Supporting Information

Solvent-promoted photochemical carbonylation of benzylic C-H Bonds under iron catalysis

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1.General information

Unless otherwise noted, all of the reagents were purchased from commercial suppliers and used without purification. All commercially available compounds were purchased from Energy Chemical, Macklin, Bidepharm or Adamas. TLC was carried out on SiO_2 (silica gel 60 F254, Merck), and the spots were located with UV light (254 nm). Flash chromatography was carried out on SiO_2 (silica gel 60, 200-300 mesh). NMR spectra were measured on a Bruker magnetic resonance spectrometer (^1H at 400 MHz, ^{13}C at 100 MHz). 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). $CDCl_3$ were used as a solvent. MS data were obtained on an Agilent 5975C inert 350 EI mass spectrometer (GC-MS); X-Ray single-crystal diffraction data were collected on an Agilent Technologies Gemini single-crystal diffractometer.

The photocatalytic reactions were performed on Beijing Roger tech Ltd with 450 nm 5 W blue LED, and the temperature of the heated reactor was set to indicate temperature.

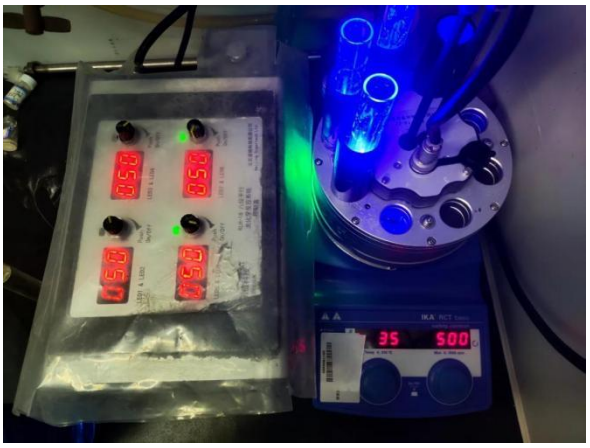


Figure 1. Setup for photocatalytic reactions

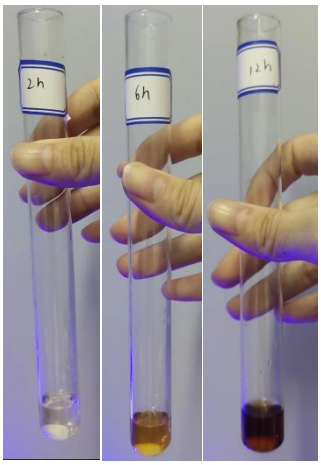
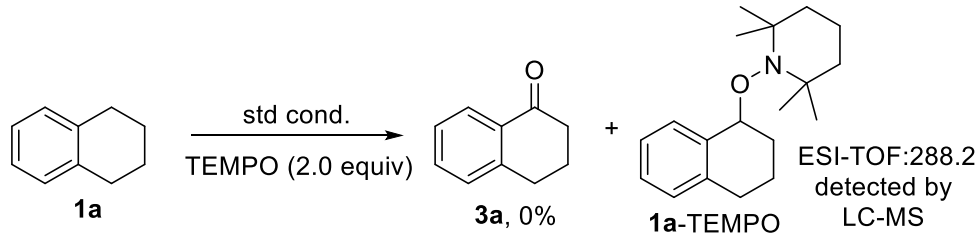
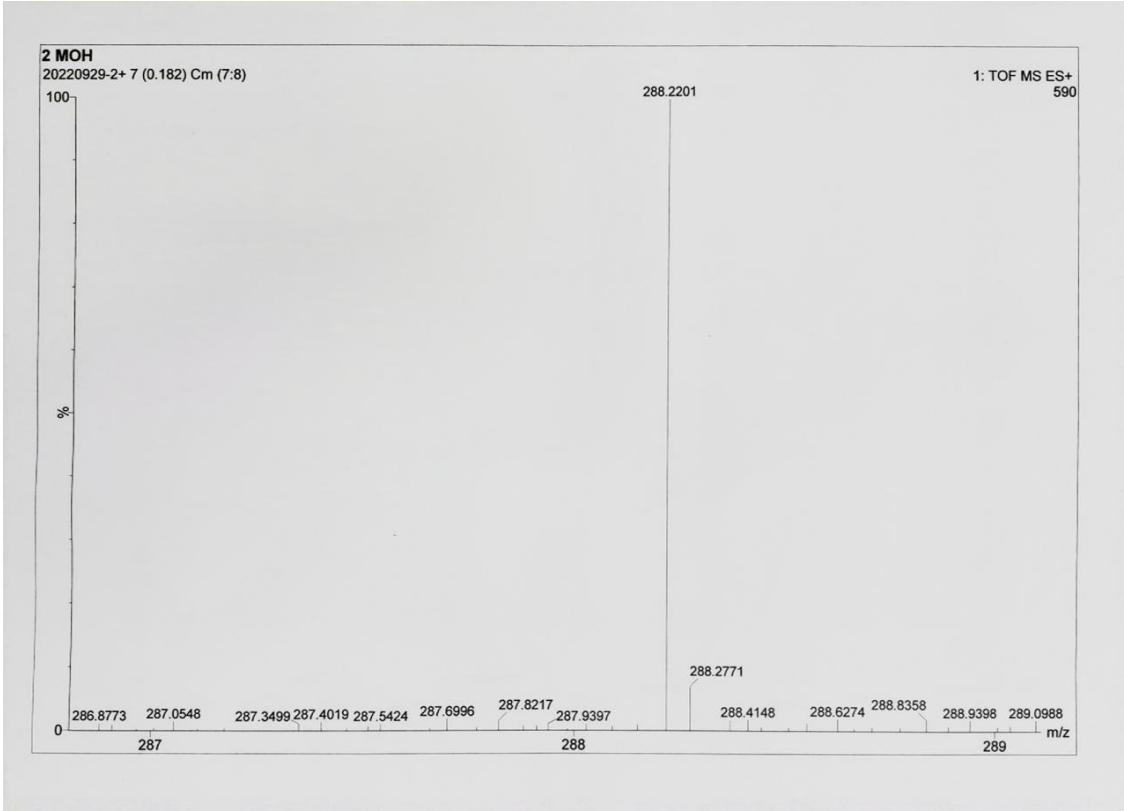


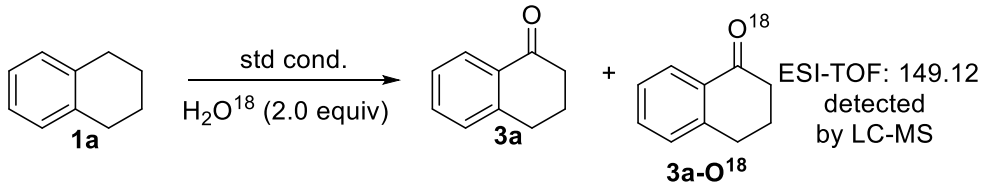
Figure 2. Color of oxidation reaction in methanol solution

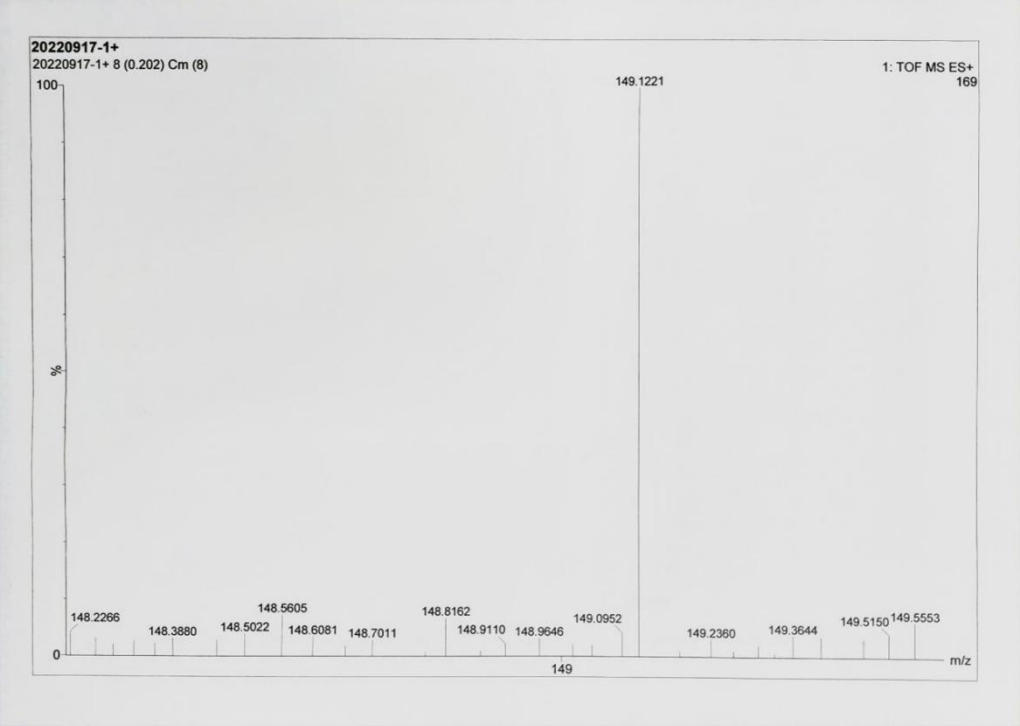
2.Mechanistic Studies



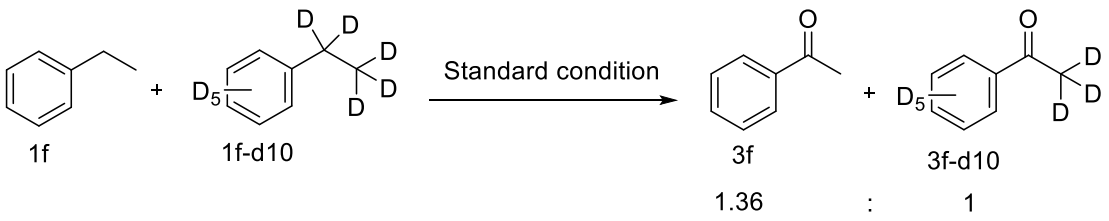


^{18}O-Labeling experiment for the oxidation of 1,2,3,4- Tetrahydronaphthalene

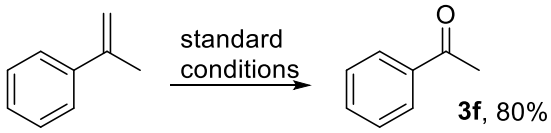




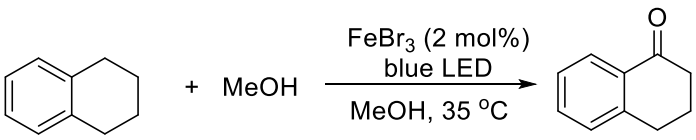
KIE study



Control experiment from styrene to ketone:



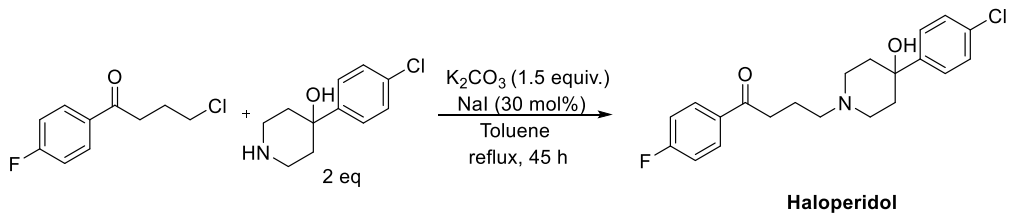
3. Synthetic procedure for photochemical carbonylation under iron catalysis



1,2,3,4-Tetrahydronaphthalene (0.8 mmol, 1.0 equiv.), $FeBr_3$ (0.02 equiv) and MeOH (2 mL) was added to an oven-dried glass tube equipped with magnetic stirring bar. The vessel placed in blue 5 W LED (450 nm). The reaction mixture was irradiated with for 12 h under air atmosphere. After irradiation, the reaction mixture was transferred to a 25 mL round-bottom flask and the solvent was concentrated in vacuo. The pure product was obtained by flash column chromatography on silica gel (petroleum ether/ethyl acetate 10%-20%).

4. Synthetic applications

[4-(4-Chlorophenyl)-4-hydroxy-1-piperidinyl]-1-(4-fluorophenyl)-1-butanone(haloperidol)

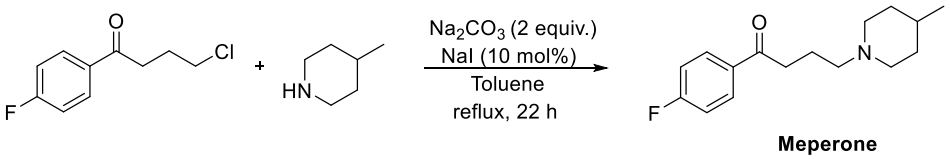


Haloperidol

To an 10 mL vial equipped with a stir bar was added alkyl chloride **1z** (0.2 mmol，1.0 equiv.), 4-(4-chlorophenyl)-4-hydroxypiperidine (0.4mmol,2.0 equiv.), and anhydrous potassium iodide (0.06 mmol, 0.03 equiv.). The vial was sealed after 2 mL of anhydrous toluene was added. The mixture was stirred at 130 ^oC for 45 h. After cooling to room temperature, the reaction mixture was diluted with aq. $NaHCO_3$ and EtOAc, and the aqueous layer was extracted with three portions of EtOAc. The combined organic layers were washed with brine, dried over Na_2SO_4, filtered, and concentrated. The residue was purified by flash chromatography (eluent: DCM/MeOH = 10/1 with 1% Et_3N) provided the title compound (56.13 mg, 78% yield) as a white solid[1]. ^1H NMR (400 MHz, $CDCl_3$) δ 8.01-7.97 (m, 2H), 7.38 (d, J = 8.0 Hz, 2H), 7.29 (d, J = 7.8 Hz, 2H), 7.18-7.08 (m, 2H), 3.02-2.94 (m, 2H), 2.84-2.75 (m, 2H), 2.51-2.46 (m, 2H), 2.45-2.36 (m, 2H), 1.96-2.05 (m, 4H), 1.68 (d, J = 13.2 Hz, 3H);$^{13}C\{^1H\}$ NMR (100 MHz, $CDCl_3$) δ 198.33, 146.81, 133.59 (d, J = 3.0 Hz), 132.73,

130.67 (d, *J* = 9.2 Hz), 128.36, 126.06, 115.72 (d, *J* = 21.65 Hz), 71.05, 57.80, 49.29, 38.29, 36.23, 21.78;^{19}F NMR (376 MHz, $CDCl_3$) δ -105.53.

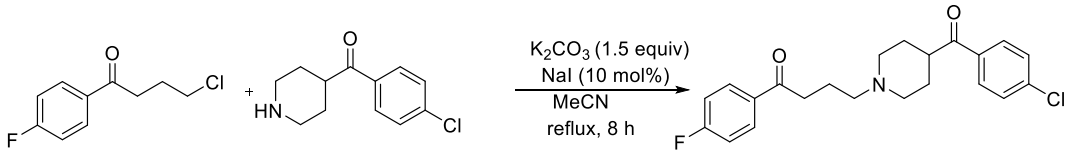
(4-Fluorophenyl)-4-(4-methylpiperidin-1-yl)butan-1-one (Melperone)



Meperone

To an 10 mL vial equipped with a stir bar was added alkyl chloride **1z** (0.2 mmol，1.0 equiv.), 4-methylpiperidine (0.4 mmol, 2 equiv.), Na_2CO_3 (0.4 mmol, 2.0 equiv.), and NaI (0.04 mmol, 0.1 equiv.). The vial was sealed after 2 mL of anhydrous toluene was added. The mixture was stirred at 120 ºC for 22 h. After cooling to room temperature,ransfer to a separatory funnel and dilute with aqueous saturated $NaHCO_3$ and EtOAc, and the aqueous layer was extracted with three portions of EtOAc. The combined organic layers were washed with brine, dried over Na_2SO_4, filtered, and concentrated. The residue was purified by flash chromatography (eluent: DCM/MeOH = 10/1 with 1% Et_3N) provided the title compound (43.65 mg, 83% yield) as a red solid[2].(43.65 mg, 83%) . ^{1}H NMR (400 MHz, $CDCl_3$)δ 7.90-8.01 (m, 2H), 7.02-7.12 (m, 2H), 2.87-2.96 (m, 2H), 2.81 (d, *J* = 9.9 Hz, 2H), 2.24-2.40 (m, 2H), 1.93-1.83 (m, 4H), 1.53 (d, *J* = 12.2 Hz, 2H), 1.27 (s, 1H), 1.06-1.17 (m, 2H), 0.81-0.87 (m, 3H);^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 198.46, 165.56 (d, *J* = 250.1 Hz), 133.54, 130.63 (d, *J* = 9.3 Hz), 115.58 (d, *J* = 21.63 Hz), 58.02, 53.85, 36.31, 34.16, 30.73, 21.85, 21.81 (d, *J* = 7.2 Hz).

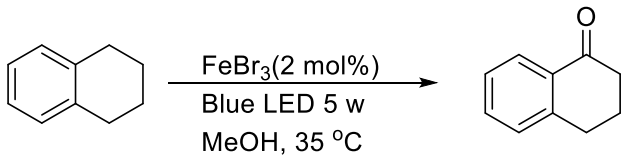
4-[4-(4-Fluorobenzoyl)-1-piperidinyl]-1-(4-fluorophenyl)-1-butan one(Lenperone)



The reaction of alkyl chloride **1z** (0.2 mmol, 1.0 equiv.), (4-chlorophenyl) (piperidin-4-yl)methanone (0.3 mmol, 1.5 equiv.), NaI (0.01 mmol, 0.1 equiv), and K_2CO_3 (0.3 mmol, 1.5 equiv.) in MeCN (5 mL).The reaction mixture was refluxe for 8

h.After completion of the reaction, the solvent was removed under reduced pressure and the residue was purified by flash column chromatography on silica gel to afford the desired product. (eluent: DCM/MeOH =10/1). Yelllow solid[3].(55.68 mg, 72%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.02-7.95 (m, 2H), 7.95-7.89 (m, 2H), 7.16-7.03 (m, 4H), 3.21-3.09 (m, 1H), 3.02-2.89 (m, 4H), 2.44-2.38 (m, 2H), 2.13-2.03 (m, 2H), 1.96-1.85(m, 2H), 1.86-1.67 (m, 4H);$^{13}C\{^{1}H\}$ NMR(100 MHz, $CDCl_3$) δ 201.03, 198.54, 165.48 (d, J = 250.3 Hz), 133.53 (d, J = 3.1 Hz), 132.38 (d, J = 2.7 Hz), 130.81 (d, J = 9.1 Hz), 130.64 (d, J = 9.2 Hz), 115.75 (d, J = 14.5 Hz), 115.53 (d, J = 14.5 Hz), 53.06, 43.62, 36.09, 28.61, 21.57.

5. Light on/off experiment



Entry	Time(h)	3a (yield%)	Entry	Time(h)	3a (yield%)
1	1	8	13	13	56
2	2	8	14	14	56
3	3	15	15	15	62
4	4	15	16	16	62
5	5	25	17	17	65
6	6	25	18	18	65
7	7	37	19	19	71
8	8	37	20	20	71
9	9	45	21	21	76
10	10	45	22	22	76
11	11	50	23	23	84
12	12	50	24	24	84

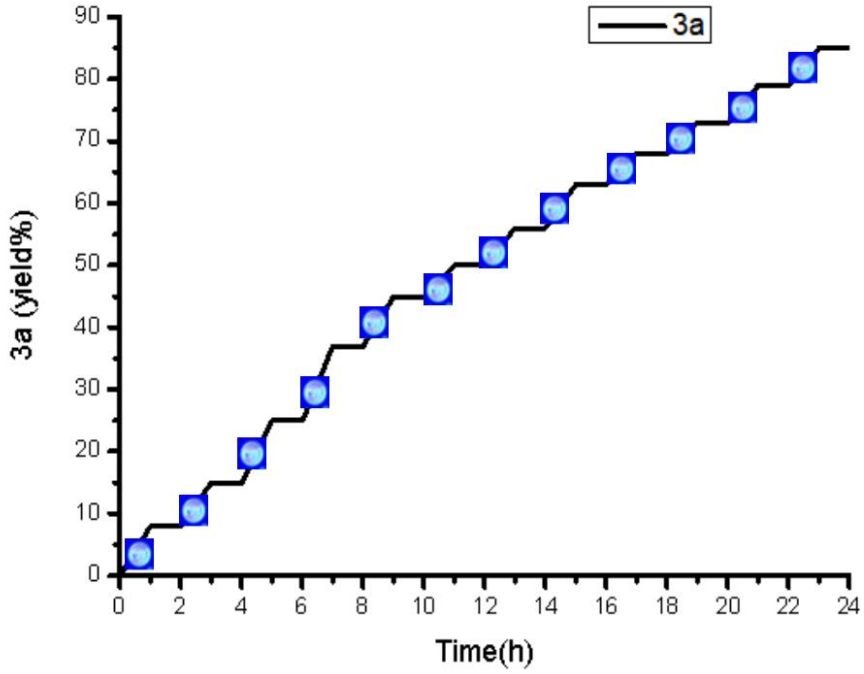


Figure 7. Light on/off experiment

6. UV/Vis absorption spectra

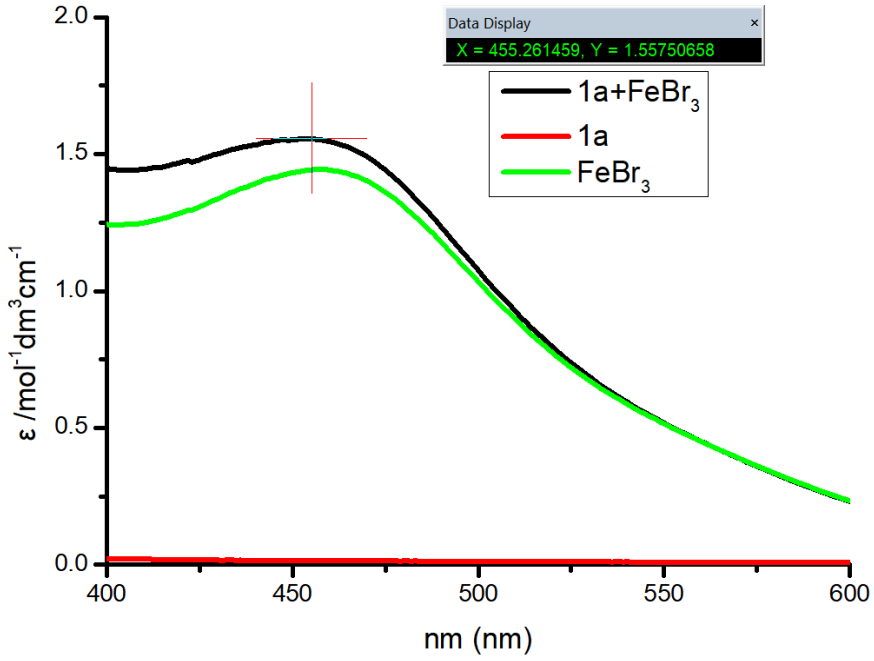
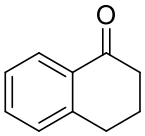
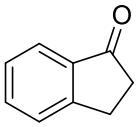


Figure 8. UV – Visible absorption spectra of $FeBr_3$ and **1a** in CH_3OH (under reaction).

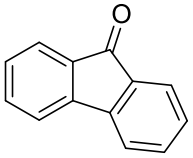
8.Characterization for all compounds



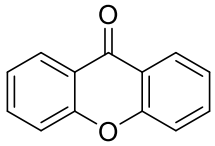
3,4-dihydronaphthalen-1(2H)-one **(3a):** The title compound was prepared according to the general procedure. Yellow liquid[4].(100.45 mg, 86%; eluent: 10%-20% ethyl acetate/ Petroleum ether);^{1}H NMR (400 MHz, $CDCl_3$) δ 7.94 (d, *J* = 7.7 Hz, 1H), 7.36 (t, *J* = 7.4Hz, 1H), 7.20 (t, *J* = 7.5 Hz, 1H), 7.15 (d, *J* = 7.4 Hz, 1H), 2.85 (t, *J* = 5.2 Hz, 2H), 2.54 (t, *J* = 6.1 Hz, 2H), 2.06-1.99 (q, 2H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 198.15, 144.43, 133.31, 132.49, 128.75, 126.98, 26.51, 39.08, 29.60, 23.23.



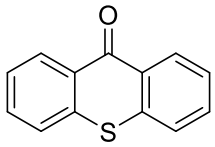
2,3-dihydro-1H-inden-1-one **(3b):** The title compound was prepared according to the general procedure. Colorless liquid[5].(98.17 mg, 93%; eluent: 10%-20% ethyl acetate/ Petroleum ether);^{1}H NMR (400 MHz, $CDCl_3$) δ 7.67 (d, *J* = 7.5 Hz, 1H), 7.51 (t, *J* = 7.3 Hz, 1H), 7.40 (d, *J* = 7.6 Hz, 1H), 7.29 (t, *J* = 7.3 Hz, 1H), 3.05 (t, *J* = 5.2 Hz, 2H), 2.60 (t, *J* = 5.8 Hz, 2H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 207.12, 155.18, 136.96, 134.59, 127.21, 126.69, 123.58, 36.17, 25.76.



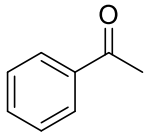
9H-fluoren-9-one **(3c):** The title compound was prepared according to the general procedure. yellow solid[4].(123.41 mg, 86%; eluent: 10%-20% ethyl acetate/ Petroleum ether);^{1}H NMR (400 MHz, $CDCl_3$) δ 7.63 (d, *J* = 7.2 Hz, 2H), 7.50-7.43 (m, 4H), 7.27 (t, *J* = 7.1 Hz, 2H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 193.83, 144.30, 134.63, 134.00, 128.98, 124.15, 120.27.



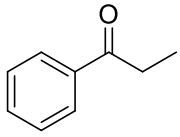
9-H-xanthen-9-one **(3d):** The title compound was prepared according to the general procedure. White solid[4].(130.21 mg, 83%; eluent: 10%-20% ethyl acetate/ Petroleum ether); ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.33 (d, *J* = 7.9 Hz, 1H), 7.71 (t, *J* = 7.3 Hz, 1H), 7.47 (d, *J* = 8.4 Hz, 1H), 7.37 (t, *J* = 7.63 Hz, 1H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 177.22, 156.14, 134.81, 126.70, 123.89, 121.81, 117.96.



9H-thioxanthen-9-one **(3e):** The title compound was prepared according to the general procedure. Yellow solid[4].(143.10 mg, 85%; eluent: 10%-20% ethyl acet ae/Petroleum ether); ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.60 (d, *J* = 8.0 Hz, 2H), 7.67-7.52 (m, 4H), 7.50-7.41 (m, 2H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 17 9.95, 137.26, 132.24, 129.84, 129.20, 126.28, 125.96.

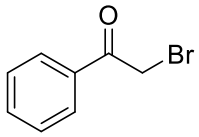


Acetophenone **(3f):** The title compound was prepared according to the general procedure. Colorless liquid[6].(80.51 mg, 84%; eluent: 10%-20% ethyl acetate/ Petroleum ether); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.95 (d, *J* = 7.4 Hz, 2H), 7.56 (t, *J* = 7.3 Hz, 1H), 7.46 (t, *J* = 7.5 Hz, 2H), 2.60 (s, 3H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 198.18, 137.07, 133.10, 128.56, 128.29, 26.63.

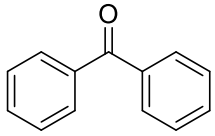


Propiophenone **(3g):** The title compound was prepared according to the general procedure. Colorless liquid[6].(65.32 mg, 61%; eluent: 10%-20% ethyl acetate/ Petroleum ether); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.97 (d, *J* = 7.4 Hz, 2H), 7.55 (t, *J* = 7.1 Hz, 1H), 7.46 (t, *J* = 7.4 Hz, 2H), 3.01 (q, *J* = 7.2 Hz, 2H), 1.23 (t, *J* = 7.2 Hz, 3H);

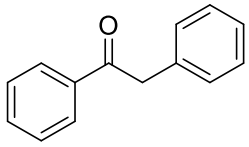
$^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$) δ 200.84, 136.87, 132.87, 128.54, 127.96, 31.78, 8.24.



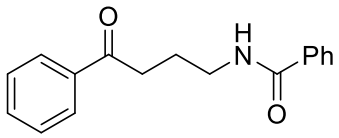
2-bromo-1-phenylethan-1-one **(3h):** The title compound was prepared according to the general procedure. Yellow liquid[4].(85.47 mg, 54%; eluent: 10%-20% ethyl acetate/ Petroleum ether); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.96 (d, *J* = 7.3 Hz, 2H), 7.58 (t, *J* = 6.6 Hz, 1H), 7.47 (t, *J* = 7.4 Hz, 2H), 4.44 (s, 3H); $^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$) δ 191.26, 133.95, 130.18, 128.89, 128.86, 128.48, 31.10.



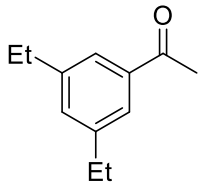
Benzophenone **(3i)**: The title compound was prepared according to the general procedure. Yellow solid[4].(123.42 mg, 85%; eluent: 10%-20% ethyl acetate/ Petroleum ether); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.79 (d, *J* = 7.2 Hz, 4H), 7.55 (t, *J* = 7.3 Hz, 2H), 7.45 (t, *J* = 7.3 Hz, 4H); $^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$) δ 196.65, 137.56, 132.43, 130.03, 128.29.



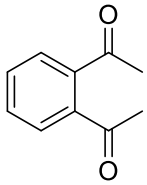
1,2-Diphenylethan-1-one **(3j):** The title compound was prepared according to the general procedure. White solid[4].(81.75 mg, 52%; eluent: 10%-20% ethyl acetate/ Petroleum ether); ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.03 (d, *J* = 7.3 Hz, 2H), 7.62- 7.53 (m, 1H), 7.47 (t, *J* = 6.9 Hz, 2H), 7.38-7.31 (m, 2H), 7.29 (m, 3H), 4.30 (s, 2H);$^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$) δ 197.63, 136.57, 134.53, 133.18, 129.47, 128.68, 128.65, 128.61, 126.89, 45.51.



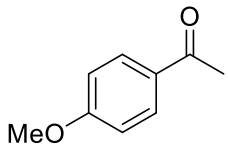
N-(4-Oxo-4-phenylbutyl)benzamide **(3k):** The title compound was prepared according to the general procedure.White solid[7].(91.89 mg, 43%; eluent: 10%-20% ethyl acetate/ Petroleum ether); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.92 (t, *J* = 3.2 Hz, 2H), 7.78 (t, *J* = 6.7 Hz, 2H), 7.56-7.46 (m, 1H), 7.47-7.41 (m, 2H),7.41-7.39(m, 2H),7.32- 7.38 (m, 2H), 7.01 (s, 1H), 3.57-3.46 (m, 2H), 3.14-3.04 (m,, 2H), 2.12-2.00 (m, 2H); ^{13}C{^{1}H} (100 MHz, $CDCl_3$) δ 200.47, 167.65, 136.59, 134.42, 133.29, 132.00, 131.34, 128.62，128.56, 128.48 , 128.05, 127.38, 126.89, 39.95, 36.33, 23.48.



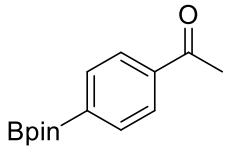
1-(3,5-Diethylphenyl)ethan-1-one **(3l):** The title compound was prepared according to the general procedure. Yellow liquid[6].(87.12 mg, 62%; eluent: 10%-20% ethyl acetate/ Petroleum ether); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.58 (s, 2H), 7.19 (s, 1H), 2.62 (q, *J* = 7.4 Hz, 4H), 2.52 (s, 3H), 1.21 (t, *J* = 7.6 Hz, 6H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 198.25, 144.55, 137.36, 132.37, 125.18, 28.70, 26.58, 15.54.



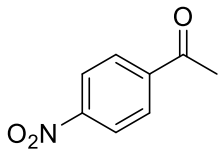
1,1'-(1,2-Phenylene)bis[ethanone] **(3m):** The title compound was prepared according to the general procedure. Yellow liquid[8].(58.01 mg, 45%; eluent: 10%-20% ethyl acetate/ Petroleum ether); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.53 (s, 4H), 2.51 (d, *J* = 2.7 Hz, 6H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 201.84, 139.43, 131.10, 127.76, 28.75.



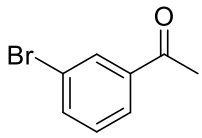
1-(4-methoxyphenyl-1-one) **(3n):** The title compound was prepared according to the general procedure. Yellow liquid[4].(106.45 mg, 89%; eluent: 10%-20% ethyl acetate/ Petroleum ether); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.92 (d, *J* = 8.8 Hz, 2H), 6.92 (d, *J* = 8.7 Hz, 2H), 3.85 (s, 3H), 2.54 (s, 3H); $^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$) δ 196.82, 163.45, 130.57, 130.26, 113.65, 55.44, 26.34.



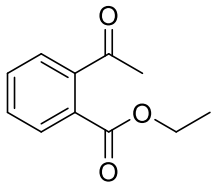
[4-(tetraMethyl-1,3,2-dioxaborlan-2-yl)phenyl]ethan-1-one **(3o):** The title compound was prepared according to the general procedure. White solid [4].(107.95 mg, 54%; eluent: 10%-20% ethyl acetate/ Petroleum ether); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.89 (d, 4H), 2.60 (s, 3H), 1.34 (s, 12H); $^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$) δ 198.46, 138.91, 134.89, 127.25, 84.18, 26.75, 24.85.



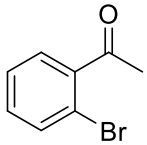
1-(4-nitrophenyl)ethan-1-one **(3p):** The title compound was prepared according to the general procedure. Yellow solid[4].(72.58 mg, 53%; eluent: 10%-20% ethyl acetate/ Petroleum ether); ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.21 (s,2H), 8.06 (s, 2H), 2.62 (s, 3H); $^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$) δ 196.42, 150.20, 141.31, 129.29, 123.75, 26.94.



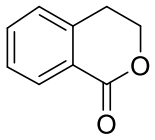
(3-Bromophenyl)ethan-1-one **(3q):** The title compound was prepared according to the general procedure. White solid[8].(133.10 mg, 84%; eluent: 10%-20% ethyl acetate/ Petroleum ether); ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.08 (s, 1H), 7.87 (d, *J* = 7.6 Hz, 1H), 7.68 (d, *J* = 7.9 Hz, 1H), 7.34 (t, *J* = 7.9 Hz, 1H), 2.59 (s, 3H); $^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$) δ 196.68, 138.74, 135.96, 131.36, 130.19, 126.84, 122.93, 26.65.



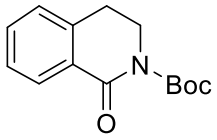
2-Acetyl-benzoic acid ethyl ester **(3r):** The title compound was prepared according to the general procedure. yellow liquid[9].(139.45 mg, 91%; eluent: 10%-20% ethyl acetate/ Petroleum ether); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.80 (d, *J* = 7.5 Hz, 1H), 7.51 -7.48 (m, 1H), 7.45-7.41(m,1H),7.37 (t, *J* = 7.36 Hz, 1H), 4.30 (q, *J* = 7.1 Hz, 2H), 2.49 (s, 3H), 1.31 (t, *J* = 7.1 Hz, 3H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 166.90, 142.66, 131.91, 129.95, 129.62, 129.00, 126.33, 61.62, 30.07, 13.96.



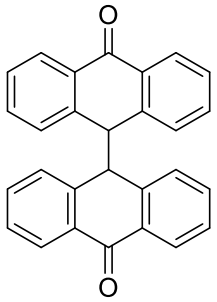
(2-Bromophenyl)ethan-1-one **(3s):** The title compound was prepared according to the general procedure. Yellow liquid[6].(55.11 mg, 35%; eluent: 10%-20% ethyl acetate/ Petroleum ether); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.58 (d, *J* = 7.9 Hz, 1H), 7.44 (d, *J* = 7.5 Hz, 1H), 7.34 (t, *J* = 7.5 Hz, 1H), 7.27 (t, *J* = 7.6 Hz, 1H), 2.60 (s, 3H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 201.36, 141.36, 133.82, 131.81, 128.91, 127.45, 118.86, 30.33.



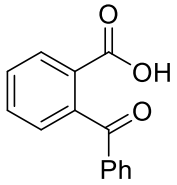
Isochroman-1-one **(3t):** The title compound was prepared according to the general procedure. Yellow liquid[4].(61.45 mg, 52%; eluent: 10%-20% ethyl acetate/ Petroleum ether); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.96 (d, *J* = 7.6 Hz, 1H), 7.44 (t, *J* = 7.3 Hz, 1H), 7.28 (t, *J* = 7.5 Hz, 1H), 7.18 (d, *J* = 7.4 Hz, 1H), 4.42 (t, *J* = 5.8 Hz, 2H), 2.96 (t, *J* = 5.7 Hz, 2H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 165.12, 139.62, 133.67, 130.11, 127.55, 127.32, 125.13, 67.33, 27.68.



tert-Butyl1-oxo-3,4-dihydroisoquinoline-2(1H)-carboxylate **(3u):** The title compound was prepared according to the general procedure. Colorless liquid[10].(65.24 mg, 33%; eluent: 10%-20% ethyl acetate/ Petroleum ether); ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.15 (d, *J* = 7.5 Hz, 1H), 7.45 (t, *J* = 7.0 Hz, 1H), 7.34 (t, *J* = 7.5 Hz, 1H), 7.20 (d, *J* = 7.4 Hz, 1H), 3.98 (t, *J* = 5.1 Hz, 2H), 2.99 (t, *J* = 5.1 Hz, 2H), 1.57 (s, 9H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 163.98, 153.12, 139.52, 132.84, 129.60, 127.20, 127.14, 83.22, 44.43, 28.31, 28.09.

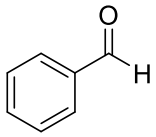


10,10'-Dianthronyl **(3v):** The title compound was prepared according to the general procedure. White solid[11].(160.51 mg, 52%; eluent: 10%-20% ethyl acetate/ Petroleum ether); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.92 (s, 4H), 7.41 (s, 8H), 6.85 (s, 4H), 4.76 (s, 2H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 183.00, 139.83, 133.72, 132.16, 128.47 , 127.90, 126.60, 54.31.

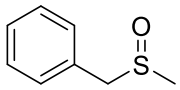


2-Benzoquinonecarboxylic acid **(3w):** The title compound was prepared according to the general procedure. White solid[9] .(125.9 mg, 70%; eluent: 10%-20% ethyl acetate/ Petroleum ether); ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.60 (s, 1H), 8.01 (t, *J* = 11.8 Hz, 1H), 7.68 (d, *J* = 7.2 Hz, 2H), 7.62 (t, *J* = 7.2 Hz, 1H), 7.51 (dd, *J* = 14.7, 7.1 Hz, 2H),

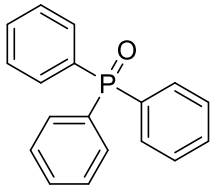
7.35(m, 3H); $^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$) δ 197.14, 170.81, 142.50, 136.93, 133.20, 130.82, 129.55, 129.37, 128.44, 127.94, 127.60.



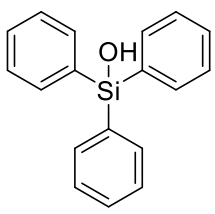
Benzaldehyde **(8):** The title compound was prepared according to the general procedure. colorless liquid[12].(27.20 mg, 32%; eluent: 10%-20% ethyl acetate/ Petroleum ether); ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.99 (s, 1H), 7.86 (d, *J* = 7.0 Hz, 2H), 7.60 (t, *J* = 7.4 Hz, 1H), 7.50 (t, *J* = 7.4 Hz, 2H); $^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$) δ 192.43, 136.33, 134.46, 129.72, 128.97.



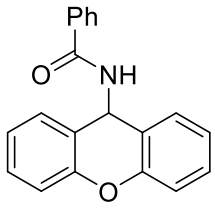
Benzyl methyl sulfoxide **(10):** The title compound was prepared according to the general procedure. White solid[13].(55.43 mg, 45%; eluent: 20%-30% ethyl acetate/ Petroleum ether); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.30 (m, 3H), 7.23 (d, *J* = 7.1 Hz, 2H), 3.99 (d, *J* = 12.8 Hz, 1H), 3.88 (d, *J* = 12.8 Hz, 1H), 2.40 (s, 3H); $^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$) δ 130.02 , 129.62, 128.93, 128.40, 60.09, 37.18.



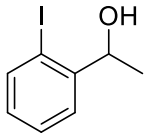
Triphenylphosphine oxide **(11):** The title compound was prepared according to the general procedure. White solid [4].(137.85 mg, 62%; eluent: 10%-20% ethyl acetate/ Petroleum ether); ^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.53-7.7.59 (m, 6H), 7.35- 7..41(m, 3H), 7.28-7.34 (m, 6H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 132.95, 131.99, 131.89, 131.87, 128.49, 128.37.



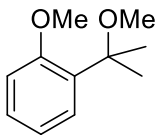
Triphenylsilanol **(13):** The title compound was prepared according to the general procedure. White solid[4].(150.31 mg, 54%; eluent: 10%-20% ethyl acetate/ Petroleum ether); ^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.65 (d, *J* = 6.7 Hz, 6H), 7.50-7.43 (m, 3H), 7.35-7.41 (m, 6H), 2.98 (s, 1H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 135.06, 130.14, 127.94.



N-9H-Xanthen-9-ylbenzamide **(16):** The title compound was prepared according to the general procedure. White solid[14].(45.56 mg, 19%; eluent: 10%-20% ethyl acetate/ Petroleum ether); ^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.75 (d, *J* = 7.2 Hz, 2H), 7.52 (d, *J* = 7.3 Hz, 2H), 7.45 (dd, *J* = 15.5, 8.4 Hz, 1H), 7.38 (t, *J* = 7.3 Hz, 2H), 7.29 (t, *J* = 7.3 Hz, 2H), 7.10 (t, *J* = 9.4 Hz, 4H), 6.71 (d, *J* = 8.5 Hz, 2H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 166.49, 151.05, 133.90, 131.75, 129.67, 129.31, 128.58, 127.06, 123.60, 121.00, 116.64, 44.18.



1-(2-Iodophenyl)ethanol **(17):** The title compound was prepared according to the general procedure. Yellow liquid[15].(39.70 mg, 20%; eluent: 10%-20% ethyl acetate/ Petroleum ether); ^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.78 (d, *J* = 7.8 Hz, 1H), 7.53 (d, *J* = 7.6 Hz, 1H), 7.36 (t, *J* = 7.4 Hz, 1H), 6.95 (t, *J* = 7.5 Hz, 1H), 5.00-5.06 (m, 1H), 2.43 (s, 1H), 1.43 (d, *J* = 6.2 Hz, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 147.46, 139.28, 129.13, 128.73, 126.33, 97.21, 73.69, 23.75.



1-Methoxy-2-(1-methoxy-1-methylethyl)benzene **(18):** The title compound was prepared according to the general procedure. Yellow liquid.(11.52 mg, 8%; eluent: 10%-20% ethyl acetate/ Petroleum ether); ^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.42 (d, *J* =

7.6 Hz, 1H), 7.24 (t, *J* = 7.6 Hz, 1H), 6.96 (d, *J* = 7.3 Hz, 1H), 6.91 (d, *J* = 8.3 Hz, 1H), 3.83 (s, 3H), 3.20 (s, 3H), 1.60 (s, 6H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 157.39, 133.32, 128.12, 127.41, 120.30, 111.62, 77.02, 55.22, 50.56, 26.57.

8. Calculation details and optimized geometry of transition state TS_{AB}

All DFT calculations included in the H-bond-assisted hydrogen atom abstraction is conducted under the tight criteria using (U)B3LYP/6-31G(d,p) in Gaussian 09 program[16]. The quintet state is carried out using unrestricted methods. The transition state **TS_{AB}** and intermediates **A** and **B** are confirmed with one or zero imaginary frequency, respectively.

TS_{AB}

Fe	-0.055949	0.123201	-0.108376
O	0.052617	1.391349	-1.692216
O	0.471321	2.583179	-1.314992
C	1.505539	1.800994	1.873063
H	1.713266	2.863353	2.031006
H	1.103250	1.379639	2.798229
H	2.432967	1.279642	1.611948
O	0.529042	1.666436	0.837714
H	0.616537	2.368195	-0.175572
Br	-2.236585	-0.471920	0.220025
Br	1.611773	-1.443158	-0.143747

9.References

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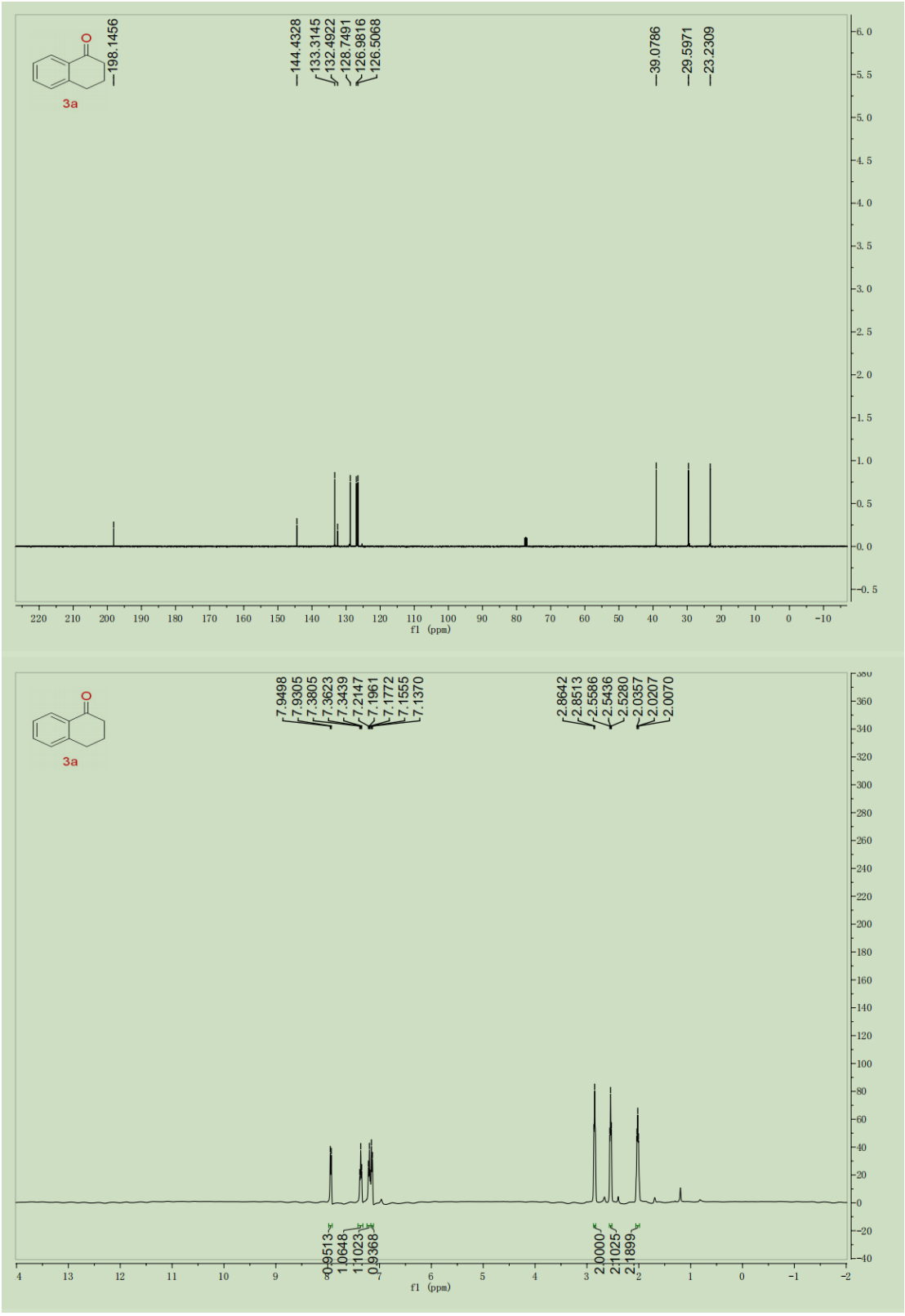
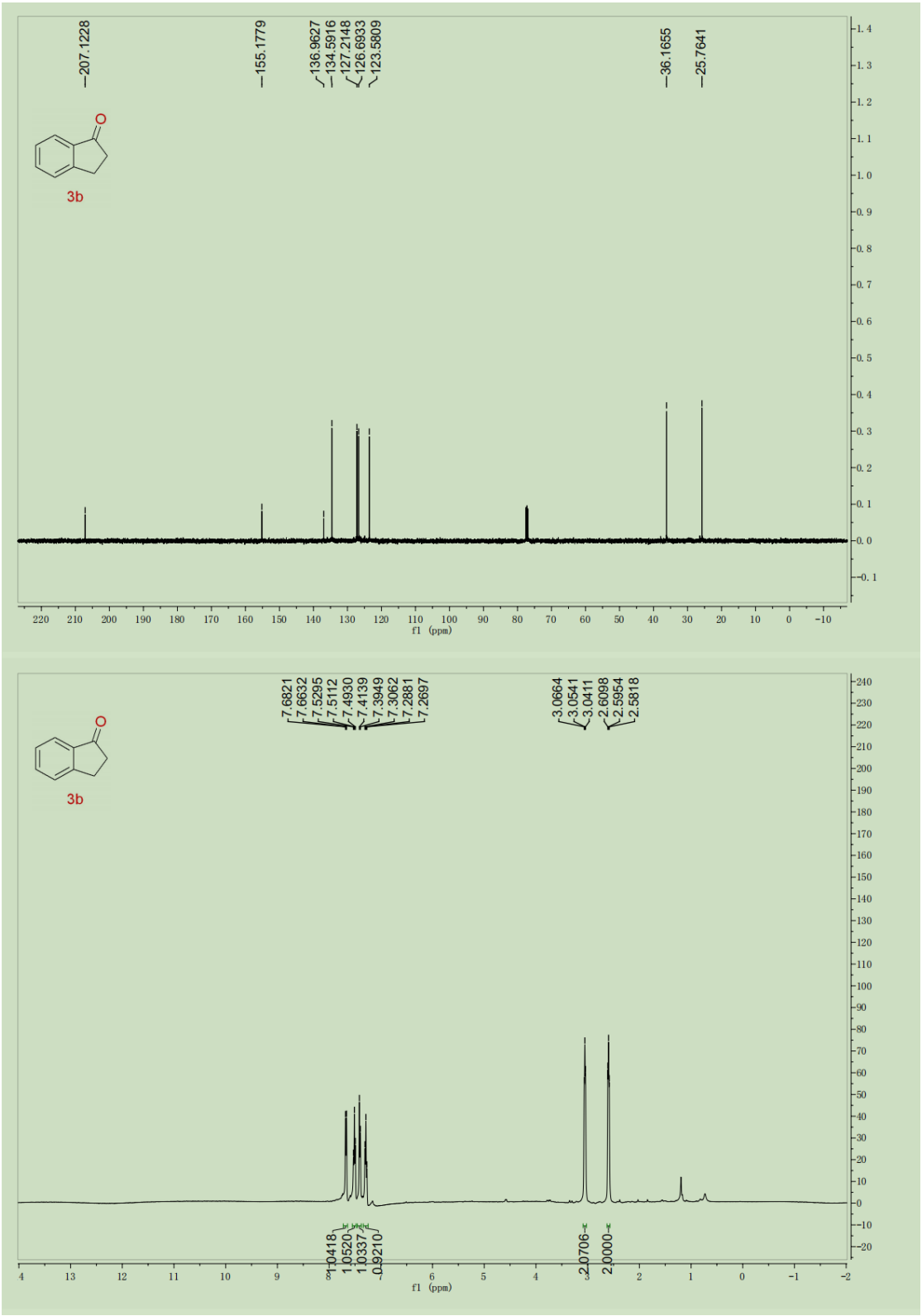
[16]M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery Jr., J. E. Peralta, F. o. Ogliaro, M. J. Bearpark, J. Heyd, E. N. Brothers, K. N. Kudin, V. N. Staroverov, R. Kobayashi, J. Normand, K. Raghavachari, A. P. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, N. J. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, d. n. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski and D. J. Fox, *Gaussian 09*, Gaussian, Inc., Wallingford, CT, USA, **2009**.

10.Copies of ^{1}H and ^{13}C NMR spectra of products

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3b
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7.2697
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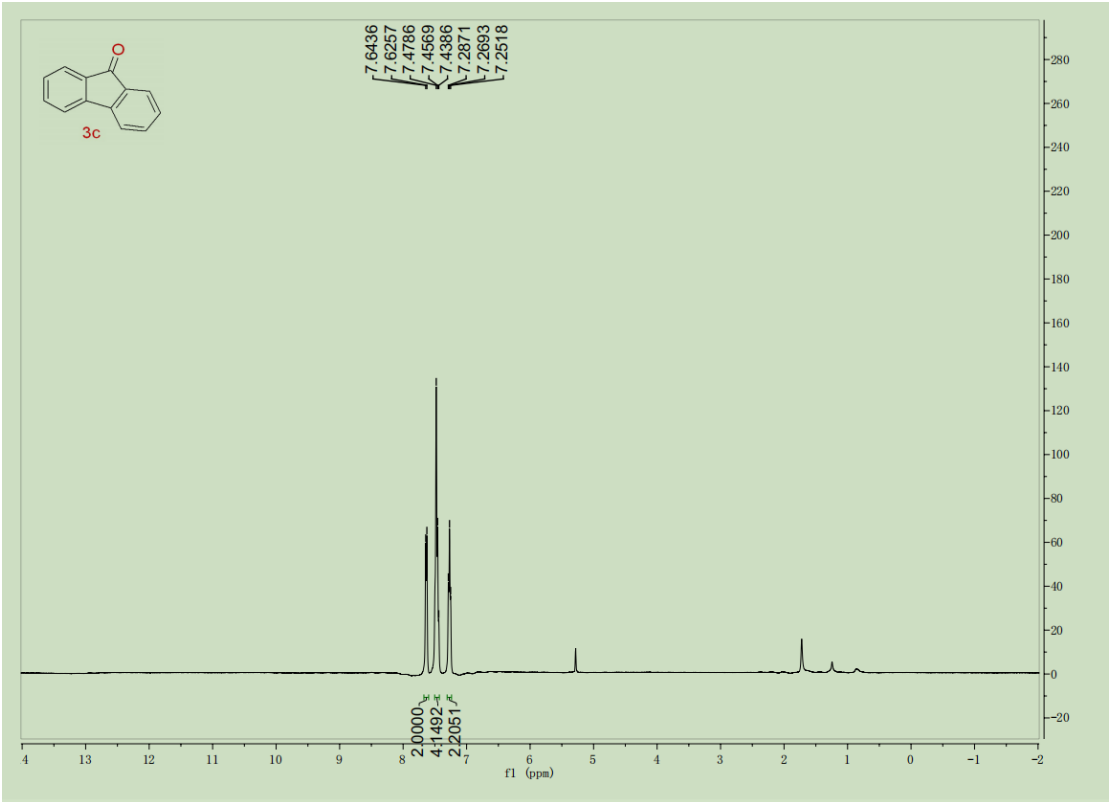
3b
f1 (ppm)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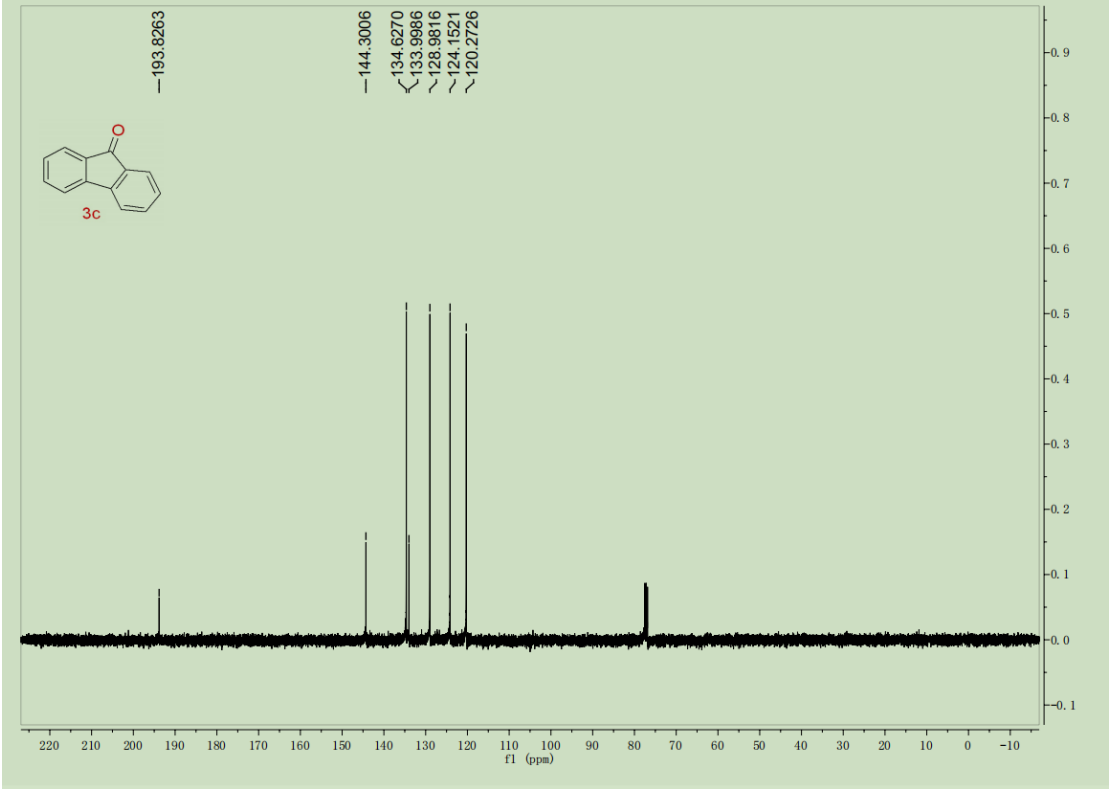
2.0000
4.1492
2.2051
f1 (ppm)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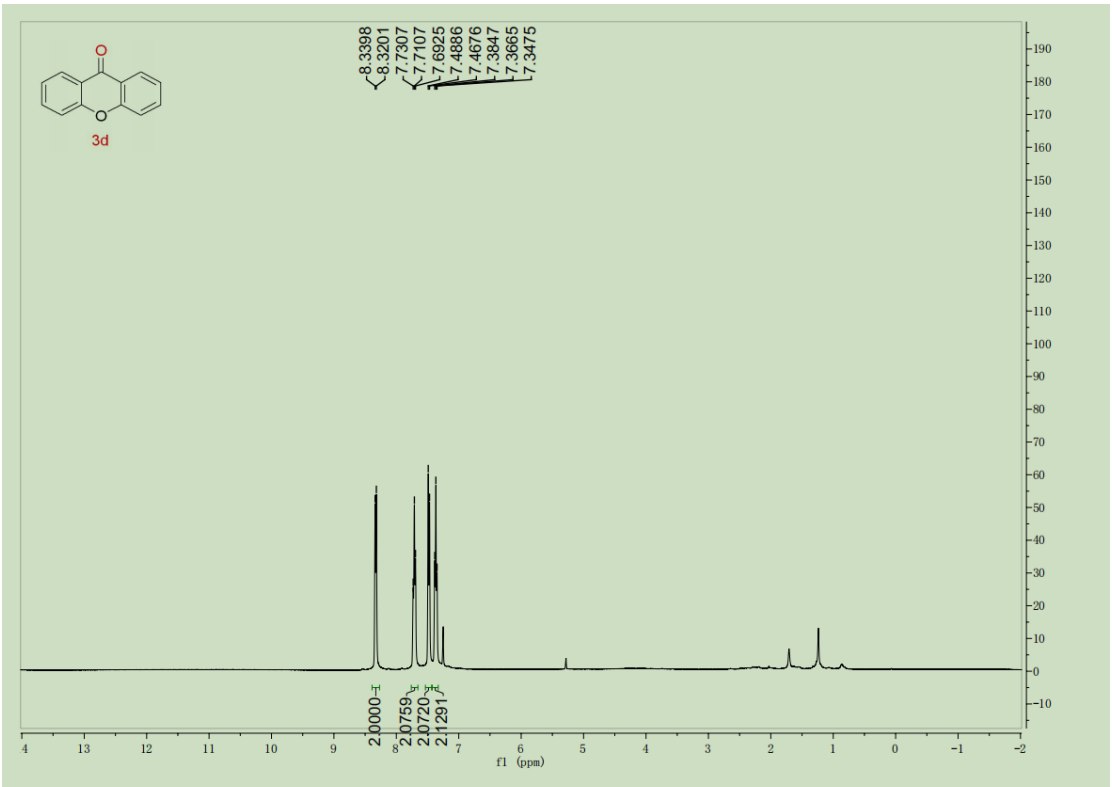
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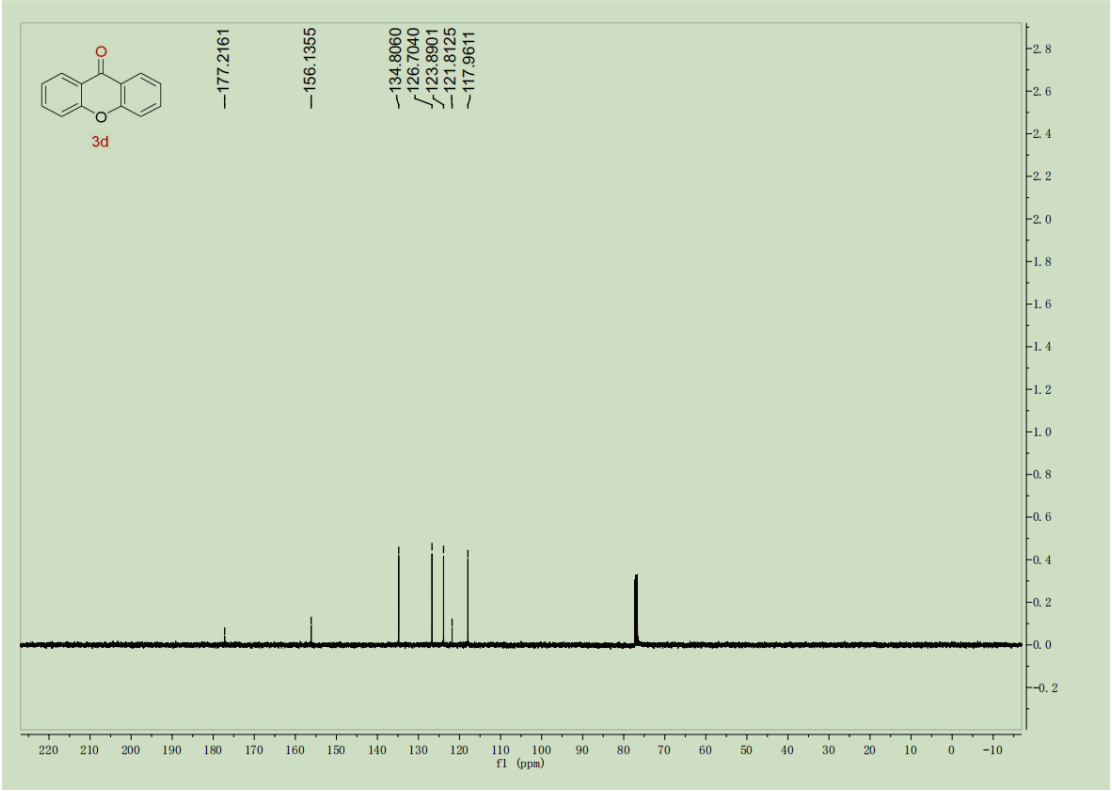
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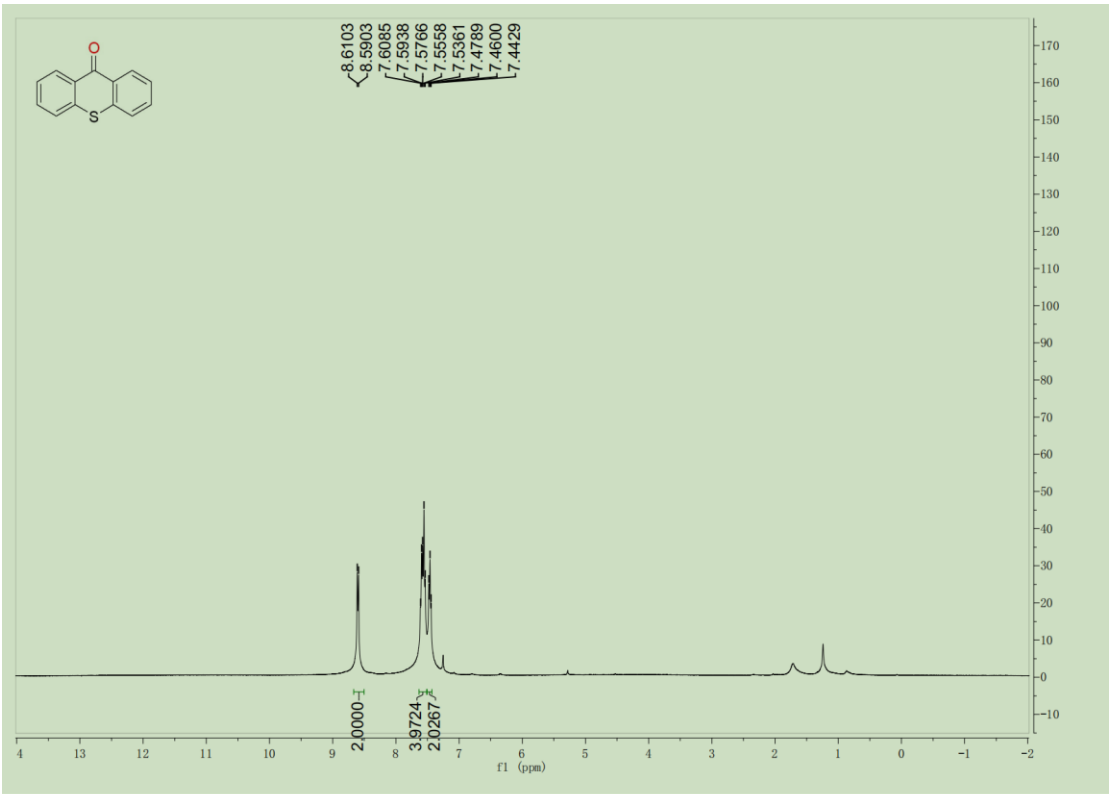
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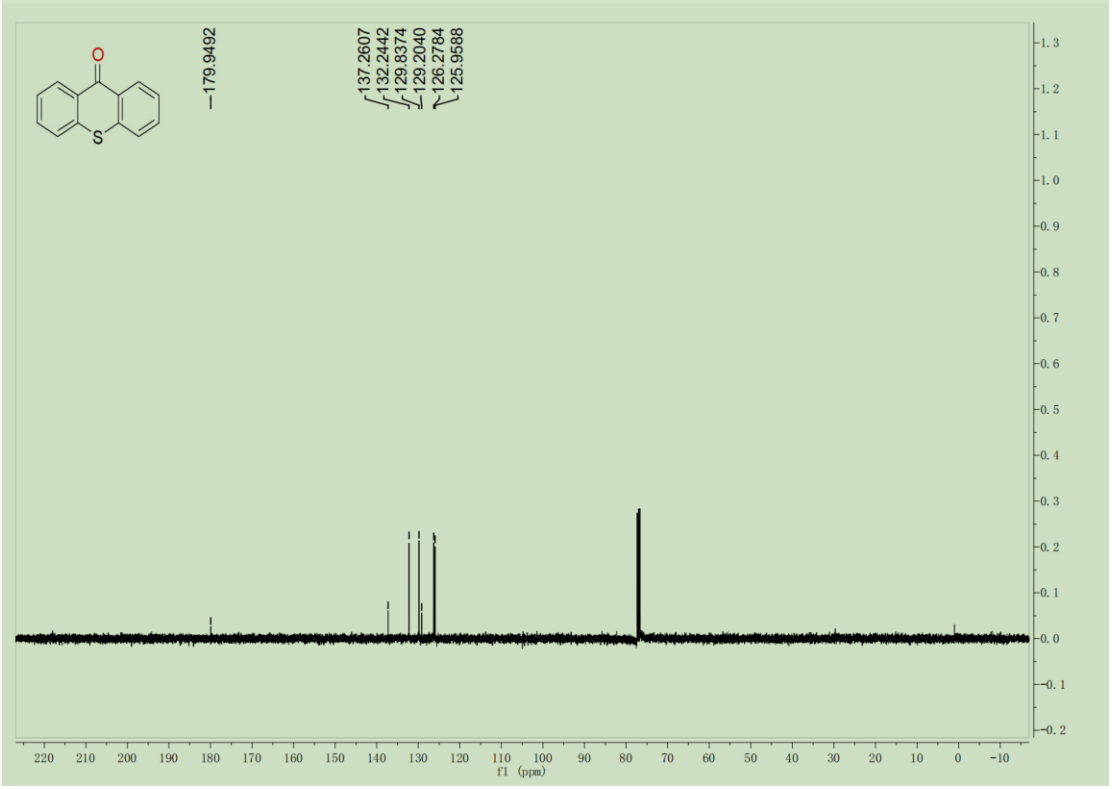
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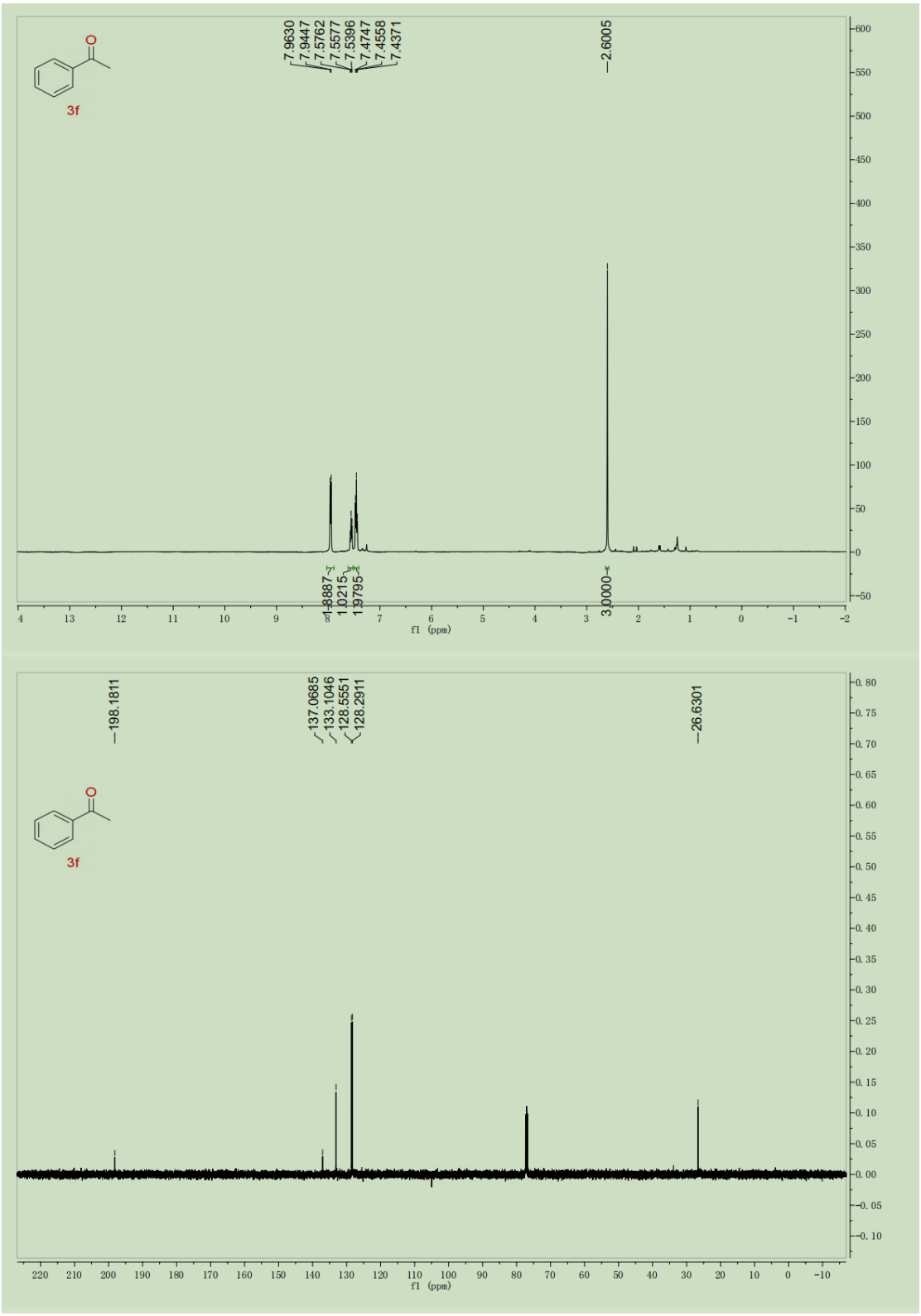
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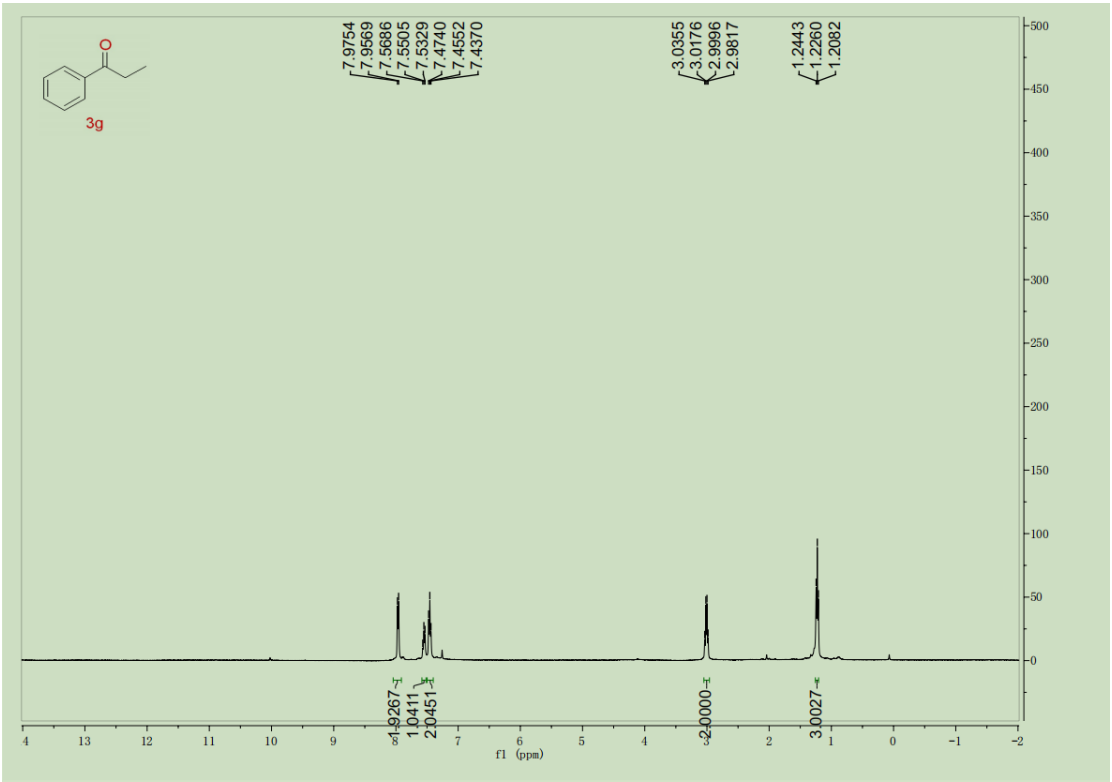
f1 (ppm)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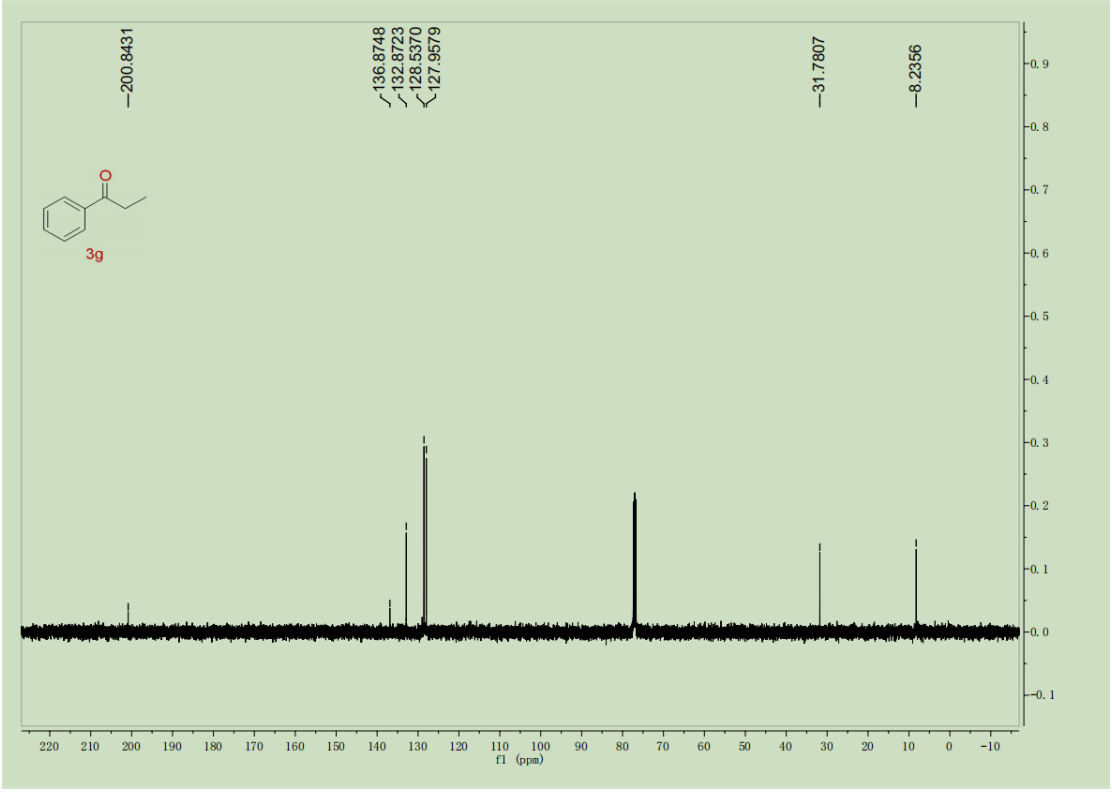
f1 (ppm)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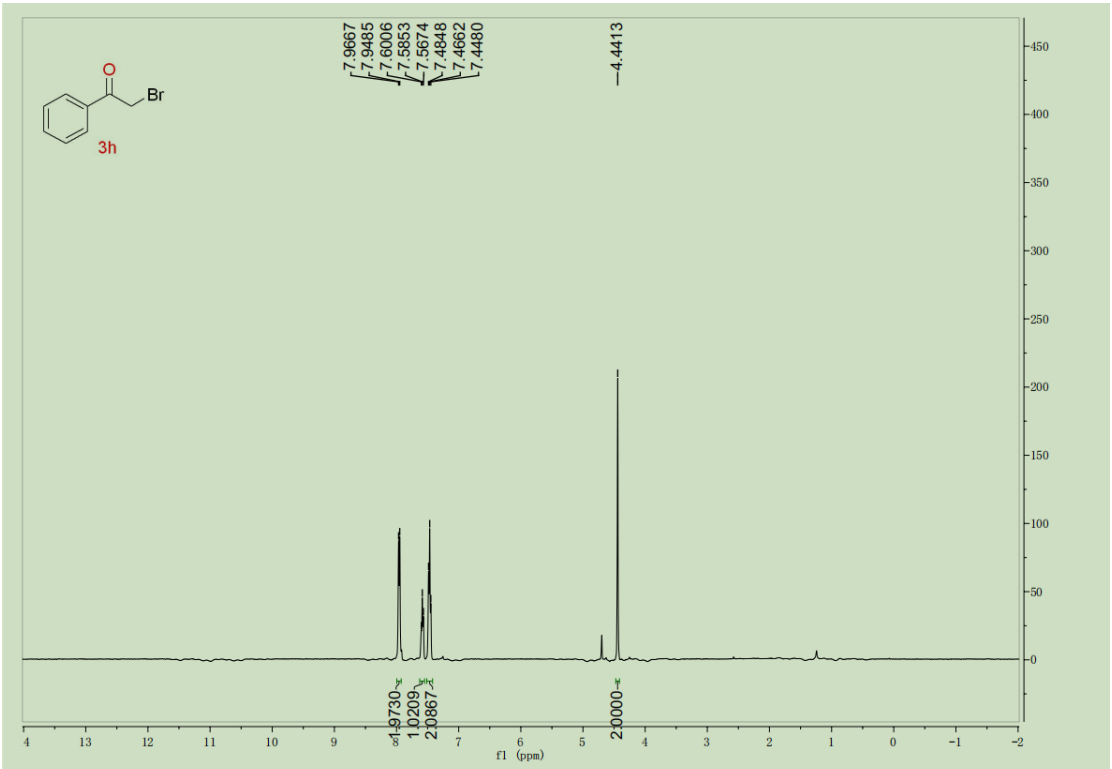
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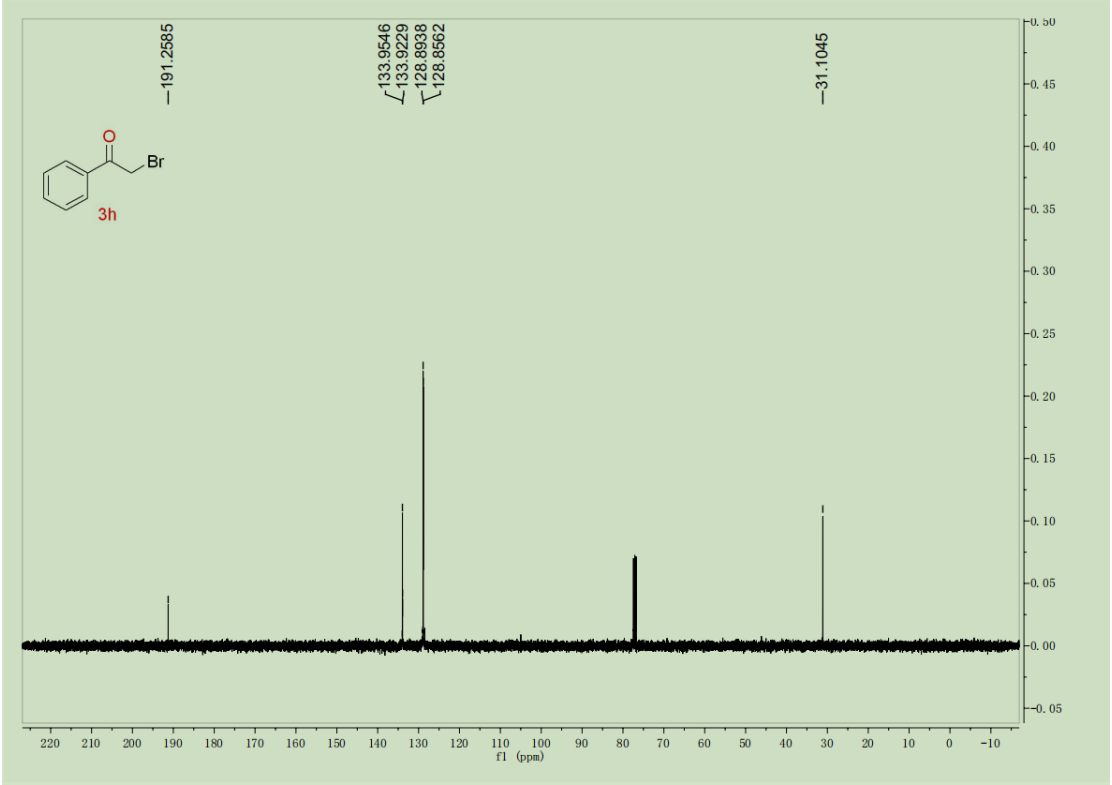
f1 (ppm)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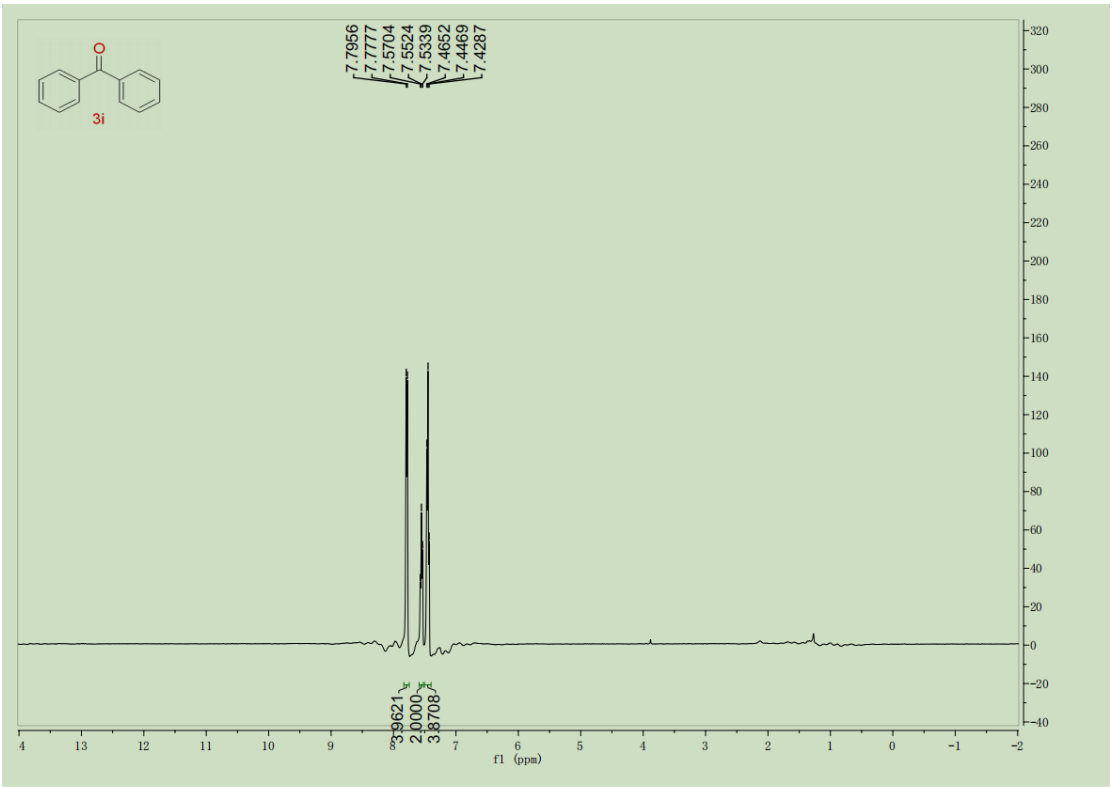
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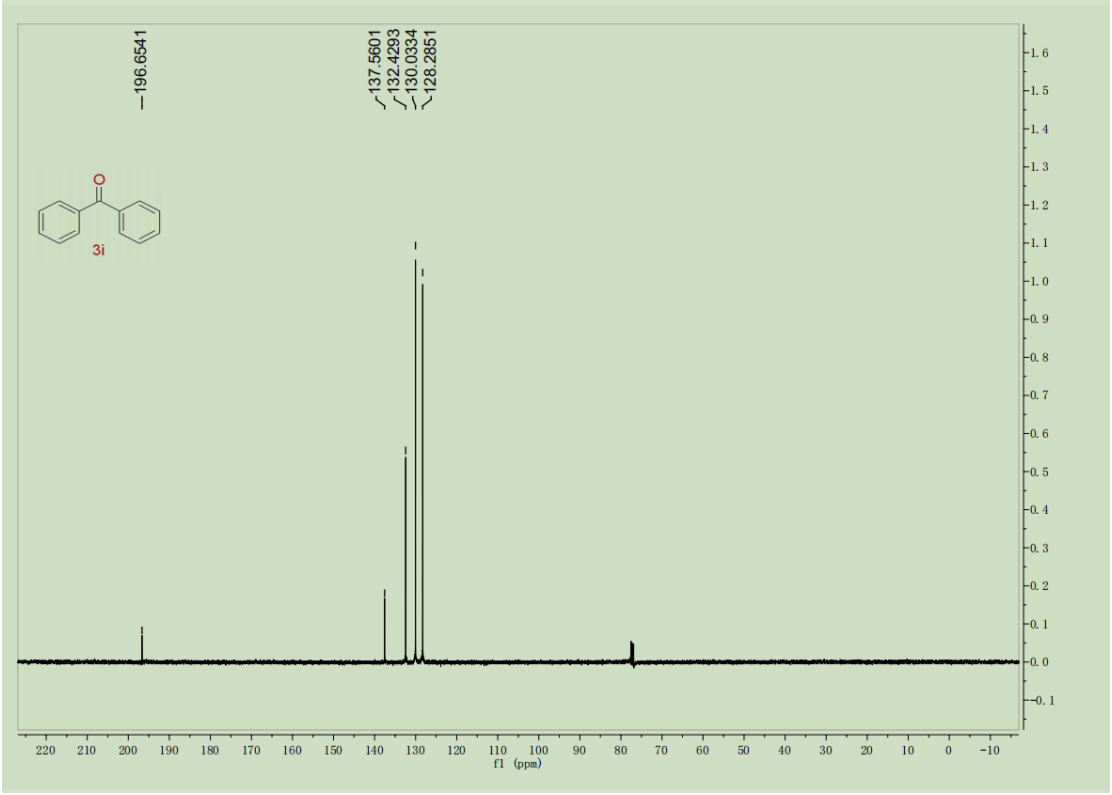
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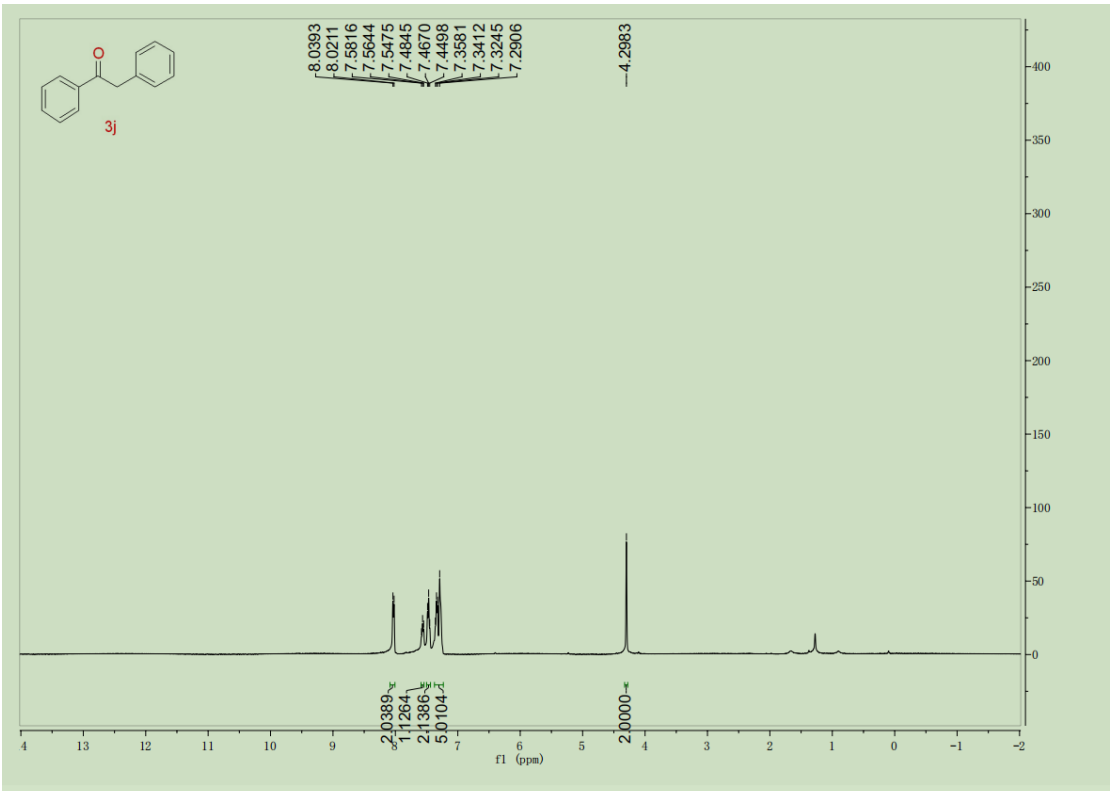
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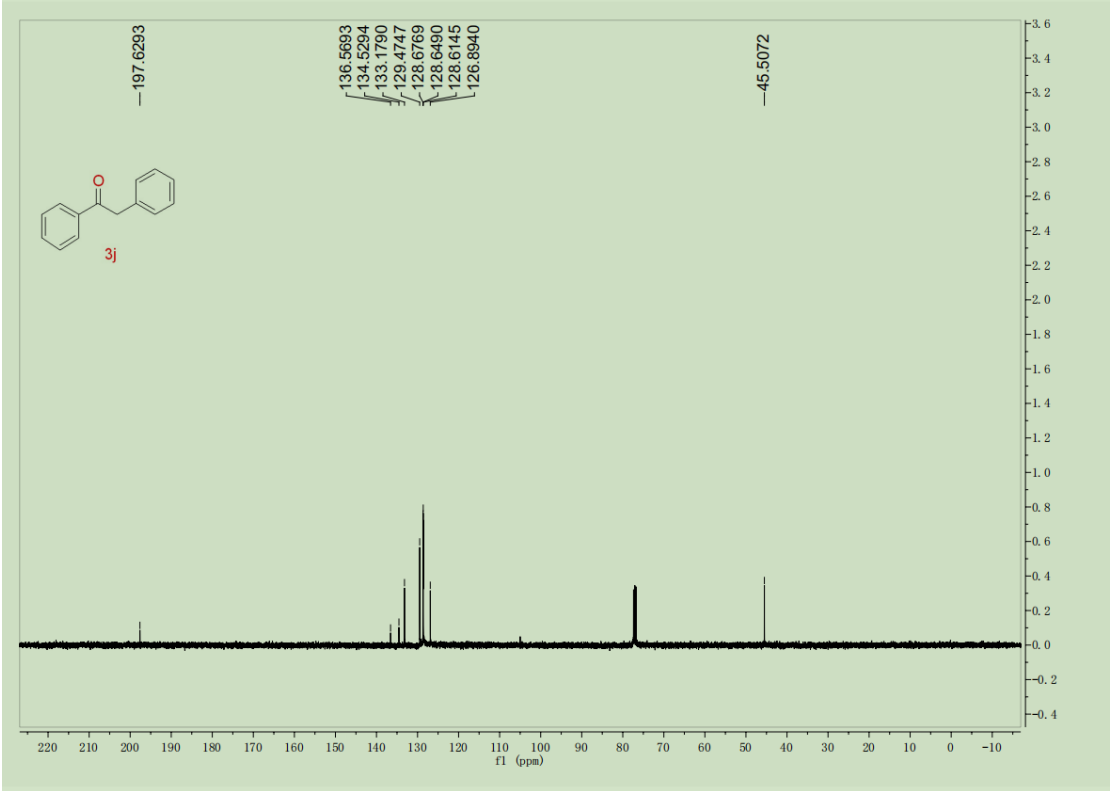
f1 (ppm)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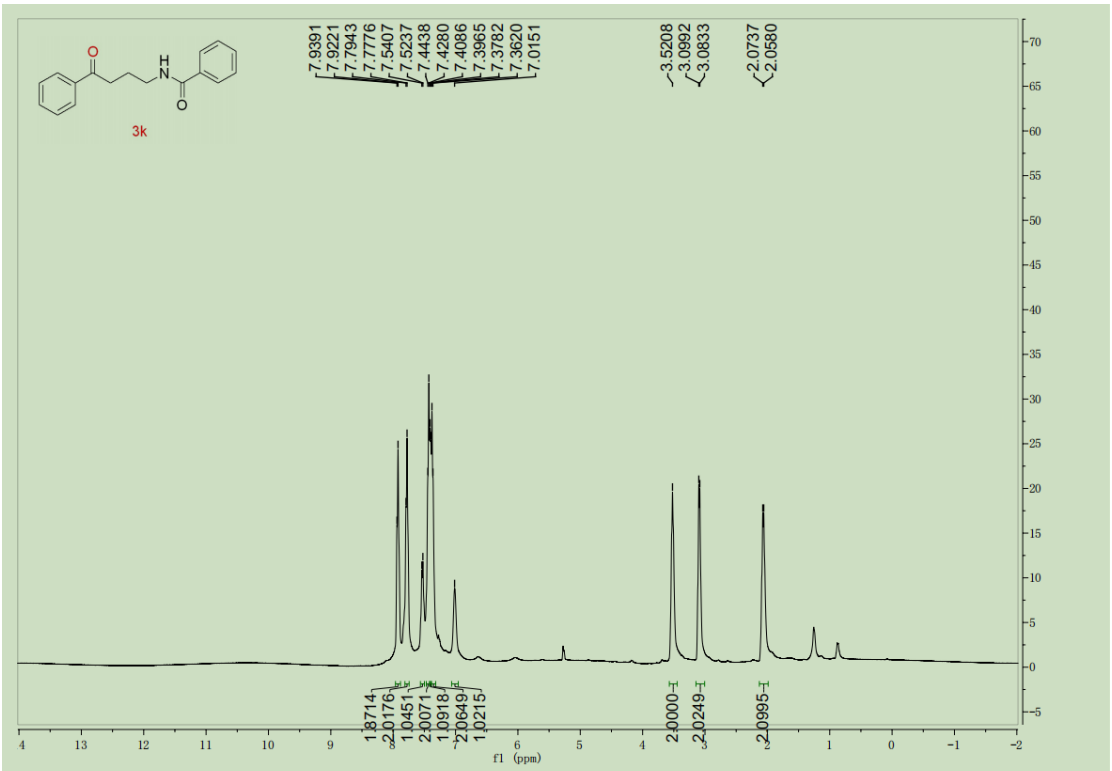
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7.3620
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3.5208
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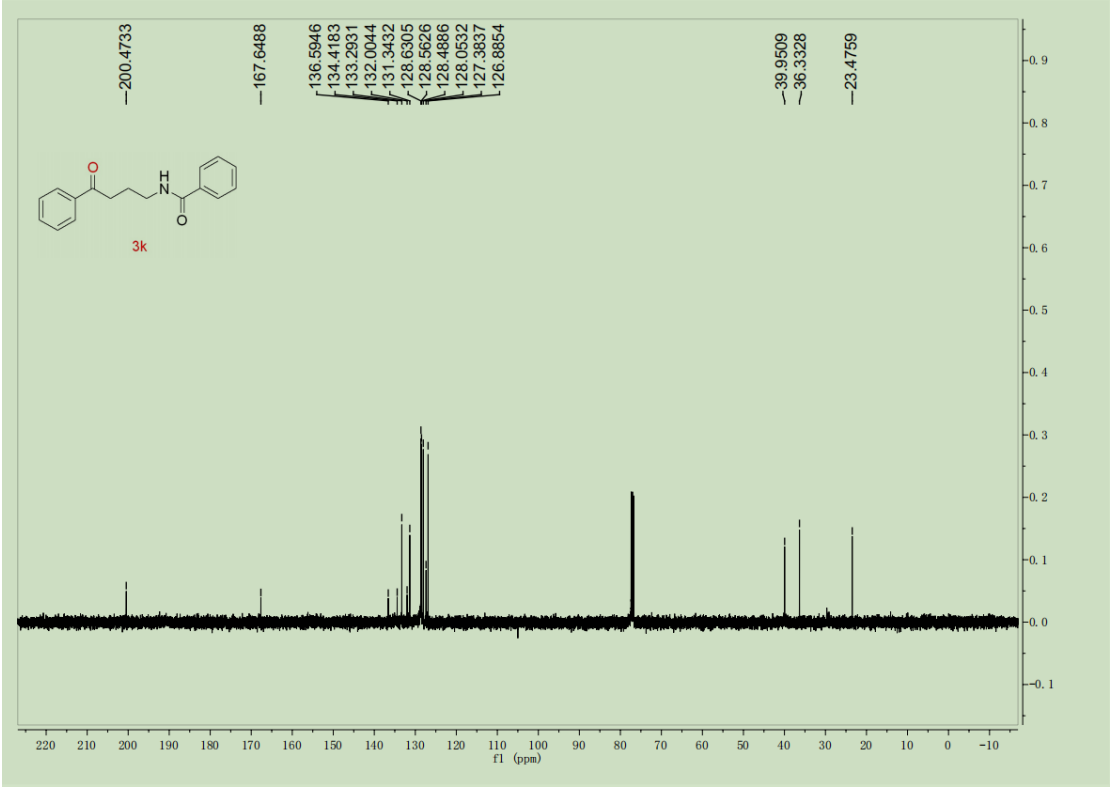
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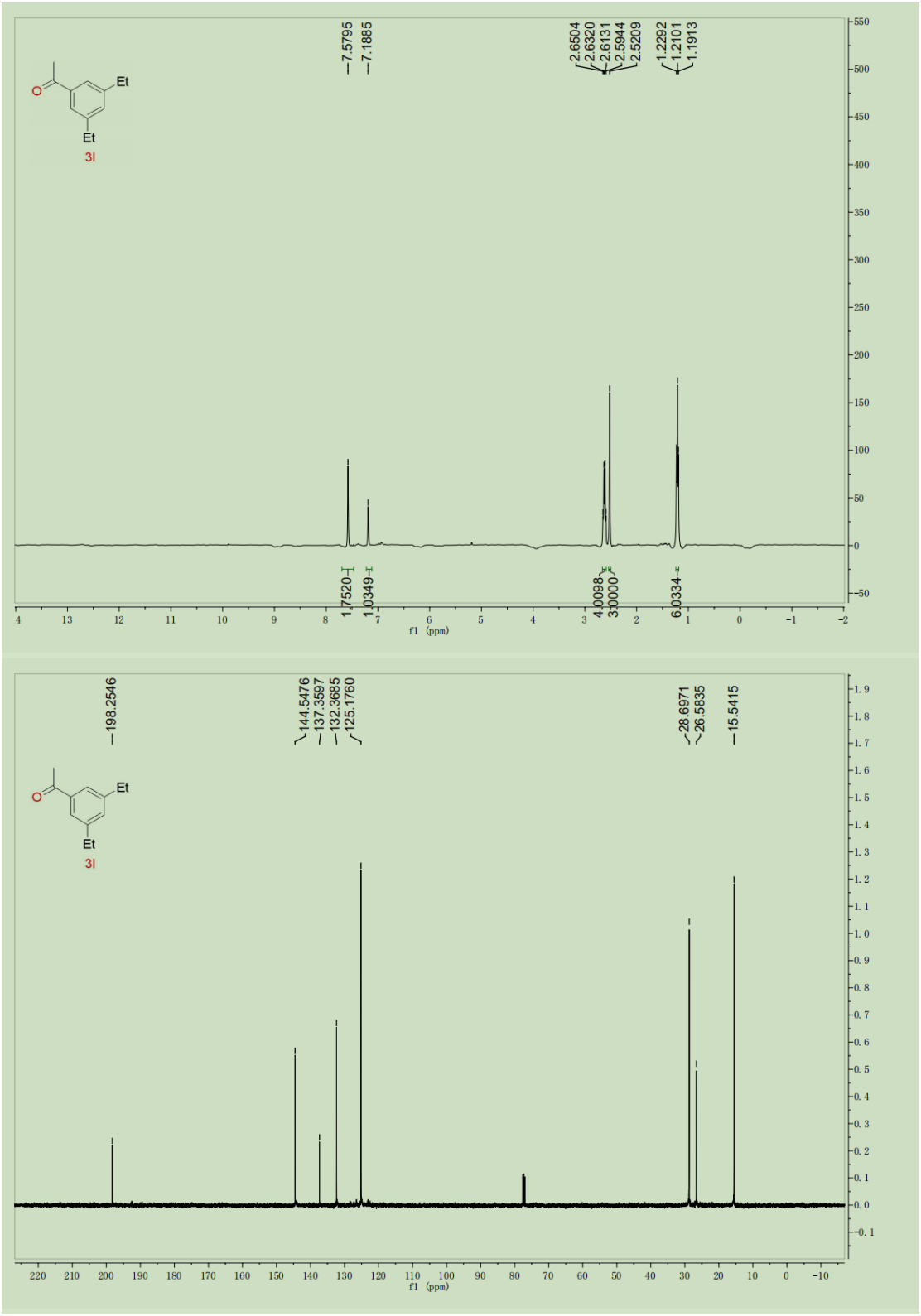
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Et
Et
O
3l
1.7520
1.0349
4.0098
3.0000
6.0334
f1 (ppm)
198.2546
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Et
O
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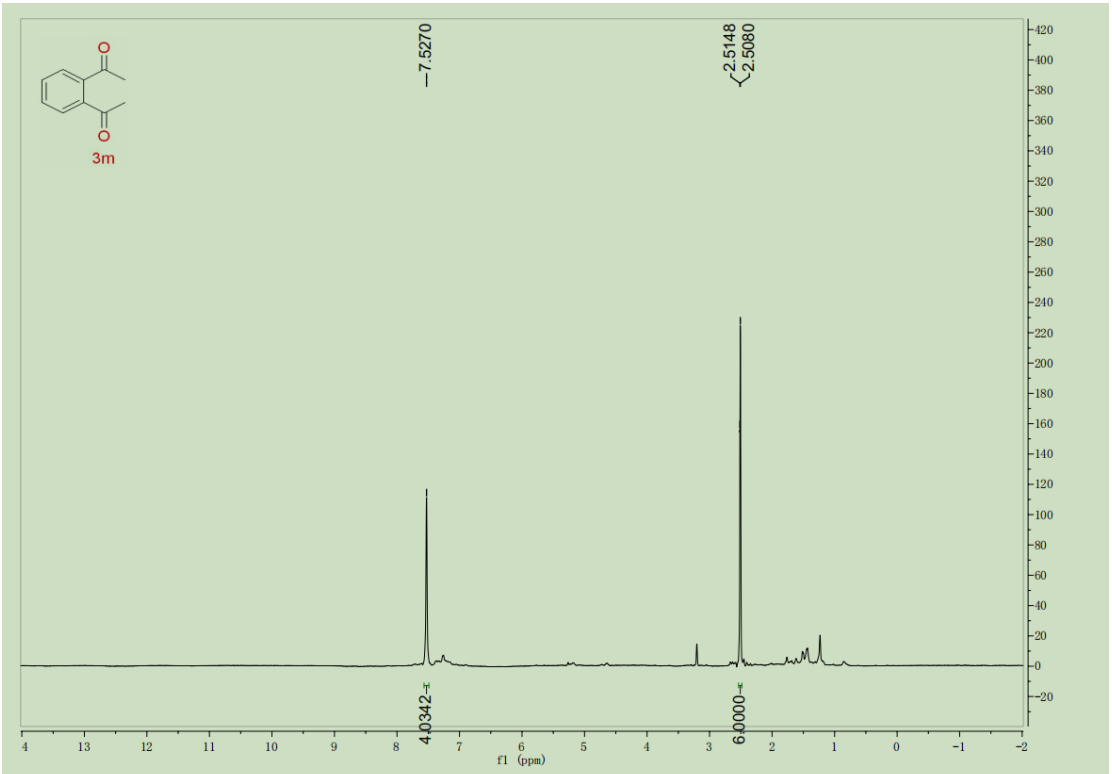
f1 (ppm)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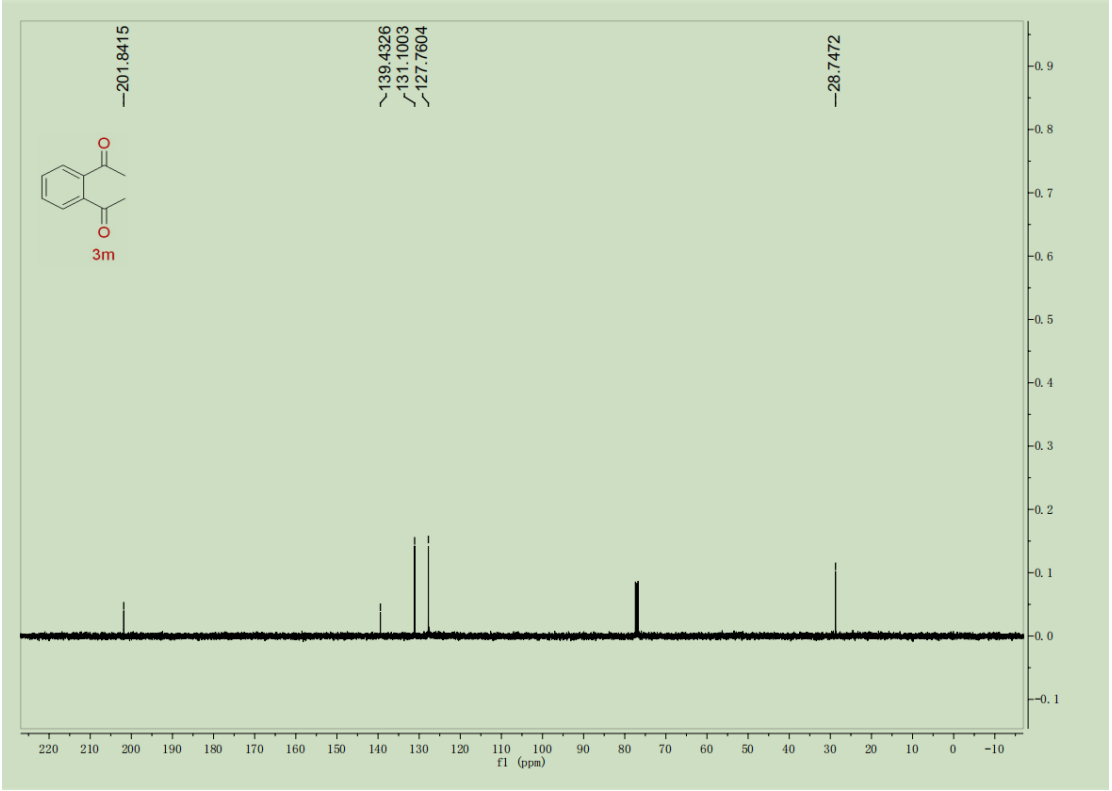
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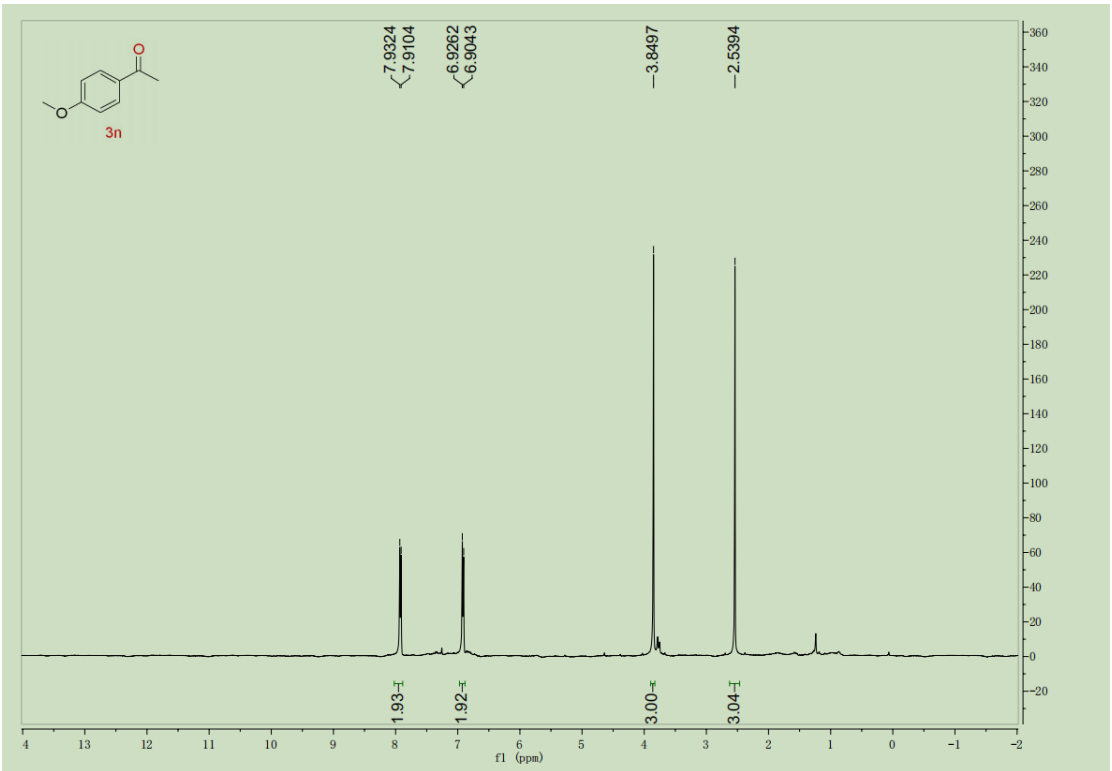
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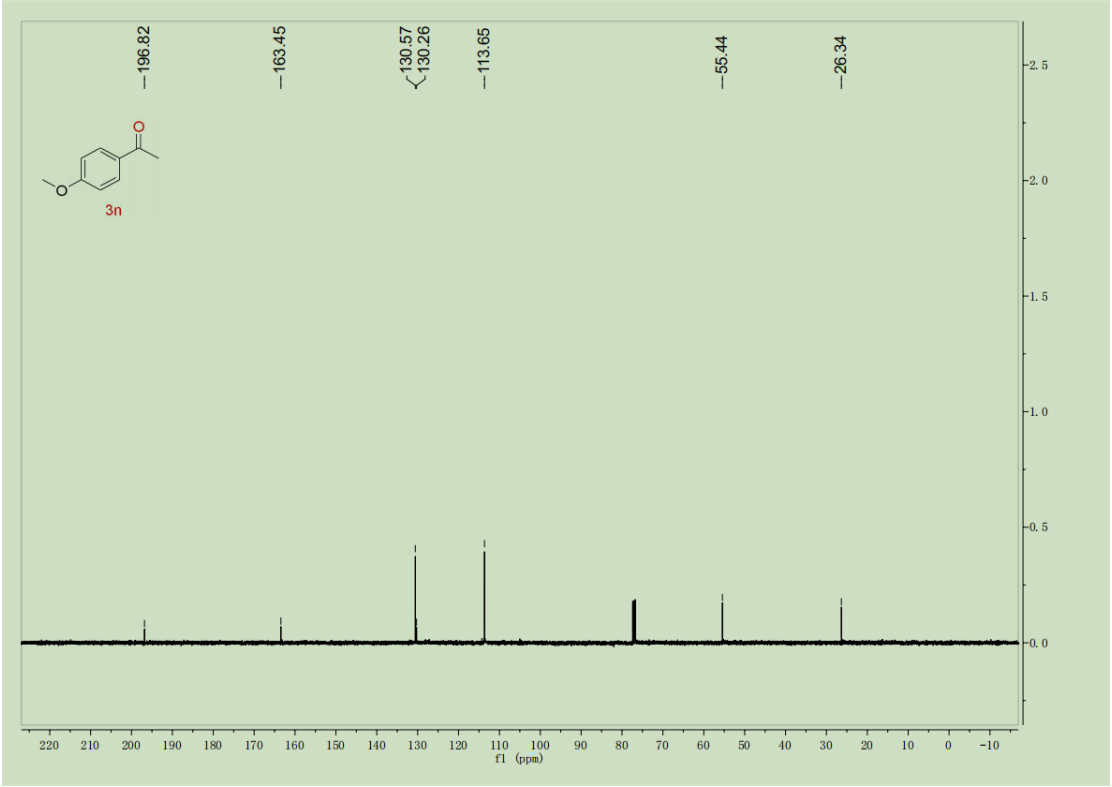
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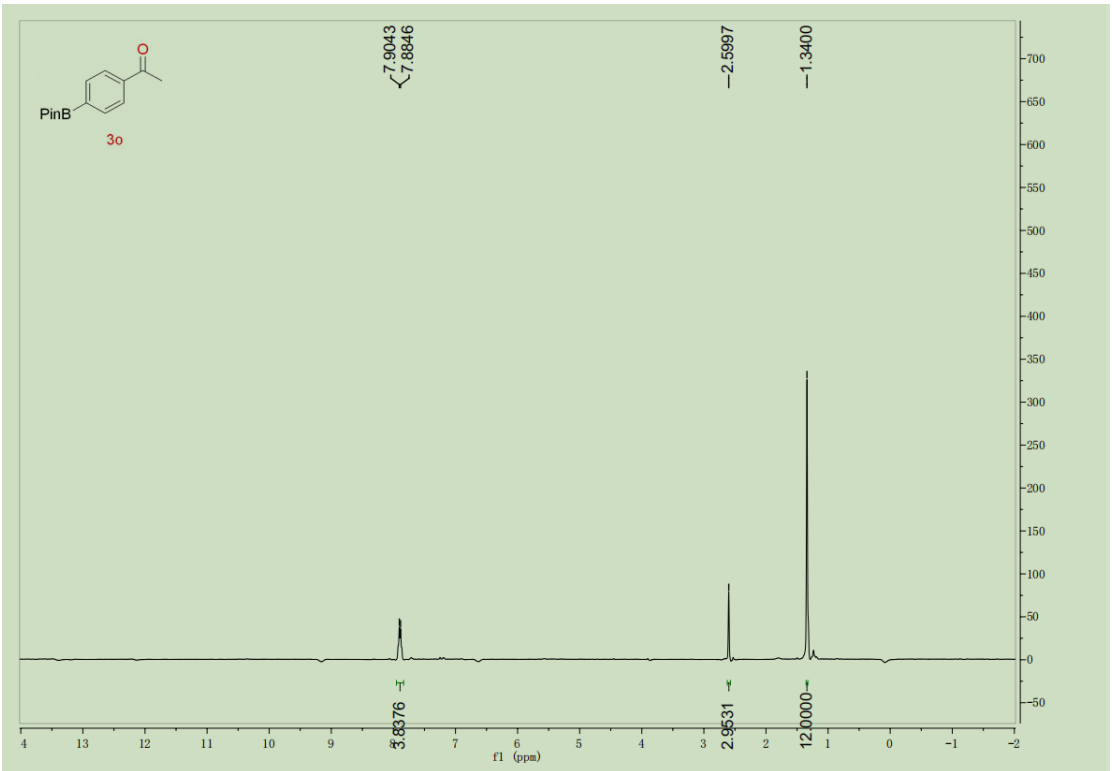
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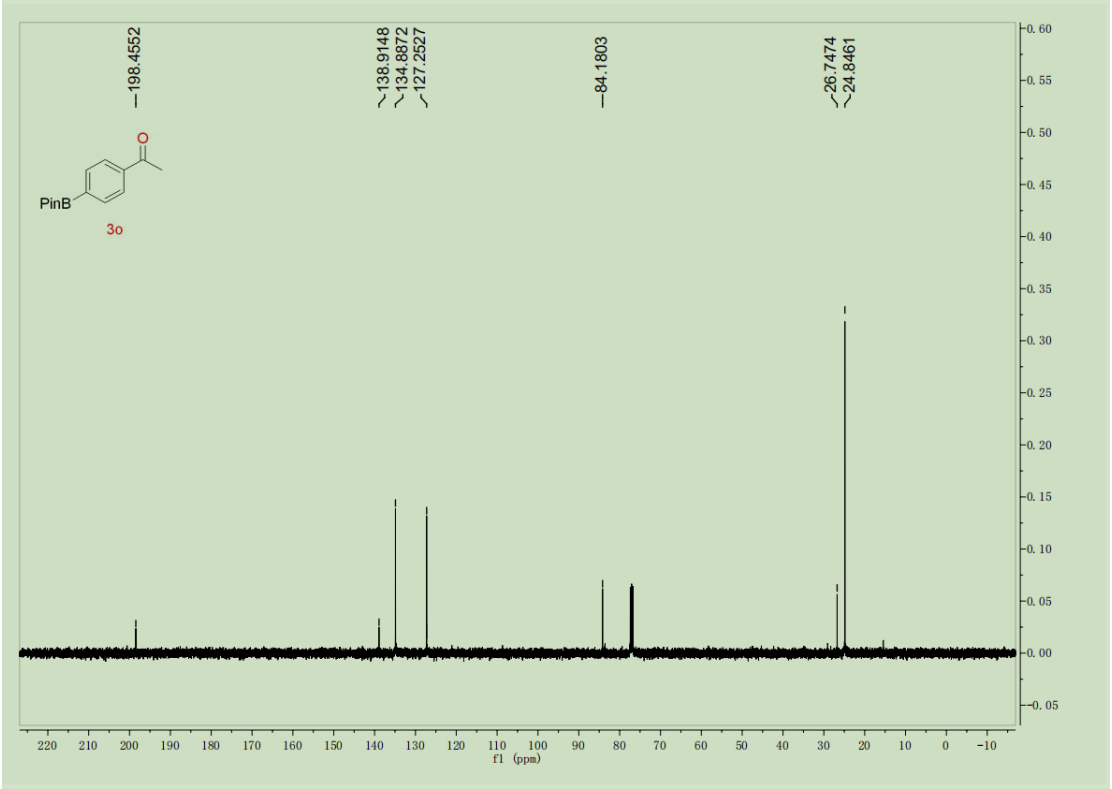
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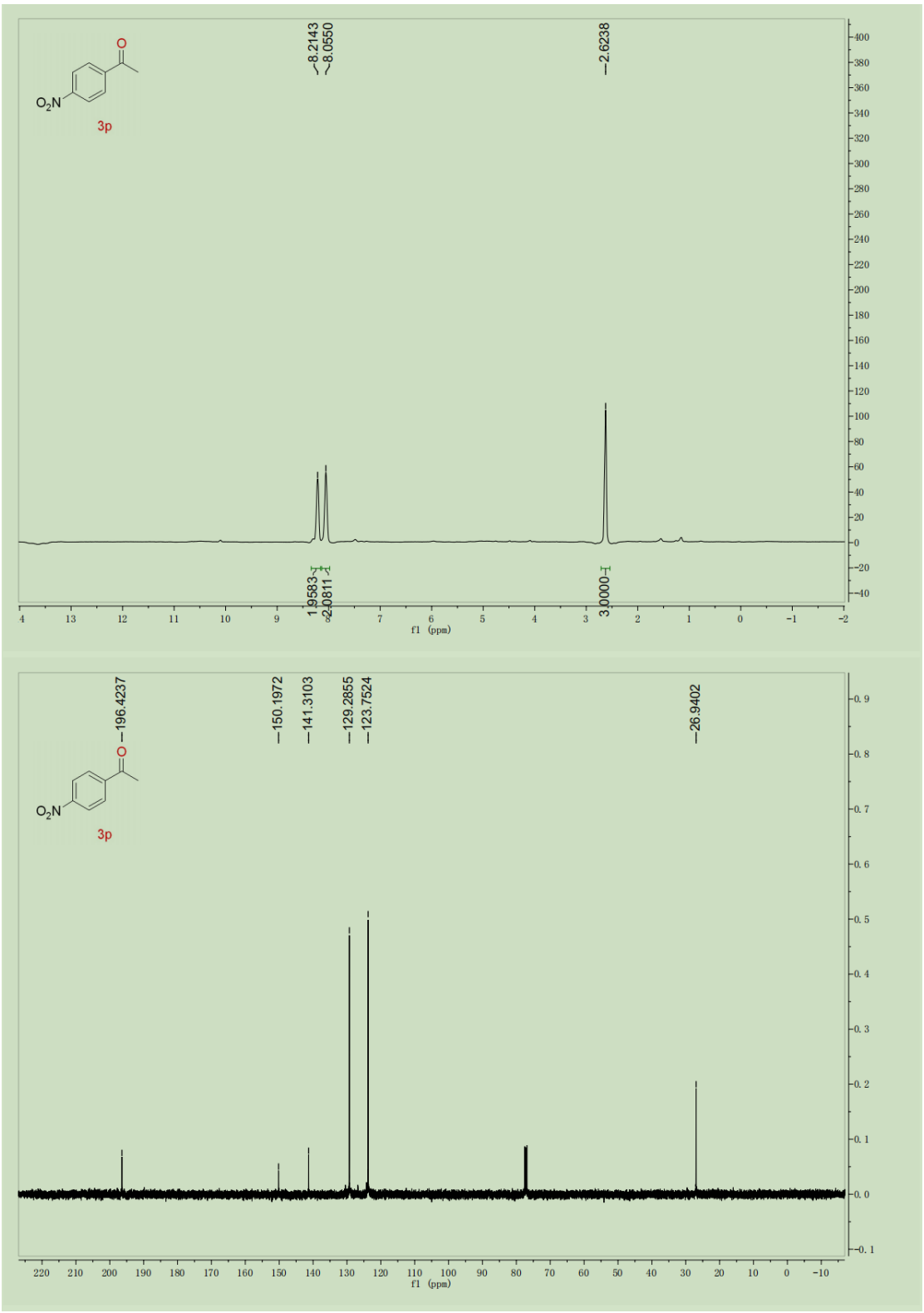
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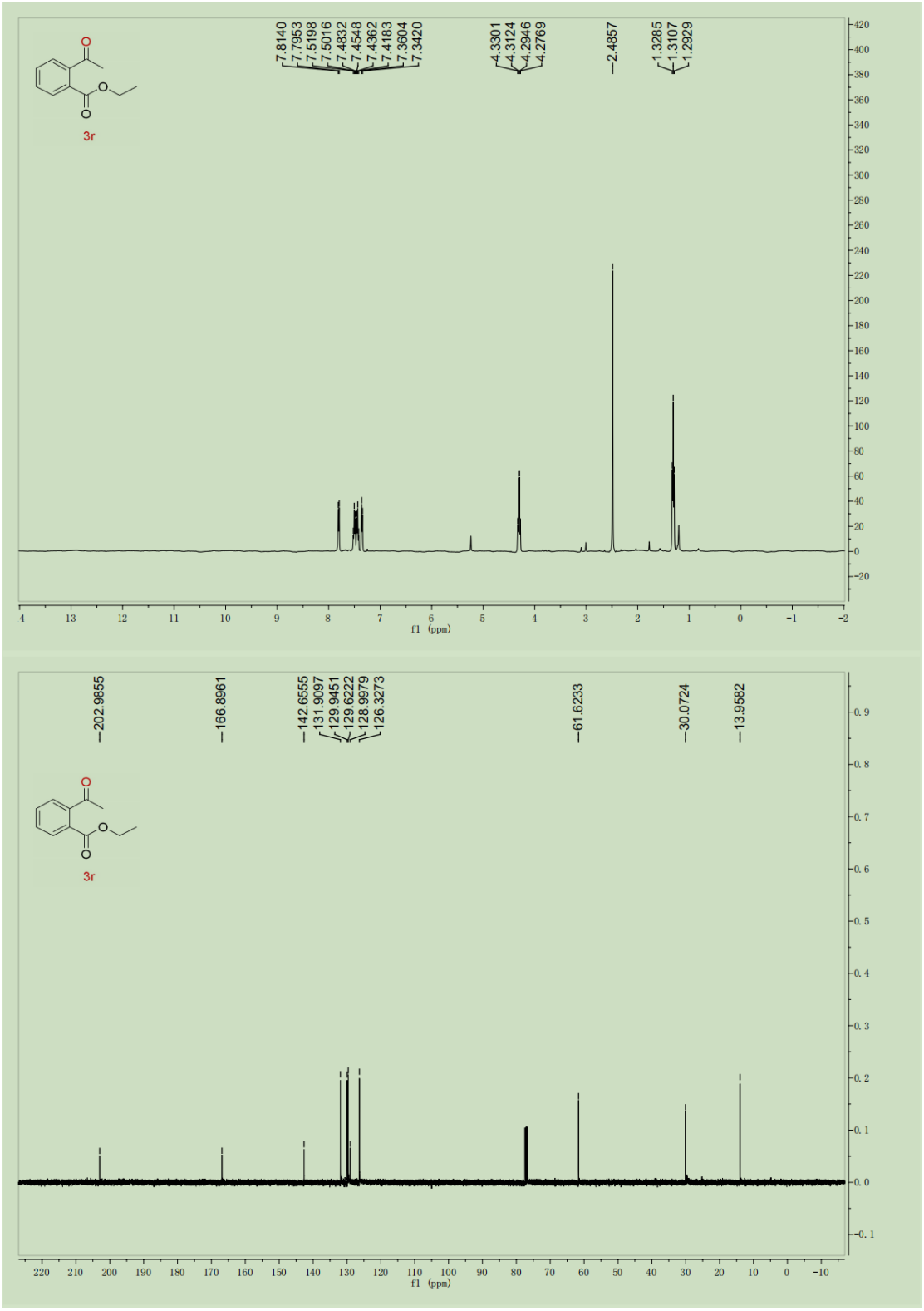
3p
f1 (ppm)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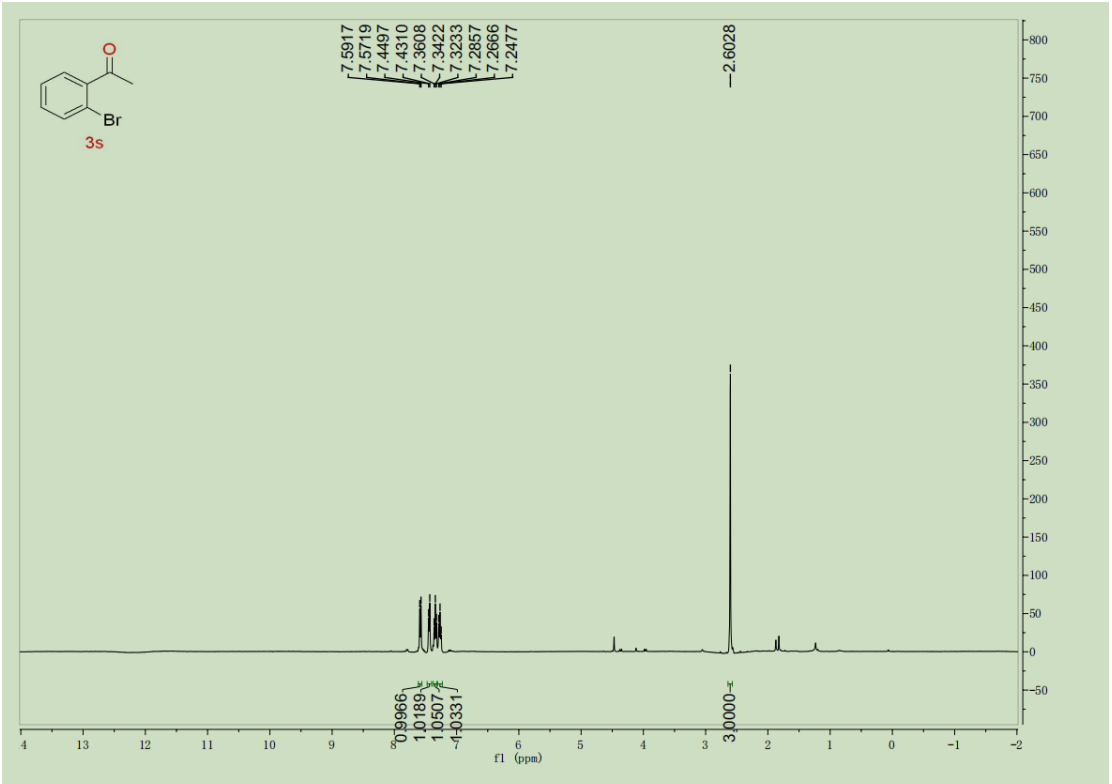
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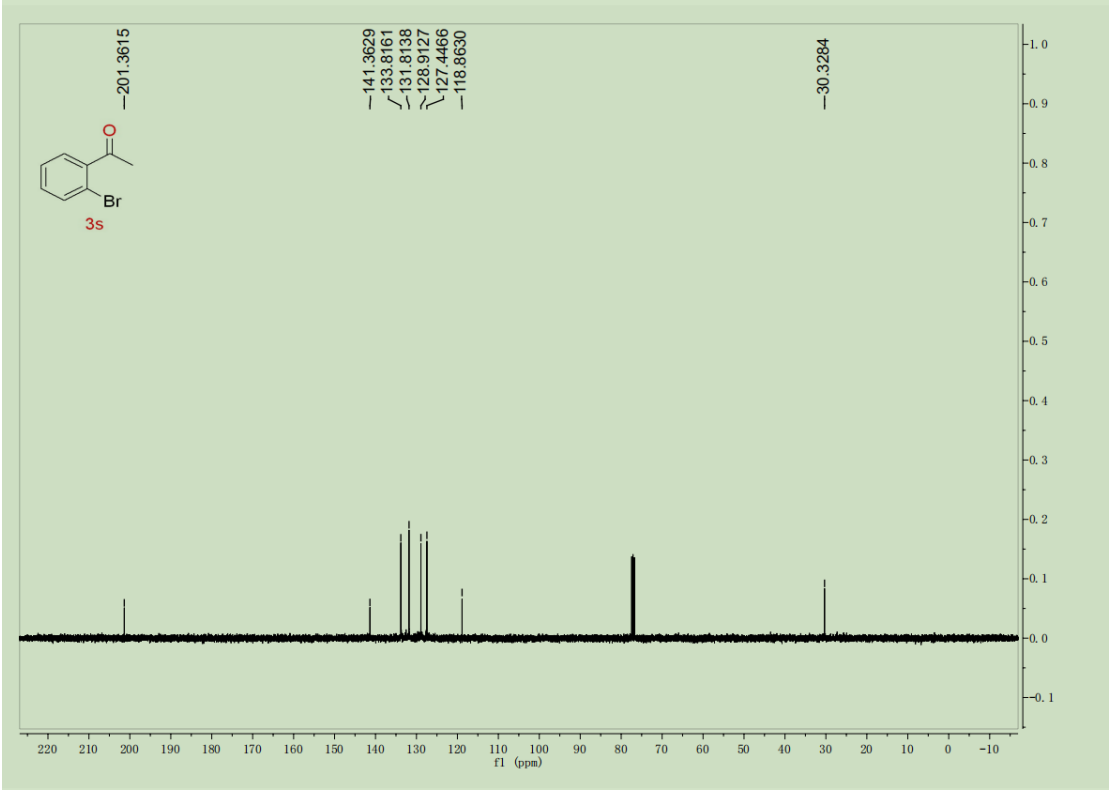
3.0000
f1 (ppm)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Br
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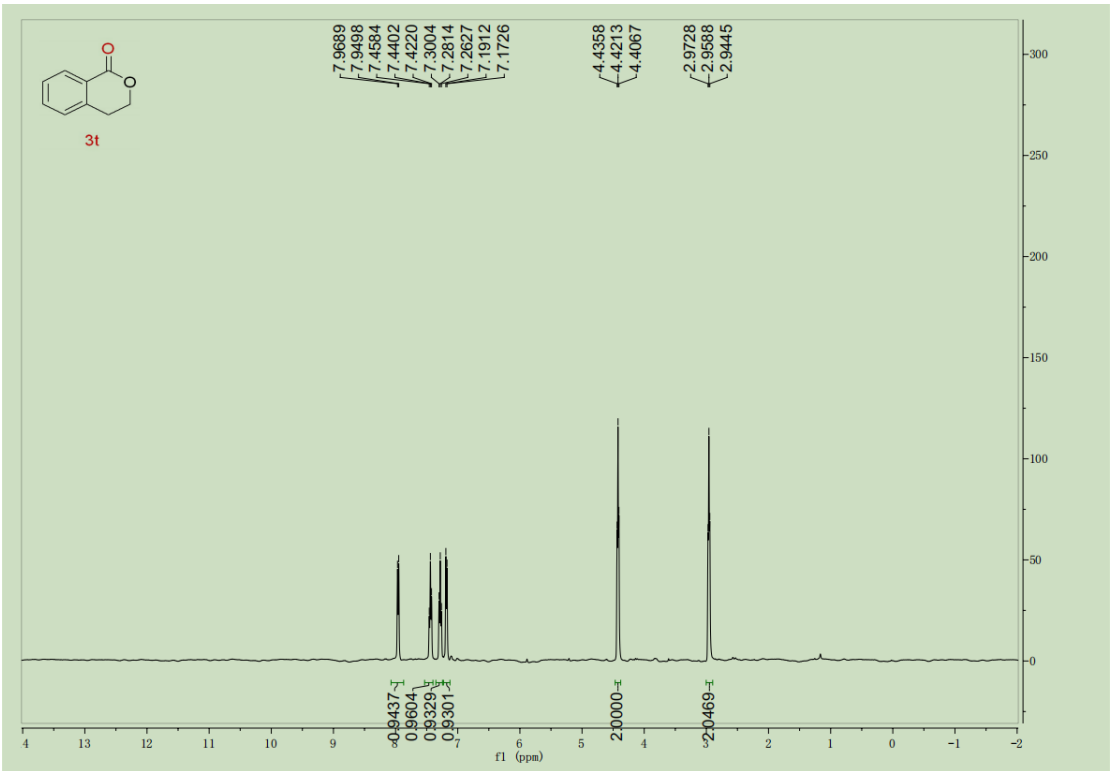
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4.4213
4.4067
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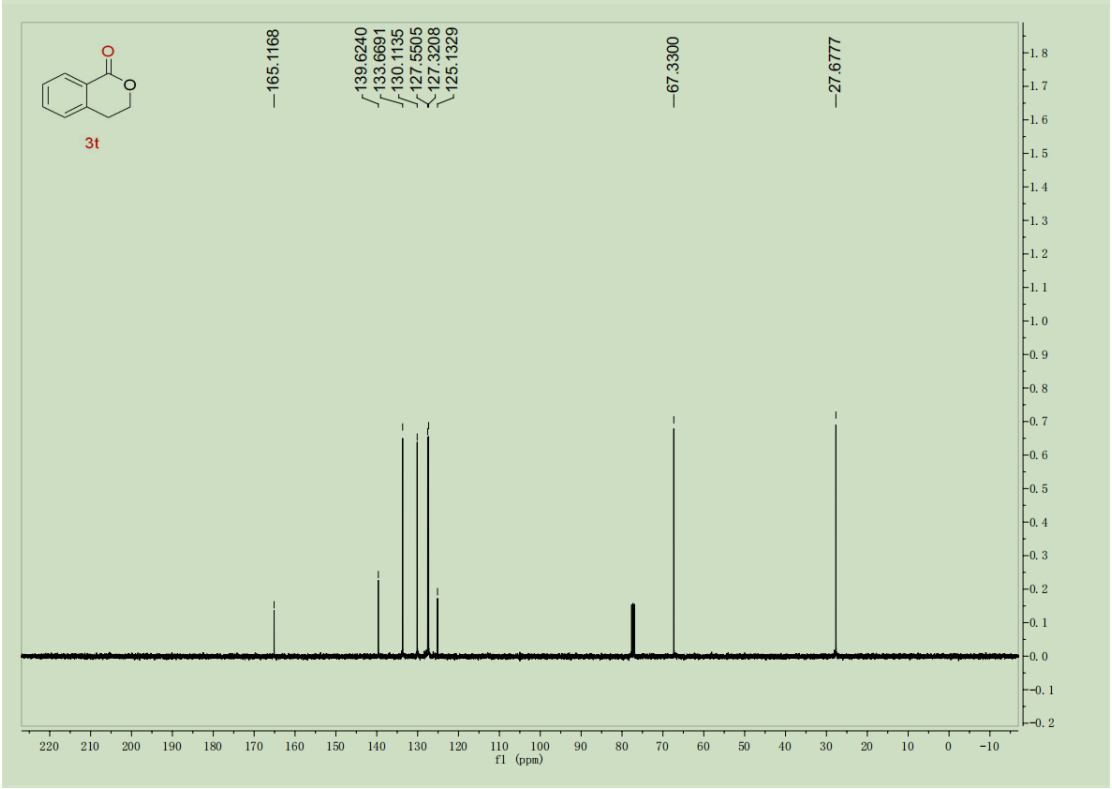
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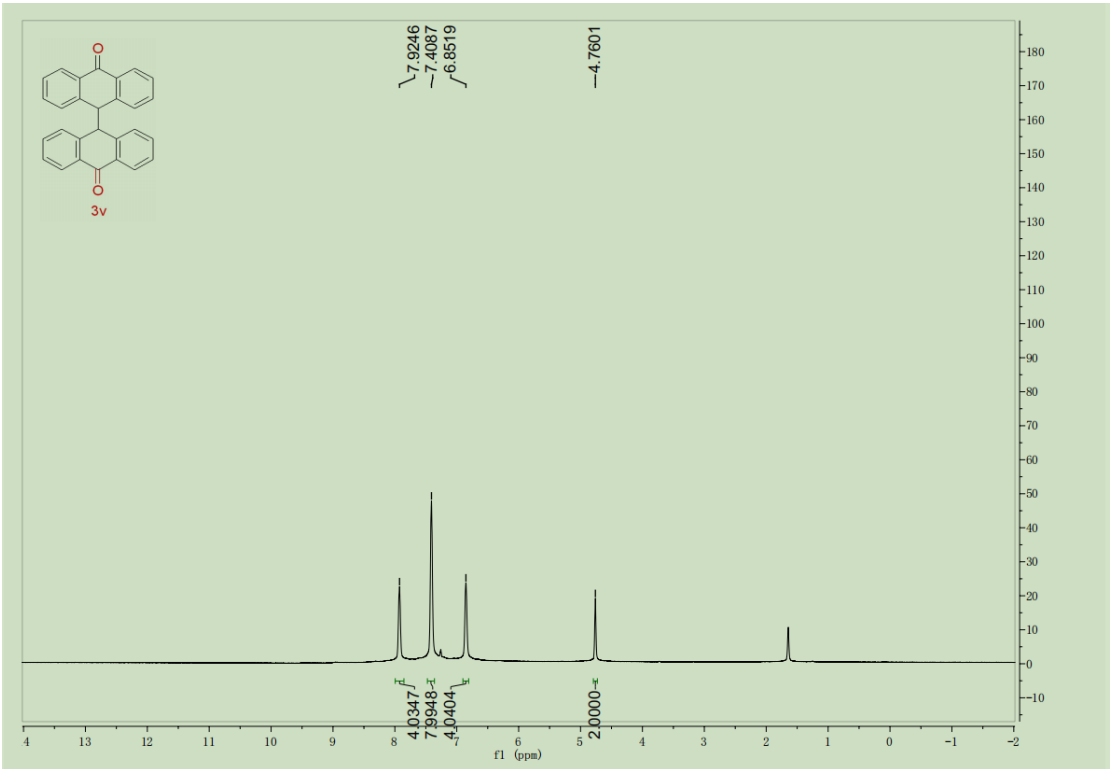
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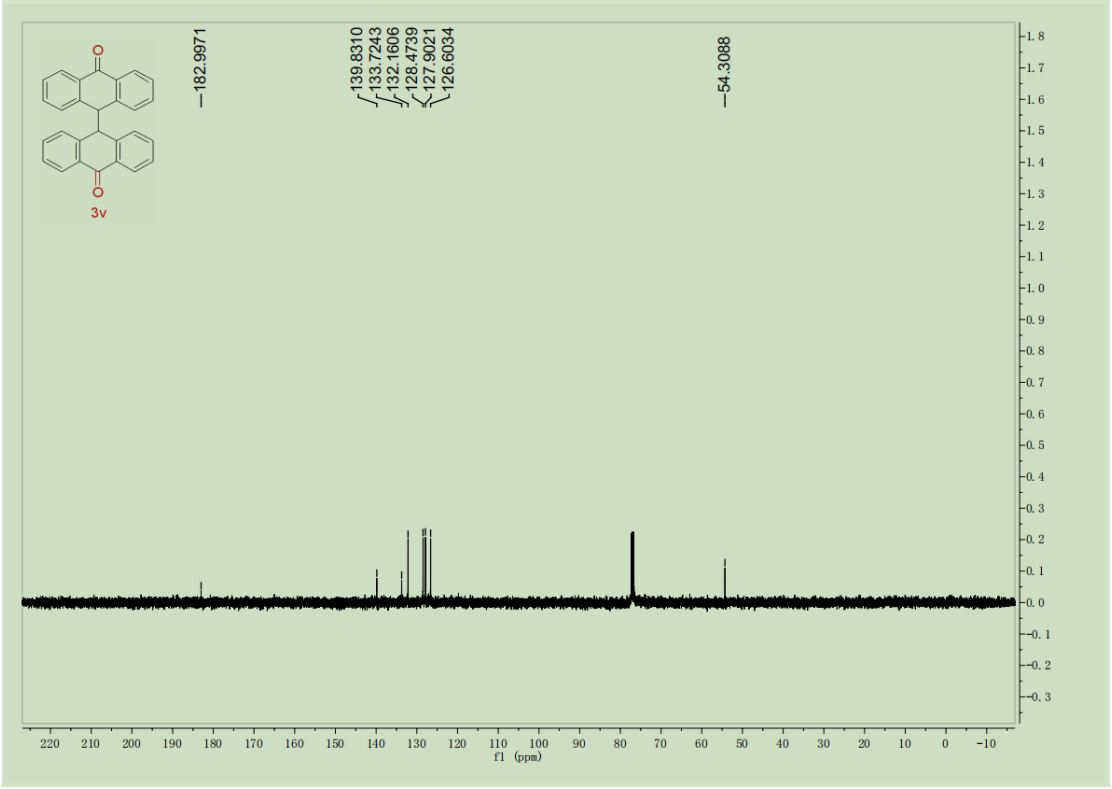
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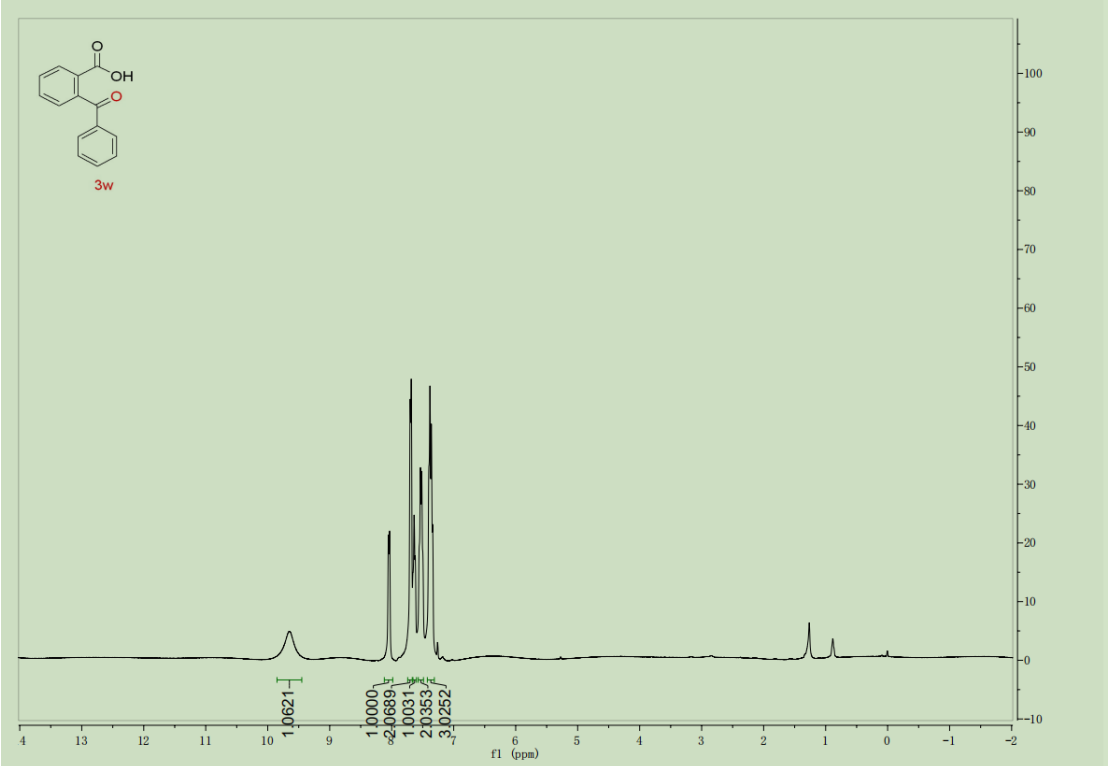
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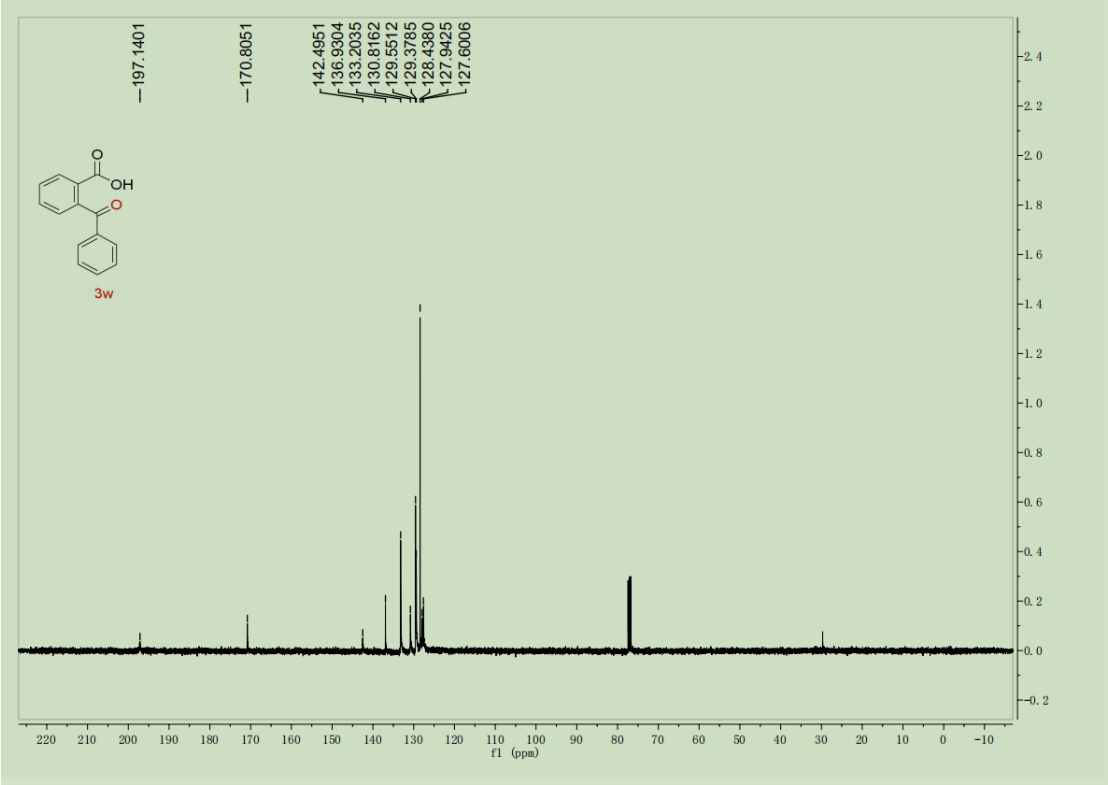
1.0000
2.0689
1.1031
2.0353
3.0252
f1 (ppm)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170.8051
142.4951
136.9304
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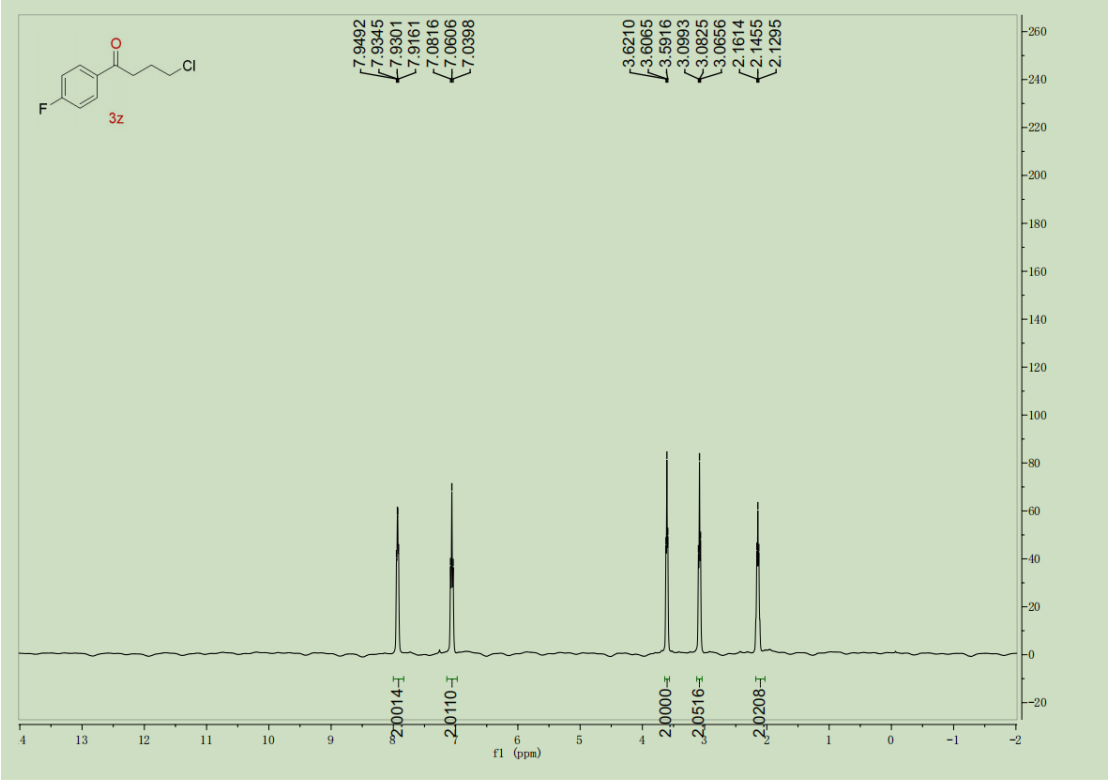
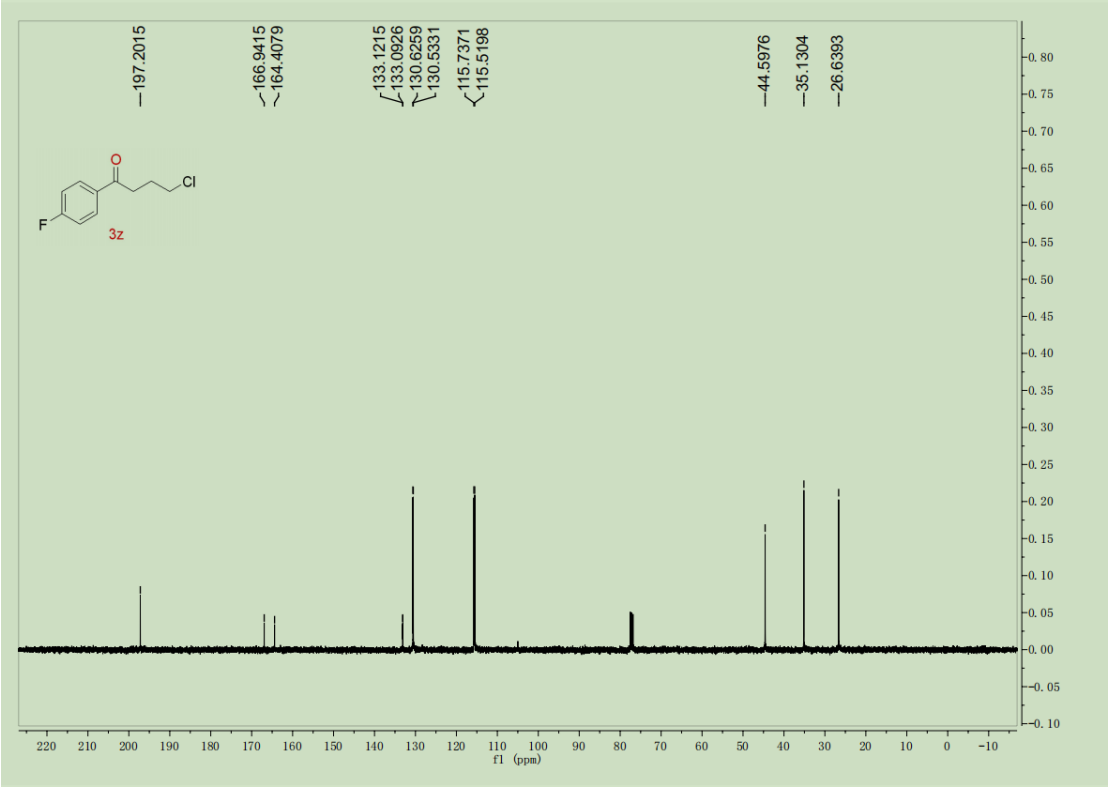
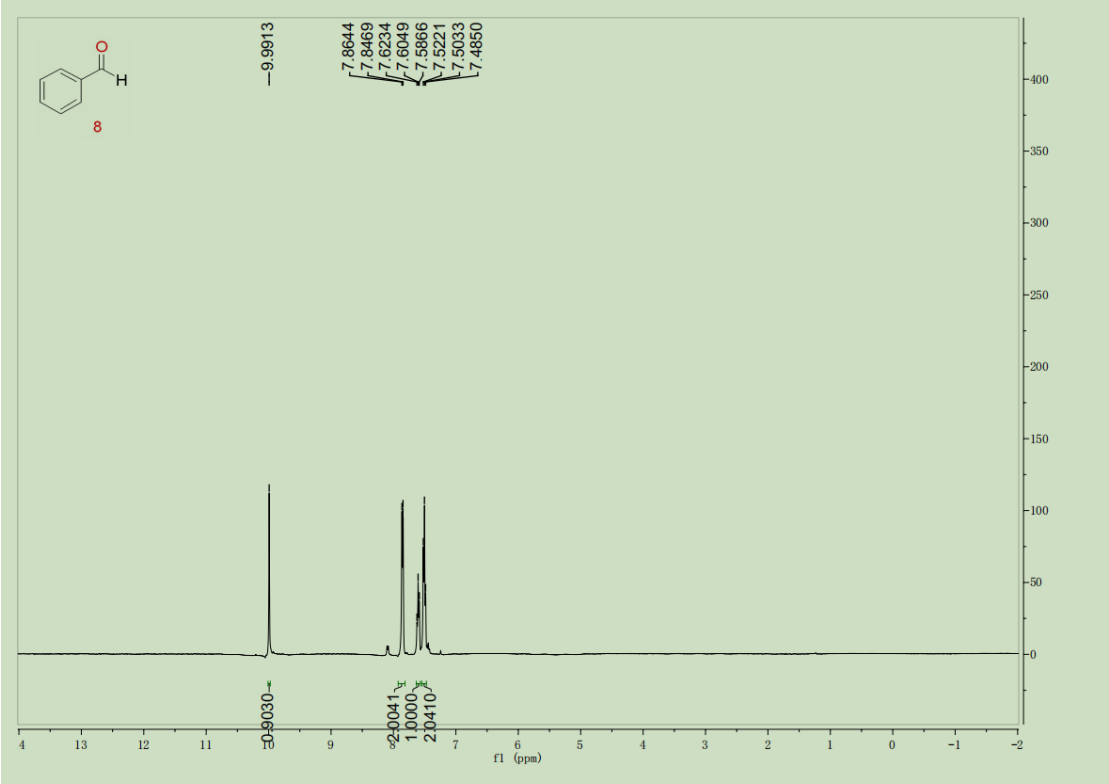
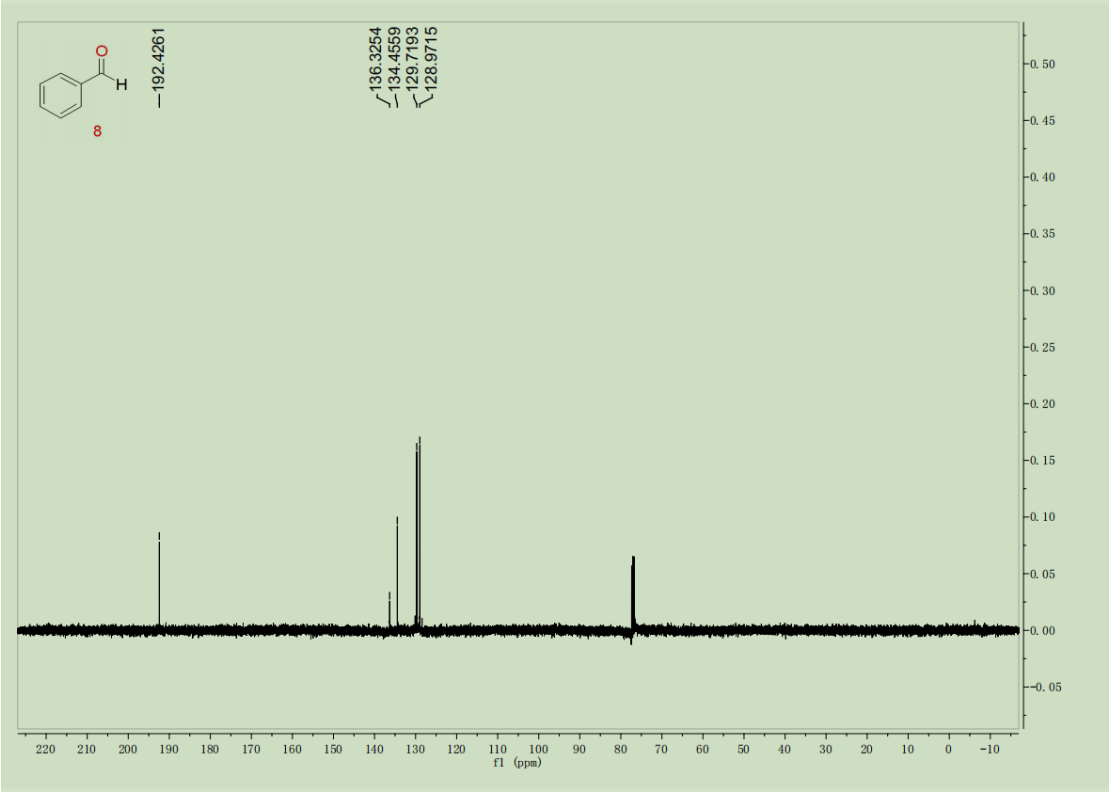
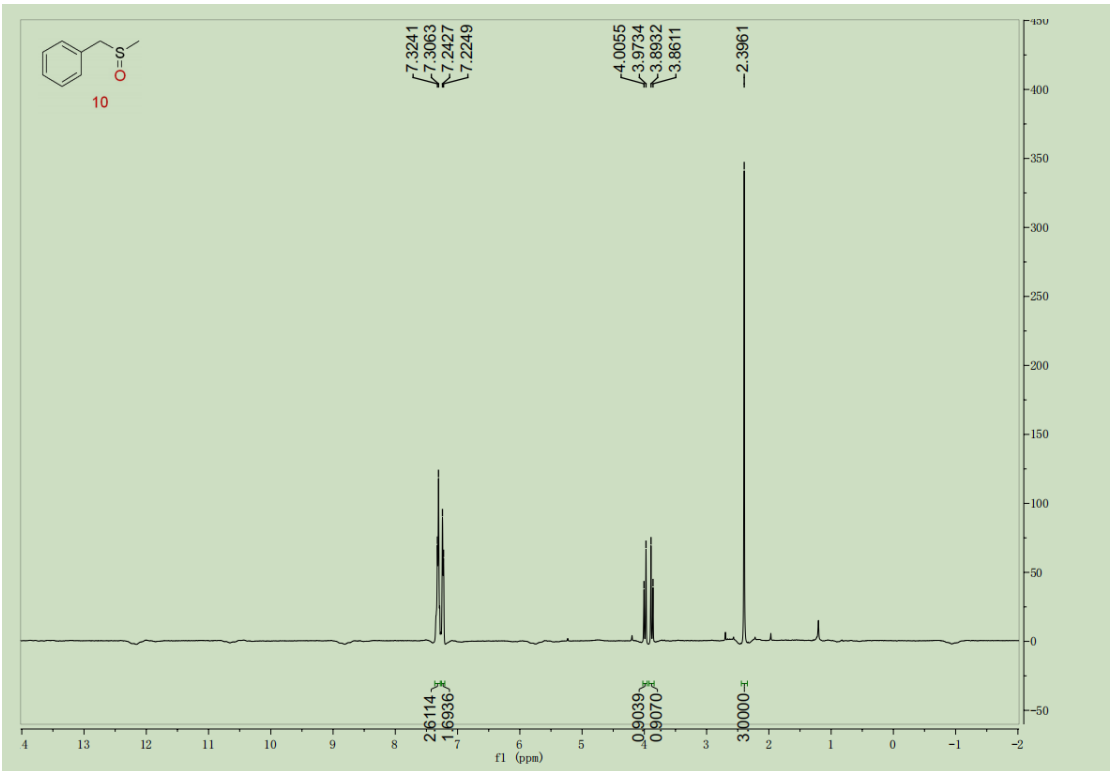
130.8162
129.5512
129.3785
128.4380
127.9425
127.6006
3w
f1 (ppm)

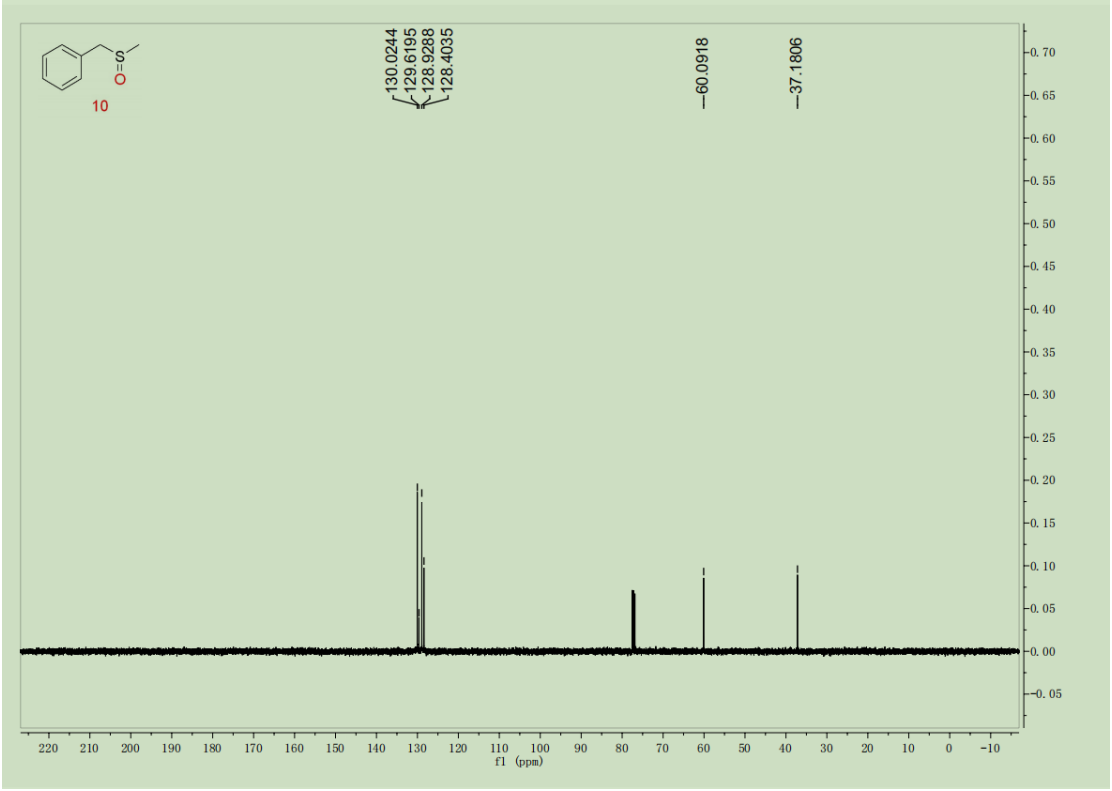

7.9492
7.9345
7.9301
7.9161
7.0816
7.0606
7.0398
3.6210
3.6065
3.5916
3.0993
3.0825
3.0656
2.1614
2.1455
2.1295
O
Cl
F
3z
2.0014
2.0110
2.0000
2.0516
2.0208
f1 (ppm)

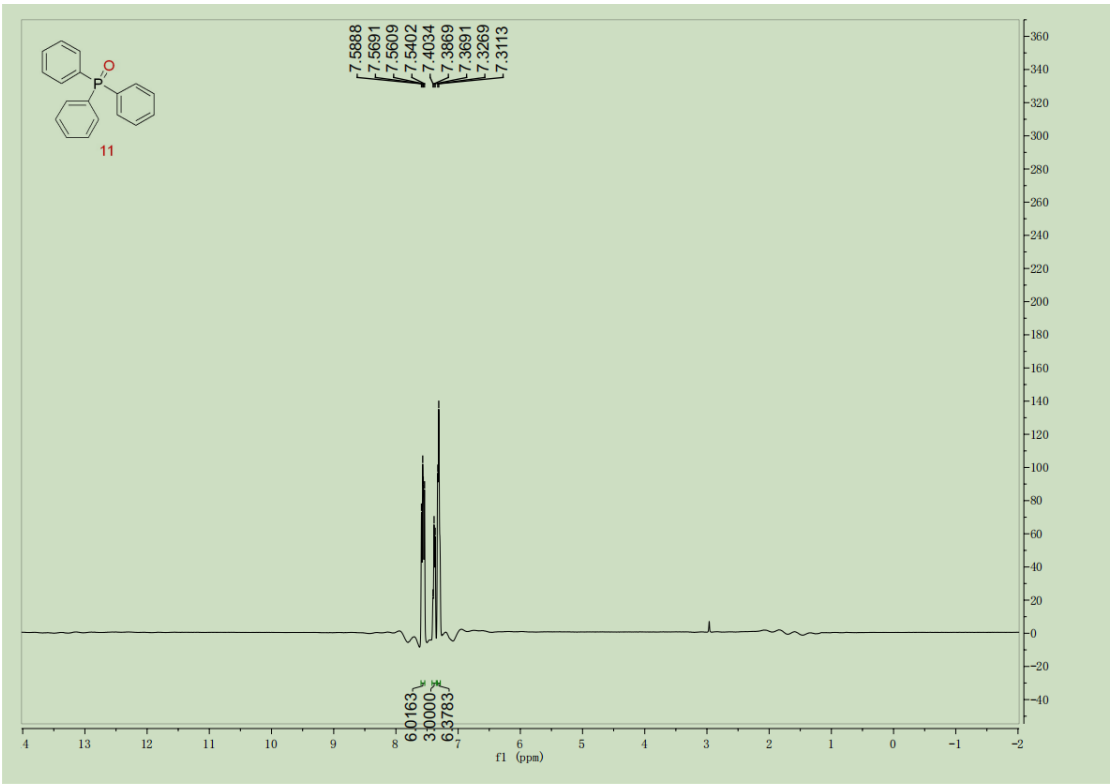

197.2015
166.9415
164.4079
133.1215
133.0926
130.6259
130.5331
115.7371
115.5198
44.5976
35.1304
26.6393
O
Cl
F
3z
f1 (ppm)

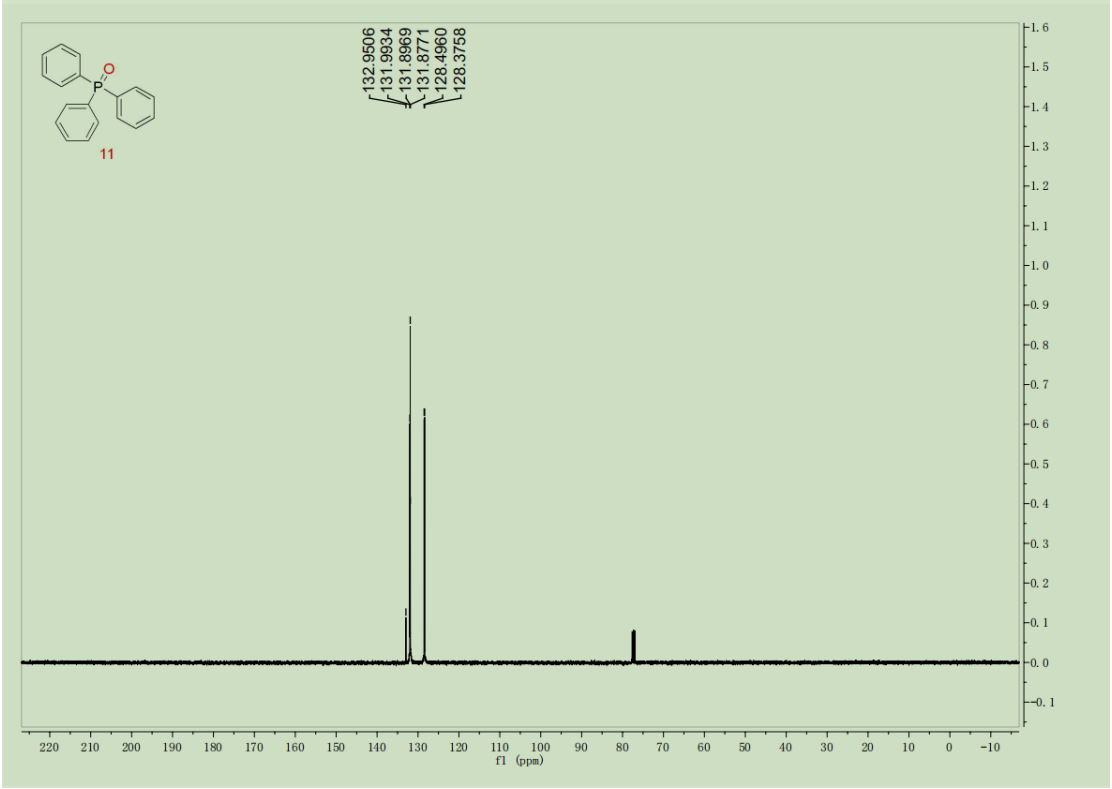

O
H
8
9.9913
7.8644
7.8469
7.6234
7.6049
7.5866
7.5221
7.5033
7.4850
0.9030
2.0041
1.0000
2.0410
f1 (ppm)

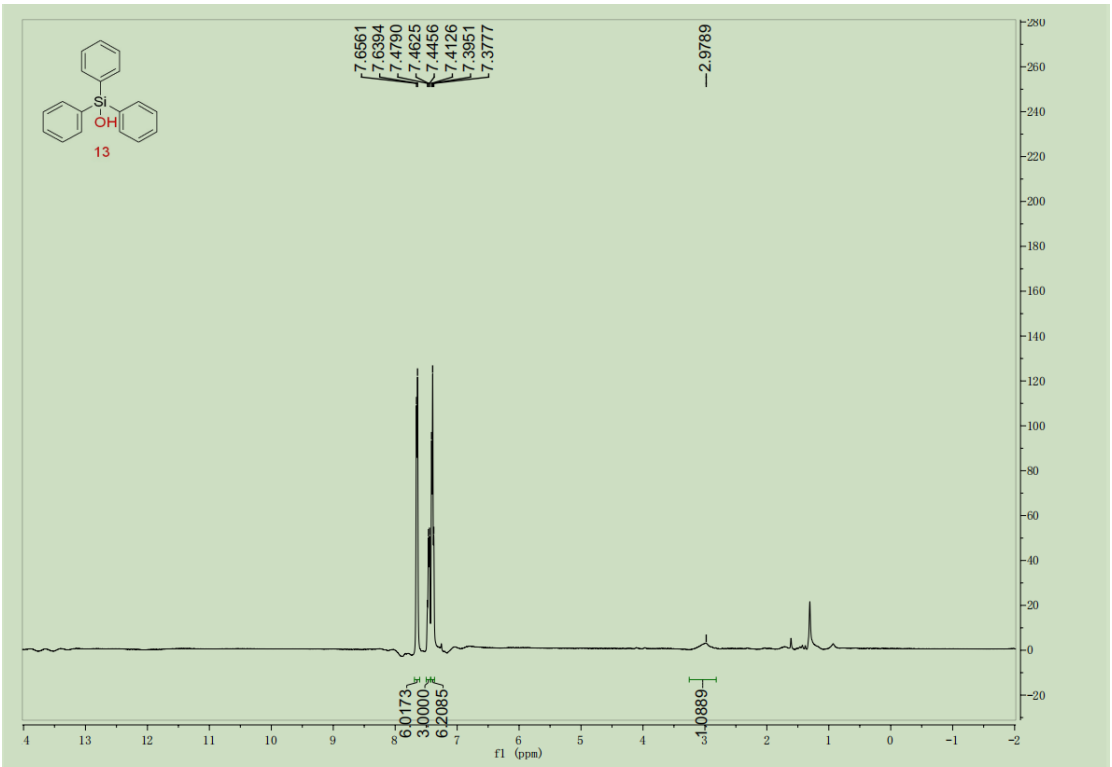

O
H
8
192.4261
136.3254
134.4559
129.7193
128.9715
f1 (ppm)

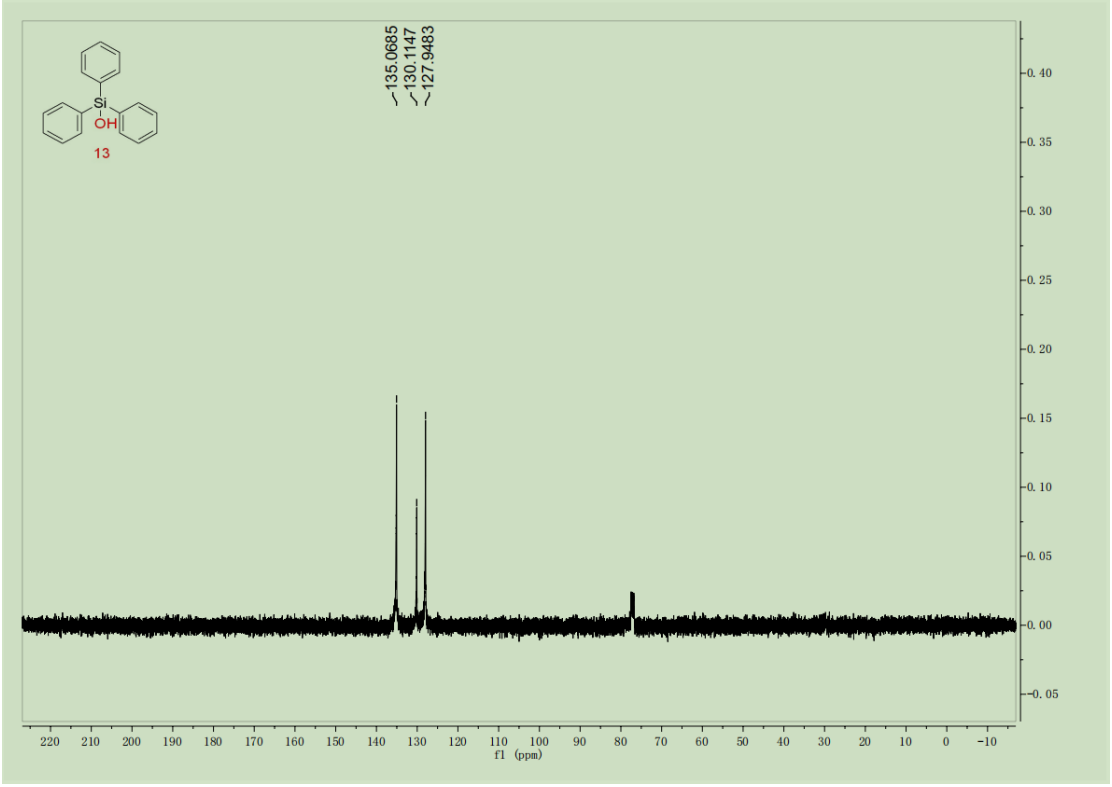

10
7.3241
7.3063
7.2427
7.2249
4.0055
3.9734
3.8932
3.8611
2.3961
2.6114
1.6936
0.9039
0.9070
3.0000
f1 (ppm)

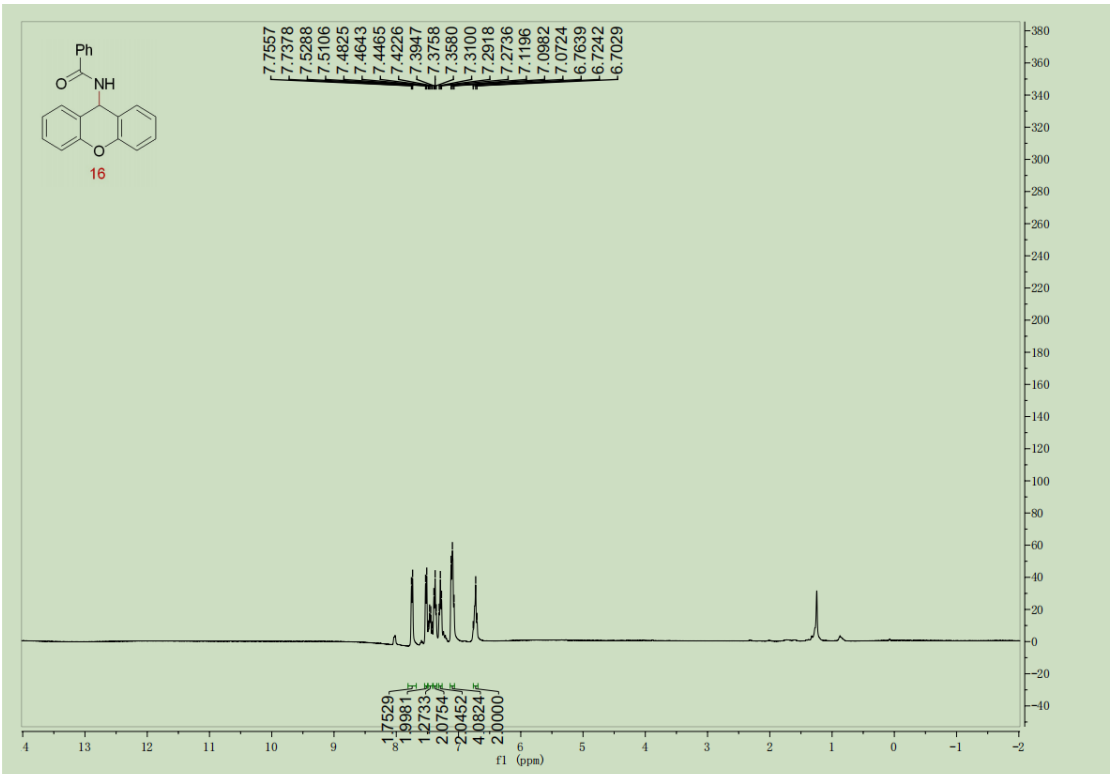

10
130.0244
129.6195
128.9288
128.4035
60.0918
37.1806
f1 (ppm)


11
7.5888
7.5691
7.5609
7.5402
7.4034
7.3869
7.3691
7.3269
7.3113
6.0163
3.0000
6.3783
f1 (ppm)


11
132.9506
131.9934
131.8969
131.8771
128.4960
128.3758
f1 (ppm)


7.6561
7.6394
7.4790
7.4625
7.4456
7.4126
7.3951
7.3777
2.9789
Si
OH
13
6.0173
3.0000
6.2085
1.0889
f1 (ppm)


135.0685
130.1147
127.9483
Si
OH
13
f1 (ppm)


Ph
O
NH
O
16
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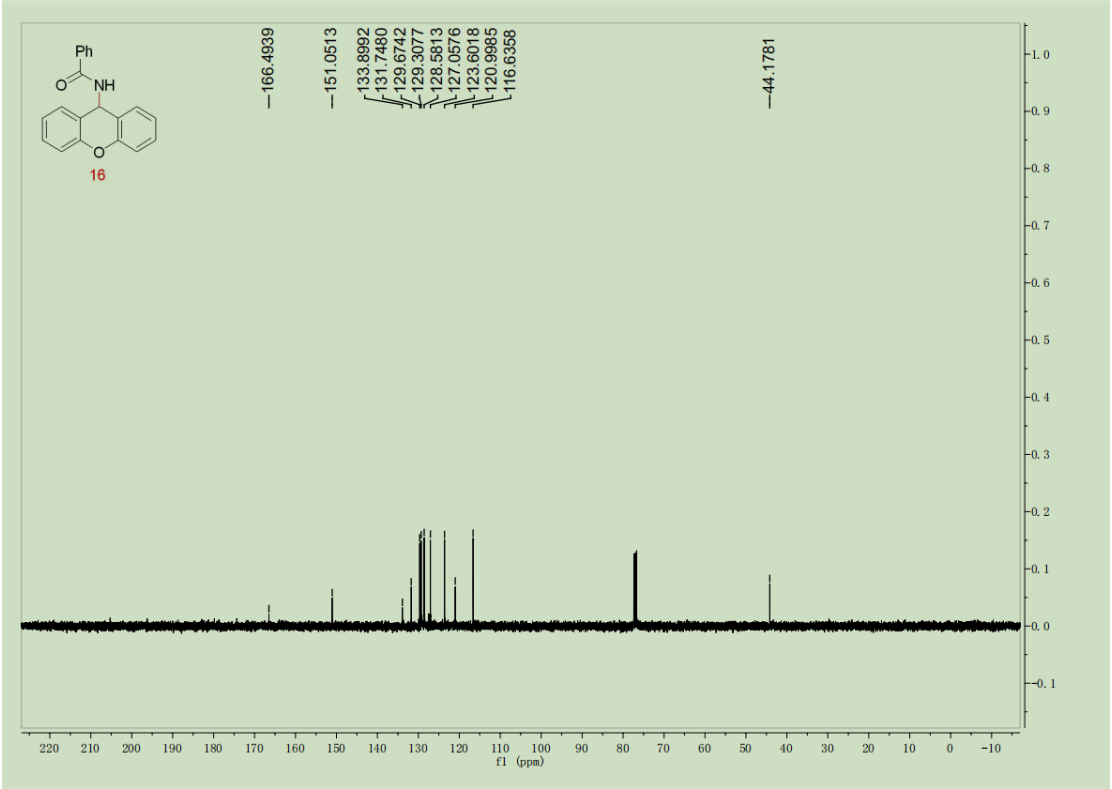
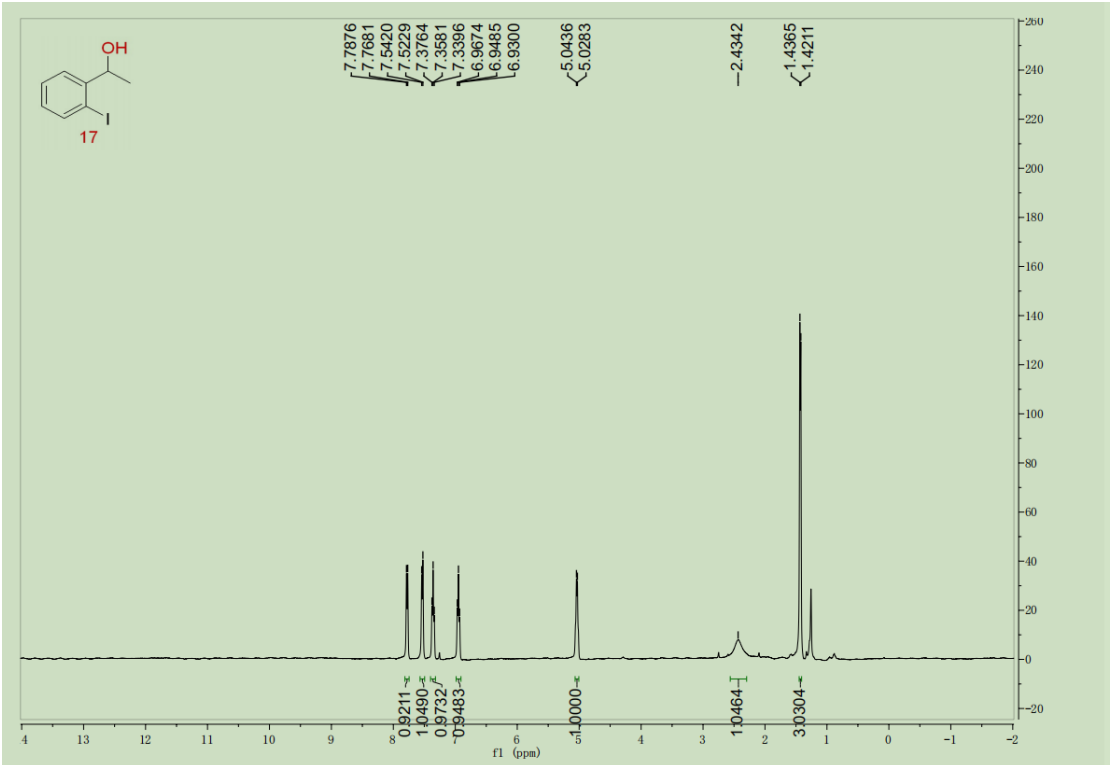
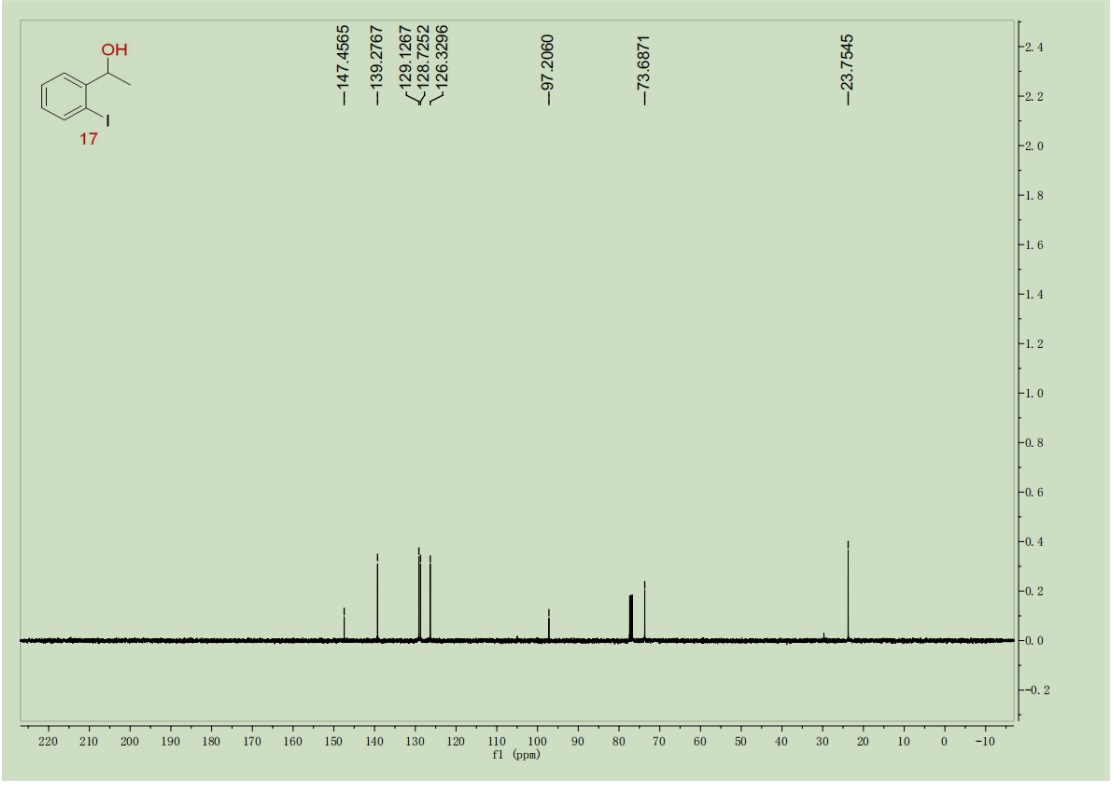
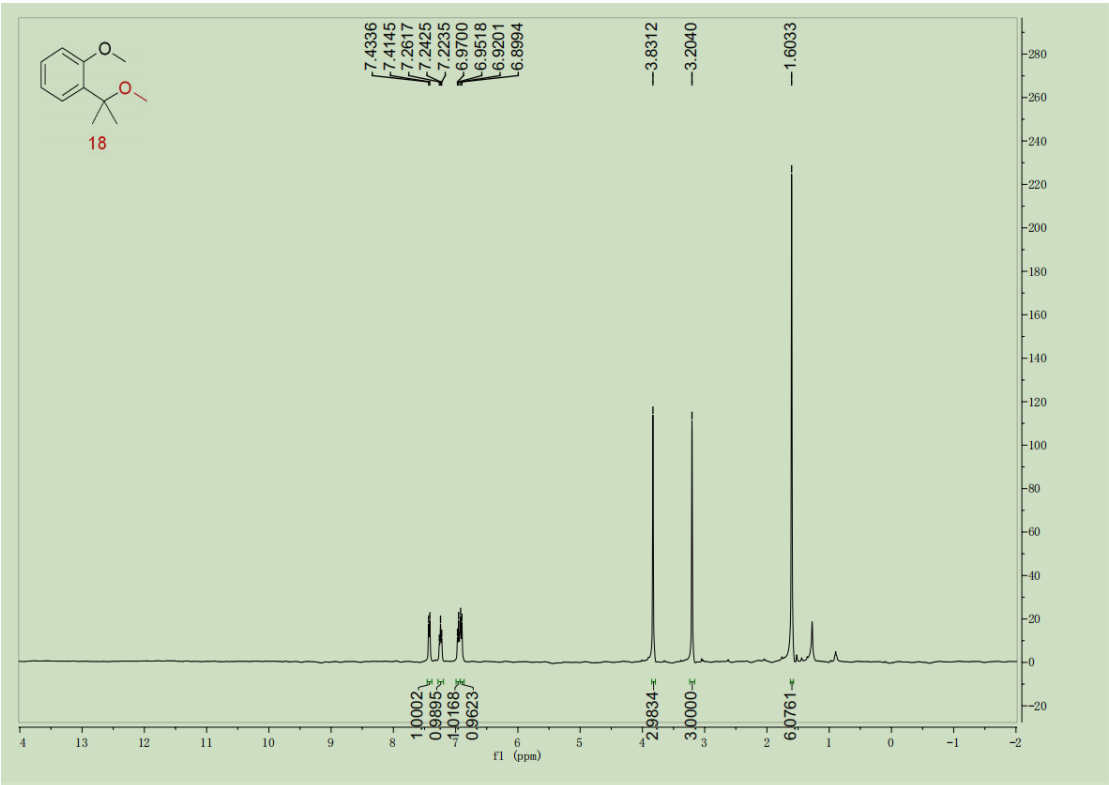
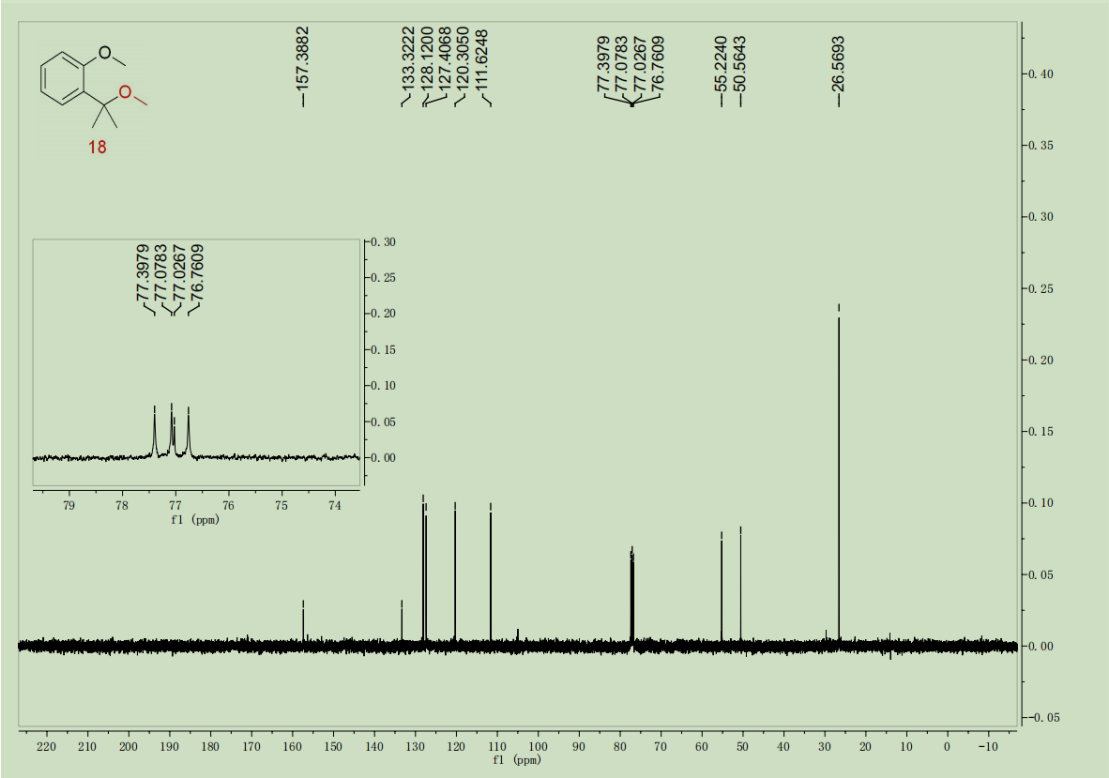
7.5288
7.5106
7.4825
7.4643
7.4465
7.4226
7.3947
7.3758
7.3580
7.3100
7.2918
7.2736
7.1196
7.0982
7.0724
6.7639
6.7242
6.7029
1.7529
1.9981
1.2733
2.0754
2.0452
4.0824
2.0000
f1 (ppm)

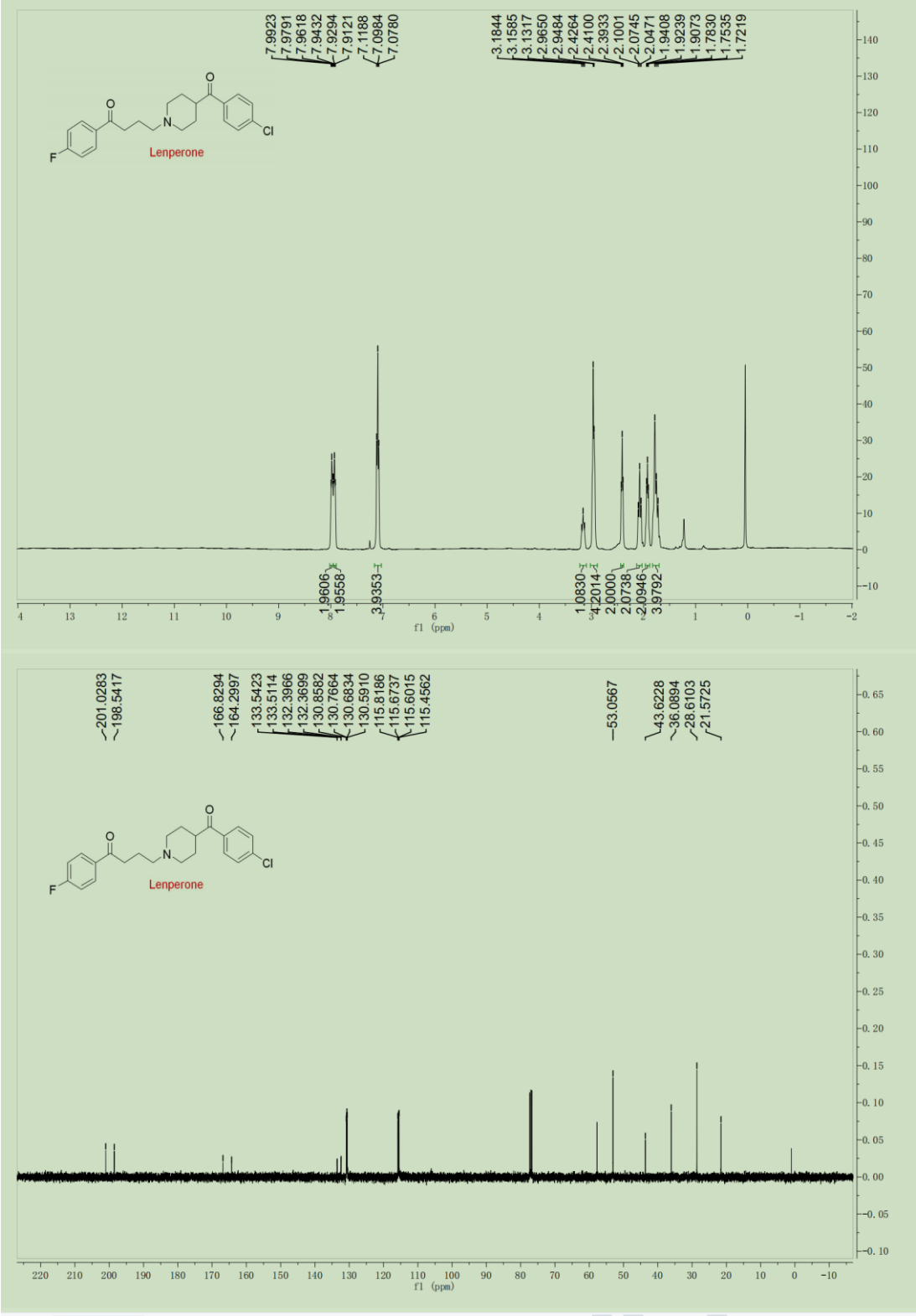

Ph
O
NH
O
16
166.4939
151.0513
133.8992
131.7480
129.6742
129.3077
128.5813
127.0576
123.6018
120.9985
116.6358
44.1781
f1 (ppm)


OH
17
7.7876
7.7681
7.5420
7.5229
7.3764
7.3581
7.3396
6.9674
6.9485
6.9300
5.0436
5.0283
2.4342
1.4365
1.4211
0.9211
1.0490
0.9732
0.9483
1.0000
1.0464
3.0304
f1 (ppm)


OH
17
147.4565
139.2767
129.1267
128.7252
126.3296
97.2060
73.6871
23.7545
f1 (ppm)


18
7.4336
7.4145
7.2617
7.2425
7.2235
6.9700
6.9518
6.9201
6.8994
3.8312
3.2040
1.6033
1.0002
0.9895
1.0168
0.9623
2.9834
3.0000
6.0761
f1 (ppm)


18
157.3882
133.3222
128.1200
127.4068
120.3050
111.6248
77.3979
77.0783
77.0267
76.7609
55.2240
50.5643
26.5693
f1 (ppm)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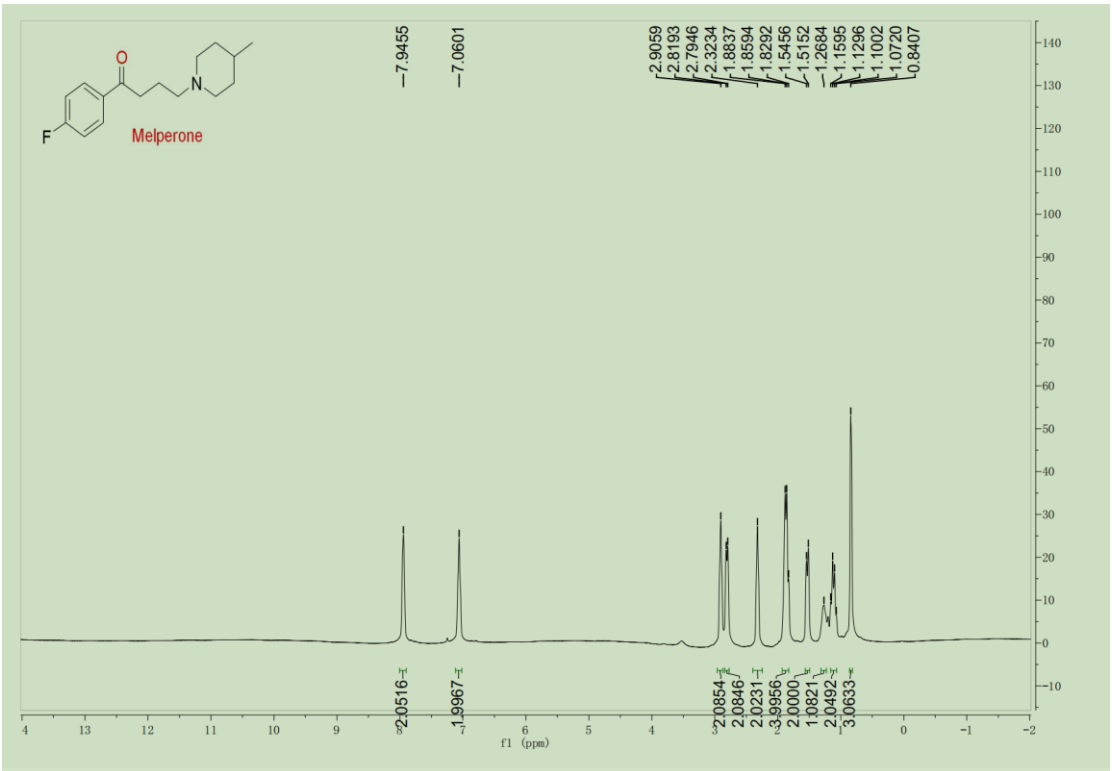
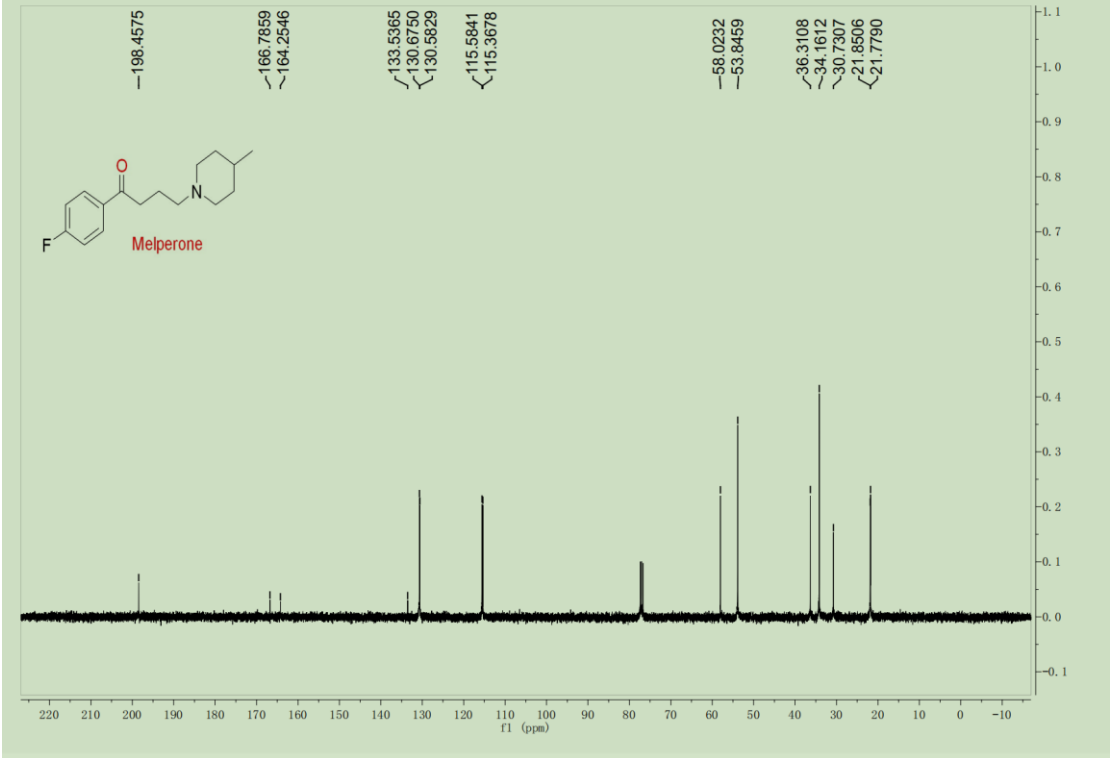
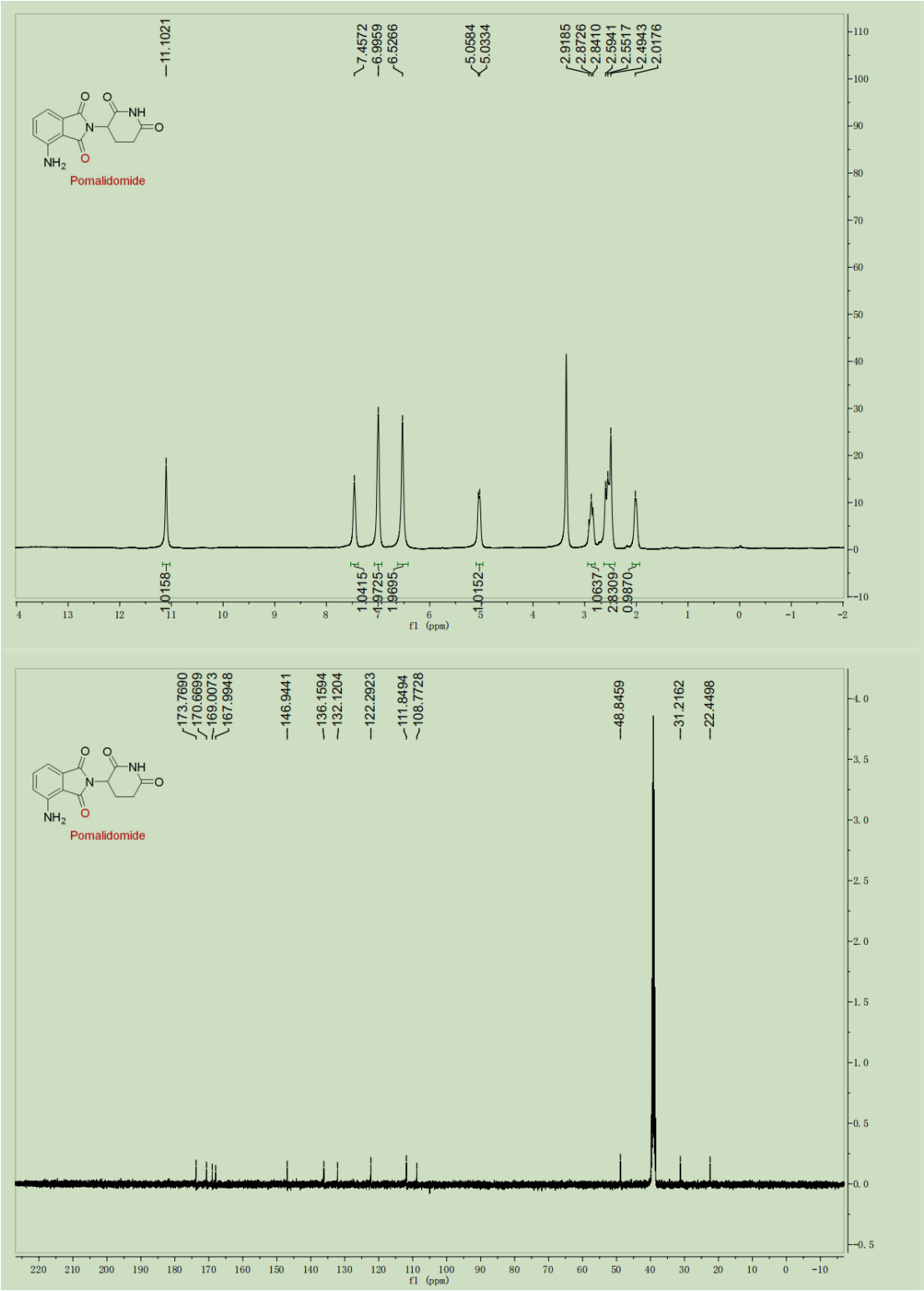
7.9618
7.9432
7.9294
7.9121
7.1188
7.0984
7.0780
3.1844
3.1585
3.1317
2.9650
2.9484
2.4264
2.4100
2.3933
2.1001
2.0745
2.0471
1.9408
1.9239
1.9073
1.7830
1.7535
1.7219
Lenperone
1.9606
1.9558
3.9353
1.0830
4.2014
2.0000
2.0738
2.0946
3.9792
f1 (ppm)
201.0283
198.5417
166.8294
164.2997
133.5423
133.5114
132.3966
132.3699
130.8582
130.7664
130.6834
130.5910
115.8186
115.6737
115.6015
115.4562
53.0567
43.6228
36.0894
28.6103
21.5725
Lenperone
f1 (ppm)


Melperone
7.9455
7.0601
2.9059
2.8193
2.7946
2.3234
1.8837
1.8594
1.8292
1.5456
1.5152
1.2684
1.1595
1.1296
1.1002
1.0720
0.8407
2.0516
1.9967
2.0854
2.0846
2.0231
3.9956
2.0000
1.0821
2.0492
3.0633
f1 (ppm)


Melperone
198.4575
166.7859
164.2546
133.5365
130.6750
130.5829
115.5841
115.3678
58.0232
53.8459
36.3108
34.1612
30.7307
21.8506
21.7790
f1 (ppm)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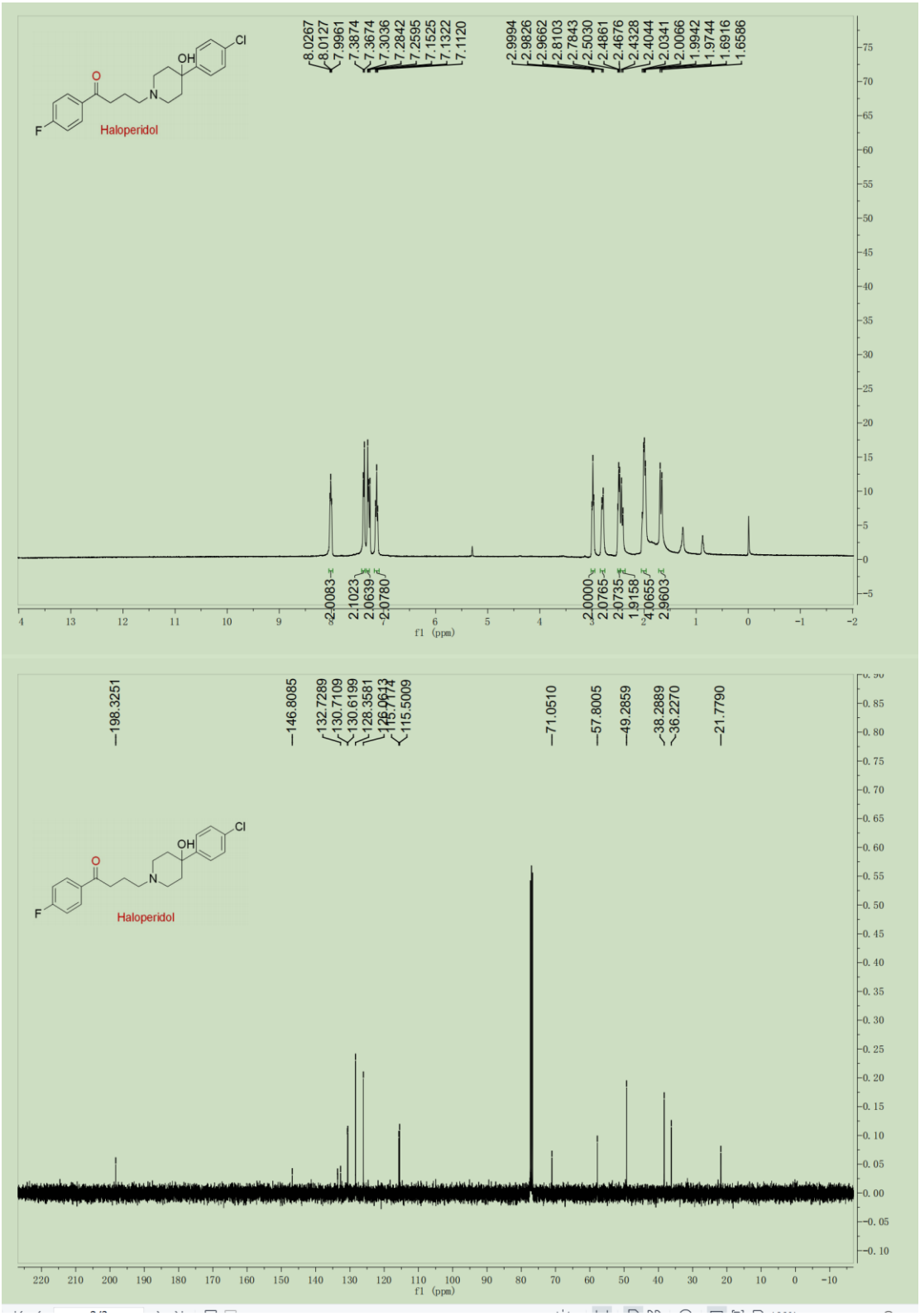
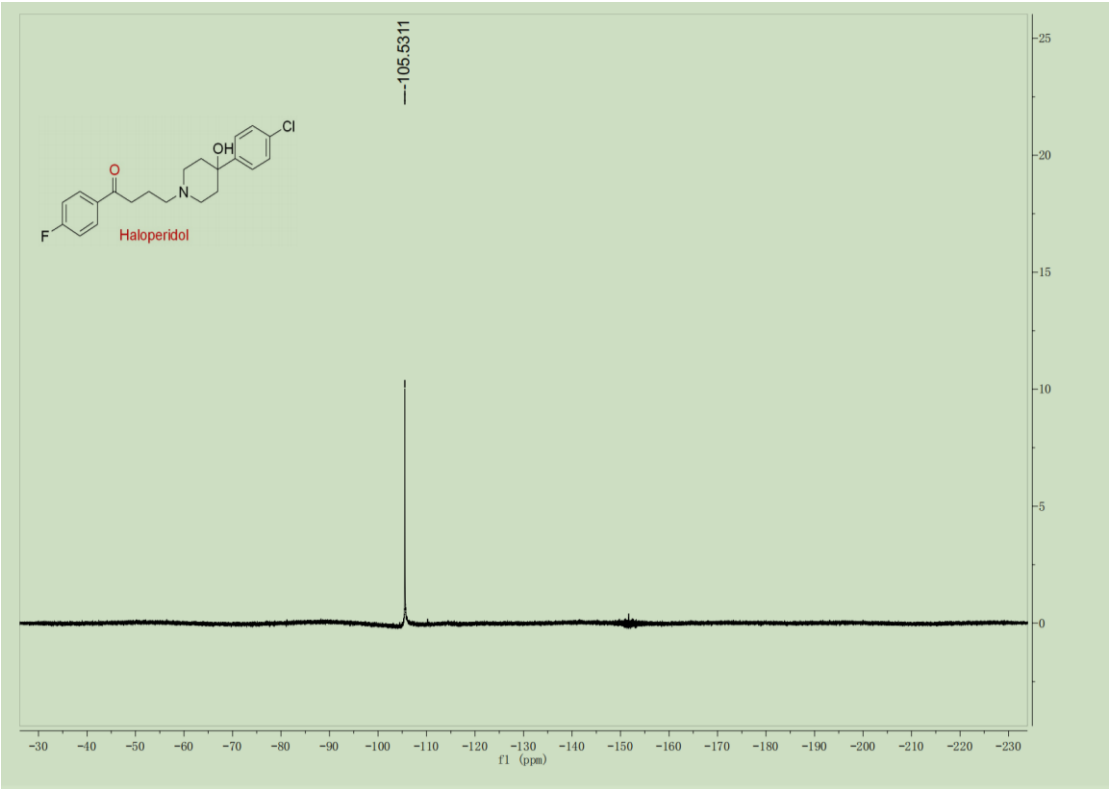
6.9959
6.5266
5.0584
5.0334
2.9185
2.8726
2.8410
2.5941
2.5517
2.4943
2.0176
1.0158
1.0415
0.9725
1.9695
1.0152
1.0637
2.8309
0.9870
f1 (ppm)
Pomalidomide
173.7690
170.6699
169.0073
167.9948
146.9441
136.1594
132.1204
122.2923
111.8494
108.7728
48.8459
31.2162
22.4498
f1 (ppm)
Pomalidomide


Haloperidol
8.0267
8.0127
7.9961
7.3874
7.3674
7.3036
7.2842
7.2595
7.1525
7.1322
7.1120
2.9994
2.9826
2.9662
2.8103
2.7843
2.5030
2.4861
2.4676
2.4328
2.4044
2.0341
2.0066
1.9942
1.9744
1.6916
1.6586
2.0083
2.1023
2.0639
2.0780
2.0000
2.0765
2.0735
1.9158
4.0655
2.9603
f1 (ppm)
Haloperidol
198.3251
146.8085
132.7289
130.7109
130.6199
128.3581
115.5009
71.0510
57.8005
49.2859
38.2889
36.2270
21.7790
f1 (ppm)


-105.5311
Cl
OH
O
N
F
Haloperidol
25
20
15
10
5
0
-30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210 -220 -230
f1 (ppm)