), 7.24 (d, *J* = 2.0 Hz, 2H), 7.03 (d, *J* = 8.0 Hz, 2H), 6.99–6.93 (m, 2H), 3.88 (s, 3H), 2.28 (s, 3H), 2.01 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 159.6, 144.2, 143.3, 137.1, 136.5, 132.6, 131.8, 129.1, 129.0, 128.4, 126.8, 124.7, 123.8, 118.8, 116.2, 112.9, 55.2, 21.5, 9.5; IR (neat) 3481, 1676, 758cm^{-1}; HRMS (EI-TOF) calcd for $C_{23}H_{21}NO_3S$ 391.1242, found 391.1245.



7d

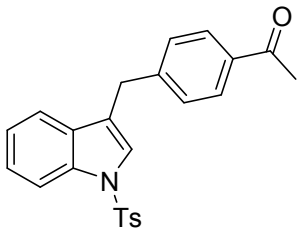
3-methyl-1-(methylsulfonyl)-2-(thiophen-2-yl)-1*H*-indole (7d): White powder, 105mg, 72% yield; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.10 (dd, *J* = 7.0, 1.0 Hz, 1H), 7.56–7.53 (m, 1H), 7.51 (dd, *J* = 5.0, 1.0 Hz, 1H), 7.40 (d, *J* = 2.0 Hz, 1H), 7.36 (dd, *J* = 5.0, 4.0 Hz, 1H), 7.20–7.16 (m, 1H), 7.15–7.12 (m, 1H), 2.85 (s, 3H), 2.19 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 136.9, 131.1, 130.8, 130.7, 129.0, 128.4, 128.1, 126.9, 125.7, 124.0, 119.4, 115.3, 40.1, 9.7; IR (neat) 3493, 1682, 759cm^{-1}; HRMS (EI-TOF) calcd for $C_{14}H_{13}NO_2S_2$ 291.0388, found 291.0386.



7e

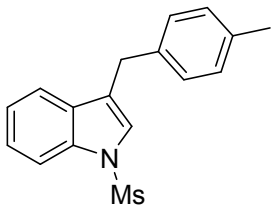
1-(4-((1-(methylsulfonyl)-1*H*-indol-3-yl)methyl)phenyl)ethanone (7e): White powder, 134mg, 82% yield; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.89 (d, *J* = 8.0 Hz, 3H), 7.44 (d, *J* = 8.0 Hz, 1H), 7.35 (d, *J* = 8.0 Hz, 3H), 7.28 – 7.24 (m, 1H), 7.15 (s, 1H), 4.09 (s, 2H), 3.06 (s, 3H), 2.57 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 197.7, 144.5,

135.6, 135.4, 130.4, 128.9, 128.8, 125.2, 123.7, 123.4, 121.2, 119.9, 113.2, 40.5, 31.4, 26.6; IR (neat) 3483, 1691, 745cm^{-1}; HRMS (EI-TOF) calcd for $C_{18}H_{17}NO_3S$ 327.0929, found 327.0928.



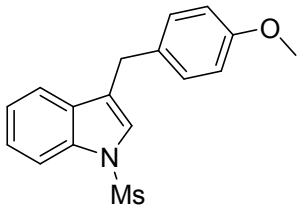
7f

1-(4-((1-tosyl-1*H*-indol-3-yl)methyl)phenyl)ethanone (7f): White powder, 155mg, 77% yield; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.97 (d, *J* = 8.0 Hz, 1H), 7.86 (d, *J* = 8.0 Hz, 2H), 7.72 (d, *J* = 8.0 Hz, 2H), 7.32–7.28 (m, 2H), 7.27 (d, *J* = 8.0 Hz, 3H), 7.20 (d, *J* = 8.0 Hz, 2H), 7.16 (s, 1H), 4.04 (s, 2H), 2.56 (s, 3H), 2.32 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 197.8, 144.9, 144.7, 135.5, 135.4, 135.1, 130.5, 129.8, 128.8, 128.7, 126.7, 124.9, 124.1, 123.2, 121.3, 119.6, 113.8, 31.4, 26.6, 21.6; IR (neat) 3488, 1693, 741cm^{-1}; HRMS (EI-TOF) calcd for $C_{24}H_{21}NO_3S$ 403.1242, found 403.1246.



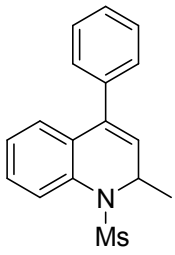
7g

3-(4-methylbenzyl)-1-(methylsulfonyl)-1*H*-indole (7g): White powder, 124mg, 83% yield; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.89 (d, *J* = 8.0 Hz, 1H), 7.50 (d, *J* = 8.0 Hz, 1H), 7.34 (d, *J* = 7.0 Hz, 1H), 7.29–7.24 (m, 1H), 7.16 (d, *J* = 8.0 Hz, 2H), 7.11 (dd, *J* = 6.0, 2.0 Hz, 3H), 4.00 (s, 2H), 3.03 (s, 3H), 2.33 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 136.0, 135.7, 135.5, 130.8, 129.3, 128.6, 125.0, 123.5, 123.3, 122.7, 120.0, 113.2, 40.4, 31.0, 21.0; IR (neat) 3485, 1692, 738cm^{-1}; HRMS (EI-TOF) calcd for $C_{17}H_{17}NO_2S$ 299.0980, found 299.0981.



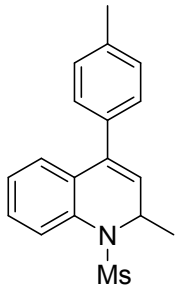
7h

3-(4-methoxybenzyl)-1-(methylsulfonyl)-1*H*-indole (7h): White powder, 134mg, 85% yield; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.89 (d, *J* = 8.0 Hz, 1H), 7.49 (d, *J* = 8.0 Hz, 1H), 7.35 (t, *J* = 8.0 Hz, 1H), 7.25 (d, *J* = 7.0 Hz, 1H), 7.18 (d, *J* = 9.0 Hz, 2H), 7.10 (s, 1H), 6.84 (d, *J* = 9.0 Hz, 2H), 3.98 (s, 2H), 3.78 (s, 3H), 3.03 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 158.2, 135.5, 130.8, 130.7, 129.7, 125.0, 123.5, 123.3, 122.9, 120.0, 114.0, 113.2, 55.3, 40.4, 30.5; IR (neat) 3482, 1687, 765cm^{-1}; HRMS (EI-TOF) calcd for $C_{17}H_{17}NO_3S$ 315.0929, found 315.0925.



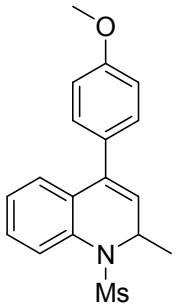
7i

2-methyl-1-(methylsulfonyl)-4-phenyl-1,2-dihydroquinoline (7i): White powder, 117mg, 78% yield; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.58–7.50 (m, 2H), 7.45–7.39 (m, 3H), 7.38 (d, *J* = 8.0 Hz, 1H), 7.31–7.24 (m, 2H), 7.15 (dd, *J* = 8.0, 1.0 Hz, 1H), 6.87 (d, *J* = 2.0 Hz, 1H), 5.45 (m, 1H), 2.83 (s, 3H), 1.51 (d, *J* = 6.0 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 141.8, 138.9, 135.6, 130.8, 130.0, 128.9, 128.4, 127.5, 124.6, 120.6, 119.4, 115.8, 62.0, 36.3, 20.7; IR (neat) 3487, 1674, 768cm^{-1}; HRMS (EI-TOF) calcd for $C_{17}H_{17}NO_2S$ 299.0980, found 299.0979.



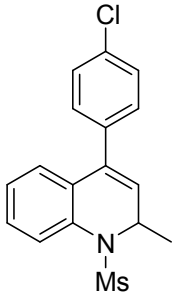
7j

2-methyl-1-(methylsulfonyl)-4-*p*-tolyl-1,2-dihydroquinoline (7j): White powder, 114mg, 73% yield; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.52 (dd, *J* = 11.0, 8.0 Hz, 2H), 7.32 (d, *J* = 8.0 Hz, 2H), 7.27 (dd, *J* = 11.0, 4.0 Hz, 1H), 7.19 (d, *J* = 8.0 Hz, 2H), 7.13 (m, 1H), 6.84 (d, *J* = 2.0 Hz, 1H), 5.44 (m, 1H), 2.82 (s, 3H), 2.36 (s, 3H), 1.52 (d, *J* = 6.0 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 141.6, 137.9, 137.6, 132.7, 131.0, 129.8, 129.6, 128.4, 124.6, 120.5, 119.4, 115.8, 62.1, 36.2, 21.3, 20.6; IR (neat) 3490, 1676, 769cm^{-1}; HRMS (EI-TOF) calcd for $C_{18}H_{19}NO_2S$ 313.1136, found 313.1132.



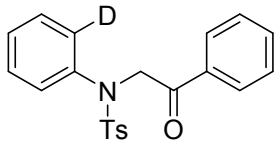
7k

4-(4-methoxyphenyl)-2-methyl-1-(methylsulfonyl)-1,2-dihydroquinoline (7k): White powder, 117mg, 71% yield; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.51 (t, *J* = 7.0 Hz, 2H), 7.36 (d, *J* = 9.0 Hz, 2H), 7.26 (dd, *J* = 9.0, 2.0 Hz, 1H), 7.13 (t, *J* = 7.0 Hz, 1H), 6.92 (d, *J* = 9.0 Hz, 2H), 6.81 (d, *J* = 2.0 Hz, 1H), 5.41 (m, 1H), 3.83 (s, 3H), 2.82 (s, 3H), 1.52 (d, *J* = 6.0 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 159.0, 141.4, 136.6, 131.2, 129.9, 129.5, 128.2, 124.6, 120.3, 119.1, 115.8, 114.3, 62.0, 55.3, 36.2, 20.6; IR (neat) 3493, 1678, 775cm^{-1}; HRMS (EI-TOF) calcd for $C_{18}H_{19}NO_3S$ 329.1086, found 329.1083.



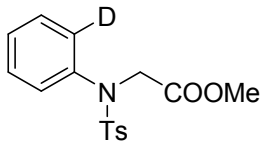
7l

4-(4-chlorophenyl)-2-methyl-1-(methylsulfonyl)-1,2-dihydroquinoline (7l): White powder, 133mg, 80% yield; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.52 (dd, *J* = 10.0, 8.0 Hz, 2H), 7.35 (s, 4H), 7.32–7.27 (m, 1H), 7.14 (m, 1H), 6.81 (d, *J* = 2.0 Hz, 1H), 5.39 (m, 1H), 2.84 (s, 3H), 1.50 (d, *J* = 6.0 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 141.9, 139.6, 134.1, 133.2, 130.4, 130.3, 129.6, 129.1, 124.6, 120.7, 118.0, 115.7, 61.9, 36.5, 20.5; IR (neat) 3497, 1686, 779cm^{-1}; HRMS (EI-TOF) calcd for $C_{17}H_{16}ClNO_2S$ 333.0590, found 333.0592.



9

***d*$_1$-4-methyl-*N*-(2-oxo-2-phenylethyl)-*N*-phenylbenzenesulfonamide (9):** White powder, 97mg, 53% yield; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.92 (dd, *J* = 5.0, 3.0 Hz, 2H), 7.59–7.53 (m, 2H), 7.45 (m, 2H), 7.28–7.23 (m, 5H), 7.15 (dd, *J* = 7.0, 3.0 Hz, 2H), 5.04 (s, 2H), 2.42 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 193.7, 143.7, 139.6, 135.3, 134.9, 133.7, 129.4, 129.3, 129.1, 128.7, 128.2, 128.1, 127.9, 57.6, 21.6; IR (neat) 3508, 1695, 763cm^{-1}; HRMS (EI-TOF) calcd for $C_{21}H_{18}DNO_3S$ 366.1148, found 366.1150.

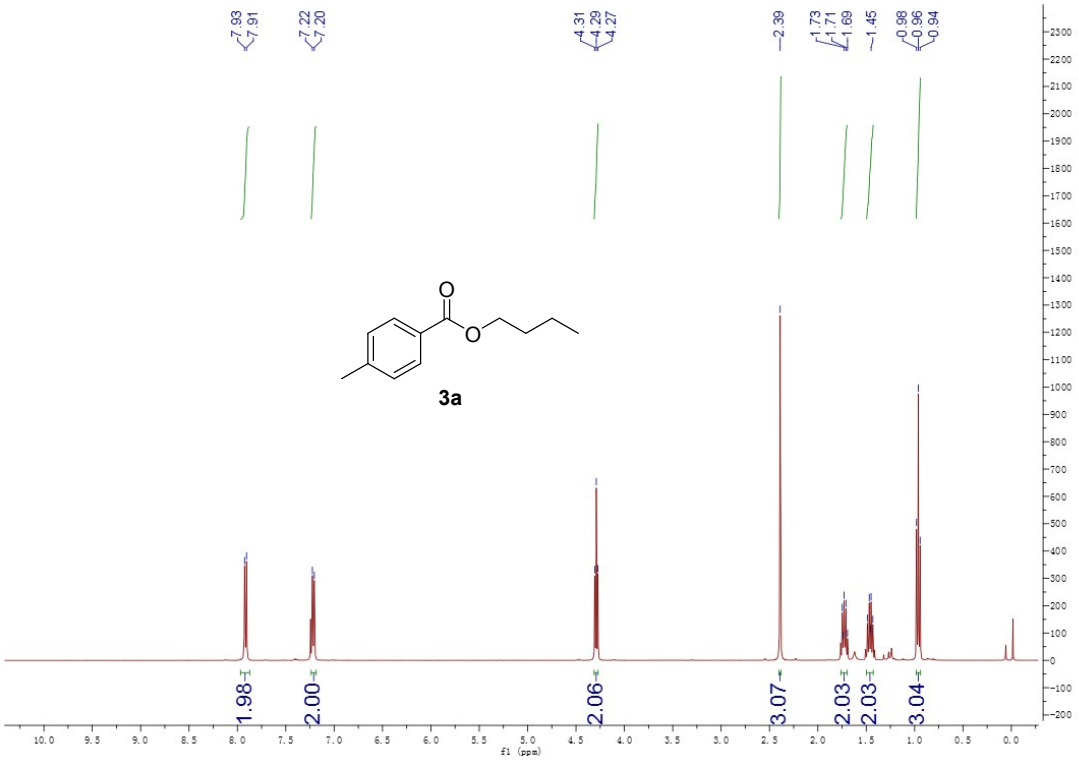


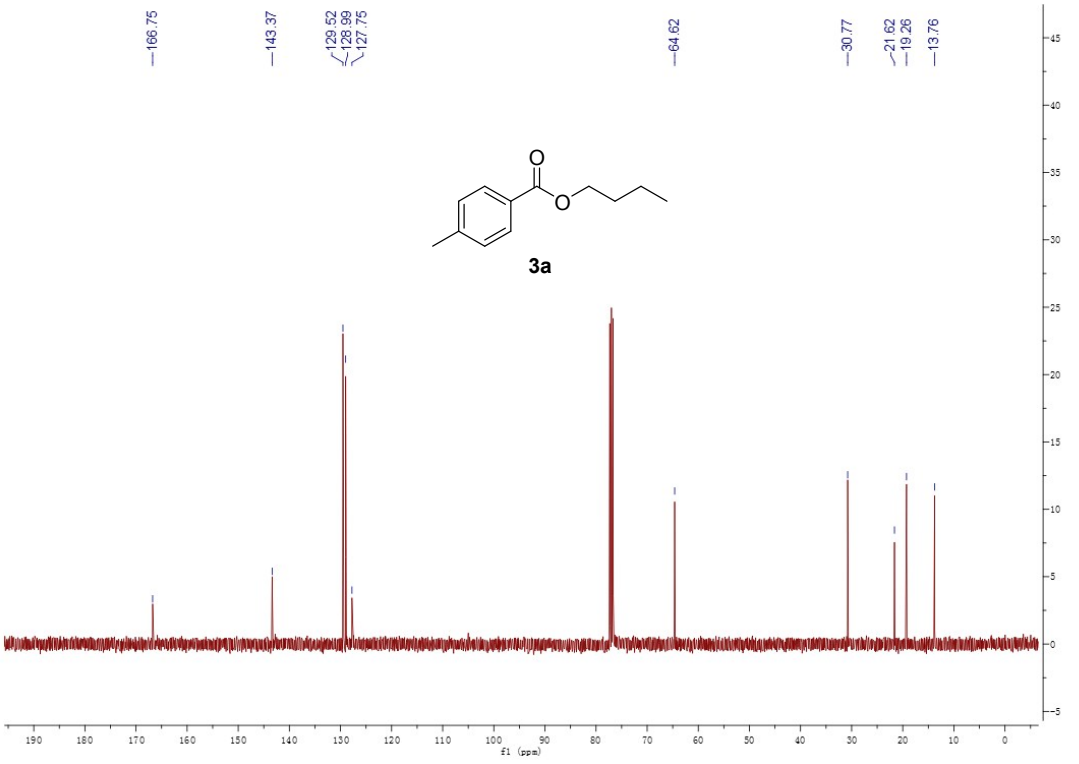
11

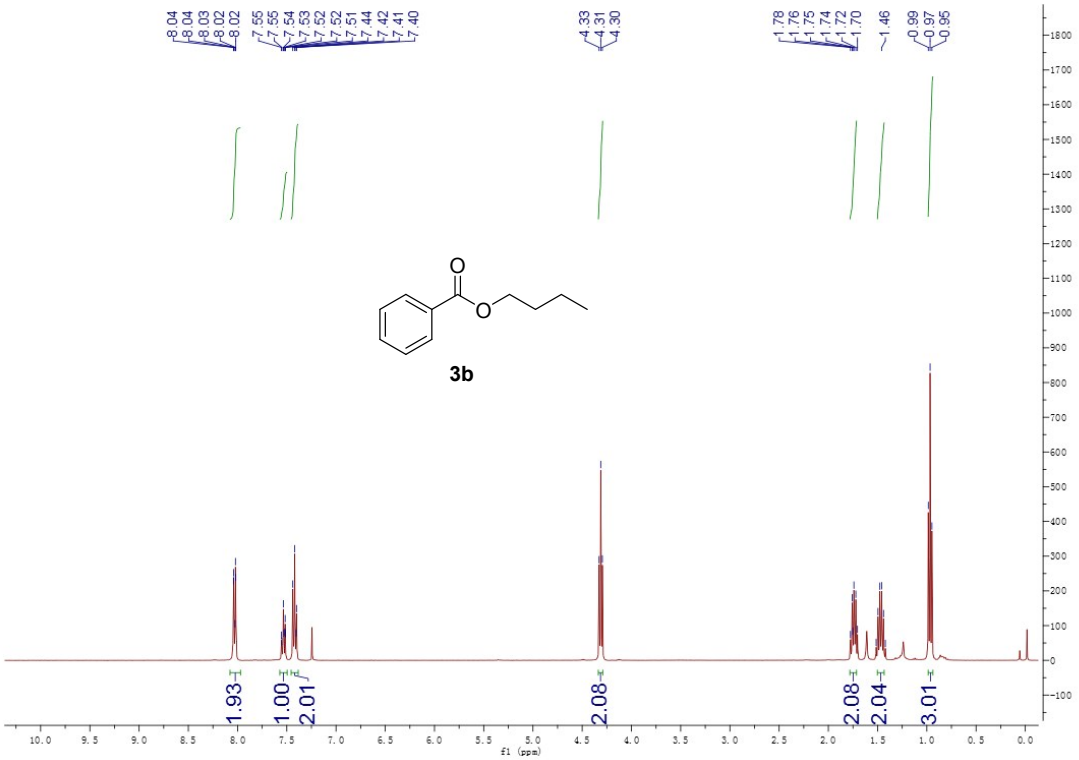
***d*$_1$-methyl 2-(4-methyl-*N*-phenylphenylsulfonamido)acetate (11):** White

powder, 82mg, 51% yield; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.52 (d, *J* = 8.0 Hz, 1H), 7.27 (m, 3H), 7.24–7.21 (m, 2H), 7.20–7.14 (m, 2H), 4.39 (s, 2H), 3.67 (s, 3H), 2.39 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 169.3, 143.7, 139.8, 135.7, 129.4, 129.3, 129.2, 128.8, 128.2, 127.7, 52.5, 21.6; IR (neat) 3516, 1688, 752cm^{-1}; HRMS (EI-TOF) calcd for $C_{16}H_{16}DNO_4S$ 320.0941, found 3320.0944.

4 The ^{1}H and ^{13}C NMR spectra of compounds



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8.04
8.03
8.02
8.02
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7.54
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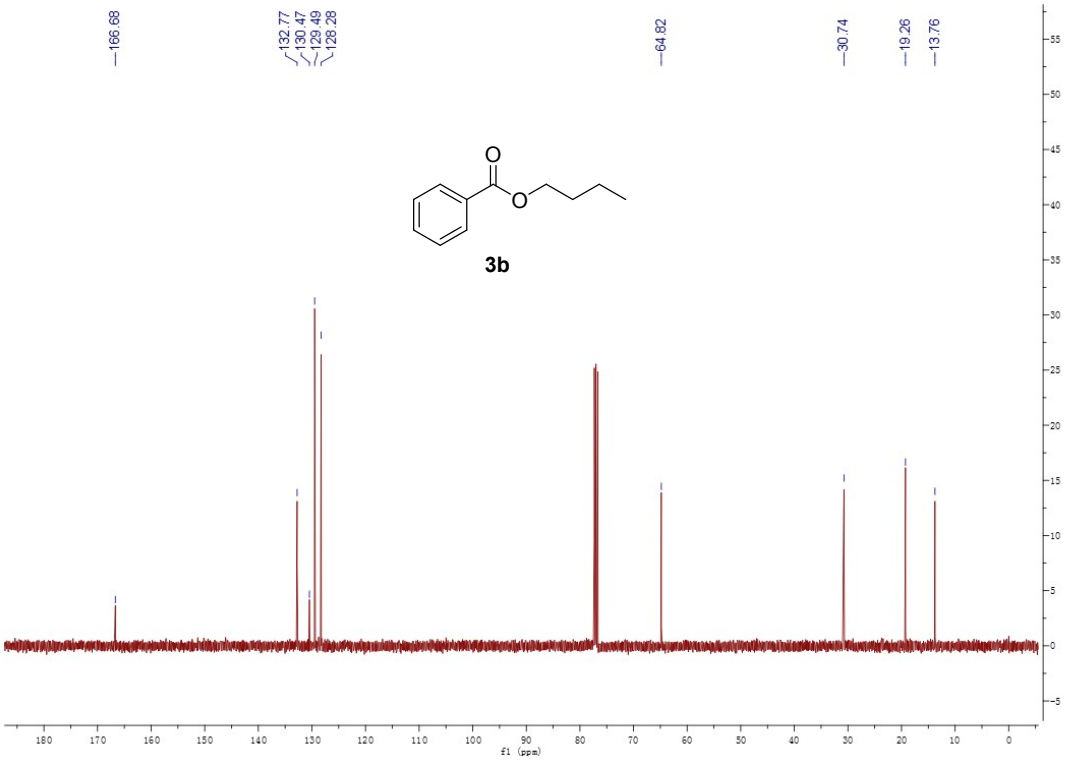
7.52
7.52
7.51
7.44
7.42
7.41
7.40
4.33
4.31
4.30
1.78
1.76
1.75
1.74
1.72
1.70
1.46
0.99
0.97
0.95
1.93
1.00
2.01
2.08
2.08
2.04
3.01
f1 (ppm)

3b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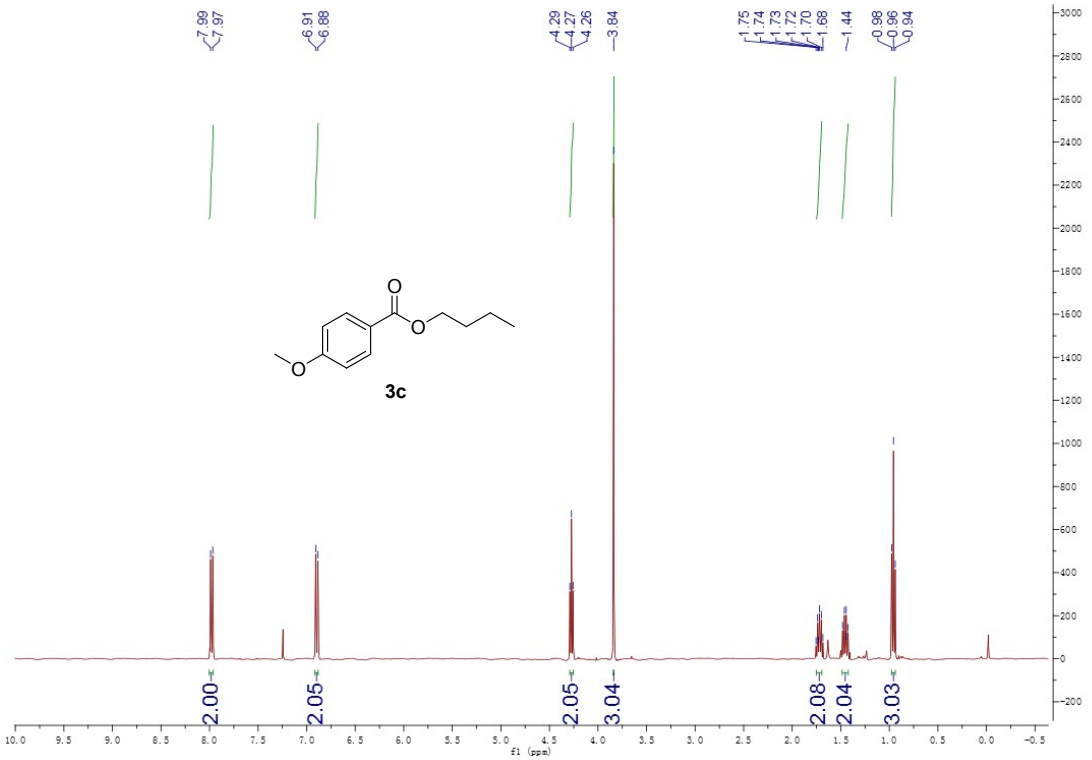
19.26
13.76
f1 (ppm)

3b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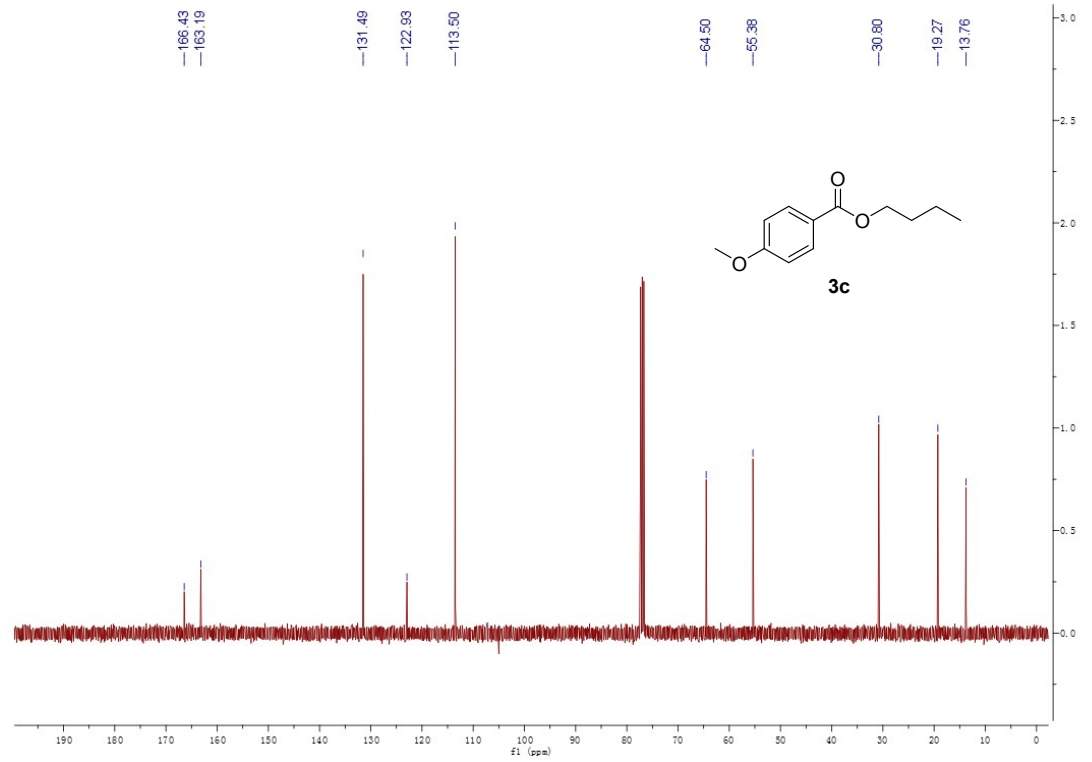
7.97
6.91
6.88
4.29
4.27
4.26
3.84
1.75
1.74
1.73
1.72
1.70
1.68
1.44
0.98
0.96
0.94
2.00
2.05
2.05
3.04
2.08
2.04
3.03
f1 (ppm)
3c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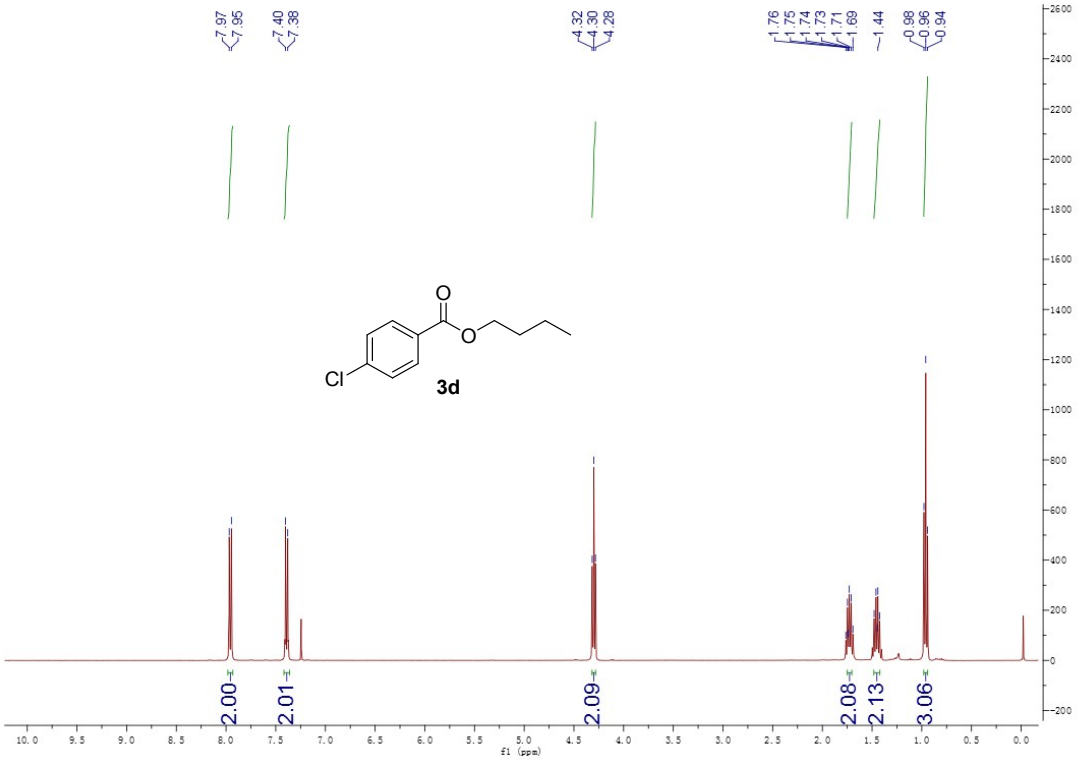
30.80
19.27
13.76
f1 (ppm)
3c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7.95
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4.32
4.30
4.28
1.76
1.75
1.74
1.73
1.71
1.69
1.44
0.98
0.96
0.94
O
O
Cl
3d
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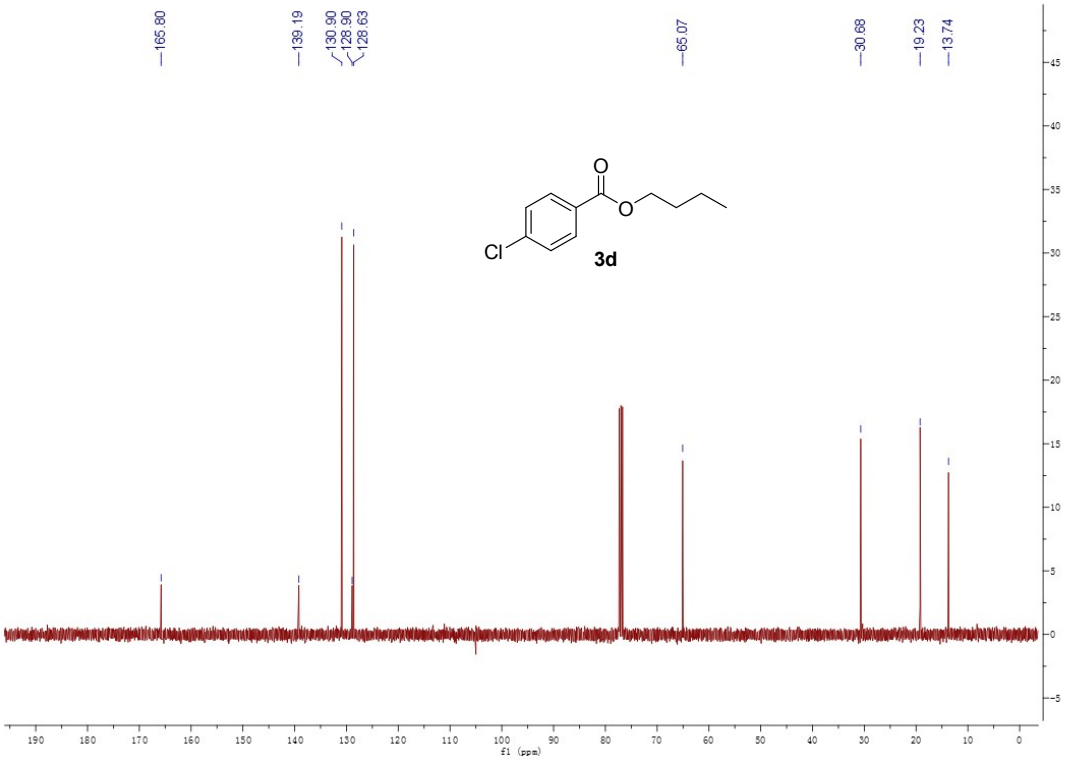
2.08
2.13
3.06
f1 (ppm)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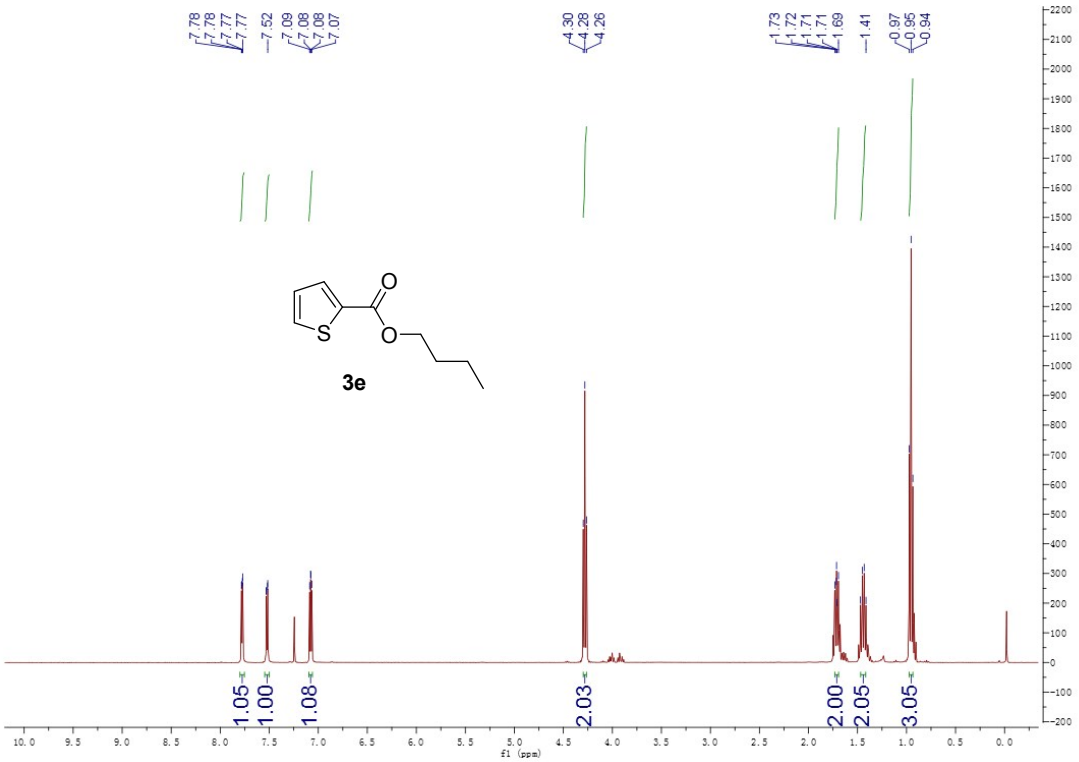
19.23
13.74
O
O
Cl
3d
f1 (ppm)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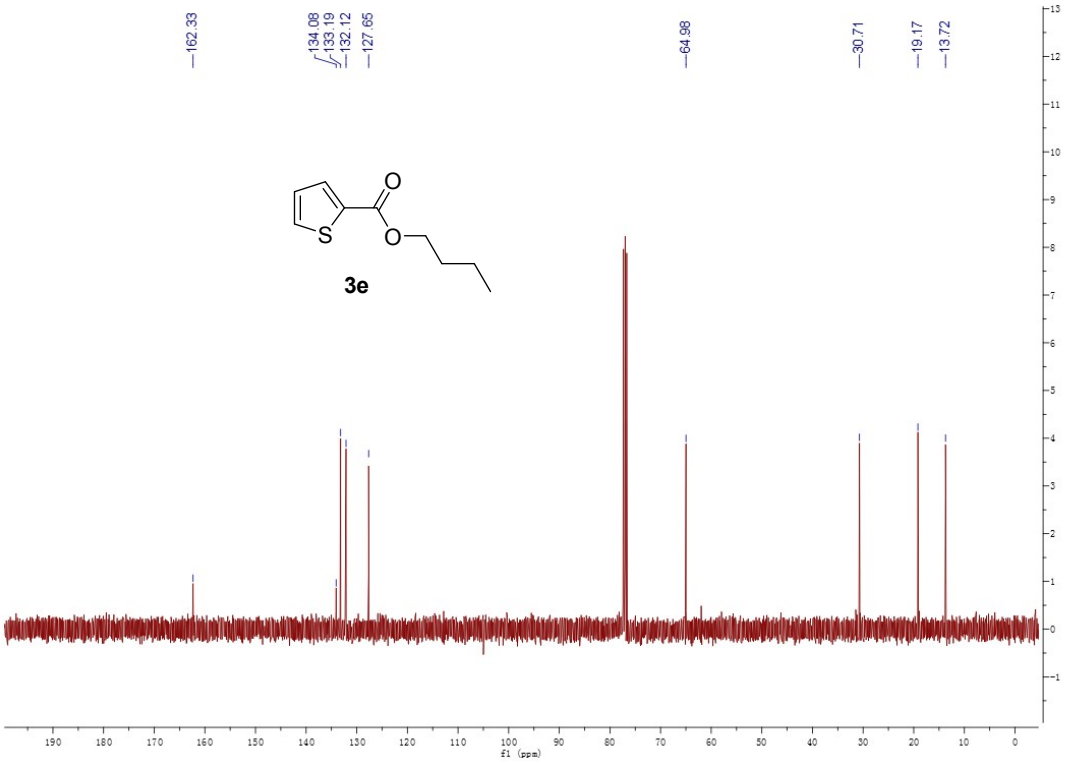
7.08
7.07
4.30
4.28
4.26
1.73
1.72
1.71
1.71
1.69
1.41
0.97
0.95
0.94
O
S
O
3e
1.05
1.00
1.08
2.03
2.00
2.05
3.05
f1 (ppm)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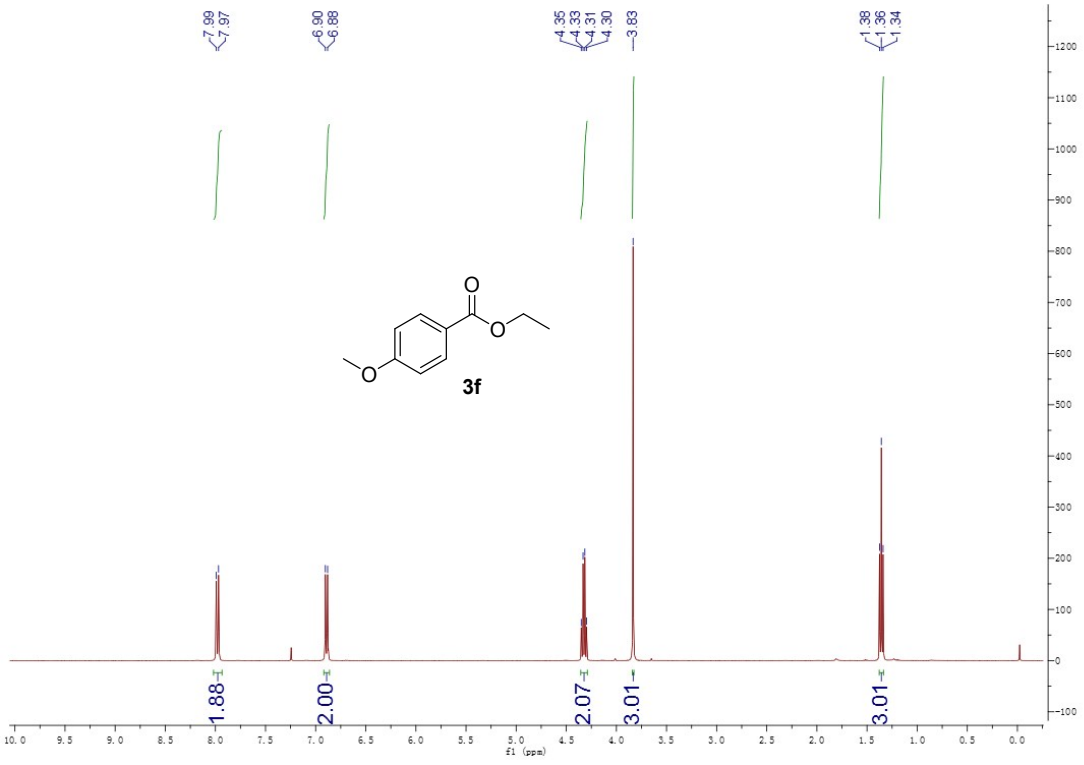
64.98
30.71
19.17
13.72
O
S
O
3e
f1 (ppm)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4.31
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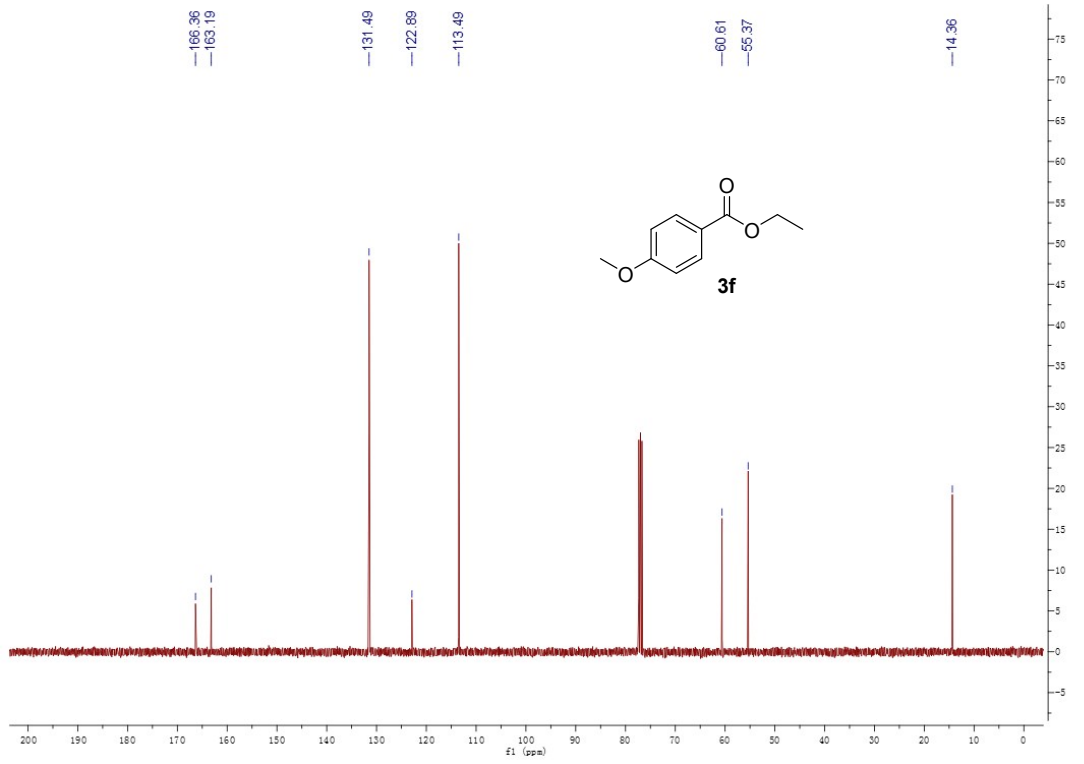
1.34
3f
1.88
2.00
2.07
3.01
3.01
f1 (ppm)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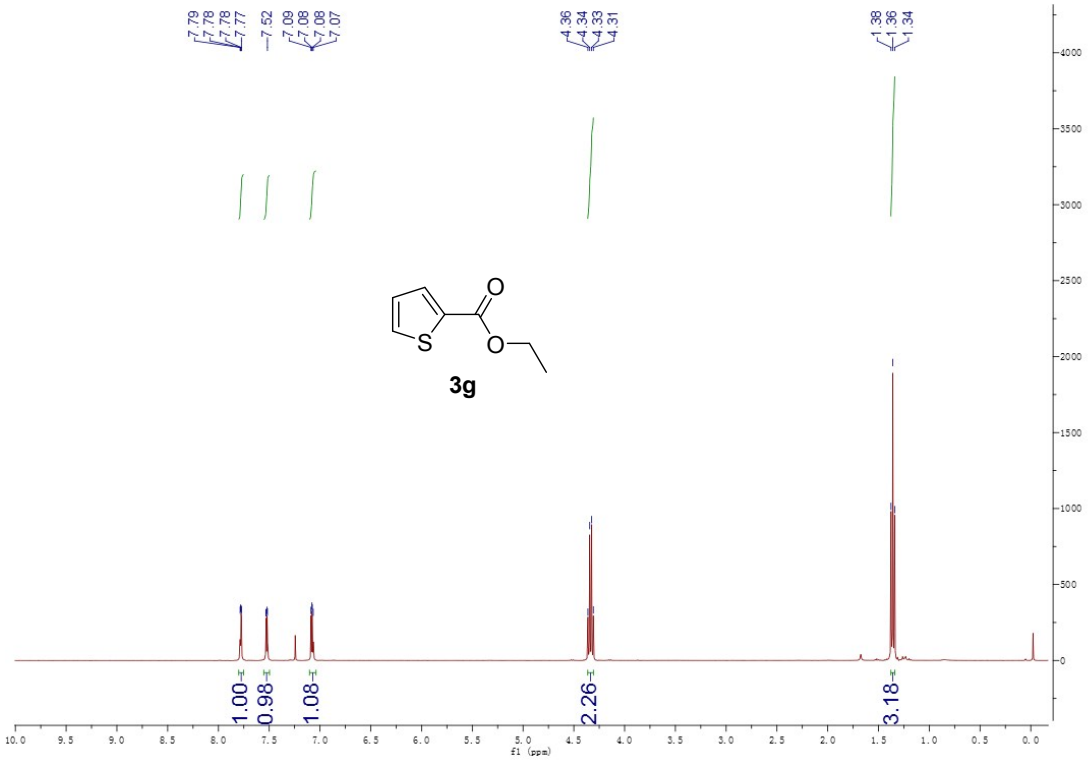
f1 (ppm)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7.08
7.08
7.07
4.36
4.34
4.33
4.31
1.38
1.36
1.34
O
S
O
3g
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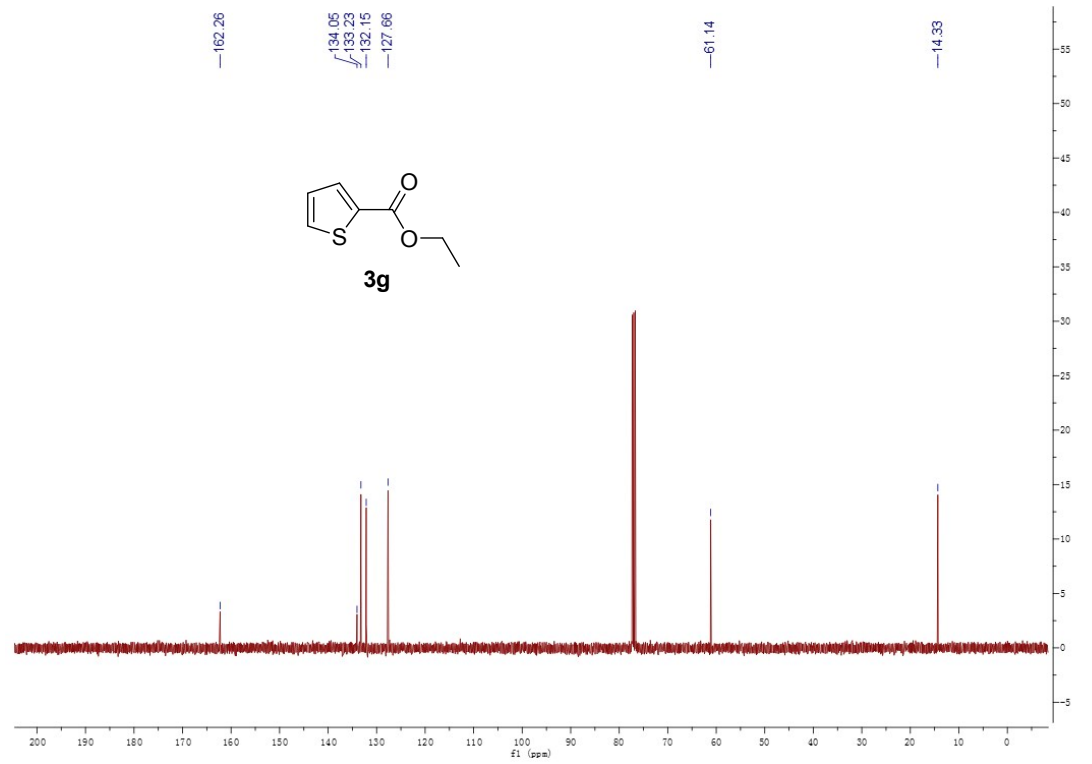
1.08
2.26
3.18
f1 (ppm)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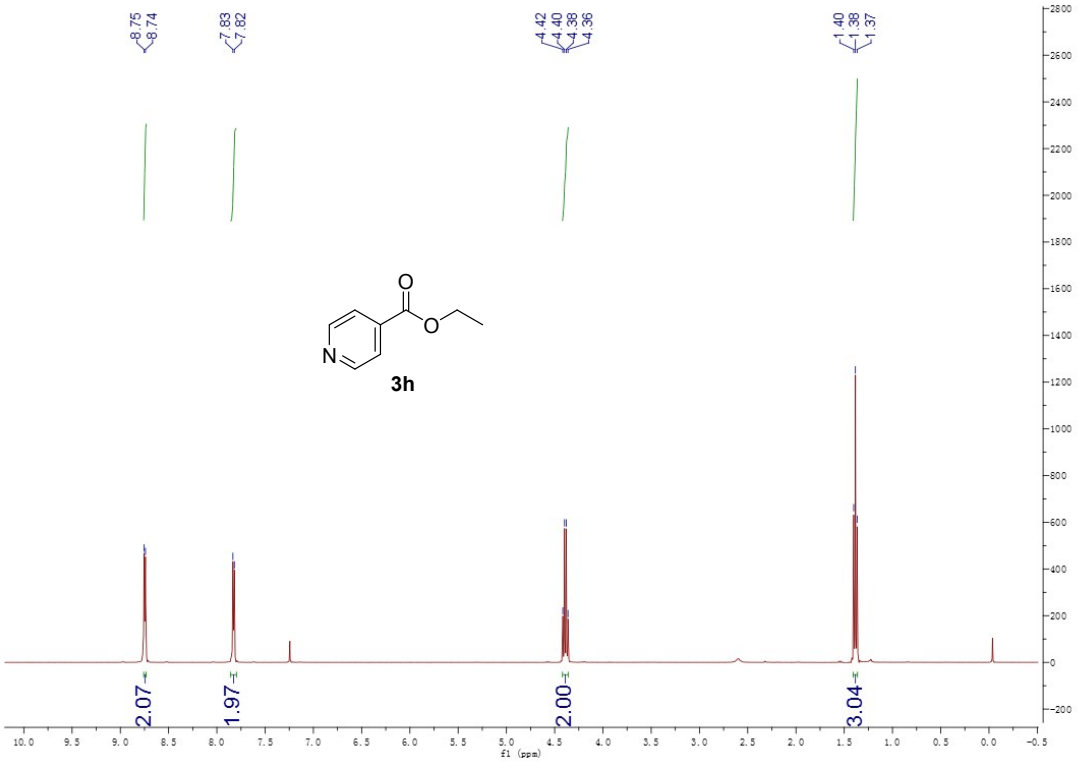
61.14
14.33
O
S
O
3g
f1 (ppm)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7.82
4.42
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4.36
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1.38
1.37
3h
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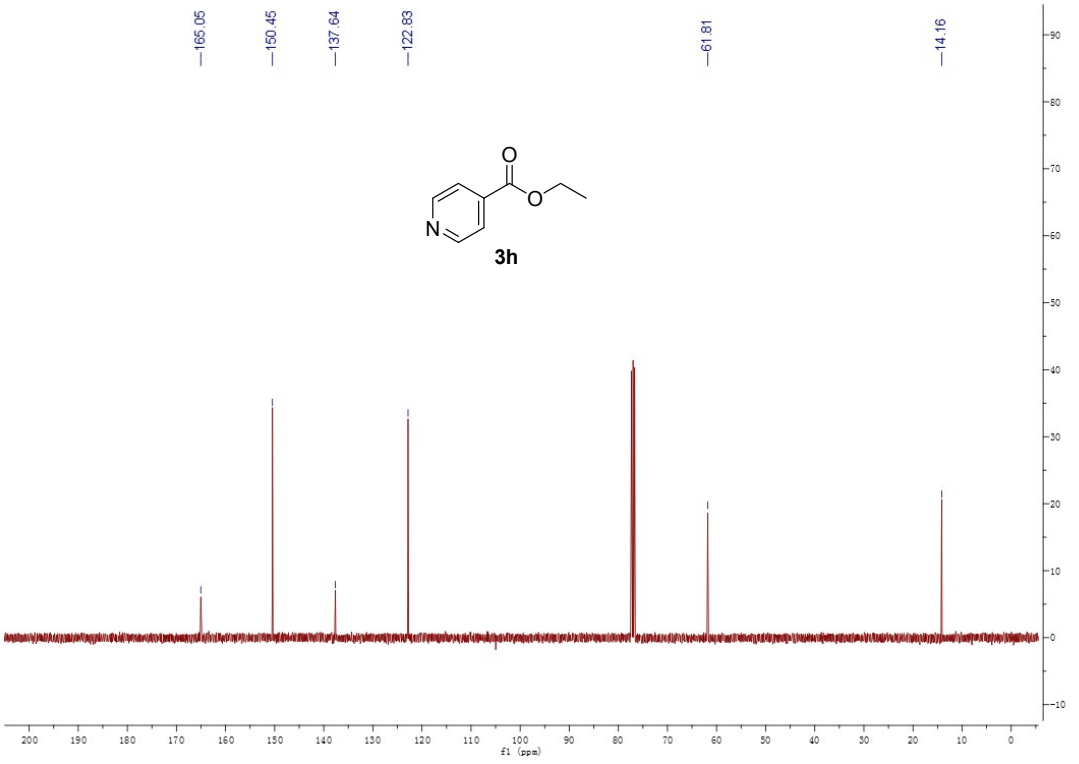
1.97
2.00
3.04
f1 (ppm)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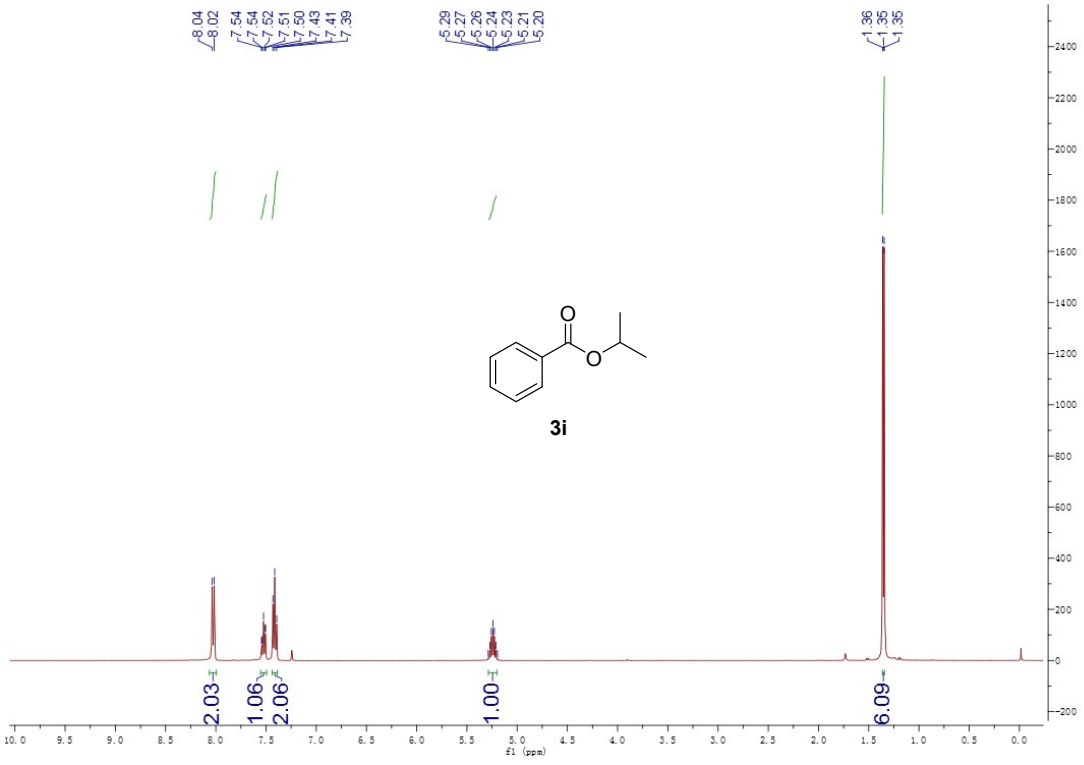
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7.39
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5.27
5.26
5.24
5.23
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2.03
1.06
2.06
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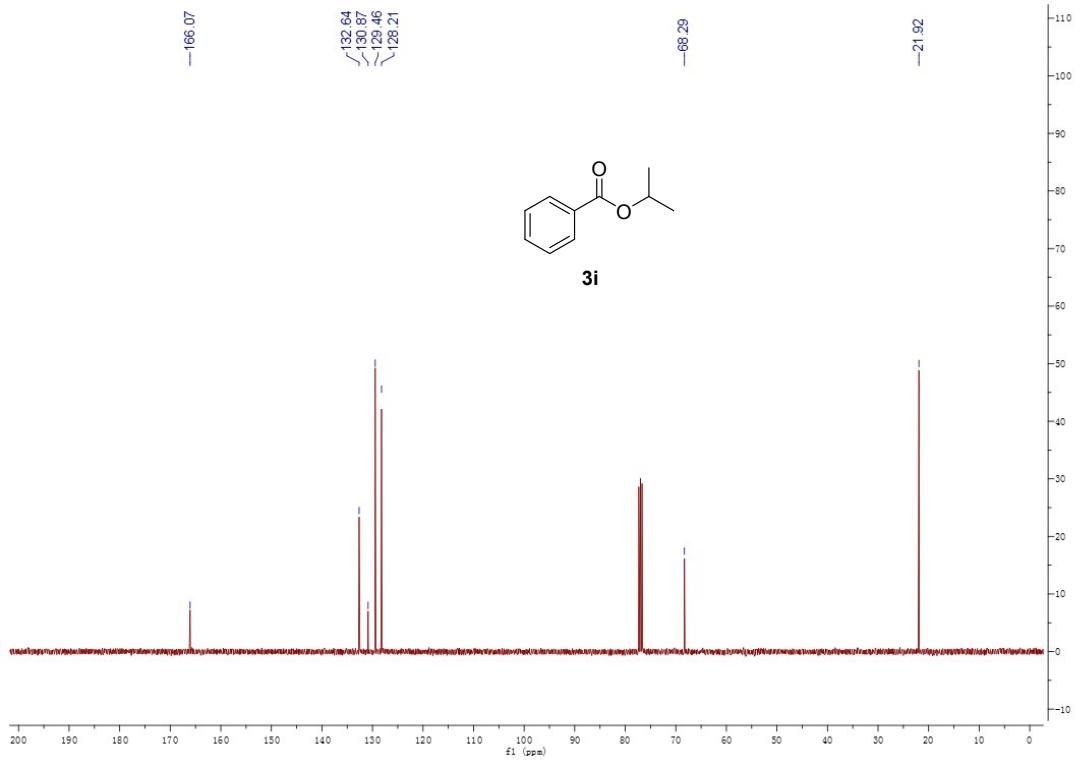
f1 (ppm)

3i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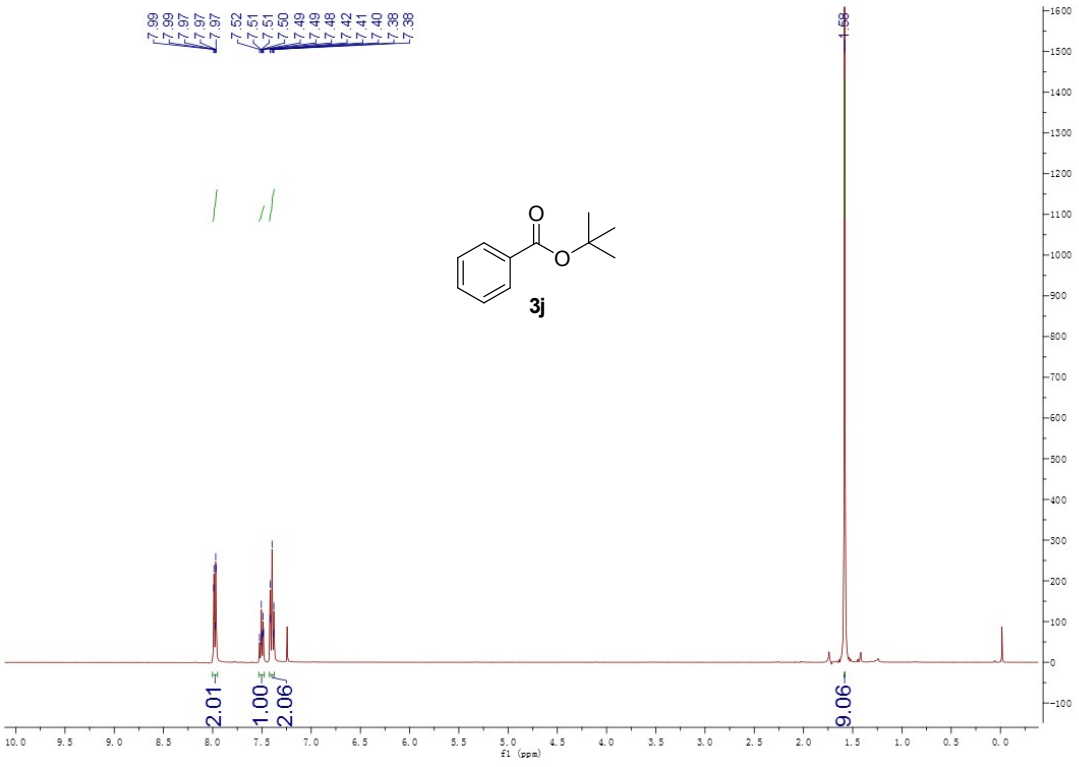
3i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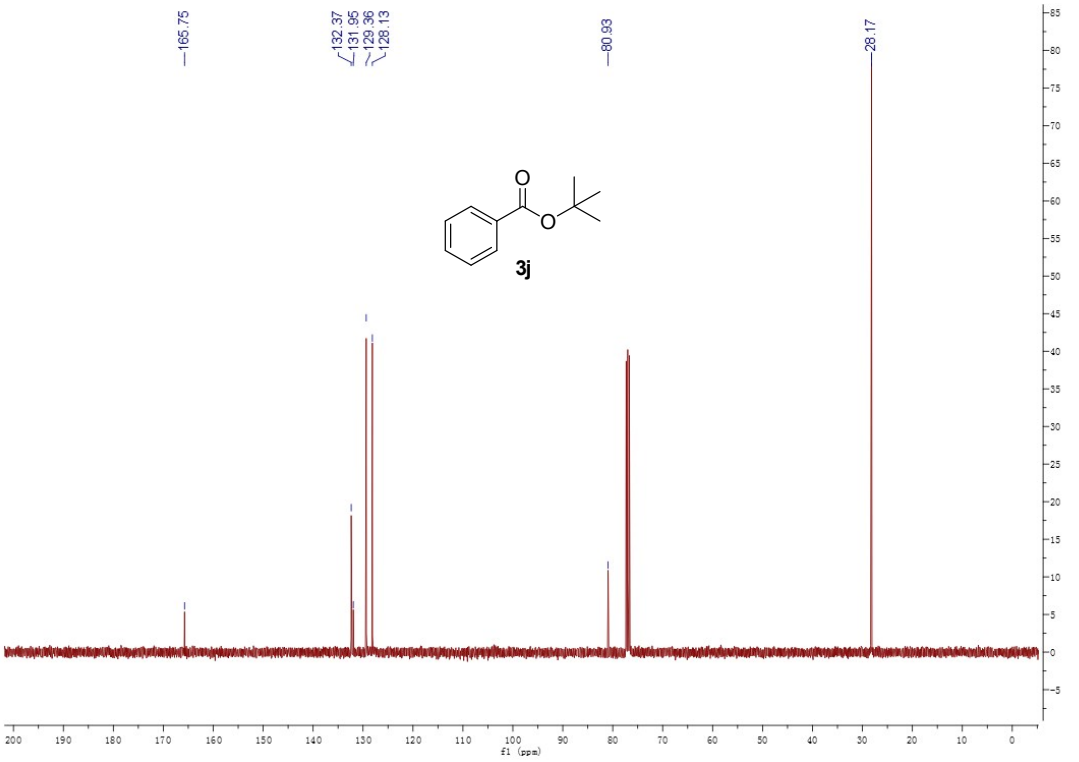
f1 (ppm)

3j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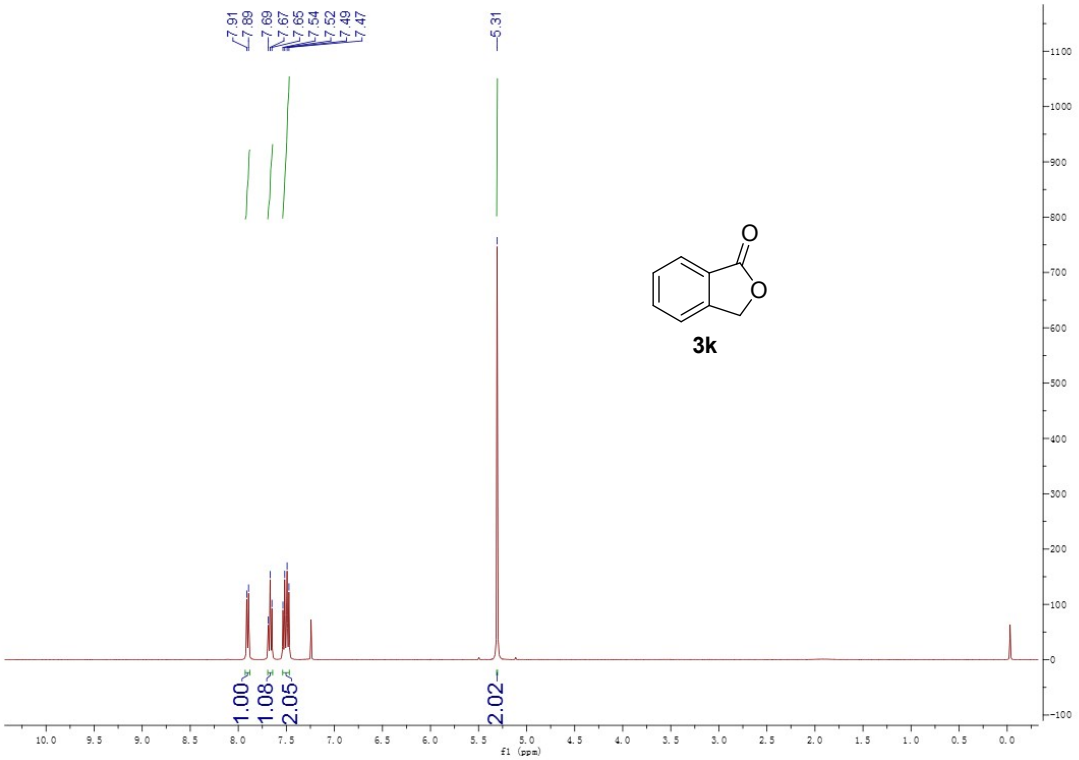
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7.47
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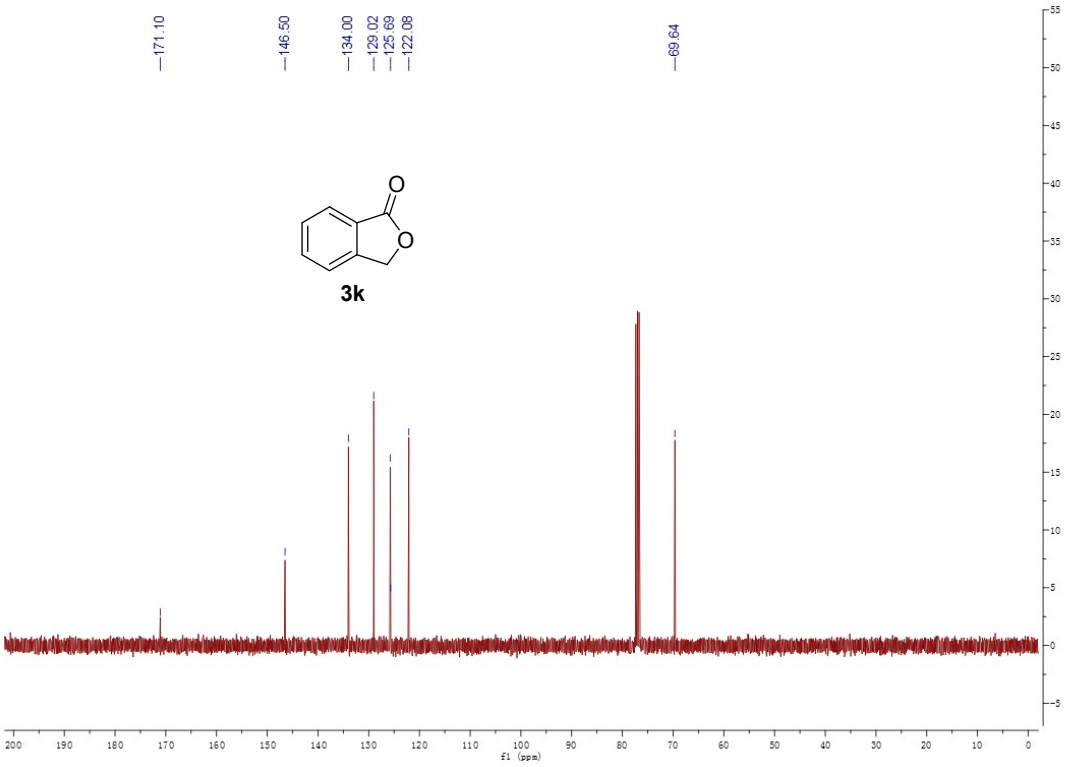
1.08
2.05
2.02
f1 (ppm)

3k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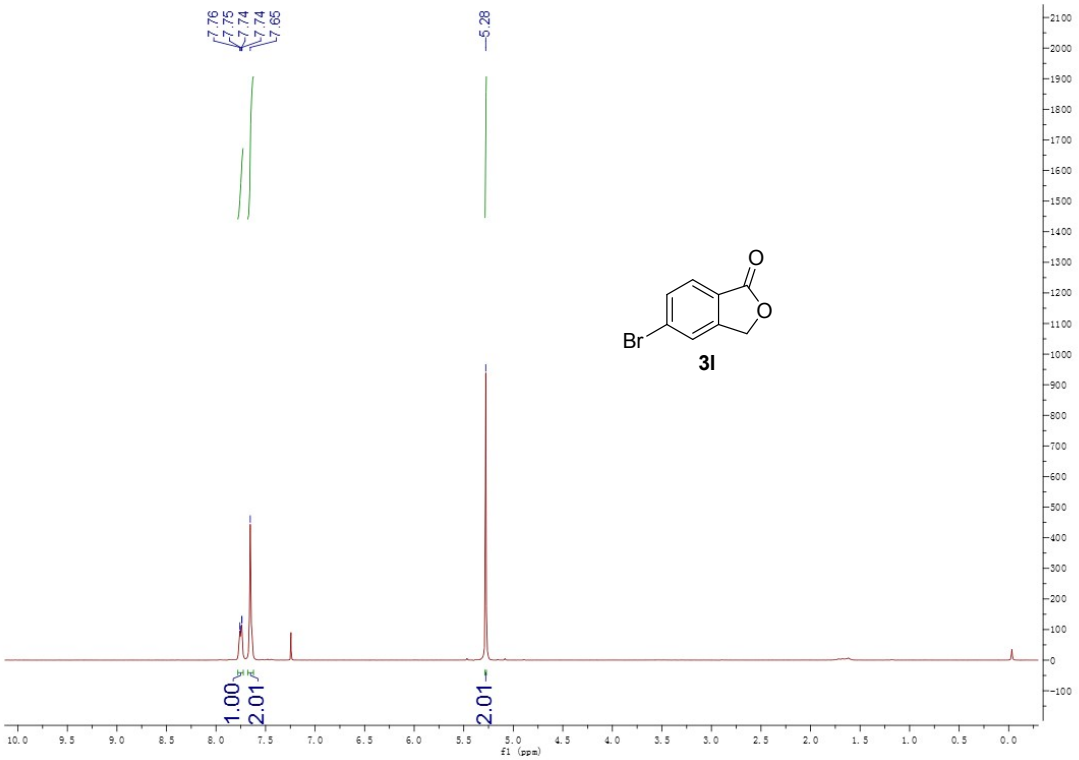
3k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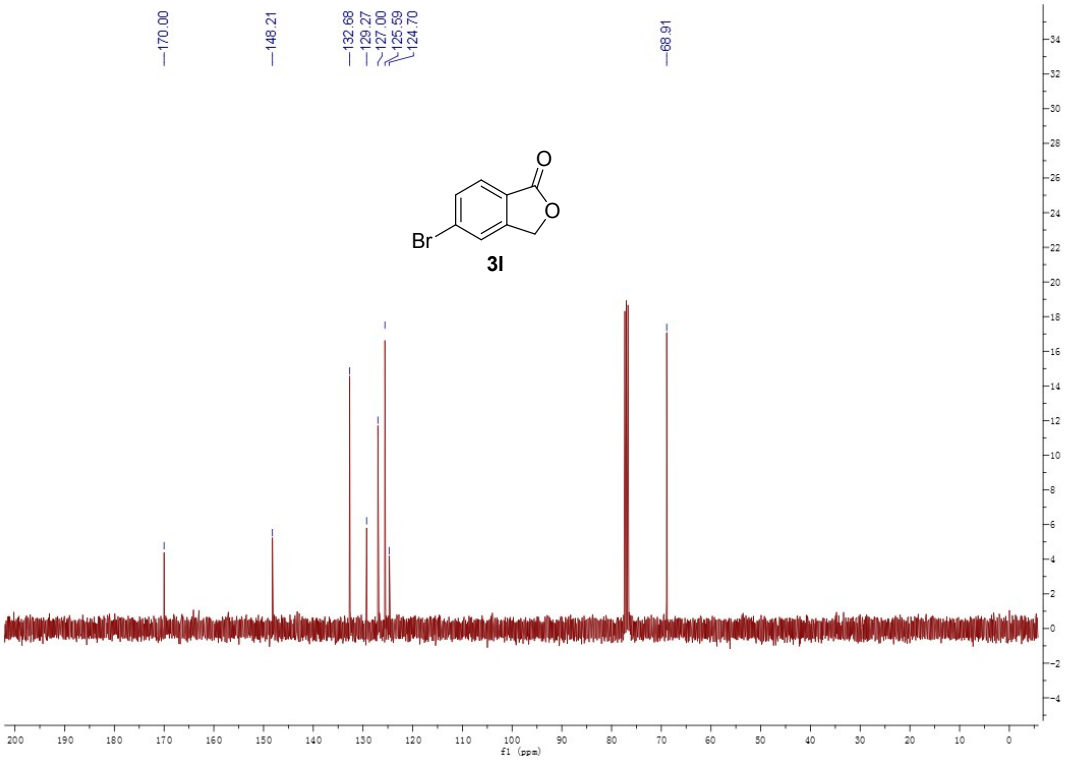
Br
O
O
3l
f1 (ppm)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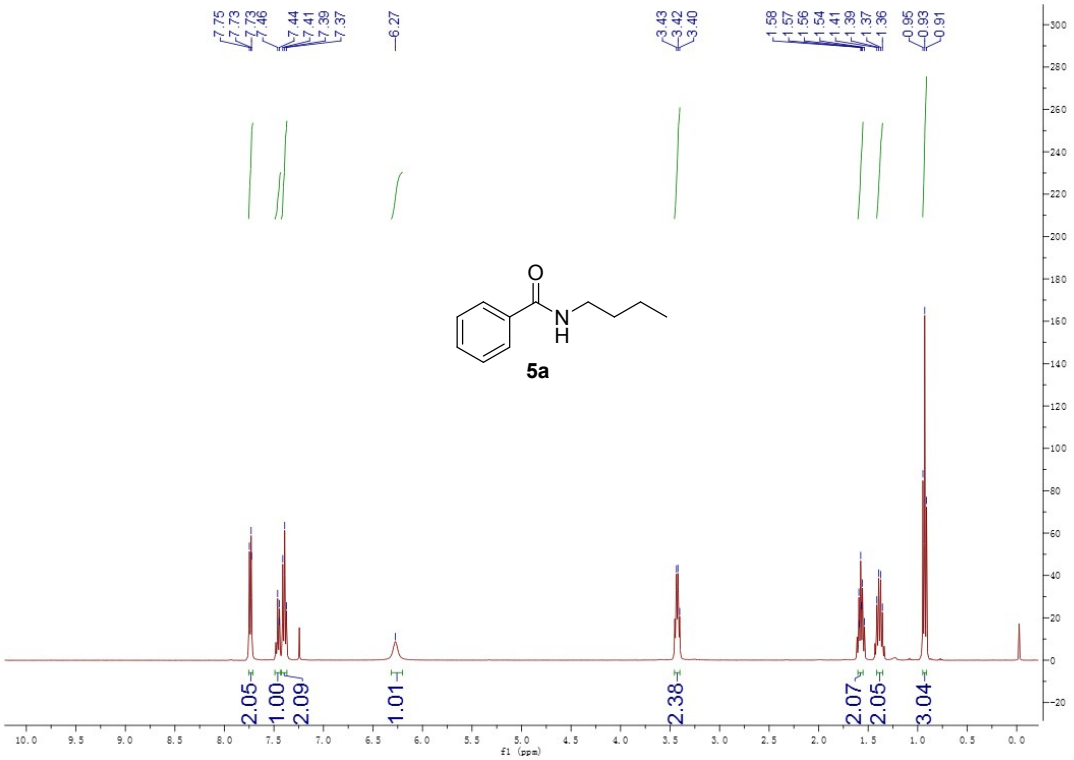
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1.57
1.56
1.54
1.41
1.39
1.37
1.36
0.95
0.93
0.91
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1.00
2.09
1.01
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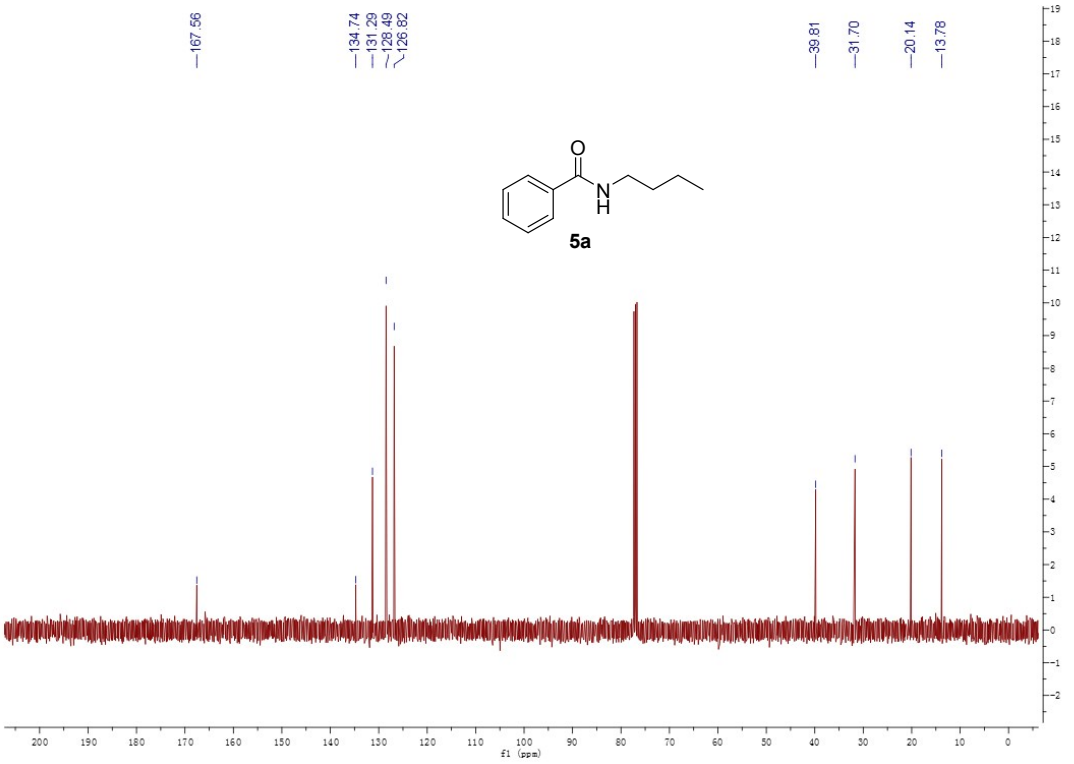
2.07
2.05
3.04
f1 (ppm)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13.78
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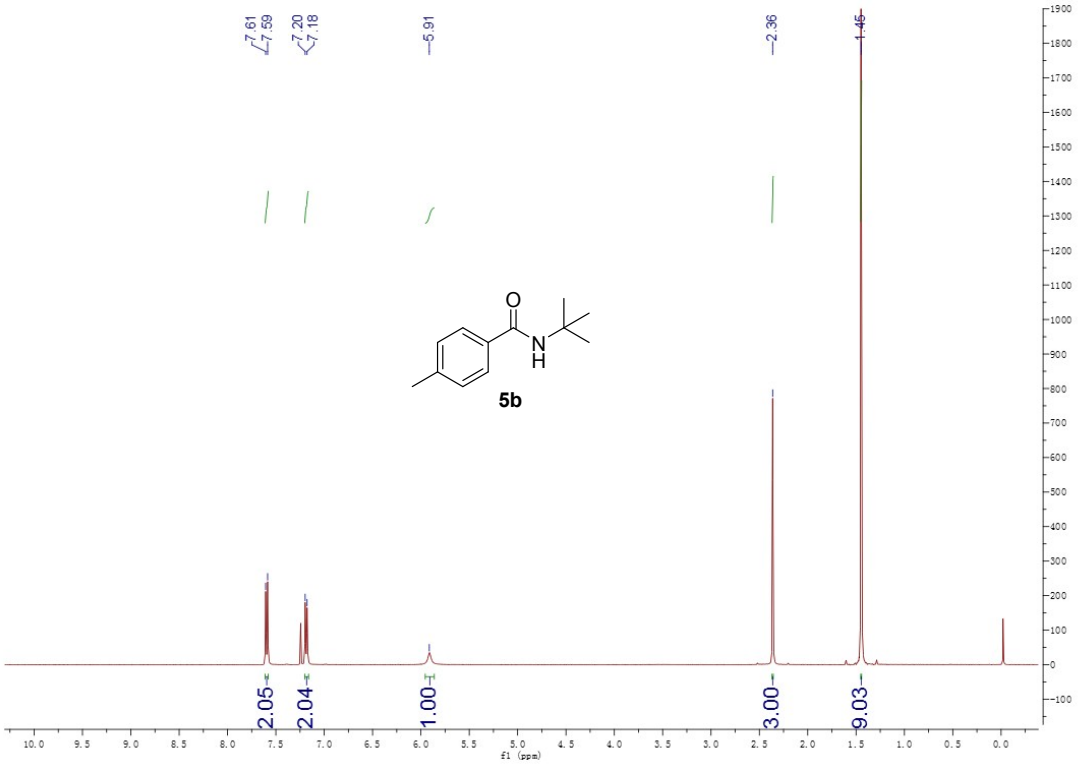
N
H
5a
f1 (ppm)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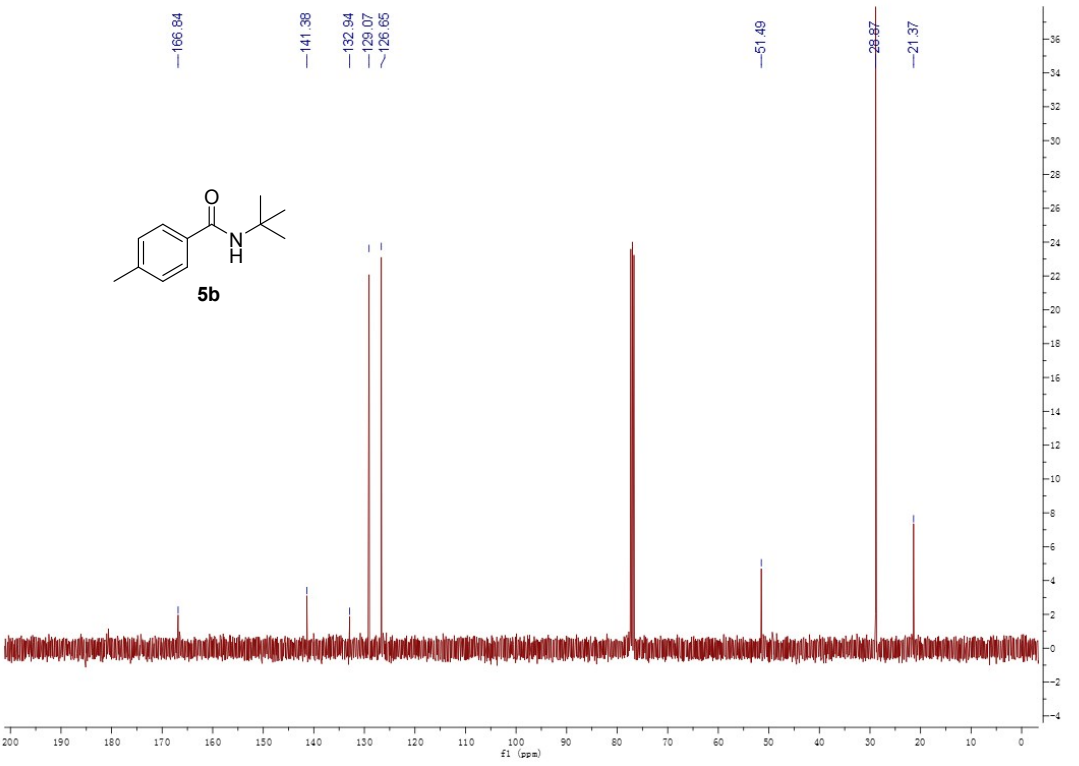
f1 (ppm)

5b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51.49
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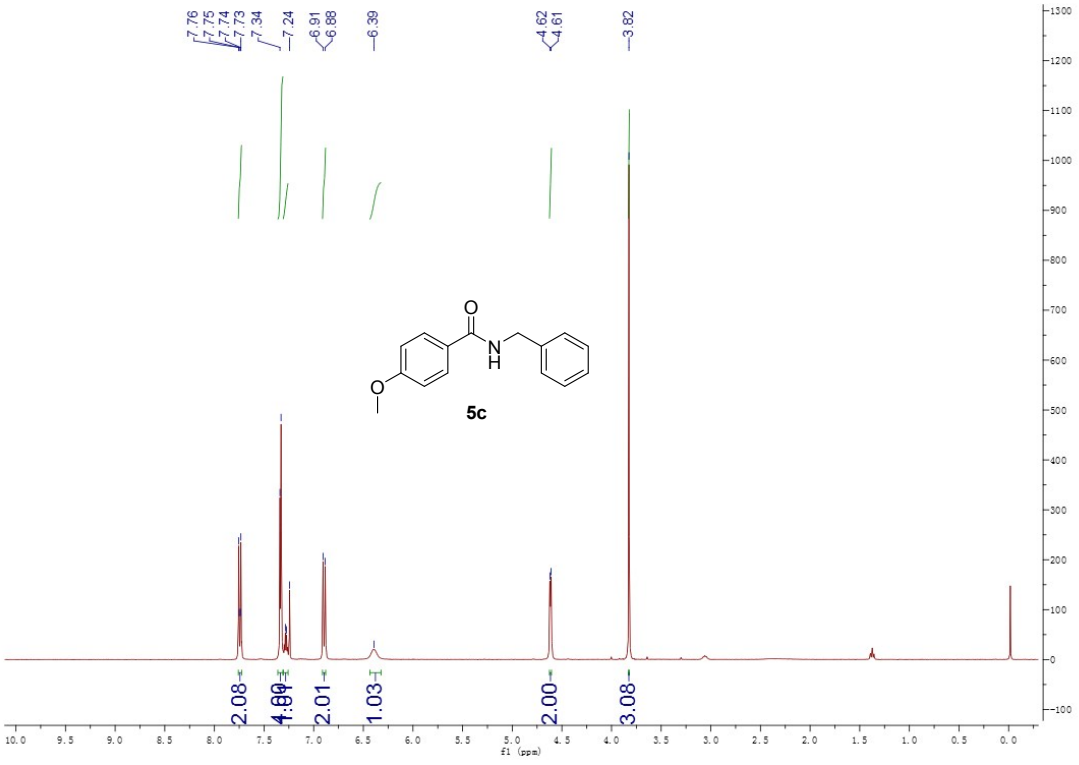
21.37
f1 (ppm)

5b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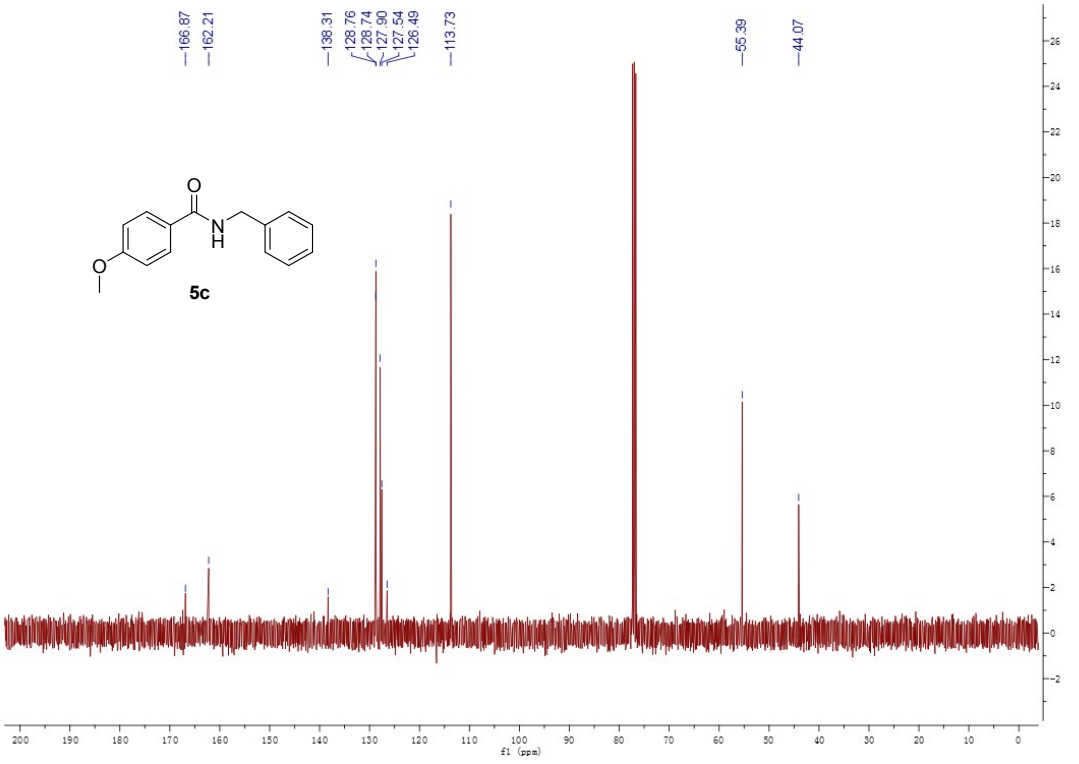
4.00
2.01
1.03
2.00
3.08
f1 (ppm)
5c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126.49
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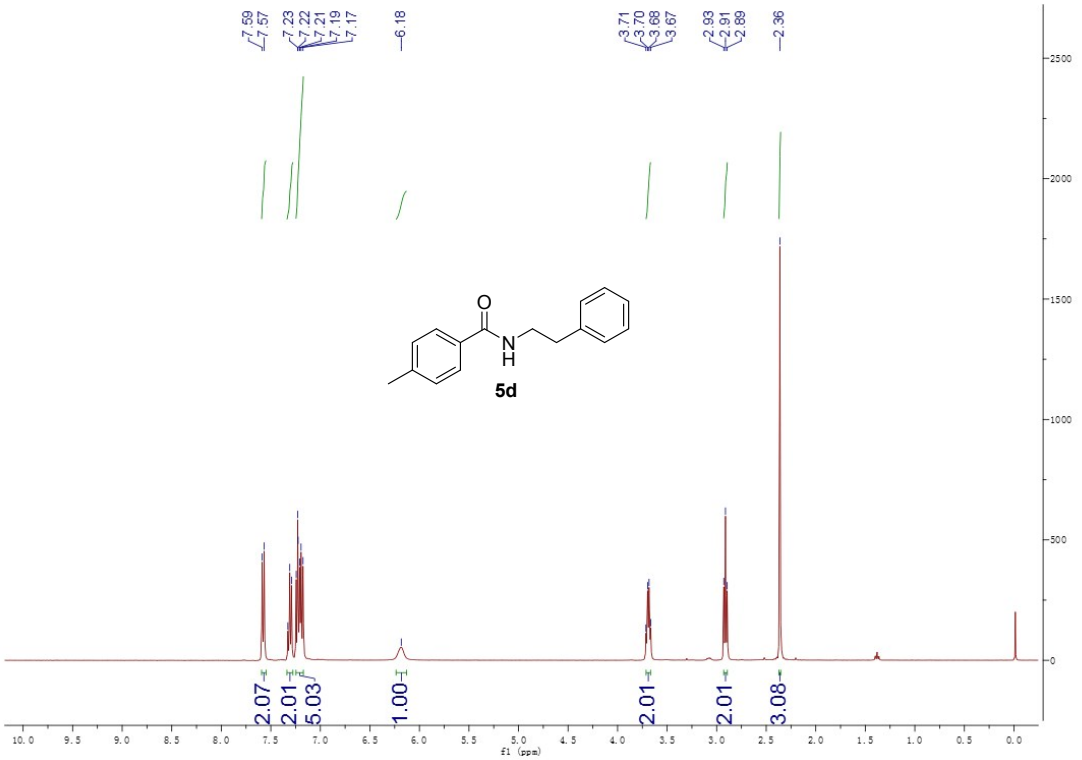
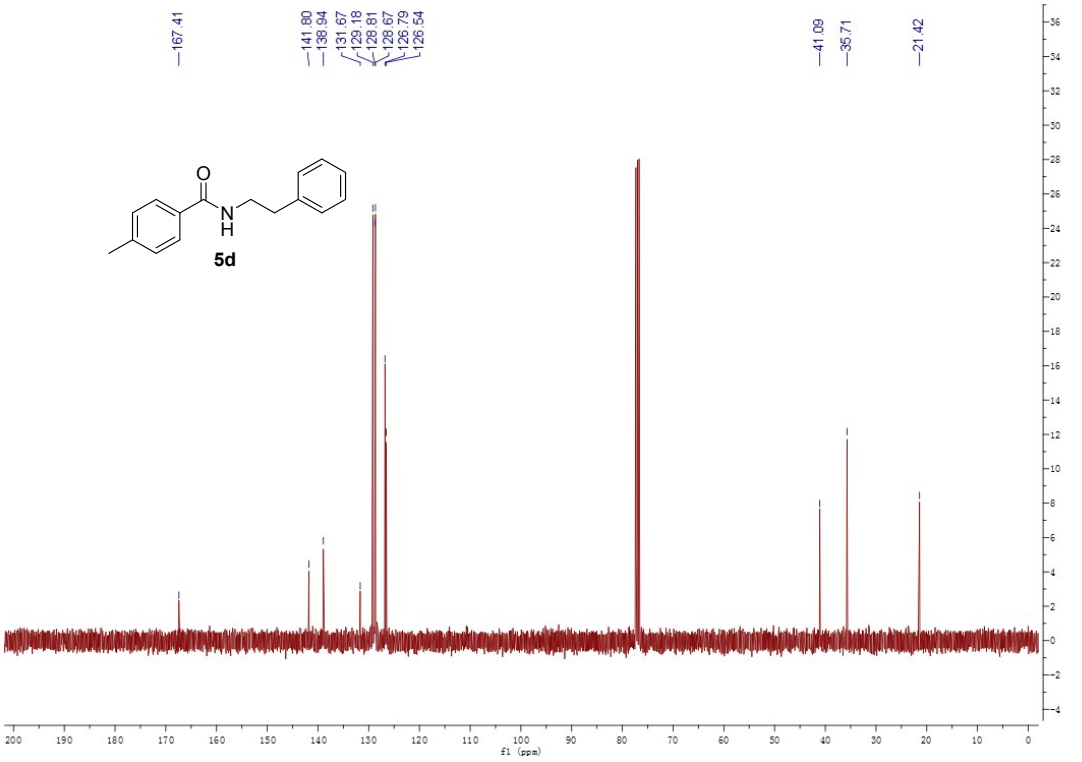
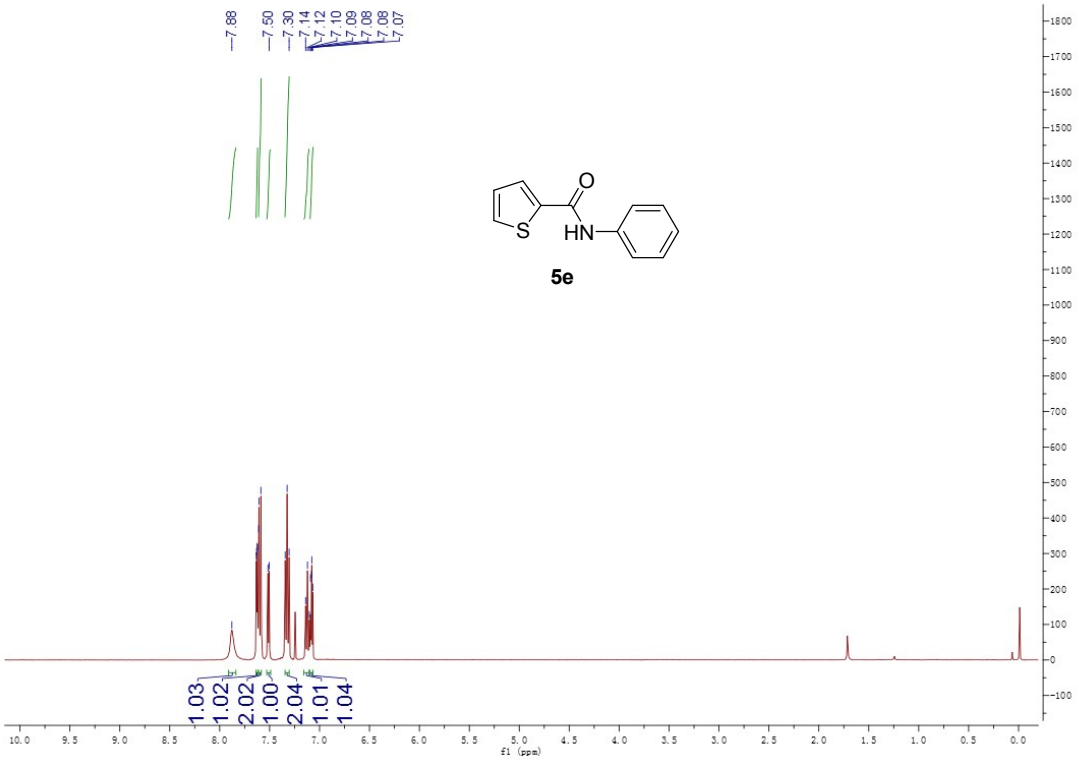
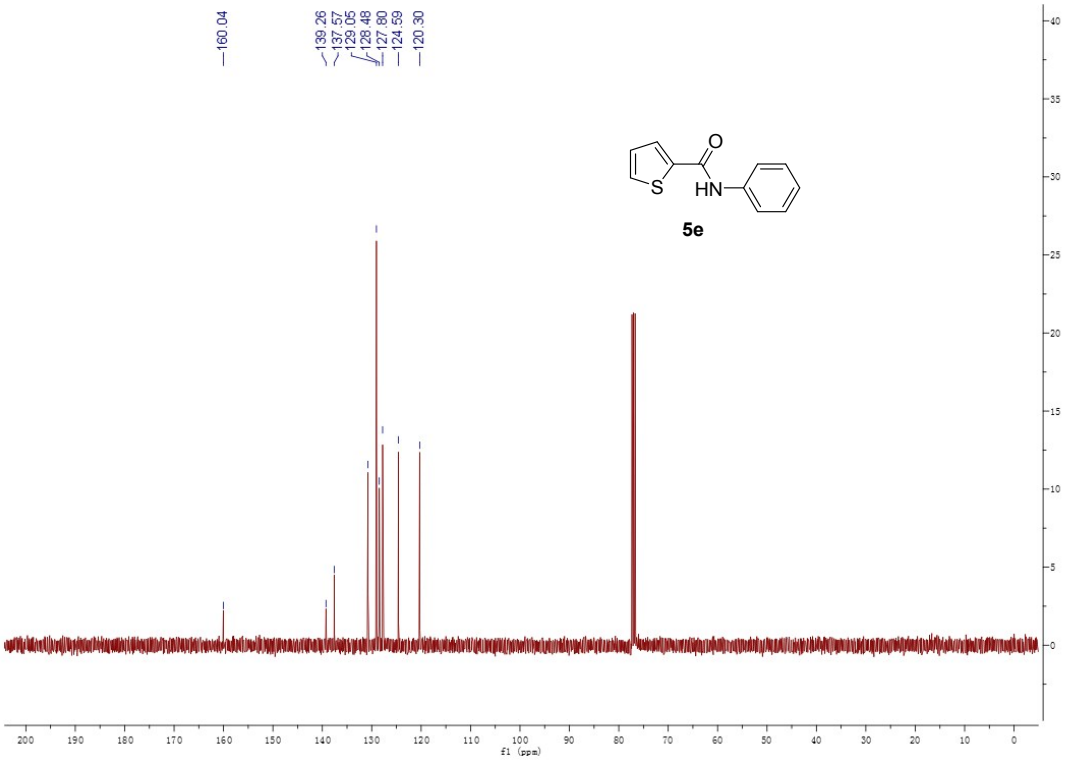
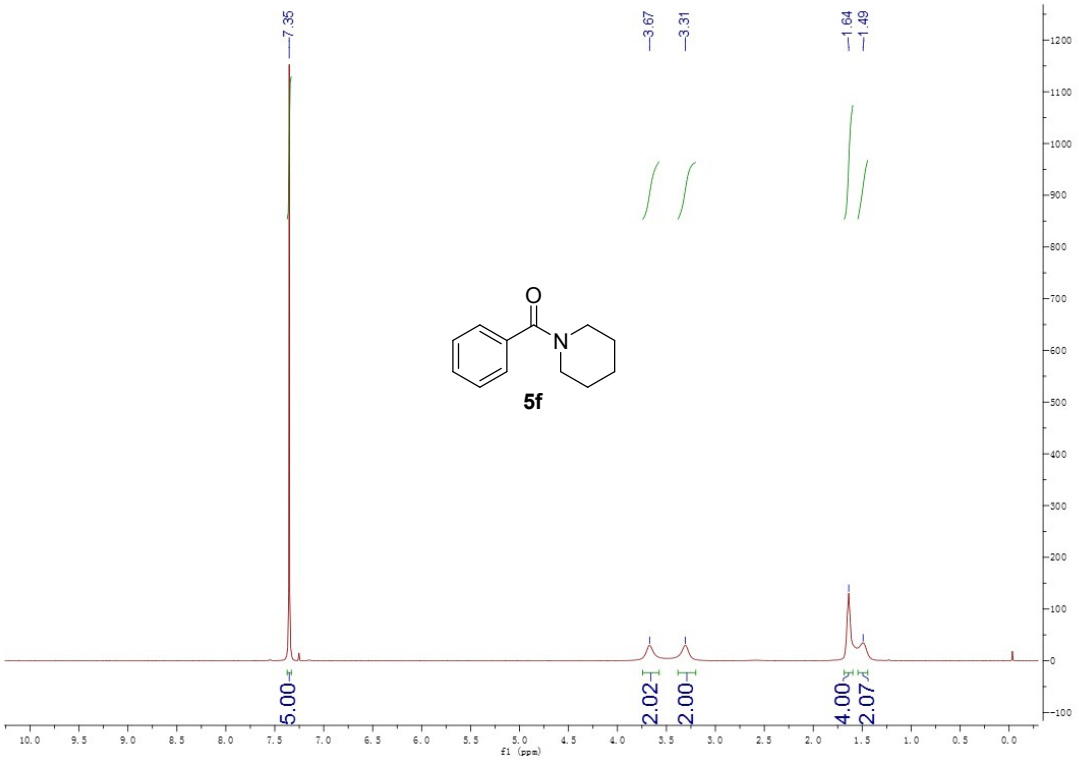
55.39
44.07
f1 (ppm)
5c


7.59
7.57
7.23
7.22
7.21
7.19
7.17
6.18
3.71
3.70
3.68
3.67
2.93
2.91
2.89
2.36
5d
2.07
2.01
5.03
1.00
2.01
2.01
3.08
f1 (ppm)

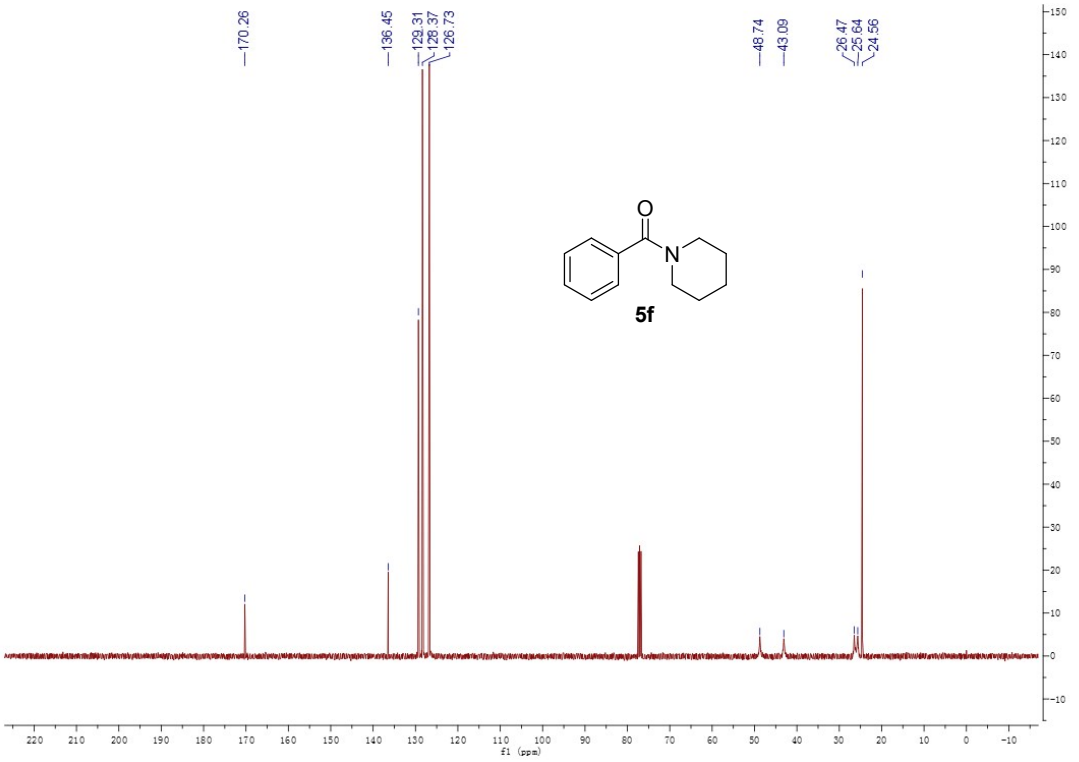

167.41
141.80
138.94
131.67
129.18
128.81
128.67
126.79
126.54
41.09
35.71
21.42
5d
f1 (ppm)


7.88
7.50
7.30
7.14
7.12
7.10
7.09
7.08
7.08
7.07
O
S
HN
5e
1.03
1.02
2.02
1.00
2.04
1.01
1.04
f1 (ppm)

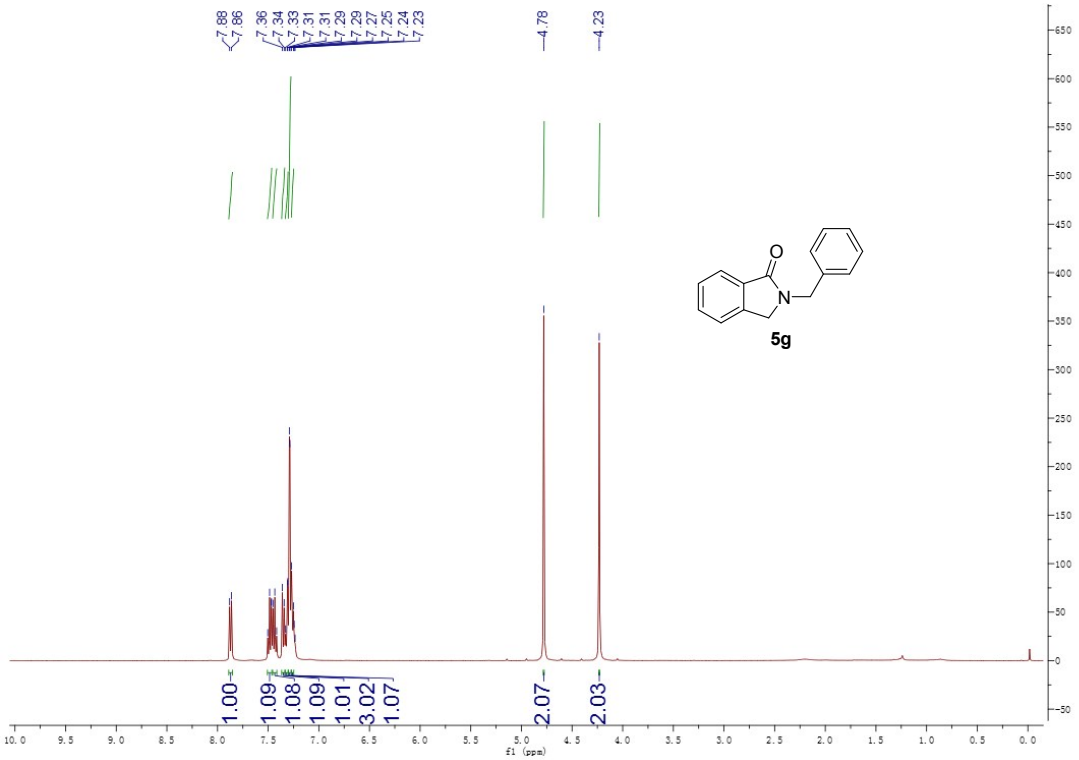

160.04
139.26
137.57
129.05
128.48
127.80
124.59
120.30
O
S
HN
5e
f1 (ppm)


7.35
3.67
3.31
1.64
1.49
5.00
2.02
2.00
4.00
2.07
f1 (ppm)

5f

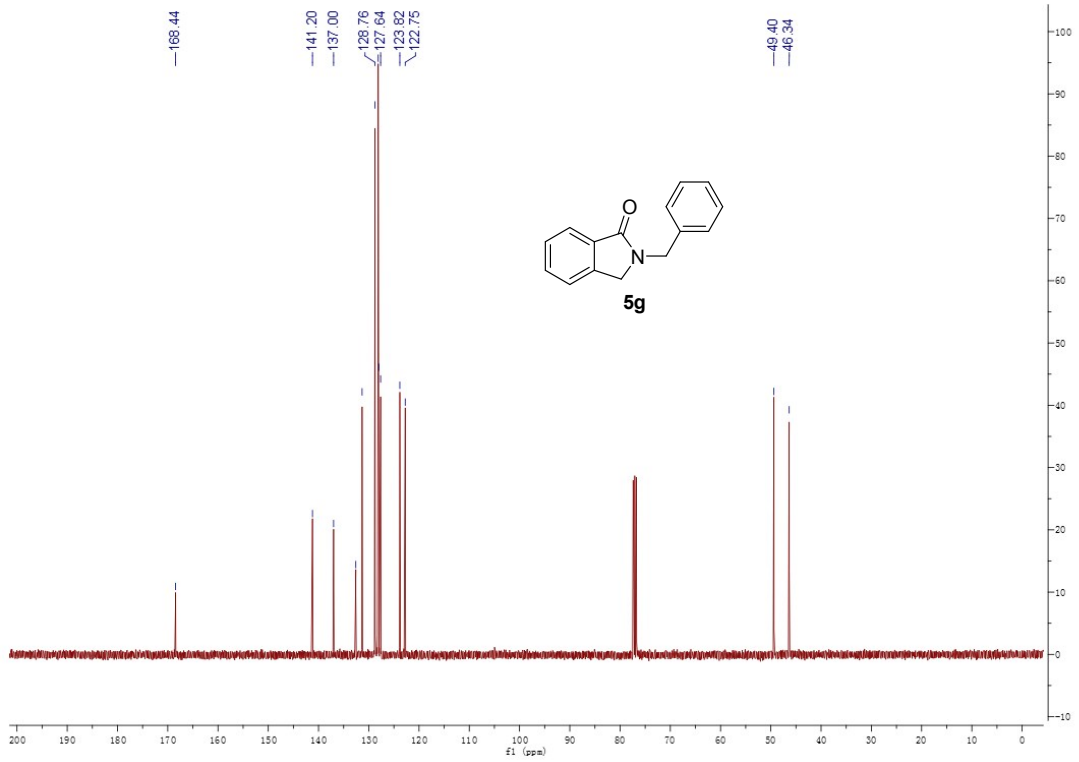

170.26
136.45
129.31
128.37
126.73
48.74
43.09
26.47
25.64
24.56
f1 (ppm)

5f


7.88
7.86
7.36
7.34
7.33
7.31
7.31
7.29
7.29
7.27
7.27
7.25
7.24
7.23
4.78
4.23
1.00
1.09
1.08
1.09
1.01
3.02
1.07
2.07
2.03
f1 (ppm)

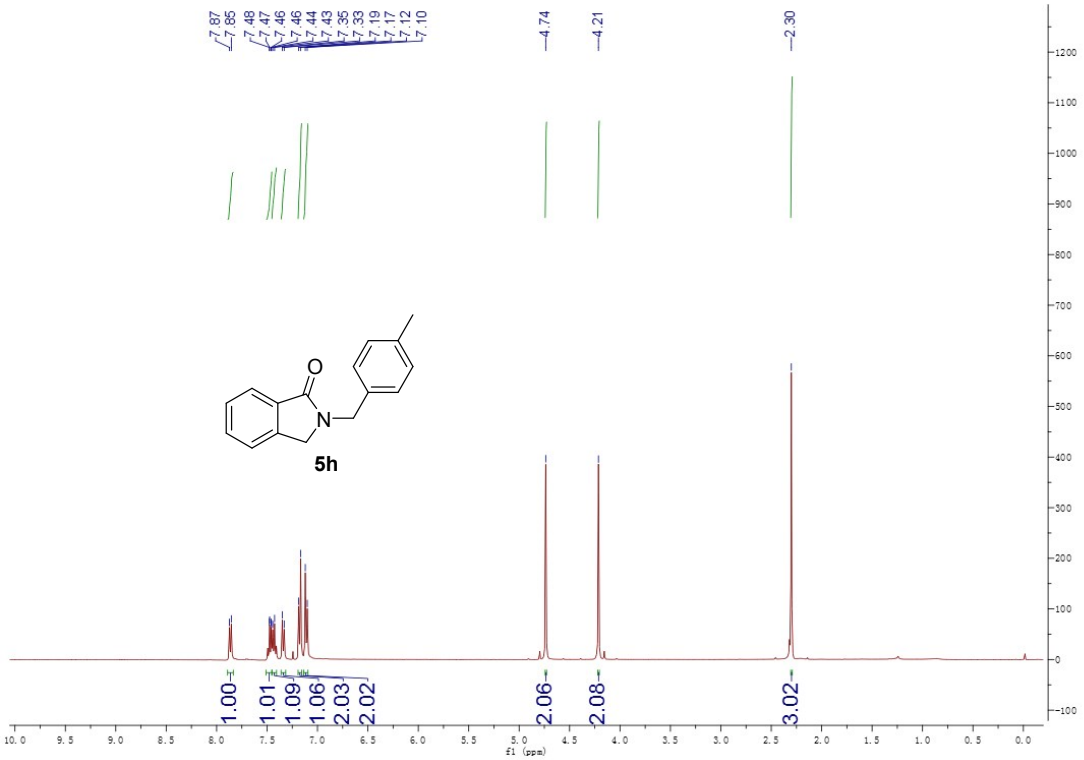
O
N

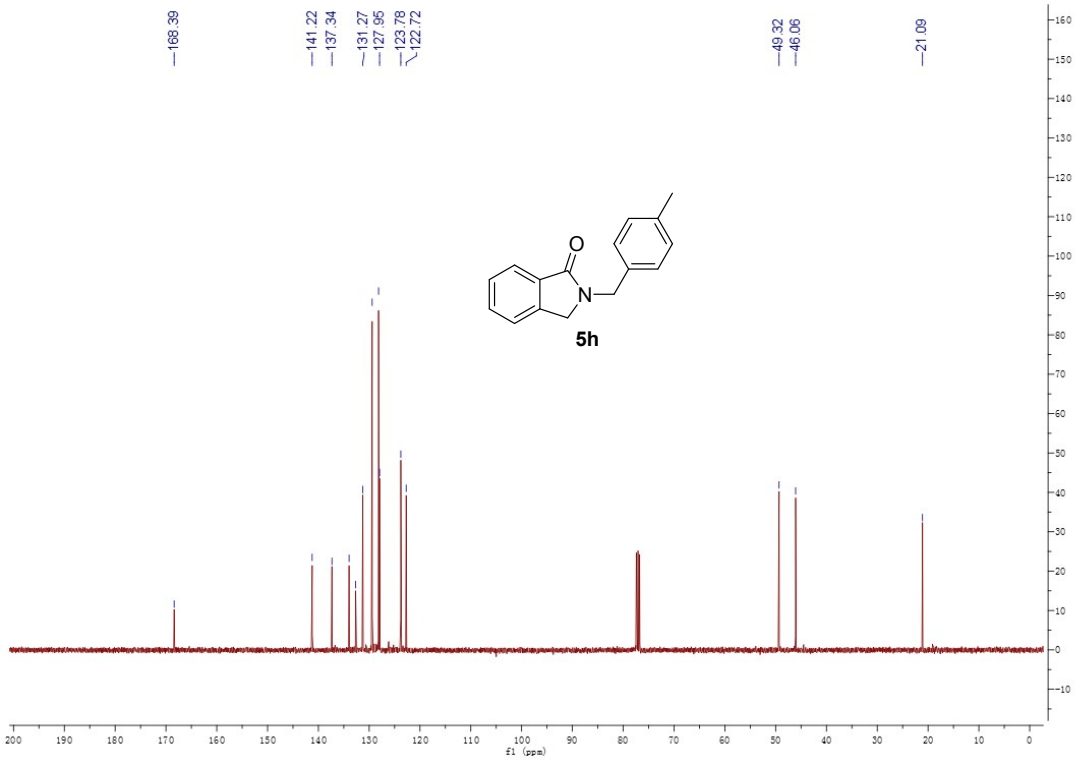
5g

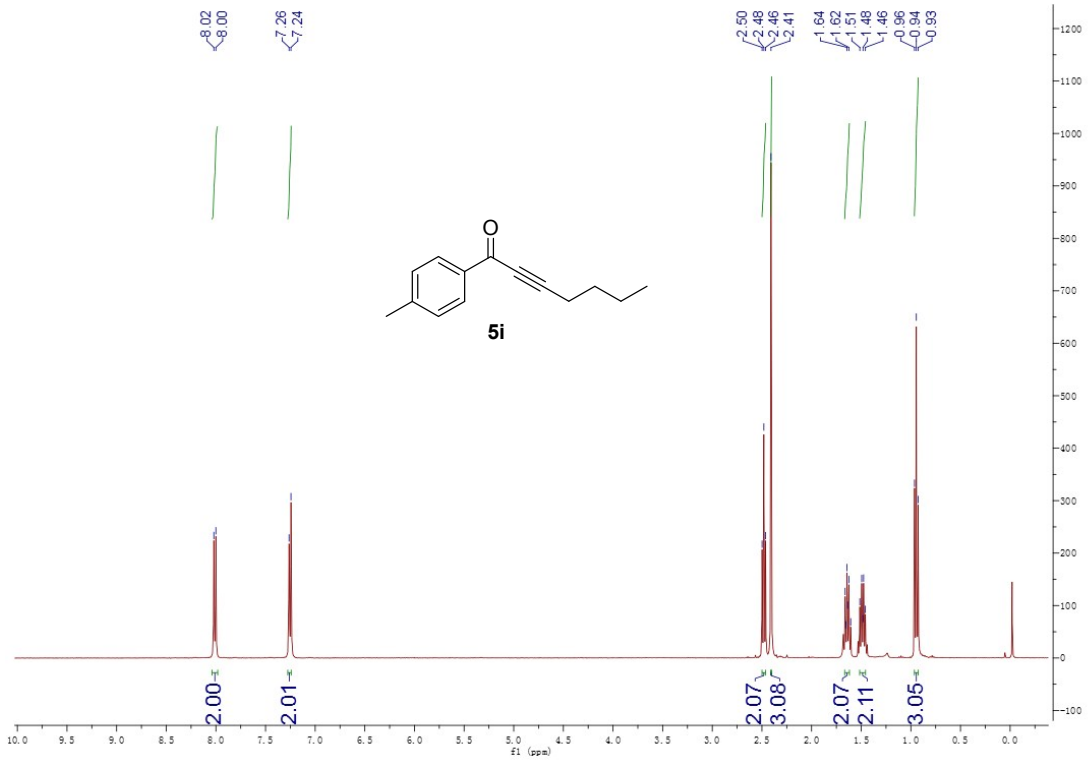

168.44
141.20
137.00
128.76
127.64
123.82
122.75
49.40
46.34
f1 (ppm)

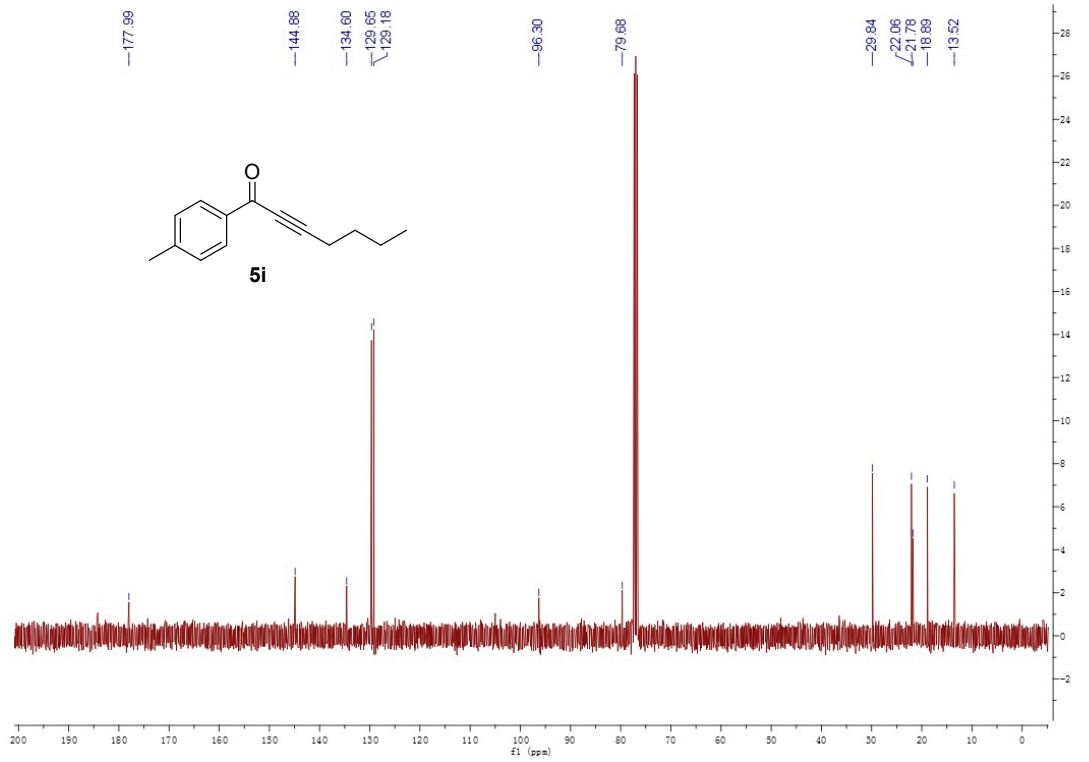
O
N

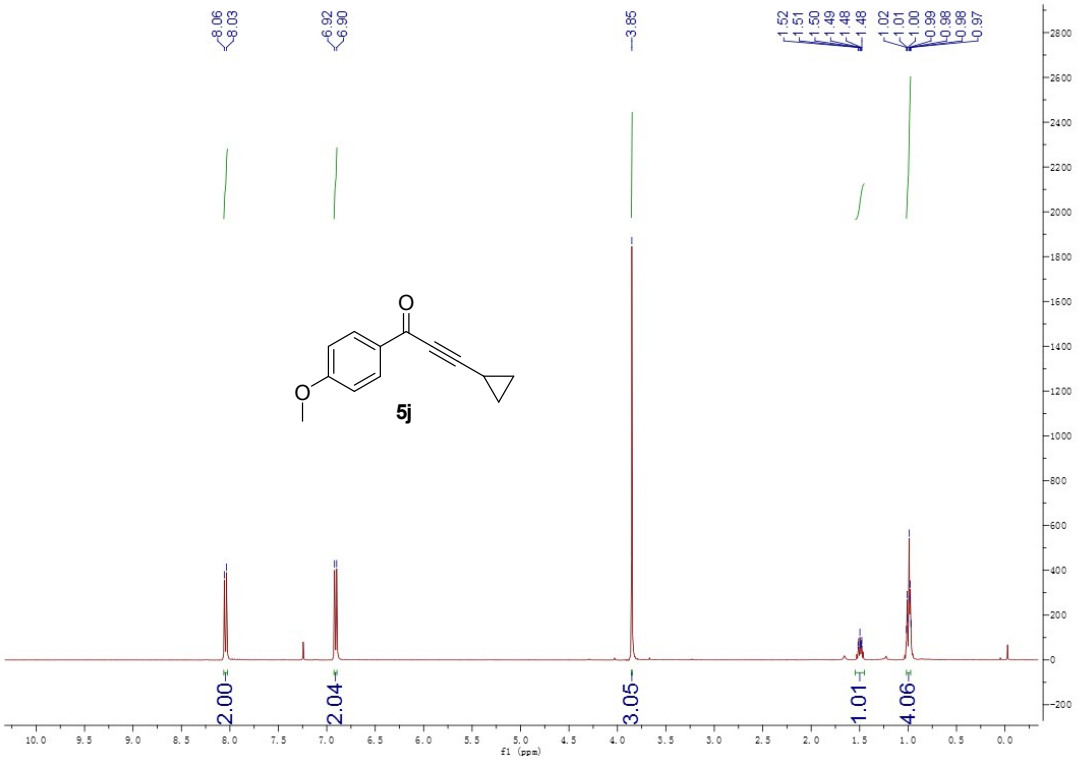
5g

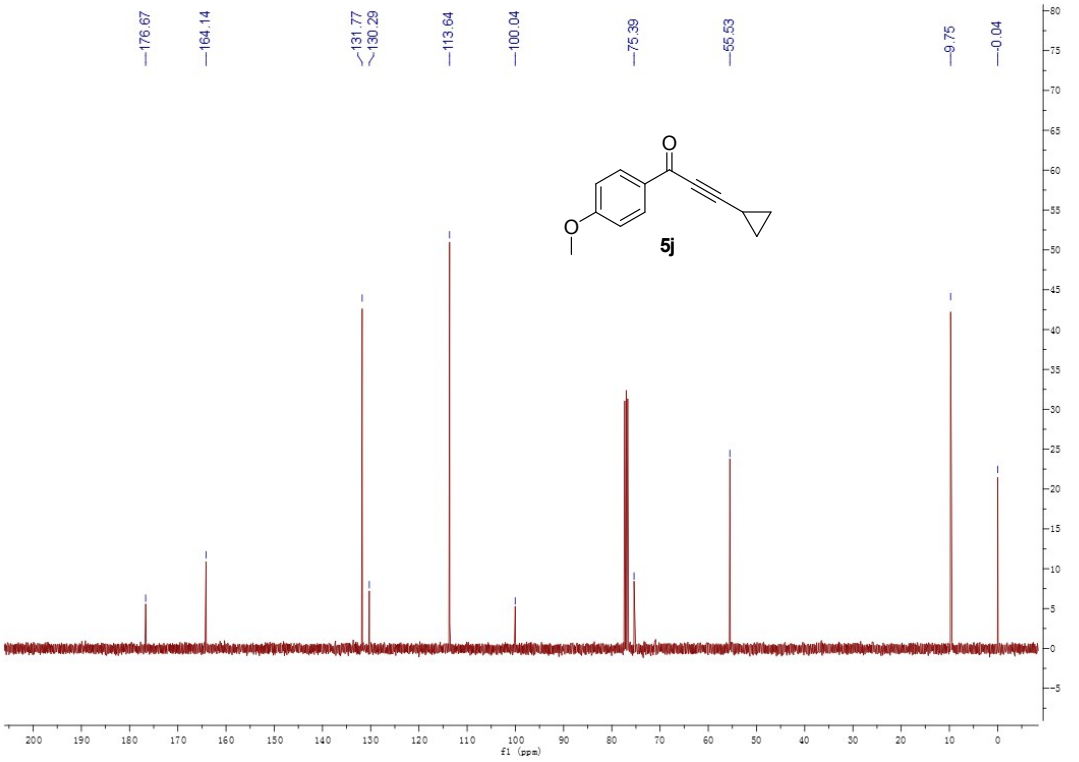

7.87
7.85
7.48
7.47
7.46
7.46
7.44
7.43
7.35
7.33
7.19
7.17
7.12
7.10
4.74
4.21
2.30
O
N
5h
1.00
1.01
1.09
1.06
2.03
2.02
2.06
2.08
3.02
f1 (ppm)

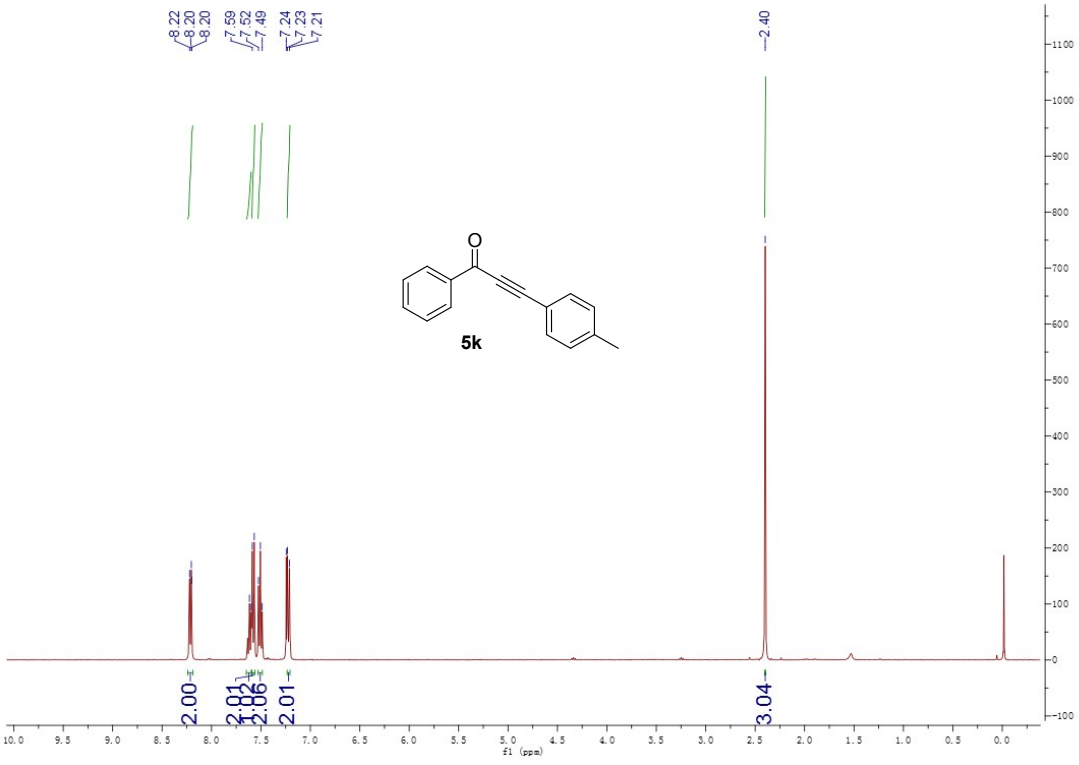

168.39
141.22
137.34
131.27
127.95
123.78
122.72
49.32
46.06
21.09
O
N
5h
f1 (ppm)

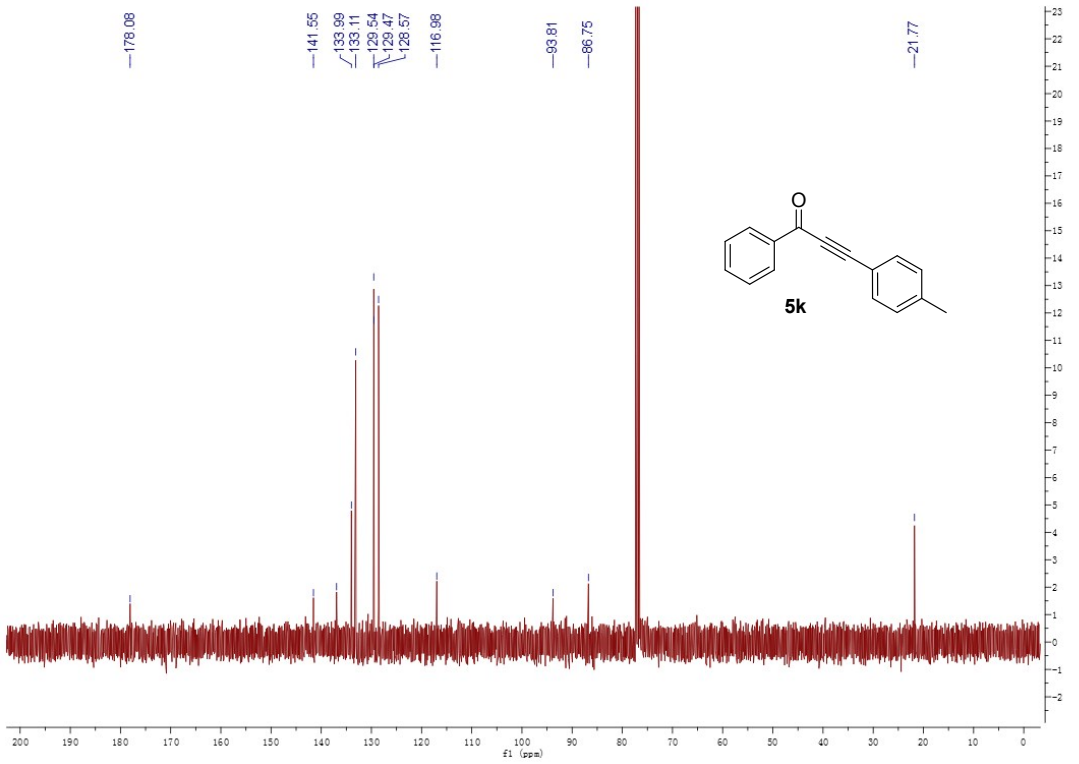

8.02
8.00
7.26
7.24
2.50
2.48
2.46
2.41
1.64
1.62
1.51
1.48
1.46
0.96
0.94
0.93
O
5i
2.00
2.01
2.07
3.08
2.07
2.11
3.05
f1 (ppm)


177.99
144.88
134.60
129.65
129.18
96.30
79.68
29.84
22.06
21.78
18.89
13.52
O
5i
f1 (ppm)


8.06
8.03
6.92
6.90
3.85
1.52
1.51
1.50
1.49
1.48
1.48
1.02
1.01
1.00
0.99
0.98
0.98
0.97
O
O
5j
2.00
2.04
3.05
1.01
4.06
f1 (ppm)


176.67
164.14
131.77
130.29
113.64
100.04
75.39
55.53
9.75
0.04
O
O
5j
f1 (ppm)


8.22
8.20
8.20
7.59
7.52
7.49
7.24
7.23
7.21
2.40
O
5k
2.00
2.01
2.02
2.06
2.01
3.04
f1 (ppm)


178.08
141.55
133.99
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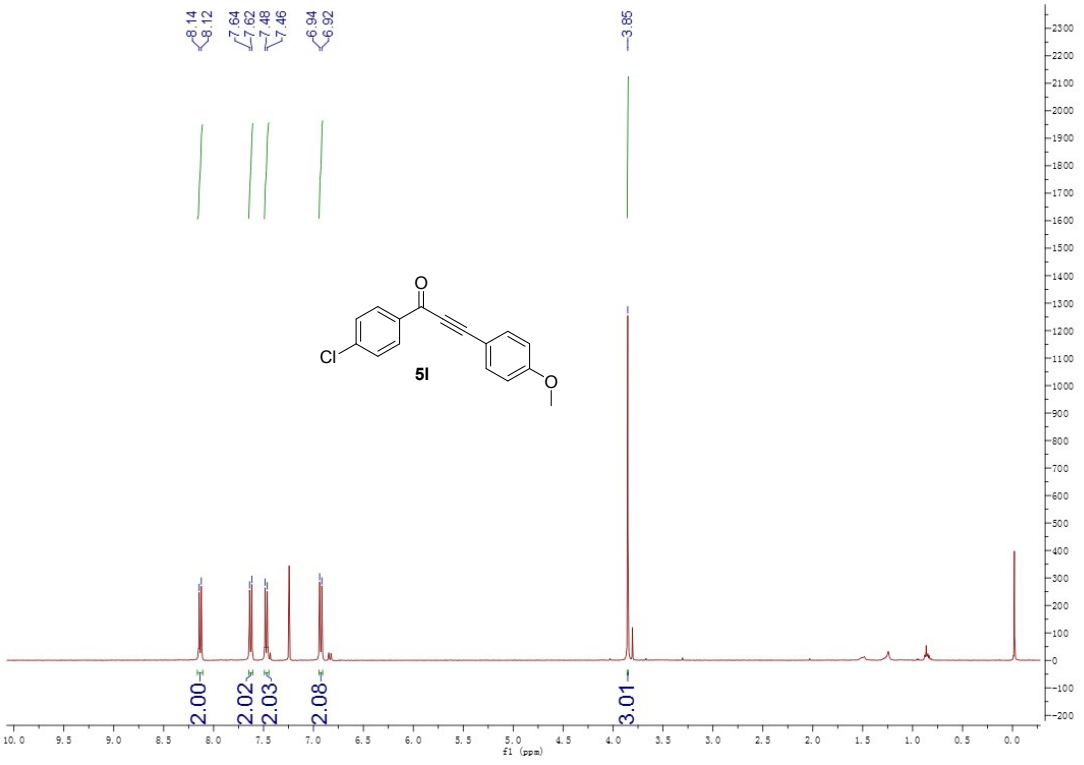
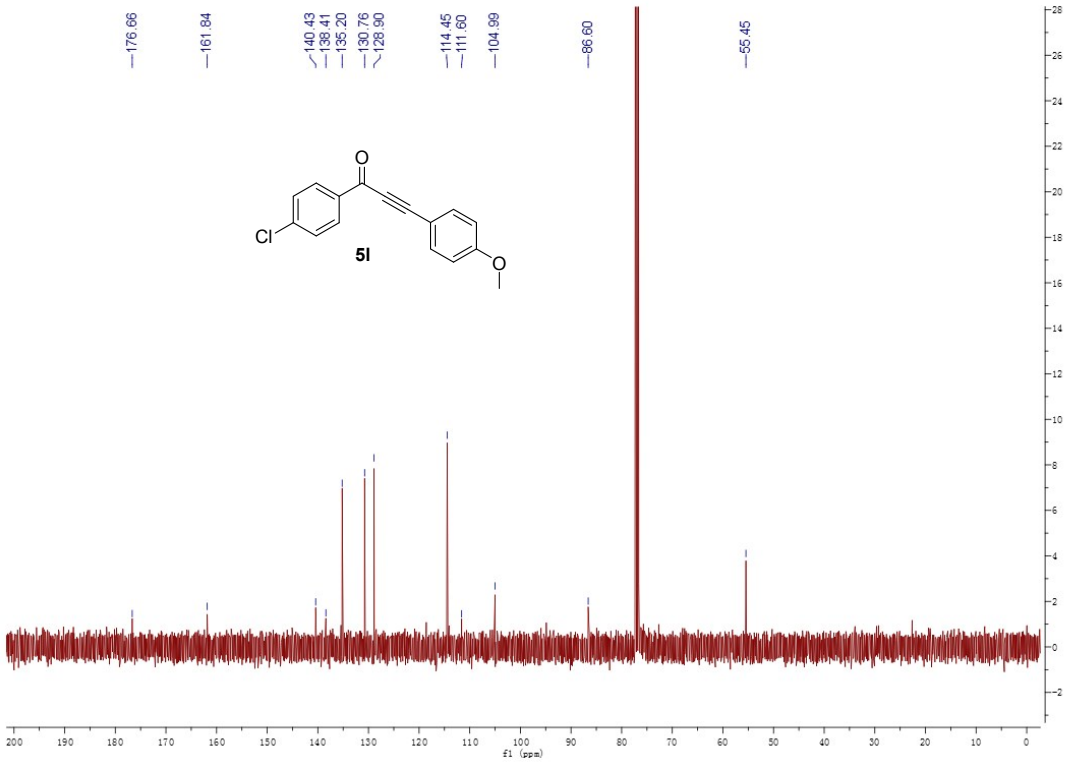
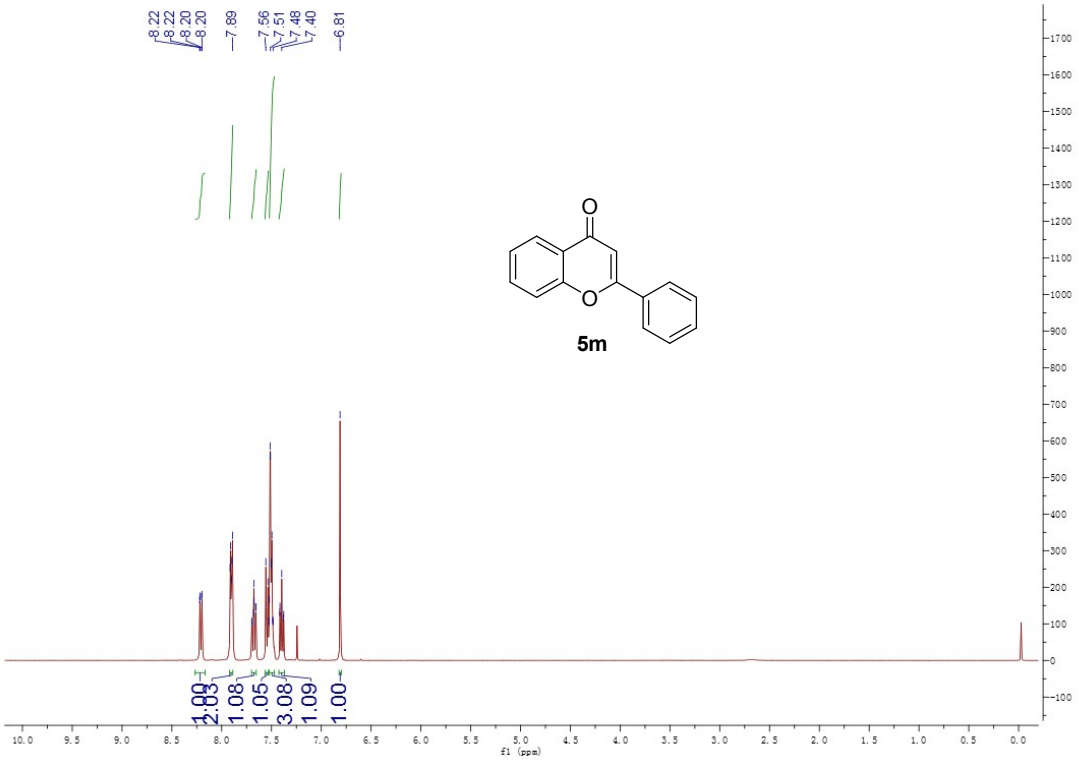
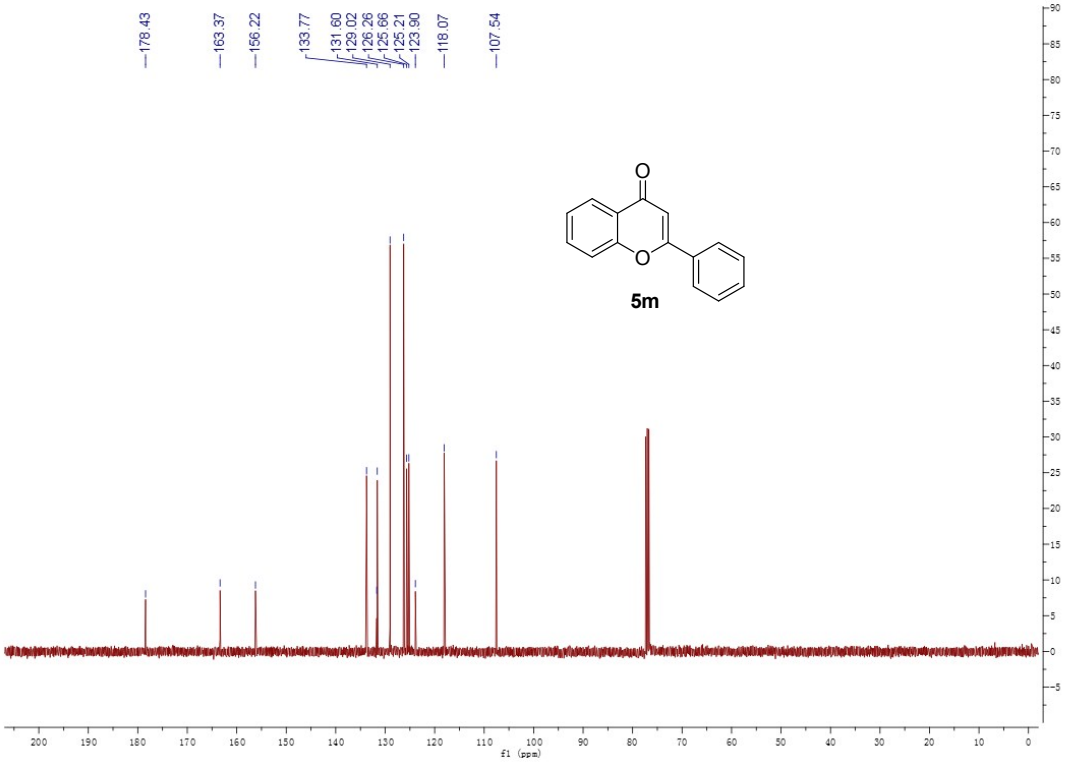
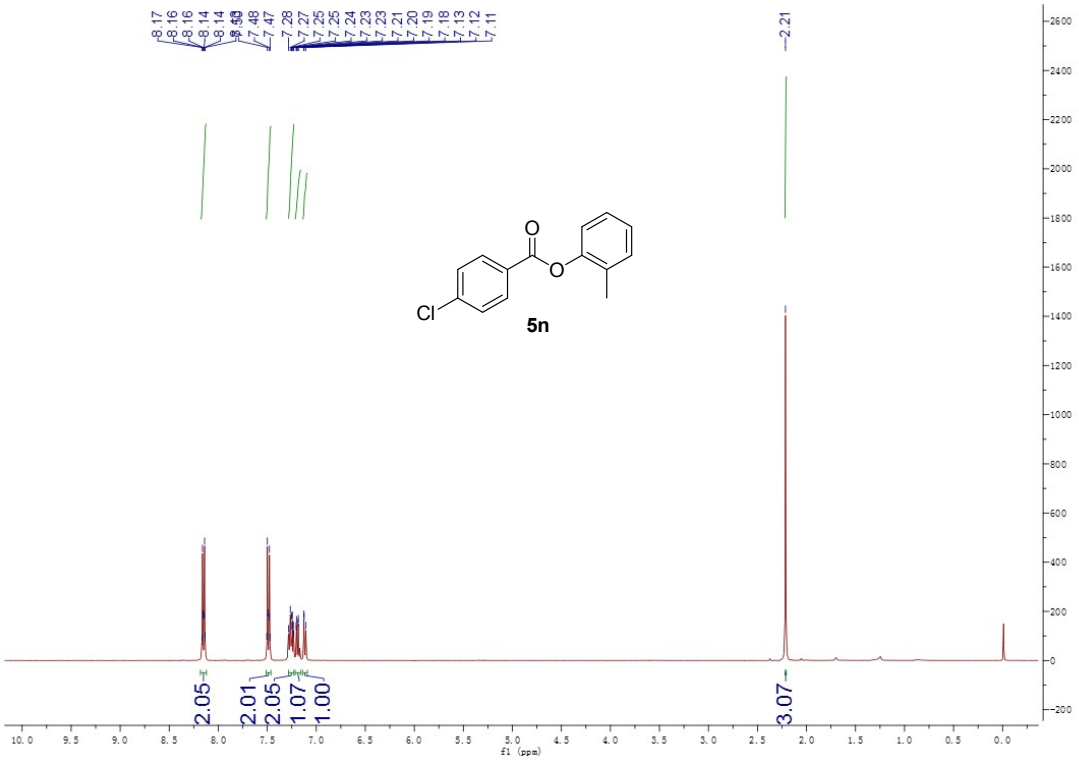
129.54
129.47
128.57
116.98
93.81
86.75
21.77
O
5k
f1 (ppm)

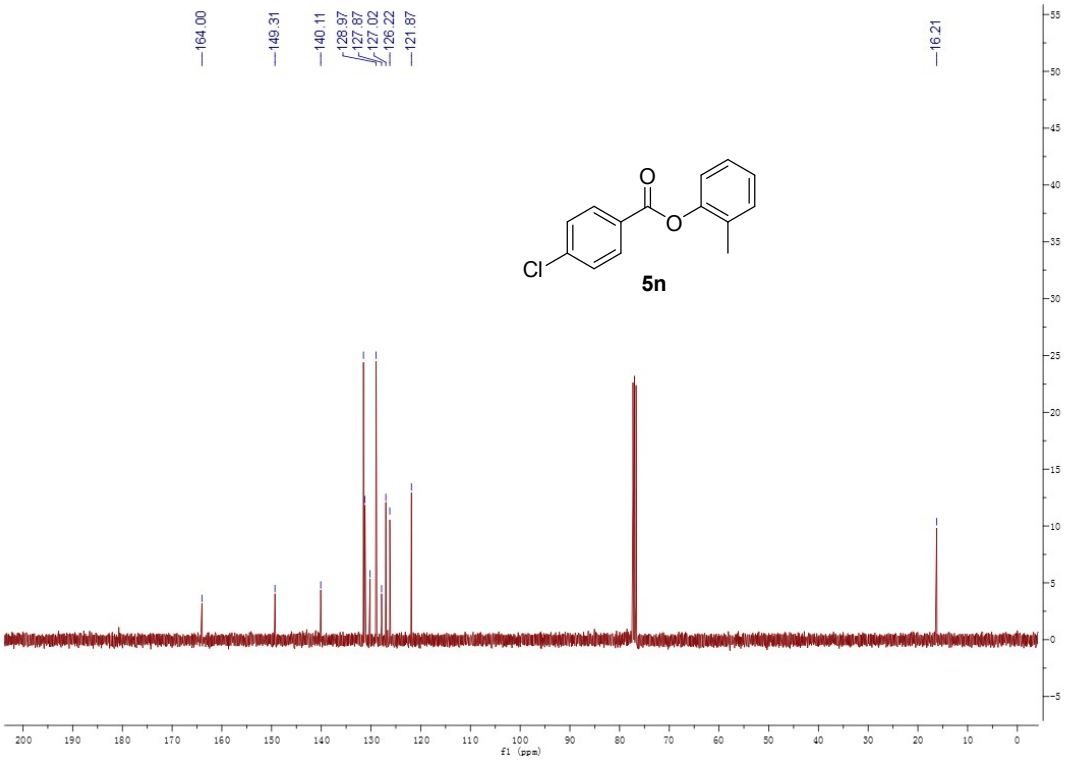

8.14
8.12
7.64
7.62
7.48
7.46
6.94
6.92
3.85
O
Cl
O
5l
2.00
2.02
2.03
2.08
3.01
f1 (ppm)

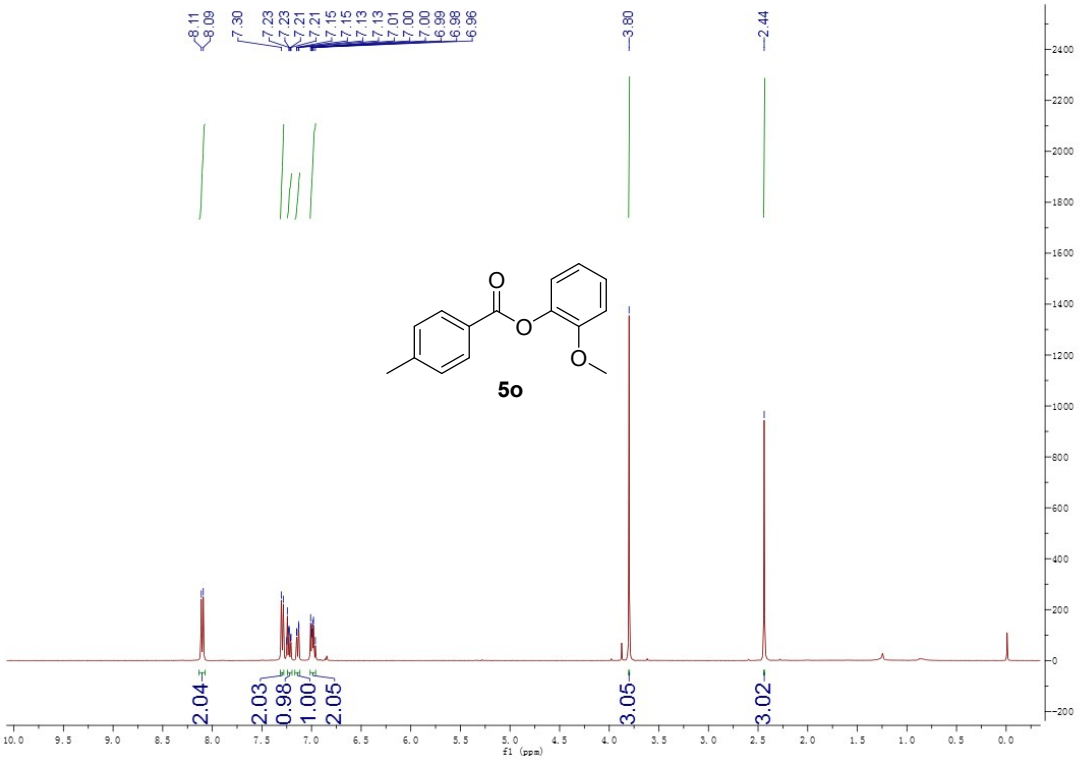

176.66
161.84
140.43
138.41
135.20
130.76
128.90
114.45
111.60
104.99
86.60
55.45
O
Cl
O
5l
f1 (ppm)

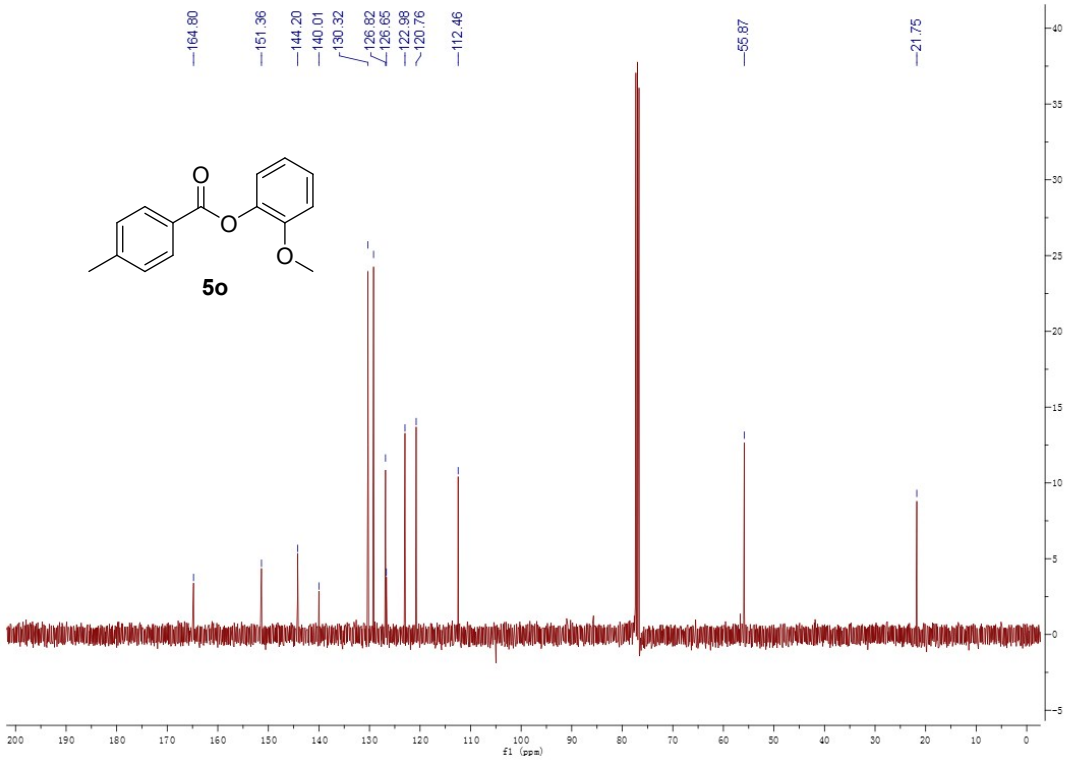

8.22
8.22
8.20
8.20
7.89
7.56
7.51
7.48
7.40
6.81
O
O
5m
1.00
2.03
1.08
1.05
3.08
1.09
1.00
f1 (ppm)

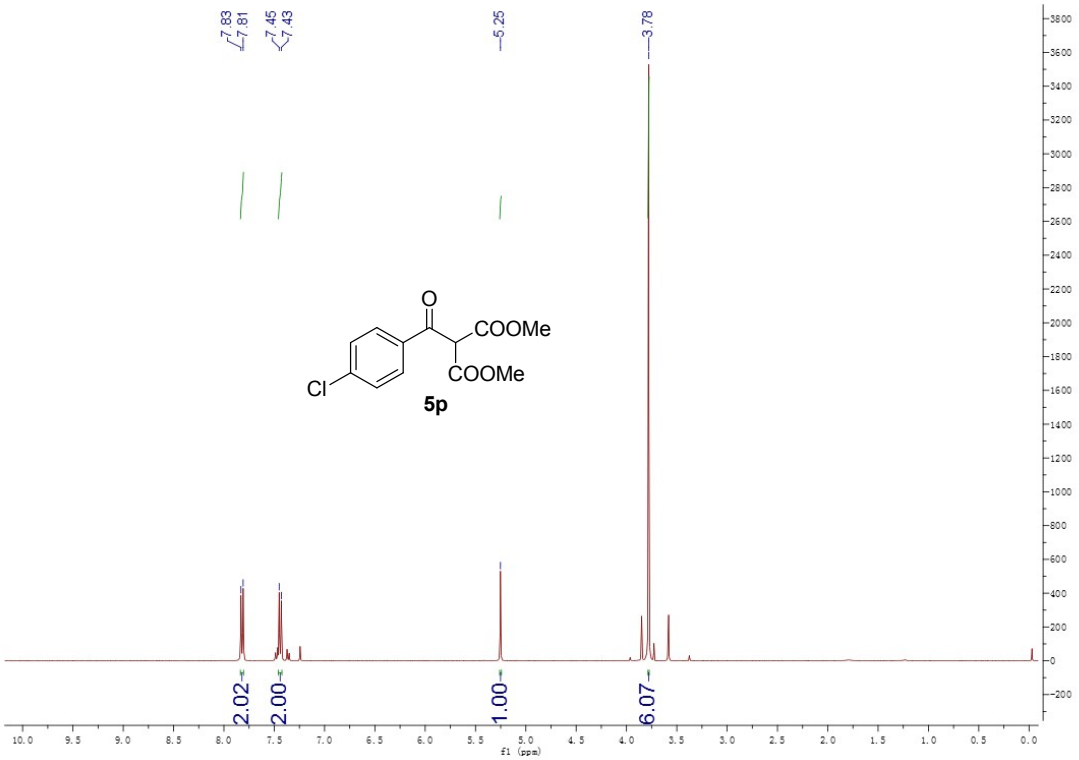

178.43
163.37
156.22
133.77
131.60
129.02
126.26
125.66
125.21
123.90
118.07
107.54
O
O
5m
f1 (ppm)

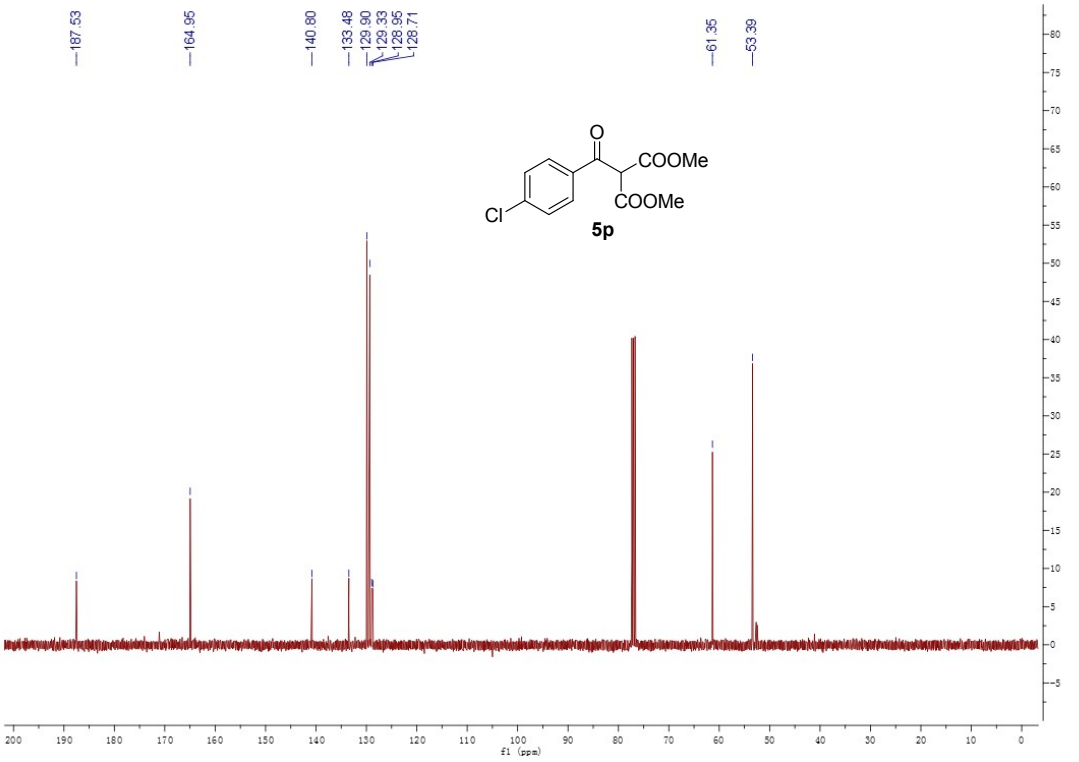

8.17
8.16
8.16
8.14
8.14
7.48
7.47
7.28
7.27
7.25
7.25
7.24
7.23
7.23
7.21
7.20
7.19
7.18
7.13
7.12
7.11
2.21
O
O
Cl
5n
2.05
2.01
2.05
1.07
1.00
3.07
f1 (ppm)

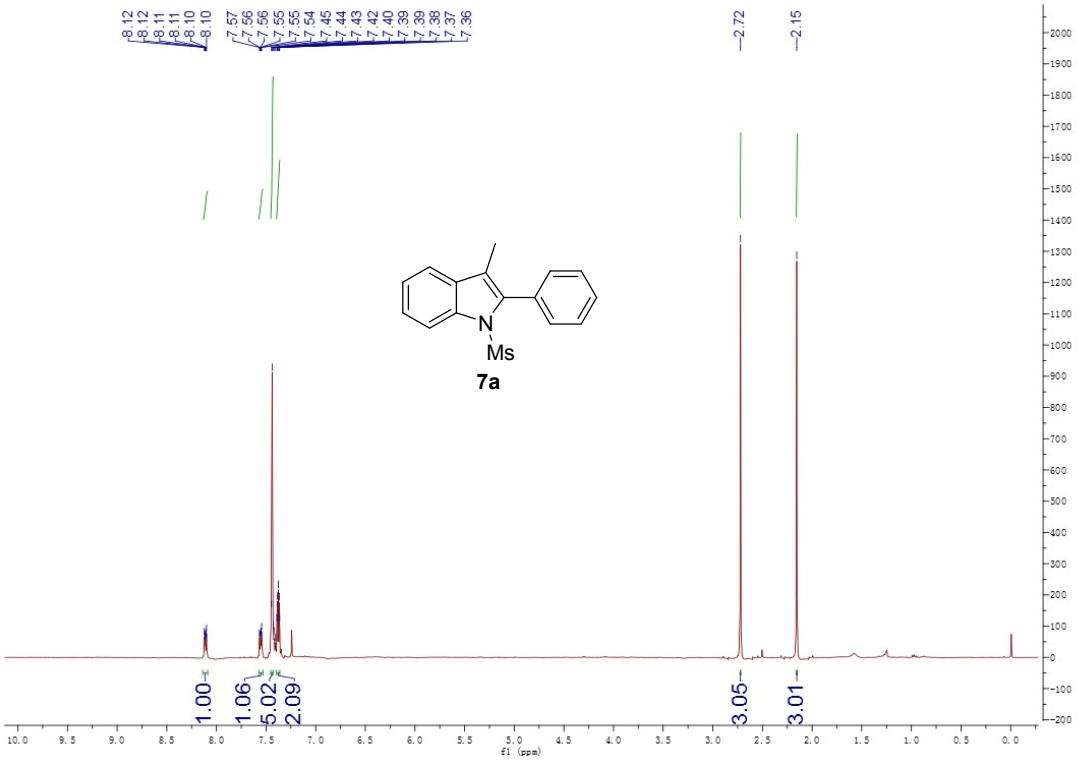

164.00
149.31
140.11
128.97
127.87
127.02
126.22
121.87
16.21
O
O
Cl
5n
f1 (ppm)


8.11
8.09
7.30
7.23
7.23
7.21
7.21
7.15
7.15
7.13
7.13
7.01
7.00
7.00
6.99
6.98
6.96
3.80
2.44
O
O
O
5o
2.04
2.03
0.98
1.00
2.05
3.05
3.02
f1 (ppm)

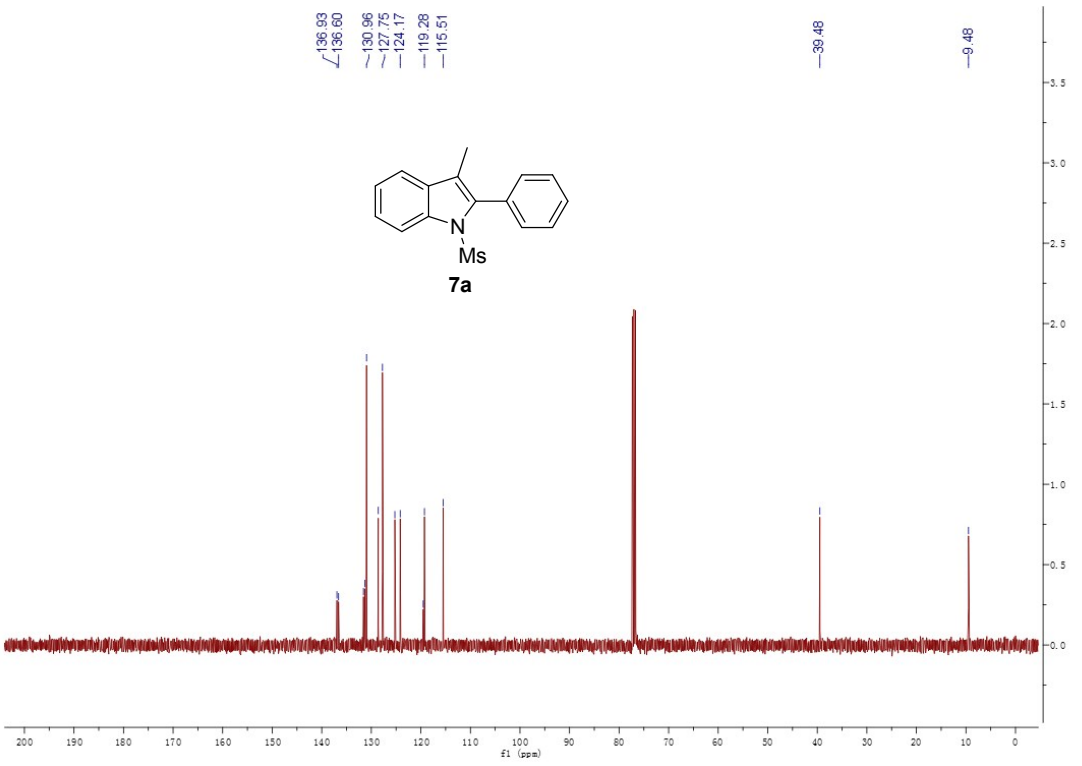

164.80
151.36
144.20
140.01
130.32
126.82
126.65
122.98
120.76
112.46
55.87
21.75
O
O
O
5o
f1 (ppm)


7.83
7.81
7.45
7.43
5.25
3.78
O
COOMe
COOMe
Cl
5p
2.02
2.00
1.00
6.07
f1 (ppm)


187.53
164.95
140.80
133.48
129.90
129.33
128.95
128.71
61.35
53.39
O
COOMe
COOMe
Cl
5p
f1 (ppm)


8.12
8.12
8.11
8.11
8.10
8.10
7.57
7.56
7.56
7.55
7.55
7.54
7.45
7.44
7.43
7.42
7.40
7.39
7.39
7.38
7.37
7.36
2.72
2.15
N
Ms
1.00
1.06
5.02
2.09
3.05
3.01
f1 (ppm)

7a


136.93
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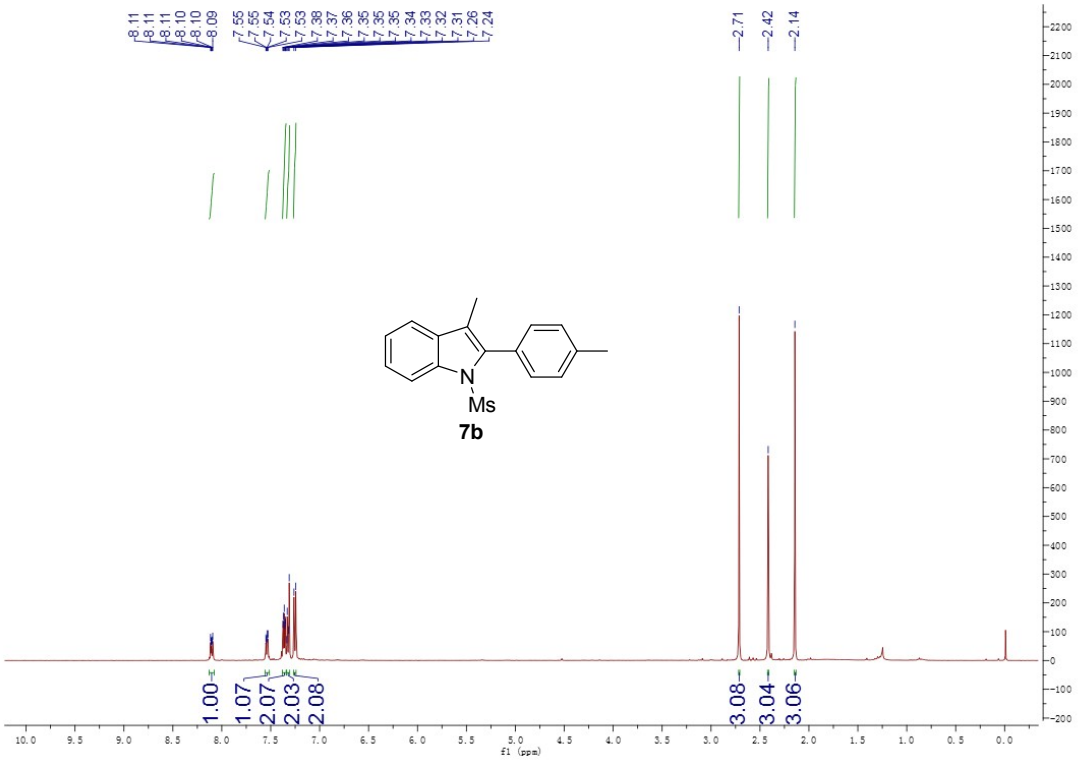
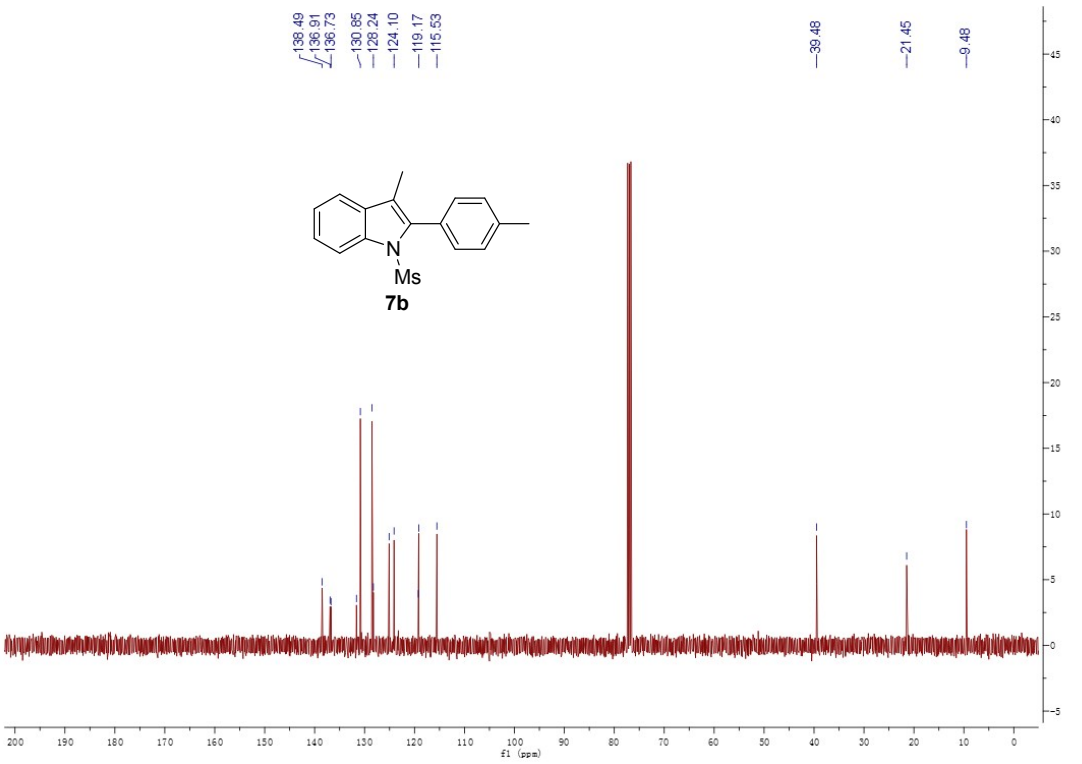
127.75
124.17
119.28
115.51
39.48
9.48
N
Ms
f1 (ppm)

7a


8.11
8.11
8.11
8.10
8.10
8.09
7.55
7.55
7.54
7.53
7.53
7.38
7.37
7.36
7.35
7.35
7.35
7.34
7.33
7.32
7.31
7.26
7.24
2.71
2.42
2.14
N
Ms
1.00
1.07
2.07
2.03
2.08
3.08
3.04
3.06
f1 (ppm)

7b


138.49
136.91
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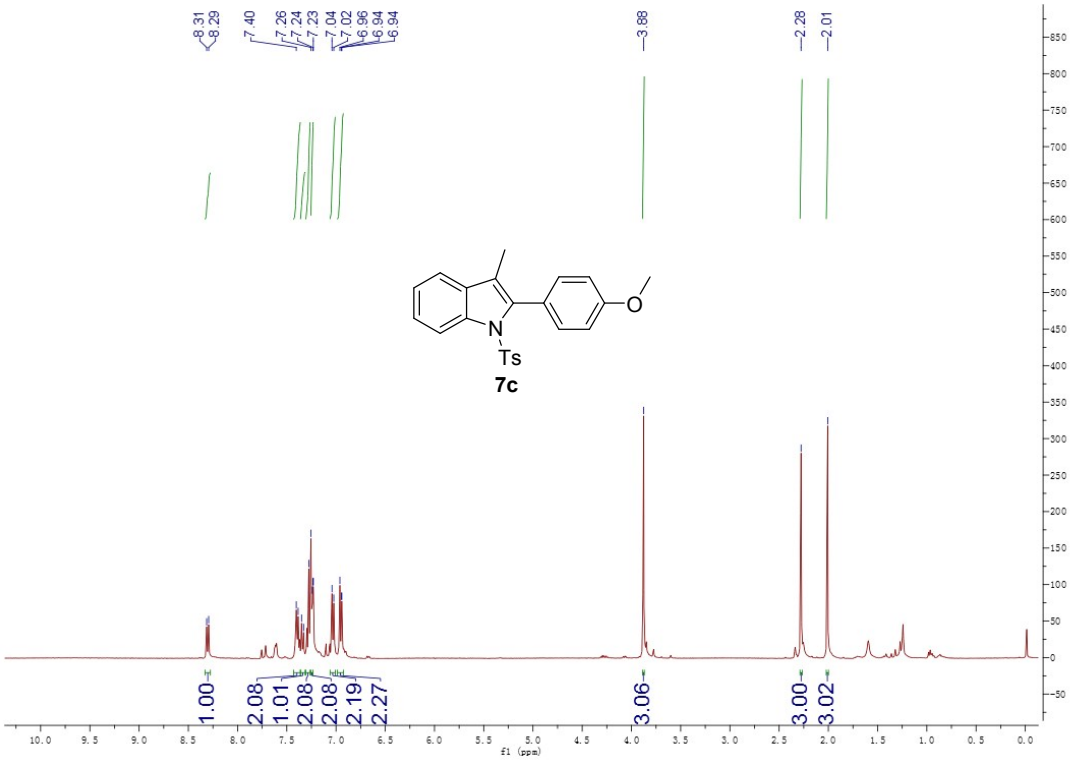
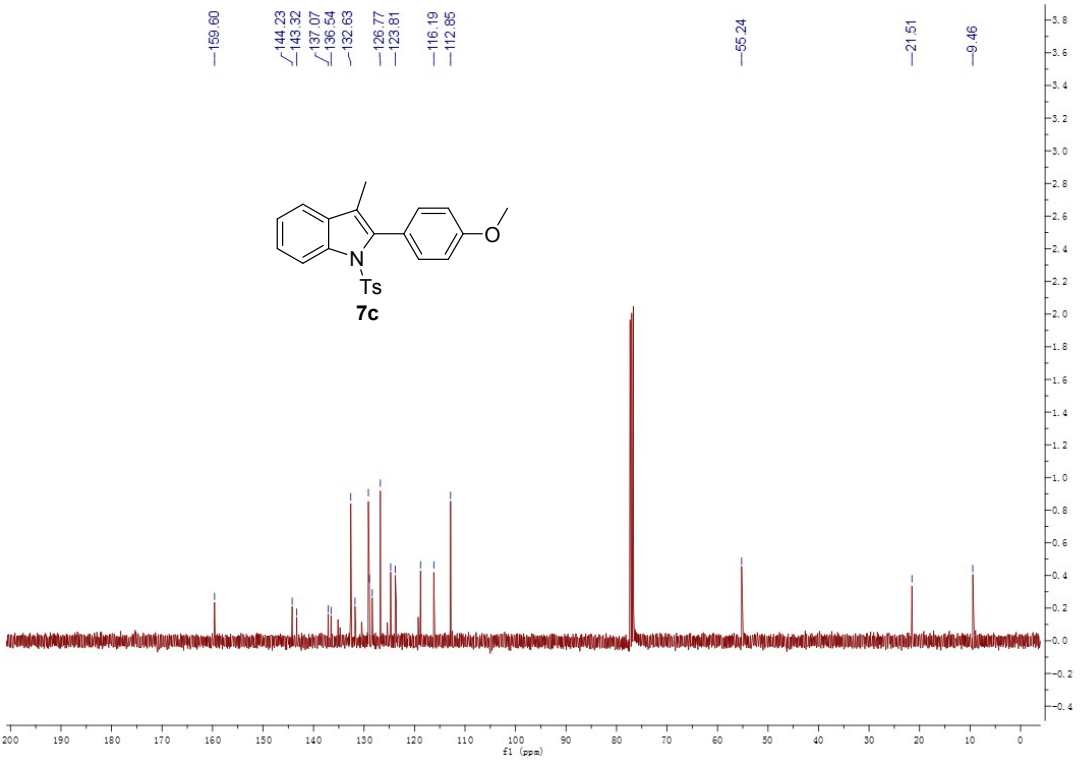
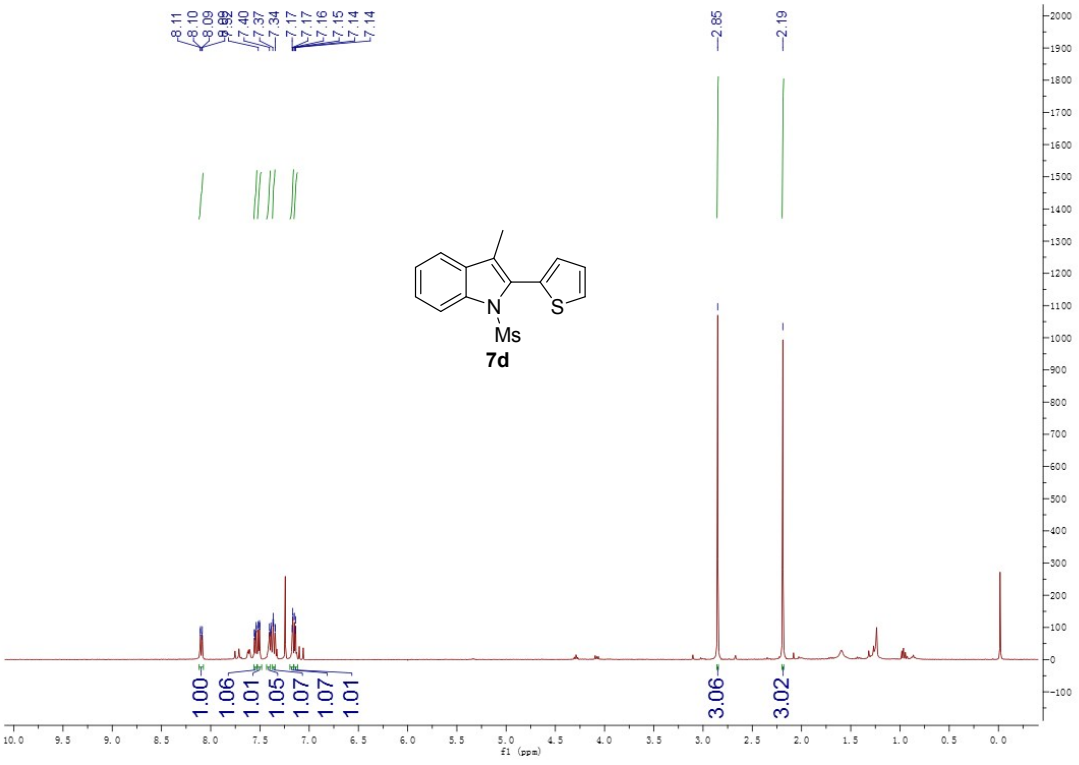
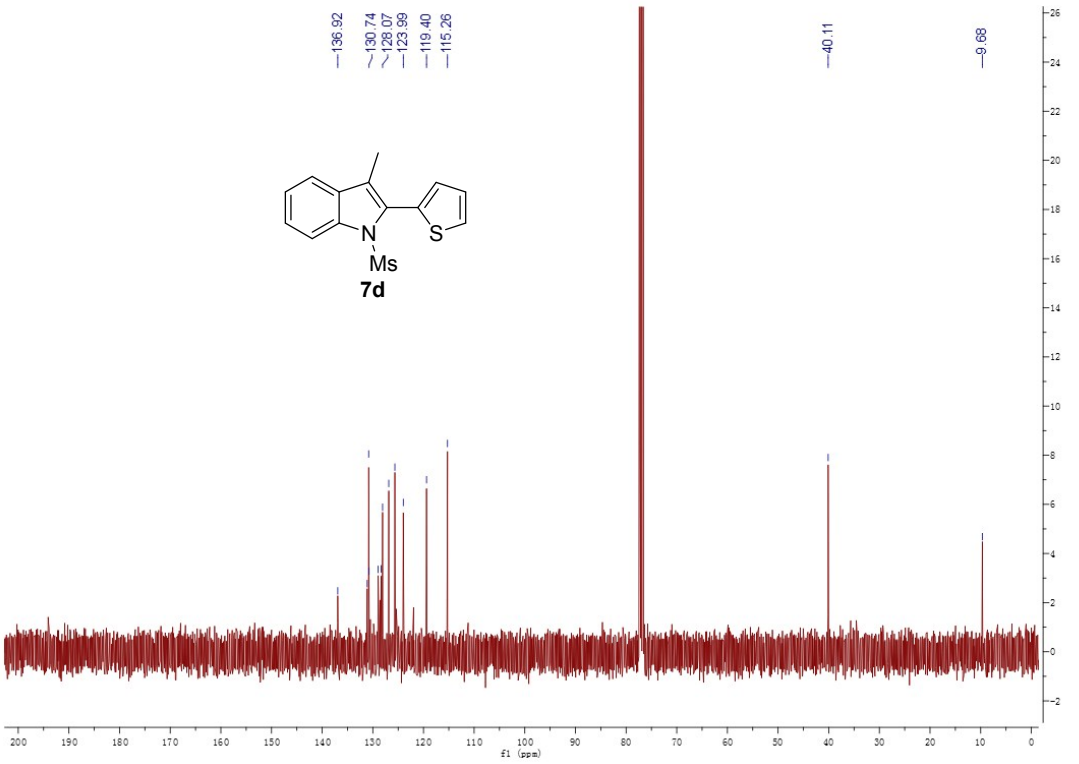
130.85
128.24
124.10
119.17
115.53
39.48
21.45
9.48
N
Ms
f1 (ppm)

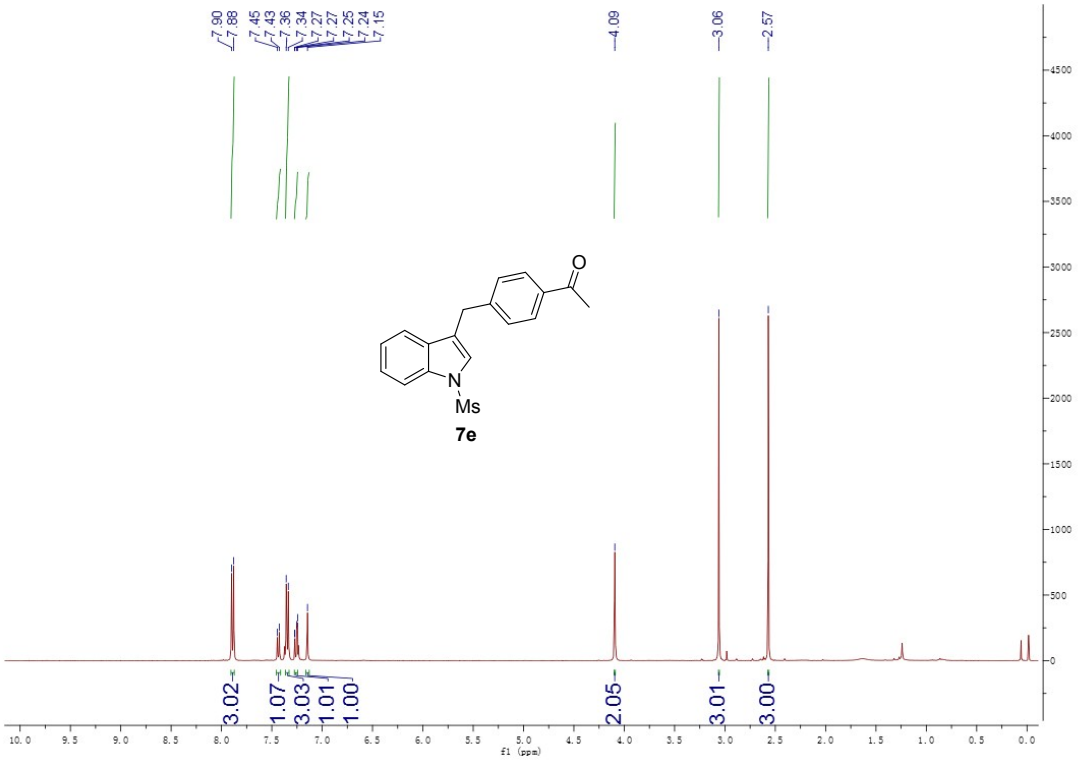
7b

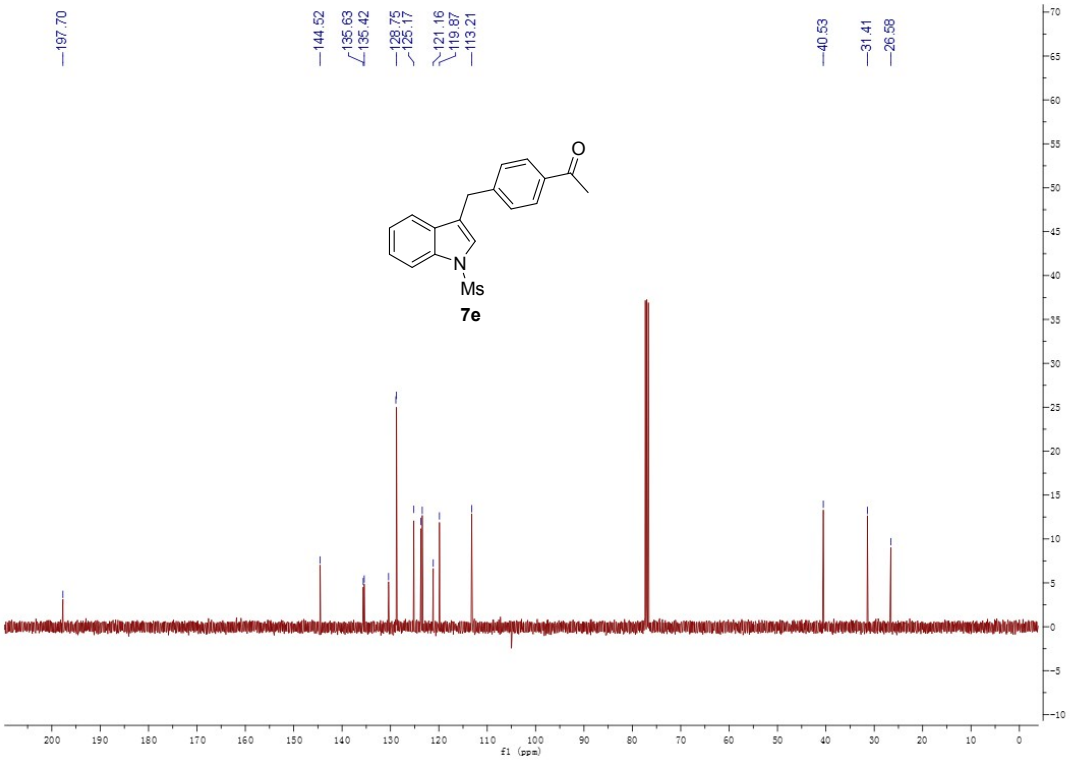

8.31
8.29
7.40
7.26
7.24
7.23
7.04
7.02
6.96
6.94
6.94
3.88
2.28
2.01
O
N
Ts
7c
1.00
2.08
1.01
2.08
2.08
2.19
2.27
3.06
3.00
3.02
f1 (ppm)


159.60
144.23
143.32
137.07
136.54
132.63
126.77
123.81
116.19
112.85
55.24
21.51
9.46
O
N
Ts
7c
f1 (ppm)


8.11
8.10
8.09
7.40
7.37
7.34
7.17
7.17
7.16
7.15
7.14
7.14
2.85
2.19
N
Ms
S
7d
1.00
1.06
1.01
1.05
1.07
1.07
1.01
3.06
3.02
f1 (ppm)


136.92
130.74
128.07
123.99
119.40
115.26
40.11
9.68
N
Ms
S
7d
f1 (ppm)


7.90
7.88
7.45
7.43
7.36
7.34
7.27
7.27
7.25
7.24
7.15
4.09
3.06
2.57
O
N
Ms
7e
3.02
1.07
3.03
1.01
1.00
2.05
3.01
3.00
f1 (ppm)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144.52
135.63
135.42
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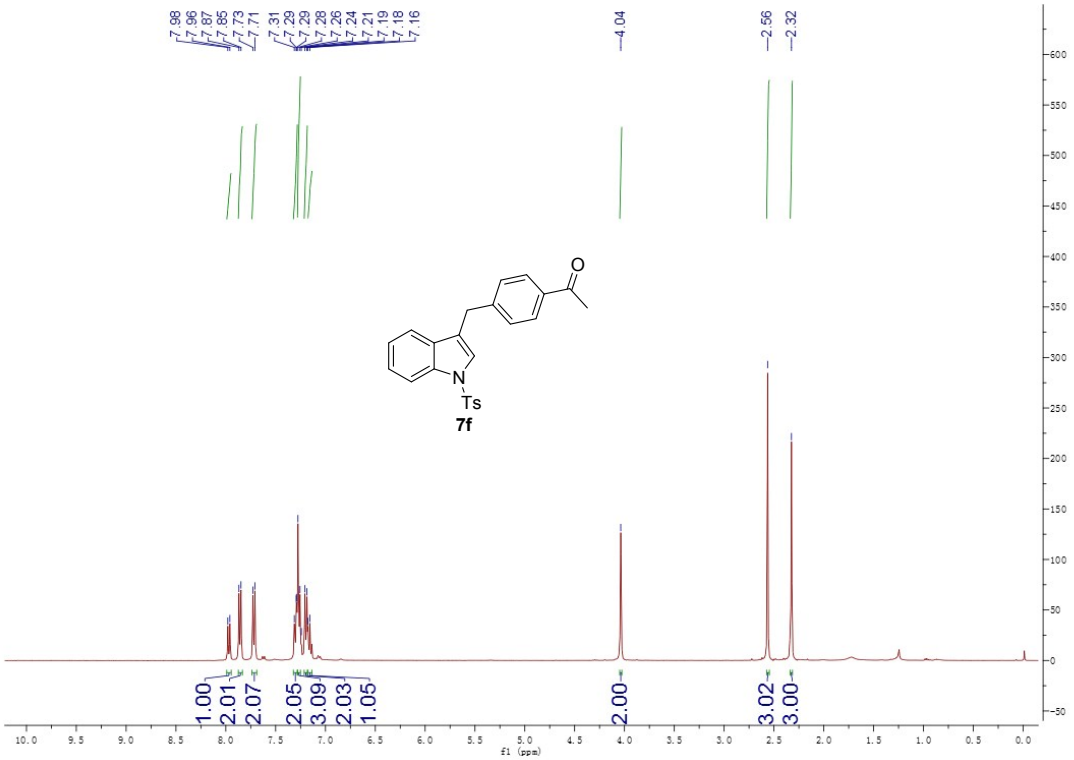
121.16
119.87
113.21
40.53
31.41
26.58
O
N
Ms
7e
f1 (ppm)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7.71
7.31
7.29
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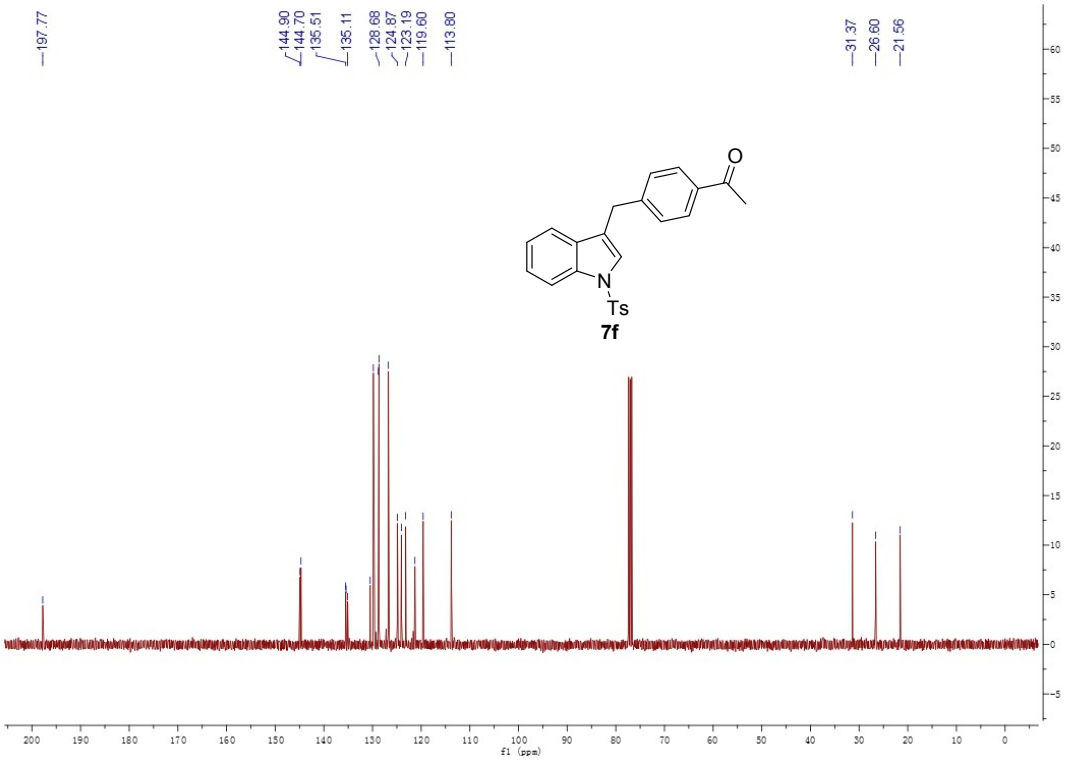
7.28
7.26
7.24
7.21
7.19
7.18
7.16
4.04
2.56
2.32
O
N
Ts
7f
1.00
2.01
2.07
2.05
3.09
2.03
1.05
2.00
3.02
3.00
f1 (ppm)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135.51
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128.68
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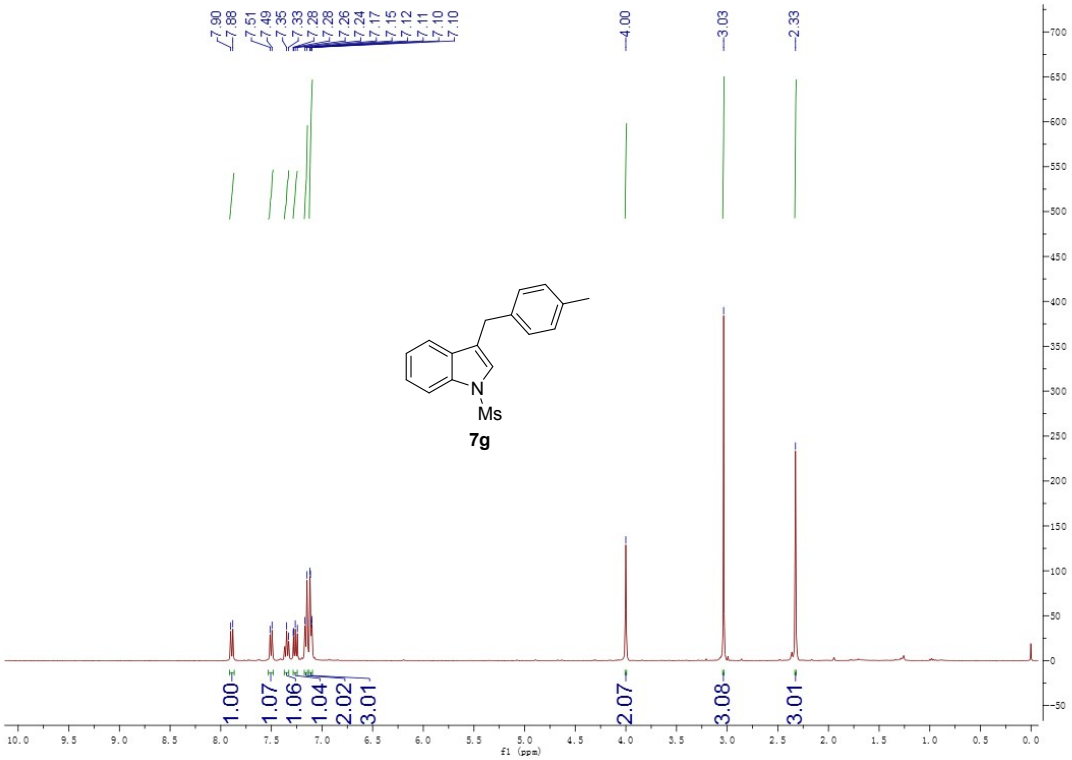
123.19
119.60
113.80
31.37
26.60
21.56
O
N
Ts
7f
f1 (ppm)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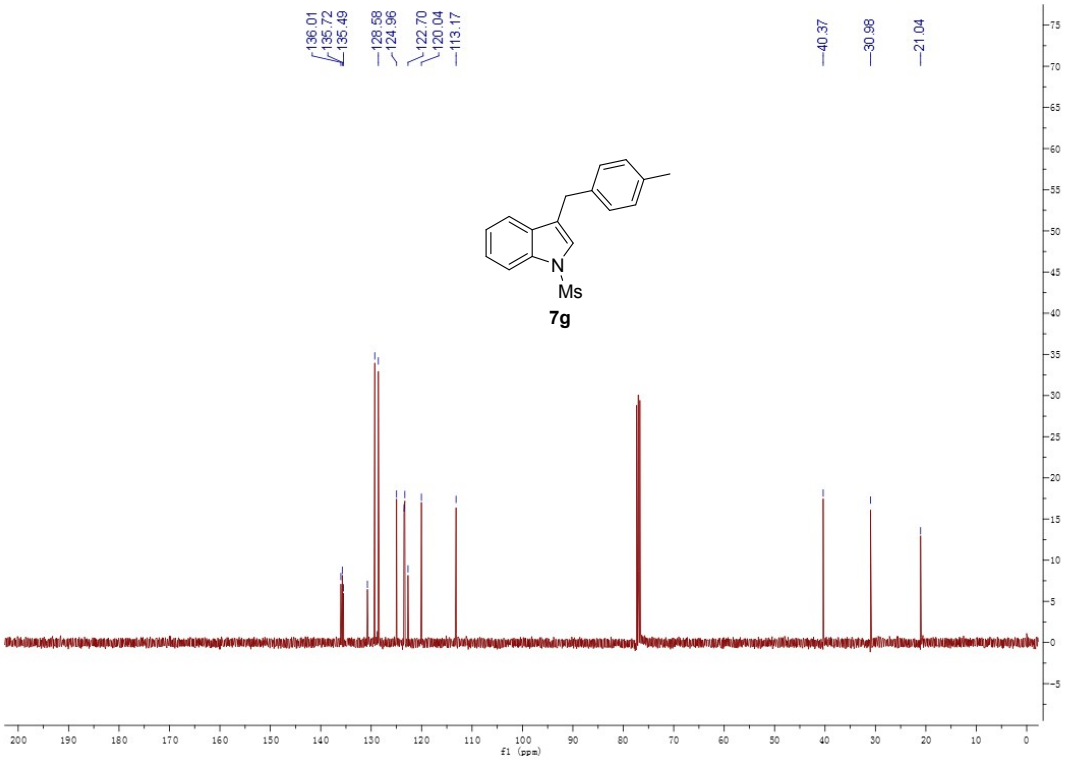
7.33
7.28
7.28
7.26
7.24
7.17
7.15
7.12
7.11
7.10
7.10
4.00
3.03
2.33
N
Ms
1.00
1.07
1.06
1.04
2.02
3.01
2.07
3.08
3.01
f1 (ppm)

7g


136.01
135.72
135.49
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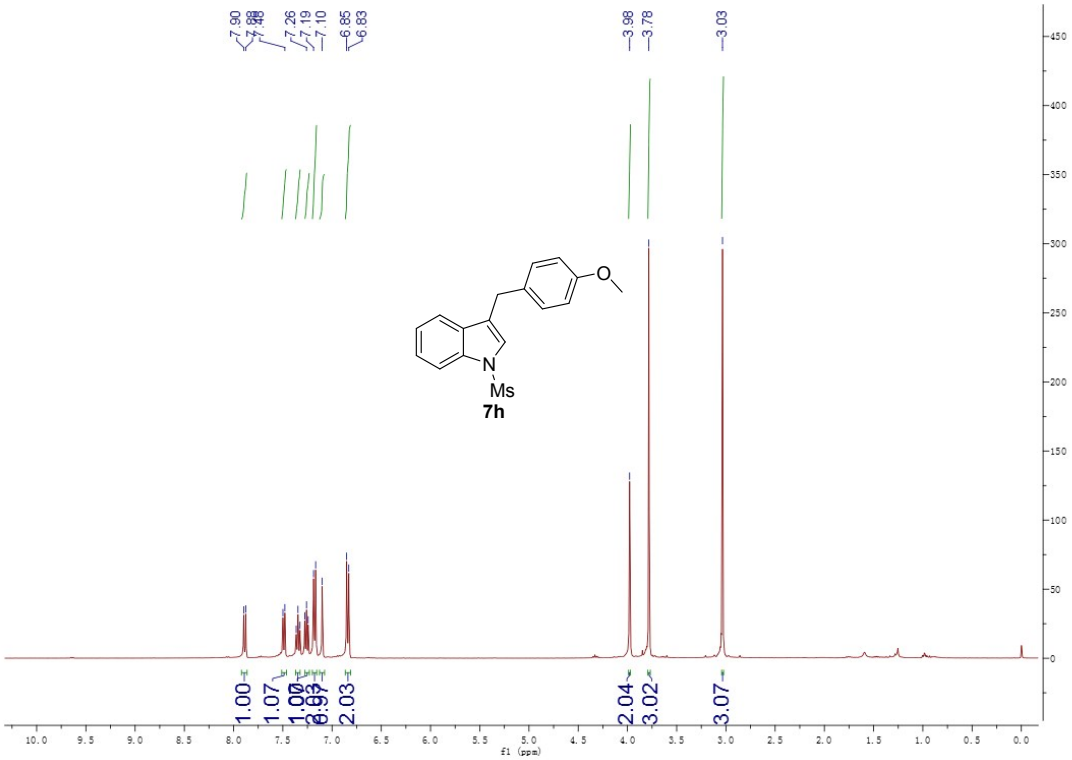
122.70
120.04
113.17
40.37
30.98
21.04
N
Ms
f1 (ppm)

7g


7.90
7.26
7.19
7.10
6.85
6.83
3.98
3.78
3.03
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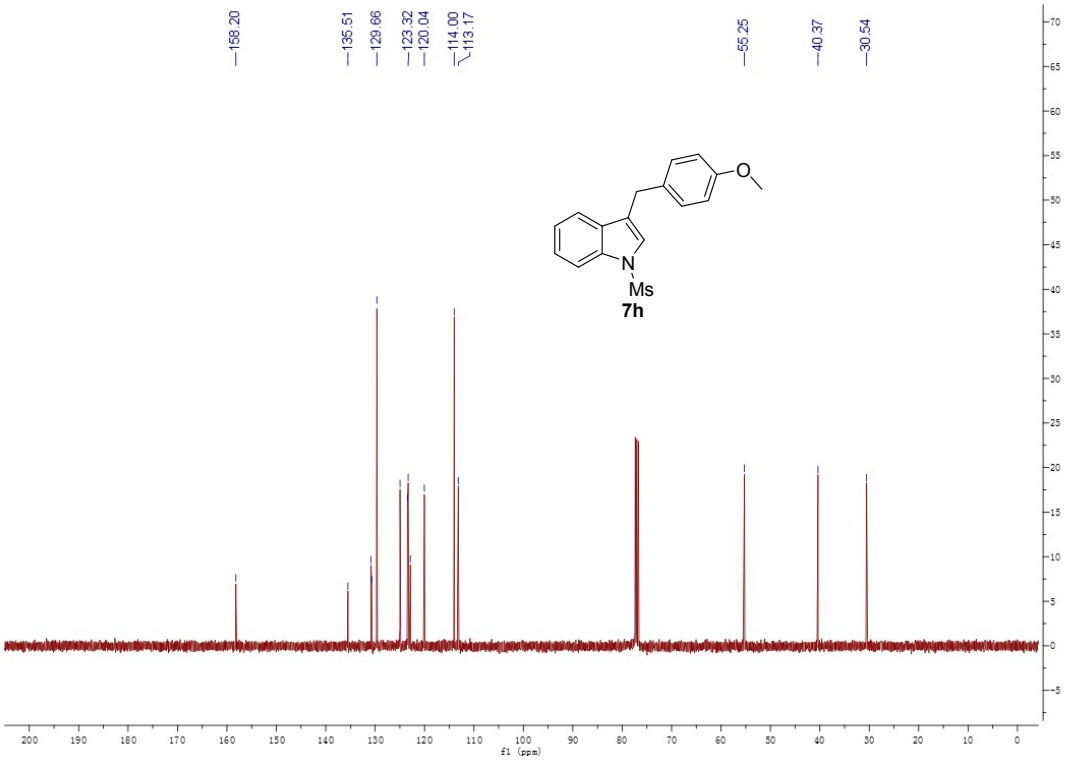
N
Ms
7h
1.00
1.07
2.03
2.04
3.02
3.07
f1 (ppm)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135.51
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114.00
113.17
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30.54
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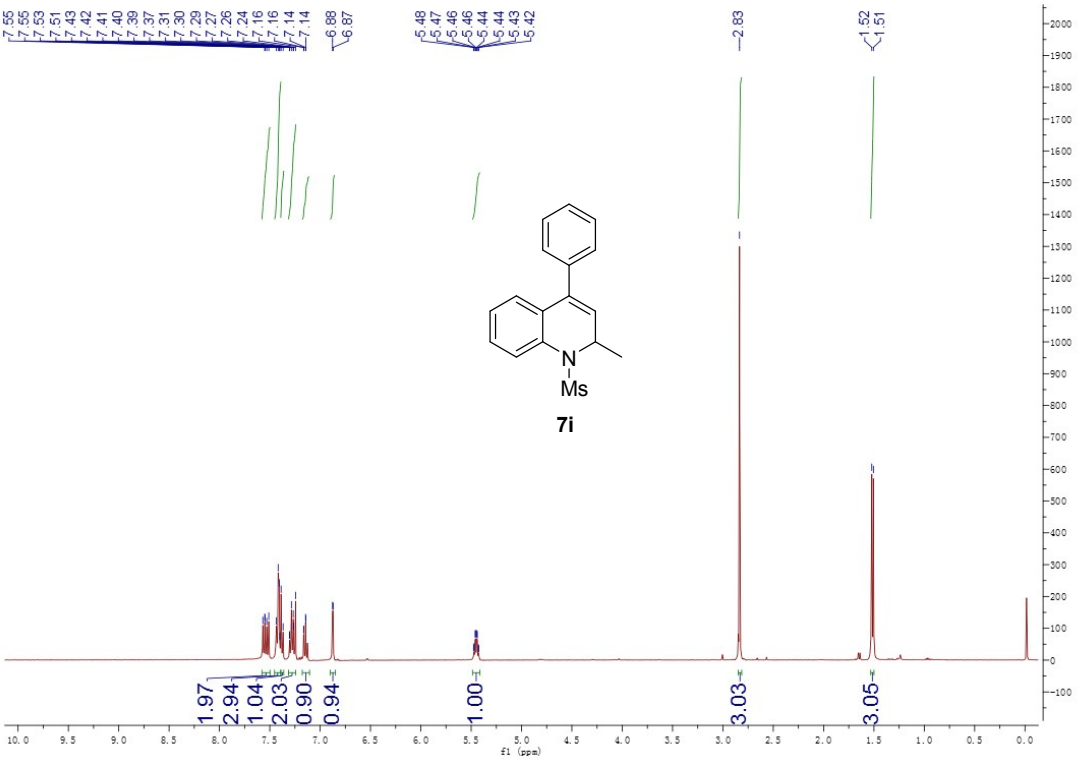
N
Ms
7h
f1 (ppm)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7.55
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7.51
7.43
7.42
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7.40
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7.37
7.31
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7.29
7.27
7.26
7.24
7.16
7.16
7.14
7.14
6.88
6.87
5.48
5.47
5.46
5.46
5.44
5.44
5.43
5.42
2.83
1.52
1.51
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Ms
7i
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1.04
2.03
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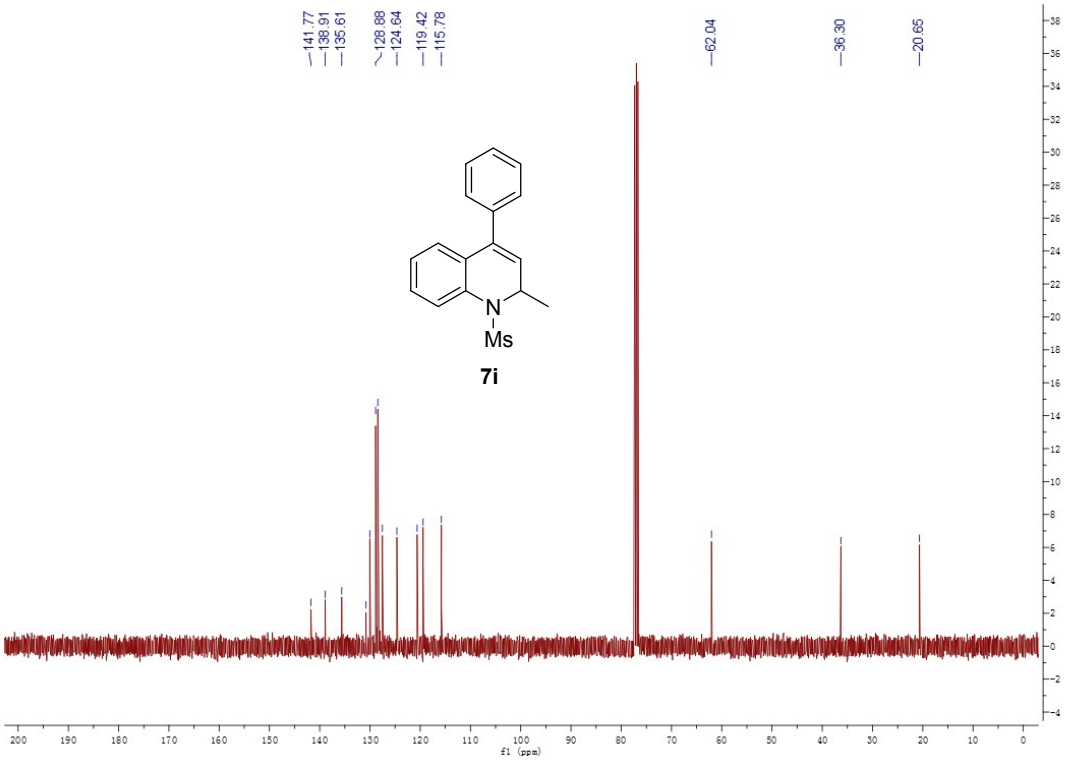
0.94
1.00
3.03
3.05
f1 (ppm)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138.91
135.61
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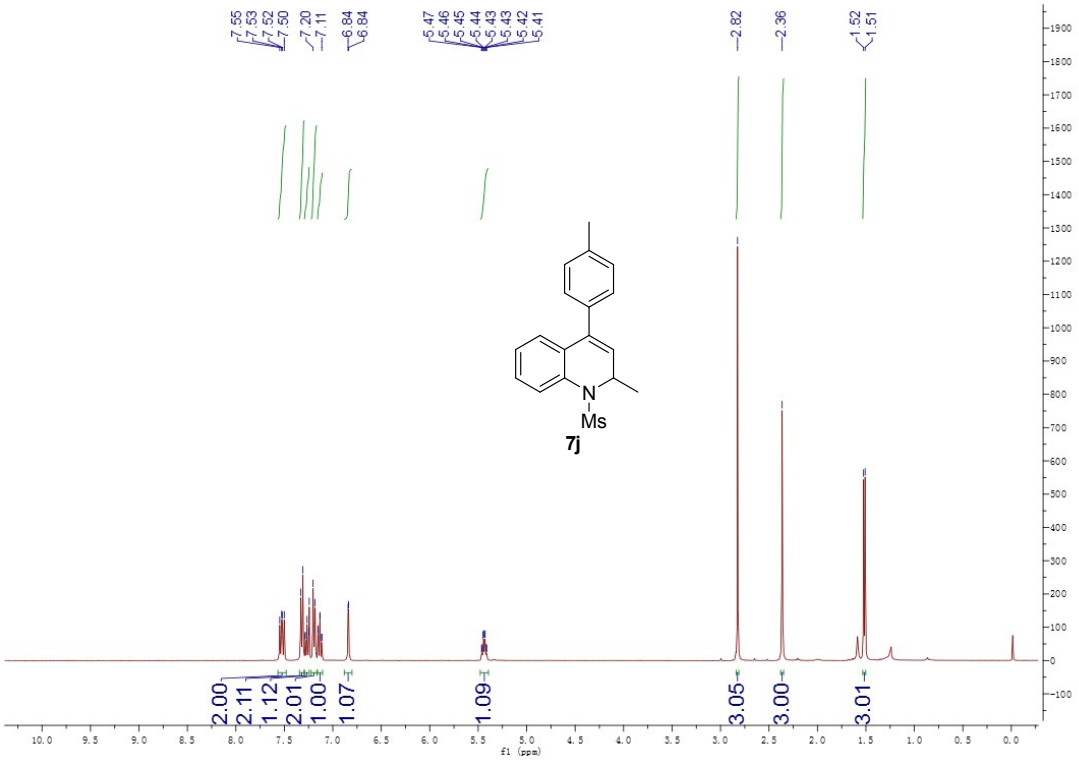
124.64
119.42
115.78
62.04
36.30
20.65
N
Ms
7i
f1 (ppm)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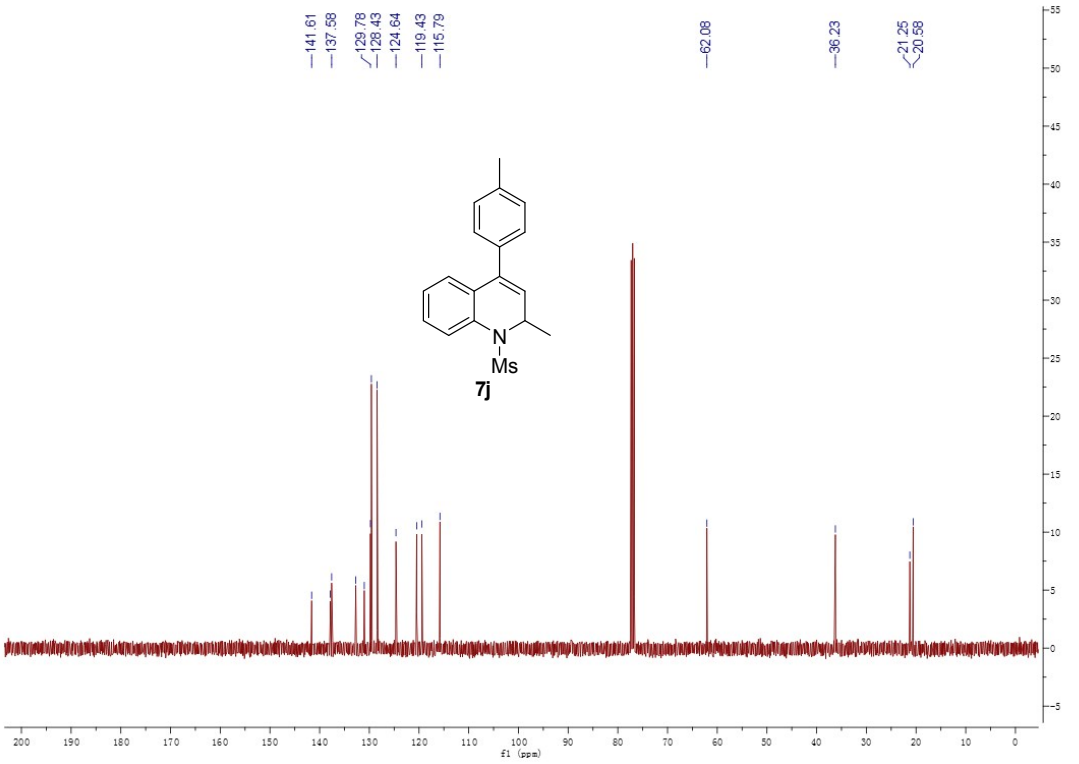
7.52
7.50
7.20
7.11
6.84
6.84
5.47
5.46
5.45
5.44
5.43
5.43
5.42
5.41
2.82
2.36
1.52
1.51
N
Ms
7j
2.00
2.11
1.12
2.01
1.00
1.07
1.09
3.05
3.00
3.01
f1 (ppm)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137.58
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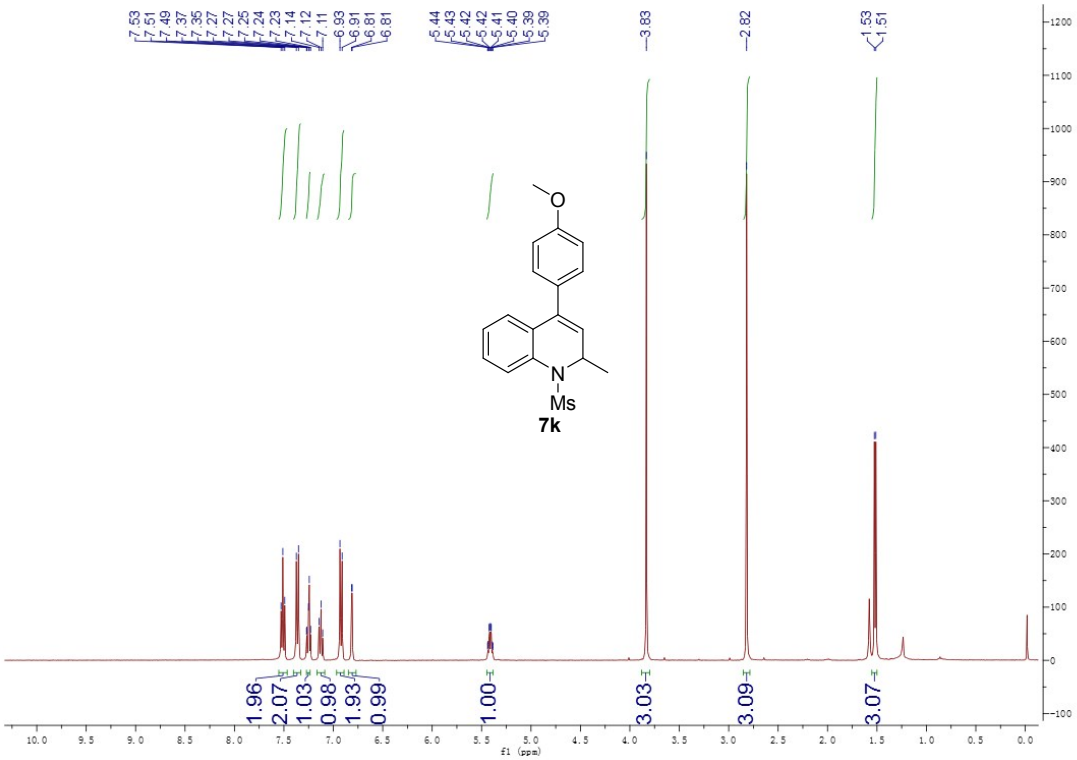
115.79
62.08
36.23
21.25
20.58
N
Ms
7j
f1 (ppm)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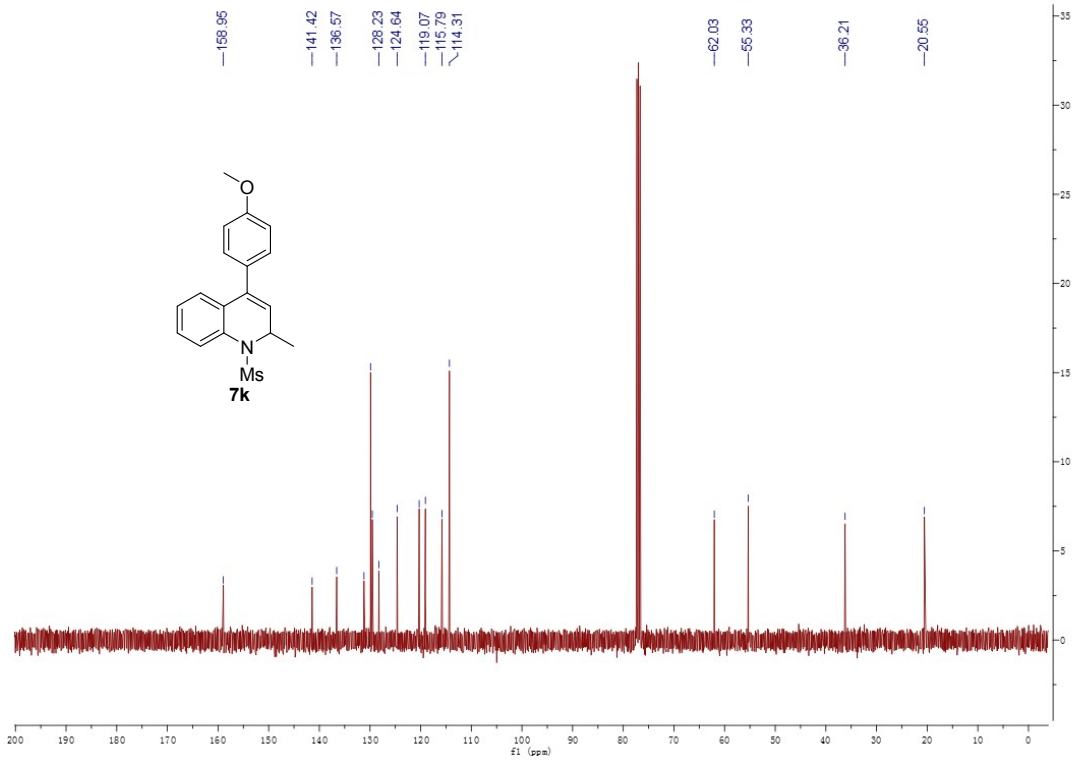
7.35
7.27
7.27
7.25
7.24
7.23
7.14
7.12
7.11
6.93
6.91
6.81
6.81
5.44
5.43
5.42
5.42
5.41
5.40
5.39
5.39
3.83
2.82
1.53
1.51
O
N
Ms
7k
1.96
2.07
1.03
0.98
1.93
0.99
1.00
3.03
3.09
3.07
f1 (ppm)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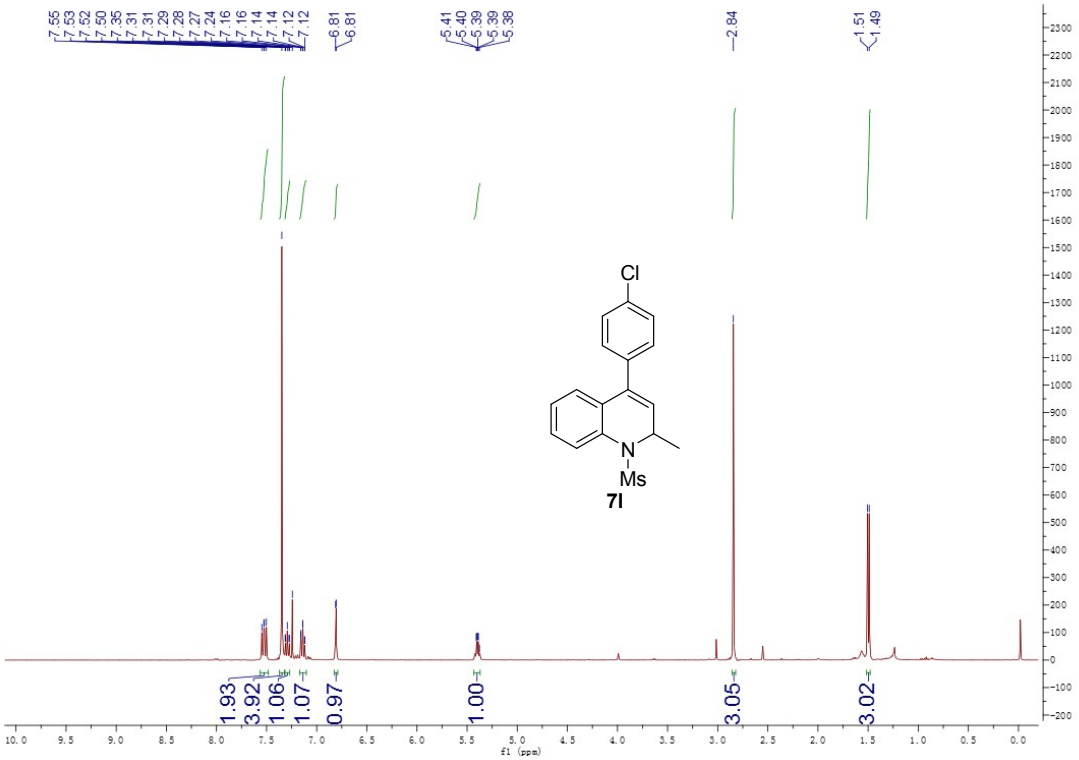
114.31
62.03
55.33
36.21
20.55
O
N
Ms
7k
f1 (ppm)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7.53
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7.35
7.31
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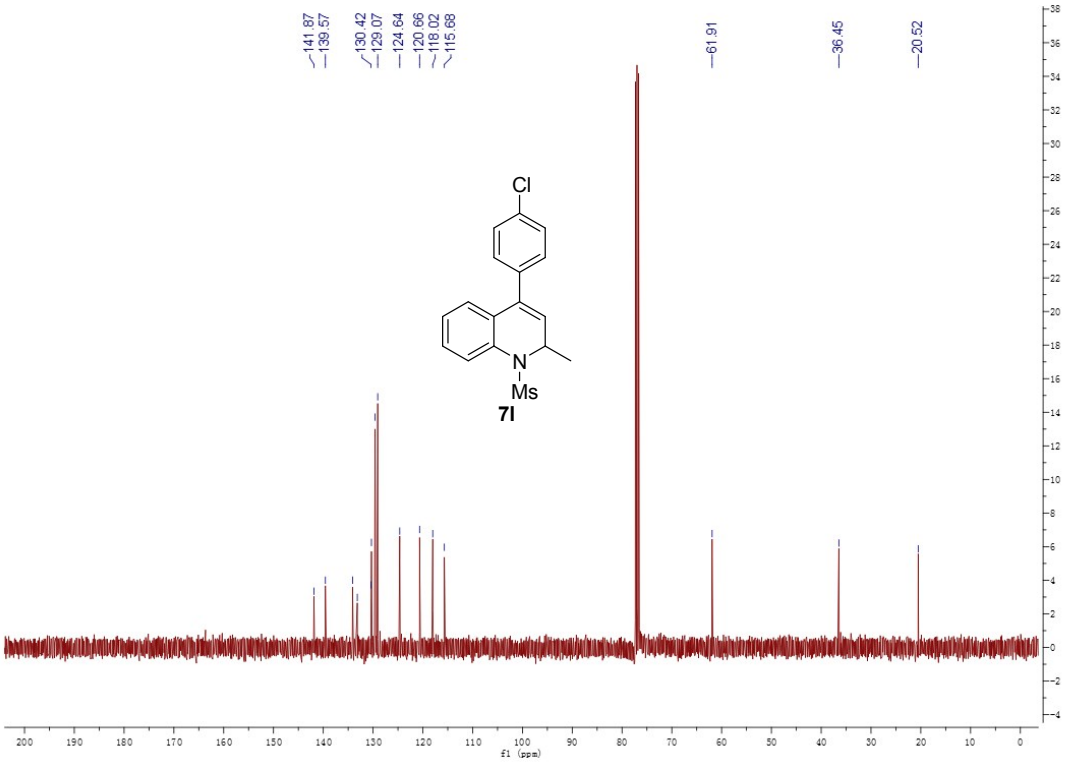
7.29
7.28
7.27
7.24
7.16
7.16
7.14
7.14
7.12
7.12
6.81
6.81
5.41
5.40
5.39
5.39
5.38
2.84
1.51
1.49
Cl
N
Ms
7l
1.93
3.92
1.06
1.07
0.97
1.00
3.05
3.02
f1 (ppm)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61.91
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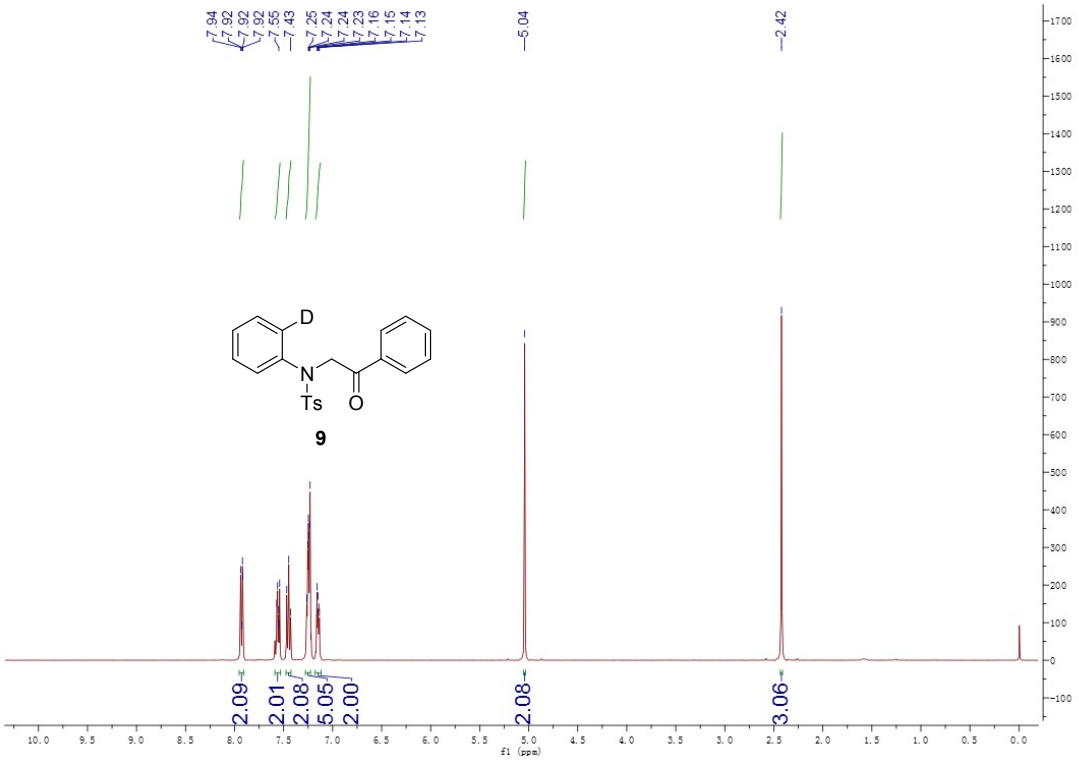
20.52
Cl
N
Ms
7l
f1 (ppm)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7.92
7.92
7.92
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7.43
7.25
7.24
7.24
7.23
7.16
7.15
7.14
7.13
5.04
2.42
D
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Ts
O
9
2.09
2.01
2.08
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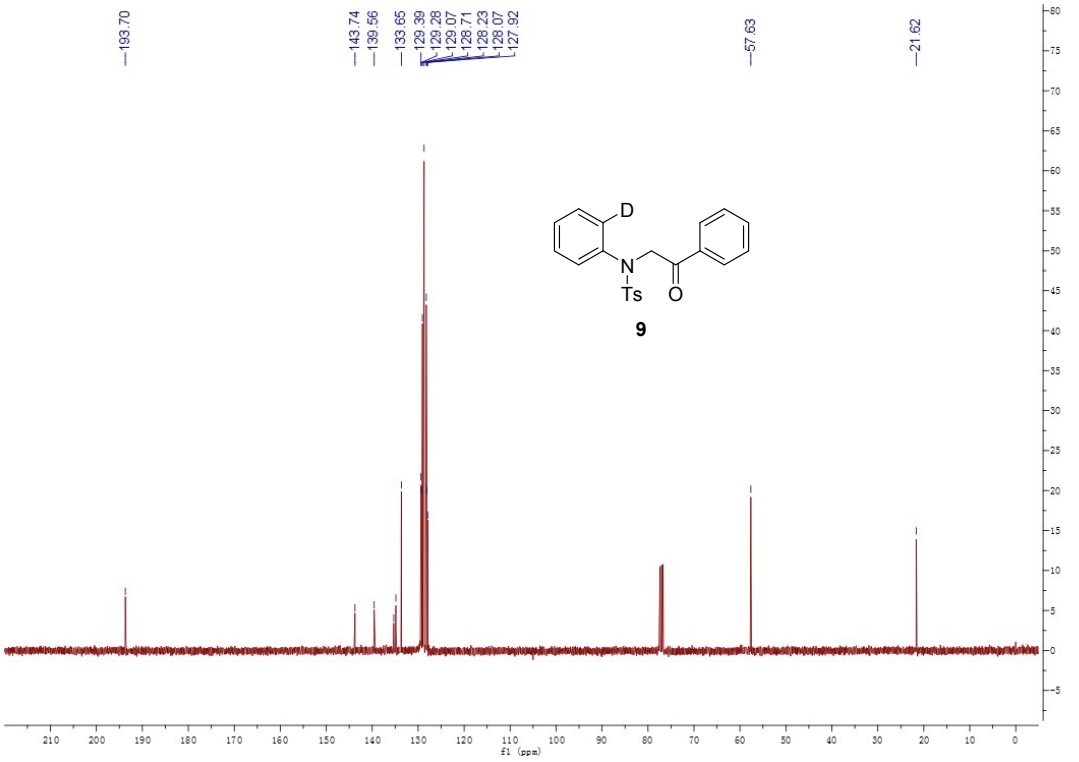
2.00
2.08
3.06
f1 (ppm)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D
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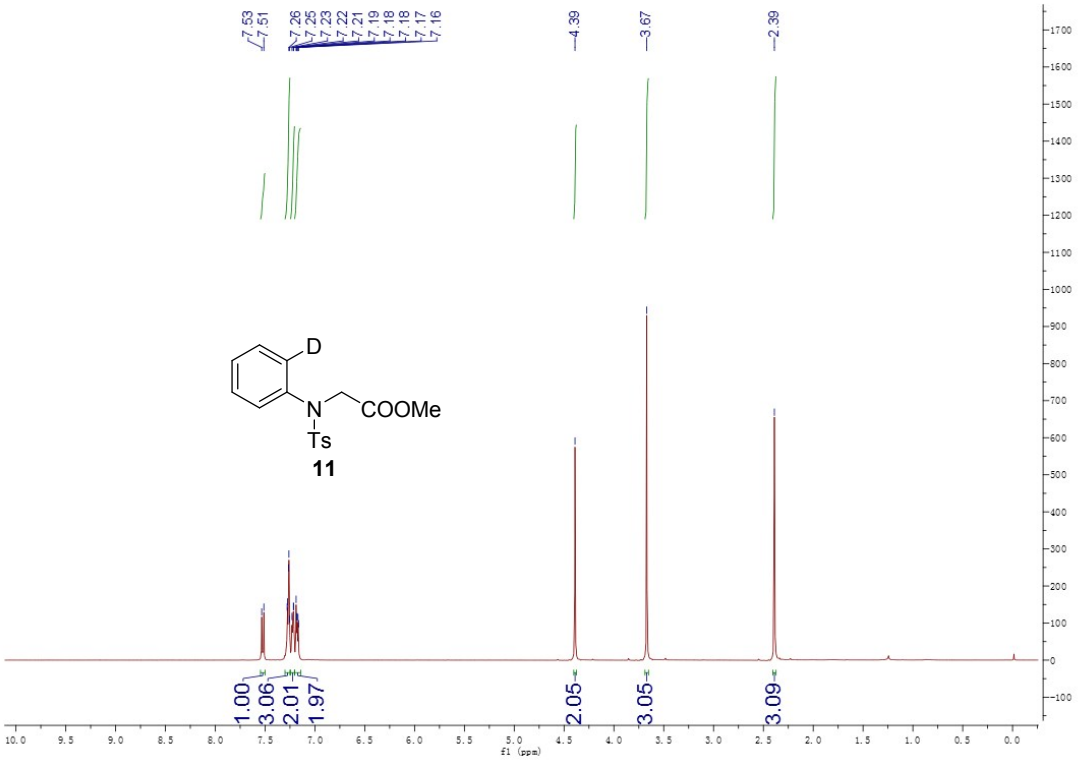
Ts
O
9
f1 (ppm)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7.18
7.18
7.17
7.16
4.39
3.67
2.39
D
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COOMe
Ts
11
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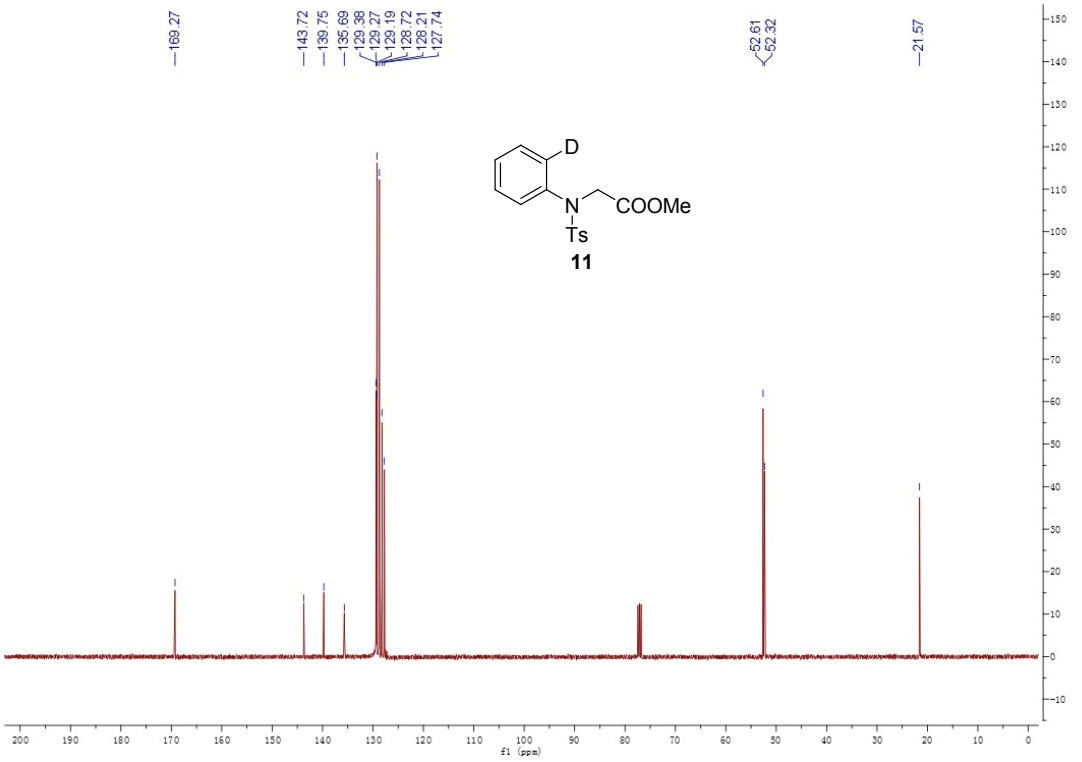
3.06
2.01
1.97
2.05
3.05
3.09
f1 (ppm)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135.69
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129.27
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128.72
128.21
127.74
52.61
52.32
21.57
D
N
COOMe
Ts
11
f1 (ppm)