

Supporting Information for

Nitro - a Traceless Directing Group Switching the Site-Selectivity of Styrene Derivatives in [4 + 2] Annulation

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1. General information

Unless otherwise noted, chemicals and solvents were purchased with the highest purity grade available and were used without further purification. Purification of products was conducted by column chromatography on silica gel (200-300 mesh, from Qingdao, China). NMR spectra were measured on a Bruker ARX400 (^1H at 400 MHz, ^{13}C at 101 MHz, ^{19}F at 471 or 376 MHz) magnetic resonance spectrometer. Chemical shifts (δ) are reported in ppm using tetramethylsilane as internal standard (s = singlet, d = doublet, t = triplet, q = quartet, dd = doublet of doublets, td = triplet of doublets, dt = doublet of triplets, ddd = doublet of doublet of doublets, m = multiplet), and coupling constants (J) were reported in Hertz (Hz). HRMS data were obtained on a VG ZAB-HS mass spectrometer, Bruker Apex IV FTMS spectrometer.

The structure of our products were idea derivation of DFT calculations suggested mechanism and identified by comparing known products with literatures.

the spectra of **3b** are in accordance with those of the compound reported in the literature Adv. Synth. Catal. 2013, 355, 2044 and Org. Lett. 2021, 23, 3593-3598 .

the spectra of **3q** are in accordance with those of the compound reported in the literature Adv. Synth. Catal. 2013, 355, 2044 .

the spectra of **3g** are in accordance with those of the compound reported in the literature J. Med. Chem. 2004, 47, 2574

the spectra of **5g** are in accordance with those of the compound reported in the literature Org.Lett.2020, 22, 2230–2234

the spectra of **5z** are in accordance with those of the compound reported in the literature Synthesis, 2011, # 10, art. no. H19211SS, p. 1547

2. General Procedure

General procedure for the synthesis of quinolones via two-component 4+2 annulation

To a 20 mL test tube with a stir bar was charged with 0.3 mmol alkene **1**, 0.36 mmol oxalic monoamide, 0.03mmol AgNO_3 and 1.2 mmol $\text{K}_2\text{S}_2\text{O}_8$ followed by 2mL acquis acetone (v/v 1/1). The resulting mixture was reacted at 65°C overnight. or monitored by TLC. Upon completion, the reaction mixture was concentrated under reduced pressure. The residue was chromatographed through silica gel eluting with PE/EA to give the desired product **3** and **5**.

Substituted 2-(methyl(phenyl)amino)-2-oxoacetic acid (**1**), cinnamate (**2**) and (2-nitroalk-1-en-1-yl)benzene were commercial available from Jiangsu YUNPU New Pharmaceutical Material Technology Co., Ltd.

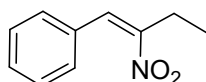
Procedure for synthesis of ethyl 2-nitro-3-phenylacrylate

To a round bottom flask were added. To the stirred ice cooled solution of ethyl cinnamate (5.68 mmol) and anhydrous CH_3CN (50 ml) were slowly added $(\text{NH}_4)_2\text{Ce}(\text{NO}_3)_6$ (17.0 mmol) and NaNO_2 (17.0 mmol). The reaction mixture was allowed to warm to room temperature naturely and stirred for 22 h, then filtered through Celite and the filter pad was washed with CH_3CN . The combined filtrate and washings were poured into cold water, extracted with

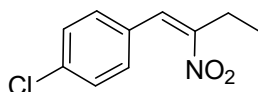
DCM, dried over Na_2SO_4 , filtered, and concentrated. The residue was separated by silica gel flash chromatography to offer the ethyl 2-nitro-3-phenylacrylate.

General procedure for synthesis of (2-nitroalk-1-en-1-yl)benzene

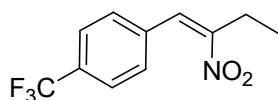
To a stirred mixture solution of aldehyde derivative (10 mmol) and nitroalkane (10 mmol) in methanol (5 mL) at 0 °C was added an aqueous solution of sodium hydroxide (15 mmol) over a period of 30 min. The stirring was continued for another half an hour in the temperature range from 0 to 5 °C. The mixture was allowed to warm to room temperature. Completion of the reaction was confirmed through monitoring by TLC (10–12 h). The post reaction mixture was mixed with water (20 mL) and poured over crushed ice containing concentrated HCl (2 mL). The yellow precipitate was filtered, dried in a vacuum desiccator, and crystallized from hot EtOH. The desired nitroolefins were obtained. Similarly, other nitroolefins were also synthesized.



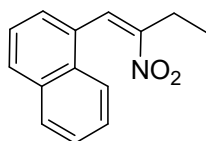
(2-nitrobut-1-en-1-yl)benzene was synthesized following the general procedure, benzaldehyde (1.06 g, 10 mmol) and nitroalkane (0.89 g, 10 mmol), was used to give (2-nitrobut-1-en-1-yl)benzene (0.49 g, 28%). white solid. The spectra are in accordance with those of the compound reported in the literature (European Journal of Organic Chemistry, 2020, vol. 2020, # 26, p. 4059 – 4066). ^1H NMR (400 MHz, CDCl_3) δ 8.05 (s, 1H), 7.57 – 7.40 (m, 5H), 2.90 (q, J = 7.4 Hz, 2H), 1.31 (t, J = 7.4 Hz, 3H). ^{13}C NMR (101 MHz, CDCl_3) δ 153.37 , 133.15 , 132.42 , 129.99 , 129.66 , 129.02 , 20.75 , 12.53 .



1-chloro-4-(2-nitrobut-1-en-1-yl)benzene was synthesized following the general procedure, 4-chlorobenzaldehyde (1.40 g, 10 mmol) and nitroalkane (0.89 g, 10 mmol), was used to give 1-chloro-4-(2-nitrobut-1-en-1-yl)benzene (0.83 g, 39%). white solid. The spectra are in accordance with those of the compound reported in the literature (Tetrahedron, 2009, vol. 65, # 23, p. 4578 – 4592) ^1H NMR (400 MHz, CDCl_3) δ 7.97 (s, 1H), 7.44 (d, J = 8.5 Hz, 2H), 7.35 (d, J = 8.5 Hz, 2H), 2.84 (q, J = 7.4 Hz, 2H), 1.28 (t, J = 7.4 Hz, 4H). ^{13}C NMR (101 MHz, CDCl_3) δ 153.65 , 136.15 , 131.81 , 130.82 (d, J = 6.0 Hz), 129.34 , 20.72 , 12.45 .

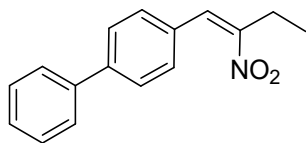


1-(2-nitrobut-1-en-1-yl)-4-(trifluoromethyl)benzene was synthesized following the general procedure, 4-trifluoromethylbenzaldehyde (1.74 g, 10 mmol) and nitroalkane (0.89 g, 10 mmol), was used to give 1-(2-nitrobut-1-en-1-yl)-4-(trifluoromethyl)benzene (0.36 g, 24 %). white solid. ^1H NMR (400 MHz, CDCl_3) δ 8.01 (s, 1H), 7.72 (d, J = 8.2 Hz, 2H), 7.52 (d, J = 8.1 Hz, 2H), 2.84 (q, J = 7.4 Hz, 2H), 1.28 (t, J = 7.4 Hz, 4H). ^{13}C NMR (101 MHz, CDCl_3) δ 154.95 , 136.02 , 131.55 (q, J = 31.9 Hz), 131.23 , 129.65 , 125.91 (q, J = 3.7 Hz), 123.68 (q, J = 272.4 Hz), 20.70 , 12.52 . ^{19}F NMR (376 MHz, CDCl_3) δ -62.97.



1-(2-nitrobut-1-en-1-yl)naphthalene was synthesized following the general procedure, 1-naphthaldehyde (1.56 g, 10 mmol) and nitroalkane (0.89 g, 10 mmol), was used to give 1-(2-nitrobut-1-en-1-yl)naphthalene (1.31 g, 57 %). white solid. The spectra are in accordance with those of the compound reported in the literature (European

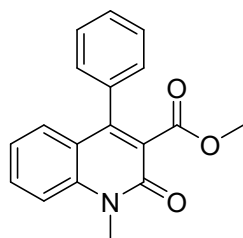
Journal of Organic Chemistry, 2020, vol. 2020, # 26, p. 4059 – 4066). ^1H NMR (400 MHz, CDCl_3) δ 8.49 (s, 1H), 7.92 – 7.82 (m, 3H), 7.57 – 7.46 (m, 3H), 7.39 (d, $J = 7.1$ Hz, 1H), 2.72 (q, $J = 7.4$ Hz, 2H), 1.18 (t, $J = 7.4$ Hz, 3H). ^{13}C NMR (101 MHz, CDCl_3) δ 154.94, 133.51, 131.53, 131.48, 130.17, 129.90, 128.81, 127.12, 126.69, 126.49, 125.29, 124.21, 20.96, 12.87.



4-(2-nitrobut-1-en-1-yl)-1,1'-biphenyl was synthesized following the general procedure, [1,1'-biphenyl]-4-carbaldehyde (1.82 g, 10 mmol) and nitroalkane (0.89 g, 10 mmol), was used to give 4-(2-nitrobut-1-en-1-yl)-1,1'-biphenyl (1.09 g, 43 %). white solid. The spectra are in accordance with those of the compound reported in the literature (Tetrahedron Letters, 2013, vol. 54, # 24, p. 3194 – 3198). ^1H NMR (400 MHz, CDCl_3) δ 8.05 (s, 1H), 7.68 (d, $J = 8.2$ Hz, 2H), 7.62 (d, $J = 7.5$ Hz, 2H), 7.48 (dd, $J = 15.5, 8.0$ Hz, 4H), 7.39 (t, $J = 7.3$ Hz, 1H), 2.92 (q, $J = 7.4$ Hz, 2H), 1.31 (t, $J = 7.4$ Hz, 3H). ^{13}C NMR (101 MHz, CDCl_3) δ 153.14, 142.87, 139.85, 132.87, 131.23, 130.35, 129.03, 128.12, 127.64, 127.11, 20.91, 12.54.

Other (2-nitroalk-1-en-1-yl)benzene were commercial available from Jiangsu YUNPU New Pharmaceutical Material Technology Co., Ltd.

3. Physical data



3a

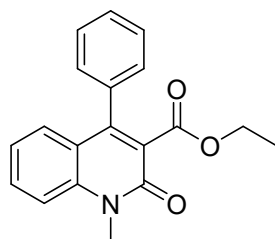
methyl 1-methyl-2-oxo-4-phenyl-1,2-dihydroquinoline-3-carboxylate

Pale yellow solid, prepared according to the general procedure from 2-(methyl(phenyl)amino)-2-oxoacetic acid (65 mg, 0.36 mmol) and methyl cinnamate (49 mg, 0.3 mmol), 12 h, 65 mg, 74 % yield.

^1H NMR (400 MHz, Chloroform-*d*) δ 7.55 (ddd, $J = 8.7, 7.2, 1.6$ Hz, 1H), 7.44 – 7.35 (m, 4H), 7.31 – 7.24 (m, 3H), 7.09 (ddd, $J = 8.2, 7.1, 1.1$ Hz, 1H), 3.73 (s, 3H), 3.53 (s, 3H).

^{13}C NMR (101 MHz, Chloroform-*d*) δ 166.24, 159.04, 148.20, 139.91, 134.42, 131.67, 128.90, 128.81, 128.41, 126.45, 122.41, 120.23, 114.39, 52.27, 29.71.

HRMS (ESI): calcd for $\text{C}_{18}\text{H}_{16}\text{NO}_3^+$ $[\text{M}+\text{H}]^+$: 294.1125; found: 294.1131.



3b

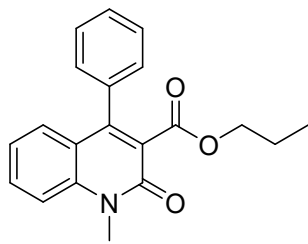
ethyl 1-methyl-2-oxo-4-phenyl-1,2-dihydroquinoline-3-carboxylate

Pale yellow solid, prepared according to the general procedure from 2-(methyl(phenyl)amino)-2-oxoacetic acid (65 mg, 0.36 mmol) and ethyl cinnamate (53 mg, 0.3 mmol), 12 h, 74.6 mg, 81 % yield. (the spectra of **3b** are in accordance with those of the compound reported in the literature Adv. Synth. Catal. 2013, 355, 2044 and Org. Lett. 2021, 23, 3593-3598)

^1H NMR (400 MHz, CDCl_3) δ 7.56 – 7.51 (m, 1H), 7.42 – 7.34 (m, 4H), 7.31 – 7.24 (m, 3H), 7.08 (t, $J = 7.6$ Hz, 1H), 4.01 (q, $J = 7.1$ Hz, 2H), 3.73 (s, 3H), 0.90 (t, $J = 7.1$ Hz, 3H).

^{13}C NMR (101 MHz, CDCl_3) δ 165.62, 159.04, 147.96, 139.88, 134.47, 131.58, 129.05 – 128.64 (m), 128.35, 122.37, 120.31, 114.36, 61.31, 29.73, 13.75.

HRMS (ESI): calcd for $\text{C}_{19}\text{H}_{18}\text{NO}_3^+$ $[\text{M}+\text{H}]^+$: 308.1281; found: 308.1288.



3c

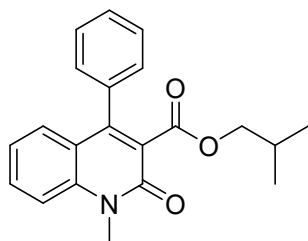
propyl 1-methyl-2-oxo-4-phenyl-1,2-dihydroquinoline-3-carboxylate

Pale yellow solid, prepared according to the general procedure from 2-(methyl(phenyl)amino)-2-oxoacetic acid (65 mg, 0.36 mmol) and propyl cinnamate (57 mg, 0.3 mmol), 12 h, 75 mg, 78 % yield.

¹H NMR (400 MHz, Chloroform-*d*) δ 7.54 (ddd, *J* = 8.6, 7.1, 1.6 Hz, 1H), 7.42 – 7.34 (m, 4H), 7.32 – 7.25 (m, 3H), 7.08 (ddd, *J* = 8.2, 7.0, 1.1 Hz, 1H), 3.91 (t, *J* = 6.7 Hz, 2H), 3.73 (s, 3H), 1.32 (h, *J* = 7.1 Hz, 2H), 0.66 (t, *J* = 7.4 Hz, 3H).

¹³C NMR (101 MHz, Chloroform-*d*) δ 165.82, 159.06, 147.78, 139.89, 134.50, 131.56, 128.97, 128.92, 128.87, 128.76, 128.39, 122.36, 120.31, 114.35, 67.02, 29.72, 21.64, 10.28.

HRMS (ESI): calcd for C₂₀H₂₀NO₃⁺ [M+H]⁺: 322.1438; found: 322.1449.



3d

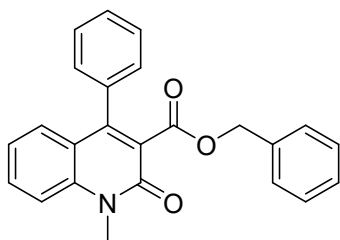
isobutyl 1-methyl-2-oxo-4-phenyl-1,2-dihydroquinoline-3-carboxylate

Pale yellow solid, prepared according to the general procedure from 2-(methyl(phenyl)amino)-2-oxoacetic acid (65 mg, 0.36 mmol) and isobutyl cinnamate (61 mg, 0.3 mmol), 12 h, 77 mg, 77 % yield.

¹H NMR (400 MHz, Chloroform-*d*) δ 7.53 (ddd, *J* = 8.6, 7.1, 1.6 Hz, 1H), 7.40 – 7.34 (m, 4H), 7.32 – 7.24 (m, 3H), 7.08 (ddd, *J* = 8.1, 7.1, 1.1 Hz, 1H), 3.77 – 3.67 (m, 5H), 1.61 (dq, *J* = 13.4, 6.7 Hz, 1H), 0.66 (d, *J* = 6.7 Hz, 6H).

¹³C NMR (101 MHz, Chloroform-*d*) δ 165.87, 159.06, 147.62, 139.87, 134.47, 131.53, 128.97, 128.87, 128.74, 128.42, 126.82, 122.34, 120.28, 114.34, 71.57, 29.71, 27.45, 18.94.

HRMS (ESI): calcd for C₂₁H₂₂NO₃⁺ [M+H]⁺: 336.1594; found: 336.1589.



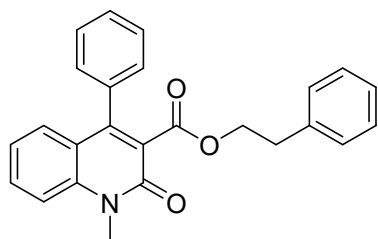
3e

benzyl 1-methyl-2-oxo-4-phenyl-1,2-dihydroquinoline-3-carboxylate

Pale yellow solid, prepared according to the general procedure from 2-(methyl(phenyl)amino)-2-oxoacetic acid (65 mg, 0.36 mmol) and benzyl cinnamate (72 mg, 0.3 mmol), 12 h, 78.6 mg, 71 % yield. $^1\text{H NMR}$ (400 MHz, Chloroform-*d*) δ 7.53 (ddd, $J = 8.6, 7.1, 1.6$ Hz, 1H), 7.37 – 7.28 (m, 4H), 7.23 (ddd, $J = 8.3, 5.4, 1.7$ Hz, 3H), 7.17 (dt, $J = 4.7, 3.0$ Hz, 3H), 7.07 (ddd, $J = 8.2, 7.0, 1.1$ Hz, 1H), 6.98 (dd, $J = 6.6, 2.9$ Hz, 2H), 4.98 (s, 2H), 3.72 (s, 3H).

$^{13}\text{C NMR}$ (101 MHz, Chloroform-*d*) δ 165.59, 159.06, 148.16, 139.92, 135.27, 134.25, 131.69, 128.91, 128.79, 128.44, 128.40, 128.38, 128.07, 122.42, 120.26, 114.39, 67.21, 29.78.

HRMS (ESI): calcd for $\text{C}_{24}\text{H}_{20}\text{NO}_3^+$ $[\text{M}+\text{H}]^+$: 370.1438; found: 370.1449.



3f

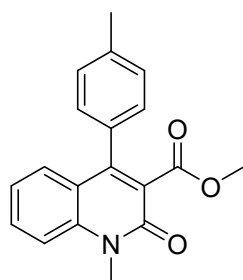
phenethyl 1-methyl-2-oxo-4-phenyl-1,2-dihydroquinoline-3-carboxylate

Pale yellow solid, prepared according to the general procedure from 2-(methyl(phenyl)amino)-2-oxoacetic acid (65 mg, 0.36 mmol) and phenethyl cinnamate (76 mg, 0.3 mmol), 12 h, 86 mg, 75 % yield.

$^1\text{H NMR}$ (400 MHz, Chloroform-*d*) δ 7.53 (ddd, $J = 8.7, 7.1, 1.6$ Hz, 1H), 7.39 – 7.29 (m, 4H), 7.25 (dd, $J = 8.1, 1.5$ Hz, 1H), 7.19 (ddd, $J = 12.6, 5.8, 3.8$ Hz, 4H), 7.14 – 7.10 (m, 1H), 7.08 (t, $J = 7.6$ Hz, 1H), 7.05 – 7.00 (m, 2H), 4.14 (t, $J = 7.4$ Hz, 2H), 3.73 (s, 3H), 2.59 (t, $J = 7.3$ Hz, 2H).

$^{13}\text{C NMR}$ (101 MHz, Chloroform-*d*) δ 165.70, 159.04, 148.03, 139.91, 137.63, 134.38, 131.65, 128.90, 128.86, 128.77, 128.44, 128.40, 126.51, 126.46, 122.41, 120.25, 114.39, 65.83, 34.55, 29.74.

HRMS (ESI): calcd for $\text{C}_{25}\text{H}_{22}\text{NO}_3^+$ $[\text{M}+\text{H}]^+$: 384.1594; found: 384.1590.



3g

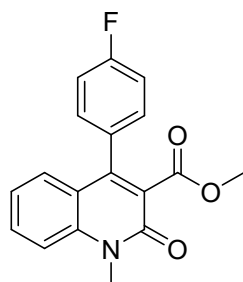
methyl 1-methyl-2-oxo-4-(p-tolyl)-1,2-dihydroquinoline-3-carboxylate

Pale yellow solid, prepared according to the general procedure from 2-(methyl(phenyl)amino)-2-oxoacetic acid (65 mg, 0.36 mmol) and methyl 3-(p-tolyl)acrylate (53 mg, 0.3 mmol), 12 h, 56 mg, 61 % yield. (the spectra of **3g** are in accordance with those of the compound reported in the literature J. Med. Chem. 2004, 47, 2574)

$^1\text{H NMR}$ (400 MHz, Chloroform-*d*) δ 7.53 (ddd, $J = 8.6, 7.1, 1.5$ Hz, 1H), 7.35 (dd, $J = 8.5, 1.0$ Hz, 1H), 7.30 (dd, $J = 8.0, 1.5$ Hz, 1H), 7.18 (q, $J = 8.0$ Hz, 4H), 7.08 (ddd, $J = 8.2, 7.1, 1.0$ Hz, 1H), 3.72 (s, 3H), 3.56 (s, 3H), 2.35 (s, 3H).

^{13}C NMR (101 MHz, Chloroform-*d*) δ 166.42, 159.12, 148.36, 139.90, 138.82, 131.59, 131.41, 129.13, 128.87, 128.73, 126.43, 122.35, 120.42, 114.36, 52.30, 29.69, 21.38.

HRMS (ESI): calcd for $\text{C}_{19}\text{H}_{18}\text{NO}_3^+$ $[\text{M}+\text{H}]^+$: 308.1281; found: 308.1282.



3h

methyl 4-(4-fluorophenyl)-1-methyl-2-oxo-1,2-dihydroquinoline-3-carboxylate

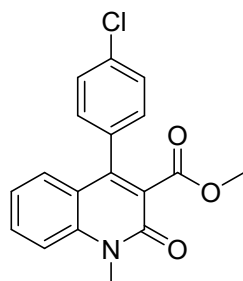
Pale yellow solid, prepared according to the general procedure from 2-(methyl(phenyl)amino)-2-oxoacetic acid (65 mg, 0.36 mmol) and methyl 3-(4-fluorophenyl)acrylate (54 mg, 0.3 mmol), 12 h, 80 mg, 86 % yield.

^1H NMR (400 MHz, Chloroform-*d*) δ 7.55 (t, $J = 7.9$ Hz, 1H), 7.37 (d, $J = 8.5$ Hz, 1H), 7.30 – 7.19 (m, 3H), 7.15 – 7.06 (m, 3H), 3.72 (s, 3H), 3.56 (s, 3H).

^{13}C NMR (101 MHz, Chloroform-*d*) δ 166.15, 163.00 (d, $J = 249.1$ Hz), 158.93, 147.15, 139.91, 131.82, 130.80 (d, $J = 8.5$ Hz), 130.30 (d, $J = 3.6$ Hz), 128.54, 126.81, 122.53, 120.16, 115.66 (d, $J = 21.8$ Hz), 114.50, 52.38, 29.75.

^{19}F NMR (377 MHz, Chloroform-*d*) δ -112.04.

HRMS (ESI): calcd for $\text{C}_{18}\text{H}_{15}\text{FNO}_3^+$ $[\text{M}+\text{H}]^+$: 312.1030; found: 312.1033.



3i

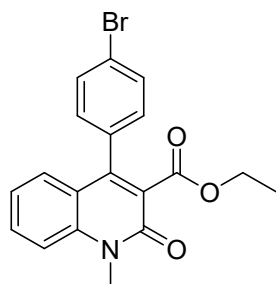
methyl 4-(4-chlorophenyl)-1-methyl-2-oxo-1,2-dihydroquinoline-3-carboxylate

Pale yellow solid, prepared according to the general procedure from 2-(methyl(phenyl)amino)-2-oxoacetic acid (65 mg, 0.36 mmol) and methyl 3-(4-chlorophenyl)acrylate (59 mg, 0.3 mmol), 12 h, 80.6 mg, 82 % yield.

^1H NMR (400 MHz, Chloroform-*d*) δ 7.64 (ddd, $J = 8.7, 7.1, 1.6$ Hz, 1H), 7.50 – 7.43 (m, 3H), 7.33 – 7.27 (m, 3H), 7.19 (ddd, $J = 8.1, 7.1, 1.1$ Hz, 1H), 3.81 (s, 3H), 3.66 (s, 3H).

^{13}C NMR (101 MHz, Chloroform-*d*) δ 166.03, 158.87, 146.92, 139.91, 135.15, 132.79, 131.86, 130.27, 128.79, 128.48, 126.64, 122.55, 119.92, 114.52, 52.44, 29.76.

HRMS (ESI): calcd for $\text{C}_{18}\text{H}_{15}\text{ClNO}_3^+$ $[\text{M}+\text{H}]^+$: 328.0735; found: 328.0742.



3j

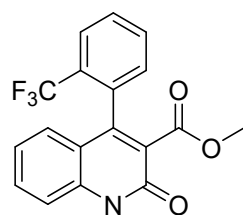
ethyl 4-(4-bromophenyl)-1-methyl-2-oxo-1,2-dihydroquinoline-3-carboxylate

Pale yellow solid, prepared according to the general procedure from 2-(methyl(phenyl)amino)-2-oxoacetic acid (65 mg, 0.36 mmol) and ethyl 3-(4-bromophenyl)acrylate (53 mg, 0.3 mmol), 12 h, 71.8 mg, 62 % yield.

^1H NMR (400 MHz, Chloroform-*d*) δ 7.60 – 7.50 (m, 3H), 7.36 (d, J = 8.5 Hz, 1H), 7.23 – 7.15 (m, 3H), 7.12 – 7.07 (m, 1H), 4.05 (q, J = 7.2 Hz, 2H), 3.72 (s, 3H), 0.97 (t, J = 7.1 Hz, 3H).

^{13}C NMR (101 MHz, Chloroform-*d*) δ 165.43, 158.86, 146.66, 139.90, 133.35, 131.81, 131.66, 130.67, 128.42, 126.78, 123.28, 122.53, 119.90, 114.50, 61.50, 29.77, 13.84.

HRMS (ESI): calcd for $\text{C}_{19}\text{H}_{17}\text{BrNO}_3^+$ $[\text{M}+\text{H}]^+$: 386.0386; found: 386.0377.



3k

methyl 1-methyl-2-oxo-4-(2-(trifluoromethyl)phenyl)-1,2-dihydroquinoline-3-carboxylate

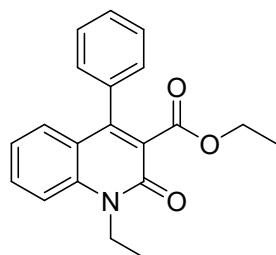
Pale yellow solid, prepared according to the general procedure from 2-(methyl(phenyl)amino)-2-oxoacetic acid (65 mg, 0.36 mmol) and methyl 3-(2-(trifluoromethyl)phenyl)acrylate (69 mg, 0.3 mmol), 12 h, 41.1 mg, 38 % yield.

^1H NMR (400 MHz, Chloroform-*d*) δ 7.37 (d, J = 8.5 Hz, 1H), 7.28 – 7.23 (m, 1H), 7.10 – 7.04 (m, 1H), 6.89 (dd, J = 8.1, 1.5 Hz, 1H), 3.74 (s, 3H), 3.51 (s, 3H).

^{13}C NMR (101 MHz, Chloroform-*d*) δ 165.48, 158.75, 146.86, 139.58, 132.48, 131.90, 131.66, 130.95, 129.30, 129.06 (q, J = 30.8 Hz), 128.75, 126.69 (q, J = 4.5 Hz), 126.10, 123.59 (q, J = 274.4 Hz), 122.41, 120.32, 114.33, 52.17, 29.82.

^{19}F NMR (376 MHz, Chloroform-*d*) δ -58.90.

HRMS (ESI): calcd for $\text{C}_{19}\text{H}_{15}\text{F}_3\text{NO}_3^+$ $[\text{M}+\text{H}]^+$: 362.0999; found: 362.1003.



3l

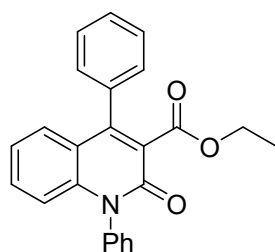
ethyl 1-ethyl-2-oxo-4-phenyl-1,2-dihydroquinoline-3-carboxylate

Pale yellow solid, prepared according to the general procedure from 2-(ethyl(phenyl)amino)-2-oxoacetic acid (70mg, 0.36 mmol) and ethyl cinnamate (53 mg, 0.3 mmol), 11 h, 80 mg, 83 % yield.

$^1\text{H NMR}$ (400 MHz, CDCl_3) δ 7.58 – 7.49 (m, 1H), 7.42 – 7.35 (m, 4H), 7.31 – 7.25 (m, 3H), 7.07 (t, $J = 7.6$ Hz, 1H), 4.37 (q, $J = 7.1$ Hz, 2H), 4.01 (q, $J = 7.1$ Hz, 2H), 1.36 (t, $J = 7.1$ Hz, 3H), 0.90 (t, $J = 7.1$ Hz, 3H).

$^{13}\text{C NMR}$ (101 MHz, CDCl_3) δ 165.69 , 158.52 , 147.85 , 138.89 , 134.56 , 131.49 , 128.86 (d, $J = 15.5$ Hz), 128.33 , 126.67 , 122.10 , 120.54 , 114.20 , 61.29 , 37.73 , 13.74 , 12.66 .

HRMS (ESI): calcd for $\text{C}_{20}\text{H}_{20}\text{NO}_3^+$ $[\text{M}+\text{H}]^+$: 322.1438; found: 322.1432.



3m

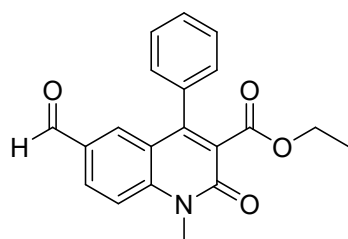
ethyl 2-oxo-1,4-diphenyl-1,2-dihydroquinoline-3-carboxylate

Pale yellow solid, prepared according to the general procedure from 2-(diphenylamino)-2-oxoacetic acid (87 mg, 0.36 mmol) and ethyl cinnamate (53 mg, 0.3 mmol), 13 h, 60.9 mg, 55 % yield.

$^1\text{H NMR}$ (400 MHz, Chloroform-*d*) δ 7.54 (dd, $J = 8.3, 6.7$ Hz, 2H), 7.49 – 7.40 (m, 4H), 7.37 (dd, $J = 7.2, 2.5$ Hz, 2H), 7.32 – 7.26 (m, 4H), 7.04 (ddd, $J = 8.2, 7.0, 1.1$ Hz, 1H), 6.68 (d, $J = 8.4$ Hz, 1H), 4.01 (q, $J = 7.1$ Hz, 2H), 0.93 (t, $J = 7.1$ Hz, 3H).

$^{13}\text{C NMR}$ (101 MHz, Chloroform-*d*) δ 165.39, 158.94, 148.79, 141.01, 137.16, 134.50, 131.08, 130.19, 129.08, 128.95, 128.90, 128.43, 128.32, 127.10, 122.51, 120.06, 116.24, 61.38, 13.78.

HRMS (ESI): calcd for $\text{C}_{24}\text{H}_{20}\text{NO}_3^+$ $[\text{M}+\text{H}]^+$: 370.1438; found: 370.1441.



3n

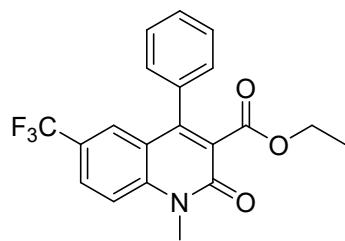
ethyl 6-formyl-1-methyl-2-oxo-4-phenyl-1,2-dihydroquinoline-3-carboxylate

Pale yellow solid, prepared according to the general procedure from 2-((4-formylphenyl)(methyl)amino)-2-oxoacetic acid (75 mg, 0.36 mmol) and ethyl cinnamate (53 mg, 0.3 mmol), 11 h, 70.4 mg, 70 % yield.

$^1\text{H NMR}$ (400 MHz, CDCl_3) δ 9.81 (s, 1H), 8.06 (dd, $J = 8.8, 1.9$ Hz, 1H), 7.75 (d, $J = 1.8$ Hz, 1H), 7.50 (d, $J = 8.8$ Hz, 1H), 7.47 – 7.42 (m, 3H), 7.33 – 7.27 (m, 2H), 4.03 (q, $J = 7.1$ Hz, 2H), 3.77 (s, 3H), 0.91 (t, $J = 7.1$ Hz, 3H).

$^{13}\text{C NMR}$ (101 MHz, CDCl_3) δ 190.39 , 164.98 , 159.05 , 147.95 , 143.77 , 133.52 , 132.25 , 130.94 , 130.69 , 129.39 , 128.77 (d, $J = 14.9$ Hz), 127.61 , 120.29 , 115.25 , 61.56 , 30.19 , 13.72 .

HRMS (ESI): calcd for $C_{20}H_{18}NO_4^+$ $[M+H]^+$: 336.1230; found: 336.1237.



3o

ethyl 1-methyl-2-oxo-4-phenyl-6-(trifluoromethyl)-1,2-dihydroquinoline-3-carboxylate

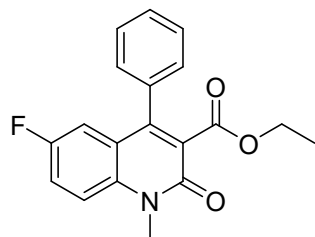
Pale yellow solid, prepared according to the general procedure from 2-(methyl(4-(trifluoromethyl)phenyl)amino)-2-oxoacetic acid (89 mg, 0.36 mmol) and ethyl cinnamate (53 mg, 0.3 mmol), 12 h, 82 mg, 73 % yield.

1H NMR (400 MHz, $CDCl_3$) δ 7.76 (dd, $J = 8.9, 1.8$ Hz, 1H), 7.52 (s, 1H), 7.46 (d, $J = 9.0$ Hz, 1H), 7.45 – 7.39 (m, 3H), 7.30 – 7.26 (m, 2H), 4.02 (q, $J = 7.1$ Hz, 2H), 3.75 (s, 3H), 0.91 (t, $J = 7.1$ Hz, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 165.02, 158.94, 147.56, 141.85, 133.41, 129.39, 128.82, 128.69, 127.98 – 127.83 (m), 125.98 (q, $J = 4.2$ Hz), 124.68 (q, $J = 33.5$ Hz), 123.74 (q, $J = 271.8$ Hz), 120.11, 114.99, 61.56, 30.03, 13.73.

^{19}F NMR (376 MHz, $CDCl_3$) δ -61.97.

HRMS (ESI): calcd for $C_{20}H_{17}F_3NO_3^+$ $[M+H]^+$: 376.1155; found: 376.1148.



3p

ethyl 6-fluoro-1-methyl-2-oxo-4-phenyl-1,2-dihydroquinoline-3-carboxylate

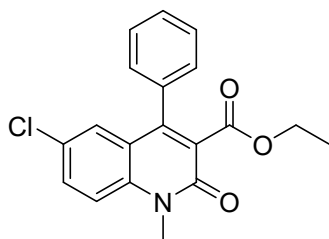
Pale yellow solid, prepared according to the general procedure from 2-((4-fluorophenyl)(methyl)amino)-2-oxoacetic acid (71 mg, 0.36 mmol) and ethyl cinnamate (53 mg, 0.3 mmol), 12 h, 77 mg, 79 % yield.

1H NMR (400 MHz, $CDCl_3$) δ 7.45 – 7.38 (m, 3H), 7.34 (dd, $J = 9.2, 4.6$ Hz, 1H), 7.30 – 7.24 (m, 3H), 6.94 (dd, $J = 9.3, 2.8$ Hz, 1H), 4.02 (q, $J = 7.1$ Hz, 2H), 3.73 (s, 3H), 0.90 (t, $J = 7.1$ Hz, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 158.71, 157.90 (d, $J = 242.7$ Hz), 147.01 (d, $J = 3.1$ Hz), 136.44, 133.90, 129.15, 128.81, 128.57, 127.78, 121.42 (d, $J = 8.1$ Hz), 119.37 (d, $J = 24.0$ Hz), 115.97 (d, $J = 8.0$ Hz), 113.89 (d, $J = 23.9$ Hz), 61.45, 30.00, 13.74.

^{19}F NMR (377 MHz, $CDCl_3$) δ -119.80.

HRMS (ESI): calcd for $C_{19}H_{17}FNO_3^+$ $[M+H]^+$: 326.1187; found: 326.1190.



3q

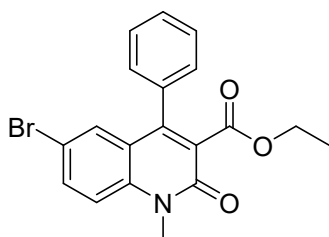
ethyl 6-chloro-1-methyl-2-oxo-4-phenyl-1,2-dihydroquinoline-3-carboxylate

Pale yellow solid, prepared according to the general procedure from 2-((4-chlorophenyl)(methyl)amino)-2-oxoacetic acid (77 mg, 0.36 mmol) and ethyl cinnamate (53 mg, 0.3 mmol), 12 h, 76.7 mg, 75 % yield. (the spectra of **3q** are in accordance with those of the compound reported in the literature Adv. Synth. Catal. 2013, 355, 2044)

$^1\text{H NMR}$ (400 MHz, CDCl_3) δ 7.48 (dd, $J = 9.0, 2.4$ Hz, 1H), 7.44 – 7.39 (m, 3H), 7.28 (ddd, $J = 9.2, 6.3, 5.9$ Hz, 3H), 7.22 – 7.17 (m, 1H), 4.01 (q, $J = 7.1$ Hz, 2H), 3.71 (s, 3H), 0.90 (t, $J = 7.1$ Hz, 3H).

$^{13}\text{C NMR}$ (101 MHz, CDCl_3) δ 165.21 , 158.70 , 146.89 , 138.41 , 133.71 , 131.59 , 129.19 , 128.85 , 128.59 , 128.12 , 127.75 (d, $J = 6.5$ Hz), 121.49 , 115.86 , 61.47 , 29.92 , 13.73 .

HRMS (ESI): calcd for $\text{C}_{19}\text{H}_{17}\text{ClNO}_3^+$ $[\text{M}+\text{H}]^+$: 342.0891; found: 342.0890.



3r

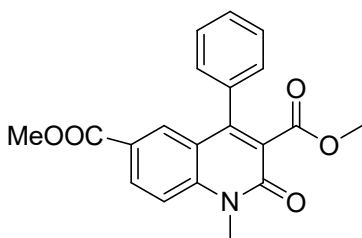
ethyl 6-bromo-1-methyl-2-oxo-4-phenyl-1,2-dihydroquinoline-3-carboxylate

Pale yellow solid, prepared according to the general procedure from 2-((4-bromophenyl)(methyl)amino)-2-oxoacetic acid (93 mg, 0.36 mmol) and ethyl cinnamate (53 mg, 0.3 mmol), 12 h, 77.6 mg, 67 % yield.

$^1\text{H NMR}$ (400 MHz, CDCl_3) δ 7.61 (dd, $J = 9.0, 2.3$ Hz, 1H), 7.41 (dd, $J = 6.5, 3.5$ Hz, 3H), 7.35 (d, $J = 2.2$ Hz, 1H), 7.29 – 7.22 (m, 3H), 4.01 (q, $J = 7.1$ Hz, 2H), 3.70 (s, 3H), 0.90 (t, $J = 7.1$ Hz, 3H).

$^{13}\text{C NMR}$ (101 MHz, CDCl_3) δ 165.18 , 158.68 , 146.83 , 138.82 , 134.35 , 133.67 , 130.79 , 129.20 , 128.85 , 128.60 , 127.69 , 121.92 , 116.13 , 115.52 , 61.47 , 29.88 , 13.73 .

HRMS (ESI): calcd for $\text{C}_{19}\text{H}_{17}\text{BrNO}_3^+$ $[\text{M}+\text{H}]^+$: 386.0386; found: 386.0389.



3s

dimethyl 1-methyl-2-oxo-4-phenyl-1,2-dihydroquinoline-3,6-dicarboxylate

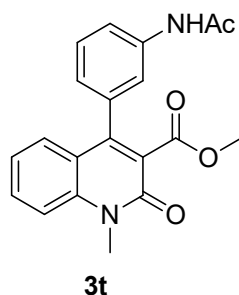
Pale yellow solid, prepared according to the general procedure from 2-((4-(methoxycarbonyl)phenyl)(methyl)amino)-2-oxoacetic acid (85 mg, 0.36 mmol) and ethyl cinnamate (49

mg, 0.3 mmol), 12 h, 81.1 mg, 77 % yield.

^1H NMR (400 MHz, CDCl_3) δ 8.17 (dd, $J = 8.9, 1.9$ Hz, 1H), 7.97 (d, $J = 1.9$ Hz, 1H), 7.45 – 7.39 (m, 4H), 7.28 (dd, $J = 6.6, 3.0$ Hz, 2H), 3.77 (s, 3H), 3.74 (s, 3H), 3.54 (s, 3H).

^{13}C NMR (101 MHz, CDCl_3) δ 165.92 (d, $J = 18.6$ Hz), 159.07, 148.35, 142.78, 133.70, 132.29, 130.78, 129.31, 128.70 (d, $J = 8.7$ Hz), 127.16, 124.31, 119.84, 114.53, 52.35 (d, $J = 9.5$ Hz), 30.05.

HRMS (ESI): calcd for $\text{C}_{20}\text{H}_{18}\text{NO}_5^+$ $[\text{M}+\text{H}]^+$: 352.1179; found: 352.1190.



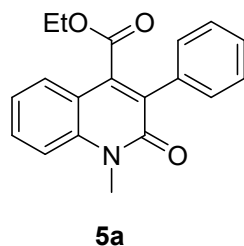
methyl 4-(3-acetamidophenyl)-1-methyl-2-oxo-1,2-dihydroquinoline-3-carboxylate

Pale yellow solid, prepared according to the general procedure from 2-(methyl(phenyl)amino)-2-oxoacetic acid (65 mg, 0.36 mmol) and methyl 3-(3-acetamidophenyl)acrylate (66 mg, 0.3 mmol), 12 h, 45.3 mg, 43 % yield.

^1H NMR (400 MHz, CDCl_3) δ 7.78 (s, 1H), 7.74 (d, $J = 8.1$ Hz, 1H), 7.52 (t, $J = 7.8$ Hz, 1H), 7.33 (d, $J = 7.5$ Hz, 2H), 7.31 – 7.25 (m, 2H), 7.08 (t, $J = 7.6$ Hz, 1H), 6.97 (d, $J = 7.4$ Hz, 1H), 3.70 (s, 3H), 3.52 (s, 3H), 2.10 (s, 3H).

^{13}C NMR (101 MHz, CDCl_3) δ 168.79, 166.31, 159.05, 147.84, 139.77, 138.35, 134.89, 131.78, 129.20, 128.81, 126.19, 124.35, 122.56, 120.33, 119.92 (d, $J = 17.6$ Hz), 114.41, 52.40, 29.78, 24.57.

HRMS (ESI): calcd for $\text{C}_{20}\text{H}_{19}\text{N}_2\text{O}_4^+$ $[\text{M}+\text{H}]^+$: 351.1345; found: 352.1363.



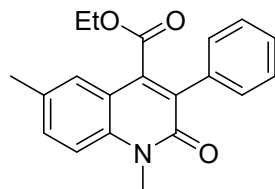
ethyl 1-methyl-2-oxo-3-phenyl-1,2-dihydroquinoline-4-carboxylate

Pale yellow solid, prepared according to the general procedure from 2-(methyl(phenyl)amino)-2-oxoacetic acid (65 mg, 0.36 mmol) and ethyl 2-nitro-3-phenylacrylate (67 mg, 0.3 mmol), 12 h, 62.1 mg, 56 % yield.

^1H NMR (400 MHz, Chloroform-*d*) δ 7.65 – 7.58 (m, 2H), 7.45 – 7.36 (m, 6H), 7.29 (d, $J = 7.6$ Hz, 1H), 4.13 (q, $J = 7.1$ Hz, 2H), 3.80 (s, 3H), 0.95 (t, $J = 7.1$ Hz, 3H).

^{13}C NMR (101 MHz, Chloroform-*d*) δ 166.50, 161.29, 140.27, 139.66, 134.80, 130.97, 129.54, 128.38, 128.04, 126.50, 122.68, 117.23, 114.48, 61.78, 30.28, 13.61.

HRMS (ESI): calcd for $\text{C}_{19}\text{H}_{18}\text{NO}_3^+$ $[\text{M}+\text{H}]^+$: 308.1281; found: 308.1275.



5b

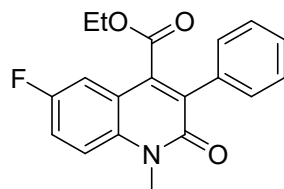
ethyl 1,6-dimethyl-2-oxo-3-phenyl-1,2-dihydroquinoline-4-carboxylate

yellow solid, prepared according to the general procedure from 2-(methyl(*p*-tolyl)amino)-2-oxoacetic acid (70 mg, 0.36 mmol) and ethyl 2-nitro-3-phenylacrylate (67 mg, 0.3 mmol), 10 h, 48.1 mg, 50 % yield.

^1H NMR (400 MHz, CDCl_3) δ 7.45 – 7.30 (m, 8H), 4.13 (q, $J = 7.1$ Hz, 2H), 3.78 (s, 3H), 2.43 (s, 3H), 0.94 (t, $J = 7.1$ Hz, 3H).

^{13}C NMR (101 MHz, CDCl_3) δ 166.63, 161.12, 140.03, 137.72, 134.94, 132.27 (d, $J = 4.8$ Hz), 130.61, 129.56, 128.28, 128.00, 126.12, 117.09, 114.39, 61.73, 30.26, 20.80, 13.59.

HRMS (ESI): calcd for $\text{C}_{20}\text{H}_{20}\text{NO}_3^+$ $[\text{M}+\text{H}]^+$: 322.1438; found: 322.1431.



5c

ethyl 6-fluoro-1-methyl-2-oxo-3-phenyl-1,2-dihydroquinoline-4-carboxylate

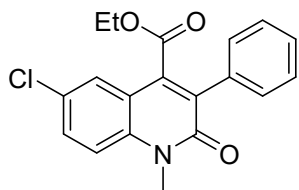
Pale yellow solid, prepared according to the general procedure from 2-((4-fluorophenyl)(methyl)amino)-2-oxoacetic acid (71 mg, 0.36 mmol) and ethyl 2-nitro-3-phenylacrylate (67 mg, 0.3 mmol), 10 h, 42.9 mg, 44 % yield.

^1H NMR (400 MHz, Chloroform-*d*) δ 7.40 (d, $J = 4.5$ Hz, 5H), 7.37 (d, $J = 3.4$ Hz, 1H), 7.36 – 7.30 (m, 2H), 4.12 (q, $J = 7.1$ Hz, 2H), 3.79 (s, 3H), 0.94 (t, $J = 7.1$ Hz, 3H).

^{13}C NMR (101 MHz, Chloroform-*d*) δ 166.12, 160.89, 158.02 (d, $J = 242.8$ Hz), 139.26 (d, $J = 3.6$ Hz), 136.25, 134.63, 132.21, 129.42, 128.58, 128.09, 118.77 (d, $J = 23.6$ Hz), 118.09 (d, $J = 8.7$ Hz), 116.04 (d, $J = 8.1$ Hz), 111.92 (d, $J = 24.0$ Hz), 61.97, 30.55, 13.55.

^{19}F NMR (376 MHz, Chloroform-*d*) δ -119.71.

HRMS (ESI): calcd for $\text{C}_{19}\text{H}_{17}\text{FNO}_3^+$ $[\text{M}+\text{H}]^+$: 326.1187; found: 326.1191.



5d

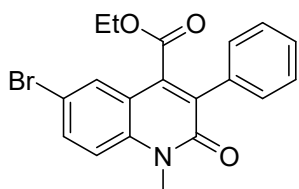
ethyl 6-chloro-1-methyl-2-oxo-3-phenyl-1,2-dihydroquinoline-4-carboxylate

Pale yellow solid, prepared according to the general procedure from 2-((4-chlorophenyl)(methyl)amino)-2-oxoacetic acid (77 mg, 0.36 mmol) and ethyl 2-nitro-3-phenylacrylate (67 mg, 0.3 mmol), 10 h, 44 mg, 43 % yield.

$^1\text{H NMR}$ (400 MHz, CDCl_3) δ 7.59 (d, $J = 2.2$ Hz, 1H), 7.56 (dd, $J = 8.9, 2.3$ Hz, 1H), 7.42 – 7.38 (m, 5H), 7.36 (d, $J = 9.0$ Hz, 1H), 4.13 (q, $J = 7.1$ Hz, 2H), 3.78 (s, 3H), 0.93 (t, $J = 7.1$ Hz, 3H).

$^{13}\text{C NMR}$ (101 MHz, CDCl_3) δ 166.00, 160.92, 139.08, 138.18, 134.50, 132.09, 130.95, 129.42, 128.61, 128.18 (d, $J = 16.7$ Hz), 125.79, 118.27, 115.85, 62.02, 30.46, 13.54.

HRMS (ESI): calcd for $\text{C}_{19}\text{H}_{17}\text{ClNO}_3^+$ $[\text{M}+\text{H}]^+$: 342.0891; found: 342.0900.



5e

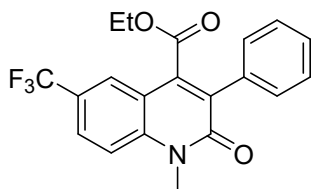
ethyl 6-bromo-1-methyl-2-oxo-3-phenyl-1,2-dihydroquinoline-4-carboxylate

Pale yellow solid, prepared according to the general procedure from 2-((4-bromophenyl)(methyl)amino)-2-oxoacetic acid (93 mg, 0.36 mmol) and ethyl 2-nitro-3-phenylacrylate (67 mg, 0.3 mmol), 10 h, 42.7 mg, 37 % yield.

$^1\text{H NMR}$ (400 MHz, CDCl_3) δ 7.73 (d, $J = 2.1$ Hz, 1H), 7.69 (dd, $J = 9.0, 2.1$ Hz, 1H), 7.40 (s, 5H), 7.30 (d, $J = 9.0$ Hz, 1H), 4.13 (q, $J = 7.1$ Hz, 2H), 3.77 (s, 3H), 0.93 (t, $J = 7.1$ Hz, 3H).

$^{13}\text{C NMR}$ (101 MHz, CDCl_3) δ 165.97, 160.90, 139.01, 138.58, 134.47, 133.70, 132.02, 129.42, 128.70 (d, $J = 17.4$ Hz), 128.09, 121.03, 118.72, 116.10, 115.61, 62.03, 30.42, 13.53.

HRMS (ESI): calcd for $\text{C}_{19}\text{H}_{17}\text{BrNO}_3^+$ $[\text{M}+\text{H}]^+$: 386.0386; found: 386.0379.



5f

1-methyl-3-phenyl-4-propionyl-6-(trifluoromethyl)quinolin-2(1H)-one

Pale yellow solid, prepared according to the general procedure from 2-(methyl(4-(trifluoromethyl)phenyl)amino)-2-oxoacetic acid (89 mg, 0.36 mmol) and ethyl 2-nitro-3-phenylacrylate

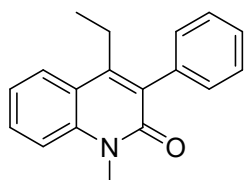
(67 mg, 0.3 mmol), 11 h, 69.7 mg, 62 % yield.

$^1\text{H NMR}$ (400 MHz, CDCl_3) δ 7.87 (s, 1H), 7.83 (d, $J = 8.9$ Hz, 1H), 7.52 (d, $J = 9.0$ Hz, 1H), 7.41 (s, 5H), 4.15 (q, $J = 7.1$ Hz, 2H), 3.82 (s, 3H), 0.95 (t, $J = 7.1$ Hz, 3H).

$^{13}\text{C NMR}$ (101 MHz, CDCl_3) δ 165.81, 161.19, 141.57, 139.67, 134.26, 132.34, 129.38, 128.75, 128.16, 127.25 (d, $J = 3.4$ Hz), 124.88 (d, $J = 33.6$ Hz), 123.97 (d, $J = 4.1$ Hz), 123.80 (d, $J = 271.7$ Hz), 116.94, 115.01, 62.14, 30.57, 13.53.

$^{19}\text{F NMR}$ (376 MHz, CDCl_3) δ -61.94.

HRMS (ESI): calcd for $\text{C}_{20}\text{H}_{17}\text{F}_3\text{NO}_3^+$ $[\text{M}+\text{H}]^+$: 376.1155; found: 376.156.



5g

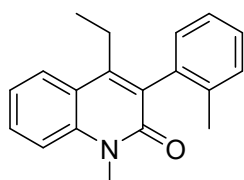
4-ethyl-1-methyl-3-phenylquinolin-2(1H)-one

Pale yellow solid, prepared according to the general procedure from 2-(methyl(phenyl)amino)-2-oxoacetic acid (65 mg, 0.36 mmol) and (2-nitrobut-1-en-1-yl)benzene (53 mg, 0.3 mmol), 12 h, 56.8 mg, 72 % yield. (the spectra of **5g** are in accordance with those of the compound reported in the literature Org.Lett.2020, 22, 2230–2234)

$^1\text{H NMR}$ (400 MHz, Chloroform-*d*) δ 7.76 (dd, $J = 8.1, 1.5$ Hz, 1H), 7.51 (ddd, $J = 8.5, 7.1, 1.4$ Hz, 1H), 7.42 – 7.33 (m, 3H), 7.33 – 7.27 (m, 1H), 7.24 – 7.20 (m, 1H), 7.20 – 7.16 (m, 2H), 3.69 (s, 3H), 2.64 (q, $J = 7.5$ Hz, 2H), 1.10 (t, $J = 7.5$ Hz, 3H).

$^{13}\text{C NMR}$ (101 MHz, Chloroform-*d*) δ 161.98, 148.20, 139.74, 136.94, 132.10, 130.06, 129.54, 128.39, 127.44, 125.75, 122.01, 120.17, 114.57, 29.87, 23.04, 14.64.

HRMS (ESI): calcd for $\text{C}_{18}\text{H}_{18}\text{NO}^+$ $[\text{M}+\text{H}]^+$: 264.1383; found: 264.1391.



5h

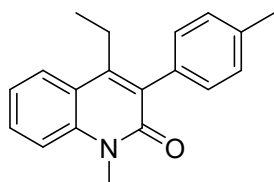
4-ethyl-1-methyl-3-(o-tolyl)quinolin-2(1H)-one

Pale yellow solid, prepared according to the general procedure from 2-(methyl(phenyl)amino)-2-oxoacetic acid (65 mg, 0.36 mmol) and 1-methyl-2-(2-nitrobut-1-en-1-yl)benzene (57 mg, 0.3 mmol), 12 h, 54.8 mg, 66 % yield.

$^1\text{H NMR}$ (400 MHz, Chloroform-*d*) δ 7.83 (dd, $J = 8.1, 1.5$ Hz, 1H), 7.59 (ddd, $J = 8.6, 7.1, 1.4$ Hz, 1H), 7.44 (dd, $J = 8.6, 1.1$ Hz, 1H), 7.32 – 7.23 (m, 5H), 7.12 – 7.06 (m, 1H), 3.77 (s, 3H), 2.77 (dq, $J = 13.1, 7.6$ Hz, 1H), 2.51 (dq, $J = 13.2, 7.6$ Hz, 1H), 2.13 (s, 3H), 1.12 (t, $J = 7.6$ Hz, 3H).

$^{13}\text{C NMR}$ (101 MHz, Chloroform-*d*) δ 161.33, 148.29, 139.83, 136.57, 136.45, 131.72, 130.10, 129.99, 129.44, 127.77, 125.87, 125.67, 121.94, 120.13, 114.58, 29.85, 22.96, 19.72, 13.96.

HRMS (ESI): calcd for $\text{C}_{19}\text{H}_{20}\text{NO}^+$ $[\text{M}+\text{H}]^+$: 278.1539; found: 278.1539.



5i

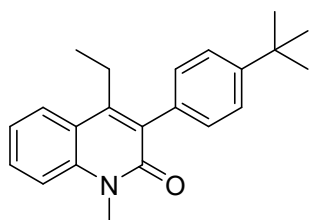
4-ethyl-1-methyl-3-(p-tolyl)quinolin-2(1H)-one

Pale yellow solid, prepared according to the general procedure from 2-(methyl(phenyl)amino)-2-oxoacetic acid (65 mg, 0.36 mmol) and 1-methyl-4-(2-nitrobut-1-en-1-yl)benzene (57 mg, 0.3 mmol), 12 h, 64.8 mg, 78 % yield.

¹H NMR (400 MHz, CDCl₃) δ 7.82 (d, *J* = 8.1 Hz, 1H), 7.57 (t, *J* = 7.8 Hz, 1H), 7.41 (d, *J* = 8.5 Hz, 1H), 7.27 (dd, *J* = 15.5, 6.5 Hz, 3H), 7.14 (d, *J* = 7.8 Hz, 2H), 3.75 (s, 3H), 2.73 (q, *J* = 7.5 Hz, 2H), 2.40 (s, 3H), 1.17 (t, *J* = 7.5 Hz, 3H).

¹³C NMR (101 MHz, CDCl₃) δ 162.08, 148.09, 139.68, 137.00, 133.89, 132.08, 129.92, 129.35, 129.11, 125.69, 121.93, 120.19, 114.52, 29.87, 23.05, 21.35, 14.67.

HRMS (ESI): calcd for C₁₉H₂₀NO⁺ [M+H]⁺: 278.1539; found: 278.1533.



5j

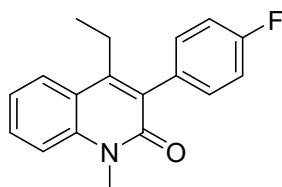
3-(4-(tert-butyl)phenyl)-4-ethyl-1-methylquinolin-2(1H)-one

Pale yellow solid, prepared according to the general procedure from 2-(methyl(phenyl)amino)-2-oxoacetic acid (65 mg, 0.36 mmol) and (Z)-1-(tert-butyl)-4-(2-nitrobut-1-en-1-yl)benzene (70 mg, 0.3 mmol), 12 h, 77.5 mg, 81 % yield.

¹H NMR (400 MHz, Chloroform-*d*) δ 7.83 (dd, *J* = 8.1, 1.5 Hz, 1H), 7.57 (ddd, *J* = 8.5, 7.1, 1.5 Hz, 1H), 7.47 – 7.43 (m, 2H), 7.42 (dd, *J* = 8.5, 1.2 Hz, 1H), 7.31 – 7.27 (m, 1H), 7.20 – 7.16 (m, 2H), 3.75 (s, 3H), 2.74 (q, *J* = 7.5 Hz, 2H), 1.36 (s, 9H), 1.19 (t, *J* = 7.5 Hz, 3H).

¹³C NMR (101 MHz, Chloroform-*d*) δ 162.09, 149.98, 148.10, 139.67, 133.75, 132.08, 129.89, 129.10, 125.72, 125.25, 121.90, 120.24, 114.50, 34.59, 31.41, 29.84, 23.07, 14.78.

HRMS (ESI): calcd for C₂₂H₂₆NO⁺ [M+H]⁺: 320.2009; found: 320.2014.



5k

4-ethyl-3-(4-fluorophenyl)-1-methylquinolin-2(1H)-one

Pale yellow solid, prepared according to the general procedure from 2-(methyl(phenyl)amino)-2-

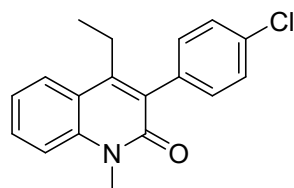
oxoacetic acid (65 mg, 0.36 mmol) and 1-fluoro-4-(2-nitrobut-1-en-1-yl)benzene (59 mg, 0.3 mmol), 12 h, 64.9 mg, 77 % yield.

^1H NMR (400 MHz, CDCl_3) δ 7.83 (d, $J = 8.0$ Hz, 1H), 7.59 (t, $J = 7.8$ Hz, 1H), 7.43 (d, $J = 8.5$ Hz, 1H), 7.31 (d, $J = 7.6$ Hz, 1H), 7.24 (dt, $J = 8.3, 6.6$ Hz, 2H), 7.14 (t, $J = 8.7$ Hz, 2H), 3.76 (s, 3H), 2.72 (q, $J = 7.5$ Hz, 2H), 1.17 (t, $J = 7.6$ Hz, 3H).

^{13}C NMR (101 MHz, CDCl_3) δ 162.23 (d, $J = 245.8$ Hz), 161.90, 148.59, 139.71, 132.72 (d, $J = 3.4$ Hz), 131.28 (d, $J = 8.0$ Hz), 131.01, 130.21, 125.75, 122.08, 120.02, 115.39 (d, $J = 21.3$ Hz), 114.60, 29.89, 23.02, 14.57.

^{19}F NMR (376 MHz, Chloroform-*d*) δ -115.07.

HRMS (ESI): calcd for $\text{C}_{18}\text{H}_{17}\text{FNO}^+$ $[\text{M}+\text{H}]^+$: 282.1289; found: 282.1286.



5l

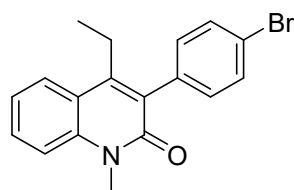
3-(4-chlorophenyl)-4-ethyl-1-methylquinolin-2(1H)-one

Pale yellow solid, prepared according to the general procedure from 2-(methyl(phenyl)amino)-2-oxoacetic acid (65 mg, 0.36 mmol) and 1-chloro-4-(2-nitrobut-1-en-1-yl)benzene (64 mg, 0.3 mmol), 12 h, 64.2 mg, 72 % yield.

^1H NMR (400 MHz, CDCl_3) δ 7.83 (d, $J = 8.0$ Hz, 1H), 7.59 (dd, $J = 10.9, 8.3$ Hz, 3H), 7.43 (d, $J = 8.5$ Hz, 1H), 7.30 (t, $J = 7.6$ Hz, 1H), 7.14 (d, $J = 8.3$ Hz, 2H), 3.76 (s, 3H), 2.71 (q, $J = 7.5$ Hz, 2H), 1.17 (t, $J = 7.5$ Hz, 3H).

^{13}C NMR (101 MHz, CDCl_3) δ 161.64, 148.50, 139.73, 135.83, 131.59, 131.36, 130.83, 130.31, 125.75, 122.13, 121.65, 119.96, 114.62, 29.88, 23.02, 14.60.

HRMS (ESI): calcd for $\text{C}_{18}\text{H}_{17}\text{ClNO}^+$ $[\text{M}+\text{H}]^+$: 298.0993; found: 298.0981.



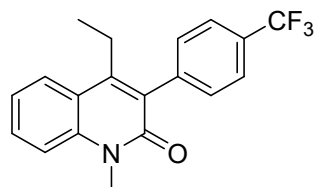
5m

3-(4-bromophenyl)-4-ethyl-1-methylquinolin-2(1H)-one

Pale yellow solid, prepared according to the general procedure from 2-(methyl(phenyl)amino)-2-oxoacetic acid (65 mg, 0.36 mmol) and 1-bromo-4-(2-nitrobut-1-en-1-yl)benzene (77 mg, 0.3 mmol), 12 h, 66.5 mg, 65 % yield.

^1H NMR (400 MHz, CDCl_3) δ 7.83 (d, $J = 8.1$ Hz, 1H), 7.60 (t, $J = 7.8$ Hz, 1H), 7.47 – 7.39 (m, 3H), 7.30 (t, $J = 7.7$ Hz, 1H), 7.20 (d, $J = 8.2$ Hz, 2H), 3.76 (s, 3H), 2.71 (q, $J = 7.5$ Hz, 2H), 1.17 (t, $J = 7.5$ Hz, 3H).

^{13}C NMR (101 MHz, CDCl_3) δ 161.71 , 148.55 , 139.73 , 135.33 , 133.43 , 130.93 (d, $J = 19.2$ Hz), 130.29 , 128.65 , 125.75 , 122.11 , 119.97 , 114.62 , 29.89 , 23.02 , 14.59 .
HRMS (ESI): calcd for $\text{C}_{18}\text{H}_{17}\text{BrNO}^+$ $[\text{M}+\text{H}]^+$: 342.0488; found: 342.0479.



5n

4-ethyl-1-methyl-3-(4-(trifluoromethyl)phenyl)quinolin-2(1H)-one

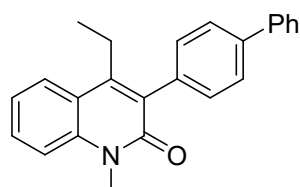
Pale yellow solid, prepared according to the general procedure from 2-(methyl(phenyl)amino)-2-oxoacetic acid (65 mg, 0.36 mmol) and 1-(2-nitrobut-1-en-1-yl)-4-(trifluoromethyl)benzene (74 mg, 0.3 mmol), 11 h, 57.7 mg, 79 % yield.

^1H NMR (400 MHz, CDCl_3) δ 7.85 (d, $J = 8.0$ Hz, 1H), 7.71 (d, $J = 8.0$ Hz, 2H), 7.62 (t, $J = 7.8$ Hz, 1H), 7.45 (d, $J = 8.4$ Hz, 1H), 7.39 (d, $J = 7.9$ Hz, 2H), 7.32 (t, $J = 7.6$ Hz, 1H), 3.77 (s, 3H), 2.70 (q, $J = 7.5$ Hz, 2H), 1.18 (t, $J = 7.6$ Hz, 3H).

^{13}C NMR (101 MHz, CDCl_3) δ 161.51 , 148.67 , 140.77 , 139.79 , 130.68, 130.49 , 130.10 , 129.61 (q, $J = 23.9$ Hz) , 125.79 , 125.39 (q, $J = 3.8$ Hz), 124.27 (q, $J = 272.4$ Hz) , 122.22 , 119.87 , 114.68 , 29.87 , 23.03 , 14.60 .

^{19}F NMR (376 MHz, CDCl_3) δ -62.52 .

HRMS (ESI): calcd for $\text{C}_{19}\text{H}_{17}\text{F}_3\text{NO}^+$ $[\text{M}+\text{H}]^+$: 332.1257; found: 332.1255.



5o

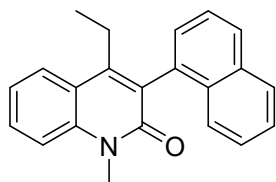
3-([1,1'-biphenyl]-4-yl)-4-ethyl-1-methylquinolin-2(1H)-one

Pale yellow solid, prepared according to the general procedure from 2-(methyl(phenyl)amino)-2-oxoacetic acid (65 mg, 0.36 mmol) and 4-(2-nitrobut-1-en-1-yl)-1,1'-biphenyl (76 mg, 0.3 mmol), 12 h, 53.9 mg, 53 % yield.

^1H NMR (400 MHz, CDCl_3) δ 7.85 (d, $J = 8.0$ Hz, 1H), 7.67 (t, $J = 7.8$ Hz, 4H), 7.60 (t, $J = 7.8$ Hz, 1H), 7.45 (dd, $J = 13.0, 5.4$ Hz, 3H), 7.32 (tt, $J = 12.8, 6.4$ Hz, 4H), 3.78 (s, 3H), 2.78 (q, $J = 7.5$ Hz, 2H), 1.22 (t, $J = 7.5$ Hz, 3H).

^{13}C NMR (101 MHz, CDCl_3) δ 162.06 , 148.32 , 141.11 , 140.25 , 139.73 , 135.92 , 131.73 , 130.02 (d, $J = 10.3$ Hz), 128.75 , 127.18 (d, $J = 2.2$ Hz), 125.75 , 122.01 , 120.16 , 114.57 , 29.88 , 23.10 , 14.72 .

HRMS (ESI): calcd for $\text{C}_{24}\text{H}_{22}\text{NO}^+$ $[\text{M}+\text{H}]^+$: 340.1696; found: 340.1700.



5p

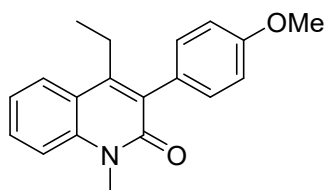
4-ethyl-1-methyl-3-(naphthalen-1-yl)quinolin-2(1H)-one

Pale yellow solid, prepared according to the general procedure from 2-(methyl(phenyl)amino)-2-oxoacetic acid (65 mg, 0.36 mmol) and 1-(2-nitrobut-1-en-1-yl)naphthalene (68 mg, 0.3 mmol), 12 h, 63.9 mg, 68 % yield.

$^1\text{H NMR}$ (400 MHz, CDCl_3) δ 7.88 (t, $J = 9.5$ Hz, 3H), 7.66 – 7.60 (m, 1H), 7.59 – 7.52 (m, 2H), 7.47 (dd, $J = 16.3, 8.3$ Hz, 2H), 7.40 – 7.29 (m, 3H), 3.79 (s, 3H), 2.72 (dq, $J = 15.1, 7.5$ Hz, 1H), 2.46 (dq, $J = 15.1, 7.6$ Hz, 1H), 1.08 (t, $J = 7.6$ Hz, 3H).

$^{13}\text{C NMR}$ (101 MHz, CDCl_3) δ 161.76, 149.75, 140.02, 134.65, 133.82, 132.20, 130.31 (d, $J = 15.8$ Hz), 128.43, 128.12, 127.07, 126.22, 125.81 (d, $J = 3.6$ Hz), 125.58, 125.21, 122.06, 120.13, 114.69, 29.91, 23.41, 14.52.

HRMS (ESI): calcd for $\text{C}_{22}\text{H}_{20}\text{NO}^+$ $[\text{M}+\text{H}]^+$: 314.1539; found: 314.1540.



5q

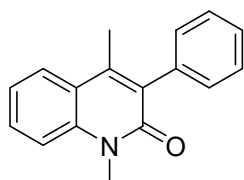
4-ethyl-3-(4-methoxyphenyl)-1-methylquinolin-2(1H)-one

Pale yellow solid, prepared according to the general procedure from 2-(methyl(phenyl)amino)-2-oxoacetic acid (65 mg, 0.36 mmol) and 1-methoxy-4-(2-nitrobut-1-en-1-yl)benzene (62 mg, 0.3 mmol), 12 h, 64.2 mg, 73 % yield.

$^1\text{H NMR}$ (400 MHz, Chloroform-*d*) δ 7.83 (d, $J = 8.1$ Hz, 1H), 7.57 (t, $J = 7.9$ Hz, 1H), 7.42 (d, $J = 8.4$ Hz, 1H), 7.29 (d, $J = 7.7$ Hz, 1H), 7.18 (d, $J = 8.1$ Hz, 2H), 6.99 (d, $J = 8.3$ Hz, 2H), 3.85 (s, 3H), 3.76 (s, 3H), 2.74 (q, $J = 7.5$ Hz, 2H), 1.18 (t, $J = 7.5$ Hz, 3H).

$^{13}\text{C NMR}$ (101 MHz, Chloroform-*d*) δ 162.21, 158.88, 148.33, 139.65, 131.72, 130.69, 129.93, 129.11, 125.71, 121.96, 120.22, 114.52, 113.88, 55.27, 29.90, 23.04, 14.64.

HRMS (ESI): calcd for $\text{C}_{19}\text{H}_{20}\text{NO}_2^+$ $[\text{M}+\text{H}]^+$: 294.1489; found: 294.1488.



5r

1,4-dimethyl-3-phenylquinolin-2(1H)-one

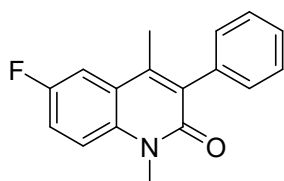
Pale yellow solid, prepared according to the general procedure from 2-(methyl(phenyl)amino)-2-

oxoacetic acid (65 mg, 0.36 mmol) and (2-nitroprop-1-en-1-yl)benzene (49 mg, 0.3 mmol), 12 h, 62.7 mg, 84 % yield.

$^1\text{H NMR}$ (400 MHz, CDCl_3) δ 7.83 (d, $J = 8.0$ Hz, 1H), 7.61 (t, $J = 7.8$ Hz, 1H), 7.43 (dt, $J = 13.8, 7.3$ Hz, 4H), 7.33 – 7.26 (m, 3H), 3.79 (s, 3H), 2.35 (s, 3H).

$^{13}\text{C NMR}$ (101 MHz, CDCl_3) δ 161.71, 142.36, 139.17, 136.83, 132.49, 130.10 (d, $J = 6.8$ Hz), 128.21, 127.45, 125.68, 122.00, 121.58, 114.24, 29.82, 16.89.

HRMS (ESI): calcd for $\text{C}_{17}\text{H}_{16}\text{NO}^+$ $[\text{M}+\text{H}]^+$: 250.1226; found: 250.1213.



5s

6-fluoro-1,4-dimethyl-3-phenylquinolin-2(1H)-one

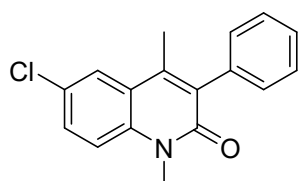
Pale yellow solid, prepared according to the general procedure from 2-((4-fluorophenyl)(methyl)amino)-2-oxoacetic acid (71 mg, 0.36 mmol) and (2-nitroprop-1-en-1-yl)benzene (49 mg, 0.3 mmol), 12 h, 63.3 mg, 79 % yield.

$^1\text{H NMR}$ (400 MHz, CDCl_3) δ 7.43 – 7.34 (m, 3H), 7.30 (dd, $J = 8.8, 5.9$ Hz, 2H), 7.25 (dd, $J = 7.5, 2.6$ Hz, 1H), 7.19 (dd, $J = 6.2, 2.0$ Hz, 2H), 3.69 (s, 3H), 2.22 (s, 3H).

$^{13}\text{C NMR}$ (101 MHz, CDCl_3) δ 161.37, 161.37, 157.93 (d, $J = 241.2$ Hz), 141.46 (d, $J = 3.1$ Hz), 136.48, 135.73 (d, $J = 1.0$ Hz), 133.69, 129.92, 128.26, 127.65, 122.71 (d, $J = 7.9$ Hz), 117.64 (d, $J = 23.6$ Hz), 115.69 (d, $J = 8.1$ Hz), 111.16 (d, $J = 23.3$ Hz), 30.12, 16.97.

$^{19}\text{F NMR}$ (376 MHz, CDCl_3) δ -120.80.

HRMS (ESI): calcd for $\text{C}_{17}\text{H}_{15}\text{FNO}^+$ $[\text{M}+\text{H}]^+$: 268.1132; found: 268.1138.



5t

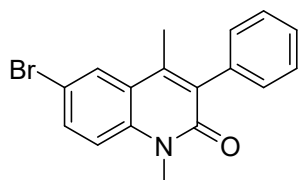
6-chloro-1,4-dimethyl-3-phenylquinolin-2(1H)-one

Pale yellow solid, prepared according to the general procedure from 2-((4-chlorophenyl)(methyl)amino)-2-oxoacetic acid (77 mg, 0.36 mmol) and (2-nitroprop-1-en-1-yl)benzene (49 mg, 0.3 mmol), 12 h, 57.7 mg, 68 % yield.

$^1\text{H NMR}$ (400 MHz, CDCl_3) δ 7.69 (d, $J = 2.3$ Hz, 1H), 7.46 (dd, $J = 9.0, 2.3$ Hz, 1H), 7.38 (t, $J = 7.3$ Hz, 2H), 7.31 (d, $J = 7.3$ Hz, 1H), 7.27 (d, $J = 9.0$ Hz, 1H), 7.18 (d, $J = 5.7$ Hz, 2H), 3.68 (s, 3H), 2.23 (s, 3H).

$^{13}\text{C NMR}$ (101 MHz, CDCl_3) δ 161.39, 141.34, 137.72, 136.35, 133.61, 129.95 (d, $J = 8.6$ Hz), 128.26, 127.63 (d, $J = 10.6$ Hz), 125.18, 122.82, 115.60, 30.00, 16.89.

HRMS (ESI): calcd for $\text{C}_{17}\text{H}_{15}\text{ClNO}^+$ $[\text{M}+\text{H}]^+$: 284.0837; found: 284.0834.



5u

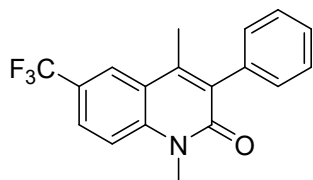
6-bromo-1,4-dimethyl-3-phenylquinolin-2(1H)-one

Pale yellow solid, prepared according to the general procedure from 2-((4-bromophenyl)(methyl)amino)-2-oxoacetic acid (93 mg, 0.36 mmol) and (2-nitroprop-1-en-1-yl)benzene (49 mg, 0.3 mmol), 12 h, 60.8 mg, 62 % yield.

^1H NMR (400 MHz, CDCl_3) δ 7.84 (d, $J = 2.3$ Hz, 1H), 7.59 (dd, $J = 9.0, 2.2$ Hz, 1H), 7.38 (tt, $J = 7.8, 1.5$ Hz, 2H), 7.31 (ddd, $J = 7.5, 3.9, 1.4$ Hz, 1H), 7.24 – 7.16 (m, 3H), 3.67 (s, 3H), 2.23 (s, 3H).

^{13}C NMR (101 MHz, CDCl_3) δ 161.37, 141.29, 138.12, 136.32, 133.58, 132.76, 129.91, 128.24 (d, $J = 5.9$ Hz), 127.69, 123.27, 115.90, 115.01, 29.96, 16.89.

HRMS (ESI): calcd for $\text{C}_{17}\text{H}_{15}\text{BrNO}^+$ $[\text{M}+\text{H}]^+$: 328.0332; found: 328.0337.



5v

1,4-dimethyl-3-phenyl-6-(trifluoromethyl)quinolin-2(1H)-one

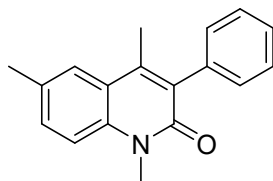
Pale yellow solid, prepared according to the general procedure from 2-(methyl(4-(trifluoromethyl)phenyl)amino)-2-oxoacetic acid (89 mg, 0.36 mmol) and (2-nitroprop-1-en-1-yl)benzene (49 mg, 0.3 mmol), 12 h, 49.5 mg, 76 % yield.

^1H NMR (400 MHz, Chloroform-*d*) δ 8.00 – 7.95 (m, 1H), 7.73 (dd, $J = 8.9, 2.1$ Hz, 1H), 7.45 – 7.36 (m, 3H), 7.35 – 7.30 (m, 1H), 7.21 – 7.18 (m, 2H), 3.72 (s, 3H), 2.29 (s, 3H).

^{13}C NMR (101 MHz, Chloroform-*d*) δ 161.68, 142.07, 141.26, 136.10, 133.84, 129.88, 128.36, 127.84, 126.50 (q, $J = 3.6$ Hz), 124.21 (q, $J = 272.0$ Hz), 124.16 (q, $J = 33.0$ Hz), 123.13 (q, $J = 4.2$ Hz), 121.39, 114.68, 30.12, 16.89.

^{19}F NMR (377 MHz, Chloroform-*d*) δ -61.65.

HRMS (ESI): calcd for $\text{C}_{18}\text{H}_{15}\text{F}_3\text{NO}^+$ $[\text{M}+\text{H}]^+$: 218.1100; found: 218.1092.



5w

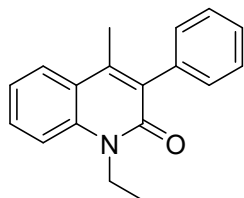
1,4,6-trimethyl-3-phenylquinolin-2(1H)-one

Pale yellow solid, prepared according to the general procedure from 2-(methyl(*p*-tolyl)amino)-2-oxoacetic acid (70 mg, 0.36 mmol) and (2-nitroprop-1-en-1-yl)benzene (49 mg, 0.3 mmol), 12 h, 52.9 mg, 67 % yield.

^1H NMR (400 MHz, CDCl_3) δ 7.51 (s, 1H), 7.40 – 7.34 (m, 2H), 7.34 – 7.25 (m, 2H), 7.23 (d, $J = 8.6$ Hz, 1H), 7.20 – 7.16 (m, 2H), 3.67 (s, 3H), 2.39 (s, 3H), 2.23 (s, 3H).

^{13}C NMR (101 MHz, CDCl_3) δ 161.57, 142.09, 137.08 (d, $J = 17.2$ Hz), 132.45, 131.31 (d, $J = 13.1$ Hz), 130.08, 128.17, 127.37, 125.58, 121.48, 114.15, 29.80, 20.96, 16.89.

HRMS (ESI): calcd for $\text{C}_{18}\text{H}_{18}\text{NO}^+$ $[\text{M}+\text{H}]^+$: 264.1383; found: 264.1392.



5x

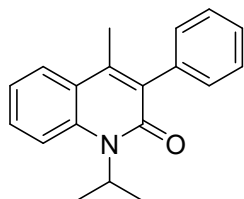
1-ethyl-4-methyl-3-phenylquinolin-2(1H)-one

Pale yellow solid, prepared according to the general procedure from 2-(ethyl(phenyl)amino)-2-oxoacetic acid (70 mg, 0.36 mmol) and (2-nitroprop-1-en-1-yl)benzene (49 mg, 0.3 mmol), 12 h, 52.9 mg, 67 % yield.

^1H NMR (400 MHz, Chloroform-*d*) δ 7.75 (dd, $J = 8.1, 1.5$ Hz, 1H), 7.50 (ddd, $J = 8.6, 7.1, 1.5$ Hz, 1H), 7.40 – 7.33 (m, 3H), 7.32 – 7.25 (m, 1H), 7.23 – 7.17 (m, 3H), 4.33 (q, $J = 7.1$ Hz, 2H), 2.26 (s, 3H), 1.31 (t, $J = 7.1$ Hz, 3H).

^{13}C NMR (101 MHz, Chloroform-*d*) δ 161.14, 142.23, 138.14, 136.78, 132.48, 130.18, 130.08, 128.17, 127.41, 125.91, 121.86, 121.77, 114.11, 37.73, 16.97, 12.78.

HRMS (ESI): calcd for $\text{C}_{18}\text{H}_{18}\text{NO}^+$ $[\text{M}+\text{H}]^+$: 264.1383; found: 264.1388.



5y

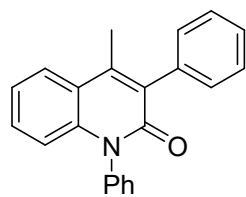
1-isopropyl-4-methyl-3-phenylquinolin-2(1H)-one

Pale yellow solid, prepared according to the general procedure from 2-(isopropyl(phenyl)amino)-2-oxoacetic acid (75 mg, 0.36 mmol) and (2-nitroprop-1-en-1-yl)benzene (49 mg, 0.3 mmol), 12 h, 36.6 mg, 44 % yield.

^1H NMR (400 MHz, Chloroform-*d*) δ 7.73 (dd, $J = 8.1, 1.6$ Hz, 1H), 7.55 (d, $J = 8.7$ Hz, 1H), 7.45 (ddd, $J = 8.7, 7.1, 1.6$ Hz, 1H), 7.39 – 7.33 (m, 2H), 7.30 – 7.25 (m, 1H), 7.22 – 7.15 (m, 3H), 5.43 (m, 1H), 2.23 (s, 3H), 1.59 (d, $J = 7.0$ Hz, 6H).

^{13}C NMR (101 MHz, Chloroform-*d*) δ 162.02, 141.92, 137.00, 130.14, 129.35, 129.17, 128.24, 128.20, 127.34, 125.99, 122.40, 121.54, 19.96, 16.98.

HRMS (ESI): calcd for $\text{C}_{19}\text{H}_{20}\text{NO}^+$ $[\text{M}+\text{H}]^+$: 278.1539; found: 278.1549.



5z

4-methyl-1,3-diphenylquinolin-2(1H)-one

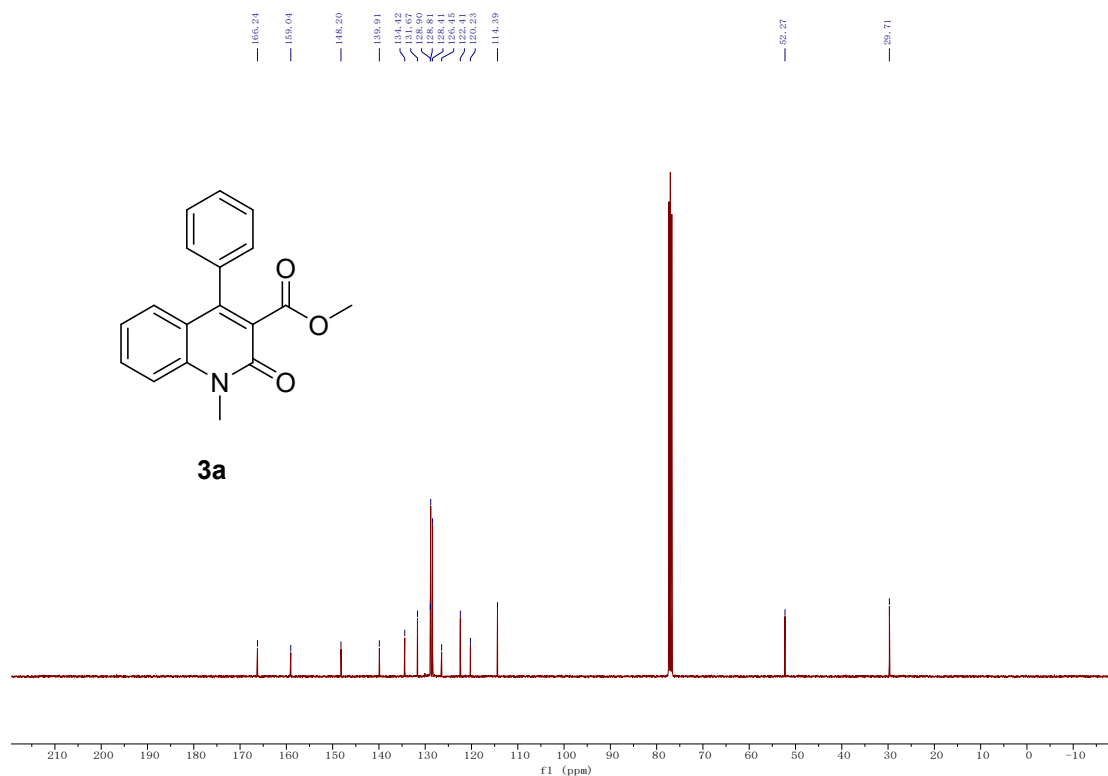
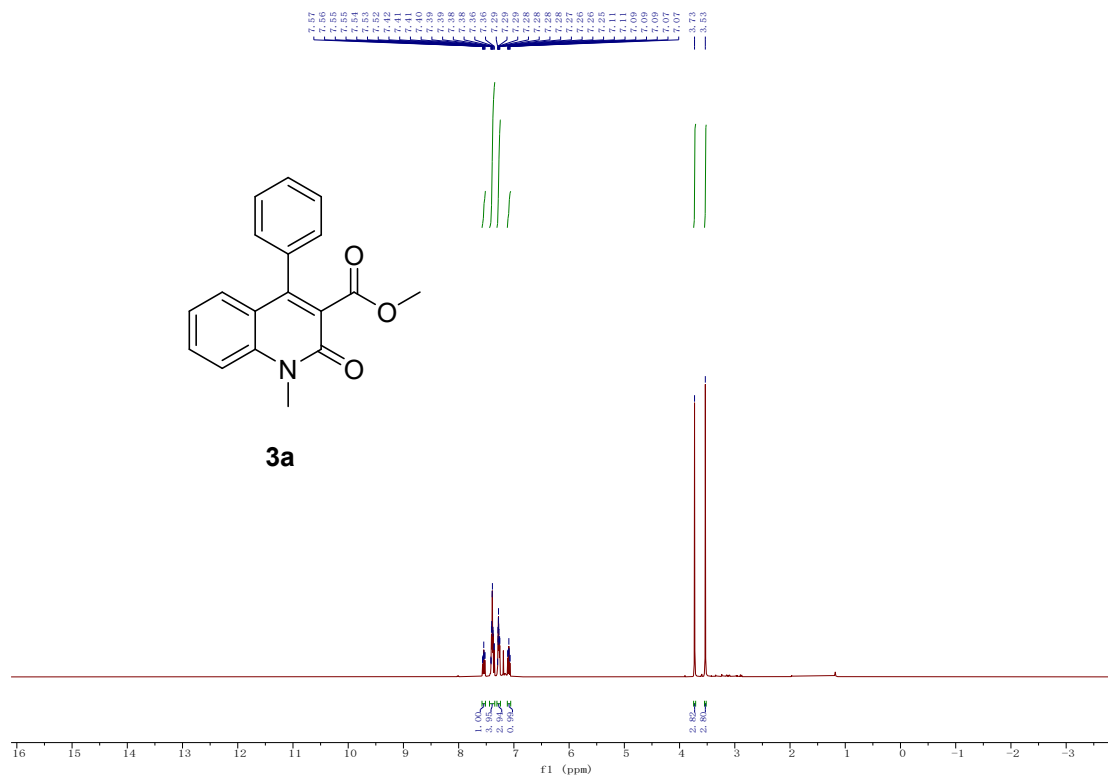
Pale yellow solid, prepared according to the general procedure from 2-(diphenylamino)-2-oxoacetic acid (87 mg, 0.36 mmol) and (2-nitroprop-1-en-1-yl)benzene (49 mg, 0.3 mmol), 12 h, 33.6 mg, 36 % yield. (the spectra of **5z** are in accordance with those of the compound reported in the literature Synthesis, 2011, # 10, art. no. H19211SS, p. 1547)

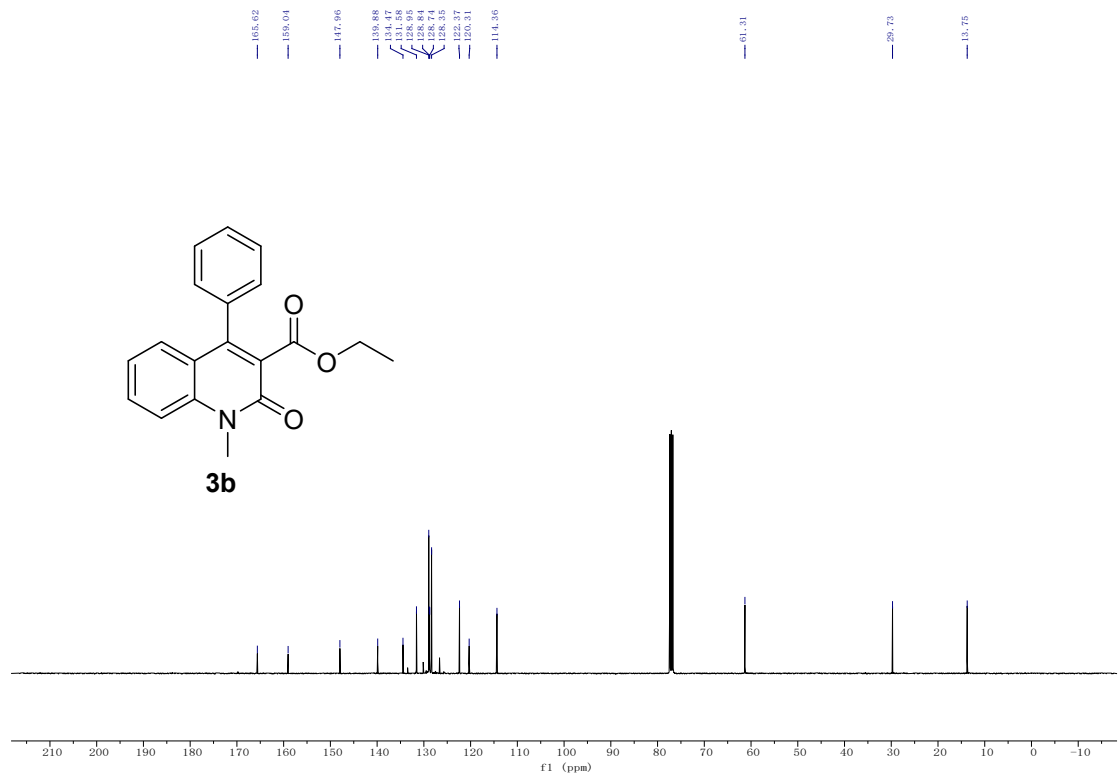
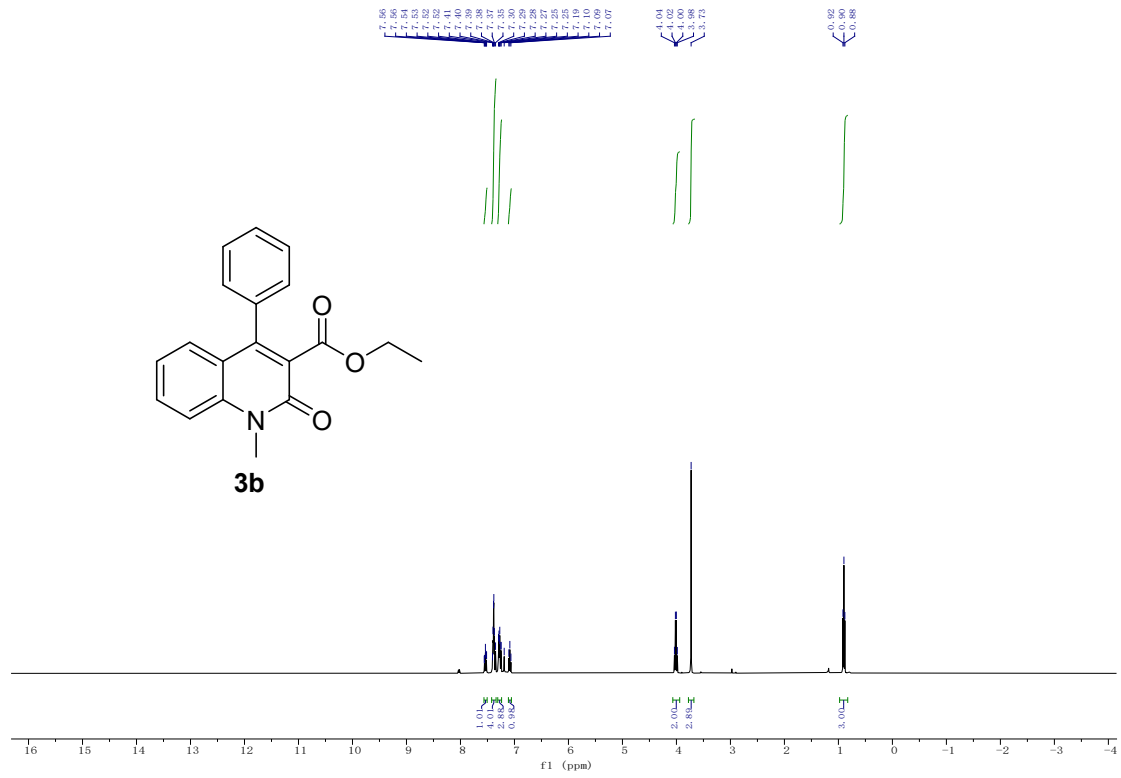
^1H NMR (400 MHz, Chloroform-*d*) δ 7.76 (dd, $J = 8.1, 1.5$ Hz, 1H), 7.49 (dd, $J = 8.3, 6.8$ Hz, 2H), 7.43 – 7.38 (m, 1H), 7.37 – 7.32 (m, 2H), 7.29 – 7.22 (m, 6H), 7.20 – 7.15 (m, 1H), 6.66 (dd, $J = 8.5, 1.2$ Hz, 1H), 2.36 (s, 3H).

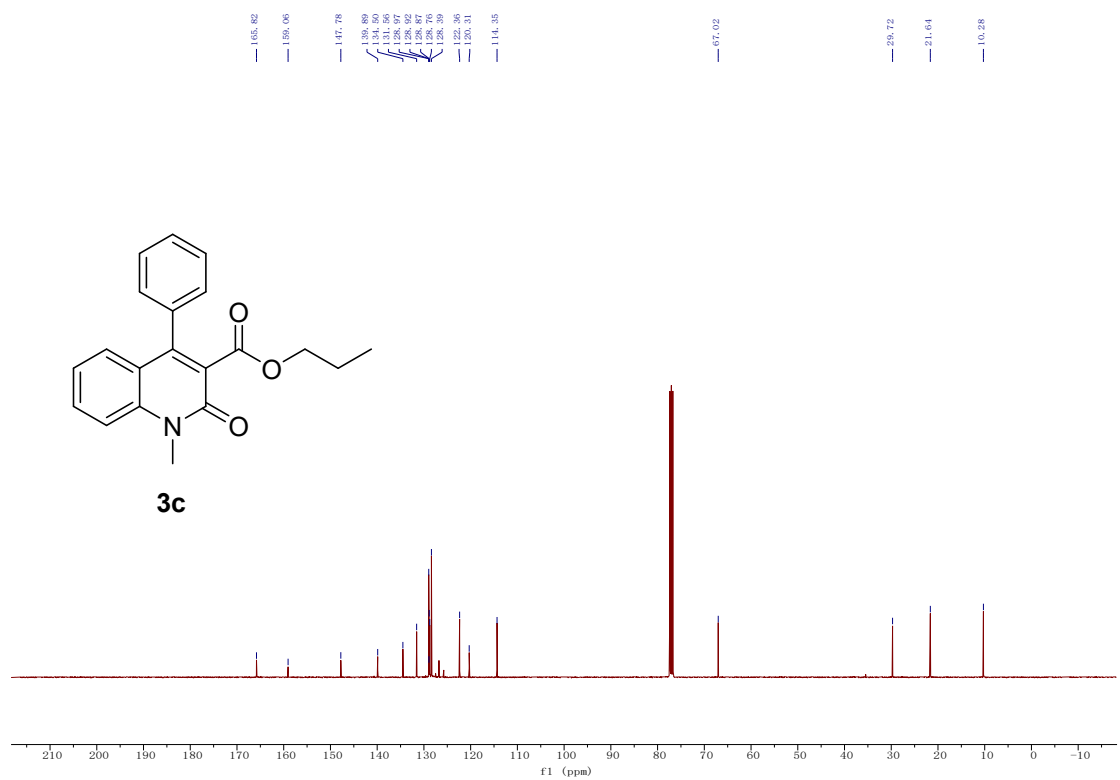
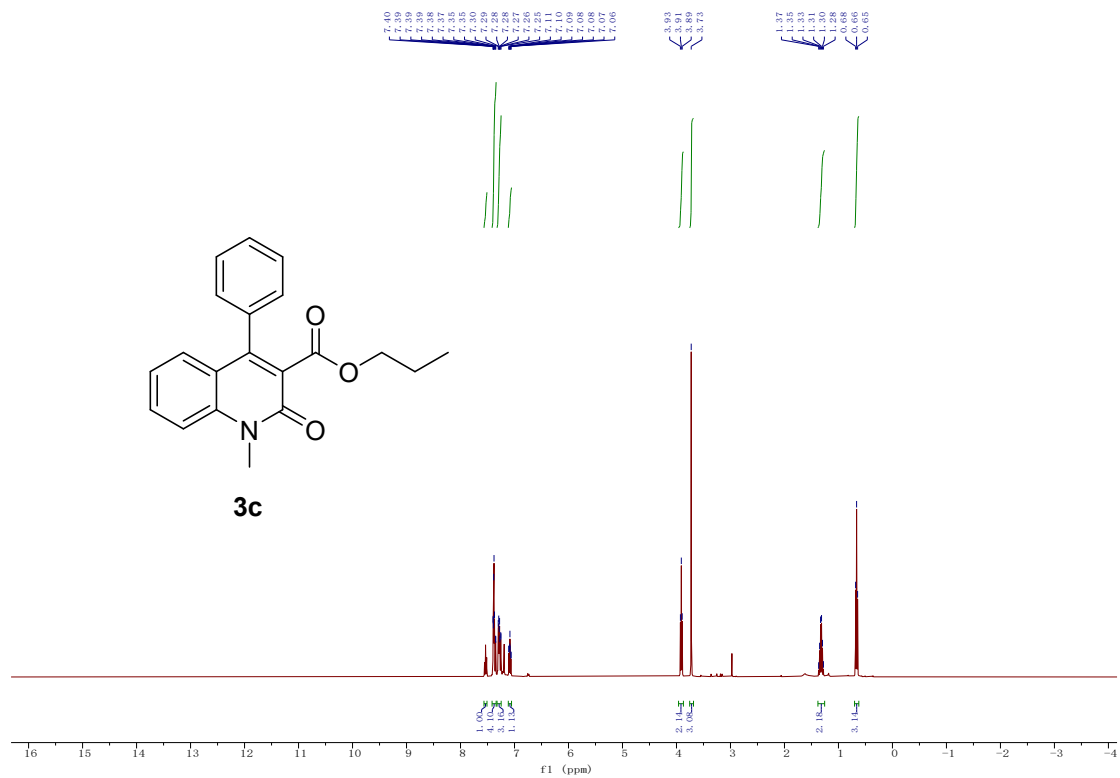
^{13}C NMR (101 MHz, Chloroform-*d*) δ 161.61, 143.22, 140.18, 138.10, 136.11, 132.74, 130.46, 129.98, 129.66, 129.05, 128.61, 128.01, 127.49, 125.37, 122.22, 121.40, 116.15, 17.20.

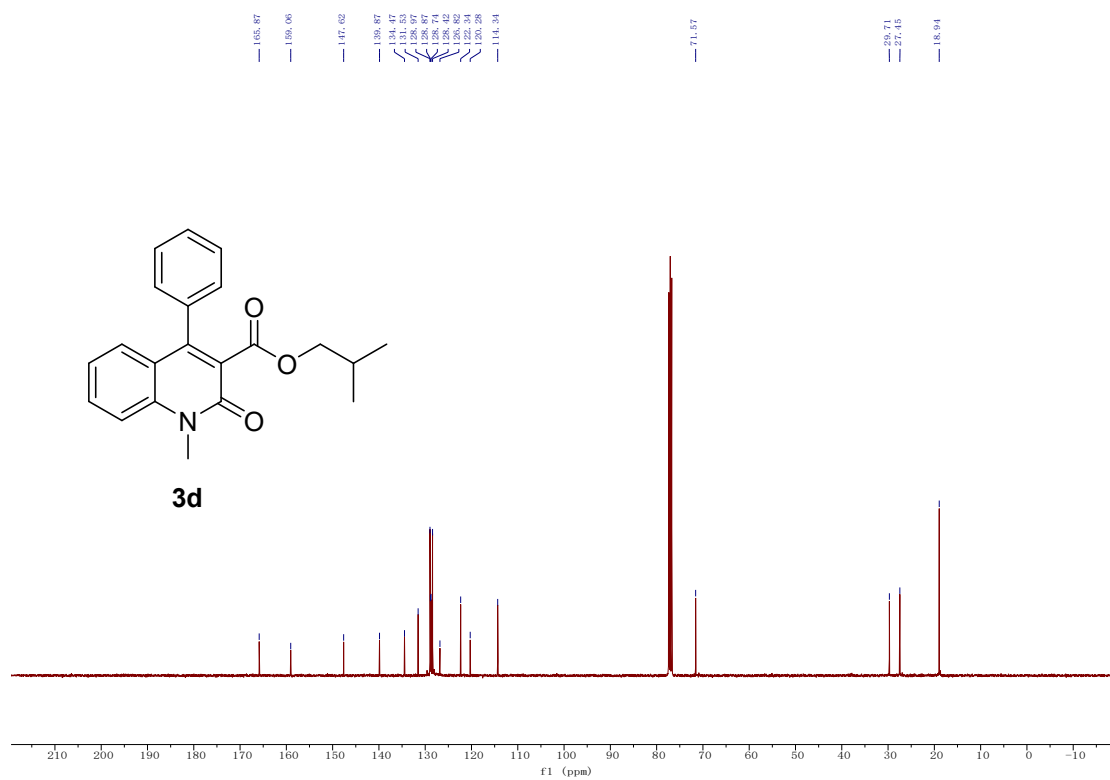
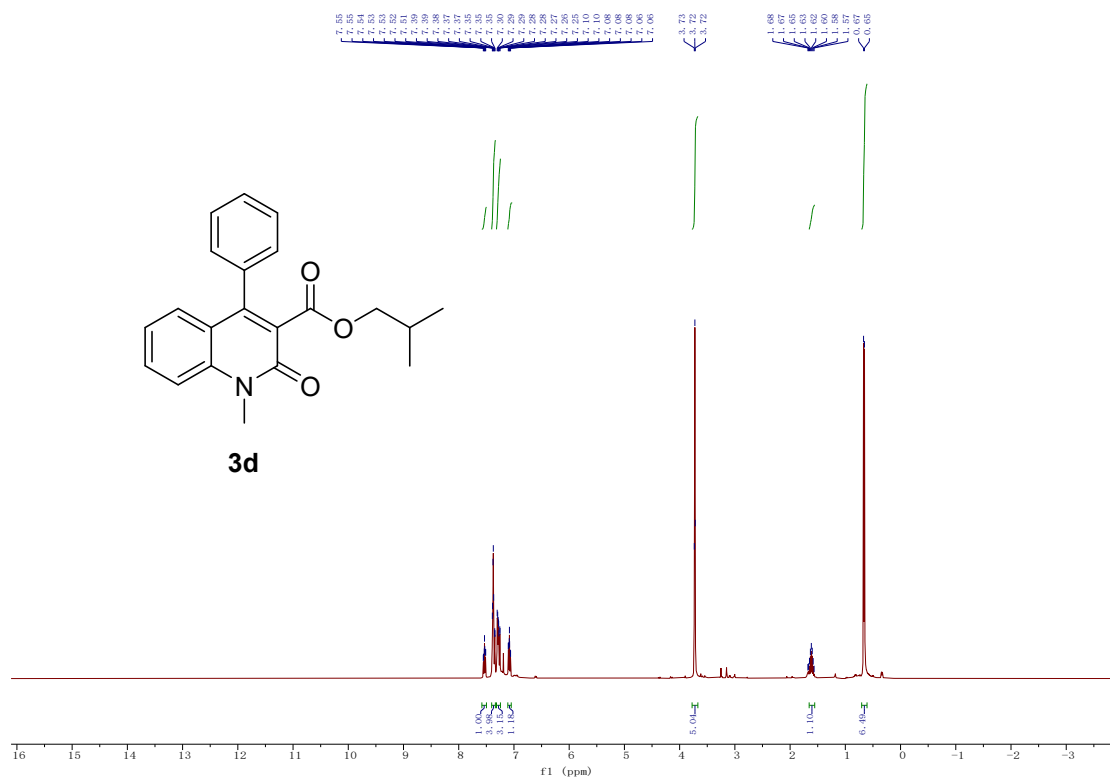
HRMS (ESI): calcd for $\text{C}_{22}\text{H}_{18}\text{NO}^+$ $[\text{M}+\text{H}]^+$: 312.1383; found: 312.1375.

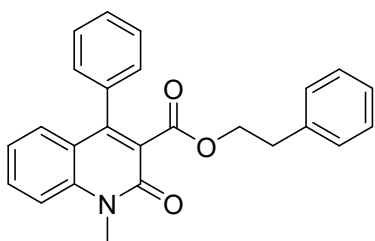
4. NMR spectra



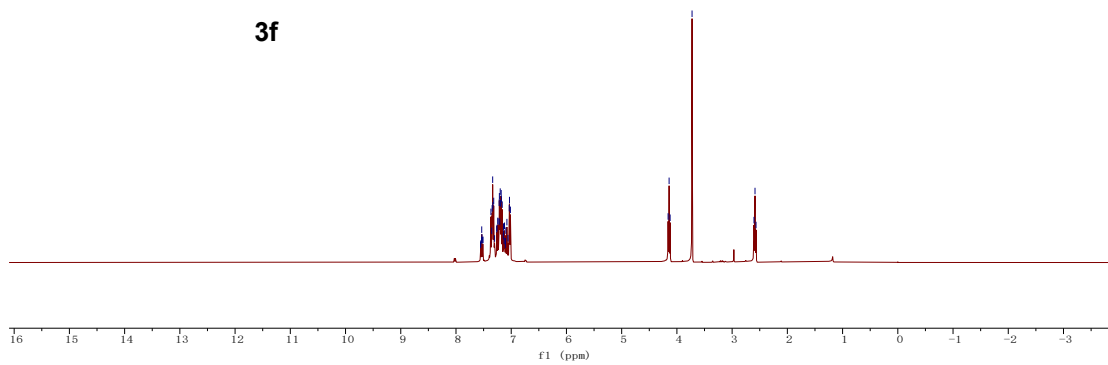


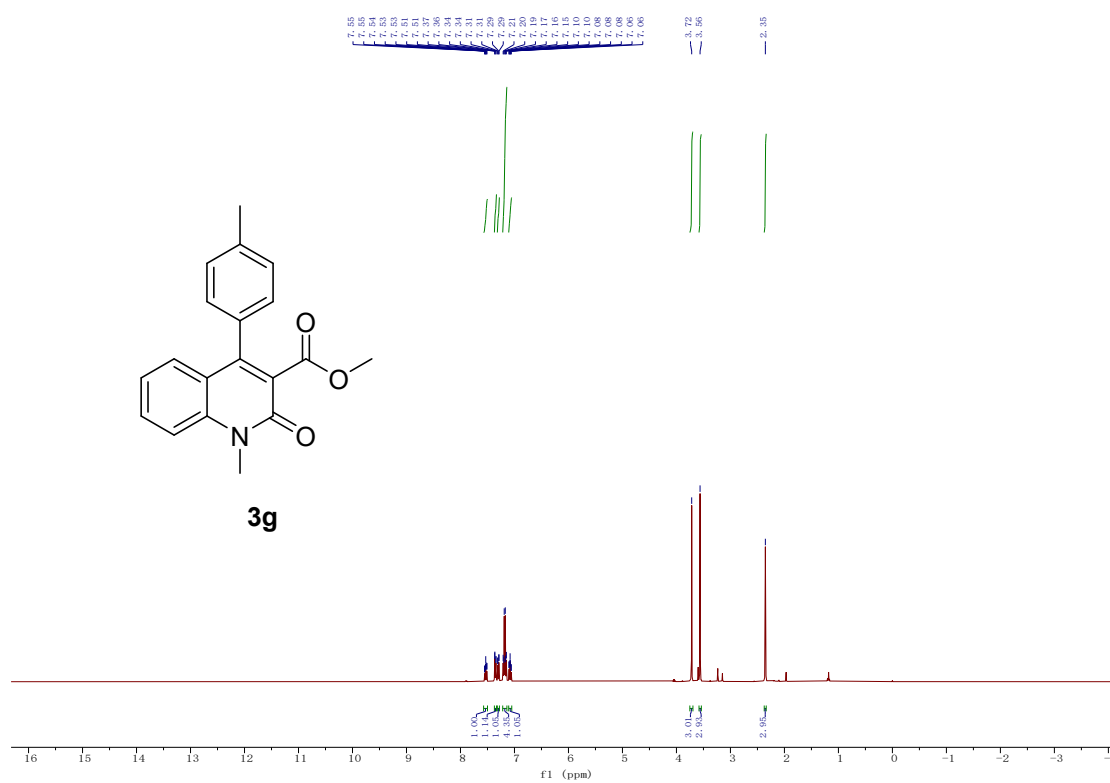
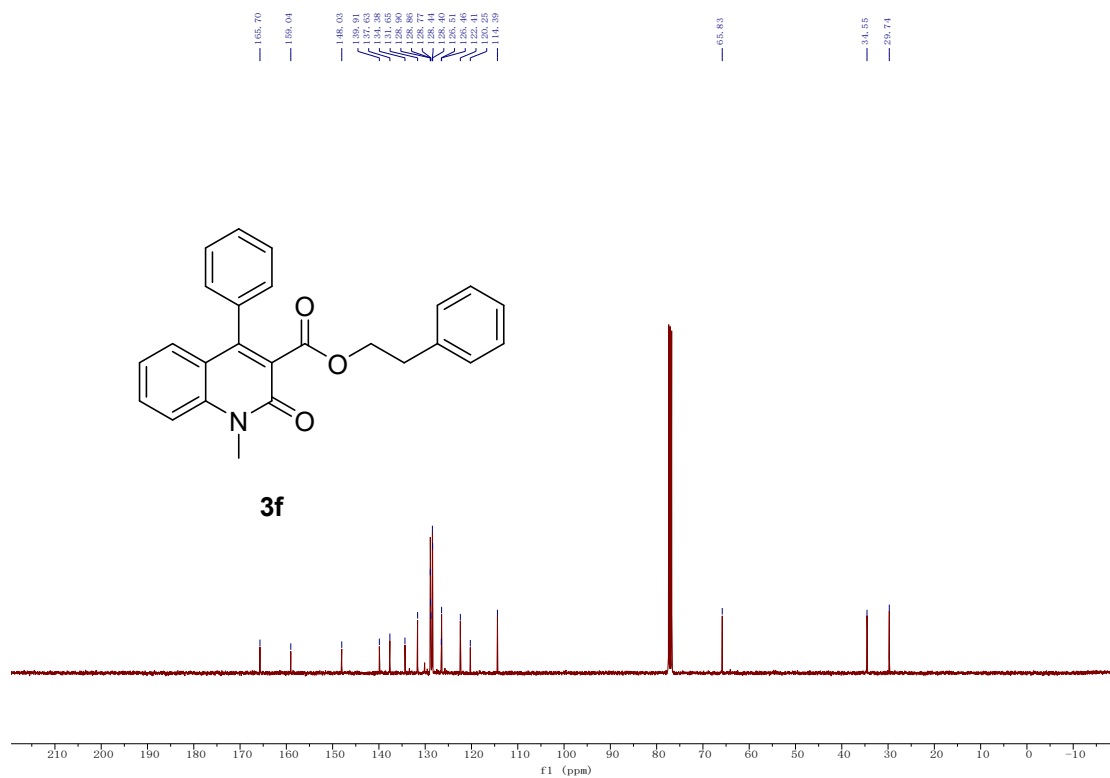


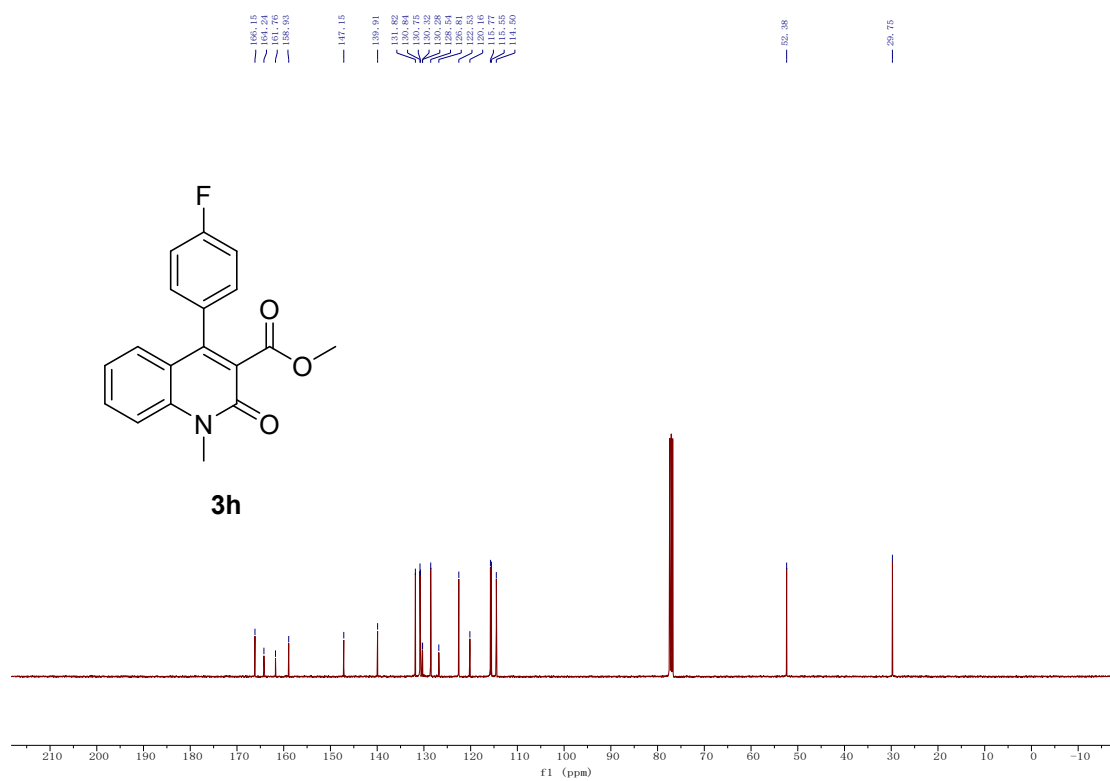


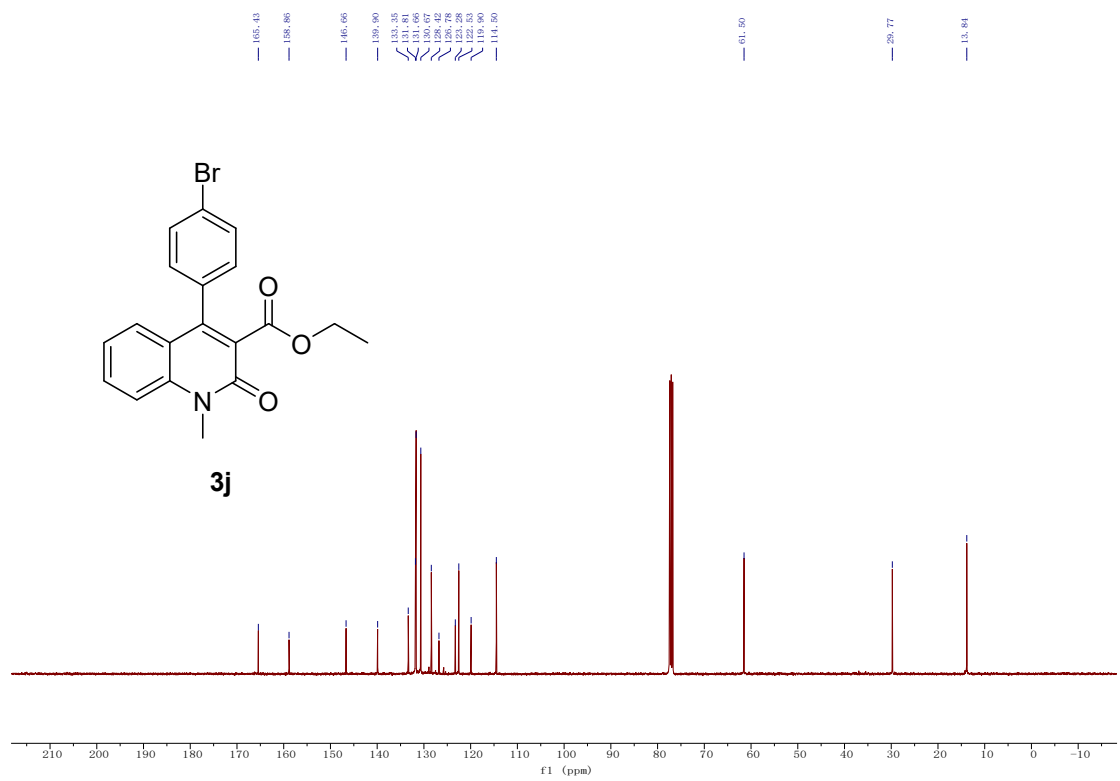
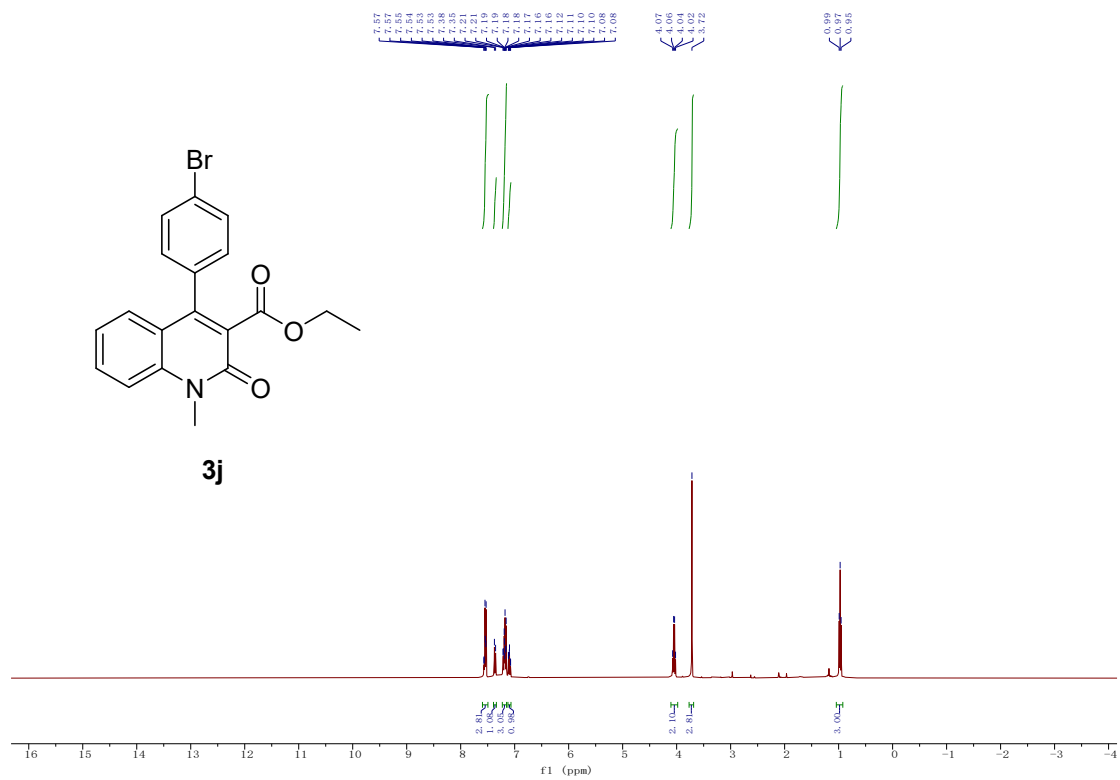


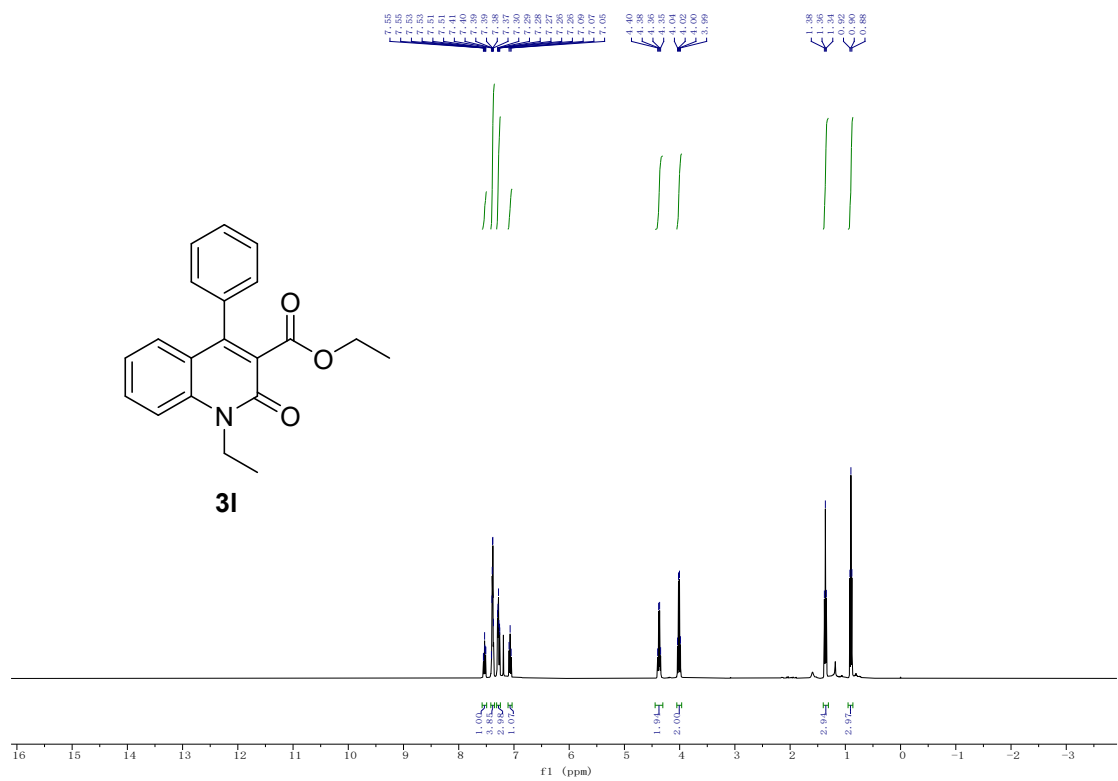
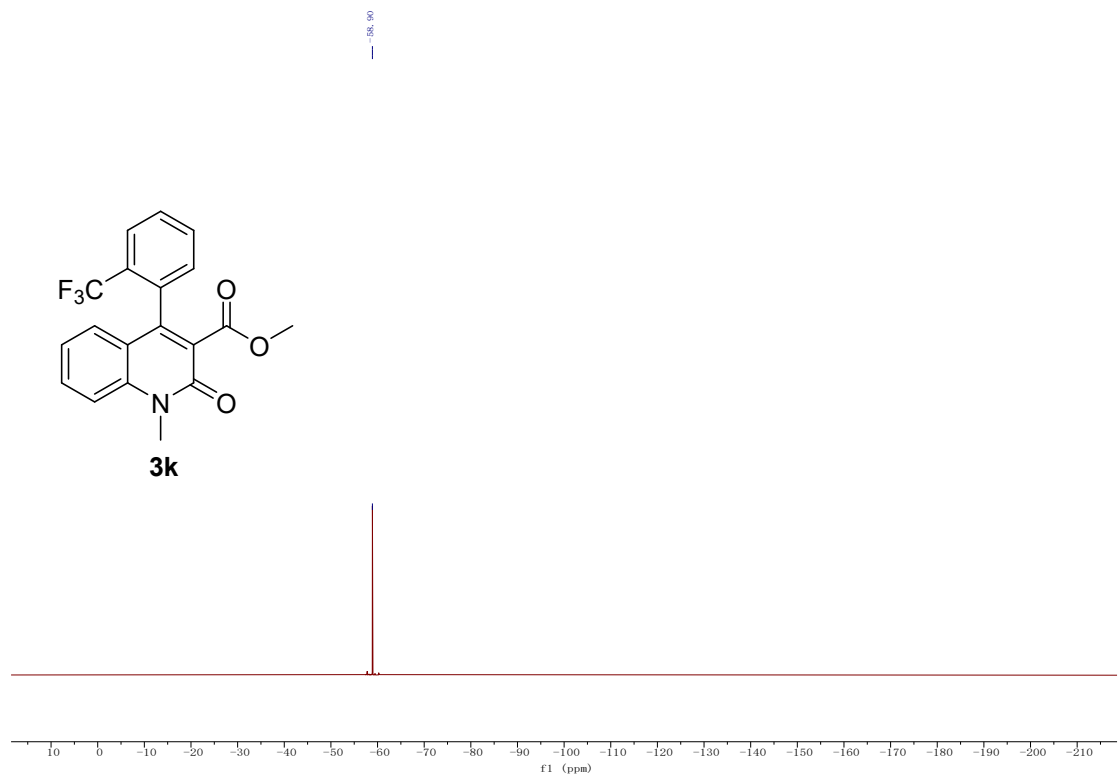
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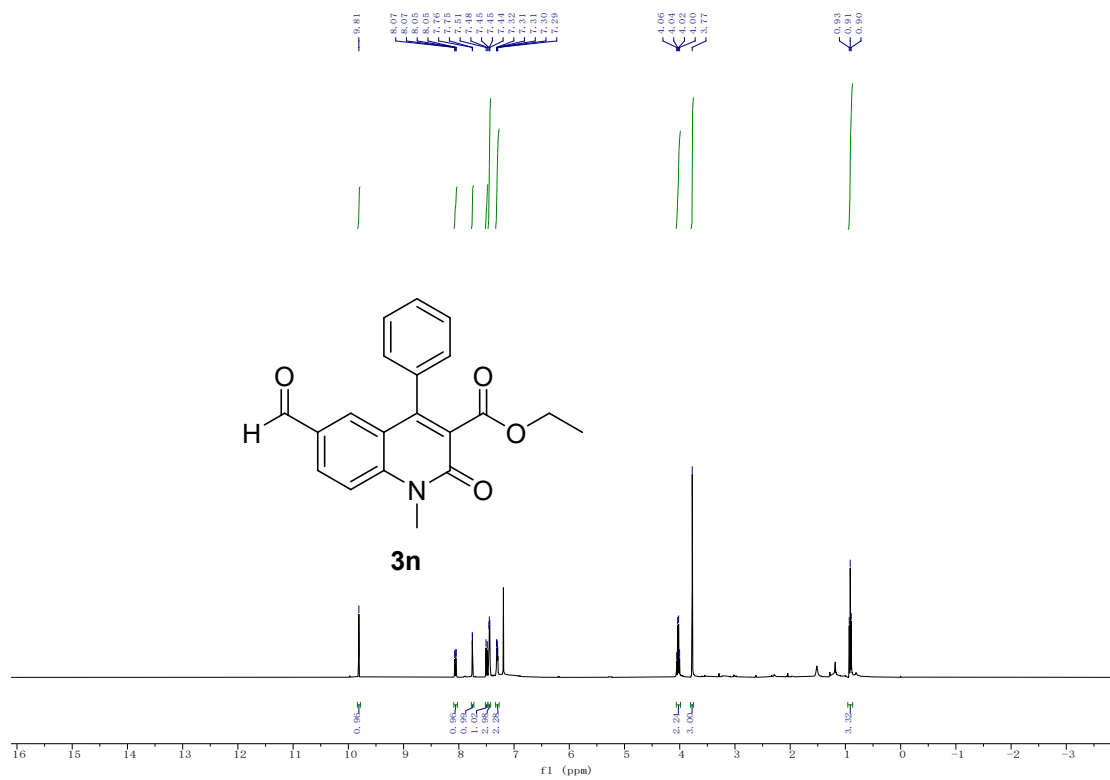
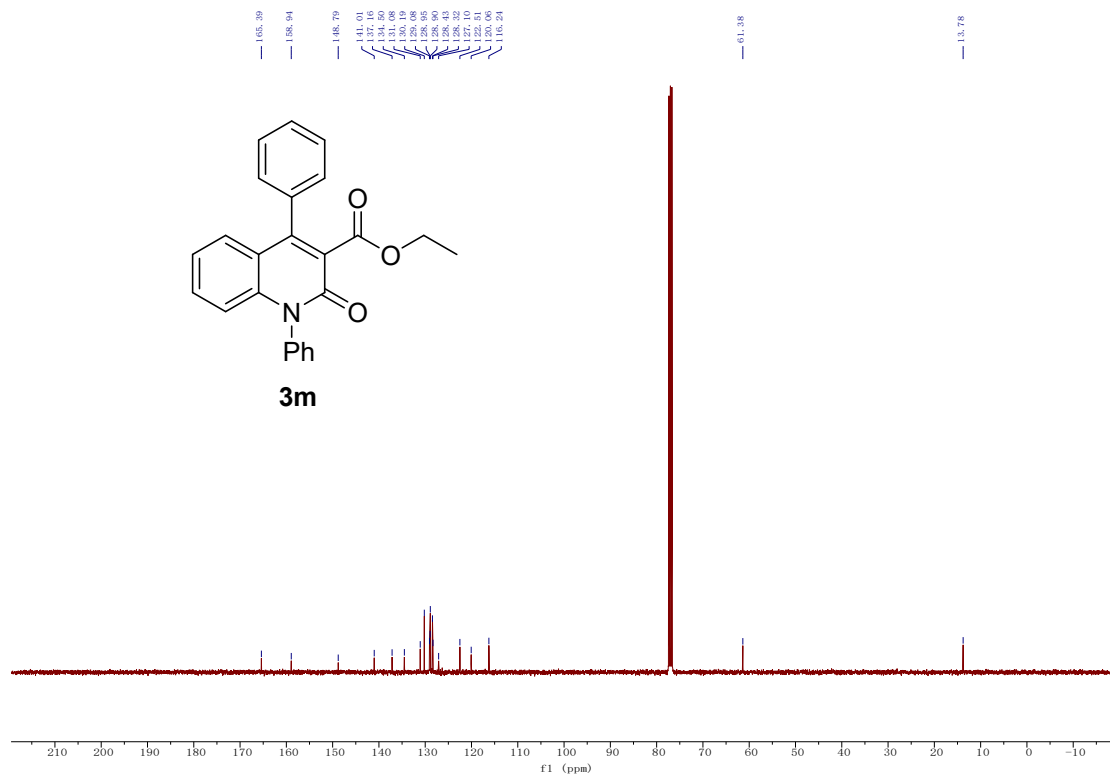


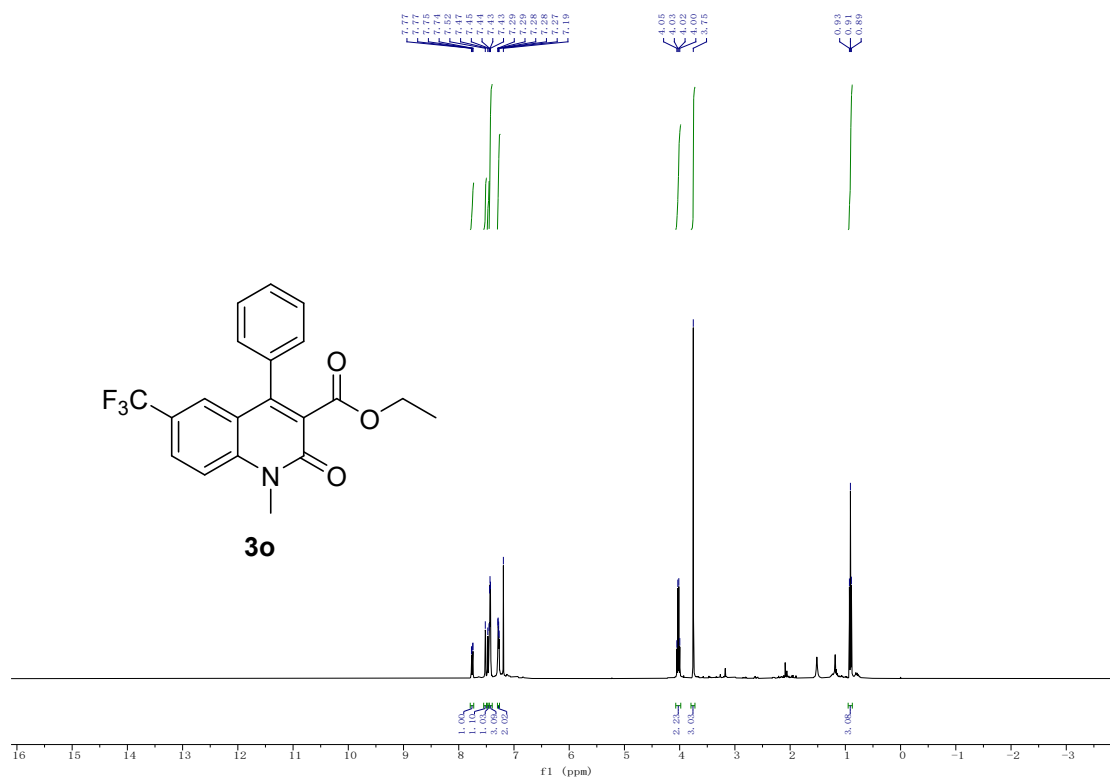
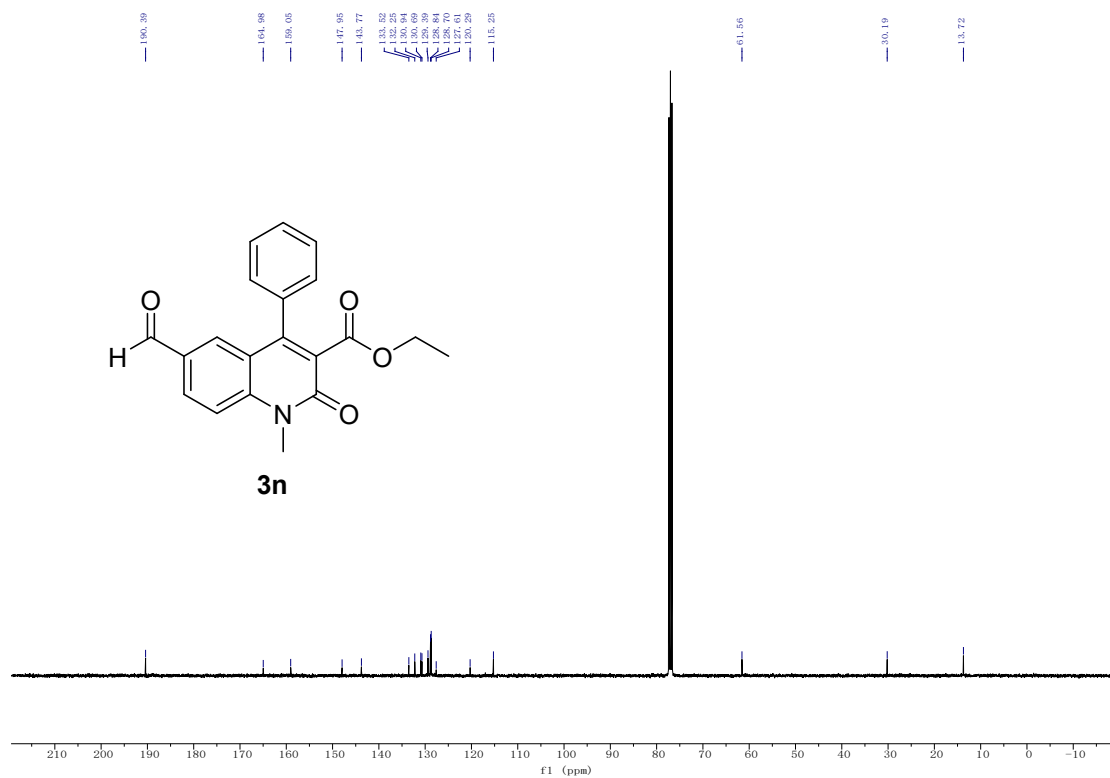


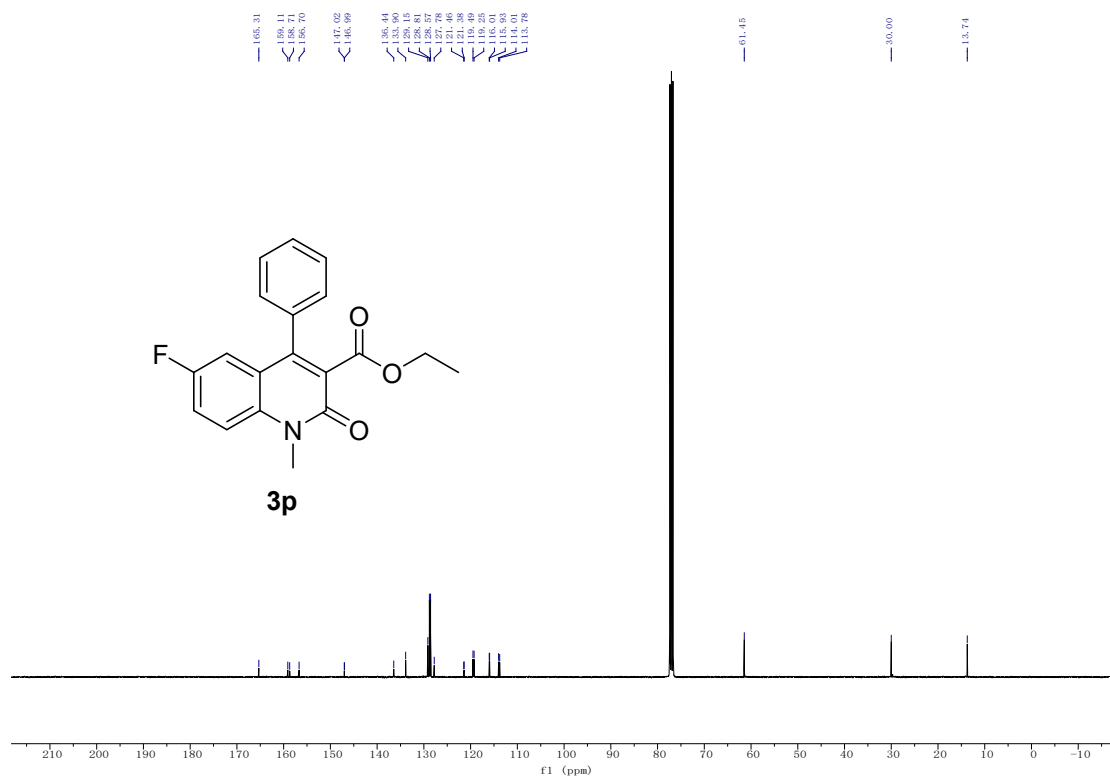
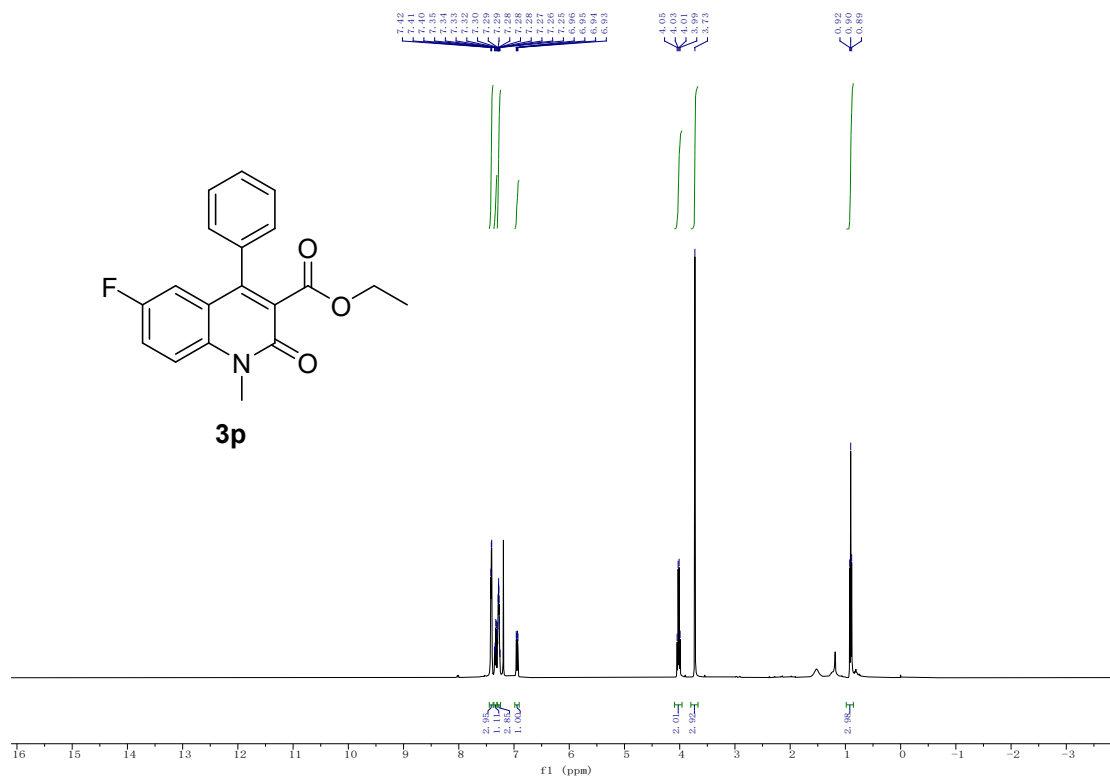


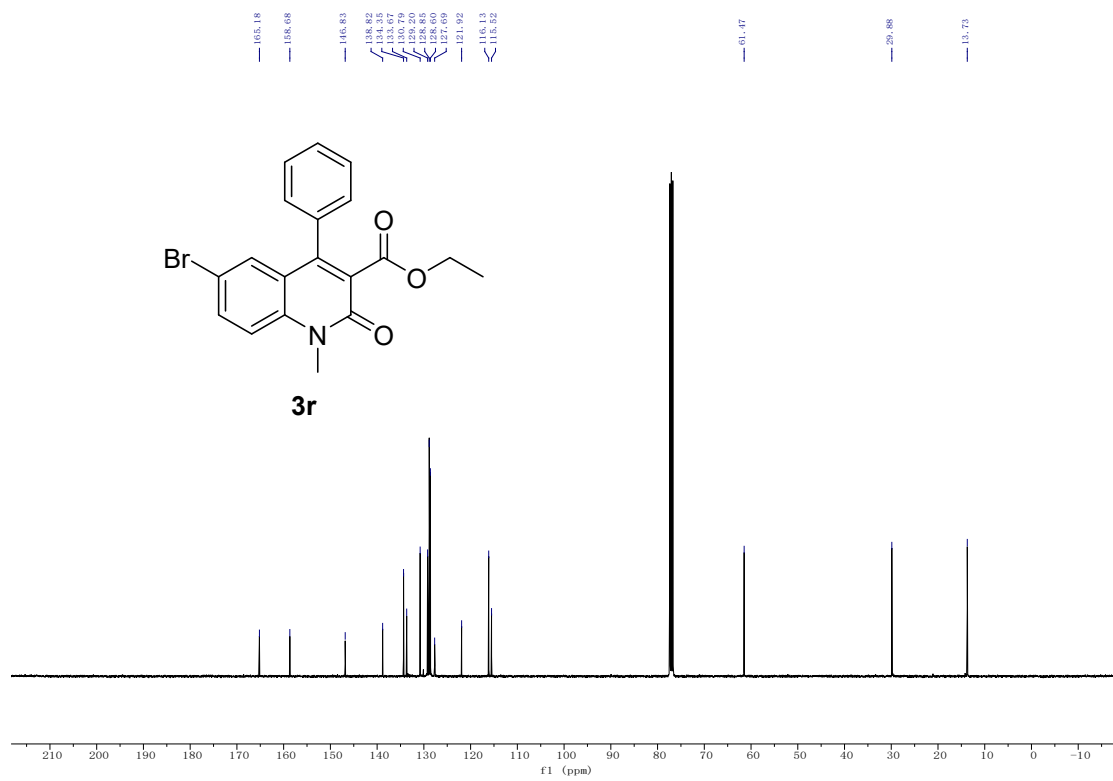
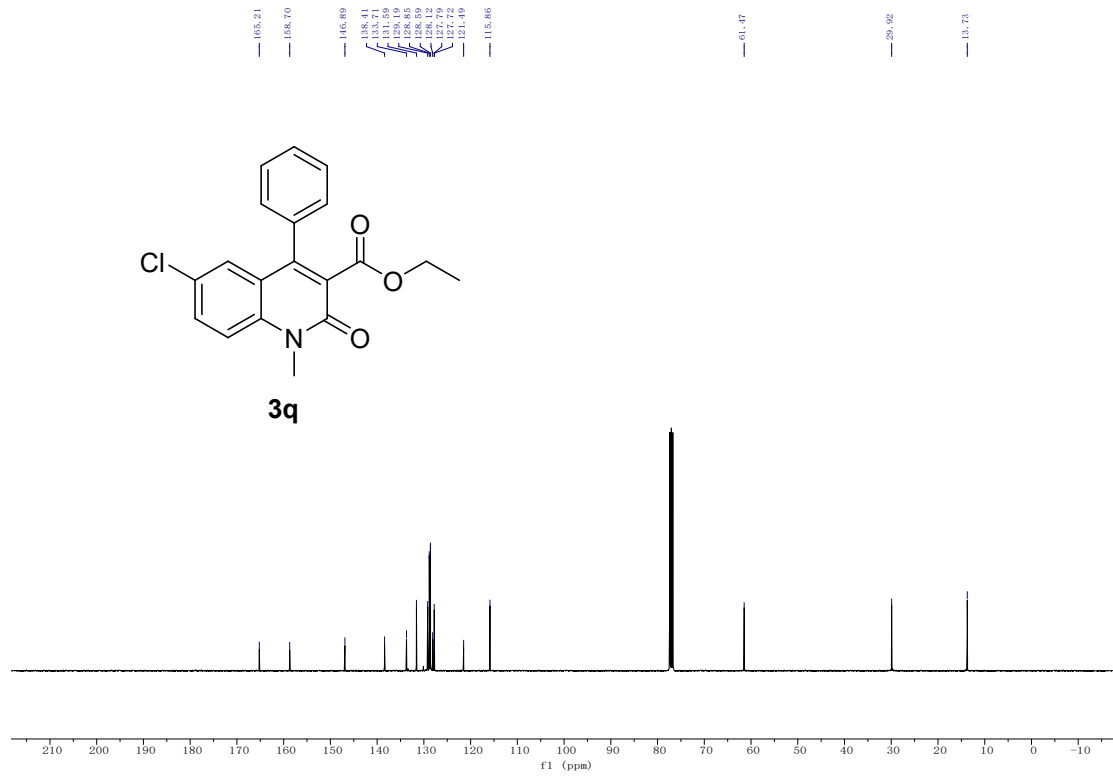


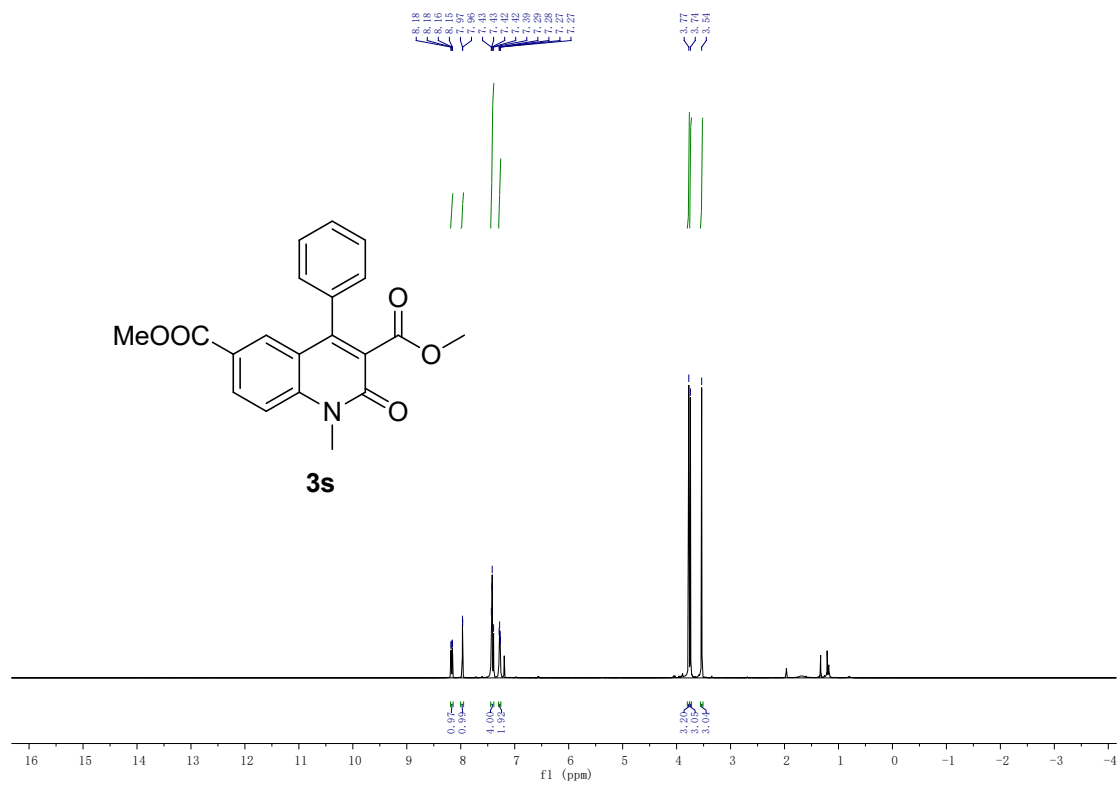


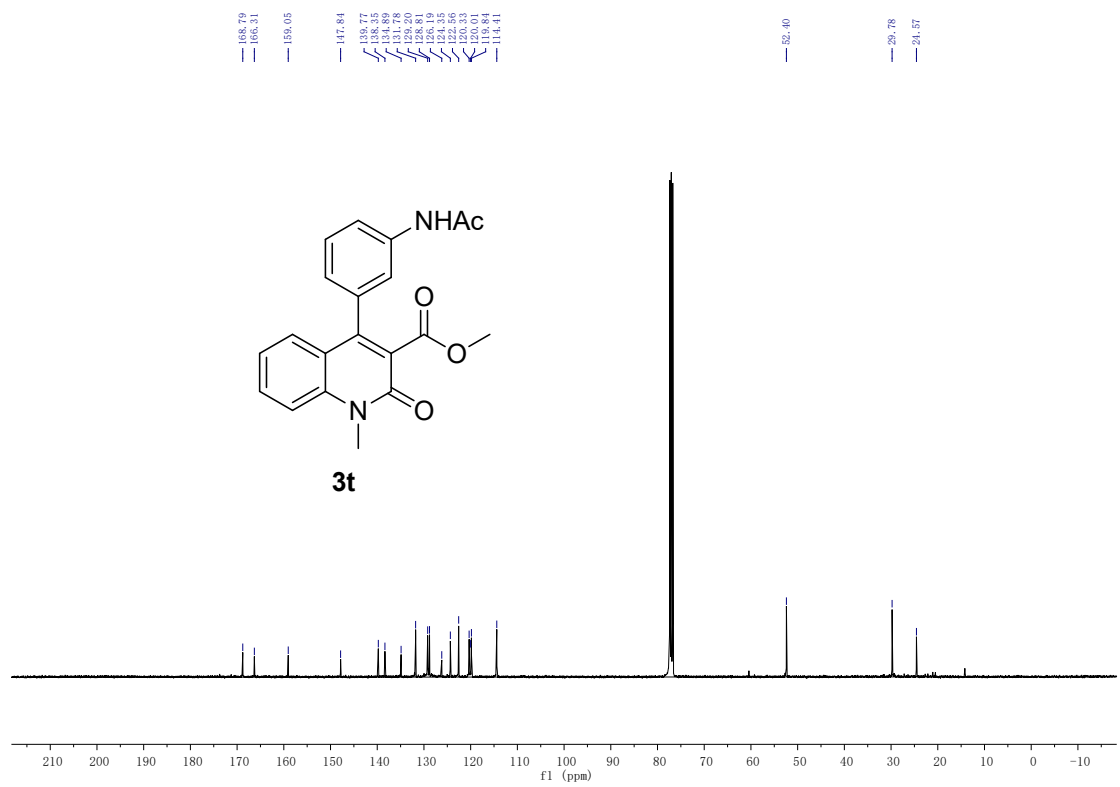
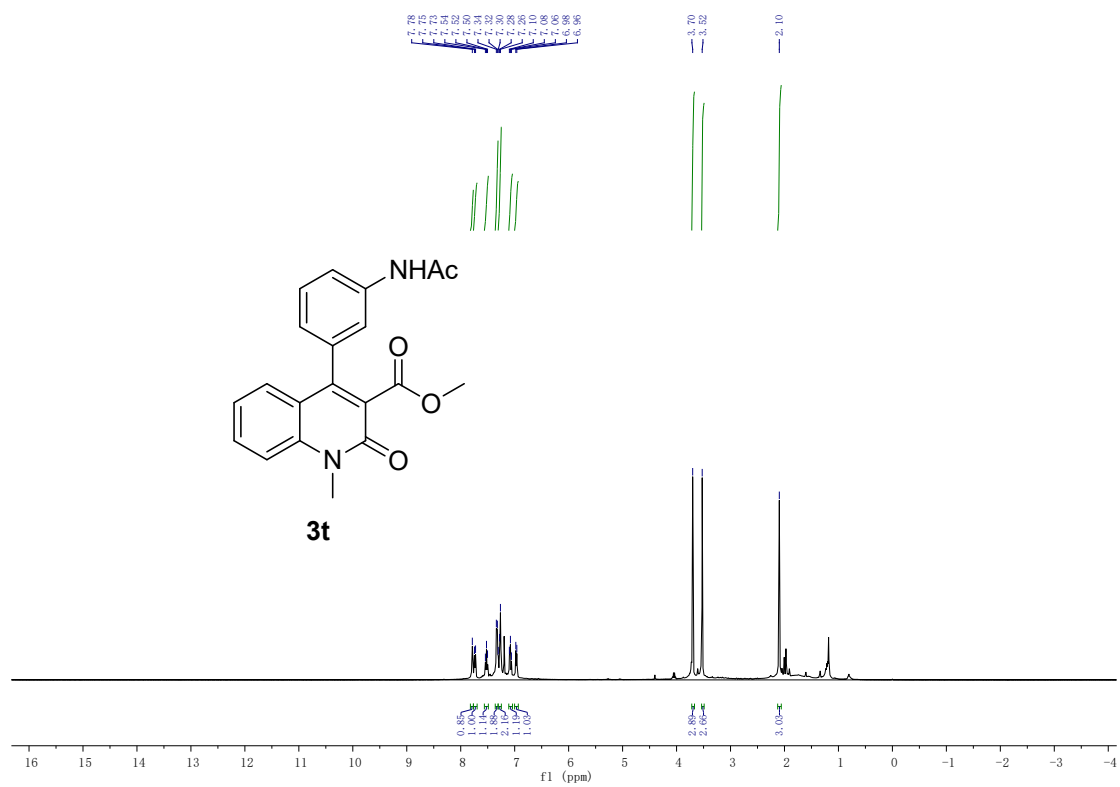


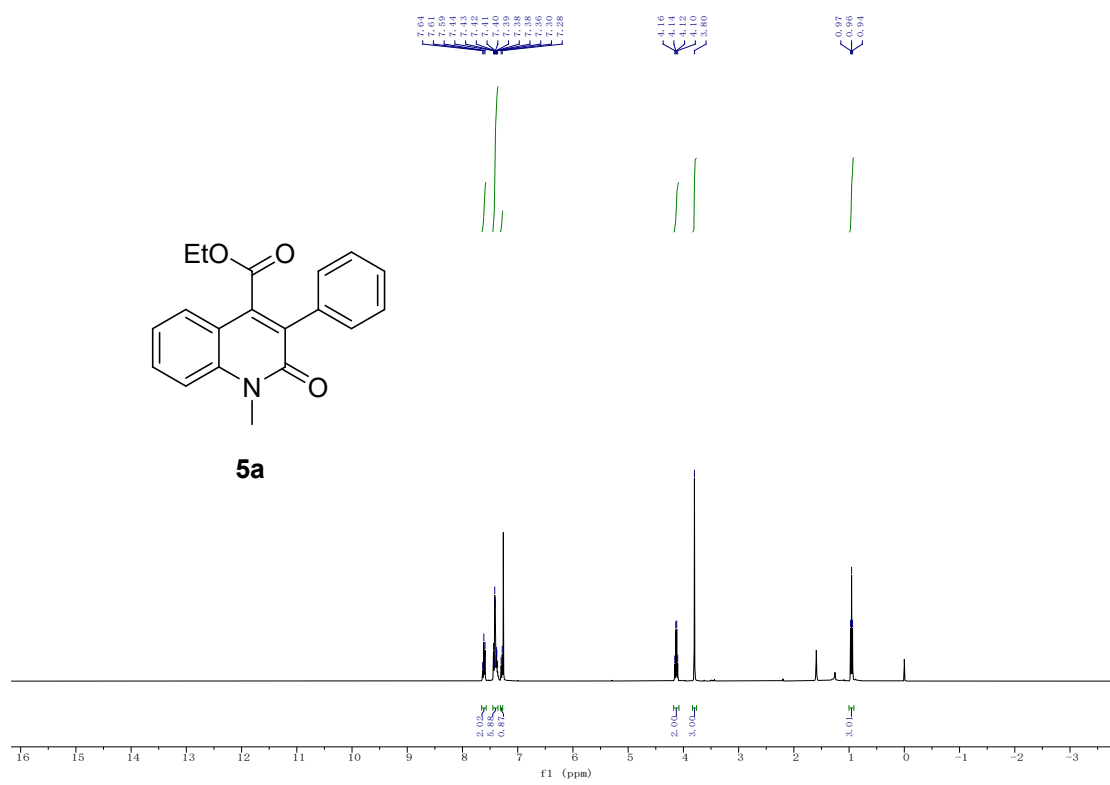


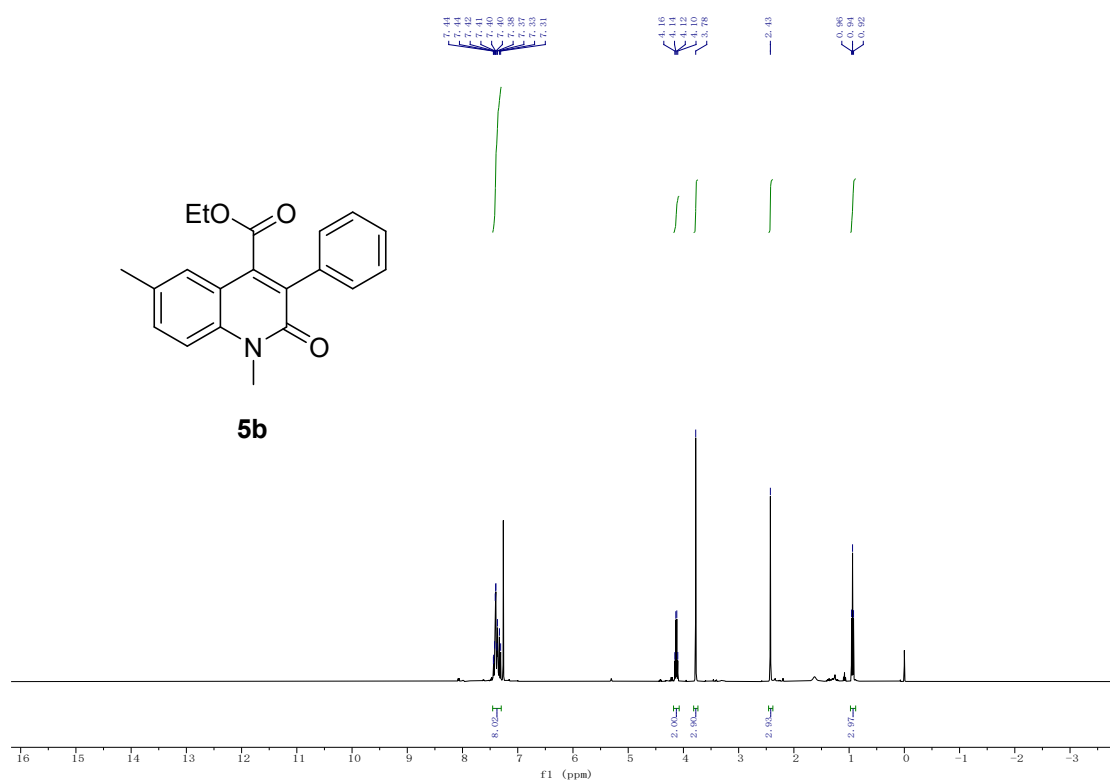
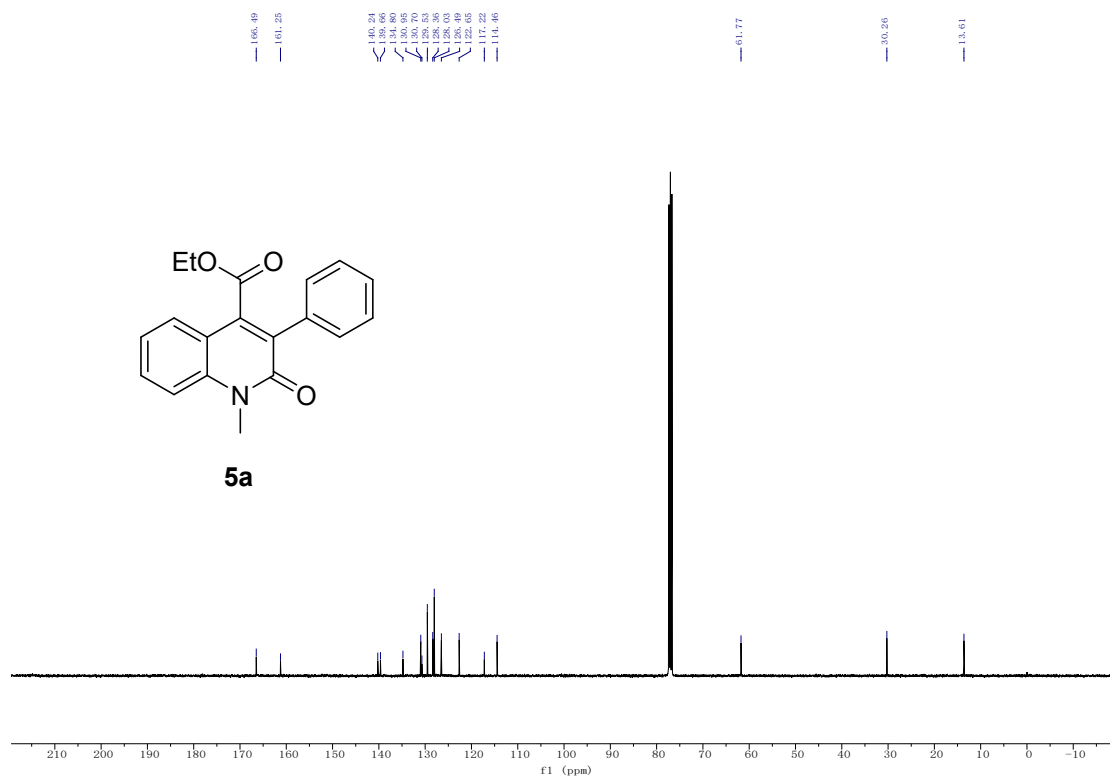


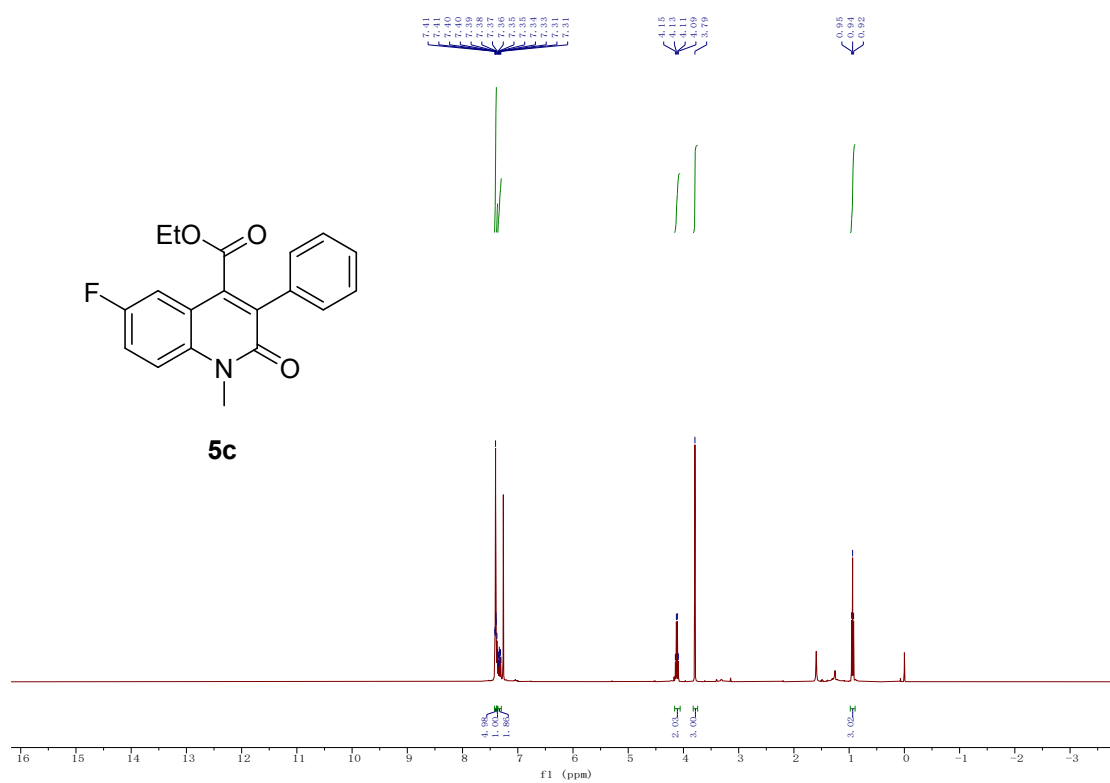
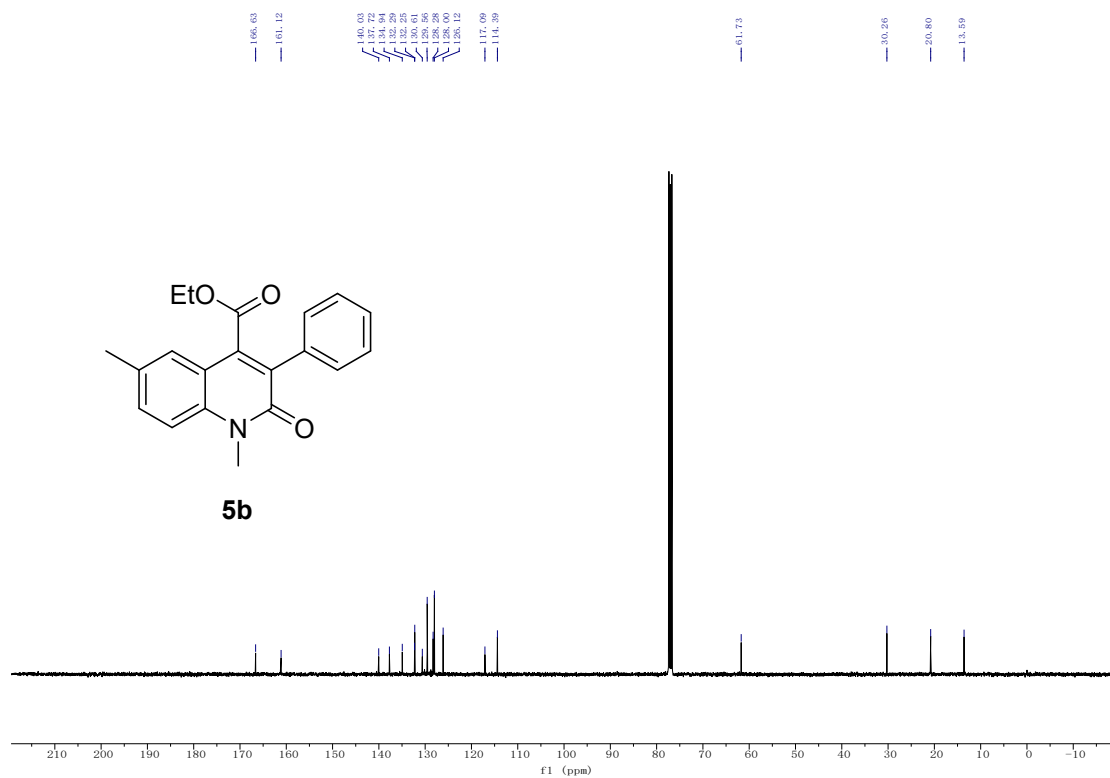


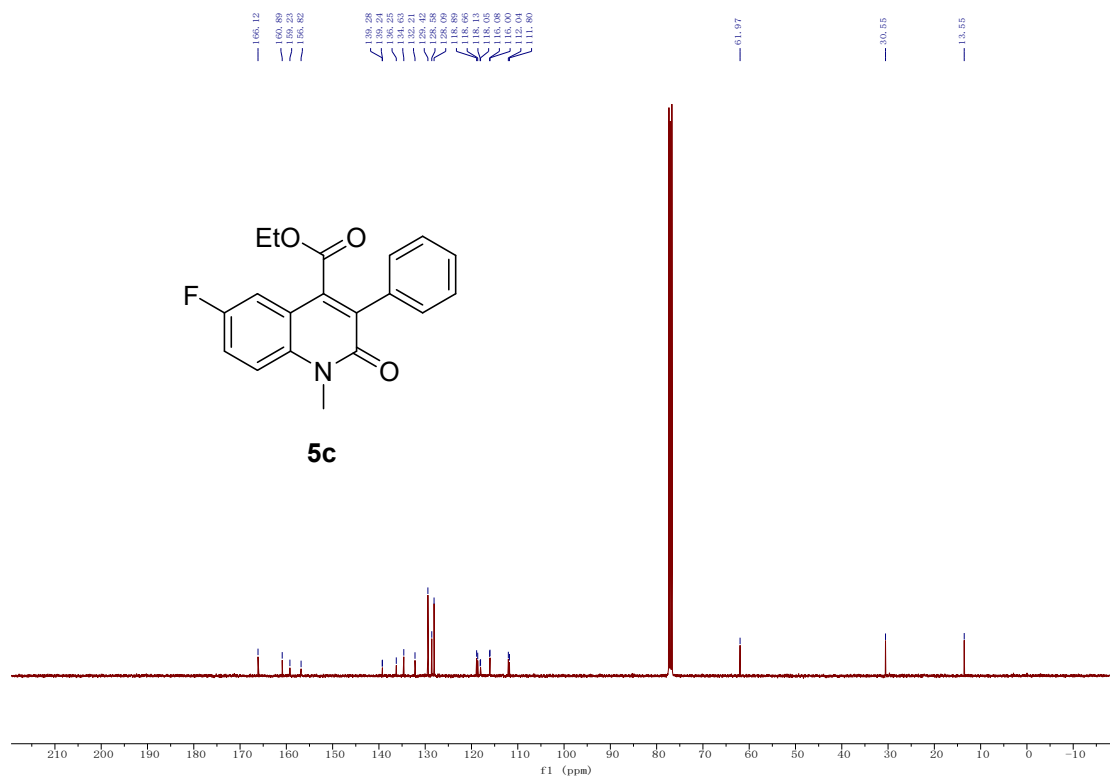


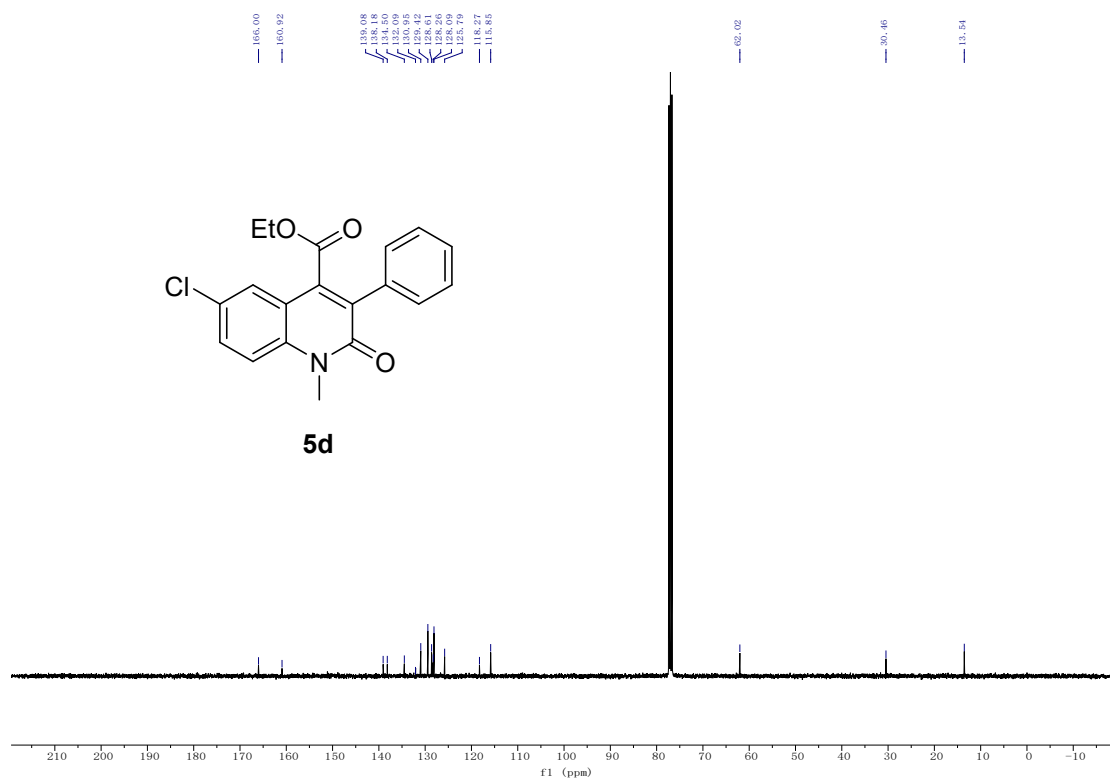
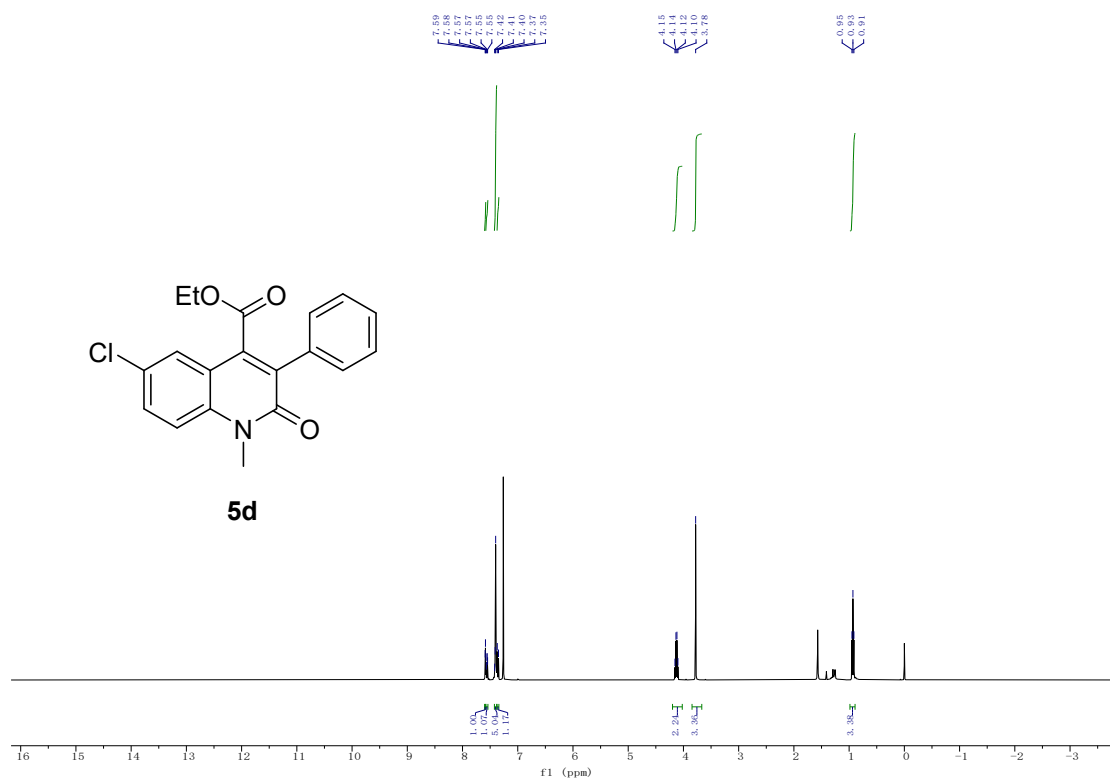


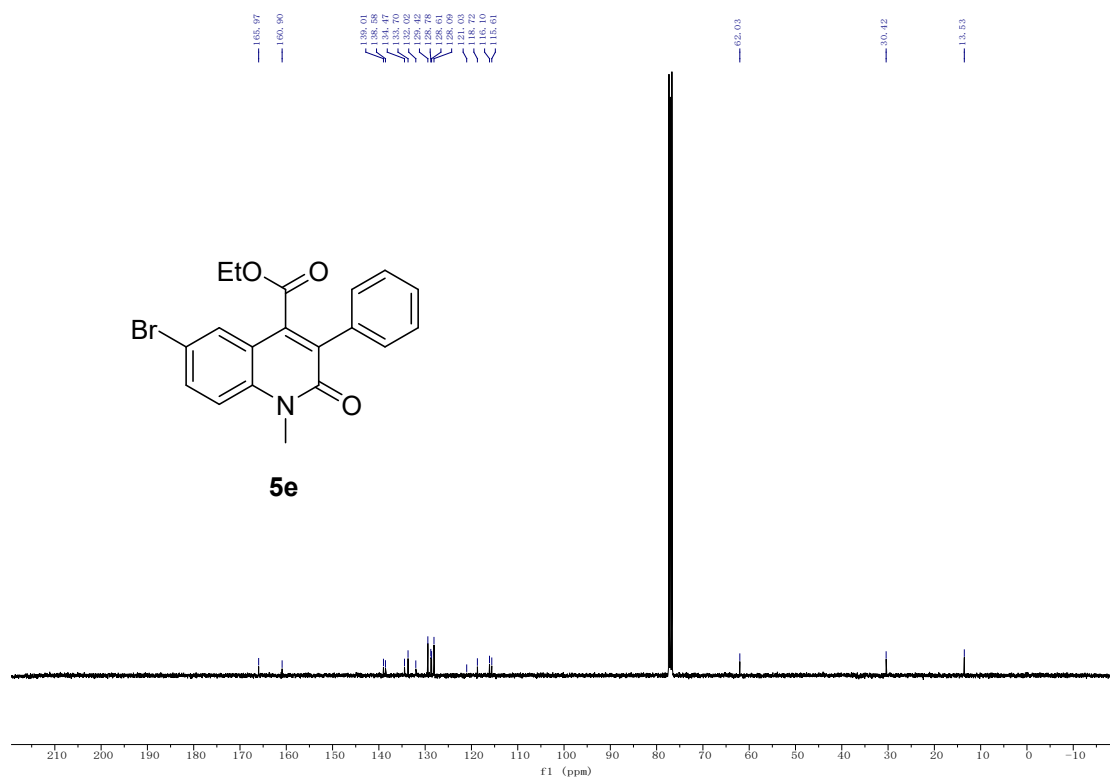
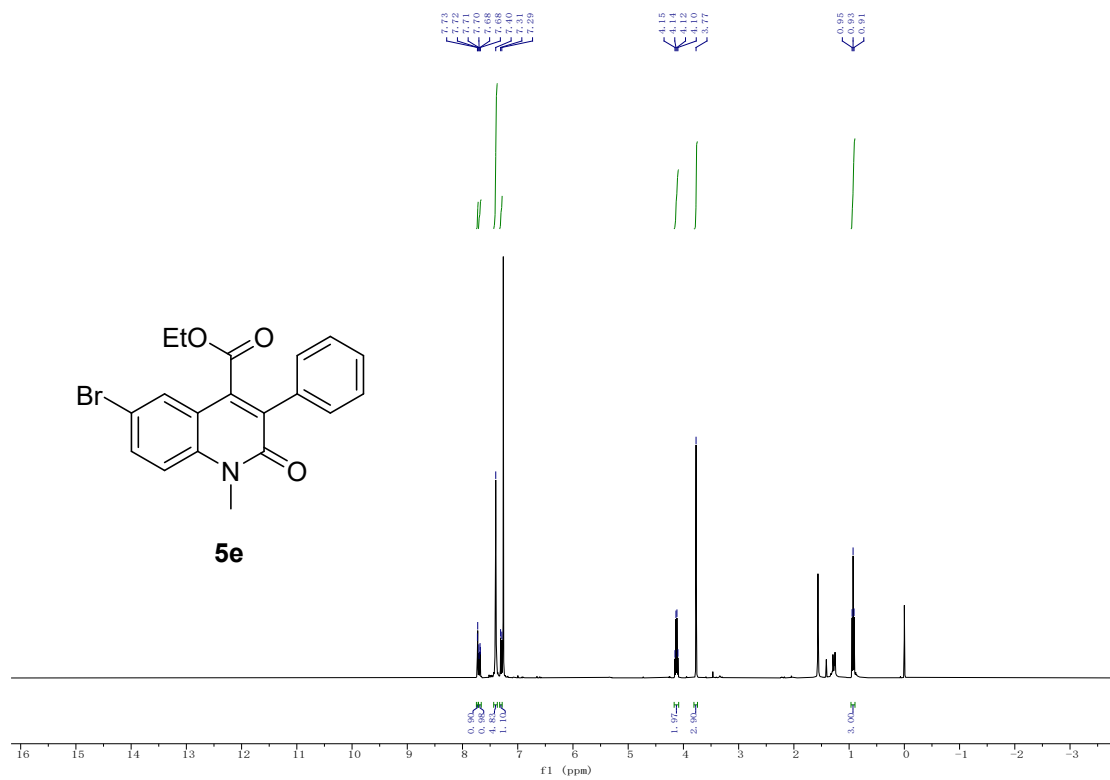


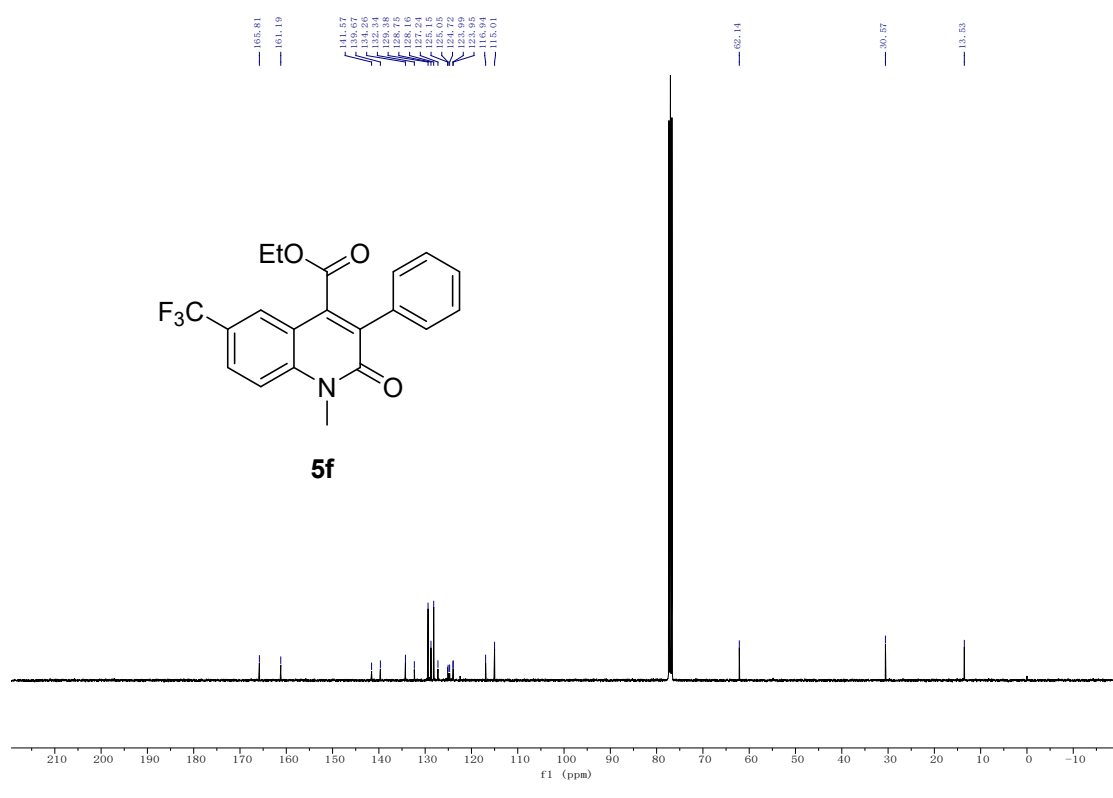
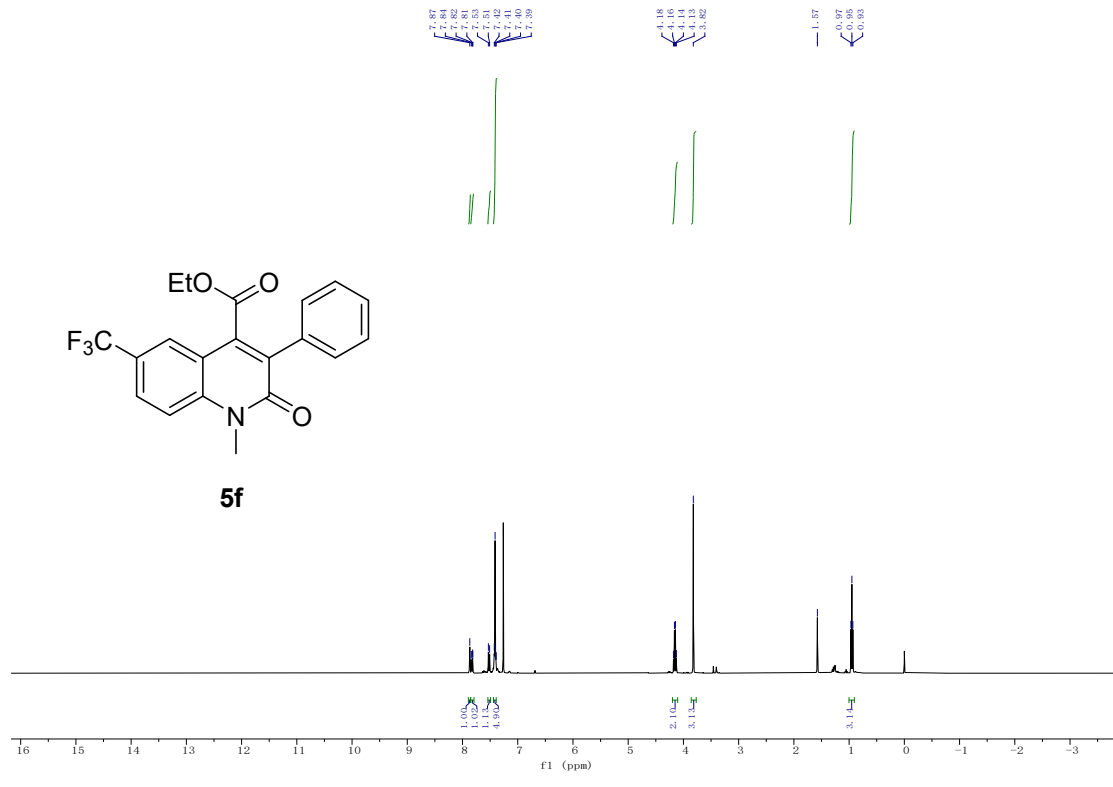




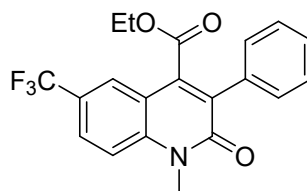




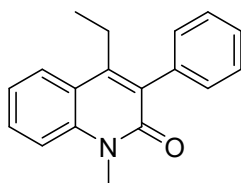
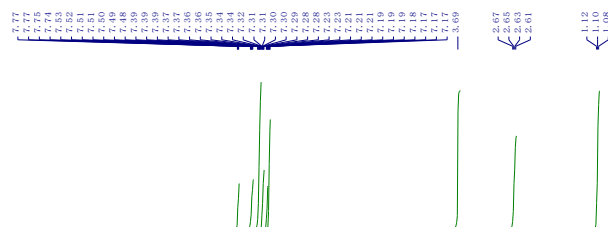
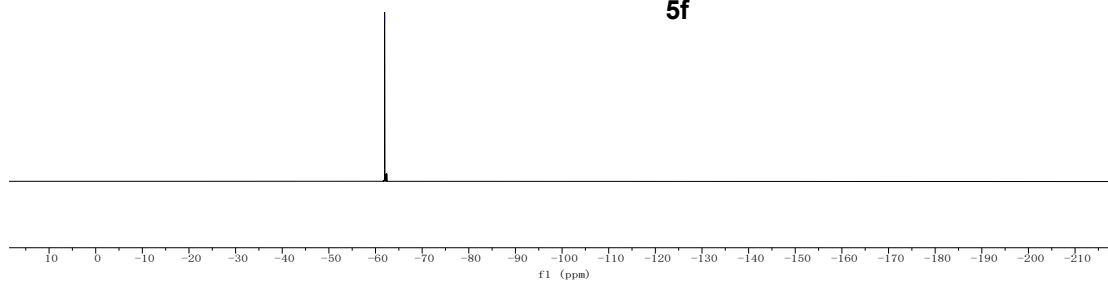




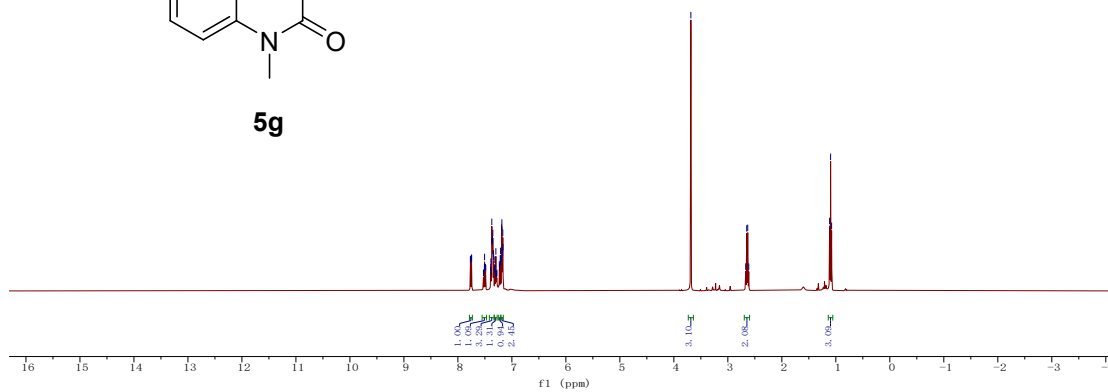
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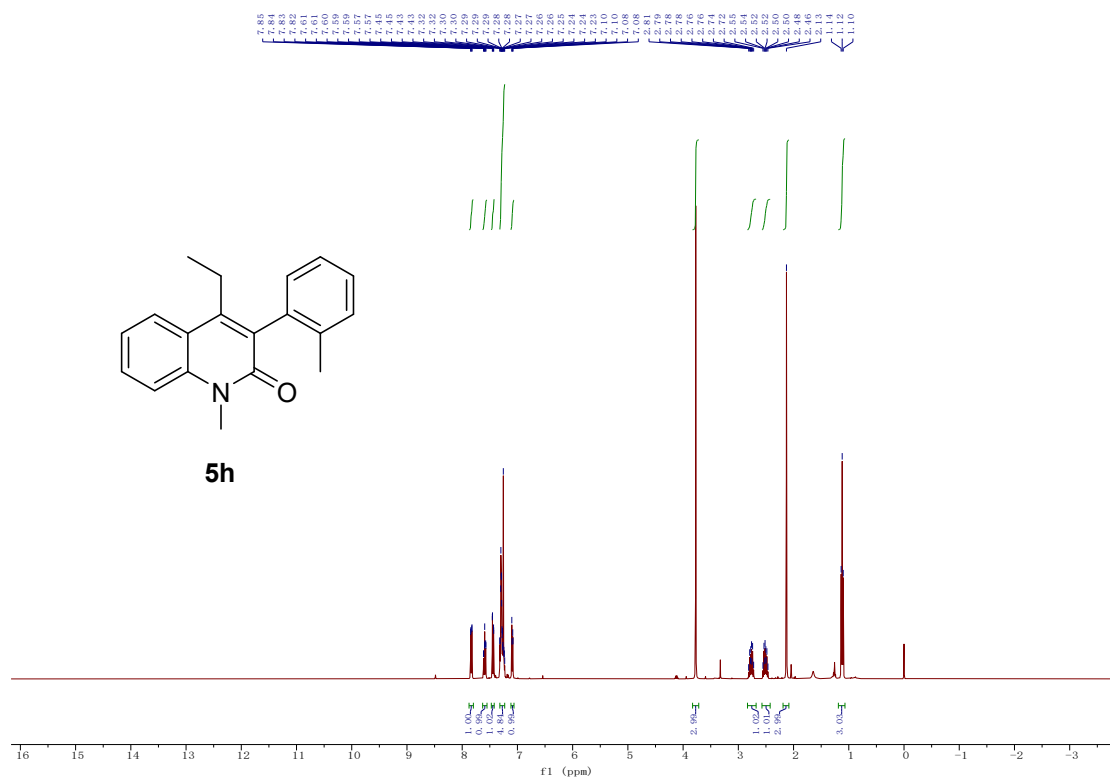
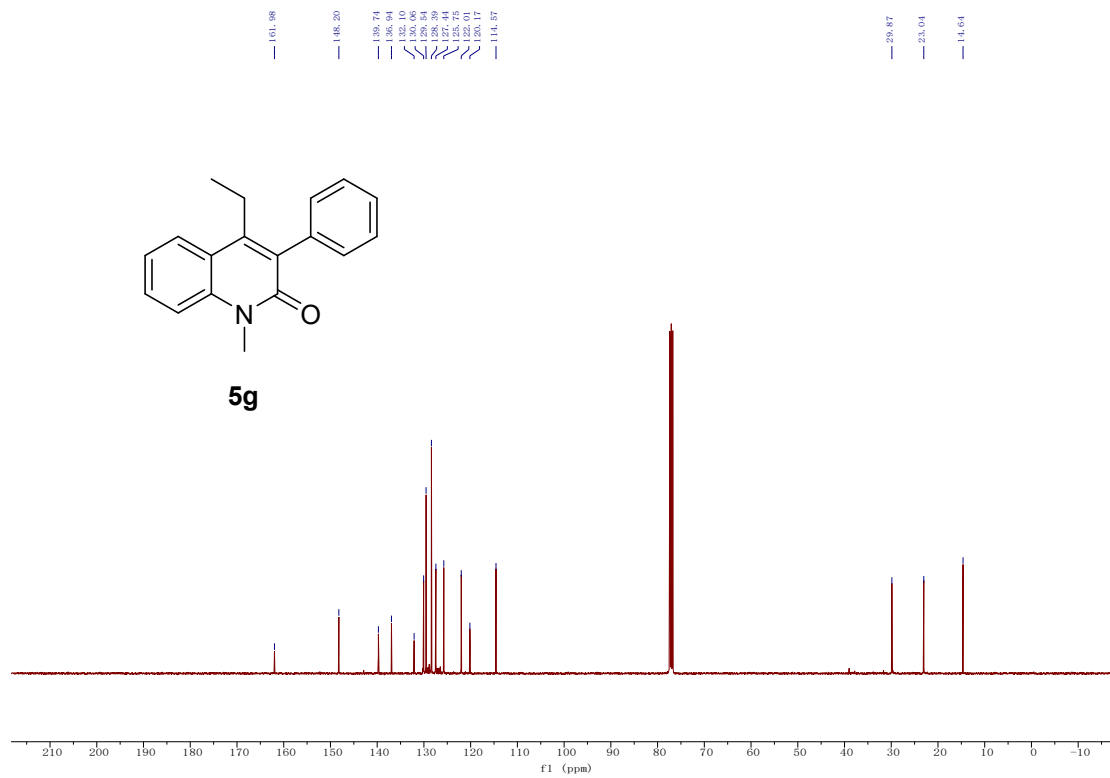


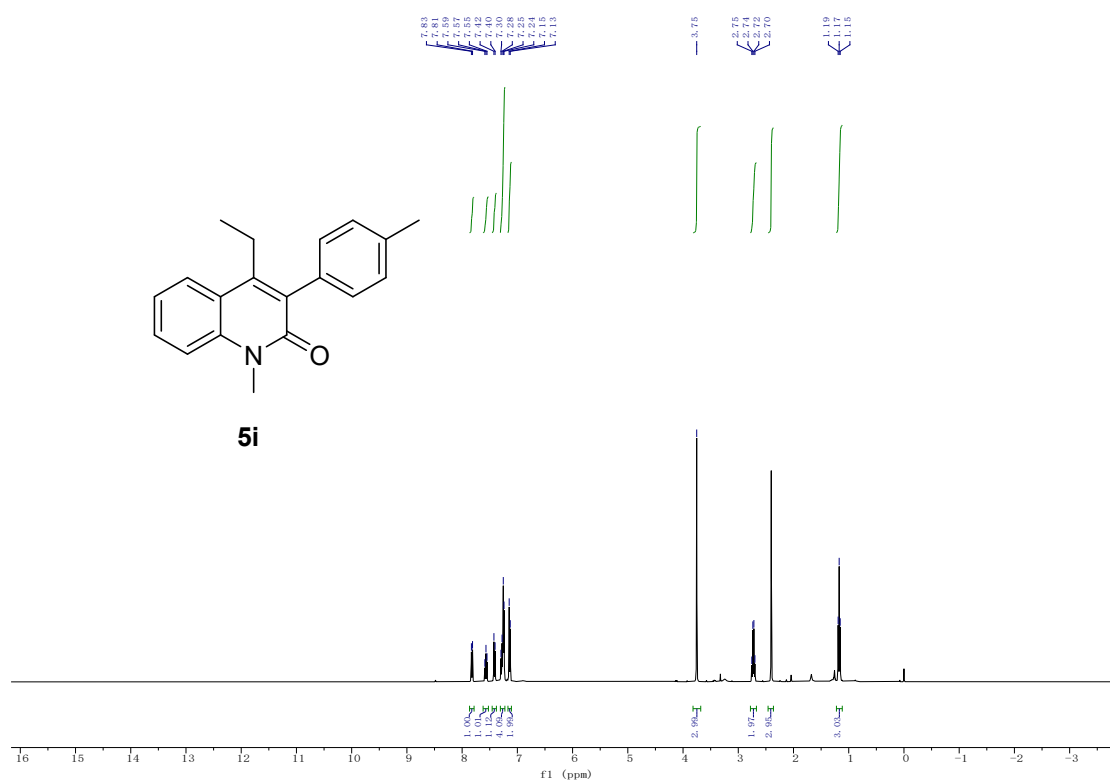
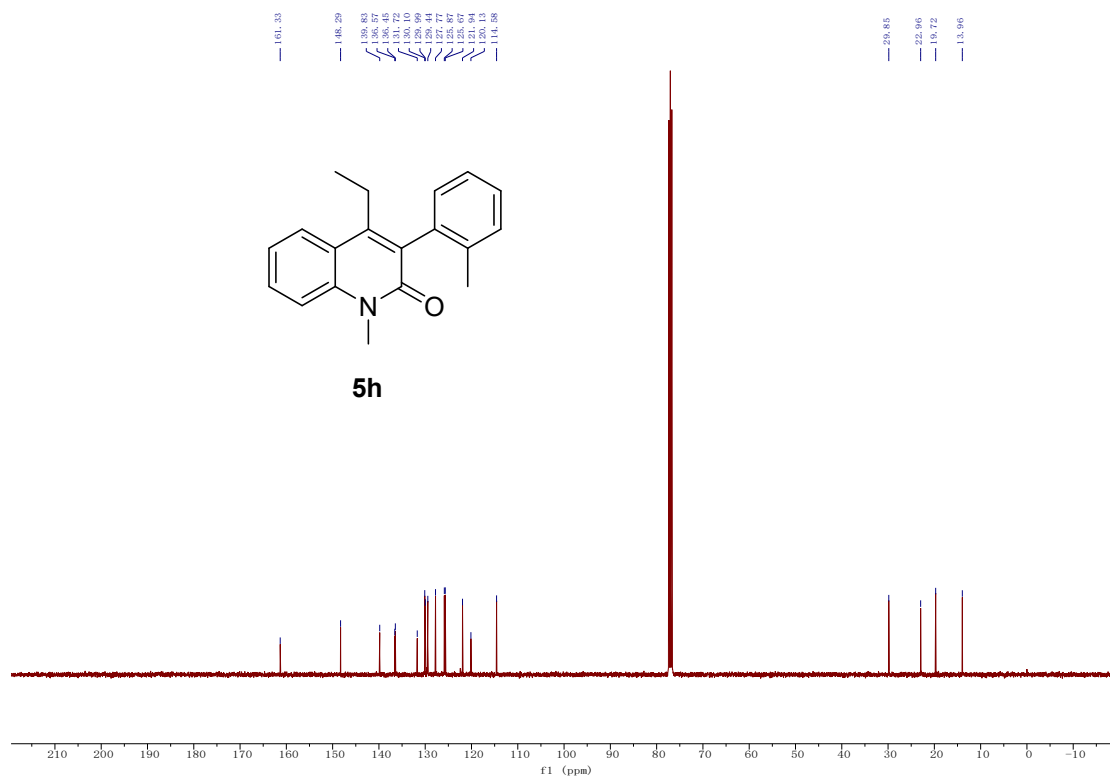
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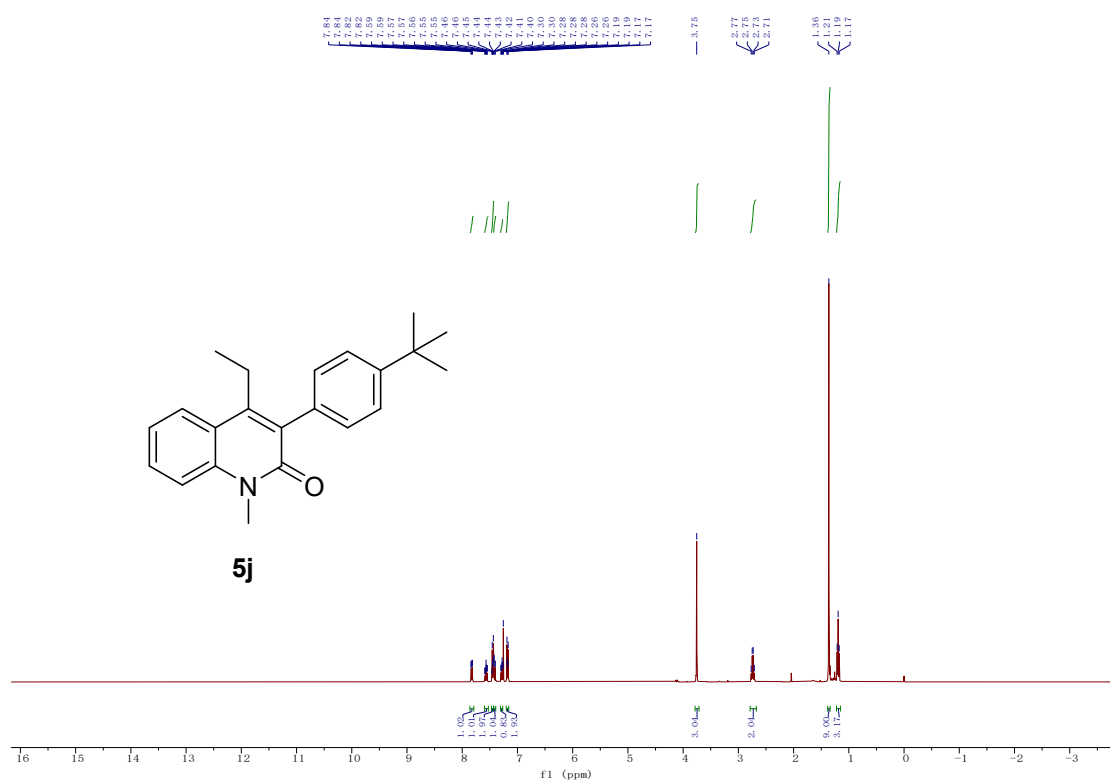
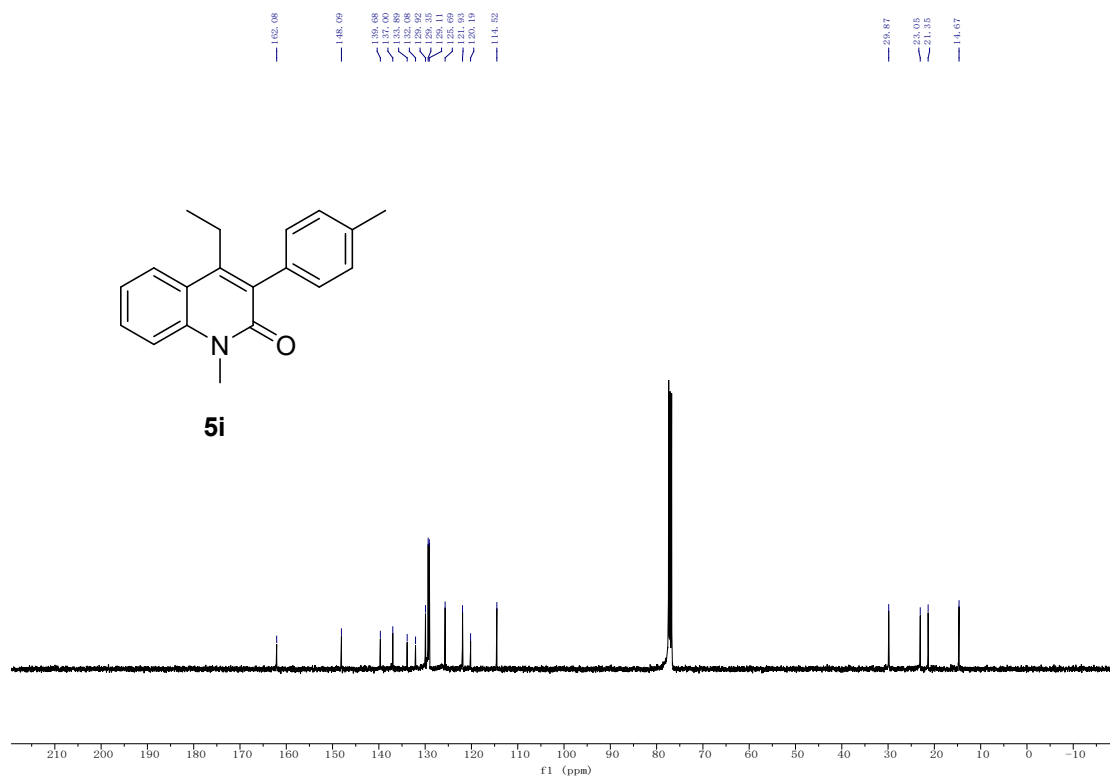


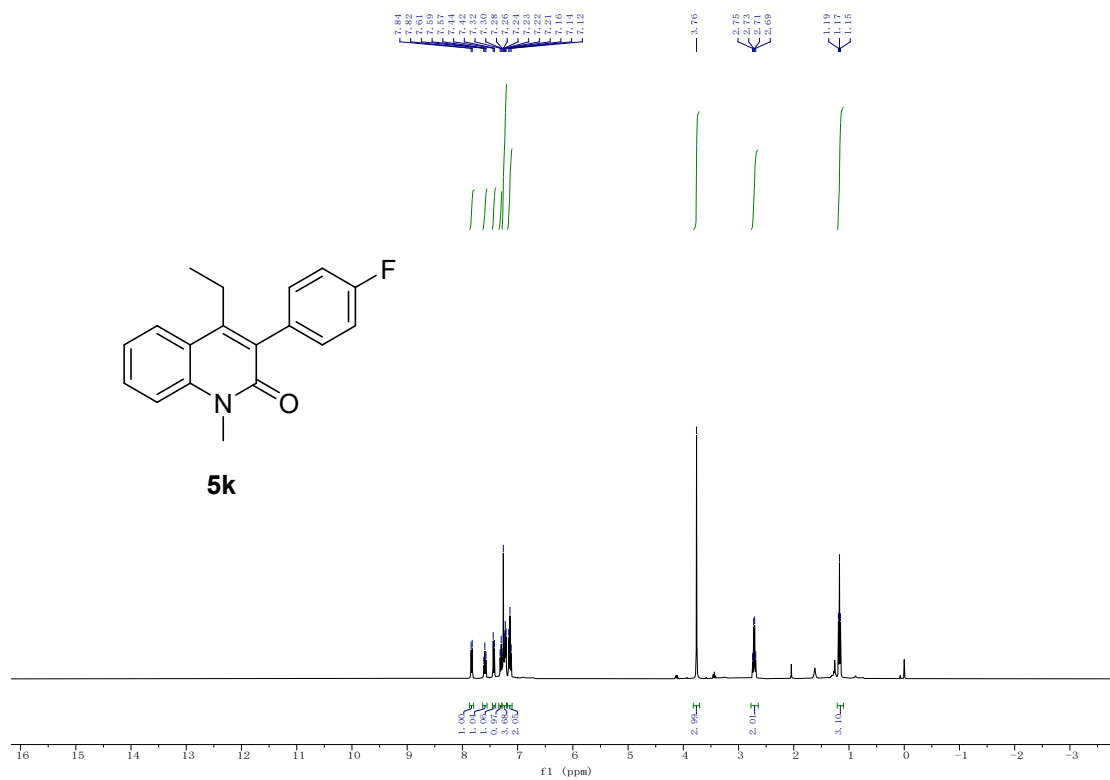
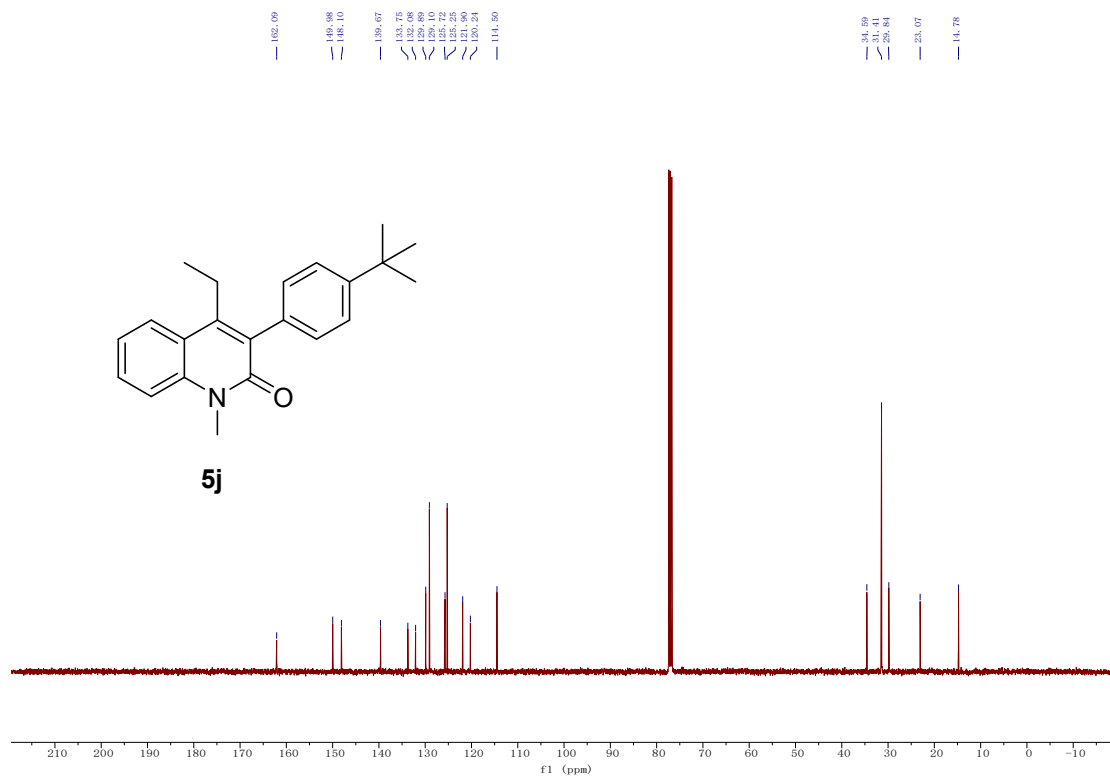
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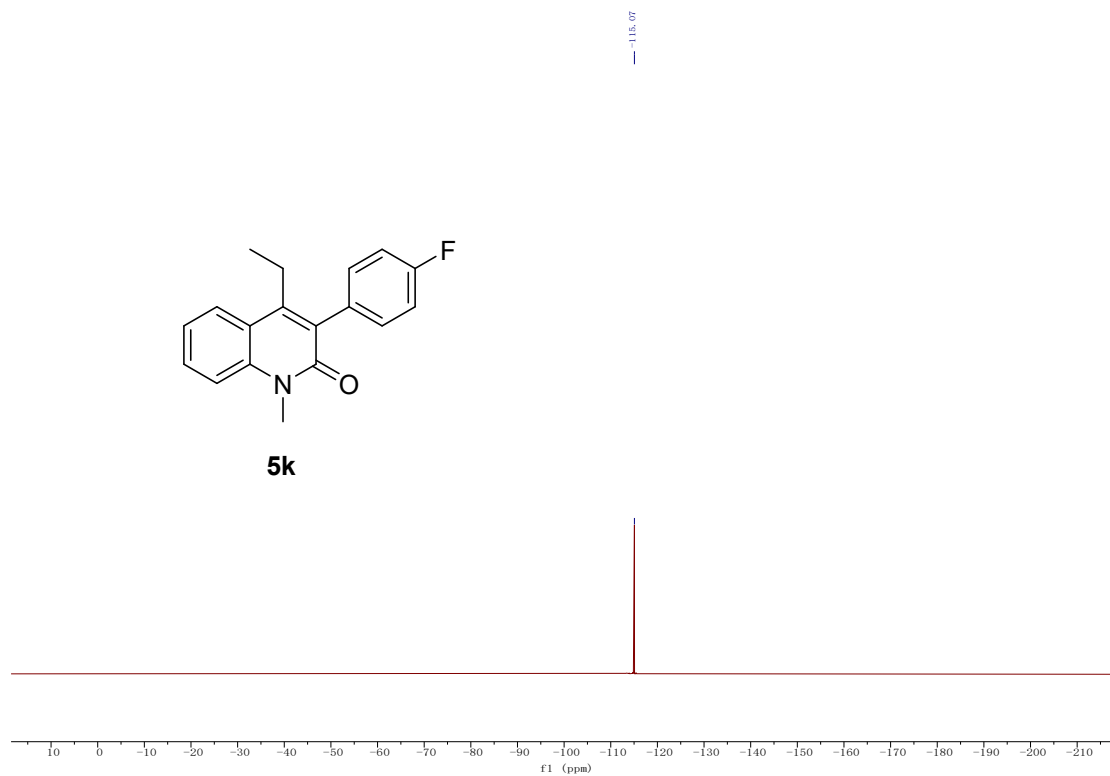
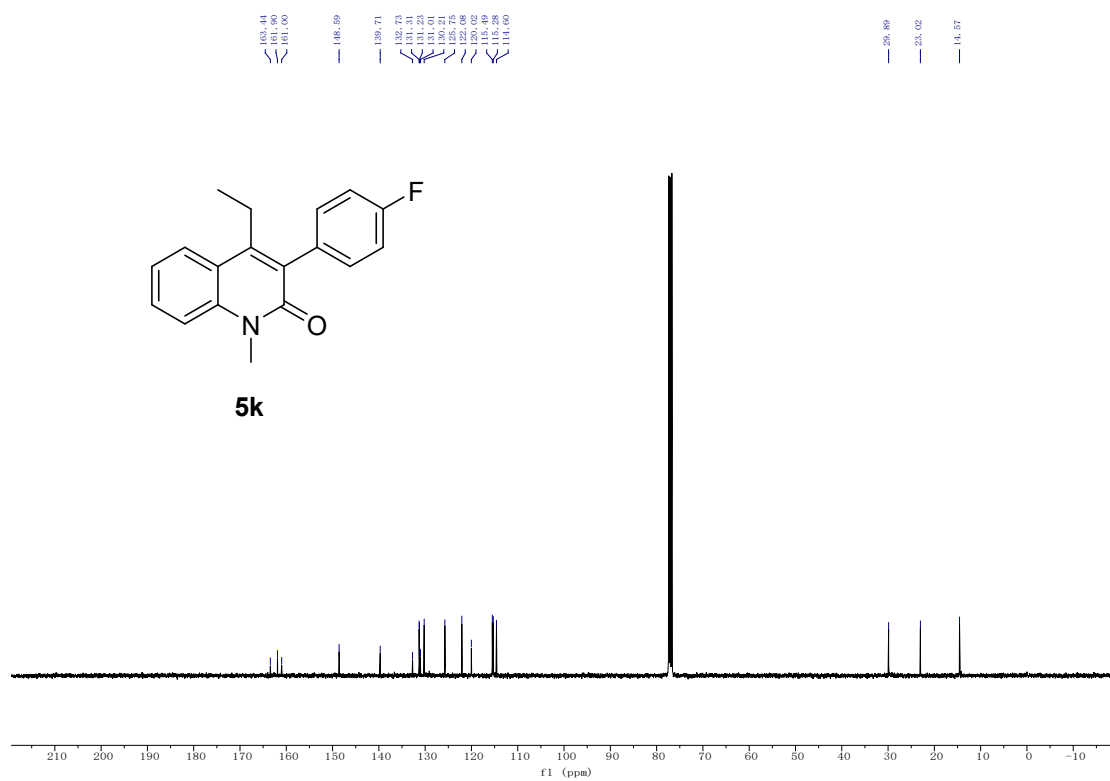


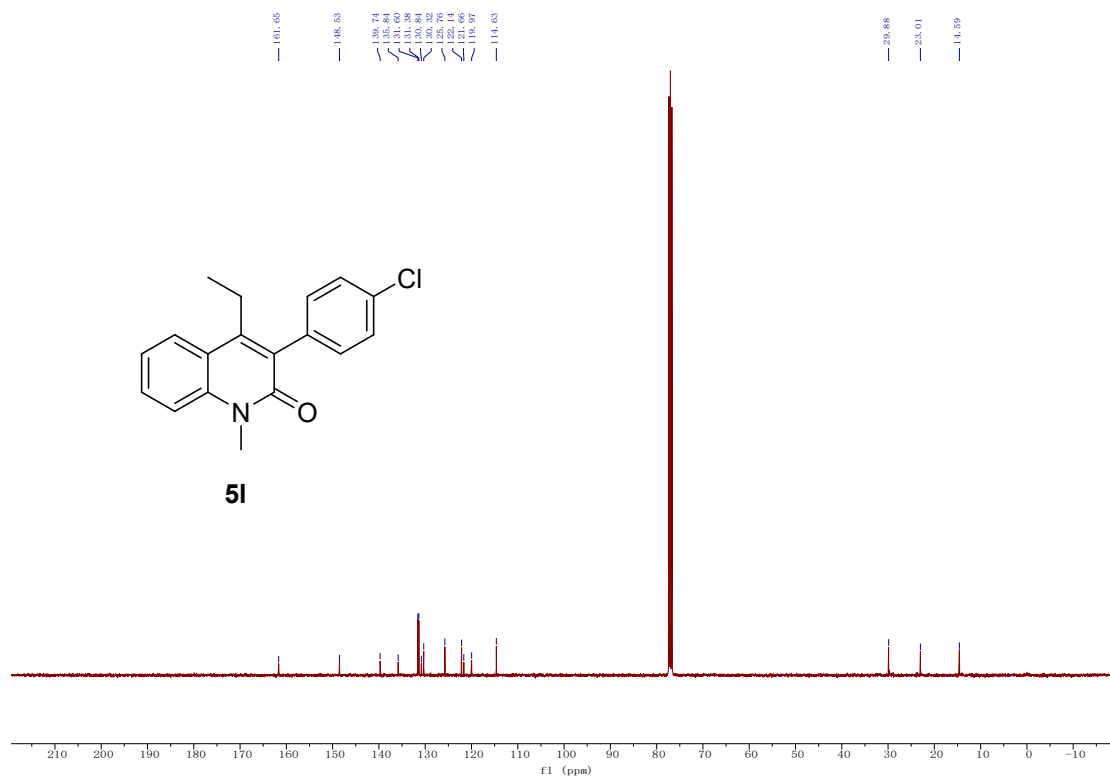
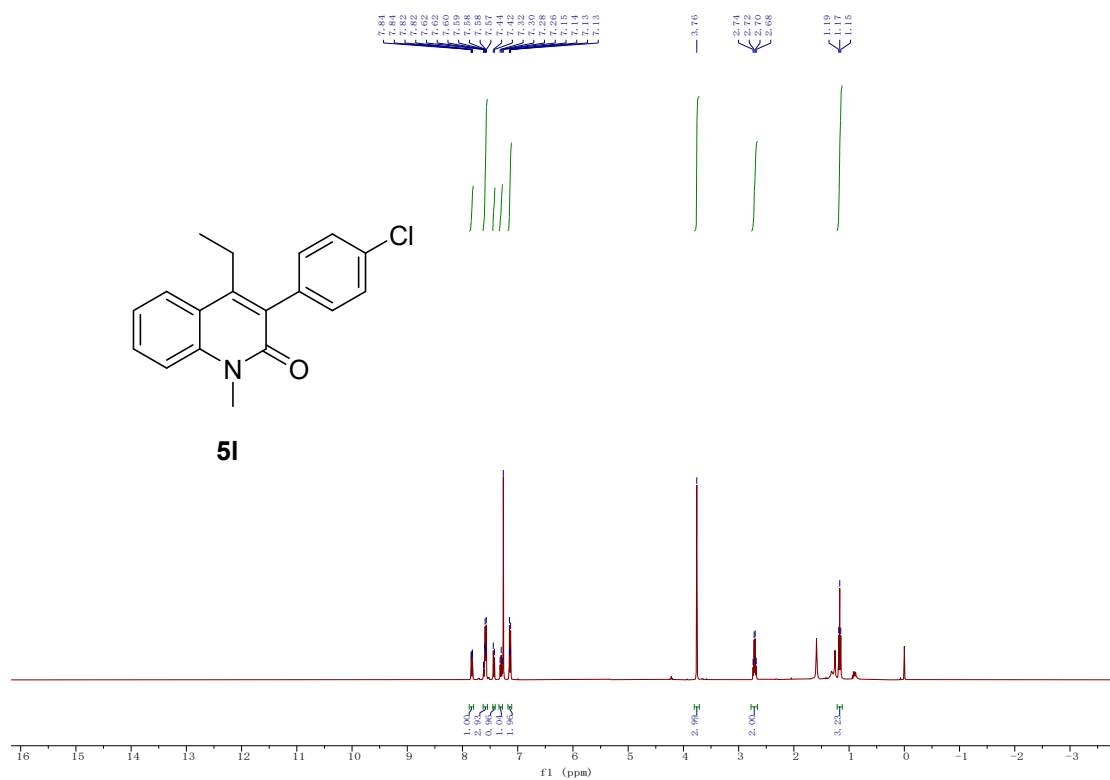


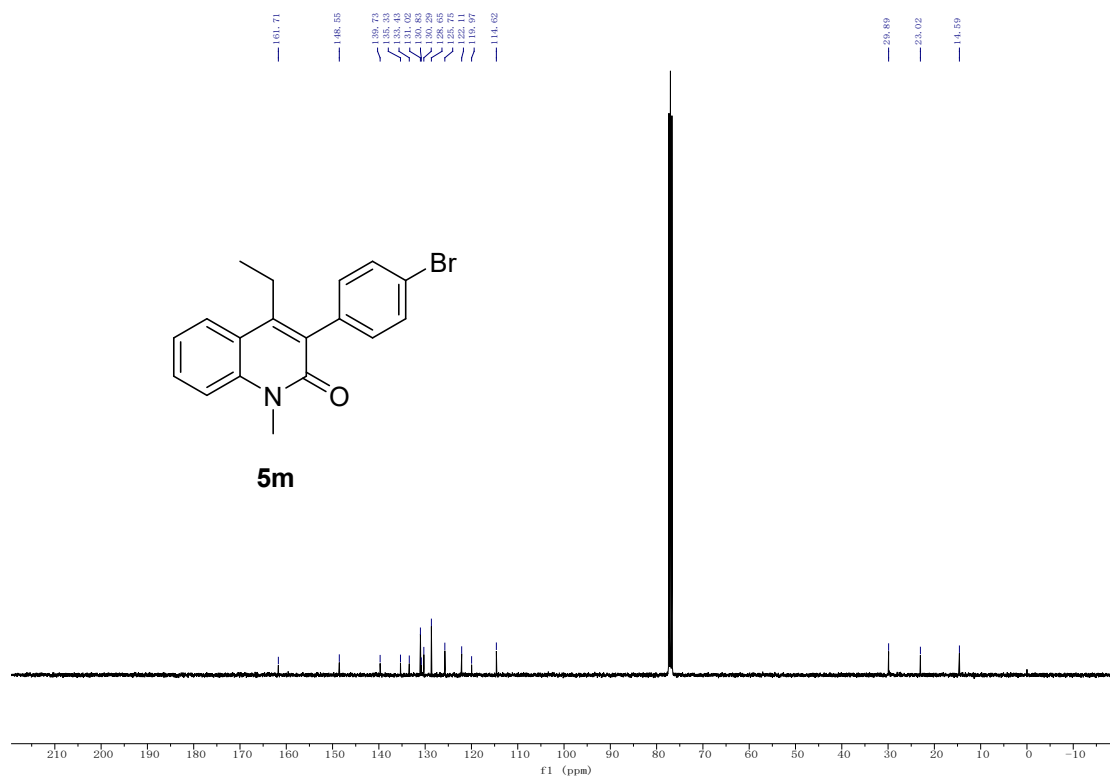
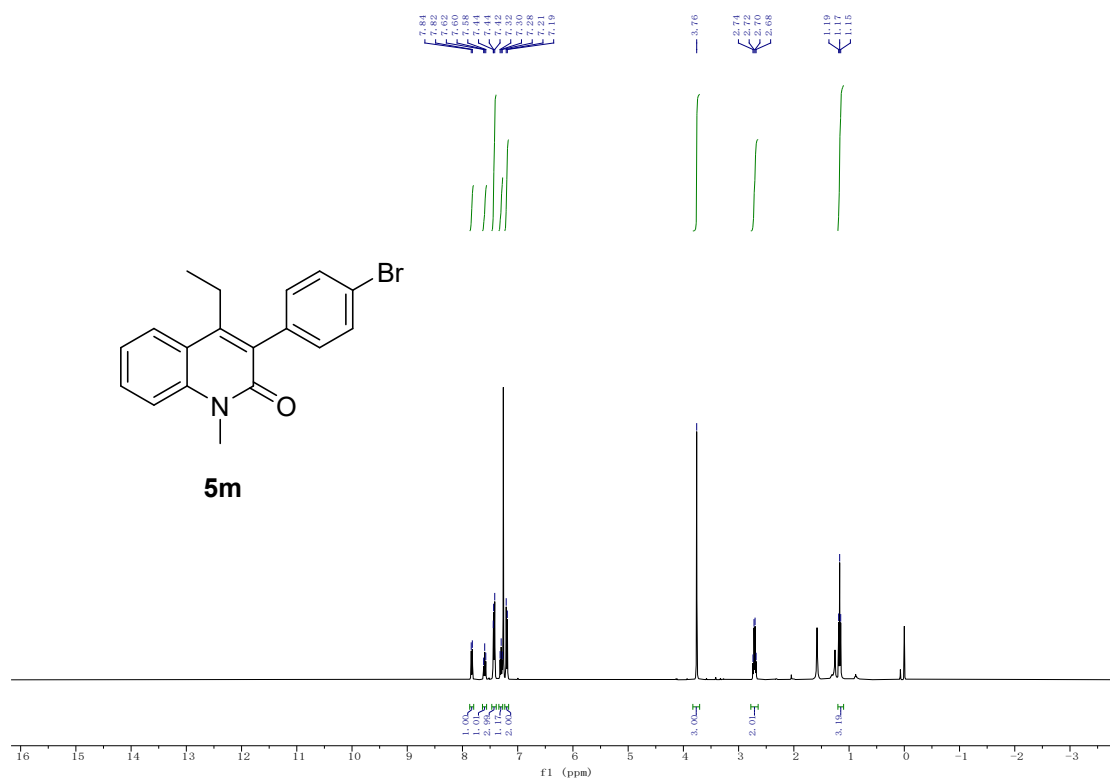


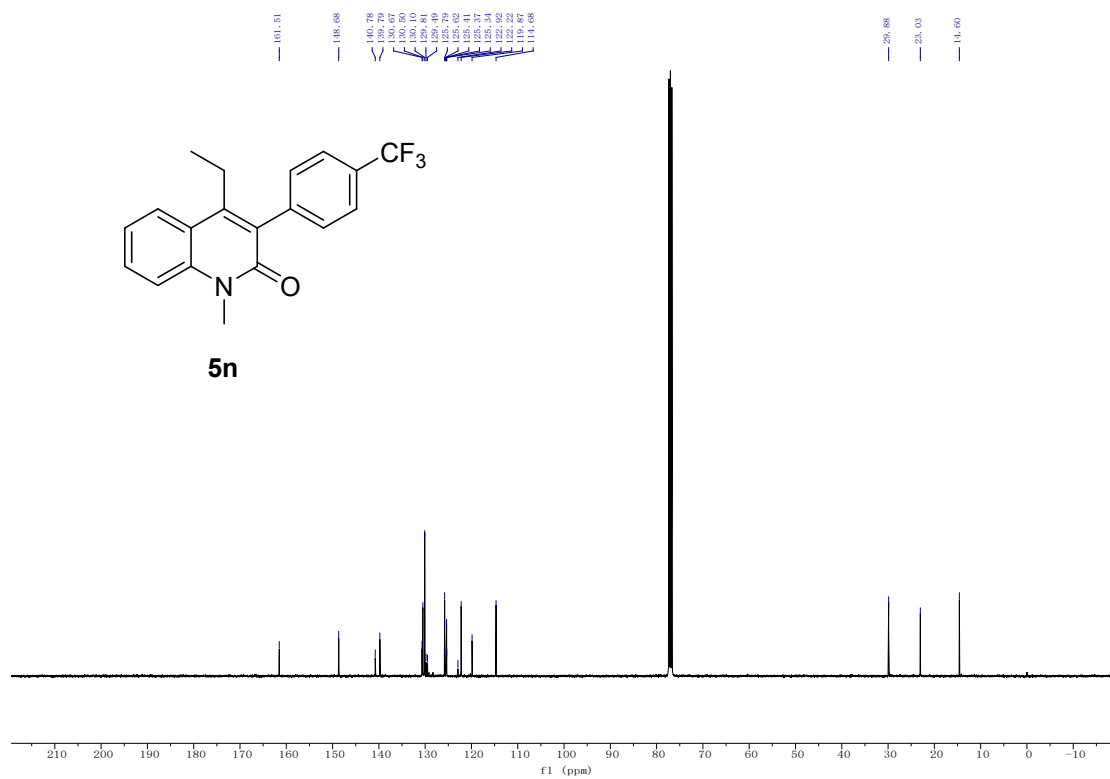
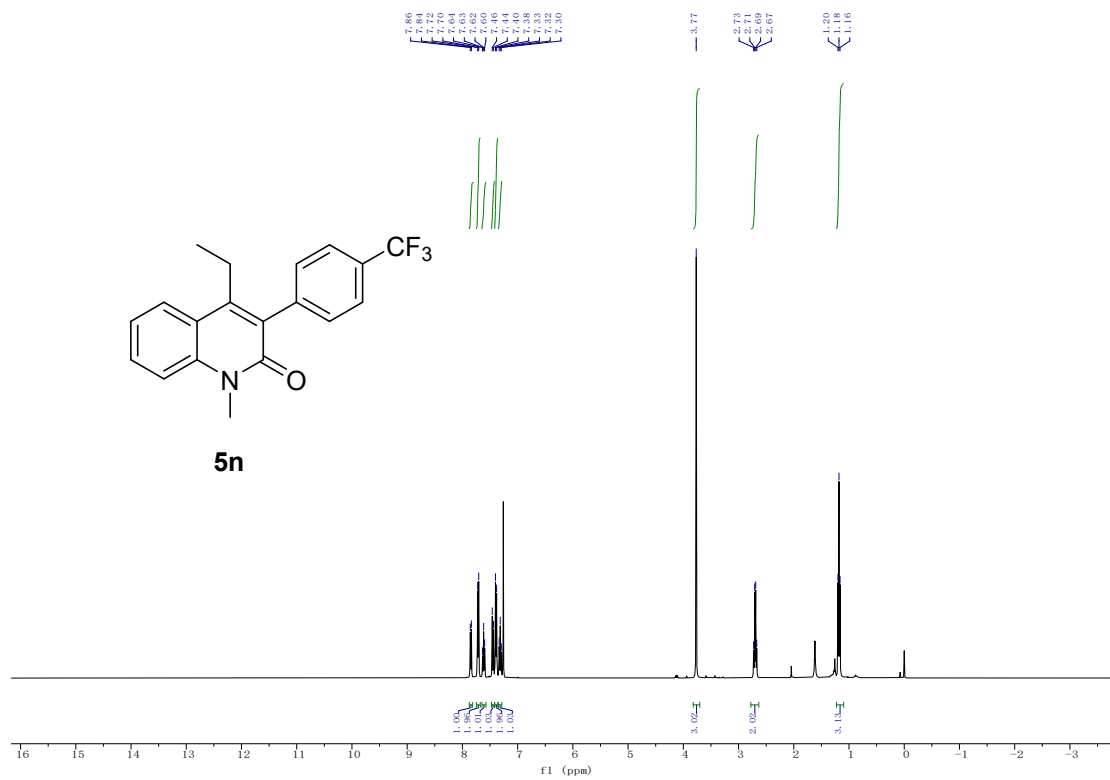


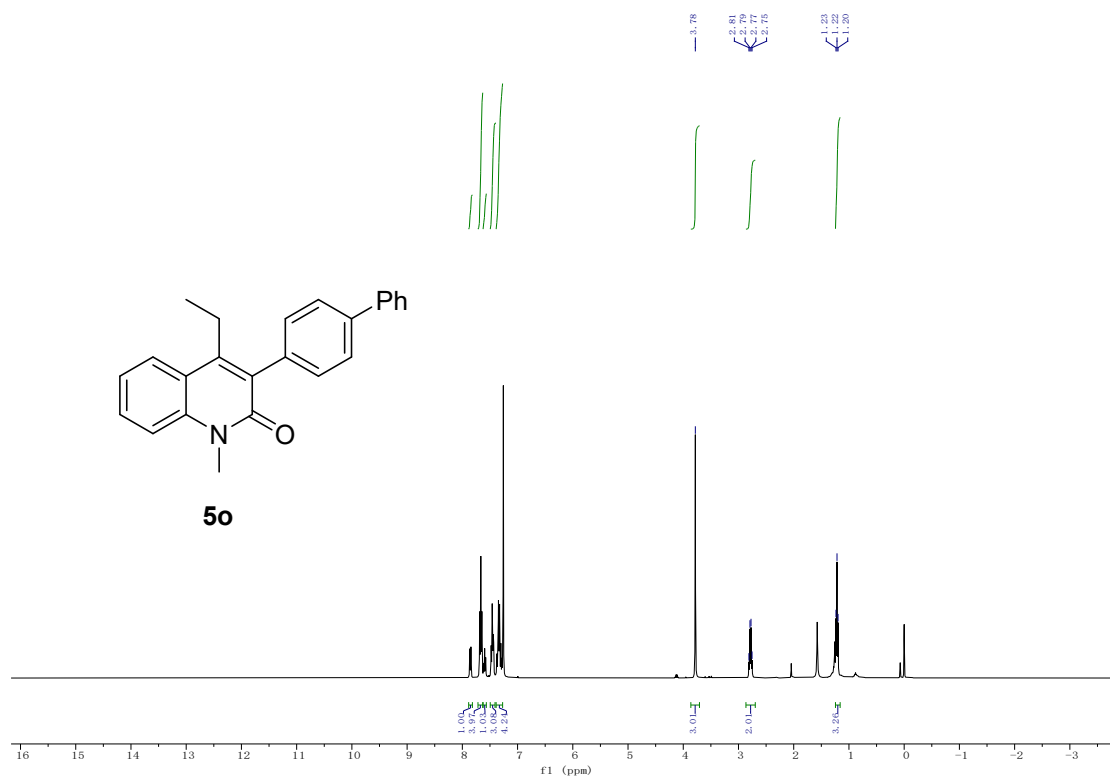
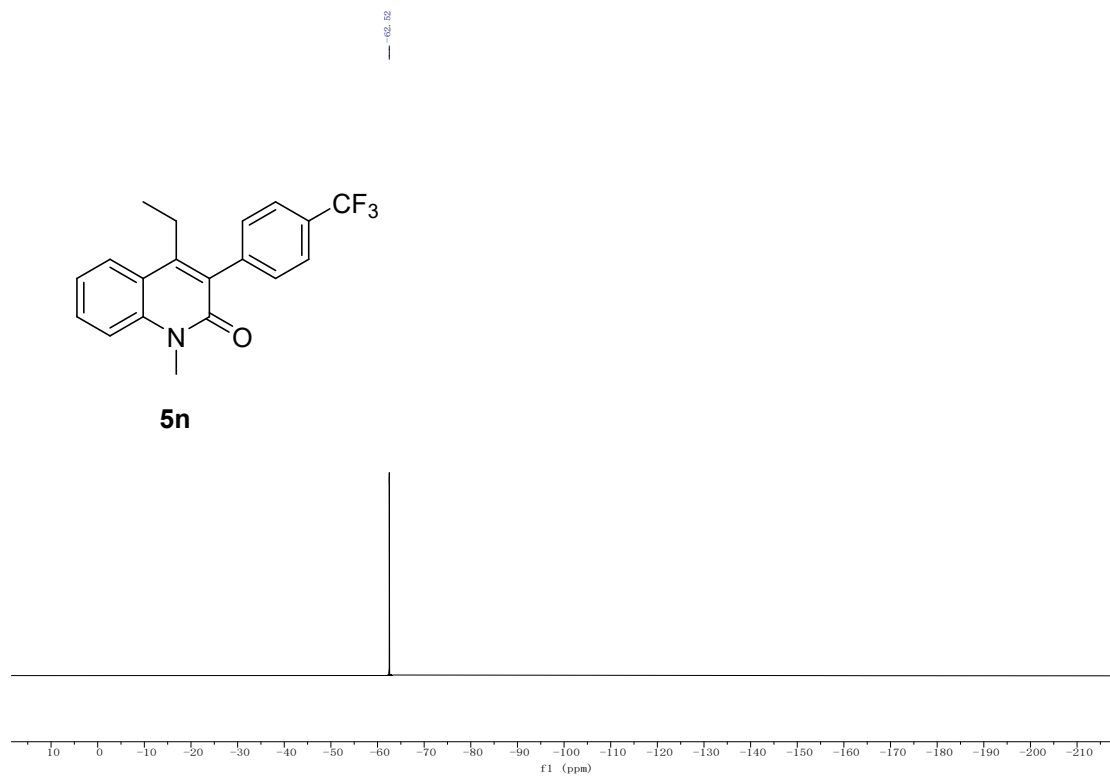


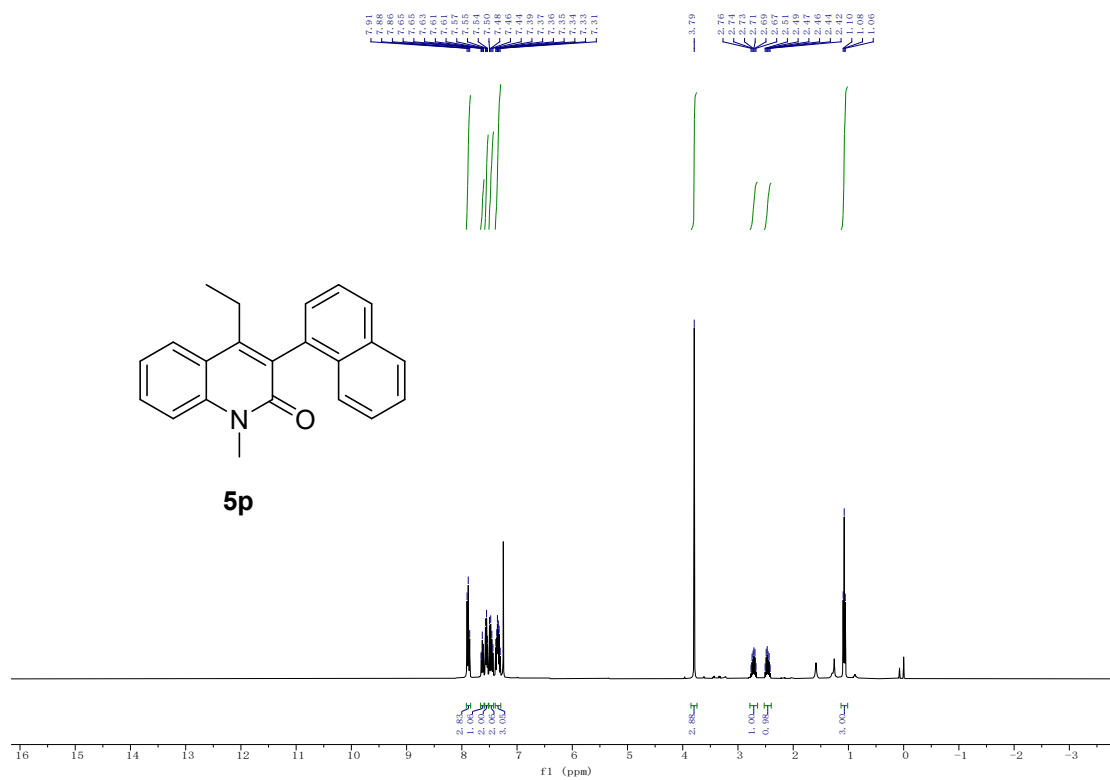
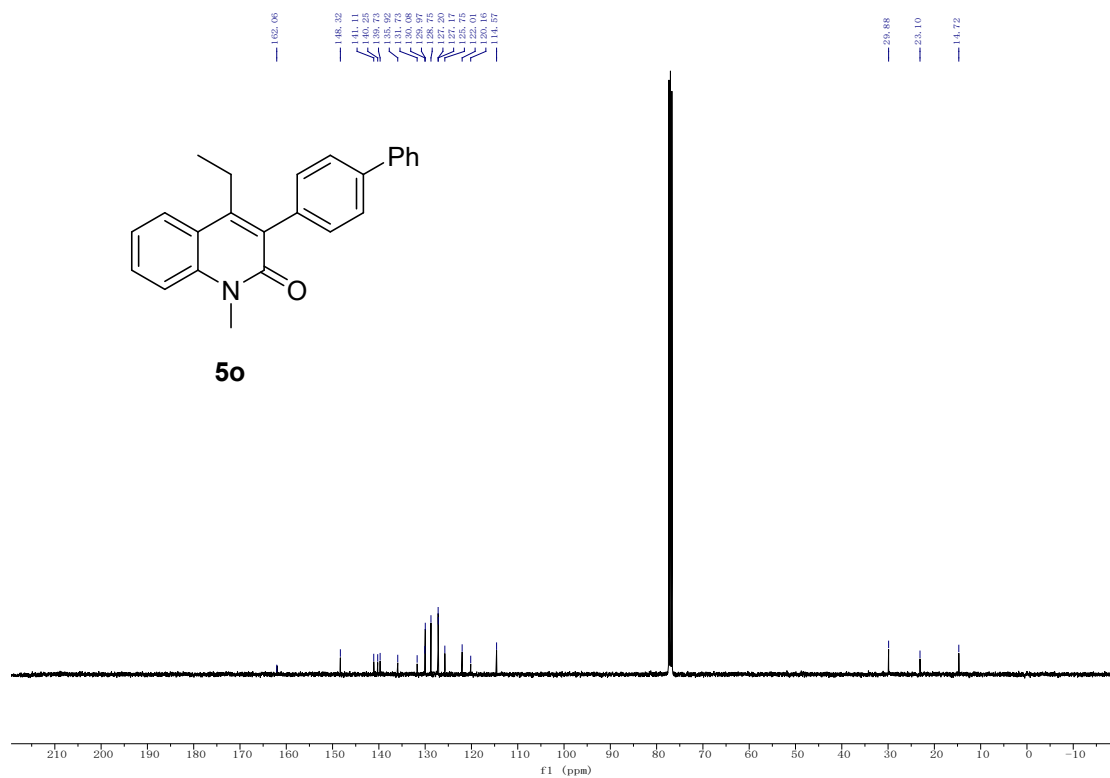


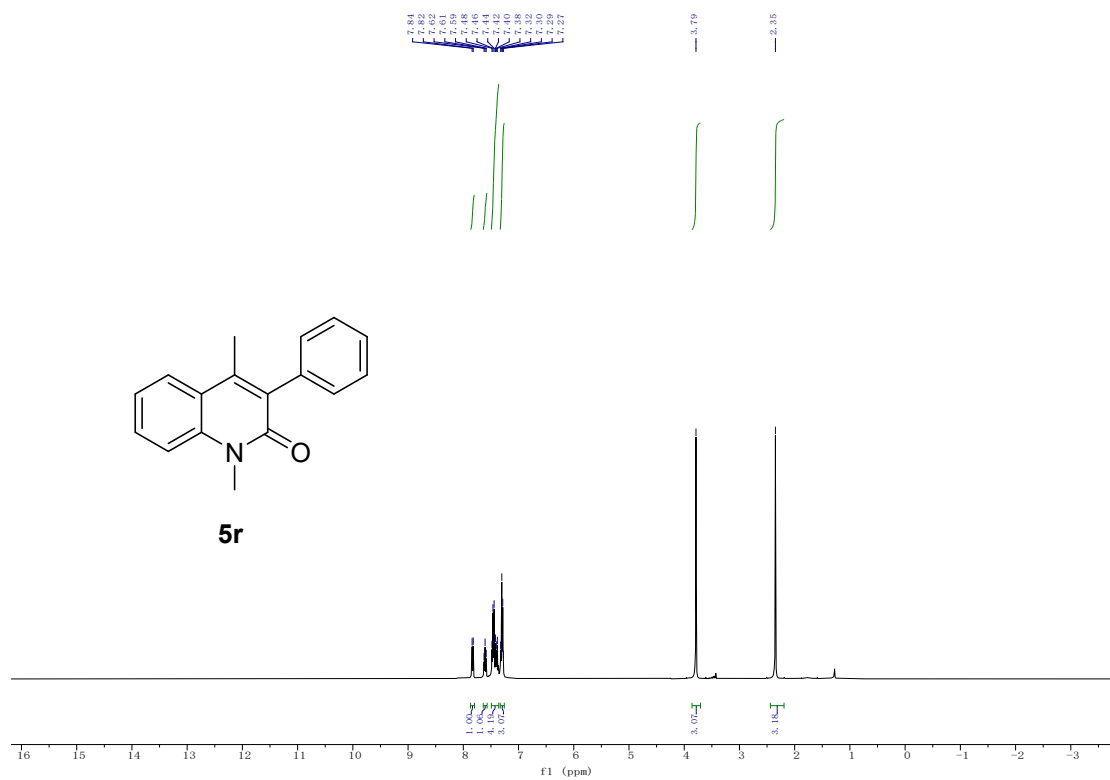
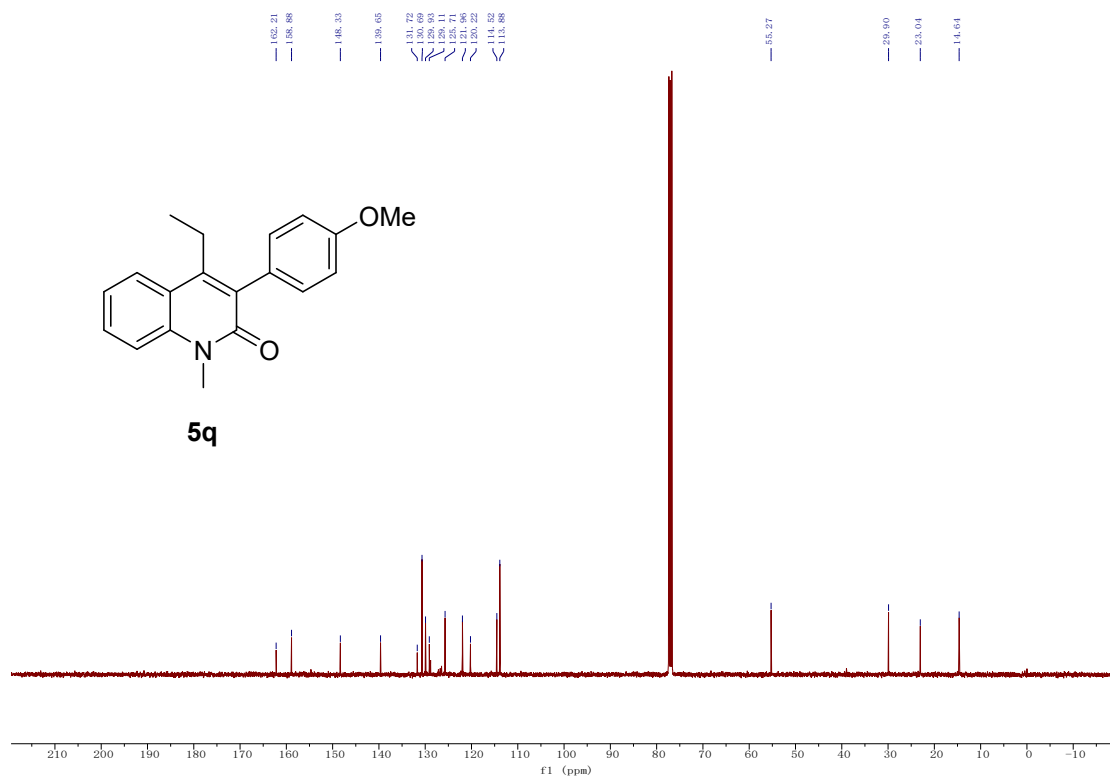


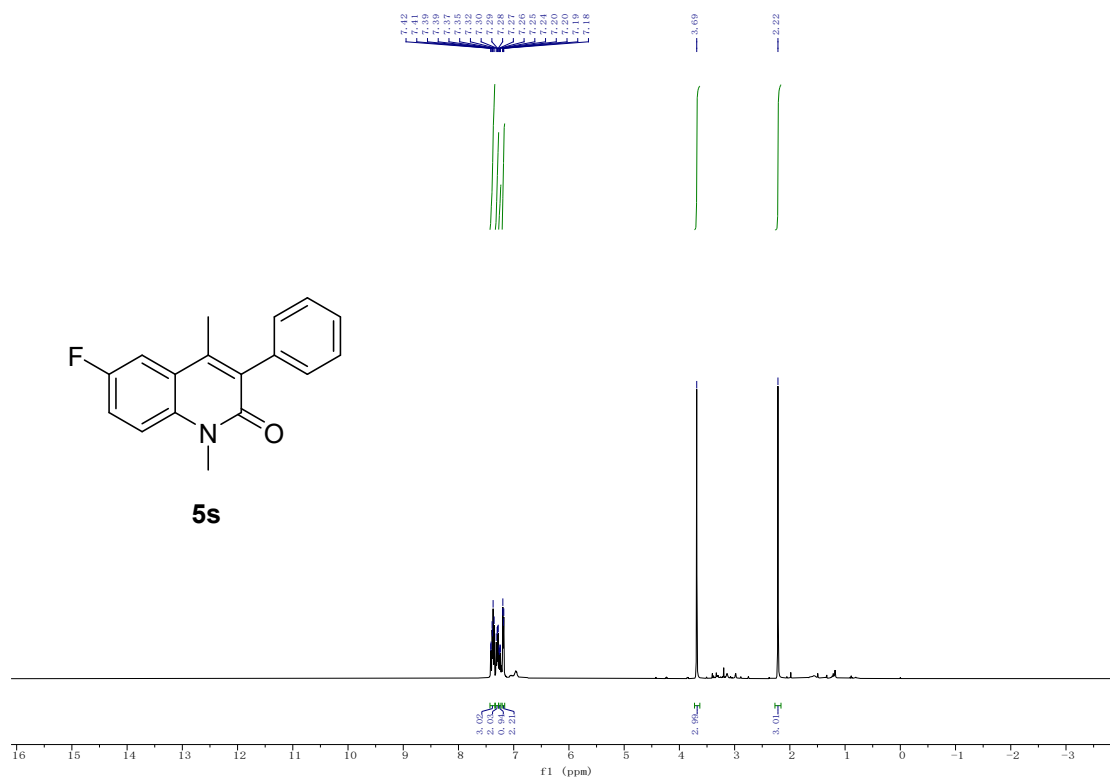
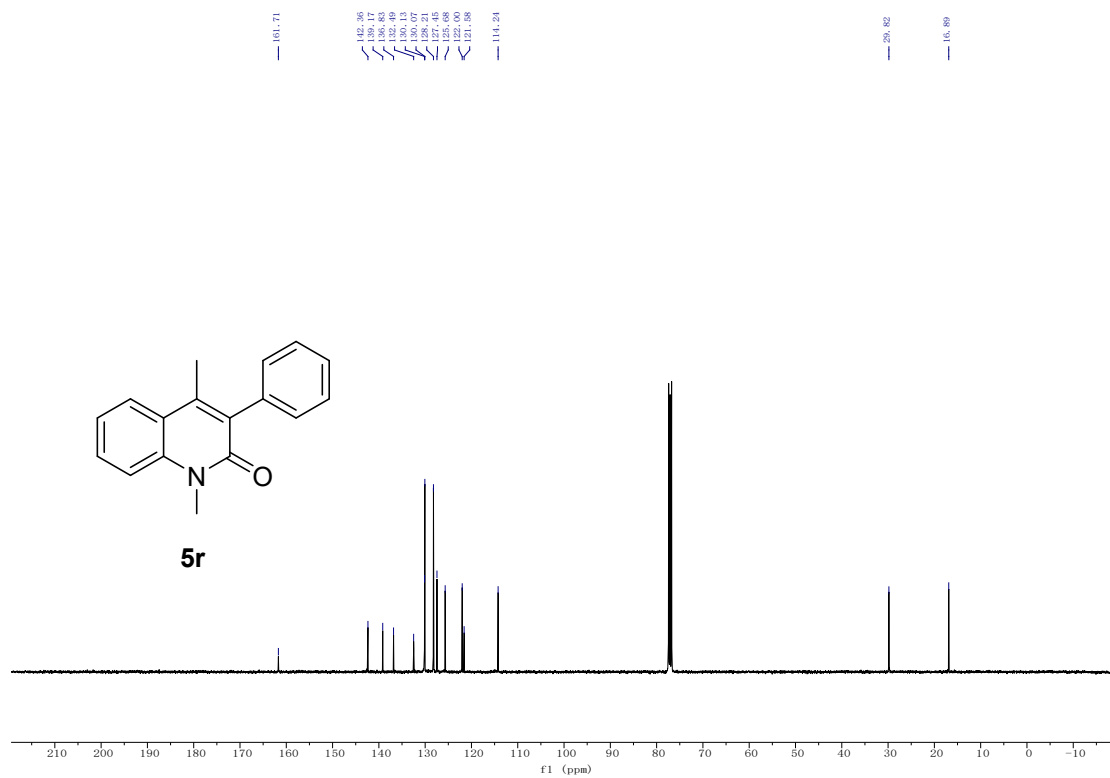


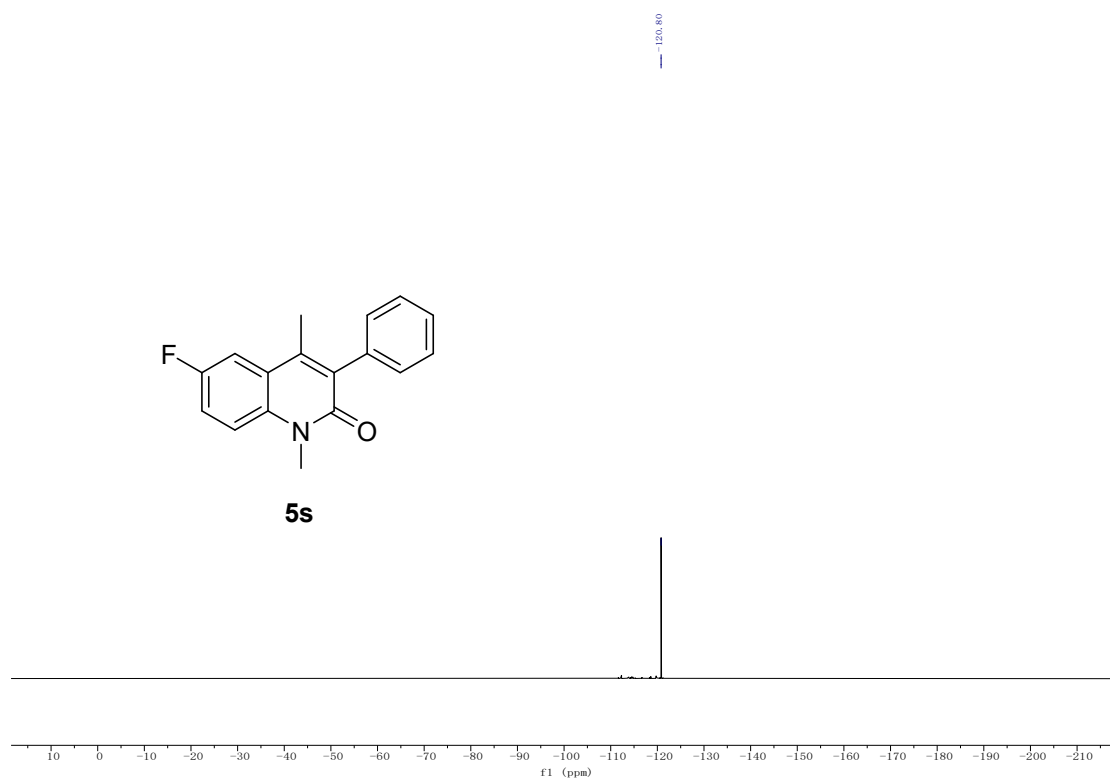
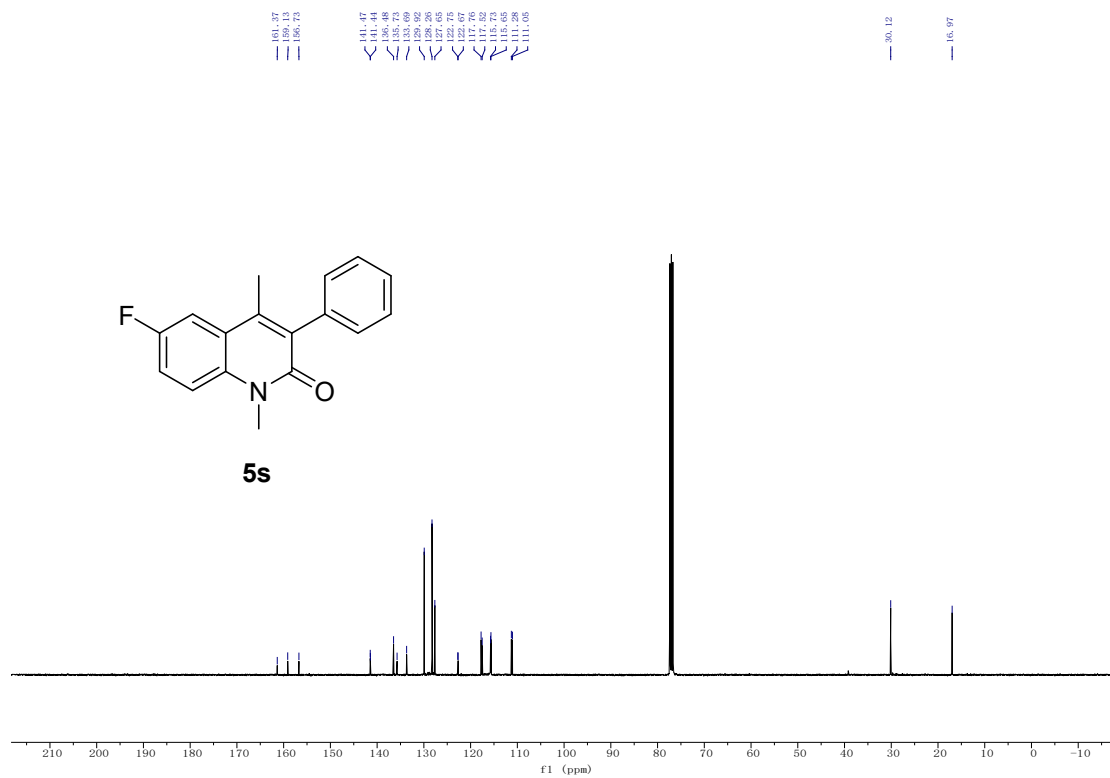


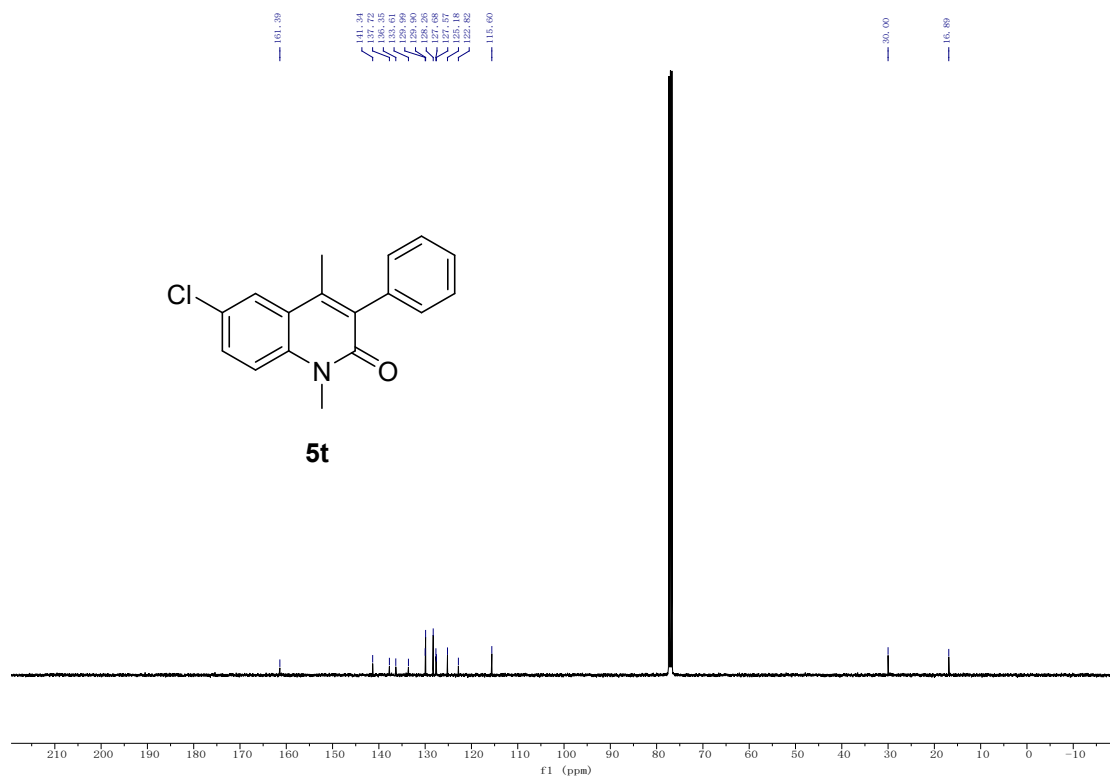
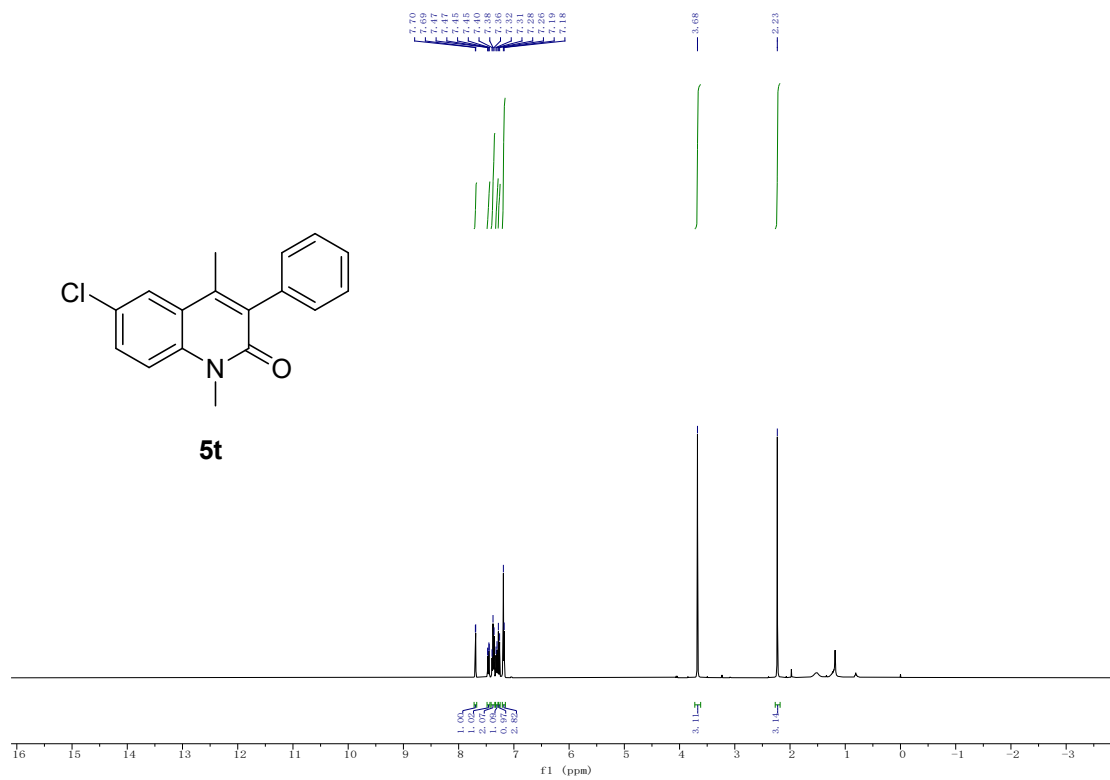


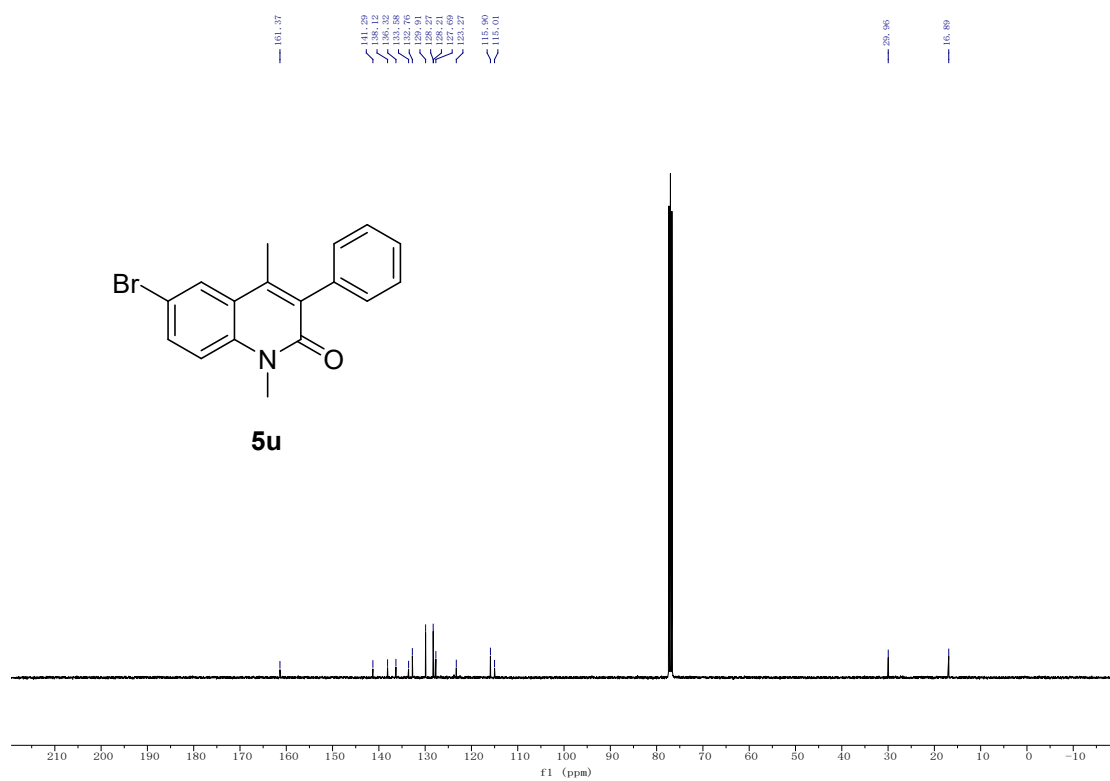
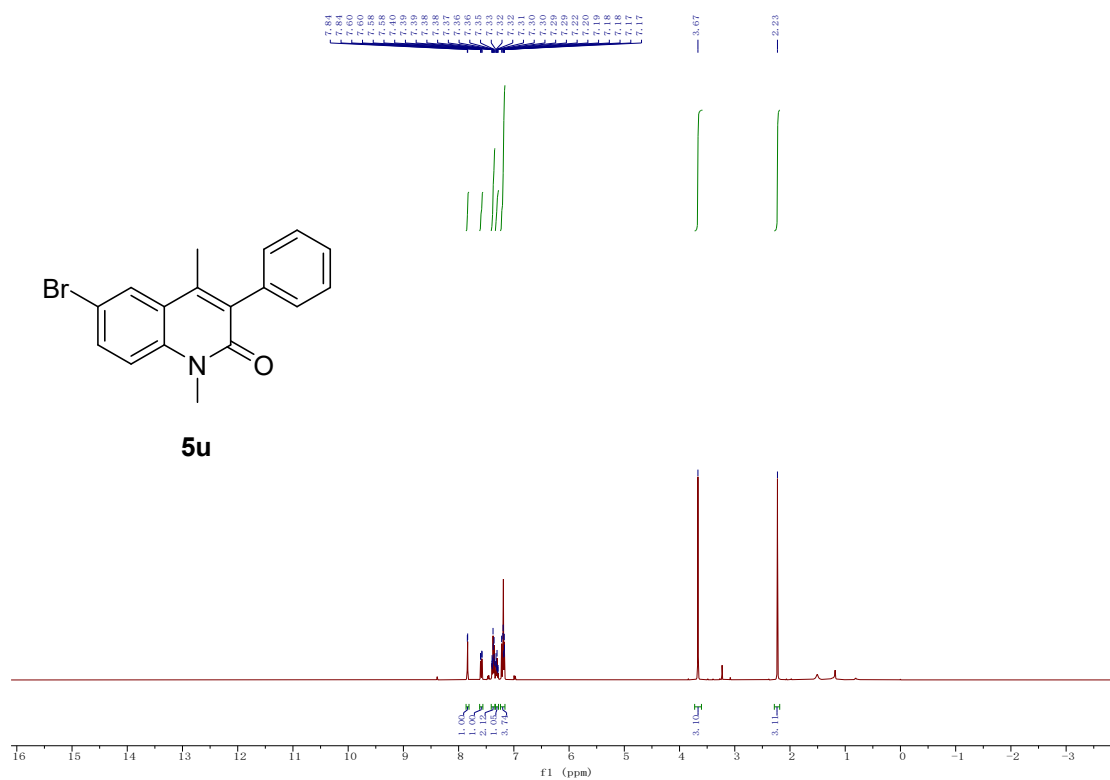


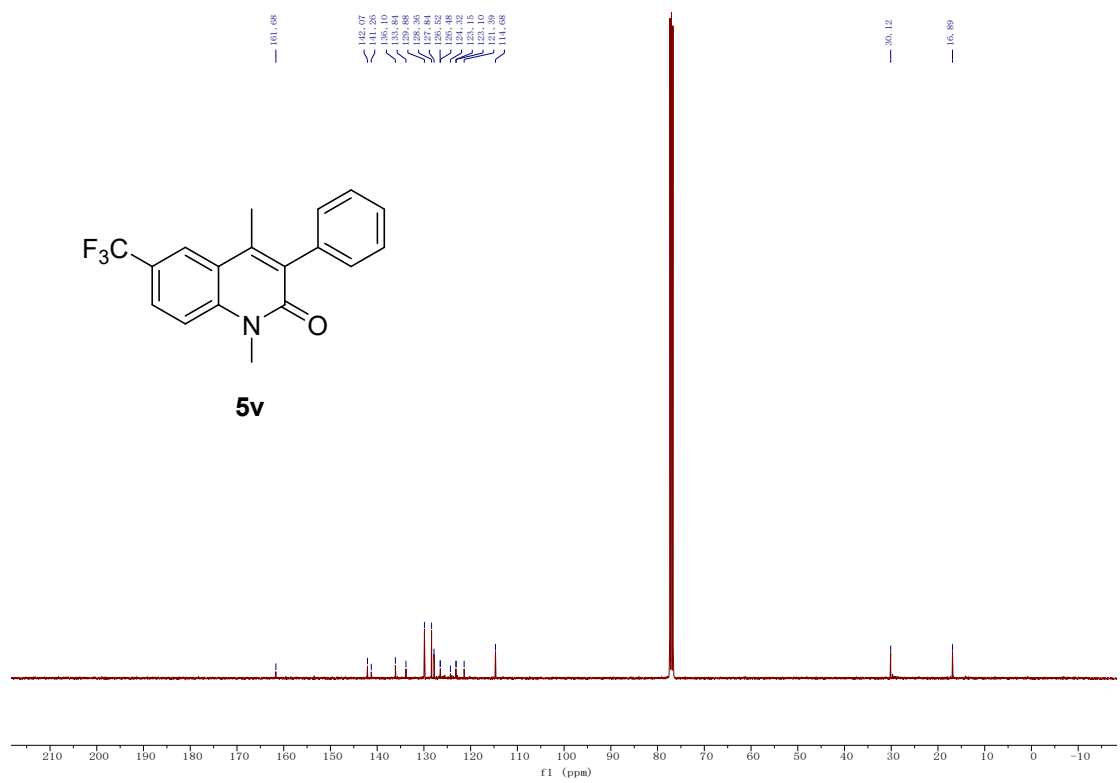
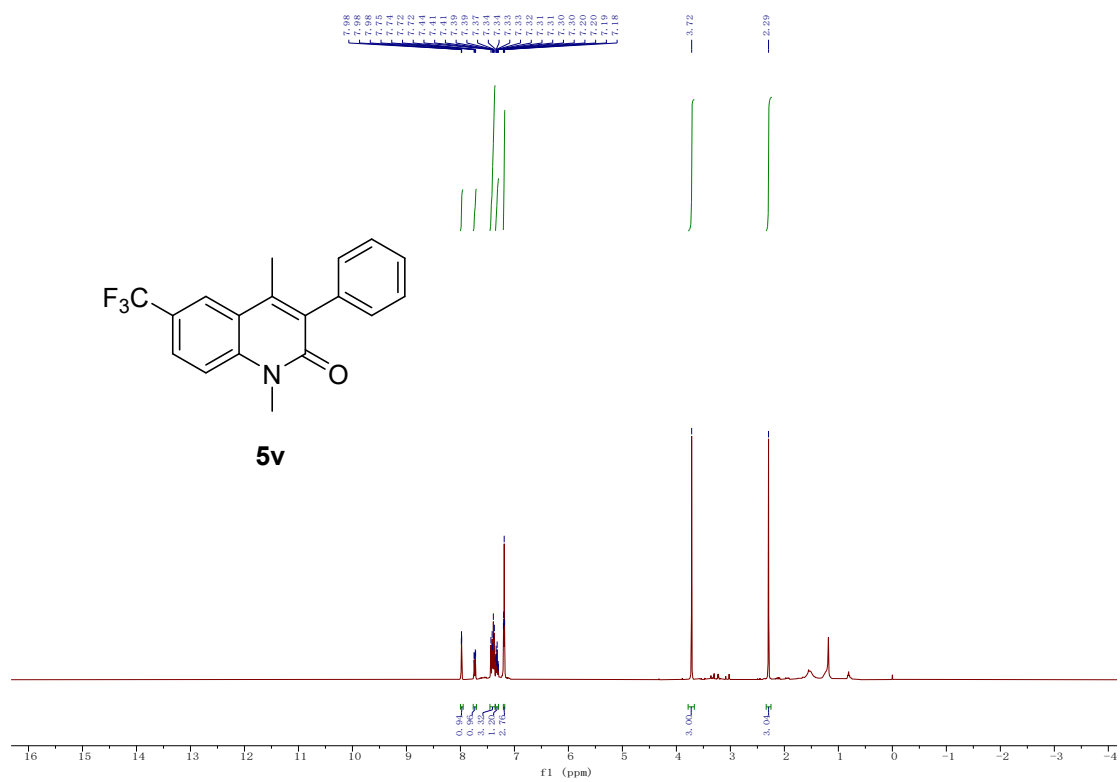


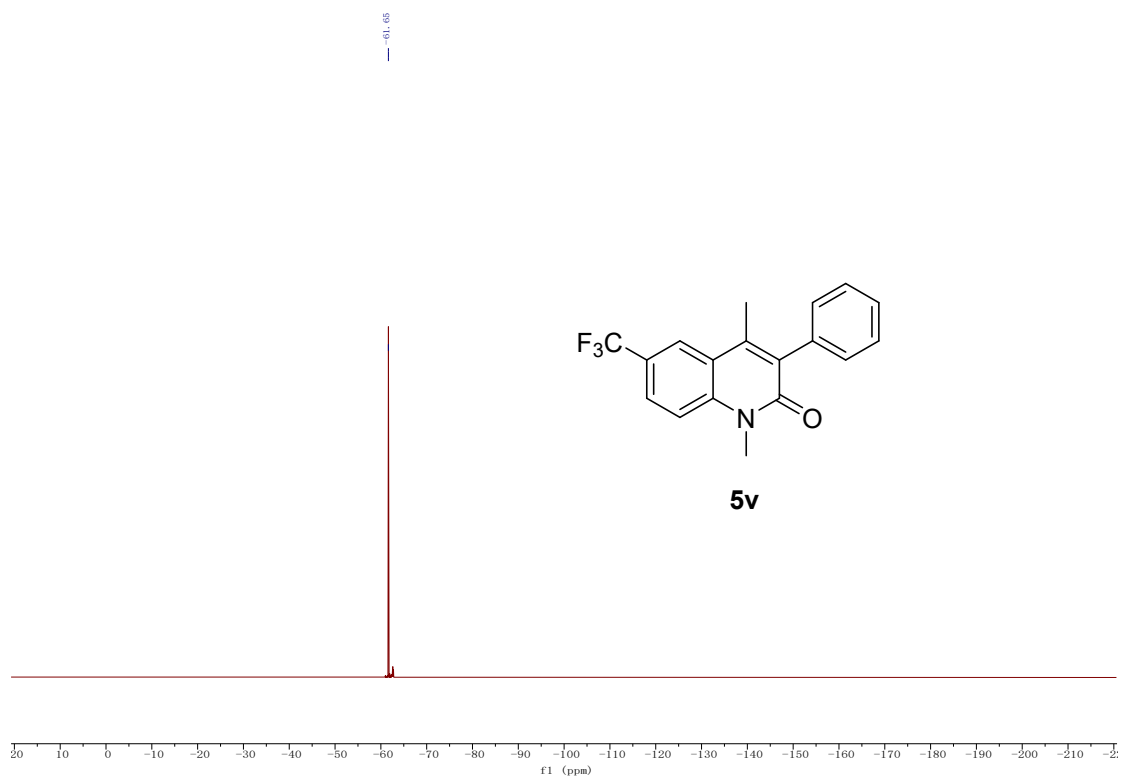


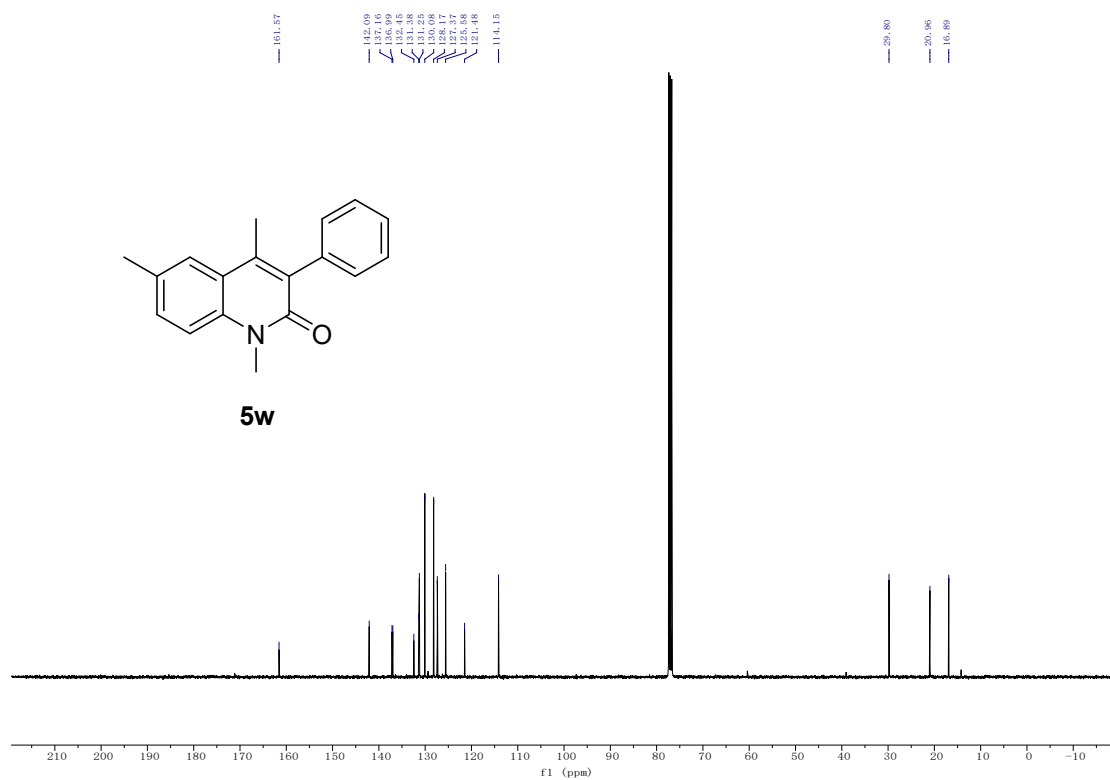
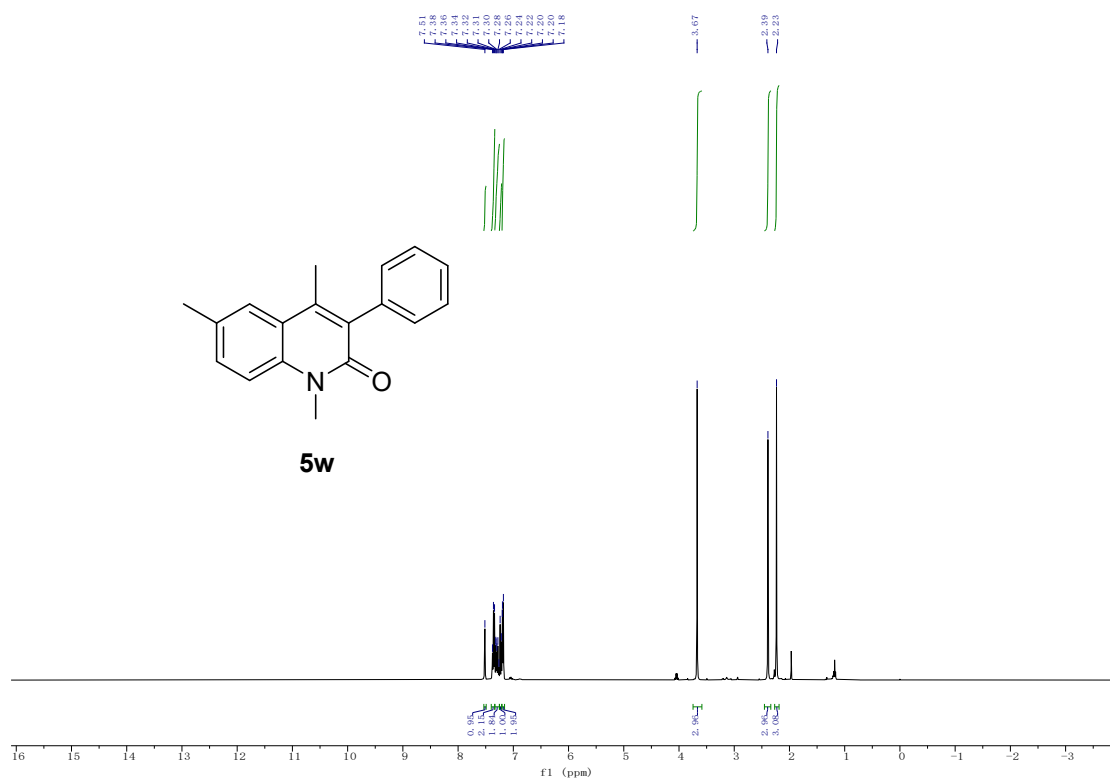


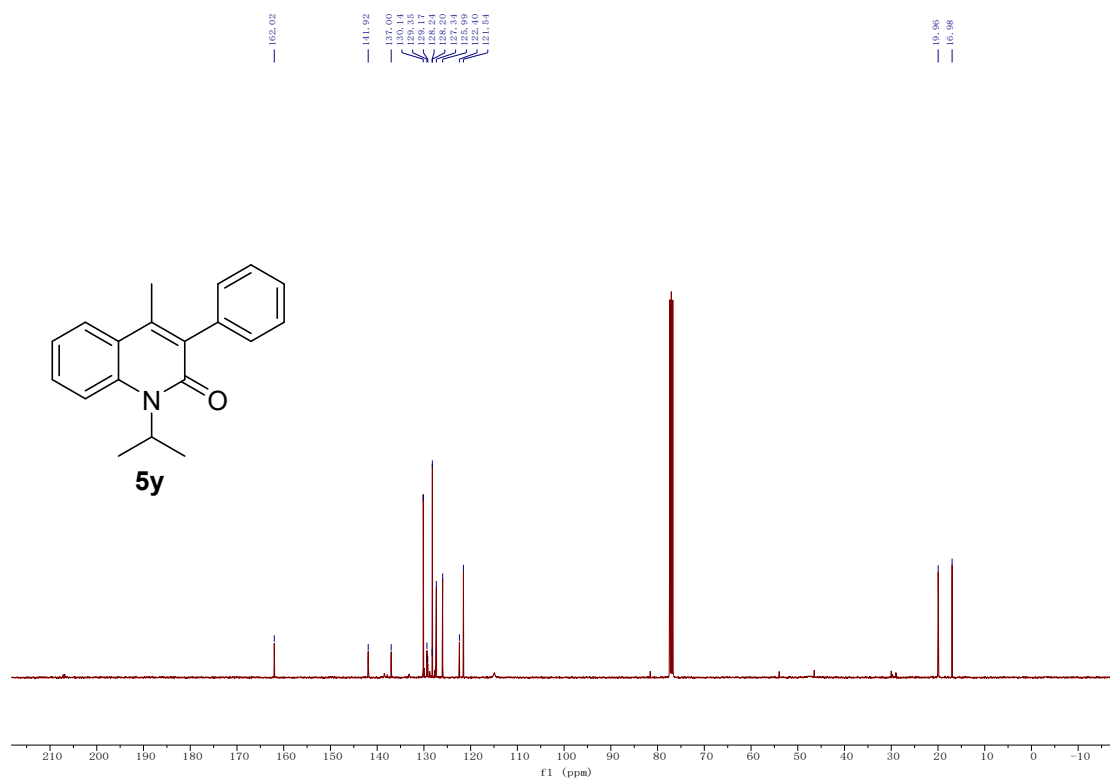
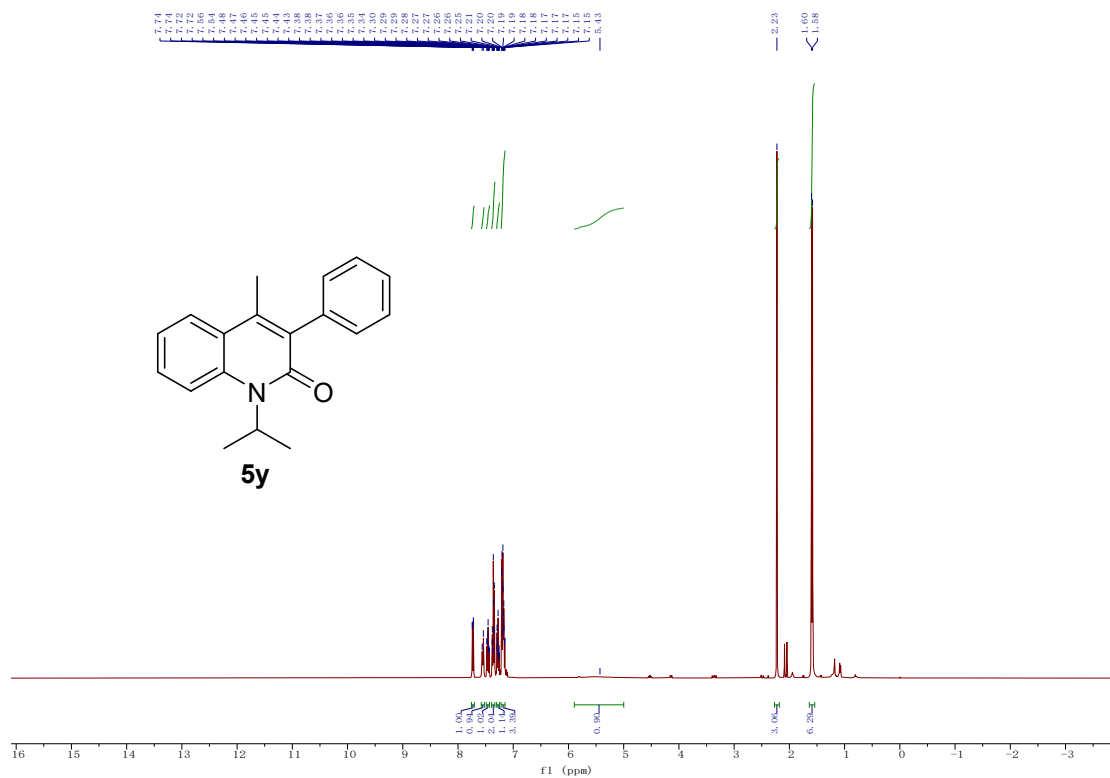


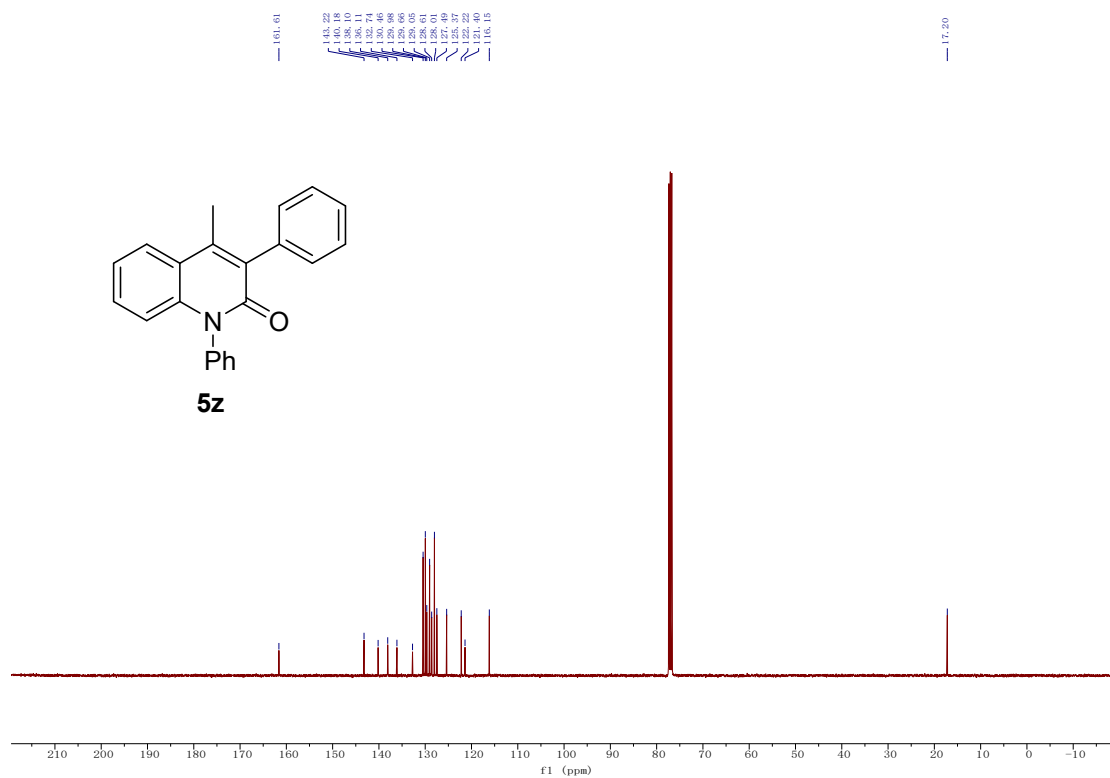
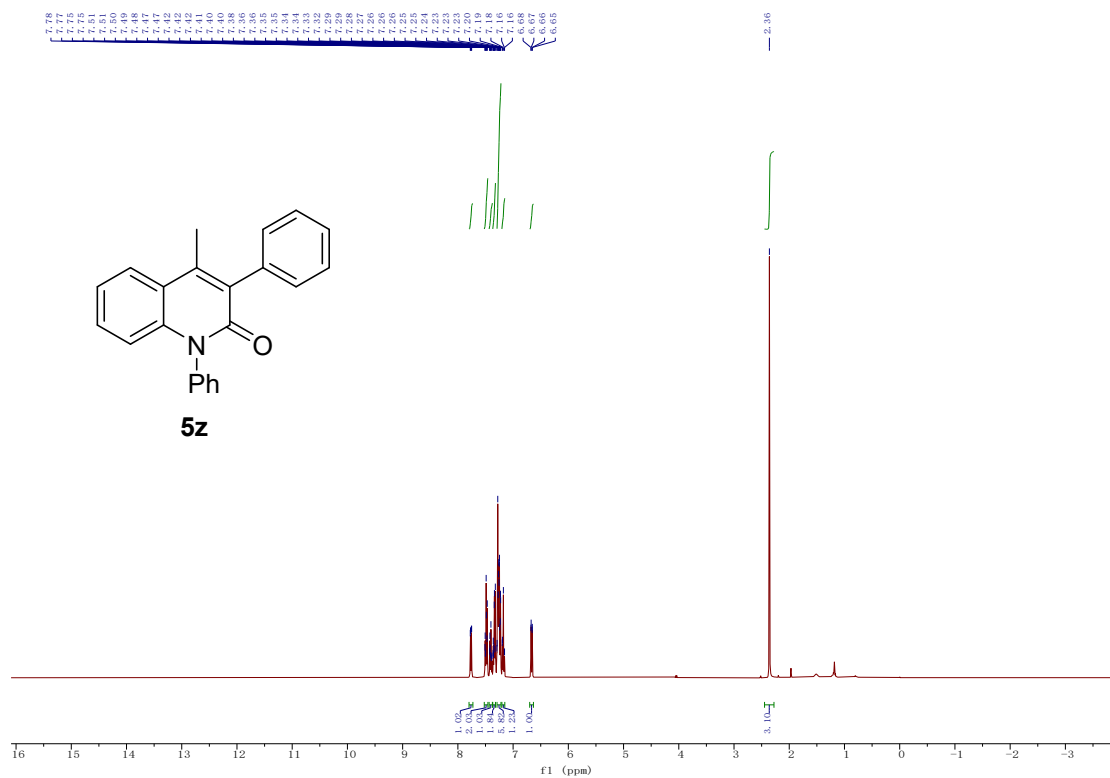












Computational Details

All calculations were implemented in Gaussian 16.¹ All of the molecular geometries were optimized without constraints at the B3LYP/6-31G(d) level.² Vibrational frequency calculations were carried out at the same level to verify all the stationary points as minima (zero imaginary frequencies) and transition states (one imaginary frequency). Single point calculations were performed at the B3LYP/6-311+G(d,p) level using the SMD³ solvation model. The dielectric constant $\epsilon=49.4240$ was used approximately according to the volume ratio of the mixed solvent (acetone:water=1:1) and the properties of acetone ($\epsilon=20.493$) and water ($\epsilon=78.355$).⁴ Intrinsic reaction coordinate (IRC) calculations⁵ were carried out to make sure the transition states indeed connect two relevant minima. Computed structures are illustrated using CYLview.⁶

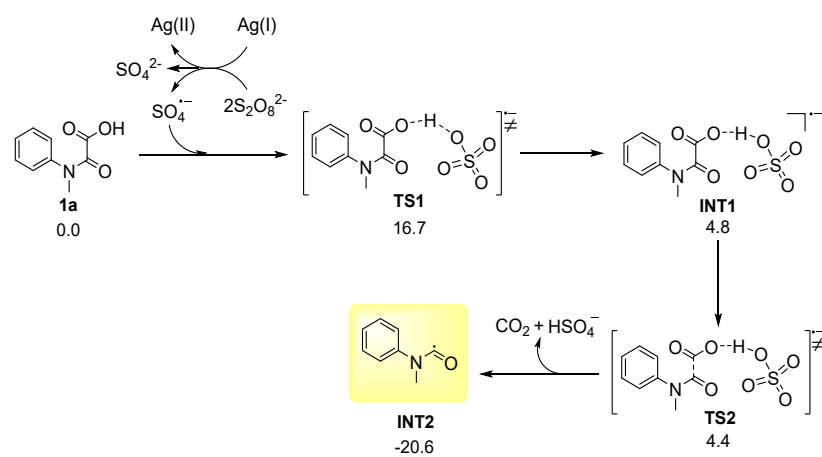


Figure S1. Intermediates and transition states with relative free energies in the decarboxylation process.

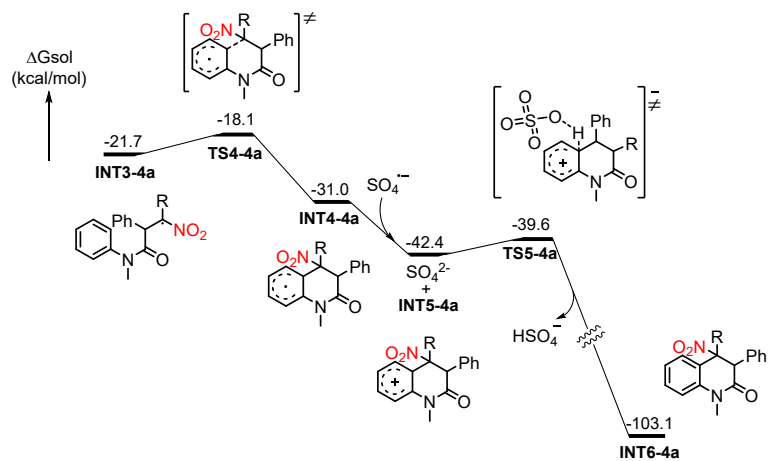


Figure S2. Gibbs free energy profile for the radical cycladdition of INT3-4a.

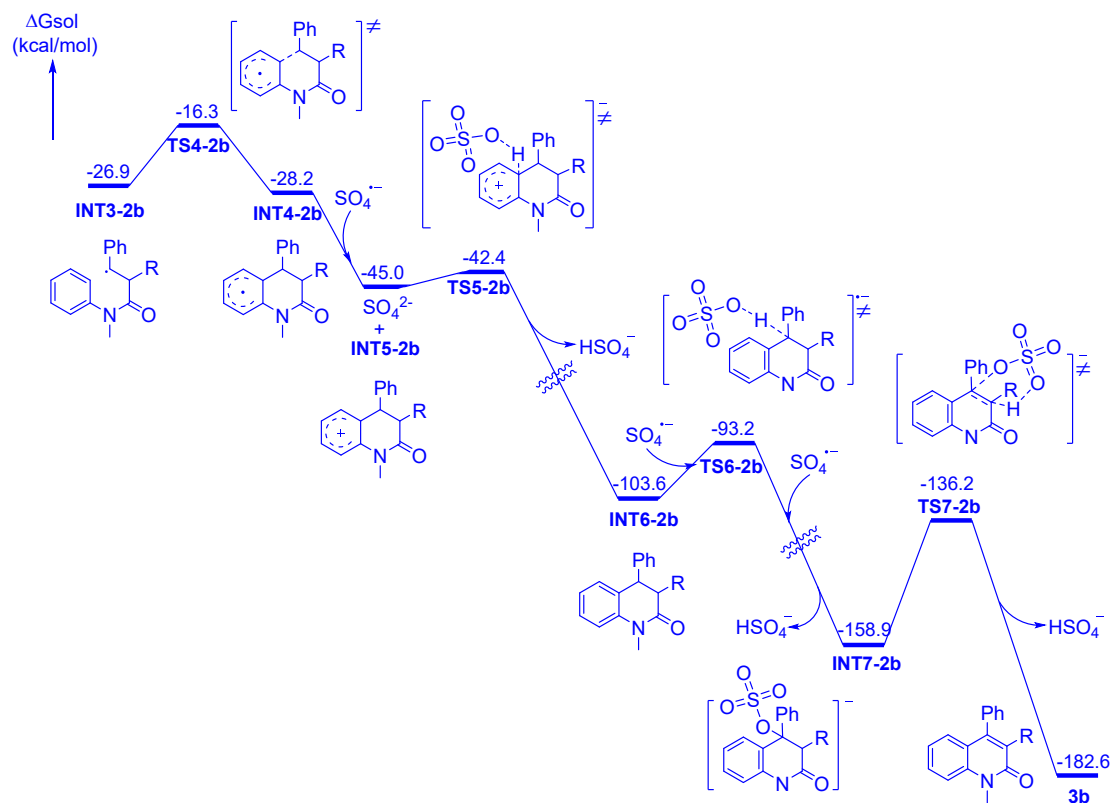


Figure S3. Gibbs free energy profile for the radical cycloaddition and rearomatization of **INT3-2b**.

Table S1. Energetics of Computed Intermediates and TSs.

Complex	SCF-Done Energy	Single Point Energy in Solvent	Free Energy Corrections in Solvent	with Imaginary Frequency
1a	-628.673910	-629.048930	-628.918519	
2b	-576.684818	-577.064774	-576.899357	
4a	-781.173694	-781.623342	-781.459556	
TS1	-1327.704253	-1328.308358	-1328.177913	-346.91
INT1	-1327.745908	-1328.332092	-1328.196899	
TS2	-1327.746332	-1328.33253	-1328.197582	-114.21
INT2	-439.481476	-439.7577229	-439.6483609	
TS3-4a	-1220.614394	-1221.380266	-1221.085086	-223.77
TS3-4a'	-1220.60914	-1221.373772	-1221.078851	-248.60
INT3-4a	-1220.687437	-1221.405454	-1221.109600	
INT3-4a'	-1220.686376	-1221.403189	-1221.106581	
TS3-2b	-1016.12457	-1016.82053	-1016.525982	-344.23
TS3-2b'	-1016.125758	-1016.818826	-1016.521212	-392.32
INT3-2b	-1016.202014	-1016.854473	-1016.557656	
INT3-2b'	-1016.196268	-1016.845213	-1016.546245	
TS4-4a	-1220.687638	-1221.405345	-1221.103905	-419.22

TS4-2b	-1016.144683	-1016.841818	-1016.540844	-534.08
INT4-4a	-1220.710634	-1221.427355	-1221.124531	
INT4-2b	-1016.212234	-1016.862365	-1016.559856	
INT5-4a	-1220.492886	-1221.267586	-1220.962621	
INT5-2b	-1016.004953	-1016.71242	-1016.406502	
TS5-4a	-1919.743394	-1920.722359	-1920.409257	-960.60
TS5-2b	-1715.251705	-1716.168307	-1715.853408	-1132.29
INT6-4a	-1220.16917	-1220.874691	-1220.580909	
INT6-2b	-1015.676624	-1016.315855	-1016.021555	
TS6-4a	-1919.159484	-1920.122794	-1919.825185	-1895.69
TS6'-4a	-1919.864884	-1920.786168	-1920.475874	-1048.52
5a	-1014.488739	-1015.099514	-1014.827435	
TS6-2b	-1714.663699	-1715.572174	-1715.275958	-1644.02
INT7-2b	-1714.179837	-1715.019693	-1714.72221	
TS7-2b	-1714.094235	-1714.977157	-1714.68602	-742.81
3b	-1014.48992	-1015.102203	-1014.830457	
S ₂ O ₈ ²⁻	-1397.979634	-1398.545218	-1398.549589	
SO ₄ ⁺	-699.025882	-699.2567125	-699.2710315	
SO ₄ ²⁻	-698.923341	-699.4388511	-699.4510791	
HSO ₄ ⁻	-699.668366	-699.9269407	-699.9294917	
H ₂ SO ₄	-700.17362	-700.3591178	-700.3493588	
NO ₂ ⁻	-205.11392	-205.3194717	-205.3351737	
NO ₂ [•]	-205.064907	-205.064907	-205.1581974	
CO ₂	-188.570988	-188.650484	-188.65961	

Cartesian Coordinates

3b			
C	-1.45103300	1.23761600	-0.05690700
C	-0.97033400	2.54603300	-0.33590700
C	-1.82078400	3.64900500	-0.13053400
C	-3.10734400	3.46396900	0.35520800
C	-3.58023300	2.18168900	0.65744700
C	-2.75458800	1.08829400	0.45420100
H	-1.47419300	4.65128500	-0.34530800
H	-3.74499700	4.33001700	0.50717600
H	-4.58199900	2.04343300	1.05144800
H	-3.10509400	0.09138300	0.69385700
N	0.32828000	2.72456900	-0.79651300
C	1.22662800	1.66454200	-0.98946900
O	2.37395400	1.85382300	-1.38962400
C	0.82316500	4.06633900	-1.09419700
H	1.84765500	3.95666600	-1.44308400
H	0.21361700	4.53421000	-1.87356800
H	0.80320100	4.69127100	-0.19560900
C	1.64441700	-0.79171300	-1.02882300
C	0.70005000	0.33210000	-0.71201100
C	-0.57072800	0.10727000	-0.28011500
C	-1.03661600	-1.28253000	-0.02566500
C	-0.38753500	-2.07574100	0.93001400
C	-2.10384000	-1.82594300	-0.75404400

C	-0.80054900	-3.38839300	1.15369800
H	0.44285300	-1.65848900	1.49035500
C	-2.51092500	-3.13986800	-0.53251800
H	-2.59929600	-1.21967800	-1.50630400
C	-1.86217400	-3.92338400	0.42369900
H	-0.29225200	-3.99263600	1.89973700
H	-3.33141900	-3.55405900	-1.11134900
H	-2.18148800	-4.94717100	0.59623400
O	1.58213900	-1.47540700	-2.02480300
O	2.55998200	-0.94284900	-0.05509500
C	3.54967100	-1.97127900	-0.28810000
H	4.06565600	-1.75009400	-1.22697300
H	3.03521000	-2.93035500	-0.40606300
C	4.49087300	-1.96485600	0.89950900
H	5.26485800	-2.72834200	0.76630000
H	4.97804200	-0.99034800	1.00153200
H	3.95042900	-2.17939200	1.82728200

5a

C	1.71526900	-0.58065300	-0.73757200
C	2.67120300	0.30007500	-0.16842700
C	4.03403500	-0.05028400	-0.19529300
C	4.43873500	-1.24421100	-0.77478400
C	3.50251800	-2.11743100	-1.34150900
C	2.15870900	-1.78494200	-1.32013300
H	4.77592300	0.60806800	0.23683500
H	5.49531500	-1.49547700	-0.78629100
H	3.82531600	-3.04721900	-1.79879900
H	1.42877300	-2.44288200	-1.77498400
N	2.24794300	1.48927200	0.41342300
C	0.90541900	1.88993900	0.48251500
O	0.58893900	2.94157700	1.03533700
C	3.23177100	2.39571100	1.00269000
H	2.68727400	3.25767000	1.38050700
H	3.76123900	1.90356600	1.82471900
H	3.95580900	2.71431400	0.24649100
C	-4.21002600	2.13492400	-0.19371700
C	-3.48300000	2.20319100	0.99734000
C	-2.13313300	1.86141400	1.01998400
C	-1.49289300	1.42640200	-0.14917700
C	-2.22439800	1.38290800	-1.34573200
C	-3.57409000	1.72961500	-1.36786700
H	-5.26169700	2.40718800	-0.20786900
H	-3.96954500	2.52678400	1.91319200
H	-1.56975700	1.92281600	1.94291100
H	-1.73046100	1.07577500	-2.26268500
H	-4.12456900	1.69094800	-2.30365500
C	-0.07906800	0.98178900	-0.13156500
C	0.32205200	-0.20674200	-0.67470300
C	-0.70750200	-1.15630200	-1.22511900
O	-0.71672200	-1.57886500	-2.36378300
O	-1.61364800	-1.46975600	-0.28930000
C	-2.80181500	-2.16180500	-0.74058800
H	-3.08925800	-1.75489000	-1.71346300
H	-2.55804600	-3.22109100	-0.87342000
C	-3.86964500	-1.93717500	0.31137900
H	-4.79142300	-2.45269400	0.02041300
H	-3.54887800	-2.32461700	1.28347500

H	-4.08180700	-0.86887800	0.41428000
CO ₂			
C	-0.69047600	1.23809500	0.00000000
O	0.47864600	1.23809500	0.00000000
O	-1.85959900	1.23809500	0.00000000
H ₂ SO ₄			
S	-0.27432300	0.24052400	0.04248200
O	0.19462200	0.90127600	-1.36947900
O	0.20299000	1.13917100	1.07005000
O	-1.89325900	0.37861200	-0.05506100
O	-0.00187100	-1.17895600	-0.00101400
H	-2.13475100	1.27501700	0.24758200
H	0.15190100	0.20483500	-2.05253600
HSO ₄ ⁻			
S	-0.21574100	0.37404500	-0.04868400
O	0.24396600	1.01870200	-1.29560100
O	0.02639100	1.15777900	1.19338600
O	-1.92257300	0.44105300	-0.14796600
O	0.08293400	-1.06893900	0.05256700
H	-2.12843000	0.96985300	0.63989800
INT1			
C	1.85257100	-1.13910600	-0.01909800
C	1.89345500	0.24363300	-0.20513600
C	3.09262500	0.95293300	-0.13218600
C	4.27887600	0.26710400	0.12612600
C	4.25938700	-1.11785400	0.30156500
C	3.05016100	-1.81204600	0.22647900
H	0.89955300	-1.66610900	-0.07018200
H	3.08898300	2.02925600	-0.27286200
H	5.21592300	0.81478600	0.18445500
H	5.18468200	-1.65311700	0.50004400
H	3.02891100	-2.88858500	0.37200600
N	0.66627300	0.95498500	-0.47574400
C	0.24790400	1.82892900	0.43167900
O	0.73949500	2.24116900	1.45325700
C	-0.12243600	0.58170100	-1.66178600
H	-1.18857700	0.68634400	-1.46979100
H	0.18868800	1.19165000	-2.51585900
H	0.03620400	-0.47755700	-1.85509100
C	-1.32577000	2.63159300	0.01870900
O	-1.04616000	3.47522100	-0.80951400
O	-2.20450000	2.13863700	0.69193300
H	-2.05423900	0.05874500	1.01850400
S	-2.11923900	-1.79029100	-0.11039500
O	-2.95223600	-2.71875400	0.67164900
O	-0.89571000	-2.40160100	-0.69733800
O	-2.86308600	-0.89518900	-1.03279400
O	-1.45419300	-0.71083400	1.00729000
INT2			
C	-1.81307200	-0.10285200	-0.69588900
C	-0.60912100	0.20067100	-0.04234700
C	-0.45939400	1.45640900	0.56664700
C	-1.49994800	2.37995400	0.51572700

C	-2.69815300	2.08038300	-0.13350600
C	-2.84517600	0.83416000	-0.73729900
H	-1.95944000	-1.06233600	-1.17519000
H	0.46267800	1.70356200	1.07351800
H	-1.36582400	3.34662700	0.99269100
H	-3.50362600	2.80760400	-0.16753200
H	-3.76888900	0.57843800	-1.24859100
N	0.43947600	-0.77258300	-0.00941900
C	1.64138500	-0.59360500	0.58998500
O	2.10498000	0.33886800	1.19544900
C	0.23537700	-2.06735000	-0.65935300
H	1.14308800	-2.65396800	-0.51984300
H	-0.60984300	-2.59991500	-0.21081000
H	0.04979700	-1.94077900	-1.73115200

INT3-2b

C	-3.81471500	0.27531600	-2.10091200
C	-2.63913000	0.91706500	-1.69397500
C	-2.66533300	2.28658400	-1.40448600
C	-3.85886800	2.99526200	-1.52174200
C	-5.03079400	2.35820100	-1.93302100
C	-5.00236100	0.99507000	-2.22394700
H	-3.80512200	-0.78927400	-2.31167400
H	-1.76063900	2.78283000	-1.08184900
H	-3.86829500	4.05758300	-1.29483400
H	-5.95631600	2.91892400	-2.02493600
H	-5.90675400	0.48315800	-2.54038800
N	-1.42523900	0.16251200	-1.61423700
C	-0.60224800	0.29934800	-0.51467200
O	-0.77351900	1.12786200	0.36229000
C	-1.17545600	-0.82359900	-2.67390100
H	-0.11216400	-0.87010900	-2.90744500
H	-1.53621200	-1.82574900	-2.40583200
H	-1.70530300	-0.49631100	-3.56937400
C	-1.28736300	-3.82291600	3.32891700
C	-0.20174700	-3.12942500	3.88143000
C	0.50112200	-2.20907900	3.12219900
C	0.14919900	-1.94450300	1.76787100
C	-0.96167300	-2.65653400	1.23257100
C	-1.66010400	-3.57444000	2.00237300
H	-1.83859500	-4.54280500	3.92637100
H	0.08976000	-3.31204700	4.91210700
H	1.34040500	-1.67089500	3.55472600
H	-1.28177800	-2.46620000	0.21283000
H	-2.50776100	-4.10044300	1.57154000
C	0.89193800	-1.00355800	1.02153300
H	1.66516900	-0.42993000	1.51699800
C	0.60448700	-0.69345100	-0.41430800
C	1.77421900	-0.05858900	-1.15763200
O	2.04447100	-0.29054600	-2.32000600
O	2.43903900	0.82115000	-0.39735700
C	3.52558200	1.52837600	-1.04200900
H	4.25679500	0.79580100	-1.39703400
H	3.12696600	2.05253600	-1.91576200
C	4.10988000	2.47848400	-0.01686600
H	4.93486100	3.04404800	-0.46286000
H	3.35162800	3.18582800	0.33237200
H	4.49485500	1.92968900	0.84832400

H	0.37639700	-1.61294400	-0.95560300
INT3-2b'			
C	-2.30168500	1.69751500	-2.48282400
C	-2.09672100	1.06148800	-1.25037500
C	-2.57576000	1.65994800	-0.07814000
C	-3.23678200	2.88567500	-0.14852500
C	-3.43982600	3.52048600	-1.37417600
C	-2.97190600	2.91796400	-2.54177100
H	-1.92219900	1.24818900	-3.39442100
H	-2.41384800	1.17530700	0.87342900
H	-3.60110800	3.34243600	0.76731600
H	-3.95800500	4.47382800	-1.41906700
H	-3.11847000	3.39996700	-3.50419600
N	-1.39482400	-0.18309900	-1.23334700
C	-0.38068900	-0.38798200	-0.31475800
O	-0.26140600	0.27003500	0.70592600
C	-1.69141300	-1.12688800	-2.31453300
H	-1.43150500	-2.13887500	-2.00333600
H	-2.76793500	-1.09841400	-2.50151400
H	-1.16668600	-0.89394500	-3.24701800
C	-0.59828400	-5.44696600	0.64133400
C	-1.24248000	-4.31020700	1.12898600
C	-0.83974700	-3.04068000	0.71538800
C	0.20845900	-2.88598100	-0.20088400
C	0.85867300	-4.03319600	-0.67293000
C	0.45881500	-5.30292800	-0.25730700
H	-0.91254600	-6.43561300	0.96300300
H	-2.06105200	-4.40776600	1.83644000
H	-1.33726400	-2.16394500	1.11721400
H	1.69435400	-3.93893700	-1.36012000
H	0.97726600	-6.17930500	-0.63590900
C	0.66653500	-1.49590300	-0.63447200
H	1.49035400	-1.19132400	0.02780800
C	1.15199100	-1.41594500	-2.04706600
C	1.44196600	-0.15284700	-2.70298300
O	1.54391700	-0.02177900	-3.91643900
O	1.51034700	0.87246300	-1.82314600
C	1.49838500	2.20776400	-2.37101500
H	2.46875600	2.40541300	-2.83895000
H	0.73308900	2.25555700	-3.15140900
C	1.20095500	3.15502200	-1.22555300
H	1.17520200	4.18602200	-1.59469300
H	0.23382200	2.91825000	-0.77363600
H	1.96949600	3.08169900	-0.44996700
H	1.14285100	-2.28292900	-2.69604700
INT3-4a			
C	-3.85804000	1.55764300	-2.64789100
C	-3.59524000	0.57757000	-1.69004400
C	-4.58043700	0.18861800	-0.78373200
C	-5.84082600	0.78455500	-0.83513400
C	-6.10914300	1.76843600	-1.78756500
C	-5.11619700	2.15536700	-2.69042100
H	-3.07364800	1.84465900	-3.34011800
H	-4.35099600	-0.57007500	-0.04099300
H	-6.60899500	0.48442400	-0.12827100
H	-7.08952400	2.23456000	-1.82551900

H	-5.32235200	2.92271000	-3.43091900
N	-2.31629600	-0.08044600	-1.66665000
C	-1.23786000	0.65840800	-1.26598300
O	-1.34226900	1.80144500	-0.84309900
C	-2.28929100	-1.39353200	-2.30683300
H	-1.32513800	-1.87634400	-2.17215000
H	-3.05007200	-2.03312600	-1.85049400
H	-2.50010800	-1.30062800	-3.37762200
C	0.32156100	-3.57808000	1.19042100
C	-0.27950300	-2.41082200	1.66725300
C	-0.32063700	-1.26862200	0.87113300
C	0.23439600	-1.28271100	-0.41353800
C	0.83715500	-2.45054200	-0.88746700
C	0.87826800	-3.59397800	-0.08748200
H	0.35336600	-4.46845900	1.81148100
H	-0.71541900	-2.38843600	2.66198400
H	-0.78515300	-0.35906000	1.24304500
H	1.25449700	-2.48019400	-1.88973400
H	1.34499100	-4.49740100	-0.46935300
C	0.17717600	0.01477500	-1.23200200
H	0.74045900	0.75742500	-0.65808100
C	0.88854800	-0.05159300	-2.53966100
C	2.33900700	0.09193500	-2.69705500
O	2.92110200	0.07955000	-3.76579700
O	2.92834400	0.25905900	-1.49700500
C	4.36561500	0.43120800	-1.52168700
H	4.80868700	-0.43165300	-2.02798500
H	4.59839200	1.32195700	-2.11339500
C	4.82297700	0.55516500	-0.08305000
H	5.91007400	0.68207400	-0.05024800
H	4.35880700	1.42030300	0.40037100
H	4.56052100	-0.34209600	0.48578800
N	0.17595600	-0.34982200	-3.76543200
O	-0.65749100	0.47095800	-4.14581300
O	0.44314800	-1.41160500	-4.32190700

INT3-4a'

C	-3.73224800	0.70224000	-2.53205500
C	-2.69483100	1.06507400	-1.67040500
C	-2.58033300	2.38833300	-1.23385200
C	-3.50168800	3.33983700	-1.66204400
C	-4.54478700	2.98010800	-2.51854800
C	-4.65711900	1.65952300	-2.95021500
H	-3.81152300	-0.32072200	-2.88445100
H	-1.76950700	2.66354100	-0.57024900
H	-3.40694000	4.36643700	-1.32020000
H	-5.26314800	3.72532900	-2.84716900
H	-5.46044300	1.36938400	-3.62114900
N	-1.77830200	0.06607600	-1.19538100
C	-0.44256200	0.27594500	-1.41108100
O	-0.00257600	1.28911800	-1.93676600
C	-2.36870000	-1.20908400	-0.78853300
H	-1.73109100	-1.71464600	-0.07088100
H	-3.32188500	-0.99812000	-0.30044500
H	-2.53400900	-1.87173500	-1.64303800
C	-0.40838200	-4.26463300	3.16924400
C	0.01100100	-3.02346900	3.66485300
C	0.31485700	-1.99267200	2.79351200

C	0.21997600	-2.15081700	1.37700700
C	-0.21051200	-3.42479700	0.90107200
C	-0.51628600	-4.44787200	1.78627600
H	-0.64800500	-5.07549300	3.85020500
H	0.09822600	-2.86546400	4.73599500
H	0.63853100	-1.03196300	3.18467500
H	-0.30621000	-3.61865000	-0.15768300
H	-0.84099600	-5.40635900	1.39167600
C	0.54066900	-1.01170200	0.59694500
H	0.80865700	-0.11957500	1.15112400
C	0.62101000	-0.75669900	-0.87548500
C	1.98049900	-0.07351000	-1.24455100
O	2.60484300	-0.33341600	-2.23970100
O	2.32030400	0.82302900	-0.31630700
C	3.45152500	1.66527100	-0.65554300
H	4.32707300	1.02656300	-0.80222800
H	3.22641800	2.16193400	-1.60332600
C	3.63342200	2.64680000	0.48315800
H	4.47839300	3.30933000	0.26823500
H	2.73673900	3.26069200	0.61224100
H	3.83649200	2.12309900	1.42275900
N	0.61759900	-2.02344500	-1.72808600
O	1.47484000	-2.85364400	-1.47046500
O	-0.22771000	-2.11483500	-2.61267800

INT4-2b

C	-0.65425400	0.82418400	1.20051300
C	-1.01399600	1.69999200	0.03583300
C	-2.23906600	2.31559300	-0.06415400
C	-3.22497600	2.13999900	0.93033700
C	-2.96385900	1.31591300	2.05419000
C	-1.76362400	0.68686600	2.19755700
H	0.22770200	1.25788000	1.70217300
H	-2.46945400	2.93548000	-0.92343200
H	-4.18578800	2.63147200	0.82261300
H	-3.73388000	1.19052800	2.81097900
H	-1.56241200	0.06142900	3.06331000
N	-0.01739700	1.84978800	-0.93980900
C	1.04519900	0.97520200	-1.09687000
O	1.92537800	1.16135800	-1.92794100
C	-0.12034400	2.94488600	-1.90420300
H	0.83291400	3.02094900	-2.42239800
H	-0.91421000	2.74754700	-2.63351600
H	-0.34312000	3.87457700	-1.37476300
C	2.36496400	-0.16306800	0.63325400
C	1.10088100	-0.28341000	-0.21231700
H	1.25682300	-1.10519500	-0.91490500
C	-0.13529000	-0.55342400	0.66683400
H	0.18824200	-1.12646200	1.54235100
C	-1.22281600	-1.33982700	-0.03331100
C	-1.98485400	-2.25508400	0.70334800
C	-1.53511100	-1.15310800	-1.38588400
C	-3.02996400	-2.96261100	0.11247300
H	-1.75368000	-2.41292100	1.75358400
C	-2.57842400	-1.86116000	-1.98235500
H	-0.96288900	-0.45453000	-1.98771700
C	-3.33135600	-2.76687500	-1.23573600
H	-3.60548000	-3.66931000	0.70395100

H	-2.80114600	-1.70325700	-3.03399800
H	-4.14312400	-3.31862200	-1.70121900
O	2.43611500	0.43958900	1.68600200
O	3.39218500	-0.80485700	0.06395400
C	4.66819200	-0.68166000	0.73789000
H	4.57503400	-1.10564600	1.74263700
H	4.90198200	0.38171000	0.84397700
C	5.69151200	-1.41431900	-0.10558400
H	6.67843800	-1.34442500	0.36410900
H	5.42990400	-2.47247000	-0.20502100
H	5.75068500	-0.97709400	-1.10681600

INT4-4a

C	1.15429900	-0.35502200	-0.78418300
C	2.28495800	0.44661700	-0.16845200
C	3.59953000	0.15311200	-0.44997400
C	3.96133300	-0.93769000	-1.26720900
C	2.95883500	-1.78699700	-1.79368600
C	1.63844200	-1.55208100	-1.55883700
H	0.58890200	0.29515800	-1.47326300
H	4.38910900	0.75557700	-0.01733700
H	5.00992500	-1.13565700	-1.45995500
H	3.24765300	-2.64657000	-2.39207300
H	0.87560200	-2.20236500	-1.96555200
N	1.93524400	1.50722400	0.68425200
C	0.73460600	1.57360400	1.38096700
O	0.54049400	2.40076400	2.25691800
C	2.97130700	2.44963500	1.10351400
H	2.48138600	3.27388300	1.61635300
H	3.67972700	1.97505400	1.79305200
H	3.51009100	2.81084300	0.22469800
C	-3.25433400	2.67786600	-1.56183100
C	-3.68286800	1.77913500	-0.58487200
C	-2.75419100	1.13716500	0.23212000
C	-1.38399900	1.37630000	0.07723200
C	-0.96277200	2.28995600	-0.89708900
C	-1.89184300	2.93501100	-1.71207400
H	-3.97797500	3.17996500	-2.19731700
H	-4.74208500	1.57809200	-0.45412500
H	-3.09238800	0.43529000	0.98811500
H	0.09288700	2.51726700	-1.00945100
H	-1.54857000	3.64237500	-2.46141400
C	-0.39442600	0.63250100	0.96800600
H	-0.90170300	0.37404000	1.89832700
C	0.13361500	-0.68495400	0.33895200
N	-1.09380000	-1.41585200	-0.19419800
O	-1.83711600	-1.88627400	0.66077500
O	-1.30536400	-1.41488700	-1.39869700
C	0.79172000	-1.63869000	1.34159800
O	0.92763100	-2.82240100	1.15032400
O	1.27583600	-0.95838700	2.38840100
C	2.10030200	-1.69629300	3.32496300
H	1.44508300	-2.34048000	3.91900000
H	2.78071400	-2.33395500	2.75486700
C	2.82749500	-0.67106600	4.17059400
H	3.43611000	-1.17660900	4.92752400
H	3.48740700	-0.05770800	3.54863700
H	2.11818800	-0.00921400	4.67633400

INT5-2b

C	-0.58382700	0.63574300	1.13984900
C	-0.93545600	1.62492300	0.08663100
C	-2.05555600	2.46040600	0.26600100
C	-2.86584700	2.29451600	1.37176700
C	-2.62271400	1.31660500	2.38070900
C	-1.54419600	0.50532100	2.25457700
H	0.34987200	1.03668500	1.60651300
H	-2.31397700	3.20698300	-0.47220400
H	-3.73548900	2.93842400	1.47079000
H	-3.29690500	1.23733000	3.22587300
H	-1.31181100	-0.24053500	3.00882900
N	-0.15477400	1.71915900	-1.01234500
C	0.87967800	0.77184000	-1.32419000
O	1.54463600	0.91642100	-2.32011200
C	-0.38930700	2.77889100	-2.01290000
H	0.40864800	2.71601300	-2.74767200
H	-1.35260400	2.62204400	-2.50479300
H	-0.36604300	3.75459400	-1.52456900
C	2.32517100	-0.03011000	0.48764900
C	1.10442500	-0.39447000	-0.36815300
H	1.36999700	-1.24622200	-0.99559200
C	-0.11346600	-0.71680600	0.51193400
H	0.22094400	-1.35016800	1.34060700
C	-1.24796100	-1.42184800	-0.21293400
C	-2.19519600	-2.11952700	0.54889800
C	-1.40620000	-1.37845700	-1.60324900
C	-3.28371300	-2.74085200	-0.05767900
H	-2.07224500	-2.19480200	1.62636300
C	-2.49637700	-2.00220100	-2.21365500
H	-0.67619500	-0.88581700	-2.23734800
C	-3.44031600	-2.67873300	-1.44398200
H	-4.00149600	-3.28387800	0.54925100
H	-2.59788200	-1.96454100	-3.29382600
H	-4.28474300	-3.16686200	-1.92012200
O	2.28264100	0.80761400	1.37595700
O	3.39147100	-0.71793000	0.13349500
C	4.63839700	-0.42840900	0.85293500
H	4.46585400	-0.63706200	1.91186700
H	4.84407000	0.63891500	0.74004400
C	5.71444000	-1.30200200	0.24836400
H	6.66286600	-1.11132900	0.76040000
H	5.47019000	-2.36230600	0.36075400
H	5.84663100	-1.08195700	-0.81481200

INT5-4a

C	1.19639000	-0.37303600	-0.80794500
C	2.33596100	0.56960500	-0.51980300
C	3.51799400	0.44294700	-1.26904900
C	3.70140600	-0.64435800	-2.10551800
C	2.74451500	-1.68357300	-2.25172400
C	1.56493800	-1.59041100	-1.58928400
H	0.51680400	0.18664700	-1.48566600
H	4.31730300	1.16231100	-1.16031000
H	4.63908000	-0.71652700	-2.64991800
H	2.96894400	-2.54168900	-2.87442800
H	0.79972900	-2.34737600	-1.69708400

N	2.20187600	1.53220600	0.41909900
C	1.04994500	1.65538500	1.28919500
O	1.04451500	2.49454200	2.15021000
C	3.29202900	2.50066300	0.65471600
H	2.96180000	3.17528200	1.43980100
H	4.19425300	1.97564200	0.97629900
H	3.48777900	3.06452700	-0.25967800
C	-3.13506500	2.53465900	-1.49527100
C	-3.49513100	1.68932600	-0.44446100
C	-2.51527400	1.13134000	0.37351700
C	-1.16253500	1.40736600	0.14259100
C	-0.80718100	2.26723800	-0.90576200
C	-1.79059000	2.82704700	-1.72151300
H	-3.90037700	2.97220100	-2.12822500
H	-4.54058200	1.46757200	-0.25583000
H	-2.80168700	0.47568500	1.19076400
H	0.23173900	2.53870200	-1.07598000
H	-1.50490300	3.49861300	-2.52494100
C	-0.12293600	0.73348000	1.03002500
H	-0.55871800	0.54000500	2.01052200
C	0.38598200	-0.61580300	0.46972200
N	-0.85842600	-1.46278900	0.19110200
O	-1.38899300	-1.94732200	1.17934800
O	-1.25730600	-1.53280800	-0.96231300
C	1.25415100	-1.43283400	1.45368700
O	1.97937400	-2.31596600	1.04934000
O	1.11984700	-1.02368700	2.70072000
C	1.86365500	-1.76558800	3.72866500
H	1.50725700	-2.79801700	3.70245200
H	2.91896000	-1.75415400	3.44442100
C	1.59601200	-1.08036400	5.04905200
H	2.13966400	-1.60270000	5.84240700
H	1.93278900	-0.03953900	5.02851500
H	0.53000900	-1.10116900	5.29247000

INT6-2b

C	-0.58322600	0.30208800	0.81843700
C	-0.10281200	1.17337000	-0.17984700
C	-0.12652200	2.55626900	0.04125700
C	-0.61994200	3.06570800	1.24288400
C	-1.09011300	2.20867700	2.23542100
C	-1.06451200	0.83111800	2.01239300
H	0.24662300	3.23668300	-0.71467600
H	-0.62858100	4.14063900	1.39873200
H	-1.47119800	2.60428400	3.17166100
H	-1.42783100	0.14690800	2.77475100
N	0.37340700	0.63880600	-1.39642700
C	0.84454400	-0.66114000	-1.49494400
O	1.30149600	-1.11902900	-2.53012100
C	0.53746800	1.50526900	-2.55611700
H	0.71750400	0.86624100	-3.41846100
H	-0.36898900	2.09783400	-2.70777000
H	1.39289400	2.18030600	-2.43022500
C	1.93487600	-1.24338100	0.72704700
C	0.76017700	-1.48498300	-0.21852300
H	0.79071400	-2.53490800	-0.51525900
C	-0.54868700	-1.18430800	0.55695200
H	-0.47548600	-1.71277800	1.51294000

C	-1.76078700	-1.72556600	-0.19339100
C	-1.99050600	-3.10741100	-0.18467200
C	-2.63417300	-0.90345300	-0.91010000
C	-3.06448000	-3.65750100	-0.88029000
H	-1.32043100	-3.75562700	0.37607500
C	-3.71093500	-1.45200800	-1.60896100
H	-2.48027900	0.17031700	-0.91457000
C	-3.92921300	-2.82875200	-1.59829800
H	-3.22898200	-4.73117800	-0.85890700
H	-4.38078800	-0.79852200	-2.16103700
H	-4.76811600	-3.25421400	-2.14161500
O	2.13214200	-1.90881600	1.71959200
O	2.66811300	-0.17946400	0.36341500
C	3.69992800	0.25076200	1.28136600
H	4.55457500	-0.42632000	1.18330800
H	3.31485200	0.16542800	2.30072000
C	4.04778400	1.67907500	0.91149900
H	4.82792900	2.05980500	1.57918900
H	4.41425200	1.73705600	-0.11824700
H	3.16524500	2.32044000	1.00256600

INT6-4a

C	1.39243400	-0.60375600	-0.49167400
C	2.25192800	0.50244700	-0.31780200
C	3.33814000	0.66095700	-1.19082200
C	3.58426100	-0.27442300	-2.19262200
C	2.76325600	-1.39017200	-2.33377300
C	1.67883600	-1.55158600	-1.47571100
H	3.99502500	1.51513300	-1.09071600
H	4.43064900	-0.12765300	-2.85710400
H	2.96217100	-2.13178000	-3.10033500
H	1.04214200	-2.42060500	-1.56966900
N	2.05313800	1.42775700	0.73055100
C	0.89690600	1.47118100	1.49132400
O	0.75368500	2.23944000	2.42698000
C	3.11147800	2.37606200	1.06681900
H	2.81762100	2.87152800	1.98963400
H	4.05923400	1.84814900	1.20831800
H	3.23220600	3.12744000	0.27874600
C	-2.95003800	2.55125600	-1.67197800
C	-3.43058400	1.88807900	-0.54345600
C	-2.54217200	1.26063700	0.32823200
C	-1.16491600	1.28387500	0.08284800
C	-0.68910300	1.95421600	-1.05101000
C	-1.57768200	2.58299600	-1.92116400
H	-3.63992500	3.04131600	-2.35294300
H	-4.49671000	1.85800800	-0.33846300
H	-2.91849700	0.73795500	1.20243600
H	0.37295300	1.98843700	-1.26327800
H	-1.19445500	3.09808200	-2.79736400
C	-0.24285200	0.55845500	1.05504900
H	-0.80428500	0.35074100	1.96471400
C	0.27971200	-0.79435300	0.50806900
N	-0.97025500	-1.49999800	-0.04367400
O	-1.75965100	-1.87475100	0.81852600
O	-1.14760300	-1.56695500	-1.24828300
C	0.81956100	-1.74237200	1.59736100
O	0.95552300	-2.93162000	1.43956000

O	1.19379400	-1.05007200	2.67771200
C	1.83718800	-1.79742400	3.74172800
H	1.11287000	-2.51351800	4.14050000
H	2.66939100	-2.36153300	3.31094400
C	2.28656600	-0.78598100	4.77565800
H	2.76652500	-1.30078200	5.61445100
H	3.00328800	-0.08138800	4.34282400
H	1.43434600	-0.21530000	5.15605200

INT7-2b

C	1.58913300	0.90330000	-0.27052500
C	2.59437300	0.09890800	0.30340000
C	3.83399600	0.67963000	0.61982500
C	4.08610900	2.02155100	0.34584400
C	3.10935400	2.80930700	-0.25637900
C	1.87635700	2.23555800	-0.56299700
H	4.60712400	0.08197300	1.08609200
H	5.05508600	2.44299300	0.60246400
H	3.30235500	3.85160100	-0.49448100
H	1.11282300	2.82897600	-1.05377700
N	2.38603300	-1.26700000	0.55254600
C	1.13848100	-1.86195500	0.52827400
O	0.95384600	-3.00668700	0.91122300
C	3.51525300	-2.12629600	0.86959200
H	3.15515400	-3.15225000	0.83372500
H	4.30900900	-1.98115000	0.13062900
H	3.91087500	-1.92093400	1.87289100
C	-0.69689100	-0.54927600	1.43445000
C	-0.03843000	-0.98438500	0.13579100
C	0.28908500	0.27143700	-0.74308600
C	-0.92627700	1.20855100	-0.68095500
C	-1.07064300	2.18146200	0.31657400
C	-1.97113100	1.01165100	-1.59090700
C	-2.23251600	2.95079600	0.39819300
H	-0.27866900	2.32674300	1.04242800
C	-3.13177500	1.77946600	-1.50585800
H	-1.87309100	0.23215500	-2.33820400
C	-3.26868400	2.75476300	-0.51529000
H	-2.32280700	3.70526200	1.17635800
H	-3.93575700	1.61081700	-2.21813900
H	-4.17338300	3.35566200	-0.45601900
O	-0.11344300	-0.09112400	2.39669500
O	-2.03240000	-0.71085500	1.37877000
C	-2.78434100	-0.15389700	2.47052200
H	-2.38687100	0.83863400	2.69972300
H	-2.64738000	-0.78602200	3.35561700
C	-4.23207400	-0.09154600	2.02316100
H	-4.85698100	0.31807900	2.82569300
H	-4.32205300	0.55080200	1.14234100
H	-4.60382200	-1.08873900	1.76617900
S	0.35422300	-1.56723400	-2.84548100
O	0.71483000	-1.23680200	-4.22854100
O	0.53394700	-0.01313300	-2.12745900
O	-1.07337800	-1.90342800	-2.61367900
O	1.31014000	-2.41426900	-2.10271400
H	-0.73833600	-1.61188500	-0.41622500

NO₂⁻

N	-2.59724800	0.18489300	0.00000000
O	-3.19125700	1.30917700	0.00000000
O	-1.32658400	0.23260800	0.00000000
NO ₂ •			
N	-2.49343500	0.28163700	0.00000000
O	-3.13064100	1.30229200	0.00000000
O	-1.31584100	0.03454500	0.00000000
S ₂ O ₈ ²⁻			
S	-1.78362400	-0.38284900	1.21126800
O	-0.81408200	0.73854300	0.34268200
O	-0.87276300	-1.28426800	1.94534000
O	-2.49675000	0.61114000	2.05006200
O	-2.62644100	-1.05607100	0.19695600
S	1.50372300	0.80280500	-0.84245300
O	2.03657700	-0.08186400	-1.90719100
O	1.18333600	2.17945700	-1.28348200
O	-0.00849500	0.00964500	-0.65330700
O	2.21266700	0.72450900	0.45072400
SO ₄ ⁻			
S	-0.37473700	0.38366400	-0.03543300
O	0.17341200	1.07010400	-1.22517500
O	0.23511000	0.93263400	1.27021600
O	-1.85215700	0.35624300	0.02105500
O	0.22804200	-1.02508900	0.13733800
SO ₄ ²⁻			
S	-0.31806400	0.34350100	0.00000000
O	0.19029800	1.06244000	-1.24521500
O	0.19029800	1.06244000	1.24521500
O	-1.84314400	0.34353900	0.00000000
O	0.19028100	-1.09436300	0.00000000
TS1			
C	3.25970100	-1.52698100	0.26762500
C	2.87175300	-0.22786100	-0.10226000
C	3.87334500	0.71915300	-0.38447800
C	5.21728300	0.36550800	-0.29034600
C	5.59922200	-0.92784600	0.07437400
C	4.60919800	-1.87014500	0.35058800
H	2.50639000	-2.26947400	0.50626800
H	3.59057600	1.72308400	-0.66743400
H	5.97467100	1.11304000	-0.51491400
H	6.65074700	-1.19535500	0.14145900
H	4.88172800	-2.88220700	0.64097200
N	1.49321300	0.08986600	-0.21781000
C	1.00013800	1.33271400	0.14888200
O	1.68861600	2.28080600	0.49613900
C	0.54627900	-0.99133800	-0.52841000
H	-0.35043500	-0.58226900	-0.98905200
H	1.01845800	-1.67636200	-1.23703500
H	0.23762900	-1.53857700	0.36802700
C	-0.55879800	1.44582900	0.09841200
O	-1.03398600	1.88907400	-0.94984400
O	-1.10247600	1.03835900	1.16815100
H	-2.50969200	0.79501400	1.01978500

S	-3.89167100	-0.56143200	-0.05125600
O	-4.70098500	0.05100600	-1.15317000
O	-4.76320200	-1.55428200	0.64483300
O	-2.62376300	-1.14788800	-0.54762300
O	-3.55102300	0.56201900	1.00031000

TS2

C	1.89689000	-1.17283400	-0.01884600
C	1.93958700	0.21020900	-0.20357700
C	3.13868200	0.91850700	-0.12352400
C	4.32344300	0.23132500	0.13907300
C	4.30208700	-1.15383600	0.31222000
C	3.09259100	-1.84729200	0.23118500
H	0.94191900	-1.69620400	-0.07275000
H	3.13560700	1.99513600	-0.26246200
H	5.26073300	0.77803700	0.20296600
H	5.22611900	-1.69005100	0.51410100
H	3.07040700	-2.92395500	0.37604300
N	0.71265900	0.92228400	-0.47458300
C	0.27187700	1.76484900	0.45092300
O	0.73749100	2.16496200	1.48683700
C	-0.06352700	0.56514600	-1.67322900
H	-1.13174100	0.65994600	-1.48746800
H	0.25021900	1.19153600	-2.51450400
H	0.10420200	-0.48928700	-1.88430900
C	-1.38397600	2.62365700	0.01261300
O	-1.07684300	3.42814600	-0.83386400
O	-2.23219200	2.14908500	0.72411500
H	-2.04631000	0.06744600	1.06157400
S	-2.10643700	-1.76097700	-0.09898100
O	-2.96491900	-2.67979200	0.66683000
O	-0.88464700	-2.38691700	-0.67208400
O	-2.82532700	-0.84994200	-1.02605600
O	-1.44054700	-0.69704100	1.03367900

TS3-2b

C	3.52029800	1.01481300	0.93141000
C	2.48526300	1.28482500	0.02370900
C	2.79590900	1.51230700	-1.32512500
C	4.12309200	1.46178000	-1.74807800
C	5.15489000	1.19534300	-0.84662300
C	4.84433500	0.97402400	0.49449500
H	3.30258100	0.82629000	1.97649100
H	2.00650200	1.72021000	-2.03412900
H	4.34794000	1.64115500	-2.79592000
H	6.18645400	1.16169000	-1.18504700
H	5.63268800	0.76230300	1.21185400
N	1.12975700	1.32638400	0.49958200
C	0.07377500	1.00622000	-0.29012700
O	0.00248400	0.83551400	-1.47647600
C	0.88710100	1.65459600	1.90986000
H	-0.15252200	1.95449300	2.03890800
H	1.09929000	0.80299700	2.56845400
H	1.53628300	2.48679100	2.19420300
C	0.43470600	-4.79982700	0.00669700
C	-0.75887700	-4.69339500	-0.71296600
C	-1.48033700	-3.50414500	-0.69749400
C	-1.03685500	-2.38970800	0.04740900

C	0.17874400	-2.51316700	0.75832800
C	0.90032000	-3.70108100	0.73716800
H	1.00267100	-5.72588500	-0.00894600
H	-1.12394200	-5.53857200	-1.29042000
H	-2.40615400	-3.42431200	-1.26224900
H	0.57233200	-1.66180400	1.30578100
H	1.83708200	-3.77042400	1.28389400
C	-1.81898500	-1.17155600	0.03652100
H	-2.60158300	-1.09750900	-0.71297800
C	-1.58873400	-0.07217100	0.83753500
C	-2.48036100	1.10694300	0.87160900
O	-2.43903700	1.96778500	1.73776000
O	-3.33513600	1.15111900	-0.17105500
C	-4.19290200	2.31092500	-0.23746600
H	-4.81169900	2.34854000	0.66557000
H	-3.56877400	3.21083500	-0.24739200
C	-5.02440400	2.17682300	-1.49890200
H	-5.69365200	3.03817600	-1.59992800
H	-4.37969300	2.13066200	-2.38227200
H	-5.63251300	1.26691300	-1.46765300
H	-0.98994400	-0.17388000	1.73510500

TS3-2b'

C	2.81716200	-0.42783300	1.26578900
C	1.91607100	-1.19359200	0.51494000
C	2.38932000	-2.16476300	-0.37426200
C	3.76375200	-2.36087000	-0.51094500
C	4.66760400	-1.60715200	0.24019000
C	4.18862400	-0.64282400	1.12873800
H	2.45342100	0.35448400	1.92372500
H	1.68644600	-2.74528100	-0.95879600
H	4.12622000	-3.11393700	-1.20515800
H	5.73642200	-1.76776900	0.13169300
H	4.88206600	-0.04204900	1.71072400
N	0.50694900	-0.94508000	0.65104900
C	-0.26445300	-0.78373500	-0.44901700
O	-0.08373100	-1.13868900	-1.58322400
C	-0.03981300	-0.69010600	1.98669700
H	-1.12705000	-0.75920900	1.94049800
H	0.33653300	-1.46260800	2.66297000
H	0.24099700	0.29486000	2.37024100
C	-5.46383900	-1.10366900	-0.00714300
C	-4.74880300	-1.12883300	-1.20689900
C	-3.51960900	-0.48066500	-1.30246500
C	-2.97808900	0.20822400	-0.20304900
C	-3.70509600	0.22071300	0.99957600
C	-4.93574500	-0.42695100	1.09481200
H	-6.42350600	-1.60742200	0.06926500
H	-5.14879900	-1.65511800	-2.06941600
H	-2.95474500	-0.51646000	-2.23027900
H	-3.31432500	0.74424200	1.86728500
H	-5.48487100	-0.40126400	2.03236000
C	-1.65707200	0.85877700	-0.35670800
H	-1.31751300	0.96292500	-1.38257500
C	-1.10453500	1.74432300	0.56275000
C	0.24599000	2.28153900	0.42720900
O	0.86491300	2.80887500	1.34314700
O	0.78073500	2.04678700	-0.79828700

C	2.18031000	2.34930700	-0.97883900
H	2.28826300	3.42895200	-1.13632400
H	2.72295800	2.08596100	-0.06723000
C	2.65735100	1.54145600	-2.17166500
H	3.72035700	1.73448900	-2.35363700
H	2.52246400	0.47199300	-1.98316300
H	2.09519400	1.80621700	-3.07298600
H	-1.53929000	1.90668300	1.54212300

TS3-4a

C	3.26745300	-1.75876800	-0.46929800
C	2.95167500	-0.39562800	-0.44585200
C	3.97209900	0.55832400	-0.35634000
C	5.30350900	0.14682000	-0.29342500
C	5.62433800	-1.21073300	-0.31181400
C	4.60150900	-2.15720200	-0.39806800
H	2.47873100	-2.49716400	-0.53977200
H	3.73187000	1.61567400	-0.32841100
H	6.08890700	0.89427300	-0.22391000
H	6.66158900	-1.52879900	-0.26063500
H	4.83943200	-3.21696000	-0.41963500
N	1.58211500	0.05121300	-0.53061700
C	0.61759900	-0.59797300	0.14146600
O	0.63014400	-1.63620300	0.74734800
C	1.29427200	1.28447500	-1.27894700
H	0.25702700	1.27300500	-1.60457500
H	1.47420600	2.17372500	-0.66738800
H	1.94396500	1.30458600	-2.15643500
C	-0.30784600	4.43390300	1.42449300
C	0.26976200	3.35234100	2.09506200
C	-0.10520400	2.05344600	1.76679400
C	-1.04758800	1.79985900	0.75065900
C	-1.63407800	2.89705900	0.09850000
C	-1.26608900	4.19860300	0.43694800
H	-0.02053300	5.45083200	1.67684300
H	1.00546500	3.52083900	2.87655700
H	0.34538600	1.21392100	2.29111200
H	-2.38003100	2.74988500	-0.67071300
H	-1.73341000	5.03338700	-0.07774100
C	-1.37620400	0.38032800	0.48734600
H	-1.31327100	-0.23936800	1.37429800
C	-2.22061900	-0.19405900	-0.45674600
C	-2.62607600	-1.62046100	-0.37711500
O	-3.00026000	-2.29034100	-1.31707100
O	-2.44844200	-2.09668300	0.87390700
C	-2.52006600	-3.53240100	1.02953500
H	-3.57145500	-3.83657000	0.98268700
H	-1.99700000	-4.00333300	0.19202000
C	-1.87622700	-3.85883700	2.36341700
H	-1.89276300	-4.94086500	2.53368100
H	-0.83771400	-3.51400900	2.36930900
H	-2.41131500	-3.37097000	3.18476000
N	-2.61501600	0.46580200	-1.68364700
O	-1.76818300	1.13179700	-2.30107400
O	-3.78477200	0.34445800	-2.03709600

TS3-4a'

C	3.48210500	-2.27037600	0.38139100
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C	2.95020000	-1.09804700	-0.16723700
C	3.78107400	-0.21583700	-0.86779400
C	5.13548900	-0.51031600	-1.01150600
C	5.67050200	-1.68196500	-0.47161100
C	4.83804200	-2.55940000	0.22289000
H	2.84802100	-2.94984700	0.94076900
H	3.37027500	0.69357700	-1.28872100
H	5.77343900	0.17968400	-1.55677700
H	6.72647500	-1.90709100	-0.59007600
H	5.24161400	-3.47128600	0.65423700
N	1.54231500	-0.82152500	-0.02540800
C	1.13209000	0.42032900	0.30049600
O	1.76141800	1.43820300	0.40835600
C	0.61274700	-1.95414100	-0.01739900
H	-0.36600700	-1.62279700	-0.34796700
H	0.98110700	-2.70537000	-0.71901700
H	0.51876500	-2.39130400	0.98037300
C	-4.46782700	-2.98796000	-1.05040100
C	-4.32250200	-2.00653600	-2.03523000
C	-3.48430700	-0.92048800	-1.81665200
C	-2.76565300	-0.77217000	-0.60533600
C	-2.92466700	-1.77983700	0.37791100
C	-3.76223400	-2.86623700	0.15052500
H	-5.12213700	-3.83892200	-1.21688500
H	-4.86285600	-2.08998900	-2.97412900
H	-3.37687600	-0.16044300	-2.58670200
H	-2.38614800	-1.73220800	1.31523800
H	-3.86657600	-3.62543400	0.92072200
C	-1.93291700	0.40415700	-0.47521100
H	-1.89599300	1.04724800	-1.34976400
C	-1.13373200	0.85760600	0.56198800
C	-0.76793900	2.30872000	0.67410200
O	-0.59622700	2.87544700	1.72771800
O	-0.62094900	2.86319500	-0.53968800
C	-0.06523200	4.20200200	-0.54219100
H	-0.76727500	4.87598100	-0.04078900
H	0.86288000	4.18254600	0.03604900
C	0.16517600	4.58118800	-1.99155400
H	0.58902500	5.58947500	-2.04974700
H	0.86343700	3.88304100	-2.46408700
H	-0.77426100	4.56775200	-2.55388700
N	-1.34063100	0.28038000	1.93150400
O	-2.37938500	0.59892300	2.49223200
O	-0.49125500	-0.48086300	2.39205600

TS4-2b

C	-0.63705300	1.05877600	1.35023000
C	-0.98066500	1.67394300	0.10201200
C	-2.30414100	1.95823200	-0.20672600
C	-3.31659400	1.70970000	0.73146500
C	-2.99736200	1.17286500	1.99137200
C	-1.68338400	0.89136600	2.31314900
H	0.37263400	1.20581900	1.72523400
H	-2.56203100	2.35250500	-1.18443700
H	-4.34831300	1.93181600	0.47684500
H	-3.78478200	1.00824500	2.72199800
H	-1.42313900	0.51301500	3.29784800
N	0.05294900	1.85219900	-0.84547900

C	1.09172700	0.96235100	-1.03122100
O	1.97296400	1.16499700	-1.85705400
C	-0.03343200	2.96709800	-1.79451700
H	0.97618500	3.25211200	-2.08822400
H	-0.59028300	2.68158500	-2.69517500
H	-0.53688800	3.80449200	-1.30779800
C	2.40126100	-0.27921600	0.64829400
C	1.14300400	-0.36483200	-0.21482600
H	1.33878200	-1.10997500	-0.99363100
C	-0.05817700	-0.77735300	0.61315900
H	0.20456300	-1.20151200	1.57930400
C	-1.20946500	-1.39394400	-0.03273600
C	-2.13862400	-2.11616300	0.74656600
C	-1.48303700	-1.24042400	-1.40862700
C	-3.28213900	-2.66562800	0.17760700
H	-1.95118800	-2.23591400	1.81064400
C	-2.62717200	-1.79522700	-1.97684200
H	-0.79471600	-0.68716700	-2.04098700
C	-3.53386200	-2.50841700	-1.18916600
H	-3.98042000	-3.21985000	0.79952800
H	-2.81257200	-1.66895600	-3.04048300
H	-4.42596500	-2.93967700	-1.63503600
O	2.44117300	0.21050600	1.76055800
O	3.46007400	-0.80041800	0.01886200
C	4.73174700	-0.68243900	0.70509500
H	4.66636000	-1.21588300	1.65932200
H	4.91091600	0.37475800	0.92533900
C	5.78640600	-1.26636600	-0.21420800
H	6.77254800	-1.19563900	0.25740000
H	5.57733100	-2.31987100	-0.42567900
H	5.81241300	-0.72190000	-1.16305900

TS4-4a

C	1.35787800	-0.17308200	-1.02513700
C	2.33026200	0.43482400	-0.16237100
C	3.58205400	-0.15334600	-0.00410600
C	3.90722000	-1.32215000	-0.70106900
C	2.97825200	-1.91660500	-1.57183300
C	1.74007800	-1.33624500	-1.75964100
H	0.58549100	0.45439100	-1.45629400
H	4.30136100	0.27886000	0.68228300
H	4.88477300	-1.77205700	-0.55795500
H	3.24519200	-2.81804500	-2.11420900
H	1.01943400	-1.76151000	-2.44795300
N	1.94919300	1.55810000	0.59734600
C	0.73584200	1.65407400	1.27205400
O	0.55473800	2.53592900	2.09517500
C	2.98808200	2.48632000	1.05009800
H	2.52571200	3.45434300	1.23576400
H	3.45407800	2.14788500	1.98338500
H	3.74550400	2.57073500	0.26951500
C	-3.41258200	2.65491900	-1.50073700
C	-3.78775000	1.72682000	-0.52884700
C	-2.81991100	1.11507700	0.26486100
C	-1.46403800	1.41340700	0.09037500
C	-1.09617000	2.35312900	-0.87840500
C	-2.06470200	2.96940700	-1.66996200
H	-4.16676100	3.13463600	-2.11770500

H	-4.83543100	1.48011700	-0.38418100
H	-3.11619400	0.38902200	1.01652200
H	-0.05201400	2.62243100	-1.00715400
H	-1.76336800	3.69897300	-2.41607700
C	-0.43326300	0.69835800	0.95936300
H	-0.88649600	0.55279100	1.94652300
C	-0.04139800	-0.68445000	0.44526600
N	-1.14204900	-1.38088900	-0.25683400
O	-1.87877200	-2.06417500	0.45340500
O	-1.29786200	-1.19470600	-1.46026300
C	0.72792800	-1.60847900	1.30870000
O	0.91690800	-2.78291700	1.07330000
O	1.29831900	-0.92734800	2.32848500
C	2.28308800	-1.65098100	3.09888400
H	1.77265700	-2.43191700	3.67072300
H	2.97397700	-2.13730500	2.40430000
C	2.97554000	-0.64262100	3.99297800
H	3.71396700	-1.14750400	4.62463800
H	3.49271600	0.11392700	3.39372700
H	2.25451500	-0.13286100	4.63899700

TS5-2b

C	-0.37253100	-0.33020300	0.80587400
C	-1.17141100	0.46568200	1.73620300
C	-1.64214000	-0.08422500	2.90636100
C	-1.51556100	-1.48944500	3.12324800
C	-0.90788300	-2.32118100	2.23161300
C	-0.25249100	-1.77888900	1.07180600
H	0.87095100	0.02310700	1.01180800
H	-2.17118800	0.50626000	3.64282600
H	-1.97366700	-1.90609000	4.01900100
H	-0.87299100	-3.39375200	2.39321900
H	-0.19191700	-2.40942400	0.19126000
N	-1.44650400	1.81345700	1.41599300
C	-1.27235300	2.36443900	0.15216300
O	-1.74549900	3.45284500	-0.15022200
C	-2.10779400	2.65473500	2.40863000
H	-2.14838800	3.66664800	2.01172400
H	-3.12837400	2.30491800	2.60862400
H	-1.53574500	2.63904200	3.34092000
C	1.01226700	2.11549600	-0.72310000
C	-0.42565600	1.58291000	-0.83771100
H	-0.78403100	1.86299800	-1.83309700
C	-0.48130100	0.04510300	-0.68752400
H	0.40800700	-0.35693500	-1.17675700
C	-1.69290900	-0.57994000	-1.35768800
C	-1.49873600	-1.66270700	-2.22752200
C	-3.00617000	-0.14892300	-1.11562100
C	-2.58206800	-2.29784200	-2.83817700
H	-0.48415100	-2.00838600	-2.41180100
C	-4.08957800	-0.77719400	-1.72936000
H	-3.18697400	0.68137400	-0.43927300
C	-3.88293100	-1.85553300	-2.59364500
H	-2.40712000	-3.13806900	-3.50636800
H	-5.09909900	-0.42445000	-1.53002700
H	-4.72889500	-2.34595000	-3.06986300
O	1.38974500	2.91602700	0.10383600
O	1.77181000	1.58393400	-1.68851600

C	3.20553600	1.74461300	-1.53768300
H	3.45299700	1.53731400	-0.49495400
H	3.46449100	2.78486500	-1.77174600
C	3.85534100	0.74775900	-2.47772200
H	4.94664700	0.82255700	-2.39933400
H	3.54567900	-0.26297400	-2.19621500
H	3.56702800	0.94139300	-3.51810400
S	2.55692100	-1.44299100	0.61603900
O	2.27546200	-1.72904600	-0.81957800
O	2.19566300	0.05059000	0.92349600
O	1.52231200	-2.22306100	1.49831600
O	3.92072500	-1.73862700	1.07000800

TS5-4a

C	-0.44563700	-0.58075800	-0.17872800
C	-1.23334500	-0.44505000	1.05110200
C	-2.17761900	-1.36497300	1.41360800
C	-2.56084800	-2.40326400	0.49070000
C	-1.94340000	-2.58215900	-0.69177800
C	-0.73818700	-1.79278300	-1.06106500
H	0.84977500	-1.08747500	0.38459800
H	-2.68532100	-1.31385000	2.36811500
H	-3.40453800	-3.03494800	0.76405100
H	-2.27093600	-3.34092300	-1.39654300
H	-0.77044700	-1.50257400	-2.11206000
N	-0.98590600	0.67961000	1.88871200
C	-0.52328700	1.88443100	1.40642200
O	-0.57270000	2.92028300	2.06141200
C	-1.52896300	0.69052600	3.24316500
H	-1.08482200	1.52884700	3.77689200
H	-2.61956200	0.81657500	3.23793900
H	-1.27830100	-0.25122000	3.73702300
C	4.46823900	2.03521700	0.60094000
C	3.84133000	2.88073200	-0.31610600
C	2.45764800	2.83026300	-0.48030600
C	1.68125400	1.93553100	0.26723800
C	2.31656700	1.10058700	1.19304800
C	3.70091100	1.14524300	1.35288300
H	5.54830600	2.06590200	0.72386400
H	4.42866100	3.57754200	-0.90939400
H	1.97345700	3.47326200	-1.20924000
H	1.73761800	0.40091300	1.78341200
H	4.17581200	0.47017000	2.05919900
C	0.17057500	1.89465300	0.04597500
H	-0.12175700	2.84025400	-0.41361400
C	-0.29672500	0.74928300	-0.90188000
N	0.72687200	0.73659300	-2.04824100
O	0.70125900	1.72765800	-2.78212600
O	1.52393700	-0.18058900	-2.12806600
C	-1.64912700	1.03769300	-1.56252100
O	-2.01767100	0.60584600	-2.63333500
O	-2.43988400	1.70506000	-0.69215600
C	-3.86461700	1.67309000	-0.91086200
H	-4.14846100	2.58229000	-1.45394800
H	-4.10664700	0.80948200	-1.53587000
C	-4.51684400	1.59362900	0.45912600
H	-5.60914200	1.60693100	0.36326100
H	-4.20990500	0.66754500	0.95570900

H	-4.20716200	2.43929400	1.08223700
S	1.25235000	-3.21086800	0.17312400
O	0.34749600	-3.89379800	1.10127300
O	1.66897200	-1.80409900	0.74815800
O	2.42334300	-3.93475300	-0.30782500
O	0.44418000	-2.76797000	-1.16542000

TS6-2b

C	0.90274700	0.31929500	0.98187200
C	2.29957800	0.48551200	0.89077900
C	3.10288400	0.20703500	2.00512900
C	2.52180900	-0.22731300	3.19783300
C	1.13941500	-0.38290900	3.29458500
C	0.33603600	-0.11144900	2.18825100
H	4.17990500	0.31578300	1.95053500
H	3.16213900	-0.44486100	4.04966600
H	0.68588000	-0.72690700	4.22002400
H	-0.74227900	-0.25718300	2.22651800
N	2.87575300	0.97598900	-0.30857200
C	2.19727600	1.02007000	-1.51320900
O	2.69827000	1.48047700	-2.53207800
C	4.25382500	1.45185200	-0.29724400
H	4.44467900	1.93474300	-1.25388000
H	4.39850900	2.16677200	0.51965300
H	4.95731800	0.61973100	-0.16919100
C	0.88207800	-1.03903800	-1.99870500
C	0.78674800	0.42448000	-1.53907100
H	0.26197800	0.94737200	-2.33737500
C	0.03785200	0.56504600	-0.20272400
H	-0.73075600	-0.46233700	-0.19072300
C	-0.89786200	1.73176400	-0.13581500
C	-1.99362600	1.78692700	-1.01530400
C	-0.70639700	2.78475700	0.77287900
C	-2.86200000	2.87411900	-0.99249000
H	-2.20201000	0.94130000	-1.66188900
C	-1.57085600	3.87828500	0.78405800
H	0.12806000	2.74344300	1.46627600
C	-2.65056300	3.92843500	-0.10025100
H	-3.72067800	2.88384800	-1.65831800
H	-1.40208700	4.69075500	1.48746600
H	-3.33180200	4.77620200	-0.08337800
O	0.51738700	-1.43982900	-3.07872400
O	1.40966700	-1.79722500	-1.02410100
C	1.17862900	-3.22467900	-1.09216800
H	1.99337000	-3.67825700	-1.67054600
H	0.23456700	-3.39538700	-1.61334400
C	1.12210700	-3.72315100	0.34001300
H	1.00046700	-4.81288600	0.35273900
H	2.03950200	-3.46412600	0.88057100
H	0.26766600	-3.26299200	0.84222900
S	-2.86772300	-1.45086000	0.33051300
O	-2.76964800	-0.65809100	1.58223700
O	-3.15184100	-2.90089400	0.52465400
O	-3.66678400	-0.80040400	-0.73198400
O	-1.33070500	-1.58745800	-0.22697300

TS6'-4a

C	1.26608100	-1.63518200	0.39519800
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C	1.69722900	-1.74048100	-0.94378300
C	3.00027900	-2.20739300	-1.19588300
C	3.83556700	-2.57795100	-0.14822800
C	3.39845400	-2.49698800	1.17415600
C	2.11443100	-2.02766700	1.43079100
H	3.36744200	-2.26062200	-2.21208200
H	4.84003900	-2.92835400	-0.37210400
H	4.04737500	-2.79219700	1.99337300
H	1.75553200	-1.96403600	2.45183700
N	0.84431800	-1.39563000	-1.99320700
C	-0.28858600	-0.60232100	-1.78064800
O	-0.88124000	-0.11987800	-2.77020200
C	1.30439100	-1.54073100	-3.36811100
H	0.46815600	-1.28380600	-4.01342700
H	2.12869100	-0.84866100	-3.56917800
H	1.61715600	-2.57396500	-3.54923500
C	-4.44362200	1.67796900	0.22886800
C	-3.26575200	2.27757900	0.67088800
C	-2.03579200	1.66058700	0.44021200
C	-1.95632600	0.42458600	-0.21767700
C	-3.14895100	-0.15800500	-0.67258400
C	-4.37750500	0.46086300	-0.45245800
H	-5.40394400	2.15824300	0.40269600
H	-3.29789700	3.23704000	1.18177800
H	-1.12030900	2.15583500	0.74342300
H	-3.09990500	-1.10189500	-1.20010100
H	-5.28876300	-0.01139400	-0.81273500
C	-0.61783700	-0.24311900	-0.41735400
H	0.37189200	0.89385400	-0.34198500
C	-0.14514200	-1.17810600	0.65286000
N	-0.97564200	-2.56194000	0.71216500
O	-0.74694500	-3.30304800	1.66076900
O	-1.70571500	-2.83537000	-0.23232400
C	-0.38851800	-0.52843400	2.02287100
O	-1.32730300	-0.74132200	2.75245800
O	0.54527400	0.41261400	2.23595900
C	0.29217100	1.34522900	3.30453200
H	-0.73119100	1.71823400	3.19945200
H	0.36060100	0.81771300	4.26271200
C	1.32499500	2.44704400	3.16488300
H	1.15132500	3.22397100	3.91842600
H	2.33589800	2.04889500	3.30007600
H	1.26852900	2.88897200	2.16608800
S	1.27746200	2.42817500	-1.77272600
O	-0.21572900	2.50630800	-2.40423200
O	2.05582000	1.47269300	-2.57065100
O	1.73090600	3.80867200	-1.67386100
O	1.04449700	1.85973800	-0.33093900
H	-0.52965700	1.58541100	-2.63373300

TS6-4a

C	1.13827100	-1.03193900	0.98056800
C	1.79741100	-1.48163300	-0.17857600
C	3.19118700	-1.65142000	-0.13133700
C	3.89410400	-1.41301500	1.04258000
C	3.23208700	-1.00991200	2.20244800
C	1.85741100	-0.81878300	2.15731100
H	3.73330800	-1.93059600	-1.02401900

H	4.97428900	-1.53561600	1.04442500
H	3.78092100	-0.82515300	3.12124500
H	1.32593900	-0.48985900	3.04384700
N	1.07955700	-1.78509100	-1.34763000
C	-0.23511500	-1.38701800	-1.55050800
O	-0.84230600	-1.65725100	-2.58055700
C	1.78928900	-2.33803300	-2.49751100
H	1.04709900	-2.56705700	-3.25889800
H	2.49033400	-1.59053000	-2.88015900
H	2.31766400	-3.25358000	-2.21074400
C	-4.96141500	0.64240100	-0.90704500
C	-3.99526800	1.58265500	-0.54913800
C	-2.65885400	1.20357000	-0.42991200
C	-2.26363500	-0.12396500	-0.66078600
C	-3.24119700	-1.05845300	-1.04058600
C	-4.57644300	-0.67709600	-1.15528000
H	-6.00481100	0.93564700	-0.99964700
H	-4.27641700	2.61765300	-0.37030100
H	-1.90639900	1.94622200	-0.19065300
H	-2.94447500	-2.07880700	-1.23876100
H	-5.32008700	-1.41687300	-1.44268700
C	-0.82240500	-0.51241600	-0.48396500
H	-0.14940100	0.62116400	-0.80329700
C	-0.35319900	-0.81378200	0.93423100
N	-0.97572600	-2.16654700	1.46218900
O	-0.79970800	-2.42652100	2.64361000
O	-1.51670000	-2.90736400	0.64831600
C	-0.86710200	0.29185600	1.88490700
O	-1.83535600	0.21144500	2.60431100
O	-0.11612600	1.37272300	1.69550600
C	-0.52626900	2.62111800	2.29278700
H	-1.61272600	2.71722400	2.19033200
H	-0.29177200	2.58131400	3.36361700
C	0.24099100	3.71051000	1.56564100
H	0.02523600	4.68555400	2.01930400
H	1.31379600	3.50699000	1.60468800
H	-0.03075700	3.72912900	0.50704800
S	1.88859500	1.83498500	-1.33114100
O	1.87473800	3.20490600	-1.94061500
O	2.35421000	0.76185900	-2.23755700
O	2.46150900	1.78077100	0.02799000
O	0.26284500	1.68956100	-1.21525000

TS7-2b

C	1.66925200	0.89414700	-0.29425300
C	2.81311300	0.27299800	0.24927100
C	4.06978000	0.88909300	0.06830600
C	4.18816300	2.07913400	-0.64263100
C	3.05944500	2.69088200	-1.18671200
C	1.81705600	2.08888200	-1.00421900
H	4.95958700	0.43905200	0.49110000
H	5.17153700	2.52832300	-0.76485300
H	3.14252700	3.61708600	-1.74889200
H	0.92966000	2.54605000	-1.42873600
N	2.70318800	-0.91859200	0.96179900
C	1.46098600	-1.40340900	1.44741100
O	1.46394100	-2.31446200	2.27444300
C	3.90088700	-1.61187500	1.40597000

H	3.58014000	-2.55175300	1.85159500
H	4.56631200	-1.80297800	0.55607800
H	4.45109400	-1.03615900	2.16383400
C	-0.95716000	-0.91105100	1.71849000
C	0.24661400	-0.85615200	0.85183700
H	-0.08741800	-1.99719300	-0.06159400
C	0.29799000	0.23789800	-0.20573300
C	-0.77029400	1.32172800	-0.00705000
C	-0.77220500	2.03092600	1.20317800
C	-1.70325100	1.66230900	-0.98853700
C	-1.69903800	3.04515800	1.43521500
H	-0.05228400	1.76862100	1.97277700
C	-2.62911000	2.68357000	-0.75702000
H	-1.72816600	1.10459300	-1.91402400
C	-2.63513200	3.37837100	0.45254800
H	-1.68902400	3.57450800	2.38520900
H	-3.35508800	2.92716300	-1.52962200
H	-3.36097100	4.16873600	0.63055400
O	-1.02137200	-0.92638100	2.93364500
O	-2.07458100	-0.92921800	0.93661200
C	-3.33171400	-0.75664500	1.59524600
H	-3.28601800	0.13342200	2.23461400
H	-3.52114600	-1.61971900	2.24573100
C	-4.37912300	-0.62023300	0.50283500
H	-5.38236700	-0.55046500	0.94202700
H	-4.18548700	0.27657200	-0.09199100
H	-4.33650800	-1.48035300	-0.17160600
S	-0.68076600	-1.59783600	-2.11010300
O	-0.05571400	-2.00871900	-3.36257400
O	0.18329000	-0.28423900	-1.64123200
O	-2.10614100	-1.25774400	-2.14264000
O	-0.35492000	-2.62228300	-0.97301200
1a			
C	-1.98351400	-0.27166000	-0.13951800
C	-0.65411800	0.11873700	0.03802400
C	-0.32920800	1.47449200	0.12824500
C	-1.33553700	2.43357100	0.03560800
C	-2.66349600	2.04782800	-0.15541500
C	-2.98465600	0.69299500	-0.24305800
H	-2.23318600	-1.32769800	-0.18255000
H	0.70302800	1.76761900	0.27999700
H	-1.07893300	3.48634100	0.10865100
H	-3.44408700	2.79906000	-0.23114800
H	-4.01640000	0.38314900	-0.38126300
N	0.37506900	-0.87894900	0.10418700
C	1.21422700	-0.88404000	1.18439000
O	1.11594200	-0.15311500	2.15747500
C	0.54049100	-1.76689300	-1.05236900
H	0.92953000	-2.73737500	-0.74386700
H	-0.43527600	-1.91697300	-1.51514500
H	1.22442000	-1.33379900	-1.78915800
C	2.41570500	-1.83425100	1.10384600
O	3.19001000	-1.88324200	0.17314900
O	2.56099200	-2.53262300	2.24169700
H	3.39401600	-3.03424200	2.15012600
2b			
C	-4.34545700	-1.00716700	0.11924500

C	-3.30045900	-0.63987200	0.96687200
C	-2.71583100	0.61832300	0.84445500
C	-3.16101600	1.53406600	-0.12440400
C	-4.21621700	1.14783900	-0.97177100
C	-4.80013200	-0.10752200	-0.85014700
H	-4.80469200	-1.98720200	0.21087700
H	-2.94078400	-1.33215300	1.72262900
H	-1.90137100	0.90437600	1.50516400
H	-4.58025800	1.83485800	-1.72904400
H	-5.61370300	-0.38874200	-1.51269000
C	-2.50815600	2.84014000	-0.20492100
H	-1.70722800	3.00795500	0.51139300
C	-2.79246300	3.83846100	-1.06070400
C	-2.08853100	5.13264700	-1.08271200
O	-2.35311900	6.03053000	-1.86103000
O	-1.11252200	5.22569000	-0.14601900
C	-0.39033700	6.47290900	-0.12307900
H	0.06613400	6.63658200	-1.10458900
H	-1.09862200	7.28964900	0.04970500
C	0.64615700	6.37391600	0.97890400
H	1.22227200	7.30375300	1.03437000
H	0.16818200	6.20544200	1.94924900
H	1.33980900	5.54876100	0.78818500
H	-3.57359000	3.76307600	-1.80997600

4a

C	-4.75692900	-0.78300000	0.27135100
C	-3.76468600	-0.77370900	-0.71196800
C	-2.98670500	0.35995600	-0.92050600
C	-3.19232100	1.51397200	-0.14004700
C	-4.17755300	1.48078300	0.86482800
C	-4.95987800	0.34817200	1.06338500
H	-5.36152000	-1.67189500	0.42586900
H	-3.59105700	-1.65796000	-1.31767600
H	-2.19987900	0.32821600	-1.66344900
H	-4.33191500	2.36147800	1.48267600
H	-5.72194000	0.34554400	1.83692800
C	-2.43651500	2.75289200	-0.29312100
H	-2.48175800	3.43772800	0.54925200
C	-1.70802800	3.20577200	-1.32694800
N	-1.57620400	2.44908700	-2.58728100
O	-2.50399600	2.52302000	-3.38250600
O	-0.54724700	1.79575600	-2.73379500
C	-0.98290600	4.49586600	-1.38016300
O	-0.39120100	4.88949900	-2.36305500
O	-1.07463500	5.16879100	-0.21767500
C	-0.41283500	6.45696100	-0.19188300
H	0.64747800	6.30685200	-0.41547300
H	-0.83610600	7.08155000	-0.98423400
C	-0.63306500	7.04656900	1.18610600
H	-0.14638800	8.02532000	1.25119400
H	-1.70064600	7.17824300	1.38856800
H	-0.20986400	6.39863600	1.96004500

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