Supporting Information

Regioselective Annulation of *N*-Methylpyridinium Ylides with Alkenes Enabled by Palladium Catalysis: Access to 3-Unsubstituted Indolizine Derivatives

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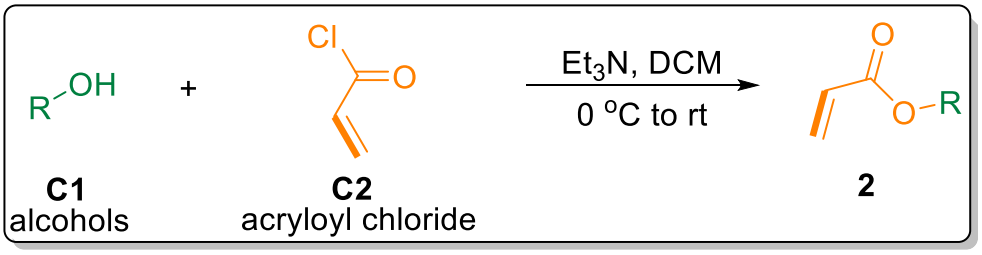
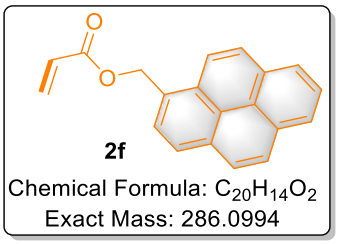
1. General information

Unless otherwise noted, solvents were distilled with a proper drying reagent and stored in a molecular sieve. Copper(I) oxide (98%+) were obtained from the commercial vendor (Bidepharm®) and used without further purification. SafeDry DMAc (dimethylacetamide, water ≤ 50 ppm) and $Pd(OAc)_2$ (99%+, Pd: 47%+) was purchased from Adamas-beta®. The other catalysts and reagents were purchased from commercial vendors and used directly without further purification. All *N*-methylpyridinium ylides were synthesized according to the reported literatures.[1] Column chromatography purifications performed using 300 – 400 mesh silica gel. NMR spectra (^1H and ^{13}C NMR) were recorded on 400 or 600 MHz spectrometers (Bruker ADVANCE III). Chemical shifts were reported relative to the residual solvent peak ($CHCl_3$ in $CDCl_3$). The following abbreviations (or combinations thereof) were used to explain multiplicities: s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet. Coupling constants (*J*) were reported in the Hertz unit (Hz). High-resolution mass spectra (HRMS) were obtained by the ESI model from an ab sciex 500R QTOF or Waters Xevo G2-S QTOF instrument.

2. Preparation of compounds 2f, 2l, 2m, 2n, and 2o



To a 50 mL round flask was charged with alcohols **C1** (1.0 g), Et_3N (2.0 equiv) and 20 mL DCM. Then the acryloyl chloride **C2** (1.5 equiv) was added into the above mixture under an ice water bath. Next, the reaction mixture was vigorously stirred at rt. After the reaction was complete as monitored by TLC, the mixture was extracted with DCM. The organic layer was combined, dried over Na_2SO_4, and evaporated to give the residue. The crude product was separated by column chromatography (eluent: ethyl acetate/ petroleum ether) on silica gel to give the compound **2**.

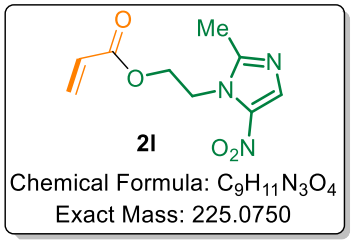


pyren-1-ylmethyl acrylate (2f): The compound **2f** was prepared according to the above procedure as a white solid (1.1 g, 90%), m.p. = 77.1–78.7 °C.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.30 (d, *J* = 9.2 Hz, 1H), 8.25 – 7.99 (m, 8H), 6.46 (dd, *J* = 17.3, 1.5 Hz, 1H), 6.19 (dd, *J* = 17.3, 10.4 Hz, 1H), 5.93 (s, 2H), 5.84 (dd, *J* = 10.4, 1.5 Hz, 1H).

^{13}C NMR (101 MHz, Chloroform-*d*) δ 166.2, 131.8, 131.3, 131.2, 130.7, 129.6, 128.8, 128.3, 128.3, 127.9, 127.8, 127.4, 126.1, 125.6, 125.5, 124.9, 124.6, 122.9, 64.9.

HRMS (ESI) *m/z*: $[M + Na]^+$ Calcd for $C_{20}H_{14}O_2Na$ 309.0886; found: 309.0881.



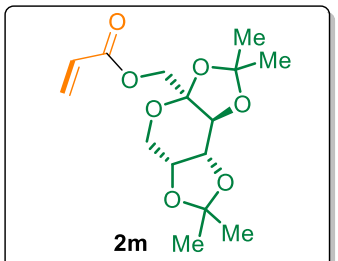
Chemical Formula: $C_9H_{11}N_3O_4$
Exact Mass: 225.0750

2-(2-methyl-5-nitro-1*H*-imidazol-1-yl)ethyl acrylate (2l): The compound **2l** was prepared according to the above procedure as a light yellow solid (986.2 mg, 75%), m.p. = 132.9–133.1 °C.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.96 (d, *J* = 1.6 Hz, 1H), 6.38 (dq, *J* = 17.3, 1.6 Hz, 1H), 6.06 (ddd, *J* = 17.2, 10.5, 1.3 Hz, 1H), 5.89 (dt, *J* = 10.4, 1.4 Hz, 1H), 4.64 (dd, *J* = 5.7, 4.6 Hz, 2H), 4.56 – 4.47 (m, 2H), 2.50 (s, 3H).

^{13}C NMR (101 MHz, Chloroform-*d*) δ 165.4, 150.9, 138.5, 133.2, 132.3, 127.3, 62.5, 45.1, 14.3.

HRMS (ESI) *m/z*: $[M + Na]^+$ Calcd for $C_9H_{11}N_3O_4Na$ 248.0642; found: 248.0641.



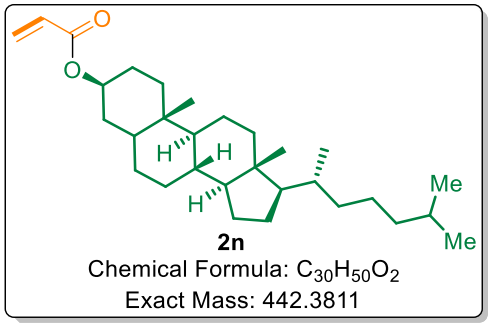
Chemical Formula: $C_{15}H_{22}O_7$
Exact Mass: 314.1366

((3a*S*,5a*R*,8a*R*,8b*S*)-2,2,7,7-tetramethyltetrahydro-3a*H*-bis([1,3]dioxolo)[4,5-b:4',5'-*d*]pyran-3a-yl)methyl acrylate (2m): The compound **2m** was prepared according to the above procedure as a light yellow oil (844.9 mg, 70%).

^{1}H NMR (400 MHz, Chloroform-*d*) δ 6.25 (dd, *J* = 17.4, 1.5 Hz, 1H), 5.96 (dd, *J* = 17.3, 10.4 Hz, 1H), 5.67 (dd, *J* = 10.4, 1.5 Hz, 1H), 4.42 (dd, *J* = 7.9, 2.6 Hz, 1H), 4.30 (d, *J* = 11.7 Hz, 1H), 4.16 (d, *J* = 2.7 Hz, 1H), 4.04 (dd, *J* = 7.9, 1.8 Hz, 1H), 3.90 (d, *J* = 11.8 Hz, 1H), 3.70 (dd, *J* = 12.9, 2.0 Hz, 1H), 3.54 (d, *J* = 12.9 Hz, 1H), 1.33 (s, 3H), 1.26 (s, 3H), 1.18 (s, 3H), 1.13 (s, 3H).

^{13}C NMR (101 MHz, Chloroform-*d*) δ 164.9, 131.1, 128.0, 108.8, 108.4, 101.4, 70.6, 70.2, 69.9, 64.7, 61.0, 26.3, 25.7, 25.1, 23.9.

HRMS (ESI) *m/z*: $[M + Na]^+$ Calcd for $C_{15}H_{22}O_7Na$ 337.1258; found: 337.1265.



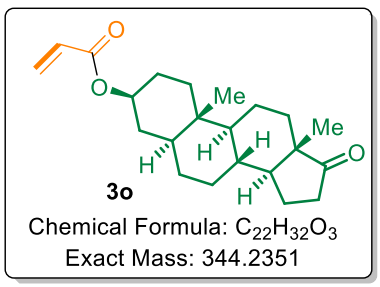
2n
Chemical Formula: $C_{30}H_{50}O_2$
Exact Mass: 442.3811

(3*S*,8*R*,9*S*,10*S*,13*R*,14*S*,17*R*)-10,13-dimethyl-17-((*R*)-6-methylheptan-2-yl)hexadecahydro-1*H*-cyclopenta[*a*]phenanthren-3-yl acrylate (2n): The compound **2n** was prepared according to the above procedure as a white solid (910.6 mg, 80%), m.p. = 91.6–93.2 ºC.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 6.30 (dd, *J* = 17.3, 1.6 Hz, 1H), 6.01 (dd, *J* = 17.3, 10.4 Hz, 1H), 5.70 (dd, *J* = 10.4, 1.6 Hz, 1H), 4.75 – 4.63 (m, 1H), 1.94 – 1.86 (m, 1H), 1.82 – 1.62 (m, 3H), 1.53 – 1.52 (m, 2H), 1.53 – 1.37 (m, 4H), 1.33 – 1.12 (m, 10H), 1.11 – 0.89 (m, 9H), 0.86 – 0.73 (m, 13H), 0.63 – 0.53 (m, 4H).

^{13}C NMR (101 MHz, Chloroform-*d*) δ 165.7, 130.0, 129.2, 73.9, 56.4, 56.3, 54.2, 44.7, 42.6, 40.0, 39.5, 36.8, 36.2, 35.8, 35.5, 34.0, 32.0, 28.6, 28.3, 28.0, 27.5, 24.2, 23.9, 22.8, 22.6, 21.2, 18.7, 12.3, 12.1.

HRMS (ESI) *m/z*: $[M + Na]^+$ Calcd for $C_{30}H_{50}O_2Na$ 465.3703; found: 465.3700.



3o
Chemical Formula: $C_{22}H_{32}O_3$
Exact Mass: 344.2351

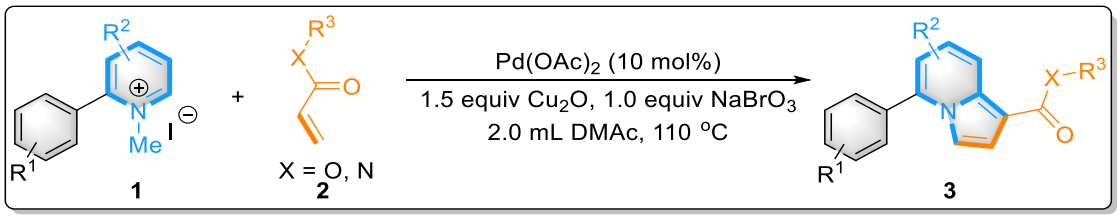
(3*S*,5*S*,8*R*,9*S*,10*S*,13*S*,14*S*)-10,13-dimethyl-17-oxohexadecahydro-1*H*-cyclopenta[*a*]phenanthren-3-yl acrylate (2o): The compound **2o** was prepared according to the above procedure as a white solid (651.9 mg, 55%), m.p. = 170.3–171.6 ^{o}C.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 6.38 (dt, *J* = 17.3, 1.4 Hz, 1H), 6.09 (ddd, *J* = 17.3, 10.5, 1.2 Hz, 1H), 5.80 (dt, *J* = 10.4, 1.4 Hz, 1H), 4.78 (ddt, *J* = 16.3, 11.2, 5.0 Hz, 1H), 2.49 – 2.38 (m, 1H), 2.13 – 2.01 (m, 1H), 1.98 – 1.73 (m, 5H), 1.71 – 1.62 (m, 2H), 1.61 – 1.37 (m, 4H), 1.37 – 1.18 (m, 6H), 1.12 – 0.93 (m, 2H), 0.86 (d, *J* = 2.4 Hz, 6H), 0.73 (td, *J* = 11.3, 3.9 Hz, 1H).

^{13}C NMR (101 MHz, Chloroform-*d*) δ 165.8, 130.2, 129.1, 73.7, 54.3, 51.4, 47.8, 44.7, 36.7, 35.9, 35.7, 35.0, 33.9, 31.5, 30.8, 28.3, 27.4, 21.8, 20.5, 13.8, 12.2.

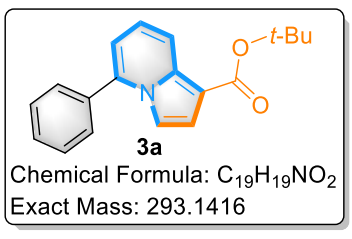
HRMS (ESI) *m/z*: $[M + Na]^+$ Calcd for $C_{22}H_{32}O_3Na$ 367.2244; found: 367.2241.

3. General procedure for the synthesis of indolizines



To a 15 mL Schlenk tube was charged with **1** (0.20 mmol), Pd(OAc) (4.5 mg, 0.02 mmol), **2** (0.8 mmol), $NaBrO_3$ (30.2 mg, 0.2 mmol, 1.0 equiv), Cu_2O (42.9 mg, 0.30 mmol, 1.5 equiv) and DMAc (dimethylacetamide, 2.0 mL) under an air atmosphere. The tube was evacuated and filled with Ar (1 atm), and stirred at rt for proper mixing of the reactants. Then the mixture heated at 110 ℃ (oil bath) with vigorous stirring for 24 h. After that, the reaction mixture was cooled to rt, diluted with ethyl acetate, washed with water, dried by anhydrous sodium sulfate and concentrated in *vacuo* to give the residue. The crude product was separated by column chromatography on silica gel (elution solvent: EtOAc/petroleum ether = 1/30 to 1/10) to afford the title compound **3**.

4. Spectroscopic data of the title compounds

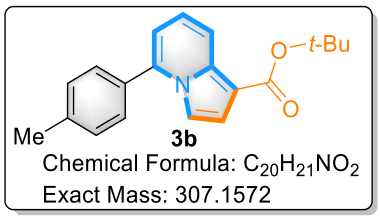


***tert*-butyl 5-phenylindolizine-1-carboxylate (3a):** The title compound **3a** was prepared according to the general procedure as a white oil (48.7 mg, 85%).

^{1}H NMR (600 MHz, Chloroform-*d*) δ 8.18 (d, *J* = 9.1 Hz, 1H), 7.60 – 7.47 (m, 5H), 7.25 (dd, *J* = 5.4, 2.0 Hz, 1H), 7.18 (d, *J* = 3.1 Hz, 1H), 7.10 (dd, *J* = 9.1, 6.8 Hz, 1H), 6.62 (d, *J* = 6.8 Hz, 1H), 1.64 (s, 9H).

^{13}C NMR (151 MHz, Chloroform-*d*) δ 164.7, 138.0, 136.3, 134.7, 129.5, 129.1, 128.7, 122.3, 118.9, 116.1, 113.0, 111.9, 106.1, 79.5, 28.7.

HRMS (ESI) *m/z*: $[M + H]^+$ Calcd for $C_{19}H_{20}NO_2$ 294.1489; found: 294.1490.

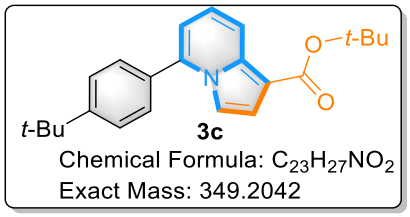


***tert*-butyl 5-(p-tolyl)indolizine-1-carboxylate (3b):** The title compound **3b** was prepared according to the general procedure as a yellow oil (49.0 mg, 80%).

^{1}H NMR (600 MHz, Chloroform-*d*) δ 8.16 (dd, *J* = 9.1, 1.2 Hz, 1H), 7.49 – 7.42 (m, 2H), 7.33 (d, *J* = 7.9 Hz, 2H), 7.26 (d, *J* = 1.9 Hz, 1H), 7.17 (d, *J* = 3.1 Hz, 1H), 7.09 (dd, *J* = 9.1, 6.8 Hz, 1H), 6.60 (dd, *J* = 6.8, 1.3 Hz, 1H), 2.45 (s, 3H), 1.64 (s, 9H).

^{13}C NMR (151 MHz, Chloroform-*d*) δ 164.8, 139.6, 138.2, 136.3, 131.9, 129.8, 128.5, 122.4, 118.6, 116.0, 112.9, 112.0, 106.0, 79.5, 28.7, 21.4.

HRMS (ESI) *m/z*: $[M + H]^+$ Calcd for $C_{20}H_{22}NO_2$ 308.1645; found: 308.1644.

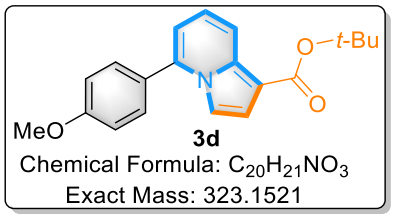


***tert*-butyl 5-(4-(*tert*-butyl)phenyl)indolizine-1-carboxylate (3c)**: The title compound **3c** was prepared according to the general procedure as a white solid (60.7 mg, 87%), m.p. = 159.9–160.8 °C.

^{1}H NMR (600 MHz, Chloroform-*d*) δ 8.20 – 8.13 (m, 1H), 7.57 – 7.47 (m, 4H), 7.30 (dd, *J* = 3.1, 0.6 Hz, 1H), 7.17 (d, *J* = 3.1 Hz, 1H), 7.09 (dd, *J* = 9.1, 6.8 Hz, 1H), 6.61 (dd, *J* = 6.8, 1.3 Hz, 1H), 1.64 (s, 9H), 1.39 (s, 9H).

^{13}C NMR (151 MHz, Chloroform-*d*) δ 164.8, 152.7, 138.2, 136.3, 131.8, 128.3, 126.0, 122.4, 118.6, 116.0, 112.9, 112.1, 106.0, 79.5, 34.9, 31.3, 28.7.

HRMS (ESI) *m/z*: $[M + H]^+$ Calcd for$C_{23}H_{28}NO_2$ 350.2115; found: 350.2104.



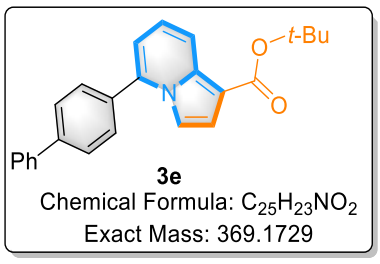
3d
Chemical Formula: $C_{20}H_{21}NO_3$
Exact Mass: 323.1521

***tert*-butyl 5-(4-methoxyphenyl)indolizine-1-carboxylate (3d):** The title compound **3d** was prepared according to the general procedure as a white solid (54.8 mg, 85%), m.p. = 108.8–109.1 °C.

^{1}H NMR (600 MHz, Chloroform-*d*) δ 8.16 (dt, *J* = 9.1, 0.9 Hz, 1H), 7.53 – 7.47 (m, 2H), 7.25 (s, 1H), 7.18 (d, *J* = 3.1 Hz, 1H), 7.09 (dd, *J* = 9.1, 6.8 Hz, 1H), 7.06 – 6.97 (m, 2H), 6.59 (dd, *J* = 6.8, 1.3 Hz, 1H), 3.89 (s, 3H), 1.64 (s, 9H).

^{13}C NMR (151 MHz, Chloroform-*d*) δ 164.8, 160.4, 137.9, 136.3, 130.0, 127.1, 122.4, 118.5, 116.0, 114.5, 112.8, 111.9, 106.0, 79.5, 55.4, 28.7.

HRMS (ESI) *m/z*: $[M + H]^+$ Calcd for $C_{20}H_{22}NO_3$ 324.1594; found: 324.1596.



3e
Chemical Formula: $C_{25}H_{23}NO_2$
Exact Mass: 369.1729

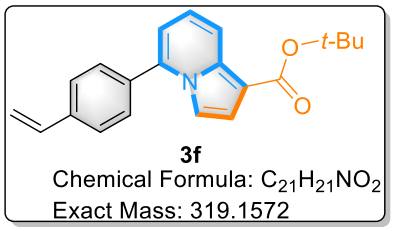
***tert*-butyl 5-([1,1'-biphenyl]-4-yl)indolizine-1-carboxylate (3e):** The title compound **3e** was prepared according to the general procedure as a light yellow solid (55.4 mg,

75%), m.p. = 160.1–161.2 °C.

^{1}H NMR (600 MHz, Chloroform-*d*) δ 8.20 (d, *J* = 9.2 Hz, 1H), 7.77 – 7.72 (m, 2H), 7.66 (dt, *J* = 6.6, 1.2 Hz, 4H), 7.52 – 7.47 (m, 2H), 7.44 – 7.38 (m, 1H), 7.36 – 7.32 (m, 1H), 7.21 (d, *J* = 3.1 Hz, 1H), 7.12 (dd, *J* = 9.1, 6.8 Hz, 1H), 6.67 (dd, *J* = 6.8, 1.3 Hz, 1H).

^{13}C NMR (151 MHz, Chloroform-*d*) δ 164.7, 142.4, 140.2, 137.8, 136.3, 133.6, 129.1, 129.0, 127.9, 127.8, 127.2, 122.3, 118.9, 116.2, 113.1, 112.0, 106.2, 79.6, 28.7.

HRMS (ESI) *m/z*: $[M + H]^+$ Calcd for $C_{25}H_{24}NO_2$ 370.1802; found: 370.1791.

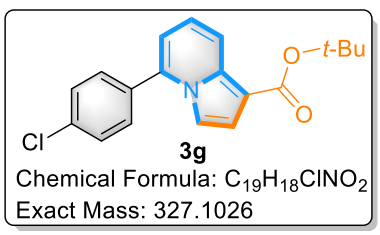


***tert*-butyl 5-(4-vinylphenyl)indolizine-1-carboxylate (3f):** The title compound **3f** was prepared according to the general procedure as a yellow oil (49.1 mg, 77%).

^{1}H NMR (600 MHz, Chloroform-*d*) δ 8.18 (dd, *J* = 9.1, 1.3 Hz, 1H), 7.60 – 7.52 (m, 4H), 7.28 (d, *J* = 3.1 Hz, 1H), 7.18 (d, *J* = 3.1 Hz, 1H), 7.10 (dd, *J* = 9.1, 6.8 Hz, 1H), 6.79 (dd, *J* = 17.6, 10.9 Hz, 1H), 6.62 (dd, *J* = 6.8, 1.3 Hz, 1H), 5.86 (dd, *J* = 17.6, 0.7 Hz, 1H), 5.37 (dd, *J* = 10.8, 0.7 Hz, 1H), 1.64 (s, 9H).

^{13}C NMR (151 MHz, Chloroform-*d*) δ 164.7, 138.8, 137.8, 136.3, 136.0, 134.0, 128.8, 126.9, 122.3, 118.9, 116.2, 115.4, 113.0, 111.9, 106.1, 79.6, 28.7.

HRMS (ESI) *m/z*: $[M + H]^+$ Calcd for $C_{21}H_{22}NO_2$ 320.1645; found: 320.1645.



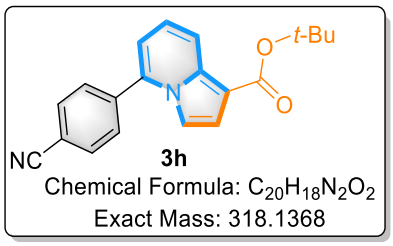
***tert*-butyl 5-(4-chlorophenyl)indolizine-1-carboxylate (3g):** The title compound **3g**

was prepared according to the general procedure as a yellow oil (53.0 mg, 81%).

^{1}H NMR (600 MHz, Chloroform-*d*) δ 8.20 (dd, *J* = 9.1, 1.2 Hz, 1H), 7.52 (d, *J* = 1.6 Hz, 4H), 7.22 – 7.17 (m, 2H), 7.09 (dd, *J* = 9.1, 6.8 Hz, 1H), 6.60 (dd, *J* = 6.8, 1.3 Hz, 1H), 1.64 (s, 9H).

^{13}C NMR (151 MHz, Chloroform-*d*) δ 164.6, 136.7, 136.2, 135.6, 133.1, 130.1, 129.5, 122.1, 119.2, 116.3, 113.2, 111.7, 106.4, 79.7, 28.7.

HRMS (ESI) *m/z*: $[M + H]^+$ Calcd for $C_{19}H_{19}ClNO_2$ 328.1099; found: 328.1101.

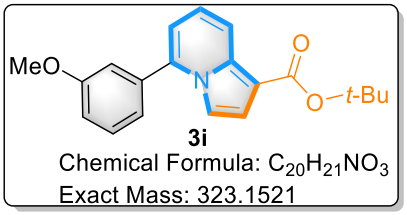


***tert*-butyl 5-(4-cyanophenyl)indolizine-1-carboxylate (3h):** The title compound **3h** was prepared according to the general procedure as a yellow oil (44.5 mg, 70%).

^{1}H NMR (600 MHz, Chloroform-*d*) δ 8.24 (dd, *J* = 9.2, 1.2 Hz, 1H), 7.87 – 7.82 (m, 2H), 7.76 – 7.71 (m, 2H), 7.23 – 7.17 (m, 2H), 7.11 (dd, *J* = 9.1, 6.8 Hz, 1H), 6.64 (dd, *J* = 6.8, 1.3 Hz, 1H), 1.64 (s, 9H).

^{13}C NMR (151 MHz, Chloroform-*d*) δ 164.4, 139.1, 136.1, 135.8, 133.0, 129.4, 121.9, 120.1, 118.2, 116.7, 113.8, 113.4, 111.5, 106.9, 79.9, 28.6.

HRMS (ESI) *m/z*: $[M + H]^+$ Calcd for $C_{20}H_{19}N_2O_2$ 319.1441; found: 319.1443.

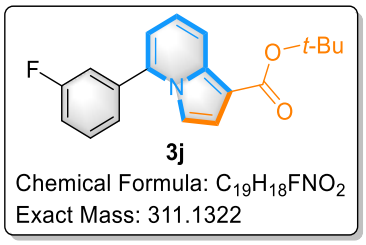


***tert*-butyl 5-(3-methoxyphenyl)indolizine-1-carboxylate (3i):** The title compound **3i** was prepared according to the general procedure as a yellow oil (53.0 mg, 82%).

^{1}H NMR (600 MHz, Chloroform-*d*) δ 8.18 (ddd, *J* = 9.1, 1.3, 0.6 Hz, 1H), 7.47 – 7.41 (m, 1H), 7.28 (dd, *J* = 3.1, 0.6 Hz, 1H), 7.18 (d, *J* = 3.1 Hz, 1H), 7.16 (ddd, *J* = 7.6, 1.6, 0.9 Hz, 1H), 7.12 – 7.08 (m, 2H), 7.04 (ddd, *J* = 8.4, 2.6, 1.0 Hz, 1H), 6.63 (dd, *J* = 6.8, 1.3 Hz, 1H), 3.85 (s, 3H), 1.64 (s, 9H).

^{13}C NMR (151 MHz, Chloroform-*d*) δ 164.7, 160.1, 137.9, 136.2, 136.0, 130.2, 122.2, 120.9, 118.9, 116.1, 115.1, 114.2, 112.9, 112.1, 106.1, 79.5, 55.4, 28.7.

HRMS (ESI) *m/z*: $[M + H]^+$ Calcd for $C_{20}H_{22}NO_3$ 324.1594; found: 324.1589.



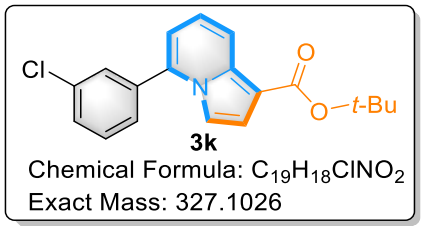
3j
Chemical Formula: $C_{19}H_{18}FNO_2$
Exact Mass: 311.1322

***tert*-butyl 5-(3-fluorophenyl)indolizine-1-carboxylate (3j):** The title compound **3j** was prepared according to the general procedure as a yellow oil (52.3 mg, 84%).

^{1}H NMR (600 MHz, Chloroform-*d*) δ 8.21 (d, *J* = 9.1 Hz, 1H), 7.51 (td, *J* = 8.0, 5.9 Hz, 1H), 7.42 – 7.36 (m, 1H), 7.30 (dt, *J* = 9.3, 2.1 Hz, 1H), 7.25 – 7.18 (m, 3H), 7.10 (dd, *J* = 9.1, 6.8 Hz, 1H), 6.63 (dd, *J* = 6.8, 1.3 Hz, 1H), 1.64 (s, 9H).

^{13}C NMR (151 MHz, Chloroform-*d*) δ 164.6, 163.0 (d, J_{C-F} = 247.64 Hz),136.6 (t, J_{C-F} = 9.06 Hz), 136.2, 130.9 (d, J_{C-F} = 7.55 Hz), 124.4 (d, J_{C-F} = 3.02 Hz), 122.1, 119.4, 116.6 (d, J_{C-F} = 21.14 Hz), 116.4, 115.9 (d, J_{C-F} = 21.14 Hz), 113.2, 111.8, 106.4, 79.7, 28.65.

HRMS (ESI) *m/z*: $[M + H]^+$ Calcd for $C_{19}H_{19}FNO_2$ 312.1394; found: 312.1395.



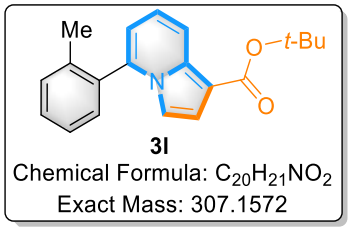
3k
Chemical Formula: $C_{19}H_{18}ClNO_2$
Exact Mass: 327.1026

***tert*-butyl 5-(3-chlorophenyl)indolizine-1-carboxylate (3k):** The title compound **3k** was prepared according to the general procedure as a yellow oil (52.3 mg, 80%).

^{1}H NMR (600 MHz, Chloroform-*d*) δ 8.24 – 8.18 (m, 1H), 7.57 (d, *J* = 1.5 Hz, 1H), 7.53 – 7.45 (m, 3H), 7.23 – 7.18 (m, 2H), 7.09 (dd, *J* = 9.1, 6.7 Hz, 1H), 6.61 (dt, *J* = 6.8, 1.0 Hz, 1H), 1.64 (s, 9H).

^{13}C NMR (151 MHz, Chloroform-*d*) δ 164.6, 136.4, 136.2, 135.2, 130.5, 129.7, 128.8, 126.8, 122.1, 119.4, 116.4, 113.3, 111.8, 106.5, 79.7, 28.7.

HRMS (ESI) *m/z* Calcd for $C_{19}H_{19}ClNO_2$ $(M + H)^+$: 328.1099, found: 328.1100.



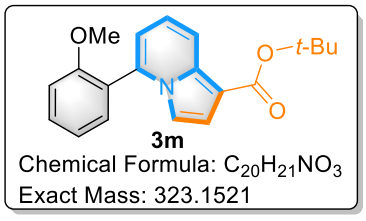
3l
Chemical Formula: $C_{20}H_{21}NO_2$
Exact Mass: 307.1572

***tert*-butyl 5-(o-tolyl)indolizine-1-carboxylate (3l):** The title compound **3l** was prepared according to the general procedure as a yellow solid (51.0 mg, 83%), m.p. = 122.4–123.8 ºC.

^{1}H NMR (600 MHz, Chloroform-*d*) δ 8.20 (dd, *J* = 9.1, 1.3 Hz, 1H), 7.42 (td, *J* = 7.5, 1.6 Hz, 1H), 7.38 – 7.27 (m, 3H), 7.16 (d, *J* = 3.0 Hz, 1H), 7.12 (dd, *J* = 9.1, 6.7 Hz, 1H), 6.70 (dd, *J* = 3.0, 0.6 Hz, 1H), 6.59 (dd, *J* = 6.7, 1.3 Hz, 1H), 2.06 (s, 3H), 1.64 (s, 9H).

^{13}C NMR (151 MHz, Chloroform-*d*) δ 164.7, 137.7, 137.2, 135.8, 134.0, 130.6, 129.9, 129.7, 126.5, 122.1, 118.7, 116.2, 112.8, 112.1, 106.0, 79.5, 28.7, 18.9.

HRMS (ESI) *m/z*: $[M + H]^+$ Calcd for $C_{20}H_{22}NO_2$ 308.1645; found: 308.1637.



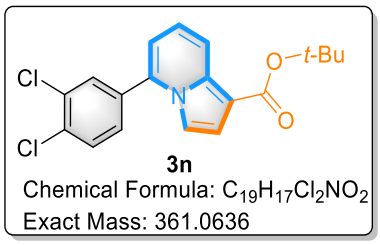
3m
Chemical Formula: $C_{20}H_{21}NO_3$
Exact Mass: 323.1521

***tert*-butyl 5-(2-methoxyphenyl)indolizine-1-carboxylate (3m):** The title compound **3m** was prepared according to the general procedure as a white oil (58.2 mg, 90%).

^{1}H NMR (600 MHz, Chloroform-*d*) δ 8.19 (dt, *J* = 9.1, 1.5 Hz, 1H), 7.50 (ddd, *J* = 8.3, 7.5, 1.8 Hz, 1H), 7.34 (dd, *J* = 7.4, 1.8 Hz, 1H), 7.17 – 7.13 (m, 1H), 7.13 – 7.06 (m, 2H), 7.04 (dd, *J* = 8.4, 1.0 Hz, 1H), 6.82 (d, *J* = 3.0 Hz, 1H), 6.63 (dd, *J* = 6.8, 1.3 Hz, 1H).

^{13}C NMR (151 MHz, Chloroform-*d*) δ 164.8, 157.4, 135.9, 135.7, 131.4, 131.2, 123.5, 121.9, 121.1, 118.7, 115.7, 113.4, 112.9, 111.1, 105.7, 79.4, 55.5, 28.7.

HRMS (ESI) *m/z*: $[M + H]^+$ Calcd for $C_{20}H_{22}NO_3$ 324.1594; found: 324.1591.

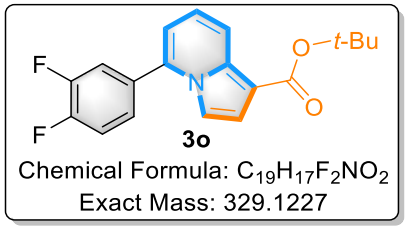


***tert*-butyl 5-(3,4-dichlorophenyl)indolizine-1-carboxylate (3n)**: The title compound **3n** was prepared according to the general procedure as a light yellow solid (41.2 mg, 57%), m.p. = 138.9–139.1 °C.

^{1}H NMR (600 MHz, Chloroform-*d*) δ 8.21 (dd, *J* = 9.1, 1.2 Hz, 1H), 7.69 (d, *J* = 2.1 Hz, 1H), 7.62 (d, *J* = 8.2 Hz, 1H), 7.44 (dd, *J* = 8.2, 2.1 Hz, 1H), 7.22 – 7.17 (m, 2H), 7.09 (dd, *J* = 9.1, 6.7 Hz, 1H), 6.61 (dd, *J* = 6.8, 1.3 Hz, 1H), 1.64 (s, 9H).

^{13}C NMR (151 MHz, Chloroform-*d*) δ 164.5, 136.1, 135.4, 134.5, 133.9, 133.6, 131.3, 130.7, 127.9, 121.9, 119.7, 116.6, 113.5, 111.6, 106.7, 79.8, 28.6.

HRMS (ESI) *m/z*: $[M + H]^+$ Calcd for $C_{19}H_{18}Cl_2NO_2$ 362.0709; found: 362.0714.

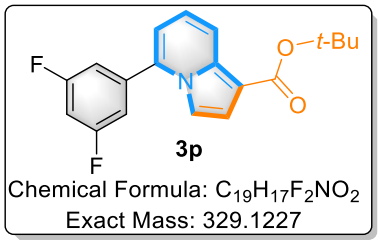


***tert*-butyl 5-(3,4-difluorophenyl)indolizine-1-carboxylate (3o):** The title compound **3o** was prepared according to the general procedure as a white viscous oil (45.4 mg, 69%).

^{1}H NMR (600 MHz, Chloroform-*d*) δ 8.21 (d, *J* = 8.6 Hz, 1H), 7.46 – 7.37 (m, 1H), 7.37 – 7.26 (m, 2H), 7.24 – 7.18 (m, 2H), 7.09 (dd, *J* = 9.1, 6.8 Hz, 1H), 6.60 (dd, *J* = 6.8, 1.3 Hz, 1H), 1.64 (s, 9H).

^{13}C NMR (151 MHz, Chloroform-*d*) δ 164.5, 150.8 (ddd, $J_{C\text{-}F}$ = 12.08 MHz, $J_{C\text{-}F}$ = 48.32 MHz, $J_{C\text{-}F}$ = 251.42 MHz), 136.2, 135.7, 131.5 (t, $J_{C\text{-}F}$ = 6.04 MHz), 125.2 (q, $J_{C\text{-}F}$ = 3.02 MHz), 122.0, 119.5, 118.20 (q, $J_{C\text{-}F}$ = 16.61 MHz), 116.5, 113.4, 111.5, 106.6, 79.7, 28.6.

HRMS (ESI) *m/z*: $[M + H]^+$ Calcd for $C_{19}H_{18}F_2NO_2$ 330.1300; found: 330.1305.

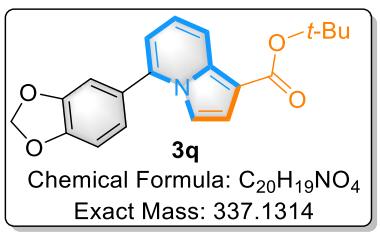


***tert*-butyl 5-(3,5-difluorophenyl)indolizine-1-carboxylate (3p):** The title compound **3p** was prepared according to the general procedure as a dark green oil (44.8 mg, 68%).

^{1}H NMR (600 MHz, Chloroform-*d*) δ 8.22 (d, *J* = 9.1 Hz, 1H), 7.23 (dd, *J* = 17.1, 3.1 Hz, 2H), 7.16 – 7.11 (m, 2H), 7.09 (dd, *J* = 9.1, 6.8 Hz, 1H), 6.97 (td, *J* = 8.8, 4.4 Hz, 1H), 6.63 (d, *J* = 6.8 Hz, 1H), 1.64 (s, 9H).

^{13}C NMR (151 MHz, Chloroform-*d*) δ 164.5, 163.5 (dd, $J_{C\text{-}F}$ = 13.59, 238.58 Hz), 137.6 (t, $J_{C\text{-}F}$ = 10.57 Hz), 136.1, 135.4 (t, $J_{C\text{-}F}$ = 3.02 Hz), 121.8, 119.9, 116.6, 113.4, 111.9 (dd, $J_{C\text{-}F}$ = 6.04, 15.10 Hz), 111.6, 106.8, 105.1 (t, $J_{C\text{-}F}$ = 25.67 Hz), 79.8, 28.6.

HRMS (ESI) *m/z*: $[M + H]^+$ Calcd for $C_{19}H_{18}F_2NO_2$ 330.1300; found: 330.1305.



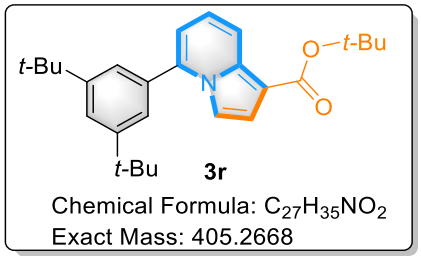
***tert*-butyl 5-(benzo[d][1,3]dioxol-5-yl)indolizine-1-carboxylate (3q):** The title

compound **3q** was prepared according to the general procedure as a yellow-brown oil (53.3 mg, 79%).

^{1}H NMR (600 MHz, Chloroform-*d*) δ 8.19 – 8.12 (m, 1H), 7.27 (dd, *J* = 3.1, 0.6 Hz, 1H), 7.18 (d, *J* = 3.1 Hz, 1H), 7.09 – 7.02 (m, 3H), 6.95 (d, *J* = 7.9 Hz, 1H), 6.58 (dd, *J* = 6.8, 1.3 Hz, 1H), 6.06 (s, 2H), 1.64 (s, 9H).

^{13}C NMR (151 MHz, Chloroform-*d*) δ 164.7, 148.6, 148.2, 137.6, 136.3, 128.4, 122.8, 122.3, 118.7, 116.1, 112.9, 112.0, 109.0, 109.0, 106.1, 101.6, 79.5, 28.7.

HRMS (ESI) *m/z*: $[M + H]^+$ Calcd for $C_{20}H_{20}NO_4$ 338.1387; found: 338.1378.

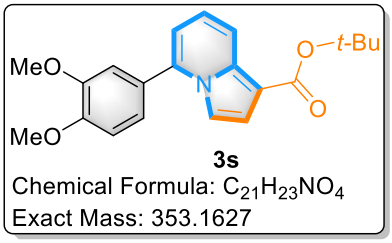


***tert*-butyl 5-(3,5-di-*tert*-butylphenyl)indolizine-1-carboxylate (3r):** The title compound **3r** was prepared according to the general procedure as a yellow oil (66.5 mg, 82%).

^{1}H NMR (600 MHz, Chloroform-*d*) δ 8.18 (d, *J* = 9.1 Hz, 1H), 7.57 – 7.53 (m, 1H), 7.40 (d, *J* = 1.7 Hz, 2H), 7.27 (dd, *J* = 3.1, 1.6 Hz, 1H), 7.19 (dd, *J* = 3.1, 1.5 Hz, 1H), 7.11 (ddd, *J* = 8.7, 6.8, 1.5 Hz, 1H), 6.65 (d, *J* = 6.7 Hz, 1H), 1.64 (d, *J* = 1.7 Hz, 9H), 1.37 (d, *J* = 1.8 Hz, 18H).

^{13}C NMR (151 MHz, Chloroform-*d*) δ 164.8, 151.7, 139.2, 136.4, 134.0, 123.4, 122.9, 122.4, 118.5, 116.0, 112.8, 112.1, 105.9, 79.5, 35.1, 31.4, 28.7.

HRMS (ESI) *m/z*: $[M + H]^+$ Calcd for $C_{27}H_{36}NO_2$ 406.2741; found: 406.2718.



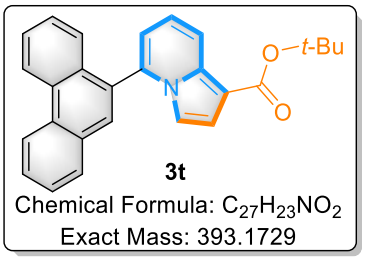
3s
Chemical Formula: $C_{21}H_{23}NO_4$
Exact Mass: 353.1627

***tert*-butyl 5-(3,4-dimethoxyphenyl)indolizine-1-carboxylate (3s):** The title compound **3s** was prepared according to the general procedure as a light yellow oil (59.3 mg, 84%).

^{1}H NMR (600 MHz, Chloroform-*d*) δ 8.17 (ddd, *J* = 9.0, 1.3, 0.6 Hz, 1H), 7.29 (dd, *J* = 3.1, 0.6 Hz, 1H), 7.19 (d, *J* = 3.1 Hz, 1H), 7.15 (dd, *J* = 8.2, 2.0 Hz, 1H), 7.12 – 7.08 (m, 1H), 7.08 – 7.06 (m, 1H), 7.01 (d, *J* = 8.2 Hz, 1H), 6.61 (dd, *J* = 6.8, 1.3 Hz, 1H), 3.96 (s, 3H), 3.90 (s, 3H), 1.64 (s, 9H).

^{13}C NMR (151 MHz, Chloroform-*d*) δ 164.7, 150.0, 149.3, 137.9, 136.3, 127.2, 122.3, 121.5, 118.6, 116.1, 112.8, 112.0, 111.6, 111.5, 106.0, 79.5, 56.1, 56.0, 28.7.

HRMS (ESI) *m/z*: $[M + H]^+$ Calcd for $C_{21}H_{24}NO_4$ 354.1700; found: 354.1690.



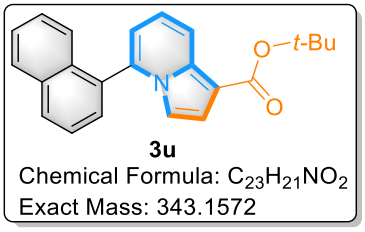
3t
Chemical Formula: $C_{27}H_{23}NO_2$
Exact Mass: 393.1729

***tert*-butyl 5-(phenanthren-9-yl)indolizine-1-carboxylate (3t):** The title compound **3t** was prepared according to the general procedure as a yellow oil (60.5 mg, 77%).

^{1}H NMR (600 MHz, Chloroform-*d*) δ 8.82 – 8.73 (m, 2H), 8.36 – 8.30 (m, 1H), 7.92 (dd, *J* = 7.9, 1.4 Hz, 1H), 7.87 (s, 1H), 7.75 (ddd, *J* = 8.3, 7.0, 1.4 Hz, 1H), 7.67 (dddd, *J* = 11.8, 8.0, 7.0, 1.2 Hz, 2H), 7.43 (ddd, *J* = 8.1, 6.9, 1.2 Hz, 1H), 7.30 (dd, *J* = 8.3, 1.3 Hz, 1H), 7.21 (dd, *J* = 9.2, 6.7 Hz, 1H), 7.09 (d, *J* = 3.1 Hz, 1H), 6.86 (dd, *J* = 6.6, 1.3 Hz, 1H), 6.66 – 6.62 (m, 1H), 1.65 (s, 9H).

^{13}C NMR (151 MHz, Chloroform-*d*) δ 164.8, 136.6, 135.9, 131.3, 131.0, 130.9, 130.6, 129.5, 129.4, 129.2, 127.9, 127.3, 127.3, 127.2, 125.9, 123.3, 122.8, 122.1, 119.3, 116.2, 114.1, 113.2, 106.1, 79.6, 28.7.

HRMS (ESI) *m/z*: $[M + H]^+$ Calcd for $C_{27}H_{24}NO_2$ 394.1802; found: 394.1794.

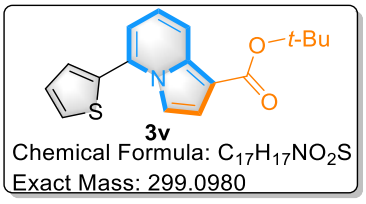


***tert*-butyl 5-(naphthalen-1-yl)indolizine-1-carboxylate (3u):** The title compound **3u** was prepared according to the general procedure as a yellow oil (48.04 mg, 70%).

^{1}H NMR (600 MHz, Chloroform-*d*) δ 8.22 (d, *J* = 9.1 Hz, 1H), 8.05 (s, 1H), 7.99 (d, *J* = 8.4 Hz, 1H), 7.92 (dd, *J* = 12.9, 7.6 Hz, 2H), 7.66 (dd, *J* = 8.4, 1.9 Hz, 1H), 7.62 – 7.54 (m, 2H), 7.29 (t, *J* = 2.4 Hz, 1H), 7.20 (t, *J* = 2.3 Hz, 1H), 7.14 (ddd, *J* = 8.8, 6.7, 1.6 Hz, 1H), 6.73 (d, *J* = 6.7 Hz, 1H), 1.65 (d, *J* = 1.7 Hz, 9H).

^{13}C NMR (151 MHz, Chloroform-*d*) δ 164.7, 138.0, 136.3, 133.6, 133.5, 132.1, 128.8, 128.4, 128.3, 127.9, 127.2, 126.9, 125.7, 122.4, 119.0, 116.2, 113.4, 112.0, 106.2, 79.6, 28.7.

HRMS (ESI) *m/z*: $[M + H]^+$ Calcd for $C_{23}H_{22}NO_2$ 344.1645; found: 344.1637.

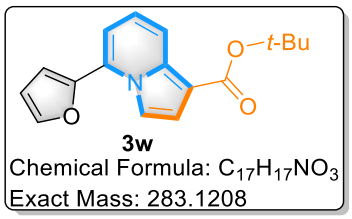


***tert*-butyl 5-(thiophen-2-yl)indolizine-1-carboxylate (3v):** The title compound **3v** was prepared according to the general procedure as a yellow oil (44.9 mg, 75%).

^{1}H NMR (600 MHz, Chloroform-*d*) δ 8.20 (dd, *J* = 9.1, 1.2 Hz, 1H), 7.60 (d, *J* = 3.1 Hz, 1H), 7.54 – 7.42 (m, 2H), 7.23 (d, *J* = 3.1 Hz, 1H), 7.22 – 7.17 (m, 1H), 7.06 (dd, *J* = 9.0, 6.8 Hz, 1H), 6.80 (dd, *J* = 6.8, 1.2 Hz, 1H), 1.64 (s, 9H).

^{13}C NMR (151 MHz, Chloroform-*d*) δ 164.6, 136.3, 135.4, 131.2, 128.0, 127.7, 127.1, 121.7, 119.4, 116.4, 114.5, 112.3, 106.6, 79.7, 28.7.

HRMS (ESI) *m/z*: $[M + H]^+$ Calcd for $C_{17}H_{18}NO_2S$ 300.1053; found: 300.1059.

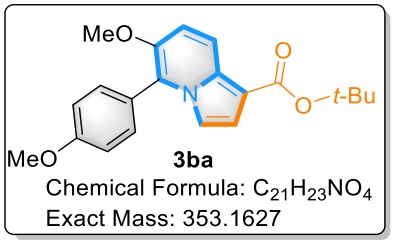


***tert*-butyl 5-(furan-2-yl)indolizine-1-carboxylate (3w):** The title compound **3w** was prepared according to the general procedure as a brown oil (38.5 mg, 68%).

^{1}H NMR (600 MHz, Chloroform-*d*) δ 8.21 (d, *J* = 8.9 Hz, 1H), 7.82 – 7.77 (m, 1H), 7.62 (s, 1H), 7.29 (dd, *J* = 3.1, 1.6 Hz, 1H), 7.11 – 7.01 (m, 2H), 6.92 (dd, *J* = 3.5, 1.6 Hz, 1H), 6.61 (dt, *J* = 3.5, 1.8 Hz, 1H), 1.64 (s, 9H).

^{13}C NMR (151 MHz, Chloroform-*d*) δ 164.6, 147.8, 143.3, 136.3, 128.2, 121.4, 119.4, 116.7, 112.9, 112.2, 111.7, 110.6, 106.3, 79.7, 28.7.

HRMS (ESI) *m/z*: $[M + H]^+$ Calcd for $C_{17}H_{18}NO_3$ 284.1281; found: 284.1282.

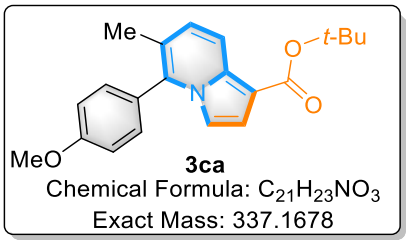


***tert*-butyl 6-methoxy-5-(4-methoxyphenyl)indolizine-1-carboxylate (3ba):** The title compound **3ba** was prepared according to the general procedure as a white oil (37.4 mg, 53%).

^{1}H NMR (600 MHz, Chloroform-*d*) δ 8.16 (d, *J* = 9.7 Hz, 1H), 7.44 – 7.33 (m, 2H), 7.13 – 7.05 (m, 4H), 6.94 (d, *J* = 3.0 Hz, 1H), 3.89 (s, 3H), 3.72 (s, 3H), 1.63 (s, 9H).

^{13}C NMR (151 MHz, Chloroform-*d*) δ 164.7, 160.2, 145.1, 133.3, 131.3, 126.2, 123.0, 119.1, 116.1, 114.9, 114.6, 112.3, 105.7, 79.4, 58.7, 55.4, 28.7.

HRMS (ESI) *m/z*: $[M + H]^+$ Calcd for $C_{21}H_{24}NO_4$ 354.1700; found: 354.1696.

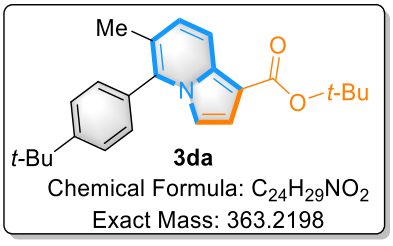


***tert*-butyl 5-(4-methoxyphenyl)-6-methylindolizine-1-carboxylate (3ca):** The title compound **3ca** was prepared according to the general procedure as a light yellow oil (41.1 mg, 61%).

^{1}H NMR (600 MHz, Chloroform-*d*) δ 8.08 (d, *J* = 9.1 Hz, 1H), 7.28 – 7.26 (m, 2H), 7.09 – 7.06 (m, 2H), 7.05 (d, *J* = 3.0 Hz, 1H), 7.00 (d, *J* = 9.2 Hz, 1H), 6.73 (dd, *J* = 3.0, 0.6 Hz, 1H), 3.90 (s, 3H), 2.08 (s, 3H), 1.62 (s, 9H).

^{13}C NMR (151 MHz, Chloroform-*d*) δ 164.9, 160.1, 135.2, 134.6, 131.0, 126.1, 125.8, 119.7, 118.3, 115.4, 114.9, 112.5, 105.5, 79.3, 55.4, 28.7, 18.1.

HRMS (ESI) *m/z*: $[M + H]^+$ Calcd for $C_{21}H_{24}NO_3$ 338.1751; found: 338.1739.

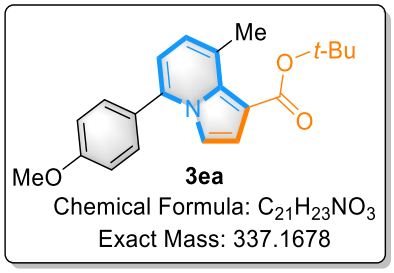


***tert*-butyl 5-(4-(tert-butyl)phenyl)-6-methylindolizine-1-carboxylate (3da):** The title compound **3da** was prepared according to the general procedure as a light yellow oil (36.3 mg, 50%).

^{1}H NMR (600 MHz, Chloroform-*d*) δ 8.08 (d, *J* = 9.2 Hz, 1H), 7.57 – 7.53 (m, 2H), 7.29 – 7.26 (m, 2H), 7.05 (d, *J* = 3.1 Hz, 1H), 7.01 (d, *J* = 9.2 Hz, 1H), 6.75 – 6.72 (m, 1H), 2.08 (s, 3H), 1.63 (s, 9H), 1.40 (s, 9H).

^{13}C NMR (151 MHz, Chloroform-*d*) δ 164.9, 152.3, 135.1, 134.9, 130.6, 129.3, 126.3, 126.1, 119.5, 118.3, 115.4, 112.7, 105.5, 79.3, 34.9, 31.3, 28.7, 18.1.

HRMS (ESI) *m/z*: $[M + H]^+$ Calcd for $C_{24}H_{30}NO_2$ 364.2271; found: 364.2269.

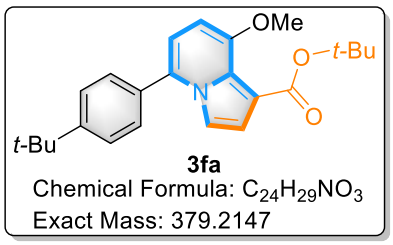


***tert*-butyl 5-(4-methoxyphenyl)-8-methylindolizine-1-carboxylate (3ea):** The title compound **3ea** was prepared according to the general procedure as a brown oil (54.6 mg, 81%).

^{1}H NMR (600 MHz, Chloroform-*d*) δ 7.47 – 7.41 (m, 2H), 7.21 (dd, *J* = 3.1, 0.9 Hz, 1H), 7.13 (dd, *J* = 3.1, 1.2 Hz, 1H), 7.04 – 6.99 (m, 2H), 6.81 (dq, *J* = 6.8, 1.1 Hz, 1H), 6.47 (d, *J* = 6.9 Hz, 1H), 3.88 (s, 3H), 2.76 (s, 3H), 1.60 (s, 9H).

^{13}C NMR (151 MHz, Chloroform-*d*) δ 164.7, 160.2, 135.7, 135.0, 130.2, 128.7, 127.4, 123.3, 117.3, 114.5, 112.9, 111.8, 108.1, 79.5, 55.4, 28.5, 22.0.

HRMS (ESI) *m/z*: $[M + H]^+$ Calcd for $C_{21}H_{24}NO_3$ 338.1751; found: 338.1734.

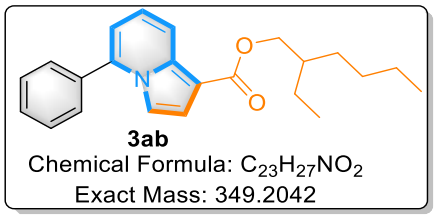


***tert*-butyl 5-(4-(*tert*-butyl)phenyl)-8-methoxyindolizine-1-carboxylate (3fa):** The title compound **3fa** was prepared according to the general procedure as a yellow oil (59.1 mg, 78%).

^{1}H NMR (600 MHz, Chloroform-*d*) δ 7.52 – 7.43 (m, 4H), 7.25 (s, 1H), 7.07 (d, *J* = 3.0 Hz, 1H), 6.49 (d, *J* = 7.6 Hz, 1H), 6.36 (d, *J* = 7.7 Hz, 1H), 3.98 (s, 3H), 1.61 (s, 9H), 1.38 (s, 9H).

^{13}C NMR (151 MHz, Chloroform-*d*) δ 164.6, 152.1, 151.4, 132.0, 131.4, 128.6, 127.4, 125.9, 116.5, 112.8, 112.5, 108.6, 99.2, 79.5, 55.5, 34.8, 31.3, 28.5.

HRMS (ESI) *m/z*: $[M + H]^+$ Calcd for $C_{24}H_{30}NO_3$ 380.2220; found: 380.2226.

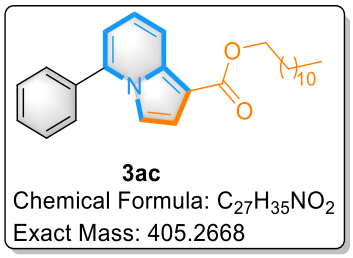


2-ethylhexyl 5-phenylindolizine-1-carboxylate (3ab): The title compound **3ab** was prepared according to the general procedure as a yellow oil (47.5 mg, 68%).

^{1}H NMR (600 MHz, Chloroform-*d*) δ 8.23 (dd, *J* = 9.1, 1.4 Hz, 1H), 7.60 – 7.56 (m, 2H), 7.55 – 7.48 (m, 3H), 7.28 – 7.20 (m, 2H), 7.14 (dd, *J* = 9.1, 6.8 Hz, 1H), 6.65 (dd, *J* = 6.8, 1.3 Hz, 1H), 4.30 – 4.22 (m, 2H), 1.75 (p, *J* = 6.1 Hz, 1H), 1.54 – 1.31 (m, 8H), 0.97 (t, *J* = 7.5 Hz, 3H), 0.91 (t, *J* = 7.1 Hz, 3H).

^{13}C NMR (151 MHz, Chloroform-*d*) δ 165.3, 138.1, 136.6, 134.7, 129.6, 129.2, 128.7, 122.6, 118.8, 116.0, 113.2, 112.2, 104.6, 66.0, 39.1, 30.8, 29.1, 24.2, 23.1, 14.1, 11.2.

HRMS (ESI) *m/z*: $[M + H]^+$ Calcd for $C_{23}H_{28}NO2$ 350.2115; found: 350.2102.



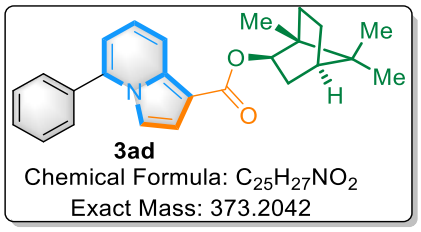
3ac
Chemical Formula: $C_{27}H_{35}NO_2$
Exact Mass: 405.2668

dodecyl 5-phenylindolizine-1-carboxylate (3ac): The title compound **3ac** was prepared according to the general procedure as a brown oil (50.2 mg, 62%).

^{1}H NMR (600 MHz, Chloroform-*d*) δ 8.23 (d, *J* = 9.1 Hz, 1H), 7.59 (d, *J* = 7.3 Hz, 2H), 7.52 (dq, *J* = 13.8, 7.1 Hz, 3H), 7.27 (d, *J* = 2.8 Hz, 1H), 7.22 (d, *J* = 3.0 Hz, 1H), 7.14 (t, *J* = 7.9 Hz, 1H), 6.65 (d, *J* = 6.8 Hz, 1H), 4.32 (t, *J* = 6.7 Hz, 2H), 1.79 (p, *J* = 7.0 Hz, 2H), 1.47 (p, *J* = 7.4 Hz, 2H), 1.36 (q, *J* = 7.1 Hz, 2H), 1.27 (d, *J* = 11.8 Hz, 15H), 0.88 (t, *J* = 6.8 Hz, 3H).

^{13}C NMR (151 MHz, Chloroform-*d*) δ 165.2, 138.1, 136.7, 134.7, 129.6, 129.2, 128.7, 122.6, 118.8, 115.9, 113.2, 112.2, 104.5, 63.8, 31.9, 29.7, 29.7, 29.6, 29.6, 29.4, 29.1, 26.2, 22.7, 14.13.

HRMS (ESI) *m/z*: $[M + H]^+$ Calcd for $C_{27}H_{36}NO_2$ 406.2741; found: 406.2727.



3ad
Chemical Formula: $C_{25}H_{27}NO_2$
Exact Mass: 373.2042

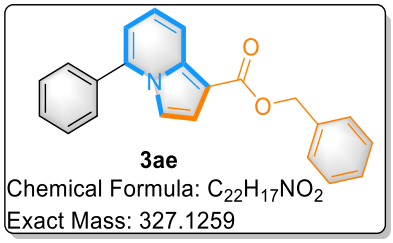
(1*R*,2*R*,4*R*)-1,7,7-trimethylbicyclo[2.2.1]heptan-2-yl 5-phenylindolizine-1-carboxylate (3ad): The title compound **3ad** was prepared according to the general procedure as a yellow oil (52.2 mg, 70%).

^{1}H NMR (600 MHz, Chloroform-*d*) δ 8.29 – 8.23 (m, 1H), 7.60 – 7.55 (m, 2H), 7.55 – 7.48 (m, 3H), 7.25 (d, *J* = 3.0 Hz, 1H), 7.17 (d, *J* = 3.1 Hz, 1H), 7.13 (dd, *J* = 9.1, 6.8 Hz, 1H), 6.64 (dd, *J* = 6.8, 1.3 Hz, 1H), 4.94 (dd, *J* = 6.6, 5.0 Hz, 1H), 1.96 – 1.92 (m, 2H), 1.79 (p, *J* = 2.0 Hz, 1H), 1.74 (tdt, *J* = 9.5, 3.5, 1.8 Hz, 1H), 1.61 (td, *J* = 12.2, 4.3

Hz, 1H), 1.27 (ddd, *J* = 17.1, 8.5, 3.9 Hz, 1H), 1.18 – 1.12 (m, 4H), 0.98 (s, 3H), 0.89 (s, 3H).

^{13}C NMR (151 MHz, Chloroform-*d*) δ 164.7, 138.1, 136.7, 134.7, 129.6, 129.2, 128.7, 122.6, 118.7, 115.9, 113.2, 112.1, 104.8, 80.1, 48.9, 47.0, 45.2, 39.3, 34.0, 27.2, 20.3, 20.2, 11.8.

HRMS (ESI) *m/z*: $[M + H]^+$ Calcd for $C_{25}H_{28}NO_2$ 374.2115; found: 374.2100.

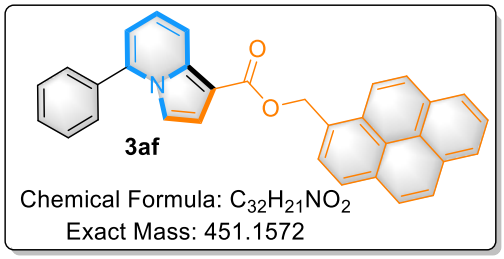


benzyl 5-phenylindolizine-1-carboxylate (3ae): The title compound **3ae** was prepared according to the general procedure as a brown oil (53.0mg, 81%).

^{1}H NMR (600 MHz, Chloroform-*d*) δ 8.24 (dd, *J* = 9.1, 1.2 Hz, 1H), 7.60 – 7.56 (m, 2H), 7.55 – 7.50 (m, 3H), 7.50 – 7.47 (m, 2H), 7.38 (t, *J* = 7.5 Hz, 2H), 7.34 – 7.30 (m, 1H), 7.26 (dd, *J* = 8.5, 2.7 Hz, 2H), 7.14 (dd, *J* = 9.1, 6.8 Hz, 1H), 6.66 (dd, *J* = 6.8, 1.3 Hz, 1H), 5.39 (s, 2H).

^{13}C NMR (151 MHz, Chloroform-*d*) δ 164.8, 138.2, 137.2, 137.0, 134.6, 129.6, 129.2, 128.7, 128.5, 128.0, 127.9, 122.9, 118.8, 116.1, 113.3, 112.4, 104.0, 65.3.

HRMS (ESI) *m/z*: $[M + H]^+$ Calcd for $C_{22}H_{18}NO_2$ 328.1332; found: 328.1326.



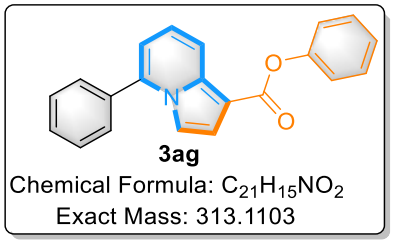
pyren-1-ylmethyl 5-phenylindolizine-1-carboxylate (3af): The title compound **3af** was prepared according to the general procedure as a light yellow solid (55.0 mg, 61%),

m.p. = 180.8–181.3 °C.

^{1}H NMR (600 MHz, Chloroform-*d*) δ 8.45 (d, *J* = 9.2 Hz, 1H), 8.23 – 8.15 (m, 6H), 8.09 – 8.05 (m, 2H), 8.01 (t, *J* = 7.6 Hz, 1H), 7.56 – 7.46 (m, 5H), 7.25 – 7.23 (m, 2H), 7.05 (dd, *J* = 9.1, 6.8 Hz, 1H), 6.61 (dd, *J* = 6.9, 1.3 Hz, 1H), 6.10 (s, 2H).

^{13}C NMR (151 MHz, Chloroform-*d*) δ 164.94, 138.19, 136.96, 134.54, 131.58, 131.27, 130.82, 130.07, 129.65, 129.59, 129.14, 128.67, 128.04, 127.66, 127.64, 127.46, 126.02, 125.38, 125.36, 124.71, 123.34, 122.98, 118.80, 116.19, 113.33, 112.41, 103.97, 64.03.

HRMS (ESI) *m/z*: $[M + H]^+$ Calcd for $C_{32}H_{22}NO_2$ 452.1645; found: 452.1631.

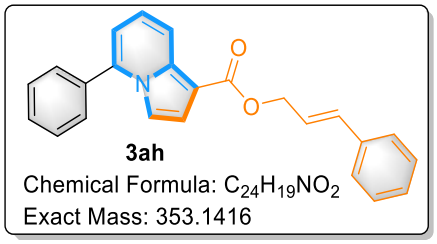


phenyl 5-phenylindolizine-1-carboxylate (3ag): The title compound **3ag** was prepared according to the general procedure as a brown oil (45.1 mg, 72%).

^{1}H NMR (600 MHz, Chloroform-*d*) δ 8.30 (d, *J* = 9.0 Hz, 1H), 7.63 – 7.60 (m, 2H), 7.59 – 7.51 (m, 3H), 7.45 – 7.41 (m, 2H), 7.39 – 7.33 (m, 2H), 7.28 – 7.24 (m, 3H), 7.24 – 7.19 (m, 1H), 6.73 (dd, *J* = 6.8, 1.3 Hz, 1H).

^{13}C NMR (151 MHz, Chloroform-*d*) δ 163.2, 151.2, 138.5, 137.7, 134.5, 129.7, 129.3, 129.2, 128.7, 125.3, 123.5, 122.2, 118.8, 116.4, 113.7, 112.8, 103.2.

HRMS (ESI) *m/z*: $[M + H]^+$ Calcd for $C_{21}H_{16}NO_2$ 314.1176; found: 314.1172.



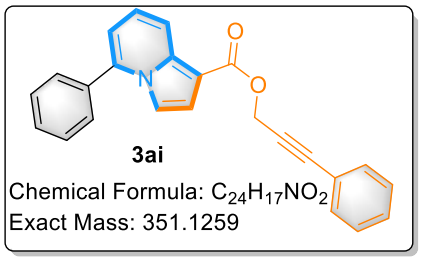
cinnamyl 5-phenylindolizine-1-carboxylate (3ah): The title compound **3ah** was

prepared according to the general procedure as a white solid (45.9 mg, 65%), m.p. = 111.8–112.1 °C.

^{1}H NMR (600 MHz, Chloroform-*d*) δ 8.29 – 8.22 (m, 1H), 7.61 – 7.58 (m, 2H), 7.57 – 7.49 (m, 3H), 7.46 – 7.41 (m, 2H), 7.33 (dd, *J* = 8.5, 6.9 Hz, 2H), 7.28 (dd, *J* = 3.1, 0.6 Hz, 1H), 7.27 – 7.24 (m, 2H), 7.16 (dd, *J* = 9.0, 6.8 Hz, 1H), 6.75 (dt, *J* = 15.9, 1.5 Hz, 1H), 6.67 (dd, *J* = 6.9, 1.3 Hz, 1H), 6.47 (dt, *J* = 15.9, 6.3 Hz, 1H), 5.00 (dd, *J* = 6.3, 1.4 Hz, 2H).

^{13}C NMR (151 MHz, Chloroform-*d*) δ 164.8, 138.2, 136.9, 136.6, 134.6, 133.4, 129.6, 129.2, 128.7, 128.6, 127.9, 126.6, 124.5, 122.9, 118.8, 116.0, 113.3, 112.4, 104.0, 64.2.

HRMS (ESI) *m/z*: $[M + H]^+$ Calcd for $C_{24}H_{20}NO_2$ 354.1489; found: 354.1473.

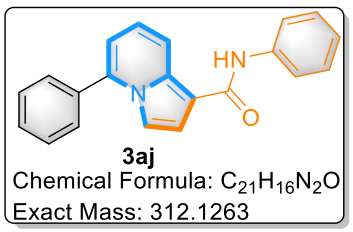


3-phenylprop-2-yn-1-yl 5-phenylindolizine-1-carboxylate (3ai): The title compound **3ai** was prepared according to the general procedure as a white solid (49.2 mg, 70%), m.p. = 102.5–103.6 °C.

^{1}H NMR (600 MHz, Chloroform-*d*) δ 8.28 (dd, *J* = 9.1, 1.2 Hz, 1H), 7.61 – 7.57 (m, 2H), 7.57 – 7.47 (m, 5H), 7.31 (qd, *J* = 4.9, 2.6 Hz, 3H), 7.30 – 7.26 (m, 2H), 7.18 (dd, *J* = 9.1, 6.8 Hz, 1H), 6.68 (dd, *J* = 6.9, 1.2 Hz, 1H), 5.17 (s, 2H).

^{13}C NMR (151 MHz, Chloroform-*d*) δ 164.1, 138.3, 137.2, 134.5, 132.0, 129.6, 129.2, 128.7, 128.6, 128.3, 123.2, 122.6, 118.8, 116.1, 113.5, 112.5, 103.4, 85.9, 84.2, 52.0.

HRMS (ESI) *m/z*: $[M + H]^+$ Calcd for $C_{24}H_{18}NO_2$ 352.1332; found: 352.1328.

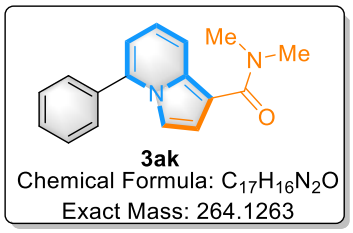


***N*,5-diphenylindolizine-1-carboxamide (3aj):** The title compound **3aj** was prepared according to the general procedure as a yellow oil (25.0 mg, 40%).

^{1}H NMR (600 MHz, Chloroform-*d*) δ 8.46 (d, *J* = 9.1 Hz, 1H), 7.66 (d, *J* = 8.0 Hz, 2H), 7.62 – 7.51 (m, 6H), 7.36 (t, *J* = 7.7 Hz, 2H), 7.32 (d, *J* = 3.1 Hz, 1H), 7.17 – 7.08 (m, 2H), 7.00 (d, *J* = 3.1 Hz, 1H), 6.67 (d, *J* = 6.7 Hz, 1H).

^{13}C NMR (151 MHz, Chloroform-*d*) δ 163.2, 138.7, 137.8, 136.5, 134.6, 129.6, 129.2, 129.0, 128.7, 123.6, 122.5, 119.9, 119.3, 113.5, 111.9, 111.7, 107.1.

HRMS (ESI) *m/z*: $[M + H]^+$ Calcd for $C_{21}H_{17}N_2O$ 313.1335; found: 313.1337.

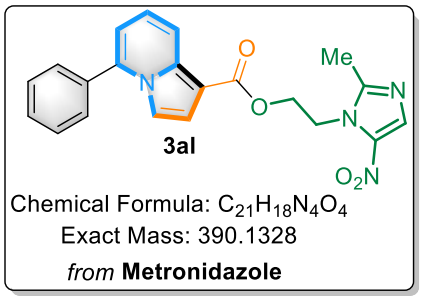


***N*,*N*-dimethyl-5-phenylindolizine-1-carboxamide (3ak):** The title compound **3ak** was prepared according to the general procedure as a yellow-brown oil (20.1 mg, 38%).

^{1}H NMR (600 MHz, Chloroform-*d*) δ 7.94 (ddd, *J* = 9.1, 1.3, 0.6 Hz, 1H), 7.61 – 7.57 (m, 2H), 7.55 – 7.48 (m, 3H), 7.27 – 7.26 (m, 1H), 7.00 (dd, *J* = 9.1, 6.7 Hz, 1H), 6.90 (d, *J* = 3.0 Hz, 1H), 6.56 (dd, *J* = 6.7, 1.3 Hz, 1H), 3.19 (s, 6H).

^{13}C NMR (151 MHz, Chloroform-*d*) δ 167.9, 137.3, 135.5, 135.0, 129.4, 129.1, 128.6, 120.7, 118.9, 114.3, 112.6, 110.8, 107.4, 29.7.

HRMS (ESI) *m/z*: $[M + H]^+$ Calcd for $C_{17}H_{17}N_2O$ 265.1335; found: 265.1332.

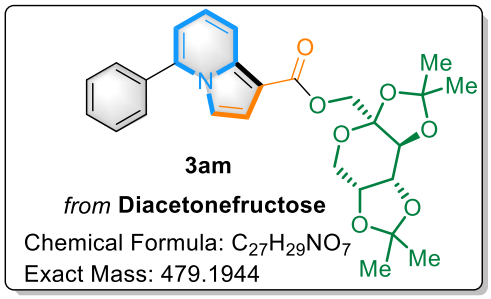


2-(2-methyl-5-nitro-1*H*-imidazol-1-yl)ethyl 5-phenylindolizine-1-carboxylate (3al): The title compound **3al** was prepared according to the general procedure as a yellow-brown oil (30.2 mg, 40%).

^{1}H NMR (600 MHz, Chloroform-*d*) δ 8.13 – 8.08 (m, 1H), 7.99 (s, 1H), 7.61 – 7.50 (m, 5H), 7.26 – 7.25 (m, 1H), 7.18 (dd, *J* = 9.0, 6.8 Hz, 1H), 7.05 (d, *J* = 3.2 Hz, 1H), 6.70 (dd, *J* = 6.8, 1.3 Hz, 1H), 4.75 – 4.65 (m, 4H), 2.48 (s, 3H).

^{13}C NMR (151 MHz, Chloroform-*d*) δ 164.0, 151.2, 138.5, 137.4, 134.3, 133.3, 129.8, 129.2, 128.7, 123.6, 118.4, 115.6, 113.7, 112.8, 102.6, 61.3, 45.9, 14.4.

HRMS (ESI) *m/z*: $[M + H]^+$ Calcd for $C_{21}H_{19}N_4O_4$ 391.1401; found: 391.1405.



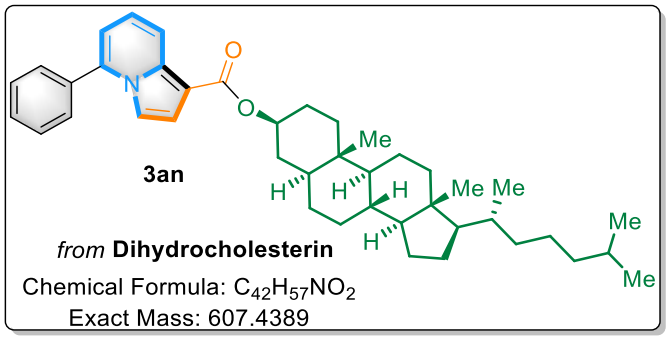
((3a*S*,5a*R*,8a*R*,8b*S*)-2,2,7,7-tetramethyltetrahydro-3a*H*-bis([1,3]dioxolo)[4,5-b:4',5'-d]pyran-3a-yl)methyl 5-phenylindolizine-1-carboxylate (3am): The title compound **3am** was prepared according to the general procedure as a light yellow solid (60.4 mg, 63%), m.p. = 142.6–143.1 ºC.

^{1}H NMR (600 MHz, Chloroform-*d*) δ 8.31 (dd, *J* = 9.2, 1.2 Hz, 1H), 7.61 – 7.57 (m, 2H), 7.56 – 7.48 (m, 3H), 7.26 (d, *J* = 3.5 Hz, 2H), 7.21 (d, *J* = 3.1 Hz, 1H), 7.16 (dd, *J* = 9.1, 6.8 Hz, 1H), 6.67 (dd, *J* = 6.8, 1.3 Hz, 1H), 4.69 (d, *J* = 11.7 Hz, 1H), 4.66 (dd,

J = 7.9, 2.6 Hz, 1H), 4.53 (d, *J* = 2.6 Hz, 1H), 4.36 (d, *J* = 11.7 Hz, 1H), 4.27 (dd, *J* = 8.0, 1.7 Hz, 1H), 3.98 (dd, *J* = 13.0, 1.9 Hz, 1H), 3.84 – 3.79 (m, 1H), 1.55 (s, 3H), 1.52 (s, 3H), 1.40 (s, 3H), 1.36 (s, 3H).

^{13}C NMR (151 MHz, Chloroform-*d*) δ 164.0, 138.2, 134.5, 129.6, 129.2, 128.7, 123.0, 118.9, 115.7, 113.5, 112.3, 109.2, 108.8, 103.5, 102.1, 71.0, 70.5, 70.3, 63.6, 61.3, 26.6, 26.0, 25.6, 24.1.

HRMS (ESI) *m/z*: $[M + H]^+$ Calcd for $C_{27}H_{30}NO_7$ 480.2017; found: 480.2020.

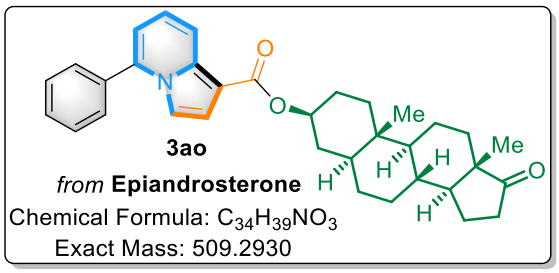


(3*S*,8*R*,9*S*,10*S*,13*R*,14*S*,17)-10,13-dimethyl-17-((*R*)-6-methylheptan-2-yl)hexadecahydro-1*H*-cyclopenta[*a*]phenanthren-3-yl 5-phenylindolizine-1-carboxylate (3an): The title compound **3an** was prepared according to the general procedure as a light yellow solid (60.8 mg, 55%), m.p. = 200.1–200.6 ºC.

^{1}H NMR (600 MHz, Chloroform-*d*) δ 8.22 (dd, *J* = 9.2, 1.3 Hz, 1H), 7.59 – 7.48 (m, 5H), 7.27 – 7.24 (m, 1H), 7.21 (d, *J* = 3.1 Hz, 1H), 7.12 (dd, *J* = 9.1, 6.8 Hz, 1H), 6.63 (dd, *J* = 6.8, 1.3 Hz, 1H), 4.97 (tt, *J* = 11.3, 4.9 Hz, 1H), 1.99 (tt, *J* = 12.7, 3.7 Hz, 2H), 1.86 – 1.75 (m, 3H), 1.72 – 1.63 (m, 2H), 1.62 – 1.48 (m, 5H), 1.39 – 1.23 (m, 9H), 1.18 – 1.07 (m, 6H), 1.05 – 0.96 (m, 3H), 0.91 (d, *J* = 6.6 Hz, 3H), 0.89 (s, 3H), 0.87 (d, *J* = 2.8 Hz, 3H), 0.86 (d, *J* = 2.8 Hz, 3H), 0.73 – 0.64 (m, 4H).

^{13}C NMR (151 MHz, Chloroform-*d*) δ 164.8, 138.1, 136.6, 134.7, 129.5, 129.1, 128.7, 122.5, 118.9, 116.0, 113.1, 112.1, 104.9, 72.8, 56.5, 56.3, 54.3, 44.9 42.6, 40.1, 39.5, 37.0, 36.2, 35.8, 35.6, 35.6, 34.6, 32.1, 28.7, 28.3, 28.0, 24.3, 23.9, 22.9, 22.6, 21.3, 18.7, 12.4, 12.1.

HRMS (ESI) *m/z*: $[M + H]^+$ Calcd for $C_{42}H_{58}NO_2$ 608.4462; found: 608.4452.



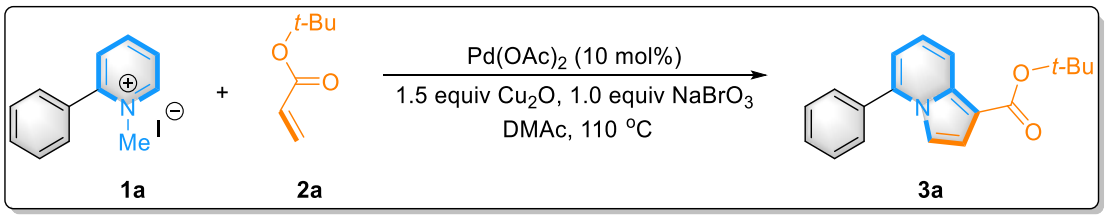
(3*S*,5S,8*R*,9*S*,10*S*,13*S*,14*S*)-10,13-dimethyl-17-oxohexadecahydro-1*H*-cyclopenta[a]phenanthren-3-yl 5-phenylindolizine-1-carboxylate (3ao): The title compound **3ao** was prepared according to the general procedure as a light yellow solid (48.9 mg, 48%), m.p. = 204.6–204.8 ºC.

^{1}H NMR (600 MHz, Chloroform-*d*) δ 8.22 (dd, *J* = 9.1, 1.3 Hz, 1H), 7.62 – 7.48 (m, 5H), 7.26 (d, *J* = 3.0 Hz, 1H), 7.21 (d, *J* = 3.1 Hz, 1H), 7.13 (dd, *J* = 9.0, 6.8 Hz, 1H), 6.64 (dd, *J* = 6.8, 1.3 Hz, 1H), 4.97 (tt, *J* = 11.3, 4.9 Hz, 1H), 2.49 – 2.38 (m, 1H), 2.08 (dt, *J* = 19.2, 9.1 Hz, 1H), 2.04 – 1.99 (m, 1H), 1.98 – 1.91 (m, 1H), 1.85 – 1.77 (m, 4H), 1.73 – 1.66 (m, 2H), 1.60 – 1.47 (m, 3H), 1.42 – 1.23 (m, 6H), 1.18 – 1.10 (m, 1H), 1.06 – 0.97 (m, 1H), 0.92 (s, 3H), 0.87 (s, 3H), 0.81 – 0.73 (m, 1H).

^{13}C NMR (151 MHz, Chloroform-*d*) δ 164.7, 138.1, 136.6, 134.6, 129.6, 129.1, 128.7, 122.6, 118.9, 116.0, 113.2, 112.2, 72.6, 54.4, 51.4, 47.8, 44.8, 36.9, 35.9, 35.8, 35.1, 34.5, 31.6, 30.9, 28.4, 28.0, 21.8, 20.5, 13.8, 12.4.

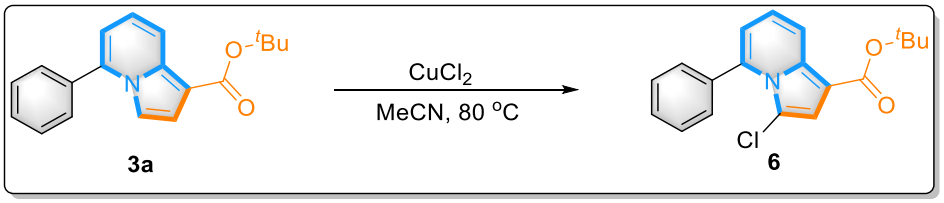
HRMS (ESI) *m/z*: $[M + H]^+$ Calcd for $C_{34}H_{40}NO_3$ 510.3003; found: 510.3004.

5. Gram-scale synthesis



To a 150 mL Schlenk tube was charged with **1a** (1.2 g, 4.04 mmol), Pd(OAc) (89.8 mg, 0.4 mmol), **2a** (2.07 g, 16.2 mmol), $NaBrO_3$ (610.0 mg, 4.04 mmol, 1.0 equiv), Cu_2O (866.6 mg, 6.06 mmol, 1.5 equiv) and DMAc (dimethylacetamide, 40.0 mL) under an air atmosphere. The tube was evacuated and filled with Ar (1 atm), and stirred at rt for 1 min for proper mixing of the reactants. Then the mixture heated at 110 ℃ (oil bath) with vigorous stirring for 24 h. After that, the reaction mixture was cooled to rt, diluted with ethyl acetate, washed with water, dried by anhydrous sodium sulfate and concentrated in *vacuo* to give the residue. The crude product was separated by column chromatography on silica gel (elution solvent: EtOAc/petroleum ether = 1/20) to afford the title compound **3a** (924 mg, 78%).

6. Synthesis of compound 6



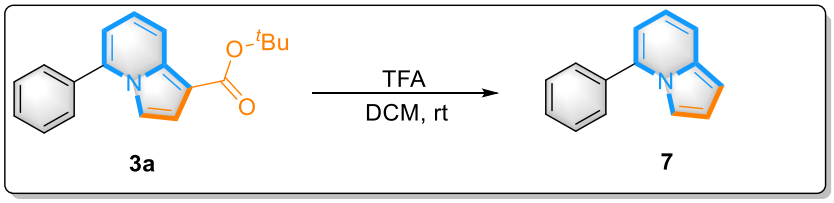
Synthesis method:[2] Indolizine **3a** (58.6 mg, 0.2 mmol) and $CuCl_2$ (40.3 mg, 0.3 mmol) were added to a flask. Then MeCN (1 mL) was added through a syringe and the mixture was stirred at 80 °C for 24 hours under air atmosphere. After the reaction was complete, the reaction was quenched with saturated NH_4Cl solution and extracted with EtOAc. The combined organic layers were washed with water, brine, then dried over Na_2SO_4. The solvents were evaporated under reduced pressure, and the residue was subjected to flash column chromatography with ethyl acetate/petroleum ether (1 : 20) as eluent to obtain the desired product **6** as a solid. (38.5 mg, 62% yield), m.p. = 179.8–180.1 °C.

^{1}H NMR (600 MHz, Chloroform-*d*) δ 8.29 (dd, *J* = 9.1, 1.4 Hz, 1H), 7.49 – 7.37 (m, 5H), 7.11 (s, 1H), 7.06 (dd, *J* = 9.1, 6.8 Hz, 1H), 6.60 (dd, *J* = 6.8, 1.4 Hz, 1H), 1.62 (s, 9H).

^{13}C NMR (151 MHz, Chloroform-*d*) δ 163.8, 137.7, 136.7, 135.0, 129.8, 128.9, 127.5, 121.5, 119.0, 117.0, 116.6, 110.1, 105.6, 80.0, 28.6.

HRMS (ESI) *m/z*: $[M + H]^+$ Calcd for $C_{19}H_{19}ClNO_2$ 328.1099; found: 328.1092.

7. Synthesis of compound 7



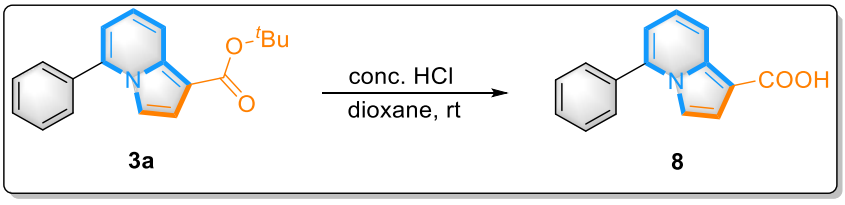
Synthesis method: A solution of indolizine **3a** (58.6 mg, 0.2 mmol) and TFA (15 μL, 0.2 mmol) in DCM (2 mL) was stirred at rt for 19 h. After the reaction was complete, the reaction mixture was concentrated to give the crude. The crude product was purified by flash column chromatography on silica gel (EtOAc/Petroleum = 50/1) to obtain the desired compound **7** as a dark green oil (18.5 mg, 48%).

^{1}H NMR (600 MHz, Chloroform-*d*) δ 7.65 – 7.61 (m, 2H), 7.53 – 7.45 (m, 3H), 7.39 (dt, *J* = 9.0, 0.9 Hz, 1H), 7.37 – 7.34 (m, 1H), 6.78 – 6.72 (m, 2H), 6.52 (dd, *J* = 3.9, 1.4 Hz, 1H), 6.41 (dd, *J* = 6.6, 1.3 Hz, 1H).

^{13}C NMR (151 MHz, Chloroform-*d*) δ 136.98, 135.68, 134.00, 129.07, 128.98, 128.54, 118.29, 117.31, 113.27, 111.15, 111.11, 99.54.

HRMS (ESI) *m/z*: $[M + H]^+$ Calcd for $C_{14}H_{12}N$ 194.0964; found: 194.0967.

8. Synthesis of compound 8



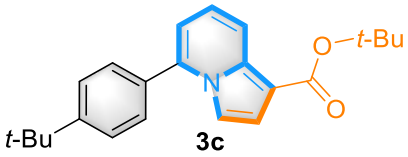
Synthesis method: A solution of indolizine **3a** (58.6 mg, 0.2 mmol) and conc. HCl (13 μL, 0.4 mmol) in DCM (2 mL) was stirred at rt for 24 h. After the reaction was complete, the reaction mixture was concentrated to give the crude. The crude product was purified by flash column chromatography on silica gel (EtOAc/Petroleum = 1/1) to obtain the desired compound **8** as a black oil (35.5 mg, 75%).

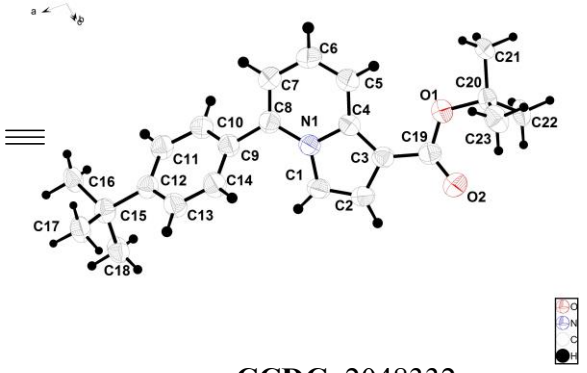
^{1}H NMR (600 MHz, Chloroform-*d*) δ 8.29 (d, *J* = 9.0 Hz, 1H), 7.60 (dd, *J* = 7.9, 1.7 Hz, 2H), 7.58 – 7.49 (m, 3H), 7.31 – 7.27 (m, 2H), 7.23 – 7.18 (m, 1H), 6.71 (dd, *J* = 6.8, 1.3 Hz, 1H).

^{13}C NMR (151 MHz, Chloroform-*d*) δ 168.9, 138.4, 134.5, 129.7, 129.2, 128.7, 123.4, 118.9, 116.6, 113.6, 112.8, 103.2.

HRMS (ESI) *m/z*: $[M + H]^+$ Calcd for $C_{15}H_{12}NO_2$ 238.0863; found: 238.0857.

9. X-ray crystallographic data of compound 3c





CCDC: 2048332

Figure S1 Molecular Structure of compound **3c**

Table S1 Crystal data and structure refinement for 3c

Identification code	**3c**
Empirical formula	$C_{23}H_{27}NO_2$
Formula weight	349.45
Temperature/K	293.15
Crystal system	monoclinic
Space group	$P2_1/c$
a/Å	17.6069(3)
b/Å	11.3574(2)
c/Å	10.3434(2)
α/°	90
β/°	102.098(2)
γ/°	90
Volume/Å^3	2022.42(6)
Z	4
ρ_{calc}g/cm^3	1.148
μ/mm^{-1}	0.567
F(000)	752.0
Radiation	Cu Kα (λ = 1.54184)
2Θ range for data collection/°	5.134 to 148.182
Index ranges	$-21 \leq h \leq 21$, $-13 \leq k \leq 12$, $-12 \leq l \leq 10$
Reflections collected	10931
Independent reflections	3976 [R_{int} = 0.0346, R_{sigma} = 0.0357]
Data/restraints/parameters	3976/0/242

Table S1 continued	
Goodness-of-fit on F^2	1.040
Final R indexes [I>=2σ (I)]	R_1 = 0.0471, wR_2 = 0.1398
Final R indexes [all data]	R_1 = 0.0543, wR_2 = 0.1465
Largest diff. peak/hole / e $Å^{-3}$	0.16/-0.17

Table S2 Bond lengths for 3c

Atom	Atom	Length/Å	Atom	Atom	Length/Å
O1	C19	1.3488(16)	C8	C9	1.4850(18)
O1	C20	1.4716(16)	C9	C10	1.385(2)
O2	C19	1.2084(17)	C9	C14	1.392(2)
N1	C1	1.3856(16)	C10	C11	1.3842(19)
N1	C4	1.4028(16)	C11	C12	1.396(2)
N1	C8	1.3907(17)	C12	C13	1.395(2)
C1	C2	1.359(2)	C12	C15	1.5315(18)
C2	C3	1.4121(18)	C13	C14	1.379(2)
C3	C4	1.4029(18)	C15	C16	1.524(2)
C3	C19	1.4516(18)	C15	C17	1.530(2)
C4	C5	1.4080(19)	C15	C18	1.524(2)
C5	C6	1.352(2)	C20	C21	1.519(3)
C6	C7	1.414(2)	C20	C22	1.511(2)
C7	C8	1.355(2)	C20	C23	1.504(3)

Table S3 Bond Angles for 3c

Atom	Atom	Atom	Angle/	Atom	Atom	Atom	Angle/
C19	O1	C20	122.22(11)	C10	C11	C12	121.47(13)
C1	N1	C4	108.65(11)	C11	C12	C15	122.42(12)
C1	N1	C8	129.35(11)	C13	C12	C11	116.79(12)
C8	N1	C4	121.94(11)	C13	C12	C15	120.75(12)
C2	C1	N1	108.41(12)	C14	C13	C12	121.81(13)
C1	C2	C3	108.92(12)	C13	C14	C9	120.90(13)
C2	C3	C19	124.29(12)	C12	C15	C17	110.40(12)
C4	C3	C2	107.07(12)	C16	C15	C12	111.81(13)
C4	C3	C19	128.62(12)	C16	C15	C17	107.69(14)
N1	C4	C5	118.14(12)	C18	C15	C12	108.09(12)
C3	C4	N1	106.94(11)	C18	C15	C16	110.64(17)
C3	C4	C5	134.92(12)	C18	C15	C17	108.16(16)
C6	C5	C4	120.04(13)	O1	C19	C3	112.18(11)
C5	C6	C7	120.34(14)	O2	C19	O1	123.76(13)
C8	C7	C6	121.42(14)	O2	C19	C3	124.05(13)
N1	C8	C9	118.83(12)	O1	C20	C21	101.83(12)

Table S3 continued							
C7	C8	N1	118.09(12)	O1	C20	C22	110.34(13)
C7	C8	C9	123.07(13)	O1	C20	C23	109.56(13)
C10	C9	C8	119.99(12)	C22	C20	C21	110.34(16)
C10	C9	C14	117.89(13)	C23	C20	C21	110.48(17)
C14	C9	C8	122.01(12)	C23	C20	C22	113.66(18)
C9	C10	C11	121.15(13)				

Table S4 Torsion Angles for 3c

A	B	C	D	Angle/°	A	B	C	D	Angle/°
N1	C1	C2	C3	-0.34(16)	C8	N1	C1	C2	178.16(13)
N1	C4	C5	C6	-1.1(2)	C8	N1	C4	C3	-178.46(12)
N1	C8	C9	C10	-129.62(14)	C8	N1	C4	C5	1.07(19)
N1	C8	C9	C14	54.18(19)	C8	C9	C10	C11	-176.20(13)
C1	N1	C4	C3	-0.77(14)	C8	C9	C14	C13	176.55(14)
C1	N1	C4	C5	178.76(13)	C9	C10	C11	C12	-0.4(2)
C1	N1	C8	C7	-177.09(14)	C10	C9	C14	C13	0.3(2)
C1	N1	C8	C9	3.8(2)	C10	C11	C12	C13	0.2(2)
C1	C2	C3	C4	-0.14(16)	C10	C11	C12	C15	-177.51(13)
C1	C2	C3	C19	178.43(13)	C11	C12	C13	C14	0.3(2)
C2	C3	C4	N1	0.55(15)	C11	C12	C15	C16	-20.3(2)
C2	C3	C4	C5	-178.86(16)	C11	C12	C15	C17	-140.17(15)
C2	C3	C19	O1	169.77(12)	C11	C12	C15	C18	101.71(19)
C2	C3	C19	O2	-10.7(2)	C12	C13	C14	C9	-0.5(3)
C3	C4	C5	C6	178.29(16)	C13	C12	C15	C16	162.11(16)
C4	N1	C1	C2	0.70(15)	C13	C12	C15	C17	42.24(19)
C4	N1	C8	C7	0.1(2)	C13	C12	C15	C18	-75.9(2)

10. Computational Studies

All the calculations were performed using the Gaussian 09 programs.[3] All of the structures were fully optimized with the B3LYP[4-5] method and Ahlrichs' split-valence def2-SVP basis set.[6] Grimmes's DFT-D3 dispersion correction was used to describe the van der waals interaction.[7] Vibrational frequency calculations were performed to ensure that a transition state has only one imaginary frequency and a local minimum has no imaginary frequency. Transition states connecting relevant minima were further examined by running intrinsic reaction coordinate (IRC) calculations.

Cartesian Coordinates And Energy

1a

C	-2.01748	0.18613	-0.59076
C	-0.62034	0.20849	-0.55415
C	0.04890	1.25461	0.09905
C	-0.69032	2.28971	0.70130
C	-2.08475	2.26366	0.65557
C	-2.75000	1.21159	0.01465
H	-2.53436	-0.63500	-1.09341
H	-0.04297	-0.59117	-1.02489
H	-0.16037	3.11886	1.18070
H	-2.65479	3.07397	1.11638
H	-3.84230	1.19423	-0.01661
C	1.53092	1.33337	0.09987
C	2.24408	1.47306	-1.07870
C	3.63851	1.68445	-1.05096

H	1.69427	1.45583	-2.01985
C	3.51070	1.74168	1.34509
C	4.26592	1.84969	0.16724
H	4.19880	1.77236	-1.98409
H	3.97571	1.74740	2.32772
H	5.32311	2.10345	0.24683
N	2.21292	1.32499	1.29469
C	1.53723	1.14793	2.58351
H	1.35399	2.14633	3.01730
H	0.59872	0.60210	2.45034
H	2.19891	0.58179	3.25265
I	2.90070	4.59498	2.02063

2a

C	-0.02359	0.38339	0.04411
O	1.15233	0.09007	0.04629
O	-0.51062	1.63443	0.04152
C	0.35496	2.81785	0.04147
C	1.21252	2.83648	-1.22728
H	1.76791	3.78562	-1.28291
H	1.92854	2.00525	-1.23104
H	0.57209	2.75876	-2.11962
C	-0.64771	3.97168	0.03733
H	-1.29223	3.92457	0.92819

H	-0.11854	4.93665	0.03704
H	-1.28818	3.92183	-0.85631
C	1.20722	2.84069	1.31378
H	1.76230	3.79004	1.36868
H	0.56286	2.76589	2.20357
H	1.92313	2.00944	1.32343
C	-1.10172	-0.64616	0.04387
H	-0.71781	-1.67000	0.04579
C	-2.41254	-0.38067	0.04185
H	-2.77558	0.65008	0.04007
H	-3.15336	-1.18507	0.04197

CH_3COOH

H	0.18879	-2.01890	-6.43166
C	-1.37258	-2.78759	-5.72391
O	-2.09274	-2.07994	-6.38143
C	-1.82179	-3.84342	-4.74615
H	-2.91699	-3.87931	-4.72052
H	-1.41454	-4.82250	-5.04227
H	-1.42412	-3.61615	-3.74494
O	-0.02413	-2.71551	-5.78712

$Pd(CH_3COO)_2$

C	-1.03762	0.92592	0.13815

O	0.19381	0.79809	-0.16042
O	-1.41614	2.08805	0.49689
C	-1.99683	-0.21649	0.04680
H	-2.68413	-0.19427	0.90431
H	-2.59775	-0.10091	-0.86969
H	-1.45316	-1.16896	0.00370
C	2.04630	4.68219	0.30919
O	2.42716	3.51809	-0.03933
O	0.81678	4.80758	0.61705
C	2.98615	5.84426	0.32598
H	3.01704	6.28748	-0.68280
H	2.63369	6.60643	1.03349
H	3.99880	5.50446	0.58281
Pd	0.50531	2.80308	0.22837

CH_3COOCu

C	3.60601	-2.25711	-7.86007
O	4.54683	-1.65698	-8.45844
O	3.01744	-1.75289	-6.85588
C	3.16837	-3.62512	-8.34156
H	3.39066	-4.36623	-7.55785
H	2.07831	-3.62914	-8.48989
H	3.68347	-3.90078	-9.26973
Cu	4.27932	-0.12935	-7.07268

CuI

I	-0.57809	0.07060	0.00000
Cu	-2.97451	0.07060	0.00000

A1

C	1.51991	2.46929	2.27066
C	0.61582	1.45001	1.96753
C	-0.60110	1.76637	1.33639
C	-0.90453	3.10762	1.03713
C	0.00265	4.11923	1.35095
C	1.22019	3.79948	1.96273
H	2.47334	2.21587	2.73959
H	0.84778	0.40512	2.18659
H	-1.86193	3.36531	0.57846
H	-0.24260	5.15911	1.12236
H	1.93470	4.59152	2.20089
C	-1.56921	0.68467	1.05965
C	-1.90953	-0.23669	2.06008
C	-2.87629	-1.20579	1.83772
H	-1.38311	-0.18047	3.00901
C	-3.15724	-0.34604	-0.37064
C	-3.53952	-1.23996	0.60656
H	-3.11005	-1.93295	2.61734

H	-3.58259	-0.35840	-1.37186
H	-4.31054	-1.97822	0.38754
N	-2.17819	0.57124	-0.15913
C	-1.71915	1.32331	-1.34897
H	-2.38256	2.17955	-1.53334
H	-1.72491	0.62478	-2.19459
I	1.71807	-0.32752	-1.08317
C	1.09837	-2.61214	1.93901
O	1.08984	-3.04035	0.71905
O	0.42989	-1.67875	2.38618
C	2.07542	-3.37443	2.82350
H	1.83548	-3.20373	3.88141
H	2.06422	-4.44793	2.58782
H	3.09192	-3.00032	2.61978
C	-2.12567	-2.84469	-1.96388
O	-1.43817	-1.79026	-2.21051
C	-3.27020	-3.20713	-2.87342
H	-3.71509	-2.30636	-3.32012
H	-2.88136	-3.83058	-3.69488
H	-4.02266	-3.79223	-2.32718
Pd	-0.04218	-2.21524	-0.69458
O	-1.82576	-3.56134	-0.97605
H	-0.68936	1.65505	-1.19041

A2-ts

C	1.14229	2.11484	2.06845
C	-0.11562	1.58459	1.76957
C	-0.89659	2.17608	0.76811
C	-0.42483	3.30410	0.07387
C	0.82352	3.83659	0.39276
C	1.60692	3.24054	1.38854
H	1.75737	1.59577	2.80438
H	-0.43727	0.67586	2.27895
H	-1.03123	3.75532	-0.71601
H	1.19402	4.70938	-0.14969
H	2.59650	3.64477	1.61410
C	-2.21966	1.59889	0.43028
C	-3.33419	1.83299	1.24185
C	-4.58772	1.33061	0.90463
H	-3.18472	2.43458	2.13880
C	-3.59347	0.35427	-1.04479
C	-4.71662	0.58941	-0.27341
H	-5.45280	1.52055	1.54362
H	-3.62361	-0.26017	-1.94287
H	-5.67582	0.18178	-0.59524
N	-2.37000	0.83408	-0.69657
C	-1.20801	0.39719	-1.49351
H	-1.49033	0.39740	-2.55605

H	-1.34787	-0.98139	-1.46036
I	2.34688	0.42947	-1.41758
C	1.88307	-1.74132	1.97735
O	1.69140	-1.98331	0.71012
O	1.32033	-0.88851	2.65118
C	2.95079	-2.65756	2.56557
H	2.96598	-2.55417	3.65847
H	2.76501	-3.70271	2.27799
H	3.93119	-2.37219	2.15239
C	-1.99914	-2.53894	-0.27472
O	-2.08205	-2.07557	-1.46364
C	-2.90556	-3.68506	0.10260
H	-2.41114	-4.62157	-0.20316
H	-3.05598	-3.71402	1.18927
H	-3.86237	-3.61746	-0.43263
Pd	0.36120	-0.88855	-0.29533
O	-1.19030	-2.09746	0.57635
H	-0.39294	1.11677	-1.38392

A3

C	-0.05887	1.13230	-3.40820
C	0.91678	0.96502	-2.42250
C	1.15252	1.99658	-1.49924
C	0.43269	3.19816	-1.59137

C	-0.53379	3.35983	-2.58723
C	-0.78842	2.32207	-3.48854
H	-0.25484	0.31838	-4.10972
H	1.48578	0.03827	-2.33681
H	0.62399	4.00331	-0.87693
H	-1.09515	4.29505	-2.65150
H	-1.55814	2.44084	-4.25480
C	2.15612	1.82351	-0.41286
C	3.50472	2.12176	-0.60806
C	4.42877	1.94959	0.41494
H	3.81189	2.45811	-1.59807
C	2.63506	1.21308	1.81841
C	3.97469	1.49886	1.65830
H	5.48895	2.14223	0.24434
H	2.23026	0.81362	2.74815
H	4.65720	1.33562	2.49282
N	1.73795	1.37426	0.81009
C	0.39762	0.84181	0.98033
H	0.12709	0.88389	2.04173
I	0.19872	-3.66022	-0.82592
C	3.33549	-1.39571	0.02273
O	2.18421	-0.92812	-0.40179
O	4.39054	-1.00557	-0.45370
C	3.29646	-2.40741	1.15821

H	4.31763	-2.63315	1.49132
H	2.70089	-2.02024	2.00194
H	2.79748	-3.32670	0.81578
Pd	0.26422	-1.15495	0.25473
H	-0.29926	1.43475	0.38705
C	-2.56766	0.18523	0.14647
O	-2.98734	0.54893	-0.92794
O	-2.61586	0.90334	1.28238
C	-3.27823	2.21260	1.36312
C	-4.75596	2.06599	0.98991
H	-5.28132	3.01248	1.19021
H	-4.87458	1.81360	-0.07109
H	-5.22412	1.27648	1.59777
C	-3.12209	2.57871	2.83831
H	-2.05692	2.61783	3.11336
H	-3.57090	3.56380	3.03579
H	-3.61768	1.83189	3.47661
C	-2.55925	3.22523	0.46886
H	-3.05014	4.20667	0.55822
H	-1.50991	3.34088	0.77868
H	-2.58040	2.91060	-0.58122
C	-1.94676	-1.16055	0.35638
H	-2.19913	-1.86690	-0.43775
C	-1.42885	-1.60956	1.56187

H	-1.42185	-0.94975	2.43248
H	-1.30639	-2.68038	1.73944

A4-ts

C	-0.08750	2.70853	-2.56844
C	0.77576	1.93627	-1.78530
C	1.33976	2.49083	-0.62606
C	1.03786	3.81532	-0.26378
C	0.18026	4.58067	-1.05663
C	-0.38290	4.02714	-2.21150
H	-0.53042	2.27010	-3.46572
H	1.02066	0.90424	-2.03872
H	1.48434	4.24936	0.63509
H	-0.04823	5.61038	-0.77163
H	-1.05800	4.62427	-2.82942
C	2.32753	1.72889	0.19082
C	3.67154	1.67274	-0.19658
C	4.61426	1.03839	0.59593
H	3.93828	2.09577	-1.16329
C	2.87911	0.56145	2.17706
C	4.20412	0.47445	1.81360
H	5.64941	0.95643	0.26255
H	2.49180	0.12155	3.09623
H	4.90325	-0.04733	2.46785

N	1.95963	1.19114	1.39428
C	0.56203	1.15963	1.83796
H	0.57074	1.60407	2.83641
I	-0.82049	-2.79053	-1.03594
C	2.87193	-1.30950	-0.85040
O	1.78611	-0.60640	-0.66405
O	3.81417	-0.87235	-1.50415
C	2.94572	-2.67832	-0.18728
H	3.96188	-3.08210	-0.28531
H	2.66068	-2.61562	0.87513
H	2.22455	-3.35911	-0.66436
Pd	0.10116	-0.89996	0.52443
H	-0.06539	1.75711	1.17406
C	-2.73825	-0.52424	1.19875
O	-3.70458	-1.18064	0.89779
O	-2.61682	0.81507	1.00932
C	-3.56907	1.58084	0.20321
C	-4.96623	1.53253	0.82820
H	-5.63321	2.22501	0.29101
H	-5.38462	0.52033	0.78065
H	-4.92099	1.84766	1.88274
C	-2.99881	2.99744	0.26223
H	-1.97743	3.02004	-0.14160
H	-3.61949	3.68533	-0.33177

H	-2.97433	3.36018	1.30180
C	-3.55060	1.04072	-1.22934
H	-4.18943	1.66649	-1.87187
H	-2.52481	1.05963	-1.62792
H	-3.91724	0.00679	-1.26293
C	-1.49615	-1.07327	1.81551
H	-1.58181	-2.12766	2.09270
C	-0.67768	-0.20309	2.63205
H	-1.18996	0.69504	2.98536
H	-0.06227	-0.67960	3.40251

A5

C	-4.54576	-0.50880	0.64561
C	-3.23918	-0.97272	0.81428
C	-2.60205	-1.67725	-0.22098
C	-3.29609	-1.91904	-1.41927
C	-4.60219	-1.45503	-1.58161
C	-5.22927	-0.74818	-0.54993
H	-5.02614	0.05201	1.45064
H	-2.68826	-0.76258	1.73272
H	-2.81865	-2.48569	-2.22167
H	-5.13408	-1.65076	-2.51562
H	-6.25012	-0.38130	-0.68092
C	-1.24153	-2.23043	0.00946

C	-1.03075	-3.11947	1.06273
C	0.22413	-3.69062	1.27635
H	-1.87769	-3.36149	1.70427
C	1.04140	-2.43044	-0.59674
C	1.26820	-3.34296	0.42841
H	0.37749	-4.38940	2.10151
H	1.86780	-2.14237	-1.26334
H	2.27735	-3.73909	0.54672
N	-0.19252	-1.90982	-0.80994
C	-0.36986	-0.90335	-1.90110
H	-0.68662	-1.46289	-2.79436
I	0.17636	0.36167	2.15013
C	4.32920	-0.91367	-1.35845
O	3.98624	-0.05352	-0.46148
O	3.58787	-1.74682	-1.89624
C	5.79807	-0.82683	-1.75294
H	5.99087	0.15301	-2.21756
H	6.43205	-0.88644	-0.85529
H	6.05433	-1.62986	-2.45599
Pd	2.15622	0.14959	0.44818
H	-1.19115	-0.25095	-1.59713
C	0.53053	2.15539	-0.93019
O	0.96354	3.19588	-0.49428
O	-0.76539	1.93844	-1.24433

C	-1.80864	2.95143	-1.05762
C	-1.49083	4.19311	-1.89567
H	-2.34400	4.88851	-1.86003
H	-0.59716	4.70451	-1.51848
H	-1.32141	3.90992	-2.94664
C	-3.05729	2.24614	-1.58791
H	-3.25189	1.32566	-1.02012
H	-3.93584	2.90271	-1.49583
H	-2.93004	1.98087	-2.64898
C	-1.95425	3.27793	0.42944
H	-2.79902	3.97017	0.57275
H	-2.14331	2.35999	1.00434
H	-1.03988	3.74298	0.81856
C	1.39598	0.96278	-1.25938
H	2.33887	1.37226	-1.64705
C	0.85242	-0.05567	-2.26110
H	0.52029	0.51022	-3.15180
H	1.68575	-0.68588	-2.59947

A6-ts

C	-4.61587	-0.79467	0.05027
C	-3.27662	-1.11932	0.27347
C	-2.70350	-2.22269	-0.38308
C	-3.48805	-2.99808	-1.24950

C	-4.82895	-2.66721	-1.46992
C	-5.39326	-1.56409	-0.82315
H	-5.05519	0.06265	0.56626
H	-2.66585	-0.52297	0.95776
H	-3.04366	-3.85962	-1.75457
H	-5.43309	-3.27442	-2.14860
H	-6.44117	-1.30598	-0.99545
C	-1.28022	-2.58146	-0.12364
C	-0.95861	-3.66088	0.68278
C	0.38747	-3.93259	0.97894
H	-1.76854	-4.26466	1.09291
C	1.05201	-1.96949	-0.33162
C	1.36135	-3.07331	0.50111
H	0.64954	-4.79509	1.59779
H	2.51817	-1.71558	-1.27047
H	2.41120	-3.23319	0.76403
N	-0.27252	-1.82199	-0.66699
C	-0.66311	-0.72130	-1.59207
H	-1.25994	-1.16948	-2.40013
I	-0.13759	0.75681	2.28407
C	4.27904	-0.92256	-1.16761
O	3.99723	-0.24507	-0.18241
O	3.42973	-1.72750	-1.76642
C	5.64382	-0.89344	-1.80670

H	5.54792	-0.55334	-2.84977
H	6.30755	-0.22183	-1.24977
H	6.06037	-1.91191	-1.83478
Pd	1.69823	0.00421	0.54446
H	-1.31057	-0.02765	-1.04454
C	0.62622	2.30351	-0.90355
O	1.27215	3.28434	-0.61499
O	-0.70408	2.27363	-1.08356
C	-1.56184	3.45739	-0.94263
C	-1.19558	4.46713	-2.03329
H	-1.89954	5.31341	-2.00875
H	-0.17827	4.85056	-1.88116
H	-1.25566	3.99669	-3.02748
C	-2.96013	2.88185	-1.16808
H	-3.18664	2.12012	-0.40693
H	-3.71600	3.67921	-1.10473
H	-3.03027	2.40980	-2.16018
C	-1.43922	4.05647	0.45921
H	-2.16911	4.87448	0.56562
H	-1.64755	3.29345	1.22199
H	-0.43137	4.45221	0.63259
C	1.25730	0.95595	-1.18349
H	2.28862	1.15760	-1.50689
C	0.51131	0.05570	-2.16694

H	0.08475	0.69580	-2.95955
H	1.22375	-0.62554	-2.65131

A7

C	-5.38351	-2.39993	0.06193
C	-4.02684	-2.18689	0.30858
C	-3.05344	-2.92006	-0.39432
C	-3.46456	-3.87602	-1.33625
C	-4.82469	-4.08498	-1.58339
C	-5.78571	-3.34755	-0.88672
H	-6.13105	-1.82817	0.61713
H	-3.71350	-1.45194	1.05447
H	-2.71174	-4.44966	-1.88225
H	-5.13279	-4.82638	-2.32459
H	-6.84867	-3.51186	-1.07933
C	-1.60643	-2.74778	-0.08993
C	-0.88725	-3.80207	0.44560
C	0.45677	-3.62267	0.81056
H	-1.39739	-4.75315	0.60102
C	0.31281	-1.30038	0.11695
C	1.03825	-2.37592	0.67421
H	1.02964	-4.45816	1.22065
H	4.04807	0.46193	0.98474
H	2.07372	-2.19102	0.95559

N	-0.97785	-1.53312	-0.28782
C	-1.65862	-0.46475	-1.07337
H	-2.66537	-0.81066	-1.32146
I	1.93160	0.78592	2.45002
C	4.59463	-0.44747	-0.60510
O	3.77375	-1.33661	-0.51258
O	4.74476	0.52890	0.28863
C	5.54513	-0.29153	-1.76824
H	6.55387	-0.03499	-1.41362
H	5.56189	-1.21305	-2.36269
H	5.19470	0.54436	-2.39550
Pd	1.14727	0.44830	-0.11998
H	-1.74564	0.42696	-0.43684
C	0.49030	1.97392	-1.76443
O	1.54535	2.46154	-1.31072
O	-0.66857	2.63355	-1.83932
C	-0.88035	3.93859	-1.18523
C	-0.00362	4.99941	-1.85323
H	-0.25183	5.99174	-1.44556
H	1.05938	4.79678	-1.67379
H	-0.18594	5.01625	-2.93908
C	-2.36147	4.20503	-1.45019
H	-2.98229	3.41649	-0.99790
H	-2.65607	5.17274	-1.01730

H	-2.56226	4.22771	-2.53203
C	-0.60560	3.81669	0.31582
H	-0.90769	4.74884	0.81753
H	-1.18715	2.98867	0.74956
H	0.45548	3.63342	0.52343
C	0.44192	0.54827	-2.09228
H	1.29974	0.21214	-2.68550
C	-0.88375	-0.13003	-2.35749
H	-1.54022	0.51911	-2.96155
H	-0.72906	-1.06055	-2.92603

A8-ts

C	-5.17877	0.10783	-2.22144
C	-4.10384	0.19661	-1.33662
C	-4.13179	-0.50104	-0.11436
C	-5.25618	-1.27969	0.20546
C	-6.32871	-1.36944	-0.68564
C	-6.29189	-0.67758	-1.89983
H	-5.15077	0.66060	-3.16350
H	-3.24277	0.82394	-1.58099
H	-5.28011	-1.82564	1.15154
H	-7.19483	-1.98507	-0.43101
H	-7.13154	-0.74743	-2.59566
C	-3.01853	-0.35640	0.85556

C	-3.24532	0.04961	2.15659
C	-2.15207	0.25138	3.02970
H	-4.26883	0.24251	2.47665
C	-0.61814	-0.26049	1.21373
C	-0.86327	0.09797	2.57320
H	-2.33332	0.55984	4.06237
H	-0.00459	0.26799	3.22336
N	-1.72411	-0.56671	0.43725
C	-1.37034	-1.27204	-0.81083
H	-2.26736	-1.72623	-1.24455
I	1.18380	2.91275	-0.40661
Pd	0.98551	0.44326	0.38295
H	-0.96022	-0.54298	-1.52548
C	2.02735	-1.86915	0.70810
O	2.71562	-1.90020	1.70845
O	2.49292	-1.96495	-0.55555
C	3.92574	-1.88700	-0.87322
C	4.64690	-3.11028	-0.30157
H	5.69546	-3.11098	-0.63781
H	4.62412	-3.10049	0.79519
H	4.16950	-4.03577	-0.65993
C	3.93018	-1.90861	-2.40122
H	3.37168	-1.04719	-2.79719
H	4.96283	-1.86204	-2.77848

H	3.46107	-2.83147	-2.77541
C	4.50697	-0.57162	-0.34755
H	5.54857	-0.47043	-0.68961
H	3.93402	0.28607	-0.73427
H	4.49228	-0.54004	0.74885
C	0.51456	-1.79843	0.75772
H	0.24429	-2.25826	1.71342
C	-0.30648	-2.31800	-0.42138
H	0.34189	-2.51577	-1.28331
H	-0.80396	-3.26075	-0.14211

A9

C	-5.20623	0.24757	-2.12170
C	-4.03271	0.17313	-1.36944
C	-4.05597	-0.39341	-0.08187
C	-5.26801	-0.86732	0.44298
C	-6.43943	-0.79445	-0.31653
C	-6.40976	-0.23968	-1.59930
H	-5.18175	0.69800	-3.11692
H	-3.09835	0.57954	-1.76676
H	-5.28783	-1.29692	1.44757
H	-7.37832	-1.17083	0.09694
H	-7.32658	-0.18003	-2.19108
C	-2.81669	-0.41082	0.73683

C	-2.68658	0.37498	1.87944
C	-1.47437	0.39522	2.60311
H	-3.52893	0.99568	2.18261
C	-0.49262	-1.06604	0.94571
C	-0.38662	-0.40280	2.21679
H	-1.40493	0.99008	3.51707
H	0.45456	-0.62623	2.87616
N	-1.74651	-1.12923	0.31146
C	-1.71948	-2.05812	-0.84072
H	-2.40581	-2.89470	-0.63036
I	0.83226	1.36409	-1.98176
Pd	0.34282	0.79519	0.54720
H	-2.06493	-1.55239	-1.74984
C	1.79880	-2.08610	0.66686
O	2.28209	-1.97446	1.77253
O	2.44441	-2.05617	-0.48647
C	3.87900	-1.71863	-0.59999
C	4.70119	-2.83212	0.04976
H	5.77279	-2.64191	-0.11623
H	4.51418	-2.87713	1.13074
H	4.45106	-3.80666	-0.39819
C	4.08390	-1.66820	-2.11211
H	3.43536	-0.89595	-2.55231
H	5.13291	-1.42839	-2.34249

H	3.83667	-2.63930	-2.56783
C	4.13989	-0.34953	0.02958
H	5.17413	-0.04459	-0.19288
H	3.45363	0.39630	-0.39818
H	4.00596	-0.37700	1.11813
C	0.29694	-2.27865	0.47762
H	0.01953	-3.12278	1.13663
C	-0.24814	-2.48579	-0.94005
H	0.28983	-1.81719	-1.62534
H	-0.13784	-3.51913	-1.29439

A10

C	-5.38822	-2.77095	0.14678
C	-4.18427	-2.23391	-0.31168
C	-3.85476	-0.89027	-0.05204
C	-4.76519	-0.09653	0.66705
C	-5.97238	-0.63483	1.12023
C	-6.28566	-1.97318	0.86535
H	-5.63295	-3.81420	-0.06806
H	-3.50091	-2.85300	-0.89888
H	-4.51094	0.94440	0.88048
H	-6.66767	-0.00655	1.68244
H	-7.22842	-2.39437	1.22302
C	-2.59972	-0.29342	-0.56654

C	-2.58226	0.83741	-1.35066
C	-1.36231	1.36058	-1.90952
H	-3.53540	1.30787	-1.59545
C	-0.19862	-0.39661	-0.71276
C	-0.14673	0.63807	-1.68014
H	-1.43495	2.05988	-2.74721
H	0.76165	0.74103	-2.27545
N	-1.38149	-0.88928	-0.25801
C	-1.16238	-1.82902	0.86817
H	-1.28762	-1.26530	1.80879
Pd	-0.24160	2.18267	-0.28256
H	-1.89705	-2.64060	0.85200
C	2.24477	-1.21798	-0.70144
O	2.52754	-0.71007	-1.76277
O	3.07060	-1.92776	0.06990
C	4.53496	-1.83573	-0.06109
C	4.94422	-0.36178	0.02299
H	6.03297	-0.28952	0.17018
H	4.67789	0.17750	-0.89516
H	4.42704	0.12308	0.86572
C	5.02703	-2.60942	1.16062
H	4.64907	-3.64314	1.13937
H	6.12702	-2.63788	1.17431
H	4.67400	-2.12717	2.08421

C	4.98491	-2.50430	-1.36080
H	6.08507	-2.50963	-1.41126
H	4.63321	-3.54738	-1.39817
H	4.59106	-1.96525	-2.23154
C	0.93004	-1.04953	0.02079
C	0.28355	-2.28511	0.66489
H	0.32032	-3.14738	-0.02087
H	0.77200	-2.57138	1.60398
C	1.80061	2.26043	1.90498
O	0.86248	2.91913	1.32947
C	2.56613	3.04463	2.96747
H	3.27886	3.71789	2.46299
H	1.88066	3.67294	3.55457
H	3.12645	2.36357	3.62213
O	2.13870	1.09190	1.65184
H	1.22694	-0.30989	0.81117

A11-ts

C	-5.26520	-2.77725	0.40140
C	-4.08604	-2.25001	-0.12702
C	-3.81041	-0.87281	-0.03149
C	-4.75052	-0.03800	0.59718
C	-5.93283	-0.56699	1.12154
C	-6.19221	-1.93752	1.02919

H	-5.46709	-3.84782	0.31377
H	-3.37816	-2.90523	-0.64104
H	-4.53851	1.03014	0.68468
H	-6.65085	0.09480	1.61238
H	-7.11498	-2.35145	1.44319
C	-2.58078	-0.29422	-0.62282
C	-2.61146	0.74498	-1.52021
C	-1.40769	1.24207	-2.14430
H	-3.58050	1.15748	-1.80314
C	-0.16869	-0.38568	-0.80788
C	-0.17213	0.58283	-1.86160
H	-1.50777	1.84872	-3.04885
H	0.72712	0.66309	-2.47453
N	-1.34552	-0.83798	-0.27981
C	-1.07689	-1.61383	0.95681
H	-1.20978	-0.92888	1.81272
Pd	-0.28342	2.25134	-0.60906
H	-1.78206	-2.44410	1.06779
C	2.28715	-1.00264	-0.68499
O	2.67526	-0.32473	-1.62063
O	3.06620	-1.85529	0.01496
C	4.52452	-1.82970	-0.08022
C	5.02892	-0.42399	0.26628
H	6.12206	-0.44023	0.39750

H	4.77617	0.29258	-0.52549
H	4.56111	-0.08427	1.20333
C	4.95209	-2.83594	0.98881
H	4.52684	-3.82790	0.77260
H	6.04904	-2.92206	1.01733
H	4.59643	-2.51599	1.97985
C	4.97750	-2.28536	-1.47012
H	6.07599	-2.36326	-1.49623
H	4.55544	-3.27632	-1.69973
H	4.64860	-1.57467	-2.23800
C	0.95220	-0.93105	-0.08052
C	0.38677	-2.04250	0.80059
H	0.45961	-3.02729	0.30626
H	0.89717	-2.11795	1.77005
C	1.57756	2.07622	1.83286
O	0.90763	2.81323	1.08042
C	2.33644	2.71433	2.98001
H	3.40478	2.75362	2.71131
H	1.97571	3.73368	3.16622
H	2.24772	2.09430	3.88351
O	1.72292	0.80670	1.73456
H	1.27580	0.10648	0.82437

A12

C	-5.59133	-2.90971	0.02110
C	-4.38324	-2.35814	-0.40791
C	-3.98840	-1.07570	0.01770
C	-4.84048	-0.35862	0.87541
C	-6.05181	-0.91051	1.30104
C	-6.42951	-2.18850	0.87916
H	-5.88603	-3.90390	-0.32465
H	-3.74628	-2.91323	-1.10105
H	-4.53705	0.63409	1.21579
H	-6.70021	-0.34094	1.97178
H	-7.37507	-2.62170	1.21483
C	-2.73045	-0.45504	-0.46624
C	-2.71856	0.76241	-1.09481
C	-1.49586	1.30601	-1.65103
H	-3.66457	1.28293	-1.24522
C	-0.31706	-0.64654	-0.73120
C	-0.28962	0.56214	-1.52450
H	-1.58980	2.05697	-2.44212
H	0.57363	0.70410	-2.17731
N	-1.53670	-1.14839	-0.31401
C	-1.31018	-2.25856	0.64019
H	-1.45168	-1.86471	1.66278
Pd	-0.20386	2.13540	-0.15617
H	-2.03277	-3.06813	0.49028

C	2.10006	-1.07799	-0.33572
O	2.53947	0.02125	-0.72778
O	2.90744	-2.06302	0.12717
C	4.35365	-1.93727	0.25006
C	4.70358	-0.87858	1.30112
H	5.78645	-0.89731	1.50194
H	4.42976	0.12858	0.96758
H	4.17547	-1.09513	2.24316
C	4.77102	-3.32801	0.73426
H	4.47558	-4.09256	0.00001
H	5.86169	-3.37529	0.87443
H	4.28183	-3.56333	1.69167
C	4.99061	-1.63034	-1.10986
H	6.08776	-1.67202	-1.02195
H	4.67540	-2.38024	-1.85217
H	4.69484	-0.63714	-1.46756
C	0.73028	-1.45037	-0.28778
C	0.15099	-2.67722	0.38243
H	0.19752	-3.56514	-0.27553
H	0.67362	-2.94251	1.31257
C	2.43781	2.98470	1.23649
O	1.20700	3.00214	1.23090
C	3.23174	3.93973	2.08894
H	3.94429	4.49030	1.45605

H	2.56108	4.63568	2.60582
H	3.82352	3.36834	2.82107
O	3.18799	2.17263	0.53947
H	2.72067	1.43506	0.02318

B2-ts

C	5.02945	-1.10728	-1.40532
C	3.83160	-0.76114	-0.77825
C	3.80006	0.32289	0.11674
C	4.97616	1.04090	0.38655
C	6.16966	0.69319	-0.25138
C	6.19675	-0.37921	-1.14819
H	5.05197	-1.95558	-2.09342
H	2.92032	-1.33952	-0.95410
H	4.95061	1.87922	1.08737
H	7.08012	1.26122	-0.04616
H	7.13150	-0.65259	-1.64383
C	2.53997	0.66334	0.82448
C	2.44319	0.52758	2.21236
C	1.24087	0.78559	2.86781
H	3.32588	0.18927	2.75582
C	0.22699	1.26136	0.72109
C	0.12952	1.14873	2.11131
H	1.16722	0.67268	3.95175

H	-0.51490	2.10717	0.11232
H	-0.84249	1.32558	2.57517
N	1.45058	1.08711	0.12829
C	1.51069	1.27612	-1.33475
H	2.49508	1.66357	-1.61898
H	0.72379	1.98587	-1.61472
I	-0.06911	-2.04301	-0.02923
C	-3.89323	-1.30030	0.18409
O	-3.06604	-0.98688	-0.78544
O	-3.77671	-0.97994	1.35444
C	-5.04991	-2.15038	-0.32907
H	-5.76001	-2.33193	0.48793
H	-5.55069	-1.64453	-1.16801
H	-4.65669	-3.10683	-0.70673
C	-2.31053	2.98333	-0.57838
O	-2.80575	1.82827	-0.50358
C	-3.22986	4.13211	-0.93055
H	-4.24181	3.77079	-1.14818
H	-3.25295	4.83950	-0.08718
H	-2.81775	4.67069	-1.79707
Pd	-1.53948	0.15820	-0.19995
O	-1.08618	3.25432	-0.36894
H	1.32484	0.31094	-1.82582

B3

C	5.59281	-0.96972	-0.62877
C	4.29139	-0.69949	-0.20458
C	3.84298	0.62998	-0.10300
C	4.72015	1.67948	-0.42075
C	6.02079	1.40365	-0.85114
C	6.45832	0.08022	-0.95676
H	5.93486	-2.00504	-0.69828
H	3.62063	-1.51919	0.06434
H	4.37480	2.71306	-0.33997
H	6.69360	2.22626	-1.10500
H	7.47605	-0.13465	-1.29151
C	2.47941	0.92491	0.40835
C	2.31047	1.65490	1.57466
C	1.02531	1.83827	2.10242
H	3.19563	2.03975	2.08139
C	0.10099	0.53797	0.25934
C	-0.05558	1.25429	1.46410
H	0.88650	2.40845	3.02431
H	-1.40583	2.08932	-2.03447
H	-1.05918	1.33472	1.88568
N	1.37095	0.43926	-0.24849
C	1.53430	-0.22789	-1.55722
H	2.41254	0.17321	-2.07396

H	0.62805	-0.05054	-2.14684
I	-0.70479	-2.55552	0.35913
C	-4.28616	-0.86953	-0.72148
O	-3.20429	-1.05054	-1.41114
O	-4.36150	-0.20279	0.31364
C	-5.50449	-1.58276	-1.28903
H	-6.41688	-1.24178	-0.78235
H	-5.57766	-1.41417	-2.37396
H	-5.38345	-2.66713	-1.13551
C	-2.23915	2.89780	-0.52572
O	-1.42156	3.77689	-0.53404
C	-3.44384	2.76086	0.34585
H	-3.33709	3.41792	1.21725
H	-4.32207	3.08044	-0.24026
H	-3.63307	1.70766	0.61557
Pd	-1.51798	-0.24876	-0.58204
O	-2.12985	1.84860	-1.42979
H	1.63071	-1.31226	-1.41308

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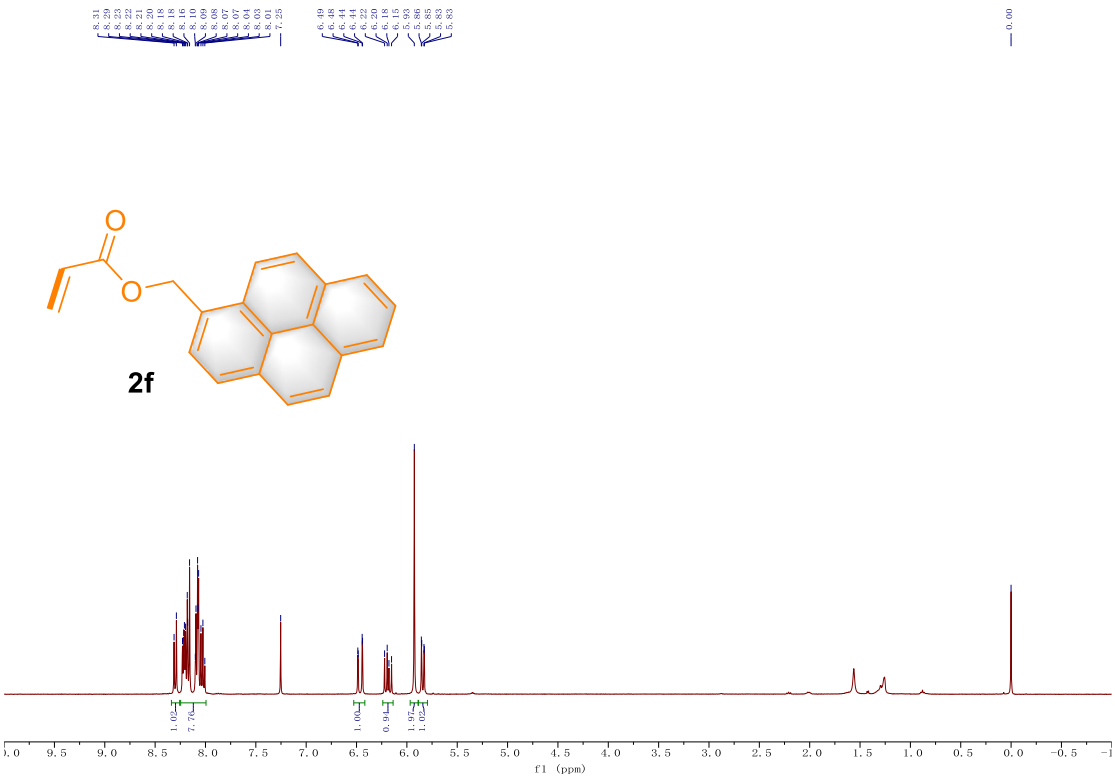
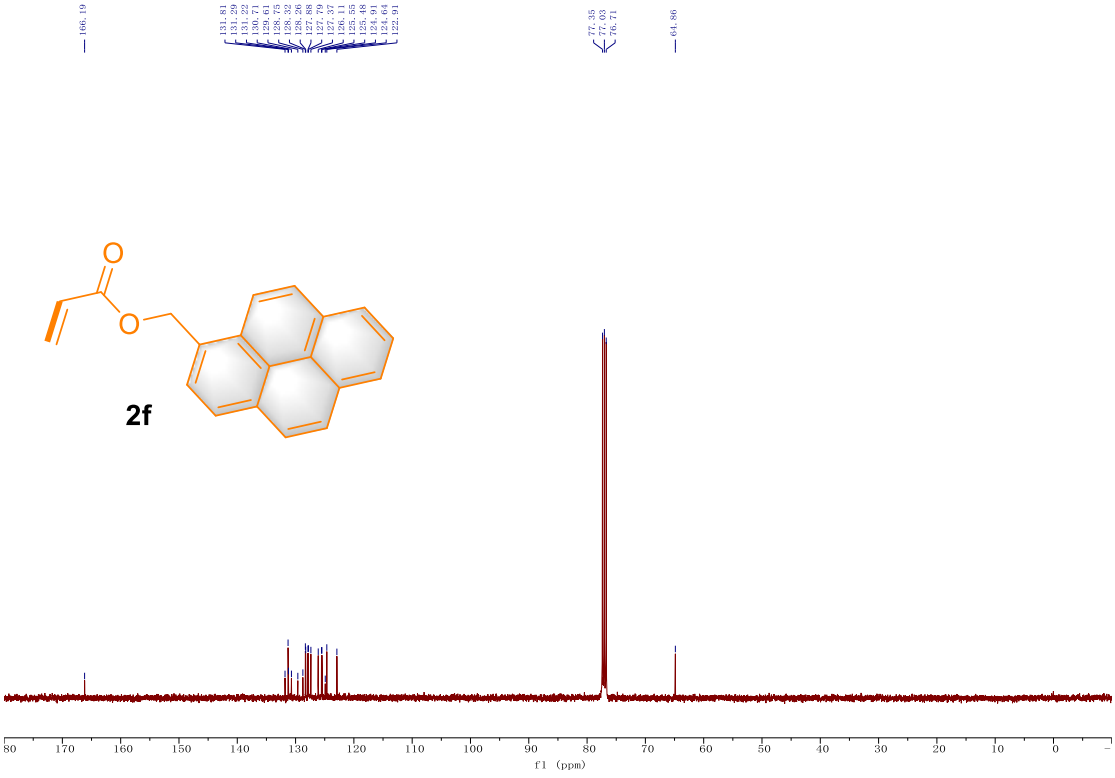
12. ^{1}H and ^{13}C NMR spectra

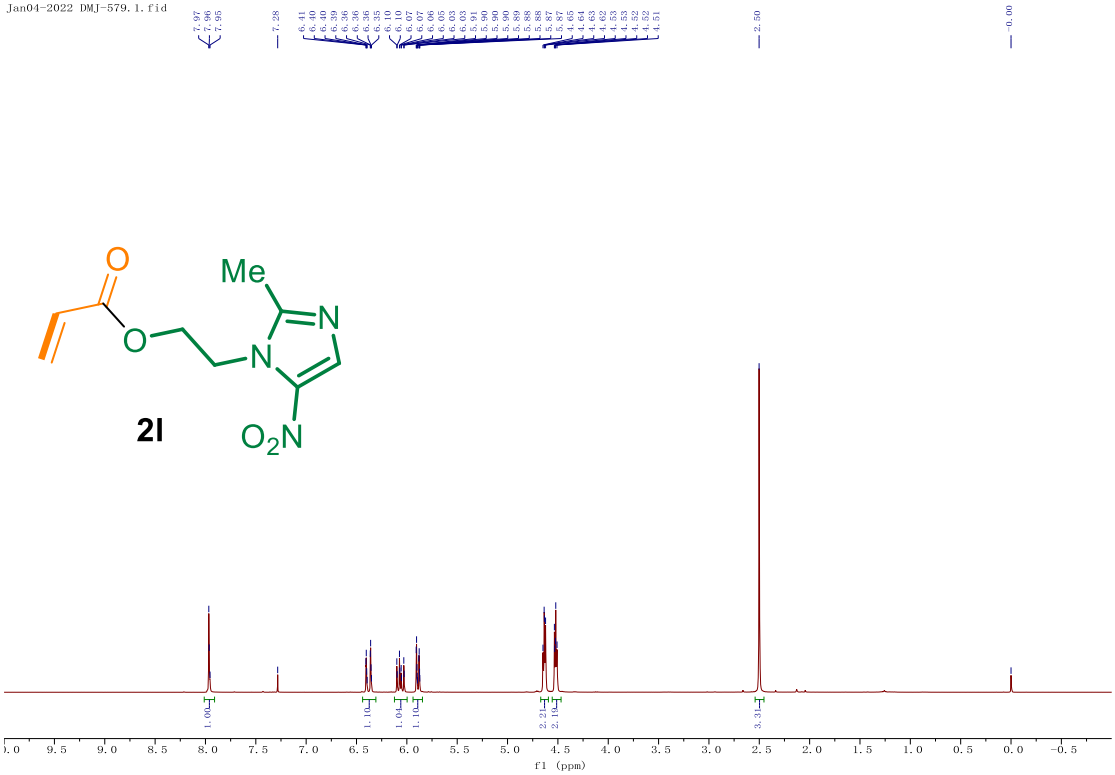
400 MHz ^{1}H NMR of **2f** in $CDCl_3$



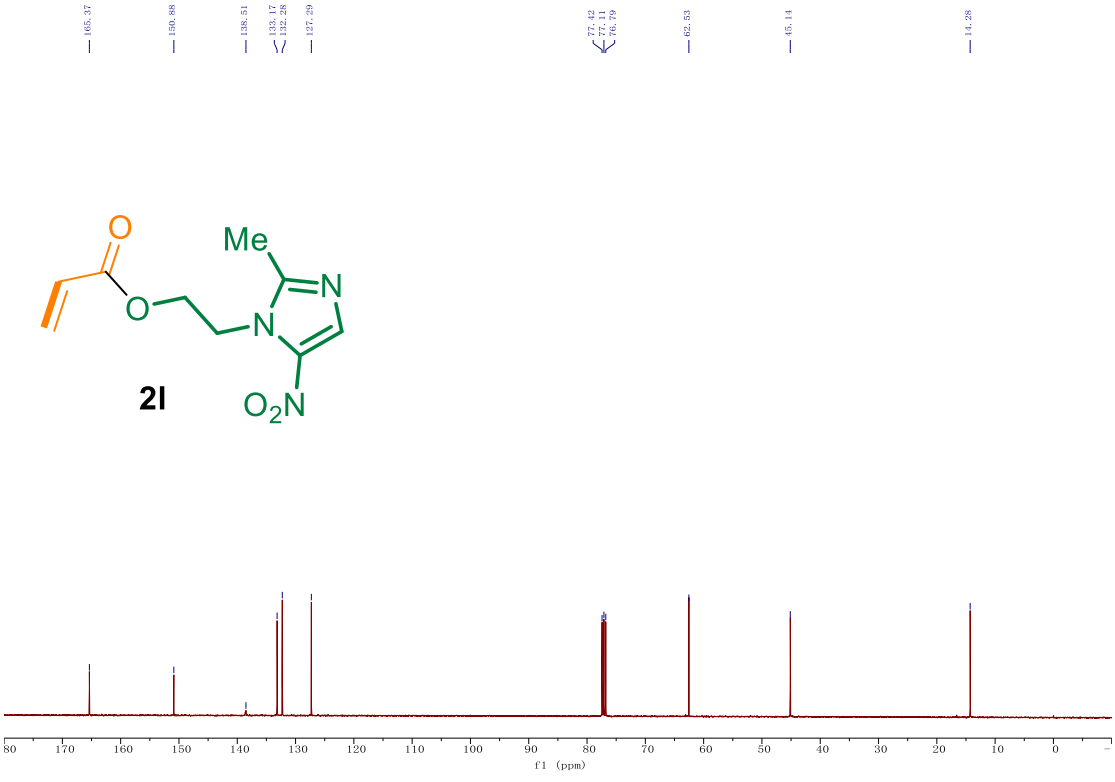
101 MHz ^{13}C NMR of **2f** in $CDCl_3$



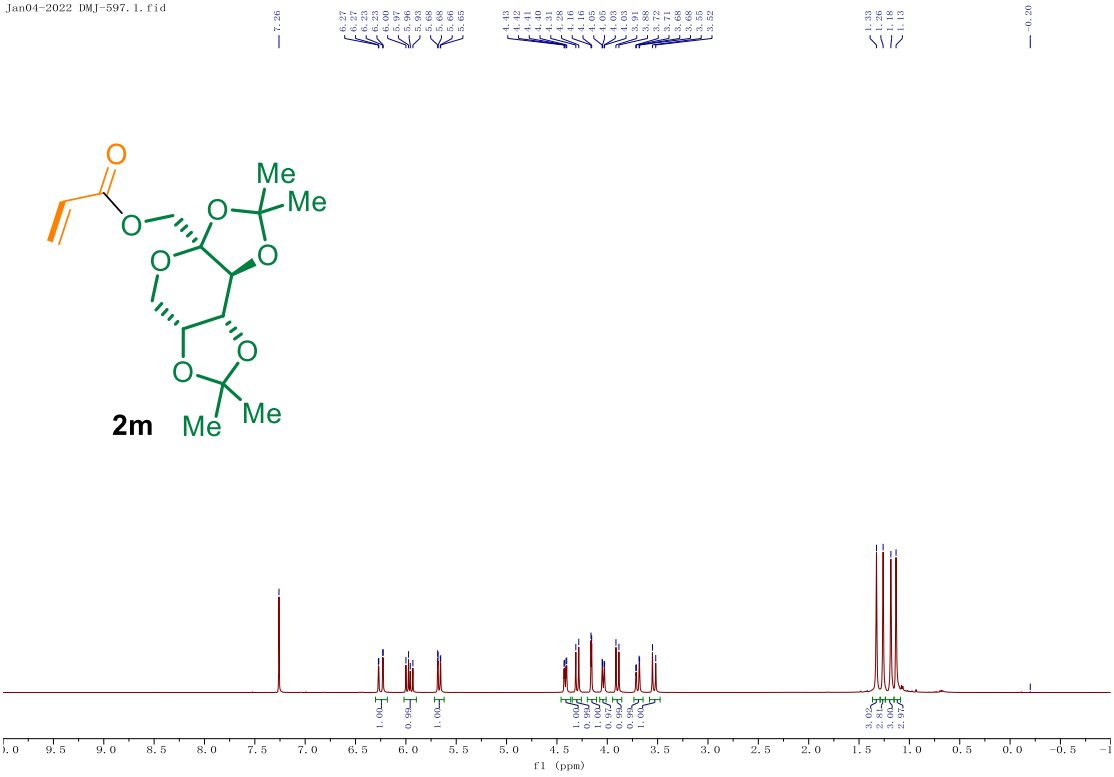
400 MHz ^{1}H NMR of **2l** in $CDCl_3$



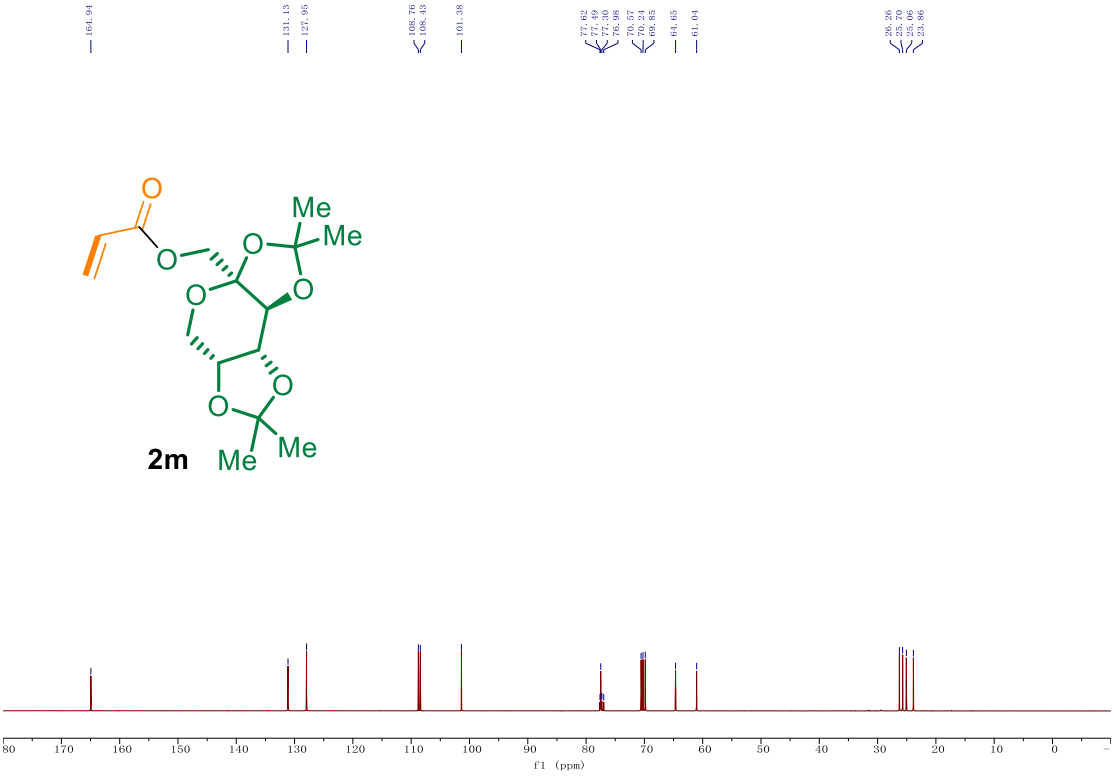
101 MHz ^{13}C NMR of **2l** in $CDCl_3$



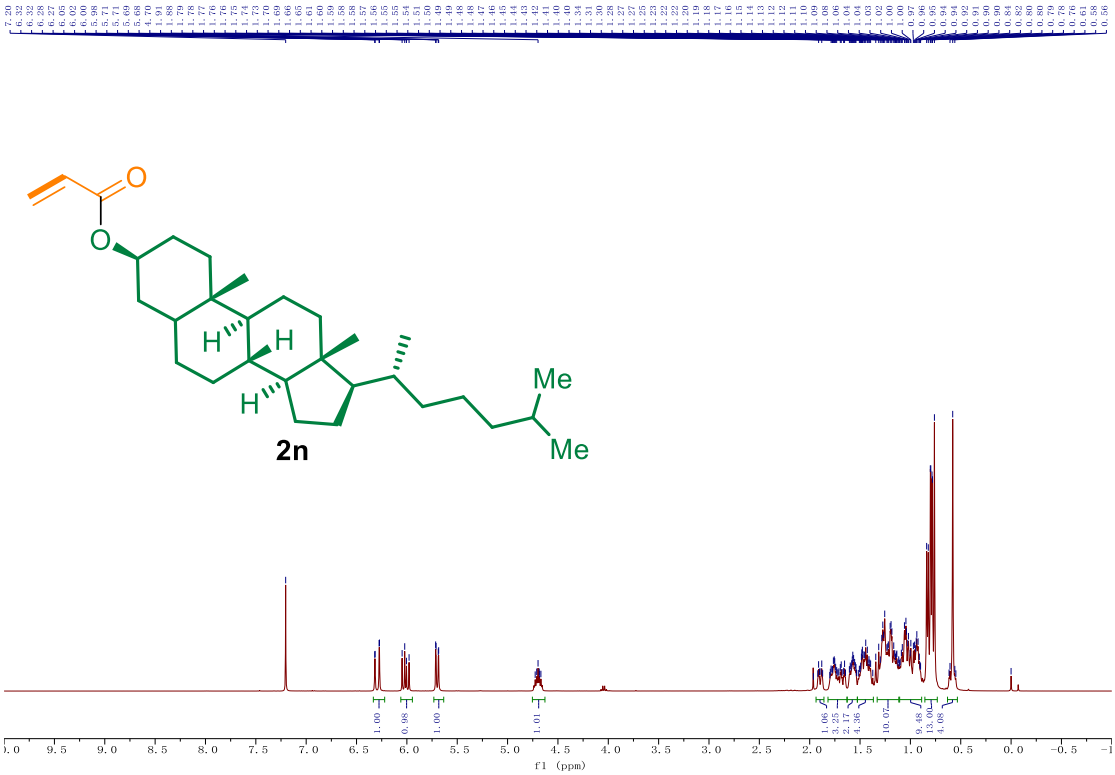
400 MHz ^{1}H NMR of **2m** in $CDCl_3$



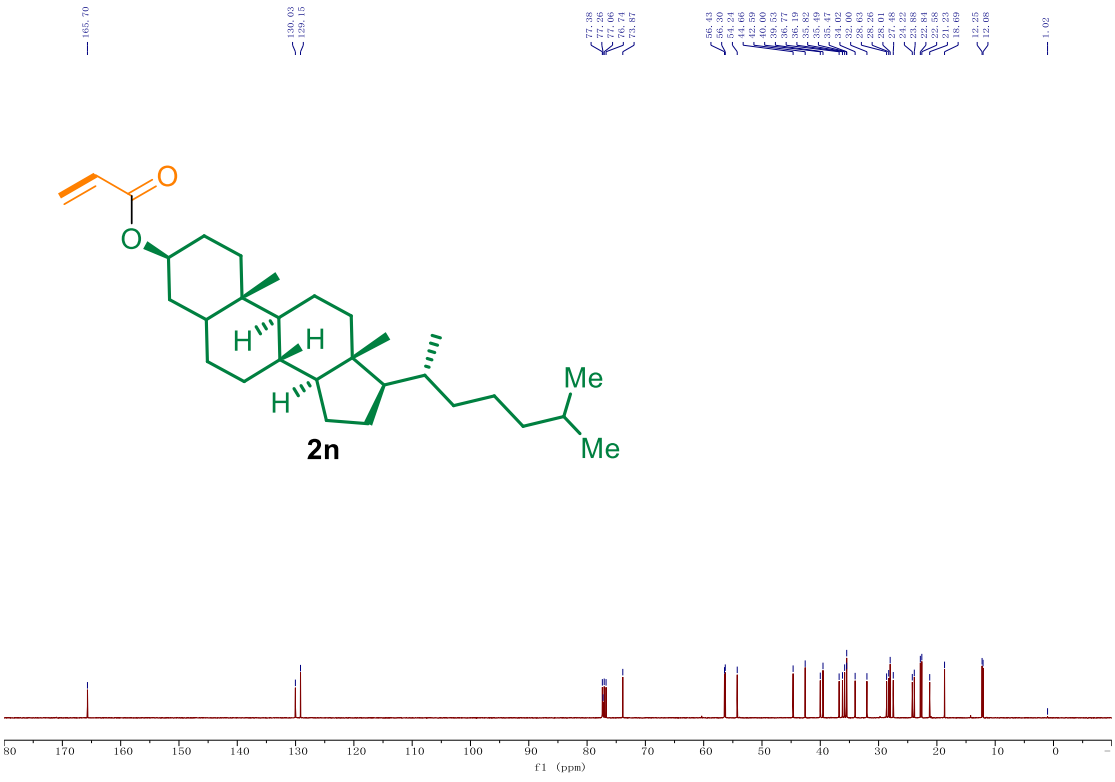
101 MHz ^{13}C NMR of **2m** in $CDCl_3$



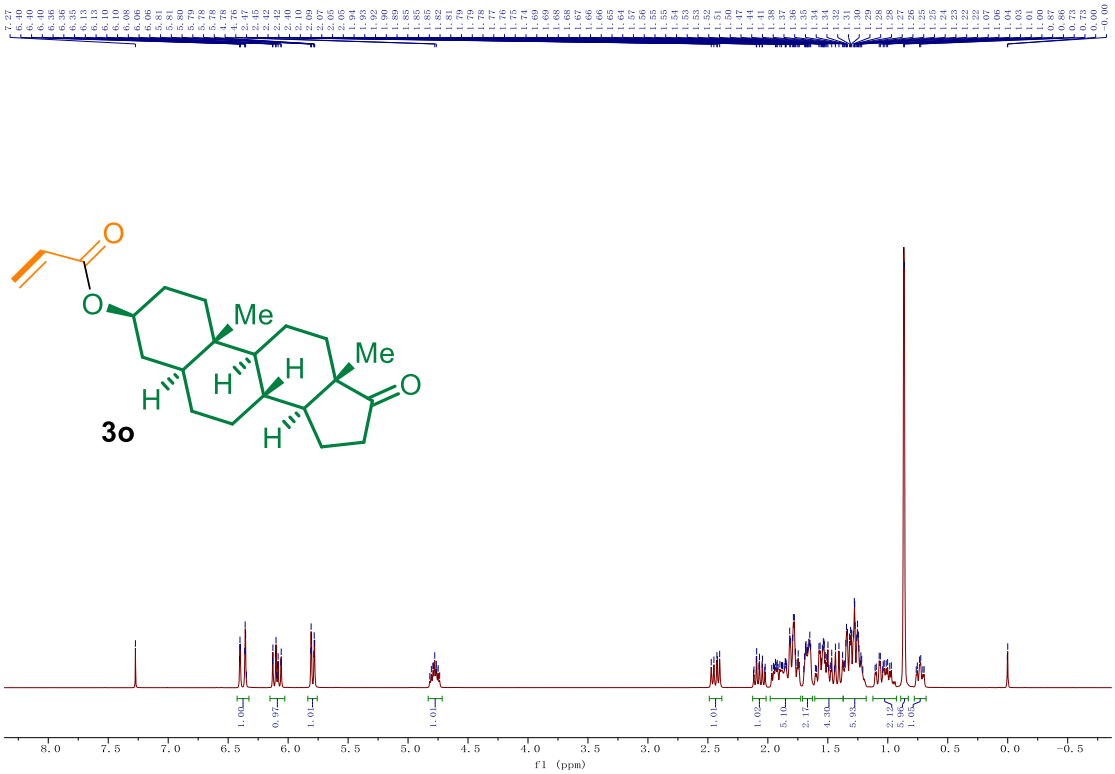
400 MHz ^{1}H NMR of **2n** in $CDCl_3$



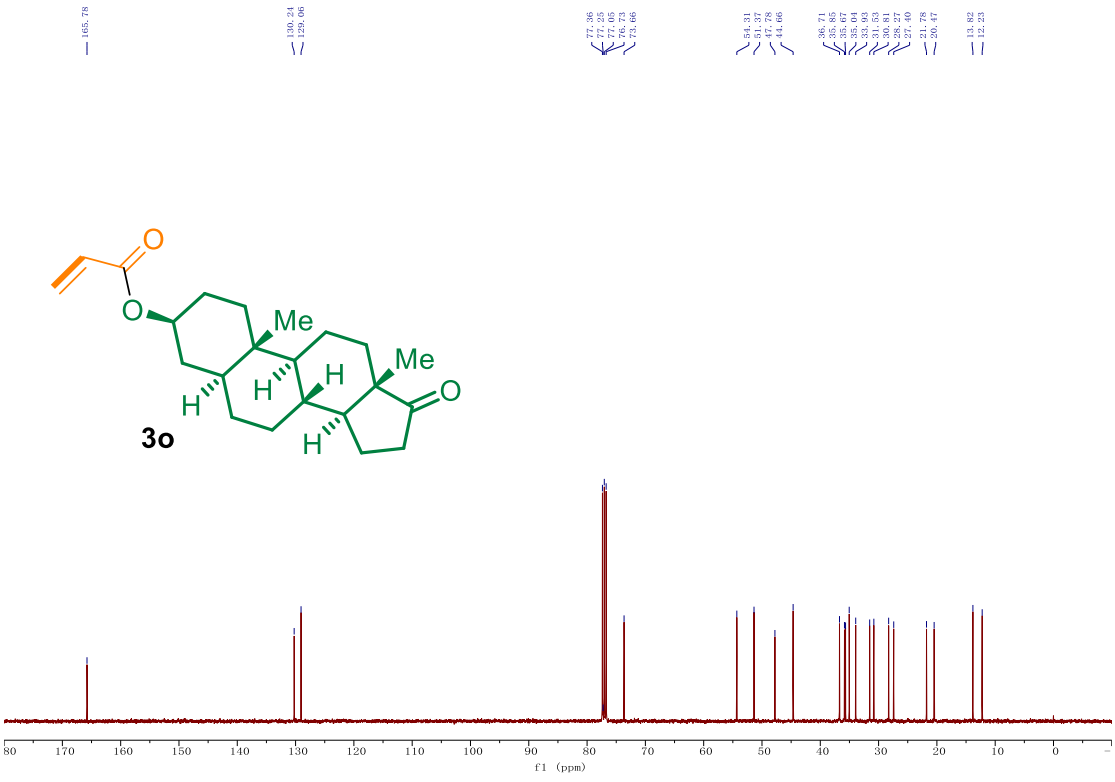
101 MHz ^{13}C NMR of **2n** in $CDCl_3$



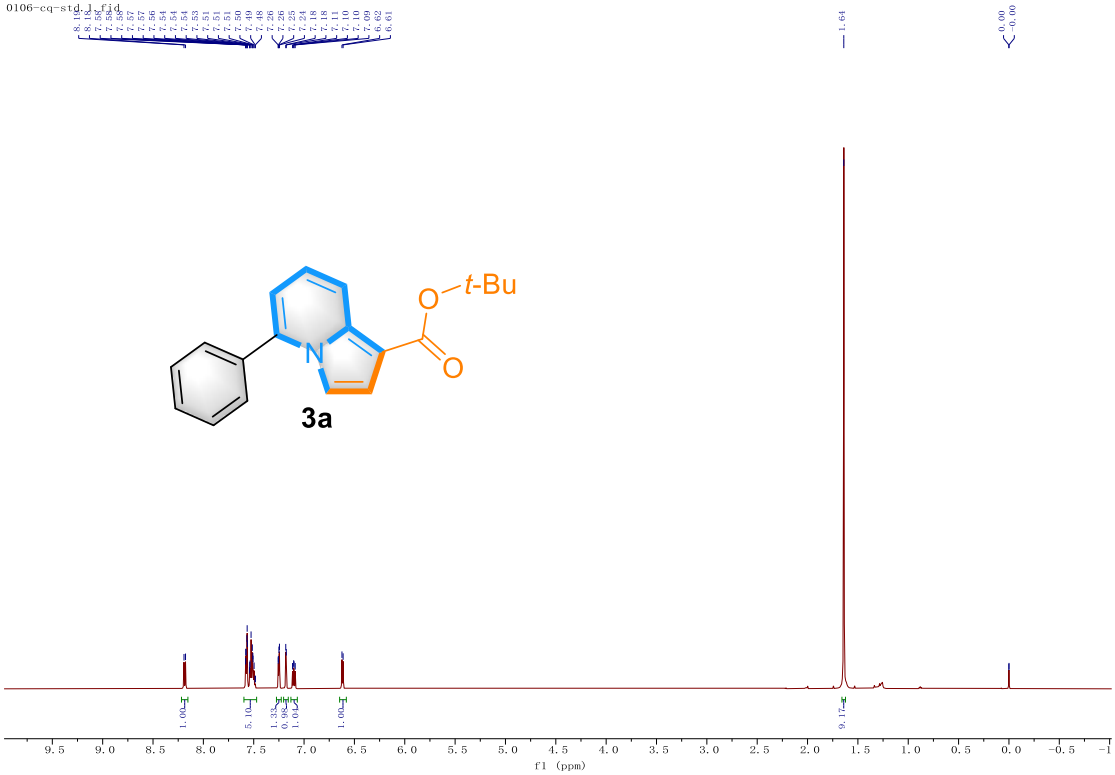
400 MHz ^{1}H NMR of **2o** in $CDCl_3$



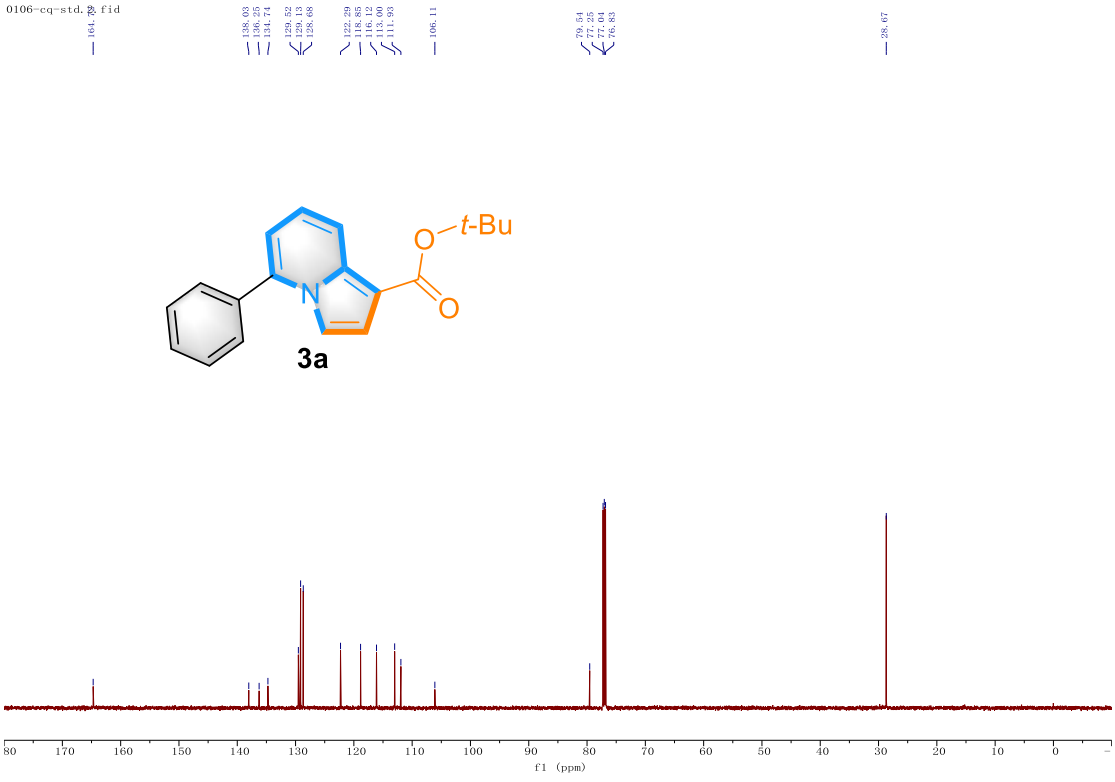
101 MHz ^{13}C NMR of **2o** in $CDCl_3$



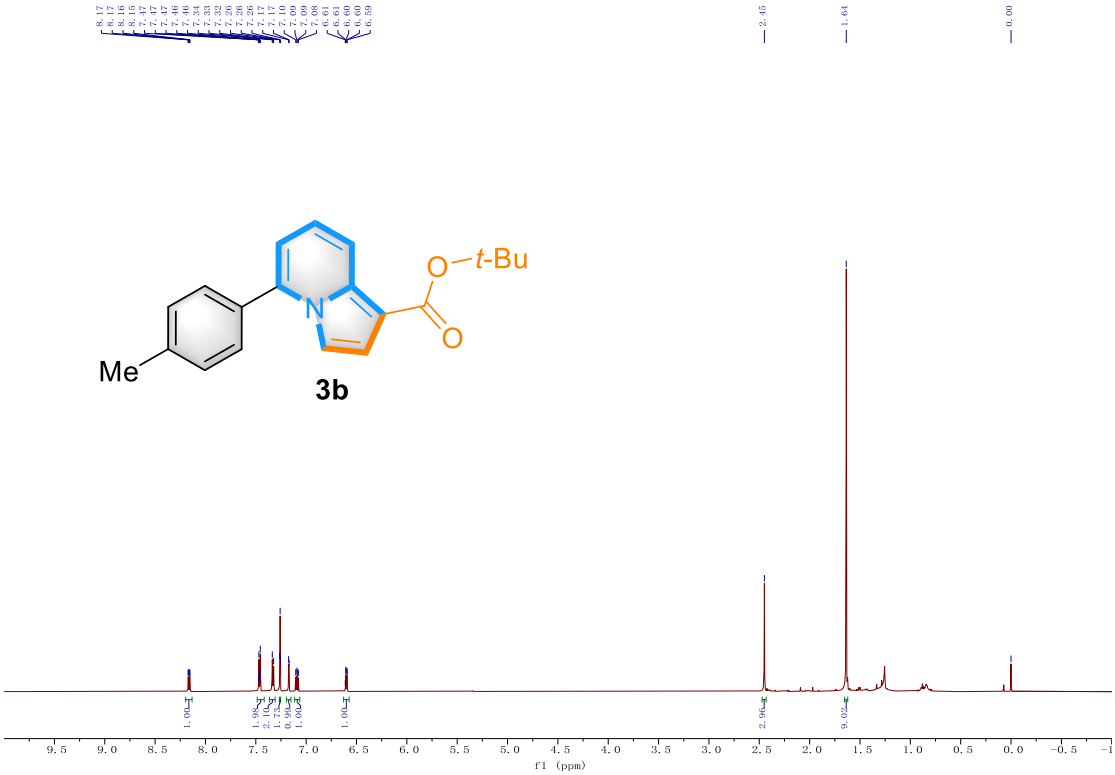
600 MHz ^{1}H NMR of **3a** in $CDCl_3$



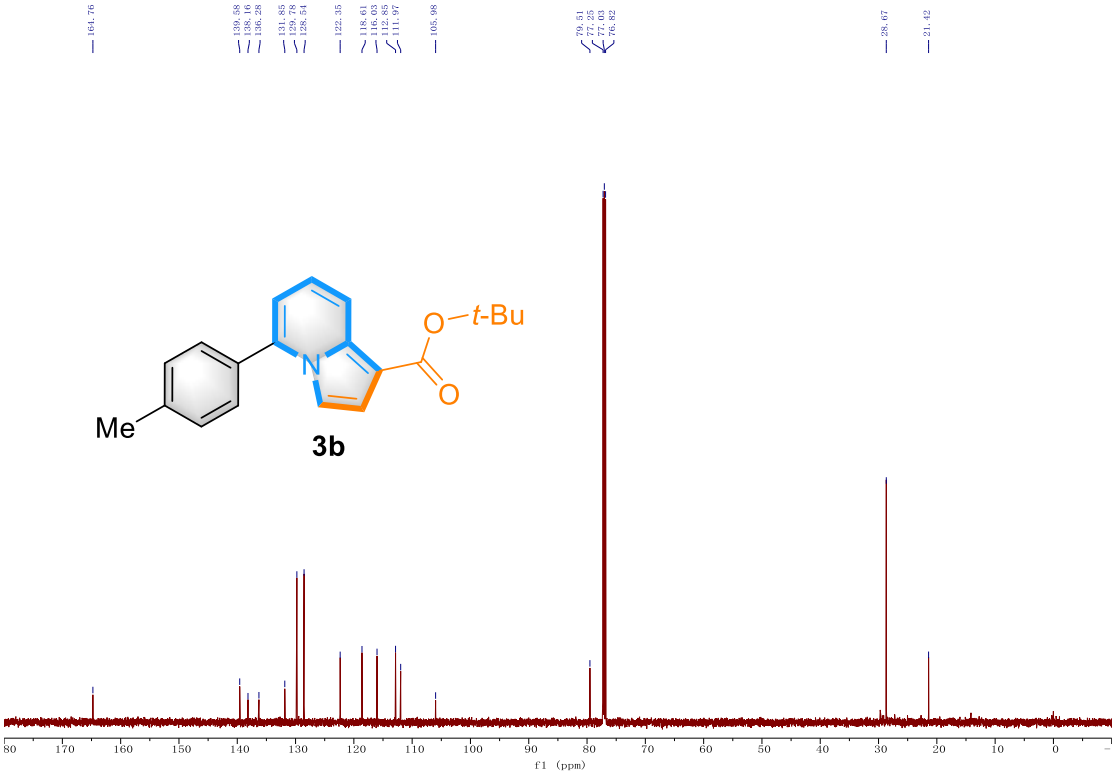
151 MHz ^{13}C NMR of **3a** in $CDCl_3$



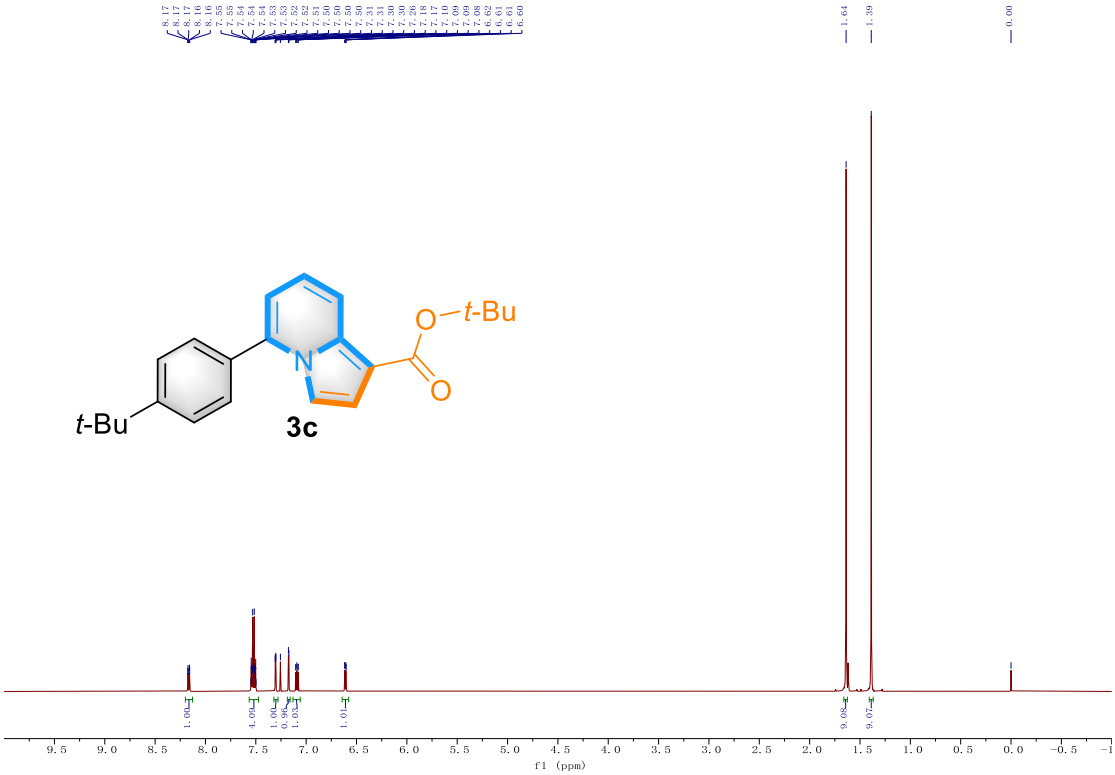
600 MHz ^{1}H NMR of **3b** in $CDCl_3$



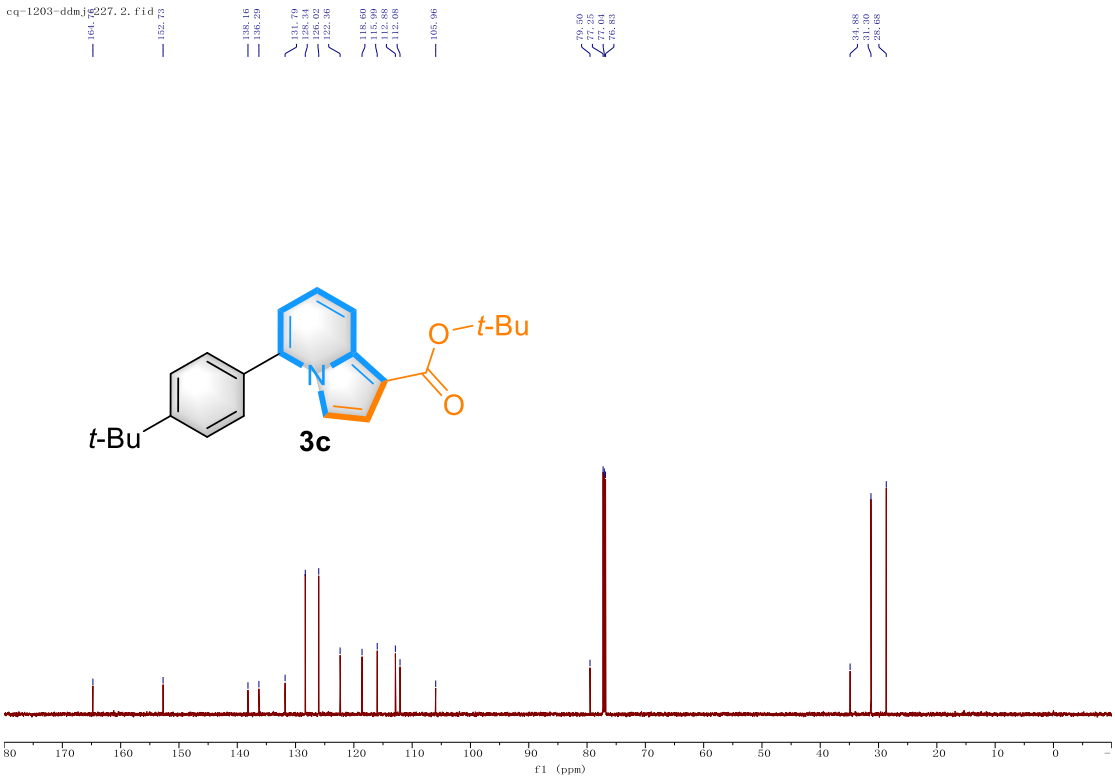
151 MHz ^{13}C NMR of **3b** in $CDCl_3$



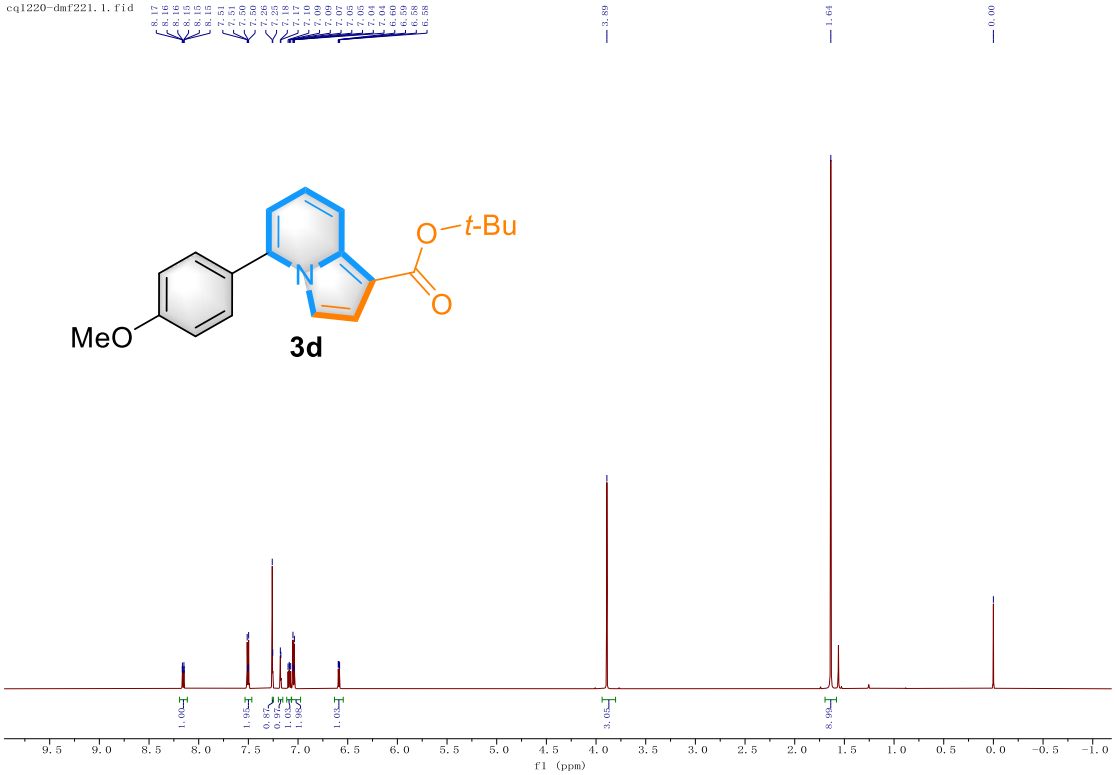
600 MHz ^{1}H NMR of **3c** in $CDCl_3$



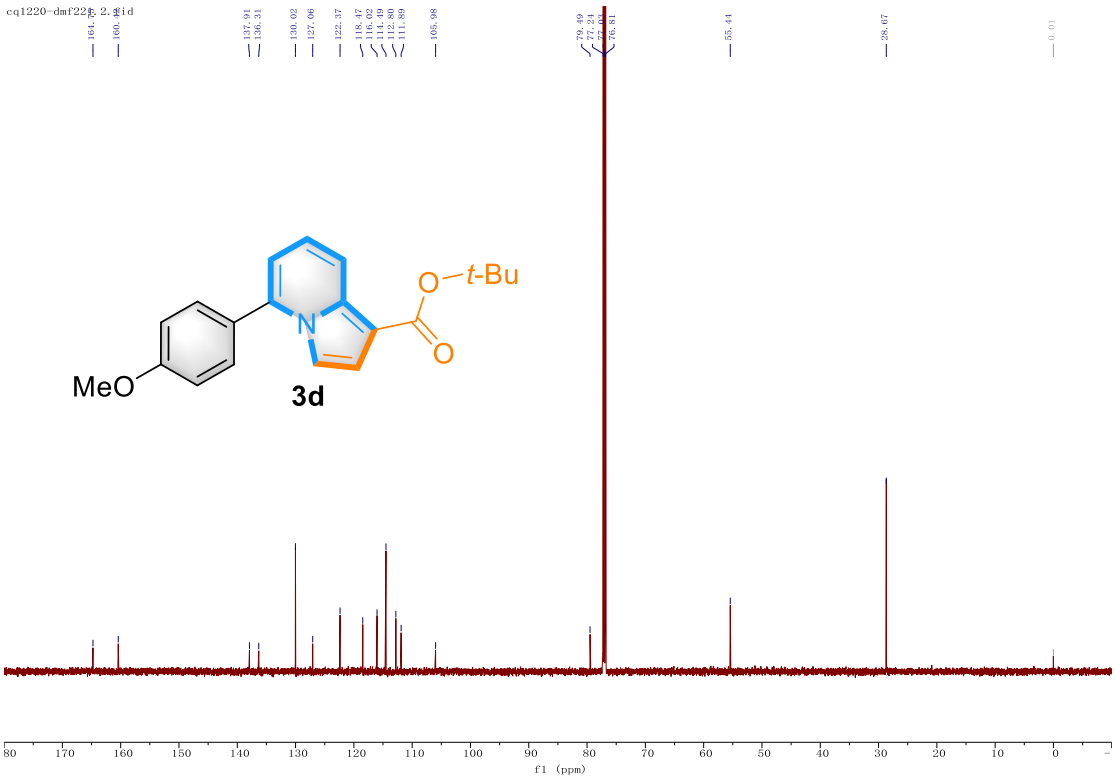
151 MHz ^{13}C NMR of **3c** in $CDCl_3$



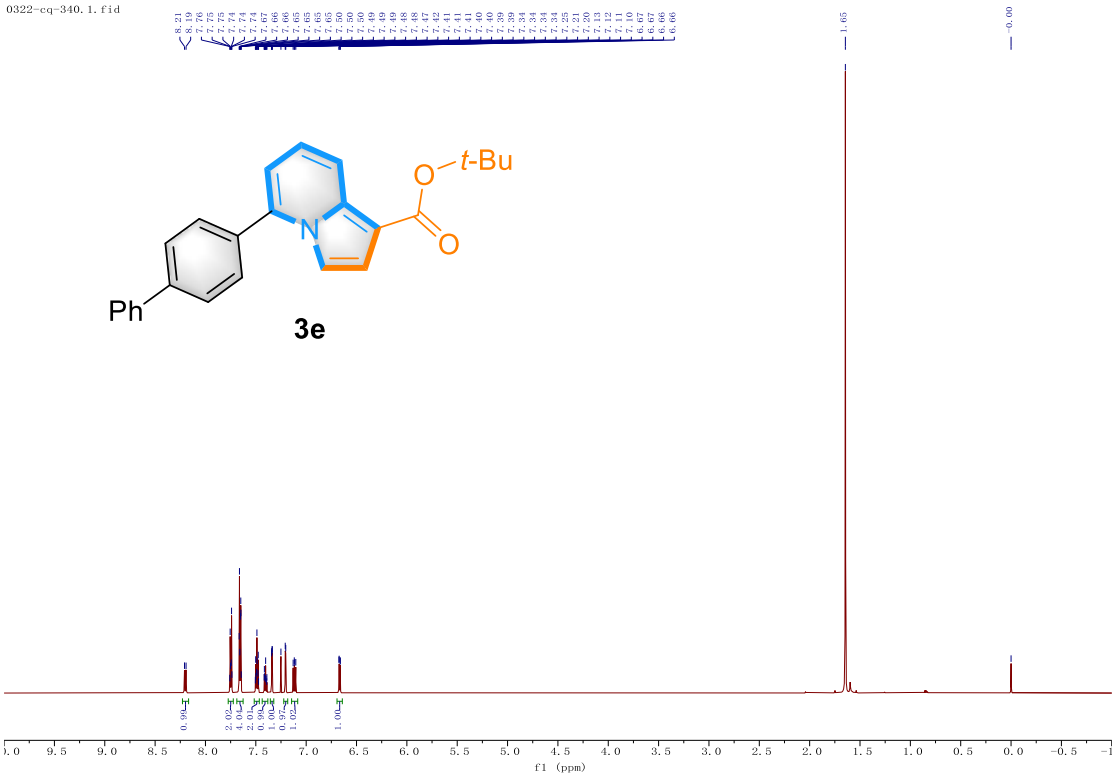
600 MHz ^{1}H NMR of **3d** in $CDCl_3$



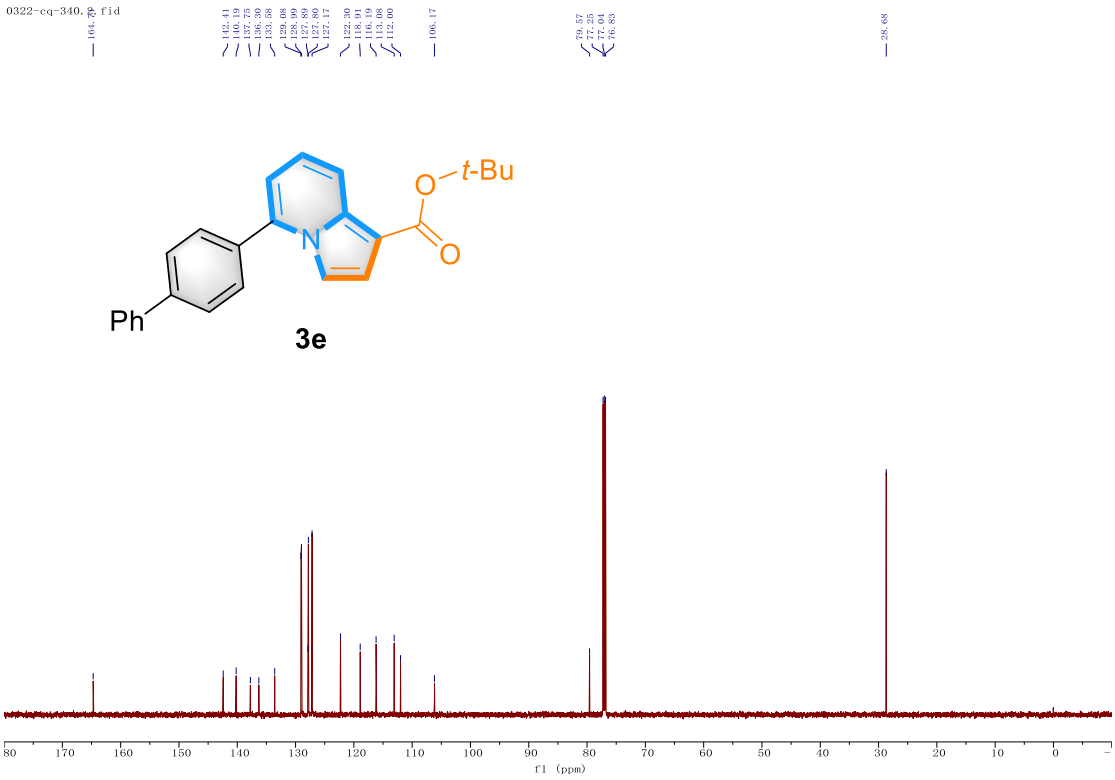
151 MHz ^{13}C NMR of **3d** in $CDCl_3$



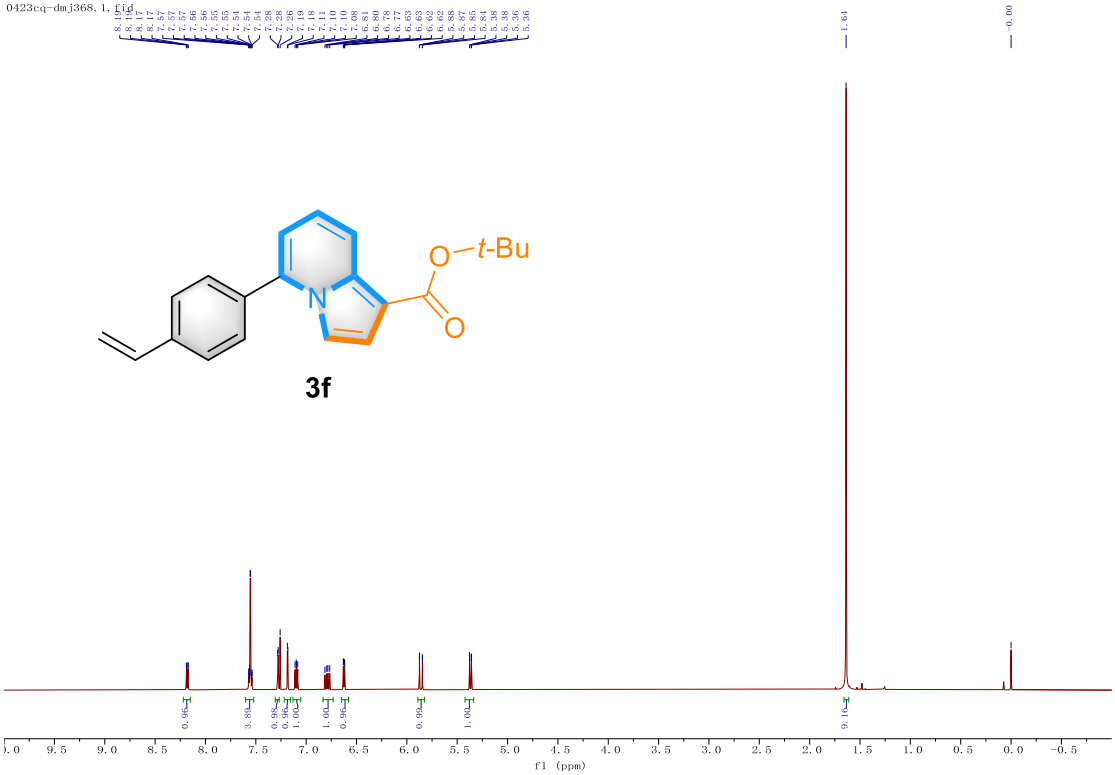
600 MHz ^{1}H NMR of **3e** in $CDCl_3$



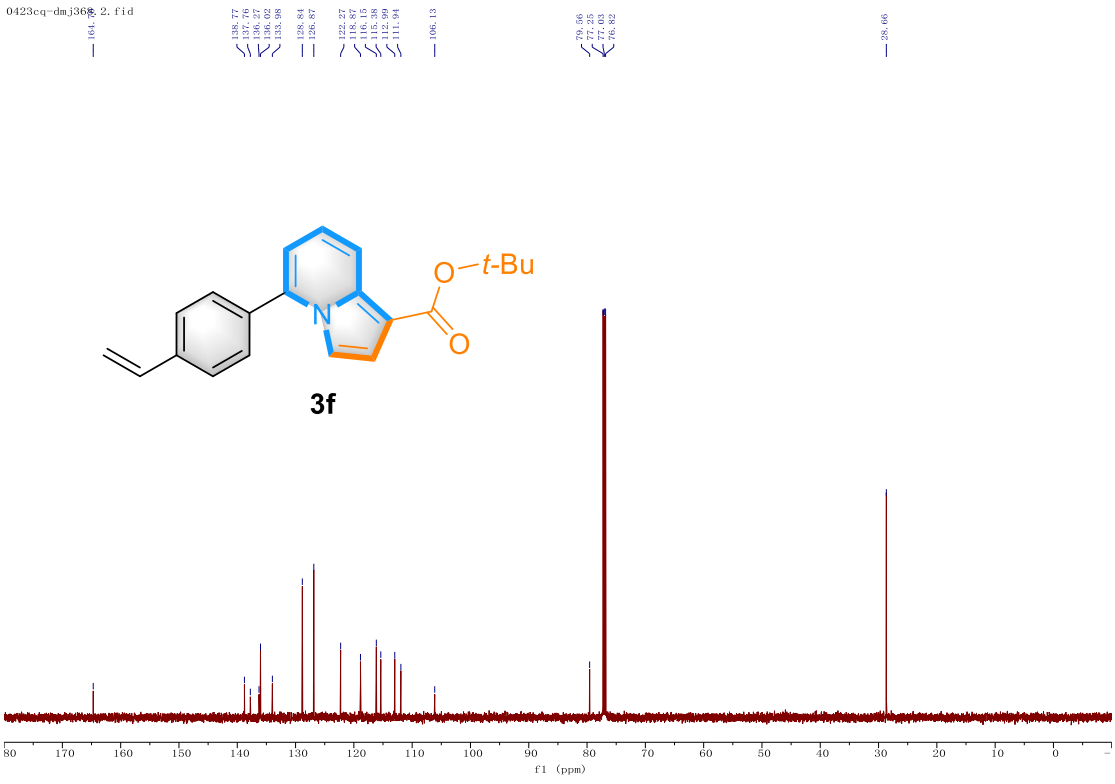
151 MHz ^{13}C NMR of **3e** in $CDCl_3$



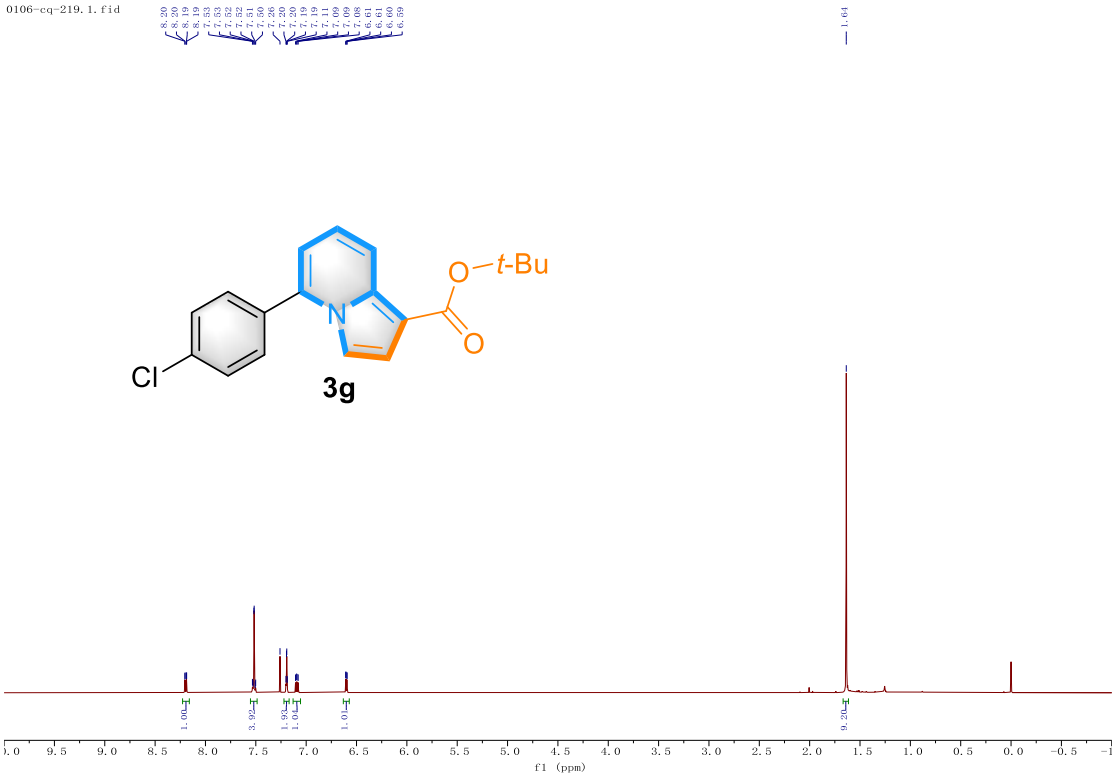
600 MHz ^{1}H NMR of **3f** in $CDCl_3$



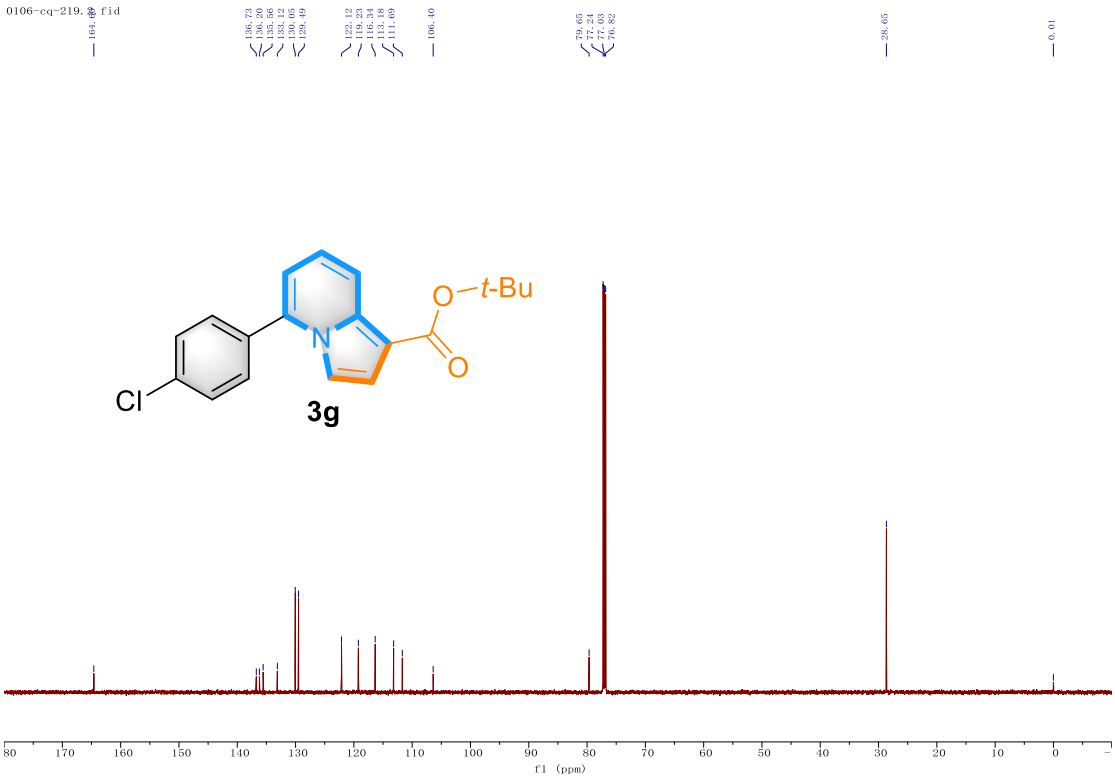
151 MHz ^{13}C NMR of **3f** in $CDCl_3$



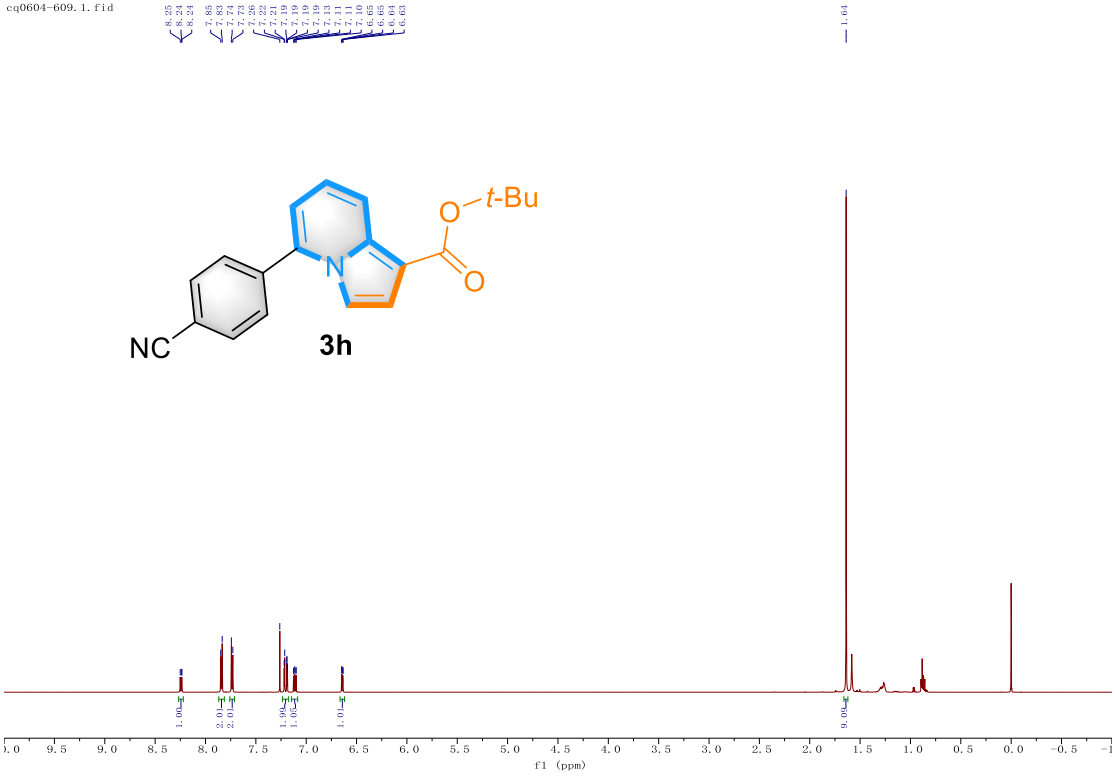
600 MHz ^{1}H NMR of **3g** in $CDCl_3$



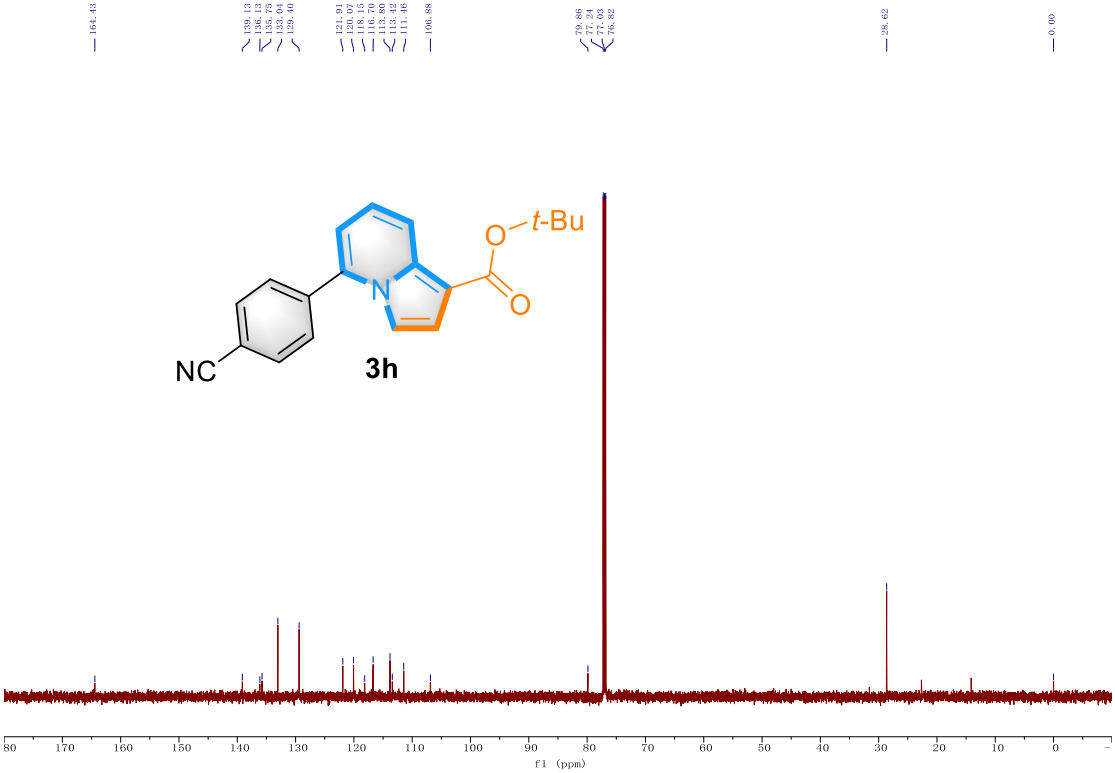
151 MHz ^{13}C NMR of **3g** in $CDCl_3$



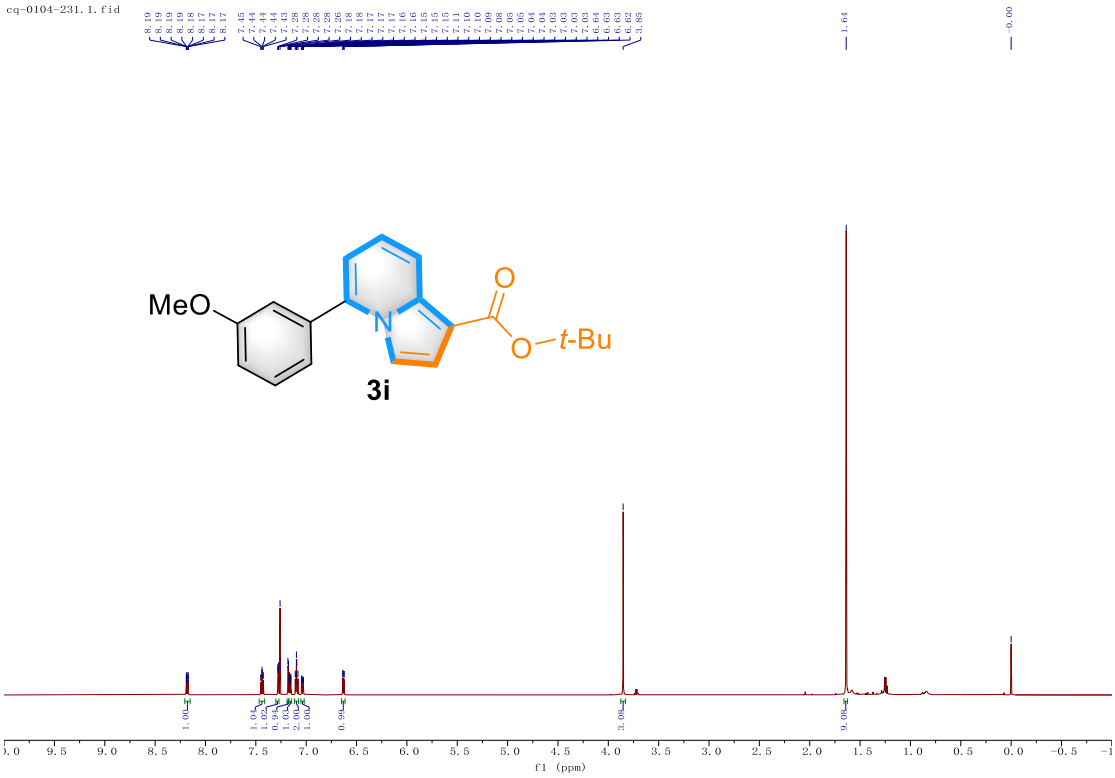
600 MHz ^{1}H NMR of **3h** in $CDCl_3$



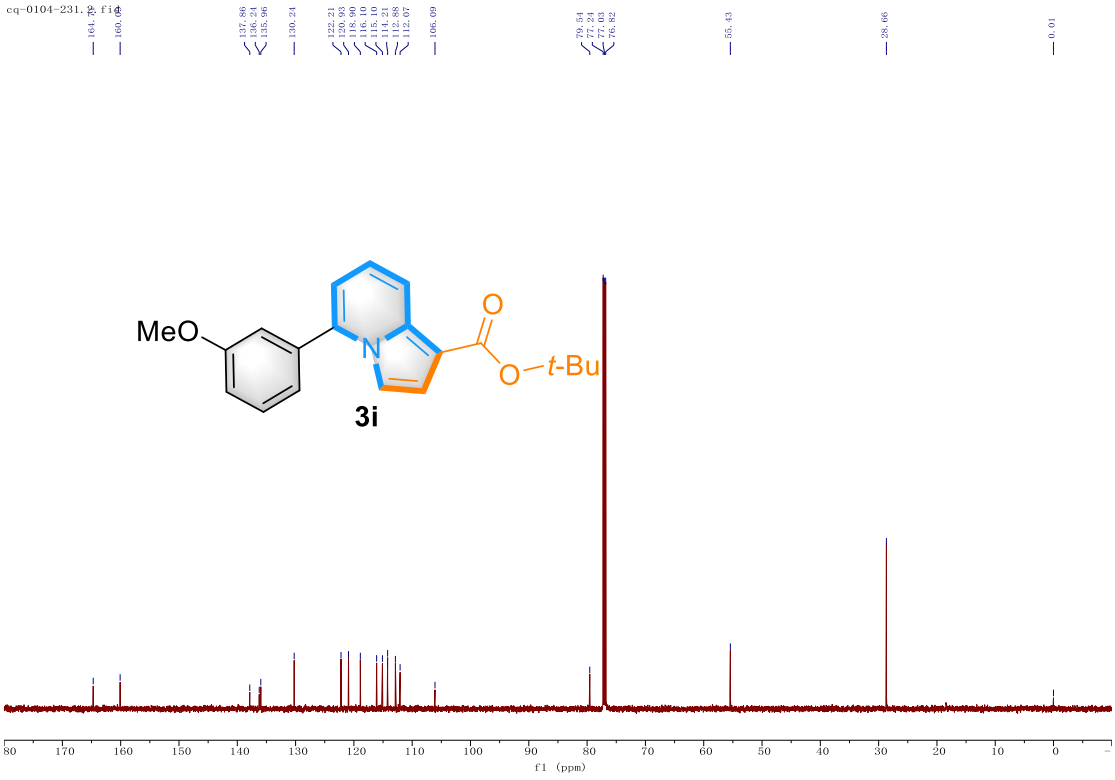
151 MHz ^{13}C NMR of **3h** in $CDCl_3$



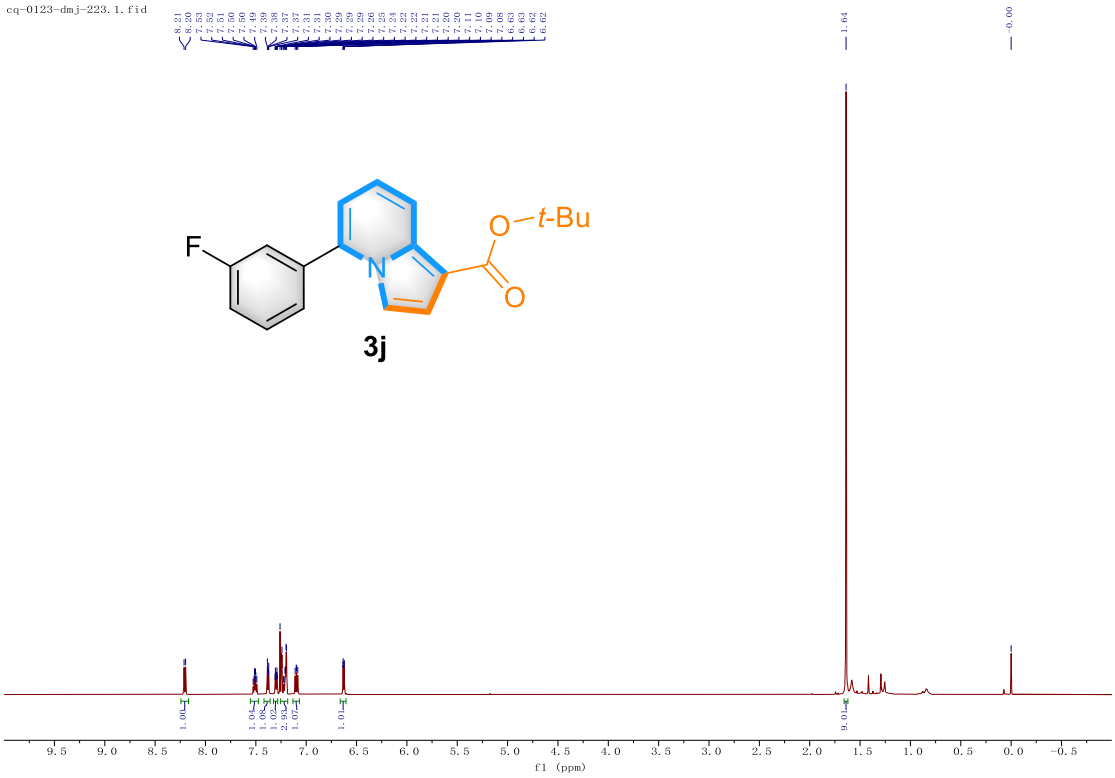
600 MHz ^{1}H NMR of **3i** in $CDCl_3$



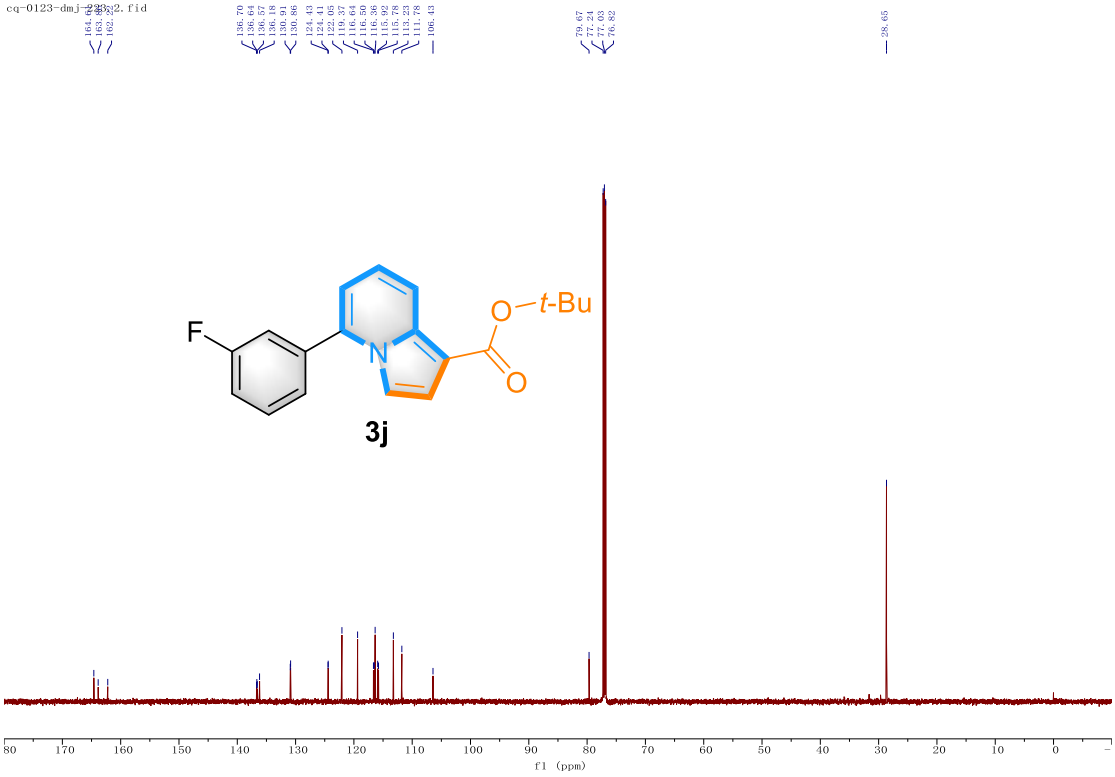
151 MHz ^{13}C NMR of **3i** in $CDCl_3$



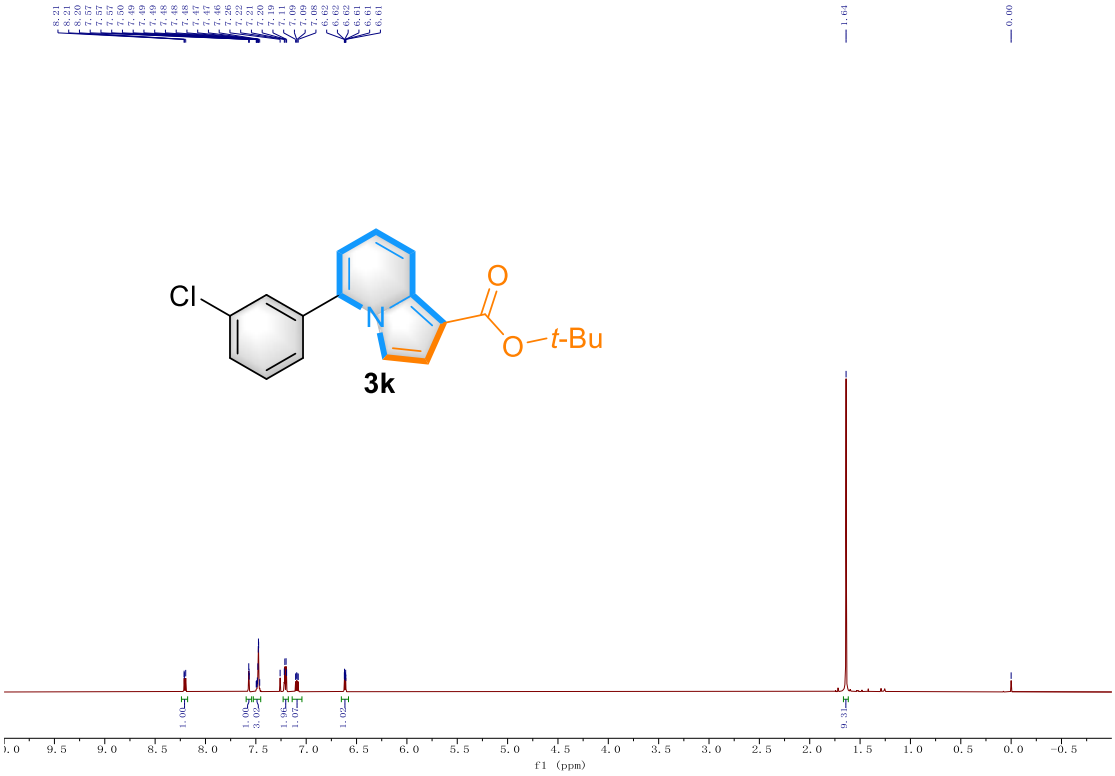
600 MHz ^{1}H NMR of **3j** in $CDCl_3$



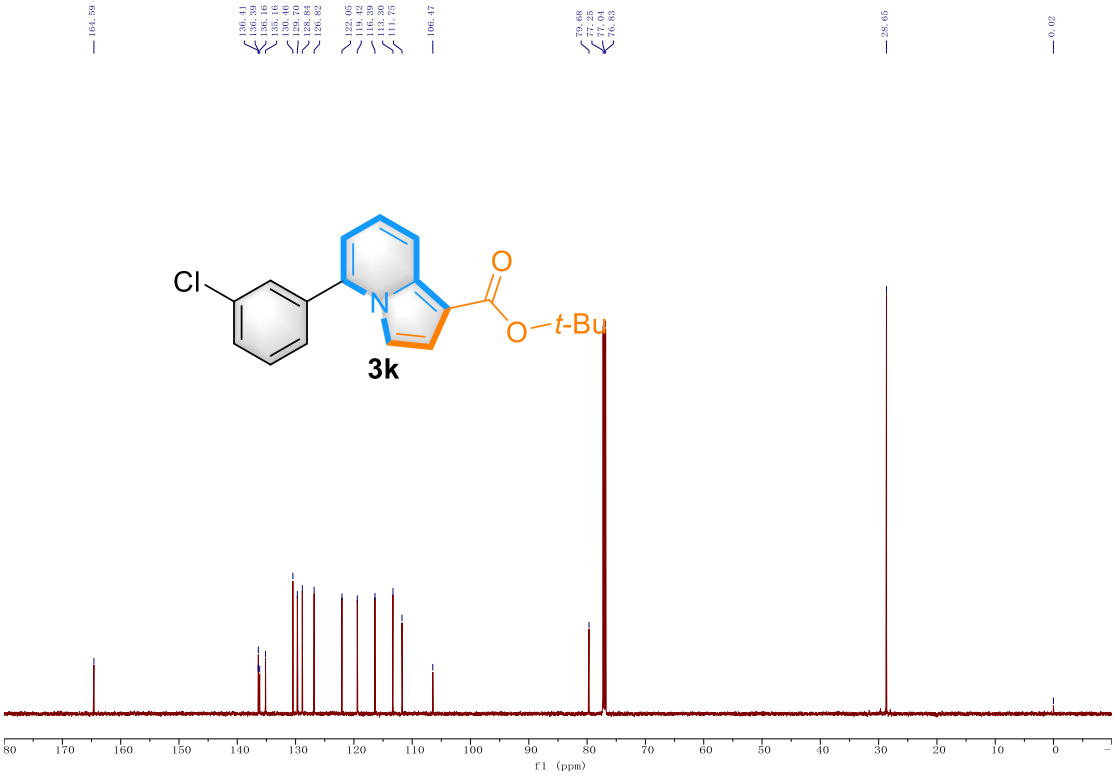
151 MHz ^{13}C NMR of **3j** in $CDCl_3$



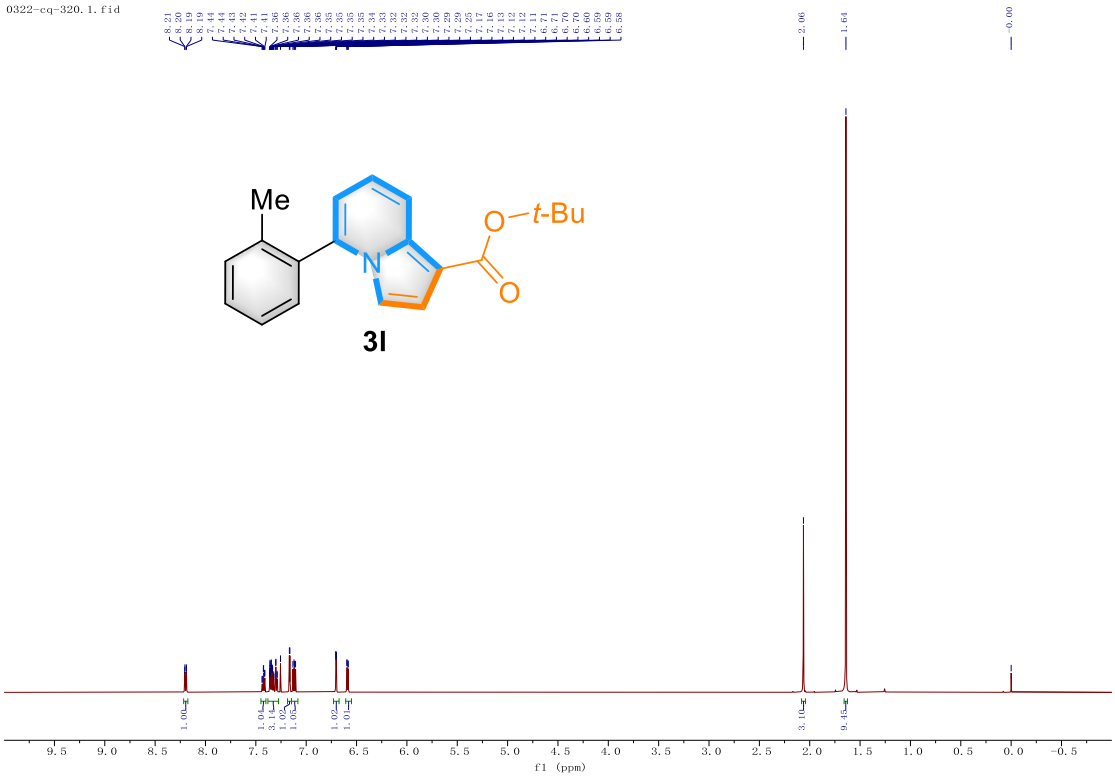
600 MHz ^{1}H NMR of **3k** in $CDCl_3$



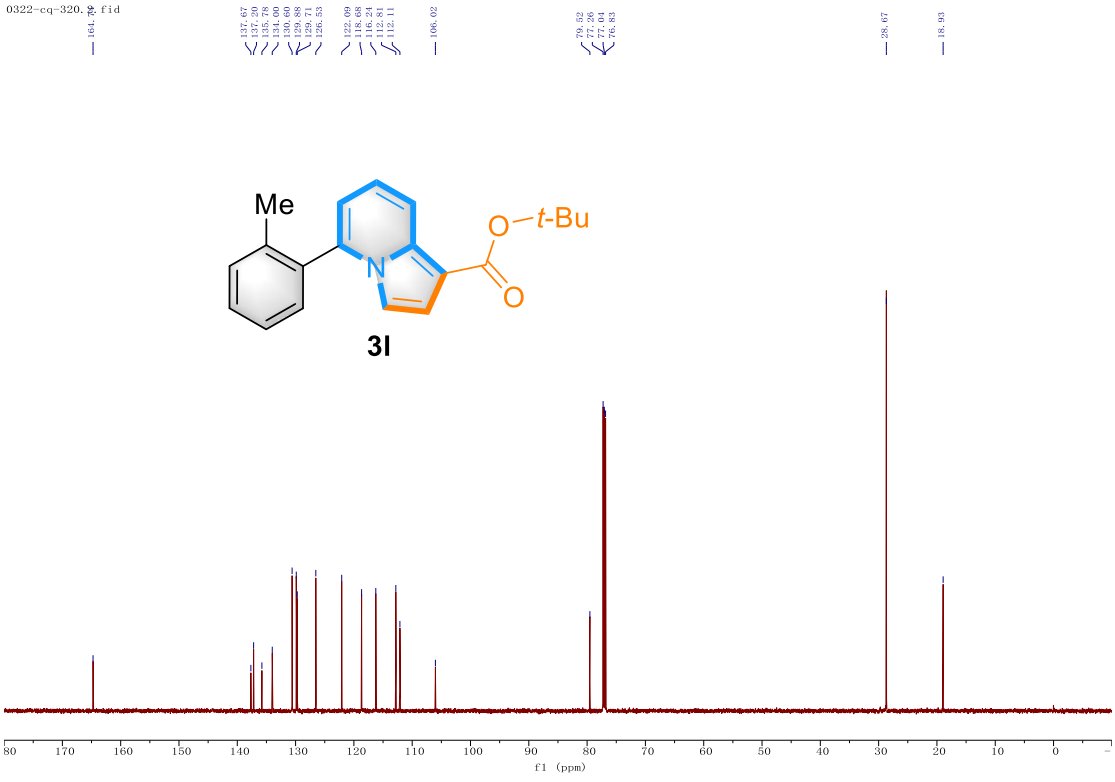
151 MHz ^{13}C NMR of **3k** in $CDCl_3$



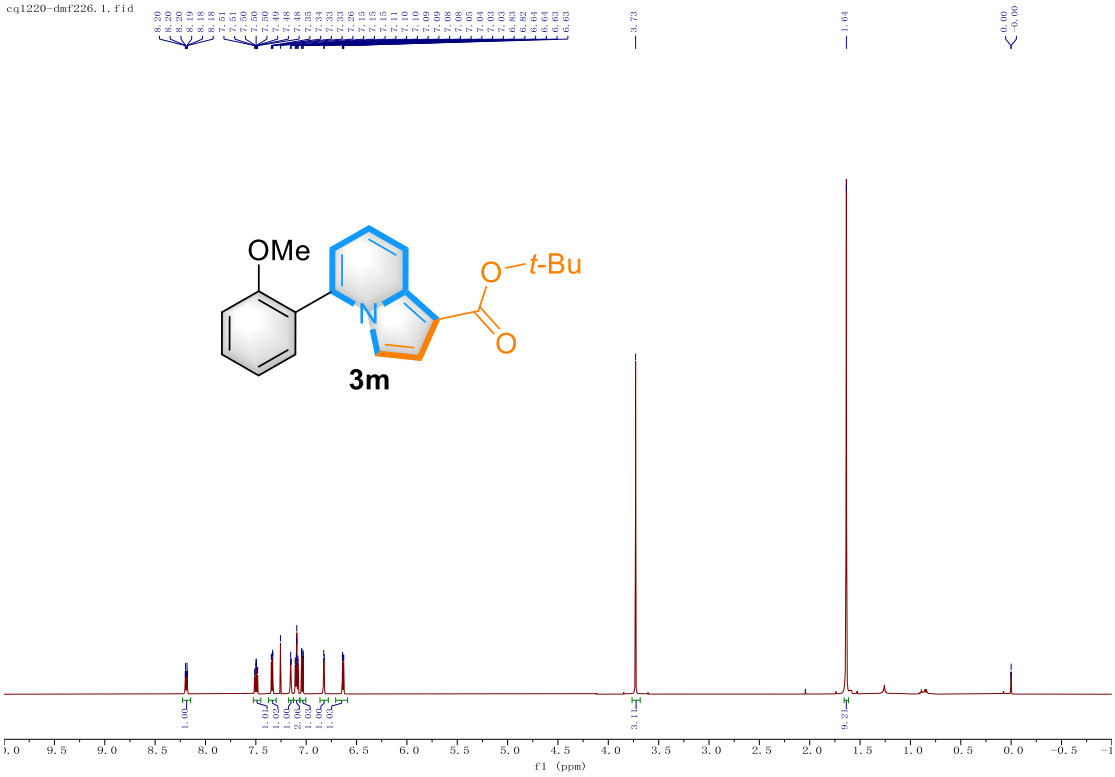
600 MHz ^{1}H NMR of **3l** in $CDCl_3$



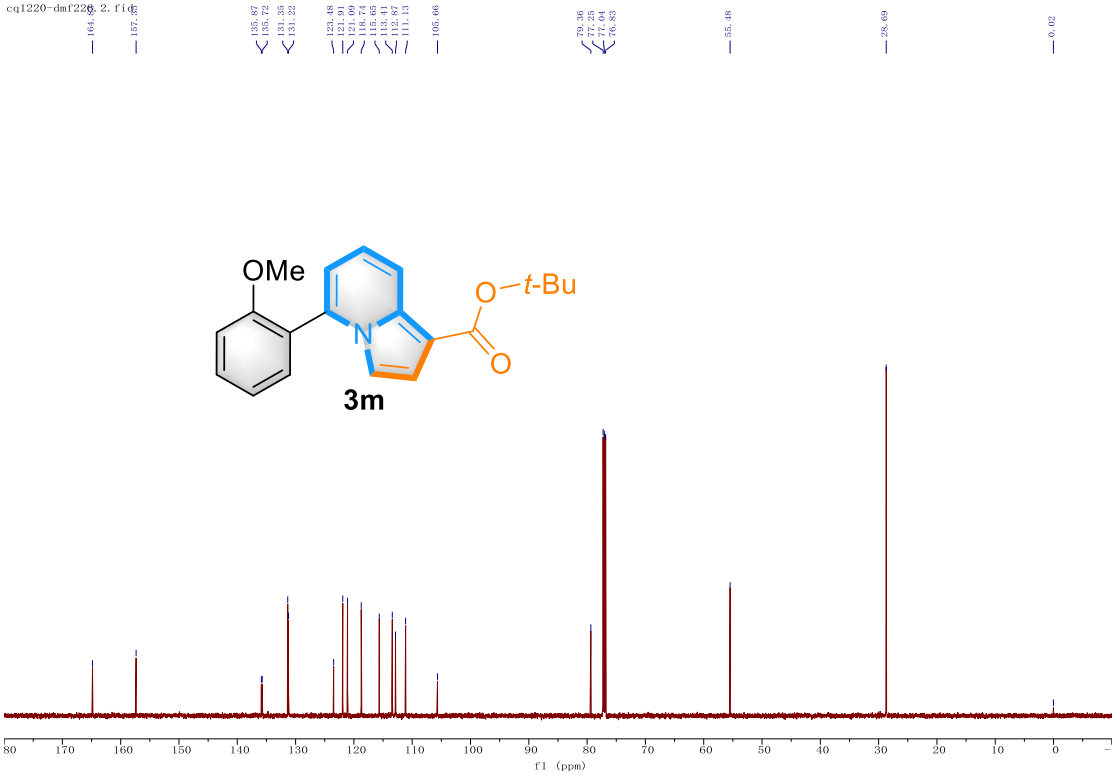
151 MHz ^{13}C NMR of **3l** in $CDCl_3$



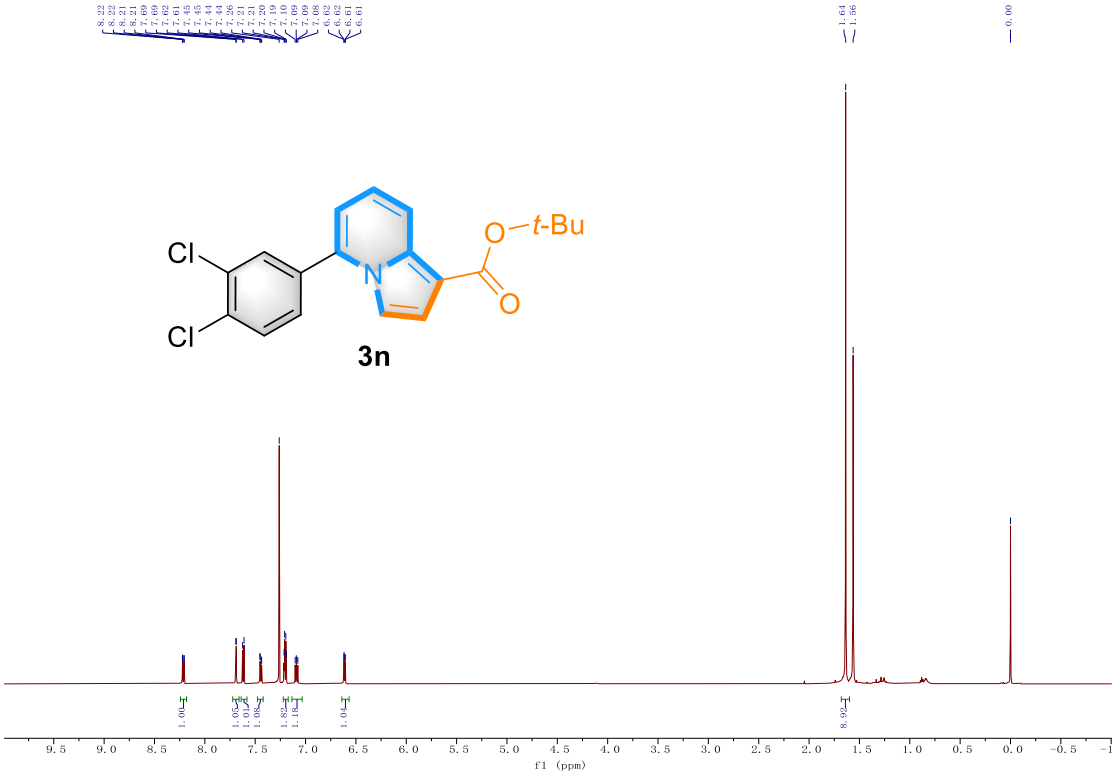
600 MHz ^{1}H NMR of **3m** in $CDCl_3$



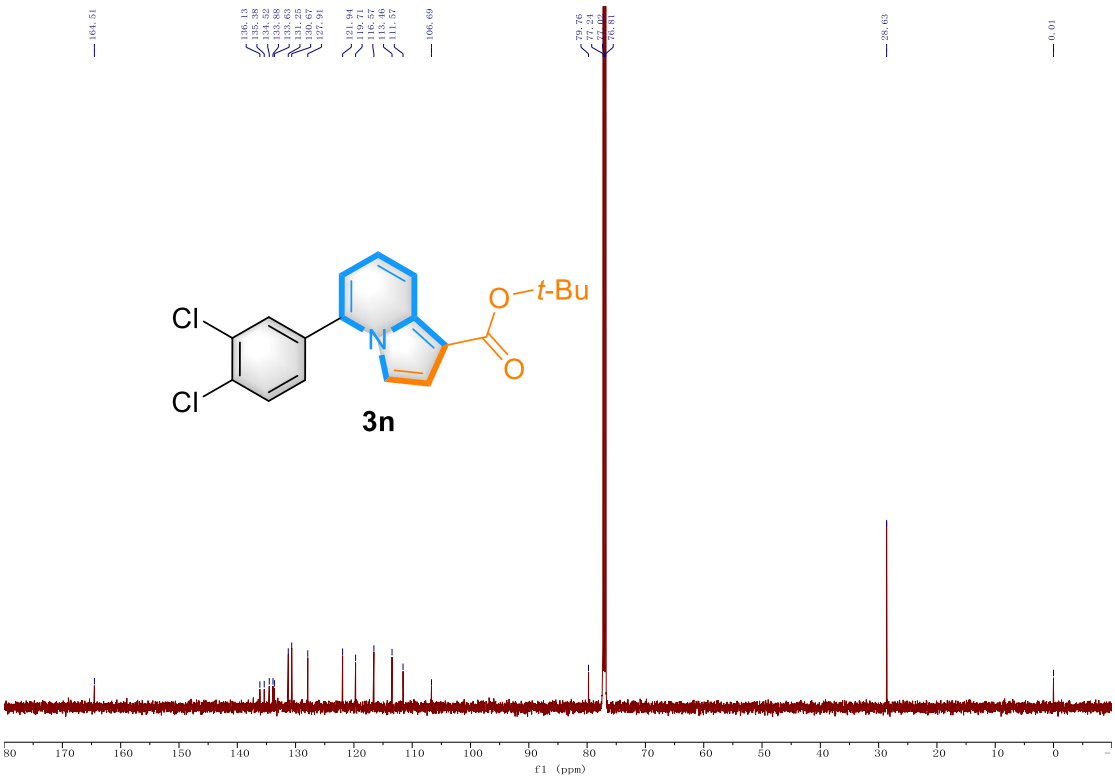
151 MHz ^{13}C NMR of **3m** in $CDCl_3$



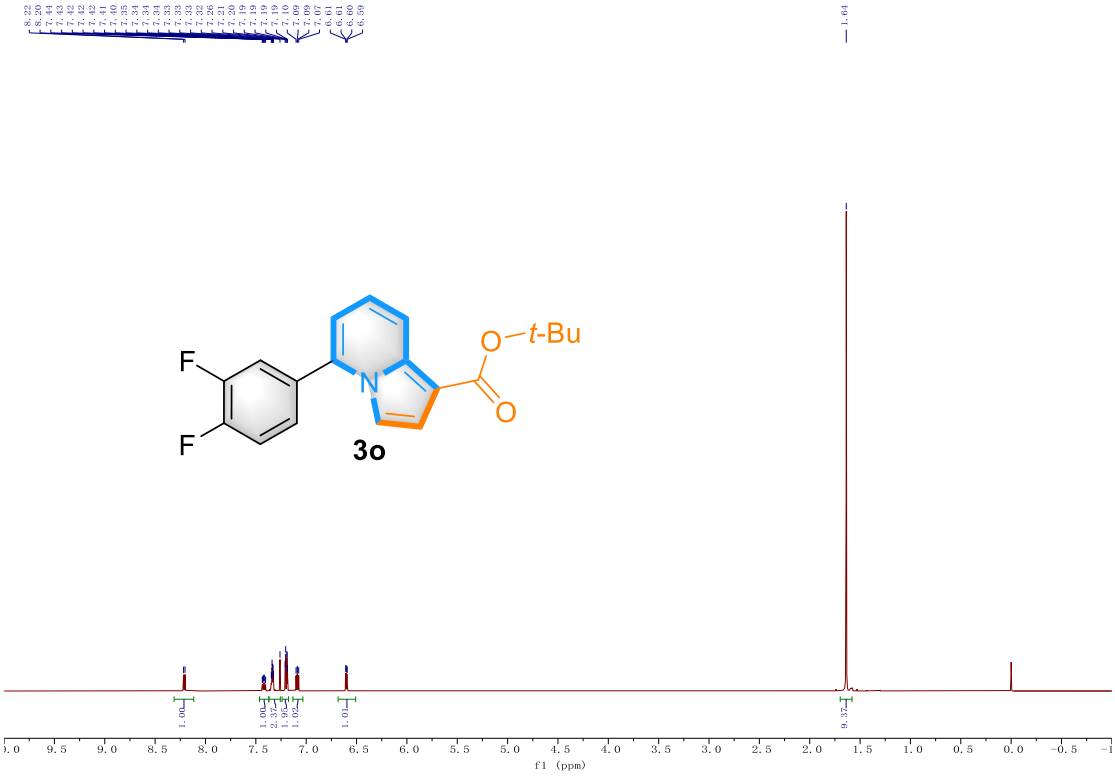
600 MHz ^{1}H NMR of **3n** in $CDCl_3$



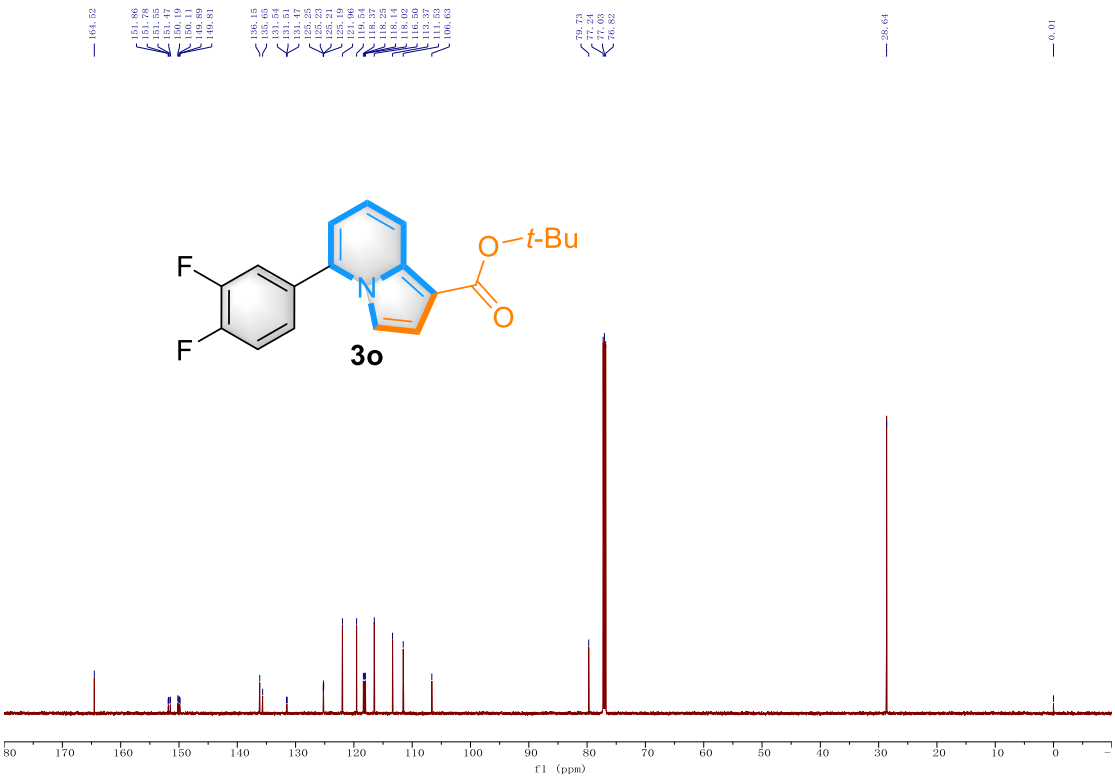
151 MHz ^{13}C NMR of **3n** in $CDCl_3$



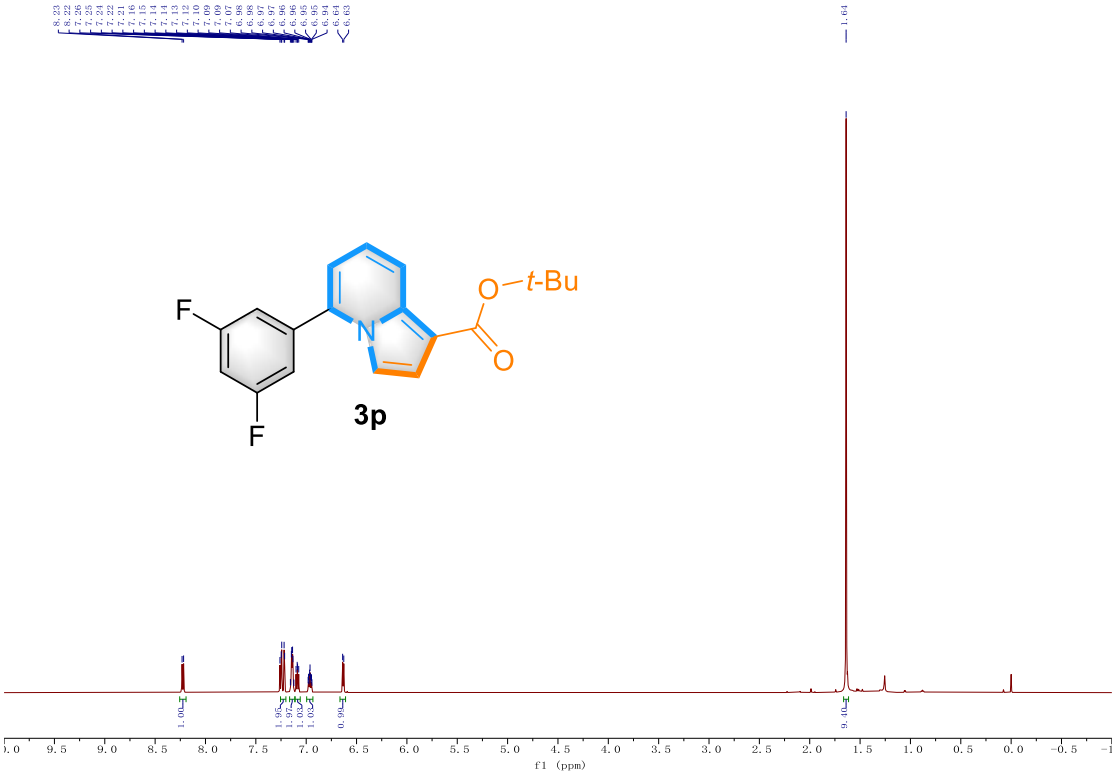
600 MHz ^{1}H NMR of **3o** in $CDCl_3$



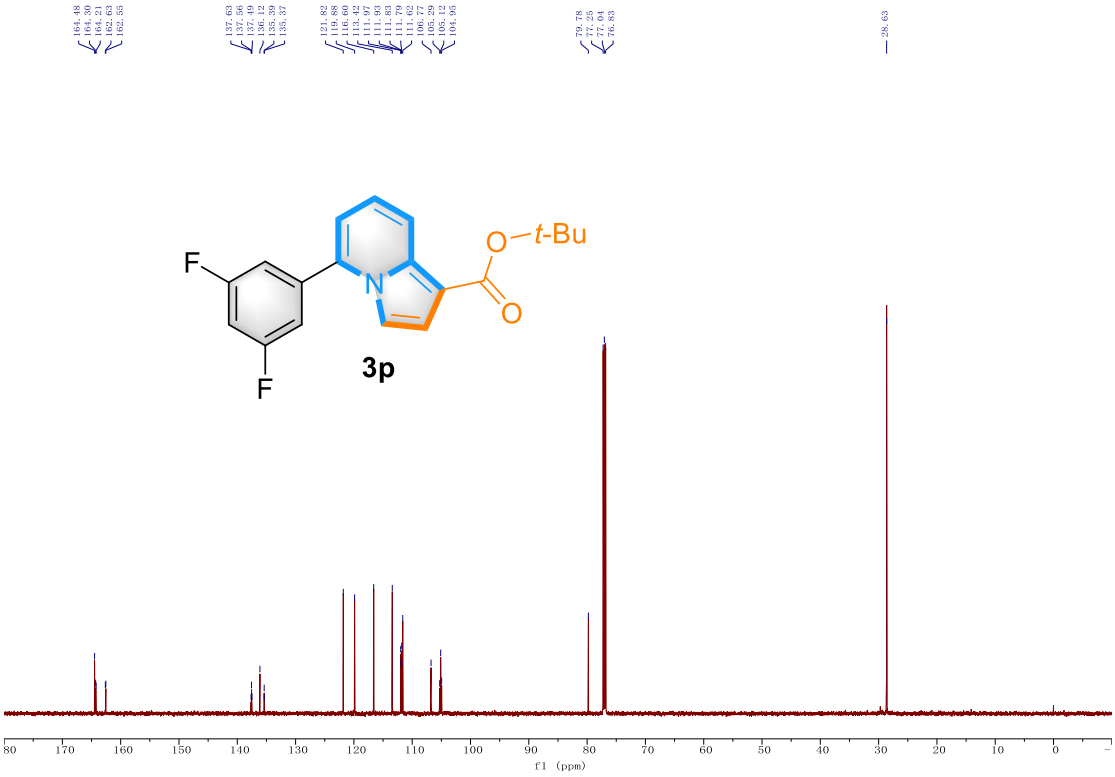
151 MHz ^{13}C NMR of **3o** in $CDCl_3$



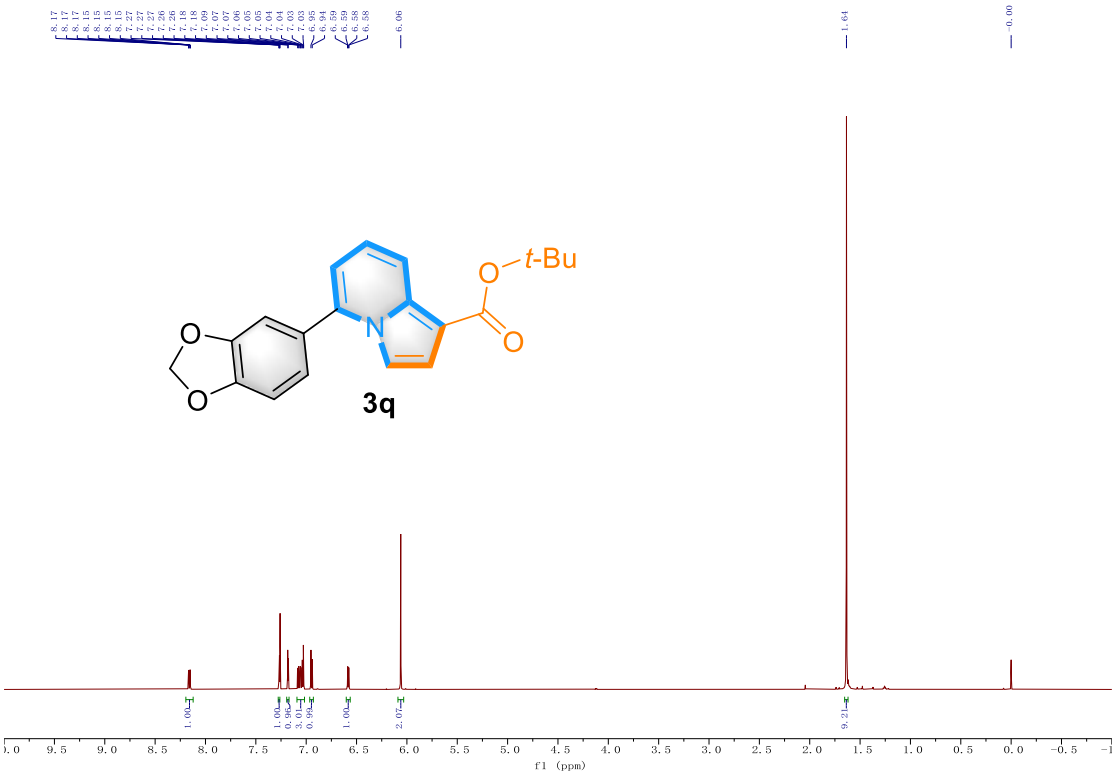
600 MHz ^{1}H NMR of **3p** in $CDCl_3$



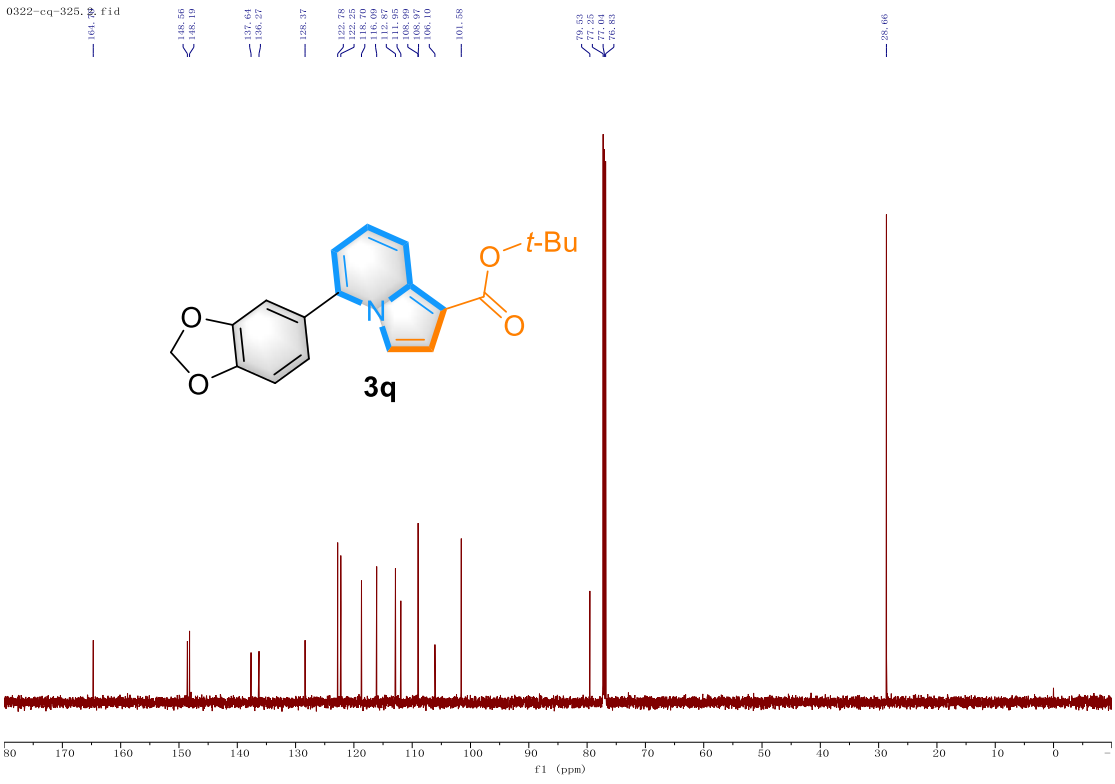
151 MHz ^{13}C NMR of **3p** in $CDCl_3$



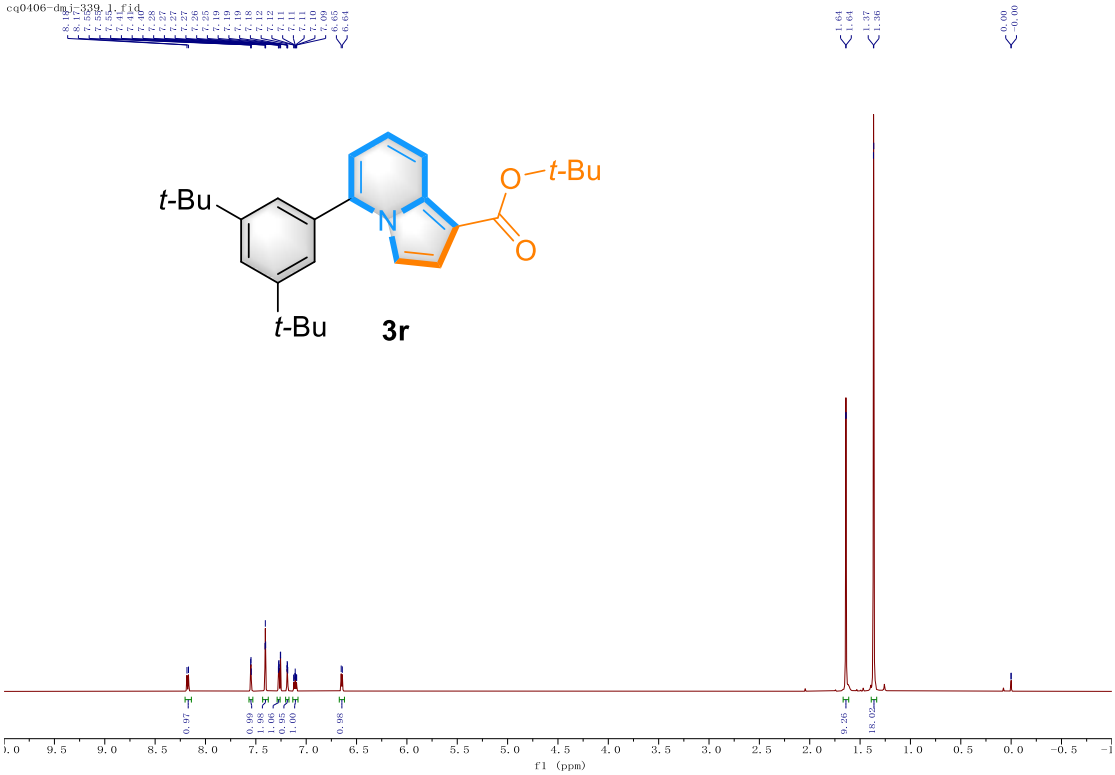
600 MHz ^{1}H NMR of **3q** in $CDCl_3$



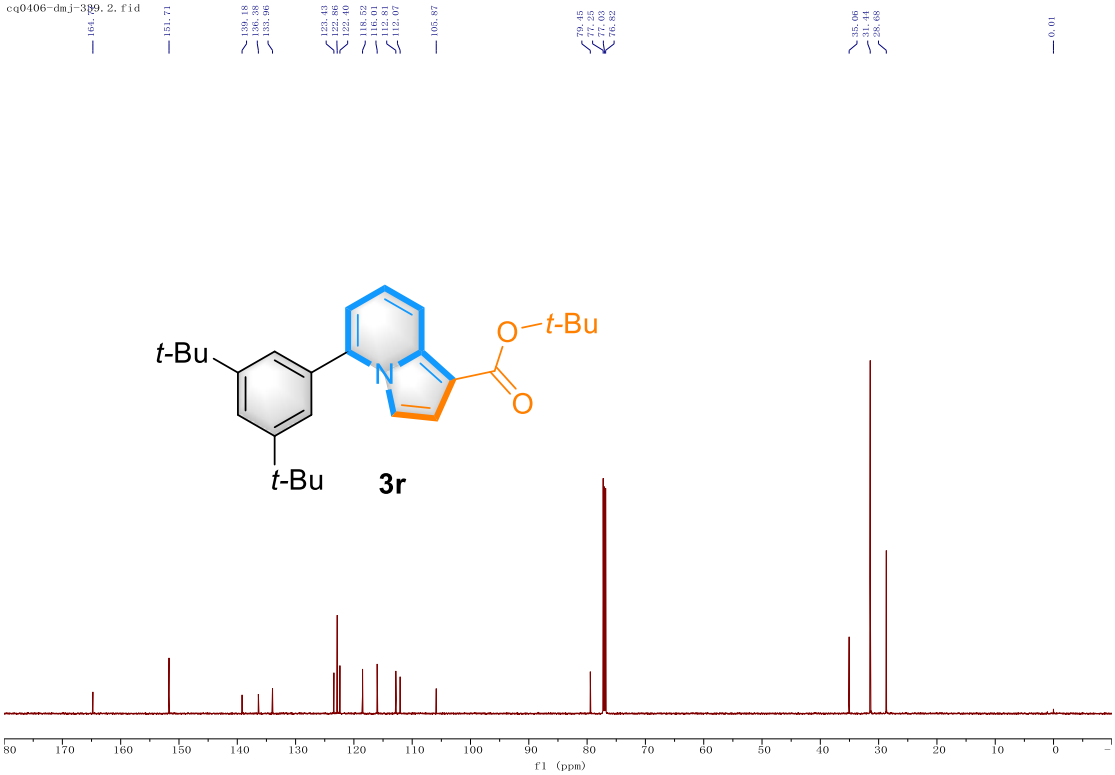
151 MHz ^{13}C NMR of **3q** in $CDCl_3$



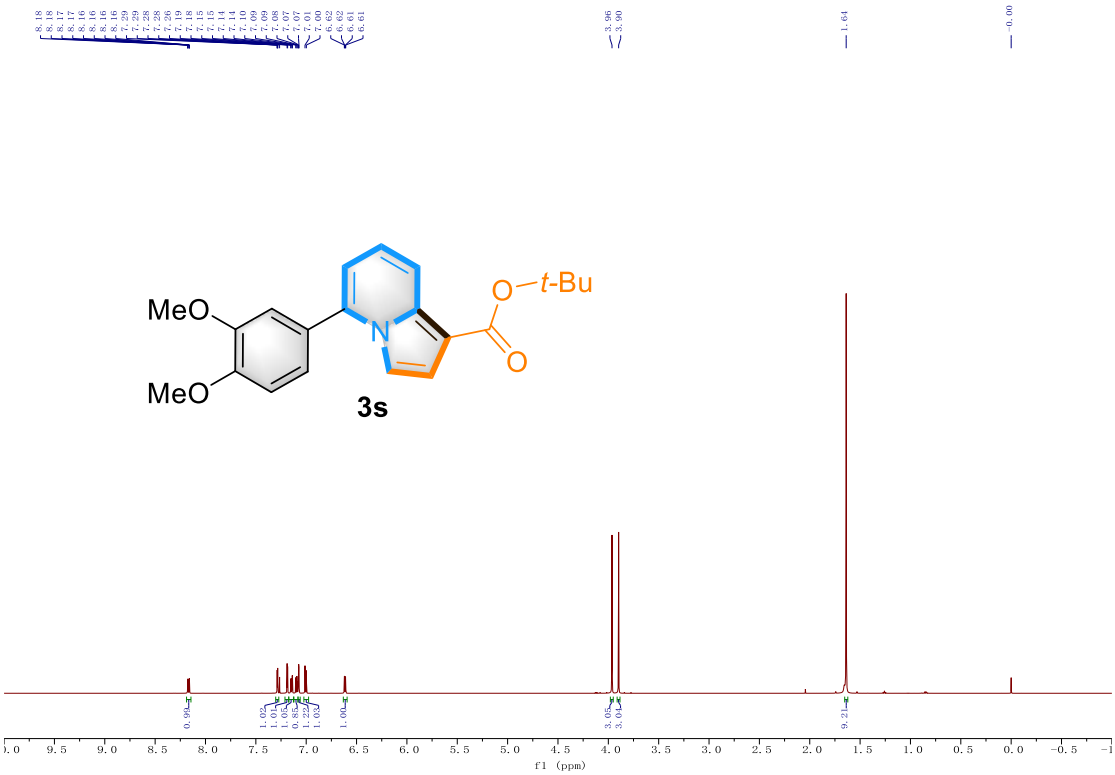
600 MHz ^{1}H NMR of **3r** in $CDCl_3$



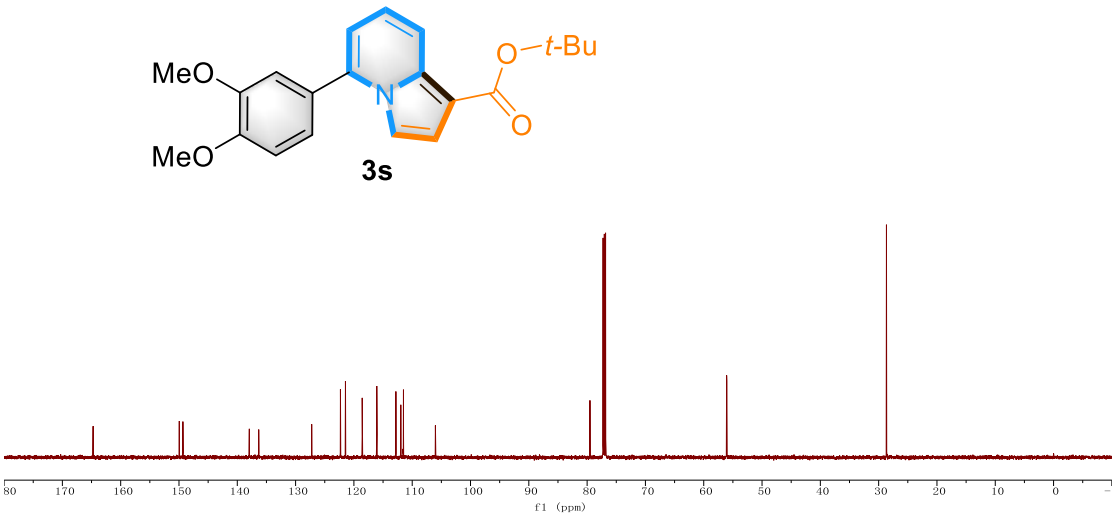
151 MHz ^{13}C NMR of **3r** in $CDCl_3$



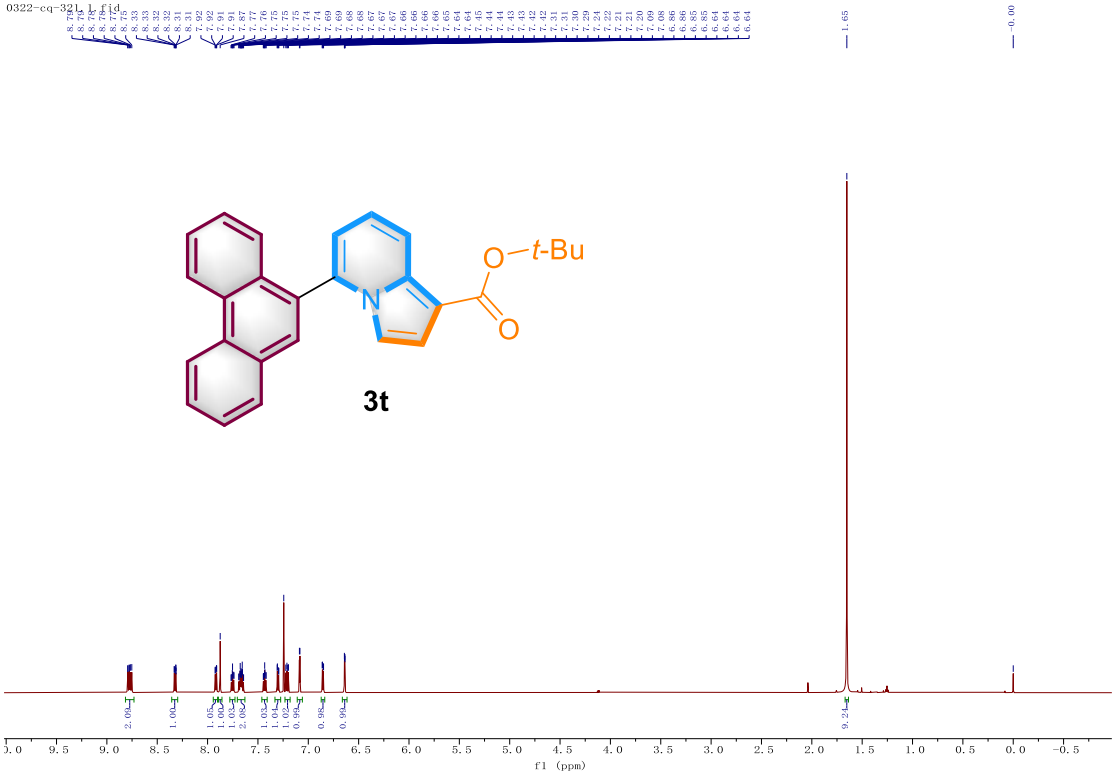
600 MHz ^{1}H NMR of **3s** in $CDCl_3$



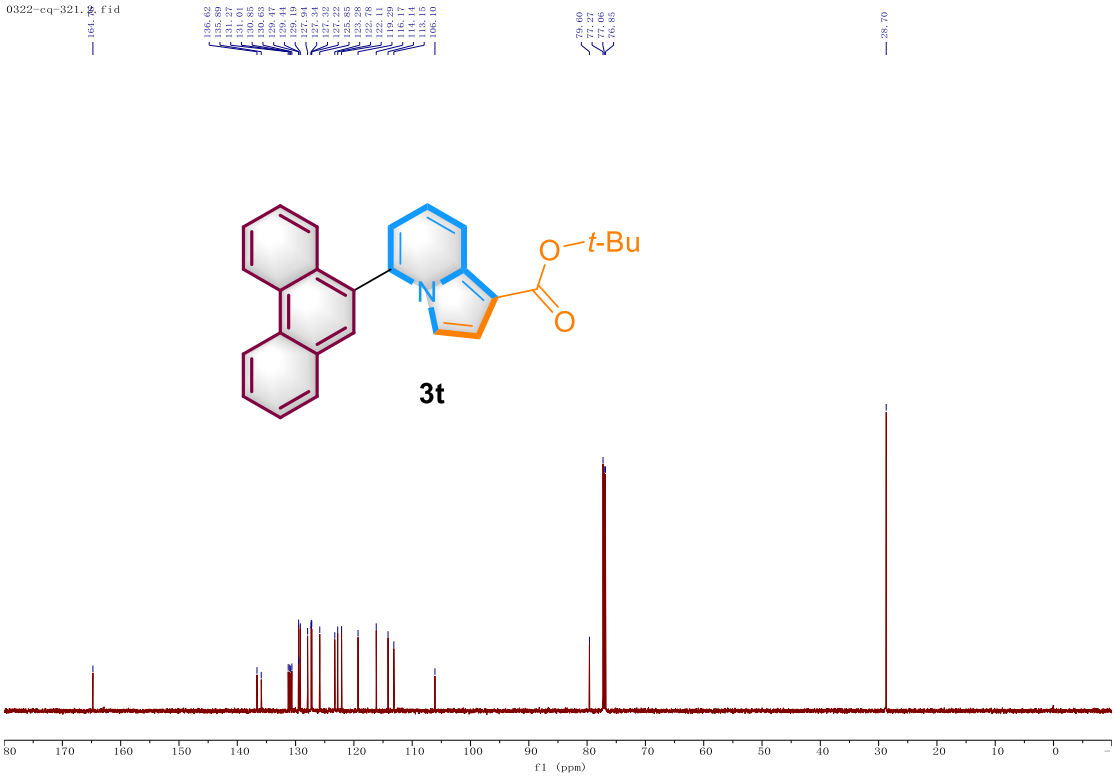
151 MHz ^{13}C NMR of **3s** in $CDCl_3$



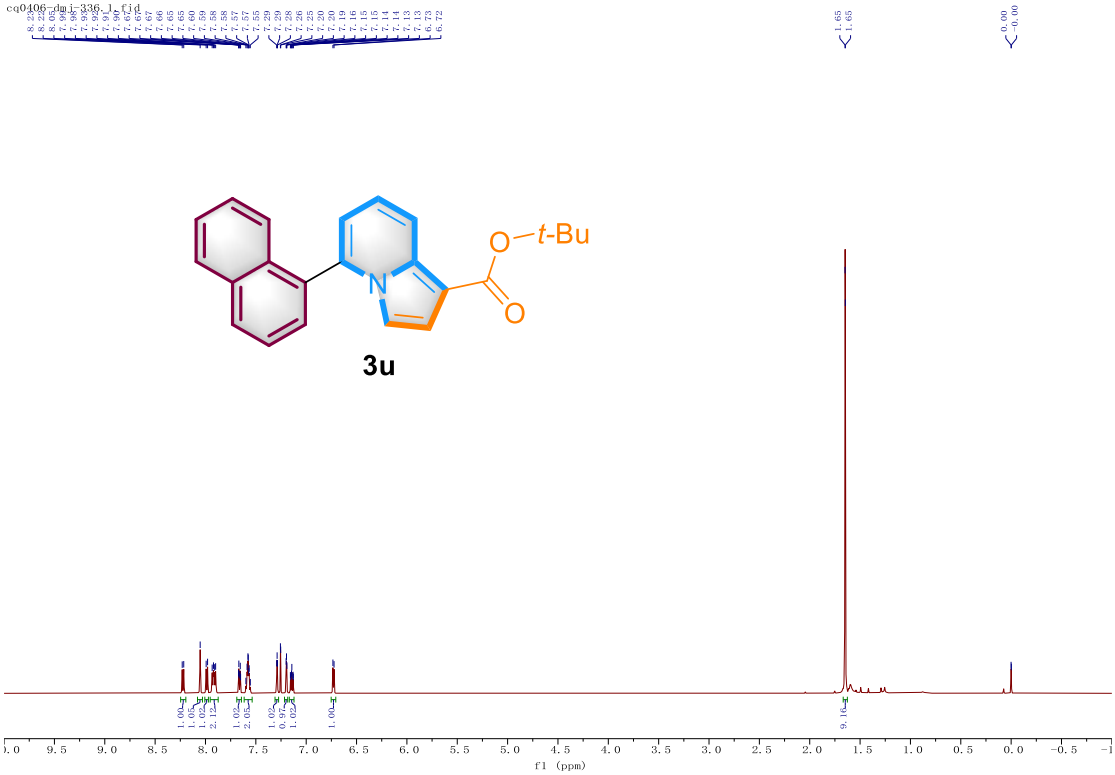
600 MHz ^{1}H NMR of **3t** in $CDCl_3$



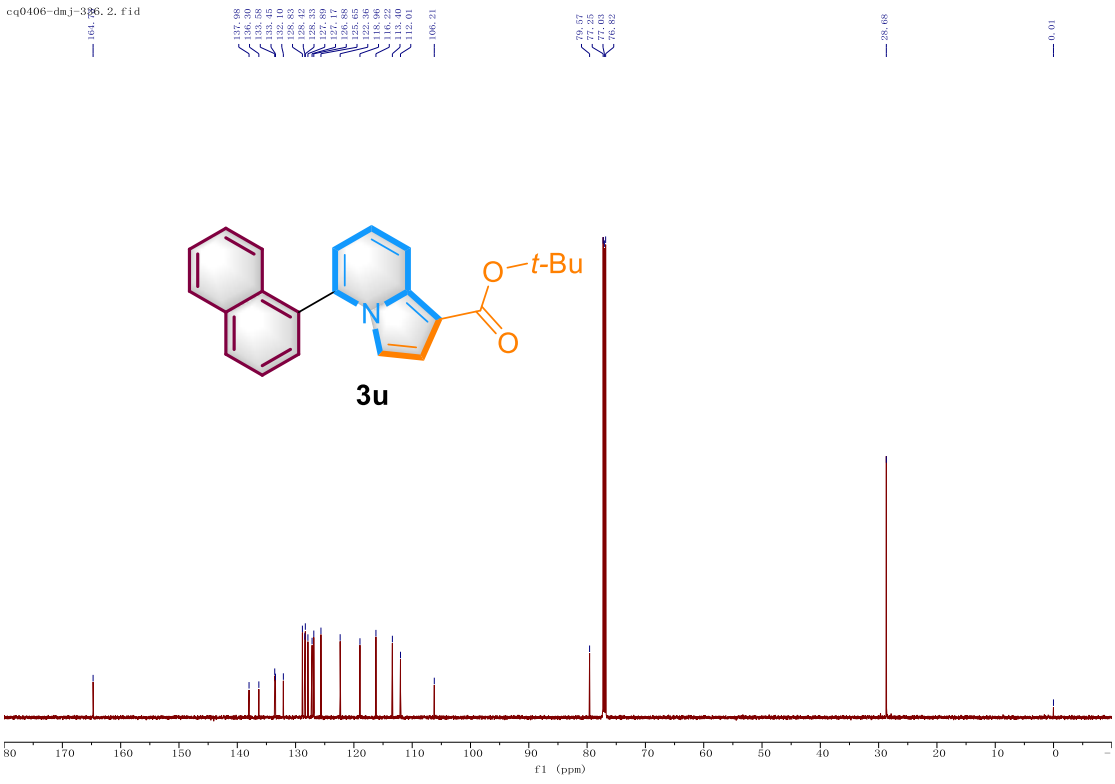
151 MHz ^{13}C NMR of **3t** in $CDCl_3$



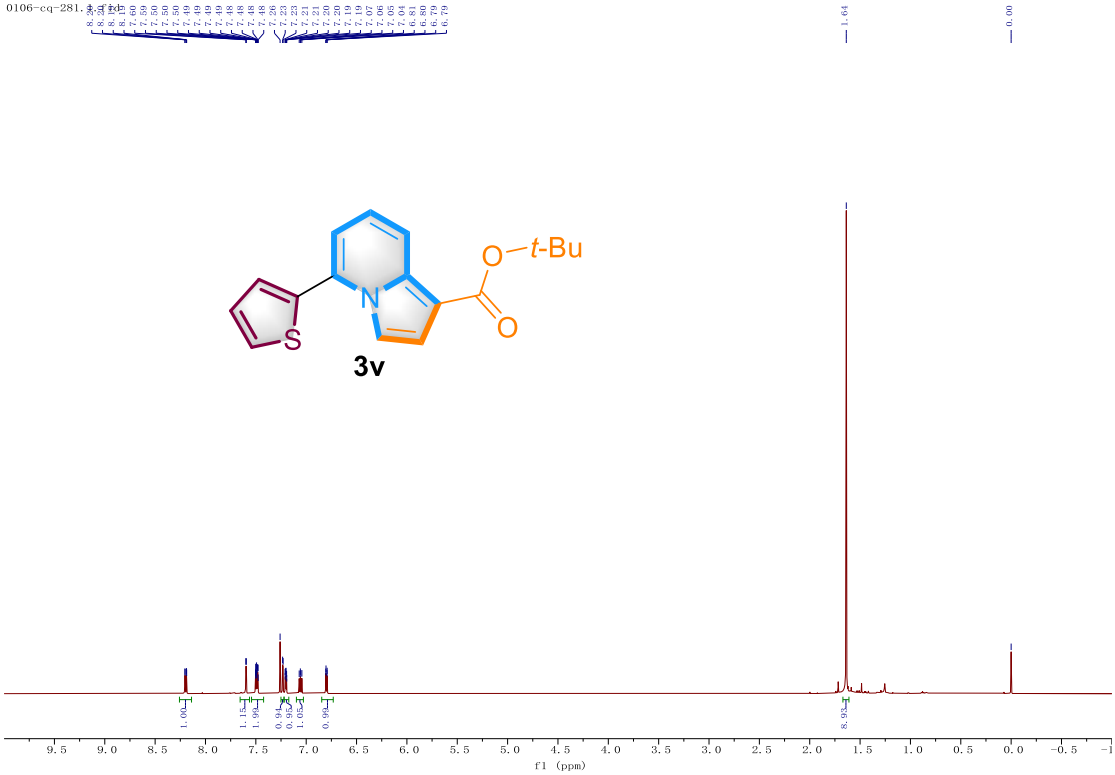
600 MHz ^{1}H NMR of **3u** in $CDCl_3$



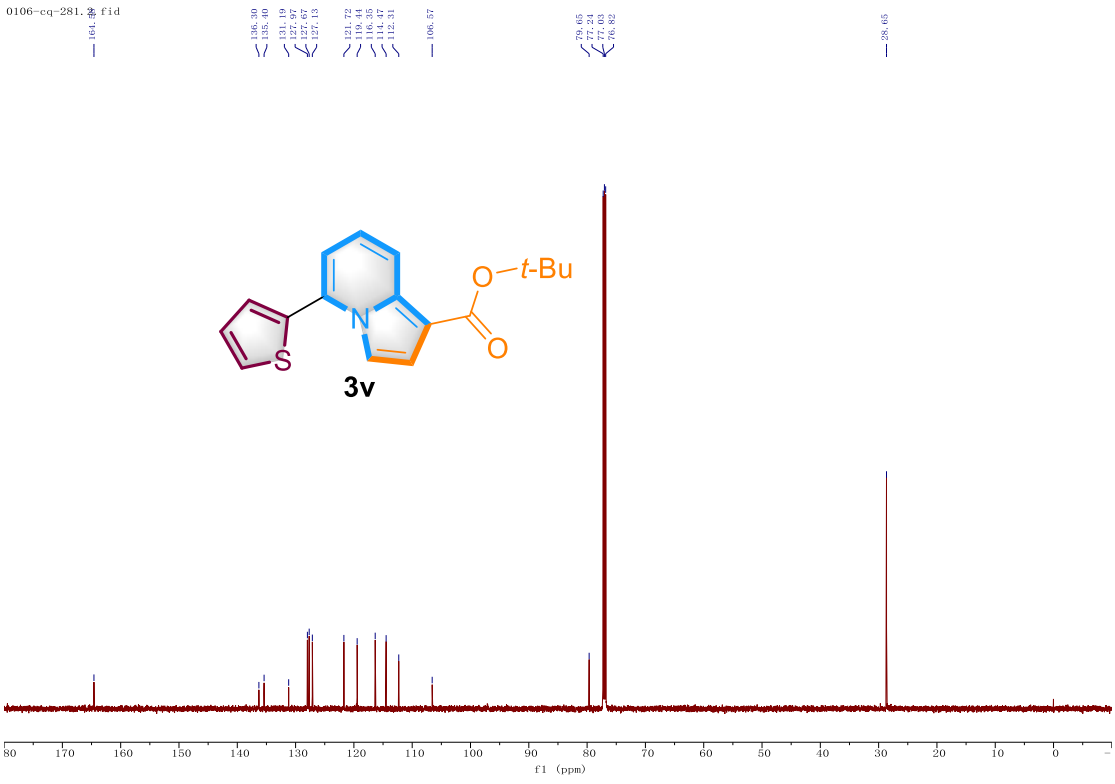
151 MHz ^{13}C NMR of **3u** in $CDCl_3$



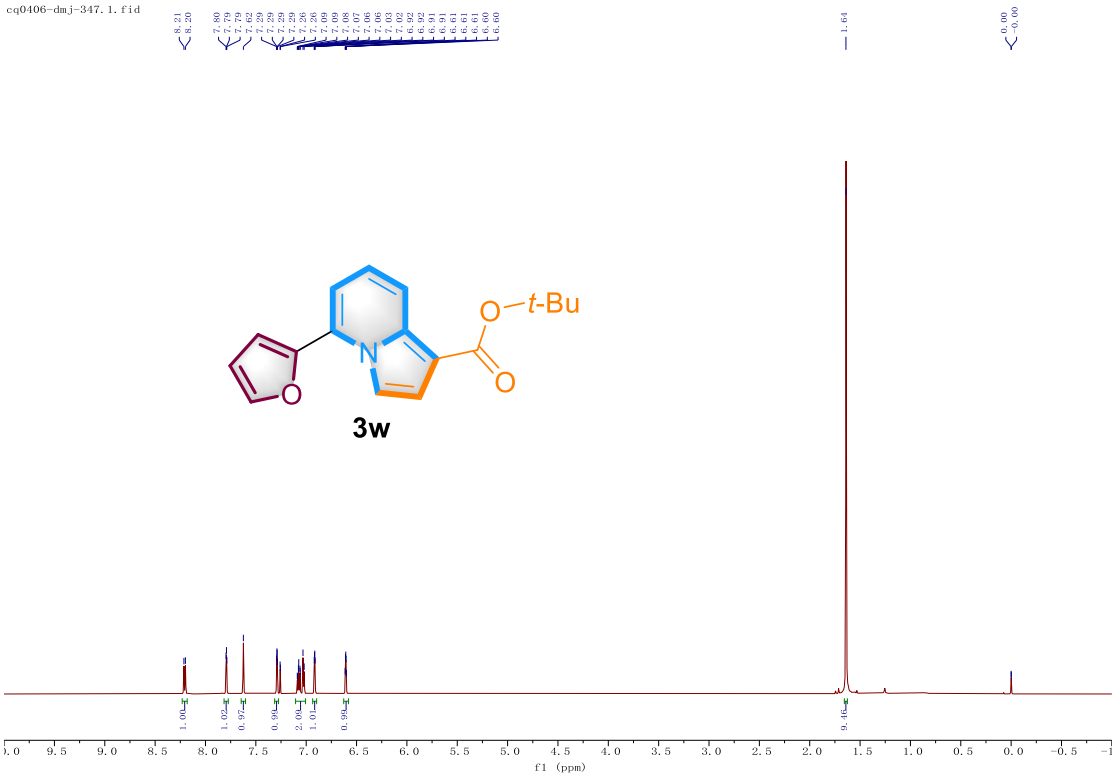
600 MHz ^{1}H NMR of **3v** in $CDCl_3$



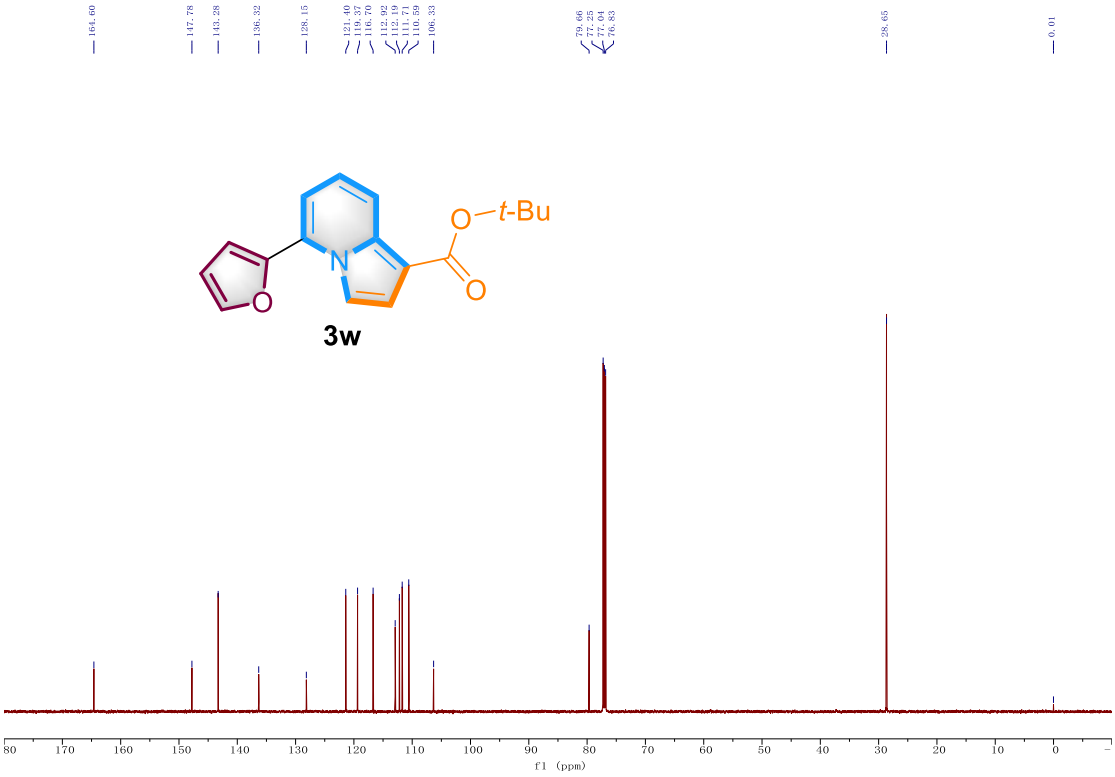
151 MHz ^{13}C NMR of **3v** in $CDCl_3$



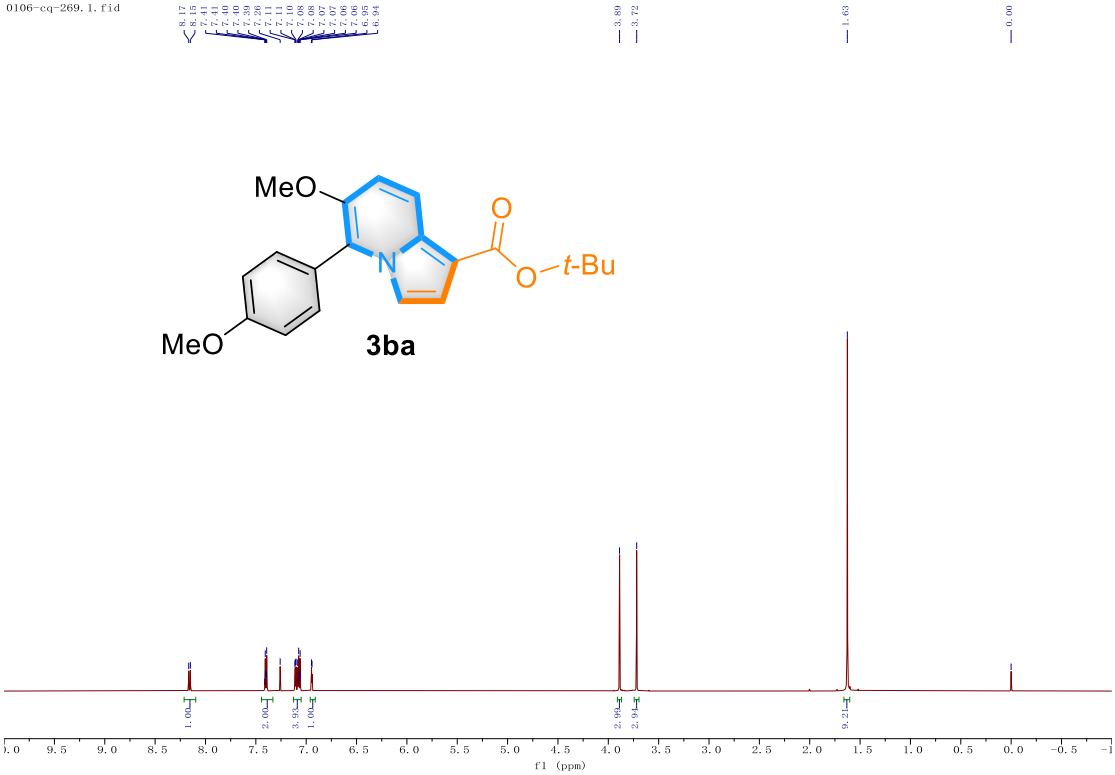
600 MHz ^{1}H NMR of **3w** in $CDCl_3$



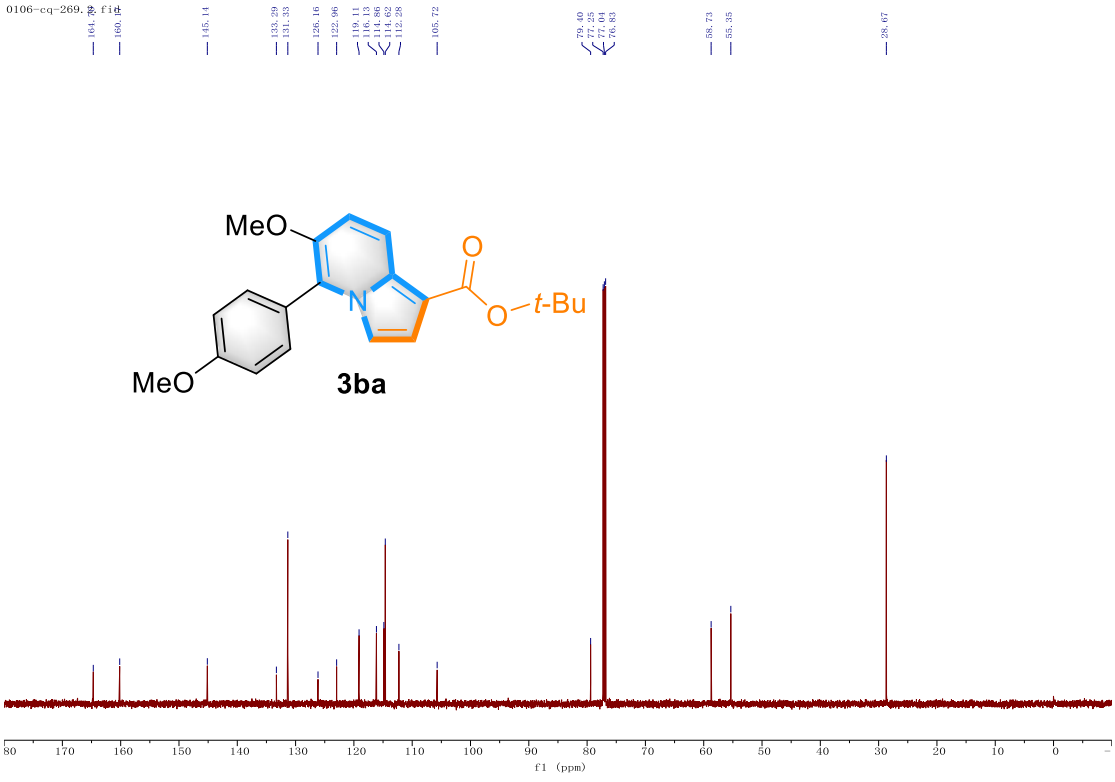
151 MHz ^{13}C NMR of **3w** in $CDCl_3$



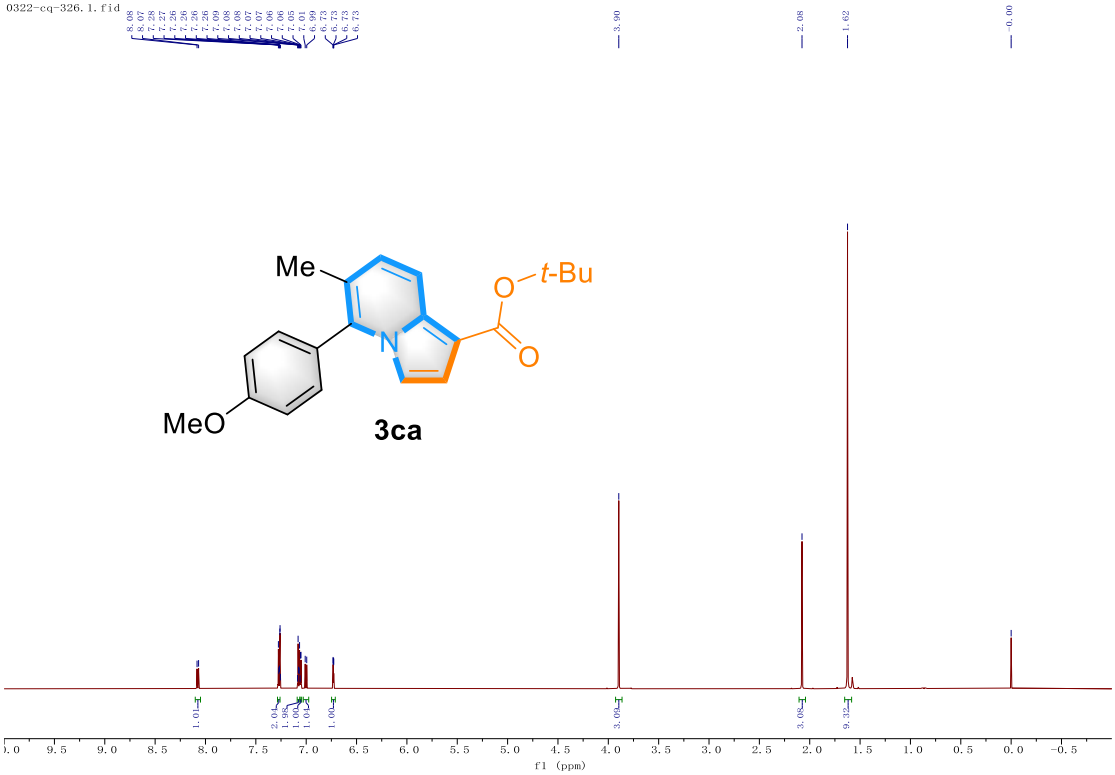
600 MHz ^{1}H NMR of **3ba** in $CDCl_3$



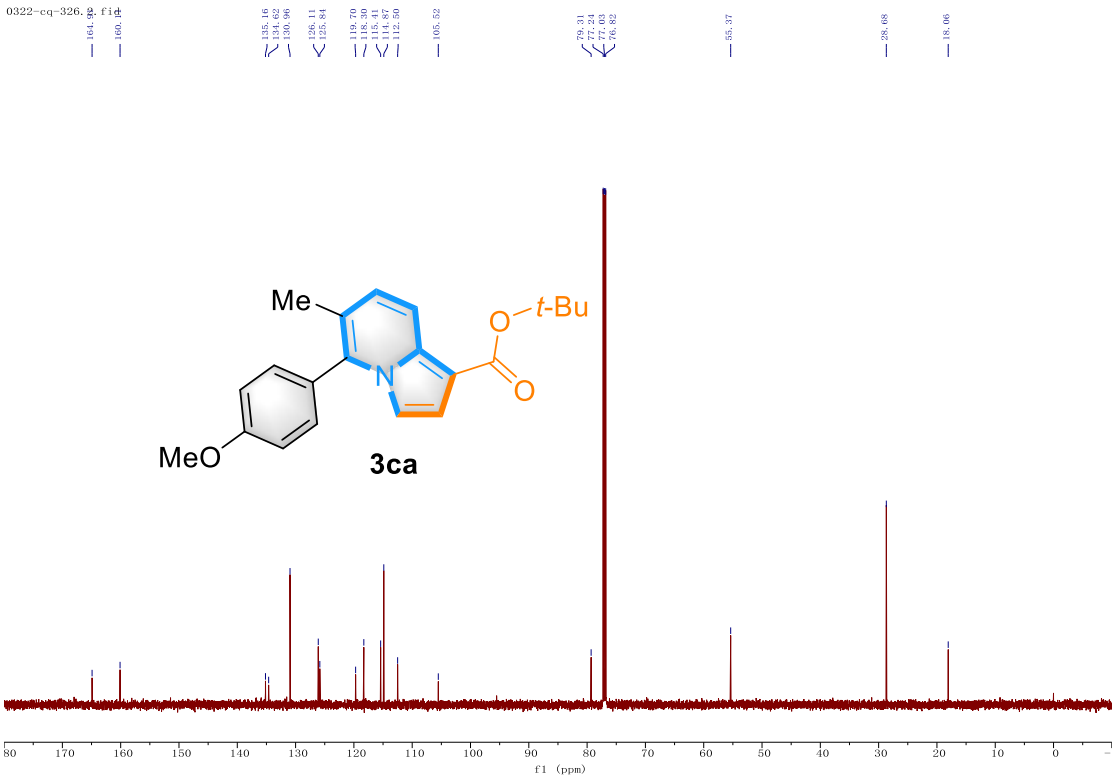
151 MHz ^{13}C NMR of **3ba** in $CDCl_3$



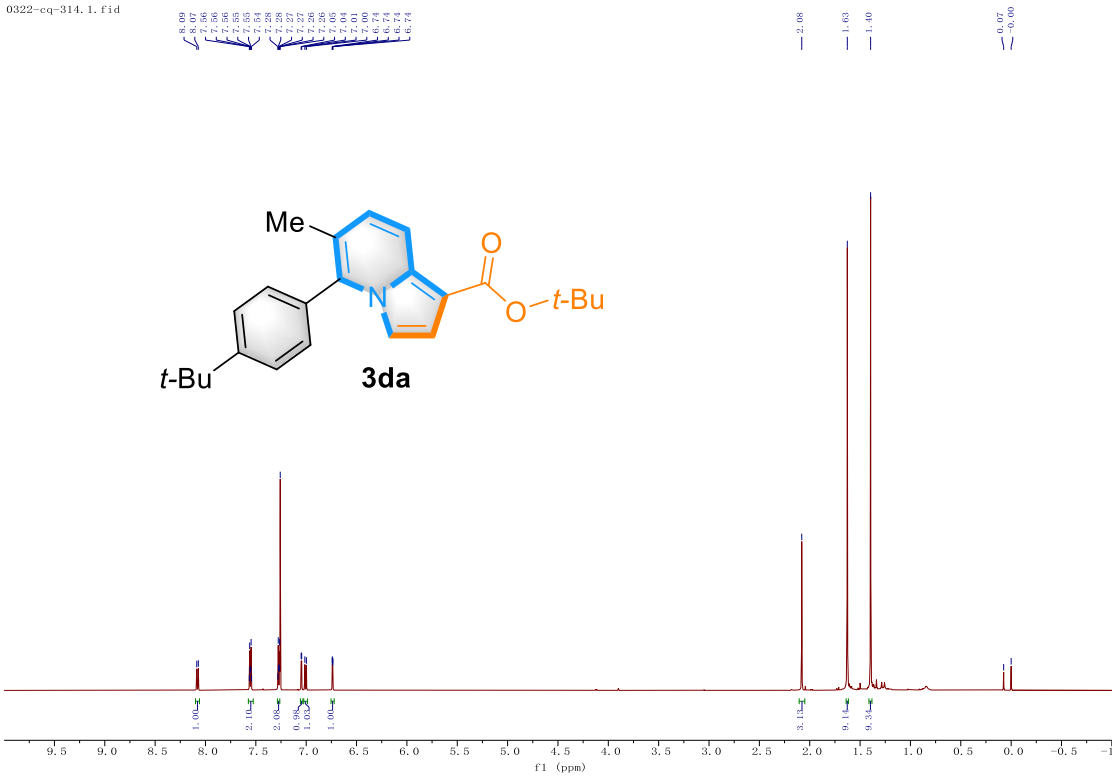
600 MHz ^{1}H NMR of **3ca** in $CDCl_3$



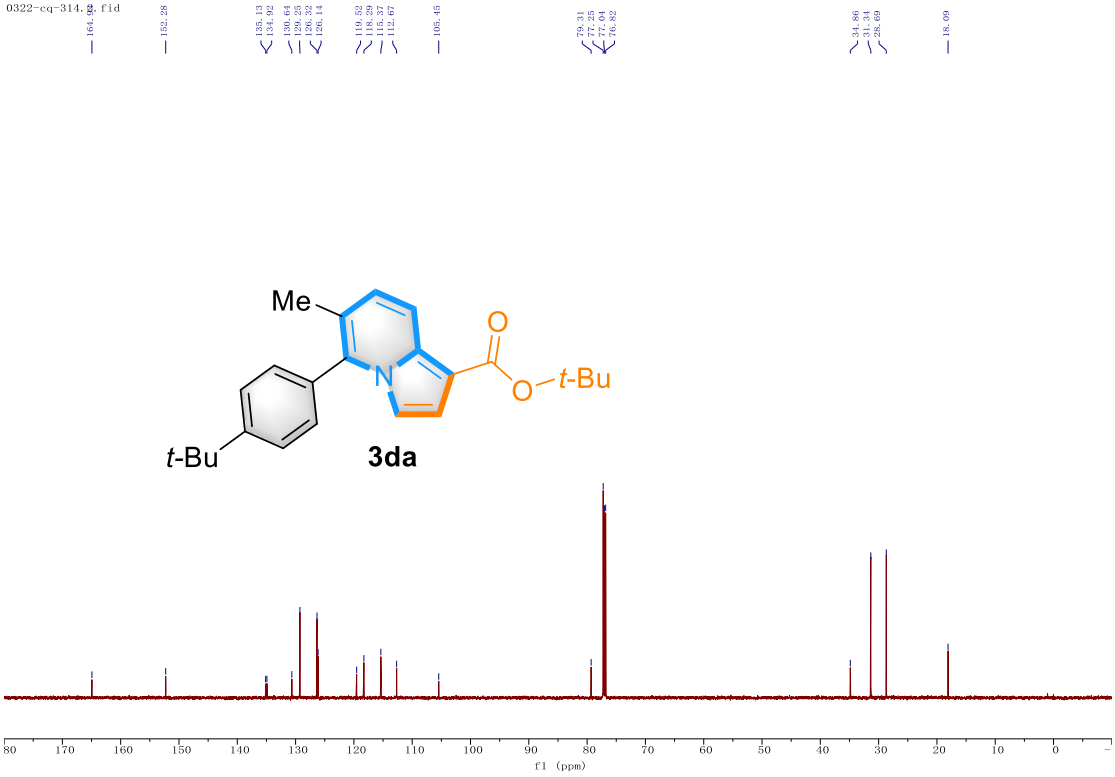
151 MHz ^{13}C NMR of **3ca** in $CDCl_3$



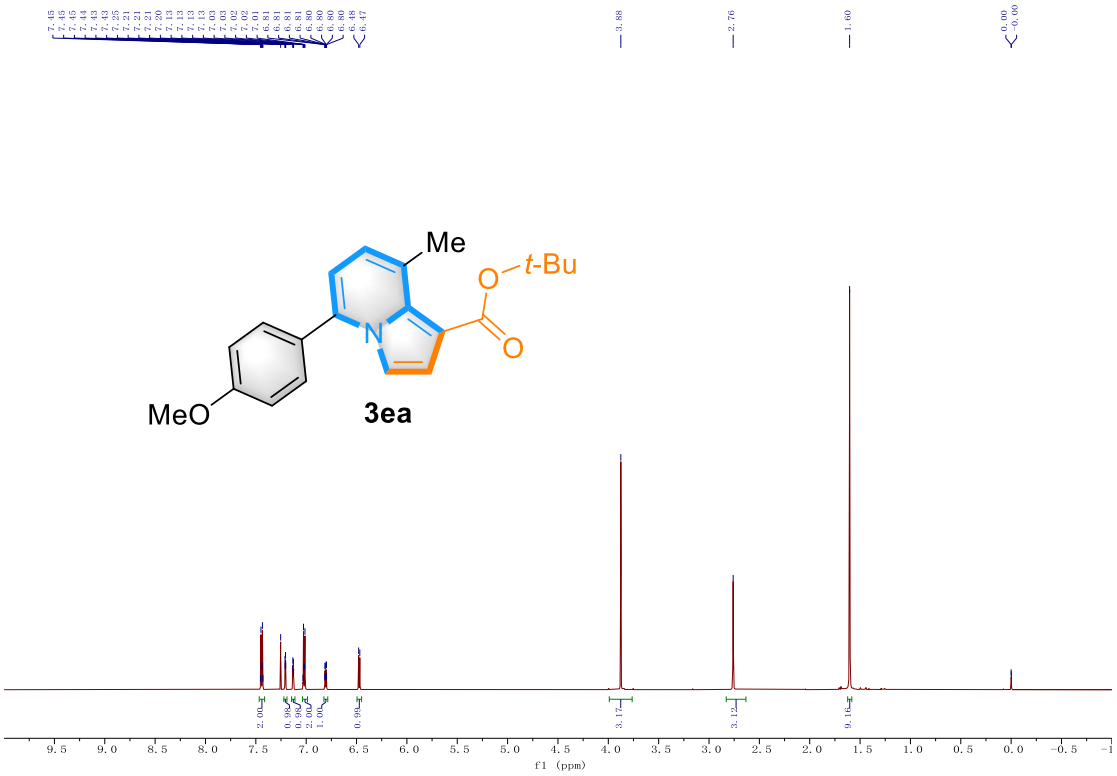
600 MHz ^{1}H NMR of **3da** in $CDCl_3$



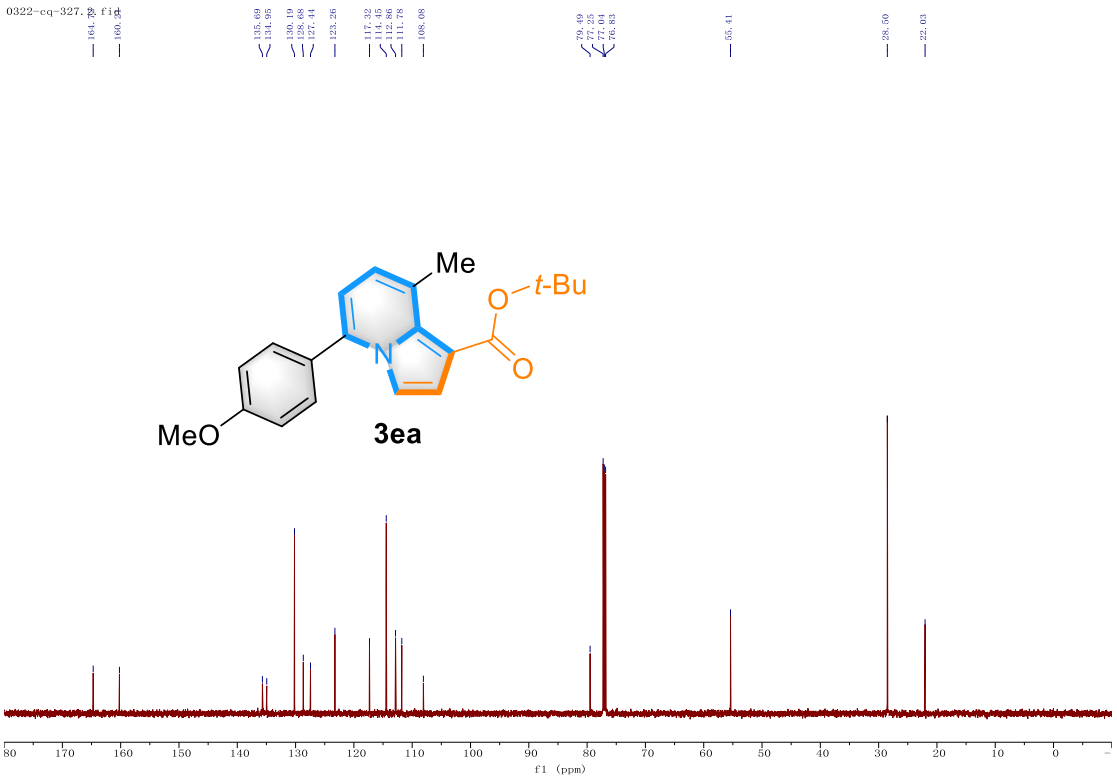
151 MHz ^{13}C NMR of **3da** in $CDCl_3$



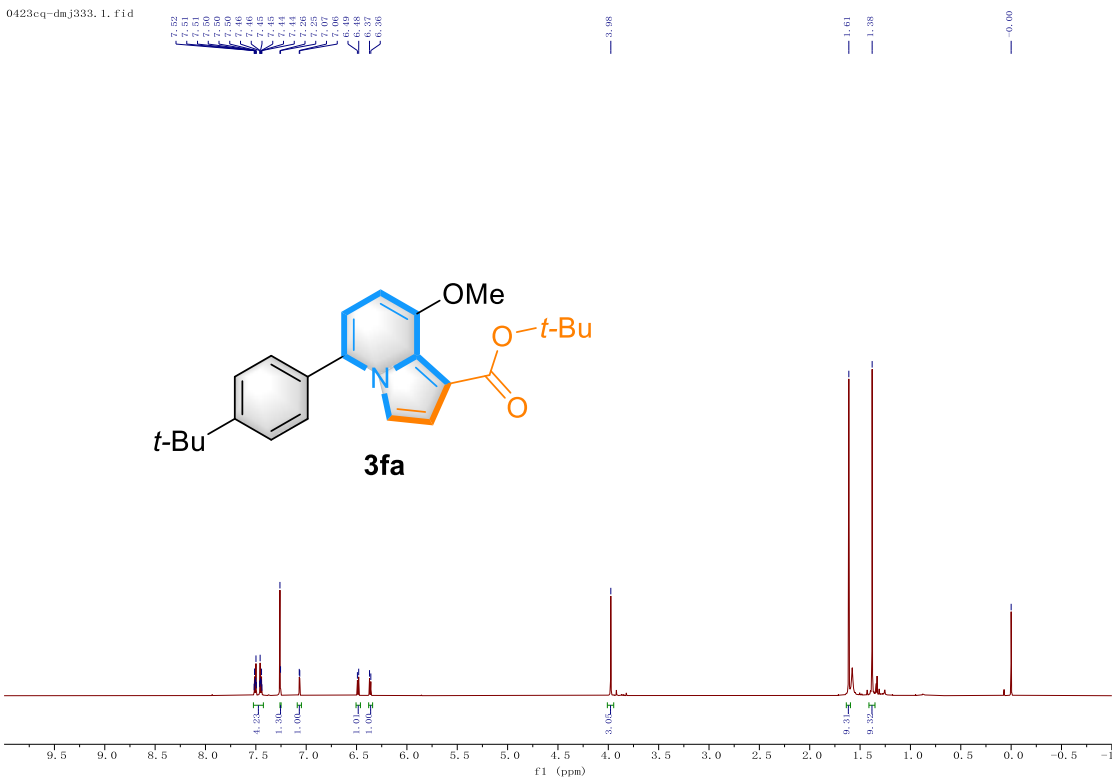
600 MHz ^{1}H NMR of **3ea** in $CDCl_3$



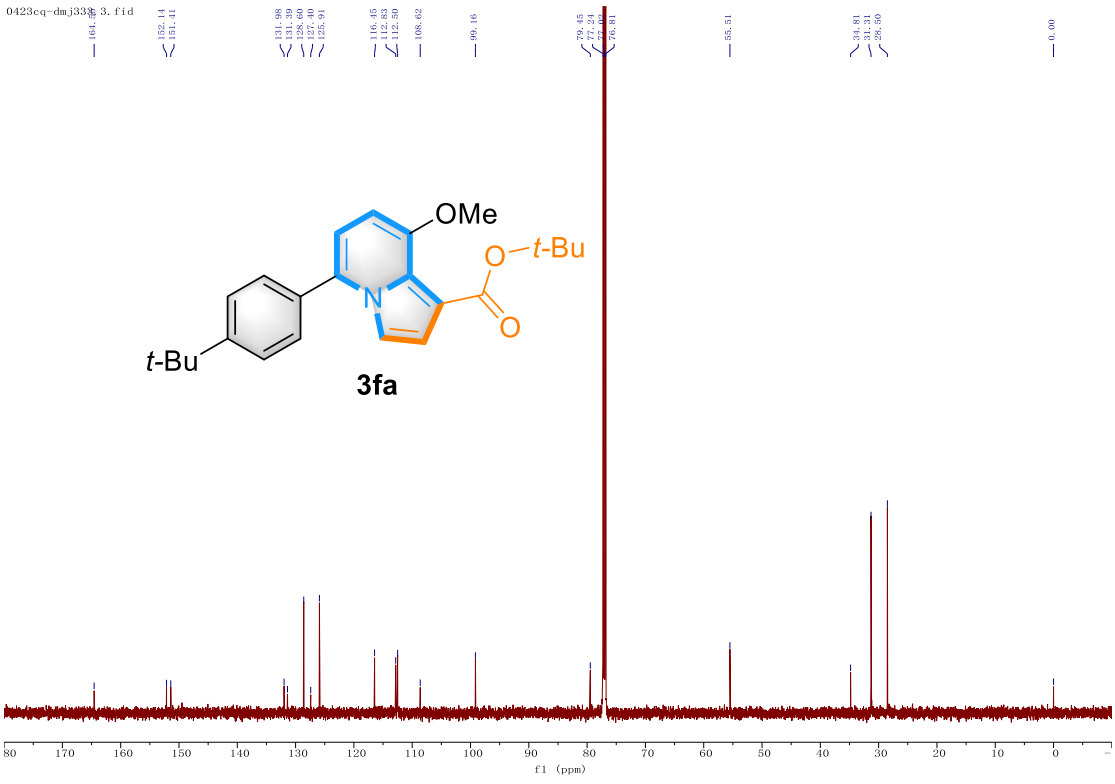
151 MHz ^{13}C NMR of **3ea** in $CDCl_3$



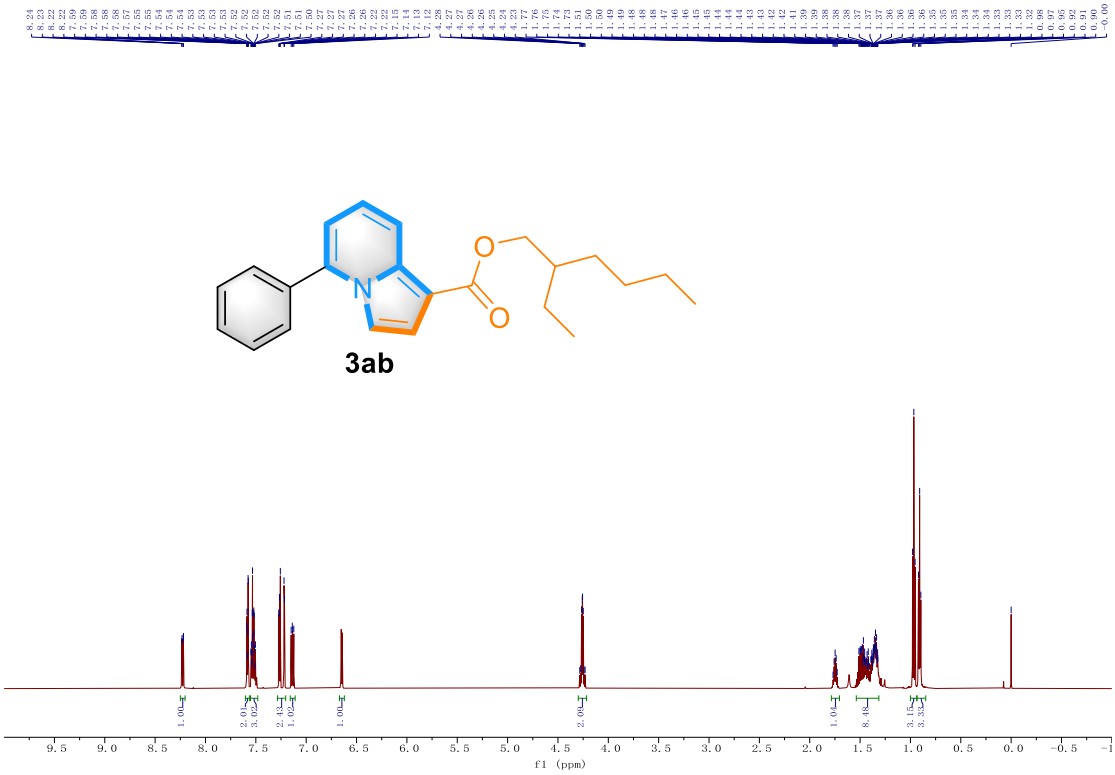
600 MHz ^{1}H NMR of **3fa** in $CDCl_3$



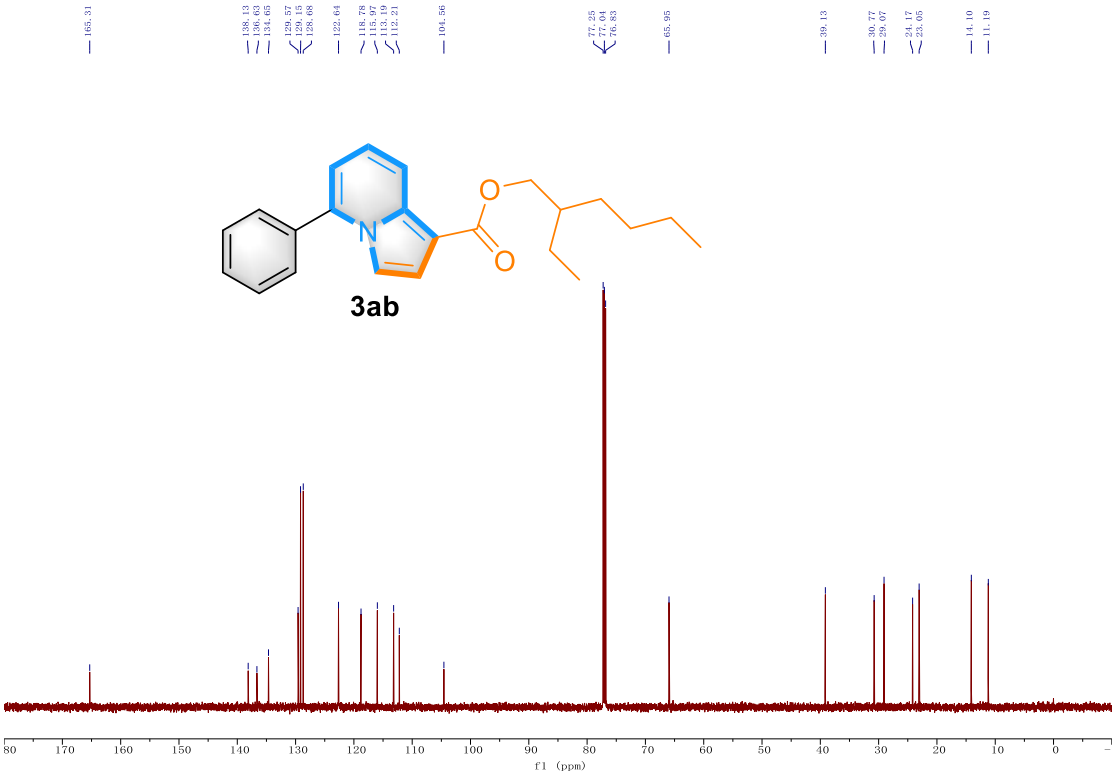
151 MHz ^{13}C NMR of **3fa** in $CDCl_3$



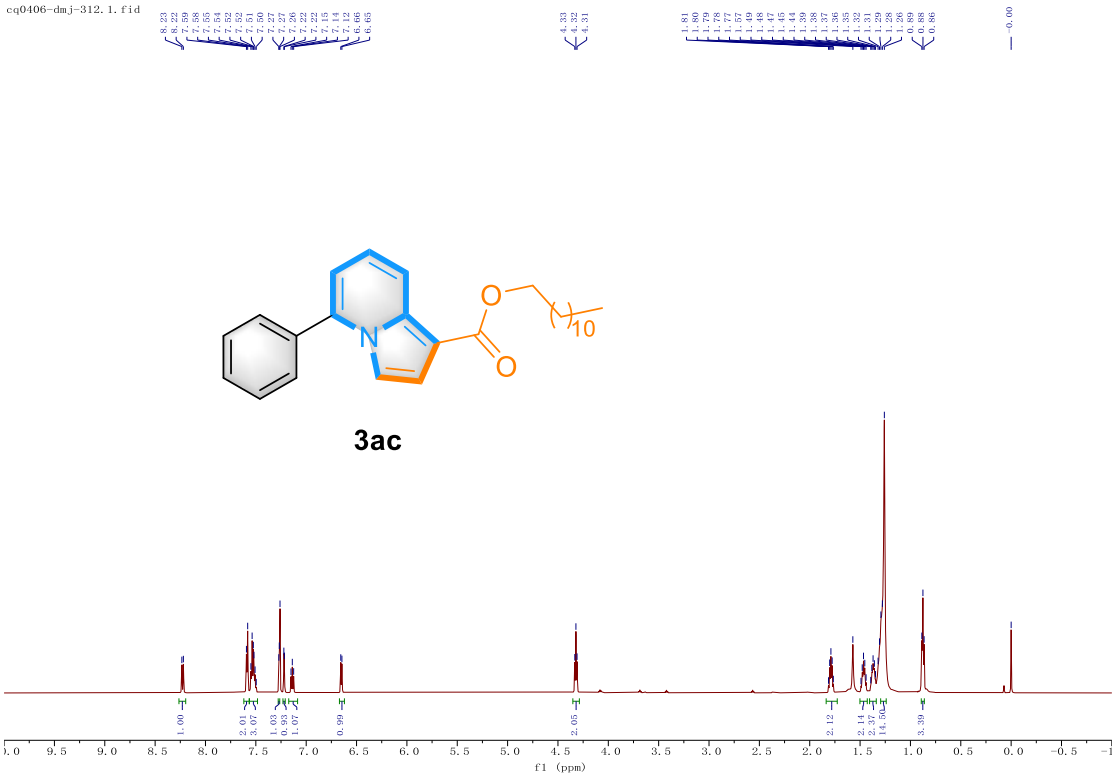
600 MHz ^{1}H NMR of **3ab** in $CDCl_3$



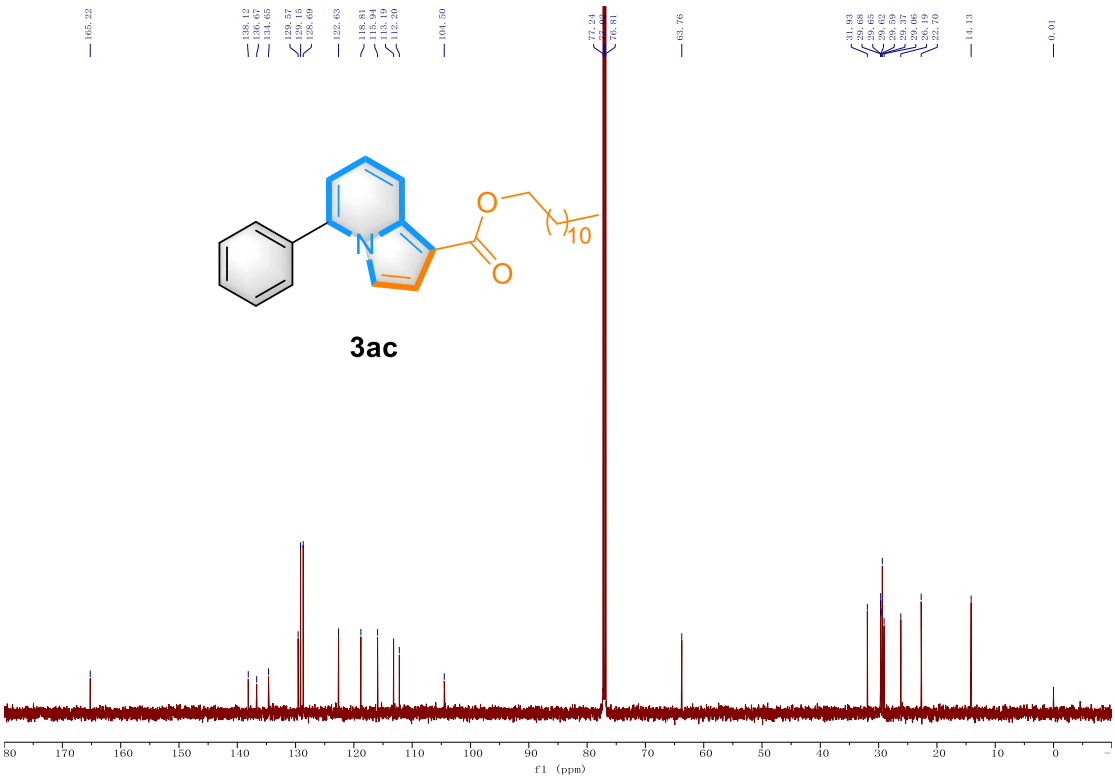
151 MHz ^{13}C NMR of **3ab** in $CDCl_3$



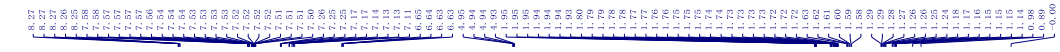
600 MHz ^{1}H NMR of **3ac** in $CDCl_3$

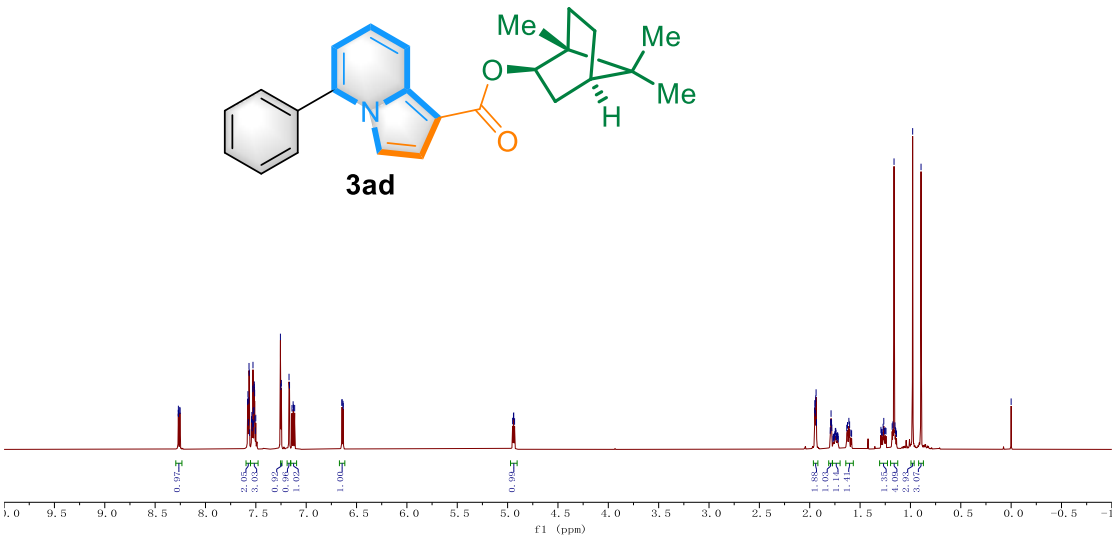


151 MHz ^{13}C NMR of **3ac** in $CDCl_3$

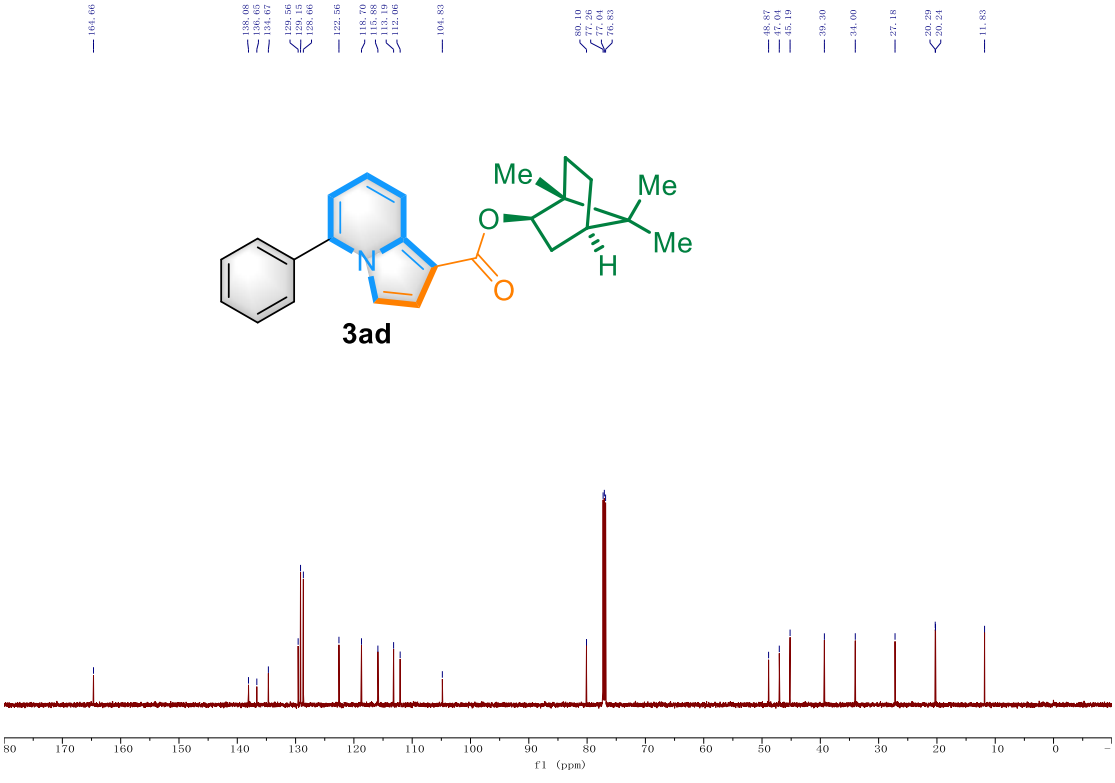


600 MHz ^{1}H NMR of **3ad** in $CDCl_3$

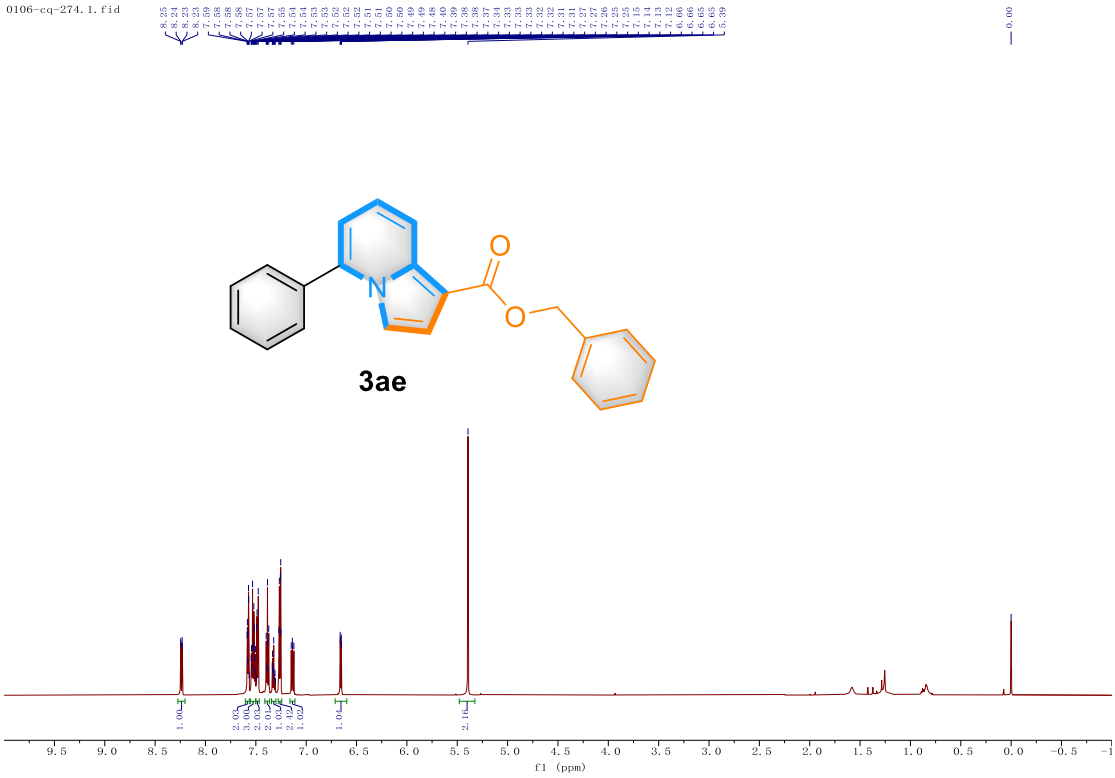




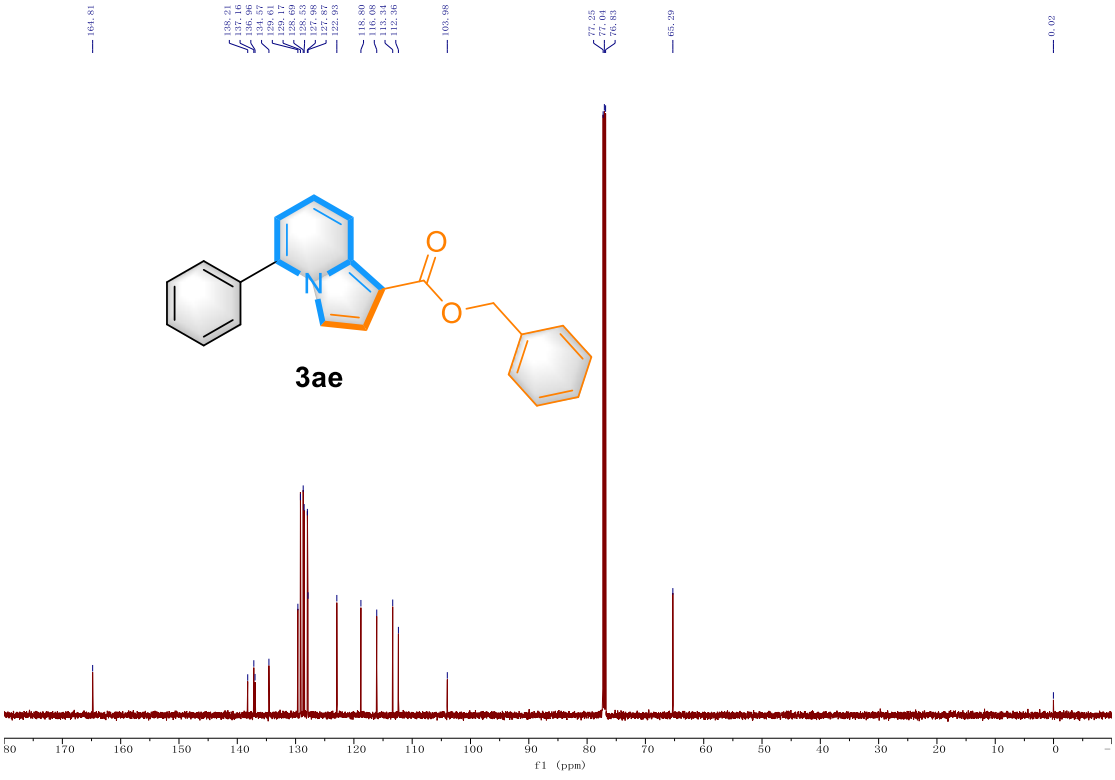
151 MHz ^{13}C NMR of **3ad** in $CDCl_3$



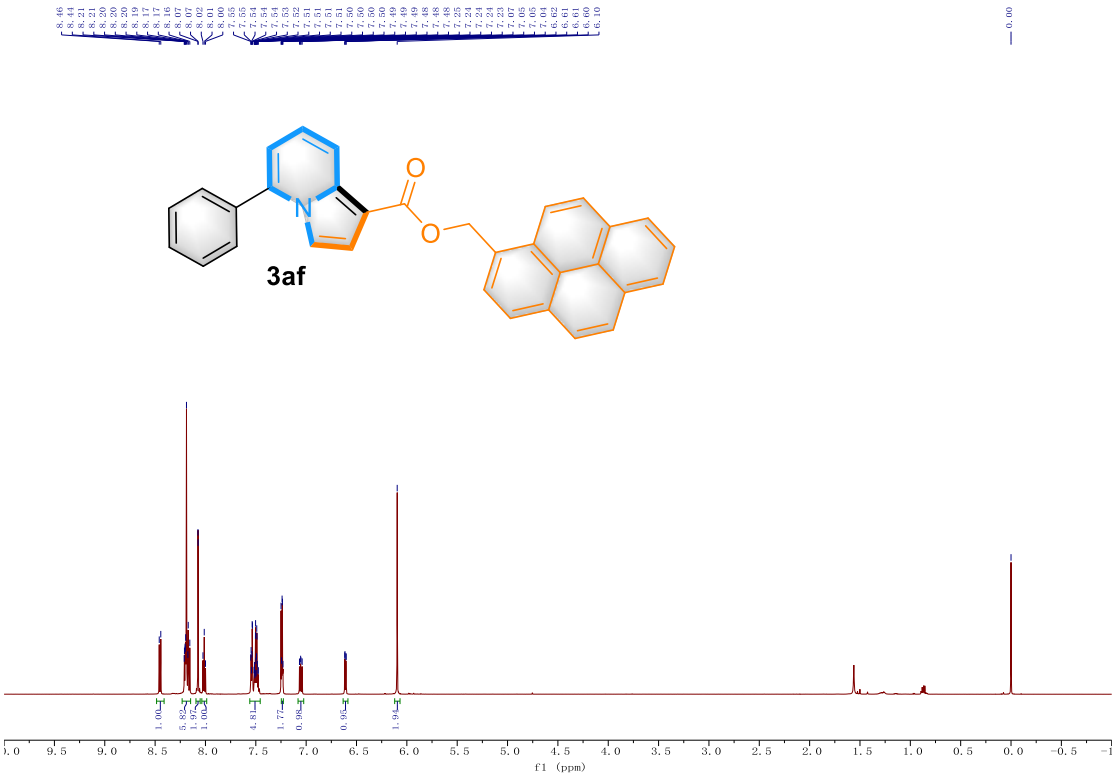
600 MHz ^{1}H NMR of **3ae** in $CDCl_3$



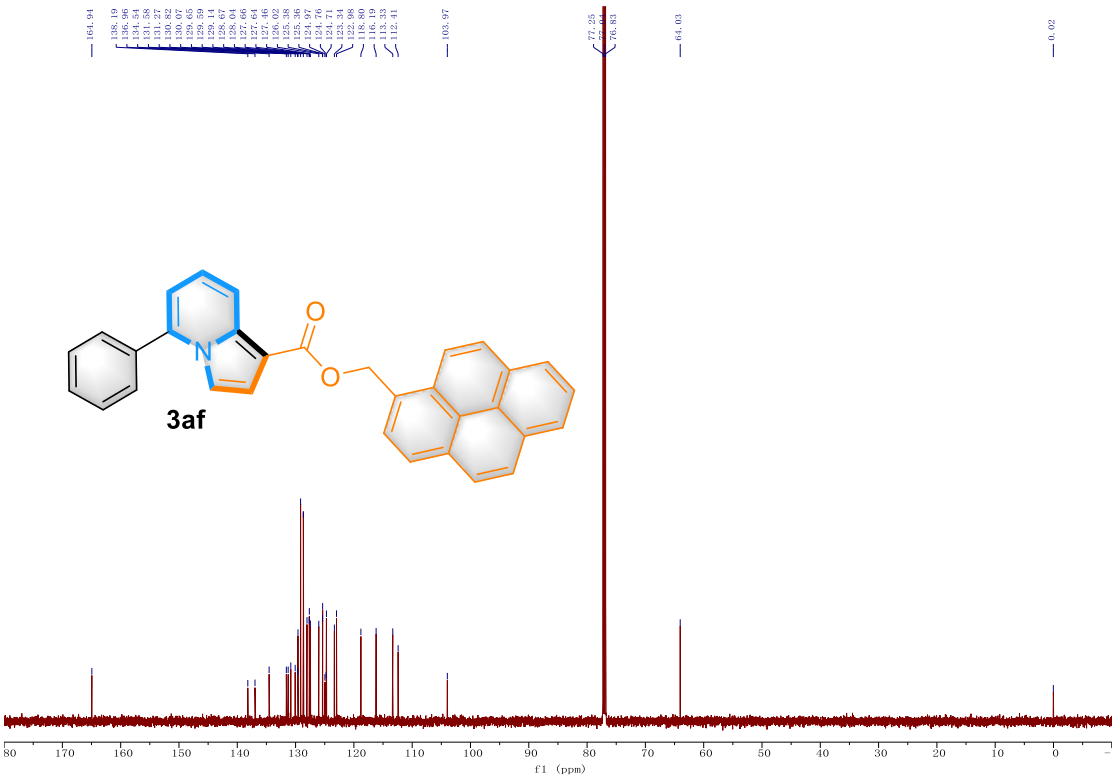
151 MHz ^{13}C NMR of **3ae** in $CDCl_3$



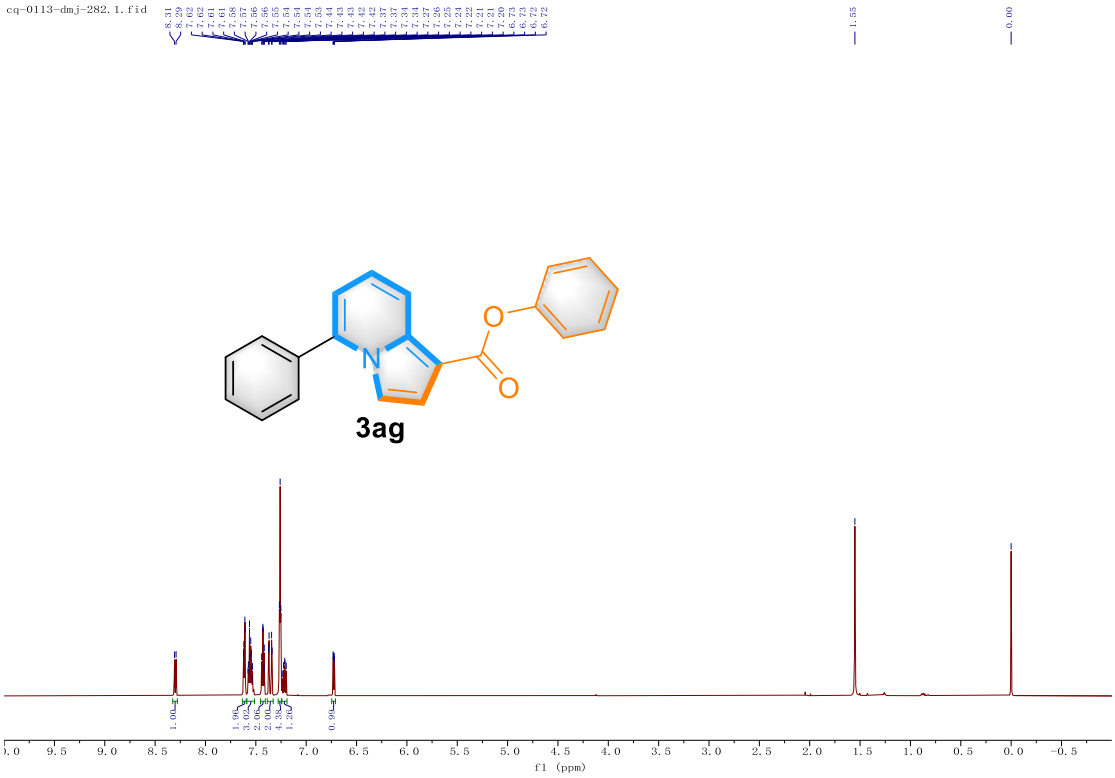
600 MHz ^{1}H NMR of **3af** in $CDCl_3$



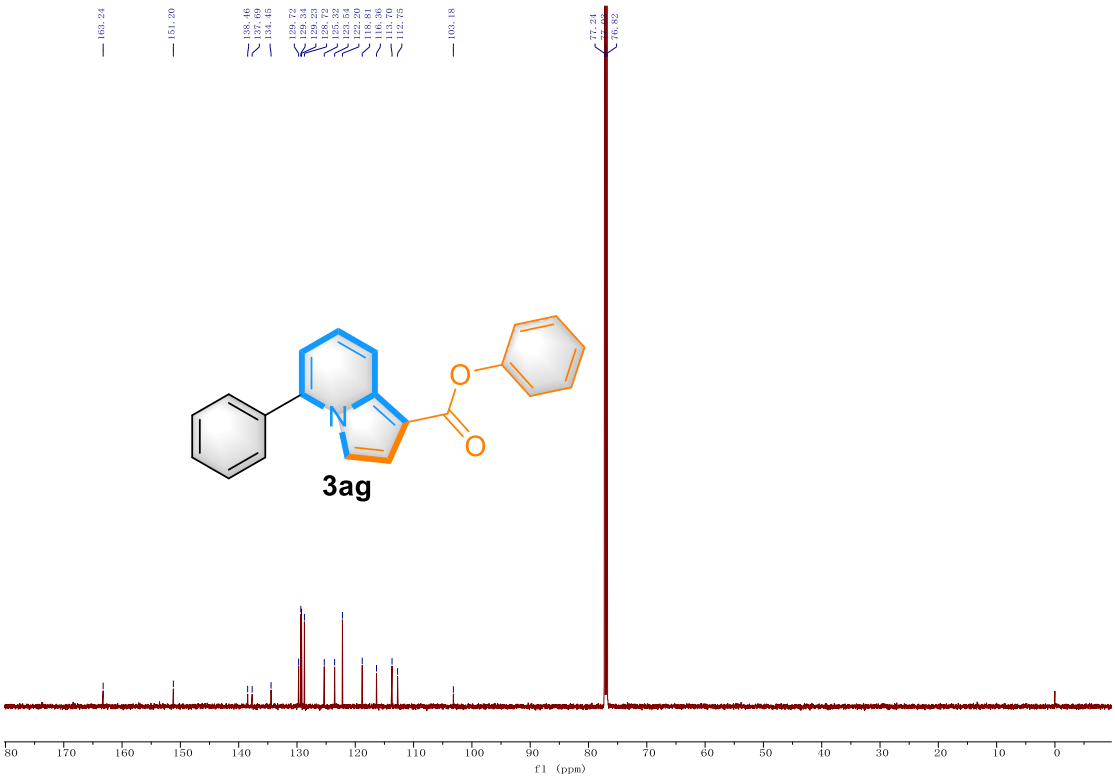
151 MHz ^{13}C NMR of **3af** in $CDCl_3$



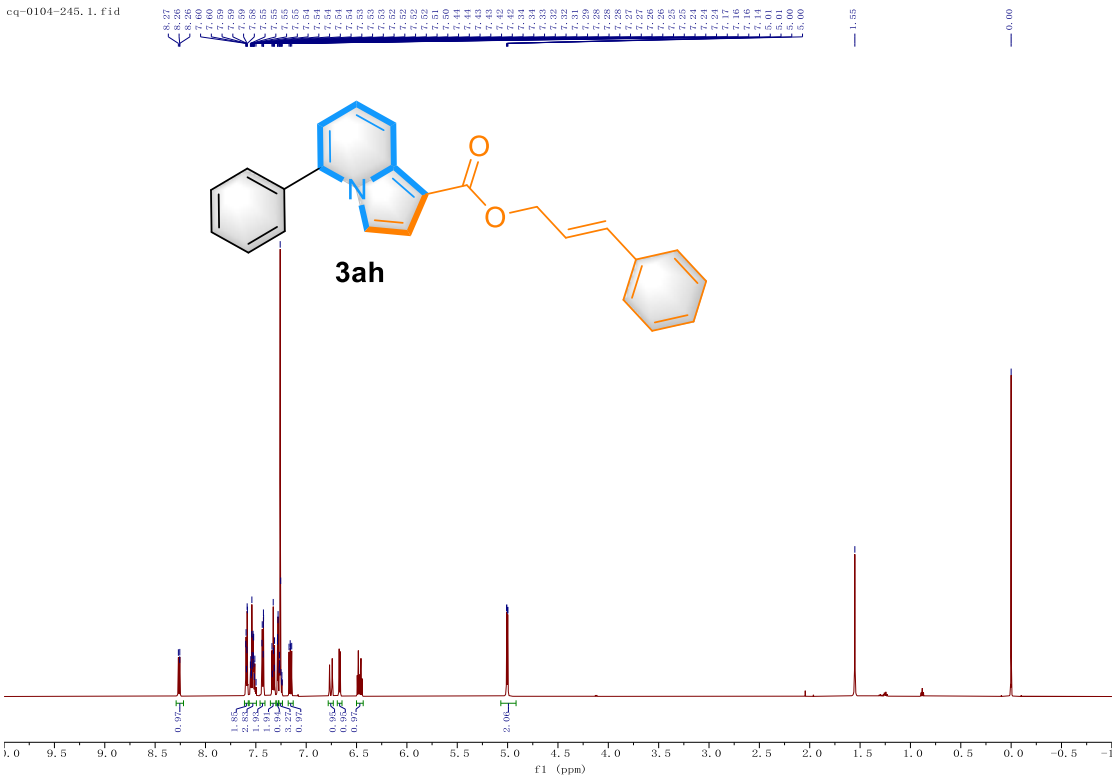
600 MHz ^{1}H NMR of **3ag** in $CDCl_3$



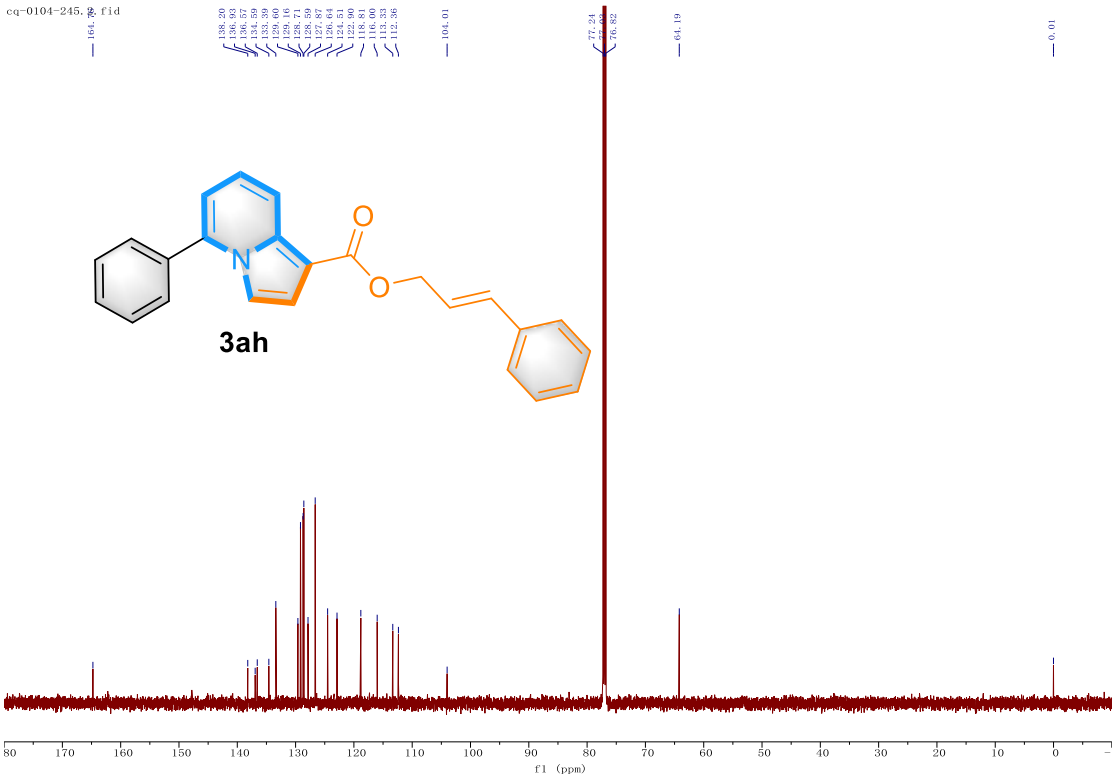
151 MHz ^{13}C NMR of **3ag** in $CDCl_3$



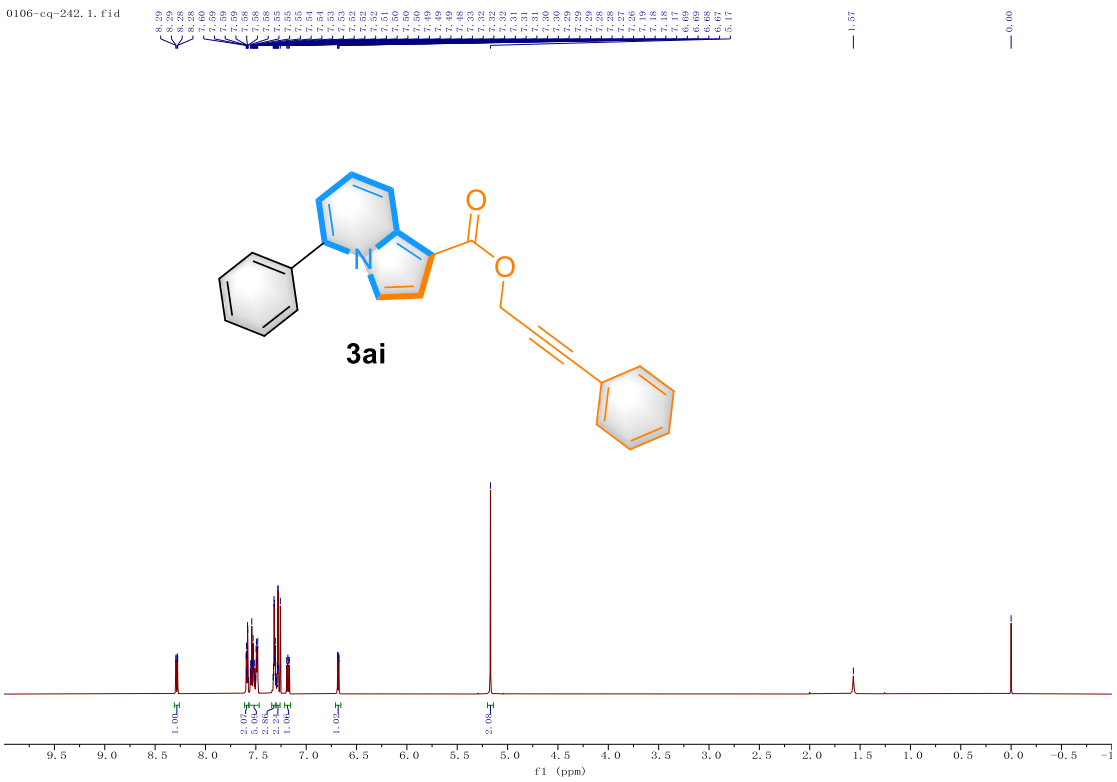
600 MHz ^{1}H NMR of **3ah** in $CDCl_3$



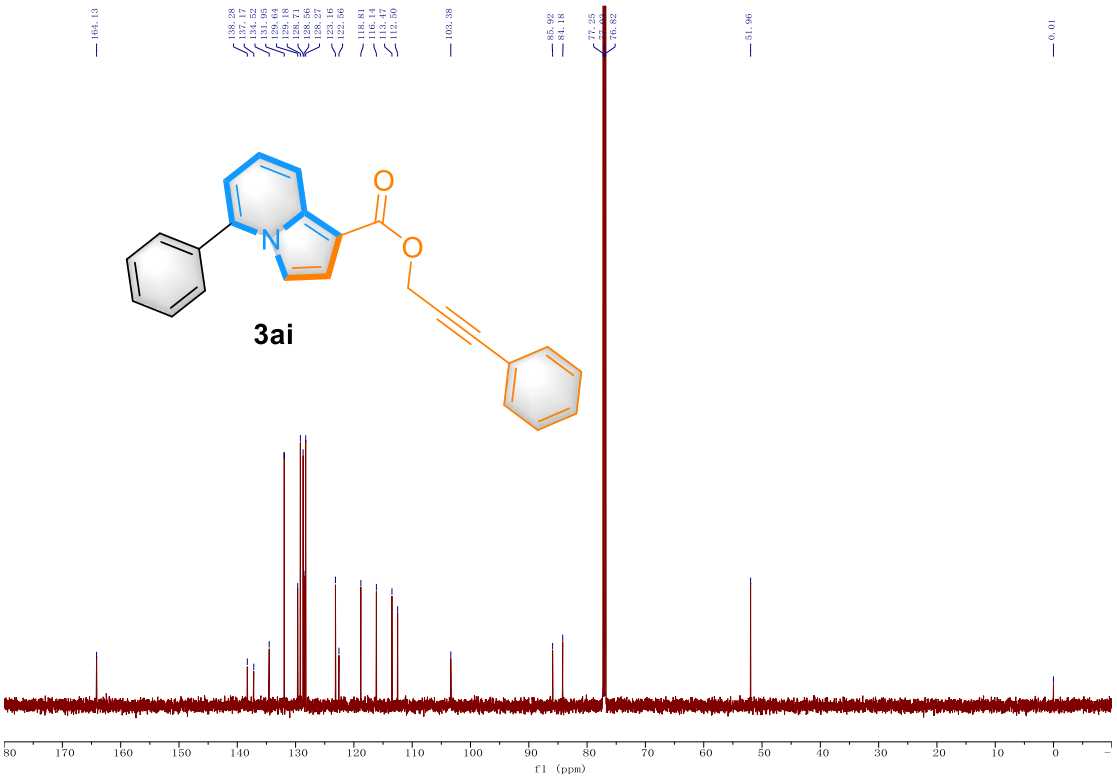
151 MHz ^{13}C NMR of **3ah** in $CDCl_3$



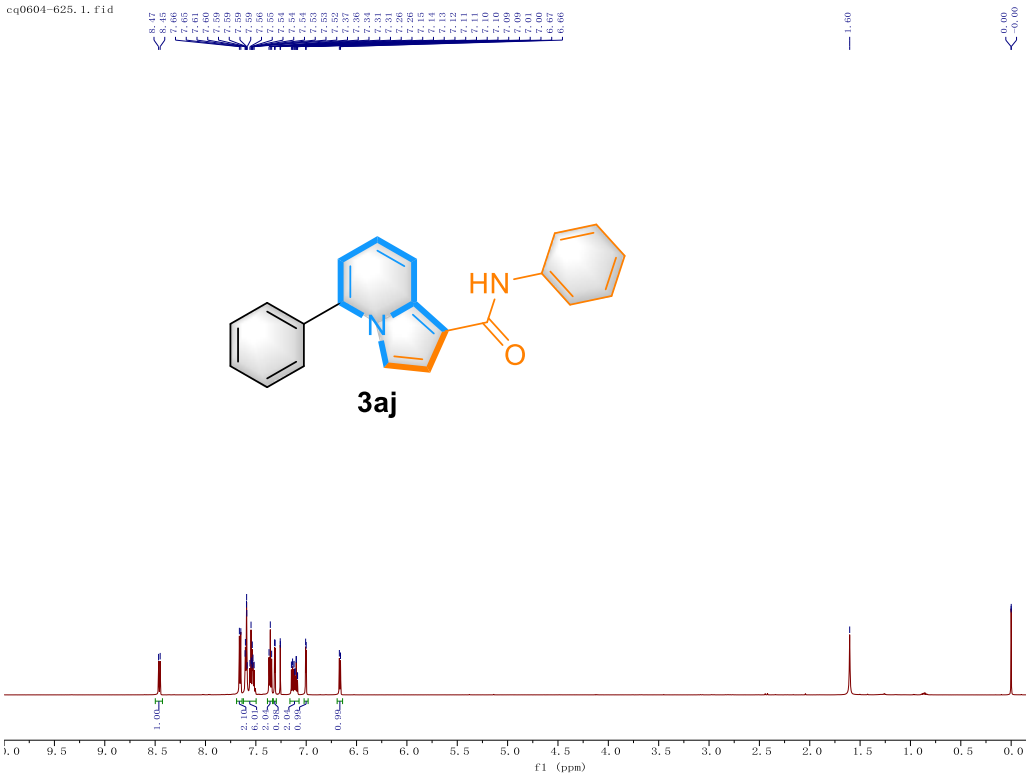
600 MHz ^{1}H NMR of **3ai** in $CDCl_3$



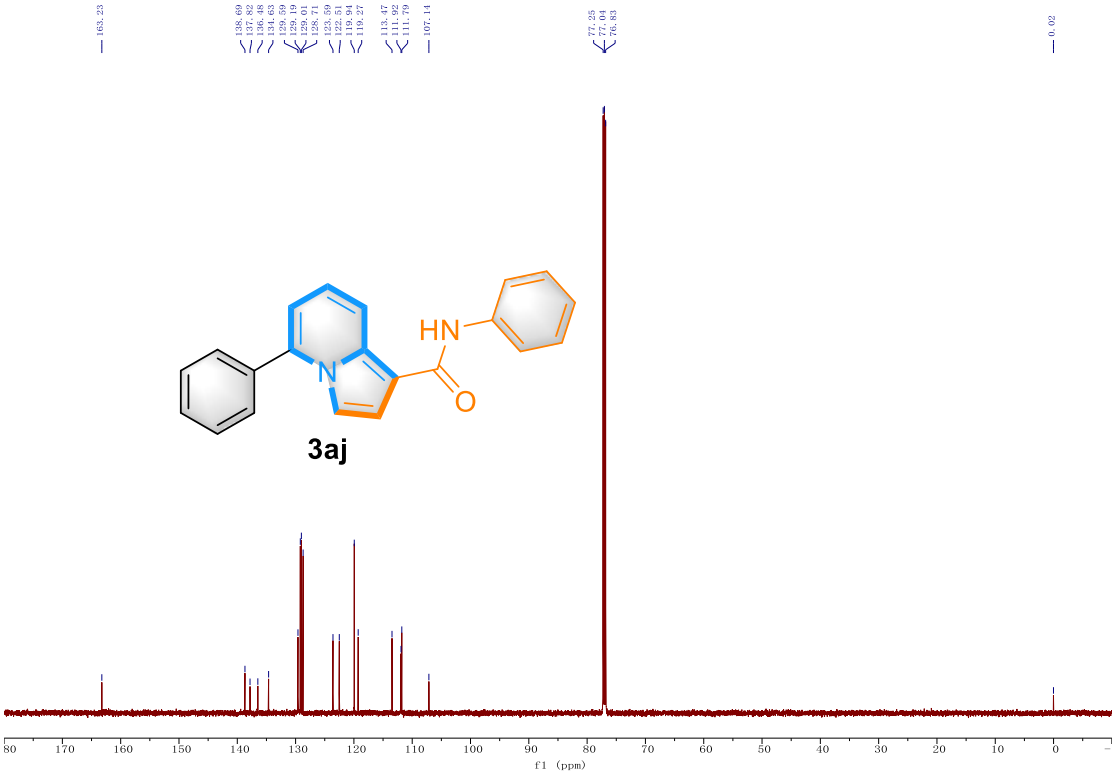
151 MHz ^{13}C NMR of **3ai** in $CDCl_3$



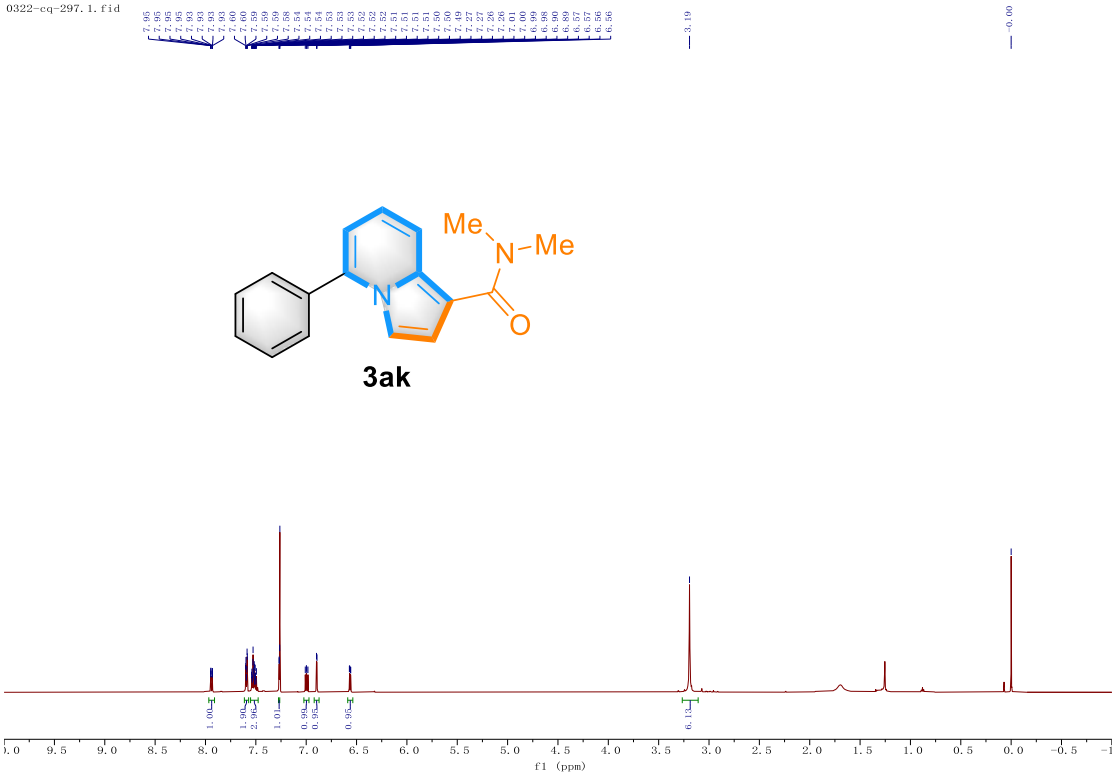
600 MHz ^{1}H NMR of **3aj** in $CDCl_3$



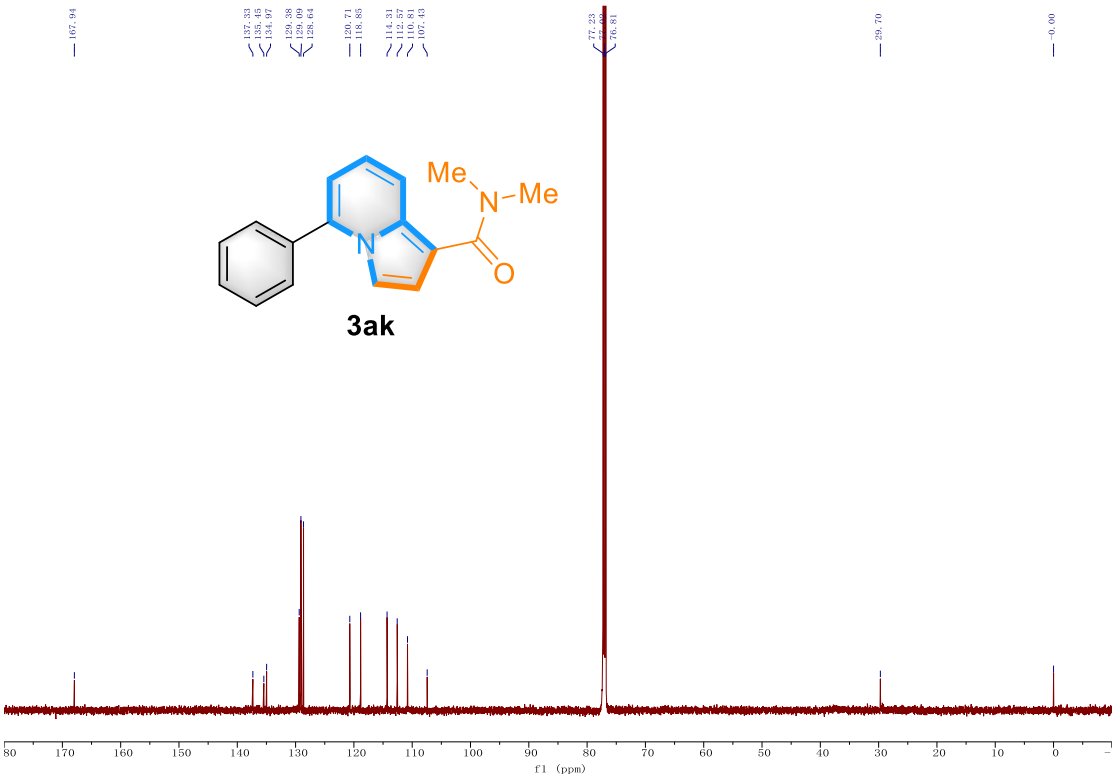
151 MHz ^{13}C NMR of **3aj** in $CDCl_3$



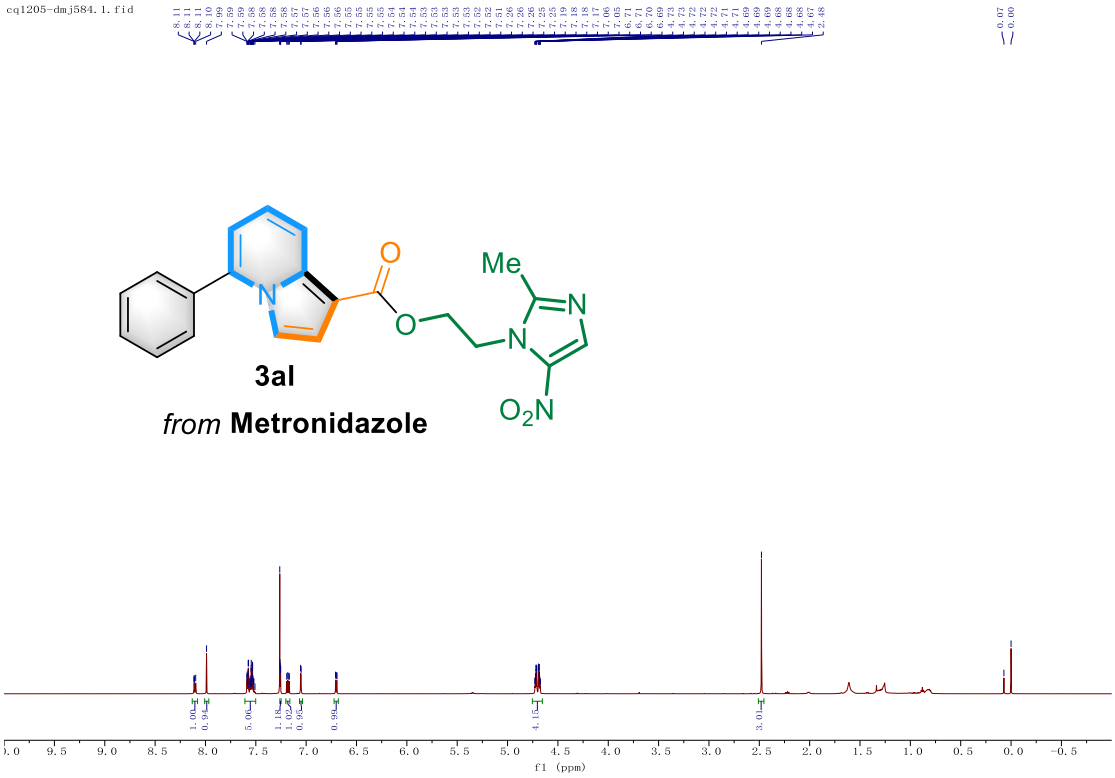
600 MHz ^{1}H NMR of **3ak** in $CDCl_3$



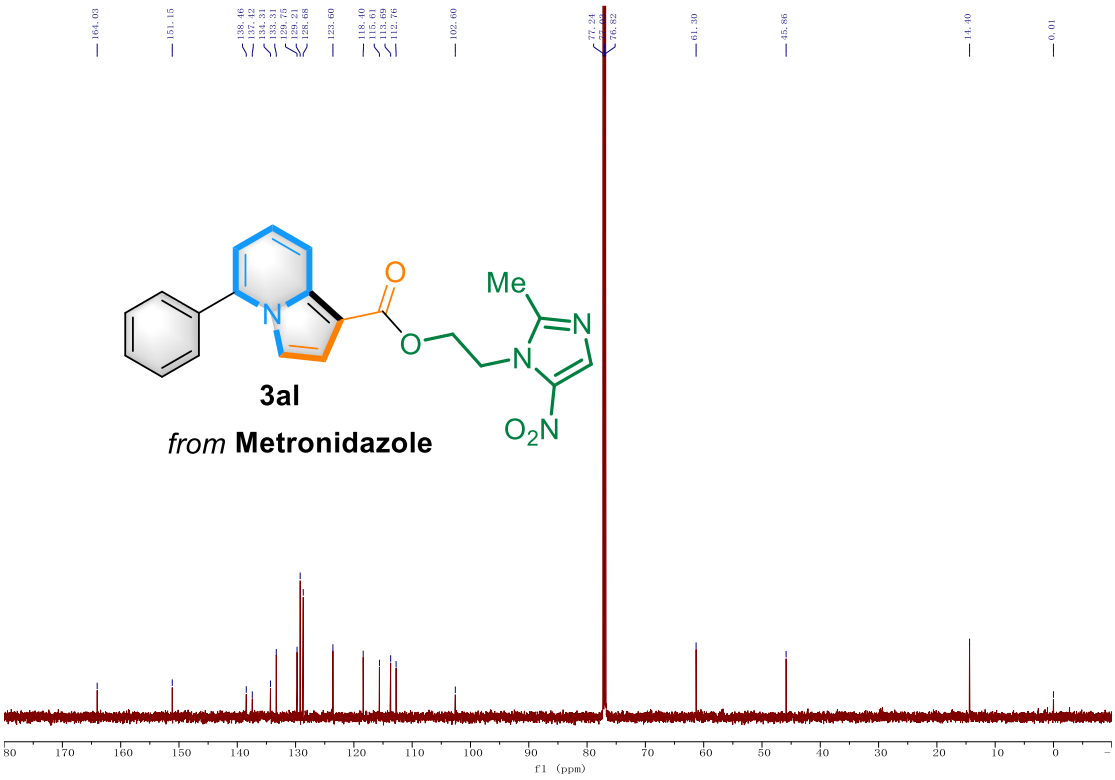
151 MHz ^{13}C NMR of **3ak** in $CDCl_3$



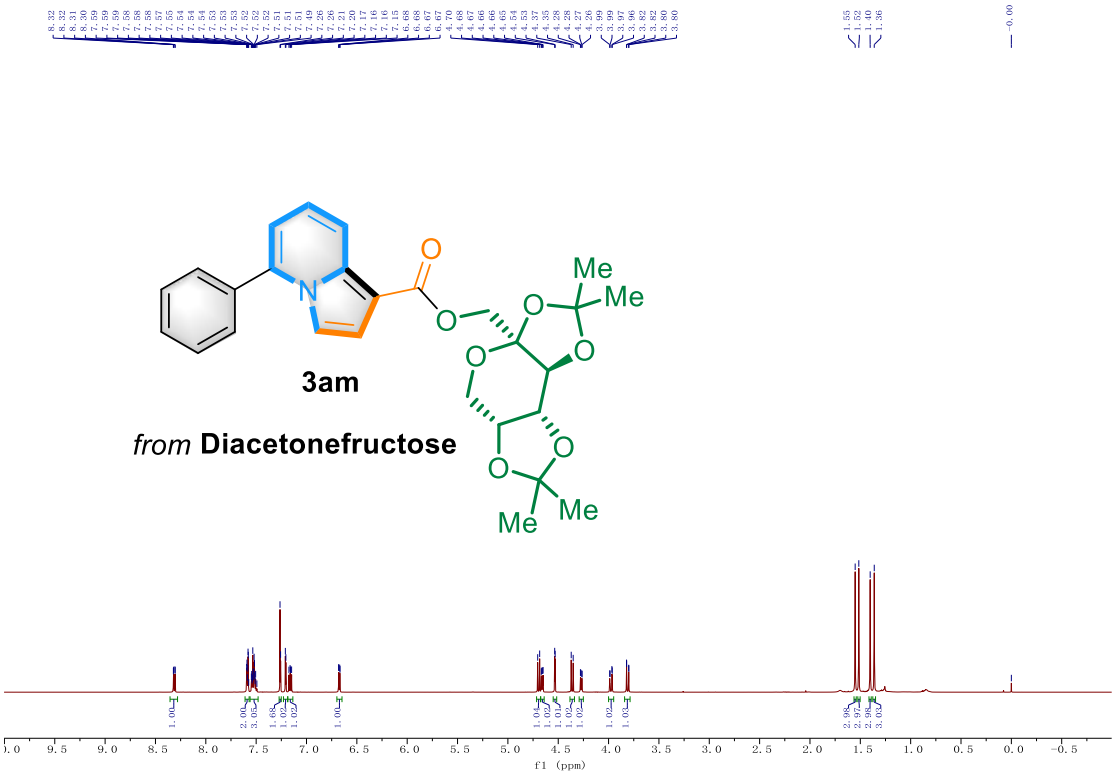
600 MHz ^{1}H NMR of **3al** in $CDCl_3$



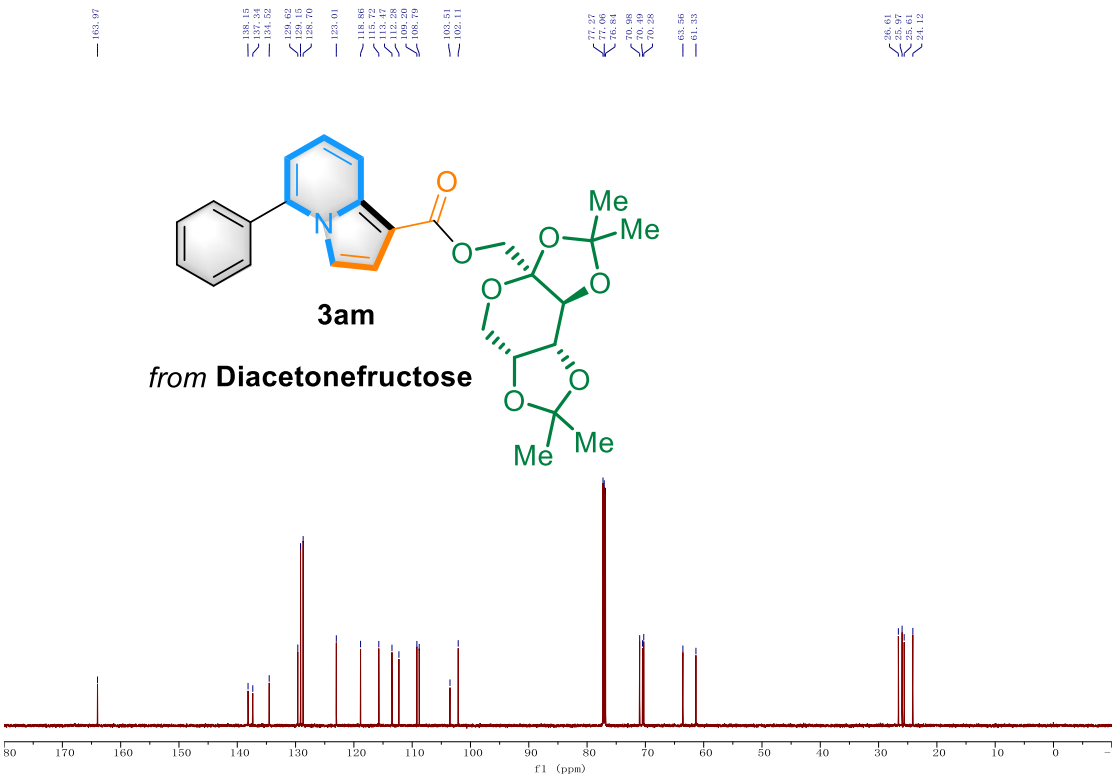
151 MHz ^{13}C NMR of **3al** in $CDCl_3$



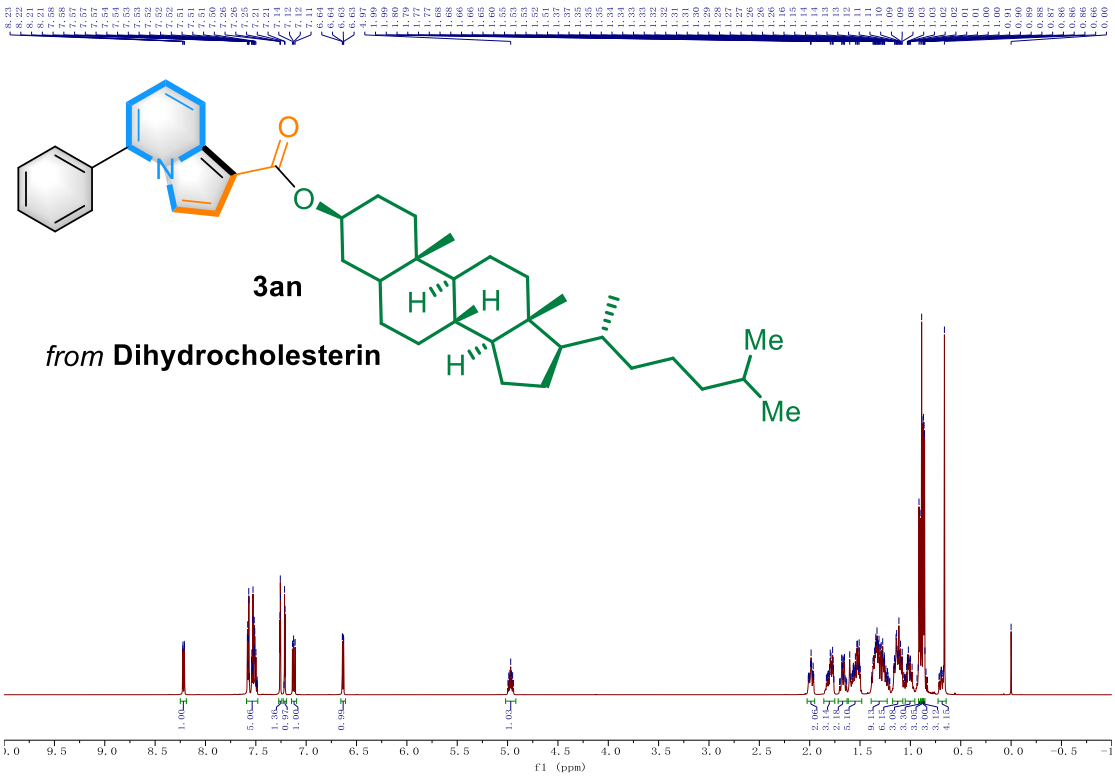
600 MHz ^{1}H NMR of **3am** in $CDCl_3$



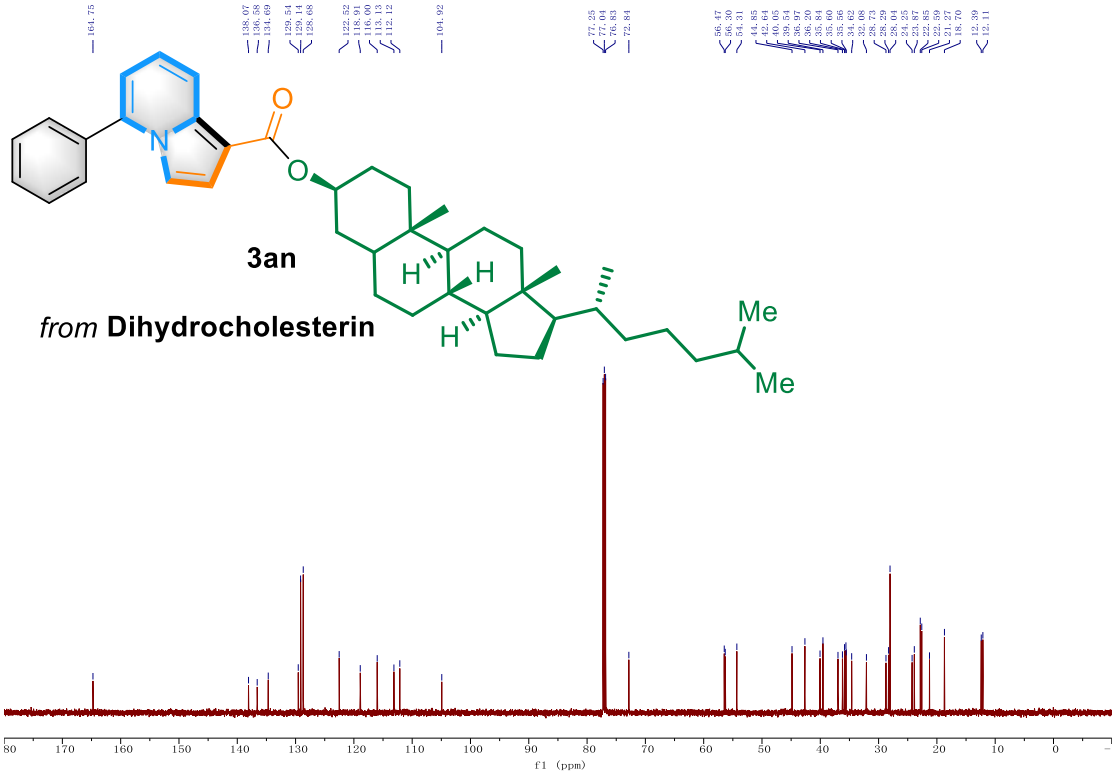
151 MHz ^{13}C NMR of **3am** in $CDCl_3$



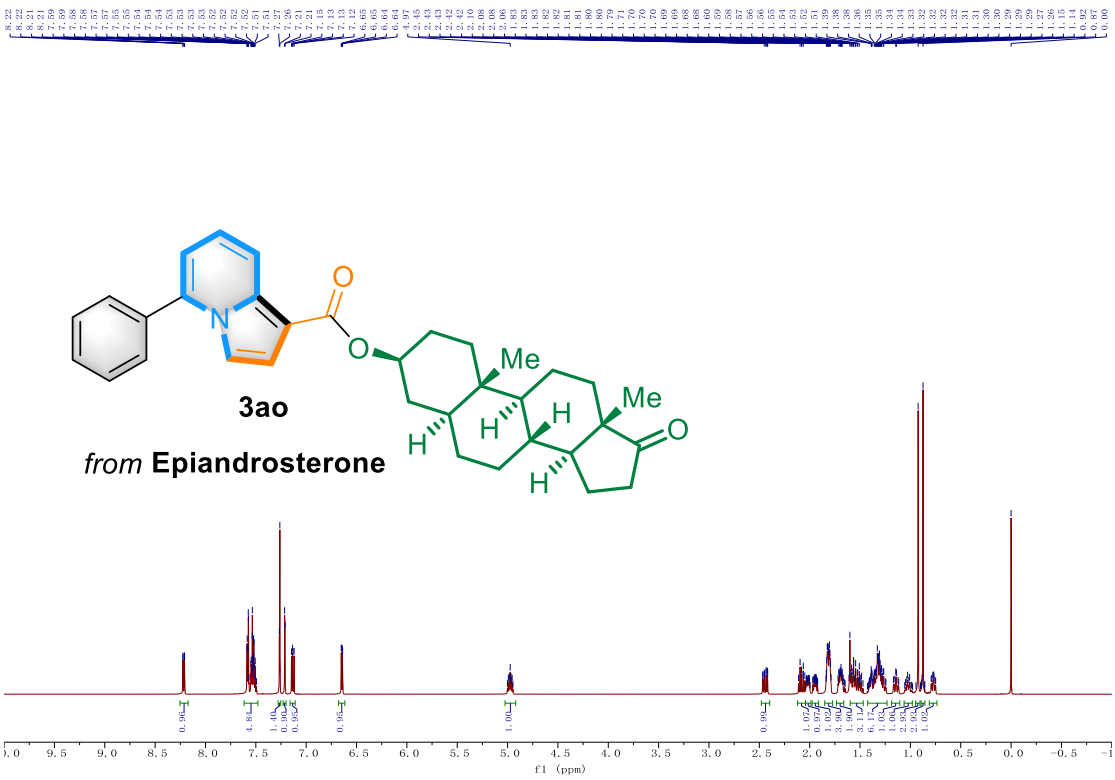
600 MHz ^{1}H NMR of **3an** in $CDCl_3$



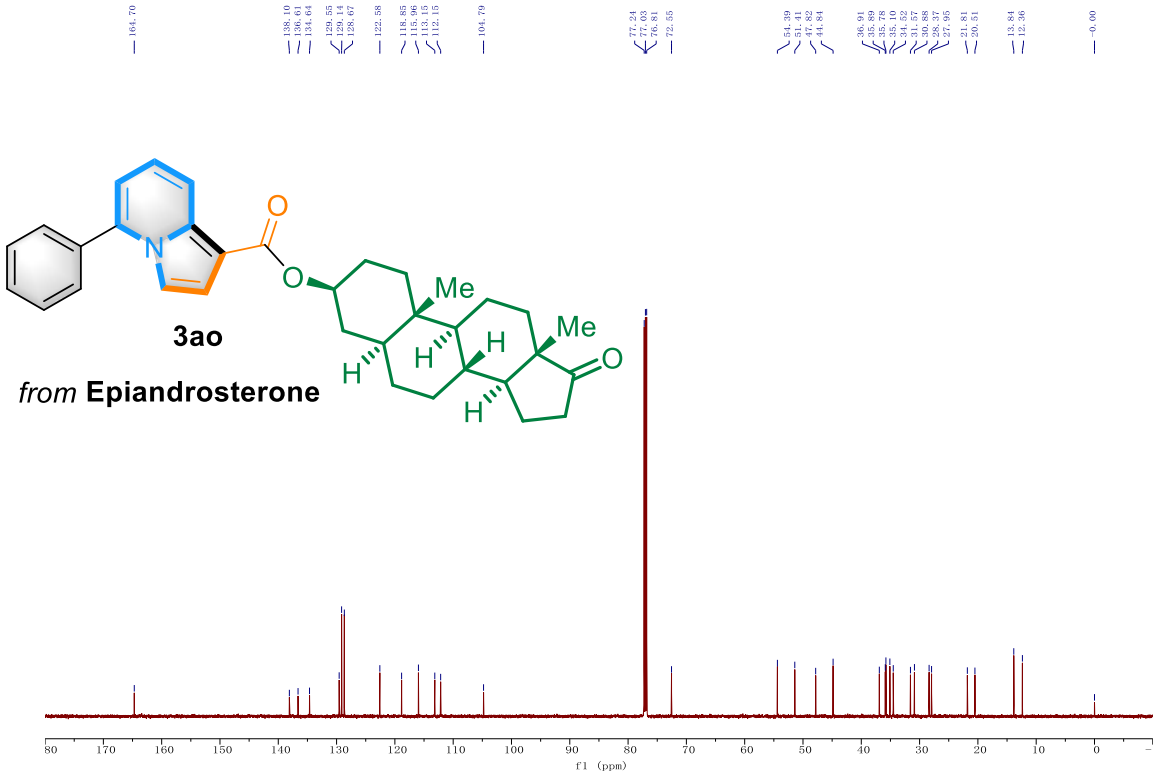
151 MHz ^{13}C NMR of **3an** in $CDCl_3$



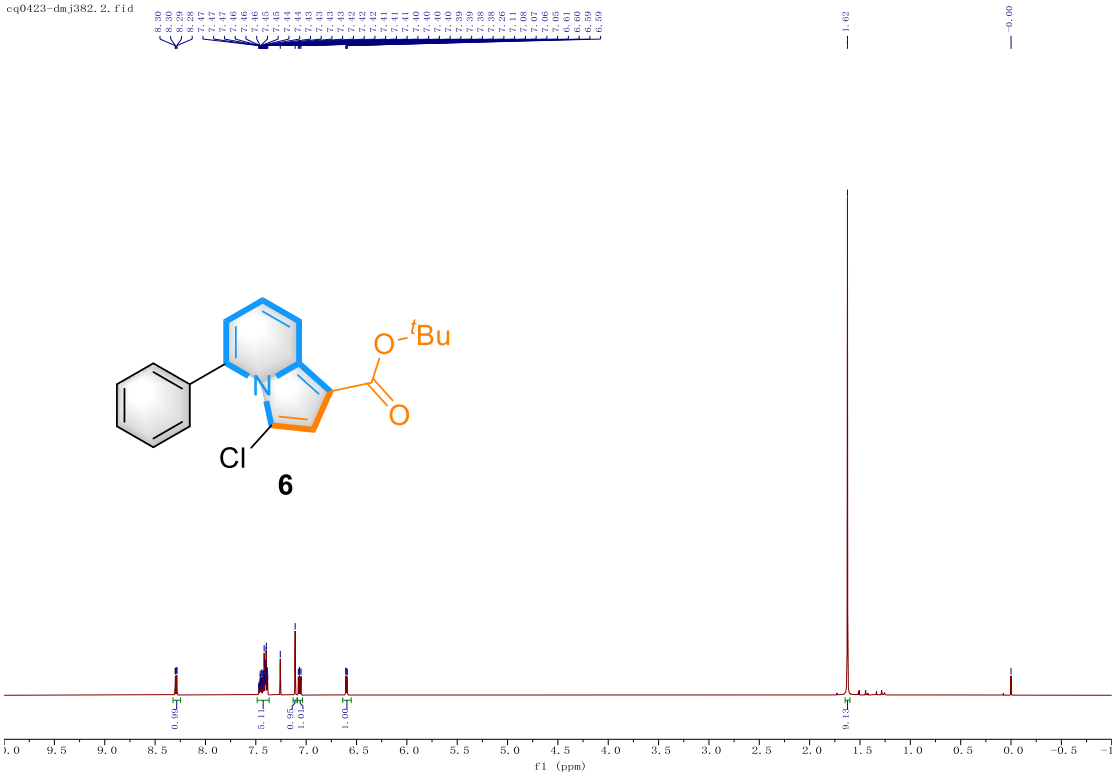
600 MHz ^{1}H NMR of **3ao** in $CDCl_3$



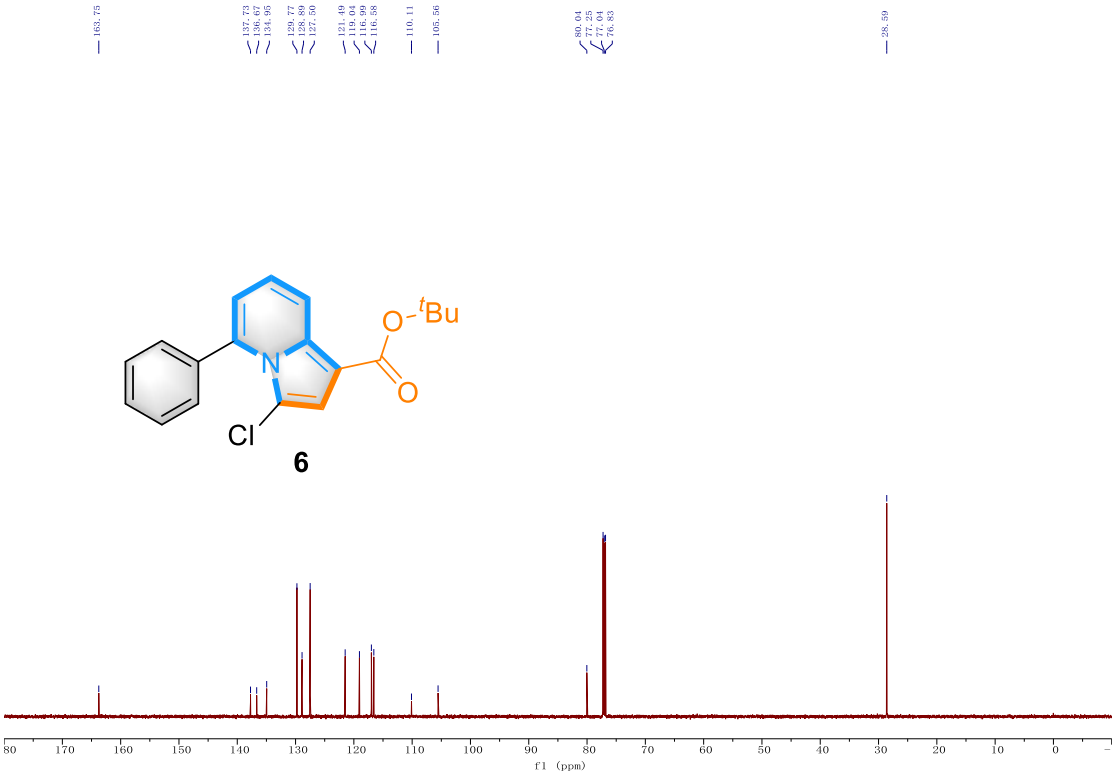
151 MHz ^{13}C NMR of **3ao** in $CDCl_3$



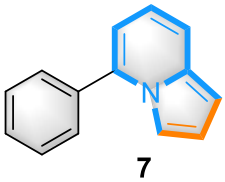
600 MHz ^{1}H NMR of **6** in $CDCl_3$



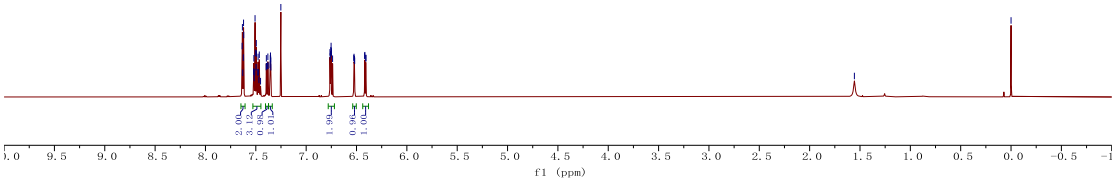
151 MHz ^{13}C NMR of **6** in $CDCl_3$



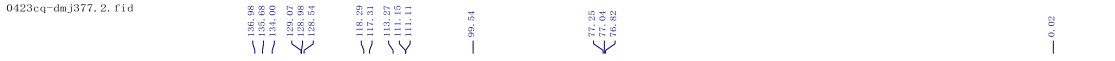
600 MHz ^{1}H NMR of **7** in $CDCl_3$

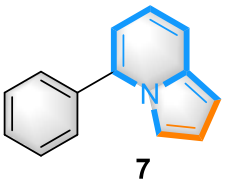


7



151 MHz ^{13}C NMR of **7** in $CDCl_3$





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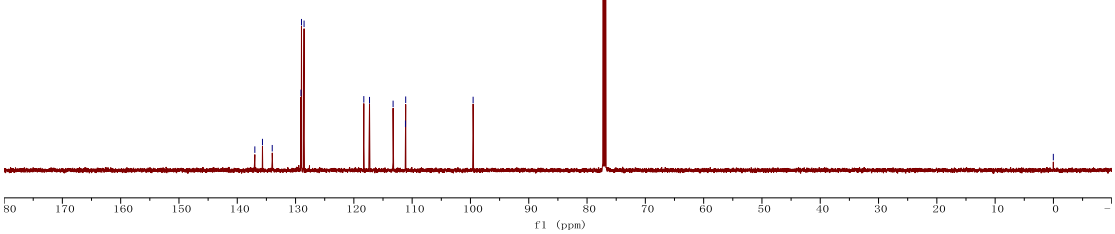
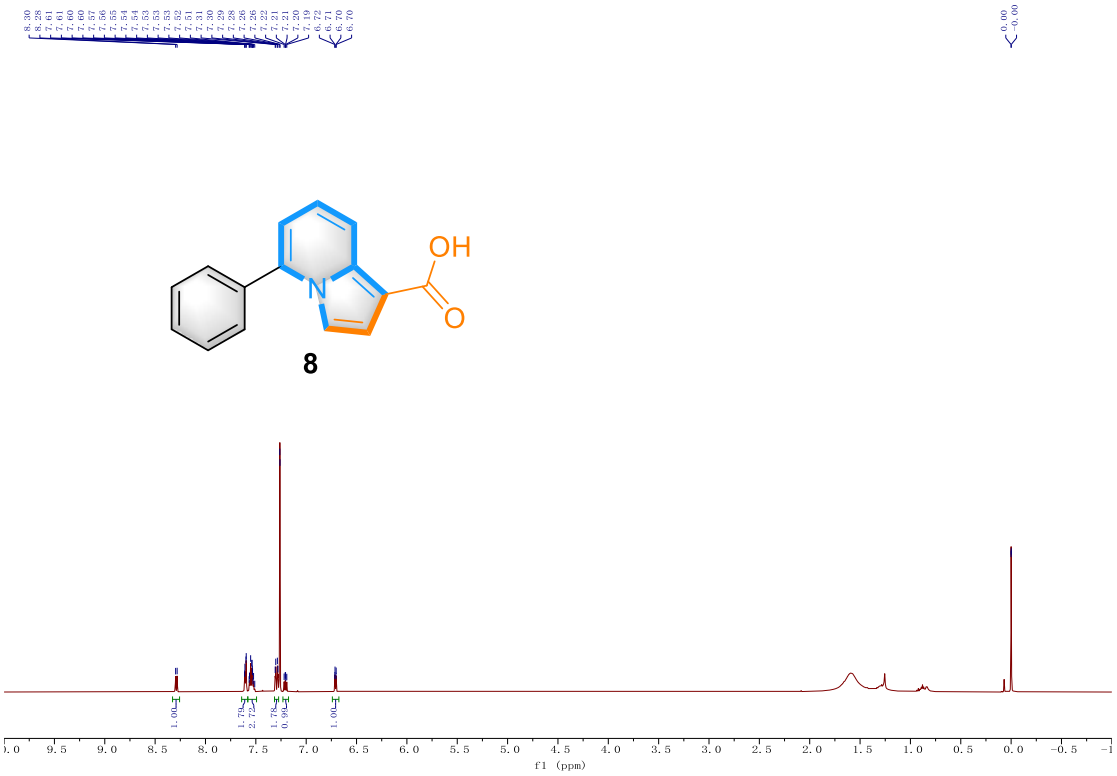


600 MHz ^{1}H NMR of **8** in $CDCl_3$



151 MHz ^{13}C NMR of **8** in $CDCl_3$