

Supporting information

Facile Synthesis of 1-Aminoindoles *via* Rh(III)-catalyzed Three-Component Annulation

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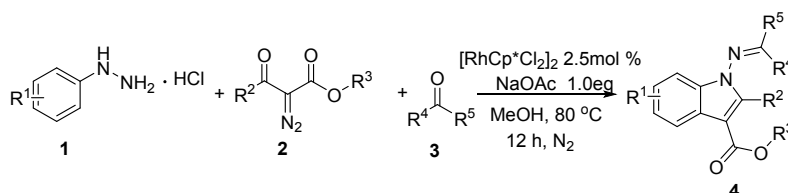
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1. General Information

All chemicals were analytically pure and used directly after purchased. All solvents were used without any particular precautions to extrude moisture. Melting points were determined in open glass capillaries and were uncorrected. ^1H NMR spectra were recorded on 400 MHz spectrometers, and ^{13}C NMR spectra were recorded on a 100 MHz spectrometer. Chemical shifts (in ppm) were referenced to tetramethylsilane ($\delta = 0$ ppm) in CDCl_3 as an internal standard at room temperature. ^{13}C NMR spectra were obtained by using the same NMR spectrometers and were calibrated with CDCl_3 ($\delta = 77.00$ ppm). High-resolution mass spectra (HRMS) were equipped with an ESI source and a TOF detector. Column chromatography was performed on silica gel (70-230 mesh ASTM) using the reported eluents. Thin-layer chromatography (TLC) was carried out on 4×15 cm plates with a layer thickness of 0.2 mm (silica gel 60 F254). Diazo compounds^[1] and phenylhydrazine hydrochloride-[D₅]^[2] were synthesized according to the previously reported procedure.

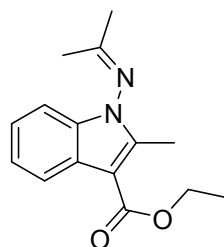
2. Typical procedure for synthesis of 4



To a test tube equipped with magnetic stir bar, phenylhydrazine hydrochloride (**1a**, 28.9 mg, 0.20 mmol), ethyl diazoacetate (**2a**, 46.8 mg, 0.30 mmol, 1.5 equiv), $[\text{RhCp}^*\text{Cl}_2]_2$ (3.09 mg, 0.005 mmol, 2.5 mmol %) and NaOAc (16.4 mg, 0.20 mmol, 1.0 equiv) were added sequentially. The tube was evacuated and backfilled with nitrogen for three cycles. Acetone (**3a**, 23.2 mg, 0.40 mmol, 2.0 equiv) was dissolved in MeOH (2.0 mL), and added under nitrogen atmosphere and the tube was sealed. The tube was immersed in an oil bath (80°C) and stirred for 12 h. After removal of the solvent under reduced pressure, purification was performed by flash column chromatography on silica gel with petroleum ether/ethyl acetate (gradient mixture ratio from 100:0 to 90:15) as eluent to afford **4a** (45 mg, 87%).

3. Characterization data of compounds 4

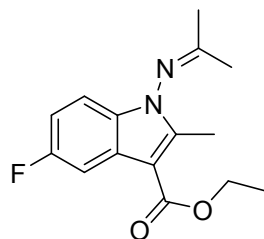
Ethyl 2-methyl-1-(propan-2-ylideneamino)-1H-indole-3-carboxylate (**4a**)



Yield: 87%, brown oil.

^1H NMR (400 MHz, CDCl_3) δ 8.15 (d, $J = 7.6$ Hz, 1H), 7.24 – 7.14 (m, 2H), 6.96 (d, $J = 7.9$ Hz, 1H), 4.40 (q, $J = 14.2, 7.1$ Hz, 2H), 2.58 (s, 3H), 2.38 (s, 3H), 1.76 (s, 3H), 1.45 (t, $J = 7.1$ Hz, 3H). ^{13}C NMR (100 MHz, CDCl_3) δ 181.1, 166.1, 141.3, 131.9, 125.0, 121.9, 121.6, 121.3, 108.8, 101.9, 59.3, 24.8, 20.0, 14.5, 11.5. HRMS (ESI): Calcd for $\text{C}_{15}\text{H}_{18}\text{N}_2\text{O}_2$ $[\text{M}+\text{H}]^+$: 259.1441; found: 259.1445.

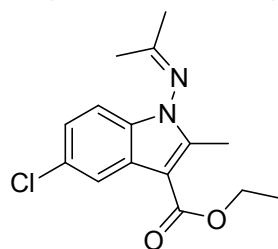
Ethyl 5-fluoro-2-methyl-1-(propan-2-ylideneamino)-1H-indole-3-carboxylate (4b)



Yield: 80%, brown oil.

¹H NMR (400 MHz, CDCl₃) δ 7.80 (dd, *J* = 9.9, 2.2 Hz, 1H), 6.93 (dd, *J* = 8.8, 2.4 Hz, 1H), 6.91 – 6.86 (m, 1H), 4.40 (q, *J* = 7.1 Hz, 2H), 2.57 (s, 3H), 2.40 (s, 3H), 1.78 (s, 3H), 1.45 (t, *J* = 7.1 Hz, 3H). **¹³C NMR (100 MHz, CDCl₃)** δ 181.5, 165.8, 159.2 (d, *J*_{CF} = 235.9 Hz), 142.5, 128.6, 125.7 (d, *J*_{CF} = 11.2 Hz), 110.2 (d, *J*_{CF} = 26.5 Hz), 109.6 (d, *J*_{CF} = 9.8 Hz), 106.8 (d, *J*_{CF} = 25.5 Hz), 102.1 (d, *J*_{CF} = 4.2 Hz), 59.5, 24.9, 20.0, 14.6, 11.6. **¹⁹F NMR (376 MHz, CDCl₃)** δ -122.01. **HRMS (ESI):** Calcd for C₁₅H₁₇FN₂O₂ [M+H]⁺: 277.1347; found: 277.1346

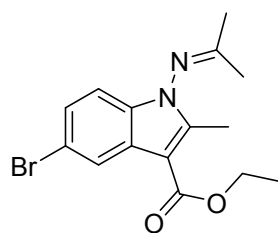
Ethyl 5-chloro-2-methyl-1-(propan-2-ylideneamino)-1H-indole-3-carboxylate (4c)



Yield: 77%, brown oil.

¹H NMR (400 MHz, CDCl₃) δ 8.12 (d, *J* = 2.0 Hz, 1H), 7.13 (dd, *J* = 8.6, 2.0 Hz, 1H), 6.88 (d, *J* = 8.6 Hz, 1H), 4.41 (q, *J* = 7.1 Hz, 2H), 2.57 (s, 3H), 2.40 (s, 3H), 1.77 (s, 3H), 1.46 (t, *J* = 7.1 Hz, 3H). **¹³C NMR (100 MHz, CDCl₃)** δ 181.6, 165.6, 142.4, 130.4, 127.5, 126.0, 122.3, 121.0, 109.90, 101.9, 59.6, 24.9, 20.0, 14.6, 11.6. **HRMS (ESI):** Calcd for C₁₅H₁₇ClN₂O₂ [M+H]⁺: 293.1051; found: 293.1032.

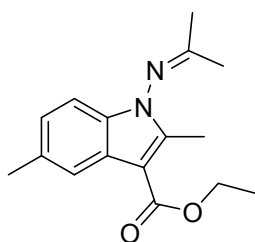
Ethyl 5-bromo-2-methyl-1-(propan-2-ylideneamino)-1H-indole-3-carboxylate (4d)



Yield: 81%, brown oil.

¹H NMR (400 MHz, CDCl₃) δ 8.28 (s, 1H), 7.26 (d, *J* = 8.6 Hz, 1H), 6.84 (d, *J* = 8.6 Hz, 1H), 4.41 (q, *J* = 7.1 Hz, 2H), 2.57 (s, 3H), 2.39 (s, 3H), 1.76 (s, 3H), 1.45 (t, *J* = 7.1 Hz, 3H). **¹³C NMR (100 MHz, CDCl₃)** δ 181.7, 165.6, 142.2, 130.7, 126.6, 124.9, 124.0, 115.3, 110.3, 101.8, 59.6, 25.0, 20.1, 14.6, 11.6. **HRMS (ESI):** Calcd for C₁₅H₁₇BrN₂O₂ [M+H]⁺: 377.0546; found: 377.0546.

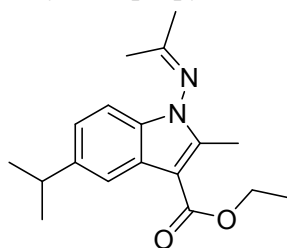
Ethyl 2,5-dimethyl-1-(propan-2-ylideneamino)-1H-indole-3-carboxylate (4e)



Yield: 74%, brown oil.

¹H NMR (400 MHz, CDCl₃) δ 7.95 (s, 1H), 7.00 (d, *J* = 8.1 Hz, 1H), 6.85 (d, *J* = 8.3 Hz, 1H), 4.41 (q, *J* = 7.0 Hz, 2H), 2.56 (s, 3H), 2.47 (s, 3H), 2.38 (s, 3H), 1.76 (s, 3H), 1.45 (t, *J* = 7.1 Hz, 3H). **¹³C NMR (100 MHz, CDCl₃)** δ 180.9, 166.2, 141.1, 131.1, 130.4, 125.3, 123.4, 121.1, 108.6, 101.4, 59.3, 24.9, 21.6, 20.0, 14.6, 11.6. **HRMS (ESI):** Calcd for C₁₆H₂₀N₂O₂ [M+H]⁺: 273.1598; found: 273.1594.

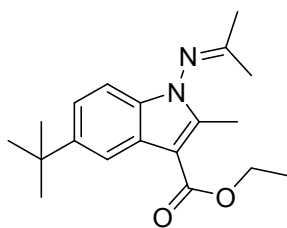
Ethyl 5-isopropyl-2-methyl-1-(propan-2-ylideneamino)-1H-indole-3-carboxylate (4f)



Yield: 51%, brown oil.

¹H NMR (400 MHz, CDCl₃) δ 8.03 (s, 1H), 7.06 (d, *J* = 8.4 Hz, 1H), 6.88 (d, *J* = 8.4 Hz, 1H), 4.41 (q, *J* = 13.7, 6.7 Hz, 2H), 3.10 – 2.98 (m, 1H), 2.56 (s, 3H), 2.38 (s, 3H), 1.78 (s, 3H), 1.46 (t, *J* = 6.7 Hz, 3H), 1.32 (d, *J* = 6.9 Hz, 6H). **¹³C NMR (100 MHz, CDCl₃)** δ 180.7, 166.2, 142.5, 141.2, 130.7, 125.2, 121.1, 118.4, 108.7, 101.7, 59.2, 34.3, 24.9, 24.5, 24.5, 20.1, 14.6, 11.6. **HRMS (ESI):** Calcd for C₁₈H₂₄N₂O₂ [M+H]⁺: 301.1911; found: 301.1912.

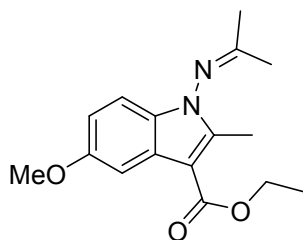
Ethyl 5-(tert-butyl)-2-methyl-1-(propan-2-ylideneamino)-1H-indole-3-carboxylate (4g)



Yield: 51%, yellow oil.

¹H NMR (400 MHz, CDCl₃) δ 8.21 (d, *J* = 1.1 Hz, 1H), 7.27 – 7.23 (m, 1H), 6.89 (d, *J* = 8.6 Hz, 1H), 4.40 (q, *J* = 7.1 Hz, 2H), 2.57 (s, 3H), 2.38 (s, 3H), 1.78 (s, 3H), 1.47 (t, *J* = 7.1 Hz, 3H), 1.40 (s, 9H). **¹³C NMR (100 MHz, CDCl₃)** δ 180.7, 166.3, 144.7, 141.3, 130.3, 124.9, 120.2, 117.3, 108.5, 101.8, 59.3, 34.7, 31.8, 24.9, 20.3, 14.6, 11.6. **HRMS (ESI):** Calcd for C₁₉H₂₆N₂O₂ [M+H]⁺: 315.2067; found: 315.2067.

Ethyl 5-methoxy-2-methyl-1-(propan-2-ylideneamino)-1H-indole-3-carboxylate (4h)

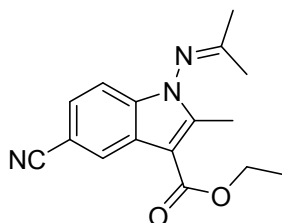


Yield: 60%, yellow oil.

¹H NMR (400 MHz, CDCl₃) δ 7.68 (d, *J* = 1.9 Hz, 1H), 6.83 (dt, *J* = 8.8, 5.4 Hz, 2H), 4.40 (q, *J* = 13.8, 6.8 Hz, 2H), 3.88 (s, 3H), 2.55 (s, 3H), 2.38 (s, 3H), 1.78 (s, 3H), 1.45 (t, *J* = 7.1 Hz, 3H).

¹³C NMR (100 MHz, CDCl₃) δ 181.0, 166.1, 155.7, 141.1, 127.2, 126.0, 111.8, 109.7, 103.42, 101.6, 59.3, 55.6, 24.9, 20.0, 14.6, 11.7. **HRMS (ESI):** Calcd for C₁₆H₂₀N₂O₃ [M+H]⁺: 289.1547; found: 289.1545.

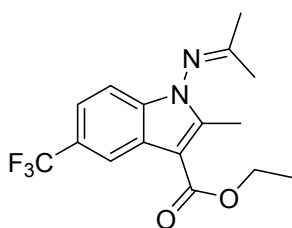
Ethyl 5-cyano-2-methyl-1-(propan-2-ylideneamino)-1H-indole-3-carboxylate (4i)



Yield: 54%, white solid, mp 105-107 °C.

¹H NMR (400 MHz, CDCl₃) δ 8.49 (d, *J* = 1.4 Hz, 1H), 7.41 (dd, *J* = 8.5, 1.5 Hz, 1H), 7.04 (d, *J* = 8.5 Hz, 1H), 4.43 (q, *J* = 7.1 Hz, 2H), 2.61 (s, 3H), 2.43 (s, 3H), 1.78 (s, 3H), 1.47 (t, *J* = 7.1 Hz, 3H). **¹³C NMR (100 MHz, CDCl₃)** δ 182.4, 165.1, 143.7, 133.3, 126.9, 125.1, 124.7, 120.5, 109.7, 104.7, 103.0, 59.9, 25.0, 20.1, 14.6, 11.6. **HRMS (ESI):** Calcd for C₁₆H₁₇N₃O₂ [M+H]⁺: 284.1394; found: 284.1394.

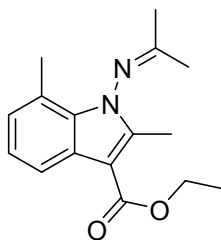
Ethyl 2-methyl-1-(propan-2-ylideneamino)-5-(trifluoromethyl)-1H-indole-3-carboxylate (4j)



Yield: 73%, white solid, mp 180-182 °C.

¹H NMR (400 MHz, CDCl₃) δ 8.47 (s, 1H), 7.41 (dd, *J* = 8.6, 1.5 Hz, 1H), 7.04 (d, *J* = 8.5 Hz, 1H), 4.43 (q, *J* = 7.1 Hz, 2H), 2.61 (s, 3H), 2.42 (s, 3H), 1.77 (s, 3H), 1.47 (t, *J* = 7.1 Hz, 3H). **¹³C NMR (100 MHz, CDCl₃)** δ 182.0, 165.5, 143.1, 133.1, 125.2 (q, *J*_{CF} = 271.7 Hz), 124.5, 123.9 (q, *J*_{CF} = 31.7 Hz), 119.2 (q, *J*_{CF} = 4.4 Hz), 118.8 (q, *J*_{CF} = 3.5 Hz), 109.1, 102.9, 59.7, 25.0, 20.1, 14.5, 11.6. **¹⁹F NMR (376 MHz, CDCl₃)** δ -60.48. **HRMS (ESI):** Calcd for C₁₆H₁₇F₃N₂O₂ [M+H]⁺: 327.1315; found: 327.1303.

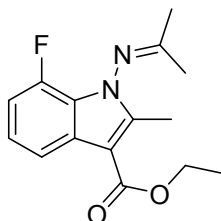
Ethyl 2,7-dimethyl-1-(propan-2-ylideneamino)-1H-indole-3-carboxylate (4k)



Yield: 85%, yellow oil.

¹H NMR (400 MHz, CDCl₃) δ 8.02 (d, *J* = 8.0 Hz, 1H), 7.08 (t, *J* = 7.6 Hz, 1H), 6.90 (d, *J* = 7.1 Hz, 1H), 4.40 (q, *J* = 7.0 Hz, 2H), 2.50 (s, 3H), 2.41 (s, 3H), 2.36 (s, 3H), 1.72 (s, 3H), 1.45 (t, *J* = 7.1 Hz, 3H). **¹³C NMR (100 MHz, CDCl₃)** δ 181.6, 166.2, 140.2, 131.4, 125.5, 124.6, 121.5, 120.3, 119.1, 101.8, 59.3, 24.7, 19.9, 19.0, 14.6, 11.3. **HRMS (ESI):** Calcd for C₁₆H₂₀N₂O₂ [M+H]⁺: 273.1598; found: 273.1602.

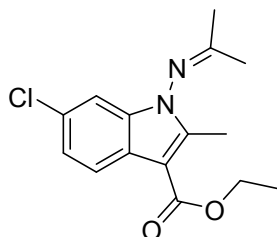
Ethyl 7-fluoro-2-methyl-1-(propan-2-ylideneamino)-1H-indole-3-carboxylate (4l)



Yield: 76%, white solid, mp 83-85 °C.

¹H NMR (400 MHz, CDCl₃) δ 7.93 (d, *J* = 8.1 Hz, 1H), 7.09 (td, *J* = 8.0, 4.7 Hz, 1H), 6.85 (dd, *J* = 12.2, 7.9 Hz, 1H), 4.40 (q, *J* = 7.1 Hz, 2H), 2.58 (s, 3H), 2.35 (s, 3H), 1.84 (s, 3H), 1.45 (t, *J* = 7.1 Hz, 3H). **¹³C NMR (100 MHz, CDCl₃)** δ 181.3, 165.8, 148.5 (d, *J* = 245.2 Hz), 142.5, 128.8 (d, *J* = 4.0 Hz), 121.6 (d, *J* = 6.6 Hz), 120.3 (d, *J* = 9.2 Hz), 117.1 (d, *J* = 3.6 Hz), 107.9 (d, *J* = 17.5 Hz), 102.7, 59.5, 24.9, 19.7 (d, *J* = 3.6 Hz), 14.6, 11.4. **¹⁹F NMR (376 MHz, CDCl₃)** δ -137.03. **HRMS (ESI):** Calcd for C₁₅H₁₇FN₂O₂ [M+H]⁺: 277.1347; found: 277.1343

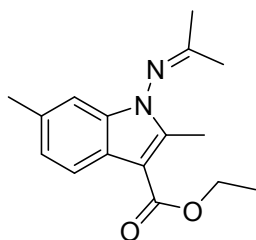
Ethyl 6-chloro-2-methyl-1-(propan-2-ylideneamino)-1H-indole-3-carboxylate (4m)



Yield: 54%, yellow oil.

¹H NMR (400 MHz, CDCl₃) δ 8.05 (d, *J* = 8.5 Hz, 1H), 7.17 (d, *J* = 8.5 Hz, 1H), 6.97 (s, 1H), 4.40 (q, *J* = 7.1 Hz, 2H), 2.56 (s, 3H), 2.40 (s, 3H), 1.78 (s, 3H), 1.44 (t, *J* = 7.1 Hz, 3H). **¹³C NMR (100 MHz, CDCl₃)** δ 181.8, 165.7, 142.0, 132.3, 127.9, 123.6, 122.3, 122.2, 108.8, 102.3, 59.5, 24.9, 20.0, 14.5, 11.5. **HRMS (ESI):** Calcd for C₁₅H₁₇ClN₂O₂ [M+H]⁺: 293.1051; found: 293.1033.

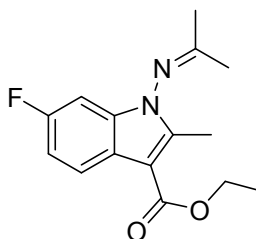
Ethyl 2,6-dimethyl-1-(propan-2-ylideneamino)-1H-indole-3-carboxylate (4n)



Yield: 69%, brown oil.

¹H NMR (400 MHz, CDCl₃) δ 8.01 (d, *J* = 8.1 Hz, 1H), 7.04 (d, *J* = 8.0 Hz, 1H), 6.75 (s, 1H), 4.39 (q, *J* = 7.0 Hz, 2H), 2.56 (s, 3H), 2.44 (s, 3H), 2.40 (s, 3H), 1.77 (s, 3H), 1.44 (t, *J* = 7.1 Hz, 3H). **¹³C NMR (100 MHz, CDCl₃)** δ 181.0, 166.2, 140.7, 132.3, 131.9, 123.3, 122.9, 121.0, 108.8, 101.8, 59.2, 24.9, 21.6, 20.0, 14.6, 11.5. **HRMS (ESI)**: Calcd for C₁₆H₂₀N₂O₂ [M+H]⁺: 273.1598; found: 273.1594.

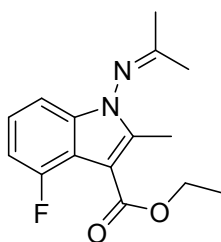
Ethyl 6-fluoro-2-methyl-1-(propan-2-ylideneamino)-1H-indole-3-carboxylate (4o)



Yield: 19%, yellow oil.

¹H NMR (400 MHz, CDCl₃) δ 8.07 (dd, *J* = 8.8, 5.4 Hz, 1H), 6.97 (ddd, *J* = 9.6, 8.8, 2.4 Hz, 1H), 6.66 (dd, *J* = 9.1, 2.3 Hz, 1H), 4.40 (q, *J* = 7.1 Hz, 2H), 2.56 (s, 3H), 2.40 (s, 3H), 1.79 (s, 3H), 1.45 (t, *J* = 7.1 Hz, 3H). **¹³C NMR (100 MHz, CDCl₃)** δ 181.6, 165.8, 159.7 (d, *J*_{CF} = 238.9 Hz), 141.9 (d, *J*_{CF} = 2.9 Hz), 131.9 (d, *J*_{CF} = 12.1 Hz), 122.4 (d, *J*_{CF} = 9.6 Hz), 121.4, 110.0 (d, *J*_{CF} = 23.8 Hz), 102.2, 95.5 (d, *J*_{CF} = 26.8 Hz), 59.5, 24.9, 20.0, 14.6, 11.6. **¹⁹F NMR (376 MHz, CDCl₃)** δ -120.47. **HRMS (ESI)**: Calcd for C₁₅H₁₇FN₂O₂ [M+H]⁺: 277.1347; found: 277.1347.

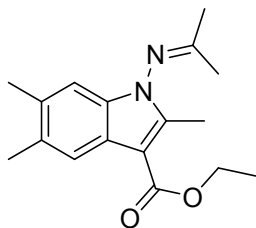
Ethyl 4-fluoro-2-methyl-1-(propan-2-ylideneamino)-1H-indole-3-carboxylate (4o')



Yield: 53%, yellow oil.

¹H NMR (400 MHz, CDCl₃) δ 7.09 (td, *J* = 8.0, 4.5 Hz, 1H), 6.87 (ddd, *J* = 11.5, 7.9, 0.7 Hz, 1H), 6.74 (dd, *J* = 8.1, 0.6 Hz, 1H), 4.38 (q, *J* = 7.1 Hz, 2H), 2.54 (s, 3H), 2.39 (s, 3H), 1.76 (s, 3H), 1.42 (t, *J* = 7.1 Hz, 3H). **¹³C NMR (100 MHz, CDCl₃)** δ 181.8, 165.2, 155.7 (d, *J*_{CF} = 252.4 Hz), 141.1, 134.5 (d, *J*_{CF} = 10.4 Hz), 122.6 (d, *J*_{CF} = 8.1 Hz), 112.8 (d, *J*_{CF} = 19.4 Hz), 107.9 (d, *J*_{CF} = 22.3 Hz), 105.0 (d, *J*_{CF} = 3.9 Hz), 101.5 (d, *J*_{CF} = 3.3 Hz), 59.8, 24.9, 20.0, 14.3, 11.6. **¹⁹F NMR (376 MHz, CDCl₃)** δ -112.25. **HRMS (ESI)**: Calcd for C₁₅H₁₇FN₂O₂ [M+H]⁺: 277.1347; found: 277.1344.

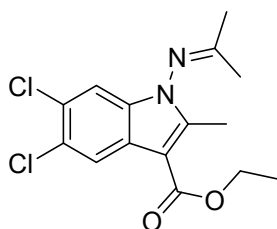
Ethyl 2,5,6-trimethyl-1-(propan-2-ylideneamino)-1H-indole-3-carboxylate (4p)



Yield: 55%, brown oil.

¹H NMR (400 MHz, CDCl₃) δ 7.90 (s, 1H), 6.73 (s, 1H), 4.40 (q, *J* = 7.1 Hz, 2H), 2.54 (s, 3H), 2.39 (s, 3H), 2.37 (s, 3H), 2.34 (s, 3H), 1.77 (s, 3H), 1.45 (t, *J* = 7.1 Hz, 3H). **¹³C NMR (100 MHz, CDCl₃)** δ 180.9, 166.3, 140.3, 131.1, 131.0, 130.4, 123.5, 121.6, 109.3, 101.4, 59.3, 24.9, 20.4, 20.2, 20.1, 14.7, 11.6. **HRMS (ESI):** Calcd for C₁₇H₂₂N₂O₂ [M+H]⁺: 287.1754; found: 287.1757.

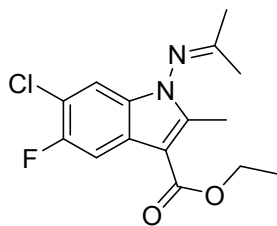
Ethyl 5,6-dichloro-2-methyl-1-(propan-2-ylideneamino)-1H-indole-3-carboxylate (4q)



Yield: 53%, yellow oil.

¹H NMR (400 MHz, CDCl₃) δ 8.21 (s, 1H), 7.08 (s, 1H), 4.40 (q, *J* = 7.1 Hz, 2H), 2.55 (s, 3H), 2.41 (s, 3H), 1.79 (s, 3H), 1.45 (t, *J* = 7.1 Hz, 3H). **¹³C NMR (100 MHz, CDCl₃)** δ 182.3, 165.3, 143.1, 130.8, 126.0, 125.8, 124.6, 122.6, 110.4, 101.9, 59.7, 25.0, 20.1, 14.6, 11.7. **HRMS (ESI):** Calcd for C₁₅H₁₆Cl₂N₂O₂ [M+H]⁺: 327.0662; found: 327.0656.

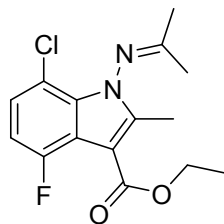
Ethyl 6-chloro-5-fluoro-2-methyl-1-(propan-2-ylideneamino)-1H-indole-3-carboxylate (4r)



Yield: 49%, brown solid, mp 108-110 °C.

¹H NMR (400 MHz, CDCl₃) δ 7.88 (d, *J* = 10.1 Hz, 1H), 7.00 (d, *J* = 6.1 Hz, 1H), 4.40 (q, *J* = 7.1 Hz, 2H), 2.55 (s, 3H), 2.41 (s, 3H), 1.79 (s, 3H), 1.45 (t, *J* = 7.1 Hz, 3H). **¹³C NMR (100 MHz, CDCl₃)** δ 182.3, 165.4, 154.3 (d, *J* = 239.3 Hz), 143.0, 128.4, 124.2 (d, *J* = 9.9 Hz), 115.7 (d, *J* = 21.6 Hz), 110.1, 108.0 (d, *J* = 25.3 Hz), 102.4 (d, *J* = 4.3 Hz), 59.7, 25.0, 20.1, 14.6, 11.7. **¹⁹F NMR (376 MHz, CDCl₃)** δ -124.22. **HRMS (ESI):** Calcd for C₁₅H₁₆ClFN₂O₂ [M+H]⁺: 311.0957; found: 311.0947.

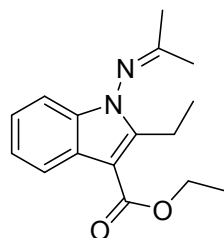
Ethyl 7-chloro-4-fluoro-2-methyl-1-(propan-2-ylideneamino)-1H-indole-3-carboxylate (4s)



Yield: 47%, yellow oil.

¹H NMR (400 MHz, CDCl₃) δ 7.05 (dd, *J* = 8.5, 3.9 Hz, 1H), 6.79 (dd, *J* = 10.6, 8.5 Hz, 1H), 4.38 (q, *J* = 7.1 Hz, 2H), 2.49 (s, 3H), 2.38 (s, 3H), 1.76 (s, 3H), 1.41 (t, *J* = 7.1 Hz, 3H). **¹³C NMR (100 MHz, CDCl₃)** δ 183.3, 164.8, 154.4 (d, *J* = 252.2 Hz), 141.7, 129.8 (d, *J* = 10.2 Hz), 124.0 (d, *J* = 8.2 Hz), 115.3 (d, *J* = 20.6 Hz), 110.8 (d, *J* = 4.0 Hz), 108.2 (d, *J* = 23.8 Hz), 102.2 (d, *J* = 3.7 Hz), 60.2, 24.8, 20.2, 14.3, 11.5. **¹⁹F NMR (376 MHz, CDCl₃)** δ -114.25. **HRMS (ESI):** Calcd for C₁₅H₁₆ClFN₂O₂ [M+H]⁺: 311.0957; found: 311.0952.

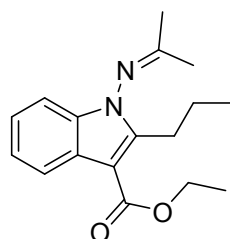
Ethyl 2-ethyl-1-(propan-2-ylideneamino)-1H-indole-3-carboxylate (4t)



Yield: 75%, yellow oil.

¹H NMR (400 MHz, CDCl₃) δ 8.17 (d, *J* = 7.8 Hz, 1H), 7.24 – 7.15 (m, 2H), 6.91 (d, *J* = 7.9 Hz, 1H), 4.41 (q, *J* = 7.1 Hz, 2H), 3.07 (q, *J* = 11.2 Hz, 2H), 2.39 (s, 3H), 1.78 (s, 3H), 1.45 (t, *J* = 7.1 Hz, 3H), 1.20 (t, *J* = 7.4 Hz, 3H). **¹³C NMR (100 MHz, CDCl₃)** δ 180.6, 165.8, 147.1, 131.7, 125.2, 122.0, 121.6, 121.5, 108.9, 101.1, 59.3, 24.9, 20.2, 18.8, 14.5, 13.0. **HRMS (ESI):** Calcd for C₁₆H₂₀N₂O₂ [M+H]⁺: 273.1598; found: 273.1598.

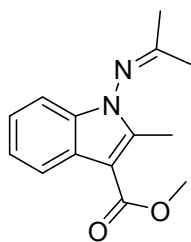
Ethyl 1-(propan-2-ylideneamino)-2-propyl-1H-indole-3-carboxylate (4u)



Yield: 65%, yellow oil.

¹H NMR (400 MHz, CDCl₃) δ 8.18 (d, *J* = 7.5 Hz, 1H), 7.20 (td, *J* = 15.0, 7.2 Hz, 2H), 6.90 (d, *J* = 7.7 Hz, 1H), 4.40 (q, *J* = 6.7 Hz, 2H), 3.18 – 2.89 (m, 2H), 2.39 (s, 3H), 1.77 (s, 3H), 1.63 (m, 2H), 1.45 (t, *J* = 7.1 Hz, 3H), 0.98 (t, *J* = 7.3 Hz, 3H). **¹³C NMR (100 MHz, CDCl₃)** δ 180.4, 165.8, 145.8, 131.6, 125.2, 122.0, 121.6, 121.5, 108.9, 101.7, 59.3, 27.2, 24.9, 22.1, 20.3, 14.5, 14.0. **HRMS (ESI):** Calcd for C₁₇H₂₂N₂O₂ [M+H]⁺: 287.1754; found: 287.1758.

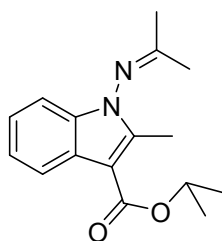
Methyl 2-methyl-1-(propan-2-ylideneamino)-1H-indole-3-carboxylate (4v)



Yield: 63%, brown oil.

¹H NMR (400 MHz, CDCl₃) δ 8.13 (d, *J* = 7.6 Hz, 1H), 7.25 – 7.14 (m, 2H), 6.96 (d, *J* = 7.9 Hz, 1H), 3.93 (s, 3H), 2.58 (s, 3H), 2.39 (s, 3H), 1.77 (s, 3H). **¹³C NMR (100 MHz, CDCl₃)** δ 181.1, 166.5, 141.4, 131.9, 125.0, 122.0, 121.7, 121.3, 108.93, 101.8, 50.6, 24.9, 20.0, 11.5. **HRMS (ESI):** Calcd for C₁₄H₁₆N₂O₂ [M+H]⁺: 245.1285; found: 245.1281.

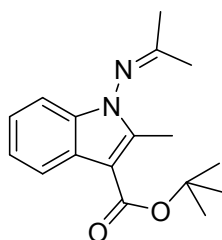
Isopropyl 2-methyl-1-(propan-2-ylideneamino)-1H-indole-3-carboxylate (4w)



Yield: 72%, brown oil.

¹H NMR (400 MHz, CDCl₃) δ 8.16 (d, *J* = 7.5 Hz, 1H), 7.25 – 7.15 (m, 2H), 6.96 (d, *J* = 8.0 Hz, 1H), 5.30 (m, *J* = 12.6, 6.2 Hz, 1H), 2.59 (s, 3H), 2.39 (s, 3H), 1.77 (s, 3H), 1.44 (s, 3H), 1.42 (s, 3H). **¹³C NMR (100 MHz, CDCl₃)** δ 181.0, 165.7, 141.3, 131.9, 125.1, 121.9, 121.6, 121.4, 108.8, 102.3, 66.5, 24.9, 22.3, 22.3, 20.0, 11.5. **HRMS (ESI):** Calcd for C₁₆H₂₀N₂O₂ [M+H]⁺: 273.1598; found: 273.1596.

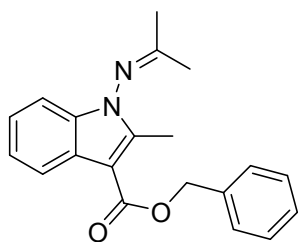
Tert-butyl 2-methyl-1-(propan-2-ylideneamino)-1H-indole-3-carboxylate (4x)



Yield: 84%, yellow oil.

¹H NMR (400 MHz, CDCl₃) δ 8.13 (d, *J* = 7.8 Hz, 1H), 7.24 – 7.13 (m, 2H), 6.95 (d, *J* = 7.6 Hz, 1H), 2.57 (s, 3H), 2.38 (s, 3H), 1.76 (s, 3H), 1.67 (s, 9H). **¹³C NMR (100 MHz, CDCl₃)** δ 180.9, 165.5, 141.0, 131.8, 125.1, 121.8, 121.5, 121.3, 108.8, 103.3, 79.6, 28.7, 24.9, 20.0, 11.5. **HRMS (ESI):** Calcd for C₁₇H₂₂N₂O₂ [M+H]⁺: 287.1754; found: 287.1756.

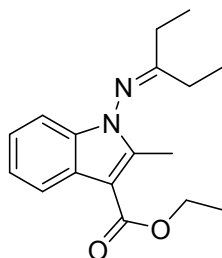
Benzyl 2-methyl-1-(propan-2-ylideneamino)-1H-indole-3-carboxylate (4y)



Yield: 52%, yellow oil.

¹H NMR (400 MHz, CDCl₃) δ 8.14 (d, *J* = 7.3 Hz, 1H), 7.49 (t, *J* = 6.8 Hz, 2H), 7.39 (t, *J* = 7.6 Hz, 2H), 7.35 – 7.30 (m, 1H), 7.24 – 7.14 (m, 2H), 6.96 (d, *J* = 7.2 Hz, 1H), 5.42 (s, 2H), 2.59 (s, 3H), 2.39 (s, 3H), 1.77 (s, 3H). **¹³C NMR (100 MHz, CDCl₃)** δ 181.2, 165.8, 141.7, 137.0, 132.0, 128.5, 128.0, 127.8, 125.0, 122.0, 121.8, 121.4, 108.9, 101.6, 65.2, 24.9, 20.1, 11.6. **HRMS (ESI):** Calcd for C₂₀H₂₀N₂O₂ [M+H]⁺: 321.1598; found: 321.1600.

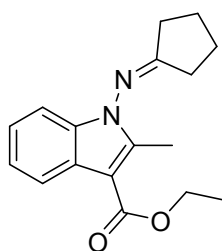
Ethyl 2-methyl-1-(pentan-3-ylideneamino)-1H-indole-3-carboxylate (4z)



Yield: 37%, yellow oil.

¹H NMR (400 MHz, CDCl₃) δ 8.15 (d, *J* = 7.4 Hz, 1H), 7.19 (dtd, *J* = 15.0, 7.2, 1.2 Hz, 2H), 6.95 (d, *J* = 7.7 Hz, 1H), 4.41 (q, *J* = 7.1 Hz, 2H), 2.70 (q, *J* = 7.4 Hz, 2H), 2.59 (s, 3H), 2.10 (q, *J* = 11.2, 5.3 Hz, 2H), 1.46 (t, *J* = 7.1 Hz, 3H), 1.38 (t, *J* = 7.4 Hz, 3H), 0.96 (t, *J* = 7.7 Hz, 3H). **¹³C NMR (100 MHz, CDCl₃)** δ 189.5, 166.1, 141.5, 132.2, 125.1, 121.9, 121.6, 121.3, 108.8, 101.9, 59.3, 29.0, 25.0, 14.6, 11.6, 11.1, 10.5. **HRMS (ESI):** Calcd for C₁₇H₂₂N₂O₂ [M+H]⁺: 287.1754; found: 287.1751.

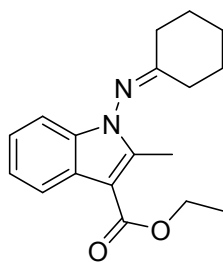
Ethyl 1-(cyclopentylideneamino)-2-methyl-1H-indole-3-carboxylate (4za)



Yield: 77%, yellow oil.

¹H NMR (400 MHz, CDCl₃) δ 8.16 (d, *J* = 7.3 Hz, 1H), 7.25 – 7.15 (m, 2H), 7.01 (d, *J* = 7.8 Hz, 1H), 4.40 (q, *J* = 7.1 Hz, 2H), 2.83 (t, *J* = 7.4 Hz, 2H), 2.62 (s, 3H), 2.12 (t, *J* = 7.2 Hz, 2H), 2.01 – 1.91 (m, 2H), 1.86 – 1.77 (m, 2H), 1.45 (t, *J* = 7.1 Hz, 3H). **¹³C NMR (100 MHz, CDCl₃)** δ 194.1, 166.1, 141.0, 131.2, 125.1, 121.9, 121.6, 121.4, 108.8, 101.8, 59.3, 33.7, 31.7, 24.5, 24.4, 14.6, 11.6. **HRMS (ESI):** Calcd for C₁₇H₂₀N₂O₂ [M+H]⁺: 285.1598; found: 285.1598.

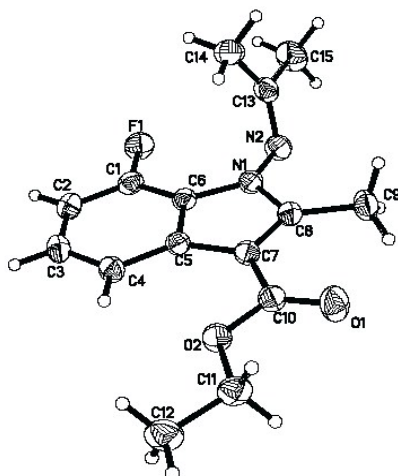
Ethyl 1-(cyclohexylideneamino)-2-methyl-1H-indole-3-carboxylate (4zb)



Yield: 56%, brown oil.

¹H NMR (400 MHz, CDCl₃) δ 8.14 (d, *J* = 7.4 Hz, 1H), 7.20 (ddd, *J* = 17.6, 11.6, 4.0 Hz, 2H), 6.99 (d, *J* = 7.7 Hz, 1H), 4.41 (q, *J* = 7.0 Hz, 2H), 2.71 (t, *J* = 6.3 Hz, 2H), 2.60 (s, 3H), 2.05 (t, *J* = 6.3 Hz, 2H), 1.95 (dt, *J* = 12.9, 6.3 Hz, 2H), 1.75 – 1.62 (m, 4H), 1.45 (t, *J* = 7.1 Hz, 3H). **¹³C NMR (100 MHz, CDCl₃)** δ 186.6, 166.2, 141.5, 132.5, 125.0, 121.9, 121.6, 121.2, 108.9, 101.8, 59.3, 35.5, 30.3, 27.8, 26.9, 25.4, 14.6, 11.5. **HRMS (ESI):** Calcd for C₁₈H₂₂N₂O₂ [M+H]⁺: 299.1754; found: 299.1756.

4. X-ray Crystallographic data of 4l



X-ray molecular structure of 4l

Table 1 Crystal data and structure refinement for 4l.

Empirical formula	C ₁₅ H ₁₇ FN ₂ O ₂
Formula weight	276.30
Temperature/K	293(2)
Crystal system	triclinic
Space group	P-1
a/Å	9.5214(8)
b/Å	9.6784(8)
c/Å	9.8861(8)
α /°	114.205(8)
β /°	92.568(7)
γ /°	116.743(8)
Volume/Å ³	712.05(12)
Z	2
$\rho_{\text{calc}}/\text{cm}^3$	1.289
μ/mm^{-1}	0.790
F(000)	292.0
Crystal size/mm ³	0.25 × 0.2 × 0.15
Radiation	CuK α (λ = 1.54184)
2 θ range for data collection/°	10.224 to 134.144
Index ranges	-11 ≤ h ≤ 11, -11 ≤ k ≤ 11, -8 ≤ l ≤ 11
Reflections collected	4970
Independent reflections	2536 [R _{int} = 0.0165, R _{sigma} = 0.0230]

Data/restraints/parameters 2536/0/186
 Goodness-of-fit on F² 1.042
 Final R indexes [I>2σ(I)] R₁ = 0.0376, wR₂ = 0.1015
 Final R indexes [all data] R₁ = 0.0440, wR₂ = 0.1075
 Largest diff. peak/hole / e Å⁻³ 0.18/-0.13

Table 2 Fractional Atomic Coordinates (×10⁴) and Equivalent Isotropic Displacement Parameters (Å²×10³) for 4l. U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{ij} tensor.

Atom	x	y	z	U(eq)
C ₁	10462.3(19)	2007.8(19)	3321.3(17)	46.5(4)
C ₂	12074(2)	2913(2)	4114.3(19)	54.0(4)
C ₃	12593.2(19)	4126(2)	5684.6(19)	53.6(4)
C ₄	11523.9(18)	4461(2)	6455.8(17)	47.0(4)
C ₅	9859.8(17)	3530.3(18)	5647.3(16)	40.0(3)
C ₆	9345.1(17)	2284.6(18)	4069.9(16)	40.7(3)
C ₇	8416.2(17)	3523.3(18)	6035.6(16)	41.4(3)
C ₈	7119.1(17)	2313.8(19)	4713.7(17)	43.8(3)
C ₉	5359.2(19)	1795(2)	4404(2)	59.6(4)
C ₁₀	8292.2(18)	4604(2)	7518.8(17)	46.2(4)
C ₁₁	9802(2)	6920(2)	10079.1(18)	57.0(4)
C ₁₂	11550(2)	8187(2)	10999(2)	70.0(5)
C ₁₃	6370.4(18)	-1196(2)	1460.6(18)	50.8(4)
C ₁₄	6878(2)	-1932(2)	2306(2)	63.1(5)
C ₁₅	5368(3)	-2431(3)	-184(2)	79.1(6)
F ₁	9955.6(12)	847.1(13)	1787.7(10)	62.9(3)
N ₁	7666.6(14)	1540.5(15)	3548.0(13)	44.1(3)
N ₂	6679.3(16)	391.6(17)	1993.8(14)	52.3(4)
O ₁	7043.5(15)	4504.8(18)	7816.6(14)	69.5(4)
O ₂	9764.4(13)	5766.9(14)	8559.8(11)	51.8(3)

Table 3 Anisotropic Displacement Parameters (Å²×10³) for 4l. The Anisotropic displacement factor exponent takes the form: -2π²[h²a^{*2}U₁₁+2hka^{*}b^{*}U₁₂+...].

Atom	U ₁₁	U ₂₂	U ₃₃	U ₂₃	U ₁₃	U ₁₂
C ₁	53.9(9)	44.3(8)	41.5(8)	15.6(7)	13.0(7)	30.0(7)
C ₂	50.2(9)	58.8(10)	61(1)	26.7(8)	21.2(8)	35.6(8)
C ₃	40.5(8)	58.3(9)	57.6(10)	24.8(8)	7.4(7)	25.5(7)
C ₄	43.0(8)	48.0(8)	40.5(8)	15.6(6)	4.1(6)	22.2(7)
C ₅	40.6(8)	38.3(7)	38.1(7)	16.2(6)	7.0(6)	20.5(6)

C ₆	41.5(8)	37.8(7)	39.2(8)	14.9(6)	6.2(6)	21.4(6)
C ₇	40.9(8)	41.1(7)	38.7(8)	16.4(6)	9.3(6)	21.1(6)
C ₈	40.1(8)	43.3(8)	44.7(8)	18.4(6)	9.1(6)	21.9(6)
C ₉	39.8(8)	65.8(10)	62.1(10)	24.1(9)	8.2(7)	25.5(8)
C ₁₀	45.2(8)	47.5(8)	43.5(8)	19.8(7)	13.0(7)	23.8(7)
C ₁₁	68.2(11)	55.5(9)	38.9(8)	13.0(7)	15.4(8)	34.2(9)
C ₁₂	78.8(13)	59.8(11)	46.9(10)	10.6(8)	4.9(9)	32(1)
C ₁₃	41.6(8)	44.9(8)	47.1(9)	11.5(7)	10.4(7)	18.0(7)
C ₁₄	64.7(11)	49.4(9)	74.8(12)	29.2(9)	26.2(9)	29.1(8)
C ₁₅	66.6(12)	65.0(12)	53.2(11)	-1.5(9)	-0.5(9)	23(1)
F ₁	70.1(6)	62.2(6)	44.8(5)	10.8(4)	17.0(5)	38.6(5)
N ₁	41.6(7)	40.0(6)	38.2(6)	9.9(5)	1.6(5)	20.3(5)
N ₂	50.6(8)	49.4(7)	39.4(7)	11.1(6)	-2.0(6)	23.2(6)
O ₁	51.4(7)	81.3(9)	57.9(7)	18.8(6)	22.0(6)	33.4(6)
O ₂	50.9(6)	53.1(6)	37.6(6)	9.9(5)	10.3(5)	27.2(5)

Table 4 Bond Lengths for 4l.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
C ₁	C ₂	1.363(2)	C ₈	C ₉	1.492(2)
C ₁	C ₆	1.384(2)	C ₈	N ₁	1.3629(19)
C ₁	F ₁	1.3578(17)	C ₁₀	O ₁	1.2089(18)
C ₂	C ₃	1.395(2)	C ₁₀	O ₂	1.3387(18)
C ₃	C ₄	1.374(2)	C ₁₁	C ₁₂	1.488(3)
C ₄	C ₅	1.4044(19)	C ₁₁	O ₂	1.4450(18)
C ₅	C ₆	1.4084(19)	C ₁₃	C ₁₄	1.483(2)
C ₅	C ₇	1.4415(19)	C ₁₃	C ₁₅	1.492(2)
C ₆	N ₁	1.3873(18)	C ₁₃	N ₂	1.281(2)
C ₇	C ₈	1.380(2)	N ₁	N ₂	1.4176(16)
C ₇	C ₁₀	1.458(2)			

Table 5 Bond Angles for 4l.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
C ₂	C ₁	C ₆	120.21(14)	C ₇	C ₈	C ₉	131.54(14)
F ₁	C ₁	C ₂	119.83(14)	N ₁	C ₈	C ₇	108.93(12)
F ₁	C ₁	C ₆	119.95(13)	N ₁	C ₈	C ₉	119.53(13)
C ₁	C ₂	C ₃	119.60(14)	O ₁	C ₁₀	C ₇	126.04(15)
C ₄	C ₃	C ₂	121.71(14)	O ₁	C ₁₀	O ₂	122.43(14)

C ₃	C ₄	C ₅	119.01(14)	O ₂	C ₁₀	C ₇	111.52(13)
C ₄	C ₅	C ₆	118.76(13)	O ₂	C ₁₁	C ₁₂	107.70(14)
C ₄	C ₅	C ₇	135.05(13)	C ₁₄	C ₁₃	C ₁₅	117.17(15)
C ₆	C ₅	C ₇	106.19(12)	N ₂	C ₁₃	C ₁₄	127.11(15)
C ₁	C ₆	C ₅	120.68(13)	N ₂	C ₁₃	C ₁₅	115.72(16)
C ₁	C ₆	N ₁	131.68(13)	C ₆	N ₁	N ₂	126.54(12)
N ₁	C ₆	C ₅	107.63(12)	C ₈	N ₁	C ₆	109.71(12)
C ₅	C ₇	C ₁₀	128.07(13)	C ₈	N ₁	N ₂	122.83(12)
C ₈	C ₇	C ₅	107.48(12)	C ₁₃	N ₂	N ₁	114.29(13)
C ₈	C ₇	C ₁₀	124.43(13)	C ₁₀	O ₂	C ₁₁	116.73(12)

Table 6 Torsion Angles for 4l.

A	B	C	D	Angle/°	A	B	C	D	Angle/°
C ₁	C ₂	C ₃	C ₄	-1.2(3)	C ₆	N ₁	N ₂	C ₁₃	76.11(19)
C ₁	C ₆	N ₁	C ₈	-176.95(15)	C ₇	C ₅	C ₆	C ₁	178.15(13)
C ₁	C ₆	N ₁	N ₂	-7.7(2)	C ₇	C ₅	C ₆	N ₁	-1.20(15)
C ₂	C ₁	C ₆	C ₅	1.5(2)	C ₇	C ₈	N ₁	C ₆	-2.52(16)
C ₂	C ₁	C ₆	N ₁	-179.35(15)	C ₇	C ₈	N ₁	N ₂	-172.23(12)
C ₂	C ₃	C ₄	C ₅	1.4(2)	C ₇	C ₁₀	O ₂	C ₁₁	179.83(13)
C ₃	C ₄	C ₅	C ₆	-0.1(2)	C ₈	C ₇	C ₁₀	O ₁	5.3(3)
C ₃	C ₄	C ₅	C ₇	-179.36(15)	C ₈	C ₇	C ₁₀	O ₂	-174.56(13)
C ₄	C ₅	C ₆	C ₁	-1.3(2)	C ₈	N ₁	N ₂	C ₁₃	-115.97(16)
C ₄	C ₅	C ₆	N ₁	179.34(12)	C ₉	C ₈	N ₁	C ₆	176.79(13)
C ₄	C ₅	C ₇	C ₈	179.04(15)	C ₉	C ₈	N ₁	N ₂	7.1(2)
C ₄	C ₅	C ₇	C ₁₀	0.7(3)	C ₁₀	C ₇	C ₈	C ₉	0.9(3)
C ₅	C ₆	N ₁	C ₈	2.31(16)	C ₁₀	C ₇	C ₈	N ₁	-179.88(13)
C ₅	C ₆	N ₁	N ₂	171.55(12)	C ₁₂	C ₁₁	O ₂	C ₁₀	-175.49(13)
C ₅	C ₇	C ₈	C ₉	-177.50(16)	C ₁₄	C ₁₃	N ₂	N ₁	2.5(2)
C ₅	C ₇	C ₈	N ₁	1.70(16)	C ₁₅	C ₁₃	N ₂	N ₁	-178.58(14)
C ₅	C ₇	C ₁₀	O ₁	-176.60(15)	F ₁	C ₁	C ₂	C ₃	178.95(14)
C ₅	C ₇	C ₁₀	O ₂	3.5(2)	F ₁	C ₁	C ₆	C ₅	-177.70(12)
C ₆	C ₁	C ₂	C ₃	-0.2(2)	F ₁	C ₁	C ₆	N ₁	1.5(2)
C ₆	C ₅	C ₇	C ₈	-0.28(15)	O ₁	C ₁₀	O ₂	C ₁₁	-0.1(2)
C ₆	C ₅	C ₇	C ₁₀	-178.62(14)					

Table 7 Hydrogen Atom Coordinates ($\text{\AA}\times 10^4$) and Isotropic Displacement Parameters ($\text{\AA}^2\times 10^3$) for 4l.

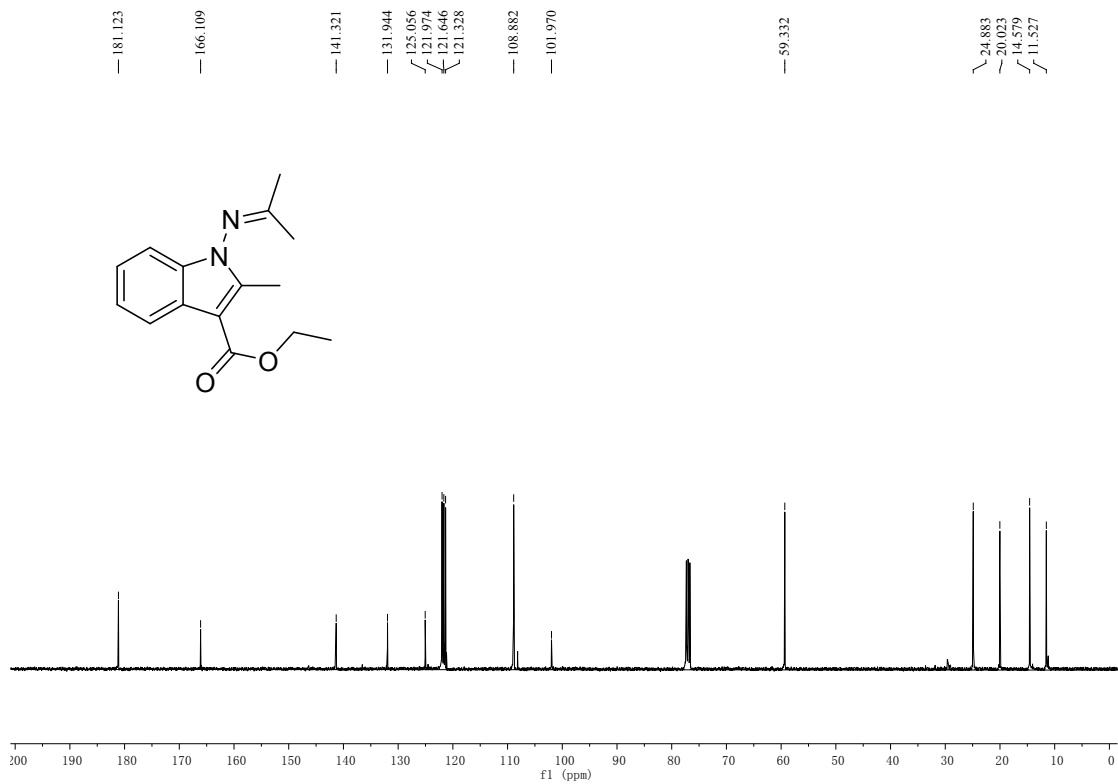
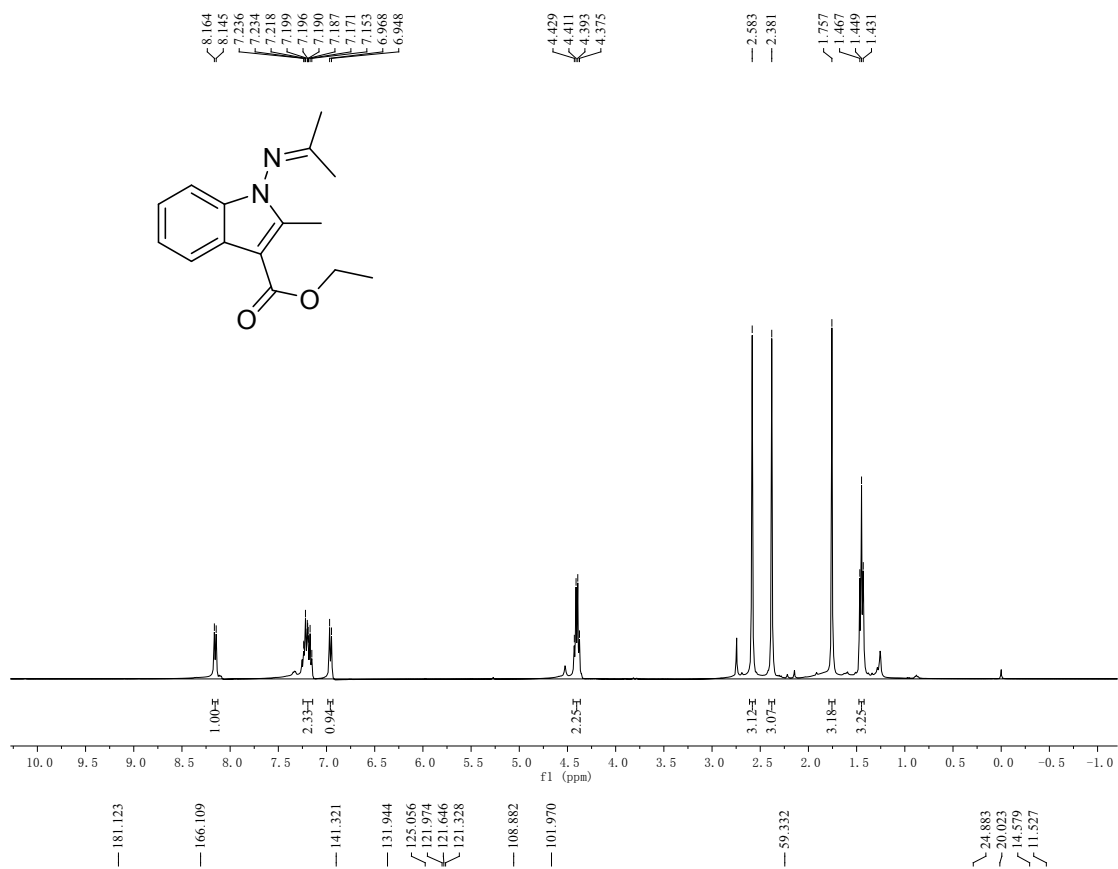
Atom	x	y	z	U(eq)
H ₂	12824	2724	3612	65
H ₃	13691	4723	6223	64
H ₄	11896	5292	7498	56
H _{9A}	5019	1763	3457	89
H _{9B}	5221	2641	5239	89
H _{9C}	4705	648	4316	89
H _{11A}	9223	6237	10573	68
H _{11B}	9277	7553	10001	68
H _{12A}	12099	8896	10528	105
H _{12B}	12069	7546	11032	105
H _{12C}	11610	8937	12032	105
H _{14A}	7643	-2244	1878	95
H _{14B}	5932	-2964	2209	95
H _{14C}	7387	-1063	3378	95
H _{15A}	5029	-1837	-576	119
H _{15B}	4418	-3438	-249	119
H _{15C}	6010	-2813	-787	119

5. Reference:

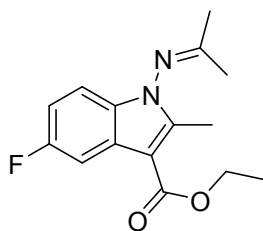
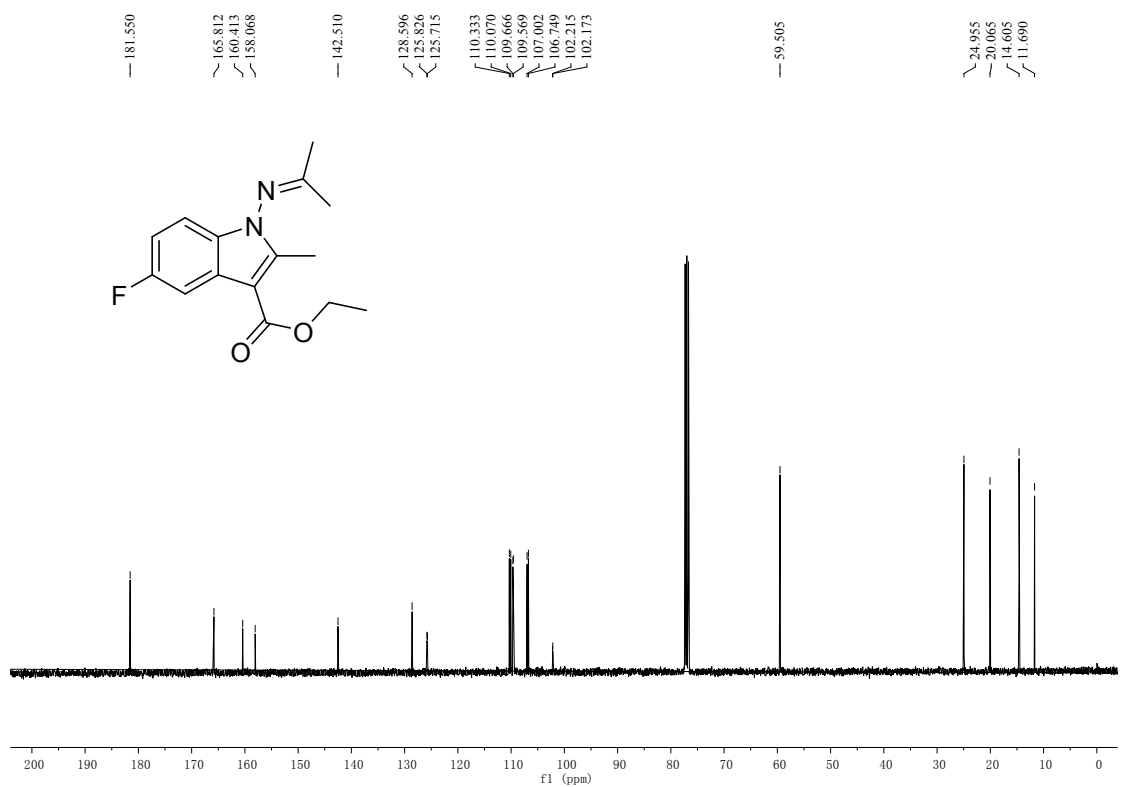
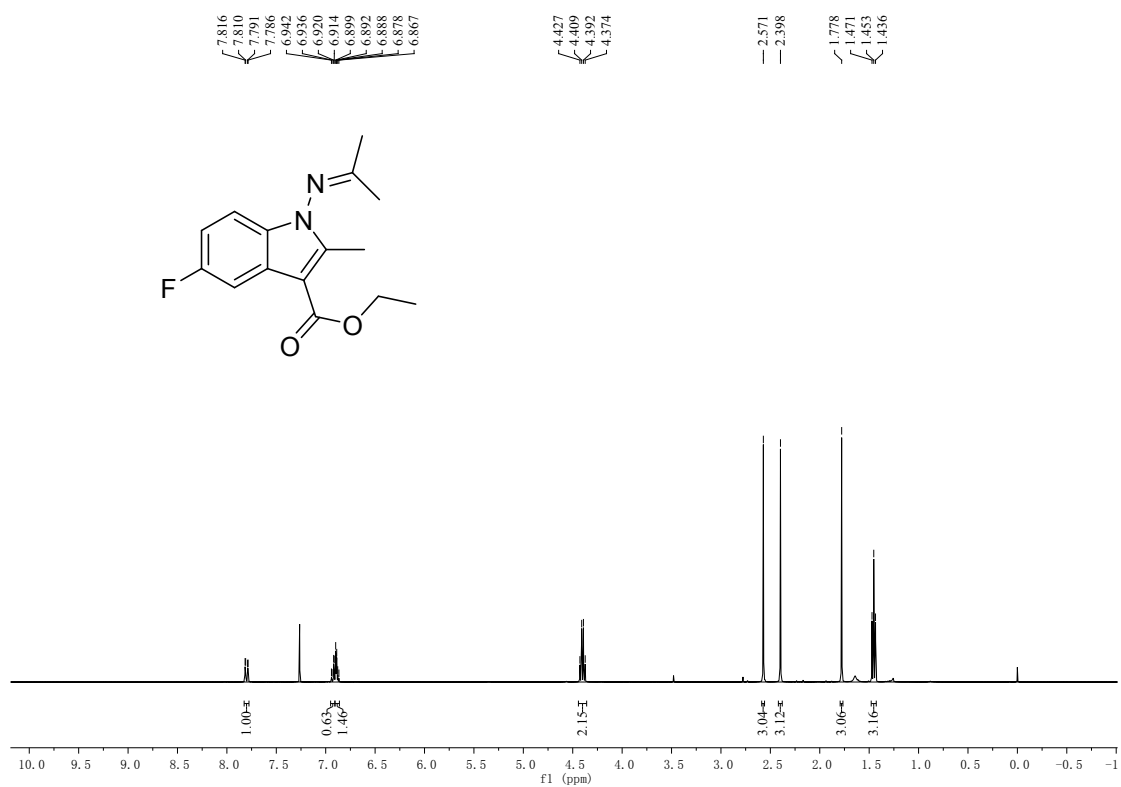
1. Koduri, N. D.; Scott, H.; Hileman, B.; Cox, J. D.; Coffin, M.; Glicksberg, L.; Hussaini, S. R., *Org. Lett.* **2012**, 14, 440.
2. Zhang, P.; Zhang, Y.; Xue, X.; Wang, C.; Wang, Z.; Huang, L. *Anal. Biochem.* **2011**, 418, 1.

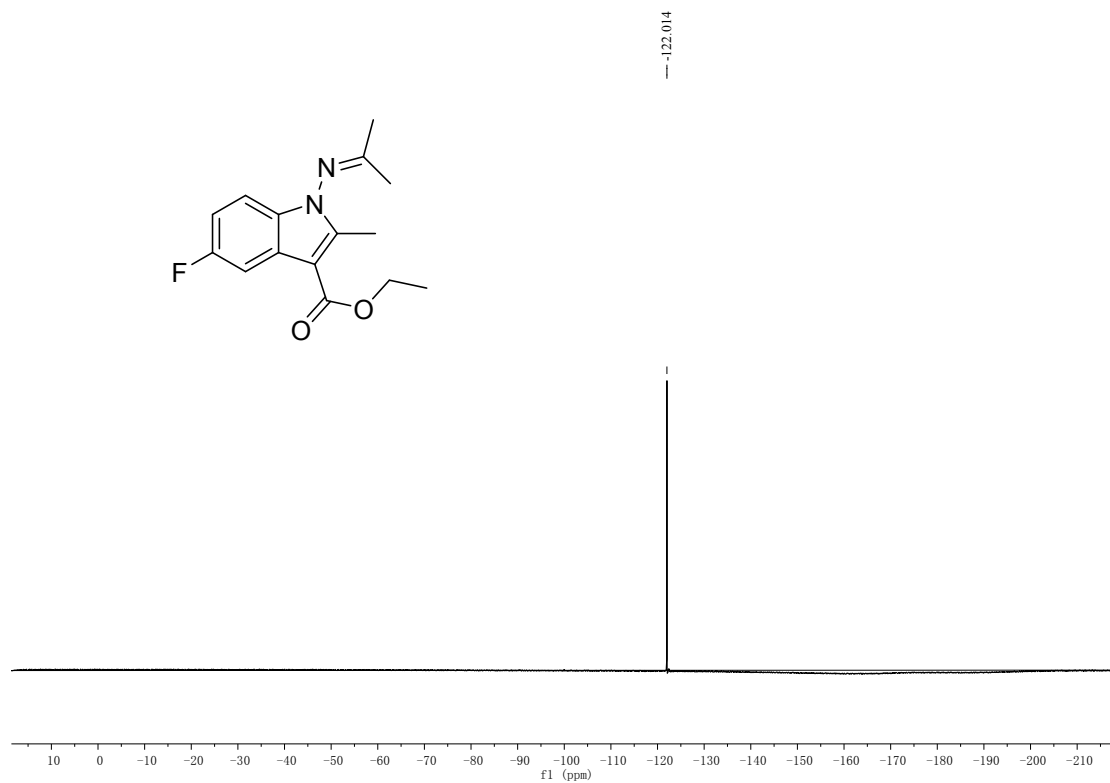
6. NMR Spectra of compounds 4

^1H , ^{13}C spectra of 4a

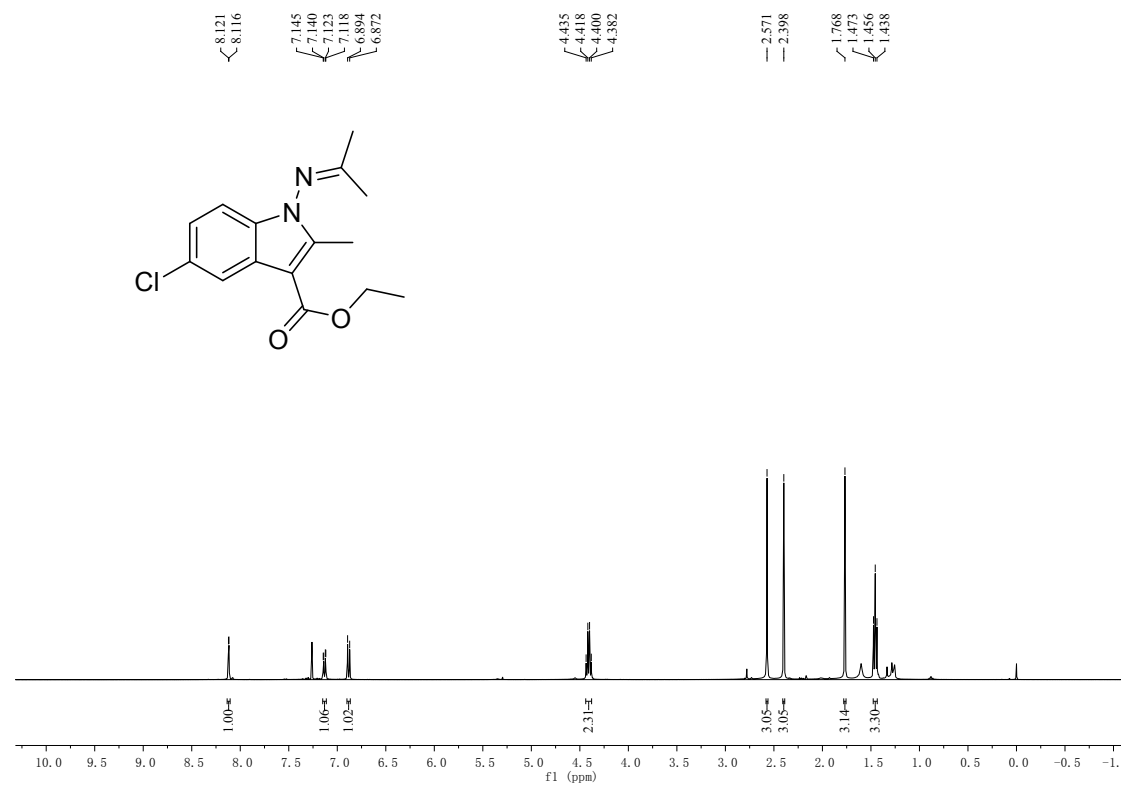


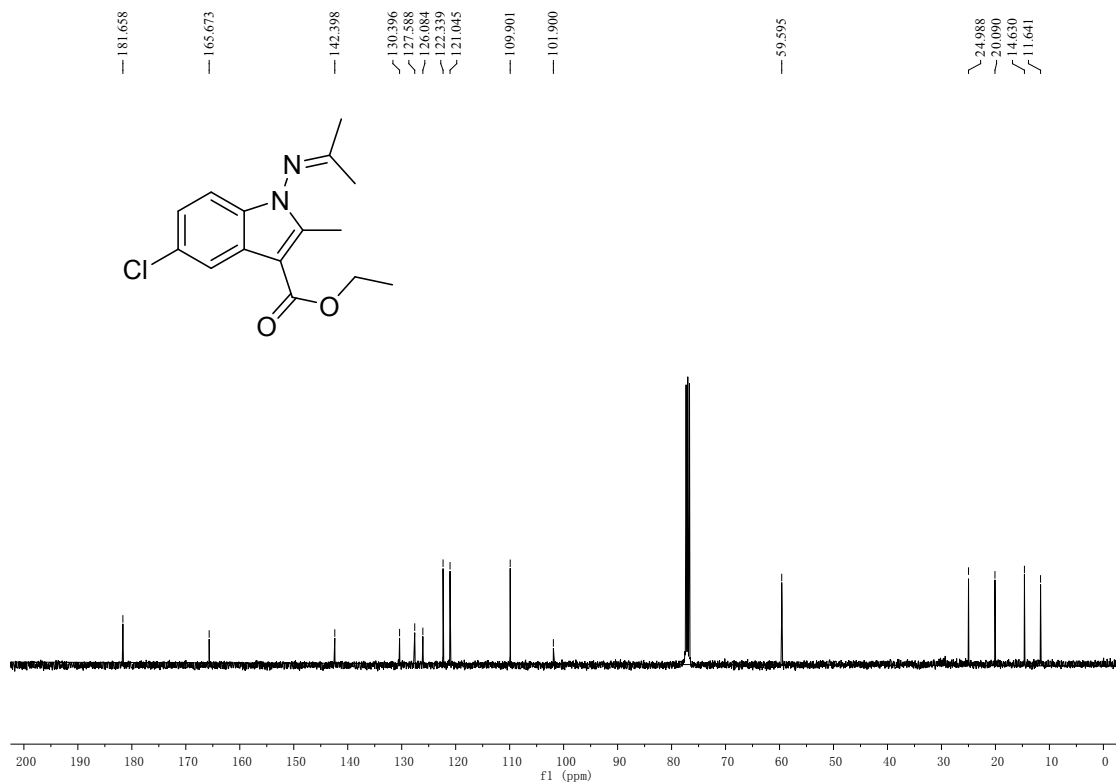
¹H, ¹³C, ¹⁹F spectra of 4b



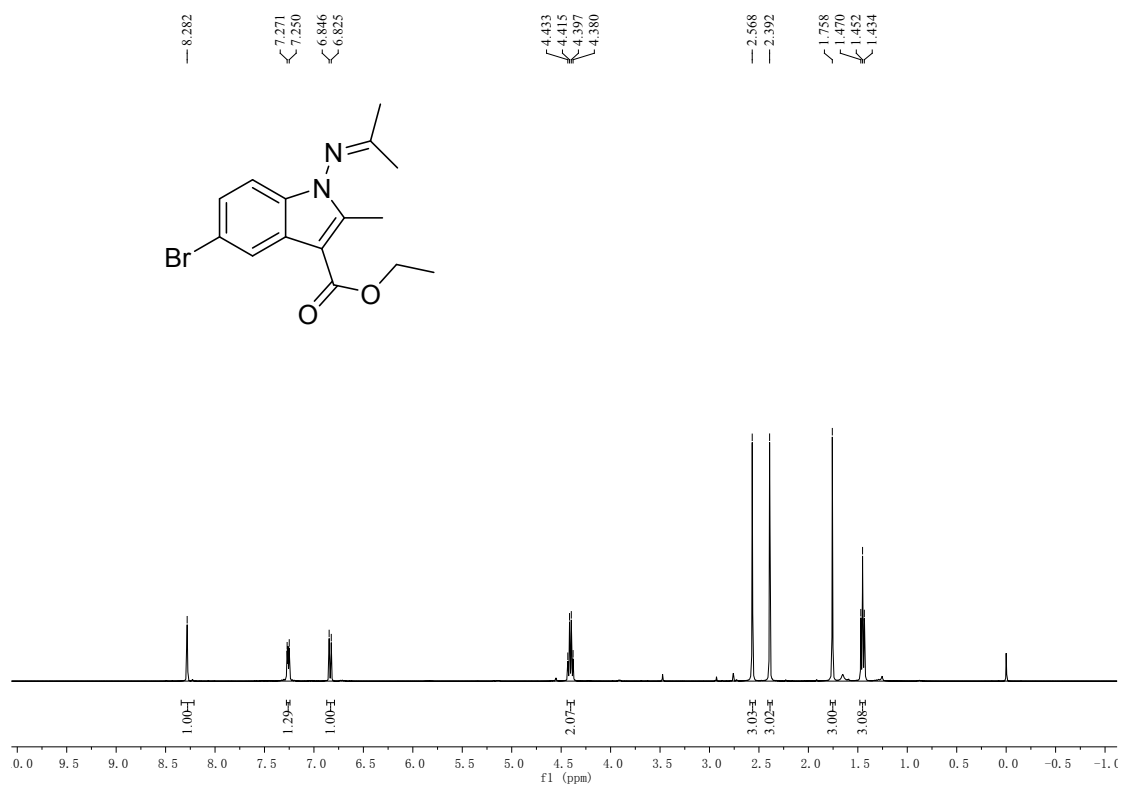


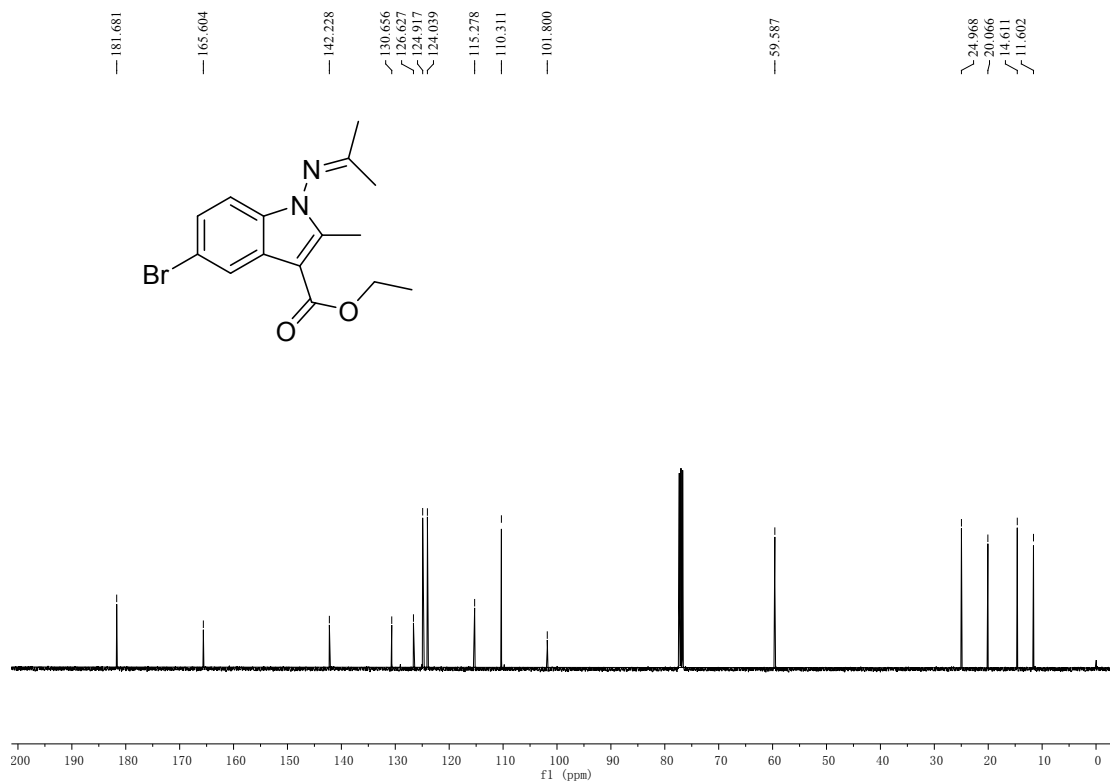
^1H , ^{13}C , spectra of 4c



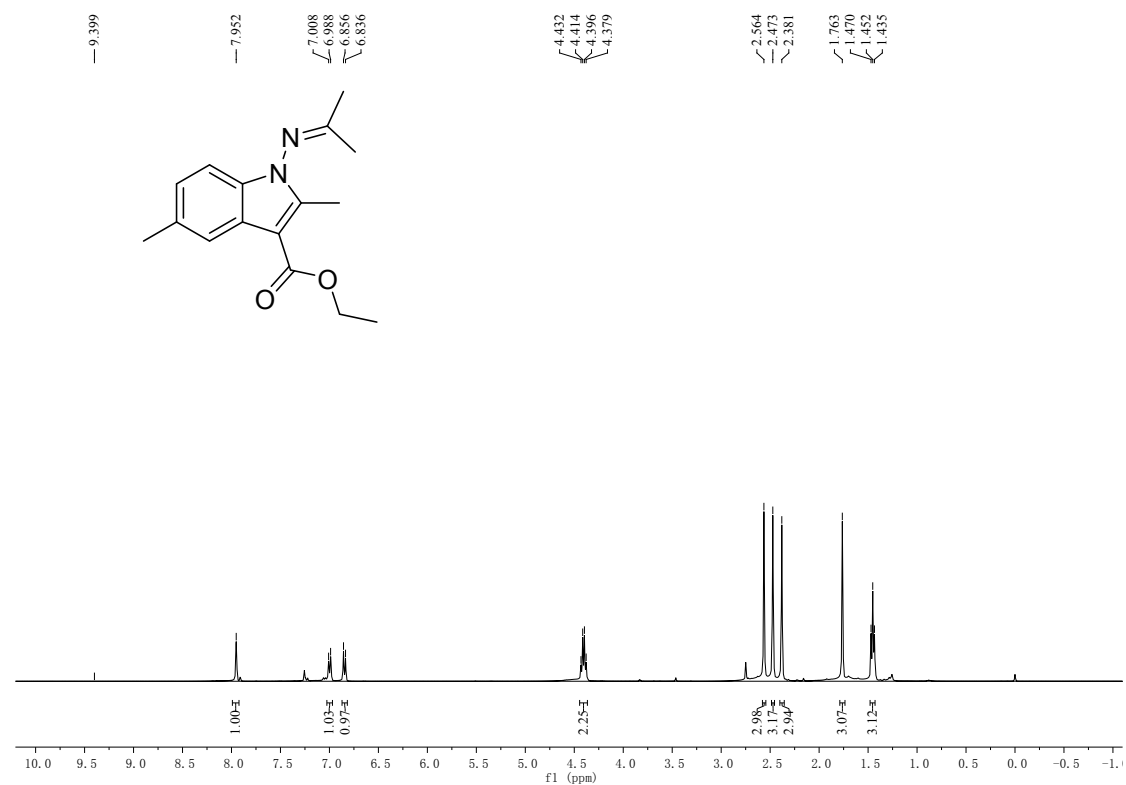


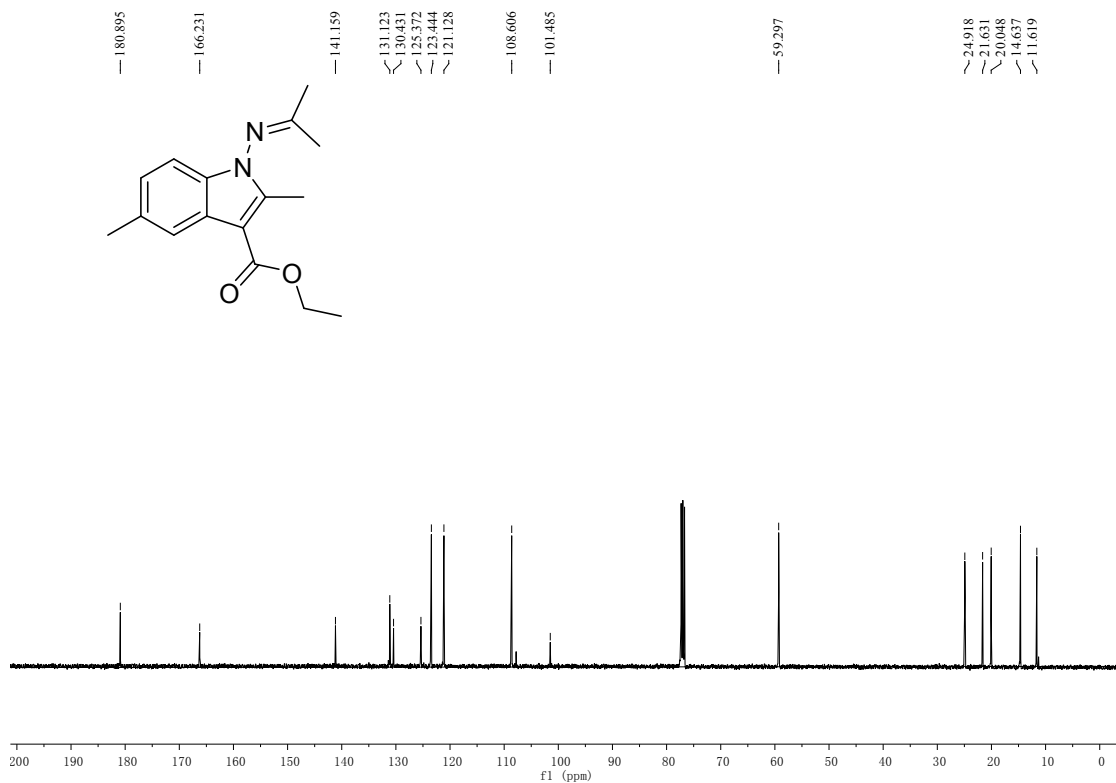
¹H, ¹³C spectra of 4d



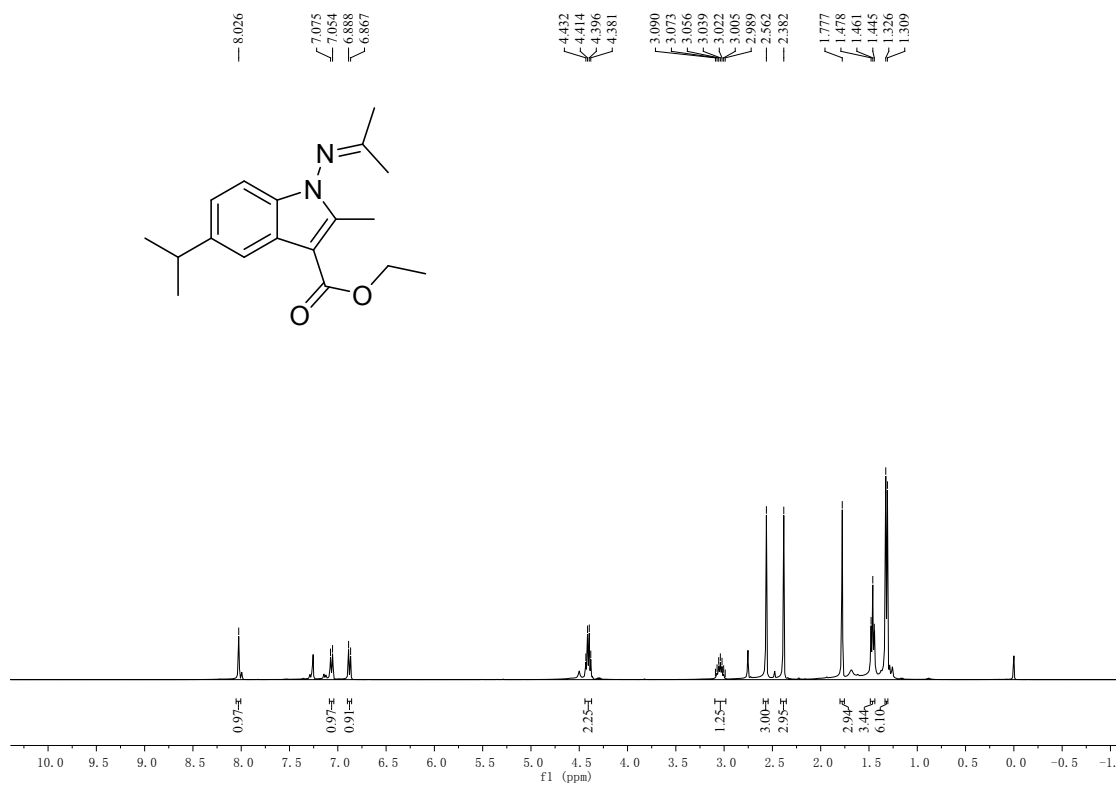


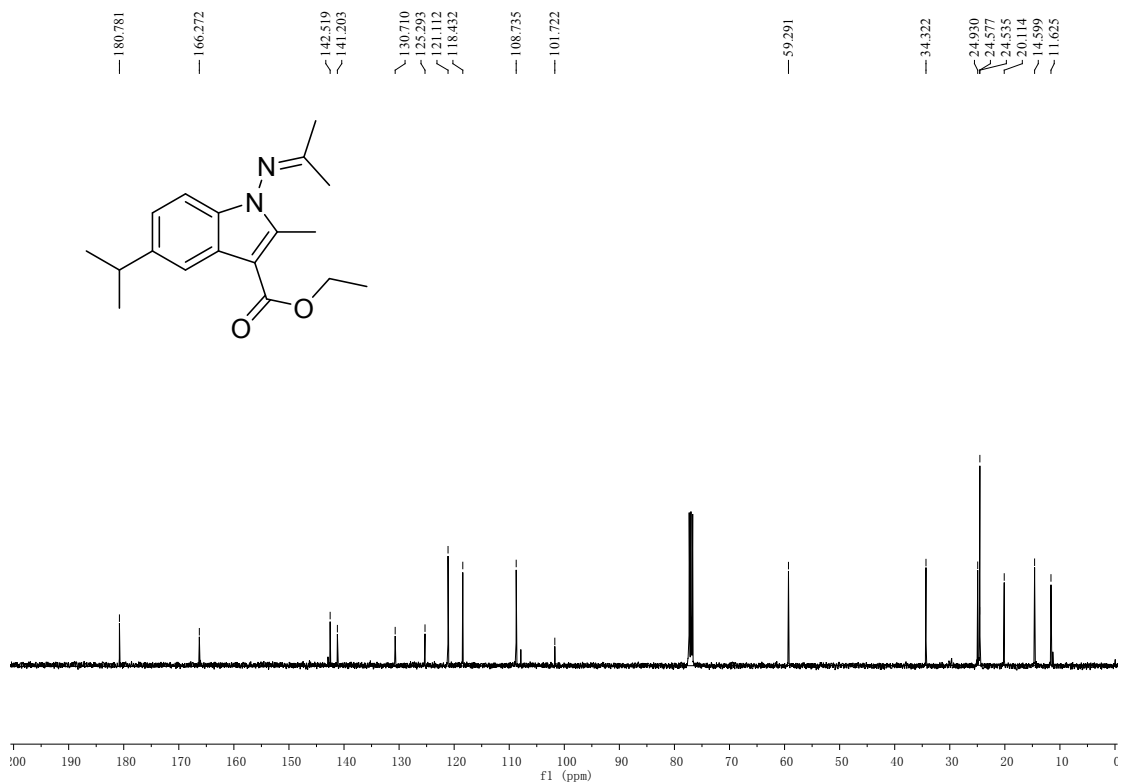
¹H, ¹³C spectra of 4e



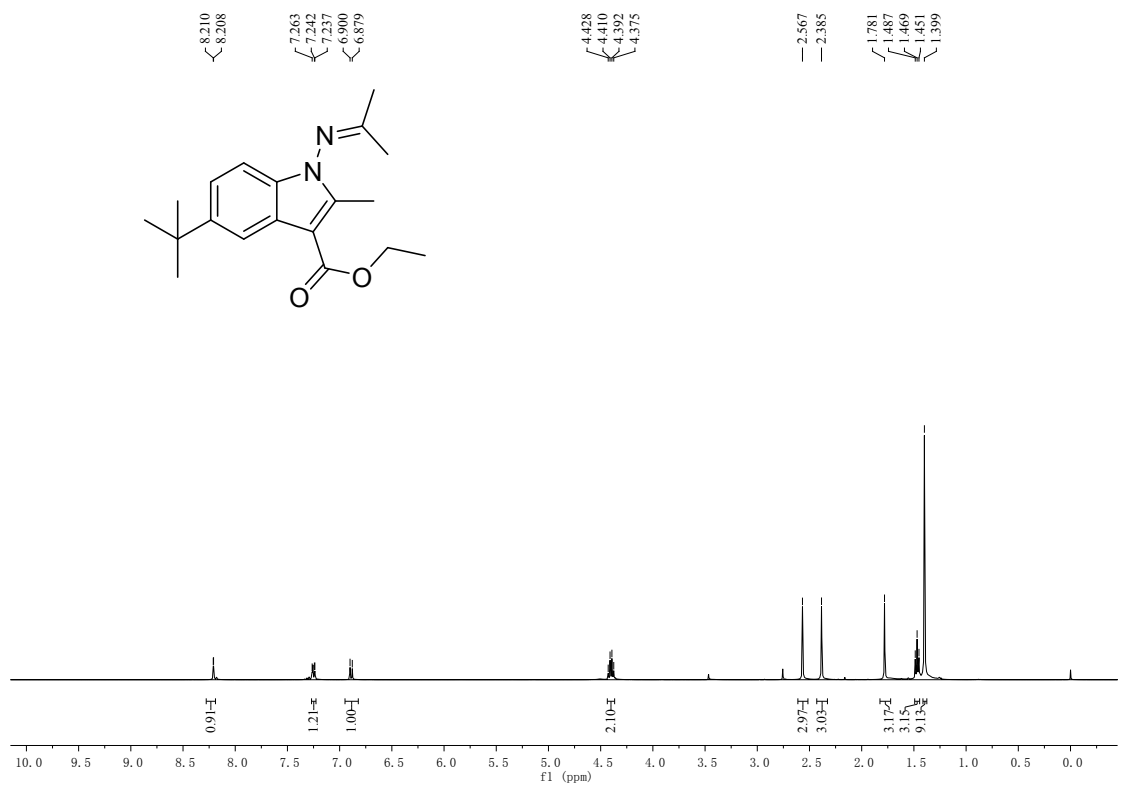


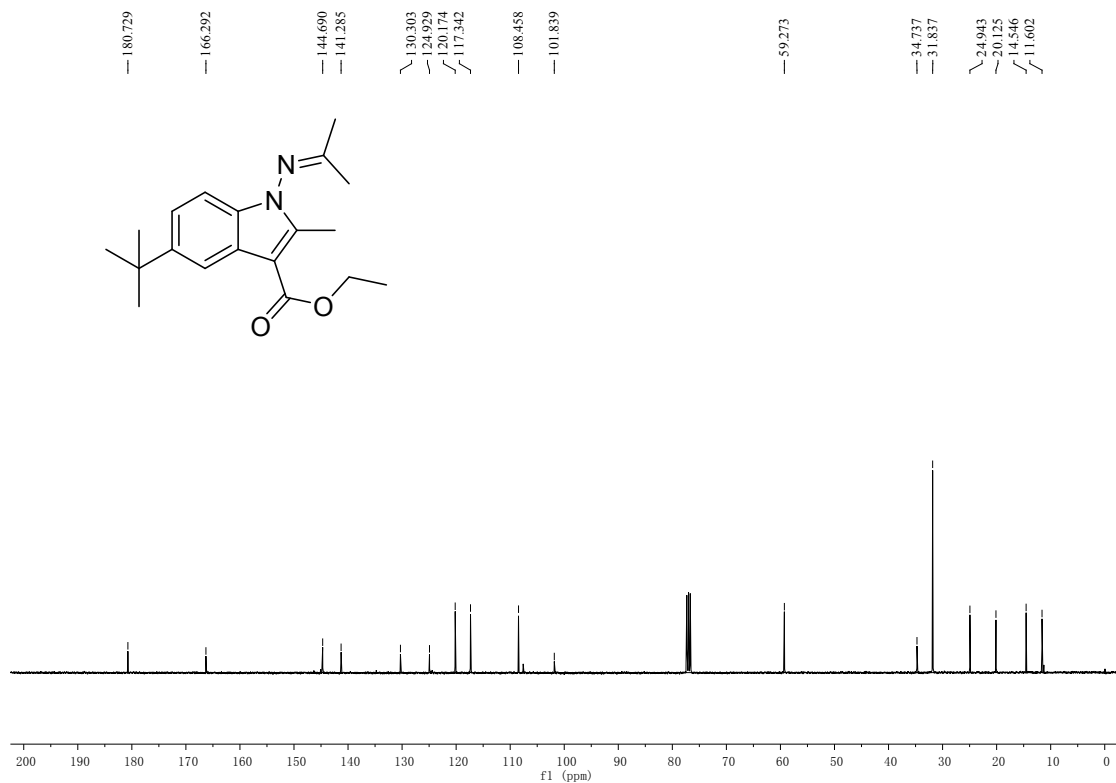
¹H, ¹³C spectra of 4f



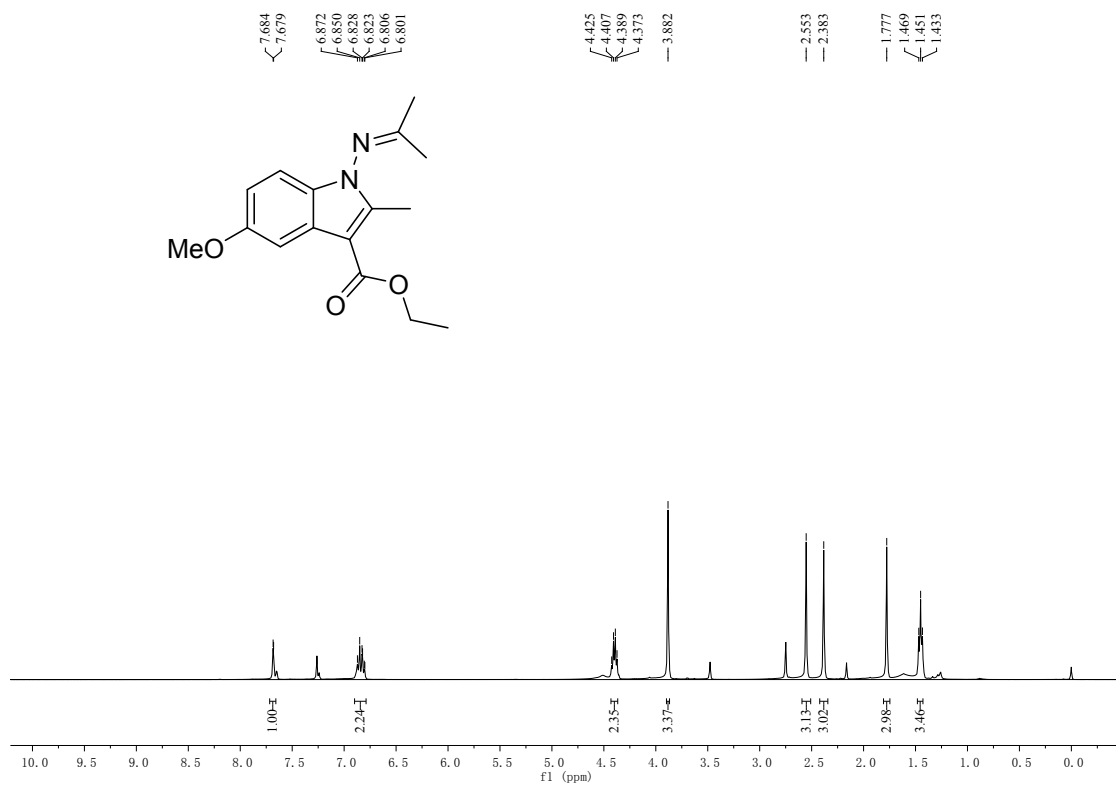


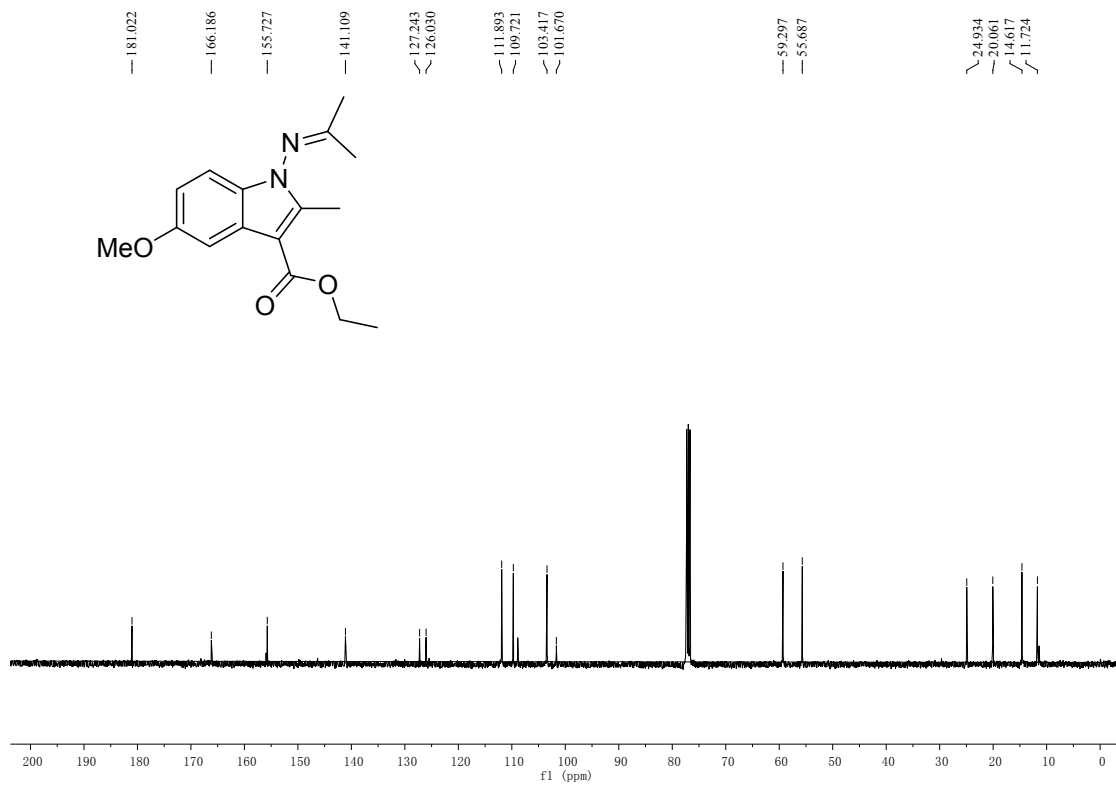
¹H, ¹³C spectra of 4g



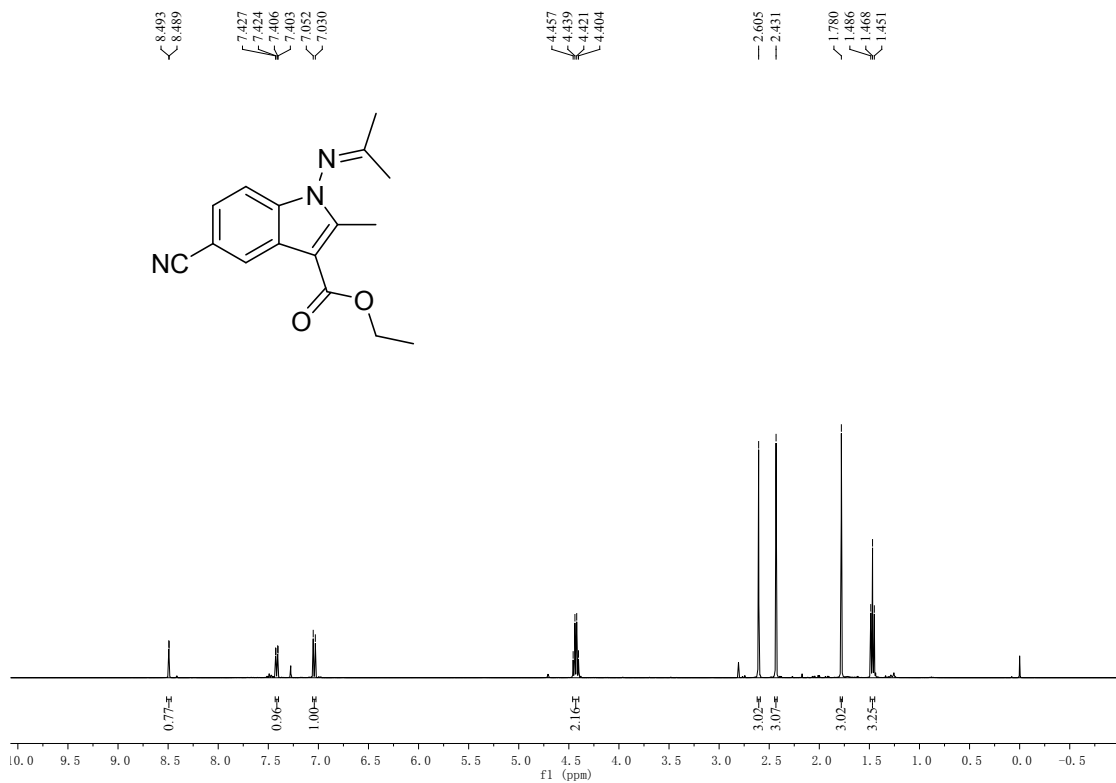


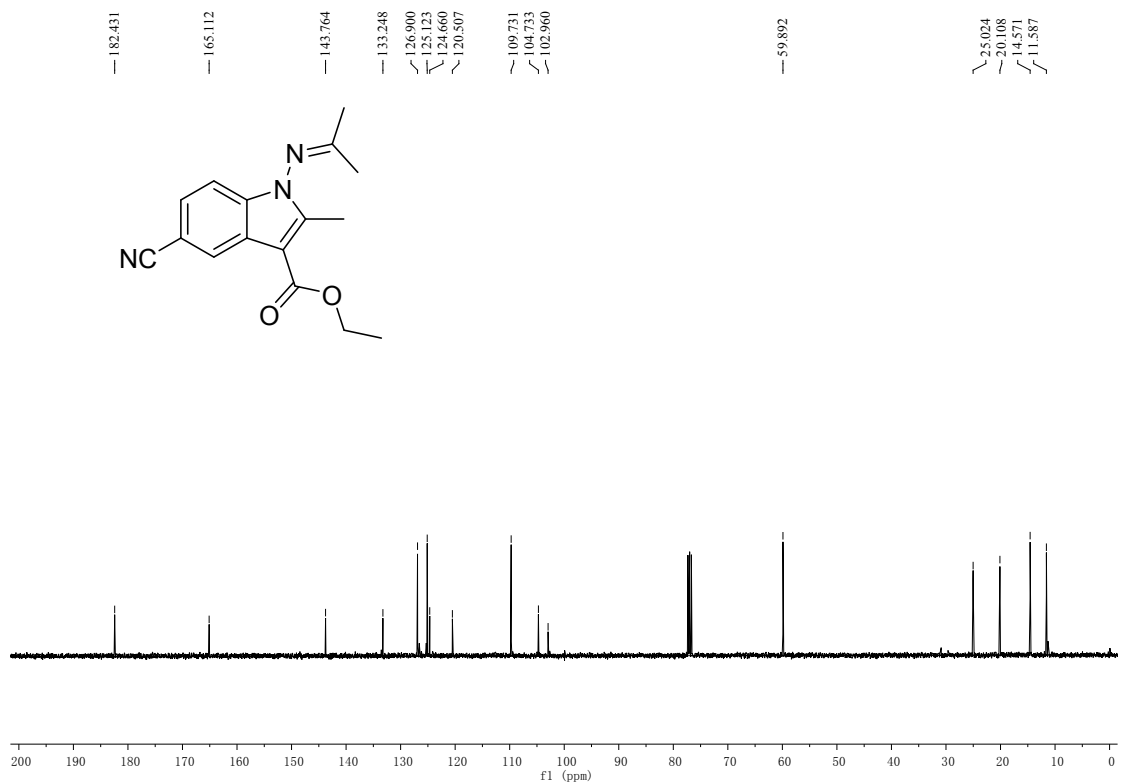
¹H, ¹³C spectra of 4h



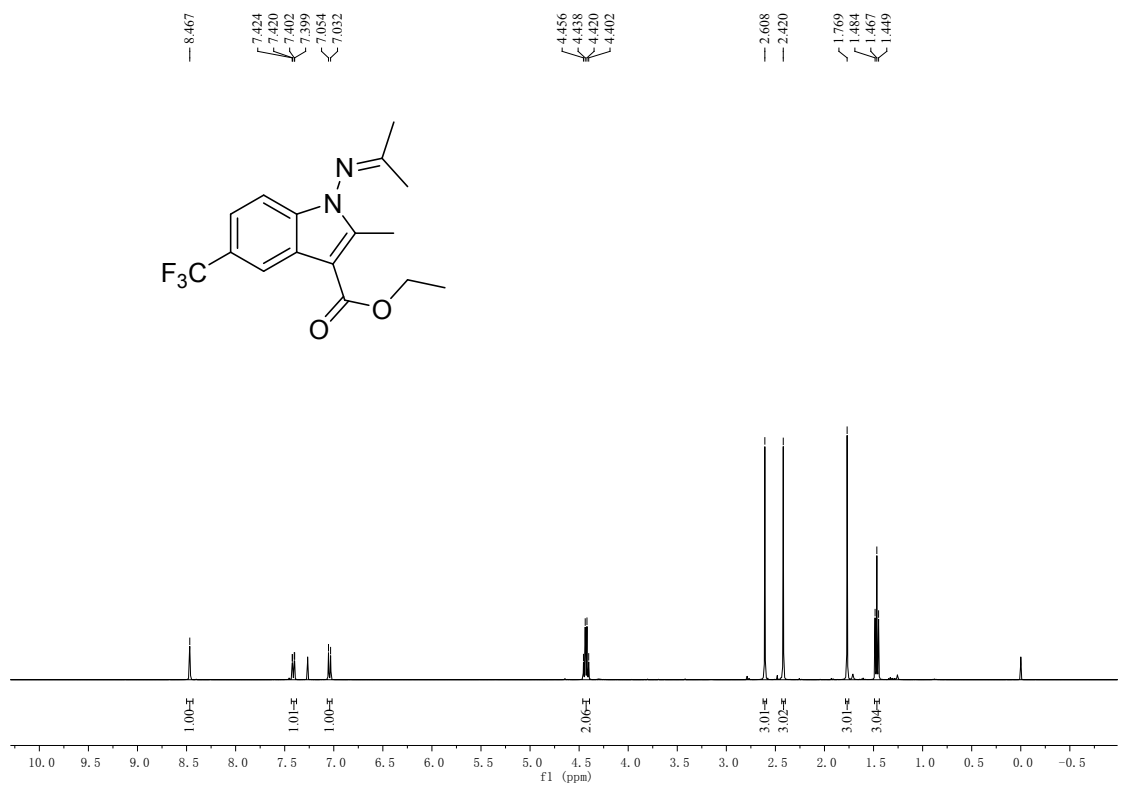


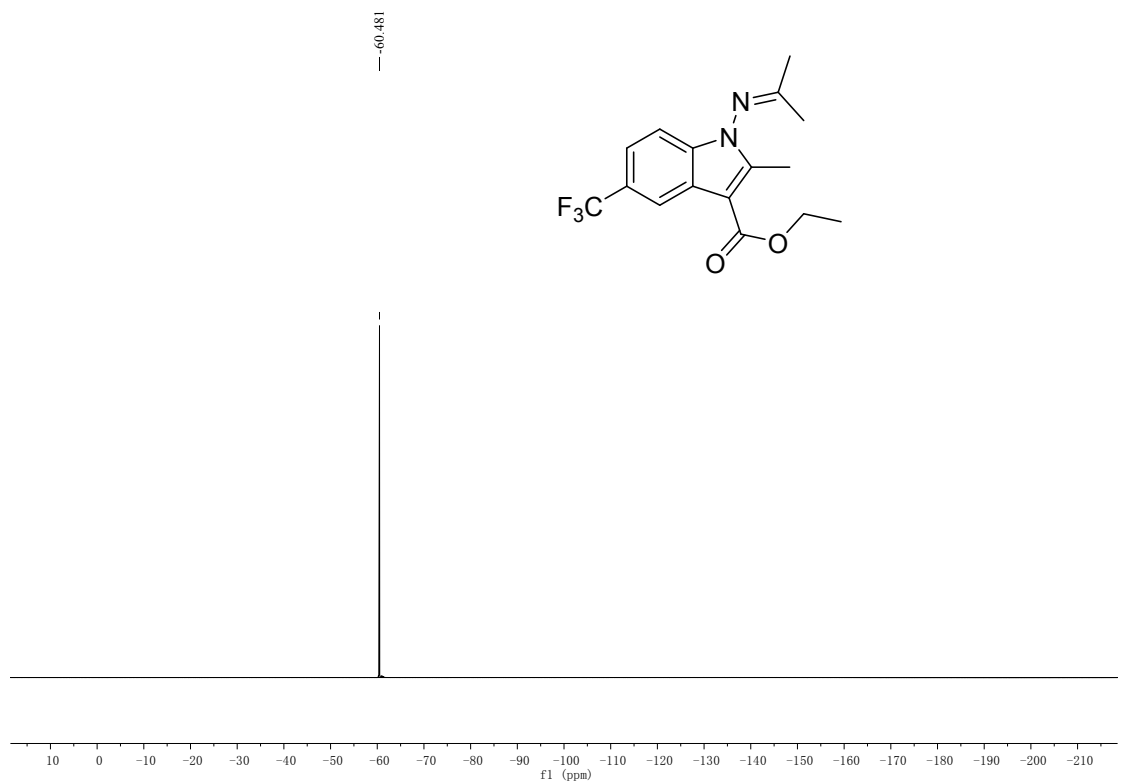
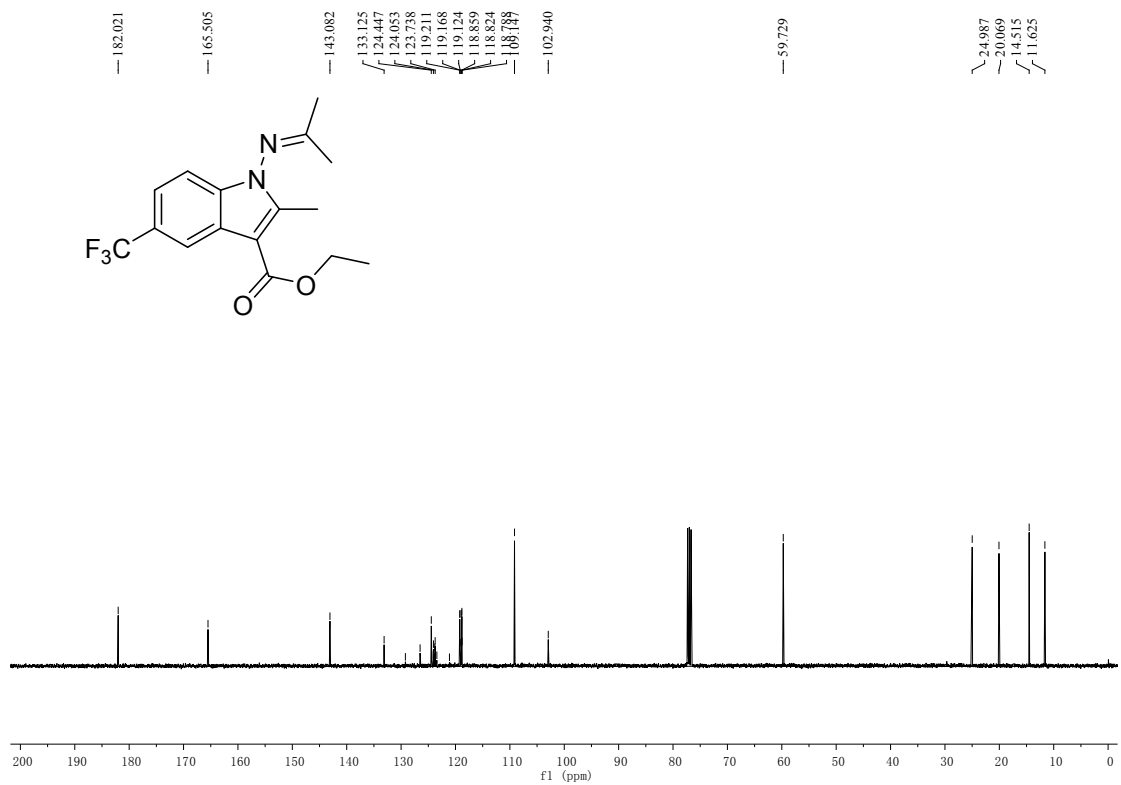
¹H, ¹³C spectra of 4i



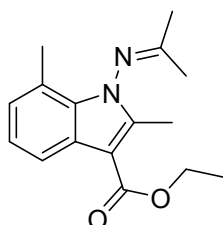
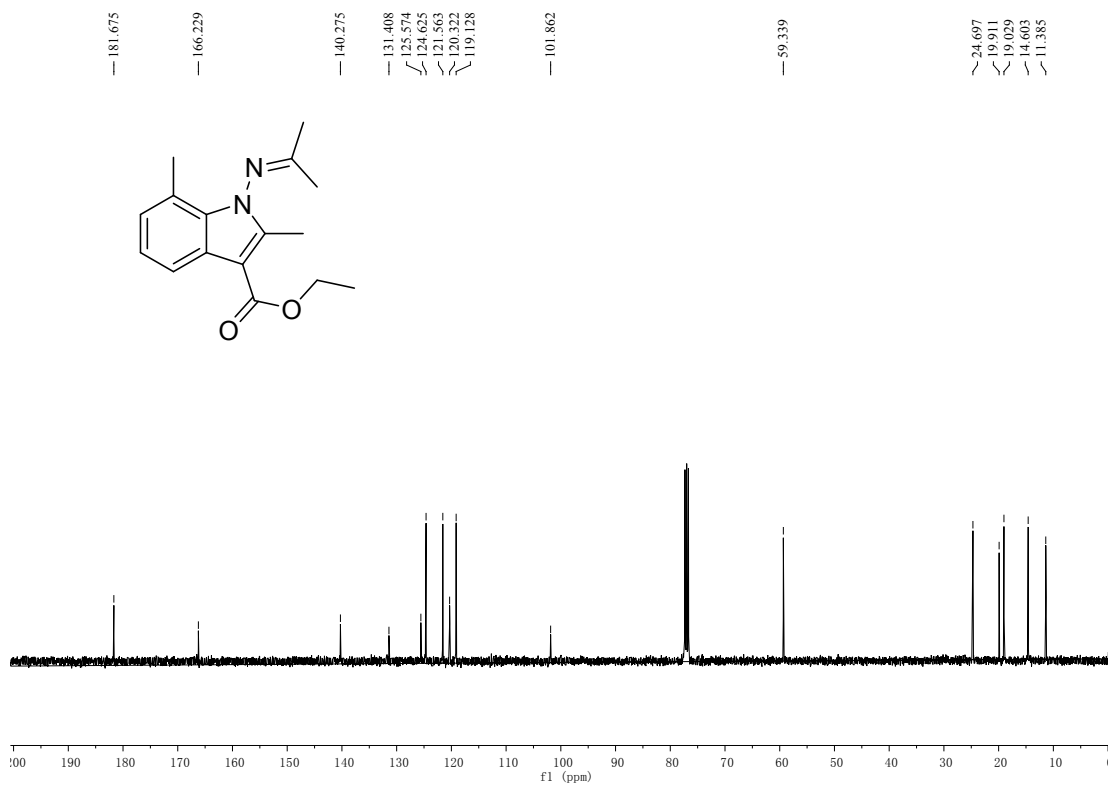
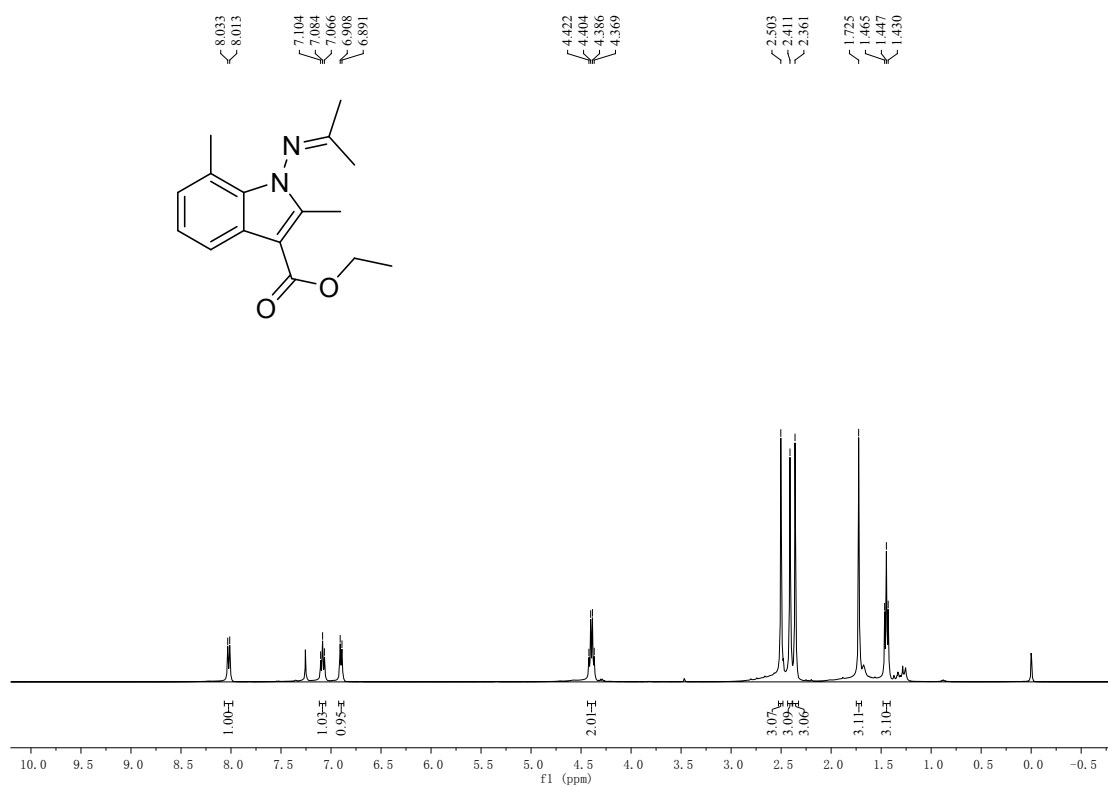


¹H, ¹³C, ¹⁹F spectra of 4j

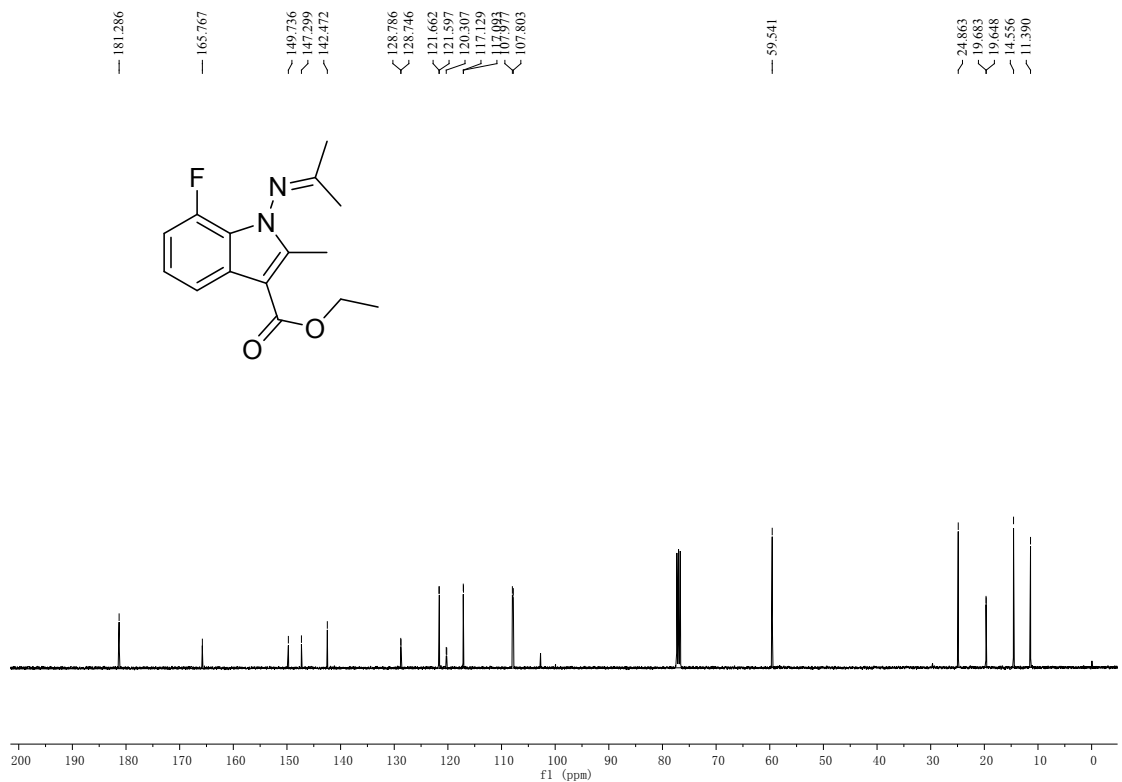
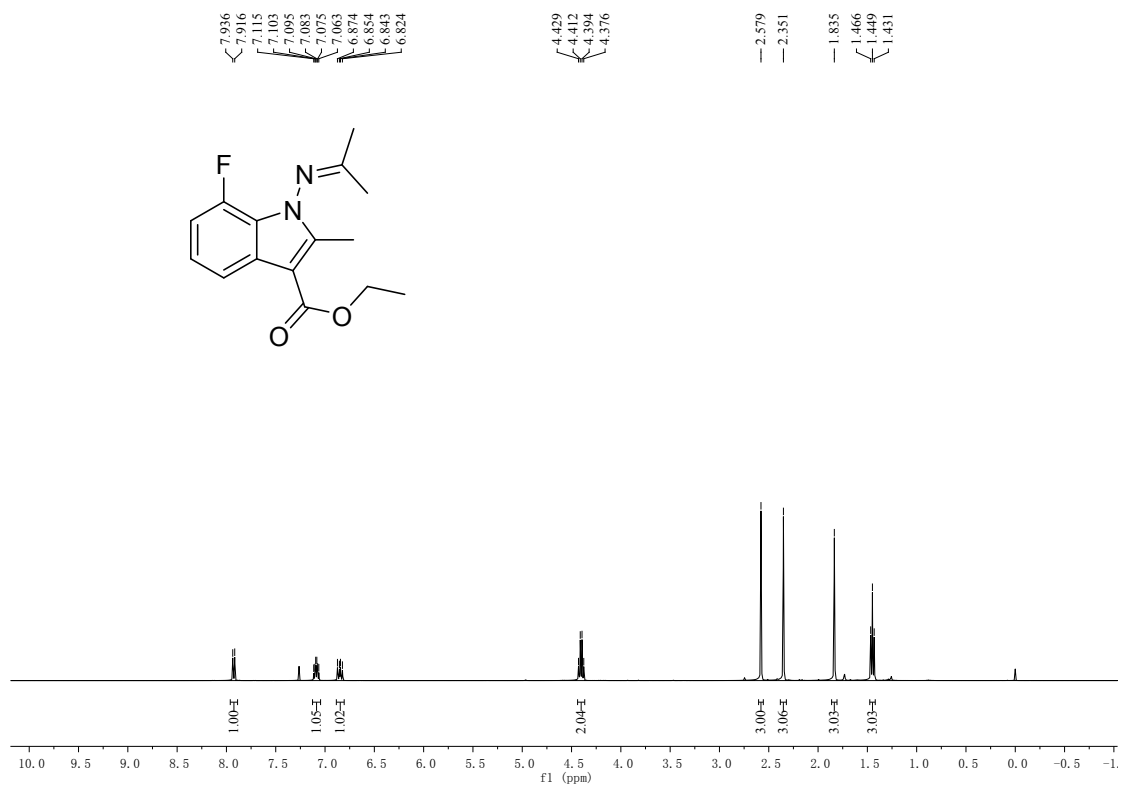


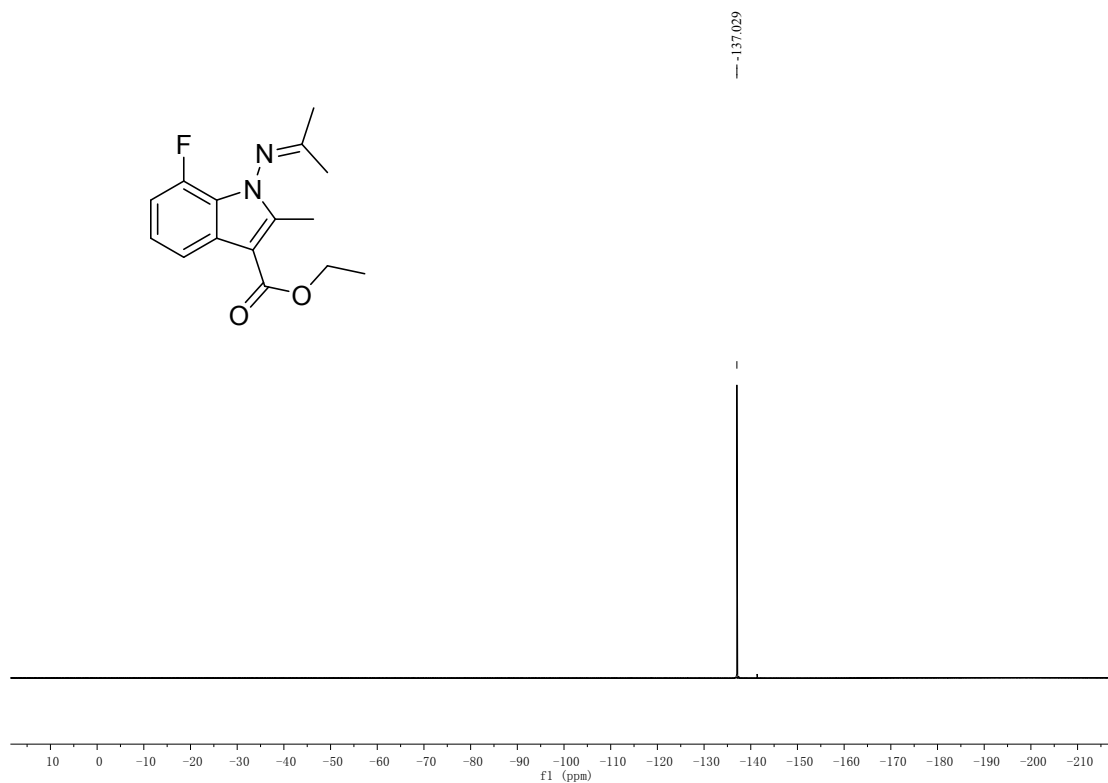


¹H, ¹³C spectra of 4k

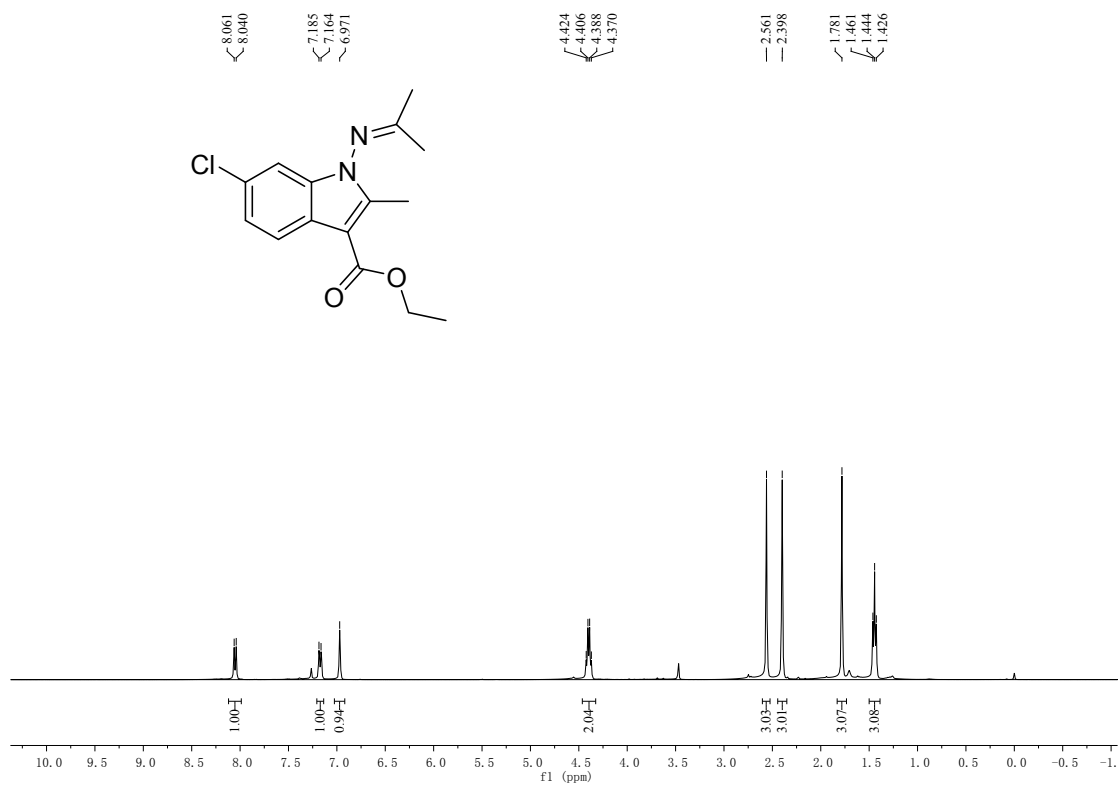


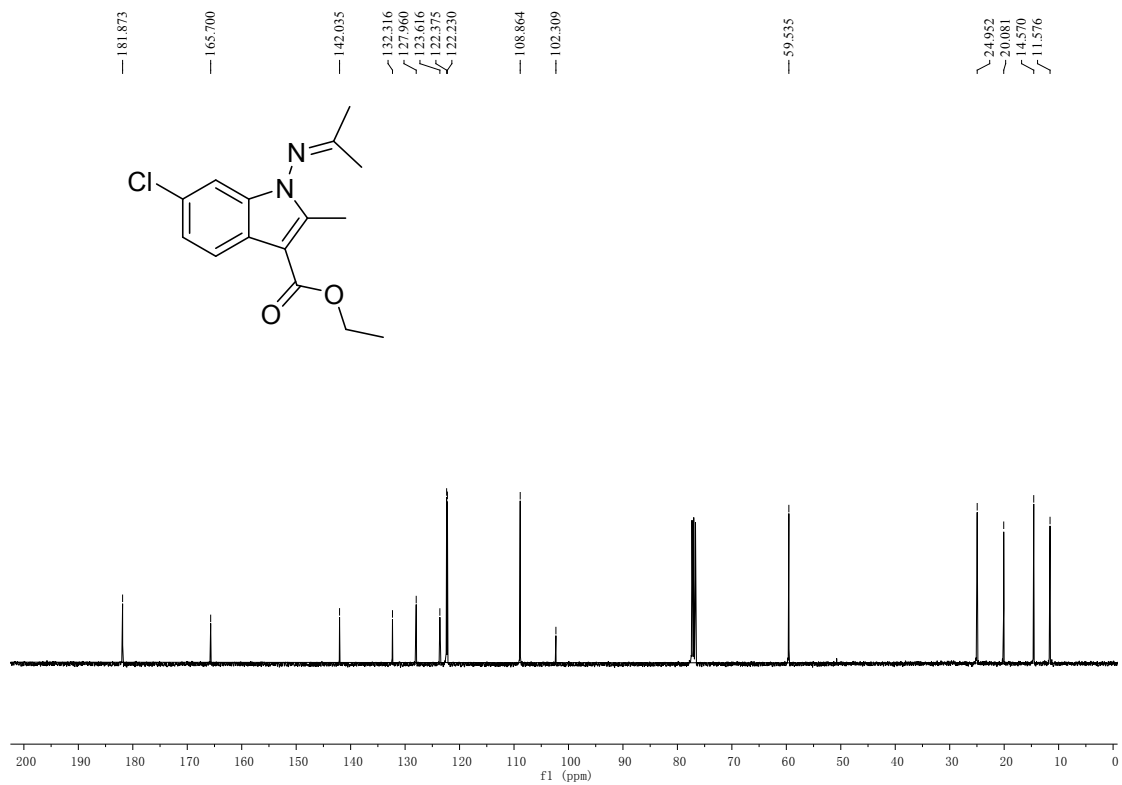
¹H, ¹³C, ¹⁹F spectra of 4l



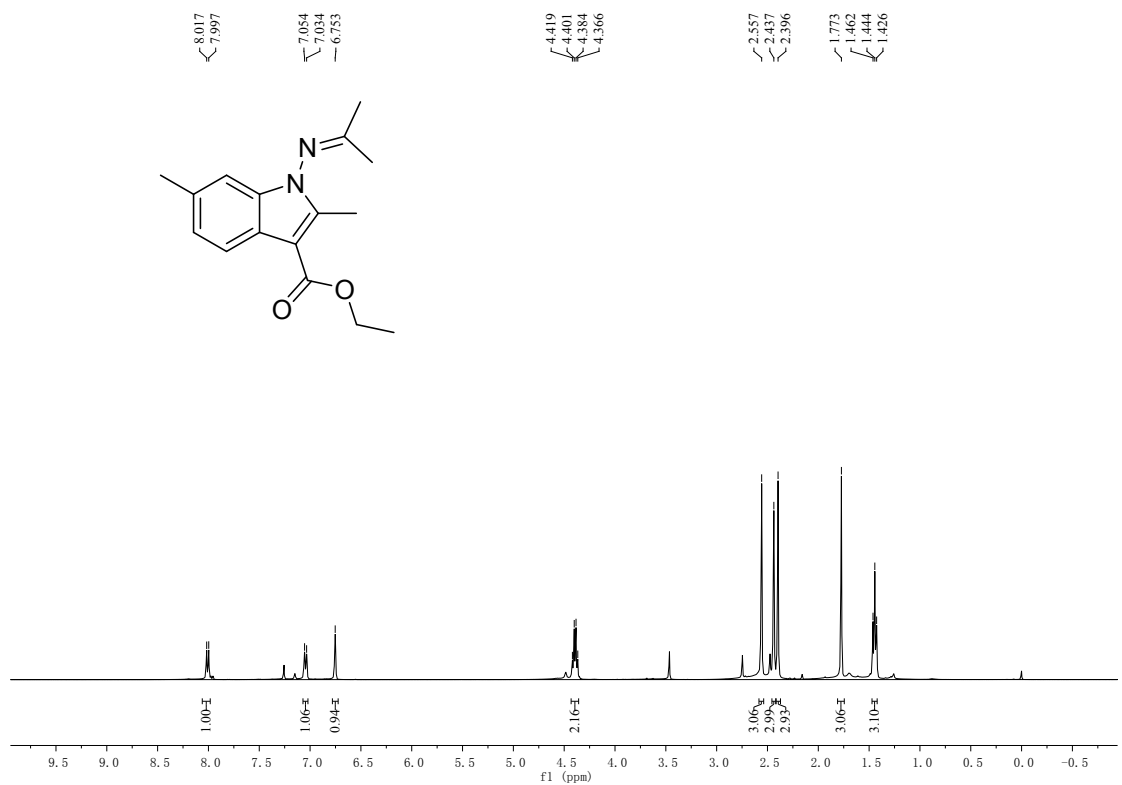


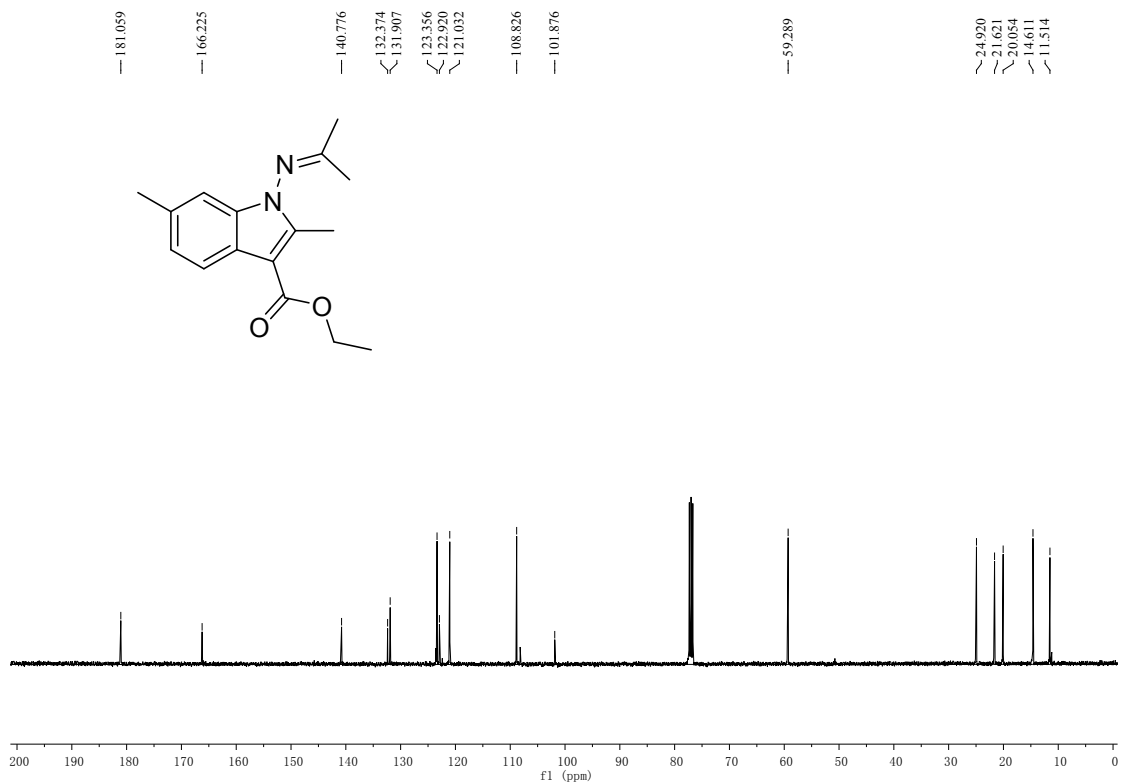
¹H, ¹³C spectra of 4m



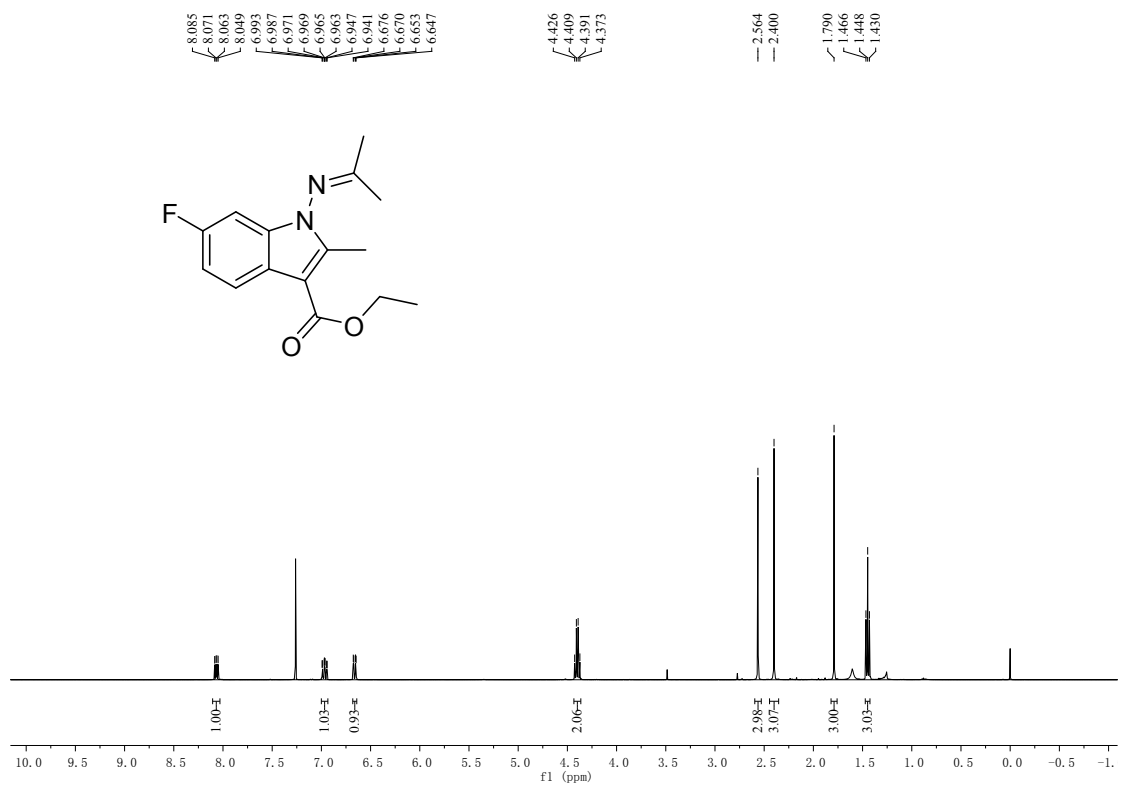


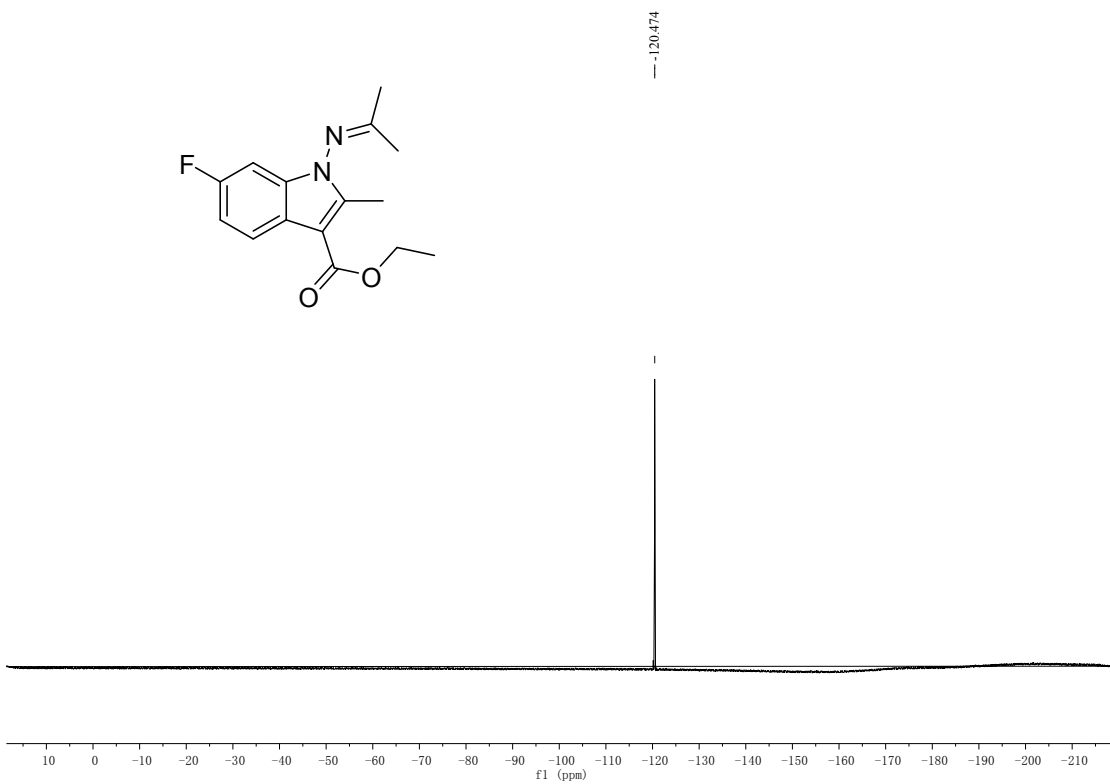
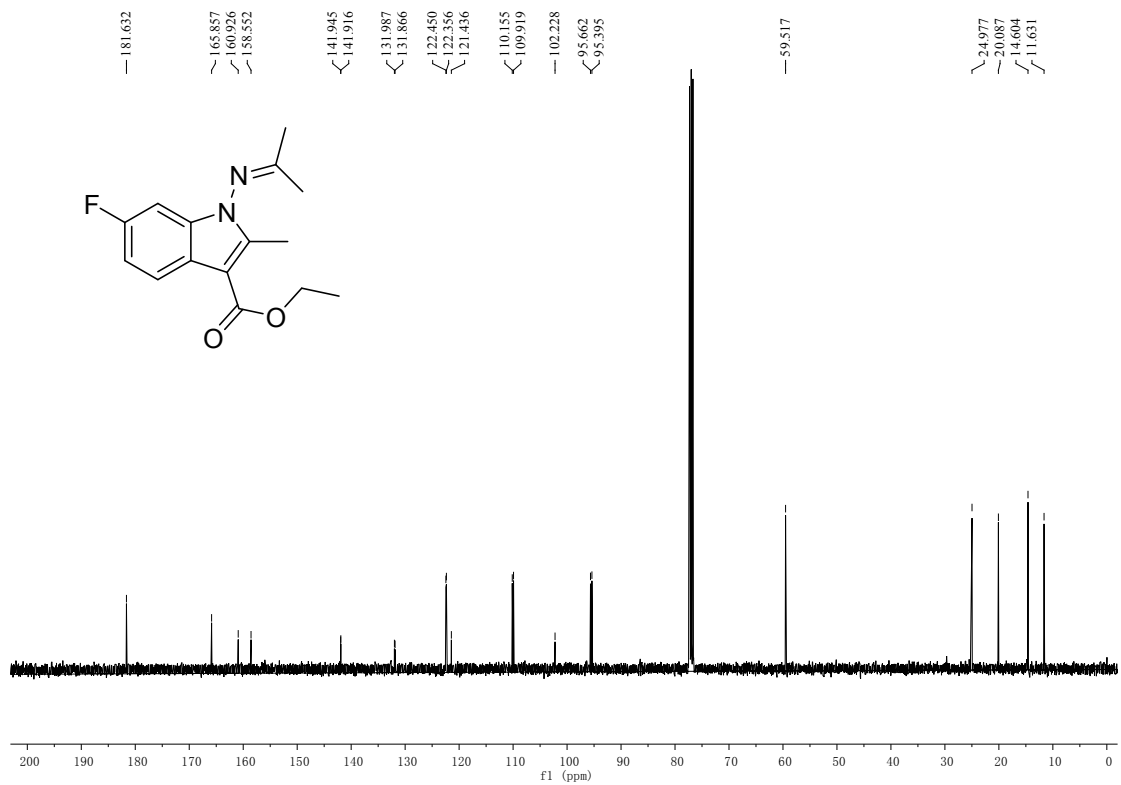
¹H, ¹³C spectra of 4n



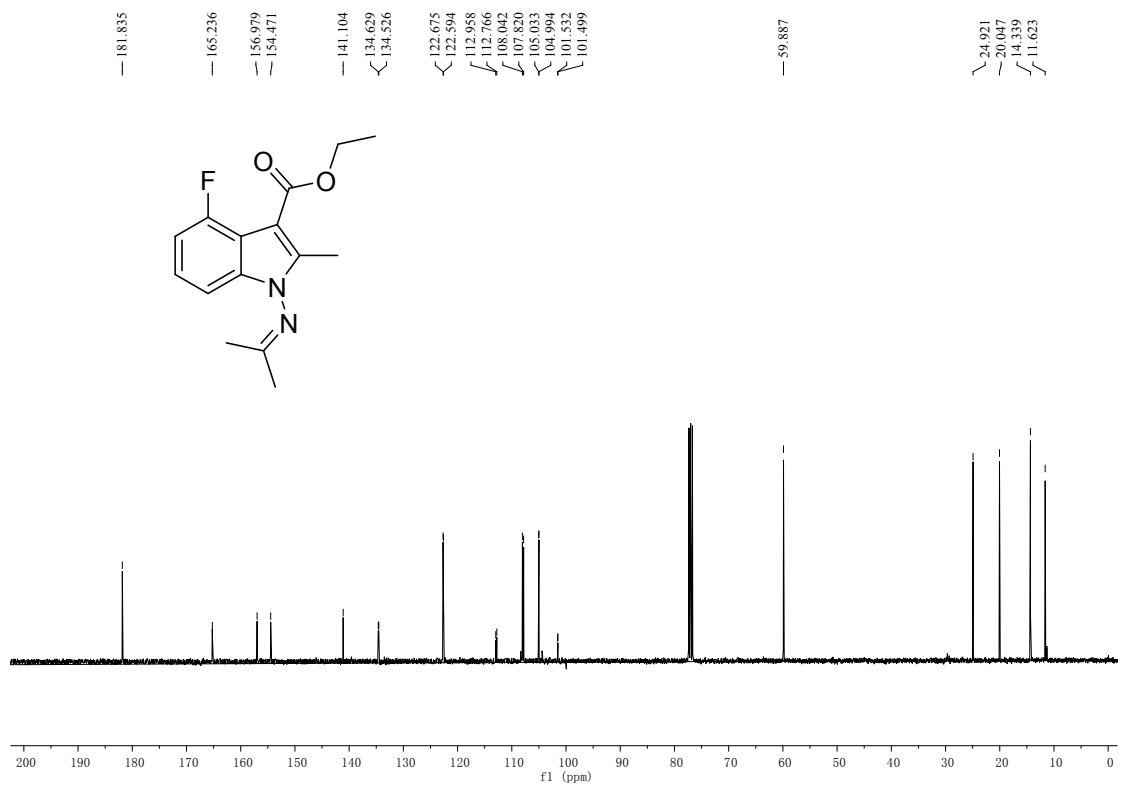
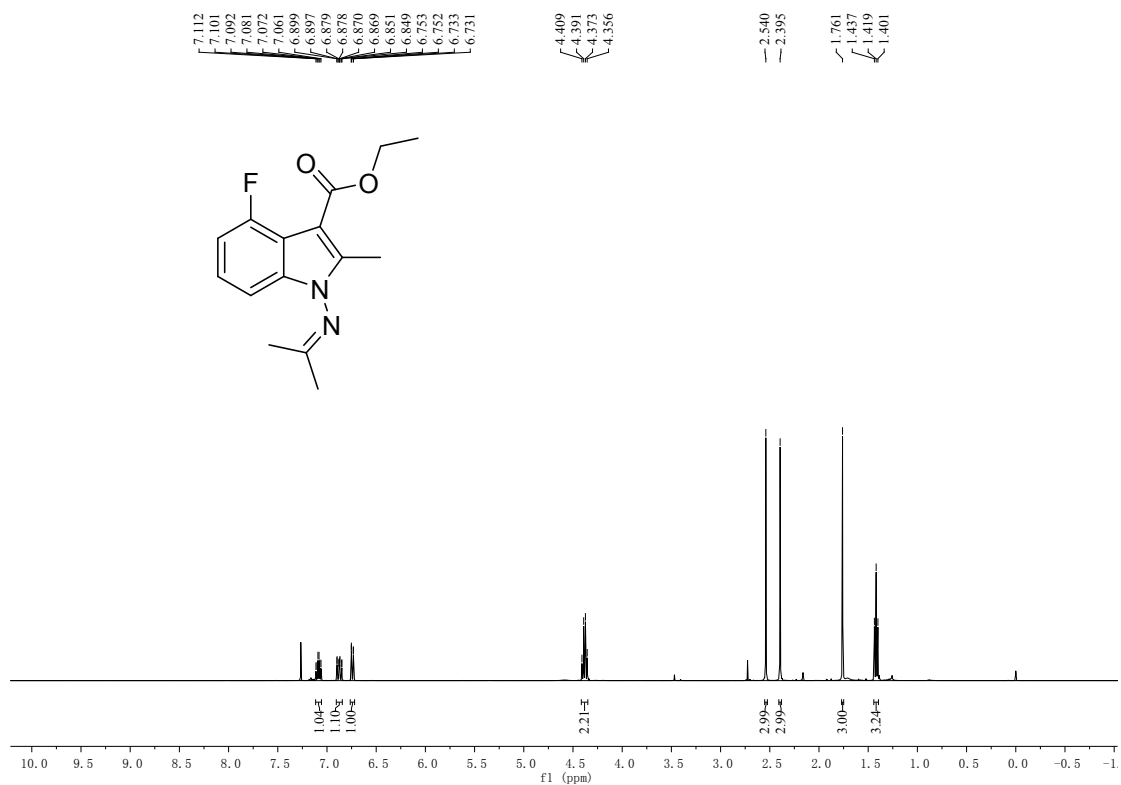


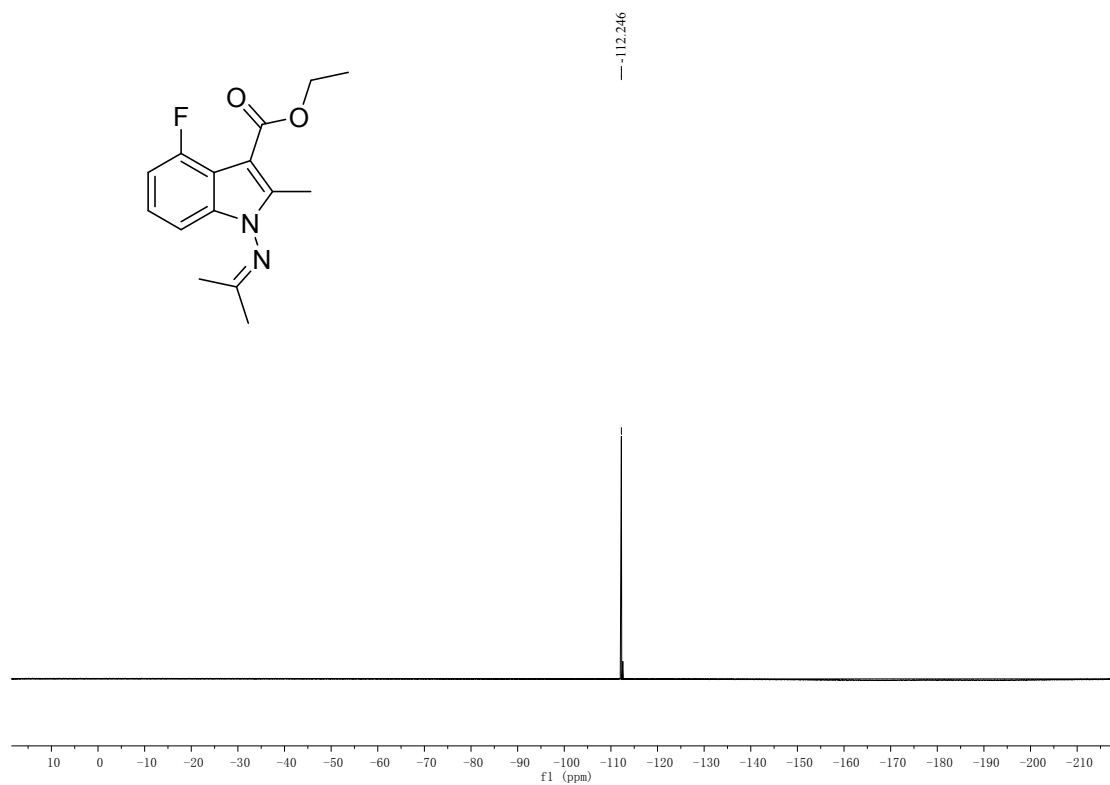
^1H , ^{13}C , ^{19}F spectra of 40



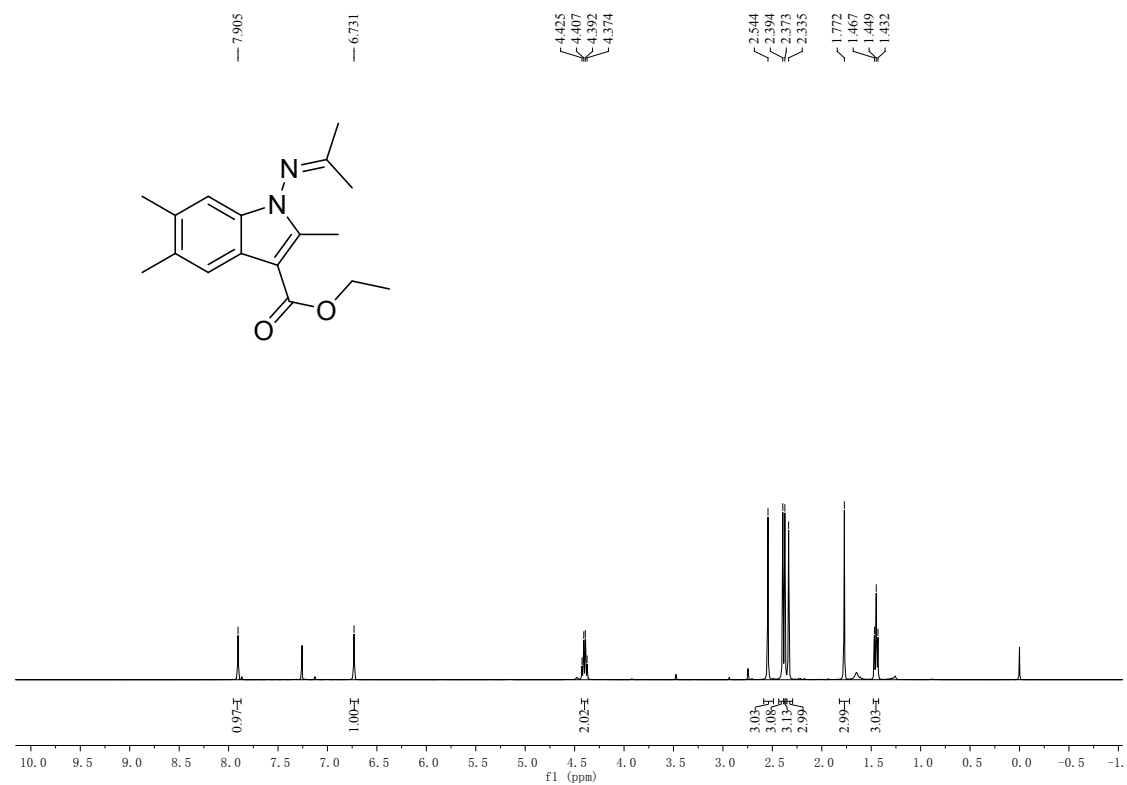


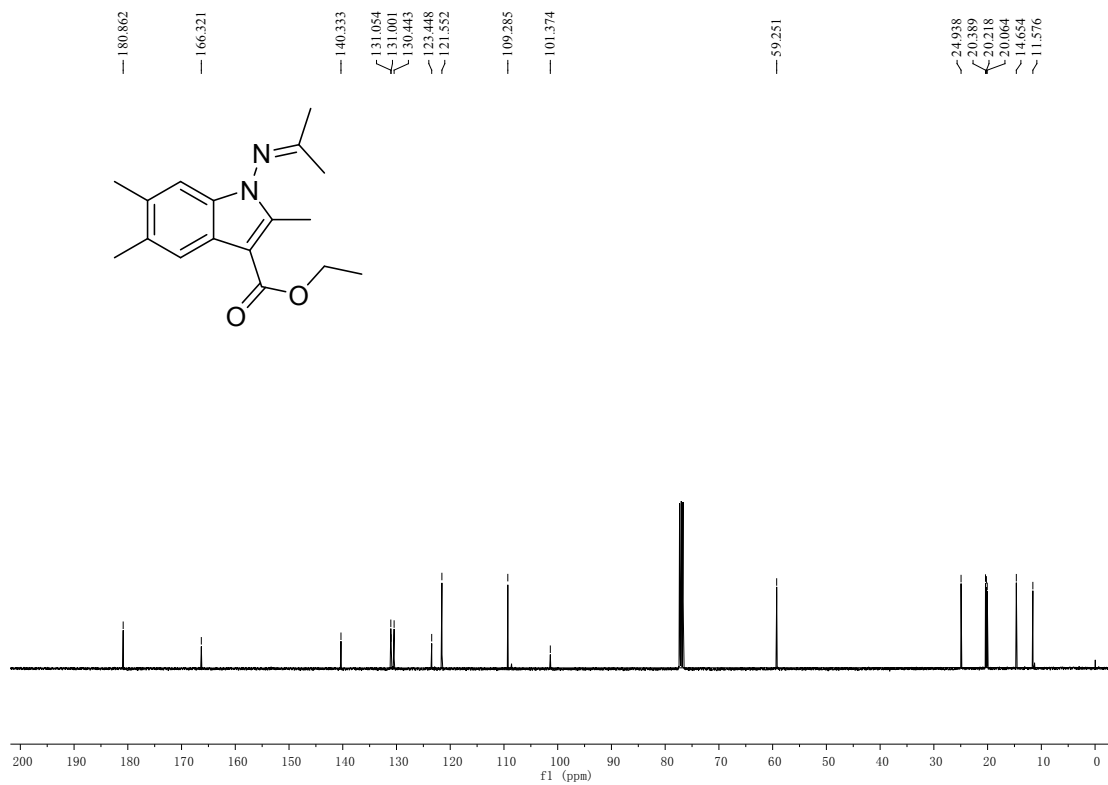
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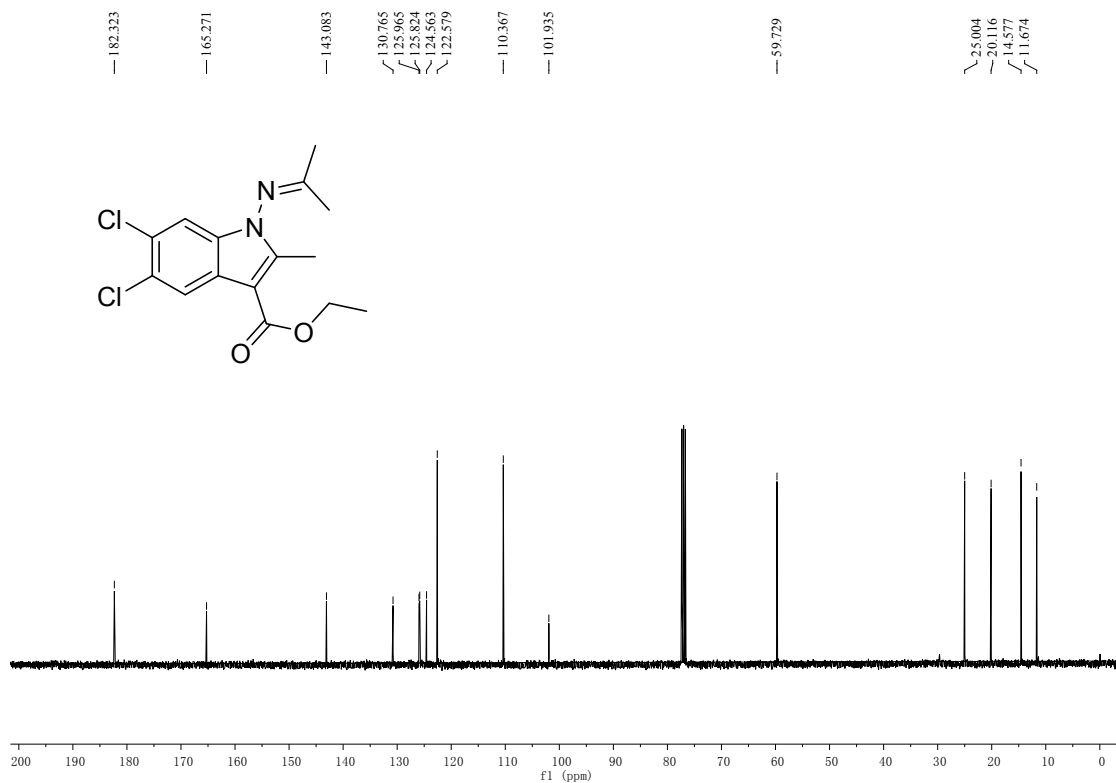
^1H , ^{13}C spectra of 4p



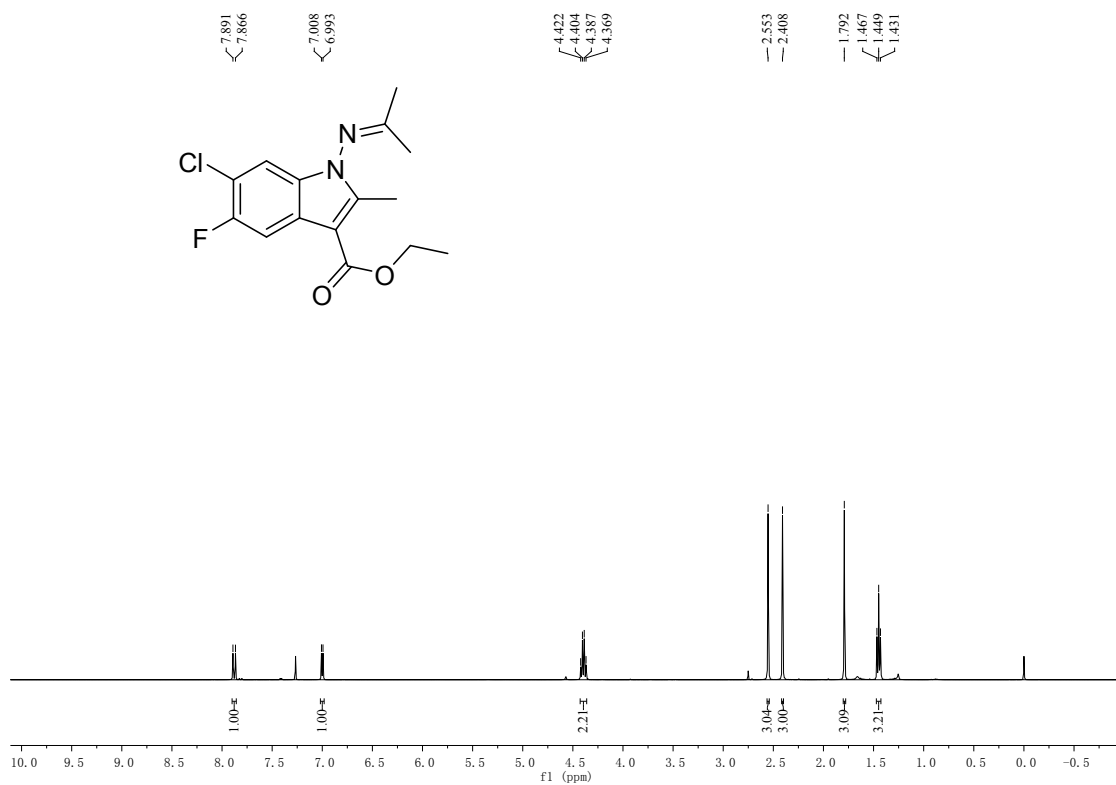


¹H, ¹³C spectra of 4q

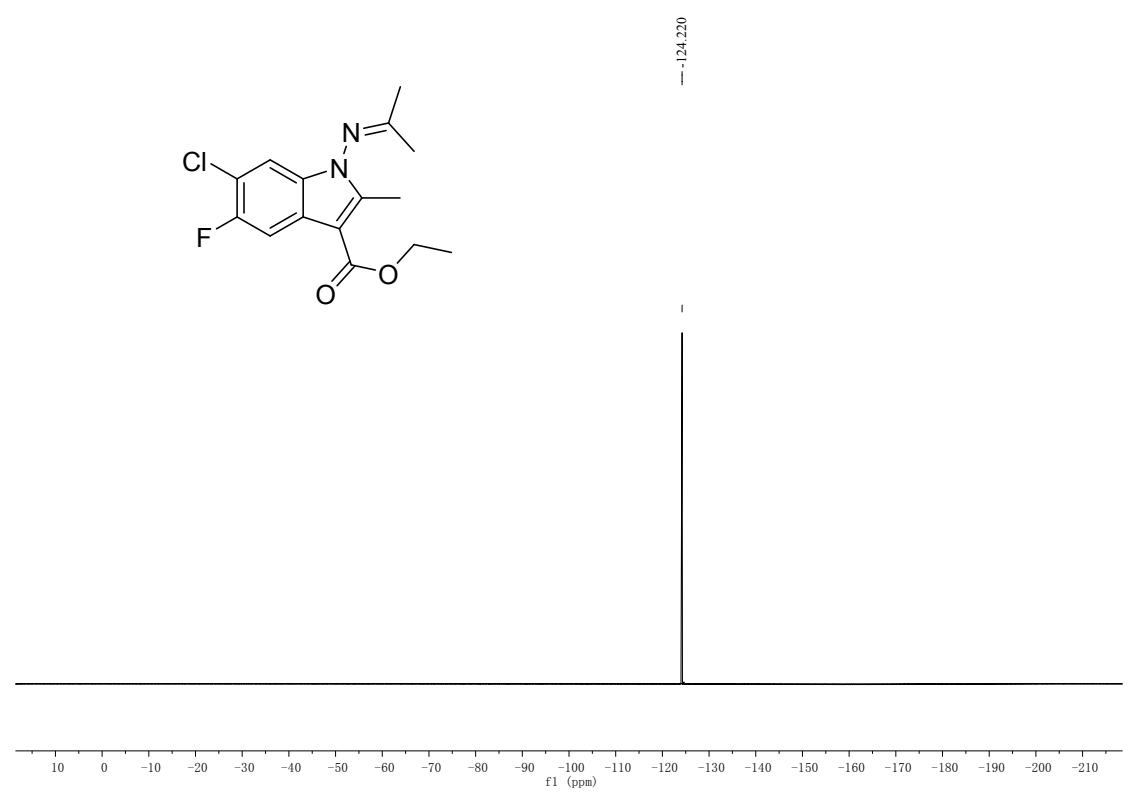
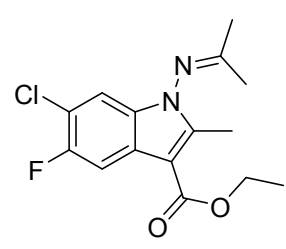
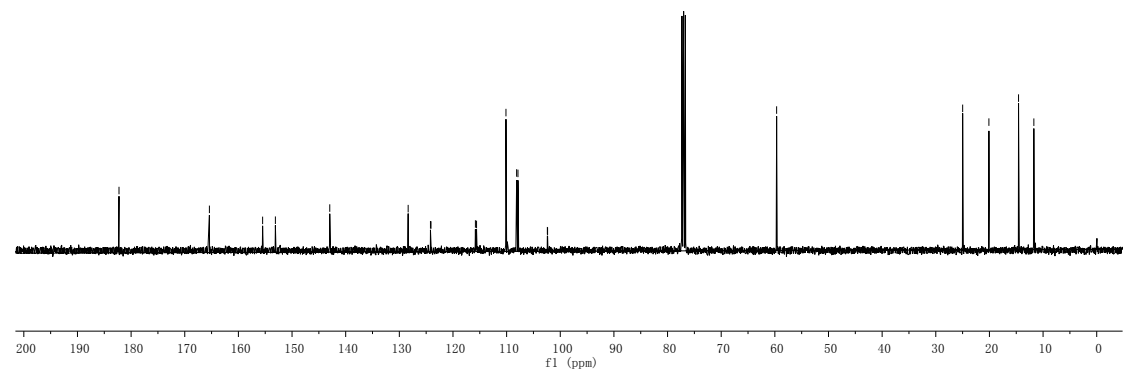
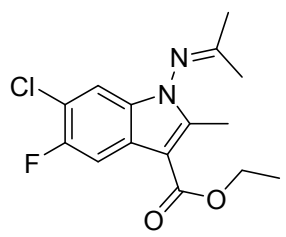




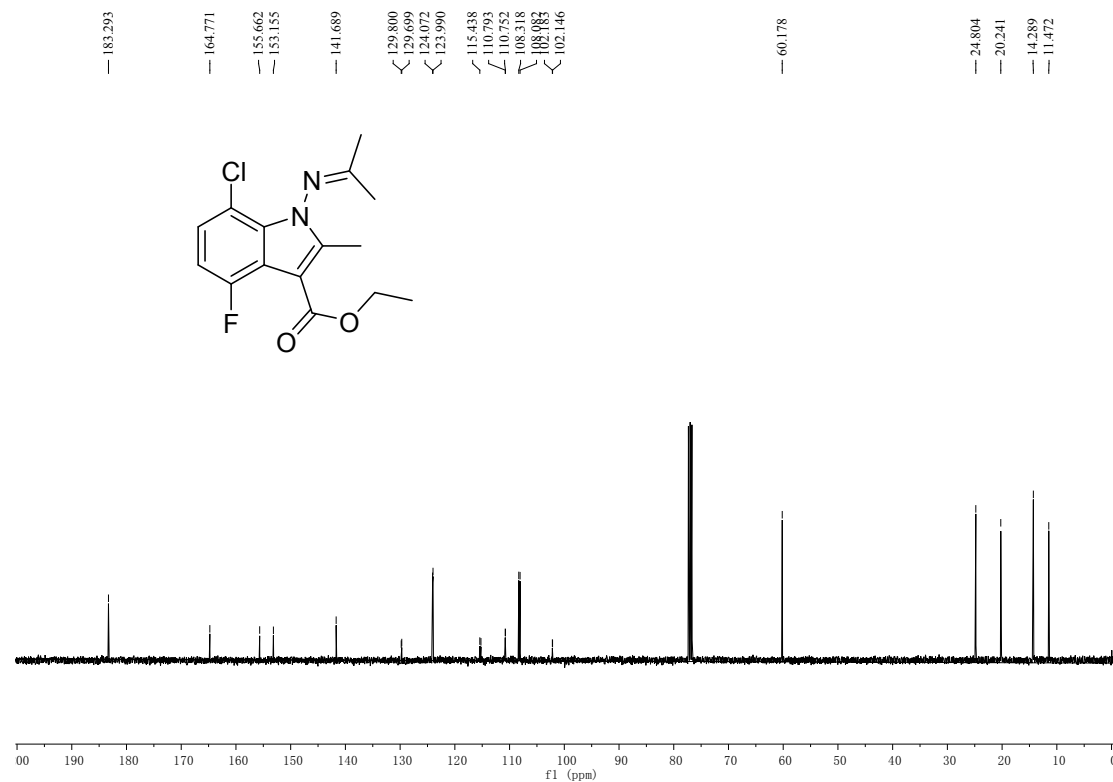
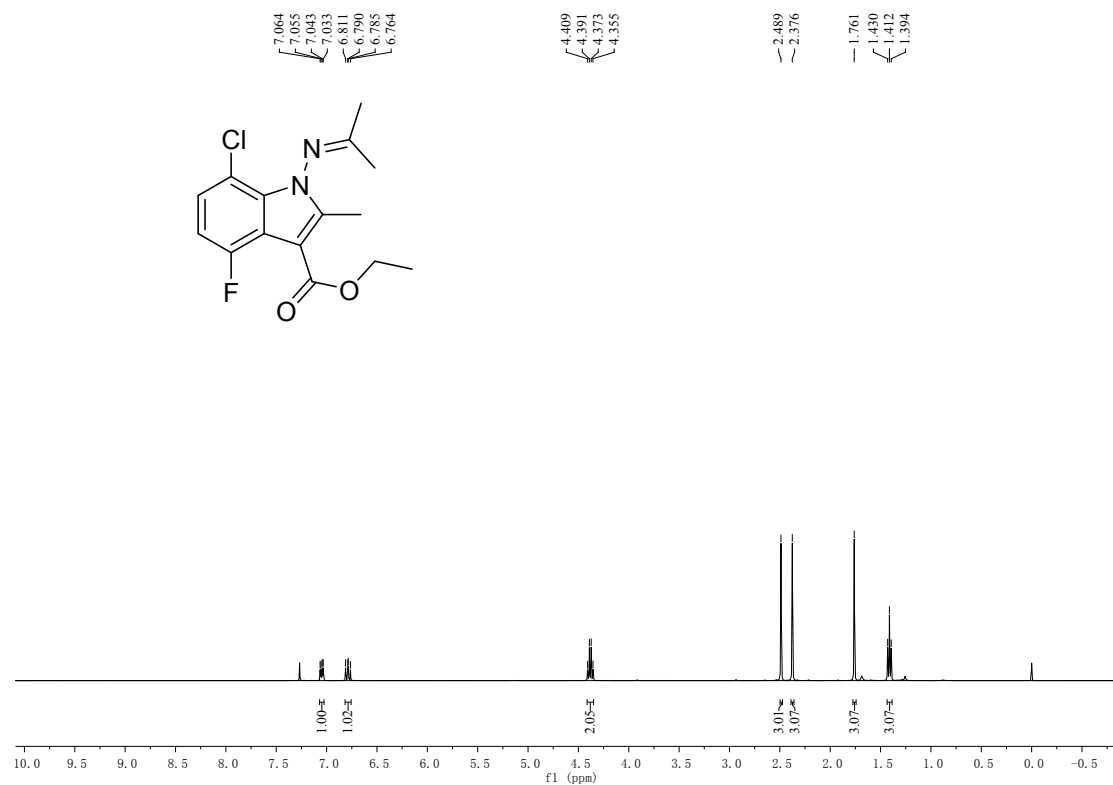
¹H, ¹³C, ¹⁹F spectra of 4r

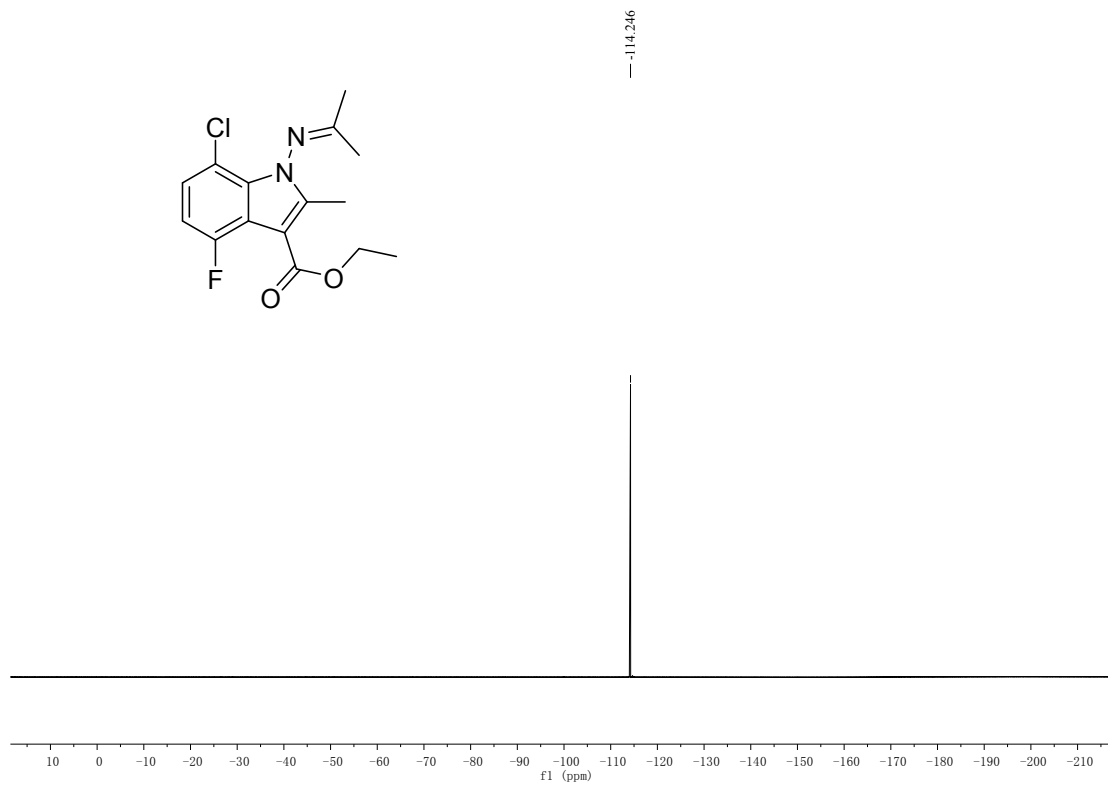


- 182.257
- 165.406
- 155.483
- 153.105
- 142.967
- 128.354
- 124.197
- 124.098
- 115.819
- 115.604
- 110.123
- 108.137
- 107.885
- 102.407
- 102.365
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- 20.098
- 14.573
- 11.718



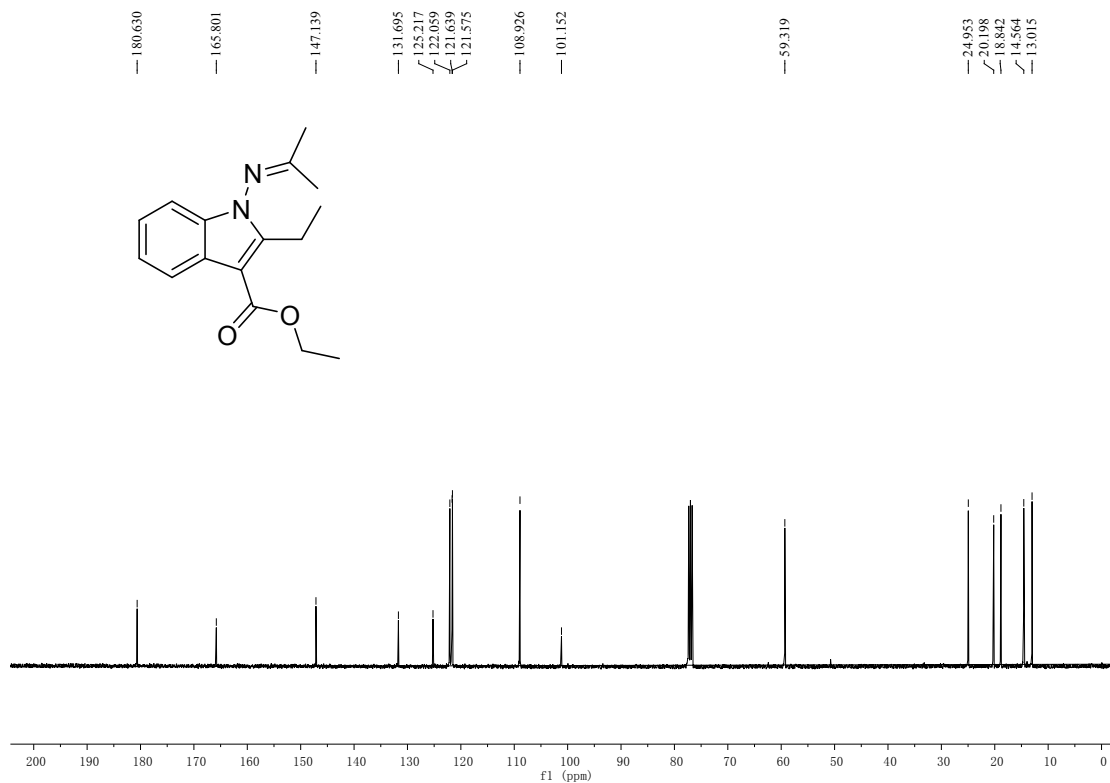
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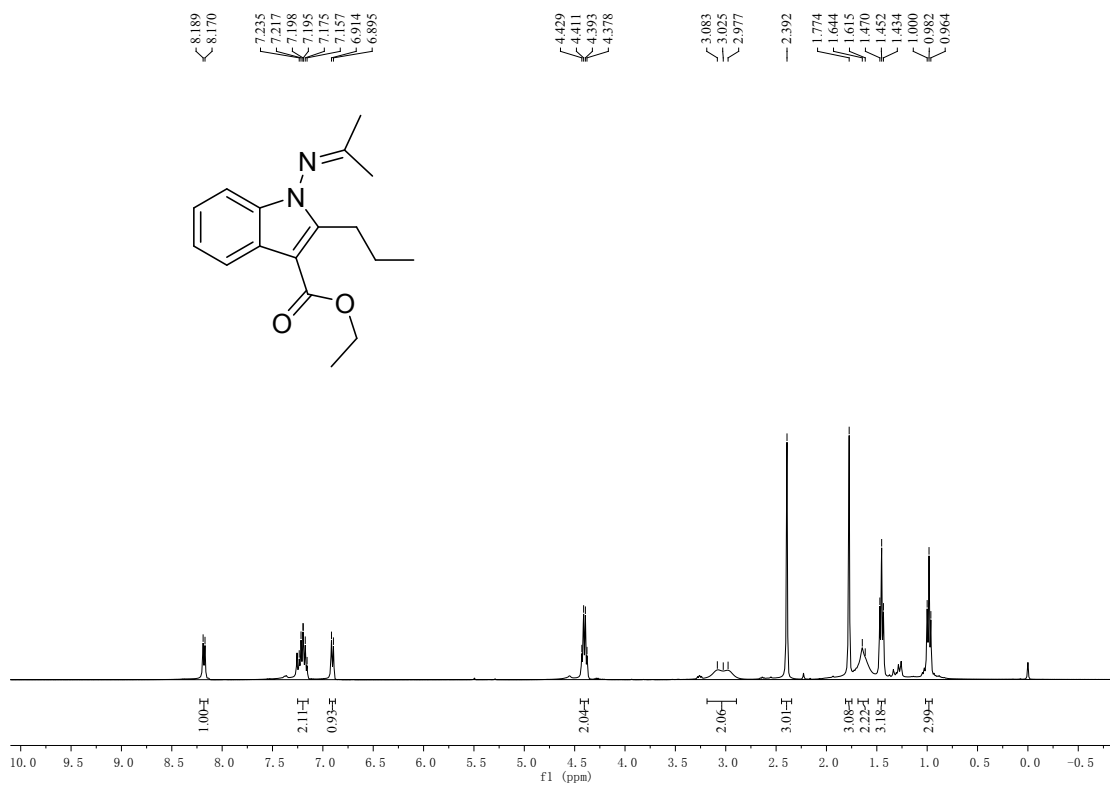


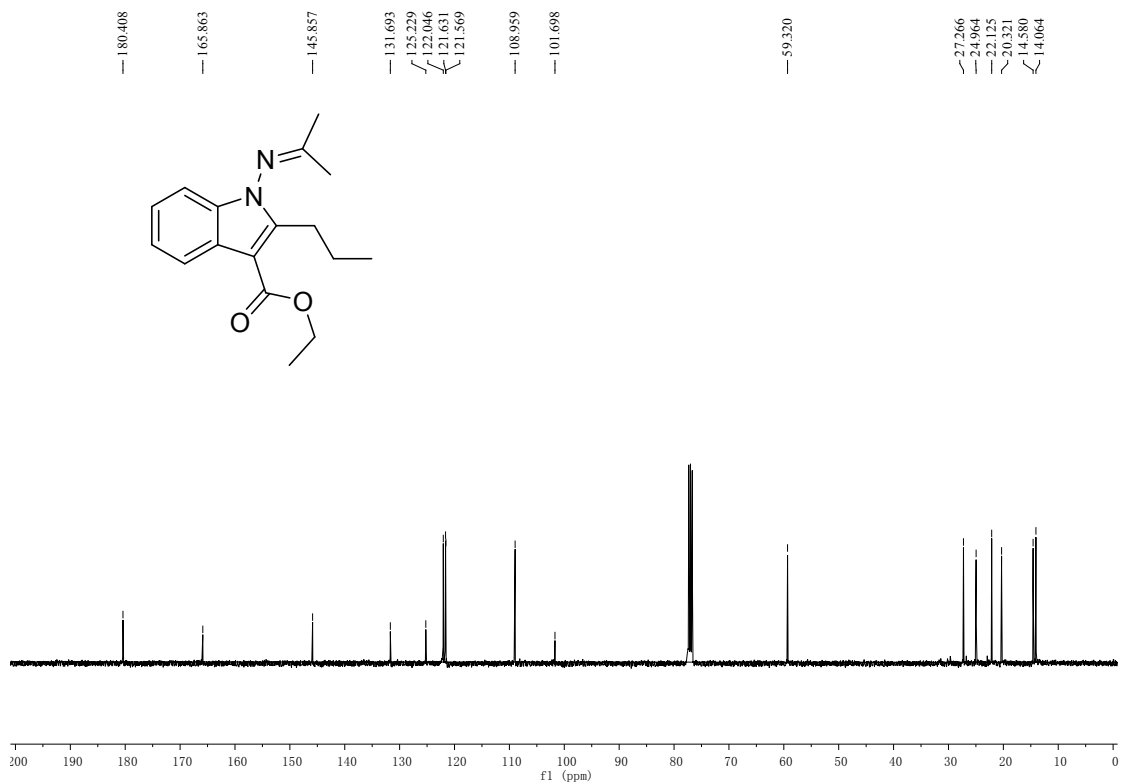
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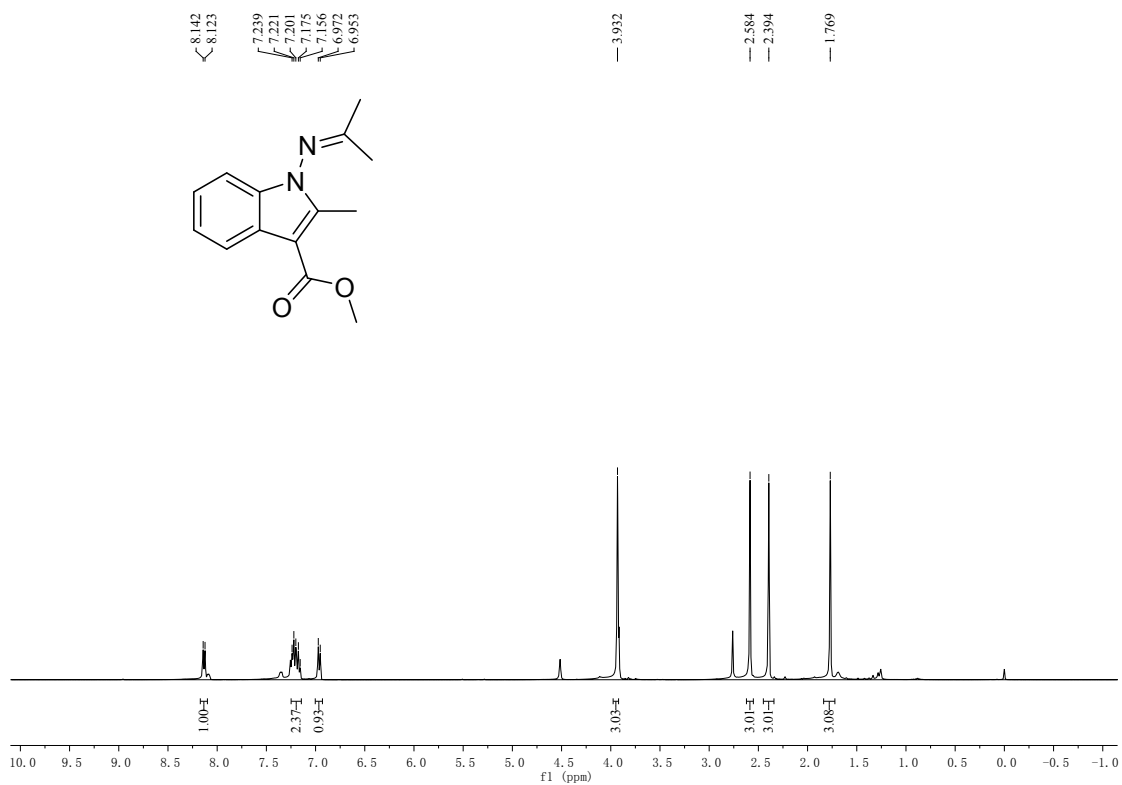


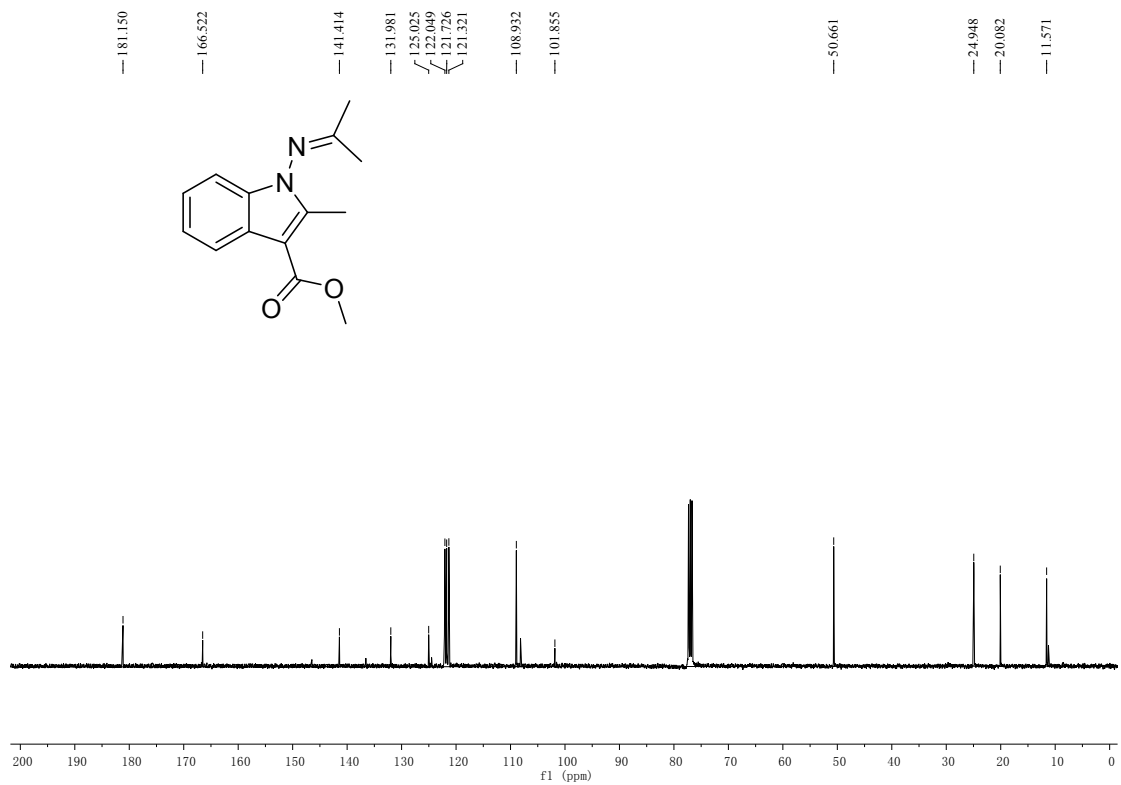
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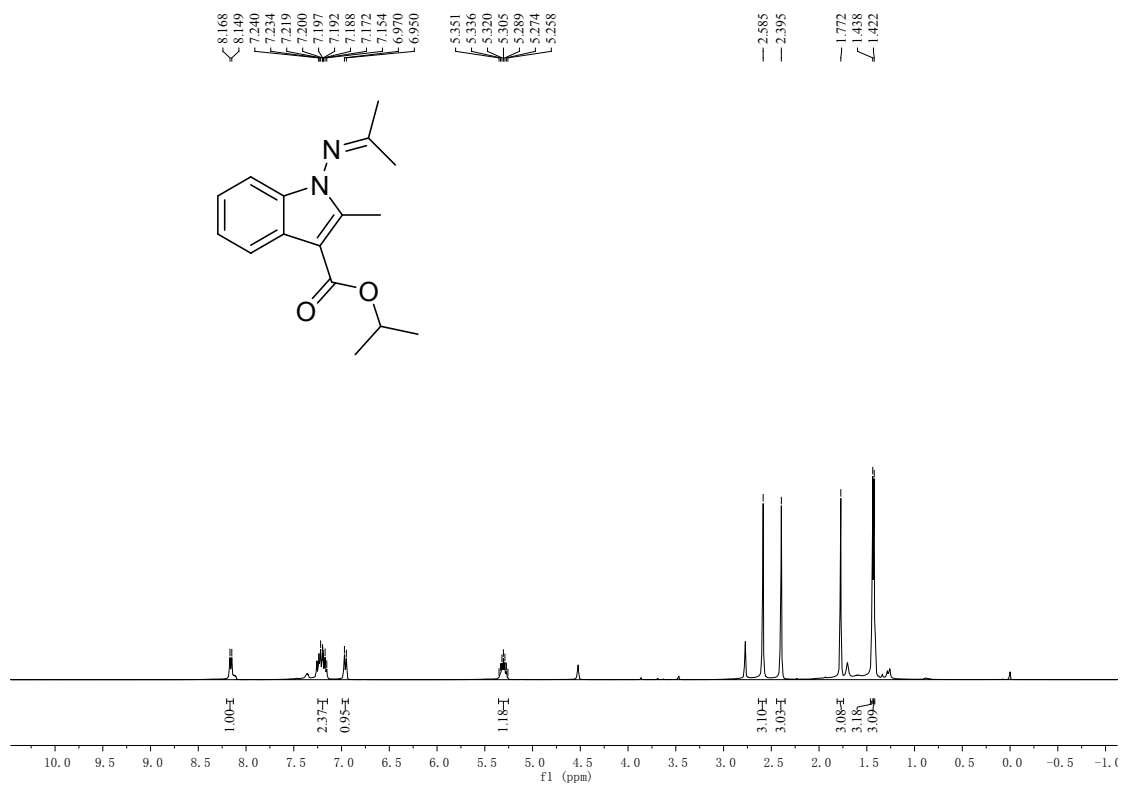


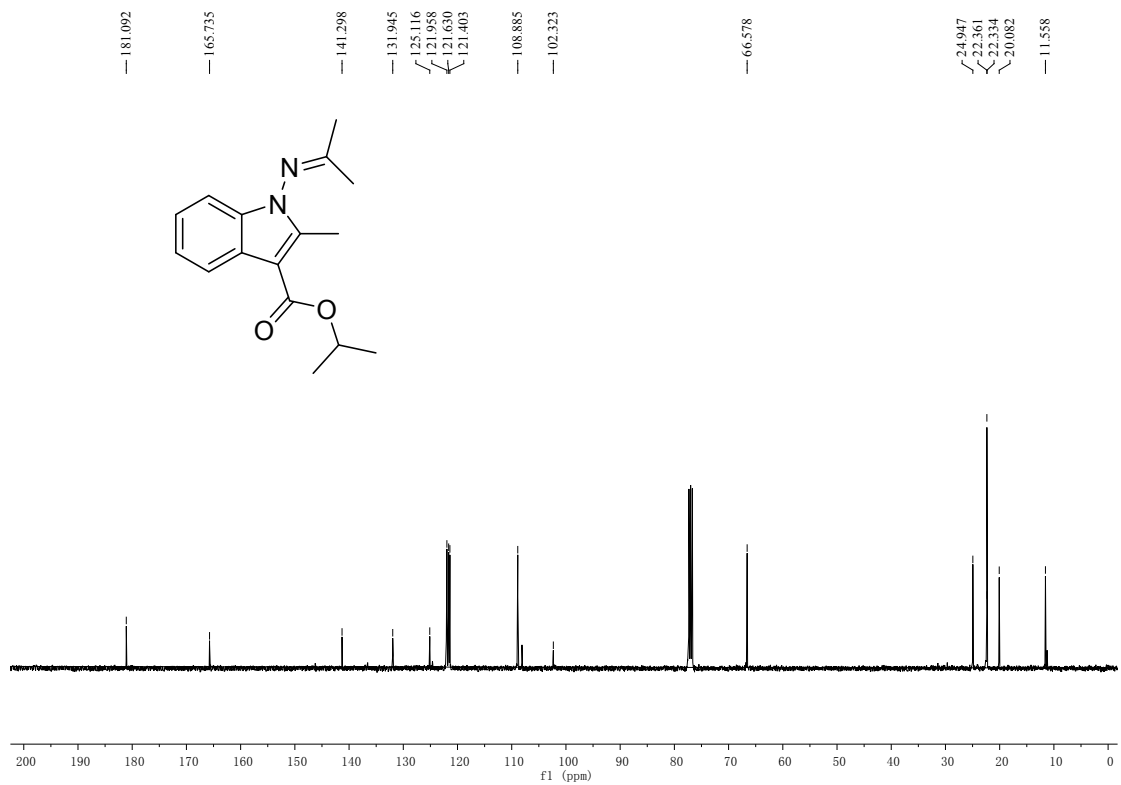
¹H, ¹³C spectra of 4v



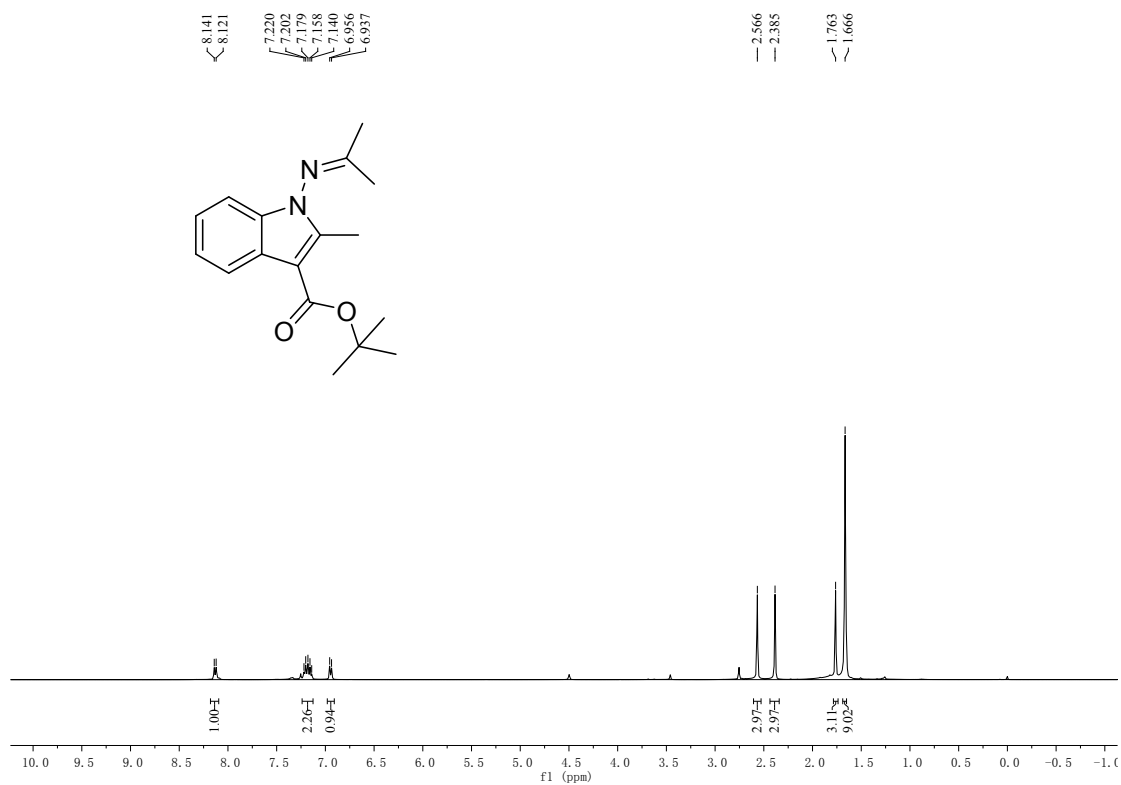


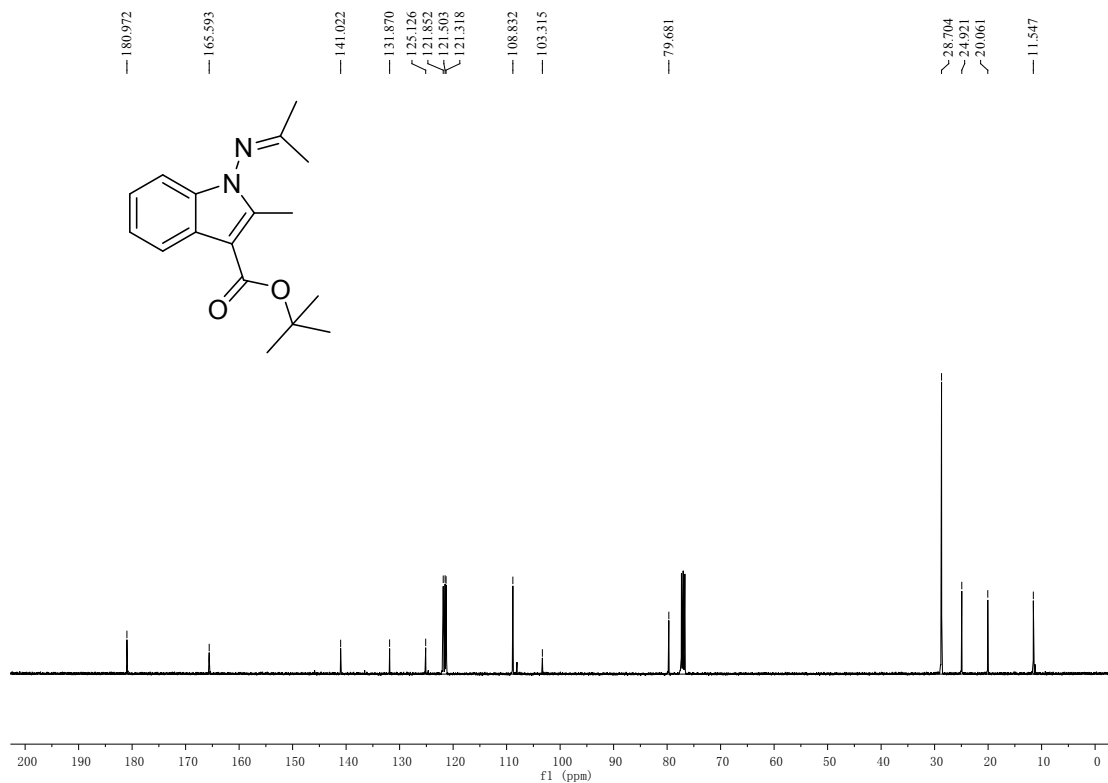
¹H, ¹³C spectra of 4w





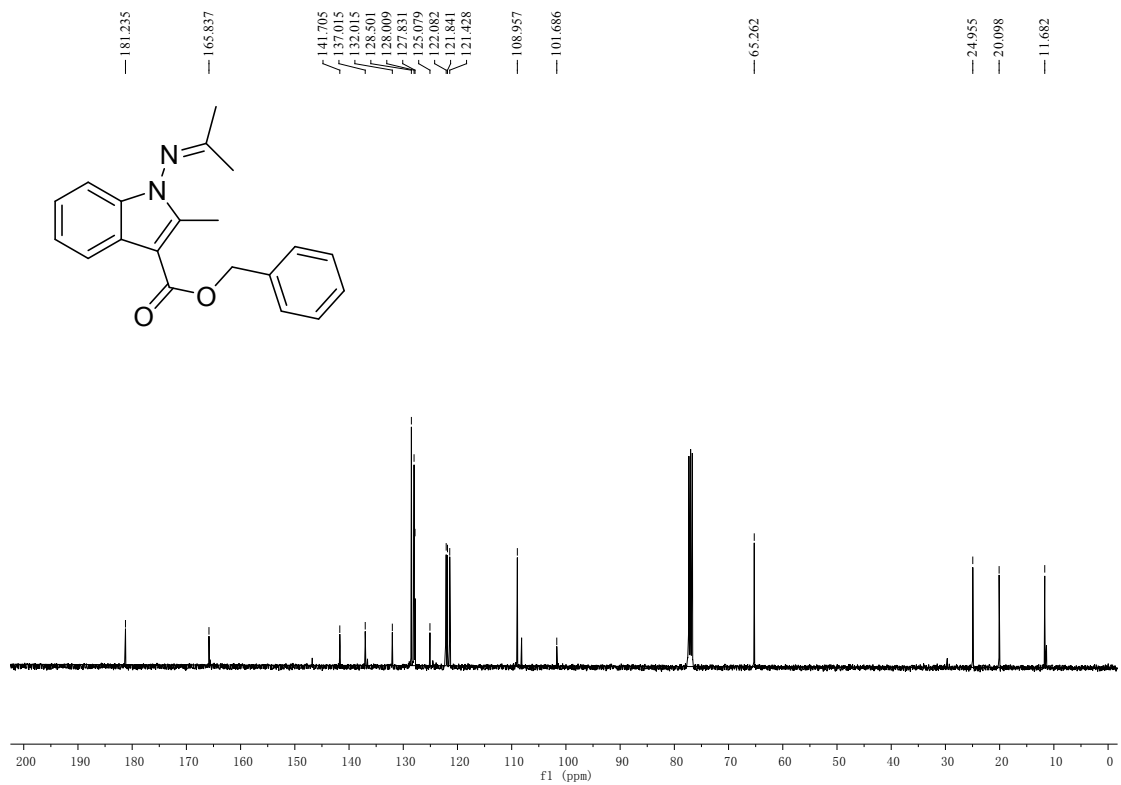
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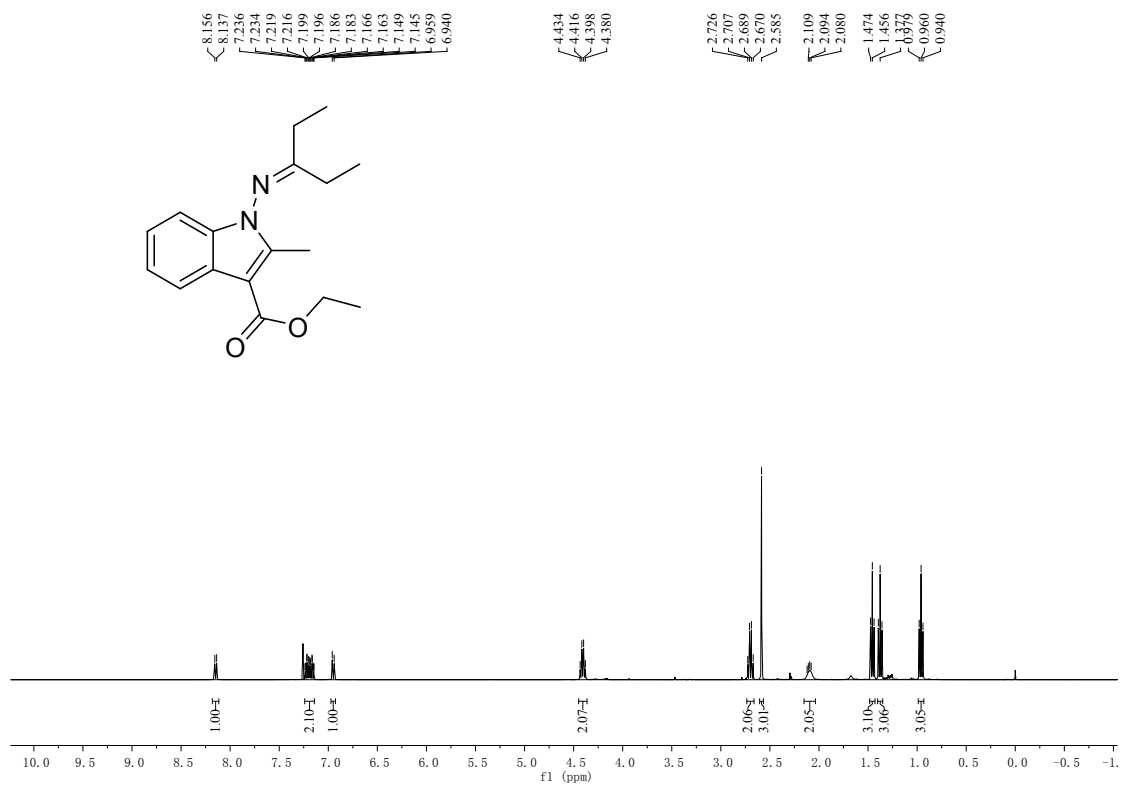


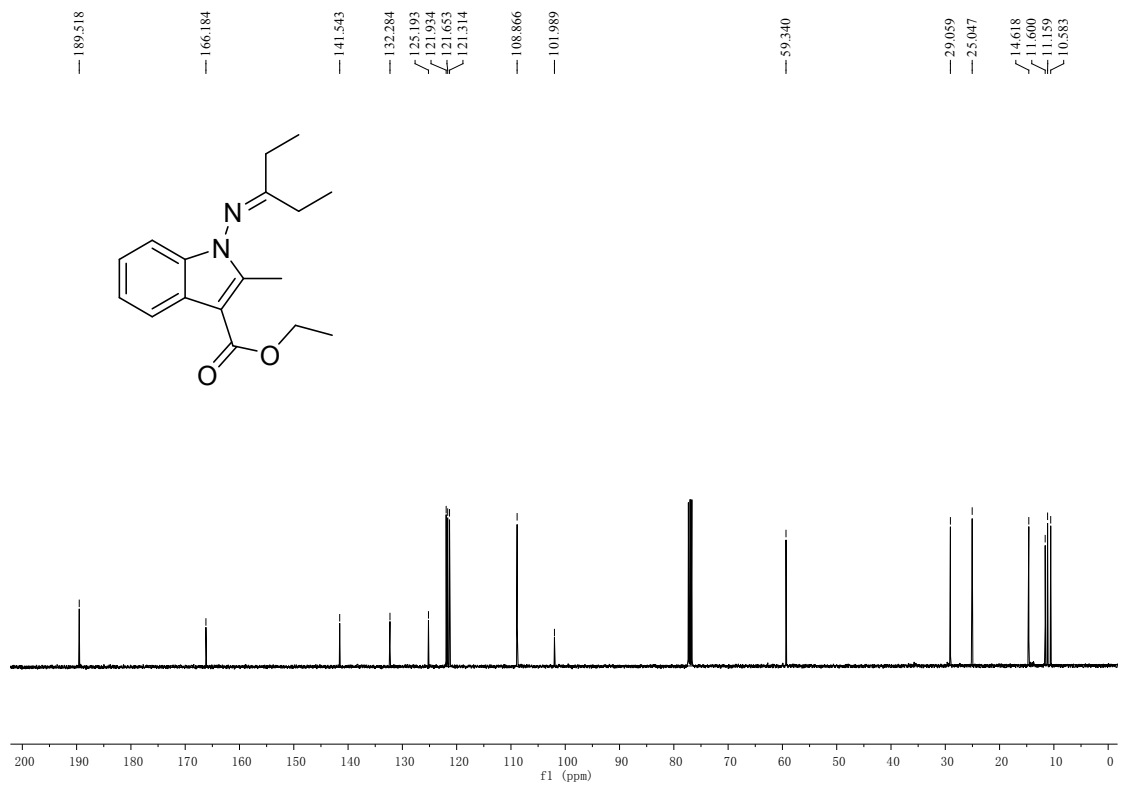
¹H, ¹³C spectra of 4y



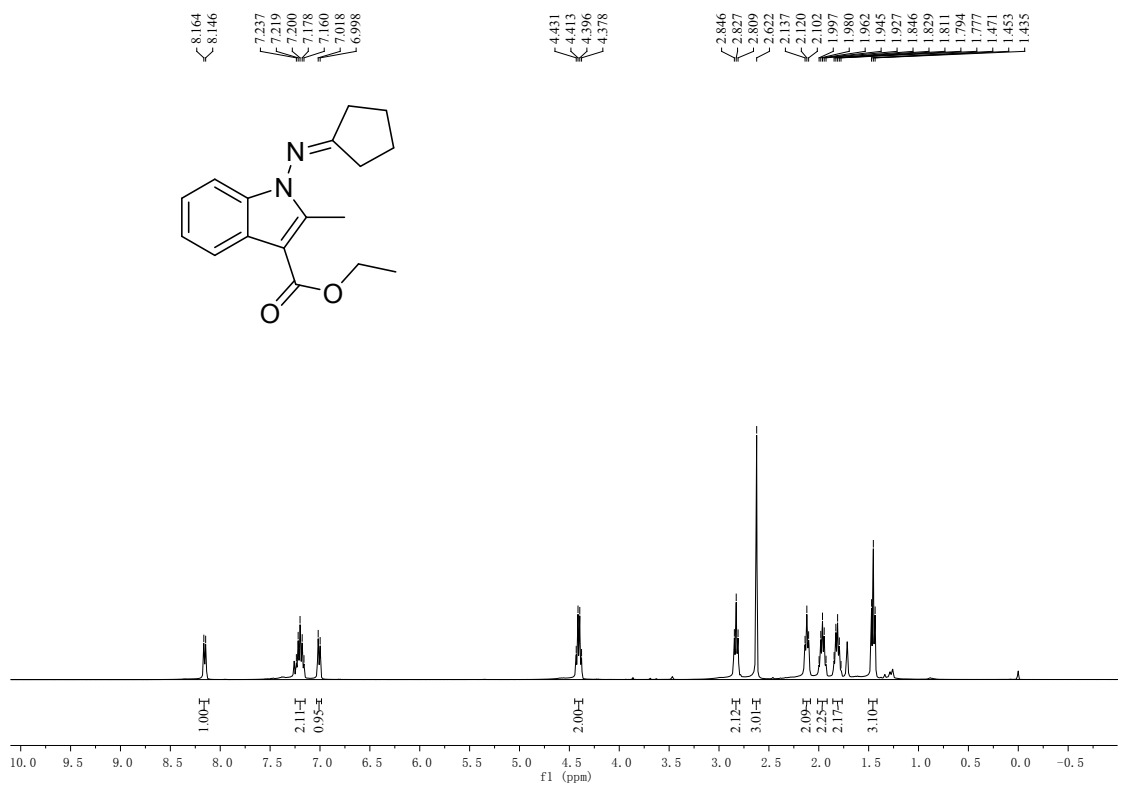


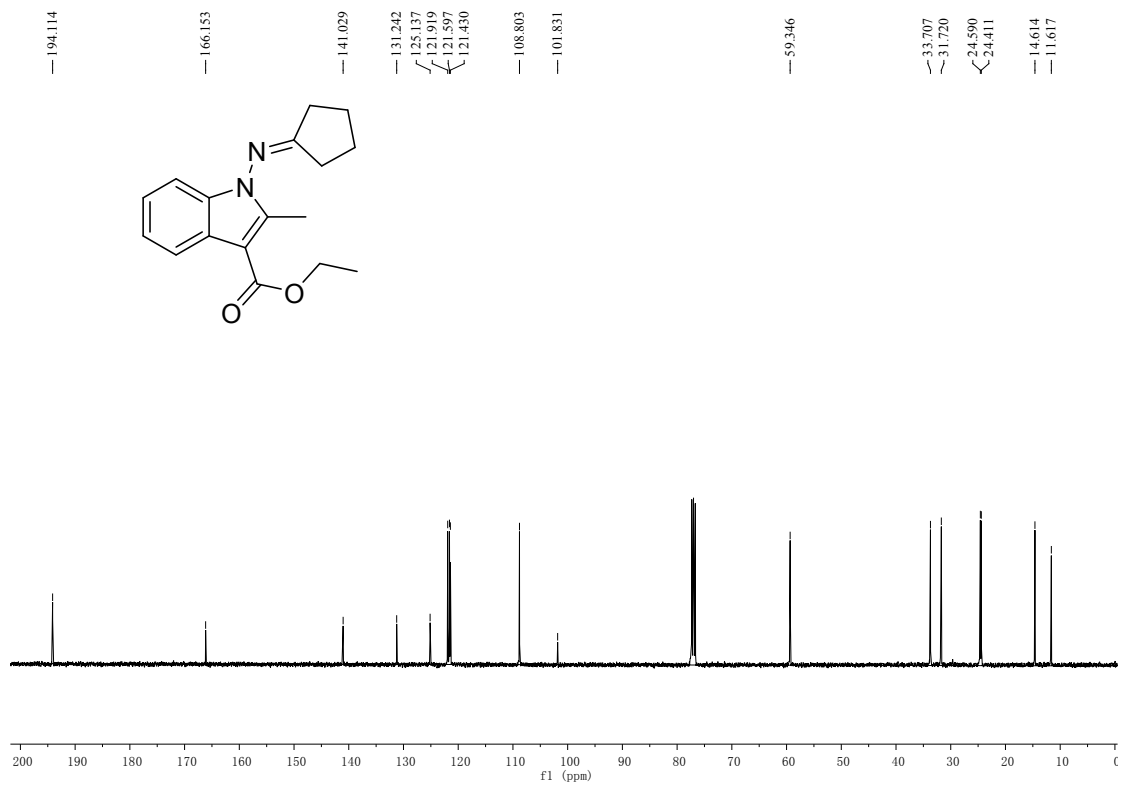
¹H, ¹³C spectra of 4z



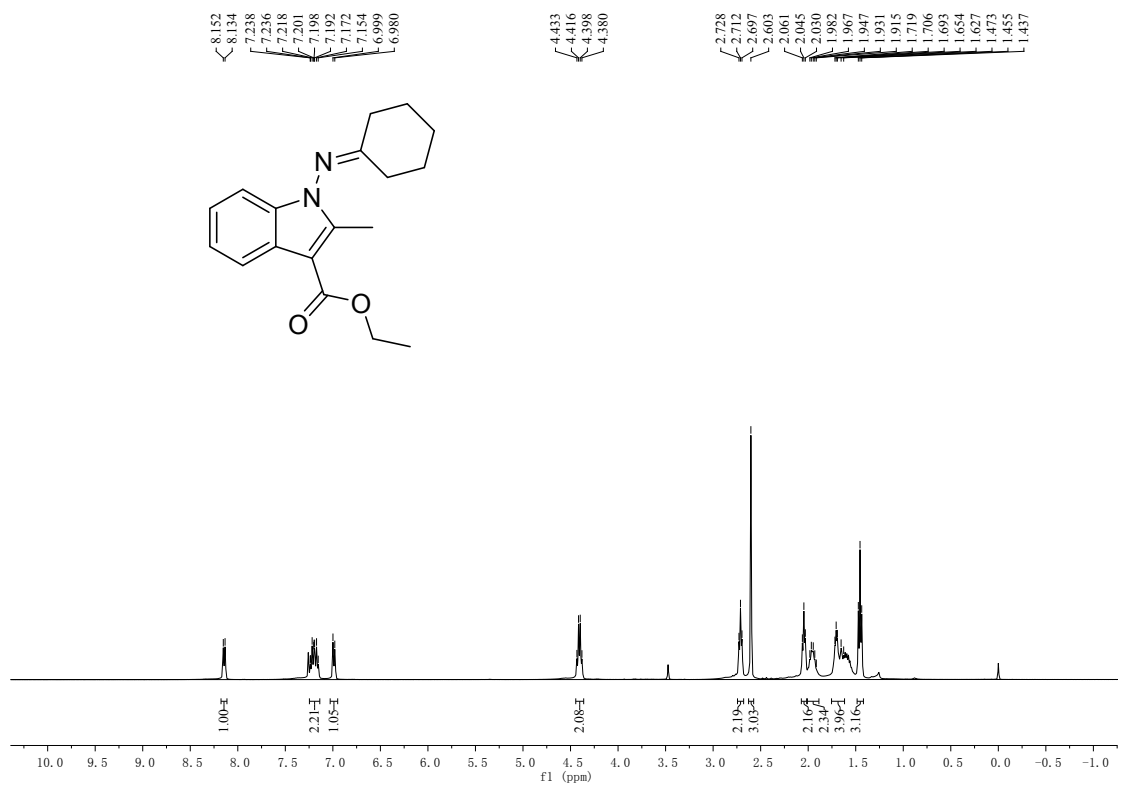


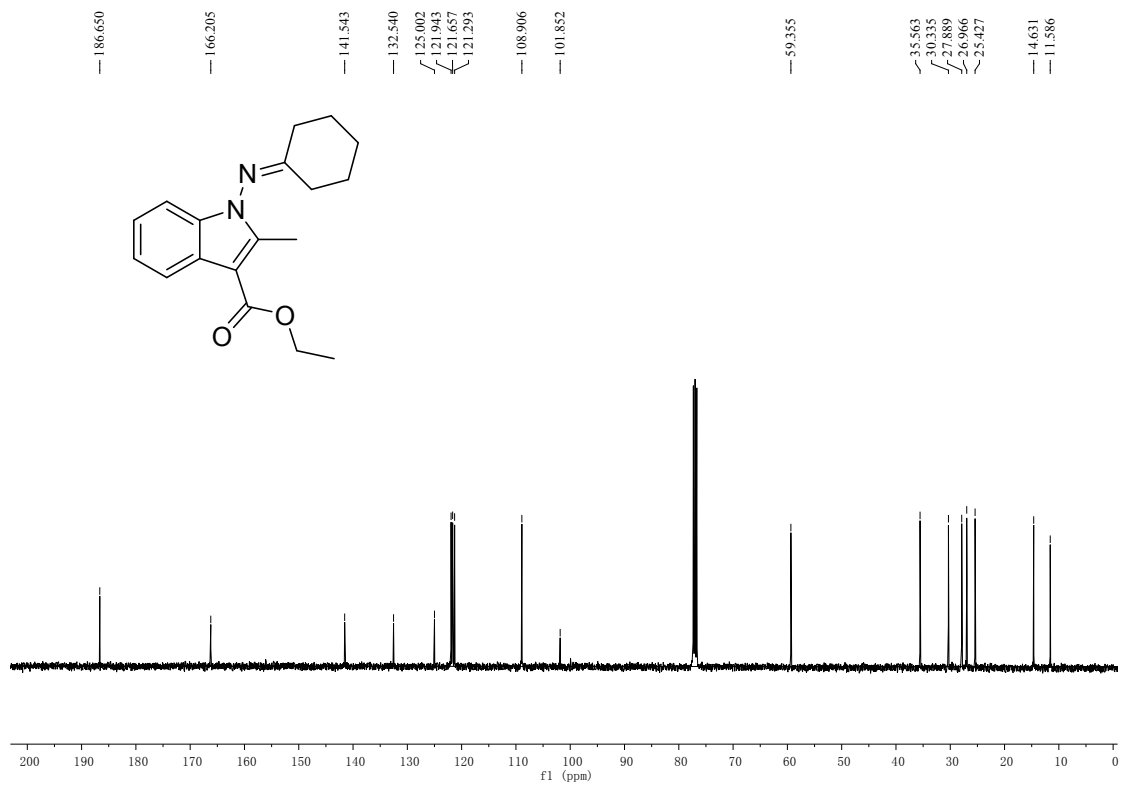
¹H, ¹³C spectra of 4za





¹H, ¹³C spectra of 4zb





¹H, ¹³C spectra of 5a

